# Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:20 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 7VD5 / pdb_00007vd5 |
| EMDB ID | : | EMD-31905 |
| Title | : | Structure of C2S2M2-type PSII-FCPII supercomplex from diatom |
| Authors | : | Nagao, R.; Kato, K.; Akita, F.; Miyazaki, N.; Shen, J.R. |
| Deposited on | : | 2021-09-06 |
| Resolution | : | 2.50 Å(reported) |
| Based on initial model | : | 6J40 |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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The following versions of software and data (see references ⓘ) were used in the production of this report:

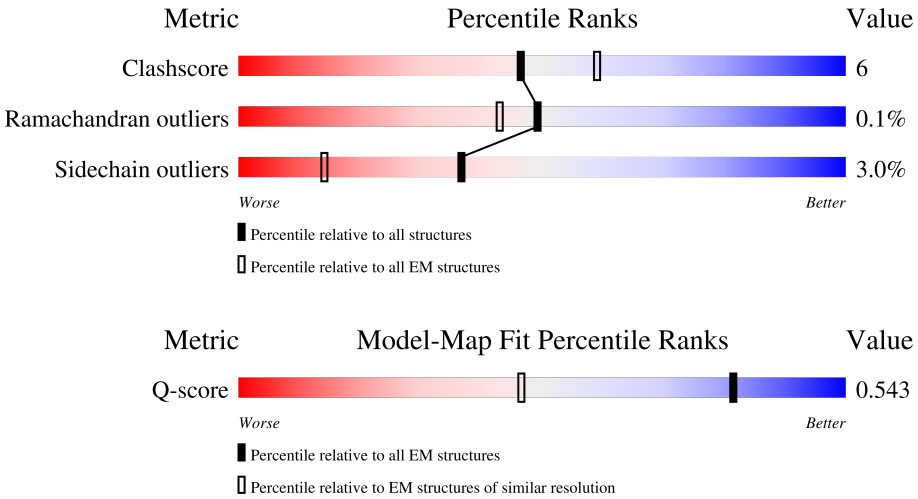
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 7115 ( 2.00 - 3.00 ) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 334 | 89% 11% |
| 1 | a | 334 | 87% 13% |
| 2 | B | 484 | 86% 14% |
| 2 | b | 484 | 87% 13% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | C | 451 | 88% 11% |
| 3 | c | 451 | 89% 11% |
| 4 | D | 341 | 87% 13% |
| 4 | d | 341 | 87% 13% |
| 5 | E | 75 | 91% 9% |
| 5 | e | 75 | 91% 9% |
| 6 | F | 28 | 89% 11% |
| 6 | f | 28 | 86% 14% |
| 7 | H | 66 | 91% 9% |
| 7 | h | 66 | 88% 12% |
| 8 | I | 35 | 91% 9% |
| 8 | i | 35 | 94% 6% |
| 9 | J | 34 | 94% 6% |
| 9 | j | 34 | 91% 9% |
| 10 | K | 37 | 81% 19% |
| 10 | k | 37 | 89% 11% |
| 11 | L | 38 | 97% |
| 11 | l | 38 | 95% 5% |
| 12 | M | 42 | 5% 95% 5% |
| 12 | m | 42 | 5% 95% 5% |
| 13 | O | 245 | 82% 16% |
| 13 | o | 245 | 80% 18% |
| 14 | T | 30 | 97% |
| 14 | t | 30 | 87% 13% |
| 15 | U | 93 | 81% 19% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | u | 93 | 82% 18% |
| 16 | V | 136 | 87% 12% |
| 16 | v | 136 | 87% 12% |
| 17 | Y | 34 | 88% 12% |
| 17 | y | 34 | 91% 9% |
| 18 | X | 37 | 5% 92% 8% |
| 18 | x | 37 | 5% 86% 14% |
| 19 | Z | 59 | 92% 8% |
| 19 | z | 59 | 97% |
| 20 | Q | 151 | 89% 11% |
| 20 | q | 151 | 87% 13% |
| 21 | W | 52 | 96% |
| 21 | w | 52 | 94% 6% |
| 22 | 0 | 31 | 97% |
| 22 | 5 | 31 | 97% |
| 23 | 1 | 30 | 100% |
| 23 | 6 | 30 | 100% |
| 24 | 11 | 176 | 86% 13% |
| 24 | 31 | 176 | 84% 16% |
| 25 | 12 | 169 | 82% 17% |
| 25 | 32 | 169 | 82% 18% |
| 26 | 13 | 169 | 6% 83% 17% |
| 26 | 33 | 169 | 5% 81% 18% |
| 27 | 14 | 172 | 80% 19% |
| 27 | 34 | 172 | 77% 22% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 28 | 15 | 170 | 75% 77% 20% |
| 28 | 35 | 170 | 75% 79% 19% |
| 29 | 16 | 179 | 12% 79% 20% |
| 29 | 36 | 179 | 12% 80% 18% |
| 30 | 17 | 176 | 21% 81% 18% |
| 30 | 37 | 176 | 21% 86% 14% |
| 31 | 18 | 168 | 78% 76% 21% |
| 31 | 38 | 168 | 80% 75% 21% |
| 32 | 19 | 227 | 8% 81% 19% |
| 32 | 39 | 227 | 8% 81% 17% |
| 33 | 20 | 155 | 41% 77% 19% |
| 33 | 40 | 155 | 47% 76% 21% |
| 34 | 21 | 162 | 94% 73% 20% |
| 34 | 41 | 162 | 94% 73% 21% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 37 | CLA | 11 | 303 | X | - | - | - |
| 37 | CLA | 11 | 305 | X | - | - | - |
| 37 | CLA | 11 | 308 | X | - | - | - |
| 37 | CLA | 11 | 310 | X | - | - | - |
| 37 | CLA | 12 | 203 | X | - | - | - |
| 37 | CLA | 12 | 204 | X | - | - | - |
| 37 | CLA | 12 | 205 | X | - | - | - |
| 37 | CLA | 12 | 207 | X | - | - | - |
| 37 | CLA | 12 | 209 | X | - | - | - |
| 37 | CLA | 12 | 212 | X | - | - | - |
| 37 | CLA | 13 | 303 | X | - | - | - |
| 37 | CLA | 13 | 305 | X | - | - | - |
| 37 | CLA | 13 | 307 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 37 | CLA | 14 | 302 | X | - | - | - |
| 37 | CLA | 14 | 305 | X | - | - | - |
| 37 | CLA | 14 | 307 | X | - | - | - |
| 37 | CLA | 14 | 308 | X | - | - | - |
| 37 | CLA | 14 | 310 | X | - | - | - |
| 37 | CLA | 15 | 305 | X | - | - | - |
| 37 | CLA | 15 | 307 | X | - | - | - |
| 37 | CLA | 15 | 308 | X | - | - | - |
| 37 | CLA | 15 | 310 | X | - | - | - |
| 37 | CLA | 16 | 303 | X | - | - | - |
| 37 | CLA | 16 | 306 | X | - | - | - |
| 37 | CLA | 16 | 307 | X | - | - | - |
| 37 | CLA | 16 | 309 | X | - | - | - |
| 37 | CLA | 17 | 304 | X | - | - | - |
| 37 | CLA | 17 | 307 | X | - | - | - |
| 37 | CLA | 17 | 309 | X | - | - | - |
| 37 | CLA | 18 | 201 | X | - | - | - |
| 37 | CLA | 18 | 203 | X | - | - | - |
| 37 | CLA | 18 | 204 | X | - | - | - |
| 37 | CLA | 18 | 206 | X | - | - | - |
| 37 | CLA | 18 | 208 | X | - | - | - |
| 37 | CLA | 18 | 209 | X | - | - | - |
| 37 | CLA | 19 | 301 | X | - | - | - |
| 37 | CLA | 19 | 302 | X | - | - | - |
| 37 | CLA | 19 | 303 | X | - | - | - |
| 37 | CLA | 19 | 304 | X | - | - | - |
| 37 | CLA | 19 | 305 | X | - | - | - |
| 37 | CLA | 19 | 306 | X | - | - | - |
| 37 | CLA | 19 | 307 | X | - | - | - |
| 37 | CLA | 19 | 309 | X | - | - | - |
| 37 | CLA | 19 | 310 | X | - | - | - |
| 37 | CLA | 20 | 303 | X | - | - | - |
| 37 | CLA | 20 | 306 | X | - | - | - |
| 37 | CLA | 20 | 307 | X | - | - | - |
| 37 | CLA | 20 | 308 | X | - | - | - |
| 37 | CLA | 21 | 202 | X | - | - | - |
| 37 | CLA | 21 | 205 | X | - | - | - |
| 37 | CLA | 21 | 206 | X | - | - | - |
| 37 | CLA | 21 | 208 | X | - | - | - |
| 37 | CLA | 21 | 209 | X | - | - | - |
| 37 | CLA | 31 | 301 | X | - | - | - |
| 37 | CLA | 31 | 304 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 37 | CLA | 31 | 306 | X | - | - | - |
| 37 | CLA | 31 | 310 | X | - | - | - |
| 37 | CLA | 32 | 202 | X | - | - | - |
| 37 | CLA | 32 | 204 | X | - | - | - |
| 37 | CLA | 32 | 205 | X | - | - | - |
| 37 | CLA | 32 | 206 | X | - | - | - |
| 37 | CLA | 32 | 208 | X | - | - | - |
| 37 | CLA | 32 | 210 | X | - | - | - |
| 37 | CLA | 32 | 213 | X | - | - | - |
| 37 | CLA | 33 | 303 | X | - | - | - |
| 37 | CLA | 33 | 305 | X | - | - | - |
| 37 | CLA | 33 | 307 | X | - | - | - |
| 37 | CLA | 34 | 302 | X | - | - | - |
| 37 | CLA | 34 | 305 | X | - | - | - |
| 37 | CLA | 34 | 307 | X | - | - | - |
| 37 | CLA | 34 | 308 | X | - | - | - |
| 37 | CLA | 34 | 310 | X | - | - | - |
| 37 | CLA | 35 | 305 | X | - | - | - |
| 37 | CLA | 35 | 307 | X | - | - | - |
| 37 | CLA | 35 | 310 | X | - | - | - |
| 37 | CLA | 36 | 303 | X | - | - | - |
| 37 | CLA | 36 | 306 | X | - | - | - |
| 37 | CLA | 36 | 307 | X | - | - | - |
| 37 | CLA | 36 | 309 | X | - | - | - |
| 37 | CLA | 37 | 303 | X | - | - | - |
| 37 | CLA | 37 | 306 | X | - | - | - |
| 37 | CLA | 37 | 308 | X | - | - | - |
| 37 | CLA | 38 | 201 | X | - | - | - |
| 37 | CLA | 38 | 203 | X | - | - | - |
| 37 | CLA | 38 | 204 | X | - | - | - |
| 37 | CLA | 38 | 208 | X | - | - | - |
| 37 | CLA | 38 | 209 | X | - | - | - |
| 37 | CLA | 39 | 301 | X | - | - | - |
| 37 | CLA | 39 | 302 | X | - | - | - |
| 37 | CLA | 39 | 303 | X | - | - | - |
| 37 | CLA | 39 | 304 | X | - | - | - |
| 37 | CLA | 39 | 305 | X | - | - | - |
| 37 | CLA | 39 | 307 | X | - | - | - |
| 37 | CLA | 39 | 309 | X | - | - | - |
| 37 | CLA | 39 | 310 | X | - | - | - |
| 37 | CLA | 40 | 205 | X | - | - | - |
| 37 | CLA | 40 | 208 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 37 | CLA | 40 | 209 | X | - | - | - |
| 37 | CLA | 40 | 210 | X | - | - | - |
| 37 | CLA | 41 | 202 | X | - | - | - |
| 37 | CLA | 41 | 205 | X | - | - | - |
| 37 | CLA | 41 | 206 | X | - | - | - |
| 37 | CLA | 41 | 208 | X | - | - | - |
| 37 | CLA | 41 | 209 | X | - | - | - |
| 37 | CLA | A | 403 | X | - | - | - |
| 37 | CLA | B | 501 | X | - | - | - |
| 37 | CLA | B | 502 | X | - | - | - |
| 37 | CLA | B | 503 | X | - | - | - |
| 37 | CLA | B | 504 | X | - | - | - |
| 37 | CLA | B | 505 | X | - | - | - |
| 37 | CLA | B | 506 | X | - | - | - |
| 37 | CLA | B | 507 | X | - | - | - |
| 37 | CLA | B | 509 | X | - | - | - |
| 37 | CLA | B | 510 | X | - | - | - |
| 37 | CLA | B | 511 | X | - | - | - |
| 37 | CLA | B | 512 | X | - | - | - |
| 37 | CLA | B | 513 | X | - | - | - |
| 37 | CLA | B | 514 | X | - | - | - |
| 37 | CLA | B | 515 | X | - | - | - |
| 37 | CLA | B | 516 | X | - | - | - |
| 37 | CLA | B | 524 | X | - | - | - |
| 37 | CLA | C | 501 | X | - | - | - |
| 37 | CLA | C | 502 | X | - | - | - |
| 37 | CLA | C | 503 | X | - | - | - |
| 37 | CLA | C | 504 | X | - | - | - |
| 37 | CLA | C | 505 | X | - | - | - |
| 37 | CLA | C | 506 | X | - | - | - |
| 37 | CLA | C | 507 | X | - | - | - |
| 37 | CLA | C | 508 | X | - | - | - |
| 37 | CLA | C | 509 | X | - | - | - |
| 37 | CLA | C | 510 | X | - | - | - |
| 37 | CLA | C | 511 | X | - | - | - |
| 37 | CLA | C | 512 | X | - | - | - |
| 37 | CLA | C | 513 | X | - | - | - |
| 37 | CLA | D | 401 | X | - | - | - |
| 37 | CLA | D | 405 | X | - | - | - |
| 37 | CLA | D | 406 | X | - | - | - |
| 37 | CLA | W | 101 | X | - | - | - |
| 37 | CLA | W | 102 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 37 | CLA | Z | 101 | X | - | - | - |
| 37 | CLA | Z | 102 | X | - | - | - |
| 37 | CLA | a | 403 | X | - | - | - |
| 37 | CLA | a | 404 | X | - | - | - |
| 37 | CLA | b | 501 | X | - | - | - |
| 37 | CLA | b | 502 | X | - | - | - |
| 37 | CLA | b | 503 | X | - | - | - |
| 37 | CLA | b | 504 | X | - | - | - |
| 37 | CLA | b | 505 | X | - | - | - |
| 37 | CLA | b | 506 | X | - | - | - |
| 37 | CLA | b | 507 | X | - | - | - |
| 37 | CLA | b | 509 | X | - | - | - |
| 37 | CLA | b | 510 | X | - | - | - |
| 37 | CLA | b | 511 | X | - | - | - |
| 37 | CLA | b | 512 | X | - | - | - |
| 37 | CLA | b | 513 | X | - | - | - |
| 37 | CLA | b | 514 | X | - | - | - |
| 37 | CLA | b | 515 | X | - | - | - |
| 37 | CLA | b | 516 | X | - | - | - |
| 37 | CLA | b | 523 | X | - | - | - |
| 37 | CLA | c | 501 | X | - | - | - |
| 37 | CLA | c | 502 | X | - | - | - |
| 37 | CLA | c | 503 | X | - | - | - |
| 37 | CLA | c | 504 | X | - | - | - |
| 37 | CLA | c | 505 | X | - | - | - |
| 37 | CLA | c | 506 | X | - | - | - |
| 37 | CLA | c | 507 | X | - | - | - |
| 37 | CLA | c | 508 | X | - | - | - |
| 37 | CLA | c | 509 | X | - | - | - |
| 37 | CLA | c | 510 | X | - | - | - |
| 37 | CLA | c | 511 | X | - | - | - |
| 37 | CLA | c | 512 | X | - | - | - |
| 37 | CLA | c | 513 | X | - | - | - |
| 37 | CLA | d | 403 | X | - | - | - |
| 37 | CLA | d | 404 | X | - | - | - |
| 37 | CLA | w | 101 | X | - | - | - |
| 37 | CLA | z | 101 | X | - | - | - |
| 37 | CLA | z | 102 | X | - | - | - |

# 2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 100884 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 334 | Total | C | N | O | S | 0 | 0 |
| | | | 2619 | 1712 | 429 | 463 | 15 | | |
| 1 | a | 334 | Total | C | N | O | S | 0 | 0 |
| | | | 2619 | 1712 | 429 | 463 | 15 | | |

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 484 | Total | C | N | O | S | 0 | 0 |
| | | | 3812 | 2494 | 645 | 660 | 13 | | |
| 2 | b | 484 | Total | C | N | O | S | 0 | 0 |
| | | | 3812 | 2494 | 645 | 660 | 13 | | |

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 451 | Total | C | N | O | S | 0 | 0 |
| | | | 3504 | 2289 | 589 | 612 | 14 | | |
| 3 | c | 451 | Total | C | N | O | S | 0 | 0 |
| | | | 3504 | 2289 | 589 | 612 | 14 | | |

- Molecule 4 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 341 | Total | C | N | O | S | 0 | 0 |
| | | | 2697 | 1781 | 441 | 465 | 10 | | |
| 4 | d | 341 | Total | C | N | O | S | 0 | 0 |
| | | | 2697 | 1781 | 441 | 465 | 10 | | |

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 5 | E | 75 | Total<br>616 | C<br>401 | N<br>102 | O<br>113 | 0 | 0 |
| 5 | e | 75 | Total<br>616 | C<br>401 | N<br>102 | O<br>113 | 0 | 0 |

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 28 | Total<br>228 | C<br>155 | N<br>39 | O<br>33 | S<br>1 | 0 | 0 |
| 6 | f | 28 | Total<br>228 | C<br>155 | N<br>39 | O<br>33 | S<br>1 | 0 | 0 |

- Molecule 7 is a protein called Photosystem II reaction center protein H.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | H | 66 | Total<br>513 | C<br>340 | N<br>83 | O<br>88 | S<br>2 | 0 | 0 |
| 7 | h | 66 | Total<br>513 | C<br>340 | N<br>83 | O<br>88 | S<br>2 | 0 | 0 |

- Molecule 8 is a protein called Photosystem II reaction center protein I.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | I | 35 | Total<br>287 | C<br>194 | N<br>45 | O<br>47 | S<br>1 | 0 | 0 |
| 8 | i | 35 | Total<br>287 | C<br>194 | N<br>45 | O<br>47 | S<br>1 | 0 | 0 |

- Molecule 9 is a protein called Photosystem II reaction center protein J.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | J | 34 | Total<br>254 | C<br>172 | N<br>38 | O<br>43 | S<br>1 | 0 | 0 |
| 9 | j | 34 | Total<br>254 | C<br>172 | N<br>38 | O<br>43 | S<br>1 | 0 | 0 |

- Molecule 10 is a protein called Photosystem II reaction center protein K.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 10 | K | 37 | Total<br>302 | C<br>212 | N<br>45 | O<br>45 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 10 | k | 37 | Total<br>302 | C<br>212 | N<br>45 | O<br>45 | 0 | 0 |

- Molecule 11 is a protein called Photosystem II reaction center protein L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | L | 38 | Total<br>310 | C<br>208 | N<br>48 | O<br>53 | S<br>1 | 0 | 0 |
| 11 | l | 38 | Total<br>310 | C<br>208 | N<br>48 | O<br>53 | S<br>1 | 0 | 0 |

- Molecule 12 is a protein called Photosystem II subunit.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 12 | M | 42 | Total<br>316 | C<br>207 | N<br>51 | O<br>58 | 0 | 0 |
| 12 | m | 42 | Total<br>316 | C<br>207 | N<br>51 | O<br>58 | 0 | 0 |

- Molecule 13 is a protein called Extrinsic protein in photosystem II.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | O | 245 | Total<br>1845 | C<br>1166 | N<br>306 | O<br>365 | S<br>8 | 0 | 0 |
| 13 | o | 245 | Total<br>1845 | C<br>1166 | N<br>306 | O<br>365 | S<br>8 | 0 | 0 |

- Molecule 14 is a protein called Photosystem II reaction center protein T.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | T | 30 | Total<br>250 | C<br>174 | N<br>36 | O<br>38 | S<br>2 | 0 | 0 |
| 14 | t | 30 | Total<br>250 | C<br>174 | N<br>36 | O<br>38 | S<br>2 | 0 | 0 |

- Molecule 15 is a protein called Extrinsic protein in photosystem II.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | U | 93 | Total<br>713 | C<br>455 | N<br>119 | O<br>137 | S<br>2 | 0 | 0 |
| 15 | u | 93 | Total<br>713 | C<br>455 | N<br>119 | O<br>137 | S<br>2 | 0 | 0 |

- Molecule 16 is a protein called Cytochrome c-550.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | V | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1037 | 647 | 180 | 206 | 4 | | |
| 16 | v | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1037 | 647 | 180 | 206 | 4 | | |

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | Y | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 250 | 166 | 41 | 40 | 3 | | |
| 17 | y | 34 | Total | C | N | O | S | 0 | 0 |
| | | | 250 | 166 | 41 | 40 | 3 | | |

- Molecule 18 is a protein called Photosystem II reaction center X protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | X | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 263 | 171 | 45 | 46 | 1 | | |
| 18 | x | 37 | Total | C | N | O | S | 0 | 0 |
| | | | 263 | 171 | 45 | 46 | 1 | | |

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | Z | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 447 | 305 | 68 | 73 | 1 | | |
| 19 | z | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 447 | 305 | 68 | 73 | 1 | | |

- Molecule 20 is a protein called Extrinsic protein in photosystem II.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | Q | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1180 | 749 | 196 | 234 | 1 | | |
| 20 | q | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1180 | 749 | 196 | 234 | 1 | | |

- Molecule 21 is a protein called Photosystem II reaction center protein W.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 21 | W | 52 | Total | C | N | O | 0 | 0 |
| | | | 422 | 273 | 65 | 84 | | |
| 21 | w | 52 | Total | C | N | O | 0 | 0 |
| | | | 422 | 273 | 65 | 84 | | |

- Molecule 22 is a protein called Unknown protein 0.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 22 | 0 | 31 | Total | C | N | O | 0 | 0 |
| | | | 155 | 93 | 31 | 31 | | |
| 22 | 5 | 31 | Total | C | N | O | 0 | 0 |
| | | | 155 | 93 | 31 | 31 | | |

- Molecule 23 is a protein called Unknown protein 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 23 | 1 | 30 | Total | C | N | O | 0 | 0 |
| | | | 150 | 90 | 30 | 30 | | |
| 23 | 6 | 30 | Total | C | N | O | 0 | 0 |
| | | | 150 | 90 | 30 | 30 | | |

- Molecule 24 is a protein called Chlorophyll a/b-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | 11 | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1343 | 852 | 228 | 256 | 7 | | |
| 24 | 31 | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1343 | 852 | 228 | 256 | 7 | | |

- Molecule 25 is a protein called Fcpb2, Fucoxanthin chlorophyll a/c-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | 12 | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1302 | 828 | 222 | 244 | 8 | | |
| 25 | 32 | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1302 | 828 | 222 | 244 | 8 | | |

- Molecule 26 is a protein called Chlorophyll a/b-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | 13 | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 220 | 246 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | 33 | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1296 | 823 | 220 | 246 | 7 | | |

- Molecule 27 is a protein called Chlorophyll a/b-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | 14 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1319 | 838 | 223 | 251 | 7 | | |
| 27 | 34 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1319 | 838 | 223 | 251 | 7 | | |

- Molecule 28 is a protein called Chlorophyll a/b-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | 15 | 170 | Total | C | N | O | S | 0 | 0 |
| | | | 1307 | 832 | 221 | 247 | 7 | | |
| 28 | 35 | 170 | Total | C | N | O | S | 0 | 0 |
| | | | 1307 | 832 | 221 | 247 | 7 | | |

- Molecule 29 is a protein called Fcpb3, Fucoxanthin chlorophyll a/c-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | 16 | 179 | Total | C | N | O | S | 0 | 0 |
| | | | 1386 | 891 | 233 | 256 | 6 | | |
| 29 | 36 | 179 | Total | C | N | O | S | 0 | 0 |
| | | | 1386 | 891 | 233 | 256 | 6 | | |

- Molecule 30 is a protein called Fcpb4, Fucoxanthin chlorophyll a/c-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | 17 | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1353 | 862 | 227 | 258 | 6 | | |
| 30 | 37 | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1353 | 862 | 227 | 258 | 6 | | |

- Molecule 31 is a protein called Chlorophyll a/b-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | 18 | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1289 | 818 | 219 | 245 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | 38 | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1289 | 818 | 219 | 245 | 7 | | |

- Molecule 32 is a protein called Fcpb5, Fucoxanthin chlorophyll a/c-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | 19 | 227 | Total | C | N | O | S | 0 | 0 |
| | | | 1746 | 1128 | 291 | 322 | 5 | | |
| 32 | 39 | 227 | Total | C | N | O | S | 0 | 0 |
| | | | 1746 | 1128 | 291 | 322 | 5 | | |

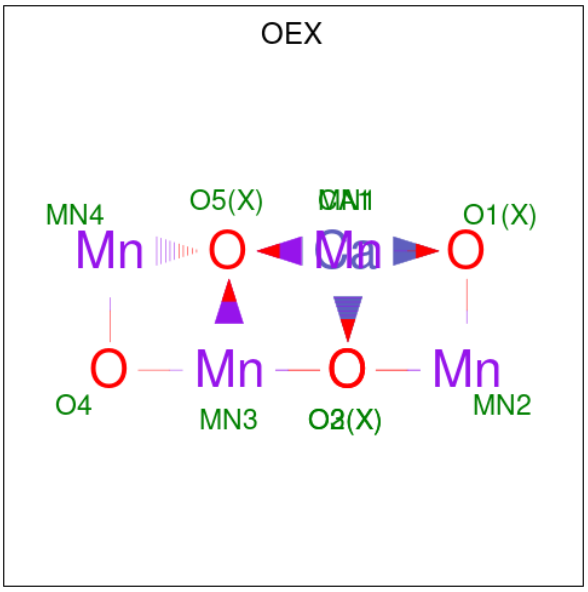
- Molecule 33 is a protein called Fcpb6, Fucoxanthin chlorophyll a/c-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | 20 | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 769 | 201 | 215 | 8 | | |
| 33 | 40 | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1193 | 769 | 201 | 215 | 8 | | |

- Molecule 34 is a protein called Fcpb7, Fucoxanthin chlorophyll a/c-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | 21 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1262 | 822 | 206 | 229 | 5 | | |
| 34 | 41 | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1262 | 822 | 206 | 229 | 5 | | |

- Molecule 35 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).

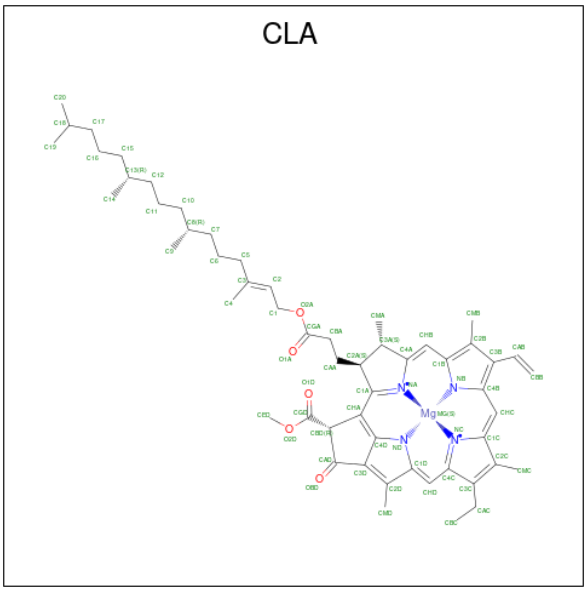



| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 35 | A | 1 | Total | Ca | Mn | O | 0 |
| | | | 10 | 1 | 4 | 5 | |
| 35 | a | 1 | Total | Ca | Mn | O | 0 |
| | | | 10 | 1 | 4 | 5 | |

- Molecule 36 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 36 | A | 1 | Total | Fe | 0 |
| | | | 1 | 1 | |
| 36 | a | 1 | Total | Fe | 0 |
| | | | 1 | 1 | |

- Molecule 37 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | A | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 62 | 52 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | B | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | C | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | D | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | D | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | D | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | D | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | Z | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | Z | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | W | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | W | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | a | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 62 | 52 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | b | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | c | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | d | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | z | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | z | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | w | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 11 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 11 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 11 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 11 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 37 | 11 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 11 | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | |
| 37 | 12 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 12 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 12 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 12 | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 37 | 12 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 37 | 12 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 12 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 13 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 13 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 37 | 13 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 13 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 37 | 13 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 13 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | 14 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 14 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 14 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 37 | 14 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 14 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 37 | 14 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 14 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 15 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 15 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 37 | 15 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 15 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 37 | 15 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 15 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 16 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 16 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 37 | 16 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 16 | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | |
| 37 | 16 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 17 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 17 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 37 | 17 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | 17 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 37 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 37 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 19 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 19 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 19 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 19 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 19 | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | |
| 37 | 19 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 19 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 19 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 19 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 20 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 37 | 20 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 37 | 20 | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | 20 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 20 | 1 | Total | C | Mg | N | O | 0 |
| | | | 47 | 37 | 1 | 4 | 5 | |
| 37 | 21 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 37 | 21 | 1 | Total | C | Mg | N | O | 0 |
| | | | 58 | 48 | 1 | 4 | 5 | |
| 37 | 21 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 21 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 21 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 21 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 21 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 31 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 31 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 31 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 31 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 31 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 37 | 31 | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | |
| 37 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 37 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 33 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 33 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 37 | 33 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 33 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 37 | 33 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 33 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 34 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 34 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 34 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 37 | 34 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 34 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 37 | 34 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 34 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 35 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 35 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 37 | 35 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 35 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 37 | 35 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 35 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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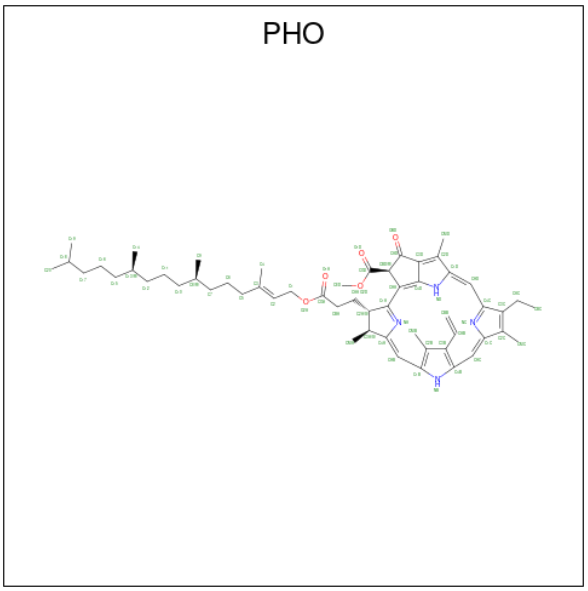
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | 36 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 36 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 37 | 36 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 36 | 1 | Total | C | Mg | N | O | 0 |
| | | | 61 | 51 | 1 | 4 | 5 | |
| 37 | 36 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 37 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 37 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 37 | 37 | 1 | Total | C | Mg | N | O | 0 |
| | | | 52 | 42 | 1 | 4 | 5 | |
| 37 | 37 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 37 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 53 | 43 | 1 | 4 | 5 | |
| 37 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 39 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 39 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 39 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 39 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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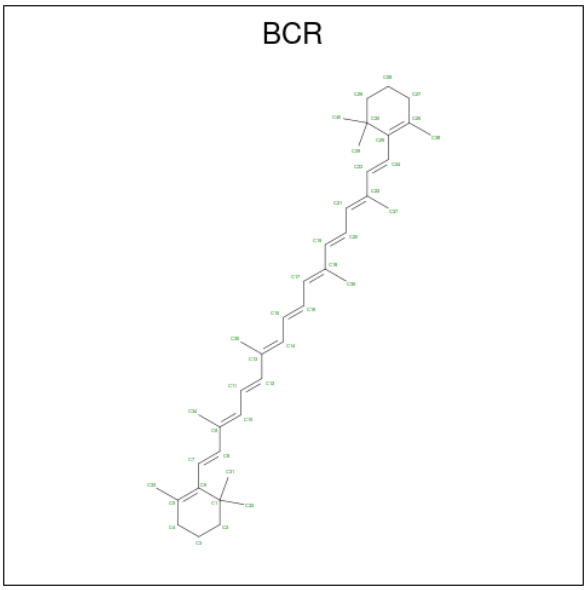
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 37 | 39 | 1 | Total | C | Mg | N | O | 0 |
| | | | 51 | 41 | 1 | 4 | 5 | |
| 37 | 39 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 39 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 39 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 39 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 40 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 37 | 40 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 46 | 1 | 4 | 5 | |
| 37 | 40 | 1 | Total | C | Mg | N | O | 0 |
| | | | 50 | 40 | 1 | 4 | 5 | |
| 37 | 40 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 40 | 1 | Total | C | Mg | N | O | 0 |
| | | | 47 | 37 | 1 | 4 | 5 | |
| 37 | 41 | 1 | Total | C | Mg | N | O | 0 |
| | | | 57 | 47 | 1 | 4 | 5 | |
| 37 | 41 | 1 | Total | C | Mg | N | O | 0 |
| | | | 58 | 48 | 1 | 4 | 5 | |
| 37 | 41 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 41 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 41 | 1 | Total | C | Mg | N | O | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | |
| 37 | 41 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 37 | 41 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

- Molecule 38 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 38 | A | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |
| 38 | D | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |
| 38 | a | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |
| 38 | a | 1 | Total | C | N | O | 0 |
| | | | 64 | 55 | 4 | 5 | |

- Molecule 39 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



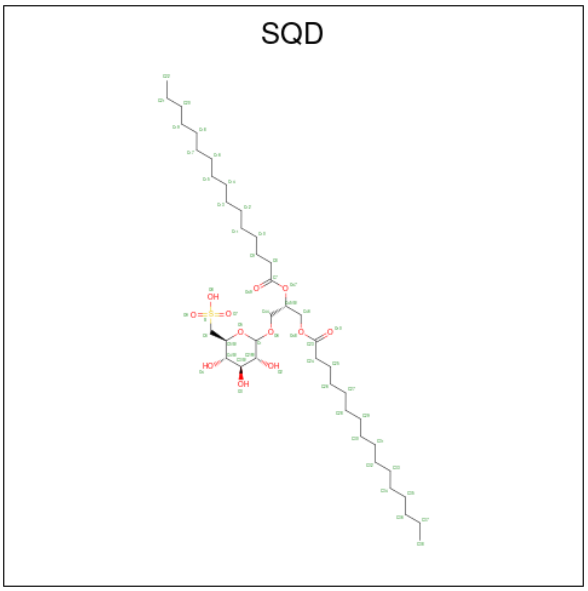
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 39 | A | 1 | Total C<br>40 40 | 0 |
| 39 | A | 1 | Total C<br>40 40 | 0 |
| 39 | B | 1 | Total C<br>40 40 | 0 |
| 39 | B | 1 | Total C<br>40 40 | 0 |
| 39 | B | 1 | Total C<br>40 40 | 0 |
| 39 | C | 1 | Total C<br>40 40 | 0 |
| 39 | C | 1 | Total C<br>40 40 | 0 |
| 39 | C | 1 | Total C<br>40 40 | 0 |
| 39 | D | 1 | Total C<br>40 40 | 0 |
| 39 | H | 1 | Total C<br>40 40 | 0 |
| 39 | K | 1 | Total C<br>40 40 | 0 |
| 39 | 0 | 1 | Total C<br>40 40 | 0 |
| 39 | a | 1 | Total C<br>40 40 | 0 |
| 39 | a | 1 | Total C<br>40 40 | 0 |
| 39 | b | 1 | Total C<br>40 40 | 0 |
| 39 | b | 1 | Total C<br>40 40 | 0 |
| 39 | b | 1 | Total C<br>40 40 | 0 |
| 39 | c | 1 | Total C<br>40 40 | 0 |
| 39 | c | 1 | Total C<br>40 40 | 0 |
| 39 | c | 1 | Total C<br>40 40 | 0 |
| 39 | d | 1 | Total C<br>40 40 | 0 |
| 39 | h | 1 | Total C<br>40 40 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 39 | y | 1 | Total C<br>40 40 | 0 |
| 39 | 5 | 1 | Total C<br>40 40 | 0 |

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



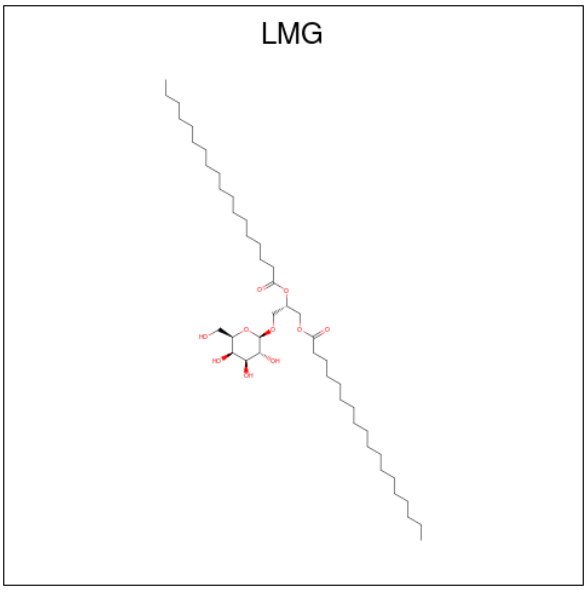

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 40 | A | 1 | Total C O S<br>54 41 12 1 | 0 |
| 40 | B | 1 | Total C O S<br>54 41 12 1 | 0 |
| 40 | B | 1 | Total C O S<br>37 24 12 1 | 0 |
| 40 | L | 1 | Total C O S<br>54 41 12 1 | 0 |
| 40 | a | 1 | Total C O S<br>54 41 12 1 | 0 |
| 40 | b | 1 | Total C O S<br>37 24 12 1 | 0 |
| 40 | 16 | 1 | Total C O S<br>54 41 12 1 | 0 |
| 40 | 17 | 1 | Total C O S<br>49 36 12 1 | 0 |
| 40 | 36 | 1 | Total C O S<br>49 36 12 1 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 40 | 40 | 1 | Total | C | O | S | 0 |
| | | | 54 | 41 | 12 | 1 | |

- Molecule 41 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



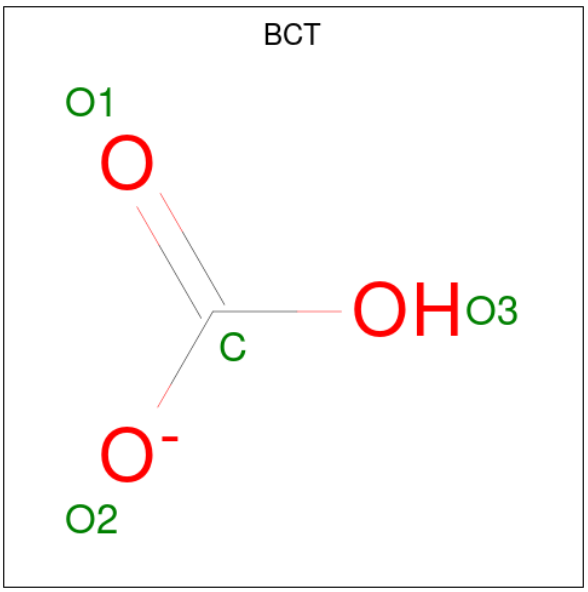

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 41 | A | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 41 | B | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 41 | B | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 41 | C | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 41 | D | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 41 | L | 1 | Total | C | O | 0 |
| | | | 40 | 30 | 10 | |
| 41 | a | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 41 | b | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 41 | b | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |
| 41 | c | 1 | Total | C | O | 0 |
| | | | 51 | 41 | 10 | |

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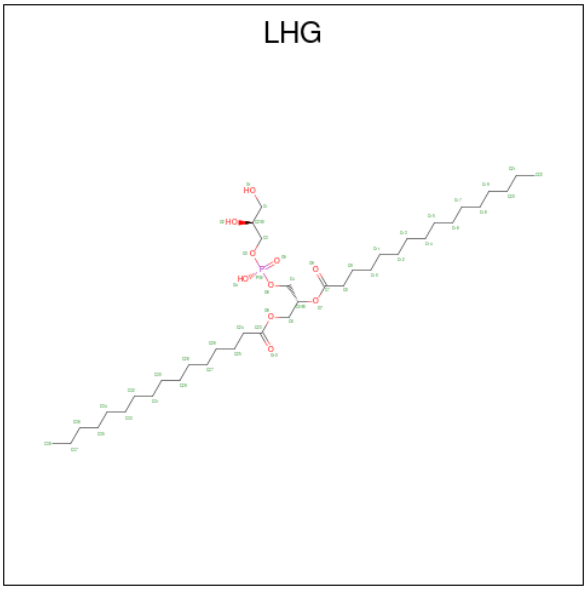
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 41 | d | 1 | Total C O<br>51 41 10 | 0 |
| 41 | l | 1 | Total C O<br>40 30 10 | 0 |
| 41 | 11 | 1 | Total C O<br>42 32 10 | 0 |
| 41 | 11 | 1 | Total C O<br>32 22 10 | 0 |
| 41 | 12 | 1 | Total C O<br>39 29 10 | 0 |
| 41 | 16 | 1 | Total C O<br>36 26 10 | 0 |
| 41 | 17 | 1 | Total C O<br>37 27 10 | 0 |
| 41 | 31 | 1 | Total C O<br>42 32 10 | 0 |
| 41 | 31 | 1 | Total C O<br>32 22 10 | 0 |
| 41 | 32 | 1 | Total C O<br>39 29 10 | 0 |
| 41 | 36 | 1 | Total C O<br>36 26 10 | 0 |
| 41 | 37 | 1 | Total C O<br>37 27 10 | 0 |

- Molecule 42 is BICARBONATE ION (CCD ID: BCT) (formula: $CHO_3$).



| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 42 | A | 1 | Total | C | O | 0 |
| | | | 4 | 1 | 3 | |
| 42 | a | 1 | Total | C | O | 0 |
| | | | 4 | 1 | 3 | |

- Molecule 43 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



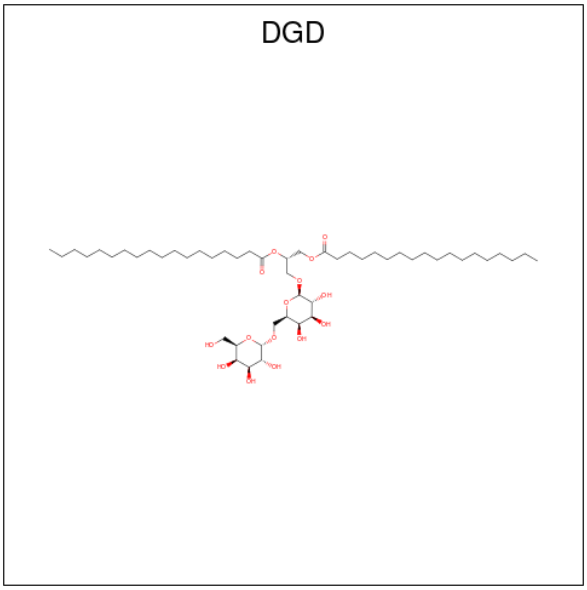

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 43 | B | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 43 | D | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 43 | D | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 43 | D | 1 | Total | C | O | P | 0 |
| | | | 46 | 35 | 10 | 1 | |
| 43 | a | 1 | Total | C | O | P | 0 |
| | | | 46 | 35 | 10 | 1 | |
| 43 | b | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 43 | d | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 43 | d | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 43 | 17 | 1 | Total | C | O | P | 0 |
| | | | 44 | 33 | 10 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 43 | 19 | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 43 | 21 | 1 | Total | C | O | P | 0 |
| | | | 35 | 25 | 9 | 1 | |
| 43 | 21 | 1 | Total | C | O | P | 0 |
| | | | 45 | 34 | 10 | 1 | |
| 43 | 37 | 1 | Total | C | O | P | 0 |
| | | | 44 | 33 | 10 | 1 | |
| 43 | 37 | 1 | Total | C | O | P | 0 |
| | | | 45 | 34 | 10 | 1 | |
| 43 | 39 | 1 | Total | C | O | P | 0 |
| | | | 49 | 38 | 10 | 1 | |
| 43 | 41 | 1 | Total | C | O | P | 0 |
| | | | 35 | 25 | 9 | 1 | |

- Molecule 44 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



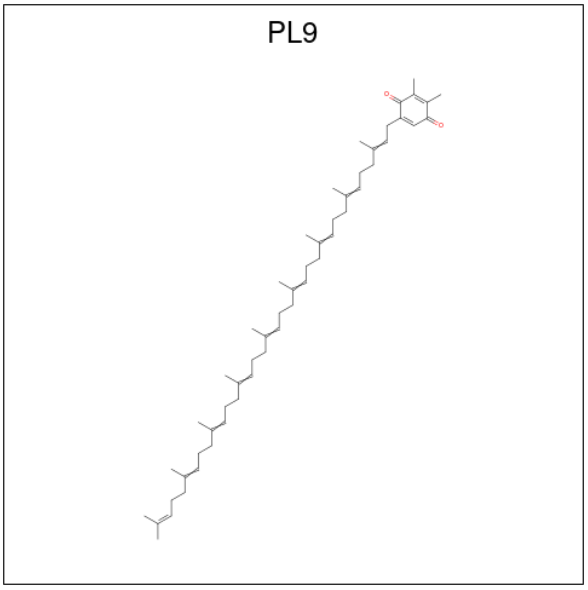

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 44 | C | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |
| 44 | C | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |
| 44 | H | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |
| 44 | J | 1 | Total | C | O | 0 |
| | | | 62 | 47 | 15 | |

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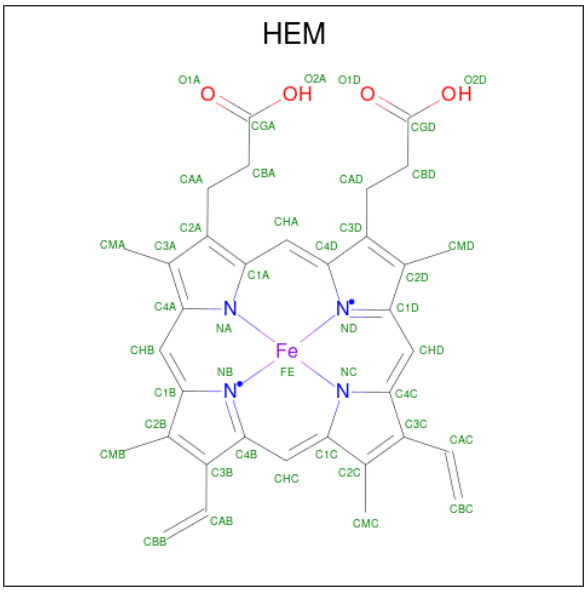
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 44 | c | 1 | Total C O<br>62 47 15 | 0 |
| 44 | c | 1 | Total C O<br>62 47 15 | 0 |
| 44 | h | 1 | Total C O<br>62 47 15 | 0 |
| 44 | j | 1 | Total C O<br>62 47 15 | 0 |

- Molecule 45 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



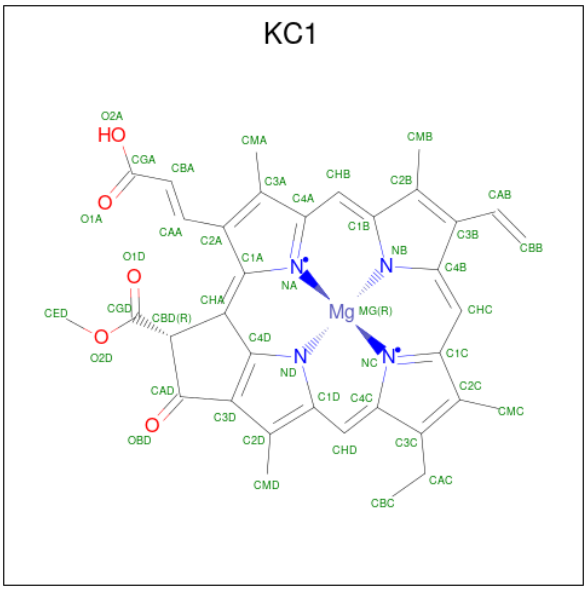

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 45 | D | 1 | Total C O<br>55 53 2 | 0 |
| 45 | D | 1 | Total C O<br>55 53 2 | 0 |
| 45 | d | 1 | Total C O<br>55 53 2 | 0 |
| 45 | d | 1 | Total C O<br>55 53 2 | 0 |

- Molecule 46 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 46 | F | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 46 | V | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 46 | f | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 46 | v | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

- Molecule 47 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 47 | 11 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 11 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 11 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 11 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 12 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 12 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 12 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 13 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 13 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 13 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 13 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 14 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 14 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 14 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 15 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 15 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 15 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 15 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 16 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 16 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 16 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 16 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 47 | 17 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 17 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 17 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 17 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 18 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 19 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 20 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 20 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 20 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 21 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 21 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 31 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 31 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 31 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 31 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 32 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 33 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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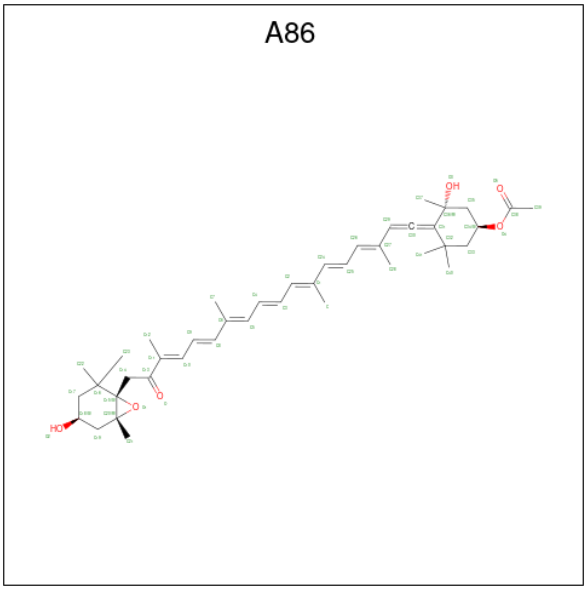
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 47 | 33 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 33 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 33 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 34 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 34 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 34 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 35 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 35 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 35 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 35 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 36 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 36 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 36 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 36 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 37 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 37 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 37 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 37 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 38 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 47 | 39 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 40 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 40 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 40 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 41 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |
| 47 | 41 | 1 | Total | C | Mg | N | O | 0 |
| | | | 45 | 35 | 1 | 4 | 5 | |

- Molecule 48 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 48 | 11 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 11 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 11 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 11 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 11 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 48 | 11 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 12 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 12 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 12 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 12 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 12 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 12 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 12 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 13 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 13 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 13 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 13 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 13 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 14 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 14 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 14 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 14 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 14 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 14 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 15 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 15 | 1 | Total C O<br>48 42 6 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 48 | 15 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 15 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 15 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 15 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 15 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 16 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 16 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 16 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 16 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 17 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 17 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 17 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 17 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 17 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 17 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 17 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 18 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 18 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 18 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 18 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 19 | 1 | Total C O<br>48 42 6 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 48 | 19 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 20 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 20 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 21 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 21 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 21 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 21 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 31 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 31 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 31 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 31 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 31 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 31 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 32 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 32 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 32 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 32 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 32 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 32 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 33 | 1 | Total C O<br>48 42 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 48 | 33 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 33 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 33 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 33 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 34 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 34 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 34 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 34 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 34 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 34 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 35 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 35 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 35 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 35 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 35 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 35 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 35 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 36 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 36 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 36 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |
| 48 | 37 | 1 | Total | C | O | 0 |
| | | | 48 | 42 | 6 | |

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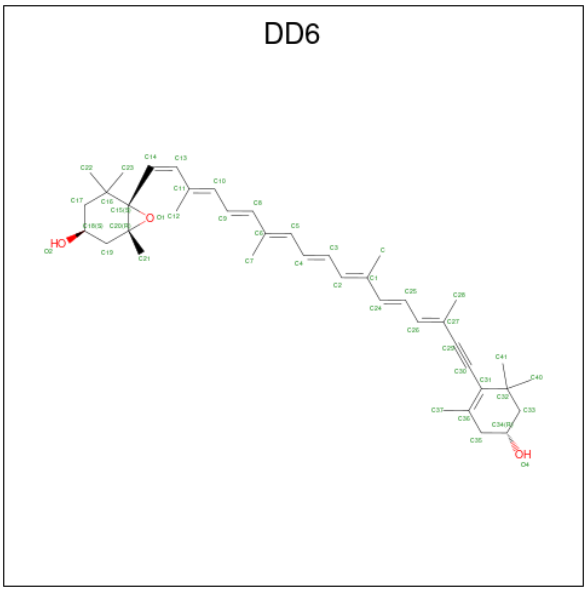
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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 48 | 37 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 37 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 37 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 37 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 37 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 37 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 38 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 38 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 38 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 38 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 39 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 39 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 40 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 40 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 40 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 41 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 41 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 41 | 1 | Total C O<br>48 42 6 | 0 |
| 48 | 41 | 1 | Total C O<br>48 42 6 | 0 |

- Molecule 49 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

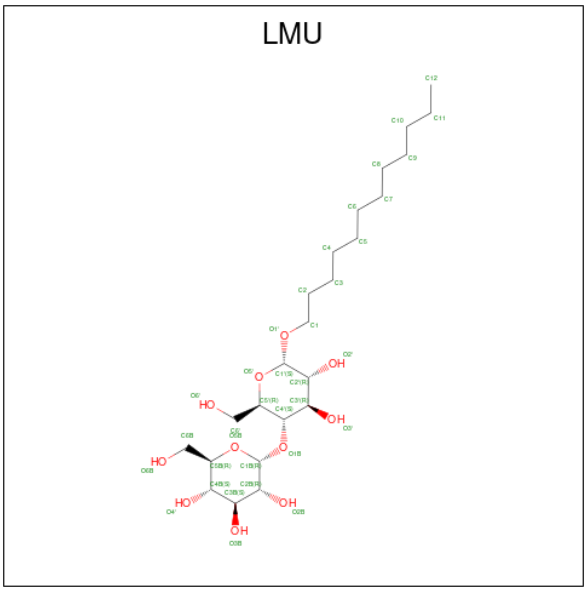
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 49 | 11 | 1 | Total C O<br>19 17 2 | 0 |
| 49 | 12 | 2 | Total C O<br>34 32 2 | 0 |
| 49 | 13 | 3 | Total C O<br>49 47 2 | 0 |
| 49 | 14 | 1 | Total C<br>16 16 | 0 |
| 49 | 15 | 2 | Total C<br>28 28 | 0 |
| 49 | 16 | 2 | Total C<br>24 24 | 0 |
| 49 | 17 | 3 | Total C O<br>54 48 6 | 0 |
| 49 | 18 | 4 | Total C<br>58 58 | 0 |
| 49 | 19 | 1 | Total C<br>12 12 | 0 |
| 49 | 31 | 1 | Total C O<br>19 17 2 | 0 |
| 49 | 32 | 2 | Total C O<br>34 32 2 | 0 |
| 49 | 33 | 3 | Total C O<br>49 47 2 | 0 |
| 49 | 34 | 1 | Total C<br>16 16 | 0 |
| 49 | 35 | 2 | Total C<br>28 28 | 0 |
| 49 | 36 | 2 | Total C<br>24 24 | 0 |
| 49 | 37 | 3 | Total C O<br>54 48 6 | 0 |
| 49 | 38 | 4 | Total C<br>58 58 | 0 |
| 49 | 39 | 1 | Total C<br>12 12 | 0 |

- Molecule 50 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 50 | 16 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 19 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 20 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 20 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 21 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 21 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 36 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 39 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 40 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 40 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 41 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |
| 50 | 41 | 1 | Total | C | O | 0 |
| | | | 43 | 40 | 3 | |

- Molecule 51 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 51 | 19 | 1 | Total C O<br>35 24 11 | 0 |
| 51 | 39 | 1 | Total C O<br>35 24 11 | 0 |

- Molecule 52 is water.

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 52 | B | 5 | Total O<br>5 5 | 0 |
| 52 | C | 3 | Total O<br>3 3 | 0 |
| 52 | D | 4 | Total O<br>4 4 | 0 |
| 52 | Z | 1 | Total O<br>1 1 | 0 |
| 52 | a | 2 | Total O<br>2 2 | 0 |
| 52 | b | 5 | Total O<br>5 5 | 0 |
| 52 | c | 3 | Total O<br>3 3 | 0 |
| 52 | d | 2 | Total O<br>2 2 | 0 |
| 52 | z | 1 | Total O<br>1 1 | 0 |
| 52 | 11 | 3 | Total O<br>3 3 | 0 |

*Continued on next page...*

*Continued from previous page...*

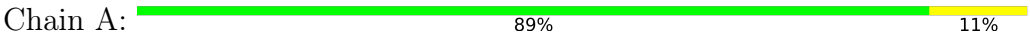
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 52 | 12 | 2 | Total O<br>2 2 | 0 |
| 52 | 13 | 1 | Total O<br>1 1 | 0 |
| 52 | 14 | 1 | Total O<br>1 1 | 0 |
| 52 | 15 | 1 | Total O<br>1 1 | 0 |
| 52 | 16 | 1 | Total O<br>1 1 | 0 |
| 52 | 17 | 2 | Total O<br>2 2 | 0 |
| 52 | 18 | 1 | Total O<br>1 1 | 0 |
| 52 | 19 | 1 | Total O<br>1 1 | 0 |
| 52 | 31 | 3 | Total O<br>3 3 | 0 |
| 52 | 32 | 2 | Total O<br>2 2 | 0 |
| 52 | 33 | 1 | Total O<br>1 1 | 0 |
| 52 | 34 | 1 | Total O<br>1 1 | 0 |
| 52 | 35 | 1 | Total O<br>1 1 | 0 |
| 52 | 36 | 1 | Total O<br>1 1 | 0 |
| 52 | 37 | 2 | Total O<br>2 2 | 0 |
| 52 | 38 | 1 | Total O<br>1 1 | 0 |
| 52 | 39 | 1 | Total O<br>1 1 | 0 |

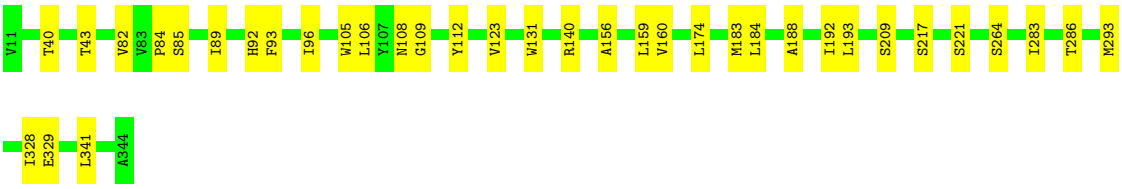
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem II protein D1

Chain A:

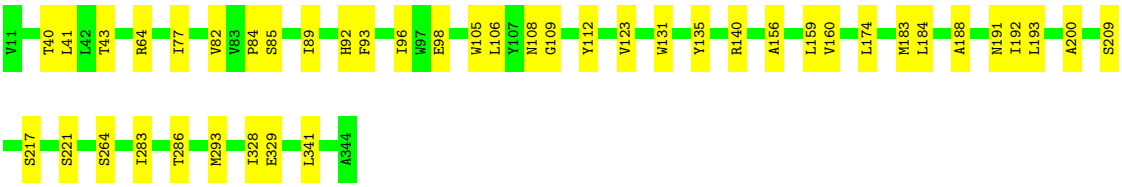



• Molecule 1: Photosystem II protein D1

Chain a:

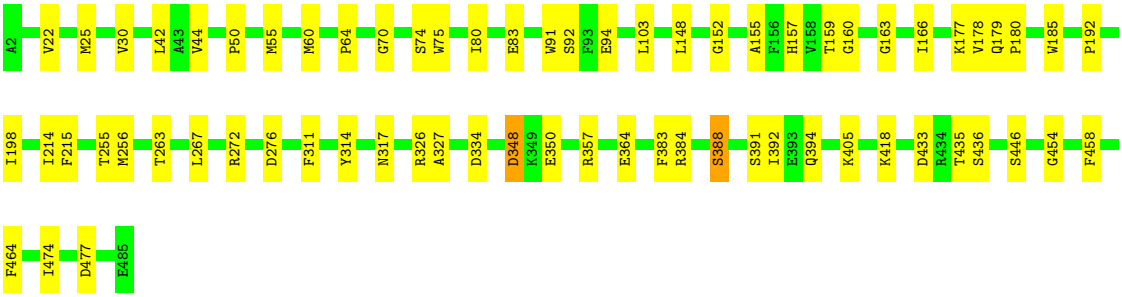



• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:

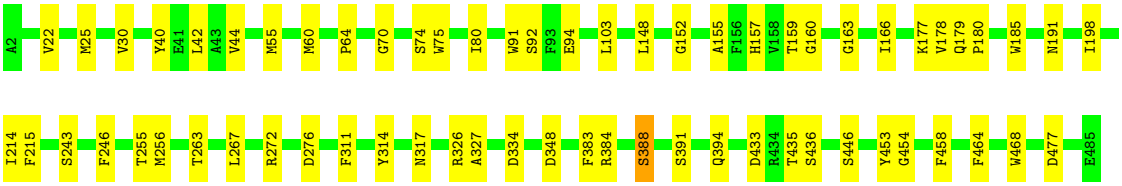



• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

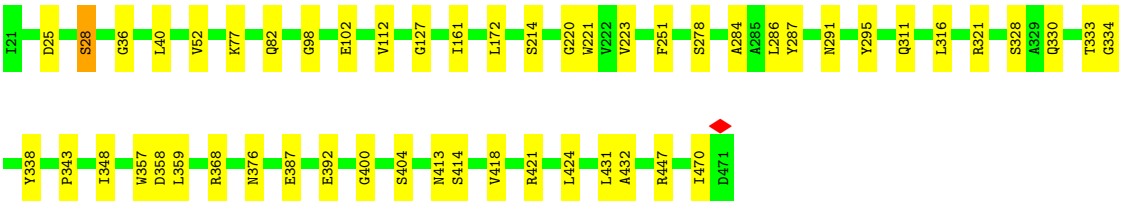





• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

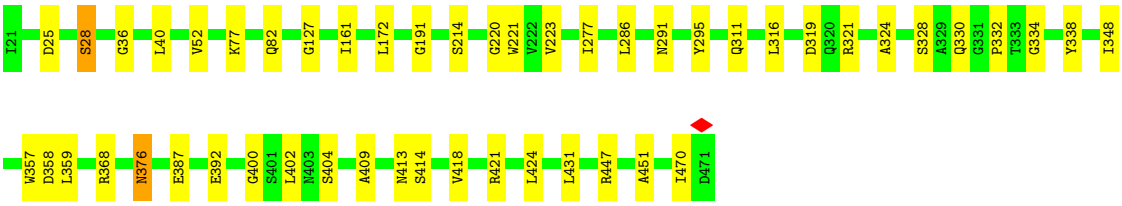



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

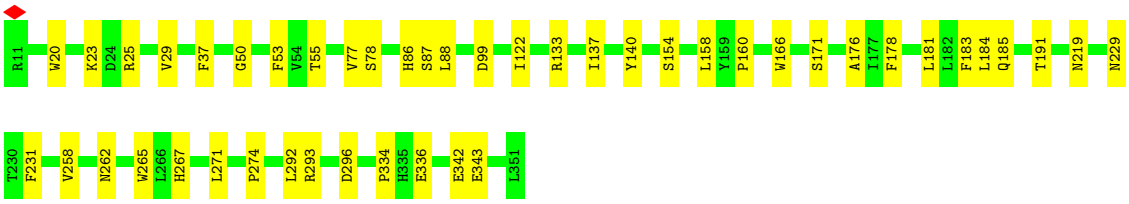



• Molecule 4: Photosystem II D2 protein

Chain D:

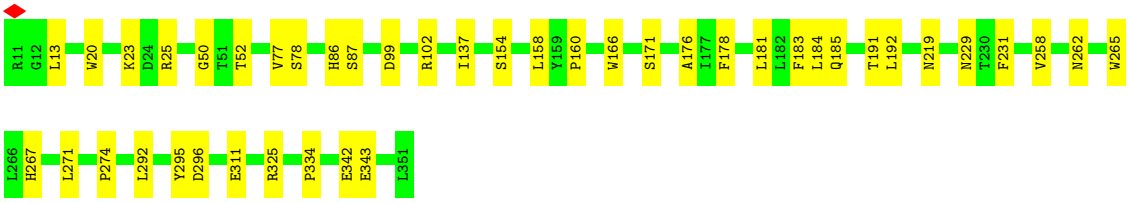



• Molecule 4: Photosystem II D2 protein

Chain d:

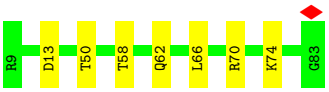



• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

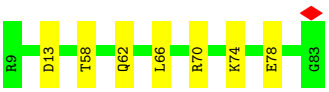



• Molecule 5: Cytochrome b559 subunit alpha

Chain e:




• Molecule 6: Cytochrome b559 subunit beta

Chain F:



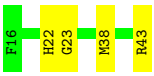




• Molecule 6: Cytochrome b559 subunit beta

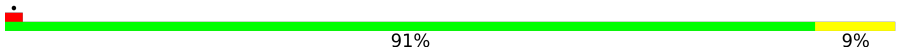
Chain f:

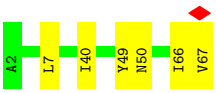



• Molecule 7: Photosystem II reaction center protein H

Chain H:

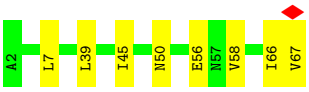



• Molecule 7: Photosystem II reaction center protein H

Chain h:

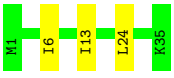



• Molecule 8: Photosystem II reaction center protein I

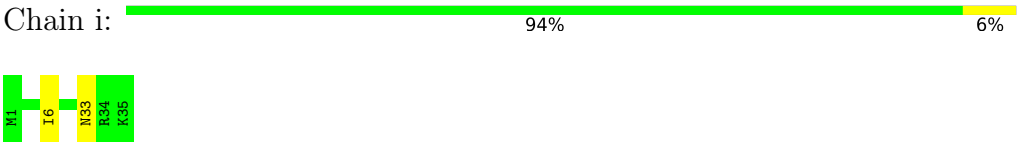
Chain I:



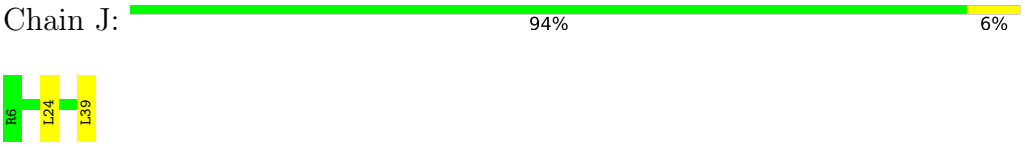

• Molecule 8: Photosystem II reaction center protein I

Chain i:



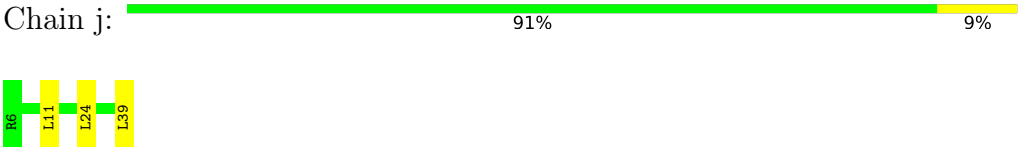

• Molecule 9: Photosystem II reaction center protein J

Chain J:



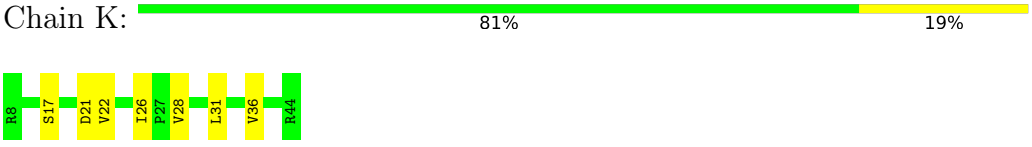

• Molecule 9: Photosystem II reaction center protein J

Chain j:



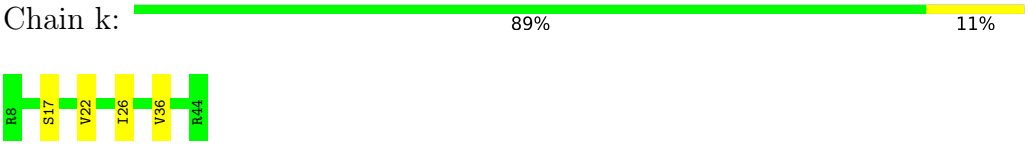

• Molecule 10: Photosystem II reaction center protein K

Chain K:



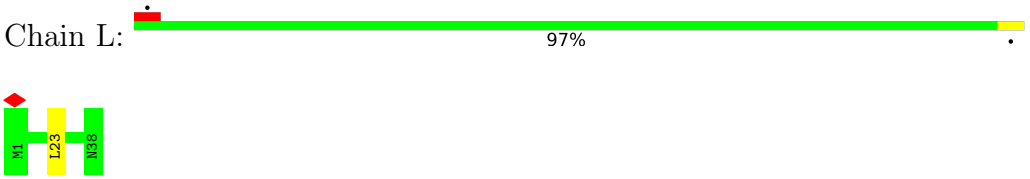

• Molecule 10: Photosystem II reaction center protein K

Chain k:



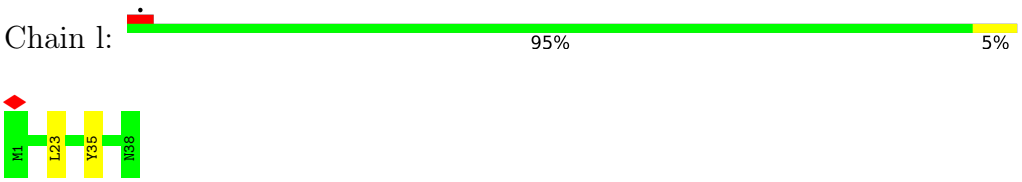

• Molecule 11: Photosystem II reaction center protein L

Chain L:



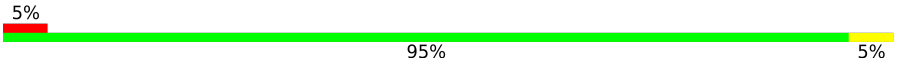

• Molecule 11: Photosystem II reaction center protein L

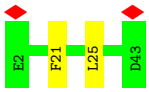
Chain l:




• Molecule 12: Photosystem II subunit

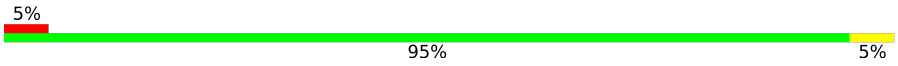
Chain M:




• Molecule 12: Photosystem II subunit

Chain m:



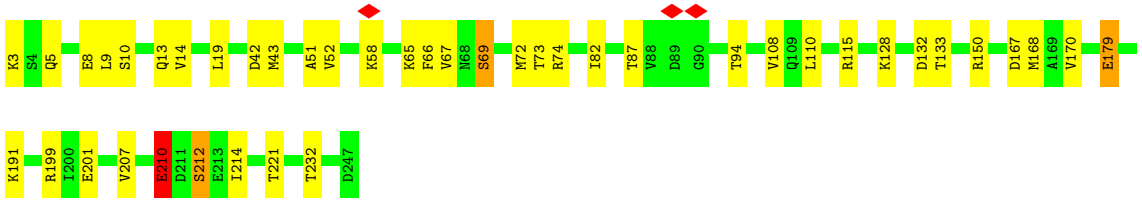




• Molecule 13: Extrinsic protein in photosystem II

Chain O:

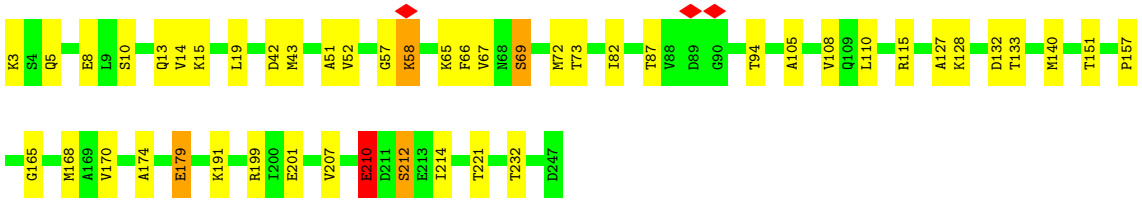



• Molecule 13: Extrinsic protein in photosystem II

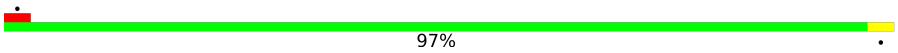
Chain o:

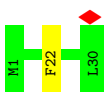



• Molecule 14: Photosystem II reaction center protein T

Chain T:

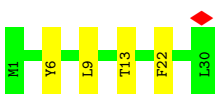



• Molecule 14: Photosystem II reaction center protein T

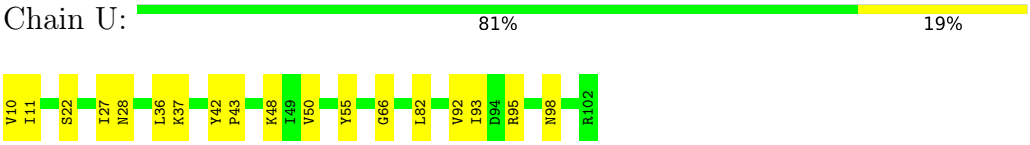
Chain t:



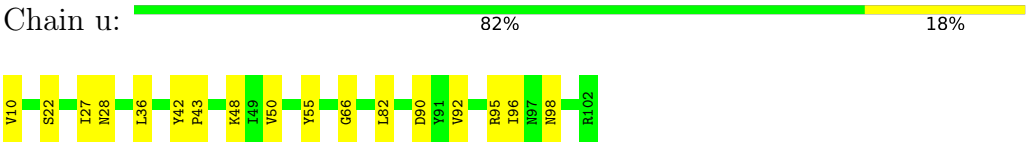
• Molecule 15: Extrinsic protein in photosystem II

Chain U:



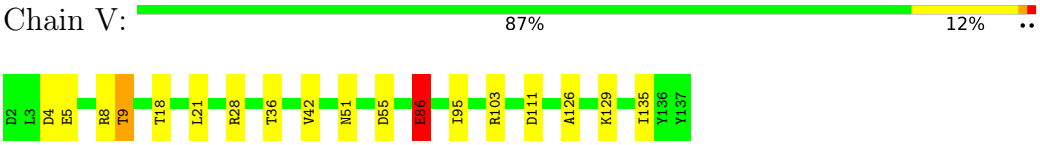

• Molecule 15: Extrinsic protein in photosystem II

Chain u:



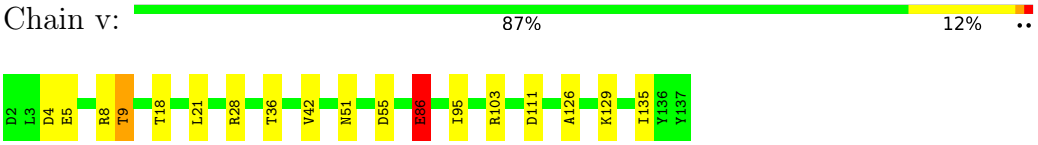

• Molecule 16: Cytochrome c-550

Chain V:



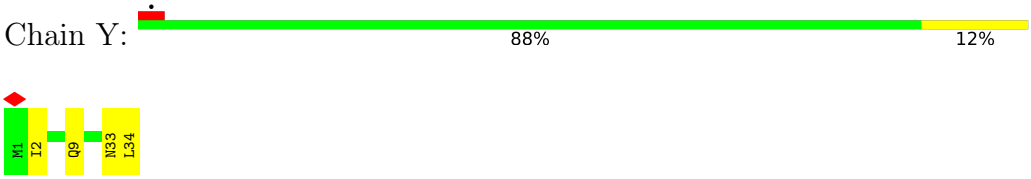

• Molecule 16: Cytochrome c-550

Chain v:



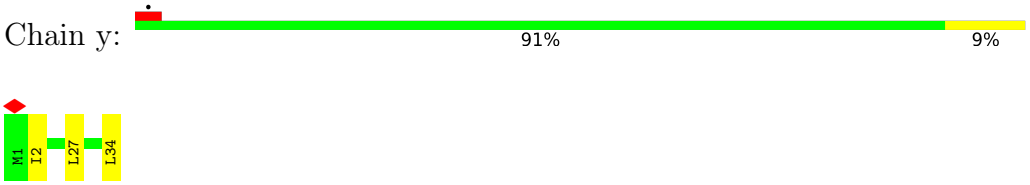

• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



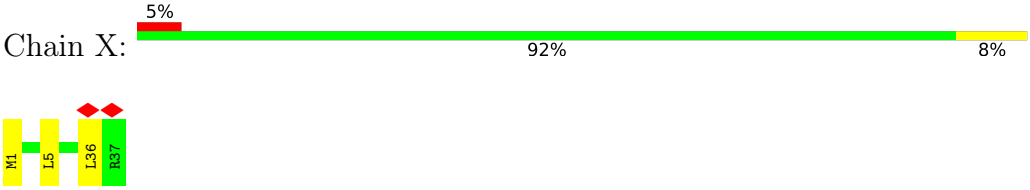

• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:




• Molecule 18: Photosystem II reaction center X protein

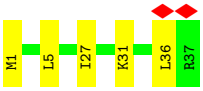
Chain X:



• Molecule 18: Photosystem II reaction center X protein

Chain x:

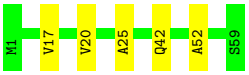



• Molecule 19: Photosystem II reaction center protein Z

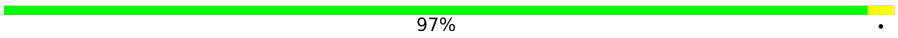
Chain Z:




• Molecule 19: Photosystem II reaction center protein Z

Chain z:







• Molecule 20: Extrinsic protein in photosystem II

Chain Q:







• Molecule 20: Extrinsic protein in photosystem II

Chain q:

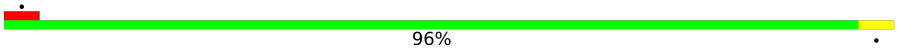


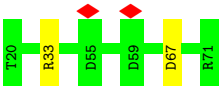




• Molecule 21: Photosystem II reaction center protein W

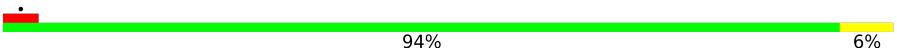
Chain W:

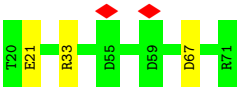



• Molecule 21: Photosystem II reaction center protein W

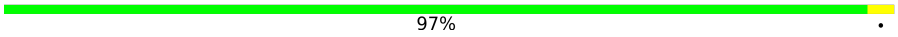
Chain w:



• Molecule 22: Unknown protein 0

Chain 0:

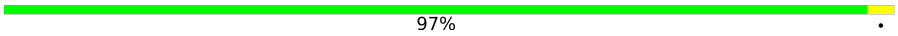






• Molecule 22: Unknown protein 0

Chain 5:

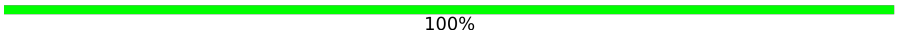






• Molecule 23: Unknown protein 1

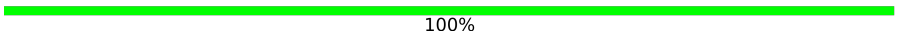
Chain 1:




There are no outlier residues recorded for this chain.

• Molecule 23: Unknown protein 1

Chain 6:




There are no outlier residues recorded for this chain.

• Molecule 24: Chlorophyll a/b-binding protein

Chain 11:



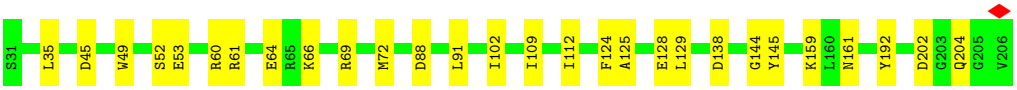




• Molecule 24: Chlorophyll a/b-binding protein

Chain 31:

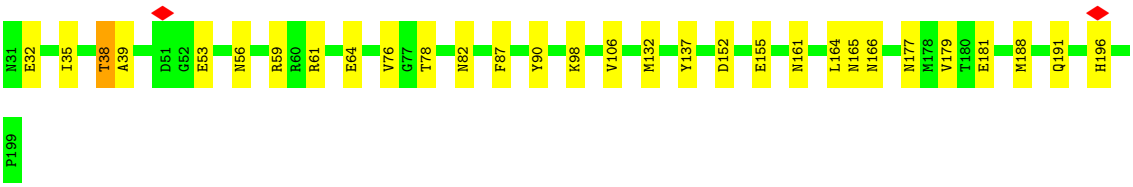



• Molecule 25: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein

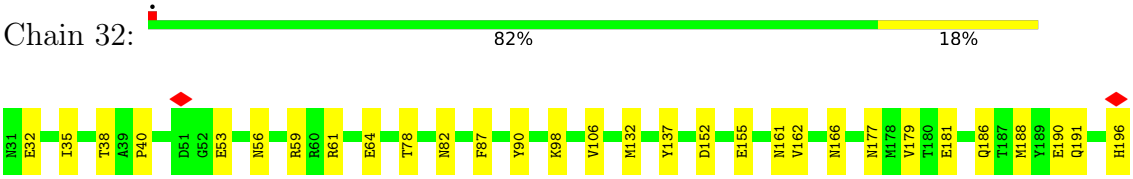
Chain 12:



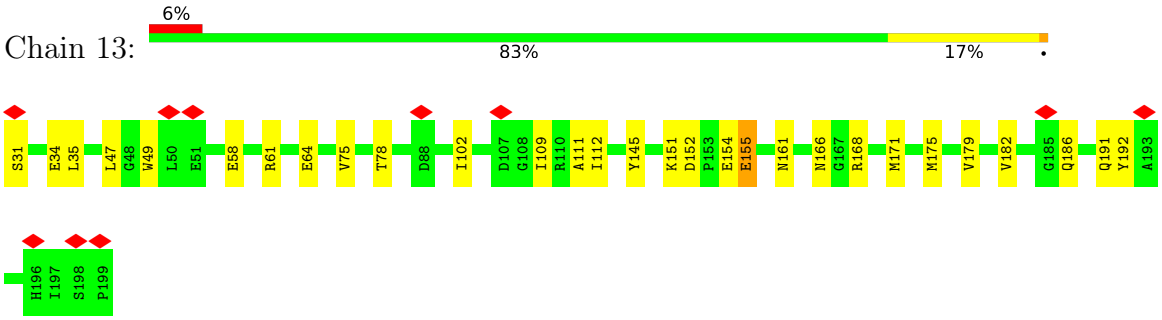
• Molecule 25: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein

Chain 32:



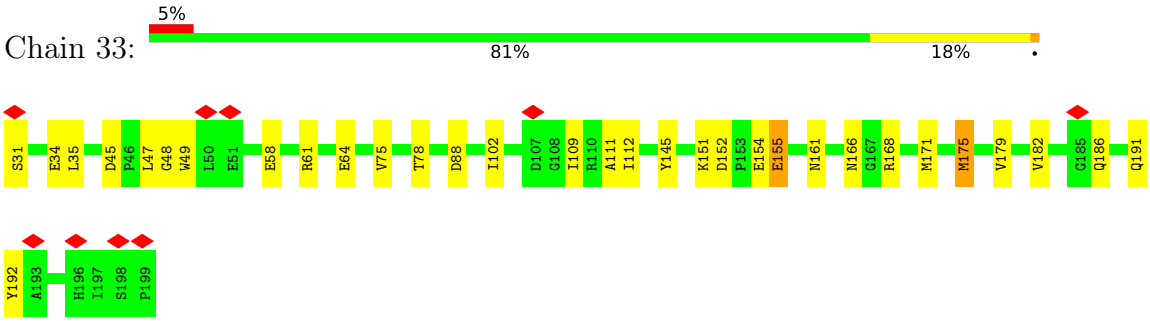

• Molecule 26: Chlorophyll a/b-binding protein

Chain 13:



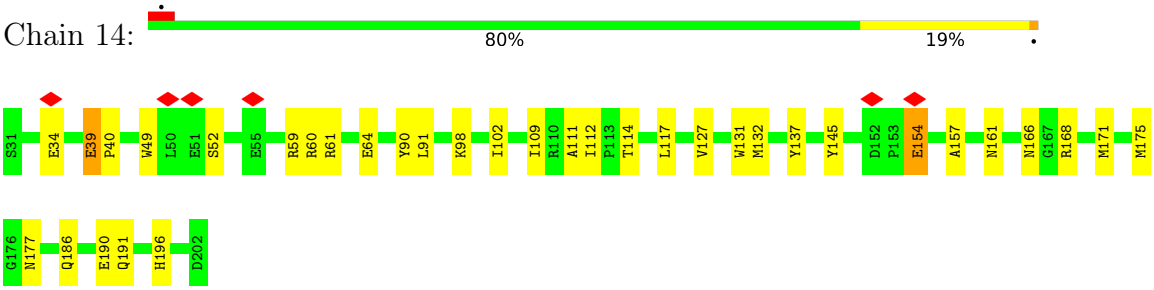

• Molecule 26: Chlorophyll a/b-binding protein

Chain 33:




• Molecule 27: Chlorophyll a/b-binding protein

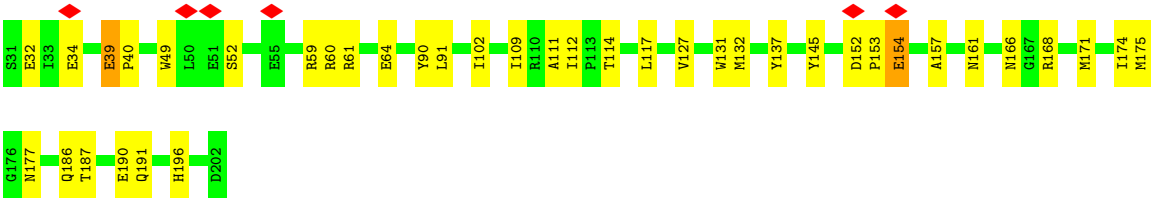
Chain 14:




• Molecule 27: Chlorophyll a/b-binding protein

Chain 34:

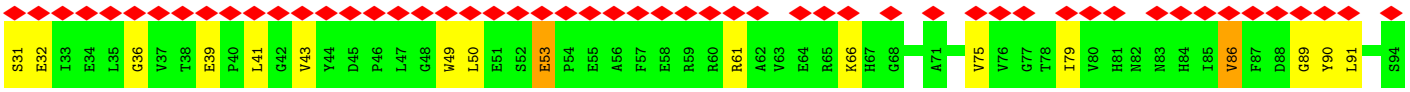


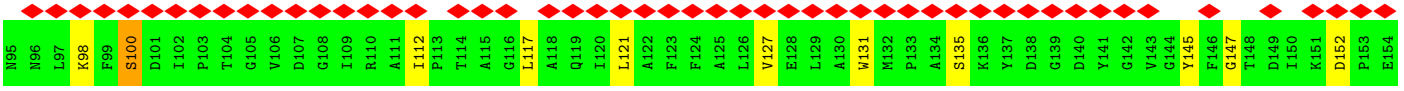


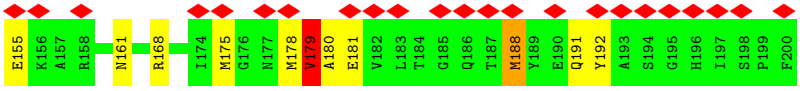

• Molecule 28: Chlorophyll a/b-binding protein

Chain 15:



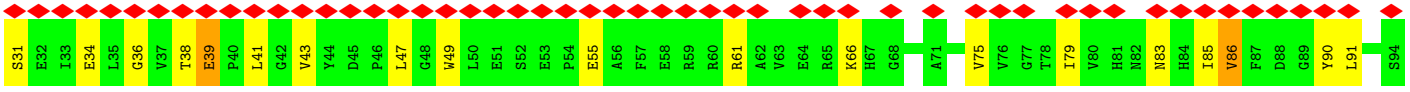



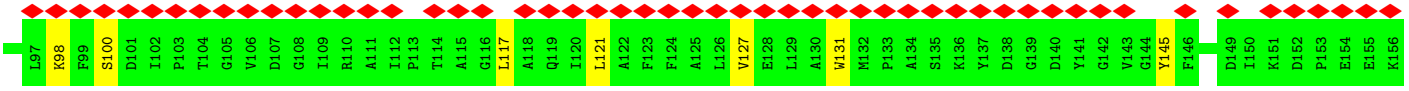



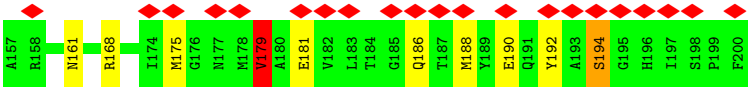

• Molecule 28: Chlorophyll a/b-binding protein

Chain 35:



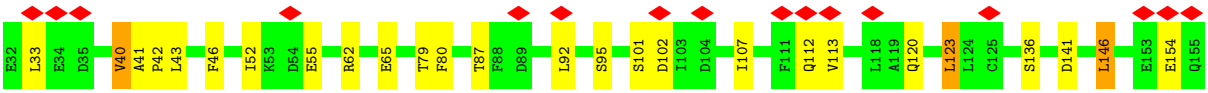



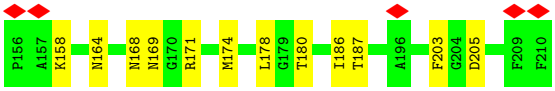




• Molecule 29: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein

Chain 16:

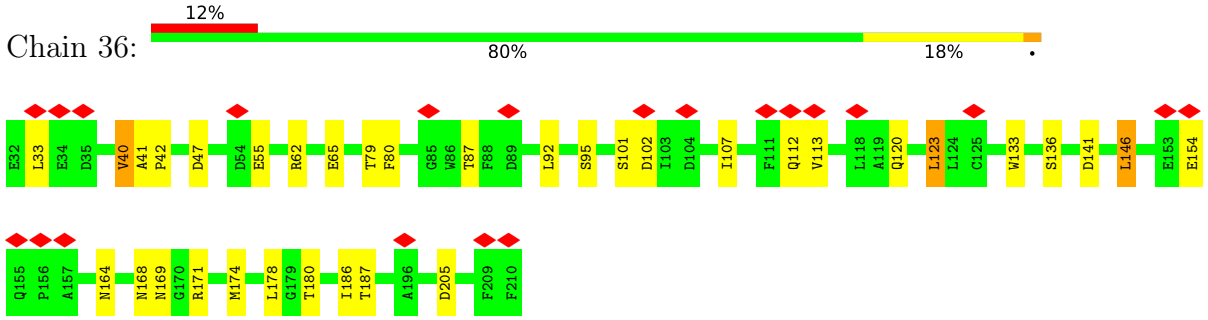


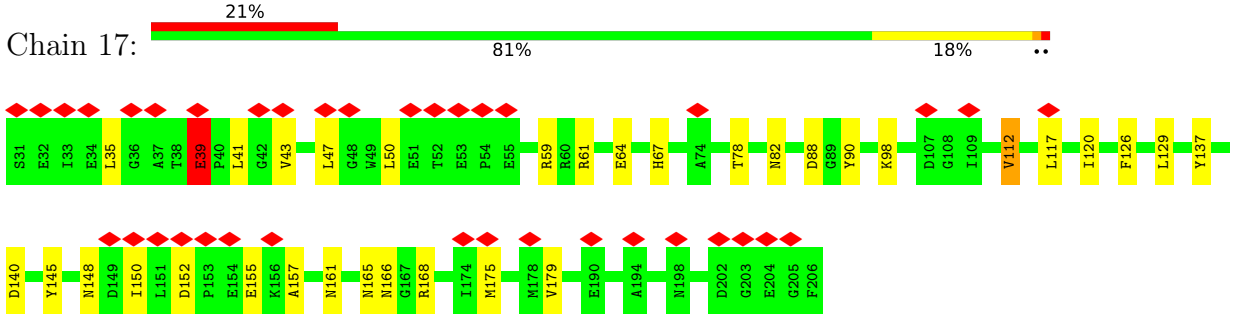

• Molecule 29: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein

Chain 36:



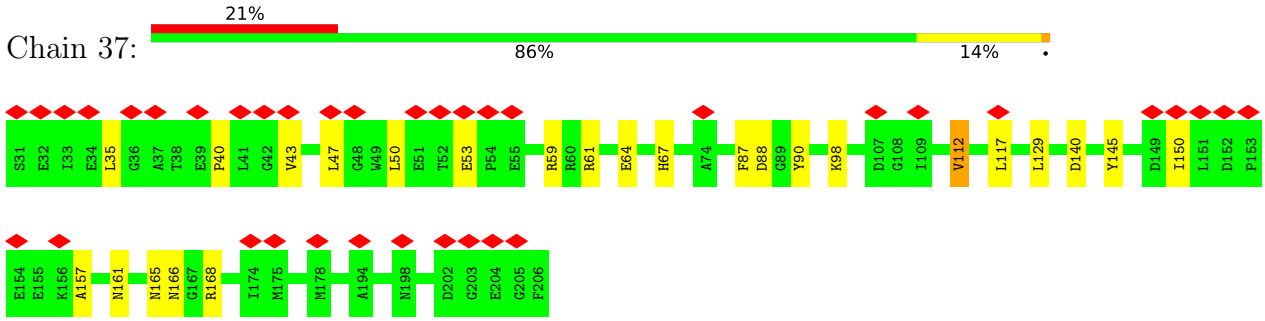

• Molecule 30: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein

Chain 17:



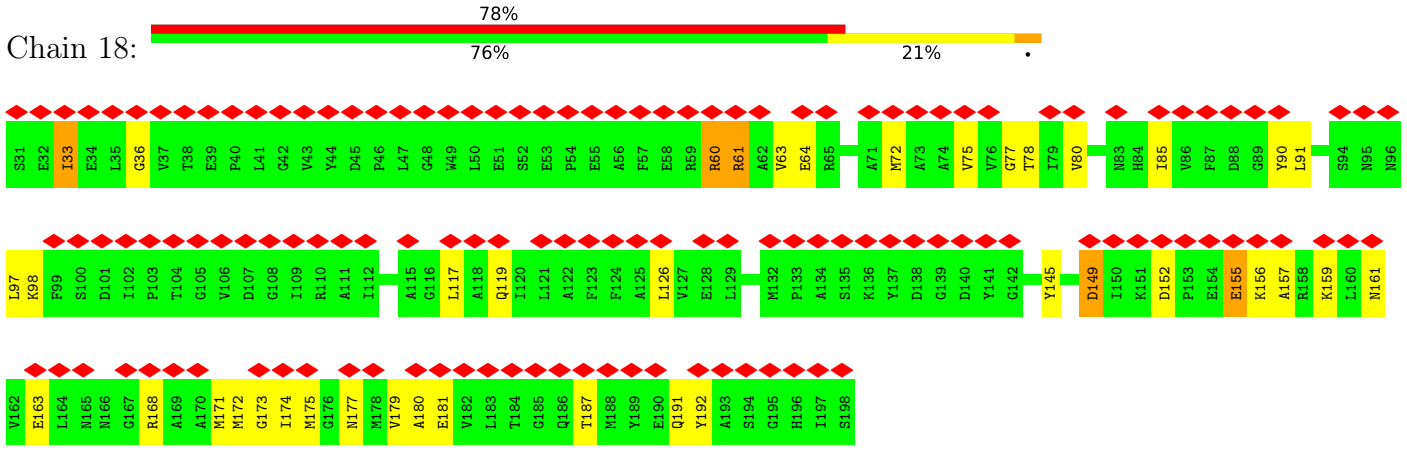

• Molecule 30: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein

Chain 37:



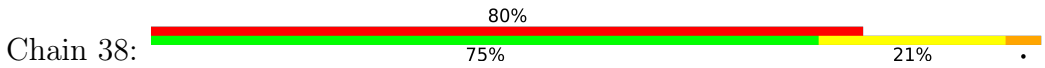

• Molecule 31: Chlorophyll a/b-binding protein

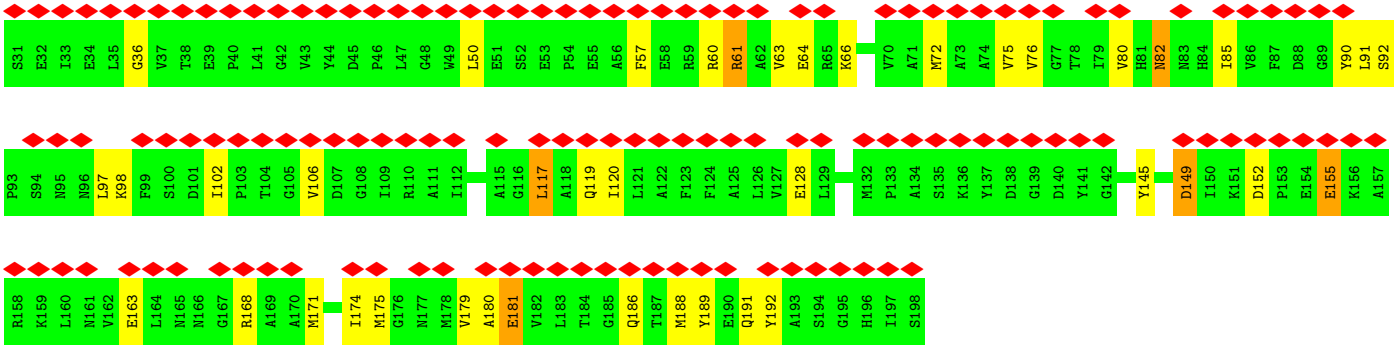
Chain 18:




• Molecule 31: Chlorophyll a/b-binding protein

Chain 38:

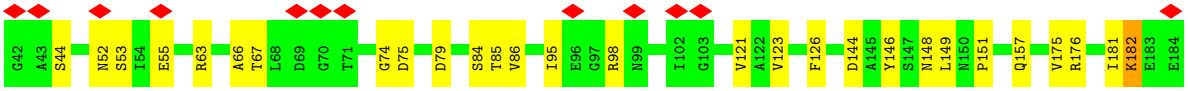





• Molecule 32: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein

Chain 19:

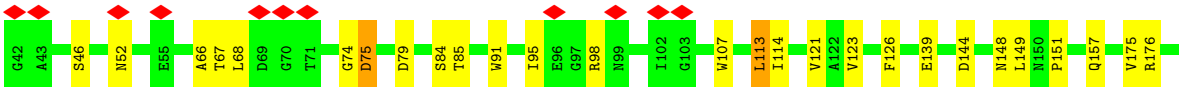



• Molecule 32: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein

Chain 39:

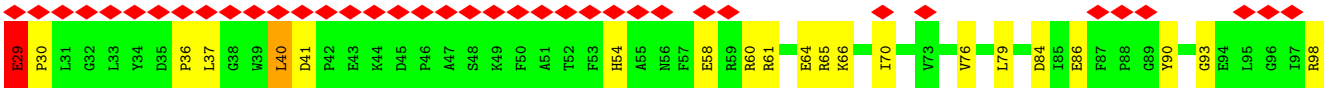



• Molecule 33: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein

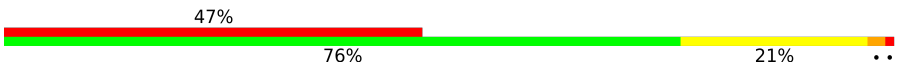
Chain 20:

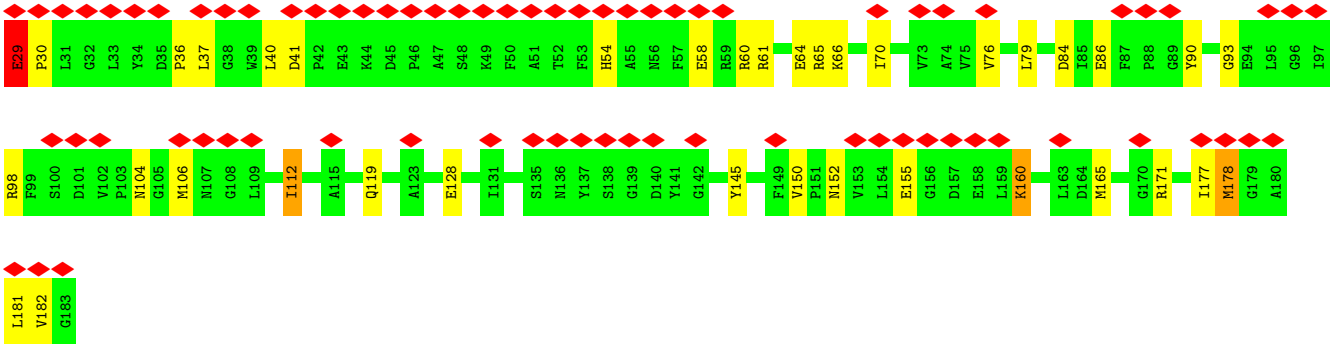



• Molecule 33: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein

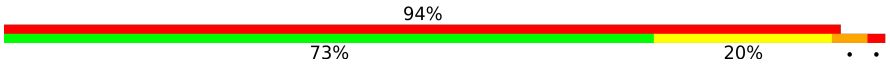
Chain 40:

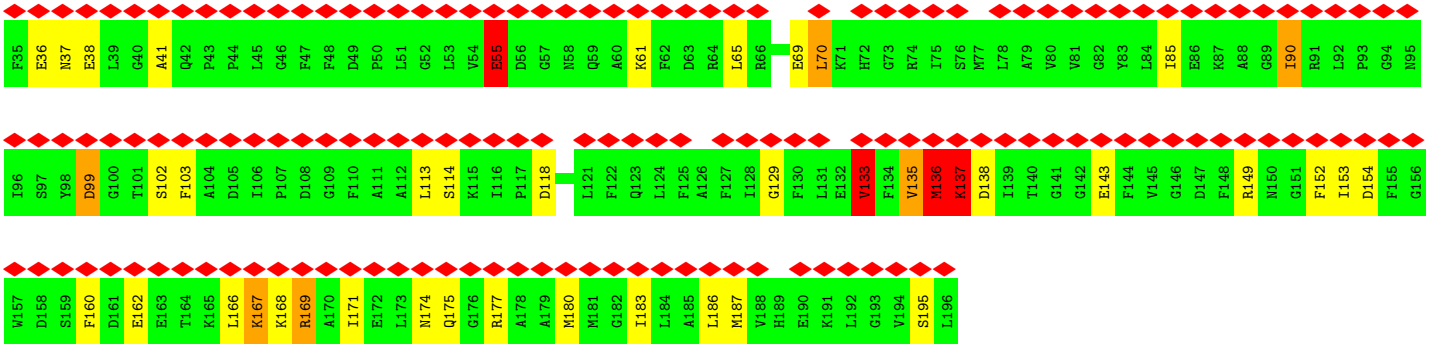





• Molecule 34: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein

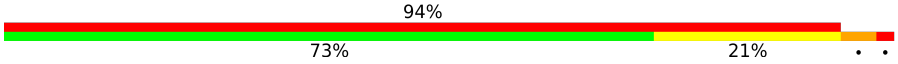
Chain 21:

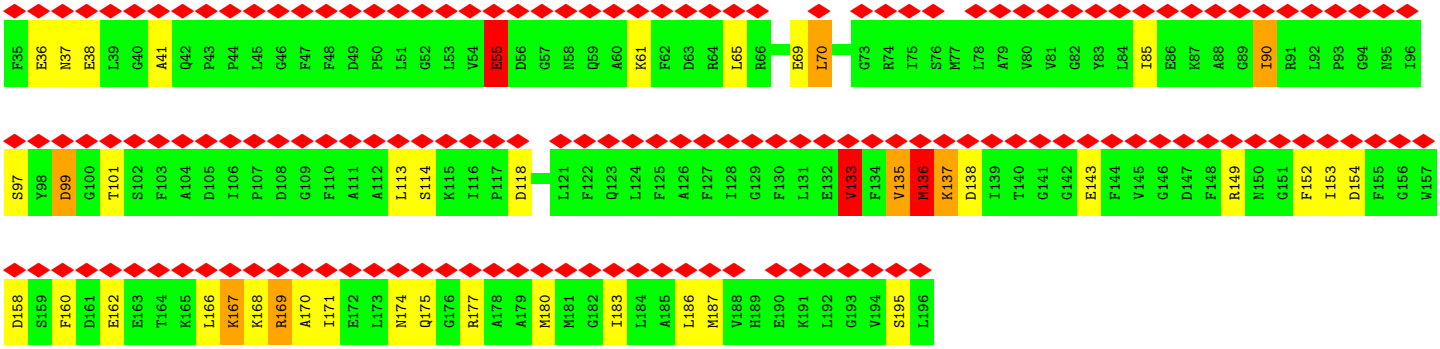



• Molecule 34: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein

Chain 41:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 210825 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 20 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 0.369 | Depositor |
| Minimum map value | -0.142 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.006 | Depositor |
| Recommended contour level | 0.045 | Depositor |
| Map size (Å) | 569.856, 569.856, 569.856 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.113, 1.113, 1.113 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, KC1, BCT, PL9, A86, LMU, OEX, DGD, SQD, DD6, HEM, BCR, FE2, PHO, CLA, LMG, LHG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.39 | 0/2702 | 0.49 | 0/3682 |
| 1 | a | 0.39 | 0/2702 | 0.49 | 0/3682 |
| 2 | B | 0.39 | 0/3942 | 0.47 | 0/5362 |
| 2 | b | 0.39 | 0/3942 | 0.47 | 0/5362 |
| 3 | C | 0.40 | 0/3620 | 0.50 | 0/4933 |
| 3 | c | 0.40 | 0/3620 | 0.50 | 0/4933 |
| 4 | D | 0.40 | 0/2789 | 0.48 | 0/3803 |
| 4 | d | 0.40 | 0/2789 | 0.48 | 0/3803 |
| 5 | E | 0.30 | 0/634 | 0.46 | 0/864 |
| 5 | e | 0.30 | 0/634 | 0.46 | 0/864 |
| 6 | F | 0.36 | 0/235 | 0.53 | 0/316 |
| 6 | f | 0.36 | 0/235 | 0.53 | 0/316 |
| 7 | H | 0.36 | 0/523 | 0.54 | 0/714 |
| 7 | h | 0.36 | 0/523 | 0.54 | 0/714 |
| 8 | I | 0.38 | 0/294 | 0.64 | 0/397 |
| 8 | i | 0.38 | 0/294 | 0.64 | 0/397 |
| 9 | J | 0.26 | 0/260 | 0.40 | 0/351 |
| 9 | j | 0.26 | 0/260 | 0.40 | 0/351 |
| 10 | K | 0.38 | 0/313 | 0.62 | 0/429 |
| 10 | k | 0.38 | 0/313 | 0.62 | 0/429 |
| 11 | L | 0.39 | 0/319 | 0.45 | 0/433 |
| 11 | l | 0.39 | 0/319 | 0.45 | 0/433 |
| 12 | M | 0.36 | 0/321 | 0.56 | 0/433 |
| 12 | m | 0.36 | 0/321 | 0.55 | 0/433 |
| 13 | O | 0.32 | 0/1875 | 0.56 | 2/2528 (0.1%) |
| 13 | o | 0.32 | 0/1875 | 0.56 | 2/2528 (0.1%) |
| 14 | T | 0.31 | 0/256 | 0.41 | 0/346 |
| 14 | t | 0.31 | 0/256 | 0.41 | 0/346 |
| 15 | U | 0.29 | 0/728 | 0.51 | 0/989 |
| 15 | u | 0.29 | 0/728 | 0.51 | 0/989 |
| 16 | V | 0.33 | 0/1056 | 0.56 | 2/1435 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 16 | v | 0.33 | 0/1056 | 0.56 | 2/1435 (0.1%) |
| 17 | Y | 0.26 | 0/252 | 0.61 | 1/341 (0.3%) |
| 17 | y | 0.26 | 0/252 | 0.61 | 1/341 (0.3%) |
| 18 | X | 0.24 | 0/263 | 0.40 | 0/355 |
| 18 | x | 0.24 | 0/263 | 0.41 | 0/355 |
| 19 | Z | 0.41 | 1/456 (0.2%) | 0.54 | 0/624 |
| 19 | z | 0.41 | 1/456 (0.2%) | 0.54 | 0/624 |
| 20 | Q | 0.28 | 0/1203 | 0.55 | 0/1623 |
| 20 | q | 0.28 | 0/1203 | 0.55 | 0/1623 |
| 21 | W | 0.35 | 0/434 | 0.53 | 0/590 |
| 21 | w | 0.35 | 0/434 | 0.53 | 0/590 |
| 24 | 11 | 0.42 | 0/1373 | 0.59 | 1/1861 (0.1%) |
| 24 | 31 | 0.41 | 0/1373 | 0.53 | 0/1861 |
| 25 | 12 | 0.39 | 0/1334 | 0.55 | 0/1810 |
| 25 | 32 | 0.37 | 0/1334 | 0.53 | 0/1810 |
| 26 | 13 | 0.41 | 0/1325 | 0.68 | 2/1797 (0.1%) |
| 26 | 33 | 0.44 | 0/1325 | 0.71 | 2/1797 (0.1%) |
| 27 | 14 | 0.41 | 1/1349 (0.1%) | 0.80 | 3/1829 (0.2%) |
| 27 | 34 | 0.42 | 1/1349 (0.1%) | 0.84 | 6/1829 (0.3%) |
| 28 | 15 | 0.35 | 0/1337 | 0.92 | 4/1813 (0.2%) |
| 28 | 35 | 0.39 | 0/1337 | 0.90 | 1/1813 (0.1%) |
| 29 | 16 | 0.30 | 0/1425 | 0.70 | 3/1930 (0.2%) |
| 29 | 36 | 0.30 | 0/1425 | 0.70 | 3/1930 (0.2%) |
| 30 | 17 | 0.36 | 0/1386 | 0.77 | 2/1879 (0.1%) |
| 30 | 37 | 0.39 | 0/1386 | 0.75 | 2/1879 (0.1%) |
| 31 | 18 | 0.49 | 0/1317 | 1.09 | 10/1785 (0.6%) |
| 31 | 38 | 0.54 | 2/1317 (0.2%) | 1.10 | 7/1785 (0.4%) |
| 32 | 19 | 0.36 | 0/1796 | 0.70 | 6/2445 (0.2%) |
| 32 | 39 | 0.38 | 0/1796 | 0.74 | 6/2445 (0.2%) |
| 33 | 20 | 0.39 | 0/1224 | 0.89 | 4/1656 (0.2%) |
| 33 | 40 | 0.39 | 0/1224 | 0.89 | 4/1656 (0.2%) |
| 34 | 21 | 0.48 | 0/1290 | 1.28 | 20/1735 (1.2%) |
| 34 | 41 | 0.48 | 0/1290 | 1.28 | 20/1735 (1.2%) |
| All | All | 0.38 | 6/75262 (0.0%) | 0.66 | 116/102176 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 3 | C | 0 | 1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 3 | c | 0 | 1 |
| 13 | O | 0 | 2 |
| 13 | o | 0 | 2 |
| 20 | Q | 0 | 1 |
| 20 | q | 0 | 1 |
| 22 | 0 | 0 | 1 |
| 22 | 5 | 0 | 1 |
| 27 | 14 | 0 | 1 |
| 27 | 34 | 0 | 1 |
| 28 | 35 | 0 | 2 |
| 29 | 16 | 0 | 1 |
| 29 | 36 | 0 | 1 |
| 32 | 19 | 0 | 1 |
| 32 | 39 | 0 | 1 |
| 33 | 20 | 0 | 3 |
| 33 | 40 | 0 | 3 |
| 34 | 21 | 0 | 3 |
| 34 | 41 | 0 | 3 |
| All | All | 0 | 30 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | Z | 20 | VAL | CA-CB | -5.48 | 1.51 | 1.54 |
| 19 | z | 20 | VAL | CA-CB | -5.45 | 1.51 | 1.54 |
| 31 | 38 | 82 | ASN | CG-OD1 | -5.41 | 1.13 | 1.23 |
| 31 | 38 | 60 | ARG | CZ-NH1 | -5.29 | 1.25 | 1.32 |
| 27 | 34 | 154 | GLU | CB-CG | -5.24 | 1.36 | 1.52 |
| 27 | 14 | 154 | GLU | CB-CG | -5.22 | 1.36 | 1.52 |

All (116) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | 21 | 70 | LEU | CA-CB-CG | 13.98 | 165.22 | 116.30 |
| 34 | 41 | 70 | LEU | CA-CB-CG | 13.96 | 165.18 | 116.30 |
| 34 | 21 | 136 | MET | CB-CG-SD | 13.02 | 151.75 | 112.70 |
| 34 | 41 | 136 | MET | CB-CG-SD | 13.02 | 151.75 | 112.70 |
| 27 | 34 | 154 | GLU | CA-CB-CG | 11.95 | 137.99 | 114.10 |
| 34 | 41 | 136 | MET | CA-CB-CG | -11.41 | 91.28 | 114.10 |
| 34 | 21 | 136 | MET | CA-CB-CG | -11.40 | 91.30 | 114.10 |
| 27 | 14 | 154 | GLU | CA-CB-CG | 10.32 | 134.75 | 114.10 |
| 34 | 21 | 169 | ARG | CA-CB-CG | 10.06 | 134.22 | 114.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 34 | 41 | 169 | ARG | CA-CB-CG | 10.05 | 134.20 | 114.10 |
| 34 | 21 | 169 | ARG | CB-CG-CD | 9.87 | 134.01 | 111.30 |
| 34 | 41 | 169 | ARG | CB-CG-CD | 9.87 | 134.01 | 111.30 |
| 34 | 41 | 38 | GLU | CA-CB-CG | 9.43 | 132.96 | 114.10 |
| 26 | 33 | 175 | MET | CG-SD-CE | -9.41 | 80.19 | 100.90 |
| 34 | 21 | 38 | GLU | CA-CB-CG | 9.39 | 132.88 | 114.10 |
| 26 | 13 | 175 | MET | CG-SD-CE | -9.24 | 80.56 | 100.90 |
| 27 | 34 | 154 | GLU | N-CA-CB | 8.64 | 124.02 | 110.46 |
| 34 | 21 | 55 | GLU | CA-CB-CG | 8.29 | 130.69 | 114.10 |
| 34 | 41 | 55 | GLU | CA-CB-CG | 8.28 | 130.67 | 114.10 |
| 31 | 38 | 180 | ALA | CA-C-N | -8.15 | 108.74 | 122.11 |
| 31 | 38 | 180 | ALA | C-N-CA | -8.15 | 108.74 | 122.11 |
| 16 | V | 86 | GLU | CA-CB-CG | 8.02 | 130.15 | 114.10 |
| 16 | v | 86 | GLU | CA-CB-CG | 7.99 | 130.08 | 114.10 |
| 31 | 38 | 60 | ARG | NE-CZ-NH2 | 7.93 | 126.34 | 119.20 |
| 27 | 14 | 154 | GLU | N-CA-CB | 7.82 | 122.74 | 110.46 |
| 13 | o | 210 | GLU | CA-CB-CG | 7.71 | 129.53 | 114.10 |
| 13 | O | 210 | GLU | CA-CB-CG | 7.69 | 129.47 | 114.10 |
| 34 | 21 | 133 | VAL | CG1-CB-CG2 | -7.34 | 94.66 | 110.80 |
| 34 | 41 | 133 | VAL | CG1-CB-CG2 | -7.33 | 94.66 | 110.80 |
| 32 | 39 | 113 | LEU | CA-C-N | -7.20 | 111.41 | 121.77 |
| 32 | 39 | 113 | LEU | C-N-CA | -7.20 | 111.41 | 121.77 |
| 34 | 21 | 135 | VAL | CG1-CB-CG2 | -7.18 | 95.00 | 110.80 |
| 34 | 41 | 135 | VAL | CG1-CB-CG2 | -7.17 | 95.02 | 110.80 |
| 31 | 18 | 60 | ARG | CG-CD-NE | 7.15 | 127.73 | 112.00 |
| 33 | 20 | 29 | GLU | CA-CB-CG | 7.12 | 128.34 | 114.10 |
| 33 | 40 | 29 | GLU | CA-CB-CG | 7.09 | 128.29 | 114.10 |
| 27 | 34 | 154 | GLU | CB-CG-CD | -7.08 | 100.57 | 112.60 |
| 28 | 15 | 53 | GLU | CA-CB-CG | 7.02 | 128.14 | 114.10 |
| 31 | 38 | 61 | ARG | CB-CG-CD | 6.90 | 127.17 | 111.30 |
| 24 | 11 | 58 | GLU | CA-CB-CG | 6.86 | 127.81 | 114.10 |
| 32 | 19 | 182 | LYS | CG-CD-CE | -6.84 | 95.56 | 111.30 |
| 32 | 19 | 248 | GLU | CA-CB-CG | -6.84 | 100.42 | 114.10 |
| 34 | 41 | 70 | LEU | CB-CG-CD1 | -6.81 | 90.28 | 110.70 |
| 34 | 21 | 70 | LEU | CB-CG-CD1 | -6.80 | 90.31 | 110.70 |
| 31 | 18 | 61 | ARG | CB-CG-CD | 6.62 | 126.54 | 111.30 |
| 34 | 21 | 69 | GLU | CA-C-N | -6.55 | 109.87 | 122.06 |
| 34 | 21 | 69 | GLU | C-N-CA | -6.55 | 109.87 | 122.06 |
| 34 | 41 | 69 | GLU | CA-C-N | -6.52 | 109.93 | 122.06 |
| 34 | 41 | 69 | GLU | C-N-CA | -6.52 | 109.93 | 122.06 |
| 32 | 19 | 74 | GLY | CA-C-N | -6.45 | 113.60 | 122.30 |
| 32 | 19 | 74 | GLY | C-N-CA | -6.45 | 113.60 | 122.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 39 | 74 | GLY | CA-C-N | -6.44 | 113.60 | 122.30 |
| 32 | 39 | 74 | GLY | C-N-CA | -6.44 | 113.60 | 122.30 |
| 33 | 20 | 112 | ILE | CG1-CB-CG2 | -6.43 | 91.41 | 110.70 |
| 33 | 40 | 112 | ILE | CG1-CB-CG2 | -6.43 | 91.41 | 110.70 |
| 32 | 39 | 248 | GLU | CA-CB-CG | -6.40 | 101.31 | 114.10 |
| 13 | O | 210 | GLU | CB-CG-CD | 6.36 | 123.42 | 112.60 |
| 13 | o | 210 | GLU | CB-CG-CD | 6.33 | 123.36 | 112.60 |
| 30 | 17 | 39 | GLU | CB-CG-CD | 6.32 | 123.34 | 112.60 |
| 34 | 41 | 99 | ASP | N-CA-CB | -6.32 | 101.24 | 110.53 |
| 34 | 21 | 99 | ASP | N-CA-CB | -6.31 | 101.26 | 110.53 |
| 28 | 15 | 50 | LEU | CA-CB-CG | 6.31 | 138.38 | 116.30 |
| 33 | 20 | 29 | GLU | CB-CG-CD | 6.20 | 123.14 | 112.60 |
| 33 | 40 | 29 | GLU | CB-CG-CD | 6.19 | 123.12 | 112.60 |
| 34 | 41 | 70 | LEU | CB-CG-CD2 | 6.11 | 129.04 | 110.70 |
| 31 | 18 | 149 | ASP | CA-CB-CG | 6.10 | 118.70 | 112.60 |
| 34 | 21 | 70 | LEU | CB-CG-CD2 | 6.10 | 129.00 | 110.70 |
| 27 | 34 | 154 | GLU | CB-CA-C | -6.04 | 98.13 | 109.72 |
| 31 | 38 | 61 | ARG | CG-CD-NE | 5.99 | 125.19 | 112.00 |
| 32 | 39 | 248 | GLU | N-CA-CB | -5.92 | 102.71 | 110.88 |
| 28 | 15 | 188 | MET | CB-CG-SD | 5.91 | 130.42 | 112.70 |
| 28 | 35 | 179 | VAL | CG1-CB-CG2 | -5.84 | 97.94 | 110.80 |
| 34 | 41 | 169 | ARG | CG-CD-NE | -5.84 | 99.15 | 112.00 |
| 34 | 21 | 169 | ARG | CG-CD-NE | -5.84 | 99.15 | 112.00 |
| 31 | 18 | 149 | ASP | CB-CA-C | 5.80 | 119.31 | 109.75 |
| 31 | 18 | 173 | GLY | CA-C-N | -5.74 | 113.53 | 122.09 |
| 31 | 18 | 173 | GLY | C-N-CA | -5.74 | 113.53 | 122.09 |
| 17 | Y | 2 | ILE | N-CA-C | -5.65 | 106.80 | 112.17 |
| 26 | 33 | 175 | MET | CA-CB-CG | -5.64 | 102.81 | 114.10 |
| 27 | 14 | 154 | GLU | CB-CG-CD | -5.62 | 103.04 | 112.60 |
| 33 | 40 | 160 | LYS | CA-CB-CG | 5.61 | 125.31 | 114.10 |
| 17 | y | 2 | ILE | N-CA-C | -5.60 | 106.85 | 112.17 |
| 33 | 20 | 160 | LYS | CA-CB-CG | 5.58 | 125.27 | 114.10 |
| 26 | 13 | 175 | MET | CA-CB-CG | -5.58 | 102.95 | 114.10 |
| 34 | 21 | 55 | GLU | CB-CG-CD | 5.50 | 121.95 | 112.60 |
| 34 | 41 | 55 | GLU | CB-CG-CD | 5.49 | 121.93 | 112.60 |
| 32 | 19 | 248 | GLU | N-CA-CB | -5.46 | 102.63 | 110.65 |
| 16 | v | 86 | GLU | CB-CG-CD | 5.36 | 121.72 | 112.60 |
| 31 | 38 | 149 | ASP | CA-CB-CG | 5.36 | 117.96 | 112.60 |
| 31 | 18 | 60 | ARG | CA-CB-CG | 5.34 | 124.79 | 114.10 |
| 29 | 16 | 101 | SER | CA-C-N | -5.33 | 114.63 | 122.83 |
| 29 | 16 | 101 | SER | C-N-CA | -5.33 | 114.63 | 122.83 |
| 16 | V | 86 | GLU | CB-CG-CD | 5.32 | 121.65 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 29 | 36 | 101 | SER | CA-C-N | -5.30 | 114.67 | 122.83 |
| 29 | 36 | 101 | SER | C-N-CA | -5.30 | 114.67 | 122.83 |
| 34 | 21 | 160 | PHE | CA-C-N | -5.28 | 114.78 | 122.86 |
| 34 | 21 | 160 | PHE | C-N-CA | -5.28 | 114.78 | 122.86 |
| 34 | 41 | 160 | PHE | CA-C-N | -5.28 | 114.78 | 122.86 |
| 34 | 41 | 160 | PHE | C-N-CA | -5.28 | 114.78 | 122.86 |
| 31 | 18 | 33 | ILE | CB-CG1-CD1 | 5.26 | 124.85 | 113.80 |
| 31 | 38 | 149 | ASP | CB-CA-C | 5.22 | 118.65 | 110.19 |
| 28 | 15 | 179 | VAL | CG1-CB-CG2 | -5.21 | 99.33 | 110.80 |
| 29 | 36 | 112 | GLN | CA-CB-CG | 5.20 | 124.50 | 114.10 |
| 29 | 16 | 112 | GLN | CA-CB-CG | 5.17 | 124.44 | 114.10 |
| 32 | 19 | 182 | LYS | CB-CG-CD | 5.17 | 123.19 | 111.30 |
| 27 | 34 | 154 | GLU | CA-C-N | -5.15 | 113.75 | 120.44 |
| 27 | 34 | 154 | GLU | C-N-CA | -5.15 | 113.75 | 120.44 |
| 30 | 37 | 87 | PHE | CA-C-N | 5.10 | 131.29 | 121.54 |
| 30 | 37 | 87 | PHE | C-N-CA | 5.10 | 131.29 | 121.54 |
| 31 | 18 | 156 | LYS | CA-CB-CG | 5.09 | 124.29 | 114.10 |
| 30 | 17 | 39 | GLU | CA-CB-CG | 5.09 | 124.28 | 114.10 |
| 34 | 21 | 168 | LYS | CA-C-N | -5.05 | 114.20 | 122.54 |
| 34 | 21 | 168 | LYS | C-N-CA | -5.05 | 114.20 | 122.54 |
| 34 | 41 | 168 | LYS | CA-C-N | -5.02 | 114.25 | 122.54 |
| 34 | 41 | 168 | LYS | C-N-CA | -5.02 | 114.25 | 122.54 |
| 31 | 18 | 60 | ARG | CD-NE-CZ | 5.00 | 131.40 | 124.40 |

There are no chirality outliers.

All (30) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | 0 | 7 | UNK | Peptide |
| 27 | 14 | 39 | GLU | Peptide |
| 29 | 16 | 146 | LEU | Peptide |
| 32 | 19 | 196 | GLY | Peptide |
| 33 | 20 | 40 | LEU | Peptide |
| 33 | 20 | 41 | ASP | Peptide |
| 33 | 20 | 86 | GLU | Peptide |
| 34 | 21 | 136 | MET | Peptide |
| 34 | 21 | 137 | LYS | Peptide |
| 34 | 21 | 41 | ALA | Peptide |
| 27 | 34 | 39 | GLU | Peptide |
| 28 | 35 | 38 | THR | Peptide |
| 28 | 35 | 39 | GLU | Peptide |
| 29 | 36 | 146 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 32 | 39 | 196 | GLY | Peptide |
| 33 | 40 | 40 | LEU | Peptide |
| 33 | 40 | 41 | ASP | Peptide |
| 33 | 40 | 86 | GLU | Peptide |
| 34 | 41 | 136 | MET | Peptide |
| 34 | 41 | 137 | LYS | Peptide |
| 34 | 41 | 41 | ALA | Peptide |
| 22 | 5 | 7 | UNK | Peptide |
| 3 | C | 220 | GLY | Peptide |
| 13 | O | 58 | LYS | Peptide |
| 13 | O | 73 | THR | Peptide |
| 20 | Q | 61 | VAL | Peptide |
| 3 | c | 220 | GLY | Peptide |
| 13 | o | 58 | LYS | Peptide |
| 13 | o | 73 | THR | Peptide |
| 20 | q | 61 | VAL | Peptide |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 2619 | 0 | 2520 | 28 | 0 |
| 1 | a | 2619 | 0 | 2520 | 35 | 0 |
| 2 | B | 3812 | 0 | 3690 | 50 | 0 |
| 2 | b | 3812 | 0 | 3690 | 48 | 0 |
| 3 | C | 3504 | 0 | 3410 | 35 | 0 |
| 3 | c | 3504 | 0 | 3410 | 36 | 0 |
| 4 | D | 2697 | 0 | 2596 | 35 | 0 |
| 4 | d | 2697 | 0 | 2596 | 34 | 0 |
| 5 | E | 616 | 0 | 602 | 6 | 0 |
| 5 | e | 616 | 0 | 602 | 6 | 0 |
| 6 | F | 228 | 0 | 234 | 4 | 0 |
| 6 | f | 228 | 0 | 234 | 5 | 0 |
| 7 | H | 513 | 0 | 541 | 7 | 0 |
| 7 | h | 513 | 0 | 541 | 8 | 0 |
| 8 | I | 287 | 0 | 306 | 5 | 0 |
| 8 | i | 287 | 0 | 306 | 2 | 0 |
| 9 | J | 254 | 0 | 266 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 9 | j | 254 | 0 | 266 | 3 | 0 |
| 10 | K | 302 | 0 | 316 | 5 | 0 |
| 10 | k | 302 | 0 | 316 | 2 | 0 |
| 11 | L | 310 | 0 | 313 | 1 | 0 |
| 11 | l | 310 | 0 | 313 | 2 | 0 |
| 12 | M | 316 | 0 | 319 | 2 | 0 |
| 12 | m | 316 | 0 | 319 | 2 | 0 |
| 13 | O | 1845 | 0 | 1841 | 26 | 0 |
| 13 | o | 1845 | 0 | 1841 | 30 | 0 |
| 14 | T | 250 | 0 | 268 | 1 | 0 |
| 14 | t | 250 | 0 | 268 | 3 | 0 |
| 15 | U | 713 | 0 | 715 | 12 | 0 |
| 15 | u | 713 | 0 | 715 | 11 | 0 |
| 16 | V | 1037 | 0 | 1031 | 15 | 0 |
| 16 | v | 1037 | 0 | 1031 | 15 | 0 |
| 17 | Y | 250 | 0 | 287 | 3 | 0 |
| 17 | y | 250 | 0 | 287 | 2 | 0 |
| 18 | X | 263 | 0 | 301 | 1 | 0 |
| 18 | x | 263 | 0 | 301 | 4 | 0 |
| 19 | Z | 447 | 0 | 490 | 4 | 0 |
| 19 | z | 447 | 0 | 490 | 1 | 0 |
| 20 | Q | 1180 | 0 | 1165 | 11 | 0 |
| 20 | q | 1180 | 0 | 1165 | 11 | 0 |
| 21 | W | 422 | 0 | 377 | 2 | 0 |
| 21 | w | 422 | 0 | 377 | 3 | 0 |
| 22 | 0 | 155 | 0 | 33 | 0 | 0 |
| 22 | 5 | 155 | 0 | 33 | 0 | 0 |
| 23 | 1 | 150 | 0 | 34 | 0 | 0 |
| 23 | 6 | 150 | 0 | 34 | 0 | 0 |
| 24 | 11 | 1343 | 0 | 1306 | 22 | 0 |
| 24 | 31 | 1343 | 0 | 1306 | 28 | 0 |
| 25 | 12 | 1302 | 0 | 1257 | 20 | 0 |
| 25 | 32 | 1302 | 0 | 1257 | 20 | 0 |
| 26 | 13 | 1296 | 0 | 1267 | 16 | 0 |
| 26 | 33 | 1296 | 0 | 1267 | 18 | 0 |
| 27 | 14 | 1319 | 0 | 1283 | 22 | 0 |
| 27 | 34 | 1319 | 0 | 1283 | 24 | 0 |
| 28 | 15 | 1307 | 0 | 1274 | 20 | 0 |
| 28 | 35 | 1307 | 0 | 1274 | 17 | 0 |
| 29 | 16 | 1386 | 0 | 1314 | 24 | 0 |
| 29 | 36 | 1386 | 0 | 1314 | 21 | 0 |
| 30 | 17 | 1353 | 0 | 1291 | 24 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 30 | 37 | 1353 | 0 | 1291 | 16 | 0 |
| 31 | 18 | 1289 | 0 | 1260 | 26 | 0 |
| 31 | 38 | 1289 | 0 | 1260 | 25 | 0 |
| 32 | 19 | 1746 | 0 | 1684 | 26 | 0 |
| 32 | 39 | 1746 | 0 | 1684 | 23 | 0 |
| 33 | 20 | 1193 | 0 | 1170 | 15 | 0 |
| 33 | 40 | 1193 | 0 | 1170 | 16 | 0 |
| 34 | 21 | 1262 | 0 | 1247 | 20 | 0 |
| 34 | 41 | 1262 | 0 | 1247 | 19 | 0 |
| 35 | A | 10 | 0 | 0 | 0 | 0 |
| 35 | a | 10 | 0 | 0 | 0 | 0 |
| 36 | A | 1 | 0 | 0 | 0 | 0 |
| 36 | a | 1 | 0 | 0 | 0 | 0 |
| 37 | 11 | 343 | 0 | 333 | 11 | 0 |
| 37 | 12 | 407 | 0 | 398 | 11 | 0 |
| 37 | 13 | 329 | 0 | 306 | 7 | 0 |
| 37 | 14 | 394 | 0 | 378 | 8 | 0 |
| 37 | 15 | 329 | 0 | 304 | 9 | 0 |
| 37 | 16 | 293 | 0 | 291 | 8 | 0 |
| 37 | 17 | 238 | 0 | 238 | 8 | 0 |
| 37 | 18 | 459 | 0 | 448 | 17 | 0 |
| 37 | 19 | 531 | 0 | 538 | 17 | 0 |
| 37 | 20 | 254 | 0 | 209 | 2 | 0 |
| 37 | 21 | 380 | 0 | 342 | 9 | 0 |
| 37 | 31 | 343 | 0 | 333 | 7 | 0 |
| 37 | 32 | 472 | 0 | 470 | 16 | 0 |
| 37 | 33 | 329 | 0 | 306 | 6 | 0 |
| 37 | 34 | 394 | 0 | 378 | 8 | 0 |
| 37 | 35 | 329 | 0 | 304 | 12 | 0 |
| 37 | 36 | 293 | 0 | 291 | 11 | 0 |
| 37 | 37 | 238 | 0 | 238 | 4 | 0 |
| 37 | 38 | 459 | 0 | 448 | 10 | 0 |
| 37 | 39 | 531 | 0 | 538 | 17 | 0 |
| 37 | 40 | 254 | 0 | 209 | 3 | 0 |
| 37 | 41 | 380 | 0 | 342 | 6 | 0 |
| 37 | A | 130 | 0 | 144 | 10 | 0 |
| 37 | B | 1102 | 0 | 1213 | 32 | 0 |
| 37 | C | 845 | 0 | 936 | 26 | 0 |
| 37 | D | 260 | 0 | 288 | 8 | 0 |
| 37 | W | 130 | 0 | 143 | 5 | 0 |
| 37 | Z | 110 | 0 | 103 | 5 | 0 |
| 37 | a | 195 | 0 | 216 | 14 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 37 | b | 1102 | 0 | 1213 | 38 | 0 |
| 37 | c | 845 | 0 | 936 | 30 | 0 |
| 37 | d | 195 | 0 | 216 | 5 | 0 |
| 37 | w | 65 | 0 | 71 | 1 | 0 |
| 37 | z | 110 | 0 | 104 | 3 | 0 |
| 38 | A | 64 | 0 | 74 | 2 | 0 |
| 38 | D | 64 | 0 | 74 | 1 | 0 |
| 38 | a | 128 | 0 | 148 | 3 | 0 |
| 39 | 0 | 40 | 0 | 56 | 5 | 0 |
| 39 | 5 | 40 | 0 | 56 | 3 | 0 |
| 39 | A | 80 | 0 | 112 | 6 | 0 |
| 39 | B | 120 | 0 | 167 | 7 | 0 |
| 39 | C | 120 | 0 | 168 | 5 | 0 |
| 39 | D | 40 | 0 | 56 | 4 | 0 |
| 39 | H | 40 | 0 | 56 | 2 | 0 |
| 39 | K | 40 | 0 | 56 | 4 | 0 |
| 39 | a | 80 | 0 | 112 | 5 | 0 |
| 39 | b | 120 | 0 | 167 | 8 | 0 |
| 39 | c | 120 | 0 | 168 | 4 | 0 |
| 39 | d | 40 | 0 | 56 | 3 | 0 |
| 39 | h | 40 | 0 | 56 | 1 | 0 |
| 39 | y | 40 | 0 | 56 | 4 | 0 |
| 40 | 16 | 54 | 0 | 77 | 1 | 0 |
| 40 | 17 | 49 | 0 | 65 | 3 | 0 |
| 40 | 36 | 49 | 0 | 65 | 3 | 0 |
| 40 | 40 | 54 | 0 | 77 | 2 | 0 |
| 40 | A | 54 | 0 | 77 | 1 | 0 |
| 40 | B | 91 | 0 | 114 | 5 | 0 |
| 40 | L | 54 | 0 | 77 | 3 | 0 |
| 40 | a | 54 | 0 | 77 | 0 | 0 |
| 40 | b | 37 | 0 | 37 | 1 | 0 |
| 41 | 11 | 74 | 0 | 88 | 0 | 0 |
| 41 | 12 | 39 | 0 | 48 | 0 | 0 |
| 41 | 16 | 36 | 0 | 42 | 1 | 0 |
| 41 | 17 | 37 | 0 | 44 | 0 | 0 |
| 41 | 31 | 74 | 0 | 88 | 0 | 0 |
| 41 | 32 | 39 | 0 | 48 | 0 | 0 |
| 41 | 36 | 36 | 0 | 42 | 0 | 0 |
| 41 | 37 | 37 | 0 | 44 | 0 | 0 |
| 41 | A | 51 | 0 | 72 | 4 | 0 |
| 41 | B | 102 | 0 | 144 | 7 | 0 |
| 41 | C | 51 | 0 | 72 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 41 | D | 51 | 0 | 72 | 2 | 0 |
| 41 | L | 40 | 0 | 50 | 2 | 0 |
| 41 | a | 51 | 0 | 72 | 4 | 0 |
| 41 | b | 102 | 0 | 144 | 8 | 0 |
| 41 | c | 51 | 0 | 72 | 3 | 0 |
| 41 | d | 51 | 0 | 72 | 2 | 0 |
| 41 | l | 40 | 0 | 50 | 1 | 0 |
| 42 | A | 4 | 0 | 0 | 1 | 0 |
| 42 | a | 4 | 0 | 0 | 1 | 0 |
| 43 | 17 | 44 | 0 | 61 | 1 | 0 |
| 43 | 19 | 49 | 0 | 74 | 10 | 0 |
| 43 | 21 | 80 | 0 | 102 | 3 | 0 |
| 43 | 37 | 89 | 0 | 124 | 4 | 0 |
| 43 | 39 | 49 | 0 | 74 | 8 | 0 |
| 43 | 41 | 35 | 0 | 39 | 0 | 0 |
| 43 | B | 49 | 0 | 74 | 0 | 0 |
| 43 | D | 144 | 0 | 213 | 6 | 0 |
| 43 | a | 46 | 0 | 65 | 3 | 0 |
| 43 | b | 49 | 0 | 74 | 0 | 0 |
| 43 | d | 98 | 0 | 148 | 3 | 0 |
| 44 | C | 124 | 0 | 164 | 4 | 0 |
| 44 | H | 62 | 0 | 82 | 2 | 0 |
| 44 | J | 62 | 0 | 81 | 1 | 0 |
| 44 | c | 124 | 0 | 164 | 4 | 0 |
| 44 | h | 62 | 0 | 82 | 3 | 0 |
| 44 | j | 62 | 0 | 81 | 2 | 0 |
| 45 | D | 110 | 0 | 157 | 5 | 0 |
| 45 | d | 110 | 0 | 157 | 5 | 0 |
| 46 | F | 43 | 0 | 30 | 2 | 0 |
| 46 | V | 43 | 0 | 30 | 2 | 0 |
| 46 | f | 43 | 0 | 30 | 2 | 0 |
| 46 | v | 43 | 0 | 30 | 2 | 0 |
| 47 | 11 | 180 | 0 | 0 | 4 | 0 |
| 47 | 12 | 135 | 0 | 0 | 0 | 0 |
| 47 | 13 | 180 | 0 | 0 | 0 | 0 |
| 47 | 14 | 135 | 0 | 0 | 0 | 0 |
| 47 | 15 | 180 | 0 | 0 | 0 | 0 |
| 47 | 16 | 180 | 0 | 0 | 1 | 0 |
| 47 | 17 | 180 | 0 | 0 | 2 | 0 |
| 47 | 18 | 135 | 0 | 0 | 1 | 0 |
| 47 | 19 | 45 | 0 | 0 | 0 | 0 |
| 47 | 20 | 135 | 0 | 0 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 47 | 21 | 90 | 0 | 0 | 0 | 0 |
| 47 | 31 | 180 | 0 | 0 | 1 | 0 |
| 47 | 32 | 135 | 0 | 0 | 0 | 0 |
| 47 | 33 | 180 | 0 | 0 | 1 | 0 |
| 47 | 34 | 135 | 0 | 0 | 0 | 0 |
| 47 | 35 | 180 | 0 | 0 | 0 | 0 |
| 47 | 36 | 180 | 0 | 0 | 1 | 0 |
| 47 | 37 | 180 | 0 | 0 | 2 | 0 |
| 47 | 38 | 135 | 0 | 0 | 2 | 0 |
| 47 | 39 | 45 | 0 | 0 | 0 | 0 |
| 47 | 40 | 135 | 0 | 0 | 2 | 0 |
| 47 | 41 | 90 | 0 | 0 | 0 | 0 |
| 48 | 11 | 288 | 0 | 0 | 11 | 0 |
| 48 | 12 | 336 | 0 | 0 | 0 | 0 |
| 48 | 13 | 240 | 0 | 0 | 1 | 0 |
| 48 | 14 | 288 | 0 | 0 | 3 | 0 |
| 48 | 15 | 336 | 0 | 0 | 1 | 0 |
| 48 | 16 | 192 | 0 | 0 | 0 | 0 |
| 48 | 17 | 336 | 0 | 0 | 0 | 0 |
| 48 | 18 | 192 | 0 | 0 | 1 | 0 |
| 48 | 19 | 96 | 0 | 0 | 0 | 0 |
| 48 | 20 | 96 | 0 | 0 | 0 | 0 |
| 48 | 21 | 192 | 0 | 0 | 0 | 0 |
| 48 | 31 | 288 | 0 | 0 | 14 | 0 |
| 48 | 32 | 336 | 0 | 0 | 0 | 0 |
| 48 | 33 | 240 | 0 | 0 | 1 | 0 |
| 48 | 34 | 288 | 0 | 0 | 3 | 0 |
| 48 | 35 | 336 | 0 | 0 | 1 | 0 |
| 48 | 36 | 144 | 0 | 0 | 0 | 0 |
| 48 | 37 | 336 | 0 | 0 | 0 | 0 |
| 48 | 38 | 192 | 0 | 0 | 1 | 0 |
| 48 | 39 | 96 | 0 | 0 | 1 | 0 |
| 48 | 40 | 144 | 0 | 0 | 0 | 0 |
| 48 | 41 | 192 | 0 | 0 | 0 | 0 |
| 49 | 11 | 19 | 0 | 0 | 0 | 0 |
| 49 | 12 | 34 | 0 | 0 | 0 | 0 |
| 49 | 13 | 49 | 0 | 0 | 0 | 0 |
| 49 | 14 | 16 | 0 | 0 | 0 | 0 |
| 49 | 15 | 28 | 0 | 0 | 0 | 0 |
| 49 | 16 | 24 | 0 | 0 | 0 | 0 |
| 49 | 17 | 54 | 0 | 0 | 0 | 0 |
| 49 | 18 | 58 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 49 | 19 | 12 | 0 | 0 | 0 | 0 |
| 49 | 31 | 19 | 0 | 0 | 0 | 0 |
| 49 | 32 | 34 | 0 | 0 | 0 | 0 |
| 49 | 33 | 49 | 0 | 0 | 0 | 0 |
| 49 | 34 | 16 | 0 | 0 | 0 | 0 |
| 49 | 35 | 28 | 0 | 0 | 0 | 0 |
| 49 | 36 | 24 | 0 | 0 | 0 | 0 |
| 49 | 37 | 54 | 0 | 0 | 0 | 0 |
| 49 | 38 | 58 | 0 | 0 | 0 | 0 |
| 49 | 39 | 12 | 0 | 0 | 0 | 0 |
| 50 | 16 | 43 | 0 | 0 | 0 | 0 |
| 50 | 19 | 43 | 0 | 0 | 2 | 0 |
| 50 | 20 | 86 | 0 | 0 | 1 | 0 |
| 50 | 21 | 86 | 0 | 0 | 0 | 0 |
| 50 | 36 | 43 | 0 | 0 | 0 | 0 |
| 50 | 39 | 43 | 0 | 0 | 2 | 0 |
| 50 | 40 | 86 | 0 | 0 | 1 | 0 |
| 50 | 41 | 86 | 0 | 0 | 0 | 0 |
| 51 | 19 | 35 | 0 | 46 | 0 | 0 |
| 51 | 39 | 35 | 0 | 46 | 0 | 0 |
| 52 | 11 | 3 | 0 | 0 | 0 | 0 |
| 52 | 12 | 2 | 0 | 0 | 0 | 0 |
| 52 | 13 | 1 | 0 | 0 | 0 | 0 |
| 52 | 14 | 1 | 0 | 0 | 0 | 0 |
| 52 | 15 | 1 | 0 | 0 | 0 | 0 |
| 52 | 16 | 1 | 0 | 0 | 0 | 0 |
| 52 | 17 | 2 | 0 | 0 | 0 | 0 |
| 52 | 18 | 1 | 0 | 0 | 0 | 0 |
| 52 | 19 | 1 | 0 | 0 | 0 | 0 |
| 52 | 31 | 3 | 0 | 0 | 0 | 0 |
| 52 | 32 | 2 | 0 | 0 | 0 | 0 |
| 52 | 33 | 1 | 0 | 0 | 0 | 0 |
| 52 | 34 | 1 | 0 | 0 | 0 | 0 |
| 52 | 35 | 1 | 0 | 0 | 0 | 0 |
| 52 | 36 | 1 | 0 | 0 | 0 | 0 |
| 52 | 37 | 2 | 0 | 0 | 0 | 0 |
| 52 | 38 | 1 | 0 | 0 | 0 | 0 |
| 52 | 39 | 1 | 0 | 0 | 0 | 0 |
| 52 | B | 5 | 0 | 0 | 0 | 0 |
| 52 | C | 3 | 0 | 0 | 0 | 0 |
| 52 | D | 4 | 0 | 0 | 0 | 0 |
| 52 | Z | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 52 | a | 2 | 0 | 0 | 0 | 0 |
| 52 | b | 5 | 0 | 0 | 0 | 0 |
| 52 | c | 3 | 0 | 0 | 0 | 0 |
| 52 | d | 2 | 0 | 0 | 0 | 0 |
| 52 | z | 1 | 0 | 0 | 0 | 0 |
| All | All | 100884 | 0 | 91037 | 1161 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:31:202:ASP:HB3 | 48:31:313:A86:C29 | 1.68 | 1.22 |
| 37:39:310:CLA:HBB2 | 43:39:314:LHG:H212 | 1.54 | 0.87 |
| 37:19:310:CLA:HBB2 | 43:19:314:LHG:H212 | 1.54 | 0.87 |
| 24:31:202:ASP:CB | 48:31:313:A86:C29 | 2.57 | 0.81 |
| 24:11:204:GLN:HG3 | 48:11:313:A86:C25 | 2.12 | 0.80 |
| 43:19:314:LHG:HC82 | 43:19:314:LHG:H272 | 1.63 | 0.80 |
| 43:39:314:LHG:HC82 | 43:39:314:LHG:H272 | 1.64 | 0.79 |
| 15:u:28:ASN:HD21 | 15:u:55:TYR:H | 1.33 | 0.76 |
| 4:d:185:GLN:HB2 | 37:d:403:CLA:HBC1 | 1.69 | 0.75 |
| 37:19:310:CLA:CBB | 43:19:314:LHG:H212 | 2.17 | 0.75 |
| 24:31:66:LYS:NZ | 24:31:128:GLU:OE2 | 2.18 | 0.74 |
| 15:U:28:ASN:HD21 | 15:U:55:TYR:H | 1.33 | 0.74 |
| 37:C:513:CLA:HBB1 | 39:C:514:BCR:H24C | 1.71 | 0.73 |
| 4:D:185:GLN:HB2 | 37:D:405:CLA:HBC1 | 1.69 | 0.73 |
| 37:c:513:CLA:HBB1 | 39:c:514:BCR:H24C | 1.71 | 0.73 |
| 37:39:310:CLA:CBB | 43:39:314:LHG:H212 | 2.16 | 0.73 |
| 8:I:6:ILE:HD13 | 48:11:313:A86:C39 | 2.18 | 0.73 |
| 19:Z:42:GLN:NE2 | 37:Z:102:CLA:O2A | 2.23 | 0.72 |
| 31:38:152:ASP:HB3 | 31:38:155:GLU:HB2 | 1.72 | 0.72 |
| 2:B:91:TRP:HE1 | 41:B:521:LMG:HC92 | 1.57 | 0.70 |
| 38:a:406:PHO:H3A | 37:d:403:CLA:H142 | 1.75 | 0.69 |
| 24:11:202:ASP:HB3 | 48:11:313:A86:C29 | 2.22 | 0.69 |
| 2:b:91:TRP:HE1 | 41:b:520:LMG:HC92 | 1.57 | 0.69 |
| 31:38:82:ASN:HB2 | 31:38:189:TYR:HB2 | 1.73 | 0.68 |
| 26:33:152:ASP:HB3 | 26:33:155:GLU:HB2 | 1.76 | 0.68 |
| 4:d:191:THR:HG23 | 37:d:403:CLA:HBC2 | 1.76 | 0.68 |
| 4:D:191:THR:HG23 | 37:D:405:CLA:HBC2 | 1.76 | 0.67 |
| 26:13:152:ASP:HB3 | 26:13:155:GLU:HB2 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:31:202:ASP:HB3 | 48:31:313:A86:C30 | 2.24 | 0.66 |
| 27:34:175:MET:HE2 | 37:34:302:CLA:HBB2 | 1.78 | 0.66 |
| 2:b:25:MET:HG2 | 39:b:517:BCR:H23C | 1.78 | 0.66 |
| 27:14:175:MET:HE2 | 37:14:302:CLA:HBB2 | 1.77 | 0.66 |
| 2:B:25:MET:HG2 | 39:B:517:BCR:H23C | 1.78 | 0.65 |
| 34:41:177:ARG:HA | 34:41:180:MET:HE2 | 1.78 | 0.65 |
| 37:19:302:CLA:H2 | 37:19:302:CLA:HED1 | 1.78 | 0.65 |
| 1:a:140:ARG:NH2 | 43:a:412:LHG:O5 | 2.30 | 0.65 |
| 38:A:404:PHO:H3A | 37:D:405:CLA:H142 | 1.78 | 0.64 |
| 37:39:302:CLA:H2 | 37:39:302:CLA:HED1 | 1.79 | 0.64 |
| 37:C:511:CLA:H42 | 17:Y:34:LEU:HA | 1.80 | 0.64 |
| 34:21:177:ARG:HA | 34:21:180:MET:HE2 | 1.77 | 0.64 |
| 29:16:120:GLN:HA | 29:16:123:LEU:HD23 | 1.79 | 0.64 |
| 31:18:145:TYR:HB2 | 37:18:208:CLA:HAA1 | 1.80 | 0.64 |
| 24:31:66:LYS:HZ1 | 24:31:128:GLU:CD | 2.06 | 0.64 |
| 29:36:120:GLN:HA | 29:36:123:LEU:HD23 | 1.79 | 0.63 |
| 33:40:29:GLU:N | 33:40:29:GLU:OE1 | 2.32 | 0.63 |
| 34:21:175:GLN:OE1 | 37:21:209:CLA:ND | 2.32 | 0.63 |
| 3:c:161:ILE:HD13 | 37:c:512:CLA:HBB1 | 1.80 | 0.63 |
| 10:k:26:ILE:HD13 | 39:y:101:BCR:HC8 | 1.81 | 0.63 |
| 10:K:26:ILE:HD13 | 39:K:101:BCR:HC8 | 1.81 | 0.63 |
| 33:40:177:ILE:HG23 | 33:40:181:LEU:HD13 | 1.81 | 0.63 |
| 33:20:29:GLU:OE1 | 33:20:29:GLU:N | 2.32 | 0.62 |
| 33:20:177:ILE:HG23 | 33:20:181:LEU:HD13 | 1.81 | 0.62 |
| 43:37:315:LHG:H121 | 32:39:175:VAL:HG22 | 1.81 | 0.62 |
| 43:17:316:LHG:H121 | 32:19:175:VAL:HG22 | 1.81 | 0.62 |
| 8:I:6:ILE:HD11 | 21:W:33:ARG:HD3 | 1.81 | 0.62 |
| 31:38:145:TYR:HB2 | 37:38:208:CLA:HAA1 | 1.81 | 0.62 |
| 1:a:131:TRP:HZ2 | 3:c:447:ARG:HG2 | 1.64 | 0.62 |
| 30:17:129:LEU:HD13 | 37:19:305:CLA:HBA1 | 1.81 | 0.62 |
| 28:35:86:VAL:HG11 | 28:35:100:SER:HB3 | 1.81 | 0.62 |
| 34:41:175:GLN:OE1 | 37:41:209:CLA:ND | 2.32 | 0.62 |
| 29:36:62:ARG:NH1 | 37:36:301:CLA:O1D | 2.33 | 0.62 |
| 3:C:161:ILE:HD13 | 37:C:512:CLA:HBB1 | 1.80 | 0.62 |
| 29:16:40:VAL:HG21 | 29:16:168:ASN:HD21 | 1.65 | 0.62 |
| 31:18:63:VAL:HG11 | 37:18:203:CLA:HAA2 | 1.81 | 0.62 |
| 31:18:152:ASP:HB3 | 31:18:155:GLU:HB2 | 1.81 | 0.62 |
| 31:38:188:MET:HA | 31:38:191:GLN:HB2 | 1.81 | 0.62 |
| 30:37:129:LEU:HD13 | 37:39:305:CLA:HBA1 | 1.81 | 0.61 |
| 41:L:102:LMG:H362 | 12:M:21:PHE:HB2 | 1.82 | 0.61 |
| 1:a:40:THR:HG23 | 37:a:407:CLA:HBB1 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:16:62:ARG:NH1 | 37:16:301:CLA:O1D | 2.33 | 0.61 |
| 24:31:204:GLN:HG2 | 48:31:313:A86:C28 | 2.31 | 0.61 |
| 27:34:186:GLN:HB3 | 27:34:190:GLU:HB2 | 1.81 | 0.61 |
| 37:c:511:CLA:H42 | 17:y:34:LEU:HA | 1.82 | 0.61 |
| 24:11:204:GLN:CG | 48:11:313:A86:C25 | 2.78 | 0.61 |
| 1:A:131:TRP:HZ2 | 3:C:447:ARG:HG2 | 1.66 | 0.61 |
| 29:36:40:VAL:HG21 | 29:36:168:ASN:HD21 | 1.65 | 0.61 |
| 25:12:38:THR:OG1 | 25:12:39:ALA:N | 2.33 | 0.61 |
| 27:14:186:GLN:HB3 | 27:14:190:GLU:HB2 | 1.82 | 0.61 |
| 29:16:41:ALA:HB1 | 32:19:98:ARG:HB3 | 1.83 | 0.61 |
| 2:B:384:ARG:NH1 | 15:U:98:ASN:O | 2.34 | 0.61 |
| 13:o:72:MET:HE1 | 13:o:115:ARG:HG2 | 1.83 | 0.61 |
| 25:32:61:ARG:NH2 | 25:32:64:GLU:OE2 | 2.34 | 0.61 |
| 33:40:119:GLN:NE2 | 40:40:202:SQD:O49 | 2.34 | 0.61 |
| 25:12:61:ARG:NH2 | 25:12:64:GLU:OE2 | 2.34 | 0.60 |
| 28:35:127:VAL:HA | 28:35:131:TRP:HB2 | 1.82 | 0.60 |
| 3:C:286:LEU:HD12 | 44:C:516:DGD:HB32 | 1.83 | 0.60 |
| 32:19:203:ASN:ND2 | 32:19:206:GLY:O | 2.35 | 0.60 |
| 1:A:40:THR:HG23 | 37:A:405:CLA:HBB1 | 1.83 | 0.60 |
| 13:O:72:MET:HE1 | 13:O:115:ARG:HG2 | 1.83 | 0.60 |
| 24:11:66:LYS:HE2 | 47:11:306:KC1:CED | 2.32 | 0.60 |
| 32:39:203:ASN:ND2 | 32:39:206:GLY:O | 2.35 | 0.60 |
| 37:A:405:CLA:H2 | 41:A:408:LMG:H132 | 1.84 | 0.60 |
| 3:c:286:LEU:HD12 | 44:c:516:DGD:HB32 | 1.83 | 0.60 |
| 24:31:61:ARG:NH1 | 24:31:64:GLU:OE2 | 2.34 | 0.60 |
| 31:38:63:VAL:HG11 | 37:38:203:CLA:HAA2 | 1.83 | 0.59 |
| 27:14:61:ARG:NH1 | 27:14:64:GLU:OE2 | 2.35 | 0.59 |
| 25:12:152:ASP:OD1 | 26:13:151:LYS:NZ | 2.35 | 0.59 |
| 25:32:186:GLN:HB3 | 25:32:190:GLU:HG3 | 1.83 | 0.59 |
| 27:34:49:TRP:HA | 27:34:52:SER:HB3 | 1.85 | 0.59 |
| 32:39:176:ARG:NH2 | 32:39:193:LEU:O | 2.35 | 0.59 |
| 25:32:152:ASP:OD1 | 26:33:151:LYS:NZ | 2.35 | 0.59 |
| 27:34:61:ARG:NH1 | 27:34:64:GLU:OE2 | 2.35 | 0.59 |
| 4:D:154:SER:HA | 4:D:158:LEU:HB2 | 1.84 | 0.59 |
| 28:15:127:VAL:HA | 28:15:131:TRP:HB2 | 1.83 | 0.59 |
| 26:33:186:GLN:O | 26:33:191:GLN:NE2 | 2.36 | 0.59 |
| 29:16:107:ILE:HG13 | 40:16:315:SQD:H441 | 1.85 | 0.59 |
| 4:d:154:SER:HA | 4:d:158:LEU:HB2 | 1.84 | 0.58 |
| 32:19:176:ARG:NH2 | 32:19:193:LEU:O | 2.35 | 0.58 |
| 2:B:30:VAL:HG12 | 37:B:505:CLA:HHD | 1.85 | 0.58 |
| 2:B:311:PHE:O | 2:B:317:ASN:ND2 | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:b:311:PHE:O | 2:b:317:ASN:ND2 | 2.36 | 0.58 |
| 13:O:69:SER:HB2 | 13:O:108:VAL:HB | 1.86 | 0.58 |
| 37:a:407:CLA:H2 | 41:a:410:LMG:H132 | 1.84 | 0.58 |
| 41:d:409:LMG:H211 | 41:d:409:LMG:H331 | 1.85 | 0.58 |
| 24:11:35:LEU:O | 24:11:161:ASN:ND2 | 2.36 | 0.58 |
| 26:13:109:ILE:HD12 | 26:13:112:ILE:HD12 | 1.85 | 0.58 |
| 27:14:49:TRP:HA | 27:14:52:SER:HB3 | 1.86 | 0.58 |
| 43:a:412:LHG:H223 | 37:c:510:CLA:H43 | 1.85 | 0.58 |
| 24:11:61:ARG:NH1 | 24:11:64:GLU:OE2 | 2.34 | 0.58 |
| 13:o:69:SER:HB2 | 13:o:108:VAL:HB | 1.86 | 0.58 |
| 28:15:145:TYR:HB2 | 37:15:307:CLA:HAA1 | 1.83 | 0.58 |
| 27:34:127:VAL:HA | 27:34:131:TRP:HB2 | 1.86 | 0.58 |
| 24:31:35:LEU:O | 24:31:161:ASN:ND2 | 2.36 | 0.58 |
| 4:D:20:TRP:O | 4:D:25:ARG:NH1 | 2.37 | 0.58 |
| 27:14:127:VAL:HA | 27:14:131:TRP:HB2 | 1.86 | 0.58 |
| 2:b:30:VAL:HG12 | 37:b:505:CLA:HHD | 1.85 | 0.58 |
| 4:d:20:TRP:O | 4:d:25:ARG:NH1 | 2.37 | 0.58 |
| 27:14:114:THR:HA | 27:14:117:LEU:HG | 1.85 | 0.58 |
| 31:18:75:VAL:HG23 | 31:18:174:ILE:HG23 | 1.86 | 0.58 |
| 25:32:191:GLN:HG3 | 25:32:196:HIS:HB2 | 1.86 | 0.58 |
| 2:b:384:ARG:NH1 | 15:u:98:ASN:O | 2.37 | 0.57 |
| 28:35:145:TYR:HB2 | 37:35:307:CLA:HAA1 | 1.84 | 0.57 |
| 29:36:107:ILE:HG13 | 40:40:202:SQD:H441 | 1.85 | 0.57 |
| 30:37:90:TYR:HA | 30:37:98:LYS:HA | 1.86 | 0.57 |
| 8:i:6:ILE:HD11 | 21:w:33:ARG:HD3 | 1.86 | 0.57 |
| 3:c:413:ASN:ND2 | 44:j:101:DGD:O4D | 2.37 | 0.57 |
| 27:34:114:THR:HA | 27:34:117:LEU:HG | 1.86 | 0.57 |
| 2:B:474:ILE:O | 4:D:133:ARG:NH1 | 2.37 | 0.57 |
| 25:12:191:GLN:HG3 | 25:12:196:HIS:HB2 | 1.86 | 0.57 |
| 1:a:341:LEU:H | 3:c:311:GLN:HE22 | 1.51 | 0.57 |
| 16:v:126:ALA:HB1 | 16:v:129:LYS:HB2 | 1.86 | 0.57 |
| 32:19:144:ASP:O | 32:19:157:GLN:NE2 | 2.38 | 0.57 |
| 16:V:126:ALA:HB1 | 16:V:129:LYS:HB2 | 1.86 | 0.57 |
| 3:C:413:ASN:ND2 | 44:J:101:DGD:O4D | 2.37 | 0.57 |
| 41:D:412:LMG:H211 | 41:D:412:LMG:H331 | 1.85 | 0.57 |
| 15:u:50:VAL:HG13 | 15:u:95:ARG:HB3 | 1.86 | 0.57 |
| 16:v:5:GLU:O | 16:v:9:THR:OG1 | 2.23 | 0.57 |
| 3:c:359:LEU:O | 3:c:368:ARG:NH2 | 2.38 | 0.57 |
| 2:B:157:HIS:HE1 | 37:B:506:CLA:NA | 2.03 | 0.57 |
| 16:v:4:ASP:N | 16:v:4:ASP:OD1 | 2.37 | 0.57 |
| 3:C:52:VAL:HG13 | 3:C:127:GLY:HA2 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:U:50:VAL:HG13 | 15:U:95:ARG:HB3 | 1.86 | 0.56 |
| 17:Y:33:ASN:N | 19:Z:25:ALA:O | 2.38 | 0.56 |
| 24:11:66:LYS:HG2 | 47:11:306:KC1:C3D | 2.34 | 0.56 |
| 24:11:69:ARG:HB3 | 37:11:307:CLA:HBC3 | 1.87 | 0.56 |
| 31:38:186:GLN:O | 31:38:191:GLN:NE2 | 2.38 | 0.56 |
| 3:C:359:LEU:O | 3:C:368:ARG:NH2 | 2.38 | 0.56 |
| 26:33:109:ILE:HD12 | 26:33:112:ILE:HD12 | 1.85 | 0.56 |
| 4:D:342:GLU:HG2 | 16:V:135:ILE:HG21 | 1.86 | 0.56 |
| 2:b:157:HIS:HE1 | 37:b:506:CLA:NA | 2.03 | 0.56 |
| 41:b:520:LMG:HO4 | 41:b:520:LMG:HO5 | 1.51 | 0.56 |
| 24:11:66:LYS:HE2 | 47:11:306:KC1:O2D | 2.04 | 0.56 |
| 30:17:90:TYR:HA | 30:17:98:LYS:HA | 1.86 | 0.56 |
| 28:35:190:GLU:O | 28:35:194:SER:OG | 2.21 | 0.56 |
| 45:d:402:PL9:H412 | 6:f:23:GLY:HA3 | 1.88 | 0.56 |
| 31:18:72:MET:HA | 31:18:75:VAL:HG12 | 1.87 | 0.56 |
| 1:A:209:SER:HB2 | 4:D:274:PRO:HB3 | 1.88 | 0.56 |
| 42:A:409:BCT:O3 | 4:D:267:HIS:CE1 | 2.58 | 0.56 |
| 16:V:5:GLU:O | 16:V:9:THR:OG1 | 2.23 | 0.56 |
| 39:0:101:BCR:H271 | 14:t:22:PHE:HB3 | 1.86 | 0.56 |
| 24:31:192:TYR:OH | 48:31:311:A86:O2 | 2.23 | 0.56 |
| 30:37:61:ARG:NH1 | 30:37:64:GLU:OE2 | 2.39 | 0.56 |
| 1:A:341:LEU:H | 3:C:311:GLN:HE22 | 1.53 | 0.56 |
| 13:o:212:SER:O | 13:o:212:SER:OG | 2.24 | 0.56 |
| 16:v:36:THR:HG22 | 46:v:201:HEM:HBB1 | 1.87 | 0.56 |
| 30:17:61:ARG:NH1 | 30:17:64:GLU:OE2 | 2.39 | 0.56 |
| 4:d:13:LEU:HD11 | 18:x:27:ILE:HG23 | 1.87 | 0.56 |
| 24:11:192:TYR:OH | 48:11:311:A86:O2 | 2.23 | 0.56 |
| 27:14:177:ASN:ND2 | 48:14:311:A86:O1 | 2.39 | 0.56 |
| 30:37:166:ASN:ND2 | 37:38:201:CLA:OBD | 2.39 | 0.56 |
| 2:b:388:SER:O | 2:b:394:GLN:NE2 | 2.39 | 0.56 |
| 24:31:112:ILE:HD11 | 37:31:304:CLA:HAA2 | 1.87 | 0.56 |
| 27:34:177:ASN:ND2 | 48:34:311:A86:O1 | 2.39 | 0.56 |
| 24:31:69:ARG:HB3 | 37:31:308:CLA:HBC3 | 1.87 | 0.55 |
| 29:36:33:LEU:HD12 | 29:36:55:GLU:HG2 | 1.89 | 0.55 |
| 25:12:166:ASN:ND2 | 37:12:210:CLA:OBD | 2.39 | 0.55 |
| 28:35:61:ARG:NH2 | 37:35:301:CLA:O1D | 2.39 | 0.55 |
| 3:c:52:VAL:HG13 | 3:c:127:GLY:HA2 | 1.88 | 0.55 |
| 32:19:95:ILE:HA | 32:19:98:ARG:HD2 | 1.88 | 0.55 |
| 42:a:411:BCT:O3 | 4:d:267:HIS:CE1 | 2.58 | 0.55 |
| 30:17:166:ASN:ND2 | 37:18:201:CLA:OBD | 2.40 | 0.55 |
| 40:36:315:SQD:H241 | 40:36:315:SQD:H81 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:O:42:ASP:N | 13:O:42:ASP:OD1 | 2.39 | 0.55 |
| 16:V:4:ASP:N | 16:V:4:ASP:OD1 | 2.37 | 0.55 |
| 13:o:8:GLU:O | 20:q:183:LYS:NZ | 2.39 | 0.55 |
| 4:D:262:ASN:HB3 | 4:D:265:TRP:HB3 | 1.89 | 0.55 |
| 5:E:70:ARG:NH2 | 7:H:50:ASN:O | 2.37 | 0.55 |
| 30:17:137:TYR:OH | 32:19:182:LYS:NZ | 2.40 | 0.55 |
| 40:17:301:SQD:H241 | 40:17:301:SQD:H81 | 1.89 | 0.55 |
| 24:31:204:GLN:CB | 48:31:313:A86:C2 | 2.85 | 0.55 |
| 25:32:166:ASN:ND2 | 37:32:211:CLA:OBD | 2.39 | 0.55 |
| 34:41:166:LEU:HA | 34:41:169:ARG:HD3 | 1.89 | 0.55 |
| 28:15:61:ARG:NH2 | 37:15:301:CLA:O1D | 2.40 | 0.55 |
| 4:d:342:GLU:HG2 | 16:v:135:ILE:HG21 | 1.88 | 0.55 |
| 48:31:313:A86:C28 | 48:31:313:A86:C24 | 2.85 | 0.55 |
| 48:11:313:A86:C23 | 48:11:313:A86:C13 | 2.85 | 0.55 |
| 25:12:78:THR:O | 25:12:82:ASN:ND2 | 2.38 | 0.55 |
| 31:38:72:MET:HA | 31:38:75:VAL:HG12 | 1.88 | 0.55 |
| 2:B:388:SER:O | 2:B:394:GLN:NE2 | 2.39 | 0.54 |
| 1:a:64:ARG:NH1 | 13:o:105:ALA:O | 2.37 | 0.54 |
| 26:13:186:GLN:O | 26:13:191:GLN:NE2 | 2.36 | 0.54 |
| 29:16:168:ASN:ND2 | 37:16:307:CLA:O1D | 2.40 | 0.54 |
| 43:19:314:LHG:C4 | 43:19:314:LHG:C3 | 2.85 | 0.54 |
| 31:38:66:LYS:NZ | 31:38:128:GLU:OE2 | 2.32 | 0.54 |
| 32:39:144:ASP:O | 32:39:157:GLN:NE2 | 2.39 | 0.54 |
| 1:a:192:ILE:HG13 | 1:a:293:MET:HE1 | 1.90 | 0.54 |
| 24:31:66:LYS:CE | 24:31:128:GLU:OE2 | 2.55 | 0.54 |
| 15:U:36:LEU:HD11 | 16:V:51:ASN:HB3 | 1.90 | 0.54 |
| 3:c:295:TYR:O | 3:c:421:ARG:NH2 | 2.39 | 0.54 |
| 24:11:112:ILE:HD11 | 37:11:303:CLA:HAA2 | 1.87 | 0.54 |
| 32:19:84:SER:HB3 | 37:19:301:CLA:HBA1 | 1.90 | 0.54 |
| 25:32:35:ILE:O | 25:32:161:ASN:ND2 | 2.41 | 0.54 |
| 28:15:178:MET:HA | 28:15:181:GLU:HG2 | 1.87 | 0.54 |
| 29:16:33:LEU:HD12 | 29:16:55:GLU:HG2 | 1.88 | 0.54 |
| 48:31:313:A86:C13 | 48:31:313:A86:C23 | 2.85 | 0.54 |
| 31:38:119:GLN:OE1 | 47:38:205:KC1:C4D | 2.51 | 0.54 |
| 1:A:192:ILE:HG13 | 1:A:293:MET:HE1 | 1.90 | 0.54 |
| 37:b:503:CLA:H191 | 7:h:39:LEU:HD12 | 1.90 | 0.54 |
| 43:39:314:LHG:C4 | 43:39:314:LHG:C3 | 2.86 | 0.54 |
| 1:A:123:VAL:HG21 | 37:A:403:CLA:H91 | 1.89 | 0.54 |
| 2:B:148:LEU:HB3 | 41:B:521:LMG:H422 | 1.89 | 0.54 |
| 1:a:123:VAL:HG21 | 37:a:403:CLA:H91 | 1.89 | 0.54 |
| 31:18:119:GLN:OE1 | 47:18:205:KC1:C4D | 2.46 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 32:19:52:ASN:HB2 | 32:19:66:ALA:HB2 | 1.90 | 0.54 |
| 2:B:477:ASP:OD1 | 2:B:477:ASP:N | 2.41 | 0.54 |
| 3:C:316:LEU:HD12 | 3:C:338:TYR:HB3 | 1.89 | 0.54 |
| 13:O:212:SER:O | 13:O:212:SER:OG | 2.24 | 0.54 |
| 1:a:183:MET:HB3 | 37:a:403:CLA:HBC2 | 1.90 | 0.54 |
| 24:31:204:GLN:HB2 | 48:31:313:A86:C2 | 2.38 | 0.54 |
| 25:32:78:THR:O | 25:32:82:ASN:ND2 | 2.38 | 0.54 |
| 2:B:177:LYS:HE2 | 2:B:179:GLN:HB3 | 1.90 | 0.54 |
| 3:C:25:ASP:OD1 | 3:C:28:SER:OG | 2.26 | 0.54 |
| 2:b:179:GLN:HE22 | 7:h:66:ILE:HB | 1.73 | 0.54 |
| 3:c:316:LEU:HD12 | 3:c:338:TYR:HB3 | 1.89 | 0.53 |
| 32:19:67:THR:HG21 | 32:19:85:THR:HA | 1.88 | 0.53 |
| 26:13:61:ARG:NH1 | 26:13:64:GLU:OE2 | 2.42 | 0.53 |
| 31:38:192:TYR:OH | 48:38:212:A86:O2 | 2.25 | 0.53 |
| 32:39:192:ASP:OD2 | 32:39:201:ARG:NH1 | 2.42 | 0.53 |
| 4:D:171:SER:HB2 | 4:D:176:ALA:HB1 | 1.90 | 0.53 |
| 2:b:148:LEU:HB3 | 41:b:520:LMG:H422 | 1.89 | 0.53 |
| 48:11:313:A86:C24 | 48:11:313:A86:C28 | 2.86 | 0.53 |
| 32:19:192:ASP:OD2 | 32:19:201:ARG:NH1 | 2.42 | 0.53 |
| 37:B:507:CLA:HMC3 | 39:B:518:BCR:HC8 | 1.91 | 0.53 |
| 32:19:55:GLU:OE2 | 32:19:63:ARG:NH1 | 2.42 | 0.53 |
| 31:38:75:VAL:HG23 | 31:38:174:ILE:HG23 | 1.91 | 0.53 |
| 4:D:53:PHE:O | 5:E:50:THR:OG1 | 2.22 | 0.53 |
| 13:o:191:LYS:O | 15:u:10:VAL:N | 2.42 | 0.53 |
| 24:11:66:LYS:CE | 47:11:306:KC1:O2D | 2.56 | 0.53 |
| 3:c:321:ARG:NH2 | 3:c:387:GLU:OE1 | 2.42 | 0.53 |
| 4:d:262:ASN:HB3 | 4:d:265:TRP:HB3 | 1.89 | 0.53 |
| 37:17:309:CLA:H151 | 37:21:206:CLA:HAC2 | 1.91 | 0.53 |
| 25:32:59:ARG:NH1 | 37:32:205:CLA:O1A | 2.42 | 0.53 |
| 32:39:52:ASN:HB2 | 32:39:66:ALA:HB2 | 1.90 | 0.53 |
| 1:A:183:MET:HB3 | 37:A:403:CLA:HBC2 | 1.90 | 0.53 |
| 2:b:42:LEU:HD13 | 2:b:94:GLU:HG3 | 1.90 | 0.53 |
| 37:c:511:CLA:H143 | 19:z:17:VAL:HG13 | 1.90 | 0.53 |
| 34:21:166:LEU:HA | 34:21:169:ARG:HD3 | 1.89 | 0.53 |
| 33:40:84:ASP:OD1 | 33:40:104:ASN:ND2 | 2.41 | 0.53 |
| 4:D:23:LYS:HB3 | 4:D:25:ARG:HH11 | 1.74 | 0.53 |
| 2:b:177:LYS:HG2 | 7:h:67:VAL:HG13 | 1.91 | 0.53 |
| 3:c:25:ASP:OD1 | 3:c:28:SER:OG | 2.26 | 0.53 |
| 4:d:23:LYS:HB3 | 4:d:25:ARG:HH11 | 1.74 | 0.53 |
| 34:21:85:ILE:HG23 | 34:21:90:ILE:HB | 1.90 | 0.53 |
| 16:V:55:ASP:N | 16:V:55:ASP:OD1 | 2.40 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:W:67:ASP:OD1 | 21:W:67:ASP:N | 2.42 | 0.53 |
| 25:12:35:ILE:O | 25:12:161:ASN:ND2 | 2.42 | 0.53 |
| 2:B:42:LEU:HD13 | 2:B:94:GLU:HG3 | 1.90 | 0.52 |
| 33:20:145:TYR:HB2 | 37:20:306:CLA:HAA1 | 1.91 | 0.52 |
| 26:33:61:ARG:NH1 | 26:33:64:GLU:OE2 | 2.42 | 0.52 |
| 34:41:85:ILE:HG23 | 34:41:90:ILE:HB | 1.90 | 0.52 |
| 1:A:184:LEU:HD21 | 4:D:185:GLN:HG2 | 1.91 | 0.52 |
| 4:d:171:SER:HB2 | 4:d:176:ALA:HB1 | 1.90 | 0.52 |
| 37:z:102:CLA:HAA2 | 33:40:152:ASN:HD22 | 1.75 | 0.52 |
| 27:14:145:TYR:HB2 | 37:14:307:CLA:HAA1 | 1.91 | 0.52 |
| 30:17:152:ASP:HB2 | 30:17:155:GLU:HB3 | 1.90 | 0.52 |
| 25:32:106:VAL:HG13 | 25:32:181:GLU:HG2 | 1.92 | 0.52 |
| 1:A:140:ARG:NH2 | 43:D:411:LHG:O5 | 2.42 | 0.52 |
| 20:Q:134:GLU:OE1 | 20:Q:137:ASN:ND2 | 2.41 | 0.52 |
| 13:o:42:ASP:OD1 | 13:o:42:ASP:N | 2.39 | 0.52 |
| 3:C:321:ARG:NH2 | 3:C:387:GLU:OE1 | 2.42 | 0.52 |
| 33:20:84:ASP:OD1 | 33:20:104:ASN:ND2 | 2.41 | 0.52 |
| 29:36:168:ASN:ND2 | 37:36:307:CLA:O1D | 2.40 | 0.52 |
| 31:38:80:VAL:HB | 31:38:85:ILE:HD13 | 1.91 | 0.52 |
| 20:q:80:ASP:OD1 | 20:q:80:ASP:N | 2.42 | 0.52 |
| 29:16:169:ASN:ND2 | 37:16:307:CLA:OBD | 2.43 | 0.52 |
| 14:T:22:PHE:HB3 | 39:5:101:BCR:H271 | 1.92 | 0.52 |
| 37:b:507:CLA:HMC3 | 39:b:518:BCR:HC8 | 1.91 | 0.52 |
| 20:q:134:GLU:OE1 | 20:q:137:ASN:ND2 | 2.41 | 0.52 |
| 31:18:192:TYR:OH | 48:18:212:A86:O2 | 2.24 | 0.52 |
| 32:39:84:SER:HB3 | 37:39:301:CLA:HBA1 | 1.90 | 0.52 |
| 13:O:8:GLU:O | 20:Q:183:LYS:NZ | 2.42 | 0.52 |
| 28:15:161:ASN:HB2 | 37:15:308:CLA:HED2 | 1.92 | 0.52 |
| 33:20:66:LYS:NZ | 50:20:312:DD6:O2 | 2.43 | 0.52 |
| 37:33:308:CLA:H11 | 27:34:132:MET:SD | 2.50 | 0.52 |
| 27:34:145:TYR:HB2 | 37:34:307:CLA:HAA1 | 1.91 | 0.52 |
| 29:36:169:ASN:ND2 | 37:36:307:CLA:OBD | 2.43 | 0.52 |
| 31:38:181:GLU:HB2 | 31:38:186:GLN:O | 2.10 | 0.52 |
| 2:B:155:ALA:O | 2:B:159:THR:OG1 | 2.28 | 0.52 |
| 2:b:177:LYS:HE2 | 2:b:179:GLN:HB3 | 1.90 | 0.52 |
| 25:12:59:ARG:NH1 | 37:12:204:CLA:O1A | 2.42 | 0.52 |
| 37:13:308:CLA:H11 | 27:14:132:MET:SD | 2.50 | 0.52 |
| 37:B:512:CLA:H171 | 37:B:513:CLA:HBB2 | 1.91 | 0.51 |
| 39:D:407:BCR:H19C | 41:D:412:LMG:H352 | 1.93 | 0.51 |
| 27:14:157:ALA:O | 27:14:161:ASN:ND2 | 2.38 | 0.51 |
| 28:35:161:ASN:HB2 | 37:35:308:CLA:HED2 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:16:171:ARG:HA | 29:16:174:MET:HE3 | 1.92 | 0.51 |
| 32:39:197:GLN:NE2 | 32:39:209:TYR:O | 2.44 | 0.51 |
| 39:d:405:BCR:H19C | 41:d:409:LMG:H352 | 1.93 | 0.51 |
| 29:16:46:PHE:HA | 32:19:86:VAL:HG21 | 1.92 | 0.51 |
| 29:16:79:THR:HG21 | 29:16:180:THR:HG21 | 1.92 | 0.51 |
| 13:O:167:ASP:OD1 | 13:O:167:ASP:N | 2.42 | 0.51 |
| 37:Z:102:CLA:HAA2 | 33:20:152:ASN:HD22 | 1.75 | 0.51 |
| 2:b:326:ARG:NH2 | 4:d:296:ASP:OD1 | 2.32 | 0.51 |
| 31:38:117:LEU:HA | 31:38:120:ILE:HG12 | 1.93 | 0.51 |
| 32:39:67:THR:HG21 | 32:39:85:THR:HA | 1.91 | 0.51 |
| 33:40:66:LYS:NZ | 50:40:214:DD6:O2 | 2.43 | 0.51 |
| 2:B:364:GLU:OE2 | 4:D:293:ARG:NH2 | 2.43 | 0.51 |
| 4:D:88:LEU:H | 7:H:50:ASN:HD21 | 1.58 | 0.51 |
| 13:O:191:LYS:O | 15:U:10:VAL:N | 2.44 | 0.51 |
| 20:q:159:SER:HB3 | 20:q:162:GLN:HG2 | 1.92 | 0.51 |
| 25:12:179:VAL:HG21 | 37:12:212:CLA:HBC3 | 1.93 | 0.51 |
| 31:18:179:VAL:HG21 | 37:18:211:CLA:HBC3 | 1.93 | 0.51 |
| 27:34:168:ARG:HA | 27:34:171:MET:HE3 | 1.93 | 0.51 |
| 29:36:171:ARG:HA | 29:36:174:MET:HE3 | 1.93 | 0.51 |
| 1:A:82:VAL:HB | 1:A:174:LEU:HB2 | 1.92 | 0.51 |
| 27:34:157:ALA:O | 27:34:161:ASN:ND2 | 2.38 | 0.51 |
| 33:40:145:TYR:HB2 | 37:40:208:CLA:HAA1 | 1.91 | 0.51 |
| 21:w:67:ASP:OD1 | 21:w:67:ASP:N | 2.42 | 0.51 |
| 32:19:197:GLN:NE2 | 32:19:209:TYR:O | 2.44 | 0.51 |
| 29:36:79:THR:HG21 | 29:36:180:THR:HG21 | 1.92 | 0.51 |
| 30:37:165:ASN:OD1 | 30:37:168:ARG:NH2 | 2.37 | 0.51 |
| 20:Q:159:SER:HB3 | 20:Q:162:GLN:HG2 | 1.91 | 0.51 |
| 37:b:505:CLA:H192 | 37:b:509:CLA:HBB2 | 1.92 | 0.51 |
| 28:15:49:TRP:HZ3 | 37:15:301:CLA:H51 | 1.75 | 0.51 |
| 26:33:47:LEU:HB3 | 26:33:49:TRP:CD1 | 2.46 | 0.51 |
| 2:B:348:ASP:OD1 | 2:B:348:ASP:N | 2.31 | 0.51 |
| 16:v:95:ILE:O | 20:q:108:TYR:OH | 2.29 | 0.51 |
| 30:17:39:GLU:HG3 | 37:18:201:CLA:HMB2 | 1.93 | 0.51 |
| 24:31:72:MET:HE1 | 37:31:308:CLA:HHC | 1.93 | 0.51 |
| 28:35:31:SER:OG | 28:35:34:GLU:OE1 | 2.29 | 0.51 |
| 31:38:168:ARG:HA | 31:38:171:MET:HE3 | 1.93 | 0.51 |
| 37:B:505:CLA:H192 | 37:B:509:CLA:HBB2 | 1.92 | 0.51 |
| 3:C:295:TYR:O | 3:C:421:ARG:NH2 | 2.39 | 0.51 |
| 34:41:174:ASN:HA | 34:41:177:ARG:HB2 | 1.92 | 0.51 |
| 37:A:405:CLA:HAA2 | 41:A:408:LMG:H111 | 1.92 | 0.50 |
| 13:O:65:LYS:HE3 | 13:O:67:VAL:HG22 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:12:106:VAL:HG13 | 25:12:181:GLU:HG2 | 1.92 | 0.50 |
| 25:32:38:THR:HG23 | 25:32:40:PRO:HD2 | 1.93 | 0.50 |
| 2:B:458:PHE:HB3 | 37:B:504:CLA:HBC2 | 1.93 | 0.50 |
| 13:O:52:VAL:HB | 13:O:110:LEU:HD21 | 1.93 | 0.50 |
| 37:b:512:CLA:H171 | 37:b:513:CLA:HBB2 | 1.91 | 0.50 |
| 4:d:334:PRO:HG2 | 5:e:66:LEU:HD21 | 1.93 | 0.50 |
| 28:35:49:TRP:HZ3 | 37:35:301:CLA:H51 | 1.76 | 0.50 |
| 3:C:112:VAL:HG22 | 37:Z:101:CLA:H8 | 1.92 | 0.50 |
| 37:a:407:CLA:HAA2 | 41:a:410:LMG:H111 | 1.92 | 0.50 |
| 41:a:410:LMG:HC72 | 3:c:214:SER:HB2 | 1.92 | 0.50 |
| 34:21:174:ASN:HA | 34:21:177:ARG:HB2 | 1.92 | 0.50 |
| 16:v:36:THR:CG2 | 46:v:201:HEM:HBB1 | 2.41 | 0.50 |
| 30:17:59:ARG:NH1 | 47:17:303:KC1:O2A | 2.45 | 0.50 |
| 37:C:511:CLA:H143 | 19:Z:17:VAL:HG13 | 1.93 | 0.50 |
| 1:a:82:VAL:HB | 1:a:174:LEU:HB2 | 1.92 | 0.50 |
| 16:v:8:ARG:NH1 | 16:v:21:LEU:O | 2.41 | 0.50 |
| 27:14:168:ARG:HA | 27:14:171:MET:HE3 | 1.93 | 0.50 |
| 8:I:6:ILE:HG21 | 48:11:313:A86:C39 | 2.41 | 0.50 |
| 1:a:84:PRO:HA | 1:a:112:TYR:CG | 2.47 | 0.50 |
| 26:33:31:SER:N | 26:33:34:GLU:OE2 | 2.44 | 0.50 |
| 43:37:321:LHG:H292 | 34:41:133:VAL:HG13 | 1.94 | 0.50 |
| 18:X:1:MET:HB3 | 18:X:5:LEU:HD23 | 1.94 | 0.50 |
| 30:17:165:ASN:ND2 | 37:18:201:CLA:O1D | 2.45 | 0.50 |
| 24:31:159:LYS:NZ | 47:31:309:KC1:O2A | 2.39 | 0.50 |
| 30:37:165:ASN:ND2 | 37:38:201:CLA:O1D | 2.44 | 0.50 |
| 37:B:502:CLA:H192 | 44:H:102:DGD:HAW1 | 1.92 | 0.50 |
| 2:b:155:ALA:O | 2:b:159:THR:OG1 | 2.28 | 0.50 |
| 2:b:198:ILE:HD13 | 37:b:503:CLA:HED2 | 1.94 | 0.50 |
| 18:x:1:MET:HB3 | 18:x:5:LEU:HD23 | 1.94 | 0.50 |
| 27:14:191:GLN:HG3 | 27:14:196:HIS:HB3 | 1.94 | 0.50 |
| 31:18:180:ALA:O | 31:18:191:GLN:NE2 | 2.45 | 0.50 |
| 2:B:44:VAL:HG23 | 2:B:60:MET:HE1 | 1.94 | 0.49 |
| 27:14:90:TYR:O | 48:14:315:A86:O3 | 2.29 | 0.49 |
| 32:39:126:PHE:HB3 | 32:39:235:LEU:HD22 | 1.94 | 0.49 |
| 37:B:508:CLA:HHC | 37:B:508:CLA:HBB1 | 1.94 | 0.49 |
| 4:D:78:SER:HA | 4:D:171:SER:HB3 | 1.95 | 0.49 |
| 37:b:508:CLA:HBB1 | 37:b:508:CLA:HHC | 1.94 | 0.49 |
| 32:19:126:PHE:HB3 | 32:19:235:LEU:HD22 | 1.94 | 0.49 |
| 24:31:45:ASP:N | 24:31:45:ASP:OD1 | 2.44 | 0.49 |
| 27:34:59:ARG:NH1 | 27:34:137:TYR:OH | 2.42 | 0.49 |
| 16:v:55:ASP:OD1 | 16:v:55:ASP:N | 2.40 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:14:59:ARG:NH1 | 27:14:137:TYR:OH | 2.42 | 0.49 |
| 28:15:36:GLY:HA2 | 28:15:168:ARG:HH12 | 1.78 | 0.49 |
| 41:B:521:LMG:O5 | 41:B:521:LMG:O4 | 2.27 | 0.49 |
| 2:b:458:PHE:HB3 | 37:b:504:CLA:HBC2 | 1.93 | 0.49 |
| 16:v:28:ARG:NH1 | 16:v:111:ASP:OD1 | 2.45 | 0.49 |
| 26:13:47:LEU:HB3 | 26:13:49:TRP:CD1 | 2.47 | 0.49 |
| 34:21:133:VAL:HG13 | 43:21:217:LHG:H292 | 1.94 | 0.49 |
| 24:31:53:GLU:OE1 | 24:31:60:ARG:NH1 | 2.42 | 0.49 |
| 27:34:90:TYR:O | 48:34:315:A86:O3 | 2.29 | 0.49 |
| 30:37:59:ARG:NH1 | 47:37:302:KC1:O2A | 2.45 | 0.49 |
| 1:A:84:PRO:HA | 1:A:112:TYR:CG | 2.47 | 0.49 |
| 37:C:506:CLA:H18 | 37:C:506:CLA:H102 | 1.95 | 0.49 |
| 13:o:52:VAL:HB | 13:o:110:LEU:HD21 | 1.93 | 0.49 |
| 25:32:179:VAL:HG21 | 37:32:213:CLA:HBC3 | 1.93 | 0.49 |
| 16:V:86:GLU:OE1 | 16:V:86:GLU:N | 2.45 | 0.49 |
| 13:o:14:VAL:HG13 | 13:o:19:LEU:HB3 | 1.94 | 0.49 |
| 13:o:65:LYS:HE3 | 13:o:67:VAL:HG22 | 1.93 | 0.49 |
| 16:v:86:GLU:OE1 | 16:v:86:GLU:N | 2.45 | 0.49 |
| 24:11:45:ASP:N | 24:11:45:ASP:OD1 | 2.44 | 0.49 |
| 31:38:61:ARG:NH1 | 31:38:64:GLU:OE2 | 2.45 | 0.49 |
| 39:C:514:BCR:HC7 | 19:Z:52:ALA:HB2 | 1.95 | 0.49 |
| 4:d:99:ASP:HB2 | 5:e:74:LYS:HE2 | 1.94 | 0.49 |
| 15:u:36:LEU:HD11 | 16:v:51:ASN:HB3 | 1.95 | 0.49 |
| 24:11:72:MET:HE1 | 37:11:307:CLA:HHC | 1.93 | 0.49 |
| 26:13:31:SER:N | 26:13:34:GLU:OE2 | 2.46 | 0.49 |
| 26:33:179:VAL:HG21 | 37:33:310:CLA:HBC3 | 1.95 | 0.49 |
| 30:37:112:VAL:HG12 | 30:37:117:LEU:HG | 1.95 | 0.49 |
| 2:B:326:ARG:NH2 | 4:D:296:ASP:OD1 | 2.39 | 0.49 |
| 4:D:178:PHE:HA | 4:D:181:LEU:HD12 | 1.94 | 0.49 |
| 16:V:28:ARG:NH1 | 16:V:111:ASP:OD1 | 2.45 | 0.49 |
| 24:11:204:GLN:HB2 | 48:11:313:A86:C25 | 2.43 | 0.49 |
| 32:39:148:ASN:ND2 | 32:39:157:GLN:OE1 | 2.39 | 0.49 |
| 2:B:198:ILE:HD13 | 37:B:503:CLA:HED2 | 1.94 | 0.49 |
| 2:B:256:MET:HA | 2:B:263:THR:HG21 | 1.95 | 0.49 |
| 20:Q:80:ASP:OD1 | 20:Q:80:ASP:N | 2.42 | 0.49 |
| 1:a:209:SER:HB2 | 4:d:274:PRO:HB3 | 1.94 | 0.49 |
| 27:14:91:LEU:HD22 | 27:14:102:ILE:HD11 | 1.94 | 0.49 |
| 25:32:32:GLU:HA | 25:32:35:ILE:HD12 | 1.95 | 0.49 |
| 29:36:47:ASP:O | 32:39:46:SER:OG | 2.24 | 0.49 |
| 3:c:330:GLN:HE21 | 3:c:334:GLY:HA2 | 1.78 | 0.48 |
| 37:c:506:CLA:H18 | 37:c:506:CLA:H102 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:u:48:LYS:NZ | 15:u:66:GLY:O | 2.42 | 0.48 |
| 30:17:112:VAL:HG12 | 30:17:117:LEU:HG | 1.93 | 0.48 |
| 32:19:148:ASN:ND2 | 32:19:157:GLN:OE1 | 2.40 | 0.48 |
| 2:B:64:PRO:HB3 | 2:B:267:LEU:HB3 | 1.95 | 0.48 |
| 4:d:78:SER:HA | 4:d:171:SER:HB3 | 1.95 | 0.48 |
| 26:13:179:VAL:HG21 | 37:13:310:CLA:HBC3 | 1.94 | 0.48 |
| 29:16:186:ILE:HG13 | 29:16:187:THR:HG23 | 1.95 | 0.48 |
| 30:17:165:ASN:OD1 | 30:17:168:ARG:NH2 | 2.37 | 0.48 |
| 31:38:91:LEU:HD22 | 31:38:102:ILE:HD11 | 1.95 | 0.48 |
| 1:A:188:ALA:HB2 | 1:A:328:ILE:HB | 1.96 | 0.48 |
| 41:A:408:LMG:HC72 | 3:C:214:SER:HB2 | 1.94 | 0.48 |
| 27:34:91:LEU:HD22 | 27:34:102:ILE:HD11 | 1.94 | 0.48 |
| 37:35:308:CLA:H12 | 29:36:133:TRP:NE1 | 2.29 | 0.48 |
| 32:39:79:ASP:OD1 | 50:39:312:DD6:O4 | 2.32 | 0.48 |
| 37:b:516:CLA:HHC | 37:b:516:CLA:HBB1 | 1.95 | 0.48 |
| 6:f:43:ARG:NH1 | 9:j:39:LEU:OXT | 2.45 | 0.48 |
| 28:35:36:GLY:HA2 | 28:35:168:ARG:HH12 | 1.78 | 0.48 |
| 32:39:95:ILE:HA | 32:39:98:ARG:HD2 | 1.95 | 0.48 |
| 2:B:464:PHE:HD2 | 37:B:511:CLA:HAC2 | 1.77 | 0.48 |
| 3:C:251:PHE:HE2 | 43:19:314:LHG:H112 | 1.78 | 0.48 |
| 37:C:508:CLA:H161 | 37:C:510:CLA:H101 | 1.95 | 0.48 |
| 45:D:404:PL9:H261 | 37:D:405:CLA:H141 | 1.96 | 0.48 |
| 30:17:88:ASP:HB2 | 40:17:301:SQD:H441 | 1.96 | 0.48 |
| 27:34:191:GLN:HG3 | 27:34:196:HIS:HB3 | 1.94 | 0.48 |
| 31:38:179:VAL:HG21 | 37:38:211:CLA:HBC3 | 1.95 | 0.48 |
| 4:D:140:TYR:OH | 43:D:409:LHG:O4 | 2.31 | 0.48 |
| 13:O:14:VAL:HG13 | 13:O:19:LEU:HB3 | 1.94 | 0.48 |
| 2:b:44:VAL:HG23 | 2:b:60:MET:HE1 | 1.94 | 0.48 |
| 2:b:464:PHE:HD2 | 37:b:511:CLA:HAC2 | 1.77 | 0.48 |
| 24:11:53:GLU:OE1 | 24:11:60:ARG:NH1 | 2.42 | 0.48 |
| 25:12:32:GLU:HA | 25:12:35:ILE:HD12 | 1.95 | 0.48 |
| 2:B:83:GLU:HA | 13:o:58:LYS:HE2 | 1.95 | 0.48 |
| 2:b:256:MET:HA | 2:b:263:THR:HG21 | 1.96 | 0.48 |
| 2:b:314:TYR:OH | 2:b:334:ASP:OD2 | 2.30 | 0.48 |
| 26:13:35:LEU:O | 26:13:161:ASN:ND2 | 2.47 | 0.48 |
| 31:18:168:ARG:HA | 31:18:171:MET:HE3 | 1.94 | 0.48 |
| 26:33:35:LEU:O | 26:33:161:ASN:ND2 | 2.47 | 0.48 |
| 37:B:524:CLA:H52 | 37:32:205:CLA:H203 | 1.95 | 0.48 |
| 16:V:36:THR:CG2 | 46:V:201:HEM:HBB1 | 2.44 | 0.48 |
| 2:b:64:PRO:HB3 | 2:b:267:LEU:HB3 | 1.95 | 0.48 |
| 3:c:223:VAL:O | 3:c:291:ASN:ND2 | 2.40 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:d:402:PL9:H261 | 37:d:403:CLA:H141 | 1.95 | 0.48 |
| 32:19:151:PRO:O | 50:19:312:DD6:O2 | 2.31 | 0.48 |
| 24:31:204:GLN:CG | 48:31:313:A86:C28 | 2.92 | 0.48 |
| 26:33:45:ASP:OD2 | 26:33:48:GLY:N | 2.46 | 0.48 |
| 32:39:151:PRO:O | 50:39:312:DD6:O2 | 2.31 | 0.48 |
| 2:b:214:ILE:HG21 | 37:b:523:CLA:HAA2 | 1.96 | 0.48 |
| 4:d:178:PHE:HA | 4:d:181:LEU:HD12 | 1.94 | 0.48 |
| 16:v:36:THR:HA | 16:v:103:ARG:HD3 | 1.96 | 0.48 |
| 37:B:515:CLA:H161 | 7:H:7:LEU:HD21 | 1.94 | 0.48 |
| 4:D:86:HIS:NE2 | 4:D:160:PRO:O | 2.43 | 0.48 |
| 3:C:330:GLN:HE21 | 3:C:334:GLY:HA2 | 1.78 | 0.47 |
| 1:a:188:ALA:HB2 | 1:a:328:ILE:HB | 1.96 | 0.47 |
| 37:b:523:CLA:H52 | 37:12:204:CLA:H203 | 1.95 | 0.47 |
| 28:15:192:TYR:OH | 48:15:311:A86:O2 | 2.31 | 0.47 |
| 37:21:206:CLA:HAA2 | 43:21:217:LHG:H102 | 1.95 | 0.47 |
| 2:B:214:ILE:HG21 | 37:B:524:CLA:HAA2 | 1.96 | 0.47 |
| 13:O:167:ASP:HB2 | 15:U:11:ILE:HG23 | 1.95 | 0.47 |
| 16:V:36:THR:HG22 | 46:V:201:HEM:HBB1 | 1.95 | 0.47 |
| 37:b:502:CLA:H102 | 37:b:509:CLA:H193 | 1.97 | 0.47 |
| 6:f:22:HIS:HE1 | 46:f:101:HEM:ND | 2.12 | 0.47 |
| 24:11:125:ALA:O | 24:11:129:LEU:HB2 | 2.14 | 0.47 |
| 33:20:90:TYR:HA | 33:20:98:ARG:HA | 1.95 | 0.47 |
| 34:41:65:LEU:HB3 | 37:41:202:CLA:HHB | 1.96 | 0.47 |
| 37:B:516:CLA:HHC | 37:B:516:CLA:HBB1 | 1.95 | 0.47 |
| 45:D:404:PL9:H412 | 6:F:23:GLY:HA3 | 1.95 | 0.47 |
| 39:d:405:BCR:H20C | 39:d:405:BCR:H361 | 1.77 | 0.47 |
| 30:37:145:TYR:HB2 | 37:37:306:CLA:HAA1 | 1.96 | 0.47 |
| 43:37:321:LHG:H102 | 37:41:206:CLA:HAA2 | 1.95 | 0.47 |
| 33:40:90:TYR:HA | 33:40:98:ARG:HA | 1.95 | 0.47 |
| 2:B:215:PHE:HB2 | 39:B:525:BCR:H272 | 1.95 | 0.47 |
| 4:D:99:ASP:HB2 | 5:E:74:LYS:HE2 | 1.96 | 0.47 |
| 5:E:58:THR:O | 5:E:62:GLN:NE2 | 2.48 | 0.47 |
| 37:c:503:CLA:H171 | 37:c:510:CLA:HBB2 | 1.97 | 0.47 |
| 30:17:145:TYR:HB2 | 37:17:307:CLA:HAA1 | 1.96 | 0.47 |
| 37:B:502:CLA:H102 | 37:B:509:CLA:H193 | 1.97 | 0.47 |
| 3:C:333:THR:O | 13:O:150:ARG:NH2 | 2.40 | 0.47 |
| 2:b:383:PHE:CZ | 13:o:165:GLY:HA2 | 2.49 | 0.47 |
| 5:e:58:THR:O | 5:e:62:GLN:NE2 | 2.48 | 0.47 |
| 31:18:172:MET:HE1 | 37:18:202:CLA:HAC1 | 1.95 | 0.47 |
| 27:34:112:ILE:HD11 | 37:34:303:CLA:H3A | 1.95 | 0.47 |
| 15:U:92:VAL:HA | 15:U:95:ARG:HD2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:Z:101:CLA:HBA1 | 37:Z:101:CLA:H42 | 1.97 | 0.47 |
| 27:14:60:ARG:HG2 | 37:14:301:CLA:HHB | 1.96 | 0.47 |
| 27:14:112:ILE:HD11 | 37:14:303:CLA:H3A | 1.95 | 0.47 |
| 37:15:301:CLA:H3A | 37:15:301:CLA:HBA2 | 1.74 | 0.47 |
| 33:40:36:PRO:HG3 | 33:40:61:ARG:HH12 | 1.80 | 0.47 |
| 2:B:50:PRO:HD2 | 13:o:57:GLY:HA3 | 1.96 | 0.47 |
| 2:B:327:ALA:HB1 | 41:B:520:LMG:HC8 | 1.97 | 0.47 |
| 37:C:503:CLA:H171 | 37:C:510:CLA:HBB2 | 1.96 | 0.47 |
| 1:a:98:GLU:HG3 | 21:w:21:GLU:HB3 | 1.96 | 0.47 |
| 2:b:327:ALA:HB1 | 41:b:519:LMG:HC8 | 1.97 | 0.47 |
| 37:b:502:CLA:H52 | 7:h:45:ILE:HG13 | 1.97 | 0.47 |
| 13:o:15:LYS:HE3 | 13:o:15:LYS:HB2 | 1.71 | 0.47 |
| 29:16:203:PHE:HB2 | 32:19:240:GLN:HB3 | 1.97 | 0.47 |
| 31:18:80:VAL:HB | 31:18:85:ILE:HD13 | 1.96 | 0.47 |
| 26:33:75:VAL:O | 26:33:78:THR:OG1 | 2.31 | 0.47 |
| 29:36:186:ILE:HG13 | 29:36:187:THR:HG23 | 1.95 | 0.47 |
| 39:D:407:BCR:H393 | 9:J:24:LEU:HD11 | 1.97 | 0.47 |
| 16:V:8:ARG:NH1 | 16:V:21:LEU:O | 2.41 | 0.47 |
| 16:V:36:THR:HA | 16:V:103:ARG:HD3 | 1.96 | 0.47 |
| 37:b:515:CLA:H161 | 7:h:7:LEU:HD21 | 1.97 | 0.47 |
| 30:17:168:ARG:HB3 | 37:17:302:CLA:HBC3 | 1.97 | 0.47 |
| 37:18:203:CLA:H11 | 37:18:203:CLA:H52 | 1.66 | 0.47 |
| 2:b:433:ASP:OD1 | 2:b:436:SER:OG | 2.30 | 0.47 |
| 37:z:101:CLA:HBA1 | 37:z:101:CLA:H42 | 1.97 | 0.47 |
| 6:F:22:HIS:HE1 | 46:F:101:HEM:ND | 2.12 | 0.47 |
| 3:c:451:ALA:O | 8:i:33:ASN:ND2 | 2.34 | 0.47 |
| 15:u:92:VAL:HA | 15:u:95:ARG:HD2 | 1.97 | 0.47 |
| 37:19:310:CLA:O2A | 43:19:314:LHG:O9 | 2.33 | 0.47 |
| 37:20:301:CLA:H41 | 37:20:301:CLA:H61 | 1.68 | 0.47 |
| 1:A:283:ILE:HA | 1:A:286:THR:HG22 | 1.97 | 0.46 |
| 3:C:330:GLN:HB3 | 15:U:93:ILE:HD11 | 1.97 | 0.46 |
| 37:D:406:CLA:H112 | 7:H:40:ILE:HD11 | 1.98 | 0.46 |
| 44:h:102:DGD:HB91 | 44:h:102:DGD:HB62 | 1.68 | 0.46 |
| 27:14:90:TYR:HA | 27:14:98:LYS:HA | 1.97 | 0.46 |
| 31:18:163:GLU:HG3 | 37:18:208:CLA:NB | 2.30 | 0.46 |
| 32:19:79:ASP:OD1 | 50:19:312:DD6:O4 | 2.32 | 0.46 |
| 2:B:272:ARG:NH2 | 2:B:276:ASP:OD2 | 2.49 | 0.46 |
| 10:K:21:ASP:OD2 | 17:Y:9:GLN:NE2 | 2.38 | 0.46 |
| 37:b:502:CLA:H203 | 44:h:102:DGD:HB82 | 1.96 | 0.46 |
| 29:16:52:ILE:HB | 32:19:44:SER:HB2 | 1.96 | 0.46 |
| 37:19:302:CLA:H62 | 37:19:302:CLA:H41 | 1.70 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:39:302:CLA:H62 | 37:39:302:CLA:H41 | 1.71 | 0.46 |
| 34:41:55:GLU:OE1 | 34:41:55:GLU:N | 2.39 | 0.46 |
| 37:a:403:CLA:H122 | 38:a:405:PHO:H3A | 1.98 | 0.46 |
| 37:c:508:CLA:H161 | 37:c:510:CLA:H101 | 1.95 | 0.46 |
| 30:17:179:VAL:HG21 | 37:17:309:CLA:HBC3 | 1.97 | 0.46 |
| 34:21:65:LEU:HB3 | 37:21:202:CLA:HHB | 1.96 | 0.46 |
| 29:36:92:LEU:HD21 | 29:36:113:VAL:HG13 | 1.98 | 0.46 |
| 30:37:168:ARG:HB3 | 37:37:301:CLA:HBC3 | 1.98 | 0.46 |
| 41:C:518:LMG:H361 | 10:K:28:VAL:HG21 | 1.97 | 0.46 |
| 1:a:159:LEU:HD21 | 44:c:516:DGD:HA51 | 1.97 | 0.46 |
| 48:31:313:A86:O | 37:32:202:CLA:HAC2 | 2.16 | 0.46 |
| 31:38:92:SER:OG | 47:38:205:KC1:O2D | 2.32 | 0.46 |
| 37:39:307:CLA:C2B | 43:39:314:LHG:HC11 | 2.45 | 0.46 |
| 43:39:314:LHG:C4 | 43:39:314:LHG:HC31 | 2.45 | 0.46 |
| 34:41:97:SER:HG | 34:41:101:THR:HG1 | 1.61 | 0.46 |
| 37:B:514:CLA:H43 | 40:B:519:SQD:H102 | 1.97 | 0.46 |
| 15:U:27:ILE:HD11 | 15:U:82:LEU:HD22 | 1.98 | 0.46 |
| 15:U:48:LYS:NZ | 15:U:66:GLY:O | 2.42 | 0.46 |
| 31:18:126:LEU:HD21 | 37:18:201:CLA:HBC3 | 1.98 | 0.46 |
| 31:18:175:MET:HE2 | 37:18:203:CLA:HBB2 | 1.98 | 0.46 |
| 33:20:36:PRO:HG3 | 33:20:61:ARG:HH12 | 1.80 | 0.46 |
| 37:33:308:CLA:H92 | 37:33:308:CLA:H62 | 1.75 | 0.46 |
| 32:39:121:VAL:HG13 | 37:39:303:CLA:HBB2 | 1.98 | 0.46 |
| 32:39:199:GLU:O | 32:39:201:ARG:N | 2.47 | 0.46 |
| 33:40:178:MET:N | 33:40:178:MET:SD | 2.88 | 0.46 |
| 34:41:167:LYS:O | 34:41:171:ILE:N | 2.49 | 0.46 |
| 2:B:70:GLY:HA2 | 2:B:178:VAL:HG11 | 1.98 | 0.46 |
| 40:L:101:SQD:H102 | 37:b:514:CLA:H43 | 1.97 | 0.46 |
| 4:d:311:GLU:HB2 | 13:o:157:PRO:HG3 | 1.98 | 0.46 |
| 3:C:98:GLY:N | 3:C:102:GLU:O | 2.41 | 0.46 |
| 2:b:255:THR:HG21 | 37:b:502:CLA:HED1 | 1.98 | 0.46 |
| 3:c:376:ASN:OD1 | 3:c:376:ASN:N | 2.47 | 0.46 |
| 5:e:70:ARG:NH2 | 7:h:50:ASN:O | 2.44 | 0.46 |
| 37:19:304:CLA:H3A | 37:19:304:CLA:HBA1 | 1.68 | 0.46 |
| 30:37:67:HIS:HE1 | 47:37:302:KC1:ND | 2.11 | 0.46 |
| 37:39:310:CLA:HBB2 | 43:39:314:LHG:C21 | 2.38 | 0.46 |
| 1:A:188:ALA:HB1 | 1:A:329:GLU:HB3 | 1.98 | 0.46 |
| 37:B:504:CLA:H193 | 39:0:101:BCR:HC8 | 1.97 | 0.46 |
| 37:W:102:CLA:H162 | 37:W:102:CLA:H122 | 1.72 | 0.46 |
| 28:15:147:GLY:O | 31:18:159:LYS:NZ | 2.42 | 0.46 |
| 28:15:152:ASP:HB3 | 28:15:155:GLU:HB3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:16:40:VAL:HG23 | 29:16:42:PRO:HD2 | 1.98 | 0.46 |
| 37:A:403:CLA:H122 | 38:D:403:PHO:H3A | 1.97 | 0.45 |
| 1:a:200:ALA:HB2 | 44:j:101:DGD:HBH2 | 1.98 | 0.45 |
| 2:b:477:ASP:OD1 | 2:b:477:ASP:N | 2.41 | 0.45 |
| 37:b:504:CLA:H193 | 39:5:101:BCR:HC8 | 1.97 | 0.45 |
| 32:19:121:VAL:HG13 | 37:19:303:CLA:HBB2 | 1.97 | 0.45 |
| 33:40:54:HIS:O | 33:40:60:ARG:NH1 | 2.49 | 0.45 |
| 1:A:217:SER:HA | 4:D:271:LEU:HD12 | 1.98 | 0.45 |
| 41:a:410:LMG:H382 | 44:c:516:DGD:HB51 | 1.98 | 0.45 |
| 37:b:523:CLA:H143 | 37:b:523:CLA:H111 | 1.78 | 0.45 |
| 33:20:178:MET:SD | 33:20:178:MET:N | 2.88 | 0.45 |
| 37:32:204:CLA:H3A | 37:32:204:CLA:HBA2 | 1.68 | 0.45 |
| 1:A:156:ALA:HA | 1:A:160:VAL:HB | 1.97 | 0.45 |
| 39:A:406:BCR:H371 | 39:A:406:BCR:H24C | 1.77 | 0.45 |
| 37:B:514:CLA:H93 | 37:B:514:CLA:H61 | 1.83 | 0.45 |
| 2:b:272:ARG:NH2 | 2:b:276:ASP:OD2 | 2.49 | 0.45 |
| 4:d:52:THR:HG22 | 6:f:38:MET:HE1 | 1.99 | 0.45 |
| 27:14:59:ARG:NH2 | 37:14:302:CLA:OBD | 2.49 | 0.45 |
| 29:16:80:PHE:HB3 | 40:17:301:SQD:H131 | 1.99 | 0.45 |
| 33:20:54:HIS:O | 33:20:60:ARG:NH1 | 2.49 | 0.45 |
| 27:34:59:ARG:NH2 | 37:34:302:CLA:OBD | 2.49 | 0.45 |
| 28:35:192:TYR:OH | 48:35:311:A86:O2 | 2.34 | 0.45 |
| 40:36:315:SQD:H441 | 30:37:88:ASP:HB2 | 1.97 | 0.45 |
| 34:41:118:ASP:OD1 | 34:41:118:ASP:N | 2.50 | 0.45 |
| 34:41:135:VAL:O | 34:41:136:MET:HG3 | 2.16 | 0.45 |
| 3:C:414:SER:HB2 | 16:V:42:VAL:HG23 | 1.99 | 0.45 |
| 1:a:283:ILE:HA | 1:a:286:THR:HG22 | 1.97 | 0.45 |
| 29:16:120:GLN:OE1 | 47:16:304:KC1:ND | 2.49 | 0.45 |
| 29:16:164:ASN:HB2 | 37:16:307:CLA:HED2 | 1.99 | 0.45 |
| 27:34:60:ARG:HG2 | 37:34:301:CLA:HHB | 1.97 | 0.45 |
| 29:36:41:ALA:HB1 | 32:39:98:ARG:HB3 | 1.97 | 0.45 |
| 31:38:163:GLU:HG3 | 37:38:208:CLA:NB | 2.30 | 0.45 |
| 37:B:504:CLA:HBB1 | 37:B:513:CLA:C2C | 2.47 | 0.45 |
| 37:C:509:CLA:H91 | 37:C:512:CLA:HBD | 1.99 | 0.45 |
| 1:a:156:ALA:HA | 1:a:160:VAL:HB | 1.97 | 0.45 |
| 2:b:70:GLY:HA2 | 2:b:178:VAL:HG11 | 1.98 | 0.45 |
| 24:31:125:ALA:O | 24:31:129:LEU:HB2 | 2.16 | 0.45 |
| 28:35:83:ASN:HB3 | 28:35:85:ILE:HD12 | 1.98 | 0.45 |
| 1:A:140:ARG:HB2 | 4:D:219:ASN:HA | 1.98 | 0.45 |
| 4:D:183:PHE:HD2 | 4:D:184:LEU:HD12 | 1.82 | 0.45 |
| 39:D:407:BCR:H20C | 39:D:407:BCR:H361 | 1.77 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:17:67:HIS:HE1 | 47:17:303:KC1:ND | 2.11 | 0.45 |
| 29:36:120:GLN:OE1 | 47:36:304:KC1:ND | 2.49 | 0.45 |
| 37:38:203:CLA:H52 | 37:38:203:CLA:H11 | 1.66 | 0.45 |
| 39:C:519:BCR:H20C | 39:C:519:BCR:H361 | 1.84 | 0.45 |
| 2:b:215:PHE:HB2 | 39:b:524:BCR:H272 | 1.98 | 0.45 |
| 37:b:504:CLA:HBB1 | 37:b:513:CLA:C2C | 2.47 | 0.45 |
| 13:o:132:ASP:OD2 | 13:o:132:ASP:N | 2.49 | 0.45 |
| 26:13:179:VAL:HA | 26:13:182:VAL:HG22 | 1.99 | 0.45 |
| 29:16:178:LEU:HG | 37:16:309:CLA:HBC2 | 1.99 | 0.45 |
| 37:19:306:CLA:H152 | 37:19:306:CLA:H112 | 1.64 | 0.45 |
| 34:21:55:GLU:OE1 | 34:21:55:GLU:N | 2.39 | 0.45 |
| 34:21:135:VAL:O | 34:21:136:MET:HG3 | 2.16 | 0.45 |
| 24:31:204:GLN:HG3 | 48:31:313:A86:C24 | 2.47 | 0.45 |
| 28:35:186:GLN:HB3 | 28:35:190:GLU:HB2 | 1.99 | 0.45 |
| 37:36:301:CLA:HBA2 | 37:36:301:CLA:H3A | 1.74 | 0.45 |
| 37:C:513:CLA:H193 | 37:Z:101:CLA:H201 | 1.99 | 0.45 |
| 37:D:406:CLA:H41 | 37:D:406:CLA:H61 | 1.68 | 0.45 |
| 13:O:132:ASP:OD2 | 13:O:132:ASP:N | 2.49 | 0.45 |
| 1:a:135:TYR:CE1 | 3:c:447:ARG:HG3 | 2.51 | 0.45 |
| 37:c:504:CLA:H62 | 37:c:504:CLA:H41 | 1.70 | 0.45 |
| 37:c:509:CLA:H91 | 37:c:512:CLA:HBD | 1.99 | 0.45 |
| 26:13:75:VAL:O | 26:13:78:THR:OG1 | 2.31 | 0.45 |
| 1:A:85:SER:HA | 1:A:109:GLY:HA3 | 1.99 | 0.45 |
| 13:O:168:MET:HE2 | 13:O:170:VAL:HA | 1.99 | 0.45 |
| 4:d:192:LEU:O | 11:l:35:TYR:OH | 2.31 | 0.45 |
| 15:u:27:ILE:HD11 | 15:u:82:LEU:HD22 | 1.98 | 0.45 |
| 29:16:92:LEU:HD21 | 29:16:113:VAL:HG13 | 1.98 | 0.45 |
| 30:17:35:LEU:O | 30:17:61:ARG:NH2 | 2.50 | 0.45 |
| 29:36:178:LEU:HG | 37:36:309:CLA:HBC2 | 1.99 | 0.45 |
| 37:36:306:CLA:H143 | 37:36:306:CLA:H111 | 1.83 | 0.45 |
| 30:37:35:LEU:O | 30:37:61:ARG:NH2 | 2.49 | 0.45 |
| 3:C:223:VAL:O | 3:C:291:ASN:ND2 | 2.40 | 0.45 |
| 43:D:411:LHG:H212 | 43:D:411:LHG:H281 | 1.99 | 0.45 |
| 13:O:43:MET:HB3 | 13:O:82:ILE:HB | 1.99 | 0.45 |
| 41:l:101:LMG:H362 | 12:m:21:PHE:HB2 | 1.99 | 0.45 |
| 31:18:91:LEU:N | 31:18:97:LEU:O | 2.50 | 0.45 |
| 43:19:314:LHG:C4 | 43:19:314:LHG:HC31 | 2.45 | 0.45 |
| 27:34:109:ILE:HD12 | 27:34:112:ILE:HD12 | 1.99 | 0.45 |
| 1:A:159:LEU:HD21 | 44:C:516:DGD:HA51 | 1.99 | 0.44 |
| 2:B:179:GLN:HE22 | 7:H:66:ILE:HB | 1.82 | 0.44 |
| 37:C:502:CLA:HBB2 | 37:C:510:CLA:H151 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:O:207:VAL:HG22 | 13:O:214:ILE:HG22 | 1.99 | 0.44 |
| 26:13:166:ASN:ND2 | 37:13:308:CLA:OBD | 2.50 | 0.44 |
| 26:33:166:ASN:ND2 | 37:33:308:CLA:OBD | 2.50 | 0.44 |
| 37:35:308:CLA:H61 | 37:35:308:CLA:H41 | 1.66 | 0.44 |
| 1:a:85:SER:HA | 1:a:109:GLY:HA3 | 1.99 | 0.44 |
| 2:b:334:ASP:OD1 | 2:b:334:ASP:N | 2.42 | 0.44 |
| 39:d:405:BCR:H393 | 9:j:24:LEU:HD11 | 2.00 | 0.44 |
| 13:o:168:MET:HE2 | 13:o:170:VAL:HA | 1.99 | 0.44 |
| 27:14:109:ILE:HD12 | 27:14:112:ILE:HD12 | 1.99 | 0.44 |
| 29:16:205:ASP:OD1 | 29:16:205:ASP:N | 2.43 | 0.44 |
| 37:32:211:CLA:H101 | 37:32:211:CLA:H62 | 1.76 | 0.44 |
| 29:36:40:VAL:HG23 | 29:36:42:PRO:HD2 | 1.98 | 0.44 |
| 29:36:80:PHE:HB3 | 40:36:315:SQD:H131 | 1.99 | 0.44 |
| 33:40:64:GLU:OE2 | 33:40:171:ARG:NE | 2.40 | 0.44 |
| 6:F:43:ARG:NH1 | 9:J:39:LEU:OXT | 2.51 | 0.44 |
| 20:q:139:LYS:HD3 | 20:q:181:THR:HG22 | 1.99 | 0.44 |
| 37:12:203:CLA:H3A | 37:12:203:CLA:HBA2 | 1.68 | 0.44 |
| 37:12:203:CLA:H142 | 37:12:203:CLA:H112 | 1.87 | 0.44 |
| 37:40:203:CLA:H61 | 37:40:203:CLA:H41 | 1.68 | 0.44 |
| 37:C:506:CLA:H18 | 37:C:506:CLA:H122 | 1.99 | 0.44 |
| 4:D:334:PRO:HG2 | 5:E:66:LEU:HD21 | 1.99 | 0.44 |
| 13:O:51:ALA:HB1 | 13:O:66:PHE:HB3 | 2.00 | 0.44 |
| 37:19:307:CLA:C2B | 43:19:314:LHG:HC11 | 2.47 | 0.44 |
| 37:33:308:CLA:H2 | 37:33:308:CLA:H61 | 1.66 | 0.44 |
| 28:35:168:ARG:HB3 | 37:35:301:CLA:HBC3 | 2.00 | 0.44 |
| 32:39:113:LEU:HD23 | 32:39:113:LEU:HA | 1.86 | 0.44 |
| 2:B:255:THR:HG21 | 37:B:502:CLA:HED1 | 1.98 | 0.44 |
| 1:a:217:SER:HA | 4:d:271:LEU:HD12 | 1.98 | 0.44 |
| 37:b:502:CLA:H62 | 37:b:502:CLA:H41 | 1.56 | 0.44 |
| 4:d:183:PHE:HD2 | 4:d:184:LEU:HD12 | 1.82 | 0.44 |
| 13:o:179:GLU:H | 13:o:179:GLU:HG2 | 1.45 | 0.44 |
| 37:11:308:CLA:H71 | 37:11:308:CLA:H112 | 1.81 | 0.44 |
| 34:21:167:LYS:O | 34:21:171:ILE:N | 2.49 | 0.44 |
| 37:21:206:CLA:HHB | 43:21:217:LHG:H312 | 2.00 | 0.44 |
| 29:36:164:ASN:HB2 | 37:36:307:CLA:HED2 | 1.99 | 0.44 |
| 37:39:306:CLA:H112 | 37:39:306:CLA:H152 | 1.64 | 0.44 |
| 37:b:501:CLA:H52 | 37:b:501:CLA:H12 | 1.79 | 0.44 |
| 37:b:502:CLA:H62 | 37:b:502:CLA:H92 | 1.86 | 0.44 |
| 31:18:36:GLY:HA3 | 31:18:168:ARG:HH22 | 1.83 | 0.44 |
| 37:19:310:CLA:H62 | 37:19:310:CLA:H41 | 1.71 | 0.44 |
| 25:32:132:MET:HG3 | 37:32:202:CLA:H12 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:404:SER:HA | 3:C:418:VAL:HG23 | 2.00 | 0.44 |
| 3:C:431:LEU:HD22 | 37:C:502:CLA:HMC2 | 1.99 | 0.44 |
| 1:a:92:HIS:NE2 | 3:c:358:ASP:OD2 | 2.38 | 0.44 |
| 43:a:412:LHG:H212 | 43:a:412:LHG:H281 | 1.99 | 0.44 |
| 37:b:523:CLA:H11 | 39:b:524:BCR:H23C | 2.00 | 0.44 |
| 29:16:158:LYS:NZ | 30:17:148:ASN:OD1 | 2.50 | 0.44 |
| 31:18:77:GLY:HA2 | 31:18:80:VAL:HG22 | 1.99 | 0.44 |
| 32:19:199:GLU:O | 32:19:201:ARG:N | 2.47 | 0.44 |
| 25:32:53:GLU:HG3 | 25:32:56:ASN:HD22 | 1.82 | 0.44 |
| 25:32:87:PHE:HE2 | 37:32:206:CLA:H11 | 1.83 | 0.44 |
| 26:33:179:VAL:HA | 26:33:182:VAL:HG22 | 2.00 | 0.44 |
| 37:39:310:CLA:O2A | 43:39:314:LHG:O9 | 2.35 | 0.44 |
| 34:41:180:MET:HA | 34:41:183:ILE:HG22 | 2.00 | 0.44 |
| 2:B:405:LYS:HE3 | 2:B:405:LYS:HB2 | 1.83 | 0.44 |
| 39:K:101:BCR:H342 | 39:K:101:BCR:H311 | 2.00 | 0.44 |
| 1:a:188:ALA:HB1 | 1:a:329:GLU:HB3 | 1.98 | 0.44 |
| 3:c:404:SER:HA | 3:c:418:VAL:HG23 | 2.00 | 0.44 |
| 4:d:229:ASN:HD21 | 4:d:231:PHE:HD2 | 1.66 | 0.44 |
| 37:12:210:CLA:H62 | 37:12:210:CLA:H101 | 1.76 | 0.44 |
| 30:17:175:MET:HG2 | 37:17:302:CLA:H191 | 1.99 | 0.44 |
| 37:19:307:CLA:H112 | 37:19:307:CLA:H72 | 1.82 | 0.44 |
| 37:32:206:CLA:H161 | 37:32:206:CLA:H122 | 1.79 | 0.44 |
| 43:37:321:LHG:H312 | 37:41:206:CLA:HHB | 2.00 | 0.44 |
| 4:D:50:GLY:HA3 | 4:D:77:VAL:HG22 | 2.00 | 0.44 |
| 37:c:506:CLA:H18 | 37:c:506:CLA:H122 | 1.99 | 0.44 |
| 37:11:308:CLA:H12 | 25:12:132:MET:HG3 | 2.00 | 0.44 |
| 34:21:118:ASP:OD1 | 34:21:118:ASP:N | 2.50 | 0.44 |
| 34:21:180:MET:HA | 34:21:183:ILE:HG22 | 2.00 | 0.44 |
| 37:32:202:CLA:H142 | 37:32:202:CLA:H111 | 1.78 | 0.44 |
| 34:41:152:PHE:HD2 | 34:41:153:ILE:HG13 | 1.83 | 0.44 |
| 37:A:405:CLA:H202 | 37:W:101:CLA:H12 | 1.99 | 0.43 |
| 2:B:74:SER:HA | 2:B:92:SER:HB2 | 2.00 | 0.43 |
| 20:Q:139:LYS:HD3 | 20:Q:181:THR:HG22 | 1.99 | 0.43 |
| 2:b:74:SER:HA | 2:b:92:SER:HB2 | 2.00 | 0.43 |
| 37:14:301:CLA:H3A | 37:14:301:CLA:HBA2 | 1.82 | 0.43 |
| 1:A:43:THR:HG23 | 39:A:406:BCR:H362 | 2.00 | 0.43 |
| 2:B:454:GLY:HA2 | 41:B:520:LMG:H212 | 2.01 | 0.43 |
| 37:B:502:CLA:H41 | 37:B:502:CLA:H62 | 1.56 | 0.43 |
| 3:C:40:LEU:HD21 | 37:C:511:CLA:H2A | 1.99 | 0.43 |
| 13:O:179:GLU:H | 13:O:179:GLU:HG2 | 1.45 | 0.43 |
| 1:a:89:ILE:HD11 | 1:a:108:ASN:HB3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:b:517:BCR:H20C | 39:b:517:BCR:H361 | 1.85 | 0.43 |
| 13:o:207:VAL:HG22 | 13:o:214:ILE:HG22 | 1.99 | 0.43 |
| 39:y:101:BCR:H342 | 39:y:101:BCR:H311 | 2.00 | 0.43 |
| 37:16:301:CLA:H142 | 37:16:301:CLA:H112 | 1.87 | 0.43 |
| 31:18:172:MET:HB2 | 31:18:172:MET:HE2 | 1.52 | 0.43 |
| 37:31:302:CLA:H3A | 37:31:302:CLA:HBA2 | 1.64 | 0.43 |
| 1:A:89:ILE:HD11 | 1:A:108:ASN:HB3 | 2.00 | 0.43 |
| 3:C:77:LYS:HE3 | 3:C:82:GLN:HG2 | 2.00 | 0.43 |
| 4:D:87:SER:O | 4:D:166:TRP:NE1 | 2.42 | 0.43 |
| 37:c:502:CLA:HBB2 | 37:c:510:CLA:H151 | 1.99 | 0.43 |
| 13:o:43:MET:HB3 | 13:o:82:ILE:HB | 1.99 | 0.43 |
| 25:12:53:GLU:HG3 | 25:12:56:ASN:HD22 | 1.82 | 0.43 |
| 34:21:137:LYS:HE2 | 34:21:137:LYS:HB3 | 1.34 | 0.43 |
| 48:39:313:A86:O | 48:39:313:A86:O2 | 2.36 | 0.43 |
| 37:B:514:CLA:H111 | 37:B:514:CLA:H152 | 1.85 | 0.43 |
| 37:B:524:CLA:H11 | 39:B:525:BCR:H23C | 2.01 | 0.43 |
| 1:a:96:ILE:HG12 | 1:a:105:TRP:CE2 | 2.53 | 0.43 |
| 1:a:106:LEU:HD11 | 39:a:408:BCR:H292 | 1.99 | 0.43 |
| 1:a:184:LEU:HD21 | 4:d:185:GLN:HG2 | 2.00 | 0.43 |
| 3:c:77:LYS:HE3 | 3:c:82:GLN:HG2 | 2.00 | 0.43 |
| 28:35:179:VAL:HG21 | 37:35:310:CLA:HBC3 | 1.99 | 0.43 |
| 1:A:183:MET:HE3 | 37:D:401:CLA:HAC1 | 2.01 | 0.43 |
| 4:D:292:LEU:HD23 | 4:D:292:LEU:HA | 1.77 | 0.43 |
| 45:D:404:PL9:H28 | 45:D:404:PL9:H322 | 1.84 | 0.43 |
| 13:O:3:LYS:HD2 | 13:O:5:GLN:HB2 | 2.01 | 0.43 |
| 1:a:191:ASN:HB2 | 3:c:409:ALA:HB1 | 2.00 | 0.43 |
| 3:c:332:PRO:HA | 13:o:151:THR:HB | 2.00 | 0.43 |
| 3:c:431:LEU:HD22 | 37:c:502:CLA:HMC2 | 1.99 | 0.43 |
| 33:20:40:LEU:HD23 | 33:20:40:LEU:HA | 1.84 | 0.43 |
| 37:31:301:CLA:H162 | 37:31:301:CLA:H122 | 1.72 | 0.43 |
| 37:35:308:CLA:H61 | 37:35:308:CLA:H92 | 1.89 | 0.43 |
| 29:36:205:ASP:OD1 | 29:36:205:ASP:N | 2.43 | 0.43 |
| 33:40:66:LYS:NZ | 33:40:128:GLU:OE2 | 2.44 | 0.43 |
| 2:B:433:ASP:OD1 | 2:B:436:SER:OG | 2.30 | 0.43 |
| 4:D:229:ASN:HD21 | 4:D:231:PHE:HD2 | 1.66 | 0.43 |
| 12:M:25:LEU:HD23 | 12:M:25:LEU:HA | 1.87 | 0.43 |
| 2:b:185:TRP:HB2 | 37:b:501:CLA:HED2 | 2.00 | 0.43 |
| 37:b:512:CLA:H61 | 37:b:512:CLA:H102 | 1.82 | 0.43 |
| 3:c:40:LEU:HD21 | 37:c:511:CLA:H2A | 1.99 | 0.43 |
| 37:13:308:CLA:H61 | 37:13:308:CLA:H2 | 1.66 | 0.43 |
| 2:B:75:TRP:HB3 | 40:B:522:SQD:H5 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:C:505:CLA:HBB1 | 37:C:505:CLA:HHC | 2.01 | 0.43 |
| 40:L:101:SQD:H101 | 39:b:517:BCR:H24C | 2.01 | 0.43 |
| 37:c:513:CLA:H91 | 37:c:513:CLA:H112 | 1.86 | 0.43 |
| 13:o:51:ALA:HB1 | 13:o:66:PHE:HB3 | 2.00 | 0.43 |
| 28:15:168:ARG:HB3 | 37:15:301:CLA:HBC3 | 2.00 | 0.43 |
| 37:15:308:CLA:H92 | 37:15:308:CLA:H41 | 2.00 | 0.43 |
| 31:18:80:VAL:O | 31:18:85:ILE:HG12 | 2.18 | 0.43 |
| 31:18:181:GLU:HG2 | 31:18:187:THR:HA | 2.00 | 0.43 |
| 33:20:178:MET:HE2 | 47:20:302:KC1:CBB | 2.49 | 0.43 |
| 24:31:49:TRP:HA | 24:31:52:SER:HB2 | 2.00 | 0.43 |
| 37:31:301:CLA:H2 | 37:31:301:CLA:HAA1 | 2.00 | 0.43 |
| 37:34:301:CLA:H3A | 37:34:301:CLA:HBA2 | 1.82 | 0.43 |
| 1:A:96:ILE:HG12 | 1:A:105:TRP:CE2 | 2.53 | 0.43 |
| 37:A:405:CLA:H92 | 37:A:405:CLA:H62 | 1.82 | 0.43 |
| 2:B:185:TRP:HB2 | 37:B:501:CLA:HED2 | 2.00 | 0.43 |
| 37:B:508:CLA:CBB | 4:D:122:ILE:HG12 | 2.49 | 0.43 |
| 44:H:102:DGD:HB62 | 44:H:102:DGD:HB91 | 1.68 | 0.43 |
| 13:O:9:LEU:HA | 20:Q:183:LYS:HZ1 | 1.83 | 0.43 |
| 16:V:9:THR:HG22 | 16:V:18:THR:HG22 | 2.01 | 0.43 |
| 20:Q:86:TYR:HA | 20:Q:94:PRO:HG3 | 2.01 | 0.43 |
| 37:W:102:CLA:H2 | 37:W:102:CLA:HAA1 | 2.00 | 0.43 |
| 16:v:9:THR:HG22 | 16:v:18:THR:HG22 | 2.01 | 0.43 |
| 39:y:101:BCR:H15C | 39:y:101:BCR:H351 | 1.90 | 0.43 |
| 37:38:208:CLA:H61 | 37:38:208:CLA:H2 | 1.67 | 0.43 |
| 33:40:178:MET:HE2 | 47:40:204:KC1:CBB | 2.49 | 0.43 |
| 1:A:106:LEU:HD11 | 39:A:406:BCR:H292 | 1.99 | 0.43 |
| 39:A:410:BCR:H11C | 39:A:410:BCR:H341 | 1.93 | 0.43 |
| 2:B:314:TYR:OH | 2:B:334:ASP:OD2 | 2.30 | 0.43 |
| 39:B:517:BCR:H24C | 40:B:519:SQD:H101 | 2.01 | 0.43 |
| 37:C:508:CLA:H111 | 10:K:31:LEU:HD21 | 2.01 | 0.43 |
| 39:b:517:BCR:H11C | 39:b:517:BCR:H341 | 1.86 | 0.43 |
| 37:c:501:CLA:H143 | 37:c:501:CLA:H161 | 1.91 | 0.43 |
| 4:d:13:LEU:HD13 | 18:x:31:LYS:HE3 | 2.01 | 0.43 |
| 4:d:102:ARG:HE | 5:e:78:GLU:HG3 | 1.84 | 0.43 |
| 20:q:86:TYR:HA | 20:q:94:PRO:HG3 | 2.01 | 0.43 |
| 37:11:301:CLA:HBA2 | 37:11:301:CLA:H3A | 1.64 | 0.43 |
| 25:12:87:PHE:HE2 | 37:12:205:CLA:H11 | 1.83 | 0.43 |
| 37:12:205:CLA:H122 | 37:12:205:CLA:H161 | 1.79 | 0.43 |
| 26:13:145:TYR:HB2 | 37:13:307:CLA:HAA1 | 2.00 | 0.43 |
| 29:16:43:LEU:HD11 | 37:19:302:CLA:H43 | 2.00 | 0.43 |
| 37:17:309:CLA:H61 | 37:17:309:CLA:H102 | 1.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:18:208:CLA:H2 | 37:18:208:CLA:H61 | 1.66 | 0.43 |
| 37:35:308:CLA:H41 | 37:35:308:CLA:H92 | 2.01 | 0.43 |
| 3:c:400:GLY:HA3 | 3:c:418:VAL:HG22 | 2.00 | 0.43 |
| 13:o:3:LYS:HD2 | 13:o:5:GLN:HB2 | 2.01 | 0.43 |
| 20:q:127:PRO:HB3 | 20:q:189:LYS:HE2 | 2.00 | 0.43 |
| 37:12:207:CLA:H3A | 37:12:207:CLA:HBA2 | 1.81 | 0.43 |
| 27:14:102:ILE:HG23 | 27:14:111:ALA:HB3 | 2.01 | 0.43 |
| 48:31:319:A86:O3 | 25:32:90:TYR:O | 2.37 | 0.43 |
| 2:B:383:PHE:N | 4:D:343:GLU:O | 2.51 | 0.42 |
| 3:C:251:PHE:CE2 | 43:19:314:LHG:H112 | 2.54 | 0.42 |
| 37:a:403:CLA:H72 | 37:a:403:CLA:H111 | 1.85 | 0.42 |
| 37:a:407:CLA:H202 | 37:w:101:CLA:H12 | 2.01 | 0.42 |
| 2:b:468:TRP:CH2 | 43:d:407:LHG:HC42 | 2.54 | 0.42 |
| 3:c:319:ASP:OD2 | 3:c:338:TYR:OH | 2.32 | 0.42 |
| 13:o:210:GLU:OE1 | 13:o:210:GLU:N | 2.31 | 0.42 |
| 48:11:319:A86:O3 | 25:12:90:TYR:O | 2.36 | 0.42 |
| 29:36:65:GLU:HA | 37:36:301:CLA:HBB1 | 2.01 | 0.42 |
| 2:B:103:LEU:HD22 | 37:B:506:CLA:H51 | 2.00 | 0.42 |
| 3:C:400:GLY:HA3 | 3:C:418:VAL:HG22 | 2.00 | 0.42 |
| 37:a:407:CLA:H62 | 37:a:407:CLA:H92 | 1.82 | 0.42 |
| 41:b:519:LMG:H361 | 41:b:519:LMG:H332 | 1.75 | 0.42 |
| 39:h:101:BCR:H15C | 39:h:101:BCR:H351 | 1.91 | 0.42 |
| 13:o:72:MET:HE3 | 13:o:72:MET:HB2 | 1.75 | 0.42 |
| 24:11:145:TYR:HB2 | 37:11:307:CLA:HAA1 | 2.01 | 0.42 |
| 26:13:168:ARG:HA | 26:13:171:MET:HE3 | 2.01 | 0.42 |
| 28:15:31:SER:OG | 28:15:32:GLU:N | 2.52 | 0.42 |
| 30:17:78:THR:O | 30:17:82:ASN:ND2 | 2.47 | 0.42 |
| 25:32:90:TYR:HA | 25:32:98:LYS:HA | 2.01 | 0.42 |
| 37:35:301:CLA:HBA2 | 37:35:301:CLA:H3A | 1.74 | 0.42 |
| 1:A:221:SER:HB3 | 4:D:137:ILE:HD12 | 2.00 | 0.42 |
| 2:B:166:ILE:HG21 | 37:B:503:CLA:HED1 | 2.01 | 0.42 |
| 2:B:350:GLU:H | 2:B:350:GLU:HG3 | 1.65 | 0.42 |
| 2:B:357:ARG:NH2 | 4:D:336:GLU:O | 2.31 | 0.42 |
| 39:B:517:BCR:H15C | 39:B:517:BCR:H351 | 1.91 | 0.42 |
| 6:F:22:HIS:HE1 | 46:F:101:HEM:C4D | 2.37 | 0.42 |
| 2:b:103:LEU:HD22 | 37:b:506:CLA:H51 | 2.00 | 0.42 |
| 37:b:505:CLA:H62 | 37:b:505:CLA:H41 | 1.78 | 0.42 |
| 3:c:172:LEU:HD11 | 37:c:512:CLA:H111 | 2.02 | 0.42 |
| 37:13:310:CLA:H3A | 37:13:310:CLA:HBA2 | 1.82 | 0.42 |
| 37:16:301:CLA:H3A | 37:16:301:CLA:HBA2 | 1.74 | 0.42 |
| 31:18:61:ARG:NH1 | 31:18:64:GLU:OE2 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:32:59:ARG:HG3 | 25:32:137:TYR:CZ | 2.55 | 0.42 |
| 26:33:145:TYR:HB2 | 37:33:307:CLA:HAA1 | 2.00 | 0.42 |
| 1:A:92:HIS:NE2 | 3:C:358:ASP:OD2 | 2.38 | 0.42 |
| 20:Q:127:PRO:HB3 | 20:Q:189:LYS:HE2 | 2.00 | 0.42 |
| 1:a:43:THR:HG23 | 39:a:408:BCR:H362 | 2.00 | 0.42 |
| 2:b:453:TYR:HB2 | 4:d:292:LEU:HD12 | 2.02 | 0.42 |
| 3:c:348:ILE:HG21 | 3:c:357:TRP:HB2 | 2.02 | 0.42 |
| 4:d:50:GLY:HA3 | 4:d:77:VAL:HG22 | 2.00 | 0.42 |
| 26:13:192:TYR:OH | 48:13:311:A86:O2 | 2.37 | 0.42 |
| 37:18:201:CLA:H62 | 37:18:201:CLA:H101 | 1.79 | 0.42 |
| 26:33:168:ARG:HA | 26:33:171:MET:HE3 | 2.01 | 0.42 |
| 26:33:192:TYR:OH | 48:33:311:A86:O2 | 2.37 | 0.42 |
| 31:38:80:VAL:O | 31:38:85:ILE:HG12 | 2.19 | 0.42 |
| 41:A:408:LMG:H382 | 44:C:516:DGD:HB51 | 2.01 | 0.42 |
| 3:C:278:SER:OG | 3:C:432:ALA:O | 2.30 | 0.42 |
| 39:a:408:BCR:H15C | 39:a:408:BCR:H351 | 1.89 | 0.42 |
| 37:c:505:CLA:HHC | 37:c:505:CLA:HBB1 | 2.01 | 0.42 |
| 20:q:130:VAL:HB | 20:q:189:LYS:HE3 | 2.02 | 0.42 |
| 31:38:91:LEU:N | 31:38:97:LEU:O | 2.50 | 0.42 |
| 38:A:404:PHO:H112 | 38:A:404:PHO:H72 | 1.88 | 0.42 |
| 37:C:503:CLA:H61 | 37:C:503:CLA:H41 | 1.64 | 0.42 |
| 37:C:512:CLA:H203 | 37:C:512:CLA:H162 | 1.80 | 0.42 |
| 39:D:407:BCR:H15C | 39:D:407:BCR:H351 | 1.88 | 0.42 |
| 37:b:504:CLA:HMB1 | 37:b:507:CLA:HHC | 2.02 | 0.42 |
| 4:d:86:HIS:NE2 | 4:d:160:PRO:O | 2.43 | 0.42 |
| 6:f:22:HIS:HE1 | 46:f:101:HEM:C4D | 2.37 | 0.42 |
| 24:11:50:LEU:HA | 24:11:50:LEU:HD23 | 1.80 | 0.42 |
| 25:12:59:ARG:HG3 | 25:12:137:TYR:CZ | 2.55 | 0.42 |
| 32:39:91:TRP:NE1 | 37:39:305:CLA:O1A | 2.45 | 0.42 |
| 2:B:192:PRO:HG3 | 7:H:49:TYR:CD1 | 2.55 | 0.42 |
| 37:B:512:CLA:H61 | 37:B:512:CLA:H102 | 1.82 | 0.42 |
| 41:B:520:LMG:H361 | 41:B:520:LMG:H332 | 1.75 | 0.42 |
| 3:C:172:LEU:HD11 | 37:C:512:CLA:H111 | 2.02 | 0.42 |
| 37:C:502:CLA:HMB2 | 37:C:504:CLA:HHC | 2.02 | 0.42 |
| 39:C:515:BCR:H20C | 39:C:515:BCR:H361 | 1.89 | 0.42 |
| 2:b:454:GLY:HA2 | 41:b:519:LMG:H212 | 2.01 | 0.42 |
| 37:c:503:CLA:H62 | 37:c:503:CLA:H102 | 1.67 | 0.42 |
| 37:11:308:CLA:HAC2 | 48:11:313:A86:O | 2.20 | 0.42 |
| 41:16:316:LMG:O5 | 41:16:316:LMG:O4 | 2.30 | 0.42 |
| 31:18:78:THR:HG21 | 31:18:177:ASN:ND2 | 2.35 | 0.42 |
| 37:21:202:CLA:H3A | 37:21:202:CLA:HBA2 | 1.77 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:31:109:ILE:HG22 | 24:31:112:ILE:HD12 | 2.02 | 0.42 |
| 28:35:90:TYR:HA | 28:35:98:LYS:HA | 2.02 | 0.42 |
| 30:37:157:ALA:O | 30:37:161:ASN:ND2 | 2.53 | 0.42 |
| 8:I:13:ILE:HD12 | 8:I:13:ILE:HA | 1.93 | 0.42 |
| 2:b:75:TRP:HB3 | 40:b:521:SQD:H5 | 2.00 | 0.42 |
| 28:15:75:VAL:O | 28:15:79:ILE:HG12 | 2.20 | 0.42 |
| 37:17:309:CLA:H51 | 37:21:206:CLA:HBB1 | 2.01 | 0.42 |
| 26:33:175:MET:HE1 | 47:33:302:KC1:CBB | 2.50 | 0.42 |
| 28:35:75:VAL:O | 28:35:79:ILE:HG12 | 2.19 | 0.42 |
| 28:35:175:MET:O | 28:35:179:VAL:HG23 | 2.20 | 0.42 |
| 30:37:40:PRO:HB3 | 37:38:201:CLA:HBB1 | 2.01 | 0.42 |
| 37:37:308:CLA:H102 | 37:37:308:CLA:H61 | 1.80 | 0.42 |
| 40:A:407:SQD:H383 | 39:K:101:BCR:H371 | 2.01 | 0.42 |
| 39:A:410:BCR:H15C | 39:A:410:BCR:H351 | 1.84 | 0.42 |
| 1:a:140:ARG:HB2 | 4:d:219:ASN:HA | 2.02 | 0.42 |
| 2:b:166:ILE:HG21 | 37:b:503:CLA:HED1 | 2.01 | 0.42 |
| 37:c:501:CLA:C1B | 37:c:501:CLA:H2 | 2.50 | 0.42 |
| 37:21:208:CLA:H142 | 37:21:208:CLA:H111 | 1.88 | 0.42 |
| 3:C:221:TRP:HE3 | 44:C:516:DGD:HB21 | 1.85 | 0.42 |
| 3:C:348:ILE:HG21 | 3:C:357:TRP:HB2 | 2.02 | 0.42 |
| 4:D:29:VAL:HA | 4:D:37:PHE:HE2 | 1.85 | 0.42 |
| 37:D:401:CLA:H141 | 37:D:401:CLA:H162 | 1.90 | 0.42 |
| 13:O:13:GLN:HE22 | 20:Q:183:LYS:NZ | 2.18 | 0.42 |
| 13:O:210:GLU:OE1 | 13:O:210:GLU:N | 2.31 | 0.42 |
| 2:b:40:TYR:HH | 41:b:519:LMG:HO5 | 1.68 | 0.42 |
| 2:b:55:MET:HE3 | 2:b:80:ILE:HD13 | 2.02 | 0.42 |
| 43:d:408:LHG:H261 | 11:l:23:LEU:HD22 | 2.02 | 0.42 |
| 13:o:199:ARG:NE | 13:o:201:GLU:OE2 | 2.41 | 0.42 |
| 24:11:49:TRP:HA | 24:11:52:SER:HB2 | 2.01 | 0.42 |
| 37:13:308:CLA:H92 | 37:13:308:CLA:H62 | 1.75 | 0.42 |
| 31:18:157:ALA:O | 31:18:161:ASN:ND2 | 2.40 | 0.42 |
| 24:31:124:PHE:O | 24:31:128:GLU:HB2 | 2.20 | 0.42 |
| 24:31:138:ASP:OD1 | 24:31:138:ASP:N | 2.53 | 0.42 |
| 24:31:145:TYR:HB2 | 37:31:308:CLA:HAA1 | 2.02 | 0.42 |
| 37:38:201:CLA:H62 | 37:38:201:CLA:H101 | 1.79 | 0.42 |
| 37:39:301:CLA:HBA2 | 37:39:301:CLA:H3A | 1.75 | 0.42 |
| 33:40:93:GLY:N | 47:40:206:KC1:O1A | 2.53 | 0.42 |
| 37:B:516:CLA:H142 | 37:B:516:CLA:H112 | 1.90 | 0.41 |
| 45:D:408:PL9:H111 | 43:D:410:LHG:H102 | 2.02 | 0.41 |
| 40:L:101:SQD:H142 | 40:L:101:SQD:H311 | 2.02 | 0.41 |
| 20:Q:130:VAL:HB | 20:Q:189:LYS:HE3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:W:101:CLA:H203 | 37:W:101:CLA:H162 | 1.88 | 0.41 |
| 1:a:221:SER:HB3 | 4:d:137:ILE:HD12 | 2.02 | 0.41 |
| 37:b:501:CLA:H92 | 37:b:501:CLA:H62 | 1.91 | 0.41 |
| 37:c:501:CLA:C2D | 37:c:503:CLA:H42 | 2.50 | 0.41 |
| 37:c:503:CLA:CHC | 37:z:101:CLA:H193 | 2.50 | 0.41 |
| 37:c:511:CLA:H41 | 17:y:27:LEU:HD13 | 2.02 | 0.41 |
| 4:d:87:SER:O | 4:d:166:TRP:NE1 | 2.41 | 0.41 |
| 45:d:406:PL9:H111 | 43:d:408:LHG:H102 | 2.02 | 0.41 |
| 5:e:74:LYS:NZ | 5:e:78:GLU:OE2 | 2.53 | 0.41 |
| 25:12:90:TYR:HA | 25:12:98:LYS:HA | 2.02 | 0.41 |
| 31:18:90:TYR:HA | 31:18:98:LYS:HA | 2.02 | 0.41 |
| 33:20:93:GLY:N | 47:20:304:KC1:O1A | 2.53 | 0.41 |
| 37:32:204:CLA:H142 | 37:32:204:CLA:H112 | 1.87 | 0.41 |
| 2:B:160:GLY:HA3 | 2:B:180:PRO:HB3 | 2.01 | 0.41 |
| 37:B:504:CLA:HBA2 | 37:B:512:CLA:H152 | 2.03 | 0.41 |
| 39:H:101:BCR:H11C | 39:H:101:BCR:H341 | 1.92 | 0.41 |
| 39:H:101:BCR:H361 | 39:H:101:BCR:H20C | 1.84 | 0.41 |
| 1:a:183:MET:HE3 | 37:a:404:CLA:HAC1 | 2.01 | 0.41 |
| 37:a:403:CLA:H142 | 37:a:403:CLA:H112 | 1.92 | 0.41 |
| 2:b:383:PHE:N | 4:d:343:GLU:O | 2.53 | 0.41 |
| 37:c:502:CLA:HMB2 | 37:c:504:CLA:HHC | 2.02 | 0.41 |
| 28:15:90:TYR:HA | 28:15:98:LYS:HA | 2.00 | 0.41 |
| 31:38:57:PHE:CE2 | 31:38:61:ARG:HB2 | 2.55 | 0.41 |
| 39:0:101:BCR:H11C | 39:0:101:BCR:H341 | 1.84 | 0.41 |
| 2:b:157:HIS:HA | 2:b:163:GLY:HA3 | 2.02 | 0.41 |
| 39:b:518:BCR:H351 | 39:b:518:BCR:H15C | 1.83 | 0.41 |
| 39:c:515:BCR:H15C | 39:c:515:BCR:H351 | 1.84 | 0.41 |
| 4:d:295:TYR:OH | 4:d:325:ARG:NH1 | 2.48 | 0.41 |
| 14:t:9:LEU:O | 14:t:13:THR:OG1 | 2.34 | 0.41 |
| 25:12:177:ASN:ND2 | 25:12:188:MET:SD | 2.93 | 0.41 |
| 32:39:182:LYS:HD2 | 32:39:182:LYS:HA | 1.87 | 0.41 |
| 2:B:177:LYS:HG2 | 7:H:67:VAL:HG13 | 2.02 | 0.41 |
| 39:a:408:BCR:H371 | 39:a:408:BCR:H24C | 1.77 | 0.41 |
| 2:b:160:GLY:HA3 | 2:b:180:PRO:HB3 | 2.01 | 0.41 |
| 3:c:324:ALA:HB2 | 15:u:96:ILE:HG21 | 2.02 | 0.41 |
| 37:12:205:CLA:HBA1 | 37:12:205:CLA:HBD | 2.02 | 0.41 |
| 27:14:166:ASN:ND2 | 37:14:308:CLA:OBD | 2.53 | 0.41 |
| 37:14:302:CLA:HBB1 | 48:14:314:A86:C4 | 2.50 | 0.41 |
| 28:15:175:MET:O | 28:15:179:VAL:HG23 | 2.20 | 0.41 |
| 29:16:65:GLU:HA | 37:16:301:CLA:HBB1 | 2.01 | 0.41 |
| 37:19:310:CLA:HBB2 | 43:19:314:LHG:C21 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:21:152:PHE:HD2 | 34:21:153:ILE:HG13 | 1.83 | 0.41 |
| 37:36:301:CLA:H142 | 37:36:301:CLA:H112 | 1.87 | 0.41 |
| 31:38:36:GLY:HA3 | 31:38:168:ARG:HH22 | 1.85 | 0.41 |
| 32:39:107:TRP:HH2 | 32:39:181:ILE:HG21 | 1.85 | 0.41 |
| 33:40:30:PRO:O | 33:40:65:ARG:NH2 | 2.49 | 0.41 |
| 39:A:406:BCR:H15C | 39:A:406:BCR:H351 | 1.89 | 0.41 |
| 39:B:518:BCR:H15C | 39:B:518:BCR:H351 | 1.83 | 0.41 |
| 3:C:36:GLY:HA3 | 37:C:511:CLA:HMD2 | 2.03 | 0.41 |
| 10:K:36:VAL:HG22 | 39:K:101:BCR:H382 | 2.02 | 0.41 |
| 13:O:94:THR:HG22 | 13:O:128:LYS:HG3 | 2.02 | 0.41 |
| 15:U:37:LYS:HA | 15:U:37:LYS:HD3 | 1.94 | 0.41 |
| 4:d:292:LEU:HD23 | 4:d:292:LEU:HA | 1.77 | 0.41 |
| 37:11:308:CLA:H111 | 37:11:308:CLA:H142 | 1.78 | 0.41 |
| 34:21:149:ARG:NH1 | 34:21:154:ASP:OD2 | 2.53 | 0.41 |
| 25:32:177:ASN:ND2 | 25:32:188:MET:SD | 2.94 | 0.41 |
| 31:38:90:TYR:HA | 31:38:98:LYS:HA | 2.02 | 0.41 |
| 34:41:149:ARG:NH1 | 34:41:154:ASP:OD2 | 2.53 | 0.41 |
| 34:41:183:ILE:HG13 | 34:41:187:MET:HE3 | 2.03 | 0.41 |
| 1:A:193:LEU:HD11 | 37:A:403:CLA:HMC2 | 2.02 | 0.41 |
| 37:C:501:CLA:H92 | 37:C:501:CLA:H62 | 1.84 | 0.41 |
| 37:C:504:CLA:H41 | 37:C:504:CLA:H62 | 1.70 | 0.41 |
| 45:D:404:PL9:H121 | 45:D:404:PL9:HC8 | 1.71 | 0.41 |
| 2:b:152:GLY:C | 37:b:506:CLA:HMC2 | 2.46 | 0.41 |
| 41:c:518:LMG:H131 | 41:c:518:LMG:H292 | 2.02 | 0.41 |
| 24:11:124:PHE:O | 24:11:128:GLU:HB2 | 2.20 | 0.41 |
| 32:19:149:LEU:HD23 | 32:19:149:LEU:HA | 1.84 | 0.41 |
| 25:32:162:VAL:HG12 | 37:32:210:CLA:HBB1 | 2.03 | 0.41 |
| 37:35:308:CLA:H142 | 37:35:308:CLA:H112 | 1.82 | 0.41 |
| 37:39:307:CLA:HHC | 37:39:307:CLA:HBB1 | 2.03 | 0.41 |
| 34:41:183:ILE:HD12 | 34:41:183:ILE:HA | 1.92 | 0.41 |
| 37:41:208:CLA:H111 | 37:41:208:CLA:H142 | 1.88 | 0.41 |
| 40:B:519:SQD:H142 | 40:B:519:SQD:H311 | 2.02 | 0.41 |
| 1:a:193:LEU:HD11 | 37:a:403:CLA:HMC2 | 2.03 | 0.41 |
| 37:b:514:CLA:H152 | 37:b:514:CLA:H111 | 1.85 | 0.41 |
| 3:c:414:SER:HB2 | 16:v:42:VAL:HG23 | 2.02 | 0.41 |
| 30:17:157:ALA:O | 30:17:161:ASN:ND2 | 2.53 | 0.41 |
| 37:18:201:CLA:H193 | 37:18:201:CLA:H161 | 1.90 | 0.41 |
| 37:21:206:CLA:H102 | 37:21:206:CLA:H62 | 1.94 | 0.41 |
| 37:39:310:CLA:H62 | 37:39:310:CLA:H41 | 1.70 | 0.41 |
| 34:41:158:ASP:OD1 | 34:41:158:ASP:N | 2.44 | 0.41 |
| 37:B:504:CLA:HMB1 | 37:B:507:CLA:HHC | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:C:501:CLA:C2D | 37:C:503:CLA:H42 | 2.50 | 0.41 |
| 39:C:515:BCR:H351 | 39:C:515:BCR:H15C | 1.84 | 0.41 |
| 1:a:77:ILE:HD11 | 14:t:6:TYR:HB3 | 2.02 | 0.41 |
| 2:b:243:SER:HA | 2:b:246:PHE:CE1 | 2.56 | 0.41 |
| 37:b:504:CLA:HBA2 | 37:b:512:CLA:H152 | 2.02 | 0.41 |
| 3:c:221:TRP:HE3 | 44:c:516:DGD:HB21 | 1.85 | 0.41 |
| 45:d:406:PL9:H422 | 45:d:406:PL9:H462 | 1.89 | 0.41 |
| 13:o:94:THR:HG22 | 13:o:128:LYS:HG3 | 2.02 | 0.41 |
| 28:15:180:ALA:O | 28:15:191:GLN:NE2 | 2.53 | 0.41 |
| 34:21:183:ILE:HD12 | 34:21:183:ILE:HA | 1.92 | 0.41 |
| 27:34:166:ASN:ND2 | 37:34:308:CLA:OBD | 2.53 | 0.41 |
| 37:34:302:CLA:HBB1 | 48:34:314:A86:C4 | 2.50 | 0.41 |
| 34:41:167:LYS:HA | 34:41:170:ALA:HB3 | 2.03 | 0.41 |
| 2:B:55:MET:HE3 | 2:B:80:ILE:HD13 | 2.02 | 0.41 |
| 2:B:157:HIS:HA | 2:B:163:GLY:HA3 | 2.02 | 0.41 |
| 2:B:392:ILE:HD12 | 2:B:418:LYS:HG2 | 2.03 | 0.41 |
| 3:C:424:LEU:HD22 | 37:C:502:CLA:HED2 | 2.03 | 0.41 |
| 37:C:501:CLA:C1B | 37:C:501:CLA:H2 | 2.50 | 0.41 |
| 37:C:510:CLA:H43 | 43:D:411:LHG:H223 | 2.02 | 0.41 |
| 38:a:405:PHO:H61 | 38:a:405:PHO:H2 | 1.84 | 0.41 |
| 2:b:191:ASN:HB2 | 7:h:58:VAL:HG13 | 2.03 | 0.41 |
| 37:c:501:CLA:H41 | 37:c:501:CLA:H61 | 1.75 | 0.41 |
| 45:d:406:PL9:H101 | 45:d:406:PL9:H122 | 1.86 | 0.41 |
| 9:j:11:LEU:HD23 | 9:j:11:LEU:HA | 1.96 | 0.41 |
| 13:o:10:SER:H | 13:o:13:GLN:NE2 | 2.19 | 0.41 |
| 20:q:120:LYS:HB3 | 20:q:120:LYS:HE2 | 1.86 | 0.41 |
| 37:11:307:CLA:HAC1 | 37:11:307:CLA:HHD | 1.85 | 0.41 |
| 37:11:308:CLA:HBB1 | 37:11:308:CLA:HHC | 2.03 | 0.41 |
| 25:12:38:THR:HB | 25:12:165:ASN:HD21 | 1.85 | 0.41 |
| 25:12:164:LEU:HD23 | 25:12:164:LEU:HA | 1.91 | 0.41 |
| 26:33:102:ILE:HG23 | 26:33:111:ALA:HB3 | 2.03 | 0.41 |
| 27:34:102:ILE:HG23 | 27:34:111:ALA:HB3 | 2.02 | 0.41 |
| 37:36:307:CLA:H72 | 37:36:307:CLA:H112 | 1.78 | 0.41 |
| 13:O:199:ARG:NE | 13:O:201:GLU:OE2 | 2.41 | 0.41 |
| 15:U:42:TYR:HA | 15:U:43:PRO:HA | 1.86 | 0.41 |
| 16:V:95:ILE:O | 20:Q:108:TYR:OH | 2.39 | 0.41 |
| 39:0:101:BCR:H20C | 39:0:101:BCR:H361 | 1.93 | 0.41 |
| 39:0:101:BCR:H371 | 39:0:101:BCR:H24C | 1.85 | 0.41 |
| 37:b:502:CLA:H93 | 44:h:102:DGD:HB52 | 2.02 | 0.41 |
| 3:c:191:GLY:HA2 | 20:q:147:TYR:CD1 | 2.56 | 0.41 |
| 3:c:277:ILE:HG12 | 37:c:502:CLA:HAC1 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:c:505:CLA:H72 | 37:c:505:CLA:H112 | 1.86 | 0.41 |
| 26:13:102:ILE:HG23 | 26:13:111:ALA:HB3 | 2.03 | 0.41 |
| 28:15:112:ILE:HD11 | 37:15:303:CLA:HAA2 | 2.03 | 0.41 |
| 32:19:207:LEU:HD23 | 32:19:207:LEU:HA | 1.89 | 0.41 |
| 33:20:64:GLU:OE2 | 33:20:171:ARG:NE | 2.40 | 0.41 |
| 27:34:152:ASP:HA | 27:34:153:PRO:HD3 | 1.85 | 0.41 |
| 30:37:50:LEU:HG | 37:37:301:CLA:HBA1 | 2.03 | 0.41 |
| 4:D:55:THR:HB | 5:E:50:THR:HG23 | 2.03 | 0.40 |
| 43:D:410:LHG:H261 | 11:L:23:LEU:HD22 | 2.03 | 0.40 |
| 37:b:514:CLA:H93 | 37:b:514:CLA:H61 | 1.83 | 0.40 |
| 37:c:504:CLA:HBB1 | 41:c:518:LMG:H422 | 2.03 | 0.40 |
| 39:c:514:BCR:H11C | 39:c:514:BCR:H341 | 1.87 | 0.40 |
| 41:c:518:LMG:H112 | 41:c:518:LMG:H142 | 1.86 | 0.40 |
| 37:d:404:CLA:H41 | 37:d:404:CLA:H61 | 1.68 | 0.40 |
| 33:20:30:PRO:O | 33:20:65:ARG:NH2 | 2.49 | 0.40 |
| 34:21:183:ILE:HG13 | 34:21:187:MET:HE3 | 2.03 | 0.40 |
| 2:B:152:GLY:C | 37:B:506:CLA:HMC2 | 2.46 | 0.40 |
| 41:L:102:LMG:H141 | 12:m:27:ILE:HD11 | 2.03 | 0.40 |
| 37:a:404:CLA:HAC1 | 37:a:404:CLA:HHD | 1.93 | 0.40 |
| 2:b:334:ASP:HB3 | 13:o:174:ALA:HB1 | 2.04 | 0.40 |
| 3:c:424:LEU:HD22 | 37:c:502:CLA:HED2 | 2.03 | 0.40 |
| 10:k:36:VAL:HG22 | 39:y:101:BCR:H382 | 2.02 | 0.40 |
| 13:o:127:ALA:HB1 | 13:o:140:MET:HG2 | 2.04 | 0.40 |
| 28:15:89:GLY:O | 28:15:98:LYS:HB2 | 2.21 | 0.40 |
| 37:18:202:CLA:H112 | 37:18:202:CLA:H152 | 1.93 | 0.40 |
| 37:39:302:CLA:H91 | 37:39:302:CLA:H112 | 1.94 | 0.40 |
| 37:41:202:CLA:H3A | 37:41:202:CLA:HBA2 | 1.77 | 0.40 |
| 3:C:284:ALA:HA | 3:C:287:TYR:HD2 | 1.86 | 0.40 |
| 13:O:10:SER:H | 13:O:13:GLN:NE2 | 2.19 | 0.40 |
| 1:a:41:LEU:HD23 | 1:a:41:LEU:HA | 1.90 | 0.40 |
| 3:c:402:LEU:HD23 | 3:c:402:LEU:HA | 1.91 | 0.40 |
| 7:h:56:GLU:H | 18:x:1:MET:HE1 | 1.87 | 0.40 |
| 24:11:109:ILE:HG22 | 24:11:112:ILE:HD12 | 2.01 | 0.40 |
| 30:17:50:LEU:HG | 37:17:302:CLA:HBA1 | 2.04 | 0.40 |
| 30:17:155:GLU:HG3 | 37:18:208:CLA:H71 | 2.03 | 0.40 |
| 32:19:53:SER:O | 32:19:63:ARG:NH2 | 2.48 | 0.40 |
| 34:21:102:SER:OG | 34:21:103:PHE:N | 2.54 | 0.40 |
| 34:21:167:LYS:HZ3 | 34:21:167:LYS:HG3 | 1.81 | 0.40 |
| 24:31:91:LEU:HD22 | 24:31:102:ILE:HD11 | 2.04 | 0.40 |
| 37:32:204:CLA:H122 | 37:32:204:CLA:H162 | 1.93 | 0.40 |
| 37:32:206:CLA:HBA1 | 37:32:206:CLA:HBD | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:34:187:THR:OG1 | 27:34:190:GLU:HG3 | 2.22 | 0.40 |
| 37:40:205:CLA:HBD | 37:40:205:CLA:HBA1 | 2.04 | 0.40 |
| 40:B:522:SQD:H441 | 39:a:408:BCR:H401 | 2.03 | 0.40 |
| 3:C:343:PRO:HB3 | 13:O:74:ARG:HD3 | 2.04 | 0.40 |
| 1:a:93:PHE:HZ | 37:a:407:CLA:HAA1 | 1.87 | 0.40 |
| 15:u:90:ASP:OD1 | 15:u:90:ASP:N | 2.54 | 0.40 |
| 39:5:101:BCR:H20C | 39:5:101:BCR:H361 | 1.93 | 0.40 |
| 28:15:61:ARG:HH22 | 37:15:301:CLA:HED3 | 1.87 | 0.40 |
| 30:17:126:PHE:HD1 | 37:19:305:CLA:H11 | 1.87 | 0.40 |
| 32:19:146:TYR:OH | 37:19:304:CLA:OBD | 2.28 | 0.40 |
| 32:39:68:LEU:HB3 | 32:39:75:ASP:OD1 | 2.22 | 0.40 |
| 1:A:93:PHE:HZ | 37:A:405:CLA:HAA1 | 1.87 | 0.40 |
| 41:B:521:LMG:H371 | 41:B:521:LMG:H402 | 1.83 | 0.40 |
| 8:I:24:LEU:HD11 | 37:W:101:CLA:HHC | 2.03 | 0.40 |
| 41:b:520:LMG:H331 | 41:b:520:LMG:H361 | 1.77 | 0.40 |
| 3:c:36:GLY:HA3 | 37:c:511:CLA:HMD2 | 2.03 | 0.40 |
| 39:c:515:BCR:H20C | 39:c:515:BCR:H361 | 1.89 | 0.40 |
| 15:u:42:TYR:HA | 15:u:43:PRO:HA | 1.86 | 0.40 |
| 28:15:86:VAL:HG11 | 28:15:100:SER:HB2 | 2.01 | 0.40 |
| 37:18:209:CLA:H193 | 37:18:209:CLA:H161 | 1.95 | 0.40 |
| 34:21:129:GLY:O | 34:21:133:VAL:HG23 | 2.22 | 0.40 |
| 24:31:144:GLY:O | 48:31:311:A86:O3 | 2.40 | 0.40 |
| 37:32:202:CLA:HBB1 | 37:32:202:CLA:HHC | 2.03 | 0.40 |
| 27:34:174:ILE:HD12 | 27:34:174:ILE:HA | 1.98 | 0.40 |
| 37:36:306:CLA:H93 | 37:36:306:CLA:H61 | 1.94 | 0.40 |
| 37:39:307:CLA:H72 | 37:39:307:CLA:H112 | 1.82 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 332/334 (99%) | 324 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | a | 332/334 (99%) | 324 (98%) | 8 (2%) | 0 | 100 | 100 |
| 2 | B | 482/484 (100%) | 467 (97%) | 15 (3%) | 0 | 100 | 100 |
| 2 | b | 482/484 (100%) | 467 (97%) | 15 (3%) | 0 | 100 | 100 |
| 3 | C | 449/451 (100%) | 431 (96%) | 18 (4%) | 0 | 100 | 100 |
| 3 | c | 449/451 (100%) | 431 (96%) | 18 (4%) | 0 | 100 | 100 |
| 4 | D | 339/341 (99%) | 327 (96%) | 12 (4%) | 0 | 100 | 100 |
| 4 | d | 339/341 (99%) | 327 (96%) | 12 (4%) | 0 | 100 | 100 |
| 5 | E | 73/75 (97%) | 73 (100%) | 0 | 0 | 100 | 100 |
| 5 | e | 73/75 (97%) | 73 (100%) | 0 | 0 | 100 | 100 |
| 6 | F | 26/28 (93%) | 26 (100%) | 0 | 0 | 100 | 100 |
| 6 | f | 26/28 (93%) | 26 (100%) | 0 | 0 | 100 | 100 |
| 7 | H | 64/66 (97%) | 63 (98%) | 1 (2%) | 0 | 100 | 100 |
| 7 | h | 64/66 (97%) | 63 (98%) | 1 (2%) | 0 | 100 | 100 |
| 8 | I | 33/35 (94%) | 31 (94%) | 2 (6%) | 0 | 100 | 100 |
| 8 | i | 33/35 (94%) | 31 (94%) | 2 (6%) | 0 | 100 | 100 |
| 9 | J | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 9 | j | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 10 | K | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 10 | k | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | L | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 11 | l | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 12 | M | 40/42 (95%) | 37 (92%) | 3 (8%) | 0 | 100 | 100 |
| 12 | m | 40/42 (95%) | 37 (92%) | 3 (8%) | 0 | 100 | 100 |
| 13 | O | 243/245 (99%) | 232 (96%) | 11 (4%) | 0 | 100 | 100 |
| 13 | o | 243/245 (99%) | 231 (95%) | 12 (5%) | 0 | 100 | 100 |
| 14 | T | 28/30 (93%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 14 | t | 28/30 (93%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 15 | U | 91/93 (98%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 15 | u | 91/93 (98%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 16 | V | 134/136 (98%) | 127 (95%) | 7 (5%) | 0 | 100 | 100 |
| 16 | v | 134/136 (98%) | 127 (95%) | 7 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 17 | Y | 32/34 (94%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 17 | y | 32/34 (94%) | 31 (97%) | 1 (3%) | 0 | 100 | 100 |
| 18 | X | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 18 | x | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 19 | Z | 57/59 (97%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 19 | z | 57/59 (97%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 20 | Q | 149/151 (99%) | 140 (94%) | 9 (6%) | 0 | 100 | 100 |
| 20 | q | 149/151 (99%) | 140 (94%) | 9 (6%) | 0 | 100 | 100 |
| 21 | W | 50/52 (96%) | 45 (90%) | 5 (10%) | 0 | 100 | 100 |
| 21 | w | 50/52 (96%) | 45 (90%) | 5 (10%) | 0 | 100 | 100 |
| 24 | 11 | 174/176 (99%) | 166 (95%) | 8 (5%) | 0 | 100 | 100 |
| 24 | 31 | 174/176 (99%) | 166 (95%) | 8 (5%) | 0 | 100 | 100 |
| 25 | 12 | 167/169 (99%) | 160 (96%) | 7 (4%) | 0 | 100 | 100 |
| 25 | 32 | 167/169 (99%) | 159 (95%) | 8 (5%) | 0 | 100 | 100 |
| 26 | 13 | 167/169 (99%) | 160 (96%) | 7 (4%) | 0 | 100 | 100 |
| 26 | 33 | 167/169 (99%) | 160 (96%) | 7 (4%) | 0 | 100 | 100 |
| 27 | 14 | 170/172 (99%) | 162 (95%) | 6 (4%) | 2 (1%) | 10 | 20 |
| 27 | 34 | 170/172 (99%) | 162 (95%) | 6 (4%) | 2 (1%) | 10 | 20 |
| 28 | 15 | 168/170 (99%) | 147 (88%) | 20 (12%) | 1 (1%) | 21 | 38 |
| 28 | 35 | 168/170 (99%) | 147 (88%) | 20 (12%) | 1 (1%) | 21 | 38 |
| 29 | 16 | 177/179 (99%) | 171 (97%) | 6 (3%) | 0 | 100 | 100 |
| 29 | 36 | 177/179 (99%) | 171 (97%) | 6 (3%) | 0 | 100 | 100 |
| 30 | 17 | 174/176 (99%) | 169 (97%) | 5 (3%) | 0 | 100 | 100 |
| 30 | 37 | 174/176 (99%) | 170 (98%) | 4 (2%) | 0 | 100 | 100 |
| 31 | 18 | 166/168 (99%) | 156 (94%) | 10 (6%) | 0 | 100 | 100 |
| 31 | 38 | 166/168 (99%) | 156 (94%) | 10 (6%) | 0 | 100 | 100 |
| 32 | 19 | 225/227 (99%) | 211 (94%) | 14 (6%) | 0 | 100 | 100 |
| 32 | 39 | 225/227 (99%) | 214 (95%) | 11 (5%) | 0 | 100 | 100 |
| 33 | 20 | 153/155 (99%) | 133 (87%) | 20 (13%) | 0 | 100 | 100 |
| 33 | 40 | 153/155 (99%) | 133 (87%) | 20 (13%) | 0 | 100 | 100 |
| 34 | 21 | 160/162 (99%) | 142 (89%) | 18 (11%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 34 | 41 | 160/162 (99%) | 142 (89%) | 18 (11%) | 0 | 100 100 |
| All | All | 9322/9450 (99%) | 8876 (95%) | 440 (5%) | 6 (0%) | 49 68 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 14 | 39 | GLU |
| 27 | 34 | 39 | GLU |
| 27 | 14 | 40 | PRO |
| 28 | 15 | 39 | GLU |
| 27 | 34 | 40 | PRO |
| 28 | 35 | 39 | GLU |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 272/272 (100%) | 271 (100%) | 1 (0%) | 84 93 |
| 1 | a | 272/272 (100%) | 271 (100%) | 1 (0%) | 84 93 |
| 2 | B | 385/385 (100%) | 379 (98%) | 6 (2%) | 55 79 |
| 2 | b | 385/385 (100%) | 379 (98%) | 6 (2%) | 55 79 |
| 3 | C | 356/356 (100%) | 351 (99%) | 5 (1%) | 59 81 |
| 3 | c | 356/356 (100%) | 351 (99%) | 5 (1%) | 59 81 |
| 4 | D | 273/273 (100%) | 272 (100%) | 1 (0%) | 84 93 |
| 4 | d | 273/273 (100%) | 272 (100%) | 1 (0%) | 84 93 |
| 5 | E | 69/69 (100%) | 68 (99%) | 1 (1%) | 59 81 |
| 5 | e | 69/69 (100%) | 68 (99%) | 1 (1%) | 59 81 |
| 6 | F | 22/22 (100%) | 22 (100%) | 0 | 100 100 |
| 6 | f | 22/22 (100%) | 22 (100%) | 0 | 100 100 |
| 7 | H | 55/55 (100%) | 55 (100%) | 0 | 100 100 |
| 7 | h | 55/55 (100%) | 55 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 8 | I | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 8 | i | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 9 | J | 27/27 (100%) | 27 (100%) | 0 | 100 | 100 |
| 9 | j | 27/27 (100%) | 27 (100%) | 0 | 100 | 100 |
| 10 | K | 32/32 (100%) | 30 (94%) | 2 (6%) | 16 | 34 |
| 10 | k | 32/32 (100%) | 30 (94%) | 2 (6%) | 16 | 34 |
| 11 | L | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 11 | l | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 12 | M | 31/31 (100%) | 31 (100%) | 0 | 100 | 100 |
| 12 | m | 31/31 (100%) | 31 (100%) | 0 | 100 | 100 |
| 13 | O | 196/198 (99%) | 188 (96%) | 8 (4%) | 27 | 53 |
| 13 | o | 196/198 (99%) | 188 (96%) | 8 (4%) | 27 | 53 |
| 14 | T | 27/27 (100%) | 27 (100%) | 0 | 100 | 100 |
| 14 | t | 27/27 (100%) | 27 (100%) | 0 | 100 | 100 |
| 15 | U | 77/77 (100%) | 76 (99%) | 1 (1%) | 61 | 82 |
| 15 | u | 77/77 (100%) | 76 (99%) | 1 (1%) | 61 | 82 |
| 16 | V | 114/114 (100%) | 112 (98%) | 2 (2%) | 51 | 77 |
| 16 | v | 114/114 (100%) | 112 (98%) | 2 (2%) | 51 | 77 |
| 17 | Y | 27/27 (100%) | 27 (100%) | 0 | 100 | 100 |
| 17 | y | 27/27 (100%) | 27 (100%) | 0 | 100 | 100 |
| 18 | X | 29/29 (100%) | 28 (97%) | 1 (3%) | 32 | 60 |
| 18 | x | 29/29 (100%) | 28 (97%) | 1 (3%) | 32 | 60 |
| 19 | Z | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |
| 19 | z | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |
| 20 | Q | 122/122 (100%) | 120 (98%) | 2 (2%) | 55 | 79 |
| 20 | q | 122/122 (100%) | 120 (98%) | 2 (2%) | 55 | 79 |
| 21 | W | 43/43 (100%) | 43 (100%) | 0 | 100 | 100 |
| 21 | w | 43/43 (100%) | 43 (100%) | 0 | 100 | 100 |
| 24 | 11 | 138/138 (100%) | 135 (98%) | 3 (2%) | 45 | 73 |
| 24 | 31 | 138/138 (100%) | 137 (99%) | 1 (1%) | 76 | 89 |
| 25 | 12 | 133/133 (100%) | 130 (98%) | 3 (2%) | 44 | 72 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 25 | 32 | 133/133 (100%) | 132 (99%) | 1 (1%) | 73 88 |
| 26 | 13 | 134/134 (100%) | 131 (98%) | 3 (2%) | 45 73 |
| 26 | 33 | 134/134 (100%) | 130 (97%) | 4 (3%) | 36 64 |
| 27 | 14 | 136/136 (100%) | 134 (98%) | 2 (2%) | 57 80 |
| 27 | 34 | 136/136 (100%) | 133 (98%) | 3 (2%) | 45 73 |
| 28 | 15 | 135/135 (100%) | 123 (91%) | 12 (9%) | 9 20 |
| 28 | 35 | 135/135 (100%) | 122 (90%) | 13 (10%) | 8 17 |
| 29 | 16 | 137/137 (100%) | 128 (93%) | 9 (7%) | 15 32 |
| 29 | 36 | 137/137 (100%) | 128 (93%) | 9 (7%) | 15 32 |
| 30 | 17 | 137/137 (100%) | 129 (94%) | 8 (6%) | 18 38 |
| 30 | 37 | 137/137 (100%) | 131 (96%) | 6 (4%) | 25 50 |
| 31 | 18 | 133/133 (100%) | 128 (96%) | 5 (4%) | 29 56 |
| 31 | 38 | 133/133 (100%) | 125 (94%) | 8 (6%) | 17 36 |
| 32 | 19 | 174/174 (100%) | 169 (97%) | 5 (3%) | 37 65 |
| 32 | 39 | 174/174 (100%) | 166 (95%) | 8 (5%) | 24 48 |
| 33 | 20 | 121/121 (100%) | 107 (88%) | 14 (12%) | 5 11 |
| 33 | 40 | 121/121 (100%) | 107 (88%) | 14 (12%) | 5 11 |
| 34 | 21 | 129/129 (100%) | 111 (86%) | 18 (14%) | 3 7 |
| 34 | 41 | 129/129 (100%) | 111 (86%) | 18 (14%) | 3 7 |
| All | All | 7560/7564 (100%) | 7333 (97%) | 227 (3%) | 37 64 |

All (227) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 264 | SER |
| 2 | B | 22 | VAL |
| 2 | B | 348 | ASP |
| 2 | B | 388 | SER |
| 2 | B | 391 | SER |
| 2 | B | 435 | THR |
| 2 | B | 446 | SER |
| 3 | C | 28 | SER |
| 3 | C | 328 | SER |
| 3 | C | 376 | ASN |
| 3 | C | 392 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 470 | ILE |
| 4 | D | 258 | VAL |
| 5 | E | 13 | ASP |
| 10 | K | 17 | SER |
| 10 | K | 22 | VAL |
| 13 | O | 69 | SER |
| 13 | O | 87 | THR |
| 13 | O | 133 | THR |
| 13 | O | 179 | GLU |
| 13 | O | 210 | GLU |
| 13 | O | 212 | SER |
| 13 | O | 221 | THR |
| 13 | O | 232 | THR |
| 15 | U | 22 | SER |
| 16 | V | 9 | THR |
| 16 | V | 86 | GLU |
| 18 | X | 36 | LEU |
| 20 | Q | 158 | SER |
| 20 | Q | 161 | THR |
| 1 | a | 264 | SER |
| 2 | b | 22 | VAL |
| 2 | b | 348 | ASP |
| 2 | b | 388 | SER |
| 2 | b | 391 | SER |
| 2 | b | 435 | THR |
| 2 | b | 446 | SER |
| 3 | c | 28 | SER |
| 3 | c | 328 | SER |
| 3 | c | 376 | ASN |
| 3 | c | 392 | GLU |
| 3 | c | 470 | ILE |
| 4 | d | 258 | VAL |
| 5 | e | 13 | ASP |
| 10 | k | 17 | SER |
| 10 | k | 22 | VAL |
| 13 | o | 69 | SER |
| 13 | o | 87 | THR |
| 13 | o | 133 | THR |
| 13 | o | 179 | GLU |
| 13 | o | 210 | GLU |
| 13 | o | 212 | SER |
| 13 | o | 221 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | o | 232 | THR |
| 15 | u | 22 | SER |
| 16 | v | 9 | THR |
| 16 | v | 86 | GLU |
| 18 | x | 36 | LEU |
| 20 | q | 158 | SER |
| 20 | q | 161 | THR |
| 24 | 11 | 58 | GLU |
| 24 | 11 | 66 | LYS |
| 24 | 11 | 88 | ASP |
| 25 | 12 | 38 | THR |
| 25 | 12 | 76 | VAL |
| 25 | 12 | 155 | GLU |
| 26 | 13 | 58 | GLU |
| 26 | 13 | 154 | GLU |
| 26 | 13 | 155 | GLU |
| 27 | 14 | 34 | GLU |
| 27 | 14 | 154 | GLU |
| 28 | 15 | 41 | LEU |
| 28 | 15 | 43 | VAL |
| 28 | 15 | 53 | GLU |
| 28 | 15 | 66 | LYS |
| 28 | 15 | 86 | VAL |
| 28 | 15 | 91 | LEU |
| 28 | 15 | 100 | SER |
| 28 | 15 | 117 | LEU |
| 28 | 15 | 121 | LEU |
| 28 | 15 | 135 | SER |
| 28 | 15 | 179 | VAL |
| 28 | 15 | 188 | MET |
| 29 | 16 | 40 | VAL |
| 29 | 16 | 87 | THR |
| 29 | 16 | 95 | SER |
| 29 | 16 | 102 | ASP |
| 29 | 16 | 123 | LEU |
| 29 | 16 | 136 | SER |
| 29 | 16 | 141 | ASP |
| 29 | 16 | 146 | LEU |
| 29 | 16 | 154 | GLU |
| 30 | 17 | 39 | GLU |
| 30 | 17 | 41 | LEU |
| 30 | 17 | 43 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | 17 | 47 | LEU |
| 30 | 17 | 112 | VAL |
| 30 | 17 | 120 | ILE |
| 30 | 17 | 140 | ASP |
| 30 | 17 | 150 | ILE |
| 31 | 18 | 33 | ILE |
| 31 | 18 | 60 | ARG |
| 31 | 18 | 117 | LEU |
| 31 | 18 | 149 | ASP |
| 31 | 18 | 155 | GLU |
| 32 | 19 | 75 | ASP |
| 32 | 19 | 123 | VAL |
| 32 | 19 | 181 | ILE |
| 32 | 19 | 208 | ASP |
| 32 | 19 | 255 | THR |
| 33 | 20 | 29 | GLU |
| 33 | 20 | 37 | LEU |
| 33 | 20 | 58 | GLU |
| 33 | 20 | 70 | ILE |
| 33 | 20 | 76 | VAL |
| 33 | 20 | 79 | LEU |
| 33 | 20 | 106 | MET |
| 33 | 20 | 112 | ILE |
| 33 | 20 | 150 | VAL |
| 33 | 20 | 155 | GLU |
| 33 | 20 | 160 | LYS |
| 33 | 20 | 165 | MET |
| 33 | 20 | 178 | MET |
| 33 | 20 | 182 | VAL |
| 34 | 21 | 36 | GLU |
| 34 | 21 | 37 | ASN |
| 34 | 21 | 55 | GLU |
| 34 | 21 | 61 | LYS |
| 34 | 21 | 70 | LEU |
| 34 | 21 | 90 | ILE |
| 34 | 21 | 99 | ASP |
| 34 | 21 | 113 | LEU |
| 34 | 21 | 114 | SER |
| 34 | 21 | 133 | VAL |
| 34 | 21 | 136 | MET |
| 34 | 21 | 137 | LYS |
| 34 | 21 | 138 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | 21 | 143 | GLU |
| 34 | 21 | 162 | GLU |
| 34 | 21 | 167 | LYS |
| 34 | 21 | 186 | LEU |
| 34 | 21 | 195 | SER |
| 24 | 31 | 88 | ASP |
| 25 | 32 | 155 | GLU |
| 26 | 33 | 58 | GLU |
| 26 | 33 | 88 | ASP |
| 26 | 33 | 154 | GLU |
| 26 | 33 | 155 | GLU |
| 27 | 34 | 32 | GLU |
| 27 | 34 | 34 | GLU |
| 27 | 34 | 154 | GLU |
| 28 | 35 | 41 | LEU |
| 28 | 35 | 43 | VAL |
| 28 | 35 | 47 | LEU |
| 28 | 35 | 55 | GLU |
| 28 | 35 | 66 | LYS |
| 28 | 35 | 86 | VAL |
| 28 | 35 | 91 | LEU |
| 28 | 35 | 117 | LEU |
| 28 | 35 | 121 | LEU |
| 28 | 35 | 179 | VAL |
| 28 | 35 | 181 | GLU |
| 28 | 35 | 188 | MET |
| 28 | 35 | 194 | SER |
| 29 | 36 | 40 | VAL |
| 29 | 36 | 87 | THR |
| 29 | 36 | 95 | SER |
| 29 | 36 | 102 | ASP |
| 29 | 36 | 123 | LEU |
| 29 | 36 | 136 | SER |
| 29 | 36 | 141 | ASP |
| 29 | 36 | 146 | LEU |
| 29 | 36 | 154 | GLU |
| 30 | 37 | 43 | VAL |
| 30 | 37 | 47 | LEU |
| 30 | 37 | 53 | GLU |
| 30 | 37 | 112 | VAL |
| 30 | 37 | 140 | ASP |
| 30 | 37 | 150 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 38 | 50 | LEU |
| 31 | 38 | 76 | VAL |
| 31 | 38 | 106 | VAL |
| 31 | 38 | 117 | LEU |
| 31 | 38 | 149 | ASP |
| 31 | 38 | 155 | GLU |
| 31 | 38 | 175 | MET |
| 31 | 38 | 181 | GLU |
| 32 | 39 | 75 | ASP |
| 32 | 39 | 114 | ILE |
| 32 | 39 | 123 | VAL |
| 32 | 39 | 139 | GLU |
| 32 | 39 | 149 | LEU |
| 32 | 39 | 181 | ILE |
| 32 | 39 | 208 | ASP |
| 32 | 39 | 255 | THR |
| 33 | 40 | 29 | GLU |
| 33 | 40 | 37 | LEU |
| 33 | 40 | 58 | GLU |
| 33 | 40 | 70 | ILE |
| 33 | 40 | 76 | VAL |
| 33 | 40 | 79 | LEU |
| 33 | 40 | 106 | MET |
| 33 | 40 | 112 | ILE |
| 33 | 40 | 150 | VAL |
| 33 | 40 | 155 | GLU |
| 33 | 40 | 160 | LYS |
| 33 | 40 | 165 | MET |
| 33 | 40 | 178 | MET |
| 33 | 40 | 182 | VAL |
| 34 | 41 | 36 | GLU |
| 34 | 41 | 37 | ASN |
| 34 | 41 | 55 | GLU |
| 34 | 41 | 61 | LYS |
| 34 | 41 | 70 | LEU |
| 34 | 41 | 90 | ILE |
| 34 | 41 | 99 | ASP |
| 34 | 41 | 113 | LEU |
| 34 | 41 | 114 | SER |
| 34 | 41 | 133 | VAL |
| 34 | 41 | 136 | MET |
| 34 | 41 | 137 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | 41 | 138 | ASP |
| 34 | 41 | 143 | GLU |
| 34 | 41 | 162 | GLU |
| 34 | 41 | 167 | LYS |
| 34 | 41 | 186 | LEU |
| 34 | 41 | 195 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 26 | ASN |
| 1 | A | 165 | GLN |
| 1 | A | 181 | ASN |
| 1 | A | 303 | ASN |
| 1 | A | 337 | HIS |
| 2 | B | 179 | GLN |
| 2 | B | 331 | ASN |
| 2 | B | 457 | ASN |
| 3 | C | 227 | ASN |
| 3 | C | 311 | GLN |
| 3 | C | 320 | GLN |
| 3 | C | 380 | ASN |
| 3 | C | 413 | ASN |
| 3 | C | 416 | ASN |
| 4 | D | 229 | ASN |
| 5 | E | 59 | GLN |
| 5 | E | 63 | GLN |
| 5 | E | 75 | GLN |
| 7 | H | 50 | ASN |
| 7 | H | 64 | ASN |
| 13 | O | 13 | GLN |
| 13 | O | 68 | ASN |
| 13 | O | 197 | GLN |
| 15 | U | 28 | ASN |
| 15 | U | 31 | ASN |
| 16 | V | 118 | HIS |
| 20 | Q | 121 | ASN |
| 20 | Q | 162 | GLN |
| 20 | Q | 192 | ASN |
| 21 | W | 24 | ASN |
| 1 | a | 26 | ASN |
| 1 | a | 165 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | a | 181 | ASN |
| 1 | a | 303 | ASN |
| 1 | a | 337 | HIS |
| 2 | b | 179 | GLN |
| 2 | b | 331 | ASN |
| 2 | b | 457 | ASN |
| 3 | c | 227 | ASN |
| 3 | c | 311 | GLN |
| 3 | c | 330 | GLN |
| 3 | c | 413 | ASN |
| 3 | c | 416 | ASN |
| 4 | d | 229 | ASN |
| 5 | e | 59 | GLN |
| 5 | e | 75 | GLN |
| 7 | h | 50 | ASN |
| 13 | o | 13 | GLN |
| 13 | o | 68 | ASN |
| 13 | o | 197 | GLN |
| 15 | u | 28 | ASN |
| 15 | u | 31 | ASN |
| 20 | q | 121 | ASN |
| 20 | q | 162 | GLN |
| 20 | q | 192 | ASN |
| 21 | w | 24 | ASN |
| 24 | 11 | 96 | ASN |
| 24 | 11 | 161 | ASN |
| 24 | 11 | 177 | ASN |
| 25 | 12 | 56 | ASN |
| 25 | 12 | 161 | ASN |
| 25 | 12 | 177 | ASN |
| 26 | 13 | 84 | HIS |
| 26 | 13 | 161 | ASN |
| 26 | 13 | 165 | ASN |
| 26 | 13 | 177 | ASN |
| 27 | 14 | 191 | GLN |
| 28 | 15 | 161 | ASN |
| 29 | 16 | 168 | ASN |
| 29 | 16 | 189 | GLN |
| 30 | 17 | 186 | GLN |
| 31 | 18 | 82 | ASN |
| 31 | 18 | 165 | ASN |
| 31 | 18 | 177 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 18 | 191 | GLN |
| 32 | 19 | 240 | GLN |
| 24 | 31 | 96 | ASN |
| 24 | 31 | 161 | ASN |
| 24 | 31 | 177 | ASN |
| 25 | 32 | 56 | ASN |
| 25 | 32 | 161 | ASN |
| 25 | 32 | 177 | ASN |
| 26 | 33 | 84 | HIS |
| 26 | 33 | 161 | ASN |
| 26 | 33 | 165 | ASN |
| 26 | 33 | 177 | ASN |
| 27 | 34 | 95 | ASN |
| 27 | 34 | 191 | GLN |
| 28 | 35 | 95 | ASN |
| 28 | 35 | 96 | ASN |
| 28 | 35 | 161 | ASN |
| 29 | 36 | 189 | GLN |
| 30 | 37 | 186 | GLN |
| 31 | 38 | 165 | ASN |
| 31 | 38 | 177 | ASN |
| 33 | 40 | 168 | ASN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 548 ligands modelled in this entry, 2 are monoatomic and 38 are unknown - leaving 508 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 48 | A86 | 41 | 214 | - | 47,50,50 | 4.40 | 24 (51%) | 51,76,76 | 6.92 | 17 (33%) |
| 50 | DD6 | 16 | 312 | - | 40,45,45 | 5.60 | 24 (60%) | 51,67,67 | 5.91 | 26 (50%) |
| 37 | CLA | 19 | 306 | 32 | 69,73,73 | 1.96 | 18 (26%) | 82,113,113 | 2.63 | 31 (37%) |
| 37 | CLA | c | 508 | - | 69,73,73 | 1.92 | 19 (27%) | 82,113,113 | 2.66 | 30 (36%) |
| 47 | KC1 | 20 | 302 | - | 49,53,53 | 3.02 | 24 (48%) | 61,89,89 | 4.05 | 36 (59%) |
| 48 | A86 | 41 | 213 | - | 47,50,50 | 4.47 | 24 (51%) | 51,76,76 | 6.79 | 15 (29%) |
| 47 | KC1 | 17 | 305 | 30 | 49,53,53 | 3.05 | 24 (48%) | 61,89,89 | 3.77 | 34 (55%) |
| 37 | CLA | C | 512 | - | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.72 | 32 (39%) |
| 37 | CLA | b | 511 | - | 69,73,73 | 1.93 | 18 (26%) | 82,113,113 | 2.66 | 32 (39%) |
| 47 | KC1 | 38 | 205 | 31 | 49,53,53 | 3.08 | 24 (48%) | 61,89,89 | 3.84 | 35 (57%) |
| 48 | A86 | 33 | 314 | - | 47,50,50 | 4.40 | 25 (53%) | 51,76,76 | 7.16 | 17 (33%) |
| 37 | CLA | b | 514 | - | 66,70,73 | 1.95 | 18 (27%) | 78,109,113 | 2.74 | 32 (41%) |
| 47 | KC1 | 11 | 309 | 24 | 49,53,53 | 2.96 | 22 (44%) | 61,89,89 | 3.73 | 36 (59%) |
| 48 | A86 | 16 | 311 | - | 47,50,50 | 4.12 | 22 (46%) | 51,76,76 | 6.32 | 21 (41%) |
| 37 | CLA | 17 | 302 | 30 | 69,73,73 | 2.01 | 20 (28%) | 82,113,113 | 2.47 | 26 (31%) |
| 47 | KC1 | 12 | 208 | 25 | 49,53,53 | 2.95 | 22 (44%) | 61,89,89 | 3.74 | 37 (60%) |
| 37 | CLA | 41 | 210 | - | 49,53,73 | 2.43 | 20 (40%) | 58,89,113 | 3.13 | 27 (46%) |
| 37 | CLA | 41 | 205 | 34 | 49,53,73 | 2.39 | 19 (38%) | 58,89,113 | 3.01 | 27 (46%) |
| 37 | CLA | b | 504 | - | 69,73,73 | 1.87 | 18 (26%) | 82,113,113 | 2.59 | 33 (40%) |
| 47 | KC1 | 38 | 210 | 31 | 49,53,53 | 3.05 | 24 (48%) | 61,89,89 | 3.82 | 35 (57%) |
| 48 | A86 | 15 | 319 | - | 47,50,50 | 4.27 | 23 (48%) | 51,76,76 | 6.00 | 19 (37%) |
| 47 | KC1 | 32 | 209 | 25 | 49,53,53 | 2.95 | 22 (44%) | 61,89,89 | 3.74 | 37 (60%) |
| 37 | CLA | 32 | 210 | 25 | 56,60,73 | 2.18 | 18 (32%) | 65,97,113 | 2.96 | 34 (52%) |
| 37 | CLA | 15 | 307 | 28 | 56,60,73 | 2.22 | 19 (33%) | 65,97,113 | 2.87 | 32 (49%) |
| 39 | BCR | C | 514 | - | 41,41,41 | 1.21 | 2 (4%) | 56,56,56 | 1.42 | 10 (17%) |
| 37 | CLA | B | 513 | - | 69,73,73 | 1.92 | 19 (27%) | 82,113,113 | 2.67 | 30 (36%) |
| 37 | CLA | 12 | 205 | - | 69,73,73 | 1.96 | 19 (27%) | 82,113,113 | 2.72 | 35 (42%) |
| 37 | CLA | 14 | 305 | - | 49,53,73 | 2.39 | 20 (40%) | 58,89,113 | 3.03 | 27 (46%) |
| 37 | CLA | 35 | 307 | 28 | 56,60,73 | 2.22 | 19 (33%) | 65,97,113 | 2.87 | 32 (49%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 37 | CLA | 41 | 202 | 34 | 61,65,73 | 2.17 | 21 (34%) | 72,103,113 | 2.83 | 30 (41%) |
| 48 | A86 | 34 | 313 | - | 47,50,50 | 4.35 | 24 (51%) | 51,76,76 | 6.23 | 17 (33%) |
| 37 | CLA | 11 | 301 | 24 | 69,73,73 | 1.93 | 19 (27%) | 82,113,113 | 2.65 | 30 (36%) |
| 37 | CLA | 11 | 308 | 52 | 69,73,73 | 1.96 | 20 (28%) | 82,113,113 | 2.61 | 32 (39%) |
| 37 | CLA | 37 | 306 | 30 | 56,60,73 | 2.21 | 18 (32%) | 65,97,113 | 2.90 | 33 (50%) |
| 41 | LMG | 37 | 316 | - | 37,37,55 | 0.96 | 2 (5%) | 45,45,63 | 1.28 | 5 (11%) |
| 47 | KC1 | 17 | 303 | - | 49,53,53 | 3.05 | 23 (46%) | 61,89,89 | 3.72 | 35 (57%) |
| 37 | CLA | 14 | 301 | 27 | 69,73,73 | 1.97 | 18 (26%) | 82,113,113 | 2.63 | 30 (36%) |
| 48 | A86 | 36 | 311 | - | 47,50,50 | 4.12 | 22 (46%) | 51,76,76 | 6.32 | 21 (41%) |
| 37 | CLA | C | 503 | - | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.78 | 34 (41%) |
| 48 | A86 | 32 | 218 | - | 47,50,50 | 4.22 | 23 (48%) | 51,76,76 | 6.22 | 21 (41%) |
| 48 | A86 | 21 | 211 | - | 47,50,50 | 4.38 | 24 (51%) | 51,76,76 | 6.78 | 12 (23%) |
| 41 | LMG | d | 409 | - | 51,51,55 | 0.89 | 3 (5%) | 59,59,63 | 1.41 | 6 (10%) |
| 37 | CLA | c | 513 | - | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.70 | 30 (36%) |
| 37 | CLA | c | 511 | 3 | 69,73,73 | 1.95 | 18 (26%) | 82,113,113 | 2.62 | 32 (39%) |
| 37 | CLA | b | 503 | - | 69,73,73 | 1.91 | 18 (26%) | 82,113,113 | 2.68 | 32 (39%) |
| 39 | BCR | b | 518 | - | 41,41,41 | 1.09 | 2 (4%) | 56,56,56 | 1.26 | 6 (10%) |
| 44 | DGD | J | 101 | - | 63,63,67 | 1.09 | 7 (11%) | 77,77,81 | 1.50 | 12 (15%) |
| 48 | A86 | 32 | 216 | - | 47,50,50 | 4.37 | 24 (51%) | 51,76,76 | 6.78 | 14 (27%) |
| 48 | A86 | 18 | 212 | - | 47,50,50 | 4.33 | 24 (51%) | 51,76,76 | 6.73 | 17 (33%) |
| 37 | CLA | c | 512 | - | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.71 | 32 (39%) |
| 47 | KC1 | 18 | 210 | 31 | 49,53,53 | 3.05 | 24 (48%) | 61,89,89 | 3.82 | 35 (57%) |
| 37 | CLA | B | 510 | 52 | 69,73,73 | 1.92 | 19 (27%) | 82,113,113 | 2.68 | 33 (40%) |
| 48 | A86 | 35 | 316 | - | 47,50,50 | 4.30 | 24 (51%) | 51,76,76 | 6.43 | 22 (43%) |
| 37 | CLA | 35 | 303 | - | 61,65,73 | 2.16 | 20 (32%) | 72,103,113 | 2.88 | 32 (44%) |
| 37 | CLA | 19 | 307 | 43 | 69,73,73 | 1.99 | 19 (27%) | 82,113,113 | 2.63 | 31 (37%) |
| 39 | BCR | c | 515 | - | 41,41,41 | 1.19 | 2 (4%) | 56,56,56 | 1.26 | 6 (10%) |
| 48 | A86 | 12 | 217 | - | 47,50,50 | 4.22 | 23 (48%) | 51,76,76 | 6.21 | 21 (41%) |
| 48 | A86 | 12 | 214 | - | 47,50,50 | 4.12 | 24 (51%) | 51,76,76 | 6.47 | 17 (33%) |
| 39 | BCR | D | 407 | - | 41,41,41 | 1.13 | 3 (7%) | 56,56,56 | 1.28 | 7 (12%) |
| 48 | A86 | 16 | 313 | - | 47,50,50 | 4.39 | 23 (48%) | 51,76,76 | 7.11 | 22 (43%) |
| 37 | CLA | 17 | 309 | 52 | 69,73,73 | 2.08 | 20 (28%) | 82,113,113 | 2.80 | 35 (42%) |
| 40 | SQD | 16 | 315 | - | 52,54,54 | 0.96 | 5 (9%) | 62,65,65 | 1.55 | 11 (17%) |
| 48 | A86 | 11 | 315 | - | 47,50,50 | 4.07 | 23 (48%) | 51,76,76 | 6.38 | 17 (33%) |
| 48 | A86 | 41 | 211 | - | 47,50,50 | 4.38 | 24 (51%) | 51,76,76 | 6.78 | 12 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 37 | CLA | w | 101 | - | 69,73,73 | 1.95 | 20 (28%) | 82,113,113 | 2.82 | 32 (39%) |
| 37 | CLA | 14 | 310 | - | 49,53,73 | 2.39 | 19 (38%) | 58,89,113 | 3.05 | 27 (46%) |
| 48 | A86 | 17 | 315 | - | 47,50,50 | 4.26 | 23 (48%) | 51,76,76 | 6.45 | 19 (37%) |
| 48 | A86 | 34 | 315 | - | 47,50,50 | 4.17 | 23 (48%) | 51,76,76 | 6.63 | 17 (33%) |
| 37 | CLA | 36 | 301 | 29 | 69,73,73 | 1.97 | 19 (27%) | 82,113,113 | 2.68 | 30 (36%) |
| 41 | LMG | 32 | 201 | - | 39,39,55 | 1.03 | 2 (5%) | 47,47,63 | 1.15 | 3 (6%) |
| 37 | CLA | 14 | 302 | - | 69,73,73 | 2.01 | 19 (27%) | 82,113,113 | 2.60 | 31 (37%) |
| 37 | CLA | 34 | 308 | 52 | 69,73,73 | 1.98 | 20 (28%) | 82,113,113 | 2.63 | 33 (40%) |
| 44 | DGD | c | 516 | - | 63,63,67 | 1.05 | 5 (7%) | 77,77,81 | 1.48 | 14 (18%) |
| 48 | A86 | 15 | 312 | - | 47,50,50 | 4.31 | 24 (51%) | 51,76,76 | 6.47 | 18 (35%) |
| 48 | A86 | 37 | 309 | - | 47,50,50 | 4.30 | 24 (51%) | 51,76,76 | 7.01 | 17 (33%) |
| 41 | LMG | C | 518 | - | 51,51,55 | 0.97 | 3 (5%) | 59,59,63 | 1.46 | 7 (11%) |
| 37 | CLA | Z | 102 | 33 | 49,53,73 | 2.43 | 20 (40%) | 58,89,113 | 3.08 | 32 (55%) |
| 37 | CLA | z | 101 | 52 | 69,73,73 | 2.01 | 19 (27%) | 82,113,113 | 2.64 | 30 (36%) |
| 48 | A86 | 14 | 313 | - | 47,50,50 | 4.35 | 24 (51%) | 51,76,76 | 6.24 | 17 (33%) |
| 39 | BCR | H | 101 | - | 41,41,41 | 1.16 | 4 (9%) | 56,56,56 | 1.25 | 5 (8%) |
| 48 | A86 | 14 | 316 | - | 47,50,50 | 4.22 | 24 (51%) | 51,76,76 | 6.14 | 21 (41%) |
| 48 | A86 | 17 | 311 | - | 47,50,50 | 4.24 | 23 (48%) | 51,76,76 | 6.29 | 19 (37%) |
| 37 | CLA | z | 102 | 33 | 49,53,73 | 2.43 | 22 (44%) | 58,89,113 | 3.08 | 32 (55%) |
| 37 | CLA | 32 | 206 | - | 69,73,73 | 1.96 | 19 (27%) | 82,113,113 | 2.73 | 33 (40%) |
| 47 | KC1 | 37 | 304 | 30 | 49,53,53 | 3.07 | 24 (48%) | 61,89,89 | 3.85 | 35 (57%) |
| 37 | CLA | C | 511 | 3 | 69,73,73 | 1.94 | 18 (26%) | 82,113,113 | 2.62 | 32 (39%) |
| 50 | DD6 | 20 | 310 | - | 40,45,45 | 5.49 | 23 (57%) | 51,67,67 | 6.37 | 25 (49%) |
| 48 | A86 | 33 | 312 | - | 47,50,50 | 4.39 | 23 (48%) | 51,76,76 | 6.58 | 18 (35%) |
| 37 | CLA | 33 | 310 | - | 49,53,73 | 2.44 | 19 (38%) | 58,89,113 | 3.06 | 28 (48%) |
| 48 | A86 | 21 | 215 | - | 47,50,50 | 4.24 | 25 (53%) | 51,76,76 | 6.86 | 16 (31%) |
| 41 | LMG | b | 519 | - | 51,51,55 | 0.82 | 1 (1%) | 59,59,63 | 1.31 | 5 (8%) |
| 37 | CLA | 39 | 304 | 32 | 49,53,73 | 2.37 | 20 (40%) | 58,89,113 | 3.10 | 27 (46%) |
| 37 | CLA | 18 | 208 | 31 | 57,61,73 | 2.18 | 19 (33%) | 67,98,113 | 2.80 | 29 (43%) |
| 37 | CLA | 21 | 206 | 34 | 69,73,73 | 1.99 | 19 (27%) | 82,113,113 | 2.65 | 30 (36%) |
| 39 | BCR | C | 515 | - | 41,41,41 | 1.19 | 2 (4%) | 56,56,56 | 1.26 | 6 (10%) |
| 48 | A86 | 12 | 202 | - | 47,50,50 | 4.10 | 21 (44%) | 51,76,76 | 6.37 | 22 (43%) |
| 40 | SQD | 40 | 202 | - | 52,54,54 | 0.96 | 5 (9%) | 62,65,65 | 1.55 | 10 (16%) |
| 37 | CLA | c | 510 | - | 69,73,73 | 1.95 | 19 (27%) | 82,113,113 | 2.70 | 29 (35%) |
| 50 | DD6 | 40 | 212 | - | 40,45,45 | 5.50 | 24 (60%) | 51,67,67 | 6.36 | 25 (49%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 37 | CLA | 31 | 302 | 24 | 69,73,73 | 1.93 | 19 (27%) | 82,113,113 | 2.65 | 30 (36%) |
| 40 | SQD | b | 521 | - | 35,37,54 | 1.18 | 6 (17%) | 45,48,65 | 1.59 | 10 (22%) |
| 46 | HEM | F | 101 | 5,6 | 50,50,50 | 1.31 | 5 (10%) | 67,82,82 | 1.12 | 4 (5%) |
| 47 | KC1 | 15 | 302 | - | 49,53,53 | 3.05 | 24 (48%) | 61,89,89 | 3.88 | 36 (59%) |
| 48 | A86 | 36 | 313 | - | 47,50,50 | 4.01 | 23 (48%) | 51,76,76 | 6.34 | 16 (31%) |
| 37 | CLA | 19 | 309 | 32 | 49,53,73 | 2.35 | 20 (40%) | 58,89,113 | 3.00 | 27 (46%) |
| 39 | BCR | h | 101 | - | 41,41,41 | 1.15 | 3 (7%) | 56,56,56 | 1.26 | 6 (10%) |
| 45 | PL9 | D | 408 | - | 55,55,55 | 1.76 | 9 (16%) | 68,69,69 | 1.39 | 11 (16%) |
| 51 | LMU | 39 | 315 | - | 36,36,36 | 1.12 | 2 (5%) | 47,47,47 | 1.04 | 2 (4%) |
| 39 | BCR | a | 413 | - | 41,41,41 | 1.10 | 2 (4%) | 56,56,56 | 1.31 | 6 (10%) |
| 37 | CLA | 12 | 212 | - | 49,53,73 | 2.38 | 20 (40%) | 58,89,113 | 3.11 | 29 (50%) |
| 37 | CLA | 15 | 308 | 52 | 69,73,73 | 2.00 | 21 (30%) | 82,113,113 | 2.62 | 30 (36%) |
| 48 | A86 | 17 | 313 | - | 47,50,50 | 4.30 | 23 (48%) | 51,76,76 | 7.01 | 20 (39%) |
| 37 | CLA | 33 | 307 | 26 | 56,60,73 | 2.22 | 19 (33%) | 65,97,113 | 2.81 | 33 (50%) |
| 42 | BCT | A | 409 | 36 | 3,3,3 | 1.21 | 0 | 2,3,3 | 4.13 | 2 (100%) |
| 37 | CLA | 35 | 301 | 28 | 69,73,73 | 2.03 | 19 (27%) | 82,113,113 | 2.65 | 27 (32%) |
| 48 | A86 | 34 | 314 | - | 47,50,50 | 4.38 | 24 (51%) | 51,76,76 | 7.03 | 18 (35%) |
| 37 | CLA | 21 | 208 | - | 69,73,73 | 2.04 | 21 (30%) | 82,113,113 | 2.63 | 30 (36%) |
| 43 | LHG | 39 | 314 | 37 | 48,48,48 | 0.29 | 0 | 51,54,54 | 0.32 | 0 |
| 37 | CLA | 32 | 211 | 52 | 69,73,73 | 1.99 | 20 (28%) | 82,113,113 | 2.58 | 30 (36%) |
| 47 | KC1 | 13 | 306 | 26 | 49,53,53 | 3.00 | 22 (44%) | 61,89,89 | 3.83 | 35 (57%) |
| 37 | CLA | 34 | 305 | - | 49,53,73 | 2.40 | 20 (40%) | 58,89,113 | 3.04 | 28 (48%) |
| 39 | BCR | y | 101 | - | 41,41,41 | 1.19 | 3 (7%) | 56,56,56 | 1.26 | 5 (8%) |
| 37 | CLA | c | 504 | 52 | 69,73,73 | 1.92 | 20 (28%) | 82,113,113 | 2.69 | 30 (36%) |
| 44 | DGD | c | 517 | - | 63,63,67 | 1.22 | 6 (9%) | 77,77,81 | 1.49 | 14 (18%) |
| 37 | CLA | 38 | 201 | 52 | 69,73,73 | 2.03 | 19 (27%) | 82,113,113 | 2.59 | 33 (40%) |
| 37 | CLA | B | 509 | - | 69,73,73 | 1.90 | 19 (27%) | 82,113,113 | 2.66 | 33 (40%) |
| 47 | KC1 | 35 | 309 | 28 | 49,53,53 | 3.06 | 24 (48%) | 61,89,89 | 3.66 | 36 (59%) |
| 37 | CLA | 31 | 310 | 52 | 55,59,73 | 2.18 | 21 (38%) | 64,96,113 | 2.88 | 30 (46%) |
| 47 | KC1 | 15 | 304 | 28 | 49,53,53 | 3.07 | 24 (48%) | 61,89,89 | 3.90 | 37 (60%) |
| 37 | CLA | 21 | 205 | 34 | 49,53,73 | 2.39 | 19 (38%) | 58,89,113 | 3.02 | 27 (46%) |
| 37 | CLA | C | 508 | - | 69,73,73 | 1.92 | 19 (27%) | 82,113,113 | 2.65 | 29 (35%) |
| 37 | CLA | 38 | 208 | 31 | 57,61,73 | 2.18 | 19 (33%) | 67,98,113 | 2.81 | 29 (43%) |
| 37 | CLA | B | 503 | - | 69,73,73 | 1.90 | 18 (26%) | 82,113,113 | 2.68 | 32 (39%) |
| 37 | CLA | C | 510 | - | 69,73,73 | 1.95 | 19 (27%) | 82,113,113 | 2.70 | 29 (35%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 44 | DGD | C | 516 | - | 63,63,67 | 1.05 | 5 (7%) | 77,77,81 | 1.48 | 14 (18%) |
| 35 | OEX | a | 401 | 1,3 | 0,15,15 | - | - | - | | |
| 43 | LHG | 41 | 201 | - | 34,34,48 | 0.76 | 1 (2%) | 37,39,54 | 1.43 | 5 (13%) |
| 48 | A86 | 12 | 216 | - | 47,50,50 | 4.23 | 23 (48%) | 51,76,76 | 6.88 | 20 (39%) |
| 37 | CLA | b | 510 | 52 | 69,73,73 | 1.92 | 19 (27%) | 82,113,113 | 2.68 | 33 (40%) |
| 47 | KC1 | 35 | 304 | 28 | 49,53,53 | 3.08 | 25 (51%) | 61,89,89 | 3.91 | 36 (59%) |
| 37 | CLA | 13 | 310 | - | 49,53,73 | 2.44 | 19 (38%) | 58,89,113 | 3.06 | 28 (48%) |
| 48 | A86 | 19 | 311 | - | 47,50,50 | 4.15 | 24 (51%) | 51,76,76 | 6.47 | 19 (37%) |
| 48 | A86 | 37 | 319 | - | 47,50,50 | 4.24 | 23 (48%) | 51,76,76 | 6.44 | 20 (39%) |
| 37 | CLA | c | 503 | - | 69,73,73 | 1.94 | 20 (28%) | 82,113,113 | 2.78 | 34 (41%) |
| 37 | CLA | C | 507 | 52 | 69,73,73 | 1.91 | 19 (27%) | 82,113,113 | 2.63 | 30 (36%) |
| 43 | LHG | 19 | 314 | 37 | 48,48,48 | 0.29 | 0 | 51,54,54 | 0.32 | 0 |
| 48 | A86 | 32 | 214 | - | 47,50,50 | 4.18 | 23 (48%) | 51,76,76 | 6.74 | 20 (39%) |
| 37 | CLA | B | 524 | - | 69,73,73 | 1.93 | 21 (30%) | 82,113,113 | 2.65 | 32 (39%) |
| 39 | BCR | B | 517 | - | 41,41,41 | 1.21 | 2 (4%) | 56,56,56 | 1.33 | 7 (12%) |
| 37 | CLA | 37 | 303 | - | 60,64,73 | 2.15 | 20 (33%) | 71,102,113 | 2.95 | 33 (46%) |
| 37 | CLA | b | 509 | - | 69,73,73 | 1.91 | 17 (24%) | 82,113,113 | 2.67 | 33 (40%) |
| 37 | CLA | 34 | 301 | 27 | 69,73,73 | 1.97 | 18 (26%) | 82,113,113 | 2.63 | 30 (36%) |
| 47 | KC1 | 32 | 207 | 25 | 49,53,53 | 2.99 | 22 (44%) | 61,89,89 | 3.73 | 32 (52%) |
| 48 | A86 | 34 | 312 | - | 47,50,50 | 4.21 | 23 (48%) | 51,76,76 | 6.60 | 22 (43%) |
| 48 | A86 | 18 | 214 | - | 47,50,50 | 4.39 | 24 (51%) | 51,76,76 | 6.79 | 19 (37%) |
| 38 | PHO | A | 404 | - | 58,69,69 | 2.05 | 11 (18%) | 55,99,99 | 1.76 | 9 (16%) |
| 37 | CLA | Z | 101 | 52 | 69,73,73 | 2.01 | 19 (27%) | 82,113,113 | 2.64 | 30 (36%) |
| 37 | CLA | 40 | 210 | - | 51,55,73 | 2.33 | 21 (41%) | 60,91,113 | 2.97 | 29 (48%) |
| 47 | KC1 | 41 | 203 | - | 49,53,53 | 3.08 | 25 (51%) | 61,89,89 | 3.84 | 33 (54%) |
| 37 | CLA | 41 | 209 | 34 | 49,53,73 | 2.43 | 20 (40%) | 58,89,113 | 3.06 | 28 (48%) |
| 43 | LHG | 37 | 315 | - | 43,43,48 | 0.63 | 0 | 46,49,54 | 1.31 | 6 (13%) |
| 39 | BCR | b | 524 | - | 41,41,41 | 1.13 | 2 (4%) | 56,56,56 | 1.33 | 7 (12%) |
| 43 | LHG | D | 410 | - | 48,48,48 | 0.76 | 1 (2%) | 51,54,54 | 1.32 | 7 (13%) |
| 41 | LMG | L | 102 | - | 40,40,55 | 0.96 | 3 (7%) | 48,48,63 | 1.33 | 4 (8%) |
| 40 | SQD | B | 519 | - | 52,54,54 | 0.93 | 4 (7%) | 62,65,65 | 1.60 | 9 (14%) |
| 37 | CLA | C | 504 | 52 | 69,73,73 | 1.92 | 20 (28%) | 82,113,113 | 2.68 | 30 (36%) |
| 37 | CLA | 14 | 303 | - | 61,65,73 | 2.13 | 19 (31%) | 72,103,113 | 3.01 | 35 (48%) |
| 48 | A86 | 15 | 315 | - | 47,50,50 | 4.28 | 24 (51%) | 51,76,76 | 6.53 | 21 (41%) |
| 43 | LHG | D | 411 | - | 45,45,48 | 0.87 | 2 (4%) | 48,51,54 | 1.25 | 7 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 48 | A86 | 19 | 313 | - | 47,50,50 | 4.34 | 25 (53%) | 51,76,76 | 7.33 | 22 (43%) |
| 40 | SQD | a | 409 | - | 52,54,54 | 0.95 | 6 (11%) | 62,65,65 | 1.64 | 10 (16%) |
| 37 | CLA | 34 | 303 | - | 61,65,73 | 2.13 | 19 (31%) | 72,103,113 | 3.00 | 35 (48%) |
| 37 | CLA | 12 | 203 | 25 | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.59 | 30 (36%) |
| 37 | CLA | c | 506 | - | 69,73,73 | 1.95 | 17 (24%) | 82,113,113 | 2.61 | 30 (36%) |
| 37 | CLA | 12 | 204 | - | 69,73,73 | 1.94 | 20 (28%) | 82,113,113 | 2.43 | 29 (35%) |
| 37 | CLA | 13 | 303 | - | 61,65,73 | 2.14 | 20 (32%) | 72,103,113 | 2.88 | 33 (45%) |
| 37 | CLA | 16 | 307 | 52 | 65,69,73 | 2.05 | 19 (29%) | 77,108,113 | 2.67 | 28 (36%) |
| 37 | CLA | B | 511 | - | 69,73,73 | 1.92 | 18 (26%) | 82,113,113 | 2.67 | 32 (39%) |
| 38 | PHO | D | 403 | - | 58,69,69 | 2.02 | 9 (15%) | 55,99,99 | 1.72 | 10 (18%) |
| 50 | DD6 | 20 | 312 | - | 40,45,45 | 5.64 | 24 (60%) | 51,67,67 | 6.11 | 28 (54%) |
| 37 | CLA | 32 | 208 | 52 | 54,58,73 | 2.25 | 19 (35%) | 64,95,113 | 3.04 | 34 (53%) |
| 37 | CLA | d | 403 | - | 69,73,73 | 1.88 | 18 (26%) | 82,113,113 | 2.80 | 32 (39%) |
| 48 | A86 | 15 | 311 | - | 47,50,50 | 4.26 | 23 (48%) | 51,76,76 | 6.55 | 14 (27%) |
| 37 | CLA | 19 | 305 | 32 | 55,59,73 | 2.21 | 19 (34%) | 64,96,113 | 2.99 | 30 (46%) |
| 48 | A86 | 15 | 316 | - | 47,50,50 | 4.33 | 23 (48%) | 51,76,76 | 6.41 | 22 (43%) |
| 37 | CLA | C | 501 | - | 69,73,73 | 1.92 | 19 (27%) | 82,113,113 | 2.73 | 32 (39%) |
| 47 | KC1 | 11 | 306 | 24 | 49,53,53 | 2.97 | 22 (44%) | 61,89,89 | 3.80 | 32 (52%) |
| 48 | A86 | 21 | 214 | - | 47,50,50 | 4.40 | 24 (51%) | 51,76,76 | 6.92 | 17 (33%) |
| 37 | CLA | D | 405 | - | 69,73,73 | 1.88 | 18 (26%) | 82,113,113 | 2.80 | 32 (39%) |
| 48 | A86 | 21 | 213 | - | 47,50,50 | 4.48 | 24 (51%) | 51,76,76 | 6.80 | 16 (31%) |
| 37 | CLA | 18 | 202 | 31 | 69,73,73 | 1.97 | 18 (26%) | 82,113,113 | 2.73 | 32 (39%) |
| 51 | LMU | 19 | 315 | - | 36,36,36 | 1.13 | 2 (5%) | 47,47,47 | 1.05 | 3 (6%) |
| 37 | CLA | 14 | 307 | 27 | 56,60,73 | 2.19 | 18 (32%) | 65,97,113 | 2.86 | 33 (50%) |
| 37 | CLA | d | 401 | 52 | 69,73,73 | 1.98 | 19 (27%) | 82,113,113 | 2.65 | 31 (37%) |
| 48 | A86 | 11 | 312 | - | 47,50,50 | 4.08 | 22 (46%) | 51,76,76 | 6.49 | 22 (43%) |
| 47 | KC1 | 13 | 304 | 26 | 49,53,53 | 3.02 | 22 (44%) | 61,89,89 | 3.81 | 35 (57%) |
| 37 | CLA | 20 | 308 | - | 51,55,73 | 2.33 | 21 (41%) | 60,91,113 | 2.97 | 29 (48%) |
| 37 | CLA | 11 | 305 | 52 | 49,53,73 | 2.34 | 20 (40%) | 58,89,113 | 3.03 | 30 (51%) |
| 37 | CLA | 33 | 308 | 52 | 69,73,73 | 2.02 | 20 (28%) | 82,113,113 | 2.60 | 29 (35%) |
| 39 | BCR | B | 525 | - | 41,41,41 | 1.13 | 2 (4%) | 56,56,56 | 1.33 | 7 (12%) |
| 48 | A86 | 36 | 310 | - | 47,50,50 | 4.09 | 23 (48%) | 51,76,76 | 6.38 | 21 (41%) |
| 48 | A86 | 17 | 312 | - | 47,50,50 | 4.31 | 24 (51%) | 51,76,76 | 6.07 | 18 (35%) |
| 48 | A86 | 11 | 313 | - | 47,50,50 | 4.03 | 22 (46%) | 51,76,76 | 5.79 | 17 (33%) |
| 37 | CLA | b | 515 | - | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.68 | 32 (39%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 37 | CLA | b | 505 | - | 69,73,73 | 1.92 | 20 (28%) | 82,113,113 | 2.72 | 30 (36%) |
| 37 | CLA | 15 | 303 | - | 61,65,73 | 2.17 | 20 (32%) | 72,103,113 | 2.86 | 33 (45%) |
| 48 | A86 | 34 | 316 | - | 47,50,50 | 4.22 | 24 (51%) | 51,76,76 | 6.15 | 21 (41%) |
| 37 | CLA | 35 | 305 | - | 49,53,73 | 2.42 | 20 (40%) | 58,89,113 | 3.01 | 28 (48%) |
| 37 | CLA | 19 | 301 | 32 | 69,73,73 | 1.99 | 19 (27%) | 82,113,113 | 2.63 | 30 (36%) |
| 41 | LMG | 36 | 314 | - | 36,36,55 | 0.94 | 1 (2%) | 44,44,63 | 1.21 | 4 (9%) |
| 37 | CLA | C | 506 | - | 69,73,73 | 1.95 | 18 (26%) | 82,113,113 | 2.61 | 30 (36%) |
| 37 | CLA | C | 509 | - | 69,73,73 | 1.97 | 18 (26%) | 82,113,113 | 2.70 | 31 (37%) |
| 50 | DD6 | 21 | 212 | - | 40,45,45 | 5.51 | 23 (57%) | 51,67,67 | 6.13 | 31 (60%) |
| 37 | CLA | 39 | 310 | 32 | 69,73,73 | 1.97 | 18 (26%) | 82,113,113 | 2.56 | 30 (36%) |
| 37 | CLA | 36 | 309 | - | 49,53,73 | 2.38 | 21 (42%) | 58,89,113 | 3.18 | 29 (50%) |
| 47 | KC1 | 12 | 211 | 25 | 49,53,53 | 3.00 | 24 (48%) | 61,89,89 | 3.71 | 38 (62%) |
| 48 | A86 | 13 | 311 | - | 47,50,50 | 4.19 | 23 (48%) | 51,76,76 | 6.64 | 20 (39%) |
| 41 | LMG | 11 | 316 | - | 42,42,55 | 1.05 | 3 (7%) | 50,50,63 | 1.22 | 3 (6%) |
| 37 | CLA | 20 | 303 | - | 60,64,73 | 2.12 | 18 (30%) | 71,102,113 | 3.01 | 37 (52%) |
| 41 | LMG | 31 | 316 | - | 42,42,55 | 1.05 | 3 (7%) | 50,50,63 | 1.22 | 3 (6%) |
| 46 | HEM | v | 201 | 16 | 50,50,50 | 1.29 | 6 (12%) | 67,82,82 | 1.23 | 6 (8%) |
| 48 | A86 | 37 | 310 | - | 47,50,50 | 4.22 | 23 (48%) | 51,76,76 | 6.28 | 18 (35%) |
| 37 | CLA | 21 | 202 | 34 | 61,65,73 | 2.17 | 20 (32%) | 72,103,113 | 2.83 | 30 (41%) |
| 47 | KC1 | 33 | 302 | - | 49,53,53 | 3.02 | 25 (51%) | 61,89,89 | 3.92 | 36 (59%) |
| 47 | KC1 | 35 | 306 | 28 | 49,53,53 | 3.06 | 24 (48%) | 61,89,89 | 3.82 | 36 (59%) |
| 37 | CLA | B | 501 | 52 | 69,73,73 | 1.96 | 19 (27%) | 82,113,113 | 2.63 | 29 (35%) |
| 37 | CLA | 32 | 204 | 25 | 69,73,73 | 1.93 | 19 (27%) | 82,113,113 | 2.59 | 30 (36%) |
| 37 | CLA | 37 | 308 | 52 | 69,73,73 | 2.07 | 20 (28%) | 82,113,113 | 2.82 | 35 (42%) |
| 43 | LHG | b | 522 | - | 48,48,48 | 0.75 | 1 (2%) | 51,54,54 | 1.29 | 6 (11%) |
| 37 | CLA | 19 | 303 | 52 | 69,73,73 | 1.98 | 21 (30%) | 82,113,113 | 2.71 | 29 (35%) |
| 47 | KC1 | 36 | 305 | 29 | 49,53,53 | 3.06 | 24 (48%) | 61,89,89 | 3.73 | 34 (55%) |
| 37 | CLA | 31 | 308 | 24 | 56,60,73 | 2.18 | 20 (35%) | 65,97,113 | 3.03 | 31 (47%) |
| 48 | A86 | 12 | 213 | - | 47,50,50 | 4.16 | 23 (48%) | 51,76,76 | 6.73 | 20 (39%) |
| 37 | CLA | 17 | 307 | 30 | 56,60,73 | 2.21 | 18 (32%) | 65,97,113 | 2.90 | 33 (50%) |
| 37 | CLA | B | 512 | - | 69,73,73 | 1.89 | 19 (27%) | 82,113,113 | 2.62 | 33 (40%) |
| 37 | CLA | c | 502 | - | 69,73,73 | 1.91 | 18 (26%) | 82,113,113 | 2.61 | 30 (36%) |
| 37 | CLA | 34 | 310 | - | 49,53,73 | 2.39 | 19 (38%) | 58,89,113 | 3.05 | 27 (46%) |
| 50 | DD6 | 41 | 212 | - | 40,45,45 | 5.51 | 23 (57%) | 51,67,67 | 6.14 | 31 (60%) |
| 37 | CLA | 40 | 209 | 33 | 49,53,73 | 2.41 | 20 (40%) | 58,89,113 | 3.00 | 28 (48%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 43 | LHG | B | 523 | - | 48,48,48 | 0.75 | 1 (2%) | 51,54,54 | 1.29 | 6 (11%) |
| 47 | KC1 | 40 | 204 | - | 49,53,53 | 3.01 | 24 (48%) | 61,89,89 | 4.05 | 36 (59%) |
| 37 | CLA | 20 | 306 | 33 | 54,58,73 | 2.25 | 18 (33%) | 64,95,113 | 2.91 | 31 (48%) |
| 41 | LMG | 11 | 317 | - | 32,32,55 | 0.97 | 1 (3%) | 40,40,63 | 1.25 | 4 (10%) |
| 37 | CLA | 16 | 306 | 29 | 69,73,73 | 2.00 | 20 (28%) | 82,113,113 | 2.54 | 31 (37%) |
| 48 | A86 | 13 | 313 | - | 47,50,50 | 4.42 | 24 (51%) | 51,76,76 | 7.22 | 18 (35%) |
| 50 | DD6 | 40 | 214 | - | 40,45,45 | 5.63 | 24 (60%) | 51,67,67 | 6.11 | 28 (54%) |
| 43 | LHG | 21 | 217 | - | 44,44,48 | 0.65 | 1 (2%) | 47,50,54 | 1.20 | 3 (6%) |
| 37 | CLA | 19 | 302 | - | 69,73,73 | 1.97 | 20 (28%) | 82,113,113 | 2.72 | 30 (36%) |
| 37 | CLA | c | 509 | - | 69,73,73 | 1.97 | 18 (26%) | 82,113,113 | 2.69 | 31 (37%) |
| 47 | KC1 | 37 | 305 | 30 | 49,53,53 | 3.04 | 23 (46%) | 61,89,89 | 3.71 | 36 (59%) |
| 35 | OEX | A | 401 | 1,3 | 0,15,15 | - | - | - | | |
| 37 | CLA | 31 | 306 | 52 | 49,53,73 | 2.34 | 20 (40%) | 58,89,113 | 3.03 | 30 (51%) |
| 47 | KC1 | 34 | 309 | 27 | 49,53,53 | 2.98 | 23 (46%) | 61,89,89 | 3.80 | 37 (60%) |
| 39 | BCR | c | 519 | - | 41,41,41 | 1.17 | 2 (4%) | 56,56,56 | 1.24 | 4 (7%) |
| 47 | KC1 | 13 | 309 | 26 | 49,53,53 | 2.99 | 25 (51%) | 61,89,89 | 3.74 | 38 (62%) |
| 37 | CLA | b | 506 | - | 69,73,73 | 1.88 | 19 (27%) | 82,113,113 | 2.76 | 31 (37%) |
| 46 | HEM | f | 101 | 5,6 | 50,50,50 | 1.31 | 6 (12%) | 67,82,82 | 1.12 | 4 (5%) |
| 48 | A86 | 35 | 311 | - | 47,50,50 | 4.26 | 23 (48%) | 51,76,76 | 6.57 | 14 (27%) |
| 48 | A86 | 35 | 313 | - | 47,50,50 | 4.36 | 24 (51%) | 51,76,76 | 6.20 | 14 (27%) |
| 37 | CLA | B | 514 | - | 66,70,73 | 1.96 | 18 (27%) | 78,109,113 | 2.74 | 32 (41%) |
| 37 | CLA | 11 | 307 | 24 | 56,60,73 | 2.18 | 20 (35%) | 65,97,113 | 3.04 | 31 (47%) |
| 47 | KC1 | 31 | 307 | 24 | 49,53,53 | 2.98 | 22 (44%) | 61,89,89 | 3.80 | 32 (52%) |
| 37 | CLA | 40 | 205 | - | 60,64,73 | 2.11 | 18 (30%) | 71,102,113 | 3.01 | 37 (52%) |
| 48 | A86 | 37 | 313 | - | 47,50,50 | 4.20 | 23 (48%) | 51,76,76 | 7.20 | 18 (35%) |
| 48 | A86 | 41 | 215 | - | 47,50,50 | 4.24 | 25 (53%) | 51,76,76 | 6.87 | 16 (31%) |
| 37 | CLA | b | 508 | - | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.61 | 29 (35%) |
| 47 | KC1 | 15 | 309 | 28 | 49,53,53 | 3.05 | 24 (48%) | 61,89,89 | 3.66 | 36 (59%) |
| 37 | CLA | 34 | 302 | - | 69,73,73 | 2.00 | 19 (27%) | 82,113,113 | 2.60 | 31 (37%) |
| 47 | KC1 | 41 | 207 | 34 | 49,53,53 | 3.04 | 25 (51%) | 61,89,89 | 3.95 | 37 (60%) |
| 47 | KC1 | 14 | 304 | 27 | 49,53,53 | 3.03 | 23 (46%) | 61,89,89 | 3.96 | 32 (52%) |
| 37 | CLA | 32 | 205 | - | 69,73,73 | 1.94 | 20 (28%) | 82,113,113 | 2.43 | 29 (35%) |
| 47 | KC1 | 31 | 303 | - | 49,53,53 | 3.00 | 21 (42%) | 61,89,89 | 3.79 | 34 (55%) |
| 39 | BCR | 5 | 101 | - | 41,41,41 | 1.15 | 3 (7%) | 56,56,56 | 1.33 | 7 (12%) |
| 37 | CLA | 38 | 206 | - | 49,53,73 | 2.42 | 20 (40%) | 58,89,113 | 3.09 | 28 (48%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 37 | CLA | 13 | 307 | 26 | 56,60,73 | 2.21 | 19 (33%) | 65,97,113 | 2.81 | 33 (50%) |
| 47 | KC1 | 13 | 302 | - | 49,53,53 | 3.02 | 25 (51%) | 61,89,89 | 3.91 | 36 (59%) |
| 41 | LMG | 16 | 316 | - | 36,36,55 | 0.94 | 1 (2%) | 44,44,63 | 1.22 | 4 (9%) |
| 47 | KC1 | 35 | 302 | - | 49,53,53 | 3.05 | 23 (46%) | 61,89,89 | 3.87 | 35 (57%) |
| 37 | CLA | 19 | 304 | 32 | 49,53,73 | 2.37 | 20 (40%) | 58,89,113 | 3.10 | 26 (44%) |
| 43 | LHG | 21 | 201 | - | 34,34,48 | 0.76 | 2 (5%) | 37,39,54 | 1.42 | 5 (13%) |
| 37 | CLA | 14 | 308 | 52 | 69,73,73 | 1.98 | 18 (26%) | 82,113,113 | 2.63 | 34 (41%) |
| 48 | A86 | 31 | 311 | - | 47,50,50 | 4.06 | 23 (48%) | 51,76,76 | 6.20 | 17 (33%) |
| 41 | LMG | 12 | 201 | - | 39,39,55 | 1.02 | 2 (5%) | 47,47,63 | 1.15 | 3 (6%) |
| 37 | CLA | 39 | 303 | 52 | 69,73,73 | 1.98 | 20 (28%) | 82,113,113 | 2.71 | 29 (35%) |
| 48 | A86 | 32 | 221 | - | 47,50,50 | 4.06 | 22 (46%) | 51,76,76 | 6.63 | 21 (41%) |
| 37 | CLA | 13 | 308 | 52 | 69,73,73 | 2.02 | 20 (28%) | 82,113,113 | 2.59 | 29 (35%) |
| 48 | A86 | 40 | 213 | - | 47,50,50 | 4.41 | 24 (51%) | 51,76,76 | 7.23 | 14 (27%) |
| 37 | CLA | 32 | 202 | 52 | 69,73,73 | 1.96 | 20 (28%) | 82,113,113 | 2.61 | 32 (39%) |
| 47 | KC1 | 33 | 309 | 26 | 49,53,53 | 3.00 | 25 (51%) | 61,89,89 | 3.74 | 38 (62%) |
| 37 | CLA | 38 | 209 | 52 | 69,73,73 | 2.02 | 20 (28%) | 82,113,113 | 2.60 | 32 (39%) |
| 47 | KC1 | 36 | 302 | - | 49,53,53 | 3.07 | 24 (48%) | 61,89,89 | 3.58 | 33 (54%) |
| 41 | LMG | 17 | 317 | - | 37,37,55 | 0.96 | 2 (5%) | 45,45,63 | 1.28 | 4 (8%) |
| 37 | CLA | 33 | 303 | - | 61,65,73 | 2.13 | 19 (31%) | 72,103,113 | 2.89 | 35 (48%) |
| 45 | PL9 | D | 404 | - | 55,55,55 | 1.16 | 5 (9%) | 68,69,69 | 1.49 | 13 (19%) |
| 37 | CLA | C | 513 | - | 69,73,73 | 1.94 | 20 (28%) | 82,113,113 | 2.71 | 30 (36%) |
| 37 | CLA | 40 | 203 | 33 | 60,64,73 | 2.16 | 21 (35%) | 71,102,113 | 2.95 | 33 (46%) |
| 41 | LMG | l | 101 | - | 40,40,55 | 0.95 | 3 (7%) | 48,48,63 | 1.33 | 4 (8%) |
| 48 | A86 | 11 | 319 | - | 47,50,50 | 4.01 | 23 (48%) | 51,76,76 | 6.23 | 17 (33%) |
| 48 | A86 | 37 | 311 | - | 47,50,50 | 4.31 | 24 (51%) | 51,76,76 | 6.05 | 18 (35%) |
| 48 | A86 | 18 | 213 | - | 47,50,50 | 4.26 | 24 (51%) | 51,76,76 | 6.90 | 21 (41%) |
| 37 | CLA | W | 101 | - | 69,73,73 | 1.95 | 20 (28%) | 82,113,113 | 2.83 | 32 (39%) |
| 40 | SQD | 17 | 301 | - | 47,49,54 | 1.01 | 5 (10%) | 57,60,65 | 1.49 | 11 (19%) |
| 37 | CLA | 18 | 211 | - | 49,53,73 | 2.42 | 20 (40%) | 58,89,113 | 3.07 | 26 (44%) |
| 37 | CLA | 31 | 301 | - | 69,73,73 | 2.02 | 20 (28%) | 82,113,113 | 2.53 | 31 (37%) |
| 37 | CLA | b | 502 | - | 69,73,73 | 1.95 | 18 (26%) | 82,113,113 | 2.75 | 31 (37%) |
| 47 | KC1 | 33 | 306 | 26 | 49,53,53 | 3.00 | 22 (44%) | 61,89,89 | 3.82 | 35 (57%) |
| 37 | CLA | W | 102 | - | 69,73,73 | 2.01 | 20 (28%) | 82,113,113 | 2.52 | 31 (37%) |
| 43 | LHG | 37 | 321 | - | 44,44,48 | 0.66 | 1 (2%) | 47,50,54 | 1.20 | 3 (6%) |
| 48 | A86 | 20 | 309 | - | 47,50,50 | 4.37 | 23 (48%) | 51,76,76 | 7.11 | 13 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 37 | CLA | 18 | 204 | - | 60,64,73 | 2.17 | 21 (35%) | 71,102,113 | 3.03 | 36 (50%) |
| 48 | A86 | 38 | 215 | - | 47,50,50 | 4.28 | 24 (51%) | 51,76,76 | 6.46 | 17 (33%) |
| 37 | CLA | B | 505 | - | 69,73,73 | 1.92 | 19 (27%) | 82,113,113 | 2.72 | 30 (36%) |
| 47 | KC1 | 31 | 309 | 24 | 49,53,53 | 2.96 | 21 (42%) | 61,89,89 | 3.72 | 37 (60%) |
| 47 | KC1 | 40 | 206 | 33 | 49,53,53 | 3.05 | 23 (46%) | 61,89,89 | 3.70 | 35 (57%) |
| 44 | DGD | h | 102 | - | 63,63,67 | 1.03 | 5 (7%) | 77,77,81 | 1.36 | 8 (10%) |
| 37 | CLA | 12 | 210 | 52 | 69,73,73 | 2.00 | 20 (28%) | 82,113,113 | 2.58 | 30 (36%) |
| 37 | CLA | 41 | 206 | 34 | 69,73,73 | 1.99 | 19 (27%) | 82,113,113 | 2.65 | 30 (36%) |
| 37 | CLA | 31 | 304 | - | 69,73,73 | 1.95 | 20 (28%) | 82,113,113 | 2.74 | 34 (41%) |
| 37 | CLA | 21 | 209 | 34 | 49,53,73 | 2.43 | 20 (40%) | 58,89,113 | 3.07 | 28 (48%) |
| 48 | A86 | 14 | 315 | - | 47,50,50 | 4.17 | 23 (48%) | 51,76,76 | 6.63 | 17 (33%) |
| 48 | A86 | 31 | 319 | - | 47,50,50 | 4.00 | 23 (48%) | 51,76,76 | 6.24 | 17 (33%) |
| 37 | CLA | 38 | 204 | - | 60,64,73 | 2.18 | 21 (35%) | 71,102,113 | 3.03 | 36 (50%) |
| 37 | CLA | 39 | 306 | 32 | 69,73,73 | 1.96 | 18 (26%) | 82,113,113 | 2.63 | 31 (37%) |
| 43 | LHG | a | 412 | - | 45,45,48 | 0.87 | 2 (4%) | 48,51,54 | 1.25 | 7 (14%) |
| 37 | CLA | B | 508 | - | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.61 | 29 (35%) |
| 37 | CLA | c | 505 | - | 69,73,73 | 1.91 | 20 (28%) | 82,113,113 | 2.70 | 32 (39%) |
| 48 | A86 | 17 | 314 | - | 47,50,50 | 4.17 | 23 (48%) | 51,76,76 | 7.19 | 17 (33%) |
| 48 | A86 | 13 | 315 | - | 47,50,50 | 4.30 | 23 (48%) | 51,76,76 | 6.33 | 19 (37%) |
| 43 | LHG | d | 407 | - | 48,48,48 | 0.72 | 1 (2%) | 51,54,54 | 1.32 | 7 (13%) |
| 37 | CLA | B | 504 | - | 69,73,73 | 1.87 | 18 (26%) | 82,113,113 | 2.59 | 33 (40%) |
| 48 | A86 | 14 | 311 | - | 47,50,50 | 4.16 | 21 (44%) | 51,76,76 | 6.95 | 20 (39%) |
| 37 | CLA | 12 | 209 | 25 | 56,60,73 | 2.18 | 18 (32%) | 65,97,113 | 2.97 | 34 (52%) |
| 48 | A86 | 35 | 315 | - | 47,50,50 | 4.28 | 24 (51%) | 51,76,76 | 6.52 | 21 (41%) |
| 37 | CLA | 15 | 310 | - | 49,53,73 | 2.43 | 20 (40%) | 58,89,113 | 3.08 | 27 (46%) |
| 37 | CLA | 20 | 307 | 33 | 49,53,73 | 2.42 | 20 (40%) | 58,89,113 | 3.00 | 28 (48%) |
| 37 | CLA | 16 | 303 | - | 61,65,73 | 2.13 | 18 (29%) | 72,103,113 | 2.87 | 32 (44%) |
| 48 | A86 | 40 | 201 | - | 47,50,50 | 4.39 | 23 (48%) | 51,76,76 | 7.12 | 22 (43%) |
| 37 | CLA | A | 405 | - | 69,73,73 | 1.94 | 17 (24%) | 82,113,113 | 2.70 | 30 (36%) |
| 40 | SQD | L | 101 | - | 52,54,54 | 0.93 | 3 (5%) | 62,65,65 | 1.60 | 9 (14%) |
| 41 | LMG | a | 410 | - | 51,51,55 | 0.88 | 2 (3%) | 59,59,63 | 1.37 | 7 (11%) |
| 47 | KC1 | 14 | 306 | 27 | 49,53,53 | 3.01 | 22 (44%) | 61,89,89 | 3.80 | 37 (60%) |
| 47 | KC1 | 16 | 308 | 29 | 49,53,53 | 3.07 | 25 (51%) | 61,89,89 | 3.71 | 36 (59%) |
| 37 | CLA | 16 | 301 | 29 | 69,73,73 | 1.97 | 19 (27%) | 82,113,113 | 2.69 | 30 (36%) |
| 37 | CLA | 36 | 307 | 52 | 65,69,73 | 2.05 | 18 (27%) | 77,108,113 | 2.68 | 28 (36%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 41 | LMG | c | 518 | - | 51,51,55 | 0.97 | 3 (5%) | 59,59,63 | 1.46 | 7 (11%) |
| 45 | PL9 | d | 406 | - | 55,55,55 | 1.76 | 9 (16%) | 68,69,69 | 1.39 | 11 (16%) |
| 48 | A86 | 31 | 313 | - | 47,50,50 | 4.08 | 22 (46%) | 51,76,76 | 5.87 | 16 (31%) |
| 48 | A86 | 13 | 312 | - | 47,50,50 | 4.38 | 23 (48%) | 51,76,76 | 6.59 | 18 (35%) |
| 48 | A86 | 35 | 319 | - | 47,50,50 | 4.27 | 23 (48%) | 51,76,76 | 6.00 | 19 (37%) |
| 37 | CLA | B | 506 | - | 69,73,73 | 1.88 | 19 (27%) | 82,113,113 | 2.76 | 30 (36%) |
| 37 | CLA | 21 | 204 | - | 62,66,73 | 2.16 | 20 (32%) | 73,104,113 | 2.93 | 35 (47%) |
| 47 | KC1 | 11 | 302 | - | 49,53,53 | 2.99 | 21 (42%) | 61,89,89 | 3.78 | 34 (55%) |
| 48 | A86 | 35 | 314 | - | 47,50,50 | 4.43 | 24 (51%) | 51,76,76 | 7.04 | 18 (35%) |
| 37 | CLA | c | 507 | 52 | 69,73,73 | 1.91 | 19 (27%) | 82,113,113 | 2.64 | 31 (37%) |
| 47 | KC1 | 40 | 207 | 33 | 49,53,53 | 3.05 | 24 (48%) | 61,89,89 | 3.77 | 32 (52%) |
| 37 | CLA | 18 | 209 | 52 | 69,73,73 | 2.02 | 20 (28%) | 82,113,113 | 2.59 | 30 (36%) |
| 37 | CLA | 13 | 305 | - | 49,53,73 | 2.41 | 20 (40%) | 58,89,113 | 3.05 | 27 (46%) |
| 48 | A86 | 12 | 220 | - | 47,50,50 | 4.05 | 22 (46%) | 51,76,76 | 6.62 | 20 (39%) |
| 37 | CLA | 15 | 305 | - | 49,53,73 | 2.42 | 20 (40%) | 58,89,113 | 3.03 | 28 (48%) |
| 48 | A86 | 37 | 314 | - | 47,50,50 | 4.26 | 23 (48%) | 51,76,76 | 6.45 | 18 (35%) |
| 38 | PHO | a | 405 | - | 58,69,69 | 2.02 | 9 (15%) | 55,99,99 | 1.72 | 10 (18%) |
| 47 | KC1 | 37 | 302 | - | 49,53,53 | 3.05 | 23 (46%) | 61,89,89 | 3.72 | 35 (57%) |
| 43 | LHG | D | 409 | - | 48,48,48 | 0.72 | 1 (2%) | 51,54,54 | 1.32 | 7 (13%) |
| 50 | DD6 | 21 | 216 | - | 40,45,45 | 5.60 | 24 (60%) | 51,67,67 | 6.13 | 27 (52%) |
| 37 | CLA | 20 | 301 | 33 | 60,64,73 | 2.16 | 21 (35%) | 71,102,113 | 2.95 | 33 (46%) |
| 37 | CLA | 39 | 309 | 32 | 49,53,73 | 2.35 | 20 (40%) | 58,89,113 | 3.02 | 27 (46%) |
| 39 | BCR | b | 517 | - | 41,41,41 | 1.22 | 2 (4%) | 56,56,56 | 1.33 | 7 (12%) |
| 50 | DD6 | 36 | 312 | - | 40,45,45 | 5.60 | 24 (60%) | 51,67,67 | 5.90 | 26 (50%) |
| 38 | PHO | a | 406 | - | 58,69,69 | 2.04 | 10 (17%) | 55,99,99 | 1.76 | 9 (16%) |
| 37 | CLA | 11 | 310 | 52 | 55,59,73 | 2.18 | 21 (38%) | 64,96,113 | 2.88 | 30 (46%) |
| 47 | KC1 | 17 | 306 | 30 | 49,53,53 | 3.04 | 23 (46%) | 61,89,89 | 3.72 | 35 (57%) |
| 41 | LMG | 31 | 317 | - | 32,32,55 | 0.97 | 1 (3%) | 40,40,63 | 1.25 | 4 (10%) |
| 48 | A86 | 20 | 311 | - | 47,50,50 | 4.40 | 24 (51%) | 51,76,76 | 7.22 | 14 (27%) |
| 48 | A86 | 38 | 212 | - | 47,50,50 | 4.33 | 24 (51%) | 51,76,76 | 6.73 | 18 (35%) |
| 43 | LHG | 17 | 316 | - | 43,43,48 | 0.63 | 0 | 46,49,54 | 1.30 | 6 (13%) |
| 37 | CLA | 19 | 310 | 32 | 69,73,73 | 1.98 | 18 (26%) | 82,113,113 | 2.57 | 30 (36%) |
| 48 | A86 | 35 | 312 | - | 47,50,50 | 4.31 | 24 (51%) | 51,76,76 | 6.47 | 18 (35%) |
| 47 | KC1 | 15 | 306 | 28 | 49,53,53 | 3.06 | 24 (48%) | 61,89,89 | 3.82 | 36 (59%) |
| 40 | SQD | A | 407 | - | 52,54,54 | 0.95 | 6 (11%) | 62,65,65 | 1.64 | 10 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 48 | A86 | 40 | 211 | - | 47,50,50 | 4.37 | 23 (48%) | 51,76,76 | 7.12 | 13 (25%) |
| 39 | BCR | A | 410 | - | 41,41,41 | 1.10 | 2 (4%) | 56,56,56 | 1.30 | 6 (10%) |
| 50 | DD6 | 39 | 312 | - | 40,45,45 | 5.37 | 22 (55%) | 51,67,67 | 5.77 | 30 (58%) |
| 37 | CLA | 17 | 304 | - | 60,64,73 | 2.16 | 20 (33%) | 71,102,113 | 2.95 | 33 (46%) |
| 37 | CLA | 38 | 202 | 31 | 69,73,73 | 2.02 | 19 (27%) | 82,113,113 | 2.68 | 32 (39%) |
| 44 | DGD | C | 517 | - | 63,63,67 | 1.21 | 6 (9%) | 77,77,81 | 1.49 | 15 (19%) |
| 48 | A86 | 18 | 215 | - | 47,50,50 | 4.26 | 24 (51%) | 51,76,76 | 6.49 | 18 (35%) |
| 37 | CLA | 12 | 207 | 52 | 54,58,73 | 2.25 | 19 (35%) | 64,95,113 | 3.04 | 33 (51%) |
| 45 | PL9 | d | 402 | - | 55,55,55 | 1.16 | 6 (10%) | 68,69,69 | 1.49 | 13 (19%) |
| 44 | DGD | j | 101 | - | 63,63,67 | 1.09 | 6 (9%) | 77,77,81 | 1.50 | 12 (15%) |
| 47 | KC1 | 18 | 207 | 31 | 49,53,53 | 3.04 | 24 (48%) | 61,89,89 | 3.82 | 38 (62%) |
| 48 | A86 | 38 | 214 | - | 47,50,50 | 4.40 | 24 (51%) | 51,76,76 | 6.83 | 19 (37%) |
| 37 | CLA | c | 501 | - | 69,73,73 | 1.92 | 19 (27%) | 82,113,113 | 2.72 | 31 (37%) |
| 47 | KC1 | 32 | 212 | 25 | 49,53,53 | 3.01 | 24 (48%) | 61,89,89 | 3.72 | 37 (60%) |
| 48 | A86 | 37 | 312 | - | 47,50,50 | 4.30 | 23 (48%) | 51,76,76 | 7.03 | 20 (39%) |
| 37 | CLA | 15 | 301 | 28 | 69,73,73 | 2.03 | 19 (27%) | 82,113,113 | 2.64 | 27 (32%) |
| 48 | A86 | 38 | 213 | - | 47,50,50 | 4.35 | 25 (53%) | 51,76,76 | 6.75 | 23 (45%) |
| 47 | KC1 | 16 | 302 | - | 49,53,53 | 3.07 | 24 (48%) | 61,89,89 | 3.58 | 33 (54%) |
| 37 | CLA | 21 | 210 | - | 49,53,73 | 2.42 | 20 (40%) | 58,89,113 | 3.13 | 27 (46%) |
| 37 | CLA | b | 507 | 52 | 69,73,73 | 1.96 | 18 (26%) | 82,113,113 | 2.60 | 30 (36%) |
| 37 | CLA | a | 407 | - | 69,73,73 | 1.94 | 17 (24%) | 82,113,113 | 2.70 | 30 (36%) |
| 47 | KC1 | 37 | 307 | 30 | 49,53,53 | 3.06 | 25 (51%) | 61,89,89 | 3.74 | 37 (60%) |
| 37 | CLA | A | 403 | - | 69,73,73 | 1.95 | 19 (27%) | 82,113,113 | 2.68 | 33 (40%) |
| 48 | A86 | 32 | 217 | - | 47,50,50 | 4.22 | 23 (48%) | 51,76,76 | 6.88 | 20 (39%) |
| 48 | A86 | 15 | 313 | - | 47,50,50 | 4.37 | 24 (51%) | 51,76,76 | 6.20 | 15 (29%) |
| 37 | CLA | D | 401 | 52 | 69,73,73 | 1.97 | 18 (26%) | 82,113,113 | 2.72 | 28 (34%) |
| 47 | KC1 | 14 | 309 | 27 | 49,53,53 | 2.98 | 23 (46%) | 61,89,89 | 3.80 | 38 (62%) |
| 37 | CLA | 41 | 208 | - | 69,73,73 | 2.04 | 21 (30%) | 82,113,113 | 2.64 | 31 (37%) |
| 46 | HEM | V | 201 | 16 | 50,50,50 | 1.29 | 6 (12%) | 67,82,82 | 1.24 | 6 (8%) |
| 39 | BCR | A | 406 | - | 41,41,41 | 1.21 | 3 (7%) | 56,56,56 | 1.32 | 7 (12%) |
| 47 | KC1 | 33 | 304 | 26 | 49,53,53 | 3.02 | 22 (44%) | 61,89,89 | 3.81 | 35 (57%) |
| 48 | A86 | 14 | 314 | - | 47,50,50 | 4.37 | 24 (51%) | 51,76,76 | 7.04 | 18 (35%) |
| 47 | KC1 | 34 | 304 | 27 | 49,53,53 | 3.03 | 23 (46%) | 61,89,89 | 3.96 | 32 (52%) |
| 48 | A86 | 33 | 315 | - | 47,50,50 | 4.30 | 24 (51%) | 51,76,76 | 6.32 | 19 (37%) |
| 37 | CLA | B | 502 | - | 69,73,73 | 1.96 | 18 (26%) | 82,113,113 | 2.76 | 31 (37%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 37 | CLA | b | 512 | - | 69,73,73 | 1.90 | 19 (27%) | 82,113,113 | 2.62 | 33 (40%) |
| 37 | CLA | 36 | 303 | - | 61,65,73 | 2.13 | 18 (29%) | 72,103,113 | 2.87 | 32 (44%) |
| 41 | LMG | b | 520 | - | 51,51,55 | 0.87 | 3 (5%) | 59,59,63 | 1.31 | 6 (10%) |
| 48 | A86 | 32 | 203 | - | 47,50,50 | 4.11 | 21 (44%) | 51,76,76 | 6.37 | 22 (43%) |
| 37 | CLA | a | 404 | 52 | 69,73,73 | 1.97 | 18 (26%) | 82,113,113 | 2.72 | 28 (34%) |
| 37 | CLA | 11 | 303 | - | 69,73,73 | 1.96 | 20 (28%) | 82,113,113 | 2.74 | 34 (41%) |
| 47 | KC1 | 21 | 207 | 34 | 49,53,53 | 3.04 | 25 (51%) | 61,89,89 | 3.95 | 36 (59%) |
| 47 | KC1 | 36 | 308 | 29 | 49,53,53 | 3.06 | 24 (48%) | 61,89,89 | 3.70 | 36 (59%) |
| 47 | KC1 | 21 | 203 | - | 49,53,53 | 3.08 | 25 (51%) | 61,89,89 | 3.83 | 33 (54%) |
| 41 | LMG | B | 521 | - | 51,51,55 | 0.87 | 3 (5%) | 59,59,63 | 1.31 | 6 (10%) |
| 47 | KC1 | 12 | 206 | 25 | 49,53,53 | 3.00 | 21 (42%) | 61,89,89 | 3.73 | 32 (52%) |
| 40 | SQD | 36 | 315 | - | 47,49,54 | 1.01 | 4 (8%) | 57,60,65 | 1.49 | 11 (19%) |
| 48 | A86 | 33 | 311 | - | 47,50,50 | 4.18 | 23 (48%) | 51,76,76 | 6.64 | 20 (39%) |
| 48 | A86 | 33 | 313 | - | 47,50,50 | 4.41 | 24 (51%) | 51,76,76 | 7.22 | 18 (35%) |
| 48 | A86 | 34 | 311 | - | 47,50,50 | 4.16 | 22 (46%) | 51,76,76 | 6.96 | 20 (39%) |
| 47 | KC1 | 16 | 304 | 29 | 49,53,53 | 3.05 | 24 (48%) | 61,89,89 | 3.90 | 36 (59%) |
| 47 | KC1 | 18 | 205 | 31 | 49,53,53 | 3.08 | 24 (48%) | 61,89,89 | 3.84 | 35 (57%) |
| 48 | A86 | 16 | 310 | - | 47,50,50 | 4.08 | 22 (46%) | 51,76,76 | 6.38 | 21 (41%) |
| 47 | KC1 | 34 | 306 | 27 | 49,53,53 | 3.00 | 22 (44%) | 61,89,89 | 3.80 | 37 (60%) |
| 37 | CLA | 39 | 305 | 32 | 55,59,73 | 2.20 | 18 (32%) | 64,96,113 | 3.00 | 31 (48%) |
| 37 | CLA | 39 | 307 | 43 | 69,73,73 | 2.03 | 20 (28%) | 82,113,113 | 2.62 | 31 (37%) |
| 47 | KC1 | 17 | 308 | 30 | 49,53,53 | 3.06 | 25 (51%) | 61,89,89 | 3.75 | 37 (60%) |
| 37 | CLA | 38 | 211 | - | 49,53,73 | 2.46 | 20 (40%) | 58,89,113 | 3.03 | 26 (44%) |
| 47 | KC1 | 11 | 304 | 24 | 49,53,53 | 3.03 | 23 (46%) | 61,89,89 | 3.76 | 34 (55%) |
| 37 | CLA | B | 515 | - | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.68 | 32 (39%) |
| 37 | CLA | 39 | 301 | 32 | 69,73,73 | 2.00 | 19 (27%) | 82,113,113 | 2.64 | 30 (36%) |
| 50 | DD6 | 41 | 216 | - | 40,45,45 | 5.61 | 24 (60%) | 51,67,67 | 6.12 | 27 (52%) |
| 37 | CLA | b | 513 | - | 69,73,73 | 1.91 | 19 (27%) | 82,113,113 | 2.66 | 30 (36%) |
| 47 | KC1 | 20 | 305 | 33 | 49,53,53 | 3.05 | 24 (48%) | 61,89,89 | 3.78 | 32 (52%) |
| 37 | CLA | 38 | 203 | - | 69,73,73 | 2.03 | 20 (28%) | 82,113,113 | 2.63 | 33 (40%) |
| 37 | CLA | C | 505 | - | 69,73,73 | 1.91 | 20 (28%) | 82,113,113 | 2.70 | 32 (39%) |
| 37 | CLA | B | 516 | - | 69,73,73 | 1.92 | 19 (27%) | 82,113,113 | 2.73 | 34 (41%) |
| 44 | DGD | H | 102 | - | 63,63,67 | 1.04 | 5 (7%) | 77,77,81 | 1.36 | 8 (10%) |
| 48 | A86 | 17 | 320 | - | 47,50,50 | 4.22 | 23 (48%) | 51,76,76 | 6.46 | 19 (37%) |
| 37 | CLA | 18 | 206 | - | 49,53,73 | 2.43 | 20 (40%) | 58,89,113 | 3.09 | 28 (48%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 37 | CLA | D | 406 | - | 69,73,73 | 1.94 | 19 (27%) | 82,113,113 | 2.72 | 31 (37%) |
| 47 | KC1 | 16 | 305 | 29 | 49,53,53 | 3.07 | 24 (48%) | 61,89,89 | 3.73 | 34 (55%) |
| 50 | DD6 | 19 | 312 | - | 40,45,45 | 5.38 | 22 (55%) | 51,67,67 | 5.77 | 30 (58%) |
| 39 | BCR | B | 518 | - | 41,41,41 | 1.10 | 2 (4%) | 56,56,56 | 1.25 | 6 (10%) |
| 48 | A86 | 31 | 315 | - | 47,50,50 | 4.07 | 23 (48%) | 51,76,76 | 6.38 | 17 (33%) |
| 47 | KC1 | 31 | 305 | 24 | 49,53,53 | 3.02 | 23 (46%) | 61,89,89 | 3.76 | 34 (55%) |
| 48 | A86 | 14 | 312 | - | 47,50,50 | 4.21 | 23 (48%) | 51,76,76 | 6.60 | 22 (43%) |
| 37 | CLA | 18 | 203 | - | 69,73,73 | 2.03 | 20 (28%) | 82,113,113 | 2.62 | 34 (41%) |
| 37 | CLA | 33 | 301 | 26 | 69,73,73 | 2.00 | 18 (26%) | 82,113,113 | 2.60 | 27 (32%) |
| 39 | BCR | d | 405 | - | 41,41,41 | 1.13 | 3 (7%) | 56,56,56 | 1.28 | 7 (12%) |
| 37 | CLA | D | 402 | 52 | 69,73,73 | 1.98 | 19 (27%) | 82,113,113 | 2.65 | 31 (37%) |
| 48 | A86 | 11 | 311 | - | 47,50,50 | 4.06 | 23 (48%) | 51,76,76 | 6.21 | 17 (33%) |
| 47 | KC1 | 20 | 304 | 33 | 49,53,53 | 3.04 | 23 (46%) | 61,89,89 | 3.69 | 34 (55%) |
| 48 | A86 | 12 | 215 | - | 47,50,50 | 4.38 | 24 (51%) | 51,76,76 | 6.79 | 14 (27%) |
| 40 | SQD | B | 522 | - | 35,37,54 | 1.19 | 6 (17%) | 45,48,65 | 1.59 | 10 (22%) |
| 37 | CLA | 13 | 301 | 26 | 69,73,73 | 2.01 | 18 (26%) | 82,113,113 | 2.60 | 28 (34%) |
| 37 | CLA | 35 | 308 | 52 | 69,73,73 | 2.01 | 21 (30%) | 82,113,113 | 2.62 | 31 (37%) |
| 37 | CLA | 40 | 208 | 33 | 54,58,73 | 2.25 | 19 (35%) | 64,95,113 | 2.91 | 30 (46%) |
| 37 | CLA | 18 | 201 | 52 | 69,73,73 | 2.00 | 20 (28%) | 82,113,113 | 2.62 | 32 (39%) |
| 37 | CLA | b | 516 | - | 69,73,73 | 1.92 | 19 (27%) | 82,113,113 | 2.73 | 34 (41%) |
| 41 | LMG | B | 520 | - | 51,51,55 | 0.82 | 1 (1%) | 59,59,63 | 1.30 | 5 (8%) |
| 47 | KC1 | 39 | 308 | - | 49,53,53 | 3.01 | 23 (46%) | 61,89,89 | 3.88 | 37 (60%) |
| 47 | KC1 | 38 | 207 | 31 | 49,53,53 | 3.05 | 25 (51%) | 61,89,89 | 3.83 | 38 (62%) |
| 37 | CLA | 33 | 305 | - | 49,53,73 | 2.41 | 20 (40%) | 58,89,113 | 3.06 | 27 (46%) |
| 48 | A86 | 31 | 312 | - | 47,50,50 | 4.08 | 22 (46%) | 51,76,76 | 6.49 | 22 (43%) |
| 48 | A86 | 32 | 215 | - | 47,50,50 | 4.11 | 24 (51%) | 51,76,76 | 6.47 | 17 (33%) |
| 48 | A86 | 16 | 314 | - | 47,50,50 | 4.01 | 23 (48%) | 51,76,76 | 6.34 | 16 (31%) |
| 43 | LHG | d | 408 | - | 48,48,48 | 0.76 | 2 (4%) | 51,54,54 | 1.31 | 7 (13%) |
| 41 | LMG | D | 412 | - | 51,51,55 | 0.89 | 3 (5%) | 59,59,63 | 1.41 | 6 (10%) |
| 39 | BCR | C | 519 | - | 41,41,41 | 1.17 | 2 (4%) | 56,56,56 | 1.24 | 4 (7%) |
| 41 | LMG | A | 408 | - | 51,51,55 | 0.88 | 2 (3%) | 59,59,63 | 1.37 | 7 (11%) |
| 48 | A86 | 31 | 314 | - | 47,50,50 | 4.17 | 23 (48%) | 51,76,76 | 7.00 | 22 (43%) |
| 48 | A86 | 39 | 311 | - | 47,50,50 | 4.15 | 23 (48%) | 51,76,76 | 6.47 | 19 (37%) |
| 48 | A86 | 39 | 313 | - | 47,50,50 | 4.40 | 26 (55%) | 51,76,76 | 7.35 | 21 (41%) |
| 48 | A86 | 11 | 314 | - | 47,50,50 | 4.18 | 23 (48%) | 51,76,76 | 7.00 | 22 (43%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 37 | CLA | 41 | 204 | - | 62,66,73 | 2.16 | 20 (32%) | 73,104,113 | 2.93 | 35 (47%) |
| 37 | CLA | b | 523 | - | 69,73,73 | 1.92 | 21 (30%) | 82,113,113 | 2.65 | 32 (39%) |
| 39 | BCR | c | 514 | - | 41,41,41 | 1.21 | 2 (4%) | 56,56,56 | 1.43 | 10 (17%) |
| 37 | CLA | 37 | 301 | 30 | 69,73,73 | 2.03 | 20 (28%) | 82,113,113 | 2.59 | 27 (32%) |
| 37 | CLA | 34 | 307 | 27 | 56,60,73 | 2.19 | 18 (32%) | 65,97,113 | 2.86 | 33 (50%) |
| 47 | KC1 | 36 | 304 | 29 | 49,53,53 | 3.05 | 24 (48%) | 61,89,89 | 3.90 | 36 (59%) |
| 37 | CLA | b | 501 | 52 | 69,73,73 | 1.96 | 19 (27%) | 82,113,113 | 2.63 | 29 (35%) |
| 37 | CLA | B | 507 | 52 | 69,73,73 | 1.96 | 19 (27%) | 82,113,113 | 2.61 | 30 (36%) |
| 48 | A86 | 13 | 314 | - | 47,50,50 | 4.41 | 24 (51%) | 51,76,76 | 7.15 | 17 (33%) |
| 37 | CLA | a | 403 | - | 69,73,73 | 1.95 | 20 (28%) | 82,113,113 | 2.68 | 33 (40%) |
| 47 | KC1 | 19 | 308 | - | 49,53,53 | 3.01 | 23 (46%) | 61,89,89 | 3.88 | 38 (62%) |
| 48 | A86 | 15 | 314 | - | 47,50,50 | 4.45 | 24 (51%) | 51,76,76 | 6.97 | 18 (35%) |
| 42 | BCT | a | 411 | 36 | 3,3,3 | 1.21 | 0 | 2,3,3 | 4.13 | 2 (100%) |
| 37 | CLA | d | 404 | - | 69,73,73 | 1.94 | 18 (26%) | 82,113,113 | 2.72 | 32 (39%) |
| 48 | A86 | 17 | 310 | - | 47,50,50 | 4.30 | 23 (48%) | 51,76,76 | 7.02 | 17 (33%) |
| 37 | CLA | 16 | 309 | - | 49,53,73 | 2.38 | 20 (40%) | 58,89,113 | 3.18 | 29 (50%) |
| 37 | CLA | 32 | 213 | - | 49,53,73 | 2.38 | 19 (38%) | 58,89,113 | 3.11 | 28 (48%) |
| 39 | BCR | K | 101 | - | 41,41,41 | 1.18 | 3 (7%) | 56,56,56 | 1.27 | 7 (12%) |
| 37 | CLA | 39 | 302 | - | 69,73,73 | 1.97 | 21 (30%) | 82,113,113 | 2.73 | 30 (36%) |
| 37 | CLA | C | 502 | - | 69,73,73 | 1.91 | 18 (26%) | 82,113,113 | 2.60 | 30 (36%) |
| 39 | BCR | a | 408 | - | 41,41,41 | 1.20 | 3 (7%) | 56,56,56 | 1.32 | 7 (12%) |
| 37 | CLA | 36 | 306 | 29 | 69,73,73 | 2.00 | 20 (28%) | 82,113,113 | 2.55 | 31 (37%) |
| 37 | CLA | 35 | 310 | - | 49,53,73 | 2.43 | 20 (40%) | 58,89,113 | 3.09 | 27 (46%) |
| 39 | BCR | 0 | 101 | - | 41,41,41 | 1.15 | 2 (4%) | 56,56,56 | 1.34 | 7 (12%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 48 | A86 | 41 | 214 | - | - | 5/34/90/90 | 0/3/3/3 |
| 50 | DD6 | 16 | 312 | - | - | 12/26/80/80 | 0/3/3/3 |
| 37 | CLA | 19 | 306 | 32 | 1/1/15/20 | 7/39/115/115 | - |
| 37 | CLA | c | 508 | - | 1/1/15/20 | 8/39/115/115 | - |
| 47 | KC1 | 20 | 302 | - | - | 7/15/71/71 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 48 | A86 | 41 | 213 | - | - | 8/34/90/90 | 0/3/3/3 |
| 47 | KC1 | 17 | 305 | 30 | - | 6/15/71/71 | - |
| 37 | CLA | C | 512 | - | 1/1/15/20 | 6/39/115/115 | - |
| 37 | CLA | b | 511 | - | 1/1/15/20 | 11/39/115/115 | - |
| 47 | KC1 | 38 | 205 | 31 | - | 6/15/71/71 | - |
| 48 | A86 | 33 | 314 | - | - | 9/34/90/90 | 0/3/3/3 |
| 37 | CLA | b | 514 | - | 1/1/14/20 | 13/36/112/115 | - |
| 47 | KC1 | 11 | 309 | 24 | - | 8/15/71/71 | - |
| 48 | A86 | 16 | 311 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | 17 | 302 | 30 | - | 12/39/115/115 | - |
| 47 | KC1 | 12 | 208 | 25 | - | 4/15/71/71 | - |
| 37 | CLA | 41 | 210 | - | - | 6/15/91/115 | - |
| 37 | CLA | 41 | 205 | 34 | 1/1/11/20 | 9/15/91/115 | - |
| 37 | CLA | b | 504 | - | 1/1/15/20 | 5/39/115/115 | - |
| 47 | KC1 | 38 | 210 | 31 | - | 8/15/71/71 | - |
| 48 | A86 | 15 | 319 | - | - | 8/34/90/90 | 0/3/3/3 |
| 47 | KC1 | 32 | 209 | 25 | - | 4/15/71/71 | - |
| 37 | CLA | 32 | 210 | 25 | 1/1/12/20 | 13/24/100/115 | - |
| 37 | CLA | 15 | 307 | 28 | 1/1/12/20 | 12/24/100/115 | - |
| 39 | BCR | C | 514 | - | - | 6/29/63/63 | 0/2/2/2 |
| 37 | CLA | B | 513 | - | 1/1/15/20 | 8/39/115/115 | - |
| 37 | CLA | 12 | 205 | - | 1/1/15/20 | 11/39/115/115 | - |
| 37 | CLA | 14 | 305 | - | 1/1/11/20 | 4/15/91/115 | - |
| 37 | CLA | 35 | 307 | 28 | 1/1/12/20 | 12/24/100/115 | - |
| 37 | CLA | 41 | 202 | 34 | 1/1/13/20 | 9/30/106/115 | - |
| 48 | A86 | 34 | 313 | - | - | 12/34/90/90 | 0/3/3/3 |
| 37 | CLA | 11 | 301 | 24 | - | 12/39/115/115 | - |
| 37 | CLA | 11 | 308 | 52 | 1/1/15/20 | 13/39/115/115 | - |
| 37 | CLA | 37 | 306 | 30 | 1/1/12/20 | 11/24/100/115 | - |
| 41 | LMG | 37 | 316 | - | - | 15/32/52/70 | 0/1/1/1 |
| 47 | KC1 | 17 | 303 | - | - | 6/15/71/71 | - |
| 37 | CLA | 14 | 301 | 27 | - | 14/39/115/115 | - |
| 48 | A86 | 36 | 311 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | C | 503 | - | 1/1/15/20 | 21/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 48 | A86 | 32 | 218 | - | - | 13/34/90/90 | 0/3/3/3 |
| 48 | A86 | 21 | 211 | - | - | 9/34/90/90 | 0/3/3/3 |
| 41 | LMG | d | 409 | - | - | 13/46/66/70 | 0/1/1/1 |
| 37 | CLA | c | 513 | - | 1/1/15/20 | 9/39/115/115 | - |
| 37 | CLA | c | 511 | 3 | 1/1/15/20 | 8/39/115/115 | - |
| 37 | CLA | b | 503 | - | 1/1/15/20 | 11/39/115/115 | - |
| 39 | BCR | b | 518 | - | - | 6/29/63/63 | 0/2/2/2 |
| 44 | DGD | J | 101 | - | - | 16/51/91/95 | 0/2/2/2 |
| 48 | A86 | 32 | 216 | - | - | 13/34/90/90 | 0/3/3/3 |
| 48 | A86 | 18 | 212 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | c | 512 | - | 1/1/15/20 | 6/39/115/115 | - |
| 47 | KC1 | 18 | 210 | 31 | - | 8/15/71/71 | - |
| 37 | CLA | B | 510 | 52 | 1/1/15/20 | 7/39/115/115 | - |
| 48 | A86 | 35 | 316 | - | - | 14/34/90/90 | 0/3/3/3 |
| 37 | CLA | 35 | 303 | - | - | 8/30/106/115 | - |
| 37 | CLA | 19 | 307 | 43 | 1/1/15/20 | 8/39/115/115 | - |
| 39 | BCR | c | 515 | - | - | 7/29/63/63 | 0/2/2/2 |
| 48 | A86 | 12 | 217 | - | - | 13/34/90/90 | 0/3/3/3 |
| 48 | A86 | 12 | 214 | - | - | 3/34/90/90 | 0/3/3/3 |
| 39 | BCR | D | 407 | - | - | 12/29/63/63 | 0/2/2/2 |
| 48 | A86 | 16 | 313 | - | - | 13/34/90/90 | 0/3/3/3 |
| 37 | CLA | 17 | 309 | 52 | 1/1/15/20 | 11/39/115/115 | - |
| 40 | SQD | 16 | 315 | - | - | 24/49/69/69 | 0/1/1/1 |
| 48 | A86 | 11 | 315 | - | - | 6/34/90/90 | 0/3/3/3 |
| 48 | A86 | 41 | 211 | - | - | 9/34/90/90 | 0/3/3/3 |
| 37 | CLA | w | 101 | - | 1/1/15/20 | 17/39/115/115 | - |
| 37 | CLA | 14 | 310 | - | 1/1/11/20 | 4/15/91/115 | - |
| 48 | A86 | 17 | 315 | - | - | 12/34/90/90 | 0/3/3/3 |
| 48 | A86 | 34 | 315 | - | - | 6/34/90/90 | 0/3/3/3 |
| 37 | CLA | 36 | 301 | 29 | - | 11/39/115/115 | - |
| 41 | LMG | 32 | 201 | - | - | 14/34/54/70 | 0/1/1/1 |
| 37 | CLA | 14 | 302 | - | 1/1/15/20 | 18/39/115/115 | - |
| 37 | CLA | 34 | 308 | 52 | 1/1/15/20 | 11/39/115/115 | - |
| 44 | DGD | c | 516 | - | - | 17/51/91/95 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 48 | A86 | 15 | 312 | - | - | 8/34/90/90 | 0/3/3/3 |
| 48 | A86 | 37 | 309 | - | - | 8/34/90/90 | 0/3/3/3 |
| 41 | LMG | C | 518 | - | - | 25/46/66/70 | 0/1/1/1 |
| 37 | CLA | Z | 102 | 33 | 1/1/11/20 | 7/15/91/115 | - |
| 37 | CLA | z | 101 | 52 | 1/1/15/20 | 20/39/115/115 | - |
| 48 | A86 | 14 | 313 | - | - | 12/34/90/90 | 0/3/3/3 |
| 39 | BCR | H | 101 | - | - | 6/29/63/63 | 0/2/2/2 |
| 48 | A86 | 14 | 316 | - | - | 13/34/90/90 | 0/3/3/3 |
| 48 | A86 | 17 | 311 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | z | 102 | 33 | 1/1/11/20 | 7/15/91/115 | - |
| 37 | CLA | 32 | 206 | - | 1/1/15/20 | 11/39/115/115 | - |
| 47 | KC1 | 37 | 304 | 30 | - | 6/15/71/71 | - |
| 37 | CLA | C | 511 | 3 | 1/1/15/20 | 8/39/115/115 | - |
| 50 | DD6 | 20 | 310 | - | - | 14/26/80/80 | 0/3/3/3 |
| 48 | A86 | 33 | 312 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | 33 | 310 | - | - | 2/15/91/115 | - |
| 48 | A86 | 21 | 215 | - | - | 6/34/90/90 | 0/3/3/3 |
| 41 | LMG | b | 519 | - | - | 15/46/66/70 | 0/1/1/1 |
| 37 | CLA | 39 | 304 | 32 | 1/1/11/20 | 6/15/91/115 | - |
| 37 | CLA | 18 | 208 | 31 | 1/1/12/20 | 13/25/101/115 | - |
| 37 | CLA | 21 | 206 | 34 | 1/1/15/20 | 15/39/115/115 | - |
| 39 | BCR | C | 515 | - | - | 7/29/63/63 | 0/2/2/2 |
| 48 | A86 | 12 | 202 | - | - | 14/34/90/90 | 0/3/3/3 |
| 40 | SQD | 40 | 202 | - | - | 24/49/69/69 | 0/1/1/1 |
| 37 | CLA | c | 510 | - | 1/1/15/20 | 12/39/115/115 | - |
| 50 | DD6 | 40 | 212 | - | - | 14/26/80/80 | 0/3/3/3 |
| 37 | CLA | 31 | 302 | 24 | - | 12/39/115/115 | - |
| 40 | SQD | b | 521 | - | - | 11/32/52/69 | 0/1/1/1 |
| 46 | HEM | F | 101 | 5,6 | - | 8/14/54/54 | - |
| 47 | KC1 | 15 | 302 | - | - | 6/15/71/71 | - |
| 48 | A86 | 36 | 313 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | 19 | 309 | 32 | 1/1/11/20 | 5/15/91/115 | - |
| 39 | BCR | h | 101 | - | - | 6/29/63/63 | 0/2/2/2 |
| 45 | PL9 | D | 408 | - | - | 9/53/73/73 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 51 | LMU | 39 | 315 | - | - | 6/21/61/61 | 0/2/2/2 |
| 39 | BCR | a | 413 | - | - | 7/29/63/63 | 0/2/2/2 |
| 37 | CLA | 12 | 212 | - | 1/1/11/20 | 7/15/91/115 | - |
| 37 | CLA | 15 | 308 | 52 | 1/1/15/20 | 10/39/115/115 | - |
| 48 | A86 | 17 | 313 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | 33 | 307 | 26 | 1/1/12/20 | 12/24/100/115 | - |
| 37 | CLA | 35 | 301 | 28 | - | 10/39/115/115 | - |
| 48 | A86 | 34 | 314 | - | - | 13/34/90/90 | 0/3/3/3 |
| 37 | CLA | 21 | 208 | - | 1/1/15/20 | 13/39/115/115 | - |
| 43 | LHG | 39 | 314 | 37 | - | 28/53/53/53 | - |
| 37 | CLA | 32 | 211 | 52 | - | 9/39/115/115 | - |
| 47 | KC1 | 13 | 306 | 26 | - | 6/15/71/71 | - |
| 37 | CLA | 34 | 305 | - | 1/1/11/20 | 4/15/91/115 | - |
| 39 | BCR | y | 101 | - | - | 15/29/63/63 | 0/2/2/2 |
| 37 | CLA | c | 504 | 52 | 1/1/15/20 | 9/39/115/115 | - |
| 44 | DGD | c | 517 | - | - | 19/51/91/95 | 0/2/2/2 |
| 37 | CLA | 38 | 201 | 52 | 1/1/15/20 | 8/39/115/115 | - |
| 37 | CLA | B | 509 | - | 1/1/15/20 | 11/39/115/115 | - |
| 47 | KC1 | 35 | 309 | 28 | - | 8/15/71/71 | - |
| 37 | CLA | 31 | 310 | 52 | 1/1/12/20 | 6/23/99/115 | - |
| 47 | KC1 | 15 | 304 | 28 | - | 6/15/71/71 | - |
| 37 | CLA | 21 | 205 | 34 | 1/1/11/20 | 9/15/91/115 | - |
| 37 | CLA | C | 508 | - | 1/1/15/20 | 8/39/115/115 | - |
| 37 | CLA | 38 | 208 | 31 | 1/1/12/20 | 13/25/101/115 | - |
| 37 | CLA | B | 503 | - | 1/1/15/20 | 11/39/115/115 | - |
| 37 | CLA | C | 510 | - | 1/1/15/20 | 12/39/115/115 | - |
| 44 | DGD | C | 516 | - | - | 17/51/91/95 | 0/2/2/2 |
| 48 | A86 | 12 | 216 | - | - | 9/34/90/90 | 0/3/3/3 |
| 43 | LHG | 41 | 201 | - | - | 19/38/38/53 | - |
| 37 | CLA | b | 510 | 52 | 1/1/15/20 | 7/39/115/115 | - |
| 47 | KC1 | 35 | 304 | 28 | - | 6/15/71/71 | - |
| 37 | CLA | 13 | 310 | - | - | 2/15/91/115 | - |
| 48 | A86 | 19 | 311 | - | - | 6/34/90/90 | 0/3/3/3 |
| 48 | A86 | 37 | 319 | - | - | 8/34/90/90 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 37 | CLA | c | 503 | - | 1/1/15/20 | 21/39/115/115 | - |
| 37 | CLA | C | 507 | 52 | 1/1/15/20 | 8/39/115/115 | - |
| 43 | LHG | 19 | 314 | 37 | - | 28/53/53/53 | - |
| 48 | A86 | 32 | 214 | - | - | 5/34/90/90 | 0/3/3/3 |
| 37 | CLA | B | 524 | - | 1/1/15/20 | 13/39/115/115 | - |
| 39 | BCR | B | 517 | - | - | 6/29/63/63 | 0/2/2/2 |
| 37 | CLA | 37 | 303 | - | 1/1/13/20 | 8/29/105/115 | - |
| 37 | CLA | b | 509 | - | 1/1/15/20 | 11/39/115/115 | - |
| 37 | CLA | 34 | 301 | 27 | - | 14/39/115/115 | - |
| 47 | KC1 | 32 | 207 | 25 | - | 6/15/71/71 | - |
| 48 | A86 | 34 | 312 | - | - | 4/34/90/90 | 0/3/3/3 |
| 48 | A86 | 18 | 214 | - | - | 12/34/90/90 | 0/3/3/3 |
| 38 | PHO | A | 404 | - | - | 6/37/103/103 | 0/5/6/6 |
| 37 | CLA | Z | 101 | 52 | 1/1/15/20 | 20/39/115/115 | - |
| 37 | CLA | 40 | 210 | - | 1/1/11/20 | 4/18/94/115 | - |
| 47 | KC1 | 41 | 203 | - | - | 4/15/71/71 | - |
| 37 | CLA | 41 | 209 | 34 | 1/1/11/20 | 6/15/91/115 | - |
| 43 | LHG | 37 | 315 | - | - | 26/48/48/53 | - |
| 39 | BCR | b | 524 | - | - | 17/29/63/63 | 0/2/2/2 |
| 43 | LHG | D | 410 | - | - | 26/53/53/53 | - |
| 41 | LMG | L | 102 | - | - | 15/35/55/70 | 0/1/1/1 |
| 40 | SQD | B | 519 | - | - | 26/49/69/69 | 0/1/1/1 |
| 37 | CLA | C | 504 | 52 | 1/1/15/20 | 9/39/115/115 | - |
| 37 | CLA | 14 | 303 | - | - | 6/30/106/115 | - |
| 48 | A86 | 15 | 315 | - | - | 8/34/90/90 | 0/3/3/3 |
| 43 | LHG | D | 411 | - | - | 26/50/50/53 | - |
| 48 | A86 | 19 | 313 | - | - | 8/34/90/90 | 0/3/3/3 |
| 40 | SQD | a | 409 | - | - | 17/49/69/69 | 0/1/1/1 |
| 37 | CLA | 34 | 303 | - | - | 6/30/106/115 | - |
| 37 | CLA | 12 | 203 | 25 | 1/1/15/20 | 14/39/115/115 | - |
| 37 | CLA | c | 506 | - | 1/1/15/20 | 13/39/115/115 | - |
| 37 | CLA | 12 | 204 | - | 1/1/15/20 | 9/39/115/115 | - |
| 37 | CLA | 13 | 303 | - | 1/1/13/20 | 11/30/106/115 | - |
| 37 | CLA | 16 | 307 | 52 | 1/1/14/20 | 13/35/111/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 37 | CLA | B | 511 | - | 1/1/15/20 | 11/39/115/115 | - |
| 38 | PHO | D | 403 | - | - | 9/37/103/103 | 0/5/6/6 |
| 50 | DD6 | 20 | 312 | - | - | 12/26/80/80 | 0/3/3/3 |
| 37 | CLA | 32 | 208 | 52 | 1/1/12/20 | 2/21/97/115 | - |
| 37 | CLA | d | 403 | - | 1/1/15/20 | 8/39/115/115 | - |
| 48 | A86 | 15 | 311 | - | - | 6/34/90/90 | 0/3/3/3 |
| 37 | CLA | 19 | 305 | 32 | 1/1/12/20 | 7/23/99/115 | - |
| 48 | A86 | 15 | 316 | - | - | 14/34/90/90 | 0/3/3/3 |
| 37 | CLA | C | 501 | - | 1/1/15/20 | 12/39/115/115 | - |
| 47 | KC1 | 11 | 306 | 24 | - | 8/15/71/71 | - |
| 48 | A86 | 21 | 214 | - | - | 5/34/90/90 | 0/3/3/3 |
| 37 | CLA | D | 405 | - | 1/1/15/20 | 8/39/115/115 | - |
| 48 | A86 | 21 | 213 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | 18 | 202 | 31 | - | 14/39/115/115 | - |
| 51 | LMU | 19 | 315 | - | - | 6/21/61/61 | 0/2/2/2 |
| 37 | CLA | 14 | 307 | 27 | 1/1/12/20 | 15/24/100/115 | - |
| 37 | CLA | d | 401 | 52 | - | 14/39/115/115 | - |
| 48 | A86 | 11 | 312 | - | - | 6/34/90/90 | 0/3/3/3 |
| 47 | KC1 | 13 | 304 | 26 | - | 7/15/71/71 | - |
| 37 | CLA | 20 | 308 | - | 1/1/11/20 | 4/18/94/115 | - |
| 37 | CLA | 11 | 305 | 52 | 1/1/11/20 | 3/15/91/115 | - |
| 37 | CLA | 33 | 308 | 52 | - | 8/39/115/115 | - |
| 39 | BCR | B | 525 | - | - | 18/29/63/63 | 0/2/2/2 |
| 48 | A86 | 36 | 310 | - | - | 5/34/90/90 | 0/3/3/3 |
| 48 | A86 | 17 | 312 | - | - | 8/34/90/90 | 0/3/3/3 |
| 48 | A86 | 11 | 313 | - | - | 6/34/90/90 | 1/3/3/3 |
| 37 | CLA | b | 515 | - | 1/1/15/20 | 5/39/115/115 | - |
| 37 | CLA | b | 505 | - | 1/1/15/20 | 6/39/115/115 | - |
| 37 | CLA | 15 | 303 | - | - | 7/30/106/115 | - |
| 48 | A86 | 34 | 316 | - | - | 13/34/90/90 | 0/3/3/3 |
| 37 | CLA | 35 | 305 | - | 1/1/11/20 | 5/15/91/115 | - |
| 37 | CLA | 19 | 301 | 32 | 1/1/15/20 | 10/39/115/115 | - |
| 41 | LMG | 36 | 314 | - | - | 14/31/51/70 | 0/1/1/1 |
| 37 | CLA | C | 506 | - | 1/1/15/20 | 13/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 37 | CLA | C | 509 | - | 1/1/15/20 | 7/39/115/115 | - |
| 50 | DD6 | 21 | 212 | - | - | 12/26/80/80 | 0/3/3/3 |
| 37 | CLA | 39 | 310 | 32 | 1/1/15/20 | 9/39/115/115 | - |
| 37 | CLA | 36 | 309 | - | 1/1/11/20 | 6/15/91/115 | - |
| 47 | KC1 | 12 | 211 | 25 | - | 6/15/71/71 | - |
| 48 | A86 | 13 | 311 | - | - | 5/34/90/90 | 0/3/3/3 |
| 41 | LMG | 11 | 316 | - | - | 19/37/57/70 | 0/1/1/1 |
| 37 | CLA | 20 | 303 | - | 1/1/13/20 | 10/29/105/115 | - |
| 41 | LMG | 31 | 316 | - | - | 19/37/57/70 | 0/1/1/1 |
| 46 | HEM | v | 201 | 16 | - | 6/14/54/54 | - |
| 48 | A86 | 37 | 310 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | 21 | 202 | 34 | 1/1/13/20 | 9/30/106/115 | - |
| 47 | KC1 | 33 | 302 | - | - | 5/15/71/71 | - |
| 47 | KC1 | 35 | 306 | 28 | - | 6/15/71/71 | - |
| 37 | CLA | B | 501 | 52 | 1/1/15/20 | 18/39/115/115 | - |
| 37 | CLA | 32 | 204 | 25 | 1/1/15/20 | 14/39/115/115 | - |
| 37 | CLA | 37 | 308 | 52 | 1/1/15/20 | 11/39/115/115 | - |
| 43 | LHG | b | 522 | - | - | 18/53/53/53 | - |
| 37 | CLA | 19 | 303 | 52 | 1/1/15/20 | 14/39/115/115 | - |
| 47 | KC1 | 36 | 305 | 29 | - | 6/15/71/71 | - |
| 37 | CLA | 31 | 308 | 24 | - | 8/24/100/115 | - |
| 48 | A86 | 12 | 213 | - | - | 5/34/90/90 | 0/3/3/3 |
| 37 | CLA | 17 | 307 | 30 | 1/1/12/20 | 11/24/100/115 | - |
| 37 | CLA | B | 512 | - | 1/1/15/20 | 8/39/115/115 | - |
| 37 | CLA | c | 502 | - | 1/1/15/20 | 9/39/115/115 | - |
| 37 | CLA | 34 | 310 | - | 1/1/11/20 | 4/15/91/115 | - |
| 50 | DD6 | 41 | 212 | - | - | 12/26/80/80 | 0/3/3/3 |
| 37 | CLA | 40 | 209 | 33 | 1/1/11/20 | 8/15/91/115 | - |
| 43 | LHG | B | 523 | - | - | 18/53/53/53 | - |
| 47 | KC1 | 40 | 204 | - | - | 7/15/71/71 | - |
| 37 | CLA | 20 | 306 | 33 | 1/1/12/20 | 5/21/97/115 | - |
| 41 | LMG | 11 | 317 | - | - | 13/27/47/70 | 0/1/1/1 |
| 37 | CLA | 16 | 306 | 29 | 1/1/15/20 | 13/39/115/115 | - |
| 48 | A86 | 13 | 313 | - | - | 18/34/90/90 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 50 | DD6 | 40 | 214 | - | - | 12/26/80/80 | 0/3/3/3 |
| 43 | LHG | 21 | 217 | - | - | 27/49/49/53 | - |
| 37 | CLA | 19 | 302 | - | 1/1/15/20 | 11/39/115/115 | - |
| 37 | CLA | c | 509 | - | 1/1/15/20 | 7/39/115/115 | - |
| 47 | KC1 | 37 | 305 | 30 | - | 9/15/71/71 | - |
| 37 | CLA | 31 | 306 | 52 | 1/1/11/20 | 3/15/91/115 | - |
| 47 | KC1 | 34 | 309 | 27 | - | 6/15/71/71 | - |
| 39 | BCR | c | 519 | - | - | 6/29/63/63 | 0/2/2/2 |
| 47 | KC1 | 13 | 309 | 26 | - | 4/15/71/71 | - |
| 37 | CLA | b | 506 | - | 1/1/15/20 | 7/39/115/115 | - |
| 46 | HEM | f | 101 | 5,6 | - | 8/14/54/54 | - |
| 48 | A86 | 35 | 311 | - | - | 6/34/90/90 | 0/3/3/3 |
| 48 | A86 | 35 | 313 | - | - | 9/34/90/90 | 0/3/3/3 |
| 37 | CLA | B | 514 | - | 1/1/14/20 | 13/36/112/115 | - |
| 37 | CLA | 11 | 307 | 24 | - | 8/24/100/115 | - |
| 47 | KC1 | 31 | 307 | 24 | - | 8/15/71/71 | - |
| 37 | CLA | 40 | 205 | - | 1/1/13/20 | 10/29/105/115 | - |
| 48 | A86 | 37 | 313 | - | - | 9/34/90/90 | 0/3/3/3 |
| 48 | A86 | 41 | 215 | - | - | 6/34/90/90 | 0/3/3/3 |
| 37 | CLA | b | 508 | - | - | 5/39/115/115 | - |
| 47 | KC1 | 15 | 309 | 28 | - | 8/15/71/71 | - |
| 37 | CLA | 34 | 302 | - | 1/1/15/20 | 18/39/115/115 | - |
| 47 | KC1 | 41 | 207 | 34 | - | 7/15/71/71 | - |
| 47 | KC1 | 14 | 304 | 27 | - | 6/15/71/71 | - |
| 37 | CLA | 32 | 205 | - | 1/1/15/20 | 9/39/115/115 | - |
| 47 | KC1 | 31 | 303 | - | - | 2/15/71/71 | - |
| 39 | BCR | 5 | 101 | - | - | 8/29/63/63 | 0/2/2/2 |
| 37 | CLA | 38 | 206 | - | - | 6/15/91/115 | - |
| 37 | CLA | 13 | 307 | 26 | 1/1/12/20 | 12/24/100/115 | - |
| 47 | KC1 | 13 | 302 | - | - | 5/15/71/71 | - |
| 41 | LMG | 16 | 316 | - | - | 14/31/51/70 | 0/1/1/1 |
| 47 | KC1 | 35 | 302 | - | - | 6/15/71/71 | - |
| 37 | CLA | 19 | 304 | 32 | 1/1/11/20 | 6/15/91/115 | - |
| 43 | LHG | 21 | 201 | - | - | 19/38/38/53 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 37 | CLA | 14 | 308 | 52 | 1/1/15/20 | 11/39/115/115 | - |
| 48 | A86 | 31 | 311 | - | - | 6/34/90/90 | 0/3/3/3 |
| 41 | LMG | 12 | 201 | - | - | 14/34/54/70 | 0/1/1/1 |
| 37 | CLA | 39 | 303 | 52 | 1/1/15/20 | 14/39/115/115 | - |
| 48 | A86 | 32 | 221 | - | - | 9/34/90/90 | 0/3/3/3 |
| 37 | CLA | 13 | 308 | 52 | - | 8/39/115/115 | - |
| 48 | A86 | 40 | 213 | - | - | 16/34/90/90 | 0/3/3/3 |
| 37 | CLA | 32 | 202 | 52 | 1/1/15/20 | 13/39/115/115 | - |
| 47 | KC1 | 33 | 309 | 26 | - | 4/15/71/71 | - |
| 37 | CLA | 38 | 209 | 52 | 1/1/15/20 | 9/39/115/115 | - |
| 47 | KC1 | 36 | 302 | - | - | 2/15/71/71 | - |
| 41 | LMG | 17 | 317 | - | - | 15/32/52/70 | 0/1/1/1 |
| 37 | CLA | 33 | 303 | - | 1/1/13/20 | 12/30/106/115 | - |
| 45 | PL9 | D | 404 | - | - | 17/53/73/73 | 0/1/1/1 |
| 37 | CLA | C | 513 | - | 1/1/15/20 | 9/39/115/115 | - |
| 37 | CLA | 40 | 203 | 33 | - | 13/29/105/115 | - |
| 41 | LMG | l | 101 | - | - | 15/35/55/70 | 0/1/1/1 |
| 48 | A86 | 11 | 319 | - | - | 7/34/90/90 | 0/3/3/3 |
| 48 | A86 | 37 | 311 | - | - | 7/34/90/90 | 0/3/3/3 |
| 48 | A86 | 18 | 213 | - | - | 9/34/90/90 | 0/3/3/3 |
| 37 | CLA | W | 101 | - | 1/1/15/20 | 17/39/115/115 | - |
| 40 | SQD | 17 | 301 | - | - | 24/44/64/69 | 0/1/1/1 |
| 37 | CLA | 18 | 211 | - | - | 4/15/91/115 | - |
| 37 | CLA | 31 | 301 | - | 1/1/15/20 | 21/39/115/115 | - |
| 37 | CLA | b | 502 | - | 1/1/15/20 | 10/39/115/115 | - |
| 47 | KC1 | 33 | 306 | 26 | - | 6/15/71/71 | - |
| 37 | CLA | W | 102 | - | 1/1/15/20 | 21/39/115/115 | - |
| 43 | LHG | 37 | 321 | - | - | 27/49/49/53 | - |
| 48 | A86 | 20 | 309 | - | - | 5/34/90/90 | 0/3/3/3 |
| 37 | CLA | 18 | 204 | - | 1/1/13/20 | 10/29/105/115 | - |
| 48 | A86 | 38 | 215 | - | - | 13/34/90/90 | 0/3/3/3 |
| 37 | CLA | B | 505 | - | 1/1/15/20 | 6/39/115/115 | - |
| 47 | KC1 | 31 | 309 | 24 | - | 8/15/71/71 | - |
| 47 | KC1 | 40 | 206 | 33 | - | 6/15/71/71 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 44 | DGD | h | 102 | - | - | 16/51/91/95 | 0/2/2/2 |
| 37 | CLA | 12 | 210 | 52 | - | 9/39/115/115 | - |
| 37 | CLA | 41 | 206 | 34 | 1/1/15/20 | 15/39/115/115 | - |
| 37 | CLA | 31 | 304 | - | 1/1/15/20 | 10/39/115/115 | - |
| 37 | CLA | 21 | 209 | 34 | 1/1/11/20 | 6/15/91/115 | - |
| 48 | A86 | 14 | 315 | - | - | 6/34/90/90 | 0/3/3/3 |
| 48 | A86 | 31 | 319 | - | - | 7/34/90/90 | 0/3/3/3 |
| 37 | CLA | 38 | 204 | - | 1/1/13/20 | 8/29/105/115 | - |
| 37 | CLA | 39 | 306 | 32 | - | 8/39/115/115 | - |
| 43 | LHG | a | 412 | - | - | 26/50/50/53 | - |
| 37 | CLA | c | 505 | - | 1/1/15/20 | 10/39/115/115 | - |
| 37 | CLA | B | 508 | - | - | 5/39/115/115 | - |
| 48 | A86 | 17 | 314 | - | - | 8/34/90/90 | 0/3/3/3 |
| 48 | A86 | 13 | 315 | - | - | 11/34/90/90 | 0/3/3/3 |
| 43 | LHG | d | 407 | - | - | 27/53/53/53 | - |
| 37 | CLA | B | 504 | - | 1/1/15/20 | 5/39/115/115 | - |
| 48 | A86 | 14 | 311 | - | - | 7/34/90/90 | 0/3/3/3 |
| 37 | CLA | 12 | 209 | 25 | 1/1/12/20 | 13/24/100/115 | - |
| 48 | A86 | 35 | 315 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | 15 | 310 | - | 1/1/11/20 | 4/15/91/115 | - |
| 37 | CLA | 20 | 307 | 33 | 1/1/11/20 | 8/15/91/115 | - |
| 37 | CLA | 16 | 303 | - | 1/1/13/20 | 10/30/106/115 | - |
| 48 | A86 | 40 | 201 | - | - | 13/34/90/90 | 0/3/3/3 |
| 37 | CLA | A | 405 | - | - | 8/39/115/115 | - |
| 40 | SQD | L | 101 | - | - | 26/49/69/69 | 0/1/1/1 |
| 41 | LMG | a | 410 | - | - | 32/46/66/70 | 0/1/1/1 |
| 47 | KC1 | 14 | 306 | 27 | - | 6/15/71/71 | - |
| 47 | KC1 | 16 | 308 | 29 | - | 4/15/71/71 | - |
| 37 | CLA | 16 | 301 | 29 | - | 11/39/115/115 | - |
| 37 | CLA | 36 | 307 | 52 | 1/1/14/20 | 13/35/111/115 | - |
| 41 | LMG | c | 518 | - | - | 25/46/66/70 | 0/1/1/1 |
| 45 | PL9 | d | 406 | - | - | 9/53/73/73 | 0/1/1/1 |
| 48 | A86 | 31 | 313 | - | - | 6/34/90/90 | 1/3/3/3 |
| 48 | A86 | 13 | 312 | - | - | 8/34/90/90 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 48 | A86 | 35 | 319 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | B | 506 | - | 1/1/15/20 | 7/39/115/115 | - |
| 37 | CLA | 21 | 204 | - | - | 12/31/107/115 | - |
| 47 | KC1 | 11 | 302 | - | - | 2/15/71/71 | - |
| 48 | A86 | 35 | 314 | - | - | 14/34/90/90 | 0/3/3/3 |
| 37 | CLA | c | 507 | 52 | 1/1/15/20 | 8/39/115/115 | - |
| 47 | KC1 | 40 | 207 | 33 | - | 12/15/71/71 | - |
| 37 | CLA | 18 | 209 | 52 | 1/1/15/20 | 10/39/115/115 | - |
| 37 | CLA | 13 | 305 | - | 1/1/11/20 | 4/15/91/115 | - |
| 48 | A86 | 12 | 220 | - | - | 9/34/90/90 | 0/3/3/3 |
| 37 | CLA | 15 | 305 | - | 1/1/11/20 | 5/15/91/115 | - |
| 48 | A86 | 37 | 314 | - | - | 12/34/90/90 | 0/3/3/3 |
| 38 | PHO | a | 405 | - | - | 9/37/103/103 | 0/5/6/6 |
| 47 | KC1 | 37 | 302 | - | - | 6/15/71/71 | - |
| 43 | LHG | D | 409 | - | - | 27/53/53/53 | - |
| 50 | DD6 | 21 | 216 | - | - | 15/26/80/80 | 0/3/3/3 |
| 37 | CLA | 20 | 301 | 33 | - | 13/29/105/115 | - |
| 37 | CLA | 39 | 309 | 32 | 1/1/11/20 | 5/15/91/115 | - |
| 39 | BCR | b | 517 | - | - | 6/29/63/63 | 0/2/2/2 |
| 50 | DD6 | 36 | 312 | - | - | 12/26/80/80 | 0/3/3/3 |
| 38 | PHO | a | 406 | - | - | 6/37/103/103 | 0/5/6/6 |
| 37 | CLA | 11 | 310 | 52 | 1/1/12/20 | 6/23/99/115 | - |
| 47 | KC1 | 17 | 306 | 30 | - | 8/15/71/71 | - |
| 41 | LMG | 31 | 317 | - | - | 13/27/47/70 | 0/1/1/1 |
| 48 | A86 | 20 | 311 | - | - | 16/34/90/90 | 0/3/3/3 |
| 48 | A86 | 38 | 212 | - | - | 8/34/90/90 | 0/3/3/3 |
| 43 | LHG | 17 | 316 | - | - | 26/48/48/53 | - |
| 37 | CLA | 19 | 310 | 32 | 1/1/15/20 | 9/39/115/115 | - |
| 48 | A86 | 35 | 312 | - | - | 8/34/90/90 | 0/3/3/3 |
| 47 | KC1 | 15 | 306 | 28 | - | 6/15/71/71 | - |
| 40 | SQD | A | 407 | - | - | 17/49/69/69 | 0/1/1/1 |
| 48 | A86 | 40 | 211 | - | - | 5/34/90/90 | 0/3/3/3 |
| 39 | BCR | A | 410 | - | - | 7/29/63/63 | 0/2/2/2 |
| 50 | DD6 | 39 | 312 | - | - | 12/26/80/80 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 37 | CLA | 17 | 304 | - | 1/1/13/20 | 8/29/105/115 | - |
| 37 | CLA | 38 | 202 | 31 | - | 14/39/115/115 | - |
| 44 | DGD | C | 517 | - | - | 19/51/91/95 | 0/2/2/2 |
| 48 | A86 | 18 | 215 | - | - | 13/34/90/90 | 0/3/3/3 |
| 37 | CLA | 12 | 207 | 52 | 1/1/12/20 | 2/21/97/115 | - |
| 45 | PL9 | d | 402 | - | - | 17/53/73/73 | 0/1/1/1 |
| 44 | DGD | j | 101 | - | - | 16/51/91/95 | 0/2/2/2 |
| 47 | KC1 | 18 | 207 | 31 | - | 6/15/71/71 | - |
| 48 | A86 | 38 | 214 | - | - | 12/34/90/90 | 0/3/3/3 |
| 37 | CLA | c | 501 | - | 1/1/15/20 | 12/39/115/115 | - |
| 47 | KC1 | 32 | 212 | 25 | - | 6/15/71/71 | - |
| 48 | A86 | 37 | 312 | - | - | 7/34/90/90 | 0/3/3/3 |
| 37 | CLA | 15 | 301 | 28 | - | 10/39/115/115 | - |
| 48 | A86 | 38 | 213 | - | - | 9/34/90/90 | 0/3/3/3 |
| 47 | KC1 | 16 | 302 | - | - | 2/15/71/71 | - |
| 37 | CLA | 21 | 210 | - | - | 6/15/91/115 | - |
| 37 | CLA | b | 507 | 52 | 1/1/15/20 | 9/39/115/115 | - |
| 37 | CLA | a | 407 | - | - | 8/39/115/115 | - |
| 47 | KC1 | 37 | 307 | 30 | - | 4/15/71/71 | - |
| 37 | CLA | A | 403 | - | 1/1/15/20 | 4/39/115/115 | - |
| 48 | A86 | 32 | 217 | - | - | 9/34/90/90 | 0/3/3/3 |
| 48 | A86 | 15 | 313 | - | - | 9/34/90/90 | 0/3/3/3 |
| 37 | CLA | D | 401 | 52 | 1/1/15/20 | 6/39/115/115 | - |
| 47 | KC1 | 14 | 309 | 27 | - | 6/15/71/71 | - |
| 37 | CLA | 41 | 208 | - | 1/1/15/20 | 13/39/115/115 | - |
| 46 | HEM | V | 201 | 16 | - | 6/14/54/54 | - |
| 39 | BCR | A | 406 | - | - | 8/29/63/63 | 0/2/2/2 |
| 47 | KC1 | 33 | 304 | 26 | - | 7/15/71/71 | - |
| 48 | A86 | 14 | 314 | - | - | 13/34/90/90 | 0/3/3/3 |
| 47 | KC1 | 34 | 304 | 27 | - | 6/15/71/71 | - |
| 48 | A86 | 33 | 315 | - | - | 11/34/90/90 | 0/3/3/3 |
| 37 | CLA | B | 502 | - | 1/1/15/20 | 10/39/115/115 | - |
| 37 | CLA | b | 512 | - | 1/1/15/20 | 8/39/115/115 | - |
| 37 | CLA | 36 | 303 | - | 1/1/13/20 | 10/30/106/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 41 | LMG | b | 520 | - | - | 24/46/66/70 | 0/1/1/1 |
| 48 | A86 | 32 | 203 | - | - | 14/34/90/90 | 0/3/3/3 |
| 37 | CLA | a | 404 | 52 | 1/1/15/20 | 6/39/115/115 | - |
| 37 | CLA | 11 | 303 | - | 1/1/15/20 | 10/39/115/115 | - |
| 47 | KC1 | 21 | 207 | 34 | - | 7/15/71/71 | - |
| 47 | KC1 | 36 | 308 | 29 | - | 4/15/71/71 | - |
| 47 | KC1 | 21 | 203 | - | - | 4/15/71/71 | - |
| 41 | LMG | B | 521 | - | - | 24/46/66/70 | 0/1/1/1 |
| 47 | KC1 | 12 | 206 | 25 | - | 6/15/71/71 | - |
| 40 | SQD | 36 | 315 | - | - | 24/44/64/69 | 0/1/1/1 |
| 48 | A86 | 33 | 311 | - | - | 5/34/90/90 | 0/3/3/3 |
| 48 | A86 | 33 | 313 | - | - | 18/34/90/90 | 0/3/3/3 |
| 48 | A86 | 34 | 311 | - | - | 7/34/90/90 | 0/3/3/3 |
| 47 | KC1 | 16 | 304 | 29 | - | 6/15/71/71 | - |
| 47 | KC1 | 18 | 205 | 31 | - | 6/15/71/71 | - |
| 48 | A86 | 16 | 310 | - | - | 5/34/90/90 | 0/3/3/3 |
| 47 | KC1 | 34 | 306 | 27 | - | 6/15/71/71 | - |
| 37 | CLA | 39 | 305 | 32 | 1/1/12/20 | 7/23/99/115 | - |
| 37 | CLA | 39 | 307 | 43 | 1/1/15/20 | 8/39/115/115 | - |
| 47 | KC1 | 17 | 308 | 30 | - | 4/15/71/71 | - |
| 37 | CLA | 38 | 211 | - | - | 4/15/91/115 | - |
| 47 | KC1 | 11 | 304 | 24 | - | 4/15/71/71 | - |
| 37 | CLA | B | 515 | - | 1/1/15/20 | 5/39/115/115 | - |
| 37 | CLA | 39 | 301 | 32 | 1/1/15/20 | 10/39/115/115 | - |
| 50 | DD6 | 41 | 216 | - | - | 15/26/80/80 | 0/3/3/3 |
| 37 | CLA | b | 513 | - | 1/1/15/20 | 8/39/115/115 | - |
| 47 | KC1 | 20 | 305 | 33 | - | 12/15/71/71 | - |
| 37 | CLA | 38 | 203 | - | 1/1/15/20 | 8/39/115/115 | - |
| 37 | CLA | C | 505 | - | 1/1/15/20 | 10/39/115/115 | - |
| 37 | CLA | B | 516 | - | 1/1/15/20 | 13/39/115/115 | - |
| 44 | DGD | H | 102 | - | - | 16/51/91/95 | 0/2/2/2 |
| 48 | A86 | 17 | 320 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | 18 | 206 | - | 1/1/11/20 | 5/15/91/115 | - |
| 37 | CLA | D | 406 | - | 1/1/15/20 | 19/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 47 | KC1 | 16 | 305 | 29 | - | 6/15/71/71 | - |
| 50 | DD6 | 19 | 312 | - | - | 12/26/80/80 | 0/3/3/3 |
| 39 | BCR | B | 518 | - | - | 6/29/63/63 | 0/2/2/2 |
| 48 | A86 | 31 | 315 | - | - | 6/34/90/90 | 0/3/3/3 |
| 47 | KC1 | 31 | 305 | 24 | - | 4/15/71/71 | - |
| 48 | A86 | 14 | 312 | - | - | 4/34/90/90 | 0/3/3/3 |
| 37 | CLA | 18 | 203 | - | 1/1/15/20 | 8/39/115/115 | - |
| 37 | CLA | 33 | 301 | 26 | - | 14/39/115/115 | - |
| 39 | BCR | d | 405 | - | - | 12/29/63/63 | 0/2/2/2 |
| 37 | CLA | D | 402 | 52 | - | 14/39/115/115 | - |
| 48 | A86 | 11 | 311 | - | - | 6/34/90/90 | 0/3/3/3 |
| 47 | KC1 | 20 | 304 | 33 | - | 6/15/71/71 | - |
| 48 | A86 | 12 | 215 | - | - | 13/34/90/90 | 0/3/3/3 |
| 40 | SQD | B | 522 | - | - | 11/32/52/69 | 0/1/1/1 |
| 37 | CLA | 13 | 301 | 26 | - | 14/39/115/115 | - |
| 37 | CLA | 35 | 308 | 52 | - | 10/39/115/115 | - |
| 37 | CLA | 40 | 208 | 33 | 1/1/12/20 | 5/21/97/115 | - |
| 37 | CLA | 18 | 201 | 52 | 1/1/15/20 | 7/39/115/115 | - |
| 37 | CLA | b | 516 | - | 1/1/15/20 | 13/39/115/115 | - |
| 41 | LMG | B | 520 | - | - | 15/46/66/70 | 0/1/1/1 |
| 47 | KC1 | 39 | 308 | - | - | 4/15/71/71 | - |
| 47 | KC1 | 38 | 207 | 31 | - | 5/15/71/71 | - |
| 37 | CLA | 33 | 305 | - | 1/1/11/20 | 4/15/91/115 | - |
| 48 | A86 | 31 | 312 | - | - | 6/34/90/90 | 0/3/3/3 |
| 48 | A86 | 32 | 215 | - | - | 3/34/90/90 | 0/3/3/3 |
| 48 | A86 | 16 | 314 | - | - | 8/34/90/90 | 0/3/3/3 |
| 43 | LHG | d | 408 | - | - | 26/53/53/53 | - |
| 41 | LMG | D | 412 | - | - | 13/46/66/70 | 0/1/1/1 |
| 39 | BCR | C | 519 | - | - | 6/29/63/63 | 0/2/2/2 |
| 41 | LMG | A | 408 | - | - | 32/46/66/70 | 0/1/1/1 |
| 48 | A86 | 31 | 314 | - | - | 9/34/90/90 | 0/3/3/3 |
| 48 | A86 | 39 | 311 | - | - | 6/34/90/90 | 0/3/3/3 |
| 48 | A86 | 39 | 313 | - | - | 7/34/90/90 | 0/3/3/3 |
| 48 | A86 | 11 | 314 | - | - | 9/34/90/90 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 37 | CLA | 41 | 204 | - | - | 12/31/107/115 | - |
| 37 | CLA | b | 523 | - | 1/1/15/20 | 13/39/115/115 | - |
| 39 | BCR | c | 514 | - | - | 6/29/63/63 | 0/2/2/2 |
| 37 | CLA | 37 | 301 | 30 | - | 12/39/115/115 | - |
| 37 | CLA | 34 | 307 | 27 | 1/1/12/20 | 15/24/100/115 | - |
| 47 | KC1 | 36 | 304 | 29 | - | 6/15/71/71 | - |
| 37 | CLA | b | 501 | 52 | 1/1/15/20 | 17/39/115/115 | - |
| 37 | CLA | B | 507 | 52 | 1/1/15/20 | 9/39/115/115 | - |
| 48 | A86 | 13 | 314 | - | - | 9/34/90/90 | 0/3/3/3 |
| 37 | CLA | a | 403 | - | 1/1/15/20 | 4/39/115/115 | - |
| 47 | KC1 | 19 | 308 | - | - | 4/15/71/71 | - |
| 48 | A86 | 15 | 314 | - | - | 14/34/90/90 | 0/3/3/3 |
| 37 | CLA | d | 404 | - | 1/1/15/20 | 19/39/115/115 | - |
| 48 | A86 | 17 | 310 | - | - | 8/34/90/90 | 0/3/3/3 |
| 37 | CLA | 16 | 309 | - | 1/1/11/20 | 6/15/91/115 | - |
| 37 | CLA | 32 | 213 | - | 1/1/11/20 | 7/15/91/115 | - |
| 39 | BCR | K | 101 | - | - | 15/29/63/63 | 0/2/2/2 |
| 37 | CLA | 39 | 302 | - | 1/1/15/20 | 11/39/115/115 | - |
| 37 | CLA | C | 502 | - | 1/1/15/20 | 9/39/115/115 | - |
| 39 | BCR | a | 408 | - | - | 8/29/63/63 | 0/2/2/2 |
| 37 | CLA | 36 | 306 | 29 | 1/1/15/20 | 13/39/115/115 | - |
| 37 | CLA | 35 | 310 | - | 1/1/11/20 | 4/15/91/115 | - |
| 39 | BCR | 0 | 101 | - | - | 8/29/63/63 | 0/2/2/2 |

All (8997) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 40 | 213 | A86 | C14-C13 | 16.10 | 1.69 | 1.51 |
| 48 | 39 | 313 | A86 | C14-C13 | 16.10 | 1.69 | 1.51 |
| 48 | 20 | 311 | A86 | C14-C13 | 16.10 | 1.69 | 1.51 |
| 48 | 35 | 319 | A86 | C14-C13 | 15.94 | 1.69 | 1.51 |
| 48 | 15 | 319 | A86 | C14-C13 | 15.94 | 1.69 | 1.51 |
| 48 | 40 | 211 | A86 | C14-C13 | 15.82 | 1.68 | 1.51 |
| 48 | 20 | 309 | A86 | C14-C13 | 15.80 | 1.68 | 1.51 |
| 48 | 19 | 313 | A86 | C14-C13 | 15.79 | 1.68 | 1.51 |
| 48 | 41 | 214 | A86 | C14-C13 | 15.79 | 1.68 | 1.51 |
| 48 | 21 | 211 | A86 | C14-C13 | 15.78 | 1.68 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 41 | 211 | A86 | C14-C13 | 15.77 | 1.68 | 1.51 |
| 48 | 21 | 214 | A86 | C14-C13 | 15.76 | 1.68 | 1.51 |
| 48 | 37 | 312 | A86 | C14-C13 | 15.73 | 1.68 | 1.51 |
| 48 | 18 | 214 | A86 | C14-C13 | 15.69 | 1.68 | 1.51 |
| 48 | 38 | 214 | A86 | C14-C13 | 15.68 | 1.68 | 1.51 |
| 48 | 35 | 314 | A86 | C14-C13 | 15.66 | 1.68 | 1.51 |
| 48 | 15 | 314 | A86 | C14-C13 | 15.65 | 1.68 | 1.51 |
| 48 | 41 | 213 | A86 | C14-C13 | 15.64 | 1.68 | 1.51 |
| 48 | 17 | 313 | A86 | C14-C13 | 15.63 | 1.68 | 1.51 |
| 48 | 21 | 213 | A86 | C14-C13 | 15.62 | 1.68 | 1.51 |
| 48 | 14 | 314 | A86 | C14-C13 | 15.60 | 1.68 | 1.51 |
| 48 | 34 | 314 | A86 | C14-C13 | 15.60 | 1.68 | 1.51 |
| 48 | 32 | 221 | A86 | C14-C13 | 15.42 | 1.68 | 1.51 |
| 48 | 17 | 310 | A86 | C14-C13 | 15.40 | 1.68 | 1.51 |
| 48 | 13 | 314 | A86 | C14-C13 | 15.40 | 1.68 | 1.51 |
| 48 | 15 | 315 | A86 | C14-C13 | 15.39 | 1.68 | 1.51 |
| 48 | 37 | 309 | A86 | C14-C13 | 15.38 | 1.68 | 1.51 |
| 48 | 37 | 319 | A86 | C14-C13 | 15.38 | 1.68 | 1.51 |
| 48 | 34 | 312 | A86 | C14-C13 | 15.38 | 1.68 | 1.51 |
| 48 | 14 | 312 | A86 | C14-C13 | 15.36 | 1.68 | 1.51 |
| 48 | 12 | 220 | A86 | C14-C13 | 15.35 | 1.68 | 1.51 |
| 48 | 15 | 311 | A86 | C14-C13 | 15.33 | 1.68 | 1.51 |
| 48 | 35 | 311 | A86 | C14-C13 | 15.33 | 1.68 | 1.51 |
| 48 | 13 | 315 | A86 | C14-C13 | 15.31 | 1.68 | 1.51 |
| 48 | 33 | 315 | A86 | C14-C13 | 15.31 | 1.68 | 1.51 |
| 48 | 33 | 314 | A86 | C14-C13 | 15.30 | 1.68 | 1.51 |
| 48 | 17 | 320 | A86 | C14-C13 | 15.30 | 1.68 | 1.51 |
| 48 | 12 | 216 | A86 | C14-C13 | 15.28 | 1.68 | 1.51 |
| 48 | 35 | 315 | A86 | C14-C13 | 15.28 | 1.68 | 1.51 |
| 48 | 32 | 217 | A86 | C14-C13 | 15.27 | 1.68 | 1.51 |
| 48 | 36 | 311 | A86 | C14-C13 | 15.25 | 1.68 | 1.51 |
| 48 | 19 | 311 | A86 | C14-C13 | 15.22 | 1.68 | 1.51 |
| 48 | 39 | 311 | A86 | C14-C13 | 15.22 | 1.68 | 1.51 |
| 48 | 15 | 316 | A86 | C14-C13 | 15.21 | 1.68 | 1.51 |
| 48 | 16 | 311 | A86 | C14-C13 | 15.20 | 1.68 | 1.51 |
| 48 | 38 | 213 | A86 | C14-C13 | 15.16 | 1.68 | 1.51 |
| 48 | 14 | 315 | A86 | C14-C13 | 15.15 | 1.68 | 1.51 |
| 48 | 33 | 312 | A86 | C14-C13 | 15.15 | 1.68 | 1.51 |
| 48 | 34 | 315 | A86 | C14-C13 | 15.14 | 1.68 | 1.51 |
| 48 | 34 | 311 | A86 | C14-C13 | 15.13 | 1.68 | 1.51 |
| 48 | 37 | 310 | A86 | C14-C13 | 15.12 | 1.68 | 1.51 |
| 48 | 17 | 312 | A86 | C14-C13 | 15.10 | 1.68 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 14 | 311 | A86 | C14-C13 | 15.10 | 1.68 | 1.51 |
| 48 | 37 | 311 | A86 | C14-C13 | 15.10 | 1.68 | 1.51 |
| 48 | 13 | 313 | A86 | C14-C13 | 15.09 | 1.68 | 1.51 |
| 48 | 13 | 311 | A86 | C14-C13 | 15.06 | 1.68 | 1.51 |
| 48 | 35 | 316 | A86 | C14-C13 | 15.06 | 1.68 | 1.51 |
| 48 | 33 | 313 | A86 | C14-C13 | 15.05 | 1.68 | 1.51 |
| 48 | 13 | 312 | A86 | C14-C13 | 15.04 | 1.68 | 1.51 |
| 48 | 38 | 212 | A86 | C14-C13 | 15.02 | 1.68 | 1.51 |
| 48 | 32 | 218 | A86 | C14-C13 | 15.01 | 1.68 | 1.51 |
| 48 | 15 | 312 | A86 | C14-C13 | 15.01 | 1.68 | 1.51 |
| 48 | 32 | 214 | A86 | C14-C13 | 14.99 | 1.68 | 1.51 |
| 48 | 18 | 213 | A86 | C14-C13 | 14.98 | 1.68 | 1.51 |
| 48 | 33 | 311 | A86 | C14-C13 | 14.98 | 1.67 | 1.51 |
| 48 | 35 | 312 | A86 | C14-C13 | 14.98 | 1.67 | 1.51 |
| 48 | 31 | 314 | A86 | C14-C13 | 14.98 | 1.67 | 1.51 |
| 48 | 36 | 310 | A86 | C14-C13 | 14.98 | 1.67 | 1.51 |
| 48 | 12 | 217 | A86 | C14-C13 | 14.97 | 1.67 | 1.51 |
| 48 | 17 | 311 | A86 | C14-C13 | 14.95 | 1.67 | 1.51 |
| 48 | 37 | 313 | A86 | C14-C13 | 14.95 | 1.67 | 1.51 |
| 48 | 14 | 316 | A86 | C14-C13 | 14.94 | 1.67 | 1.51 |
| 48 | 34 | 313 | A86 | C14-C13 | 14.94 | 1.67 | 1.51 |
| 48 | 34 | 316 | A86 | C14-C13 | 14.93 | 1.67 | 1.51 |
| 48 | 11 | 314 | A86 | C14-C13 | 14.92 | 1.67 | 1.51 |
| 48 | 11 | 315 | A86 | C14-C13 | 14.91 | 1.67 | 1.51 |
| 48 | 32 | 203 | A86 | C14-C13 | 14.90 | 1.67 | 1.51 |
| 48 | 17 | 315 | A86 | C14-C13 | 14.90 | 1.67 | 1.51 |
| 48 | 16 | 310 | A86 | C14-C13 | 14.90 | 1.67 | 1.51 |
| 48 | 17 | 314 | A86 | C14-C13 | 14.90 | 1.67 | 1.51 |
| 48 | 14 | 313 | A86 | C14-C13 | 14.89 | 1.67 | 1.51 |
| 48 | 12 | 213 | A86 | C14-C13 | 14.87 | 1.67 | 1.51 |
| 48 | 18 | 212 | A86 | C14-C13 | 14.87 | 1.67 | 1.51 |
| 48 | 37 | 314 | A86 | C14-C13 | 14.86 | 1.67 | 1.51 |
| 48 | 31 | 315 | A86 | C14-C13 | 14.86 | 1.67 | 1.51 |
| 48 | 40 | 201 | A86 | C14-C13 | 14.84 | 1.67 | 1.51 |
| 48 | 12 | 215 | A86 | C14-C13 | 14.82 | 1.67 | 1.51 |
| 48 | 32 | 216 | A86 | C14-C13 | 14.82 | 1.67 | 1.51 |
| 48 | 12 | 202 | A86 | C14-C13 | 14.82 | 1.67 | 1.51 |
| 48 | 16 | 313 | A86 | C14-C13 | 14.81 | 1.67 | 1.51 |
| 48 | 38 | 215 | A86 | C14-C13 | 14.78 | 1.67 | 1.51 |
| 50 | 20 | 312 | DD6 | C10-C11 | 14.77 | 1.70 | 1.35 |
| 48 | 11 | 319 | A86 | C14-C13 | 14.74 | 1.67 | 1.51 |
| 50 | 40 | 214 | DD6 | C10-C11 | 14.72 | 1.69 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 31 | 319 | A86 | C14-C13 | 14.66 | 1.67 | 1.51 |
| 48 | 31 | 312 | A86 | C14-C13 | 14.66 | 1.67 | 1.51 |
| 50 | 41 | 212 | DD6 | C10-C11 | 14.63 | 1.69 | 1.35 |
| 48 | 18 | 215 | A86 | C14-C13 | 14.61 | 1.67 | 1.51 |
| 48 | 11 | 312 | A86 | C14-C13 | 14.61 | 1.67 | 1.51 |
| 50 | 39 | 312 | DD6 | C10-C11 | 14.61 | 1.69 | 1.35 |
| 50 | 41 | 216 | DD6 | C10-C11 | 14.61 | 1.69 | 1.35 |
| 50 | 19 | 312 | DD6 | C10-C11 | 14.59 | 1.69 | 1.35 |
| 50 | 21 | 212 | DD6 | C10-C11 | 14.59 | 1.69 | 1.35 |
| 50 | 21 | 216 | DD6 | C10-C11 | 14.56 | 1.69 | 1.35 |
| 50 | 20 | 310 | DD6 | C10-C11 | 14.55 | 1.69 | 1.35 |
| 50 | 40 | 212 | DD6 | C10-C11 | 14.52 | 1.69 | 1.35 |
| 50 | 20 | 312 | DD6 | C36-C31 | 14.50 | 1.51 | 1.35 |
| 48 | 11 | 311 | A86 | C14-C13 | 14.50 | 1.67 | 1.51 |
| 50 | 40 | 214 | DD6 | C36-C31 | 14.48 | 1.51 | 1.35 |
| 48 | 31 | 311 | A86 | C14-C13 | 14.44 | 1.67 | 1.51 |
| 48 | 35 | 313 | A86 | C14-C13 | 14.44 | 1.67 | 1.51 |
| 48 | 15 | 313 | A86 | C14-C13 | 14.40 | 1.67 | 1.51 |
| 50 | 16 | 312 | DD6 | C10-C11 | 14.35 | 1.69 | 1.35 |
| 50 | 36 | 312 | DD6 | C10-C11 | 14.32 | 1.68 | 1.35 |
| 48 | 32 | 215 | A86 | C14-C13 | 14.31 | 1.67 | 1.51 |
| 48 | 12 | 214 | A86 | C14-C13 | 14.31 | 1.67 | 1.51 |
| 48 | 36 | 313 | A86 | C14-C13 | 14.25 | 1.67 | 1.51 |
| 48 | 16 | 314 | A86 | C14-C13 | 14.24 | 1.67 | 1.51 |
| 48 | 31 | 313 | A86 | C14-C13 | 14.17 | 1.67 | 1.51 |
| 48 | 11 | 313 | A86 | C14-C13 | 14.13 | 1.67 | 1.51 |
| 50 | 16 | 312 | DD6 | C36-C31 | 14.07 | 1.50 | 1.35 |
| 50 | 36 | 312 | DD6 | C36-C31 | 14.00 | 1.50 | 1.35 |
| 50 | 21 | 212 | DD6 | C36-C31 | 13.76 | 1.50 | 1.35 |
| 50 | 41 | 212 | DD6 | C36-C31 | 13.72 | 1.50 | 1.35 |
| 50 | 20 | 310 | DD6 | C36-C31 | 13.66 | 1.50 | 1.35 |
| 50 | 40 | 212 | DD6 | C36-C31 | 13.63 | 1.50 | 1.35 |
| 50 | 41 | 216 | DD6 | C36-C31 | 13.50 | 1.50 | 1.35 |
| 50 | 21 | 216 | DD6 | C36-C31 | 13.47 | 1.49 | 1.35 |
| 48 | 41 | 215 | A86 | C14-C13 | 13.07 | 1.65 | 1.51 |
| 48 | 21 | 215 | A86 | C14-C13 | 13.06 | 1.65 | 1.51 |
| 50 | 39 | 312 | DD6 | C36-C31 | 12.74 | 1.49 | 1.35 |
| 50 | 19 | 312 | DD6 | C36-C31 | 12.74 | 1.49 | 1.35 |
| 48 | 16 | 313 | A86 | C30-C31 | 12.12 | 1.44 | 1.30 |
| 48 | 40 | 201 | A86 | C30-C31 | 12.12 | 1.44 | 1.30 |
| 48 | 41 | 213 | A86 | C30-C31 | 11.96 | 1.44 | 1.30 |
| 48 | 21 | 213 | A86 | C30-C31 | 11.92 | 1.44 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 15 | 313 | A86 | C30-C31 | 11.85 | 1.44 | 1.30 |
| 48 | 15 | 314 | A86 | C30-C31 | 11.82 | 1.44 | 1.30 |
| 48 | 12 | 215 | A86 | C30-C31 | 11.82 | 1.44 | 1.30 |
| 48 | 35 | 313 | A86 | C30-C31 | 11.77 | 1.44 | 1.30 |
| 48 | 35 | 314 | A86 | C30-C31 | 11.75 | 1.44 | 1.30 |
| 48 | 32 | 216 | A86 | C30-C31 | 11.74 | 1.44 | 1.30 |
| 48 | 13 | 313 | A86 | C30-C31 | 11.73 | 1.44 | 1.30 |
| 48 | 33 | 312 | A86 | C30-C31 | 11.72 | 1.44 | 1.30 |
| 48 | 33 | 313 | A86 | C30-C31 | 11.70 | 1.44 | 1.30 |
| 48 | 13 | 312 | A86 | C30-C31 | 11.69 | 1.44 | 1.30 |
| 48 | 21 | 215 | A86 | C30-C31 | 11.67 | 1.44 | 1.30 |
| 50 | 36 | 312 | DD6 | C28-C27 | 11.67 | 1.58 | 1.50 |
| 48 | 41 | 215 | A86 | C30-C31 | 11.64 | 1.44 | 1.30 |
| 50 | 16 | 312 | DD6 | C28-C27 | 11.62 | 1.58 | 1.50 |
| 48 | 38 | 215 | A86 | C30-C31 | 11.53 | 1.44 | 1.30 |
| 48 | 34 | 313 | A86 | C30-C31 | 11.52 | 1.44 | 1.30 |
| 48 | 13 | 314 | A86 | C30-C31 | 11.51 | 1.44 | 1.30 |
| 48 | 18 | 215 | A86 | C30-C31 | 11.49 | 1.44 | 1.30 |
| 48 | 33 | 314 | A86 | C30-C31 | 11.49 | 1.44 | 1.30 |
| 48 | 14 | 313 | A86 | C30-C31 | 11.48 | 1.44 | 1.30 |
| 48 | 41 | 214 | A86 | C30-C31 | 11.45 | 1.43 | 1.30 |
| 48 | 21 | 214 | A86 | C30-C31 | 11.40 | 1.43 | 1.30 |
| 48 | 38 | 214 | A86 | C30-C31 | 11.40 | 1.43 | 1.30 |
| 48 | 18 | 214 | A86 | C30-C31 | 11.34 | 1.43 | 1.30 |
| 48 | 14 | 314 | A86 | C30-C31 | 11.24 | 1.43 | 1.30 |
| 48 | 34 | 314 | A86 | C30-C31 | 11.24 | 1.43 | 1.30 |
| 48 | 18 | 212 | A86 | C30-C31 | 11.21 | 1.43 | 1.30 |
| 48 | 38 | 212 | A86 | C30-C31 | 11.18 | 1.43 | 1.30 |
| 48 | 38 | 213 | A86 | C30-C31 | 11.16 | 1.43 | 1.30 |
| 48 | 15 | 312 | A86 | C30-C31 | 11.16 | 1.43 | 1.30 |
| 48 | 35 | 312 | A86 | C30-C31 | 11.14 | 1.43 | 1.30 |
| 48 | 37 | 311 | A86 | C30-C31 | 11.13 | 1.43 | 1.30 |
| 48 | 17 | 312 | A86 | C30-C31 | 11.13 | 1.43 | 1.30 |
| 48 | 21 | 211 | A86 | C30-C31 | 11.08 | 1.43 | 1.30 |
| 48 | 18 | 213 | A86 | C30-C31 | 11.08 | 1.43 | 1.30 |
| 48 | 41 | 211 | A86 | C30-C31 | 11.05 | 1.43 | 1.30 |
| 48 | 15 | 316 | A86 | C30-C31 | 11.04 | 1.43 | 1.30 |
| 48 | 33 | 315 | A86 | C30-C31 | 11.03 | 1.43 | 1.30 |
| 48 | 13 | 315 | A86 | C30-C31 | 11.03 | 1.43 | 1.30 |
| 48 | 17 | 311 | A86 | C30-C31 | 11.01 | 1.43 | 1.30 |
| 48 | 14 | 316 | A86 | C30-C31 | 11.00 | 1.43 | 1.30 |
| 48 | 34 | 316 | A86 | C30-C31 | 10.99 | 1.43 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 34 | 312 | A86 | C30-C31 | 10.96 | 1.43 | 1.30 |
| 48 | 20 | 309 | A86 | C30-C31 | 10.94 | 1.43 | 1.30 |
| 48 | 12 | 217 | A86 | C30-C31 | 10.92 | 1.43 | 1.30 |
| 48 | 32 | 218 | A86 | C30-C31 | 10.92 | 1.43 | 1.30 |
| 48 | 35 | 316 | A86 | C30-C31 | 10.92 | 1.43 | 1.30 |
| 48 | 35 | 311 | A86 | C30-C31 | 10.91 | 1.43 | 1.30 |
| 50 | 40 | 214 | DD6 | C28-C27 | 10.90 | 1.58 | 1.50 |
| 48 | 14 | 312 | A86 | C30-C31 | 10.90 | 1.43 | 1.30 |
| 48 | 37 | 309 | A86 | C30-C31 | 10.90 | 1.43 | 1.30 |
| 48 | 40 | 211 | A86 | C30-C31 | 10.90 | 1.43 | 1.30 |
| 50 | 20 | 312 | DD6 | C28-C27 | 10.89 | 1.58 | 1.50 |
| 48 | 35 | 319 | A86 | C30-C31 | 10.89 | 1.43 | 1.30 |
| 50 | 41 | 216 | DD6 | C28-C27 | 10.88 | 1.58 | 1.50 |
| 48 | 17 | 310 | A86 | C30-C31 | 10.87 | 1.43 | 1.30 |
| 48 | 15 | 319 | A86 | C30-C31 | 10.87 | 1.43 | 1.30 |
| 50 | 21 | 216 | DD6 | C28-C27 | 10.85 | 1.58 | 1.50 |
| 48 | 17 | 313 | A86 | C30-C31 | 10.84 | 1.43 | 1.30 |
| 48 | 37 | 310 | A86 | C30-C31 | 10.83 | 1.43 | 1.30 |
| 48 | 15 | 315 | A86 | C30-C31 | 10.81 | 1.43 | 1.30 |
| 48 | 35 | 315 | A86 | C30-C31 | 10.81 | 1.43 | 1.30 |
| 48 | 17 | 315 | A86 | C30-C31 | 10.81 | 1.43 | 1.30 |
| 48 | 37 | 314 | A86 | C30-C31 | 10.81 | 1.43 | 1.30 |
| 48 | 39 | 313 | A86 | C30-C31 | 10.81 | 1.43 | 1.30 |
| 50 | 40 | 212 | DD6 | C28-C27 | 10.80 | 1.58 | 1.50 |
| 48 | 14 | 311 | A86 | C30-C31 | 10.79 | 1.43 | 1.30 |
| 48 | 19 | 313 | A86 | C30-C31 | 10.76 | 1.43 | 1.30 |
| 48 | 37 | 312 | A86 | C30-C31 | 10.75 | 1.43 | 1.30 |
| 48 | 32 | 214 | A86 | C30-C31 | 10.74 | 1.43 | 1.30 |
| 50 | 20 | 310 | DD6 | C28-C27 | 10.72 | 1.58 | 1.50 |
| 48 | 12 | 213 | A86 | C30-C31 | 10.69 | 1.43 | 1.30 |
| 48 | 34 | 311 | A86 | C30-C31 | 10.68 | 1.43 | 1.30 |
| 48 | 15 | 311 | A86 | C30-C31 | 10.67 | 1.43 | 1.30 |
| 50 | 19 | 312 | DD6 | C28-C27 | 10.64 | 1.57 | 1.50 |
| 48 | 31 | 313 | A86 | C30-C31 | 10.64 | 1.43 | 1.30 |
| 48 | 17 | 320 | A86 | C30-C31 | 10.59 | 1.42 | 1.30 |
| 48 | 37 | 319 | A86 | C30-C31 | 10.56 | 1.42 | 1.30 |
| 48 | 33 | 311 | A86 | C30-C31 | 10.55 | 1.42 | 1.30 |
| 50 | 39 | 312 | DD6 | C28-C27 | 10.55 | 1.57 | 1.50 |
| 48 | 12 | 216 | A86 | C30-C31 | 10.54 | 1.42 | 1.30 |
| 48 | 32 | 217 | A86 | C30-C31 | 10.54 | 1.42 | 1.30 |
| 48 | 31 | 312 | A86 | C30-C31 | 10.54 | 1.42 | 1.30 |
| 48 | 13 | 311 | A86 | C30-C31 | 10.53 | 1.42 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 32 | 215 | A86 | C30-C31 | 10.50 | 1.42 | 1.30 |
| 48 | 11 | 314 | A86 | C30-C31 | 10.50 | 1.42 | 1.30 |
| 48 | 11 | 311 | A86 | C30-C31 | 10.49 | 1.42 | 1.30 |
| 48 | 31 | 311 | A86 | C30-C31 | 10.49 | 1.42 | 1.30 |
| 48 | 40 | 213 | A86 | C30-C31 | 10.48 | 1.42 | 1.30 |
| 48 | 20 | 311 | A86 | C30-C31 | 10.47 | 1.42 | 1.30 |
| 48 | 11 | 312 | A86 | C30-C31 | 10.45 | 1.42 | 1.30 |
| 48 | 12 | 214 | A86 | C30-C31 | 10.43 | 1.42 | 1.30 |
| 48 | 11 | 313 | A86 | C30-C31 | 10.39 | 1.42 | 1.30 |
| 48 | 31 | 314 | A86 | C30-C31 | 10.34 | 1.42 | 1.30 |
| 48 | 37 | 313 | A86 | C30-C31 | 10.25 | 1.42 | 1.30 |
| 48 | 36 | 311 | A86 | C30-C31 | 10.22 | 1.42 | 1.30 |
| 48 | 16 | 314 | A86 | C30-C31 | 10.21 | 1.42 | 1.30 |
| 48 | 16 | 311 | A86 | C30-C31 | 10.18 | 1.42 | 1.30 |
| 48 | 36 | 313 | A86 | C30-C31 | 10.16 | 1.42 | 1.30 |
| 50 | 40 | 214 | DD6 | C5-C6 | 10.11 | 1.59 | 1.35 |
| 48 | 34 | 315 | A86 | C30-C31 | 10.10 | 1.42 | 1.30 |
| 48 | 17 | 314 | A86 | C30-C31 | 10.10 | 1.42 | 1.30 |
| 50 | 20 | 312 | DD6 | C5-C6 | 10.10 | 1.59 | 1.35 |
| 48 | 11 | 315 | A86 | C30-C31 | 10.07 | 1.42 | 1.30 |
| 48 | 31 | 315 | A86 | C30-C31 | 10.07 | 1.42 | 1.30 |
| 48 | 12 | 202 | A86 | C30-C31 | 10.06 | 1.42 | 1.30 |
| 48 | 19 | 311 | A86 | C30-C31 | 10.06 | 1.42 | 1.30 |
| 48 | 14 | 315 | A86 | C30-C31 | 10.06 | 1.42 | 1.30 |
| 48 | 32 | 203 | A86 | C30-C31 | 10.04 | 1.42 | 1.30 |
| 50 | 41 | 212 | DD6 | C28-C27 | 10.04 | 1.57 | 1.50 |
| 50 | 21 | 212 | DD6 | C28-C27 | 10.04 | 1.57 | 1.50 |
| 50 | 41 | 216 | DD6 | C5-C6 | 10.03 | 1.59 | 1.35 |
| 50 | 21 | 216 | DD6 | C5-C6 | 10.02 | 1.59 | 1.35 |
| 50 | 20 | 310 | DD6 | C5-C6 | 10.01 | 1.58 | 1.35 |
| 48 | 39 | 311 | A86 | C30-C31 | 10.00 | 1.42 | 1.30 |
| 48 | 36 | 310 | A86 | C30-C31 | 9.99 | 1.42 | 1.30 |
| 48 | 16 | 310 | A86 | C30-C31 | 9.98 | 1.42 | 1.30 |
| 50 | 40 | 212 | DD6 | C5-C6 | 9.97 | 1.58 | 1.35 |
| 50 | 16 | 312 | DD6 | C5-C6 | 9.90 | 1.58 | 1.35 |
| 50 | 36 | 312 | DD6 | C5-C6 | 9.88 | 1.58 | 1.35 |
| 50 | 21 | 212 | DD6 | C5-C6 | 9.86 | 1.58 | 1.35 |
| 50 | 41 | 212 | DD6 | C5-C6 | 9.85 | 1.58 | 1.35 |
| 50 | 19 | 312 | DD6 | C5-C6 | 9.77 | 1.58 | 1.35 |
| 50 | 39 | 312 | DD6 | C5-C6 | 9.76 | 1.58 | 1.35 |
| 48 | 40 | 201 | A86 | C30-C29 | 9.74 | 1.47 | 1.31 |
| 48 | 16 | 313 | A86 | C30-C29 | 9.72 | 1.47 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 21 | 213 | A86 | C30-C29 | 9.65 | 1.47 | 1.31 |
| 48 | 12 | 220 | A86 | C30-C31 | 9.64 | 1.41 | 1.30 |
| 48 | 32 | 221 | A86 | C30-C31 | 9.64 | 1.41 | 1.30 |
| 48 | 41 | 213 | A86 | C30-C29 | 9.62 | 1.47 | 1.31 |
| 48 | 35 | 313 | A86 | C30-C29 | 9.56 | 1.47 | 1.31 |
| 48 | 13 | 312 | A86 | C30-C29 | 9.54 | 1.47 | 1.31 |
| 48 | 35 | 314 | A86 | C30-C29 | 9.54 | 1.47 | 1.31 |
| 48 | 15 | 313 | A86 | C30-C29 | 9.54 | 1.47 | 1.31 |
| 48 | 13 | 313 | A86 | C30-C29 | 9.52 | 1.47 | 1.31 |
| 48 | 15 | 314 | A86 | C30-C29 | 9.51 | 1.47 | 1.31 |
| 48 | 33 | 312 | A86 | C30-C29 | 9.50 | 1.47 | 1.31 |
| 48 | 33 | 313 | A86 | C30-C29 | 9.50 | 1.47 | 1.31 |
| 48 | 32 | 216 | A86 | C30-C29 | 9.48 | 1.47 | 1.31 |
| 48 | 11 | 319 | A86 | C30-C31 | 9.45 | 1.41 | 1.30 |
| 48 | 31 | 319 | A86 | C30-C31 | 9.45 | 1.41 | 1.30 |
| 48 | 12 | 215 | A86 | C30-C29 | 9.44 | 1.47 | 1.31 |
| 48 | 41 | 215 | A86 | C30-C29 | 9.33 | 1.47 | 1.31 |
| 48 | 34 | 313 | A86 | C30-C29 | 9.31 | 1.47 | 1.31 |
| 48 | 13 | 314 | A86 | C30-C29 | 9.31 | 1.47 | 1.31 |
| 48 | 21 | 215 | A86 | C30-C29 | 9.29 | 1.47 | 1.31 |
| 48 | 18 | 215 | A86 | C30-C29 | 9.29 | 1.47 | 1.31 |
| 48 | 14 | 313 | A86 | C30-C29 | 9.27 | 1.46 | 1.31 |
| 48 | 33 | 314 | A86 | C30-C29 | 9.27 | 1.46 | 1.31 |
| 48 | 38 | 215 | A86 | C30-C29 | 9.24 | 1.46 | 1.31 |
| 48 | 21 | 214 | A86 | C30-C29 | 9.21 | 1.46 | 1.31 |
| 48 | 34 | 314 | A86 | C30-C29 | 9.21 | 1.46 | 1.31 |
| 48 | 41 | 214 | A86 | C30-C29 | 9.20 | 1.46 | 1.31 |
| 48 | 14 | 314 | A86 | C30-C29 | 9.16 | 1.46 | 1.31 |
| 50 | 21 | 216 | DD6 | C23-C16 | 9.15 | 1.71 | 1.53 |
| 48 | 37 | 311 | A86 | C30-C29 | 9.14 | 1.46 | 1.31 |
| 48 | 17 | 312 | A86 | C30-C29 | 9.14 | 1.46 | 1.31 |
| 48 | 18 | 212 | A86 | C30-C29 | 9.12 | 1.46 | 1.31 |
| 50 | 41 | 216 | DD6 | C23-C16 | 9.11 | 1.71 | 1.53 |
| 48 | 18 | 214 | A86 | C30-C29 | 9.10 | 1.46 | 1.31 |
| 48 | 38 | 214 | A86 | C30-C29 | 9.09 | 1.46 | 1.31 |
| 48 | 38 | 212 | A86 | C30-C29 | 9.09 | 1.46 | 1.31 |
| 48 | 15 | 316 | A86 | C30-C29 | 9.08 | 1.46 | 1.31 |
| 48 | 35 | 312 | A86 | C30-C29 | 9.04 | 1.46 | 1.31 |
| 48 | 41 | 211 | A86 | C30-C29 | 9.03 | 1.46 | 1.31 |
| 48 | 38 | 213 | A86 | C30-C29 | 9.03 | 1.46 | 1.31 |
| 48 | 18 | 213 | A86 | C30-C29 | 9.01 | 1.46 | 1.31 |
| 48 | 21 | 211 | A86 | C30-C29 | 9.01 | 1.46 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 34 | 316 | A86 | C30-C29 | 9.00 | 1.46 | 1.31 |
| 48 | 13 | 315 | A86 | C30-C29 | 8.98 | 1.46 | 1.31 |
| 50 | 16 | 312 | DD6 | C13-C11 | -8.97 | 1.26 | 1.46 |
| 48 | 14 | 316 | A86 | C30-C29 | 8.96 | 1.46 | 1.31 |
| 48 | 40 | 211 | A86 | C30-C29 | 8.95 | 1.46 | 1.31 |
| 48 | 35 | 316 | A86 | C30-C29 | 8.95 | 1.46 | 1.31 |
| 48 | 37 | 309 | A86 | C30-C29 | 8.94 | 1.46 | 1.31 |
| 48 | 15 | 312 | A86 | C30-C29 | 8.94 | 1.46 | 1.31 |
| 48 | 12 | 217 | A86 | C30-C29 | 8.94 | 1.46 | 1.31 |
| 48 | 20 | 309 | A86 | C30-C29 | 8.93 | 1.46 | 1.31 |
| 50 | 36 | 312 | DD6 | C13-C11 | -8.92 | 1.26 | 1.46 |
| 48 | 33 | 315 | A86 | C30-C29 | 8.92 | 1.46 | 1.31 |
| 48 | 35 | 311 | A86 | C30-C29 | 8.91 | 1.46 | 1.31 |
| 48 | 32 | 218 | A86 | C30-C29 | 8.91 | 1.46 | 1.31 |
| 48 | 17 | 310 | A86 | C30-C29 | 8.91 | 1.46 | 1.31 |
| 48 | 35 | 315 | A86 | C30-C29 | 8.90 | 1.46 | 1.31 |
| 48 | 15 | 319 | A86 | C30-C29 | 8.89 | 1.46 | 1.31 |
| 48 | 39 | 313 | A86 | C30-C29 | 8.85 | 1.46 | 1.31 |
| 48 | 17 | 311 | A86 | C30-C29 | 8.83 | 1.46 | 1.31 |
| 48 | 35 | 319 | A86 | C30-C29 | 8.83 | 1.46 | 1.31 |
| 48 | 37 | 312 | A86 | C30-C29 | 8.83 | 1.46 | 1.31 |
| 48 | 19 | 313 | A86 | C30-C29 | 8.82 | 1.46 | 1.31 |
| 48 | 17 | 313 | A86 | C30-C29 | 8.82 | 1.46 | 1.31 |
| 48 | 17 | 315 | A86 | C30-C29 | 8.81 | 1.46 | 1.31 |
| 48 | 14 | 312 | A86 | C30-C29 | 8.81 | 1.46 | 1.31 |
| 48 | 34 | 312 | A86 | C30-C29 | 8.81 | 1.46 | 1.31 |
| 48 | 15 | 311 | A86 | C30-C29 | 8.81 | 1.46 | 1.31 |
| 48 | 12 | 216 | A86 | C30-C29 | 8.81 | 1.46 | 1.31 |
| 48 | 37 | 310 | A86 | C30-C29 | 8.80 | 1.46 | 1.31 |
| 48 | 15 | 315 | A86 | C30-C29 | 8.79 | 1.46 | 1.31 |
| 48 | 14 | 311 | A86 | C30-C29 | 8.79 | 1.46 | 1.31 |
| 48 | 34 | 311 | A86 | C30-C29 | 8.79 | 1.46 | 1.31 |
| 38 | A | 404 | PHO | C1B-C2B | 8.78 | 1.49 | 1.39 |
| 48 | 31 | 314 | A86 | C30-C29 | 8.77 | 1.46 | 1.31 |
| 48 | 37 | 314 | A86 | C30-C29 | 8.77 | 1.46 | 1.31 |
| 38 | a | 406 | PHO | C1B-C2B | 8.76 | 1.49 | 1.39 |
| 48 | 32 | 217 | A86 | C30-C29 | 8.75 | 1.46 | 1.31 |
| 48 | 31 | 313 | A86 | C30-C29 | 8.73 | 1.46 | 1.31 |
| 48 | 17 | 320 | A86 | C30-C29 | 8.73 | 1.46 | 1.31 |
| 48 | 11 | 314 | A86 | C30-C29 | 8.72 | 1.46 | 1.31 |
| 48 | 32 | 214 | A86 | C30-C29 | 8.72 | 1.46 | 1.31 |
| 48 | 12 | 214 | A86 | C30-C29 | 8.70 | 1.46 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 12 | 213 | A86 | C30-C29 | 8.69 | 1.46 | 1.31 |
| 48 | 37 | 319 | A86 | C30-C29 | 8.68 | 1.46 | 1.31 |
| 48 | 20 | 311 | A86 | C30-C29 | 8.63 | 1.45 | 1.31 |
| 48 | 13 | 311 | A86 | C30-C29 | 8.63 | 1.45 | 1.31 |
| 48 | 40 | 213 | A86 | C30-C29 | 8.62 | 1.45 | 1.31 |
| 48 | 32 | 215 | A86 | C30-C29 | 8.62 | 1.45 | 1.31 |
| 50 | 20 | 312 | DD6 | C23-C16 | 8.61 | 1.70 | 1.53 |
| 50 | 40 | 212 | DD6 | C23-C16 | 8.60 | 1.70 | 1.53 |
| 50 | 40 | 214 | DD6 | C23-C16 | 8.59 | 1.70 | 1.53 |
| 48 | 11 | 312 | A86 | C30-C29 | 8.58 | 1.45 | 1.31 |
| 48 | 33 | 311 | A86 | C30-C29 | 8.57 | 1.45 | 1.31 |
| 50 | 21 | 212 | DD6 | C13-C11 | -8.56 | 1.27 | 1.46 |
| 50 | 20 | 310 | DD6 | C23-C16 | 8.55 | 1.70 | 1.53 |
| 50 | 41 | 212 | DD6 | C13-C11 | -8.55 | 1.27 | 1.46 |
| 48 | 31 | 312 | A86 | C30-C29 | 8.55 | 1.45 | 1.31 |
| 38 | D | 403 | PHO | C1B-C2B | 8.53 | 1.48 | 1.39 |
| 48 | 37 | 313 | A86 | C30-C29 | 8.52 | 1.45 | 1.31 |
| 50 | 36 | 312 | DD6 | C23-C16 | 8.51 | 1.70 | 1.53 |
| 38 | a | 405 | PHO | C1B-C2B | 8.50 | 1.48 | 1.39 |
| 48 | 36 | 313 | A86 | C30-C29 | 8.50 | 1.45 | 1.31 |
| 48 | 31 | 311 | A86 | C30-C29 | 8.50 | 1.45 | 1.31 |
| 48 | 31 | 315 | A86 | C30-C29 | 8.50 | 1.45 | 1.31 |
| 50 | 16 | 312 | DD6 | C23-C16 | 8.49 | 1.70 | 1.53 |
| 48 | 14 | 315 | A86 | C30-C29 | 8.46 | 1.45 | 1.31 |
| 48 | 16 | 314 | A86 | C30-C29 | 8.45 | 1.45 | 1.31 |
| 48 | 11 | 311 | A86 | C30-C29 | 8.45 | 1.45 | 1.31 |
| 48 | 11 | 315 | A86 | C30-C29 | 8.44 | 1.45 | 1.31 |
| 48 | 32 | 203 | A86 | C30-C29 | 8.40 | 1.45 | 1.31 |
| 48 | 12 | 202 | A86 | C30-C29 | 8.40 | 1.45 | 1.31 |
| 48 | 17 | 314 | A86 | C30-C29 | 8.39 | 1.45 | 1.31 |
| 48 | 16 | 311 | A86 | C30-C29 | 8.39 | 1.45 | 1.31 |
| 48 | 34 | 315 | A86 | C30-C29 | 8.38 | 1.45 | 1.31 |
| 48 | 11 | 313 | A86 | C30-C29 | 8.36 | 1.45 | 1.31 |
| 48 | 36 | 311 | A86 | C30-C29 | 8.35 | 1.45 | 1.31 |
| 50 | 41 | 212 | DD6 | C23-C16 | 8.35 | 1.69 | 1.53 |
| 50 | 41 | 216 | DD6 | C13-C11 | -8.34 | 1.28 | 1.46 |
| 50 | 21 | 212 | DD6 | C23-C16 | 8.32 | 1.69 | 1.53 |
| 50 | 21 | 216 | DD6 | C13-C11 | -8.32 | 1.28 | 1.46 |
| 38 | A | 404 | PHO | C3B-C4B | 8.25 | 1.49 | 1.41 |
| 48 | 39 | 311 | A86 | C30-C29 | 8.24 | 1.45 | 1.31 |
| 48 | 19 | 311 | A86 | C30-C29 | 8.23 | 1.45 | 1.31 |
| 50 | 20 | 312 | DD6 | C13-C11 | -8.23 | 1.28 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 50 | 40 | 214 | DD6 | C13-C11 | -8.21 | 1.28 | 1.46 |
| 38 | a | 406 | PHO | C3B-C4B | 8.20 | 1.49 | 1.41 |
| 50 | 19 | 312 | DD6 | C13-C11 | -8.15 | 1.28 | 1.46 |
| 50 | 41 | 212 | DD6 | C19-C20 | 8.14 | 1.63 | 1.52 |
| 47 | 36 | 308 | KC1 | C2A-C3A | 8.13 | 1.53 | 1.37 |
| 50 | 21 | 212 | DD6 | C19-C20 | 8.12 | 1.63 | 1.52 |
| 50 | 39 | 312 | DD6 | C13-C11 | -8.12 | 1.28 | 1.46 |
| 38 | a | 405 | PHO | C3B-C4B | 8.10 | 1.49 | 1.41 |
| 38 | D | 403 | PHO | C3B-C4B | 8.09 | 1.49 | 1.41 |
| 47 | 16 | 308 | KC1 | C2A-C3A | 8.09 | 1.53 | 1.37 |
| 50 | 41 | 216 | DD6 | C19-C20 | 8.08 | 1.63 | 1.52 |
| 48 | 36 | 310 | A86 | C30-C29 | 8.07 | 1.45 | 1.31 |
| 48 | 16 | 310 | A86 | C30-C29 | 8.06 | 1.45 | 1.31 |
| 48 | 12 | 220 | A86 | C30-C29 | 8.06 | 1.45 | 1.31 |
| 48 | 32 | 221 | A86 | C30-C29 | 8.06 | 1.45 | 1.31 |
| 50 | 40 | 212 | DD6 | C13-C11 | -8.05 | 1.28 | 1.46 |
| 48 | 11 | 319 | A86 | C30-C29 | 8.03 | 1.44 | 1.31 |
| 50 | 20 | 310 | DD6 | C13-C11 | -8.03 | 1.28 | 1.46 |
| 50 | 21 | 216 | DD6 | C19-C20 | 8.02 | 1.63 | 1.52 |
| 48 | 31 | 319 | A86 | C30-C29 | 8.01 | 1.44 | 1.31 |
| 50 | 19 | 312 | DD6 | C23-C16 | 7.99 | 1.69 | 1.53 |
| 50 | 39 | 312 | DD6 | C23-C16 | 7.98 | 1.69 | 1.53 |
| 47 | 17 | 308 | KC1 | C2A-C3A | 7.98 | 1.53 | 1.37 |
| 47 | 37 | 307 | KC1 | C2A-C3A | 7.98 | 1.53 | 1.37 |
| 47 | 32 | 209 | KC1 | C2A-C3A | 7.97 | 1.53 | 1.37 |
| 47 | 36 | 302 | KC1 | C2A-C3A | 7.95 | 1.53 | 1.37 |
| 48 | 38 | 213 | A86 | C19-C20 | 7.94 | 1.63 | 1.52 |
| 47 | 12 | 208 | KC1 | C2A-C3A | 7.93 | 1.53 | 1.37 |
| 47 | 16 | 302 | KC1 | C2A-C3A | 7.92 | 1.53 | 1.37 |
| 47 | 15 | 309 | KC1 | C2A-C3A | 7.90 | 1.53 | 1.37 |
| 47 | 17 | 306 | KC1 | C2A-C3A | 7.87 | 1.53 | 1.37 |
| 50 | 19 | 312 | DD6 | C19-C20 | 7.87 | 1.63 | 1.52 |
| 50 | 39 | 312 | DD6 | C19-C20 | 7.87 | 1.63 | 1.52 |
| 48 | 15 | 315 | A86 | C19-C20 | 7.86 | 1.63 | 1.52 |
| 47 | 35 | 309 | KC1 | C2A-C3A | 7.86 | 1.53 | 1.37 |
| 50 | 16 | 312 | DD6 | C19-C20 | 7.85 | 1.63 | 1.52 |
| 47 | 17 | 303 | KC1 | C2A-C3A | 7.84 | 1.53 | 1.37 |
| 47 | 37 | 302 | KC1 | C2A-C3A | 7.84 | 1.53 | 1.37 |
| 47 | 37 | 305 | KC1 | C2A-C3A | 7.82 | 1.53 | 1.37 |
| 48 | 15 | 316 | A86 | C4-C5 | 7.82 | 1.67 | 1.43 |
| 48 | 35 | 315 | A86 | C19-C20 | 7.81 | 1.63 | 1.52 |
| 48 | 35 | 316 | A86 | C4-C5 | 7.80 | 1.67 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 50 | 36 | 312 | DD6 | C19-C20 | 7.79 | 1.63 | 1.52 |
| 47 | 32 | 212 | KC1 | C2A-C3A | 7.79 | 1.53 | 1.37 |
| 47 | 38 | 210 | KC1 | C2A-C3A | 7.78 | 1.53 | 1.37 |
| 47 | 21 | 203 | KC1 | C2A-C3A | 7.77 | 1.52 | 1.37 |
| 47 | 12 | 211 | KC1 | C2A-C3A | 7.77 | 1.52 | 1.37 |
| 48 | 13 | 313 | A86 | C4-C5 | 7.75 | 1.67 | 1.43 |
| 47 | 14 | 306 | KC1 | C2A-C3A | 7.75 | 1.52 | 1.37 |
| 47 | 34 | 306 | KC1 | C2A-C3A | 7.75 | 1.52 | 1.37 |
| 47 | 41 | 203 | KC1 | C2A-C3A | 7.75 | 1.52 | 1.37 |
| 48 | 18 | 213 | A86 | C19-C20 | 7.74 | 1.63 | 1.52 |
| 48 | 33 | 314 | A86 | C4-C5 | 7.74 | 1.67 | 1.43 |
| 47 | 18 | 210 | KC1 | C2A-C3A | 7.74 | 1.52 | 1.37 |
| 48 | 33 | 313 | A86 | C4-C5 | 7.73 | 1.67 | 1.43 |
| 48 | 16 | 313 | A86 | C4-C5 | 7.71 | 1.67 | 1.43 |
| 48 | 13 | 314 | A86 | C4-C5 | 7.71 | 1.67 | 1.43 |
| 48 | 40 | 201 | A86 | C4-C5 | 7.71 | 1.67 | 1.43 |
| 48 | 21 | 213 | A86 | C4-C5 | 7.69 | 1.67 | 1.43 |
| 48 | 21 | 211 | A86 | C4-C5 | 7.68 | 1.67 | 1.43 |
| 47 | 16 | 305 | KC1 | C2A-C3A | 7.68 | 1.52 | 1.37 |
| 48 | 40 | 213 | A86 | C4-C5 | 7.67 | 1.67 | 1.43 |
| 48 | 41 | 211 | A86 | C4-C5 | 7.67 | 1.67 | 1.43 |
| 48 | 41 | 213 | A86 | C4-C5 | 7.67 | 1.67 | 1.43 |
| 47 | 11 | 302 | KC1 | C2A-C3A | 7.67 | 1.52 | 1.37 |
| 47 | 31 | 303 | KC1 | C2A-C3A | 7.67 | 1.52 | 1.37 |
| 48 | 15 | 313 | A86 | C4-C5 | 7.66 | 1.66 | 1.43 |
| 48 | 20 | 311 | A86 | C4-C5 | 7.66 | 1.66 | 1.43 |
| 48 | 35 | 313 | A86 | C4-C5 | 7.66 | 1.66 | 1.43 |
| 47 | 37 | 304 | KC1 | C2A-C3A | 7.66 | 1.52 | 1.37 |
| 47 | 33 | 309 | KC1 | C2A-C3A | 7.66 | 1.52 | 1.37 |
| 47 | 18 | 207 | KC1 | C2A-C3A | 7.65 | 1.52 | 1.37 |
| 47 | 38 | 207 | KC1 | C2A-C3A | 7.65 | 1.52 | 1.37 |
| 48 | 38 | 215 | A86 | C4-C5 | 7.65 | 1.66 | 1.43 |
| 47 | 11 | 309 | KC1 | C2A-C3A | 7.65 | 1.52 | 1.37 |
| 47 | 20 | 305 | KC1 | C2A-C3A | 7.64 | 1.52 | 1.37 |
| 48 | 21 | 215 | A86 | C4-C5 | 7.64 | 1.66 | 1.43 |
| 48 | 40 | 211 | A86 | C4-C5 | 7.63 | 1.66 | 1.43 |
| 50 | 40 | 214 | DD6 | C9-C10 | 7.63 | 1.66 | 1.43 |
| 48 | 14 | 313 | A86 | C4-C5 | 7.62 | 1.66 | 1.43 |
| 50 | 20 | 312 | DD6 | C9-C10 | 7.62 | 1.66 | 1.43 |
| 48 | 34 | 314 | A86 | C19-C20 | 7.62 | 1.62 | 1.52 |
| 47 | 13 | 309 | KC1 | C2A-C3A | 7.62 | 1.52 | 1.37 |
| 47 | 13 | 306 | KC1 | C2A-C3A | 7.62 | 1.52 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 33 | 306 | KC1 | C2A-C3A | 7.62 | 1.52 | 1.37 |
| 47 | 31 | 309 | KC1 | C2A-C3A | 7.62 | 1.52 | 1.37 |
| 48 | 41 | 215 | A86 | C4-C5 | 7.62 | 1.66 | 1.43 |
| 48 | 20 | 309 | A86 | C4-C5 | 7.62 | 1.66 | 1.43 |
| 50 | 41 | 216 | DD6 | C9-C10 | 7.61 | 1.66 | 1.43 |
| 47 | 36 | 305 | KC1 | C2A-C3A | 7.61 | 1.52 | 1.37 |
| 50 | 21 | 216 | DD6 | C9-C10 | 7.61 | 1.66 | 1.43 |
| 48 | 34 | 313 | A86 | C4-C5 | 7.61 | 1.66 | 1.43 |
| 48 | 14 | 316 | A86 | C4-C5 | 7.60 | 1.66 | 1.43 |
| 48 | 34 | 316 | A86 | C4-C5 | 7.60 | 1.66 | 1.43 |
| 48 | 33 | 314 | A86 | C8-C6 | 7.60 | 1.62 | 1.46 |
| 48 | 19 | 313 | A86 | C4-C5 | 7.60 | 1.66 | 1.43 |
| 47 | 17 | 305 | KC1 | C2A-C3A | 7.60 | 1.52 | 1.37 |
| 48 | 12 | 217 | A86 | C4-C5 | 7.60 | 1.66 | 1.43 |
| 47 | 40 | 207 | KC1 | C2A-C3A | 7.59 | 1.52 | 1.37 |
| 47 | 11 | 306 | KC1 | C2A-C3A | 7.59 | 1.52 | 1.37 |
| 48 | 18 | 215 | A86 | C4-C5 | 7.58 | 1.66 | 1.43 |
| 48 | 32 | 218 | A86 | C4-C5 | 7.58 | 1.66 | 1.43 |
| 50 | 20 | 310 | DD6 | C9-C10 | 7.58 | 1.66 | 1.43 |
| 48 | 39 | 313 | A86 | C4-C5 | 7.58 | 1.66 | 1.43 |
| 48 | 33 | 313 | A86 | C8-C6 | 7.58 | 1.62 | 1.46 |
| 48 | 13 | 314 | A86 | C8-C6 | 7.58 | 1.62 | 1.46 |
| 48 | 16 | 313 | A86 | C8-C6 | 7.57 | 1.62 | 1.46 |
| 50 | 16 | 312 | DD6 | C9-C10 | 7.57 | 1.66 | 1.43 |
| 48 | 33 | 312 | A86 | C4-C5 | 7.57 | 1.66 | 1.43 |
| 48 | 39 | 313 | A86 | C19-C20 | 7.56 | 1.62 | 1.52 |
| 50 | 40 | 212 | DD6 | C9-C10 | 7.56 | 1.66 | 1.43 |
| 50 | 41 | 212 | DD6 | C9-C10 | 7.56 | 1.66 | 1.43 |
| 48 | 32 | 216 | A86 | C4-C5 | 7.55 | 1.66 | 1.43 |
| 48 | 37 | 314 | A86 | C4-C5 | 7.55 | 1.66 | 1.43 |
| 48 | 13 | 313 | A86 | C8-C6 | 7.55 | 1.62 | 1.46 |
| 48 | 13 | 312 | A86 | C4-C5 | 7.55 | 1.66 | 1.43 |
| 48 | 35 | 314 | A86 | C4-C5 | 7.55 | 1.66 | 1.43 |
| 48 | 40 | 213 | A86 | C19-C20 | 7.54 | 1.62 | 1.52 |
| 47 | 35 | 302 | KC1 | C2A-C3A | 7.54 | 1.52 | 1.37 |
| 50 | 36 | 312 | DD6 | C9-C10 | 7.54 | 1.66 | 1.43 |
| 50 | 21 | 212 | DD6 | C9-C10 | 7.54 | 1.66 | 1.43 |
| 48 | 21 | 214 | A86 | C19-C20 | 7.54 | 1.62 | 1.52 |
| 48 | 14 | 314 | A86 | C4-C5 | 7.54 | 1.66 | 1.43 |
| 48 | 17 | 315 | A86 | C4-C5 | 7.54 | 1.66 | 1.43 |
| 48 | 40 | 201 | A86 | C8-C6 | 7.54 | 1.62 | 1.46 |
| 48 | 14 | 314 | A86 | C19-C20 | 7.54 | 1.62 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 40 | 213 | A86 | C8-C6 | 7.53 | 1.62 | 1.46 |
| 47 | 31 | 307 | KC1 | C2A-C3A | 7.53 | 1.52 | 1.37 |
| 48 | 20 | 311 | A86 | C8-C6 | 7.53 | 1.62 | 1.46 |
| 47 | 35 | 306 | KC1 | C2A-C3A | 7.53 | 1.52 | 1.37 |
| 47 | 11 | 304 | KC1 | C2A-C3A | 7.53 | 1.52 | 1.37 |
| 48 | 15 | 314 | A86 | C4-C5 | 7.53 | 1.66 | 1.43 |
| 48 | 34 | 314 | A86 | C4-C5 | 7.53 | 1.66 | 1.43 |
| 48 | 18 | 212 | A86 | C8-C6 | 7.52 | 1.62 | 1.46 |
| 48 | 12 | 215 | A86 | C4-C5 | 7.52 | 1.66 | 1.43 |
| 48 | 38 | 212 | A86 | C8-C6 | 7.52 | 1.62 | 1.46 |
| 48 | 21 | 213 | A86 | C8-C6 | 7.51 | 1.62 | 1.46 |
| 50 | 19 | 312 | DD6 | C9-C10 | 7.51 | 1.66 | 1.43 |
| 48 | 17 | 312 | A86 | C4-C5 | 7.51 | 1.66 | 1.43 |
| 48 | 35 | 312 | A86 | C4-C5 | 7.51 | 1.66 | 1.43 |
| 48 | 40 | 211 | A86 | C8-C6 | 7.51 | 1.62 | 1.46 |
| 48 | 37 | 311 | A86 | C4-C5 | 7.50 | 1.66 | 1.43 |
| 47 | 32 | 207 | KC1 | C2A-C3A | 7.50 | 1.52 | 1.37 |
| 47 | 14 | 309 | KC1 | C2A-C3A | 7.50 | 1.52 | 1.37 |
| 48 | 41 | 214 | A86 | C19-C20 | 7.50 | 1.62 | 1.52 |
| 48 | 38 | 214 | A86 | C4-C5 | 7.50 | 1.66 | 1.43 |
| 47 | 15 | 306 | KC1 | C2A-C3A | 7.50 | 1.52 | 1.37 |
| 50 | 20 | 312 | DD6 | C19-C20 | 7.50 | 1.62 | 1.52 |
| 48 | 15 | 312 | A86 | C4-C5 | 7.49 | 1.66 | 1.43 |
| 50 | 39 | 312 | DD6 | C9-C10 | 7.49 | 1.66 | 1.43 |
| 48 | 20 | 311 | A86 | C19-C20 | 7.49 | 1.62 | 1.52 |
| 47 | 34 | 309 | KC1 | C2A-C3A | 7.49 | 1.52 | 1.37 |
| 48 | 18 | 214 | A86 | C4-C5 | 7.49 | 1.66 | 1.43 |
| 47 | 12 | 206 | KC1 | C2A-C3A | 7.49 | 1.52 | 1.37 |
| 48 | 41 | 214 | A86 | C4-C5 | 7.49 | 1.66 | 1.43 |
| 48 | 18 | 212 | A86 | C4-C5 | 7.49 | 1.66 | 1.43 |
| 48 | 15 | 311 | A86 | C4-C5 | 7.49 | 1.66 | 1.43 |
| 48 | 41 | 213 | A86 | C8-C6 | 7.48 | 1.62 | 1.46 |
| 48 | 15 | 314 | A86 | C19-C20 | 7.48 | 1.62 | 1.52 |
| 50 | 40 | 212 | DD6 | C19-C20 | 7.48 | 1.62 | 1.52 |
| 50 | 40 | 214 | DD6 | C19-C20 | 7.48 | 1.62 | 1.52 |
| 48 | 15 | 316 | A86 | C8-C6 | 7.47 | 1.61 | 1.46 |
| 50 | 20 | 310 | DD6 | C19-C20 | 7.47 | 1.62 | 1.52 |
| 47 | 31 | 305 | KC1 | C2A-C3A | 7.47 | 1.52 | 1.37 |
| 48 | 38 | 212 | A86 | C4-C5 | 7.47 | 1.66 | 1.43 |
| 48 | 38 | 214 | A86 | C19-C20 | 7.46 | 1.62 | 1.52 |
| 47 | 40 | 206 | KC1 | C2A-C3A | 7.46 | 1.52 | 1.37 |
| 47 | 15 | 302 | KC1 | C2A-C3A | 7.46 | 1.52 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 21 | 214 | A86 | C4-C5 | 7.46 | 1.66 | 1.43 |
| 48 | 13 | 315 | A86 | C4-C5 | 7.45 | 1.66 | 1.43 |
| 48 | 33 | 315 | A86 | C4-C5 | 7.45 | 1.66 | 1.43 |
| 48 | 20 | 309 | A86 | C8-C6 | 7.45 | 1.61 | 1.46 |
| 48 | 35 | 311 | A86 | C4-C5 | 7.44 | 1.66 | 1.43 |
| 48 | 35 | 316 | A86 | C8-C6 | 7.44 | 1.61 | 1.46 |
| 48 | 37 | 314 | A86 | C8-C6 | 7.43 | 1.61 | 1.46 |
| 48 | 37 | 312 | A86 | C4-C5 | 7.43 | 1.66 | 1.43 |
| 47 | 18 | 205 | KC1 | C2A-C3A | 7.43 | 1.52 | 1.37 |
| 48 | 17 | 313 | A86 | C4-C5 | 7.42 | 1.66 | 1.43 |
| 48 | 17 | 311 | A86 | C4-C5 | 7.42 | 1.66 | 1.43 |
| 47 | 20 | 304 | KC1 | C2A-C3A | 7.42 | 1.52 | 1.37 |
| 48 | 38 | 215 | A86 | C8-C6 | 7.42 | 1.61 | 1.46 |
| 47 | 38 | 205 | KC1 | C2A-C3A | 7.41 | 1.52 | 1.37 |
| 47 | 13 | 302 | KC1 | C2A-C3A | 7.41 | 1.52 | 1.37 |
| 48 | 19 | 313 | A86 | C8-C6 | 7.41 | 1.61 | 1.46 |
| 48 | 11 | 313 | A86 | C4-C5 | 7.41 | 1.66 | 1.43 |
| 48 | 17 | 315 | A86 | C8-C6 | 7.40 | 1.61 | 1.46 |
| 48 | 32 | 217 | A86 | C4-C5 | 7.40 | 1.66 | 1.43 |
| 47 | 20 | 302 | KC1 | C2A-C3A | 7.40 | 1.52 | 1.37 |
| 48 | 18 | 214 | A86 | C19-C20 | 7.40 | 1.62 | 1.52 |
| 48 | 15 | 313 | A86 | C8-C6 | 7.39 | 1.61 | 1.46 |
| 48 | 14 | 315 | A86 | C4-C5 | 7.39 | 1.66 | 1.43 |
| 48 | 37 | 310 | A86 | C4-C5 | 7.39 | 1.66 | 1.43 |
| 48 | 14 | 313 | A86 | C8-C6 | 7.39 | 1.61 | 1.46 |
| 48 | 34 | 315 | A86 | C4-C5 | 7.38 | 1.66 | 1.43 |
| 48 | 12 | 215 | A86 | C8-C6 | 7.38 | 1.61 | 1.46 |
| 48 | 32 | 216 | A86 | C8-C6 | 7.38 | 1.61 | 1.46 |
| 48 | 31 | 313 | A86 | C4-C5 | 7.37 | 1.66 | 1.43 |
| 47 | 33 | 302 | KC1 | C2A-C3A | 7.37 | 1.52 | 1.37 |
| 47 | 40 | 204 | KC1 | C2A-C3A | 7.37 | 1.52 | 1.37 |
| 48 | 12 | 216 | A86 | C4-C5 | 7.37 | 1.66 | 1.43 |
| 48 | 17 | 310 | A86 | C4-C5 | 7.37 | 1.66 | 1.43 |
| 48 | 37 | 319 | A86 | C4-C5 | 7.37 | 1.66 | 1.43 |
| 48 | 37 | 309 | A86 | C4-C5 | 7.36 | 1.66 | 1.43 |
| 48 | 34 | 313 | A86 | C8-C6 | 7.36 | 1.61 | 1.46 |
| 48 | 35 | 313 | A86 | C8-C6 | 7.36 | 1.61 | 1.46 |
| 48 | 33 | 315 | A86 | C8-C6 | 7.36 | 1.61 | 1.46 |
| 48 | 21 | 215 | A86 | C8-C6 | 7.36 | 1.61 | 1.46 |
| 48 | 35 | 319 | A86 | C4-C5 | 7.35 | 1.66 | 1.43 |
| 48 | 18 | 215 | A86 | C8-C6 | 7.35 | 1.61 | 1.46 |
| 48 | 19 | 313 | A86 | C19-C20 | 7.35 | 1.62 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 17 | 320 | A86 | C4-C5 | 7.35 | 1.66 | 1.43 |
| 48 | 13 | 311 | A86 | C4-C5 | 7.35 | 1.66 | 1.43 |
| 48 | 15 | 315 | A86 | C4-C5 | 7.35 | 1.66 | 1.43 |
| 48 | 17 | 310 | A86 | C19-C20 | 7.34 | 1.62 | 1.52 |
| 48 | 37 | 309 | A86 | C19-C20 | 7.34 | 1.62 | 1.52 |
| 48 | 12 | 213 | A86 | C4-C5 | 7.34 | 1.65 | 1.43 |
| 48 | 39 | 313 | A86 | C8-C6 | 7.34 | 1.61 | 1.46 |
| 48 | 15 | 319 | A86 | C4-C5 | 7.33 | 1.65 | 1.43 |
| 48 | 41 | 215 | A86 | C8-C6 | 7.33 | 1.61 | 1.46 |
| 48 | 33 | 312 | A86 | C8-C6 | 7.32 | 1.61 | 1.46 |
| 48 | 14 | 316 | A86 | C8-C6 | 7.32 | 1.61 | 1.46 |
| 48 | 15 | 314 | A86 | C8-C6 | 7.32 | 1.61 | 1.46 |
| 48 | 35 | 315 | A86 | C4-C5 | 7.32 | 1.65 | 1.43 |
| 48 | 16 | 310 | A86 | C4-C5 | 7.32 | 1.65 | 1.43 |
| 48 | 35 | 314 | A86 | C19-C20 | 7.32 | 1.62 | 1.52 |
| 48 | 13 | 314 | A86 | C19-C20 | 7.32 | 1.62 | 1.52 |
| 48 | 36 | 310 | A86 | C4-C5 | 7.32 | 1.65 | 1.43 |
| 48 | 35 | 314 | A86 | C8-C6 | 7.31 | 1.61 | 1.46 |
| 48 | 33 | 314 | A86 | C19-C20 | 7.31 | 1.62 | 1.52 |
| 48 | 13 | 312 | A86 | C8-C6 | 7.31 | 1.61 | 1.46 |
| 48 | 13 | 315 | A86 | C8-C6 | 7.30 | 1.61 | 1.46 |
| 48 | 33 | 311 | A86 | C4-C5 | 7.30 | 1.65 | 1.43 |
| 48 | 34 | 316 | A86 | C8-C6 | 7.30 | 1.61 | 1.46 |
| 48 | 11 | 311 | A86 | C4-C5 | 7.30 | 1.65 | 1.43 |
| 48 | 12 | 217 | A86 | C8-C6 | 7.29 | 1.61 | 1.46 |
| 48 | 21 | 211 | A86 | C8-C6 | 7.29 | 1.61 | 1.46 |
| 47 | 19 | 308 | KC1 | C2A-C3A | 7.29 | 1.52 | 1.37 |
| 48 | 11 | 314 | A86 | C4-C5 | 7.29 | 1.65 | 1.43 |
| 48 | 37 | 313 | A86 | C4-C5 | 7.28 | 1.65 | 1.43 |
| 48 | 41 | 211 | A86 | C8-C6 | 7.28 | 1.61 | 1.46 |
| 48 | 19 | 311 | A86 | C4-C5 | 7.28 | 1.65 | 1.43 |
| 47 | 33 | 304 | KC1 | C2A-C3A | 7.28 | 1.52 | 1.37 |
| 48 | 32 | 203 | A86 | C4-C5 | 7.28 | 1.65 | 1.43 |
| 48 | 18 | 214 | A86 | C8-C6 | 7.27 | 1.61 | 1.46 |
| 48 | 31 | 311 | A86 | C4-C5 | 7.27 | 1.65 | 1.43 |
| 48 | 12 | 202 | A86 | C4-C5 | 7.27 | 1.65 | 1.43 |
| 48 | 32 | 214 | A86 | C4-C5 | 7.27 | 1.65 | 1.43 |
| 48 | 31 | 314 | A86 | C4-C5 | 7.27 | 1.65 | 1.43 |
| 48 | 39 | 311 | A86 | C4-C5 | 7.27 | 1.65 | 1.43 |
| 48 | 20 | 309 | A86 | C19-C20 | 7.27 | 1.62 | 1.52 |
| 47 | 13 | 304 | KC1 | C2A-C3A | 7.27 | 1.51 | 1.37 |
| 48 | 38 | 213 | A86 | C4-C5 | 7.27 | 1.65 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 32 | 218 | A86 | C8-C6 | 7.27 | 1.61 | 1.46 |
| 48 | 34 | 314 | A86 | C8-C6 | 7.27 | 1.61 | 1.46 |
| 48 | 17 | 312 | A86 | C8-C6 | 7.26 | 1.61 | 1.46 |
| 48 | 16 | 314 | A86 | C4-C5 | 7.26 | 1.65 | 1.43 |
| 48 | 36 | 313 | A86 | C4-C5 | 7.26 | 1.65 | 1.43 |
| 48 | 15 | 312 | A86 | C8-C6 | 7.26 | 1.61 | 1.46 |
| 48 | 35 | 312 | A86 | C8-C6 | 7.26 | 1.61 | 1.46 |
| 48 | 18 | 213 | A86 | C4-C5 | 7.25 | 1.65 | 1.43 |
| 47 | 39 | 308 | KC1 | C2A-C3A | 7.25 | 1.51 | 1.37 |
| 48 | 40 | 211 | A86 | C19-C20 | 7.25 | 1.62 | 1.52 |
| 48 | 17 | 314 | A86 | C4-C5 | 7.25 | 1.65 | 1.43 |
| 48 | 14 | 314 | A86 | C8-C6 | 7.24 | 1.61 | 1.46 |
| 47 | 15 | 304 | KC1 | C2A-C3A | 7.24 | 1.51 | 1.37 |
| 47 | 35 | 304 | KC1 | C2A-C3A | 7.23 | 1.51 | 1.37 |
| 48 | 38 | 214 | A86 | C8-C6 | 7.23 | 1.61 | 1.46 |
| 48 | 13 | 313 | A86 | C19-C20 | 7.22 | 1.62 | 1.52 |
| 48 | 21 | 211 | A86 | C19-C20 | 7.22 | 1.62 | 1.52 |
| 48 | 11 | 319 | A86 | C4-C5 | 7.22 | 1.65 | 1.43 |
| 50 | 41 | 212 | DD6 | C24-C1 | 7.21 | 1.61 | 1.46 |
| 48 | 17 | 314 | A86 | C8-C6 | 7.21 | 1.61 | 1.46 |
| 48 | 11 | 312 | A86 | C4-C5 | 7.21 | 1.65 | 1.43 |
| 48 | 37 | 313 | A86 | C8-C6 | 7.21 | 1.61 | 1.46 |
| 48 | 31 | 319 | A86 | C4-C5 | 7.21 | 1.65 | 1.43 |
| 48 | 12 | 214 | A86 | C4-C5 | 7.21 | 1.65 | 1.43 |
| 48 | 32 | 215 | A86 | C4-C5 | 7.21 | 1.65 | 1.43 |
| 48 | 31 | 312 | A86 | C4-C5 | 7.20 | 1.65 | 1.43 |
| 48 | 33 | 313 | A86 | C19-C20 | 7.20 | 1.62 | 1.52 |
| 47 | 36 | 304 | KC1 | C2A-C3A | 7.19 | 1.51 | 1.37 |
| 50 | 21 | 212 | DD6 | C24-C1 | 7.19 | 1.61 | 1.46 |
| 50 | 41 | 212 | DD6 | C30-C29 | 7.18 | 1.40 | 1.20 |
| 47 | 16 | 304 | KC1 | C2A-C3A | 7.18 | 1.51 | 1.37 |
| 48 | 41 | 211 | A86 | C19-C20 | 7.18 | 1.62 | 1.52 |
| 48 | 37 | 311 | A86 | C8-C6 | 7.17 | 1.61 | 1.46 |
| 48 | 31 | 314 | A86 | C19-C20 | 7.17 | 1.62 | 1.52 |
| 50 | 21 | 212 | DD6 | C30-C29 | 7.17 | 1.40 | 1.20 |
| 48 | 41 | 214 | A86 | C8-C6 | 7.17 | 1.61 | 1.46 |
| 48 | 11 | 315 | A86 | C4-C5 | 7.17 | 1.65 | 1.43 |
| 48 | 21 | 215 | A86 | C19-C20 | 7.16 | 1.62 | 1.52 |
| 48 | 14 | 312 | A86 | C4-C5 | 7.16 | 1.65 | 1.43 |
| 48 | 34 | 312 | A86 | C4-C5 | 7.16 | 1.65 | 1.43 |
| 48 | 37 | 313 | A86 | C19-C20 | 7.16 | 1.62 | 1.52 |
| 48 | 21 | 214 | A86 | C8-C6 | 7.16 | 1.61 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 31 | 315 | A86 | C4-C5 | 7.16 | 1.65 | 1.43 |
| 48 | 11 | 314 | A86 | C19-C20 | 7.15 | 1.62 | 1.52 |
| 48 | 17 | 313 | A86 | C8-C6 | 7.15 | 1.61 | 1.46 |
| 47 | 21 | 207 | KC1 | C2A-C3A | 7.14 | 1.51 | 1.37 |
| 48 | 41 | 215 | A86 | C19-C20 | 7.14 | 1.62 | 1.52 |
| 48 | 35 | 312 | A86 | C25-C26 | 7.14 | 1.65 | 1.43 |
| 47 | 41 | 207 | KC1 | C2A-C3A | 7.14 | 1.51 | 1.37 |
| 50 | 41 | 216 | DD6 | C30-C29 | 7.14 | 1.40 | 1.20 |
| 48 | 37 | 312 | A86 | C19-C20 | 7.14 | 1.62 | 1.52 |
| 48 | 33 | 311 | A86 | C8-C6 | 7.14 | 1.61 | 1.46 |
| 48 | 18 | 212 | A86 | C19-C20 | 7.13 | 1.62 | 1.52 |
| 48 | 35 | 311 | A86 | C8-C6 | 7.13 | 1.61 | 1.46 |
| 48 | 37 | 312 | A86 | C8-C6 | 7.13 | 1.61 | 1.46 |
| 48 | 17 | 314 | A86 | C19-C20 | 7.13 | 1.62 | 1.52 |
| 50 | 21 | 216 | DD6 | C30-C29 | 7.13 | 1.40 | 1.20 |
| 48 | 16 | 311 | A86 | C4-C5 | 7.13 | 1.65 | 1.43 |
| 50 | 21 | 212 | DD6 | C30-C31 | 7.12 | 1.55 | 1.42 |
| 48 | 36 | 311 | A86 | C4-C5 | 7.12 | 1.65 | 1.43 |
| 48 | 15 | 312 | A86 | C25-C26 | 7.11 | 1.65 | 1.43 |
| 50 | 36 | 312 | DD6 | C30-C29 | 7.11 | 1.40 | 1.20 |
| 50 | 40 | 214 | DD6 | C24-C1 | 7.11 | 1.61 | 1.46 |
| 48 | 13 | 311 | A86 | C8-C6 | 7.10 | 1.61 | 1.46 |
| 48 | 14 | 311 | A86 | C8-C6 | 7.10 | 1.61 | 1.46 |
| 48 | 12 | 214 | A86 | C25-C26 | 7.10 | 1.65 | 1.43 |
| 50 | 36 | 312 | DD6 | C30-C31 | 7.10 | 1.55 | 1.42 |
| 48 | 17 | 313 | A86 | C19-C20 | 7.10 | 1.62 | 1.52 |
| 50 | 41 | 212 | DD6 | C30-C31 | 7.10 | 1.55 | 1.42 |
| 50 | 16 | 312 | DD6 | C30-C29 | 7.10 | 1.40 | 1.20 |
| 48 | 15 | 311 | A86 | C8-C6 | 7.09 | 1.61 | 1.46 |
| 48 | 32 | 215 | A86 | C25-C26 | 7.09 | 1.65 | 1.43 |
| 50 | 20 | 312 | DD6 | C24-C1 | 7.09 | 1.61 | 1.46 |
| 50 | 40 | 212 | DD6 | C24-C1 | 7.08 | 1.61 | 1.46 |
| 48 | 38 | 213 | A86 | C8-C6 | 7.07 | 1.61 | 1.46 |
| 48 | 38 | 212 | A86 | C19-C20 | 7.07 | 1.62 | 1.52 |
| 48 | 14 | 311 | A86 | C4-C5 | 7.07 | 1.65 | 1.43 |
| 50 | 20 | 310 | DD6 | C24-C1 | 7.07 | 1.61 | 1.46 |
| 48 | 34 | 311 | A86 | C4-C5 | 7.07 | 1.65 | 1.43 |
| 48 | 35 | 319 | A86 | C8-C6 | 7.06 | 1.61 | 1.46 |
| 48 | 34 | 311 | A86 | C8-C6 | 7.06 | 1.61 | 1.46 |
| 48 | 15 | 319 | A86 | C8-C6 | 7.06 | 1.61 | 1.46 |
| 50 | 16 | 312 | DD6 | C30-C31 | 7.06 | 1.55 | 1.42 |
| 48 | 11 | 313 | A86 | C8-C6 | 7.06 | 1.61 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 14 | 304 | KC1 | C2A-C3A | 7.06 | 1.51 | 1.37 |
| 47 | 34 | 304 | KC1 | C2A-C3A | 7.06 | 1.51 | 1.37 |
| 48 | 32 | 203 | A86 | C8-C6 | 7.06 | 1.61 | 1.46 |
| 48 | 15 | 313 | A86 | C25-C26 | 7.05 | 1.65 | 1.43 |
| 48 | 12 | 202 | A86 | C8-C6 | 7.05 | 1.61 | 1.46 |
| 48 | 31 | 313 | A86 | C8-C6 | 7.04 | 1.61 | 1.46 |
| 48 | 12 | 220 | A86 | C4-C5 | 7.04 | 1.65 | 1.43 |
| 48 | 35 | 313 | A86 | C25-C26 | 7.04 | 1.65 | 1.43 |
| 48 | 12 | 215 | A86 | C19-C20 | 7.03 | 1.62 | 1.52 |
| 48 | 32 | 216 | A86 | C19-C20 | 7.03 | 1.62 | 1.52 |
| 48 | 37 | 319 | A86 | C8-C6 | 7.03 | 1.61 | 1.46 |
| 48 | 17 | 320 | A86 | C8-C6 | 7.03 | 1.61 | 1.46 |
| 48 | 32 | 221 | A86 | C4-C5 | 7.03 | 1.65 | 1.43 |
| 48 | 14 | 315 | A86 | C8-C6 | 7.03 | 1.61 | 1.46 |
| 48 | 34 | 315 | A86 | C8-C6 | 7.03 | 1.61 | 1.46 |
| 48 | 33 | 312 | A86 | C19-C20 | 7.02 | 1.62 | 1.52 |
| 48 | 12 | 216 | A86 | C19-C20 | 7.02 | 1.62 | 1.52 |
| 48 | 37 | 319 | A86 | C19-C20 | 7.02 | 1.62 | 1.52 |
| 48 | 37 | 310 | A86 | C8-C6 | 7.01 | 1.61 | 1.46 |
| 48 | 19 | 311 | A86 | C8-C6 | 7.00 | 1.60 | 1.46 |
| 48 | 39 | 311 | A86 | C8-C6 | 7.00 | 1.60 | 1.46 |
| 48 | 32 | 217 | A86 | C8-C6 | 7.00 | 1.60 | 1.46 |
| 48 | 40 | 201 | A86 | C19-C20 | 7.00 | 1.62 | 1.52 |
| 48 | 13 | 312 | A86 | C25-C26 | 7.00 | 1.64 | 1.43 |
| 48 | 12 | 216 | A86 | C8-C6 | 7.00 | 1.60 | 1.46 |
| 48 | 33 | 312 | A86 | C25-C26 | 6.99 | 1.64 | 1.43 |
| 48 | 14 | 313 | A86 | C25-C26 | 6.99 | 1.64 | 1.43 |
| 48 | 13 | 312 | A86 | C19-C20 | 6.98 | 1.62 | 1.52 |
| 48 | 16 | 314 | A86 | C8-C6 | 6.98 | 1.60 | 1.46 |
| 48 | 13 | 313 | A86 | C25-C26 | 6.98 | 1.64 | 1.43 |
| 48 | 33 | 313 | A86 | C25-C26 | 6.98 | 1.64 | 1.43 |
| 50 | 40 | 214 | DD6 | C30-C29 | 6.97 | 1.39 | 1.20 |
| 50 | 20 | 312 | DD6 | C30-C29 | 6.97 | 1.39 | 1.20 |
| 48 | 37 | 311 | A86 | C25-C26 | 6.97 | 1.64 | 1.43 |
| 48 | 37 | 309 | A86 | C8-C6 | 6.96 | 1.60 | 1.46 |
| 48 | 16 | 313 | A86 | C19-C20 | 6.96 | 1.62 | 1.52 |
| 48 | 34 | 313 | A86 | C25-C26 | 6.96 | 1.64 | 1.43 |
| 50 | 20 | 312 | DD6 | C30-C31 | 6.96 | 1.55 | 1.42 |
| 48 | 12 | 215 | A86 | C25-C26 | 6.96 | 1.64 | 1.43 |
| 48 | 17 | 310 | A86 | C8-C6 | 6.96 | 1.60 | 1.46 |
| 50 | 40 | 214 | DD6 | C30-C31 | 6.96 | 1.55 | 1.42 |
| 48 | 35 | 312 | A86 | C19-C20 | 6.95 | 1.62 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 17 | 312 | A86 | C25-C26 | 6.95 | 1.64 | 1.43 |
| 48 | 32 | 216 | A86 | C25-C26 | 6.95 | 1.64 | 1.43 |
| 50 | 19 | 312 | DD6 | C24-C1 | 6.95 | 1.60 | 1.46 |
| 48 | 14 | 312 | A86 | C8-C6 | 6.95 | 1.60 | 1.46 |
| 48 | 34 | 312 | A86 | C8-C6 | 6.95 | 1.60 | 1.46 |
| 48 | 17 | 311 | A86 | C25-C26 | 6.94 | 1.64 | 1.43 |
| 48 | 41 | 213 | A86 | C25-C26 | 6.94 | 1.64 | 1.43 |
| 48 | 36 | 313 | A86 | C8-C6 | 6.94 | 1.60 | 1.46 |
| 48 | 17 | 311 | A86 | C8-C6 | 6.94 | 1.60 | 1.46 |
| 48 | 21 | 213 | A86 | C25-C26 | 6.94 | 1.64 | 1.43 |
| 48 | 15 | 312 | A86 | C19-C20 | 6.93 | 1.61 | 1.52 |
| 48 | 35 | 315 | A86 | C8-C6 | 6.93 | 1.60 | 1.46 |
| 48 | 12 | 213 | A86 | C8-C6 | 6.93 | 1.60 | 1.46 |
| 48 | 12 | 213 | A86 | C19-C20 | 6.93 | 1.61 | 1.52 |
| 48 | 20 | 311 | A86 | C25-C26 | 6.92 | 1.64 | 1.43 |
| 48 | 32 | 217 | A86 | C19-C20 | 6.92 | 1.61 | 1.52 |
| 48 | 41 | 213 | A86 | C19-C20 | 6.92 | 1.61 | 1.52 |
| 48 | 15 | 315 | A86 | C8-C6 | 6.92 | 1.60 | 1.46 |
| 50 | 41 | 216 | DD6 | C24-C1 | 6.92 | 1.60 | 1.46 |
| 48 | 16 | 311 | A86 | C8-C6 | 6.91 | 1.60 | 1.46 |
| 48 | 21 | 213 | A86 | C19-C20 | 6.91 | 1.61 | 1.52 |
| 48 | 40 | 213 | A86 | C25-C26 | 6.91 | 1.64 | 1.43 |
| 48 | 32 | 214 | A86 | C8-C6 | 6.91 | 1.60 | 1.46 |
| 48 | 32 | 214 | A86 | C19-C20 | 6.91 | 1.61 | 1.52 |
| 50 | 39 | 312 | DD6 | C24-C1 | 6.91 | 1.60 | 1.46 |
| 48 | 36 | 311 | A86 | C8-C6 | 6.90 | 1.60 | 1.46 |
| 50 | 21 | 216 | DD6 | C30-C31 | 6.90 | 1.55 | 1.42 |
| 48 | 17 | 311 | A86 | C19-C20 | 6.90 | 1.61 | 1.52 |
| 48 | 35 | 311 | A86 | C19-C20 | 6.90 | 1.61 | 1.52 |
| 50 | 20 | 310 | DD6 | C30-C29 | 6.89 | 1.39 | 1.20 |
| 50 | 21 | 216 | DD6 | C24-C1 | 6.89 | 1.60 | 1.46 |
| 48 | 15 | 311 | A86 | C19-C20 | 6.89 | 1.61 | 1.52 |
| 48 | 18 | 213 | A86 | C8-C6 | 6.88 | 1.60 | 1.46 |
| 48 | 37 | 310 | A86 | C25-C26 | 6.88 | 1.64 | 1.43 |
| 48 | 41 | 215 | A86 | C25-C26 | 6.88 | 1.64 | 1.43 |
| 50 | 41 | 216 | DD6 | C30-C31 | 6.88 | 1.55 | 1.42 |
| 48 | 13 | 311 | A86 | C19-C20 | 6.88 | 1.61 | 1.52 |
| 50 | 40 | 212 | DD6 | C30-C29 | 6.88 | 1.39 | 1.20 |
| 48 | 16 | 310 | A86 | C8-C6 | 6.87 | 1.60 | 1.46 |
| 48 | 21 | 215 | A86 | C25-C26 | 6.87 | 1.64 | 1.43 |
| 48 | 33 | 311 | A86 | C19-C20 | 6.86 | 1.61 | 1.52 |
| 48 | 36 | 310 | A86 | C8-C6 | 6.86 | 1.60 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 16 | 308 | KC1 | CBA-CAA | 6.85 | 1.53 | 1.33 |
| 48 | 15 | 311 | A86 | C25-C26 | 6.85 | 1.64 | 1.43 |
| 48 | 34 | 315 | A86 | C19-C20 | 6.85 | 1.61 | 1.52 |
| 47 | 36 | 308 | KC1 | CBA-CAA | 6.85 | 1.53 | 1.33 |
| 48 | 31 | 314 | A86 | C8-C6 | 6.84 | 1.60 | 1.46 |
| 48 | 15 | 316 | A86 | C19-C20 | 6.84 | 1.61 | 1.52 |
| 48 | 37 | 310 | A86 | C19-C20 | 6.83 | 1.61 | 1.52 |
| 48 | 13 | 314 | A86 | C25-C26 | 6.83 | 1.64 | 1.43 |
| 48 | 15 | 314 | A86 | C25-C26 | 6.82 | 1.64 | 1.43 |
| 48 | 18 | 212 | A86 | C25-C26 | 6.82 | 1.64 | 1.43 |
| 48 | 18 | 215 | A86 | C25-C26 | 6.82 | 1.64 | 1.43 |
| 48 | 11 | 314 | A86 | C8-C6 | 6.82 | 1.60 | 1.46 |
| 48 | 33 | 314 | A86 | C25-C26 | 6.82 | 1.64 | 1.43 |
| 48 | 12 | 214 | A86 | C19-C20 | 6.82 | 1.61 | 1.52 |
| 50 | 19 | 312 | DD6 | C21-C20 | -6.81 | 1.41 | 1.51 |
| 48 | 21 | 211 | A86 | C25-C26 | 6.81 | 1.64 | 1.43 |
| 50 | 39 | 312 | DD6 | C21-C20 | -6.80 | 1.41 | 1.51 |
| 48 | 35 | 311 | A86 | C25-C26 | 6.80 | 1.64 | 1.43 |
| 48 | 41 | 211 | A86 | C25-C26 | 6.80 | 1.64 | 1.43 |
| 48 | 21 | 214 | A86 | C25-C26 | 6.80 | 1.64 | 1.43 |
| 48 | 38 | 215 | A86 | C25-C26 | 6.80 | 1.64 | 1.43 |
| 48 | 35 | 314 | A86 | C25-C26 | 6.79 | 1.64 | 1.43 |
| 48 | 38 | 212 | A86 | C25-C26 | 6.79 | 1.64 | 1.43 |
| 50 | 16 | 312 | DD6 | C24-C1 | 6.79 | 1.60 | 1.46 |
| 48 | 32 | 215 | A86 | C19-C20 | 6.78 | 1.61 | 1.52 |
| 47 | 13 | 304 | KC1 | CBA-CAA | 6.78 | 1.53 | 1.33 |
| 48 | 41 | 214 | A86 | C25-C26 | 6.78 | 1.64 | 1.43 |
| 48 | 18 | 214 | A86 | C25-C26 | 6.78 | 1.64 | 1.43 |
| 48 | 15 | 316 | A86 | C25-C26 | 6.77 | 1.64 | 1.43 |
| 47 | 20 | 305 | KC1 | CBA-CAA | 6.77 | 1.53 | 1.33 |
| 48 | 15 | 313 | A86 | C19-C20 | 6.77 | 1.61 | 1.52 |
| 50 | 36 | 312 | DD6 | C24-C1 | 6.77 | 1.60 | 1.46 |
| 48 | 31 | 312 | A86 | C8-C6 | 6.77 | 1.60 | 1.46 |
| 48 | 38 | 214 | A86 | C25-C26 | 6.77 | 1.64 | 1.43 |
| 48 | 11 | 312 | A86 | C8-C6 | 6.77 | 1.60 | 1.46 |
| 48 | 14 | 314 | A86 | C25-C26 | 6.77 | 1.64 | 1.43 |
| 48 | 34 | 314 | A86 | C25-C26 | 6.77 | 1.64 | 1.43 |
| 47 | 40 | 207 | KC1 | CBA-CAA | 6.76 | 1.53 | 1.33 |
| 48 | 35 | 313 | A86 | C19-C20 | 6.76 | 1.61 | 1.52 |
| 47 | 33 | 304 | KC1 | CBA-CAA | 6.76 | 1.53 | 1.33 |
| 48 | 14 | 315 | A86 | C19-C20 | 6.75 | 1.61 | 1.52 |
| 48 | 31 | 311 | A86 | C8-C6 | 6.75 | 1.60 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 18 | 207 | KC1 | CBA-CAA | 6.75 | 1.53 | 1.33 |
| 47 | 38 | 207 | KC1 | CBA-CAA | 6.75 | 1.53 | 1.33 |
| 48 | 11 | 319 | A86 | C8-C6 | 6.75 | 1.60 | 1.46 |
| 48 | 31 | 319 | A86 | C8-C6 | 6.75 | 1.60 | 1.46 |
| 50 | 20 | 312 | DD6 | C21-C20 | -6.74 | 1.41 | 1.51 |
| 48 | 11 | 315 | A86 | C25-C26 | 6.74 | 1.64 | 1.43 |
| 48 | 31 | 315 | A86 | C25-C26 | 6.74 | 1.64 | 1.43 |
| 48 | 35 | 316 | A86 | C25-C26 | 6.74 | 1.64 | 1.43 |
| 47 | 37 | 307 | KC1 | CBA-CAA | 6.74 | 1.53 | 1.33 |
| 48 | 31 | 313 | A86 | C25-C26 | 6.74 | 1.64 | 1.43 |
| 50 | 40 | 214 | DD6 | C21-C20 | -6.73 | 1.41 | 1.51 |
| 47 | 17 | 308 | KC1 | CBA-CAA | 6.73 | 1.53 | 1.33 |
| 48 | 11 | 312 | A86 | C25-C26 | 6.73 | 1.64 | 1.43 |
| 48 | 14 | 315 | A86 | C25-C26 | 6.73 | 1.64 | 1.43 |
| 48 | 14 | 316 | A86 | C25-C26 | 6.73 | 1.64 | 1.43 |
| 48 | 16 | 313 | A86 | C25-C26 | 6.72 | 1.64 | 1.43 |
| 48 | 34 | 315 | A86 | C25-C26 | 6.72 | 1.64 | 1.43 |
| 48 | 31 | 312 | A86 | C25-C26 | 6.72 | 1.64 | 1.43 |
| 47 | 37 | 304 | KC1 | CBA-CAA | 6.72 | 1.53 | 1.33 |
| 48 | 40 | 201 | A86 | C25-C26 | 6.72 | 1.64 | 1.43 |
| 48 | 11 | 311 | A86 | C8-C6 | 6.72 | 1.60 | 1.46 |
| 48 | 12 | 217 | A86 | C25-C26 | 6.72 | 1.64 | 1.43 |
| 48 | 39 | 313 | A86 | C25-C26 | 6.72 | 1.64 | 1.43 |
| 48 | 14 | 311 | A86 | C19-C20 | 6.71 | 1.61 | 1.52 |
| 48 | 34 | 311 | A86 | C19-C20 | 6.71 | 1.61 | 1.52 |
| 48 | 19 | 313 | A86 | C25-C26 | 6.71 | 1.64 | 1.43 |
| 48 | 20 | 309 | A86 | C25-C26 | 6.71 | 1.64 | 1.43 |
| 48 | 32 | 218 | A86 | C25-C26 | 6.71 | 1.64 | 1.43 |
| 48 | 35 | 316 | A86 | C19-C20 | 6.71 | 1.61 | 1.52 |
| 48 | 35 | 315 | A86 | C25-C26 | 6.71 | 1.64 | 1.43 |
| 47 | 17 | 305 | KC1 | CBA-CAA | 6.70 | 1.53 | 1.33 |
| 48 | 33 | 315 | A86 | C25-C26 | 6.70 | 1.64 | 1.43 |
| 47 | 37 | 305 | KC1 | CBA-CAA | 6.70 | 1.53 | 1.33 |
| 47 | 19 | 308 | KC1 | CBA-CAA | 6.70 | 1.53 | 1.33 |
| 48 | 34 | 316 | A86 | C25-C26 | 6.70 | 1.64 | 1.43 |
| 48 | 17 | 313 | A86 | C25-C26 | 6.70 | 1.63 | 1.43 |
| 47 | 35 | 309 | KC1 | CBA-CAA | 6.69 | 1.53 | 1.33 |
| 48 | 11 | 319 | A86 | C25-C26 | 6.69 | 1.63 | 1.43 |
| 48 | 15 | 315 | A86 | C25-C26 | 6.69 | 1.63 | 1.43 |
| 48 | 17 | 315 | A86 | C25-C26 | 6.69 | 1.63 | 1.43 |
| 47 | 16 | 305 | KC1 | CBA-CAA | 6.69 | 1.53 | 1.33 |
| 48 | 40 | 211 | A86 | C25-C26 | 6.69 | 1.63 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 36 | 305 | KC1 | CBA-CAA | 6.69 | 1.53 | 1.33 |
| 48 | 32 | 215 | A86 | C8-C6 | 6.69 | 1.60 | 1.46 |
| 47 | 39 | 308 | KC1 | CBA-CAA | 6.69 | 1.53 | 1.33 |
| 47 | 15 | 309 | KC1 | CBA-CAA | 6.68 | 1.53 | 1.33 |
| 47 | 20 | 302 | KC1 | CBA-CAA | 6.68 | 1.53 | 1.33 |
| 48 | 13 | 315 | A86 | C25-C26 | 6.68 | 1.63 | 1.43 |
| 48 | 37 | 314 | A86 | C25-C26 | 6.67 | 1.63 | 1.43 |
| 48 | 12 | 214 | A86 | C8-C6 | 6.67 | 1.60 | 1.46 |
| 47 | 17 | 306 | KC1 | CBA-CAA | 6.67 | 1.53 | 1.33 |
| 48 | 37 | 312 | A86 | C25-C26 | 6.67 | 1.63 | 1.43 |
| 47 | 21 | 207 | KC1 | CBA-CAA | 6.67 | 1.52 | 1.33 |
| 47 | 40 | 204 | KC1 | CBA-CAA | 6.67 | 1.52 | 1.33 |
| 47 | 41 | 207 | KC1 | CBA-CAA | 6.67 | 1.52 | 1.33 |
| 48 | 19 | 311 | A86 | C25-C26 | 6.66 | 1.63 | 1.43 |
| 48 | 31 | 319 | A86 | C25-C26 | 6.66 | 1.63 | 1.43 |
| 47 | 16 | 302 | KC1 | CBA-CAA | 6.66 | 1.52 | 1.33 |
| 48 | 36 | 310 | A86 | C19-C20 | 6.66 | 1.61 | 1.52 |
| 47 | 36 | 302 | KC1 | CBA-CAA | 6.66 | 1.52 | 1.33 |
| 47 | 18 | 210 | KC1 | CBA-CAA | 6.66 | 1.52 | 1.33 |
| 48 | 15 | 319 | A86 | C25-C26 | 6.66 | 1.63 | 1.43 |
| 48 | 35 | 319 | A86 | C25-C26 | 6.65 | 1.63 | 1.43 |
| 48 | 37 | 309 | A86 | C25-C26 | 6.65 | 1.63 | 1.43 |
| 47 | 35 | 302 | KC1 | CBA-CAA | 6.65 | 1.52 | 1.33 |
| 48 | 14 | 312 | A86 | C19-C20 | 6.65 | 1.61 | 1.52 |
| 48 | 34 | 312 | A86 | C19-C20 | 6.65 | 1.61 | 1.52 |
| 47 | 15 | 302 | KC1 | CBA-CAA | 6.65 | 1.52 | 1.33 |
| 47 | 38 | 210 | KC1 | CBA-CAA | 6.64 | 1.52 | 1.33 |
| 47 | 15 | 304 | KC1 | CBA-CAA | 6.64 | 1.52 | 1.33 |
| 47 | 12 | 206 | KC1 | CBA-CAA | 6.64 | 1.52 | 1.33 |
| 47 | 32 | 207 | KC1 | CBA-CAA | 6.64 | 1.52 | 1.33 |
| 50 | 39 | 312 | DD6 | C30-C29 | 6.64 | 1.38 | 1.20 |
| 47 | 13 | 306 | KC1 | CBA-CAA | 6.64 | 1.52 | 1.33 |
| 48 | 32 | 217 | A86 | C25-C26 | 6.64 | 1.63 | 1.43 |
| 47 | 14 | 304 | KC1 | CBA-CAA | 6.63 | 1.52 | 1.33 |
| 47 | 11 | 304 | KC1 | CBA-CAA | 6.63 | 1.52 | 1.33 |
| 47 | 34 | 306 | KC1 | CBA-CAA | 6.63 | 1.52 | 1.33 |
| 48 | 11 | 314 | A86 | C25-C26 | 6.63 | 1.63 | 1.43 |
| 47 | 34 | 304 | KC1 | CBA-CAA | 6.63 | 1.52 | 1.33 |
| 47 | 14 | 306 | KC1 | CBA-CAA | 6.62 | 1.52 | 1.33 |
| 48 | 39 | 311 | A86 | C25-C26 | 6.62 | 1.63 | 1.43 |
| 48 | 11 | 311 | A86 | C25-C26 | 6.62 | 1.63 | 1.43 |
| 48 | 17 | 320 | A86 | C25-C26 | 6.62 | 1.63 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 304 | KC1 | CBA-CAA | 6.62 | 1.52 | 1.33 |
| 48 | 17 | 310 | A86 | C25-C26 | 6.62 | 1.63 | 1.43 |
| 48 | 19 | 311 | A86 | C19-C20 | 6.62 | 1.61 | 1.52 |
| 48 | 39 | 311 | A86 | C19-C20 | 6.62 | 1.61 | 1.52 |
| 48 | 31 | 315 | A86 | C8-C6 | 6.62 | 1.60 | 1.46 |
| 47 | 31 | 305 | KC1 | CBA-CAA | 6.62 | 1.52 | 1.33 |
| 47 | 33 | 306 | KC1 | CBA-CAA | 6.62 | 1.52 | 1.33 |
| 50 | 41 | 216 | DD6 | C21-C20 | -6.61 | 1.41 | 1.51 |
| 50 | 19 | 312 | DD6 | C30-C29 | 6.61 | 1.38 | 1.20 |
| 48 | 33 | 311 | A86 | C25-C26 | 6.61 | 1.63 | 1.43 |
| 48 | 12 | 216 | A86 | C25-C26 | 6.61 | 1.63 | 1.43 |
| 47 | 31 | 307 | KC1 | CBA-CAA | 6.61 | 1.52 | 1.33 |
| 48 | 11 | 315 | A86 | C8-C6 | 6.61 | 1.60 | 1.46 |
| 48 | 13 | 311 | A86 | C25-C26 | 6.61 | 1.63 | 1.43 |
| 48 | 37 | 319 | A86 | C25-C26 | 6.61 | 1.63 | 1.43 |
| 48 | 16 | 310 | A86 | C19-C20 | 6.61 | 1.61 | 1.52 |
| 47 | 36 | 304 | KC1 | CBA-CAA | 6.60 | 1.52 | 1.33 |
| 48 | 37 | 314 | A86 | C19-C20 | 6.60 | 1.61 | 1.52 |
| 47 | 18 | 205 | KC1 | CBA-CAA | 6.60 | 1.52 | 1.33 |
| 47 | 11 | 306 | KC1 | CBA-CAA | 6.60 | 1.52 | 1.33 |
| 48 | 31 | 311 | A86 | C25-C26 | 6.59 | 1.63 | 1.43 |
| 47 | 16 | 304 | KC1 | CBA-CAA | 6.59 | 1.52 | 1.33 |
| 48 | 17 | 315 | A86 | C19-C20 | 6.59 | 1.61 | 1.52 |
| 48 | 12 | 220 | A86 | C8-C6 | 6.59 | 1.60 | 1.46 |
| 47 | 33 | 309 | KC1 | CBA-CAA | 6.59 | 1.52 | 1.33 |
| 47 | 38 | 205 | KC1 | CBA-CAA | 6.59 | 1.52 | 1.33 |
| 50 | 21 | 216 | DD6 | C21-C20 | -6.59 | 1.42 | 1.51 |
| 48 | 36 | 311 | A86 | C25-C26 | 6.59 | 1.63 | 1.43 |
| 48 | 16 | 311 | A86 | C25-C26 | 6.59 | 1.63 | 1.43 |
| 47 | 37 | 302 | KC1 | CBA-CAA | 6.58 | 1.52 | 1.33 |
| 48 | 11 | 313 | A86 | C25-C26 | 6.58 | 1.63 | 1.43 |
| 48 | 17 | 320 | A86 | C19-C20 | 6.58 | 1.61 | 1.52 |
| 47 | 17 | 303 | KC1 | CBA-CAA | 6.58 | 1.52 | 1.33 |
| 48 | 32 | 221 | A86 | C8-C6 | 6.58 | 1.60 | 1.46 |
| 47 | 12 | 211 | KC1 | CBA-CAA | 6.58 | 1.52 | 1.33 |
| 48 | 14 | 312 | A86 | C25-C26 | 6.57 | 1.63 | 1.43 |
| 47 | 35 | 306 | KC1 | CBA-CAA | 6.57 | 1.52 | 1.33 |
| 47 | 32 | 212 | KC1 | CBA-CAA | 6.57 | 1.52 | 1.33 |
| 48 | 31 | 314 | A86 | C25-C26 | 6.56 | 1.63 | 1.43 |
| 47 | 31 | 303 | KC1 | CBA-CAA | 6.56 | 1.52 | 1.33 |
| 48 | 14 | 313 | A86 | C19-C20 | 6.56 | 1.61 | 1.52 |
| 47 | 15 | 306 | KC1 | CBA-CAA | 6.55 | 1.52 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 38 | 213 | A86 | C25-C26 | 6.55 | 1.63 | 1.43 |
| 50 | 40 | 212 | DD6 | C30-C31 | 6.54 | 1.54 | 1.42 |
| 48 | 34 | 313 | A86 | C19-C20 | 6.54 | 1.61 | 1.52 |
| 47 | 11 | 302 | KC1 | CBA-CAA | 6.54 | 1.52 | 1.33 |
| 48 | 34 | 312 | A86 | C25-C26 | 6.54 | 1.63 | 1.43 |
| 47 | 13 | 309 | KC1 | CBA-CAA | 6.54 | 1.52 | 1.33 |
| 47 | 13 | 302 | KC1 | CBA-CAA | 6.53 | 1.52 | 1.33 |
| 47 | 33 | 302 | KC1 | CBA-CAA | 6.53 | 1.52 | 1.33 |
| 50 | 36 | 312 | DD6 | C21-C20 | -6.53 | 1.42 | 1.51 |
| 50 | 20 | 310 | DD6 | C30-C31 | 6.53 | 1.54 | 1.42 |
| 47 | 20 | 304 | KC1 | CBA-CAA | 6.52 | 1.52 | 1.33 |
| 50 | 16 | 312 | DD6 | C21-C20 | -6.52 | 1.42 | 1.51 |
| 48 | 33 | 315 | A86 | C19-C20 | 6.52 | 1.61 | 1.52 |
| 48 | 18 | 213 | A86 | C25-C26 | 6.51 | 1.63 | 1.43 |
| 47 | 21 | 203 | KC1 | CBA-CAA | 6.51 | 1.52 | 1.33 |
| 47 | 41 | 203 | KC1 | CBA-CAA | 6.51 | 1.52 | 1.33 |
| 48 | 34 | 311 | A86 | C25-C26 | 6.51 | 1.63 | 1.43 |
| 47 | 40 | 206 | KC1 | CBA-CAA | 6.51 | 1.52 | 1.33 |
| 47 | 14 | 309 | KC1 | CBA-CAA | 6.51 | 1.52 | 1.33 |
| 48 | 32 | 221 | A86 | C19-C20 | 6.50 | 1.61 | 1.52 |
| 48 | 13 | 315 | A86 | C19-C20 | 6.50 | 1.61 | 1.52 |
| 48 | 32 | 214 | A86 | C25-C26 | 6.50 | 1.63 | 1.43 |
| 48 | 12 | 220 | A86 | C19-C20 | 6.49 | 1.61 | 1.52 |
| 48 | 37 | 313 | A86 | C25-C26 | 6.49 | 1.63 | 1.43 |
| 47 | 34 | 309 | KC1 | CBA-CAA | 6.49 | 1.52 | 1.33 |
| 48 | 14 | 311 | A86 | C25-C26 | 6.48 | 1.63 | 1.43 |
| 48 | 37 | 311 | A86 | C19-C20 | 6.46 | 1.61 | 1.52 |
| 50 | 40 | 212 | DD6 | C21-C20 | -6.45 | 1.42 | 1.51 |
| 48 | 12 | 220 | A86 | C25-C26 | 6.43 | 1.63 | 1.43 |
| 48 | 36 | 313 | A86 | C25-C26 | 6.43 | 1.63 | 1.43 |
| 47 | 31 | 309 | KC1 | CBA-CAA | 6.42 | 1.52 | 1.33 |
| 47 | 11 | 309 | KC1 | CBA-CAA | 6.42 | 1.52 | 1.33 |
| 48 | 32 | 221 | A86 | C25-C26 | 6.41 | 1.63 | 1.43 |
| 48 | 17 | 314 | A86 | C25-C26 | 6.41 | 1.63 | 1.43 |
| 48 | 12 | 202 | A86 | C25-C26 | 6.41 | 1.63 | 1.43 |
| 48 | 32 | 203 | A86 | C25-C26 | 6.41 | 1.63 | 1.43 |
| 48 | 16 | 314 | A86 | C25-C26 | 6.41 | 1.63 | 1.43 |
| 48 | 36 | 311 | A86 | C19-C20 | 6.41 | 1.61 | 1.52 |
| 48 | 12 | 213 | A86 | C25-C26 | 6.40 | 1.63 | 1.43 |
| 48 | 17 | 312 | A86 | C19-C20 | 6.40 | 1.61 | 1.52 |
| 50 | 20 | 310 | DD6 | C21-C20 | -6.39 | 1.42 | 1.51 |
| 48 | 16 | 311 | A86 | C19-C20 | 6.37 | 1.61 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 16 | 310 | A86 | C25-C26 | 6.37 | 1.62 | 1.43 |
| 48 | 35 | 319 | A86 | C19-C20 | 6.36 | 1.61 | 1.52 |
| 48 | 36 | 310 | A86 | C25-C26 | 6.36 | 1.62 | 1.43 |
| 48 | 15 | 319 | A86 | C19-C20 | 6.35 | 1.61 | 1.52 |
| 48 | 12 | 202 | A86 | C19-C20 | 6.33 | 1.61 | 1.52 |
| 48 | 32 | 203 | A86 | C19-C20 | 6.32 | 1.61 | 1.52 |
| 47 | 12 | 208 | KC1 | CBA-CAA | 6.28 | 1.51 | 1.33 |
| 47 | 32 | 209 | KC1 | CBA-CAA | 6.27 | 1.51 | 1.33 |
| 48 | 14 | 316 | A86 | C19-C20 | 6.26 | 1.61 | 1.52 |
| 50 | 21 | 212 | DD6 | C21-C20 | -6.25 | 1.42 | 1.51 |
| 48 | 31 | 312 | A86 | C19-C20 | 6.24 | 1.61 | 1.52 |
| 48 | 11 | 312 | A86 | C19-C20 | 6.21 | 1.60 | 1.52 |
| 48 | 34 | 316 | A86 | C19-C20 | 6.20 | 1.60 | 1.52 |
| 50 | 41 | 212 | DD6 | C21-C20 | -6.19 | 1.42 | 1.51 |
| 48 | 38 | 215 | A86 | C19-C20 | 6.15 | 1.60 | 1.52 |
| 48 | 12 | 217 | A86 | C19-C20 | 6.10 | 1.60 | 1.52 |
| 48 | 18 | 215 | A86 | C19-C20 | 6.08 | 1.60 | 1.52 |
| 48 | 32 | 218 | A86 | C19-C20 | 6.05 | 1.60 | 1.52 |
| 48 | 31 | 319 | A86 | C19-C20 | 6.03 | 1.60 | 1.52 |
| 47 | 15 | 302 | KC1 | O2A-CGA | 6.03 | 1.45 | 1.30 |
| 48 | 11 | 319 | A86 | C19-C20 | 6.03 | 1.60 | 1.52 |
| 48 | 11 | 315 | A86 | C19-C20 | 6.02 | 1.60 | 1.52 |
| 48 | 31 | 315 | A86 | C19-C20 | 6.02 | 1.60 | 1.52 |
| 47 | 17 | 306 | KC1 | O2A-CGA | 6.02 | 1.45 | 1.30 |
| 47 | 18 | 205 | KC1 | O2A-CGA | 6.02 | 1.45 | 1.30 |
| 47 | 38 | 205 | KC1 | O2A-CGA | 6.02 | 1.45 | 1.30 |
| 47 | 15 | 304 | KC1 | O2A-CGA | 6.02 | 1.45 | 1.30 |
| 47 | 35 | 302 | KC1 | O2A-CGA | 6.01 | 1.45 | 1.30 |
| 48 | 31 | 311 | A86 | C19-C20 | 6.01 | 1.60 | 1.52 |
| 47 | 20 | 304 | KC1 | O2A-CGA | 6.01 | 1.45 | 1.30 |
| 47 | 21 | 203 | KC1 | O2A-CGA | 6.01 | 1.45 | 1.30 |
| 47 | 40 | 206 | KC1 | O2A-CGA | 6.00 | 1.45 | 1.30 |
| 48 | 11 | 311 | A86 | C19-C20 | 5.99 | 1.60 | 1.52 |
| 47 | 15 | 306 | KC1 | O2A-CGA | 5.99 | 1.45 | 1.30 |
| 47 | 35 | 306 | KC1 | O2A-CGA | 5.99 | 1.45 | 1.30 |
| 50 | 19 | 312 | DD6 | C30-C31 | 5.99 | 1.53 | 1.42 |
| 47 | 35 | 309 | KC1 | O2A-CGA | 5.99 | 1.45 | 1.30 |
| 47 | 41 | 203 | KC1 | O2A-CGA | 5.99 | 1.45 | 1.30 |
| 47 | 13 | 306 | KC1 | O2A-CGA | 5.98 | 1.45 | 1.30 |
| 47 | 20 | 305 | KC1 | O2A-CGA | 5.98 | 1.45 | 1.30 |
| 50 | 39 | 312 | DD6 | C30-C31 | 5.98 | 1.53 | 1.42 |
| 47 | 37 | 305 | KC1 | O2A-CGA | 5.97 | 1.45 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 304 | KC1 | O2A-CGA | 5.97 | 1.45 | 1.30 |
| 47 | 40 | 204 | KC1 | O2A-CGA | 5.97 | 1.45 | 1.30 |
| 47 | 36 | 302 | KC1 | O2A-CGA | 5.97 | 1.45 | 1.30 |
| 47 | 21 | 207 | KC1 | O2A-CGA | 5.96 | 1.45 | 1.30 |
| 47 | 40 | 207 | KC1 | O2A-CGA | 5.96 | 1.45 | 1.30 |
| 47 | 36 | 304 | KC1 | O2A-CGA | 5.96 | 1.45 | 1.30 |
| 47 | 33 | 302 | KC1 | O2A-CGA | 5.96 | 1.45 | 1.30 |
| 47 | 16 | 304 | KC1 | O2A-CGA | 5.96 | 1.45 | 1.30 |
| 47 | 16 | 308 | KC1 | O2A-CGA | 5.96 | 1.45 | 1.30 |
| 47 | 15 | 309 | KC1 | O2A-CGA | 5.96 | 1.45 | 1.30 |
| 47 | 19 | 308 | KC1 | O2A-CGA | 5.96 | 1.45 | 1.30 |
| 47 | 36 | 308 | KC1 | O2A-CGA | 5.95 | 1.45 | 1.30 |
| 47 | 38 | 207 | KC1 | O2A-CGA | 5.95 | 1.45 | 1.30 |
| 47 | 34 | 306 | KC1 | O2A-CGA | 5.95 | 1.45 | 1.30 |
| 47 | 17 | 308 | KC1 | O2A-CGA | 5.95 | 1.45 | 1.30 |
| 47 | 41 | 207 | KC1 | O2A-CGA | 5.94 | 1.45 | 1.30 |
| 47 | 20 | 302 | KC1 | O2A-CGA | 5.94 | 1.45 | 1.30 |
| 47 | 13 | 302 | KC1 | O2A-CGA | 5.94 | 1.45 | 1.30 |
| 47 | 13 | 304 | KC1 | O2A-CGA | 5.94 | 1.45 | 1.30 |
| 47 | 16 | 305 | KC1 | O2A-CGA | 5.94 | 1.45 | 1.30 |
| 47 | 33 | 304 | KC1 | O2A-CGA | 5.94 | 1.45 | 1.30 |
| 47 | 41 | 203 | KC1 | C3B-C2B | 5.93 | 1.49 | 1.37 |
| 47 | 37 | 307 | KC1 | O2A-CGA | 5.93 | 1.45 | 1.30 |
| 47 | 18 | 207 | KC1 | O2A-CGA | 5.93 | 1.45 | 1.30 |
| 47 | 33 | 306 | KC1 | O2A-CGA | 5.93 | 1.45 | 1.30 |
| 47 | 17 | 305 | KC1 | O2A-CGA | 5.93 | 1.45 | 1.30 |
| 47 | 16 | 302 | KC1 | O2A-CGA | 5.93 | 1.45 | 1.30 |
| 47 | 39 | 308 | KC1 | O2A-CGA | 5.93 | 1.45 | 1.30 |
| 47 | 21 | 203 | KC1 | C3B-C2B | 5.92 | 1.49 | 1.37 |
| 47 | 37 | 304 | KC1 | O2A-CGA | 5.91 | 1.45 | 1.30 |
| 47 | 36 | 305 | KC1 | O2A-CGA | 5.91 | 1.45 | 1.30 |
| 50 | 41 | 216 | DD6 | C13-C14 | 5.90 | 1.45 | 1.32 |
| 50 | 21 | 216 | DD6 | C13-C14 | 5.90 | 1.45 | 1.32 |
| 47 | 14 | 306 | KC1 | O2A-CGA | 5.90 | 1.45 | 1.30 |
| 47 | 38 | 210 | KC1 | O2A-CGA | 5.89 | 1.45 | 1.30 |
| 47 | 11 | 304 | KC1 | O2A-CGA | 5.89 | 1.45 | 1.30 |
| 48 | 11 | 313 | A86 | C19-C20 | 5.89 | 1.60 | 1.52 |
| 47 | 18 | 210 | KC1 | O2A-CGA | 5.89 | 1.45 | 1.30 |
| 48 | 16 | 314 | A86 | C19-C20 | 5.89 | 1.60 | 1.52 |
| 47 | 31 | 305 | KC1 | O2A-CGA | 5.88 | 1.45 | 1.30 |
| 47 | 17 | 303 | KC1 | O2A-CGA | 5.87 | 1.45 | 1.30 |
| 47 | 37 | 302 | KC1 | O2A-CGA | 5.87 | 1.45 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 13 | 309 | KC1 | O2A-CGA | 5.87 | 1.45 | 1.30 |
| 48 | 31 | 313 | A86 | C19-C20 | 5.86 | 1.60 | 1.52 |
| 47 | 14 | 304 | KC1 | O2A-CGA | 5.86 | 1.45 | 1.30 |
| 47 | 33 | 309 | KC1 | O2A-CGA | 5.83 | 1.45 | 1.30 |
| 47 | 31 | 307 | KC1 | O2A-CGA | 5.83 | 1.45 | 1.30 |
| 47 | 11 | 306 | KC1 | O2A-CGA | 5.82 | 1.45 | 1.30 |
| 47 | 34 | 304 | KC1 | O2A-CGA | 5.82 | 1.45 | 1.30 |
| 48 | 36 | 313 | A86 | C19-C20 | 5.81 | 1.60 | 1.52 |
| 47 | 34 | 309 | KC1 | O2A-CGA | 5.79 | 1.45 | 1.30 |
| 47 | 14 | 309 | KC1 | O2A-CGA | 5.77 | 1.45 | 1.30 |
| 50 | 20 | 312 | DD6 | C13-C14 | 5.77 | 1.45 | 1.32 |
| 50 | 40 | 214 | DD6 | C13-C14 | 5.77 | 1.45 | 1.32 |
| 47 | 12 | 206 | KC1 | O2A-CGA | 5.76 | 1.45 | 1.30 |
| 47 | 32 | 207 | KC1 | O2A-CGA | 5.76 | 1.45 | 1.30 |
| 47 | 31 | 303 | KC1 | O2A-CGA | 5.76 | 1.45 | 1.30 |
| 47 | 32 | 212 | KC1 | O2A-CGA | 5.76 | 1.45 | 1.30 |
| 47 | 11 | 302 | KC1 | O2A-CGA | 5.76 | 1.45 | 1.30 |
| 47 | 11 | 302 | KC1 | C3B-C2B | 5.73 | 1.48 | 1.37 |
| 47 | 31 | 303 | KC1 | C3B-C2B | 5.73 | 1.48 | 1.37 |
| 47 | 12 | 211 | KC1 | O2A-CGA | 5.73 | 1.45 | 1.30 |
| 47 | 31 | 309 | KC1 | O2A-CGA | 5.68 | 1.44 | 1.30 |
| 47 | 11 | 309 | KC1 | O2A-CGA | 5.67 | 1.44 | 1.30 |
| 47 | 16 | 304 | KC1 | C3B-C2B | 5.65 | 1.48 | 1.37 |
| 47 | 20 | 305 | KC1 | C3B-C2B | 5.65 | 1.48 | 1.37 |
| 47 | 36 | 304 | KC1 | C3B-C2B | 5.64 | 1.48 | 1.37 |
| 47 | 40 | 207 | KC1 | C3B-C2B | 5.64 | 1.48 | 1.37 |
| 45 | D | 408 | PL9 | C3-C4 | -5.63 | 1.40 | 1.49 |
| 45 | d | 406 | PL9 | C3-C4 | -5.62 | 1.40 | 1.49 |
| 37 | 17 | 309 | CLA | C3C-C2C | 5.60 | 1.48 | 1.36 |
| 47 | 18 | 205 | KC1 | C3B-C2B | 5.60 | 1.48 | 1.37 |
| 47 | 35 | 304 | KC1 | C3B-C2B | 5.59 | 1.48 | 1.37 |
| 47 | 15 | 304 | KC1 | C3B-C2B | 5.59 | 1.48 | 1.37 |
| 47 | 38 | 205 | KC1 | C3B-C2B | 5.57 | 1.48 | 1.37 |
| 47 | 12 | 206 | KC1 | C3C-C2C | 5.57 | 1.48 | 1.36 |
| 47 | 32 | 207 | KC1 | C3C-C2C | 5.53 | 1.48 | 1.36 |
| 47 | 15 | 306 | KC1 | C3B-C2B | 5.51 | 1.48 | 1.37 |
| 47 | 39 | 308 | KC1 | C3B-C2B | 5.50 | 1.48 | 1.37 |
| 37 | 37 | 308 | CLA | C3C-C2C | 5.49 | 1.48 | 1.36 |
| 37 | 38 | 211 | CLA | C3C-C2C | 5.48 | 1.48 | 1.36 |
| 50 | 19 | 312 | DD6 | C13-C14 | 5.48 | 1.44 | 1.32 |
| 47 | 15 | 309 | KC1 | C3B-C2B | 5.47 | 1.48 | 1.37 |
| 47 | 35 | 309 | KC1 | C3B-C2B | 5.47 | 1.48 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 37 | 301 | CLA | C3C-C2C | 5.47 | 1.48 | 1.36 |
| 47 | 19 | 308 | KC1 | C3B-C2B | 5.47 | 1.48 | 1.37 |
| 47 | 35 | 306 | KC1 | C3B-C2B | 5.47 | 1.48 | 1.37 |
| 47 | 33 | 304 | KC1 | C3B-C2B | 5.46 | 1.48 | 1.37 |
| 50 | 39 | 312 | DD6 | C13-C14 | 5.46 | 1.44 | 1.32 |
| 47 | 18 | 210 | KC1 | C3B-C2B | 5.45 | 1.48 | 1.37 |
| 47 | 32 | 209 | KC1 | O2A-CGA | 5.45 | 1.44 | 1.30 |
| 37 | 31 | 308 | CLA | C3C-C2C | 5.45 | 1.48 | 1.36 |
| 47 | 17 | 303 | KC1 | C3B-C2B | 5.44 | 1.48 | 1.37 |
| 47 | 13 | 304 | KC1 | C3B-C2B | 5.44 | 1.48 | 1.37 |
| 47 | 38 | 207 | KC1 | C3B-C2B | 5.44 | 1.48 | 1.37 |
| 37 | 11 | 307 | CLA | C3C-C2C | 5.44 | 1.48 | 1.36 |
| 47 | 12 | 208 | KC1 | O2A-CGA | 5.44 | 1.44 | 1.30 |
| 47 | 38 | 210 | KC1 | C3B-C2B | 5.43 | 1.48 | 1.37 |
| 47 | 14 | 304 | KC1 | C3B-C2B | 5.43 | 1.48 | 1.37 |
| 37 | 33 | 307 | CLA | O2D-CGD | 5.42 | 1.46 | 1.33 |
| 47 | 14 | 304 | KC1 | C3C-C2C | 5.42 | 1.48 | 1.36 |
| 50 | 20 | 312 | DD6 | C3-C2 | 5.42 | 1.60 | 1.43 |
| 37 | 35 | 310 | CLA | C3C-C2C | 5.41 | 1.48 | 1.36 |
| 37 | 13 | 307 | CLA | O2D-CGD | 5.41 | 1.46 | 1.33 |
| 37 | 17 | 302 | CLA | C3C-C2C | 5.41 | 1.48 | 1.36 |
| 47 | 34 | 304 | KC1 | C3C-C2C | 5.41 | 1.48 | 1.36 |
| 47 | 34 | 304 | KC1 | C3B-C2B | 5.39 | 1.48 | 1.37 |
| 47 | 37 | 304 | KC1 | C3B-C2B | 5.39 | 1.48 | 1.37 |
| 50 | 40 | 214 | DD6 | C3-C2 | 5.39 | 1.59 | 1.43 |
| 37 | 15 | 310 | CLA | C3C-C2C | 5.38 | 1.48 | 1.36 |
| 37 | 41 | 202 | CLA | C3C-C2C | 5.38 | 1.48 | 1.36 |
| 37 | 21 | 202 | CLA | C3C-C2C | 5.38 | 1.48 | 1.36 |
| 47 | 41 | 207 | KC1 | C3B-C2B | 5.37 | 1.48 | 1.37 |
| 47 | 37 | 305 | KC1 | C3B-C2B | 5.37 | 1.48 | 1.37 |
| 47 | 11 | 304 | KC1 | C3B-C2B | 5.37 | 1.48 | 1.37 |
| 47 | 31 | 305 | KC1 | C3B-C2B | 5.37 | 1.48 | 1.37 |
| 37 | 21 | 210 | CLA | C3C-C2C | 5.36 | 1.48 | 1.36 |
| 47 | 13 | 306 | KC1 | C3B-C2B | 5.36 | 1.48 | 1.37 |
| 37 | 41 | 210 | CLA | C3C-C2C | 5.36 | 1.48 | 1.36 |
| 47 | 37 | 302 | KC1 | C3B-C2B | 5.35 | 1.48 | 1.37 |
| 47 | 21 | 207 | KC1 | C3B-C2B | 5.35 | 1.48 | 1.37 |
| 50 | 21 | 216 | DD6 | C3-C2 | 5.34 | 1.59 | 1.43 |
| 47 | 17 | 308 | KC1 | C3B-C2B | 5.34 | 1.48 | 1.37 |
| 50 | 41 | 216 | DD6 | C3-C2 | 5.33 | 1.59 | 1.43 |
| 47 | 33 | 306 | KC1 | C3B-C2B | 5.33 | 1.48 | 1.37 |
| 47 | 40 | 206 | KC1 | C3B-C2B | 5.32 | 1.48 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 17 | 306 | KC1 | C3B-C2B | 5.31 | 1.48 | 1.37 |
| 47 | 17 | 306 | KC1 | C3C-C2C | 5.31 | 1.48 | 1.36 |
| 47 | 37 | 305 | KC1 | C3C-C2C | 5.31 | 1.48 | 1.36 |
| 37 | z | 102 | CLA | O2D-CGD | 5.31 | 1.46 | 1.33 |
| 37 | Z | 102 | CLA | O2D-CGD | 5.31 | 1.46 | 1.33 |
| 47 | 37 | 307 | KC1 | C3B-C2B | 5.30 | 1.47 | 1.37 |
| 47 | 20 | 304 | KC1 | C3B-C2B | 5.29 | 1.47 | 1.37 |
| 37 | 31 | 301 | CLA | C3C-C2C | 5.28 | 1.48 | 1.36 |
| 37 | z | 101 | CLA | C3C-C2C | 5.28 | 1.48 | 1.36 |
| 47 | 16 | 305 | KC1 | C3B-C2B | 5.27 | 1.47 | 1.37 |
| 47 | 20 | 305 | KC1 | C3C-C2C | 5.27 | 1.48 | 1.36 |
| 37 | 35 | 305 | CLA | C3C-C2C | 5.27 | 1.48 | 1.36 |
| 37 | Z | 102 | CLA | C3C-C2C | 5.26 | 1.48 | 1.36 |
| 37 | D | 401 | CLA | C3C-C2C | 5.26 | 1.48 | 1.36 |
| 37 | 38 | 204 | CLA | O2D-CGD | 5.26 | 1.46 | 1.33 |
| 47 | 32 | 212 | KC1 | C3B-C2B | 5.25 | 1.47 | 1.37 |
| 37 | 35 | 301 | CLA | C3C-C2C | 5.25 | 1.48 | 1.36 |
| 37 | 38 | 206 | CLA | C3C-C2C | 5.25 | 1.48 | 1.36 |
| 47 | 15 | 302 | KC1 | C3C-C2C | 5.25 | 1.48 | 1.36 |
| 37 | Z | 101 | CLA | C3C-C2C | 5.25 | 1.48 | 1.36 |
| 47 | 36 | 305 | KC1 | C3B-C2B | 5.25 | 1.47 | 1.37 |
| 37 | a | 404 | CLA | C3C-C2C | 5.24 | 1.48 | 1.36 |
| 47 | 17 | 305 | KC1 | C3B-C2B | 5.24 | 1.47 | 1.37 |
| 47 | 16 | 305 | KC1 | C3C-C2C | 5.24 | 1.48 | 1.36 |
| 37 | 18 | 206 | CLA | C3C-C2C | 5.24 | 1.48 | 1.36 |
| 37 | W | 102 | CLA | C3C-C2C | 5.24 | 1.48 | 1.36 |
| 45 | d | 406 | PL9 | C7-C3 | -5.24 | 1.44 | 1.51 |
| 37 | z | 102 | CLA | C3C-C2C | 5.23 | 1.48 | 1.36 |
| 37 | 15 | 305 | CLA | C3C-C2C | 5.23 | 1.48 | 1.36 |
| 47 | 18 | 207 | KC1 | C3B-C2B | 5.23 | 1.47 | 1.37 |
| 37 | 21 | 209 | CLA | C3C-C2C | 5.23 | 1.48 | 1.36 |
| 37 | 41 | 209 | CLA | C3C-C2C | 5.23 | 1.48 | 1.36 |
| 37 | 39 | 304 | CLA | C3C-C2C | 5.22 | 1.48 | 1.36 |
| 37 | 18 | 204 | CLA | O2D-CGD | 5.22 | 1.46 | 1.33 |
| 37 | 38 | 201 | CLA | C3C-C2C | 5.22 | 1.48 | 1.36 |
| 37 | 34 | 310 | CLA | C3C-C2C | 5.22 | 1.48 | 1.36 |
| 47 | 11 | 306 | KC1 | C3B-C2B | 5.22 | 1.47 | 1.37 |
| 47 | 31 | 307 | KC1 | C3B-C2B | 5.22 | 1.47 | 1.37 |
| 47 | 14 | 309 | KC1 | C3B-C2B | 5.21 | 1.47 | 1.37 |
| 37 | 15 | 301 | CLA | C3C-C2C | 5.21 | 1.48 | 1.36 |
| 37 | 37 | 308 | CLA | O2D-CGD | 5.21 | 1.46 | 1.33 |
| 37 | 20 | 307 | CLA | C3C-C2C | 5.21 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 209 | CLA | O2D-CGD | 5.20 | 1.46 | 1.33 |
| 37 | 19 | 304 | CLA | C3C-C2C | 5.20 | 1.48 | 1.36 |
| 47 | 40 | 207 | KC1 | C3C-C2C | 5.20 | 1.48 | 1.36 |
| 37 | 16 | 309 | CLA | C3C-C2C | 5.20 | 1.48 | 1.36 |
| 47 | 36 | 308 | KC1 | C3B-C2B | 5.20 | 1.47 | 1.37 |
| 47 | 16 | 308 | KC1 | C3B-C2B | 5.20 | 1.47 | 1.37 |
| 37 | 13 | 310 | CLA | C3C-C2C | 5.20 | 1.48 | 1.36 |
| 47 | 34 | 309 | KC1 | C3B-C2B | 5.20 | 1.47 | 1.37 |
| 37 | 20 | 303 | CLA | O2D-CGD | 5.19 | 1.46 | 1.33 |
| 47 | 18 | 205 | KC1 | C3C-C2C | 5.19 | 1.48 | 1.36 |
| 37 | c | 512 | CLA | C3C-C2C | 5.19 | 1.48 | 1.36 |
| 37 | 14 | 310 | CLA | C3C-C2C | 5.19 | 1.48 | 1.36 |
| 47 | 36 | 305 | KC1 | C3C-C2C | 5.18 | 1.48 | 1.36 |
| 50 | 21 | 212 | DD6 | C13-C14 | 5.18 | 1.44 | 1.32 |
| 50 | 16 | 312 | DD6 | C13-C14 | 5.18 | 1.44 | 1.32 |
| 37 | 38 | 209 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 37 | 40 | 209 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 47 | 13 | 309 | KC1 | C3B-C2B | 5.18 | 1.47 | 1.37 |
| 47 | 33 | 309 | KC1 | C3B-C2B | 5.18 | 1.47 | 1.37 |
| 37 | 41 | 209 | CLA | O2D-CGD | 5.18 | 1.46 | 1.33 |
| 37 | 36 | 309 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 47 | 41 | 207 | KC1 | O2D-CGD | 5.18 | 1.46 | 1.33 |
| 47 | 35 | 302 | KC1 | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 37 | 12 | 212 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 37 | 38 | 209 | CLA | O2D-CGD | 5.18 | 1.46 | 1.33 |
| 47 | 12 | 211 | KC1 | C3B-C2B | 5.17 | 1.47 | 1.37 |
| 50 | 41 | 212 | DD6 | C13-C14 | 5.17 | 1.44 | 1.32 |
| 37 | 18 | 209 | CLA | O2D-CGD | 5.17 | 1.45 | 1.33 |
| 37 | 40 | 205 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 37 | C | 512 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 37 | 33 | 310 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 37 | 21 | 205 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 37 | 33 | 305 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 47 | 21 | 207 | KC1 | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 37 | 38 | 202 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 37 | 14 | 305 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 37 | 21 | 208 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 37 | 34 | 305 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 50 | 36 | 312 | DD6 | C13-C14 | 5.15 | 1.44 | 1.32 |
| 37 | 15 | 303 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 47 | 12 | 206 | KC1 | C3B-C2B | 5.15 | 1.47 | 1.37 |
| 47 | 32 | 207 | KC1 | C3B-C2B | 5.15 | 1.47 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 38 | 205 | KC1 | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 37 | 37 | 303 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 47 | 15 | 304 | KC1 | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 37 | 17 | 309 | CLA | O2D-CGD | 5.15 | 1.45 | 1.33 |
| 47 | 21 | 203 | KC1 | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 37 | 41 | 205 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 45 | D | 408 | PL9 | C7-C3 | -5.14 | 1.44 | 1.51 |
| 47 | 36 | 304 | KC1 | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 37 | 32 | 213 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 37 | 41 | 208 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 47 | 41 | 203 | KC1 | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 37 | 13 | 305 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 37 | 18 | 209 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 50 | 20 | 310 | DD6 | C3-C2 | 5.13 | 1.59 | 1.43 |
| 37 | 35 | 303 | CLA | C3C-C2C | 5.13 | 1.47 | 1.36 |
| 37 | 15 | 310 | CLA | O2D-CGD | 5.13 | 1.45 | 1.33 |
| 50 | 20 | 310 | DD6 | C13-C14 | 5.13 | 1.44 | 1.32 |
| 37 | D | 402 | CLA | C3C-C2C | 5.13 | 1.47 | 1.36 |
| 47 | 14 | 306 | KC1 | C3B-C2B | 5.13 | 1.47 | 1.37 |
| 37 | 36 | 307 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 50 | 16 | 312 | DD6 | C3-C2 | 5.12 | 1.59 | 1.43 |
| 47 | 16 | 304 | KC1 | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 37 | d | 401 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 37 | 17 | 304 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 37 | 16 | 307 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 47 | 15 | 306 | KC1 | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 47 | 35 | 304 | KC1 | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 37 | 15 | 301 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 37 | 15 | 308 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 37 | 18 | 211 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 50 | 40 | 212 | DD6 | C3-C2 | 5.12 | 1.59 | 1.43 |
| 37 | 14 | 303 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 47 | 20 | 302 | KC1 | C3B-C2B | 5.11 | 1.47 | 1.37 |
| 37 | 35 | 301 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 37 | 35 | 310 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 37 | 18 | 203 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 50 | 40 | 212 | DD6 | C13-C14 | 5.11 | 1.43 | 1.32 |
| 37 | 13 | 303 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 37 | 21 | 202 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 47 | 40 | 204 | KC1 | C3B-C2B | 5.11 | 1.47 | 1.37 |
| 37 | 38 | 203 | CLA | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 50 | 36 | 312 | DD6 | C3-C2 | 5.10 | 1.59 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 33 | 308 | CLA | C3C-C2C | 5.10 | 1.47 | 1.36 |
| 47 | 34 | 306 | KC1 | C3B-C2B | 5.10 | 1.47 | 1.37 |
| 37 | 18 | 202 | CLA | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 47 | 35 | 302 | KC1 | C3B-C2B | 5.10 | 1.47 | 1.37 |
| 47 | 33 | 302 | KC1 | C3C-C2C | 5.10 | 1.47 | 1.36 |
| 47 | 38 | 205 | KC1 | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 37 | 33 | 303 | CLA | C3C-C2C | 5.10 | 1.47 | 1.36 |
| 47 | 35 | 306 | KC1 | C3C-C2C | 5.10 | 1.47 | 1.36 |
| 37 | 13 | 305 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 37 | 21 | 205 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 37 | 21 | 204 | CLA | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 37 | z | 101 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 47 | 19 | 308 | KC1 | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 37 | 18 | 206 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 37 | 13 | 303 | CLA | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 47 | 31 | 307 | KC1 | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 37 | 34 | 303 | CLA | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 47 | 36 | 302 | KC1 | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 37 | 33 | 305 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 47 | 16 | 308 | KC1 | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 37 | Z | 101 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 37 | 37 | 301 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 37 | 32 | 208 | CLA | C3C-C2C | 5.08 | 1.47 | 1.36 |
| 37 | 20 | 308 | CLA | C3C-C2C | 5.08 | 1.47 | 1.36 |
| 37 | 21 | 208 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 47 | 35 | 304 | KC1 | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 37 | 17 | 302 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 47 | 16 | 302 | KC1 | C3B-C2B | 5.08 | 1.47 | 1.37 |
| 37 | 41 | 205 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 37 | 41 | 204 | CLA | C3C-C2C | 5.07 | 1.47 | 1.36 |
| 37 | 13 | 308 | CLA | C3C-C2C | 5.07 | 1.47 | 1.36 |
| 47 | 35 | 302 | KC1 | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 37 | 38 | 206 | CLA | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 47 | 11 | 309 | KC1 | C3B-C2B | 5.06 | 1.47 | 1.37 |
| 37 | 18 | 202 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 37 | 12 | 207 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 47 | 13 | 302 | KC1 | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 47 | 18 | 205 | KC1 | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 37 | 38 | 204 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 37 | 38 | 211 | CLA | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 37 | 31 | 310 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 37 | 40 | 210 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 41 | 202 | CLA | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 37 | 31 | 301 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 37 | 37 | 306 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 37 | 18 | 211 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 47 | 11 | 306 | KC1 | C3C-C2C | 5.05 | 1.47 | 1.36 |
| 37 | 33 | 310 | CLA | C1D-ND | 5.05 | 1.44 | 1.37 |
| 47 | 35 | 304 | KC1 | CHD-C4C | 5.05 | 1.48 | 1.38 |
| 37 | 35 | 305 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 47 | 39 | 308 | KC1 | C3C-C2C | 5.05 | 1.47 | 1.36 |
| 37 | 19 | 302 | CLA | C3C-C2C | 5.05 | 1.47 | 1.36 |
| 47 | 36 | 302 | KC1 | C3B-C2B | 5.05 | 1.47 | 1.37 |
| 37 | 17 | 307 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 37 | 16 | 301 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 37 | 16 | 306 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 37 | 39 | 302 | CLA | C3C-C2C | 5.04 | 1.47 | 1.36 |
| 47 | 14 | 304 | KC1 | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 37 | 17 | 304 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 37 | W | 102 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 47 | 36 | 308 | KC1 | C3C-C2C | 5.04 | 1.47 | 1.36 |
| 37 | 14 | 302 | CLA | C3C-C2C | 5.04 | 1.47 | 1.36 |
| 37 | 40 | 203 | CLA | C3C-C2C | 5.04 | 1.47 | 1.36 |
| 50 | 21 | 212 | DD6 | C3-C2 | 5.04 | 1.58 | 1.43 |
| 37 | 20 | 307 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 37 | 36 | 306 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 47 | 31 | 309 | KC1 | C3B-C2B | 5.04 | 1.47 | 1.37 |
| 37 | 18 | 204 | CLA | C3C-C2C | 5.04 | 1.47 | 1.36 |
| 37 | 20 | 301 | CLA | C3C-C2C | 5.03 | 1.47 | 1.36 |
| 47 | 40 | 206 | KC1 | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 37 | 41 | 206 | CLA | C3C-C2C | 5.03 | 1.47 | 1.36 |
| 37 | 18 | 203 | CLA | C3C-C2C | 5.03 | 1.47 | 1.36 |
| 47 | 35 | 306 | KC1 | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 50 | 41 | 212 | DD6 | C3-C2 | 5.03 | 1.58 | 1.43 |
| 47 | 34 | 304 | KC1 | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 47 | 37 | 304 | KC1 | CHD-C4C | 5.03 | 1.48 | 1.38 |
| 37 | 16 | 307 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 37 | 41 | 208 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 47 | 15 | 304 | KC1 | CHD-C4C | 5.03 | 1.48 | 1.38 |
| 37 | 11 | 310 | CLA | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 37 | 40 | 209 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 47 | 18 | 207 | KC1 | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 47 | 15 | 306 | KC1 | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 37 | 33 | 310 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 38 | 210 | KC1 | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 37 | 38 | 203 | CLA | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 48 | 12 | 202 | A86 | C17-C18 | -5.02 | 1.45 | 1.52 |
| 37 | B | 508 | CLA | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 47 | 13 | 302 | KC1 | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 37 | 34 | 302 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 47 | 20 | 304 | KC1 | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 37 | 21 | 206 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 37 | 38 | 202 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 37 | 41 | 210 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 47 | 36 | 304 | KC1 | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 48 | 32 | 203 | A86 | C17-C18 | -5.01 | 1.45 | 1.52 |
| 37 | 15 | 305 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 37 | 11 | 305 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 47 | 16 | 302 | KC1 | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 37 | 18 | 201 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 37 | 14 | 305 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 37 | 39 | 301 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 37 | 13 | 310 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 37 | 33 | 308 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 37 | 15 | 307 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 47 | 15 | 302 | KC1 | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 47 | 38 | 207 | KC1 | C3C-C2C | 5.00 | 1.47 | 1.36 |
| 37 | 37 | 303 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 37 | 18 | 211 | CLA | C1D-ND | 5.00 | 1.44 | 1.37 |
| 47 | 15 | 304 | KC1 | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 37 | 31 | 306 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 37 | 36 | 307 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 37 | b | 508 | CLA | C3C-C2C | 5.00 | 1.47 | 1.36 |
| 37 | 13 | 308 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 37 | 21 | 210 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 47 | 17 | 305 | KC1 | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 37 | 34 | 302 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 37 | 36 | 301 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 37 | 12 | 210 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 47 | 15 | 302 | KC1 | C3B-C2B | 4.99 | 1.47 | 1.37 |
| 37 | 19 | 301 | CLA | C3C-C2C | 4.99 | 1.47 | 1.36 |
| 37 | 19 | 303 | CLA | C3C-C2C | 4.99 | 1.47 | 1.36 |
| 37 | 39 | 303 | CLA | C3C-C2C | 4.99 | 1.47 | 1.36 |
| 37 | 41 | 206 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 37 | 19 | 310 | CLA | C3C-C2C | 4.98 | 1.47 | 1.36 |
| 37 | 35 | 307 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 18 | 210 | KC1 | C3C-C2C | 4.98 | 1.47 | 1.36 |
| 47 | 15 | 309 | KC1 | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 47 | 37 | 304 | KC1 | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 37 | 34 | 305 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 47 | 40 | 204 | KC1 | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 48 | 40 | 213 | A86 | C9-C8 | 4.98 | 1.47 | 1.34 |
| 48 | 11 | 319 | A86 | C17-C18 | -4.98 | 1.45 | 1.52 |
| 48 | 31 | 319 | A86 | C17-C18 | -4.98 | 1.45 | 1.52 |
| 47 | 16 | 304 | KC1 | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 47 | 20 | 302 | KC1 | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 37 | 21 | 206 | CLA | C3C-C2C | 4.97 | 1.47 | 1.36 |
| 37 | 35 | 308 | CLA | C3C-C2C | 4.97 | 1.47 | 1.36 |
| 47 | 14 | 306 | KC1 | C3C-C2C | 4.97 | 1.47 | 1.36 |
| 47 | 34 | 306 | KC1 | C3C-C2C | 4.97 | 1.47 | 1.36 |
| 47 | 19 | 308 | KC1 | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 37 | 40 | 210 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 37 | 38 | 201 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 37 | 39 | 306 | CLA | CHC-C1C | 4.97 | 1.48 | 1.38 |
| 37 | 34 | 308 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 37 | 40 | 203 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 37 | 14 | 302 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 48 | 33 | 313 | A86 | C9-C8 | 4.97 | 1.47 | 1.34 |
| 37 | 38 | 201 | CLA | CHC-C1C | 4.97 | 1.48 | 1.38 |
| 37 | 18 | 208 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 37 | 36 | 303 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 47 | 36 | 305 | KC1 | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 47 | 33 | 302 | KC1 | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 37 | 35 | 308 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 48 | 13 | 313 | A86 | C9-C8 | 4.96 | 1.47 | 1.34 |
| 47 | 39 | 308 | KC1 | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 47 | 13 | 309 | KC1 | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 47 | 16 | 305 | KC1 | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 48 | 20 | 311 | A86 | C9-C8 | 4.96 | 1.47 | 1.34 |
| 37 | C | 511 | CLA | C3C-C2C | 4.96 | 1.47 | 1.36 |
| 37 | 41 | 204 | CLA | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 37 | 13 | 301 | CLA | C3C-C2C | 4.96 | 1.47 | 1.36 |
| 37 | 33 | 301 | CLA | C3C-C2C | 4.96 | 1.47 | 1.36 |
| 47 | 17 | 305 | KC1 | C3C-C2C | 4.96 | 1.47 | 1.36 |
| 47 | 40 | 204 | KC1 | C3C-C2C | 4.96 | 1.47 | 1.36 |
| 37 | 11 | 305 | CLA | C3C-C2C | 4.95 | 1.47 | 1.36 |
| 37 | 31 | 306 | CLA | C3C-C2C | 4.95 | 1.47 | 1.36 |
| 37 | 21 | 204 | CLA | O2D-CGD | 4.95 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 18 | 210 | KC1 | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 37 | 39 | 310 | CLA | C3C-C2C | 4.95 | 1.47 | 1.36 |
| 37 | 33 | 303 | CLA | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 48 | 39 | 313 | A86 | C9-C8 | 4.95 | 1.47 | 1.34 |
| 48 | 21 | 213 | A86 | C9-C8 | 4.95 | 1.47 | 1.34 |
| 37 | 32 | 211 | CLA | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 47 | 13 | 304 | KC1 | C3C-C2C | 4.95 | 1.47 | 1.36 |
| 37 | 14 | 301 | CLA | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 47 | 37 | 307 | KC1 | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 37 | 39 | 309 | CLA | C3C-C2C | 4.95 | 1.47 | 1.36 |
| 47 | 16 | 302 | KC1 | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 47 | 37 | 302 | KC1 | C3C-C2C | 4.95 | 1.47 | 1.36 |
| 47 | 41 | 203 | KC1 | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 48 | 15 | 314 | A86 | C9-C8 | 4.94 | 1.47 | 1.34 |
| 37 | 14 | 308 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 37 | 19 | 305 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 37 | 39 | 305 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 50 | 39 | 312 | DD6 | C3-C2 | 4.94 | 1.58 | 1.43 |
| 48 | 13 | 315 | A86 | C9-C8 | 4.94 | 1.47 | 1.34 |
| 37 | 20 | 308 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 48 | 41 | 213 | A86 | C9-C8 | 4.94 | 1.47 | 1.34 |
| 37 | 39 | 309 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 47 | 11 | 304 | KC1 | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 47 | 17 | 308 | KC1 | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 37 | 19 | 307 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 37 | 39 | 307 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 50 | 19 | 312 | DD6 | C3-C2 | 4.94 | 1.58 | 1.43 |
| 37 | 19 | 306 | CLA | CHC-C1C | 4.94 | 1.48 | 1.38 |
| 37 | c | 511 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 47 | 17 | 308 | KC1 | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 37 | 16 | 303 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 37 | 13 | 310 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 47 | 38 | 207 | KC1 | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 37 | B | 507 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 37 | 16 | 303 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 47 | 33 | 304 | KC1 | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 37 | 35 | 303 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 48 | 35 | 314 | A86 | C9-C8 | 4.94 | 1.47 | 1.34 |
| 37 | 19 | 310 | CLA | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 47 | 17 | 303 | KC1 | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 47 | 31 | 305 | KC1 | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 47 | 33 | 309 | KC1 | C3C-C2C | 4.93 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 204 | CLA | C3C-C2C | 4.93 | 1.47 | 1.36 |
| 37 | 32 | 205 | CLA | C3C-C2C | 4.93 | 1.47 | 1.36 |
| 47 | 36 | 302 | KC1 | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 37 | 20 | 306 | CLA | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 37 | 19 | 309 | CLA | C3C-C2C | 4.93 | 1.47 | 1.36 |
| 48 | 18 | 212 | A86 | C9-C8 | 4.93 | 1.47 | 1.34 |
| 47 | 37 | 302 | KC1 | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 47 | 38 | 210 | KC1 | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 47 | 16 | 308 | KC1 | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 47 | 20 | 302 | KC1 | C3C-C2C | 4.93 | 1.47 | 1.36 |
| 37 | 14 | 303 | CLA | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 47 | 13 | 309 | KC1 | C3C-C2C | 4.93 | 1.47 | 1.36 |
| 47 | 18 | 205 | KC1 | C1D-ND | 4.93 | 1.44 | 1.37 |
| 47 | 38 | 205 | KC1 | C1D-ND | 4.93 | 1.44 | 1.37 |
| 37 | 20 | 301 | CLA | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 48 | 18 | 212 | A86 | C17-C18 | -4.93 | 1.45 | 1.52 |
| 37 | 36 | 303 | CLA | C3C-C2C | 4.93 | 1.47 | 1.36 |
| 47 | 31 | 305 | KC1 | C3C-C2C | 4.93 | 1.47 | 1.36 |
| 37 | 11 | 303 | CLA | C3C-C2C | 4.92 | 1.47 | 1.36 |
| 37 | 21 | 209 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 37 | 35 | 305 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 37 | b | 507 | CLA | C3C-C2C | 4.92 | 1.47 | 1.36 |
| 37 | 40 | 208 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 37 | 16 | 306 | CLA | C3C-C2C | 4.92 | 1.47 | 1.36 |
| 37 | C | 506 | CLA | C1B-NB | -4.92 | 1.31 | 1.37 |
| 37 | 19 | 309 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 37 | 41 | 210 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 48 | 33 | 314 | A86 | C9-C8 | 4.91 | 1.47 | 1.34 |
| 47 | 33 | 304 | KC1 | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 37 | 37 | 306 | CLA | C3C-C2C | 4.91 | 1.47 | 1.36 |
| 37 | 38 | 208 | CLA | C3C-C2C | 4.91 | 1.47 | 1.36 |
| 47 | 13 | 306 | KC1 | C3C-C2C | 4.91 | 1.47 | 1.36 |
| 50 | 40 | 214 | DD6 | C2-C1 | 4.91 | 1.47 | 1.35 |
| 47 | 13 | 306 | KC1 | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 47 | 33 | 306 | KC1 | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 37 | 41 | 209 | CLA | C1D-ND | 4.91 | 1.44 | 1.37 |
| 47 | 36 | 308 | KC1 | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 37 | 34 | 301 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 48 | 34 | 313 | A86 | C9-C8 | 4.91 | 1.47 | 1.34 |
| 37 | 34 | 303 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 37 | 20 | 303 | CLA | C3C-C2C | 4.91 | 1.47 | 1.36 |
| 47 | 20 | 304 | KC1 | CHD-C4C | 4.91 | 1.48 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 33 | 315 | A86 | C9-C8 | 4.91 | 1.47 | 1.34 |
| 47 | 20 | 304 | KC1 | C1D-ND | 4.91 | 1.44 | 1.37 |
| 47 | 15 | 309 | KC1 | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 47 | 41 | 207 | KC1 | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 37 | w | 101 | CLA | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 48 | 38 | 212 | A86 | C9-C8 | 4.90 | 1.47 | 1.34 |
| 47 | 33 | 309 | KC1 | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 37 | 38 | 211 | CLA | C1D-ND | 4.90 | 1.44 | 1.37 |
| 47 | 13 | 304 | KC1 | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 47 | 33 | 306 | KC1 | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 37 | 35 | 307 | CLA | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 47 | 21 | 203 | KC1 | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 48 | 13 | 314 | A86 | C9-C8 | 4.90 | 1.47 | 1.34 |
| 47 | 35 | 309 | KC1 | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 47 | 37 | 307 | KC1 | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 37 | 39 | 305 | CLA | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 47 | 18 | 207 | KC1 | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 47 | 40 | 206 | KC1 | C1D-ND | 4.90 | 1.44 | 1.37 |
| 37 | c | 507 | CLA | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 48 | 38 | 214 | A86 | C9-C8 | 4.90 | 1.47 | 1.34 |
| 47 | 11 | 304 | KC1 | C3C-C2C | 4.90 | 1.47 | 1.36 |
| 47 | 37 | 304 | KC1 | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 47 | 32 | 212 | KC1 | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | 19 | 305 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 47 | 16 | 302 | KC1 | C1D-ND | 4.89 | 1.44 | 1.37 |
| 47 | 21 | 207 | KC1 | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | b | 503 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | 36 | 306 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | c | 508 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | 31 | 304 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 47 | 37 | 302 | KC1 | CHD-C4C | 4.89 | 1.48 | 1.38 |
| 37 | 17 | 307 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | 15 | 305 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 37 | 40 | 205 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | 38 | 208 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 50 | 20 | 312 | DD6 | C2-C1 | 4.89 | 1.47 | 1.35 |
| 37 | 39 | 310 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 37 | B | 503 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | C | 505 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | 12 | 205 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | 12 | 210 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 37 | C | 507 | CLA | C3C-C2C | 4.88 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | b | 502 | CLA | C3C-C2C | 4.88 | 1.47 | 1.36 |
| 37 | c | 506 | CLA | C1B-NB | -4.88 | 1.31 | 1.37 |
| 37 | 38 | 203 | CLA | C1D-ND | 4.88 | 1.44 | 1.37 |
| 47 | 32 | 209 | KC1 | C3B-C2B | 4.88 | 1.47 | 1.37 |
| 37 | W | 101 | CLA | C3C-C2C | 4.88 | 1.47 | 1.36 |
| 37 | 21 | 202 | CLA | C1D-ND | 4.88 | 1.44 | 1.37 |
| 37 | 15 | 303 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 37 | 15 | 308 | CLA | C3C-C2C | 4.88 | 1.47 | 1.36 |
| 48 | 12 | 214 | A86 | C17-C18 | -4.88 | 1.45 | 1.52 |
| 47 | 35 | 304 | KC1 | C1D-ND | 4.88 | 1.44 | 1.37 |
| 47 | 15 | 302 | KC1 | CHD-C4C | 4.88 | 1.48 | 1.38 |
| 47 | 40 | 206 | KC1 | CHD-C4C | 4.88 | 1.48 | 1.38 |
| 37 | 18 | 204 | CLA | CHC-C1C | 4.88 | 1.48 | 1.38 |
| 37 | 15 | 307 | CLA | C3C-C2C | 4.88 | 1.47 | 1.36 |
| 37 | 21 | 204 | CLA | C1D-ND | 4.88 | 1.44 | 1.37 |
| 37 | D | 406 | CLA | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 47 | 31 | 309 | KC1 | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 48 | 14 | 313 | A86 | C9-C8 | 4.87 | 1.47 | 1.34 |
| 37 | 32 | 211 | CLA | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 45 | d | 406 | PL9 | C6-C1 | -4.87 | 1.40 | 1.48 |
| 47 | 17 | 303 | KC1 | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 37 | c | 503 | CLA | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 37 | 18 | 203 | CLA | C1D-ND | 4.87 | 1.44 | 1.37 |
| 37 | 35 | 303 | CLA | C1D-ND | 4.87 | 1.44 | 1.37 |
| 37 | c | 505 | CLA | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 37 | b | 523 | CLA | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 37 | C | 508 | CLA | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 47 | 11 | 309 | KC1 | C3C-C2C | 4.87 | 1.47 | 1.36 |
| 37 | B | 524 | CLA | C3C-C2C | 4.86 | 1.47 | 1.36 |
| 48 | 35 | 313 | A86 | C9-C8 | 4.86 | 1.47 | 1.34 |
| 37 | d | 404 | CLA | C3C-C2C | 4.86 | 1.47 | 1.36 |
| 37 | c | 509 | CLA | C3C-C2C | 4.86 | 1.47 | 1.36 |
| 37 | 18 | 208 | CLA | C3C-C2C | 4.86 | 1.47 | 1.36 |
| 47 | 35 | 309 | KC1 | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 47 | 12 | 208 | KC1 | C3B-C2B | 4.86 | 1.47 | 1.37 |
| 47 | 40 | 206 | KC1 | C3C-C2C | 4.86 | 1.47 | 1.36 |
| 37 | 34 | 310 | CLA | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 37 | 13 | 305 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 37 | 41 | 208 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 48 | 18 | 214 | A86 | C9-C8 | 4.85 | 1.47 | 1.34 |
| 37 | 14 | 310 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 37 | 38 | 204 | CLA | CHC-C1C | 4.85 | 1.48 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | C | 509 | CLA | C3C-C2C | 4.85 | 1.47 | 1.36 |
| 37 | 31 | 302 | CLA | CHC-C1C | 4.85 | 1.48 | 1.38 |
| 37 | B | 502 | CLA | C3C-C2C | 4.85 | 1.47 | 1.36 |
| 48 | 38 | 212 | A86 | C17-C18 | -4.85 | 1.45 | 1.52 |
| 37 | 13 | 301 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 37 | 33 | 301 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 37 | C | 510 | CLA | C3C-C2C | 4.85 | 1.47 | 1.36 |
| 37 | 39 | 307 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 37 | 35 | 301 | CLA | CHC-C1C | 4.85 | 1.48 | 1.38 |
| 47 | 38 | 205 | KC1 | CHD-C4C | 4.85 | 1.48 | 1.38 |
| 37 | 11 | 301 | CLA | CHC-C1C | 4.85 | 1.48 | 1.38 |
| 48 | 31 | 315 | A86 | C17-C18 | -4.85 | 1.45 | 1.52 |
| 45 | D | 408 | PL9 | C6-C1 | -4.85 | 1.40 | 1.48 |
| 37 | 14 | 307 | CLA | C3C-C2C | 4.85 | 1.47 | 1.36 |
| 37 | 34 | 307 | CLA | C3C-C2C | 4.85 | 1.47 | 1.36 |
| 37 | 21 | 208 | CLA | C1D-ND | 4.84 | 1.44 | 1.37 |
| 37 | 32 | 210 | CLA | C3C-C2C | 4.84 | 1.47 | 1.36 |
| 47 | 12 | 211 | KC1 | C3C-C2C | 4.84 | 1.47 | 1.36 |
| 37 | 34 | 301 | CLA | CHC-C1C | 4.84 | 1.48 | 1.38 |
| 37 | 14 | 308 | CLA | C3C-C2C | 4.84 | 1.47 | 1.36 |
| 47 | 18 | 205 | KC1 | CHD-C4C | 4.84 | 1.48 | 1.38 |
| 37 | 33 | 305 | CLA | C1D-ND | 4.84 | 1.44 | 1.37 |
| 47 | 17 | 303 | KC1 | CHD-C4C | 4.84 | 1.48 | 1.38 |
| 37 | C | 506 | CLA | C3C-C2C | 4.84 | 1.47 | 1.36 |
| 37 | 15 | 301 | CLA | CHC-C1C | 4.84 | 1.48 | 1.38 |
| 47 | 17 | 305 | KC1 | CHD-C4C | 4.84 | 1.48 | 1.38 |
| 47 | 35 | 302 | KC1 | CHD-C4C | 4.84 | 1.48 | 1.38 |
| 37 | 39 | 304 | CLA | O2D-CGD | 4.84 | 1.45 | 1.33 |
| 48 | 32 | 215 | A86 | C17-C18 | -4.84 | 1.45 | 1.52 |
| 48 | 40 | 201 | A86 | C9-C8 | 4.84 | 1.47 | 1.34 |
| 47 | 36 | 302 | KC1 | C1D-ND | 4.84 | 1.44 | 1.37 |
| 37 | 20 | 301 | CLA | CHC-C1C | 4.84 | 1.48 | 1.38 |
| 37 | 40 | 203 | CLA | CHC-C1C | 4.84 | 1.48 | 1.38 |
| 37 | C | 513 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 37 | c | 513 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 48 | 19 | 313 | A86 | C9-C8 | 4.83 | 1.47 | 1.34 |
| 37 | 41 | 204 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 37 | C | 503 | CLA | C3C-C2C | 4.83 | 1.47 | 1.36 |
| 48 | 38 | 215 | A86 | C9-C8 | 4.83 | 1.47 | 1.34 |
| 48 | 15 | 313 | A86 | C9-C8 | 4.83 | 1.47 | 1.34 |
| 47 | 15 | 304 | KC1 | C1D-ND | 4.83 | 1.44 | 1.37 |
| 47 | 21 | 207 | KC1 | CHD-C4C | 4.83 | 1.48 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 209 | CLA | C3C-C2C | 4.83 | 1.47 | 1.36 |
| 48 | 11 | 311 | A86 | C17-C18 | -4.83 | 1.45 | 1.52 |
| 48 | 31 | 311 | A86 | C17-C18 | -4.83 | 1.45 | 1.52 |
| 48 | 16 | 313 | A86 | C9-C8 | 4.83 | 1.47 | 1.34 |
| 37 | A | 405 | CLA | C3C-C2C | 4.83 | 1.47 | 1.36 |
| 37 | a | 407 | CLA | C3C-C2C | 4.83 | 1.47 | 1.36 |
| 47 | 20 | 304 | KC1 | C3C-C2C | 4.83 | 1.47 | 1.36 |
| 37 | B | 513 | CLA | C3C-C2C | 4.83 | 1.47 | 1.36 |
| 37 | c | 506 | CLA | C3C-C2C | 4.83 | 1.47 | 1.36 |
| 37 | 19 | 307 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 47 | 14 | 309 | KC1 | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 47 | 34 | 309 | KC1 | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 47 | 36 | 302 | KC1 | CHD-C4C | 4.82 | 1.48 | 1.38 |
| 37 | c | 510 | CLA | C3C-C2C | 4.82 | 1.47 | 1.36 |
| 37 | 12 | 203 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 37 | 32 | 204 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 37 | A | 403 | CLA | C3C-C2C | 4.82 | 1.47 | 1.36 |
| 37 | 34 | 308 | CLA | C3C-C2C | 4.82 | 1.47 | 1.36 |
| 47 | 16 | 304 | KC1 | C1D-ND | 4.82 | 1.44 | 1.37 |
| 37 | 18 | 201 | CLA | C3C-C2C | 4.82 | 1.47 | 1.36 |
| 37 | 14 | 307 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 37 | 34 | 307 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 37 | b | 513 | CLA | C3C-C2C | 4.82 | 1.47 | 1.36 |
| 47 | 16 | 304 | KC1 | CHD-C4C | 4.82 | 1.48 | 1.38 |
| 37 | 41 | 202 | CLA | C1D-ND | 4.82 | 1.44 | 1.37 |
| 37 | 13 | 301 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 37 | 33 | 301 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 37 | 21 | 210 | CLA | C1D-ND | 4.82 | 1.44 | 1.37 |
| 37 | 39 | 306 | CLA | C3C-C2C | 4.81 | 1.47 | 1.36 |
| 48 | 41 | 213 | A86 | O4-C38 | 4.81 | 1.45 | 1.35 |
| 47 | 36 | 304 | KC1 | CHD-C4C | 4.81 | 1.48 | 1.38 |
| 37 | 12 | 205 | CLA | O2D-CGD | 4.81 | 1.45 | 1.33 |
| 37 | 19 | 306 | CLA | O2D-CGD | 4.81 | 1.45 | 1.33 |
| 48 | 37 | 314 | A86 | C9-C8 | 4.81 | 1.47 | 1.34 |
| 37 | 20 | 307 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 37 | 15 | 303 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 37 | C | 513 | CLA | C3C-C2C | 4.81 | 1.47 | 1.36 |
| 37 | 32 | 202 | CLA | C3C-C2C | 4.81 | 1.47 | 1.36 |
| 48 | 41 | 215 | A86 | C17-C18 | -4.81 | 1.45 | 1.52 |
| 37 | z | 102 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 47 | 21 | 203 | KC1 | CHD-C4C | 4.80 | 1.48 | 1.38 |
| 48 | 13 | 313 | A86 | O4-C38 | 4.80 | 1.45 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 37 | 311 | A86 | C17-C18 | -4.80 | 1.45 | 1.52 |
| 47 | 20 | 302 | KC1 | CHD-C4C | 4.80 | 1.48 | 1.38 |
| 47 | 14 | 304 | KC1 | CHD-C4C | 4.80 | 1.48 | 1.38 |
| 47 | 34 | 304 | KC1 | CHD-C4C | 4.80 | 1.48 | 1.38 |
| 37 | 32 | 202 | CLA | O2D-CGD | 4.80 | 1.45 | 1.33 |
| 37 | 32 | 206 | CLA | C3C-C2C | 4.80 | 1.47 | 1.36 |
| 47 | 31 | 303 | KC1 | C3C-C2C | 4.80 | 1.47 | 1.36 |
| 37 | b | 507 | CLA | O2D-CGD | 4.80 | 1.45 | 1.33 |
| 37 | 19 | 304 | CLA | O2D-CGD | 4.80 | 1.45 | 1.33 |
| 47 | 41 | 207 | KC1 | CHD-C4C | 4.80 | 1.48 | 1.38 |
| 37 | b | 514 | CLA | C3C-C2C | 4.80 | 1.47 | 1.36 |
| 37 | 14 | 301 | CLA | CHC-C1C | 4.79 | 1.48 | 1.38 |
| 37 | c | 509 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 47 | 16 | 302 | KC1 | CHD-C4C | 4.79 | 1.48 | 1.38 |
| 37 | a | 403 | CLA | C3C-C2C | 4.79 | 1.47 | 1.36 |
| 37 | 12 | 212 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 47 | 41 | 203 | KC1 | CHD-C4C | 4.79 | 1.48 | 1.38 |
| 48 | 14 | 313 | A86 | O4-C38 | 4.79 | 1.45 | 1.35 |
| 37 | 32 | 206 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 37 | 40 | 203 | CLA | C1D-ND | 4.79 | 1.44 | 1.37 |
| 37 | 11 | 308 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 50 | 21 | 212 | DD6 | C2-C1 | 4.79 | 1.46 | 1.35 |
| 48 | 11 | 315 | A86 | C17-C18 | -4.79 | 1.45 | 1.52 |
| 37 | B | 509 | CLA | O2D-CGD | 4.79 | 1.45 | 1.33 |
| 37 | 20 | 301 | CLA | C1D-ND | 4.79 | 1.44 | 1.37 |
| 48 | 21 | 215 | A86 | C17-C18 | -4.79 | 1.45 | 1.52 |
| 37 | b | 515 | CLA | O2D-CGD | 4.78 | 1.45 | 1.33 |
| 37 | b | 509 | CLA | O2D-CGD | 4.78 | 1.45 | 1.33 |
| 37 | 18 | 206 | CLA | C1D-ND | 4.78 | 1.44 | 1.37 |
| 47 | 14 | 309 | KC1 | C3C-C2C | 4.78 | 1.47 | 1.36 |
| 37 | b | 515 | CLA | C3C-C2C | 4.78 | 1.47 | 1.36 |
| 37 | 39 | 306 | CLA | O2D-CGD | 4.78 | 1.45 | 1.33 |
| 48 | 21 | 213 | A86 | O4-C38 | 4.78 | 1.45 | 1.35 |
| 50 | 21 | 216 | DD6 | C2-C1 | 4.78 | 1.46 | 1.35 |
| 48 | 17 | 315 | A86 | C9-C8 | 4.78 | 1.47 | 1.34 |
| 37 | 20 | 306 | CLA | C3C-C2C | 4.78 | 1.47 | 1.36 |
| 37 | D | 402 | CLA | O2D-CGD | 4.78 | 1.45 | 1.33 |
| 37 | 11 | 308 | CLA | C3C-C2C | 4.78 | 1.47 | 1.36 |
| 37 | B | 507 | CLA | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 37 | B | 515 | CLA | C3C-C2C | 4.77 | 1.47 | 1.36 |
| 37 | 38 | 206 | CLA | C1D-ND | 4.77 | 1.44 | 1.37 |
| 47 | 37 | 304 | KC1 | C1D-ND | 4.77 | 1.44 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 37 | 305 | KC1 | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 48 | 18 | 215 | A86 | C9-C8 | 4.77 | 1.47 | 1.34 |
| 48 | 34 | 313 | A86 | O4-C38 | 4.77 | 1.45 | 1.35 |
| 37 | 12 | 207 | CLA | O2D-CGD | 4.77 | 1.45 | 1.33 |
| 37 | 34 | 301 | CLA | C3C-C2C | 4.77 | 1.47 | 1.36 |
| 48 | 33 | 313 | A86 | O4-C38 | 4.77 | 1.45 | 1.35 |
| 48 | 31 | 313 | A86 | C17-C18 | -4.77 | 1.45 | 1.52 |
| 37 | 40 | 209 | CLA | C1D-ND | 4.77 | 1.44 | 1.37 |
| 47 | 18 | 210 | KC1 | C1D-ND | 4.77 | 1.44 | 1.37 |
| 48 | 13 | 315 | A86 | C17-C18 | -4.77 | 1.45 | 1.52 |
| 47 | 38 | 210 | KC1 | C1D-ND | 4.76 | 1.44 | 1.37 |
| 37 | 38 | 202 | CLA | CHC-C1C | 4.76 | 1.48 | 1.38 |
| 47 | 15 | 306 | KC1 | CHD-C4C | 4.76 | 1.48 | 1.38 |
| 37 | C | 509 | CLA | O2D-CGD | 4.76 | 1.44 | 1.33 |
| 37 | d | 401 | CLA | O2D-CGD | 4.76 | 1.44 | 1.33 |
| 37 | C | 513 | CLA | CHC-C1C | 4.76 | 1.48 | 1.38 |
| 37 | b | 512 | CLA | O2D-CGD | 4.76 | 1.44 | 1.33 |
| 47 | 11 | 302 | KC1 | C3C-C2C | 4.76 | 1.47 | 1.36 |
| 48 | 21 | 215 | A86 | C9-C8 | 4.76 | 1.47 | 1.34 |
| 48 | 41 | 215 | A86 | C9-C8 | 4.76 | 1.47 | 1.34 |
| 37 | 32 | 213 | CLA | O2D-CGD | 4.76 | 1.44 | 1.33 |
| 37 | c | 513 | CLA | C3C-C2C | 4.76 | 1.47 | 1.36 |
| 48 | 37 | 309 | A86 | O4-C38 | 4.76 | 1.45 | 1.35 |
| 48 | 15 | 316 | A86 | C21-C20 | 4.76 | 1.58 | 1.51 |
| 37 | c | 511 | CLA | O2D-CGD | 4.76 | 1.44 | 1.33 |
| 47 | 12 | 208 | KC1 | C3C-C2C | 4.76 | 1.47 | 1.36 |
| 47 | 32 | 209 | KC1 | C3C-C2C | 4.76 | 1.47 | 1.36 |
| 47 | 13 | 302 | KC1 | C3B-C2B | 4.76 | 1.46 | 1.37 |
| 47 | 17 | 306 | KC1 | O2D-CGD | 4.76 | 1.44 | 1.33 |
| 37 | 17 | 309 | CLA | C1D-ND | 4.76 | 1.44 | 1.37 |
| 37 | 11 | 303 | CLA | O2D-CGD | 4.76 | 1.44 | 1.33 |
| 47 | 34 | 306 | KC1 | O2D-CGD | 4.76 | 1.44 | 1.33 |
| 47 | 11 | 304 | KC1 | CHD-C4C | 4.76 | 1.48 | 1.38 |
| 37 | 41 | 206 | CLA | C1D-ND | 4.76 | 1.44 | 1.37 |
| 47 | 40 | 204 | KC1 | CHD-C4C | 4.75 | 1.48 | 1.38 |
| 37 | 18 | 201 | CLA | CHC-C1C | 4.75 | 1.48 | 1.38 |
| 37 | 39 | 301 | CLA | CHC-C1C | 4.75 | 1.48 | 1.38 |
| 47 | 14 | 306 | KC1 | O2D-CGD | 4.75 | 1.44 | 1.33 |
| 47 | 12 | 211 | KC1 | CHD-C4C | 4.75 | 1.48 | 1.38 |
| 50 | 41 | 212 | DD6 | C2-C1 | 4.75 | 1.46 | 1.35 |
| 37 | 15 | 307 | CLA | CHC-C1C | 4.75 | 1.48 | 1.38 |
| 37 | 32 | 208 | CLA | O2D-CGD | 4.75 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | B | 505 | CLA | C3C-C2C | 4.75 | 1.47 | 1.36 |
| 37 | 40 | 208 | CLA | C3C-C2C | 4.75 | 1.47 | 1.36 |
| 48 | 33 | 315 | A86 | C17-C18 | -4.75 | 1.45 | 1.52 |
| 50 | 41 | 216 | DD6 | C2-C1 | 4.75 | 1.46 | 1.35 |
| 47 | 32 | 209 | KC1 | O2D-CGD | 4.75 | 1.44 | 1.33 |
| 37 | B | 512 | CLA | O2D-CGD | 4.75 | 1.44 | 1.33 |
| 47 | 34 | 309 | KC1 | C3C-C2C | 4.75 | 1.47 | 1.36 |
| 47 | 12 | 211 | KC1 | O2D-CGD | 4.75 | 1.44 | 1.33 |
| 37 | B | 514 | CLA | C3C-C2C | 4.75 | 1.47 | 1.36 |
| 37 | b | 501 | CLA | C3C-C2C | 4.75 | 1.47 | 1.36 |
| 37 | C | 511 | CLA | O2D-CGD | 4.75 | 1.44 | 1.33 |
| 47 | 33 | 302 | KC1 | C3B-C2B | 4.75 | 1.46 | 1.37 |
| 47 | 16 | 305 | KC1 | CHD-C4C | 4.74 | 1.48 | 1.38 |
| 48 | 35 | 313 | A86 | O4-C38 | 4.74 | 1.45 | 1.35 |
| 37 | 32 | 205 | CLA | O2D-CGD | 4.74 | 1.44 | 1.33 |
| 37 | 14 | 305 | CLA | C1D-ND | 4.74 | 1.44 | 1.37 |
| 37 | 34 | 305 | CLA | C1D-ND | 4.74 | 1.44 | 1.37 |
| 48 | 34 | 314 | A86 | C9-C8 | 4.74 | 1.47 | 1.34 |
| 37 | 35 | 307 | CLA | CHC-C1C | 4.74 | 1.48 | 1.38 |
| 37 | 38 | 202 | CLA | C1D-ND | 4.74 | 1.44 | 1.37 |
| 37 | 31 | 304 | CLA | O2D-CGD | 4.74 | 1.44 | 1.33 |
| 37 | c | 513 | CLA | CHC-C1C | 4.74 | 1.48 | 1.38 |
| 37 | B | 515 | CLA | O2D-CGD | 4.74 | 1.44 | 1.33 |
| 47 | 37 | 307 | KC1 | C1D-ND | 4.74 | 1.44 | 1.37 |
| 37 | a | 404 | CLA | O2D-CGD | 4.74 | 1.44 | 1.33 |
| 48 | 14 | 313 | A86 | C17-C18 | -4.74 | 1.45 | 1.52 |
| 47 | 17 | 308 | KC1 | C1D-ND | 4.74 | 1.44 | 1.37 |
| 48 | 15 | 313 | A86 | O4-C38 | 4.73 | 1.45 | 1.35 |
| 37 | 19 | 306 | CLA | C3C-C2C | 4.73 | 1.47 | 1.36 |
| 37 | 16 | 309 | CLA | O2D-CGD | 4.73 | 1.44 | 1.33 |
| 37 | B | 510 | CLA | C3C-C2C | 4.73 | 1.47 | 1.36 |
| 37 | 21 | 206 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 37 | 35 | 308 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 47 | 36 | 304 | KC1 | C1D-ND | 4.73 | 1.44 | 1.37 |
| 47 | 18 | 210 | KC1 | CHD-C4C | 4.73 | 1.48 | 1.38 |
| 47 | 38 | 210 | KC1 | CHD-C4C | 4.73 | 1.48 | 1.38 |
| 37 | b | 510 | CLA | C3C-C2C | 4.73 | 1.47 | 1.36 |
| 37 | 14 | 301 | CLA | C3C-C2C | 4.73 | 1.47 | 1.36 |
| 37 | 15 | 308 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 47 | 31 | 305 | KC1 | CHD-C4C | 4.73 | 1.48 | 1.38 |
| 48 | 17 | 310 | A86 | O4-C38 | 4.73 | 1.45 | 1.35 |
| 47 | 32 | 212 | KC1 | O2D-CGD | 4.72 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 306 | KC1 | CHD-C4C | 4.72 | 1.47 | 1.38 |
| 37 | Z | 102 | CLA | C1D-ND | 4.72 | 1.44 | 1.37 |
| 37 | 32 | 213 | CLA | C1D-ND | 4.72 | 1.44 | 1.37 |
| 48 | 12 | 215 | A86 | O4-C38 | 4.72 | 1.45 | 1.35 |
| 37 | 41 | 205 | CLA | C1D-ND | 4.72 | 1.44 | 1.37 |
| 48 | 12 | 215 | A86 | C9-C8 | 4.72 | 1.47 | 1.34 |
| 48 | 32 | 216 | A86 | C9-C8 | 4.72 | 1.47 | 1.34 |
| 37 | 36 | 309 | CLA | O2D-CGD | 4.72 | 1.44 | 1.33 |
| 37 | 40 | 208 | CLA | CHC-C1C | 4.72 | 1.47 | 1.38 |
| 37 | 19 | 303 | CLA | CHC-C1C | 4.72 | 1.47 | 1.38 |
| 37 | 39 | 303 | CLA | CHC-C1C | 4.72 | 1.47 | 1.38 |
| 37 | 35 | 310 | CLA | C1D-ND | 4.72 | 1.44 | 1.37 |
| 47 | 15 | 306 | KC1 | C1D-ND | 4.72 | 1.44 | 1.37 |
| 37 | A | 405 | CLA | O2D-CGD | 4.72 | 1.44 | 1.33 |
| 37 | 11 | 307 | CLA | O2D-CGD | 4.72 | 1.44 | 1.33 |
| 37 | 31 | 308 | CLA | O2D-CGD | 4.72 | 1.44 | 1.33 |
| 48 | 17 | 312 | A86 | C9-C8 | 4.72 | 1.47 | 1.34 |
| 48 | 37 | 311 | A86 | C9-C8 | 4.72 | 1.47 | 1.34 |
| 37 | D | 401 | CLA | O2D-CGD | 4.72 | 1.44 | 1.33 |
| 48 | 32 | 216 | A86 | O4-C38 | 4.72 | 1.45 | 1.35 |
| 47 | 12 | 208 | KC1 | O2D-CGD | 4.71 | 1.44 | 1.33 |
| 47 | 36 | 305 | KC1 | CHD-C4C | 4.71 | 1.47 | 1.38 |
| 48 | 14 | 314 | A86 | C9-C8 | 4.71 | 1.47 | 1.34 |
| 37 | C | 510 | CLA | O2D-CGD | 4.71 | 1.44 | 1.33 |
| 47 | 12 | 206 | KC1 | O2D-CGD | 4.71 | 1.44 | 1.33 |
| 37 | b | 509 | CLA | C3C-C2C | 4.71 | 1.46 | 1.36 |
| 37 | c | 502 | CLA | C3C-C2C | 4.71 | 1.46 | 1.36 |
| 37 | 12 | 204 | CLA | O2D-CGD | 4.71 | 1.44 | 1.33 |
| 47 | 32 | 207 | KC1 | O2D-CGD | 4.71 | 1.44 | 1.33 |
| 37 | B | 501 | CLA | C3C-C2C | 4.71 | 1.46 | 1.36 |
| 37 | b | 505 | CLA | C3C-C2C | 4.71 | 1.46 | 1.36 |
| 37 | 21 | 210 | CLA | CHC-C1C | 4.71 | 1.47 | 1.38 |
| 48 | 15 | 316 | A86 | C9-C8 | 4.71 | 1.47 | 1.34 |
| 47 | 40 | 204 | KC1 | C1D-ND | 4.71 | 1.44 | 1.37 |
| 37 | 19 | 301 | CLA | O2D-CGD | 4.71 | 1.44 | 1.33 |
| 37 | 39 | 301 | CLA | O2D-CGD | 4.71 | 1.44 | 1.33 |
| 37 | 16 | 301 | CLA | CHC-C1C | 4.70 | 1.47 | 1.38 |
| 47 | 20 | 302 | KC1 | C1D-ND | 4.70 | 1.44 | 1.37 |
| 47 | 38 | 207 | KC1 | C1D-ND | 4.70 | 1.44 | 1.37 |
| 37 | 41 | 210 | CLA | CHC-C1C | 4.70 | 1.47 | 1.38 |
| 37 | 19 | 304 | CLA | CHC-C1C | 4.70 | 1.47 | 1.38 |
| 37 | 39 | 304 | CLA | CHC-C1C | 4.70 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 19 | 301 | CLA | CHC-C1C | 4.70 | 1.47 | 1.38 |
| 37 | 20 | 306 | CLA | CHC-C1C | 4.70 | 1.47 | 1.38 |
| 48 | 34 | 313 | A86 | C17-C18 | -4.69 | 1.45 | 1.52 |
| 37 | 36 | 301 | CLA | CHC-C1C | 4.69 | 1.47 | 1.38 |
| 47 | 32 | 212 | KC1 | CHD-C4C | 4.69 | 1.47 | 1.38 |
| 37 | C | 502 | CLA | C3C-C2C | 4.69 | 1.46 | 1.36 |
| 47 | 21 | 207 | KC1 | CHC-C4B | 4.69 | 1.47 | 1.38 |
| 47 | 41 | 207 | KC1 | CHC-C4B | 4.69 | 1.47 | 1.38 |
| 37 | 20 | 308 | CLA | C1D-ND | 4.69 | 1.44 | 1.37 |
| 48 | 17 | 315 | A86 | C17-C18 | -4.69 | 1.45 | 1.52 |
| 37 | 18 | 202 | CLA | CHC-C1C | 4.69 | 1.47 | 1.38 |
| 47 | 11 | 309 | KC1 | O2D-CGD | 4.69 | 1.44 | 1.33 |
| 47 | 31 | 309 | KC1 | O2D-CGD | 4.69 | 1.44 | 1.33 |
| 37 | 13 | 307 | CLA | C3C-C2C | 4.69 | 1.46 | 1.36 |
| 37 | 33 | 307 | CLA | C3C-C2C | 4.69 | 1.46 | 1.36 |
| 47 | 41 | 207 | KC1 | C1D-ND | 4.69 | 1.44 | 1.37 |
| 47 | 35 | 302 | KC1 | C1D-ND | 4.69 | 1.44 | 1.37 |
| 48 | 17 | 312 | A86 | C17-C18 | -4.69 | 1.45 | 1.52 |
| 37 | c | 504 | CLA | O2D-CGD | 4.69 | 1.44 | 1.33 |
| 37 | 16 | 306 | CLA | CHC-C1C | 4.68 | 1.47 | 1.38 |
| 48 | 12 | 217 | A86 | C17-C18 | -4.68 | 1.45 | 1.52 |
| 47 | 17 | 308 | KC1 | CHD-C4C | 4.68 | 1.47 | 1.38 |
| 47 | 37 | 307 | KC1 | CHD-C4C | 4.68 | 1.47 | 1.38 |
| 48 | 32 | 218 | A86 | C17-C18 | -4.68 | 1.45 | 1.52 |
| 37 | a | 407 | CLA | O2D-CGD | 4.68 | 1.44 | 1.33 |
| 37 | c | 510 | CLA | O2D-CGD | 4.68 | 1.44 | 1.33 |
| 37 | C | 504 | CLA | O2D-CGD | 4.68 | 1.44 | 1.33 |
| 37 | b | 501 | CLA | O2D-CGD | 4.68 | 1.44 | 1.33 |
| 37 | 11 | 310 | CLA | O2D-CGD | 4.68 | 1.44 | 1.33 |
| 37 | C | 501 | CLA | C3C-C2C | 4.68 | 1.46 | 1.36 |
| 48 | 33 | 312 | A86 | C9-C8 | 4.68 | 1.46 | 1.34 |
| 37 | 38 | 209 | CLA | C1D-ND | 4.68 | 1.44 | 1.37 |
| 37 | 31 | 310 | CLA | O2D-CGD | 4.68 | 1.44 | 1.33 |
| 37 | 18 | 201 | CLA | C1D-ND | 4.68 | 1.44 | 1.37 |
| 37 | d | 403 | CLA | C3C-C2C | 4.68 | 1.46 | 1.36 |
| 48 | 11 | 313 | A86 | C17-C18 | -4.67 | 1.45 | 1.52 |
| 37 | B | 505 | CLA | O2D-CGD | 4.67 | 1.44 | 1.33 |
| 37 | B | 516 | CLA | O2D-CGD | 4.67 | 1.44 | 1.33 |
| 37 | 37 | 308 | CLA | C1D-ND | 4.67 | 1.44 | 1.37 |
| 37 | 38 | 204 | CLA | C1D-ND | 4.67 | 1.44 | 1.37 |
| 47 | 13 | 309 | KC1 | CHD-C4C | 4.67 | 1.47 | 1.38 |
| 47 | 33 | 309 | KC1 | CHD-C4C | 4.67 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 35 | 316 | A86 | C21-C20 | 4.67 | 1.58 | 1.51 |
| 37 | B | 501 | CLA | O2D-CGD | 4.67 | 1.44 | 1.33 |
| 37 | 21 | 205 | CLA | C1D-ND | 4.67 | 1.44 | 1.37 |
| 37 | 31 | 302 | CLA | O2D-CGD | 4.67 | 1.44 | 1.33 |
| 37 | D | 405 | CLA | C3C-C2C | 4.67 | 1.46 | 1.36 |
| 48 | 15 | 312 | A86 | C9-C8 | 4.67 | 1.46 | 1.34 |
| 37 | B | 509 | CLA | C3C-C2C | 4.67 | 1.46 | 1.36 |
| 37 | B | 506 | CLA | C3C-C2C | 4.67 | 1.46 | 1.36 |
| 37 | b | 523 | CLA | O2D-CGD | 4.67 | 1.44 | 1.33 |
| 37 | 40 | 210 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 37 | b | 505 | CLA | O2D-CGD | 4.66 | 1.44 | 1.33 |
| 48 | 21 | 211 | A86 | C9-C8 | 4.66 | 1.46 | 1.34 |
| 37 | c | 501 | CLA | C3C-C2C | 4.66 | 1.46 | 1.36 |
| 37 | 18 | 209 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 37 | 37 | 301 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 48 | 37 | 319 | A86 | C9-C8 | 4.66 | 1.46 | 1.34 |
| 48 | 37 | 312 | A86 | C9-C8 | 4.66 | 1.46 | 1.34 |
| 47 | 21 | 207 | KC1 | C1D-ND | 4.66 | 1.44 | 1.37 |
| 47 | 35 | 306 | KC1 | C1D-ND | 4.66 | 1.44 | 1.37 |
| 37 | 19 | 302 | CLA | O2D-CGD | 4.66 | 1.44 | 1.33 |
| 47 | 38 | 207 | KC1 | CHD-C4C | 4.66 | 1.47 | 1.38 |
| 37 | c | 506 | CLA | O2D-CGD | 4.66 | 1.44 | 1.33 |
| 48 | 14 | 315 | A86 | C9-C8 | 4.66 | 1.46 | 1.34 |
| 48 | 34 | 315 | A86 | C9-C8 | 4.66 | 1.46 | 1.34 |
| 48 | 15 | 311 | A86 | O4-C38 | 4.66 | 1.45 | 1.35 |
| 37 | 34 | 310 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 37 | 39 | 302 | CLA | O2D-CGD | 4.66 | 1.44 | 1.33 |
| 48 | 20 | 309 | A86 | C9-C8 | 4.66 | 1.46 | 1.34 |
| 37 | B | 508 | CLA | O2D-CGD | 4.66 | 1.44 | 1.33 |
| 47 | 33 | 302 | KC1 | CHD-C4C | 4.65 | 1.47 | 1.38 |
| 37 | 36 | 306 | CLA | CHC-C1C | 4.65 | 1.47 | 1.38 |
| 37 | 21 | 206 | CLA | CHC-C1C | 4.65 | 1.47 | 1.38 |
| 48 | 38 | 213 | A86 | C17-C18 | -4.65 | 1.45 | 1.52 |
| 37 | b | 506 | CLA | C3C-C2C | 4.65 | 1.46 | 1.36 |
| 48 | 35 | 316 | A86 | C9-C8 | 4.65 | 1.46 | 1.34 |
| 47 | 41 | 203 | KC1 | C1D-ND | 4.65 | 1.44 | 1.37 |
| 37 | B | 524 | CLA | O2D-CGD | 4.65 | 1.44 | 1.33 |
| 48 | 33 | 312 | A86 | C17-C18 | -4.65 | 1.45 | 1.52 |
| 47 | 13 | 302 | KC1 | CHD-C4C | 4.65 | 1.47 | 1.38 |
| 47 | 36 | 308 | KC1 | CHD-C4C | 4.65 | 1.47 | 1.38 |
| 48 | 13 | 312 | A86 | C9-C8 | 4.65 | 1.46 | 1.34 |
| 37 | 38 | 201 | CLA | C1D-ND | 4.65 | 1.44 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 17 | 306 | KC1 | CHD-C4C | 4.65 | 1.47 | 1.38 |
| 48 | 17 | 310 | A86 | C9-C8 | 4.65 | 1.46 | 1.34 |
| 37 | C | 506 | CLA | O2D-CGD | 4.65 | 1.44 | 1.33 |
| 37 | 11 | 301 | CLA | O2D-CGD | 4.65 | 1.44 | 1.33 |
| 48 | 17 | 314 | A86 | C17-C18 | -4.65 | 1.45 | 1.52 |
| 37 | 41 | 204 | CLA | CHC-C1C | 4.64 | 1.47 | 1.38 |
| 37 | W | 102 | CLA | C1D-ND | 4.64 | 1.44 | 1.37 |
| 47 | 14 | 304 | KC1 | C1A-NA | -4.64 | 1.28 | 1.38 |
| 47 | 34 | 304 | KC1 | C1A-NA | -4.64 | 1.28 | 1.38 |
| 37 | c | 504 | CLA | C3C-C2C | 4.64 | 1.46 | 1.36 |
| 37 | 13 | 305 | CLA | CHC-C1C | 4.64 | 1.47 | 1.38 |
| 47 | 16 | 308 | KC1 | CHD-C4C | 4.64 | 1.47 | 1.38 |
| 48 | 37 | 314 | A86 | C17-C18 | -4.64 | 1.45 | 1.52 |
| 48 | 37 | 311 | A86 | O4-C38 | 4.64 | 1.45 | 1.35 |
| 37 | 15 | 301 | CLA | C1D-ND | 4.64 | 1.44 | 1.37 |
| 37 | 35 | 301 | CLA | C1D-ND | 4.64 | 1.44 | 1.37 |
| 37 | 20 | 307 | CLA | CHC-C1C | 4.64 | 1.47 | 1.38 |
| 47 | 18 | 207 | KC1 | CHD-C4C | 4.64 | 1.47 | 1.38 |
| 48 | 35 | 312 | A86 | C9-C8 | 4.64 | 1.46 | 1.34 |
| 48 | 37 | 309 | A86 | C9-C8 | 4.64 | 1.46 | 1.34 |
| 37 | b | 516 | CLA | O2D-CGD | 4.64 | 1.44 | 1.33 |
| 37 | 40 | 209 | CLA | CHC-C1C | 4.64 | 1.47 | 1.38 |
| 37 | d | 403 | CLA | O2D-CGD | 4.64 | 1.44 | 1.33 |
| 37 | D | 405 | CLA | O2D-CGD | 4.63 | 1.44 | 1.33 |
| 48 | 41 | 211 | A86 | C9-C8 | 4.63 | 1.46 | 1.34 |
| 47 | 35 | 309 | KC1 | CHD-C4C | 4.63 | 1.47 | 1.38 |
| 37 | c | 505 | CLA | O2D-CGD | 4.63 | 1.44 | 1.33 |
| 37 | 15 | 310 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 47 | 21 | 203 | KC1 | C1D-ND | 4.63 | 1.43 | 1.37 |
| 48 | 40 | 211 | A86 | C9-C8 | 4.63 | 1.46 | 1.34 |
| 48 | 21 | 214 | A86 | C9-C8 | 4.63 | 1.46 | 1.34 |
| 37 | b | 502 | CLA | O2D-CGD | 4.63 | 1.44 | 1.33 |
| 48 | 32 | 218 | A86 | C9-C8 | 4.63 | 1.46 | 1.34 |
| 48 | 15 | 311 | A86 | C9-C8 | 4.63 | 1.46 | 1.34 |
| 48 | 12 | 217 | A86 | C9-C8 | 4.63 | 1.46 | 1.34 |
| 48 | 41 | 214 | A86 | C9-C8 | 4.63 | 1.46 | 1.34 |
| 37 | 33 | 305 | CLA | CHC-C1C | 4.63 | 1.47 | 1.38 |
| 48 | 39 | 313 | A86 | C19-C18 | 4.62 | 1.58 | 1.52 |
| 37 | 39 | 304 | CLA | O2A-CGA | 4.62 | 1.46 | 1.30 |
| 47 | 13 | 302 | KC1 | C1A-NA | -4.62 | 1.28 | 1.38 |
| 47 | 33 | 302 | KC1 | C1A-NA | -4.62 | 1.28 | 1.38 |
| 37 | B | 502 | CLA | O2D-CGD | 4.62 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 17 | 312 | A86 | O4-C38 | 4.62 | 1.45 | 1.35 |
| 47 | 15 | 302 | KC1 | C1D-ND | 4.62 | 1.43 | 1.37 |
| 37 | 31 | 301 | CLA | CHC-C1C | 4.62 | 1.47 | 1.38 |
| 37 | C | 504 | CLA | C3C-C2C | 4.62 | 1.46 | 1.36 |
| 48 | 17 | 313 | A86 | C9-C8 | 4.62 | 1.46 | 1.34 |
| 37 | C | 505 | CLA | O2D-CGD | 4.62 | 1.44 | 1.33 |
| 37 | 31 | 301 | CLA | C1D-ND | 4.62 | 1.43 | 1.37 |
| 48 | 35 | 315 | A86 | C9-C8 | 4.62 | 1.46 | 1.34 |
| 37 | b | 508 | CLA | O2D-CGD | 4.62 | 1.44 | 1.33 |
| 37 | 41 | 209 | CLA | CHC-C1C | 4.62 | 1.47 | 1.38 |
| 47 | 15 | 309 | KC1 | CHD-C4C | 4.62 | 1.47 | 1.38 |
| 47 | 37 | 305 | KC1 | CHD-C4C | 4.62 | 1.47 | 1.38 |
| 37 | 19 | 304 | CLA | O2A-CGA | 4.61 | 1.46 | 1.30 |
| 47 | 36 | 305 | KC1 | C1D-ND | 4.61 | 1.43 | 1.37 |
| 37 | 20 | 303 | CLA | CHC-C1C | 4.61 | 1.47 | 1.38 |
| 37 | 21 | 204 | CLA | CHC-C1C | 4.61 | 1.47 | 1.38 |
| 37 | 41 | 206 | CLA | CHC-C1C | 4.61 | 1.47 | 1.38 |
| 48 | 38 | 213 | A86 | C9-C8 | 4.61 | 1.46 | 1.34 |
| 47 | 34 | 304 | KC1 | C1D-ND | 4.61 | 1.43 | 1.37 |
| 37 | B | 506 | CLA | O2D-CGD | 4.61 | 1.44 | 1.33 |
| 37 | 38 | 206 | CLA | CHC-C1C | 4.61 | 1.47 | 1.38 |
| 37 | 17 | 302 | CLA | CHC-C1C | 4.61 | 1.47 | 1.38 |
| 37 | C | 508 | CLA | O2D-CGD | 4.61 | 1.44 | 1.33 |
| 37 | 34 | 307 | CLA | CHC-C1C | 4.61 | 1.47 | 1.38 |
| 37 | 32 | 210 | CLA | C1B-NB | -4.61 | 1.31 | 1.37 |
| 37 | 38 | 208 | CLA | CHC-C1C | 4.60 | 1.47 | 1.38 |
| 37 | 14 | 307 | CLA | CHC-C1C | 4.60 | 1.47 | 1.38 |
| 48 | 19 | 313 | A86 | O4-C38 | 4.60 | 1.45 | 1.35 |
| 37 | 18 | 202 | CLA | C1D-ND | 4.60 | 1.43 | 1.37 |
| 47 | 40 | 207 | KC1 | O2D-CGD | 4.60 | 1.44 | 1.33 |
| 47 | 33 | 302 | KC1 | CHC-C4B | 4.60 | 1.47 | 1.38 |
| 47 | 16 | 308 | KC1 | C1D-ND | 4.60 | 1.43 | 1.37 |
| 47 | 36 | 308 | KC1 | C1D-ND | 4.60 | 1.43 | 1.37 |
| 47 | 37 | 305 | KC1 | C1D-ND | 4.60 | 1.43 | 1.37 |
| 47 | 13 | 302 | KC1 | CHC-C4B | 4.60 | 1.47 | 1.38 |
| 37 | 12 | 212 | CLA | C1D-ND | 4.60 | 1.43 | 1.37 |
| 37 | 40 | 205 | CLA | C1D-ND | 4.60 | 1.43 | 1.37 |
| 48 | 19 | 311 | A86 | C9-C8 | 4.60 | 1.46 | 1.34 |
| 48 | 12 | 202 | A86 | C9-C8 | 4.60 | 1.46 | 1.34 |
| 48 | 32 | 203 | A86 | C9-C8 | 4.60 | 1.46 | 1.34 |
| 48 | 35 | 311 | A86 | C9-C8 | 4.60 | 1.46 | 1.34 |
| 48 | 37 | 313 | A86 | C17-C18 | -4.60 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | C | 501 | CLA | O2D-CGD | 4.60 | 1.44 | 1.33 |
| 37 | 18 | 208 | CLA | CHC-C1C | 4.60 | 1.47 | 1.38 |
| 37 | 21 | 205 | CLA | CHC-C1C | 4.60 | 1.47 | 1.38 |
| 37 | 14 | 310 | CLA | C1D-ND | 4.60 | 1.43 | 1.37 |
| 37 | 19 | 309 | CLA | O2A-CGA | 4.60 | 1.46 | 1.30 |
| 48 | 13 | 311 | A86 | C9-C8 | 4.60 | 1.46 | 1.34 |
| 48 | 33 | 311 | A86 | C9-C8 | 4.60 | 1.46 | 1.34 |
| 37 | 21 | 208 | CLA | CHC-C1C | 4.60 | 1.47 | 1.38 |
| 37 | 35 | 308 | CLA | CHC-C1C | 4.60 | 1.47 | 1.38 |
| 37 | c | 501 | CLA | O2D-CGD | 4.60 | 1.44 | 1.33 |
| 37 | 12 | 212 | CLA | CHC-C1C | 4.59 | 1.47 | 1.38 |
| 37 | 18 | 206 | CLA | CHC-C1C | 4.59 | 1.47 | 1.38 |
| 48 | 17 | 314 | A86 | C9-C8 | 4.59 | 1.46 | 1.34 |
| 47 | 36 | 304 | KC1 | CHC-C4B | 4.59 | 1.47 | 1.38 |
| 47 | 11 | 304 | KC1 | C1A-NA | -4.59 | 1.28 | 1.38 |
| 47 | 19 | 308 | KC1 | C1A-NA | -4.59 | 1.28 | 1.38 |
| 47 | 39 | 308 | KC1 | C1A-NA | -4.59 | 1.28 | 1.38 |
| 47 | 31 | 305 | KC1 | C1A-NA | -4.59 | 1.28 | 1.38 |
| 47 | 13 | 302 | KC1 | C1D-ND | 4.59 | 1.43 | 1.37 |
| 47 | 33 | 302 | KC1 | C1D-ND | 4.59 | 1.43 | 1.37 |
| 48 | 13 | 312 | A86 | C17-C18 | -4.59 | 1.45 | 1.52 |
| 48 | 15 | 315 | A86 | C9-C8 | 4.59 | 1.46 | 1.34 |
| 37 | 38 | 211 | CLA | CHD-C1D | 4.59 | 1.47 | 1.38 |
| 37 | 21 | 209 | CLA | CHC-C1C | 4.59 | 1.47 | 1.38 |
| 37 | 14 | 310 | CLA | O2A-CGA | 4.59 | 1.46 | 1.30 |
| 37 | 34 | 310 | CLA | O2A-CGA | 4.59 | 1.46 | 1.30 |
| 37 | b | 506 | CLA | O2D-CGD | 4.59 | 1.44 | 1.33 |
| 50 | 16 | 312 | DD6 | C2-C1 | 4.58 | 1.46 | 1.35 |
| 47 | 19 | 308 | KC1 | CHC-C4B | 4.58 | 1.47 | 1.38 |
| 47 | 12 | 206 | KC1 | CHC-C4B | 4.58 | 1.47 | 1.38 |
| 47 | 32 | 207 | KC1 | CHC-C4B | 4.58 | 1.47 | 1.38 |
| 37 | b | 511 | CLA | C3C-C2C | 4.58 | 1.46 | 1.36 |
| 48 | 39 | 313 | A86 | O4-C38 | 4.58 | 1.45 | 1.35 |
| 37 | 12 | 209 | CLA | C1B-NB | -4.58 | 1.31 | 1.37 |
| 47 | 35 | 306 | KC1 | CHC-C4B | 4.58 | 1.47 | 1.38 |
| 37 | 41 | 205 | CLA | CHC-C1C | 4.58 | 1.47 | 1.38 |
| 47 | 18 | 207 | KC1 | CHB-C1B | 4.58 | 1.47 | 1.38 |
| 37 | 20 | 303 | CLA | C1D-ND | 4.58 | 1.43 | 1.37 |
| 37 | 37 | 301 | CLA | CHC-C1C | 4.58 | 1.47 | 1.38 |
| 50 | 36 | 312 | DD6 | C2-C1 | 4.58 | 1.46 | 1.35 |
| 37 | B | 511 | CLA | C3C-C2C | 4.58 | 1.46 | 1.36 |
| 37 | c | 502 | CLA | O2D-CGD | 4.58 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | W | 102 | CLA | CHC-C1C | 4.58 | 1.47 | 1.38 |
| 37 | 38 | 211 | CLA | O2A-CGA | 4.58 | 1.45 | 1.30 |
| 47 | 16 | 305 | KC1 | C1D-ND | 4.58 | 1.43 | 1.37 |
| 47 | 18 | 205 | KC1 | CHC-C4B | 4.58 | 1.47 | 1.38 |
| 47 | 38 | 205 | KC1 | CHC-C4B | 4.58 | 1.47 | 1.38 |
| 37 | 39 | 309 | CLA | O2A-CGA | 4.58 | 1.45 | 1.30 |
| 37 | c | 508 | CLA | O2D-CGD | 4.58 | 1.44 | 1.33 |
| 37 | 32 | 210 | CLA | O2D-CGD | 4.58 | 1.44 | 1.33 |
| 48 | 37 | 310 | A86 | C9-C8 | 4.58 | 1.46 | 1.34 |
| 37 | 32 | 213 | CLA | O2A-CGA | 4.58 | 1.45 | 1.30 |
| 48 | 40 | 213 | A86 | C7-C6 | 4.58 | 1.60 | 1.50 |
| 37 | 41 | 202 | CLA | CHC-C1C | 4.58 | 1.47 | 1.38 |
| 37 | 34 | 305 | CLA | CHC-C1C | 4.57 | 1.47 | 1.38 |
| 37 | 12 | 209 | CLA | CHC-C1C | 4.57 | 1.47 | 1.38 |
| 37 | 13 | 310 | CLA | CHC-C1C | 4.57 | 1.47 | 1.38 |
| 37 | 40 | 205 | CLA | CHC-C1C | 4.57 | 1.47 | 1.38 |
| 48 | 20 | 311 | A86 | C7-C6 | 4.57 | 1.60 | 1.50 |
| 37 | 12 | 209 | CLA | O2D-CGD | 4.57 | 1.44 | 1.33 |
| 37 | 19 | 302 | CLA | C1D-ND | 4.57 | 1.43 | 1.37 |
| 37 | 41 | 208 | CLA | CHC-C1C | 4.57 | 1.47 | 1.38 |
| 47 | 11 | 306 | KC1 | O2D-CGD | 4.57 | 1.44 | 1.33 |
| 47 | 14 | 306 | KC1 | CHD-C4C | 4.57 | 1.47 | 1.38 |
| 48 | 34 | 316 | A86 | C9-C8 | 4.57 | 1.46 | 1.34 |
| 47 | 19 | 308 | KC1 | CHD-C4C | 4.57 | 1.47 | 1.38 |
| 37 | b | 514 | CLA | O2D-CGD | 4.57 | 1.44 | 1.33 |
| 47 | 11 | 302 | KC1 | O2D-CGD | 4.57 | 1.44 | 1.33 |
| 37 | 36 | 309 | CLA | CHC-C1C | 4.57 | 1.47 | 1.38 |
| 47 | 31 | 303 | KC1 | O2D-CGD | 4.56 | 1.44 | 1.33 |
| 37 | 21 | 209 | CLA | O2A-CGA | 4.56 | 1.45 | 1.30 |
| 37 | 31 | 302 | CLA | C3C-C2C | 4.56 | 1.46 | 1.36 |
| 47 | 11 | 302 | KC1 | CHD-C4C | 4.56 | 1.47 | 1.38 |
| 47 | 31 | 303 | KC1 | CHD-C4C | 4.56 | 1.47 | 1.38 |
| 48 | 39 | 311 | A86 | C9-C8 | 4.56 | 1.46 | 1.34 |
| 48 | 17 | 320 | A86 | C9-C8 | 4.56 | 1.46 | 1.34 |
| 47 | 39 | 308 | KC1 | CHC-C4B | 4.56 | 1.47 | 1.38 |
| 37 | 41 | 210 | CLA | O2A-CGA | 4.56 | 1.45 | 1.30 |
| 37 | 16 | 309 | CLA | CHC-C1C | 4.56 | 1.47 | 1.38 |
| 37 | 21 | 202 | CLA | CHC-C1C | 4.56 | 1.47 | 1.38 |
| 47 | 20 | 305 | KC1 | O2D-CGD | 4.56 | 1.44 | 1.33 |
| 47 | 11 | 309 | KC1 | CHD-C4C | 4.56 | 1.47 | 1.38 |
| 47 | 31 | 309 | KC1 | CHD-C4C | 4.56 | 1.47 | 1.38 |
| 37 | 16 | 301 | CLA | C3C-C2C | 4.56 | 1.46 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 16 | 304 | KC1 | CHC-C4B | 4.56 | 1.47 | 1.38 |
| 37 | 11 | 301 | CLA | C3C-C2C | 4.56 | 1.46 | 1.36 |
| 37 | 33 | 308 | CLA | O2A-CGA | 4.56 | 1.46 | 1.33 |
| 37 | 18 | 211 | CLA | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 37 | 13 | 301 | CLA | CHC-C1C | 4.55 | 1.47 | 1.38 |
| 37 | 32 | 213 | CLA | CHC-C1C | 4.55 | 1.47 | 1.38 |
| 37 | 33 | 301 | CLA | CHC-C1C | 4.55 | 1.47 | 1.38 |
| 47 | 39 | 308 | KC1 | CHD-C4C | 4.55 | 1.47 | 1.38 |
| 37 | 13 | 310 | CLA | CHD-C1D | 4.55 | 1.47 | 1.38 |
| 47 | 31 | 307 | KC1 | O2D-CGD | 4.55 | 1.44 | 1.33 |
| 47 | 15 | 306 | KC1 | CHC-C4B | 4.55 | 1.47 | 1.38 |
| 37 | 13 | 308 | CLA | C1D-ND | 4.55 | 1.43 | 1.37 |
| 37 | 33 | 308 | CLA | C1D-ND | 4.55 | 1.43 | 1.37 |
| 37 | 35 | 310 | CLA | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 37 | 40 | 209 | CLA | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 37 | 15 | 310 | CLA | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 37 | 12 | 212 | CLA | O2A-CGA | 4.55 | 1.45 | 1.30 |
| 47 | 14 | 309 | KC1 | CHD-C4C | 4.55 | 1.47 | 1.38 |
| 47 | 35 | 309 | KC1 | C1D-ND | 4.55 | 1.43 | 1.37 |
| 37 | 13 | 308 | CLA | O2A-CGA | 4.55 | 1.46 | 1.33 |
| 47 | 31 | 307 | KC1 | CHC-C4B | 4.55 | 1.47 | 1.38 |
| 47 | 36 | 304 | KC1 | C1A-NA | -4.55 | 1.28 | 1.38 |
| 37 | 16 | 307 | CLA | C1D-ND | 4.55 | 1.43 | 1.37 |
| 37 | 35 | 305 | CLA | CHC-C1C | 4.55 | 1.47 | 1.38 |
| 48 | 37 | 313 | A86 | C9-C8 | 4.55 | 1.46 | 1.34 |
| 37 | B | 514 | CLA | O2D-CGD | 4.55 | 1.44 | 1.33 |
| 47 | 11 | 306 | KC1 | CHC-C4B | 4.55 | 1.47 | 1.38 |
| 37 | 36 | 301 | CLA | C3C-C2C | 4.54 | 1.46 | 1.36 |
| 37 | 39 | 302 | CLA | C1D-ND | 4.54 | 1.43 | 1.37 |
| 37 | 16 | 303 | CLA | CHC-C1C | 4.54 | 1.47 | 1.38 |
| 37 | 15 | 305 | CLA | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 37 | C | 502 | CLA | O2D-CGD | 4.54 | 1.44 | 1.33 |
| 48 | 34 | 311 | A86 | C9-C8 | 4.54 | 1.46 | 1.34 |
| 48 | 15 | 316 | A86 | O4-C38 | 4.54 | 1.45 | 1.35 |
| 37 | 38 | 206 | CLA | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 47 | 33 | 304 | KC1 | CHC-C4B | 4.54 | 1.47 | 1.38 |
| 37 | 35 | 305 | CLA | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 37 | 20 | 307 | CLA | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 48 | 14 | 316 | A86 | C9-C8 | 4.54 | 1.46 | 1.34 |
| 37 | 32 | 210 | CLA | CHC-C1C | 4.54 | 1.47 | 1.38 |
| 37 | B | 503 | CLA | C1B-NB | -4.54 | 1.31 | 1.37 |
| 47 | 17 | 305 | KC1 | C1D-ND | 4.54 | 1.43 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 37 | 304 | KC1 | C1A-NA | -4.54 | 1.28 | 1.38 |
| 37 | 34 | 305 | CLA | O2A-CGA | 4.54 | 1.45 | 1.30 |
| 48 | 35 | 315 | A86 | C7-C6 | 4.54 | 1.60 | 1.50 |
| 37 | 14 | 305 | CLA | CHC-C1C | 4.54 | 1.47 | 1.38 |
| 47 | 16 | 304 | KC1 | C1A-NA | -4.54 | 1.28 | 1.38 |
| 37 | 33 | 310 | CLA | CHD-C1D | 4.54 | 1.47 | 1.38 |
| 37 | 34 | 307 | CLA | C1B-NB | -4.54 | 1.31 | 1.37 |
| 37 | 33 | 310 | CLA | CHC-C1C | 4.53 | 1.47 | 1.38 |
| 37 | 33 | 310 | CLA | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 37 | 15 | 310 | CLA | CHC-C1C | 4.53 | 1.47 | 1.38 |
| 37 | 17 | 309 | CLA | CHC-C1C | 4.53 | 1.47 | 1.38 |
| 47 | 37 | 302 | KC1 | C1D-ND | 4.53 | 1.43 | 1.37 |
| 37 | 21 | 210 | CLA | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 47 | 34 | 309 | KC1 | CHD-C4C | 4.53 | 1.47 | 1.38 |
| 37 | 14 | 305 | CLA | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 37 | 13 | 310 | CLA | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 37 | 15 | 305 | CLA | CHC-C1C | 4.53 | 1.47 | 1.38 |
| 47 | 17 | 306 | KC1 | C1D-ND | 4.53 | 1.43 | 1.37 |
| 37 | Z | 101 | CLA | C1D-ND | 4.53 | 1.43 | 1.37 |
| 37 | 36 | 303 | CLA | CHC-C1C | 4.53 | 1.47 | 1.38 |
| 37 | 41 | 209 | CLA | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 48 | 21 | 215 | A86 | C7-C6 | 4.53 | 1.60 | 1.50 |
| 37 | 21 | 205 | CLA | O2A-CGA | 4.53 | 1.45 | 1.30 |
| 37 | 36 | 303 | CLA | C1D-ND | 4.53 | 1.43 | 1.37 |
| 48 | 21 | 215 | A86 | O4-C38 | 4.53 | 1.45 | 1.35 |
| 48 | 35 | 316 | A86 | O4-C38 | 4.52 | 1.45 | 1.35 |
| 48 | 14 | 311 | A86 | C9-C8 | 4.52 | 1.46 | 1.34 |
| 47 | 13 | 304 | KC1 | CHC-C4B | 4.52 | 1.47 | 1.38 |
| 47 | 18 | 207 | KC1 | C1D-ND | 4.52 | 1.43 | 1.37 |
| 37 | b | 511 | CLA | C1B-NB | -4.52 | 1.31 | 1.37 |
| 37 | D | 402 | CLA | CHC-C1C | 4.52 | 1.47 | 1.38 |
| 37 | c | 508 | CLA | C1B-NB | -4.52 | 1.31 | 1.37 |
| 48 | 12 | 202 | A86 | O4-C38 | 4.52 | 1.45 | 1.35 |
| 48 | 32 | 203 | A86 | O4-C38 | 4.52 | 1.45 | 1.35 |
| 37 | 36 | 309 | CLA | O2A-CGA | 4.52 | 1.45 | 1.30 |
| 37 | 36 | 307 | CLA | C1D-ND | 4.52 | 1.43 | 1.37 |
| 47 | 17 | 305 | KC1 | C1A-NA | -4.52 | 1.28 | 1.38 |
| 37 | 41 | 205 | CLA | O2A-CGA | 4.51 | 1.45 | 1.30 |
| 37 | 37 | 308 | CLA | CHC-C1C | 4.51 | 1.47 | 1.38 |
| 47 | 40 | 207 | KC1 | C1D-ND | 4.51 | 1.43 | 1.37 |
| 37 | 13 | 305 | CLA | O2A-CGA | 4.51 | 1.45 | 1.30 |
| 37 | 18 | 203 | CLA | CHC-C1C | 4.51 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 14 | 307 | CLA | C1B-NB | -4.51 | 1.31 | 1.37 |
| 47 | 20 | 302 | KC1 | C1A-NA | -4.51 | 1.28 | 1.38 |
| 48 | 32 | 217 | A86 | C9-C8 | 4.51 | 1.46 | 1.34 |
| 47 | 38 | 210 | KC1 | CHC-C4B | 4.51 | 1.47 | 1.38 |
| 37 | 32 | 204 | CLA | C3C-C2C | 4.51 | 1.46 | 1.36 |
| 47 | 34 | 306 | KC1 | CHD-C4C | 4.51 | 1.47 | 1.38 |
| 37 | 14 | 302 | CLA | CHC-C1C | 4.50 | 1.47 | 1.38 |
| 37 | 18 | 209 | CLA | CHC-C1C | 4.50 | 1.47 | 1.38 |
| 48 | 17 | 320 | A86 | C21-C20 | 4.50 | 1.58 | 1.51 |
| 37 | 35 | 310 | CLA | CHC-C1C | 4.50 | 1.47 | 1.38 |
| 37 | Z | 101 | CLA | O2A-CGA | 4.50 | 1.46 | 1.33 |
| 47 | 17 | 306 | KC1 | C1A-CHA | 4.50 | 1.51 | 1.40 |
| 47 | 37 | 305 | KC1 | C1A-CHA | 4.50 | 1.51 | 1.40 |
| 37 | 38 | 209 | CLA | CHC-C1C | 4.50 | 1.47 | 1.38 |
| 48 | 15 | 319 | A86 | C9-C8 | 4.50 | 1.46 | 1.34 |
| 37 | 38 | 203 | CLA | CHC-C1C | 4.50 | 1.47 | 1.38 |
| 37 | 31 | 306 | CLA | O2A-CGA | 4.50 | 1.45 | 1.30 |
| 37 | C | 507 | CLA | O2D-CGD | 4.50 | 1.44 | 1.33 |
| 37 | b | 512 | CLA | C1B-NB | -4.50 | 1.32 | 1.37 |
| 48 | 12 | 216 | A86 | C9-C8 | 4.50 | 1.46 | 1.34 |
| 48 | 36 | 310 | A86 | C9-C8 | 4.50 | 1.46 | 1.34 |
| 37 | 11 | 305 | CLA | CHC-C1C | 4.50 | 1.47 | 1.38 |
| 47 | 40 | 204 | KC1 | C1A-NA | -4.50 | 1.28 | 1.38 |
| 47 | 15 | 309 | KC1 | CHC-C4B | 4.50 | 1.47 | 1.38 |
| 37 | 16 | 309 | CLA | O2A-CGA | 4.50 | 1.45 | 1.30 |
| 47 | 38 | 207 | KC1 | CHC-C4B | 4.50 | 1.47 | 1.38 |
| 48 | 41 | 215 | A86 | C7-C6 | 4.49 | 1.59 | 1.50 |
| 47 | 18 | 207 | KC1 | C1A-CHA | 4.49 | 1.51 | 1.40 |
| 37 | 18 | 211 | CLA | CHC-C1C | 4.49 | 1.47 | 1.38 |
| 47 | 13 | 304 | KC1 | CHD-C4C | 4.49 | 1.47 | 1.38 |
| 37 | C | 512 | CLA | O2D-CGD | 4.49 | 1.44 | 1.33 |
| 37 | 14 | 302 | CLA | C1D-ND | 4.49 | 1.43 | 1.37 |
| 37 | b | 503 | CLA | C1B-NB | -4.49 | 1.32 | 1.37 |
| 47 | 12 | 206 | KC1 | C1A-NA | -4.49 | 1.28 | 1.38 |
| 47 | 32 | 207 | KC1 | C1A-NA | -4.49 | 1.28 | 1.38 |
| 37 | 18 | 204 | CLA | C1D-ND | 4.49 | 1.43 | 1.37 |
| 47 | 38 | 210 | KC1 | C1A-CHA | 4.49 | 1.51 | 1.40 |
| 37 | c | 512 | CLA | O2D-CGD | 4.49 | 1.44 | 1.33 |
| 48 | 41 | 215 | A86 | O4-C38 | 4.49 | 1.45 | 1.35 |
| 37 | 18 | 206 | CLA | O2A-CGA | 4.49 | 1.45 | 1.30 |
| 37 | d | 401 | CLA | CHC-C1C | 4.49 | 1.47 | 1.38 |
| 47 | 18 | 210 | KC1 | C1A-CHA | 4.49 | 1.51 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 50 | 40 | 212 | DD6 | C2-C1 | 4.49 | 1.46 | 1.35 |
| 48 | 15 | 315 | A86 | C7-C6 | 4.49 | 1.59 | 1.50 |
| 48 | 19 | 311 | A86 | O4-C38 | 4.49 | 1.45 | 1.35 |
| 47 | 33 | 304 | KC1 | CHD-C4C | 4.48 | 1.47 | 1.38 |
| 47 | 15 | 302 | KC1 | CHC-C4B | 4.48 | 1.47 | 1.38 |
| 48 | 35 | 319 | A86 | C9-C8 | 4.48 | 1.46 | 1.34 |
| 48 | 16 | 313 | A86 | O4-C38 | 4.48 | 1.45 | 1.35 |
| 37 | b | 507 | CLA | C1B-NB | -4.48 | 1.32 | 1.37 |
| 47 | 17 | 303 | KC1 | C1D-ND | 4.48 | 1.43 | 1.37 |
| 37 | 18 | 204 | CLA | O2A-CGA | 4.48 | 1.46 | 1.33 |
| 37 | Z | 102 | CLA | CHC-C1C | 4.48 | 1.47 | 1.38 |
| 47 | 14 | 304 | KC1 | C1D-ND | 4.48 | 1.43 | 1.37 |
| 47 | 14 | 304 | KC1 | CHC-C4B | 4.48 | 1.47 | 1.38 |
| 37 | 37 | 303 | CLA | CHC-C1C | 4.48 | 1.47 | 1.38 |
| 47 | 35 | 309 | KC1 | CHC-C4B | 4.48 | 1.47 | 1.38 |
| 48 | 11 | 314 | A86 | O4-C38 | 4.48 | 1.45 | 1.35 |
| 48 | 16 | 310 | A86 | C9-C8 | 4.48 | 1.46 | 1.34 |
| 37 | b | 516 | CLA | C3C-C2C | 4.48 | 1.46 | 1.36 |
| 50 | 20 | 310 | DD6 | C2-C1 | 4.48 | 1.46 | 1.35 |
| 37 | c | 507 | CLA | O2D-CGD | 4.48 | 1.44 | 1.33 |
| 47 | 15 | 304 | KC1 | C1A-NA | -4.48 | 1.28 | 1.38 |
| 48 | 16 | 310 | A86 | C17-C18 | -4.48 | 1.46 | 1.52 |
| 37 | c | 509 | CLA | O2A-CGA | 4.48 | 1.46 | 1.33 |
| 37 | z | 101 | CLA | O2A-CGA | 4.48 | 1.46 | 1.33 |
| 47 | 31 | 307 | KC1 | CHD-C4C | 4.48 | 1.47 | 1.38 |
| 37 | 33 | 305 | CLA | O2A-CGA | 4.48 | 1.45 | 1.30 |
| 37 | B | 505 | CLA | CHC-C1C | 4.48 | 1.47 | 1.38 |
| 37 | b | 523 | CLA | CHC-C1C | 4.48 | 1.47 | 1.38 |
| 37 | 12 | 203 | CLA | CHC-C1C | 4.48 | 1.47 | 1.38 |
| 37 | 11 | 305 | CLA | O2A-CGA | 4.48 | 1.45 | 1.30 |
| 47 | 36 | 302 | KC1 | C1A-CHA | 4.48 | 1.51 | 1.40 |
| 48 | 35 | 313 | A86 | C17-C18 | -4.48 | 1.46 | 1.52 |
| 47 | 15 | 309 | KC1 | C1D-ND | 4.48 | 1.43 | 1.37 |
| 37 | C | 508 | CLA | C1B-NB | -4.48 | 1.32 | 1.37 |
| 37 | C | 509 | CLA | O2A-CGA | 4.48 | 1.46 | 1.33 |
| 37 | 14 | 301 | CLA | C1D-ND | 4.47 | 1.43 | 1.37 |
| 37 | 34 | 301 | CLA | C1D-ND | 4.47 | 1.43 | 1.37 |
| 48 | 39 | 311 | A86 | O4-C38 | 4.47 | 1.45 | 1.35 |
| 37 | 16 | 301 | CLA | C1D-ND | 4.47 | 1.43 | 1.37 |
| 37 | b | 504 | CLA | O2D-CGD | 4.47 | 1.44 | 1.33 |
| 37 | 19 | 310 | CLA | CHC-C1C | 4.47 | 1.47 | 1.38 |
| 37 | 19 | 305 | CLA | C1D-ND | 4.47 | 1.43 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 38 | 207 | KC1 | C1A-CHA | 4.47 | 1.51 | 1.40 |
| 37 | 33 | 303 | CLA | C1D-ND | 4.47 | 1.43 | 1.37 |
| 37 | B | 516 | CLA | C3C-C2C | 4.47 | 1.46 | 1.36 |
| 37 | d | 404 | CLA | O2D-CGD | 4.47 | 1.44 | 1.33 |
| 37 | 16 | 303 | CLA | C1D-ND | 4.47 | 1.43 | 1.37 |
| 37 | 34 | 302 | CLA | CHC-C1C | 4.47 | 1.47 | 1.38 |
| 37 | B | 513 | CLA | O2D-CGD | 4.47 | 1.44 | 1.33 |
| 48 | 14 | 316 | A86 | O4-C38 | 4.47 | 1.45 | 1.35 |
| 48 | 34 | 316 | A86 | O4-C38 | 4.47 | 1.45 | 1.35 |
| 48 | 35 | 311 | A86 | O4-C38 | 4.47 | 1.45 | 1.35 |
| 37 | 41 | 204 | CLA | CHD-C1D | 4.47 | 1.47 | 1.38 |
| 37 | 17 | 307 | CLA | CHC-C1C | 4.47 | 1.47 | 1.38 |
| 48 | 13 | 315 | A86 | C7-C6 | 4.47 | 1.59 | 1.50 |
| 48 | 32 | 218 | A86 | O4-C38 | 4.47 | 1.45 | 1.35 |
| 47 | 34 | 306 | KC1 | C1D-ND | 4.47 | 1.43 | 1.37 |
| 37 | B | 512 | CLA | C1B-NB | -4.47 | 1.32 | 1.37 |
| 47 | 35 | 309 | KC1 | C1A-CHA | 4.47 | 1.51 | 1.40 |
| 37 | 12 | 207 | CLA | CHC-C1C | 4.47 | 1.47 | 1.38 |
| 37 | 32 | 204 | CLA | CHC-C1C | 4.47 | 1.47 | 1.38 |
| 37 | B | 524 | CLA | CHC-C1C | 4.47 | 1.47 | 1.38 |
| 37 | 34 | 302 | CLA | C1D-ND | 4.46 | 1.43 | 1.37 |
| 37 | 12 | 203 | CLA | C3C-C2C | 4.46 | 1.46 | 1.36 |
| 48 | 36 | 313 | A86 | C9-C8 | 4.46 | 1.46 | 1.34 |
| 48 | 40 | 201 | A86 | O4-C38 | 4.46 | 1.45 | 1.35 |
| 37 | z | 101 | CLA | C1D-ND | 4.46 | 1.43 | 1.37 |
| 47 | 33 | 304 | KC1 | C1D-ND | 4.46 | 1.43 | 1.37 |
| 48 | 15 | 313 | A86 | C17-C18 | -4.46 | 1.46 | 1.52 |
| 37 | 17 | 304 | CLA | C1D-ND | 4.46 | 1.43 | 1.37 |
| 47 | 35 | 304 | KC1 | C1A-NA | -4.46 | 1.28 | 1.38 |
| 47 | 16 | 305 | KC1 | C1A-CHA | 4.46 | 1.51 | 1.40 |
| 47 | 36 | 305 | KC1 | C1A-CHA | 4.46 | 1.51 | 1.40 |
| 48 | 35 | 315 | A86 | O4-C38 | 4.46 | 1.45 | 1.35 |
| 37 | 31 | 306 | CLA | CHC-C1C | 4.46 | 1.47 | 1.38 |
| 48 | 31 | 311 | A86 | O4-C38 | 4.46 | 1.45 | 1.35 |
| 37 | 39 | 310 | CLA | CHC-C1C | 4.46 | 1.47 | 1.38 |
| 37 | 36 | 307 | CLA | CHC-C1C | 4.46 | 1.47 | 1.38 |
| 48 | 36 | 310 | A86 | C17-C18 | -4.46 | 1.46 | 1.52 |
| 48 | 37 | 319 | A86 | C21-C20 | 4.46 | 1.58 | 1.51 |
| 48 | 19 | 313 | A86 | C10-C11 | 4.46 | 1.46 | 1.34 |
| 37 | 41 | 204 | CLA | O2A-CGA | 4.46 | 1.46 | 1.33 |
| 48 | 41 | 214 | A86 | O4-C38 | 4.46 | 1.45 | 1.35 |
| 47 | 32 | 209 | KC1 | C1A-CHA | 4.46 | 1.51 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 18 | 212 | A86 | C21-C20 | 4.46 | 1.58 | 1.51 |
| 47 | 13 | 304 | KC1 | C1A-NA | -4.46 | 1.28 | 1.38 |
| 48 | 12 | 215 | A86 | C17-C18 | -4.46 | 1.46 | 1.52 |
| 48 | 32 | 216 | A86 | C17-C18 | -4.46 | 1.46 | 1.52 |
| 37 | 34 | 303 | CLA | C1D-ND | 4.46 | 1.43 | 1.37 |
| 48 | 11 | 311 | A86 | O4-C38 | 4.45 | 1.45 | 1.35 |
| 37 | 21 | 204 | CLA | O2A-CGA | 4.45 | 1.46 | 1.33 |
| 37 | 32 | 208 | CLA | CHC-C1C | 4.45 | 1.47 | 1.38 |
| 48 | 17 | 311 | A86 | C9-C8 | 4.45 | 1.46 | 1.34 |
| 48 | 18 | 213 | A86 | O4-C38 | 4.45 | 1.45 | 1.35 |
| 47 | 20 | 305 | KC1 | C1D-ND | 4.45 | 1.43 | 1.37 |
| 48 | 41 | 211 | A86 | C10-C11 | 4.45 | 1.46 | 1.34 |
| 47 | 31 | 303 | KC1 | C1A-NA | -4.45 | 1.28 | 1.38 |
| 37 | 38 | 204 | CLA | O2A-CGA | 4.45 | 1.46 | 1.33 |
| 48 | 37 | 314 | A86 | C7-C6 | 4.45 | 1.59 | 1.50 |
| 47 | 16 | 302 | KC1 | C1A-CHA | 4.45 | 1.51 | 1.40 |
| 48 | 13 | 311 | A86 | C17-C18 | -4.45 | 1.46 | 1.52 |
| 47 | 15 | 304 | KC1 | CHC-C4B | 4.45 | 1.47 | 1.38 |
| 47 | 16 | 305 | KC1 | CHC-C4B | 4.45 | 1.47 | 1.38 |
| 48 | 40 | 201 | A86 | C10-C11 | 4.45 | 1.46 | 1.34 |
| 48 | 14 | 312 | A86 | C9-C8 | 4.45 | 1.46 | 1.34 |
| 37 | C | 512 | CLA | O2A-CGA | 4.45 | 1.46 | 1.33 |
| 48 | 17 | 313 | A86 | C7-C6 | 4.45 | 1.59 | 1.50 |
| 47 | 18 | 205 | KC1 | C1A-NA | -4.45 | 1.28 | 1.38 |
| 47 | 38 | 205 | KC1 | C1A-NA | -4.45 | 1.28 | 1.38 |
| 37 | 37 | 306 | CLA | O2A-CGA | 4.45 | 1.46 | 1.33 |
| 47 | 37 | 304 | KC1 | CHC-C4B | 4.45 | 1.47 | 1.38 |
| 48 | 16 | 314 | A86 | O4-C38 | 4.45 | 1.45 | 1.35 |
| 37 | B | 504 | CLA | O2D-CGD | 4.44 | 1.44 | 1.33 |
| 47 | 11 | 302 | KC1 | C1A-NA | -4.44 | 1.28 | 1.38 |
| 37 | 40 | 205 | CLA | O2A-CGA | 4.44 | 1.46 | 1.33 |
| 47 | 38 | 207 | KC1 | CHB-C1B | 4.44 | 1.47 | 1.38 |
| 37 | 21 | 204 | CLA | CHD-C1D | 4.44 | 1.47 | 1.38 |
| 37 | B | 507 | CLA | C1B-NB | -4.44 | 1.32 | 1.37 |
| 47 | 11 | 306 | KC1 | CHD-C4C | 4.44 | 1.47 | 1.38 |
| 37 | B | 511 | CLA | C1B-NB | -4.44 | 1.32 | 1.37 |
| 37 | b | 505 | CLA | CHC-C1C | 4.44 | 1.47 | 1.38 |
| 37 | 37 | 306 | CLA | CHC-C1C | 4.44 | 1.47 | 1.38 |
| 47 | 34 | 304 | KC1 | CHC-C4B | 4.44 | 1.47 | 1.38 |
| 48 | 13 | 315 | A86 | O4-C38 | 4.44 | 1.45 | 1.35 |
| 48 | 21 | 214 | A86 | O4-C38 | 4.44 | 1.45 | 1.35 |
| 37 | 17 | 304 | CLA | CHC-C1C | 4.44 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 306 | KC1 | C1A-CHA | 4.44 | 1.51 | 1.40 |
| 47 | 14 | 306 | KC1 | C1D-ND | 4.44 | 1.43 | 1.37 |
| 47 | 11 | 306 | KC1 | CHB-C1B | 4.44 | 1.47 | 1.38 |
| 48 | 20 | 309 | A86 | O4-C38 | 4.44 | 1.45 | 1.35 |
| 37 | c | 512 | CLA | O2A-CGA | 4.44 | 1.46 | 1.33 |
| 48 | 16 | 314 | A86 | C9-C8 | 4.44 | 1.46 | 1.34 |
| 37 | z | 102 | CLA | CHC-C1C | 4.44 | 1.47 | 1.38 |
| 47 | 35 | 302 | KC1 | CHC-C4B | 4.44 | 1.47 | 1.38 |
| 37 | 15 | 303 | CLA | CHC-C1C | 4.44 | 1.47 | 1.38 |
| 37 | 19 | 307 | CLA | C1D-ND | 4.44 | 1.43 | 1.37 |
| 48 | 39 | 313 | A86 | C10-C11 | 4.44 | 1.46 | 1.34 |
| 48 | 18 | 213 | A86 | C9-C8 | 4.44 | 1.46 | 1.34 |
| 47 | 15 | 309 | KC1 | C1A-CHA | 4.44 | 1.51 | 1.40 |
| 37 | C | 504 | CLA | CHC-C1C | 4.44 | 1.47 | 1.38 |
| 37 | 12 | 205 | CLA | CHC-C1C | 4.44 | 1.47 | 1.38 |
| 47 | 35 | 304 | KC1 | CHC-C4B | 4.43 | 1.47 | 1.38 |
| 47 | 40 | 207 | KC1 | CHD-C4C | 4.43 | 1.47 | 1.38 |
| 48 | 31 | 313 | A86 | C9-C8 | 4.43 | 1.46 | 1.34 |
| 47 | 40 | 204 | KC1 | CHC-C4B | 4.43 | 1.47 | 1.38 |
| 37 | 16 | 307 | CLA | CHC-C1C | 4.43 | 1.47 | 1.38 |
| 48 | 17 | 315 | A86 | C7-C6 | 4.43 | 1.59 | 1.50 |
| 37 | b | 503 | CLA | O2D-CGD | 4.43 | 1.44 | 1.33 |
| 48 | 11 | 313 | A86 | C9-C8 | 4.43 | 1.46 | 1.34 |
| 48 | 12 | 217 | A86 | O4-C38 | 4.43 | 1.45 | 1.35 |
| 48 | 15 | 315 | A86 | O4-C38 | 4.43 | 1.45 | 1.35 |
| 47 | 13 | 306 | KC1 | CHD-C4C | 4.43 | 1.47 | 1.38 |
| 47 | 20 | 305 | KC1 | CHD-C4C | 4.43 | 1.47 | 1.38 |
| 47 | 33 | 306 | KC1 | CHD-C4C | 4.43 | 1.47 | 1.38 |
| 37 | D | 406 | CLA | O2D-CGD | 4.43 | 1.44 | 1.33 |
| 48 | 38 | 213 | A86 | C7-C6 | 4.43 | 1.59 | 1.50 |
| 47 | 15 | 302 | KC1 | C1A-NA | -4.43 | 1.28 | 1.38 |
| 37 | b | 513 | CLA | O2D-CGD | 4.43 | 1.44 | 1.33 |
| 47 | 20 | 302 | KC1 | CHC-C4B | 4.43 | 1.47 | 1.38 |
| 37 | 20 | 303 | CLA | O2A-CGA | 4.43 | 1.46 | 1.33 |
| 37 | b | 508 | CLA | C1B-NB | -4.43 | 1.32 | 1.37 |
| 48 | 34 | 312 | A86 | C9-C8 | 4.43 | 1.46 | 1.34 |
| 37 | C | 509 | CLA | C1B-NB | -4.43 | 1.32 | 1.37 |
| 37 | c | 504 | CLA | CHC-C1C | 4.42 | 1.47 | 1.38 |
| 37 | 39 | 305 | CLA | CHC-C1C | 4.42 | 1.47 | 1.38 |
| 48 | 16 | 313 | A86 | C10-C11 | 4.42 | 1.46 | 1.34 |
| 37 | d | 403 | CLA | CHC-C1C | 4.42 | 1.47 | 1.38 |
| 37 | B | 510 | CLA | O2D-CGD | 4.42 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 35 | 303 | CLA | CHC-C1C | 4.42 | 1.47 | 1.38 |
| 48 | 14 | 314 | A86 | C7-C6 | 4.42 | 1.59 | 1.50 |
| 48 | 34 | 314 | A86 | C7-C6 | 4.42 | 1.59 | 1.50 |
| 47 | 17 | 303 | KC1 | C1A-CHA | 4.42 | 1.51 | 1.40 |
| 47 | 37 | 302 | KC1 | C1A-CHA | 4.42 | 1.51 | 1.40 |
| 47 | 13 | 304 | KC1 | C1D-ND | 4.42 | 1.43 | 1.37 |
| 48 | 12 | 213 | A86 | C9-C8 | 4.42 | 1.46 | 1.34 |
| 47 | 31 | 307 | KC1 | CHB-C1B | 4.42 | 1.47 | 1.38 |
| 37 | b | 510 | CLA | O2D-CGD | 4.42 | 1.44 | 1.33 |
| 48 | 21 | 211 | A86 | C10-C11 | 4.42 | 1.46 | 1.34 |
| 47 | 18 | 210 | KC1 | CHC-C4B | 4.42 | 1.47 | 1.38 |
| 47 | 12 | 208 | KC1 | C1A-CHA | 4.42 | 1.51 | 1.40 |
| 48 | 36 | 313 | A86 | O4-C38 | 4.42 | 1.45 | 1.35 |
| 37 | 39 | 309 | CLA | CHC-C1C | 4.42 | 1.47 | 1.38 |
| 37 | 15 | 310 | CLA | CHD-C1D | 4.42 | 1.47 | 1.38 |
| 37 | c | 509 | CLA | C1B-NB | -4.42 | 1.32 | 1.37 |
| 37 | 36 | 309 | CLA | C1D-ND | 4.42 | 1.43 | 1.37 |
| 47 | 32 | 212 | KC1 | C1A-NA | -4.42 | 1.28 | 1.38 |
| 47 | 33 | 304 | KC1 | C1A-NA | -4.42 | 1.28 | 1.38 |
| 37 | 13 | 303 | CLA | O2A-CGA | 4.42 | 1.46 | 1.33 |
| 48 | 35 | 319 | A86 | C7-C6 | 4.42 | 1.59 | 1.50 |
| 37 | c | 503 | CLA | CHC-C1C | 4.42 | 1.47 | 1.38 |
| 37 | 16 | 309 | CLA | C1D-ND | 4.42 | 1.43 | 1.37 |
| 37 | 36 | 301 | CLA | C1D-ND | 4.42 | 1.43 | 1.37 |
| 47 | 14 | 309 | KC1 | CHC-C4B | 4.41 | 1.47 | 1.38 |
| 48 | 36 | 311 | A86 | C21-C20 | 4.41 | 1.58 | 1.51 |
| 47 | 11 | 304 | KC1 | C1D-ND | 4.41 | 1.43 | 1.37 |
| 48 | 33 | 315 | A86 | O4-C38 | 4.41 | 1.45 | 1.35 |
| 47 | 18 | 207 | KC1 | CHC-C4B | 4.41 | 1.47 | 1.38 |
| 48 | 32 | 214 | A86 | C9-C8 | 4.41 | 1.46 | 1.34 |
| 37 | 32 | 206 | CLA | CHC-C1C | 4.41 | 1.47 | 1.38 |
| 37 | 18 | 211 | CLA | CHD-C1D | 4.41 | 1.47 | 1.38 |
| 37 | 35 | 305 | CLA | CHD-C1D | 4.41 | 1.47 | 1.38 |
| 47 | 36 | 305 | KC1 | CHC-C4B | 4.41 | 1.47 | 1.38 |
| 48 | 15 | 314 | A86 | C7-C6 | 4.41 | 1.59 | 1.50 |
| 37 | 39 | 307 | CLA | C1D-ND | 4.41 | 1.43 | 1.37 |
| 37 | B | 506 | CLA | C1B-NB | -4.41 | 1.32 | 1.37 |
| 48 | 21 | 211 | A86 | O4-C38 | 4.41 | 1.44 | 1.35 |
| 48 | 37 | 314 | A86 | O4-C38 | 4.41 | 1.44 | 1.35 |
| 48 | 40 | 211 | A86 | O4-C38 | 4.41 | 1.44 | 1.35 |
| 48 | 18 | 214 | A86 | C7-C6 | 4.41 | 1.59 | 1.50 |
| 37 | 19 | 309 | CLA | CHC-C1C | 4.41 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 37 | 303 | CLA | C1D-ND | 4.41 | 1.43 | 1.37 |
| 47 | 20 | 304 | KC1 | CHB-C1B | 4.41 | 1.47 | 1.38 |
| 48 | 12 | 220 | A86 | C9-C8 | 4.41 | 1.46 | 1.34 |
| 48 | 16 | 311 | A86 | C21-C20 | 4.41 | 1.58 | 1.51 |
| 48 | 17 | 315 | A86 | O4-C38 | 4.41 | 1.44 | 1.35 |
| 37 | 38 | 208 | CLA | O2A-CGA | 4.41 | 1.46 | 1.33 |
| 37 | D | 405 | CLA | CHC-C1C | 4.41 | 1.47 | 1.38 |
| 37 | 32 | 205 | CLA | C1B-NB | -4.40 | 1.32 | 1.37 |
| 37 | 39 | 301 | CLA | C1D-ND | 4.40 | 1.43 | 1.37 |
| 47 | 15 | 306 | KC1 | C1A-CHA | 4.40 | 1.51 | 1.40 |
| 37 | B | 512 | CLA | C3C-C2C | 4.40 | 1.46 | 1.36 |
| 50 | 39 | 312 | DD6 | C2-C1 | 4.40 | 1.46 | 1.35 |
| 37 | 38 | 211 | CLA | CHC-C1C | 4.40 | 1.47 | 1.38 |
| 37 | 14 | 303 | CLA | C1D-ND | 4.40 | 1.43 | 1.37 |
| 47 | 34 | 306 | KC1 | C1A-CHA | 4.40 | 1.51 | 1.40 |
| 37 | 19 | 305 | CLA | CHC-C1C | 4.40 | 1.47 | 1.38 |
| 37 | 14 | 308 | CLA | C1D-ND | 4.40 | 1.43 | 1.37 |
| 37 | 34 | 308 | CLA | C1D-ND | 4.40 | 1.43 | 1.37 |
| 48 | 33 | 314 | A86 | C7-C6 | 4.40 | 1.59 | 1.50 |
| 37 | b | 506 | CLA | C1B-NB | -4.40 | 1.32 | 1.37 |
| 47 | 17 | 305 | KC1 | CHC-C4B | 4.40 | 1.47 | 1.38 |
| 47 | 14 | 306 | KC1 | C1A-CHA | 4.40 | 1.51 | 1.40 |
| 48 | 31 | 319 | A86 | O4-C38 | 4.40 | 1.44 | 1.35 |
| 48 | 38 | 213 | A86 | O4-C38 | 4.40 | 1.44 | 1.35 |
| 48 | 41 | 211 | A86 | O4-C38 | 4.40 | 1.44 | 1.35 |
| 47 | 14 | 306 | KC1 | CHC-C4B | 4.40 | 1.47 | 1.38 |
| 48 | 14 | 314 | A86 | O4-C38 | 4.40 | 1.44 | 1.35 |
| 48 | 34 | 314 | A86 | O4-C38 | 4.40 | 1.44 | 1.35 |
| 48 | 12 | 213 | A86 | C17-C18 | -4.40 | 1.46 | 1.52 |
| 48 | 35 | 316 | A86 | C17-C18 | -4.40 | 1.46 | 1.52 |
| 37 | 33 | 303 | CLA | O2A-CGA | 4.40 | 1.46 | 1.33 |
| 37 | 39 | 305 | CLA | C1D-ND | 4.39 | 1.43 | 1.37 |
| 37 | 17 | 309 | CLA | CHD-C1D | 4.39 | 1.47 | 1.38 |
| 48 | 35 | 312 | A86 | C7-C6 | 4.39 | 1.59 | 1.50 |
| 37 | 18 | 208 | CLA | O2A-CGA | 4.39 | 1.46 | 1.33 |
| 48 | 33 | 315 | A86 | C7-C6 | 4.39 | 1.59 | 1.50 |
| 48 | 16 | 311 | A86 | C17-C18 | -4.39 | 1.46 | 1.52 |
| 37 | 37 | 303 | CLA | O2A-CGA | 4.39 | 1.46 | 1.33 |
| 48 | 36 | 311 | A86 | C9-C8 | 4.39 | 1.46 | 1.34 |
| 37 | b | 514 | CLA | CHC-C1C | 4.39 | 1.47 | 1.38 |
| 37 | 17 | 307 | CLA | O2A-CGA | 4.39 | 1.46 | 1.33 |
| 48 | 13 | 314 | A86 | C7-C6 | 4.39 | 1.59 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | c | 505 | CLA | C1B-NB | -4.39 | 1.32 | 1.37 |
| 48 | 40 | 201 | A86 | C7-C6 | 4.39 | 1.59 | 1.50 |
| 37 | d | 404 | CLA | O2A-CGA | 4.39 | 1.46 | 1.33 |
| 48 | 32 | 221 | A86 | O4-C38 | 4.39 | 1.44 | 1.35 |
| 47 | 12 | 211 | KC1 | C1A-NA | -4.39 | 1.28 | 1.38 |
| 48 | 17 | 315 | A86 | C21-C20 | 4.39 | 1.58 | 1.51 |
| 47 | 40 | 206 | KC1 | CHB-C1B | 4.39 | 1.47 | 1.38 |
| 48 | 37 | 319 | A86 | C17-C18 | -4.39 | 1.46 | 1.52 |
| 48 | 11 | 319 | A86 | O4-C38 | 4.39 | 1.44 | 1.35 |
| 50 | 19 | 312 | DD6 | C2-C1 | 4.39 | 1.45 | 1.35 |
| 37 | B | 503 | CLA | O2D-CGD | 4.39 | 1.44 | 1.33 |
| 48 | 40 | 213 | A86 | C21-C20 | 4.39 | 1.58 | 1.51 |
| 48 | 20 | 311 | A86 | C21-C20 | 4.38 | 1.58 | 1.51 |
| 48 | 13 | 314 | A86 | O4-C38 | 4.38 | 1.44 | 1.35 |
| 48 | 16 | 313 | A86 | C7-C6 | 4.38 | 1.59 | 1.50 |
| 48 | 32 | 214 | A86 | C17-C18 | -4.38 | 1.46 | 1.52 |
| 48 | 34 | 313 | A86 | C7-C6 | 4.38 | 1.59 | 1.50 |
| 48 | 37 | 313 | A86 | C21-C20 | 4.38 | 1.58 | 1.51 |
| 37 | 37 | 301 | CLA | CHD-C1D | 4.38 | 1.47 | 1.38 |
| 48 | 12 | 216 | A86 | O4-C38 | 4.38 | 1.44 | 1.35 |
| 37 | 19 | 303 | CLA | O2D-CGD | 4.38 | 1.44 | 1.33 |
| 48 | 36 | 313 | A86 | C7-C6 | 4.38 | 1.59 | 1.50 |
| 48 | 37 | 312 | A86 | O4-C38 | 4.38 | 1.44 | 1.35 |
| 48 | 40 | 213 | A86 | O4-C38 | 4.38 | 1.44 | 1.35 |
| 37 | 19 | 301 | CLA | C1D-ND | 4.38 | 1.43 | 1.37 |
| 48 | 20 | 309 | A86 | C7-C6 | 4.38 | 1.59 | 1.50 |
| 47 | 35 | 306 | KC1 | C1A-NA | -4.38 | 1.28 | 1.38 |
| 48 | 40 | 211 | A86 | C21-C20 | 4.38 | 1.58 | 1.51 |
| 37 | 15 | 303 | CLA | CHD-C1D | 4.38 | 1.47 | 1.38 |
| 48 | 37 | 313 | A86 | O4-C38 | 4.38 | 1.44 | 1.35 |
| 48 | 37 | 310 | A86 | C17-C18 | -4.37 | 1.46 | 1.52 |
| 37 | C | 503 | CLA | CHC-C1C | 4.37 | 1.47 | 1.38 |
| 48 | 15 | 319 | A86 | C7-C6 | 4.37 | 1.59 | 1.50 |
| 48 | 12 | 220 | A86 | C17-C18 | -4.37 | 1.46 | 1.52 |
| 37 | B | 514 | CLA | CHC-C1C | 4.37 | 1.47 | 1.38 |
| 48 | 14 | 313 | A86 | C7-C6 | 4.37 | 1.59 | 1.50 |
| 48 | 21 | 214 | A86 | C7-C6 | 4.37 | 1.59 | 1.50 |
| 37 | 32 | 204 | CLA | C1D-ND | 4.37 | 1.43 | 1.37 |
| 37 | c | 512 | CLA | CHC-C1C | 4.37 | 1.47 | 1.38 |
| 37 | 15 | 305 | CLA | CHD-C1D | 4.37 | 1.47 | 1.38 |
| 37 | 35 | 310 | CLA | CHD-C1D | 4.37 | 1.47 | 1.38 |
| 37 | b | 512 | CLA | C3C-C2C | 4.37 | 1.46 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | B | 511 | CLA | O2D-CGD | 4.37 | 1.44 | 1.33 |
| 47 | 32 | 212 | KC1 | C1D-ND | 4.37 | 1.43 | 1.37 |
| 48 | 17 | 314 | A86 | C21-C20 | 4.37 | 1.58 | 1.51 |
| 48 | 17 | 311 | A86 | C17-C18 | -4.37 | 1.46 | 1.52 |
| 48 | 20 | 309 | A86 | C21-C20 | 4.37 | 1.58 | 1.51 |
| 48 | 16 | 311 | A86 | C9-C8 | 4.37 | 1.46 | 1.34 |
| 37 | 21 | 202 | CLA | CHD-C1D | 4.37 | 1.46 | 1.38 |
| 47 | 34 | 309 | KC1 | CHC-C4B | 4.37 | 1.46 | 1.38 |
| 47 | 17 | 308 | KC1 | C1A-CHA | 4.37 | 1.51 | 1.40 |
| 48 | 13 | 313 | A86 | C7-C6 | 4.37 | 1.59 | 1.50 |
| 47 | 13 | 306 | KC1 | CHC-C4B | 4.37 | 1.46 | 1.38 |
| 47 | 33 | 306 | KC1 | CHC-C4B | 4.37 | 1.46 | 1.38 |
| 48 | 32 | 221 | A86 | C9-C8 | 4.37 | 1.46 | 1.34 |
| 47 | 36 | 308 | KC1 | CHC-C4B | 4.37 | 1.46 | 1.38 |
| 37 | 14 | 303 | CLA | CHC-C1C | 4.37 | 1.47 | 1.38 |
| 37 | 34 | 303 | CLA | CHC-C1C | 4.37 | 1.47 | 1.38 |
| 48 | 33 | 314 | A86 | O4-C38 | 4.37 | 1.44 | 1.35 |
| 47 | 11 | 309 | KC1 | C1B-NB | -4.37 | 1.32 | 1.37 |
| 47 | 14 | 309 | KC1 | C1D-ND | 4.37 | 1.43 | 1.37 |
| 47 | 34 | 309 | KC1 | C1D-ND | 4.37 | 1.43 | 1.37 |
| 47 | 35 | 304 | KC1 | CHB-C1B | 4.37 | 1.46 | 1.38 |
| 48 | 35 | 311 | A86 | C17-C18 | -4.36 | 1.46 | 1.52 |
| 47 | 31 | 303 | KC1 | C1B-NB | -4.36 | 1.32 | 1.37 |
| 47 | 34 | 309 | KC1 | C1B-NB | -4.36 | 1.32 | 1.37 |
| 37 | C | 503 | CLA | O2D-CGD | 4.36 | 1.44 | 1.33 |
| 47 | 17 | 308 | KC1 | CHC-C4B | 4.36 | 1.46 | 1.38 |
| 47 | 21 | 203 | KC1 | CHC-C4B | 4.36 | 1.46 | 1.38 |
| 48 | 17 | 314 | A86 | C7-C6 | 4.36 | 1.59 | 1.50 |
| 48 | 41 | 214 | A86 | C7-C6 | 4.36 | 1.59 | 1.50 |
| 48 | 12 | 220 | A86 | O4-C38 | 4.36 | 1.44 | 1.35 |
| 48 | 16 | 314 | A86 | C7-C6 | 4.36 | 1.59 | 1.50 |
| 48 | 35 | 313 | A86 | C7-C6 | 4.36 | 1.59 | 1.50 |
| 48 | 38 | 214 | A86 | O4-C38 | 4.36 | 1.44 | 1.35 |
| 48 | 15 | 311 | A86 | C17-C18 | -4.36 | 1.46 | 1.52 |
| 37 | 17 | 304 | CLA | O2A-CGA | 4.36 | 1.46 | 1.33 |
| 48 | 38 | 212 | A86 | C7-C6 | 4.36 | 1.59 | 1.50 |
| 37 | 20 | 306 | CLA | C1D-ND | 4.36 | 1.43 | 1.37 |
| 37 | b | 511 | CLA | O2D-CGD | 4.36 | 1.43 | 1.33 |
| 48 | 17 | 312 | A86 | C7-C6 | 4.36 | 1.59 | 1.50 |
| 48 | 37 | 314 | A86 | C21-C20 | 4.36 | 1.58 | 1.51 |
| 47 | 34 | 306 | KC1 | CHC-C4B | 4.36 | 1.46 | 1.38 |
| 37 | a | 407 | CLA | CHC-C1C | 4.36 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | D | 402 | CLA | O2A-CGA | 4.36 | 1.46 | 1.33 |
| 37 | 33 | 308 | CLA | CHD-C1D | 4.36 | 1.46 | 1.38 |
| 48 | 35 | 314 | A86 | C7-C6 | 4.36 | 1.59 | 1.50 |
| 48 | 38 | 215 | A86 | O4-C38 | 4.36 | 1.44 | 1.35 |
| 37 | c | 503 | CLA | O2D-CGD | 4.36 | 1.43 | 1.33 |
| 37 | B | 502 | CLA | CHC-C1C | 4.36 | 1.47 | 1.38 |
| 37 | 19 | 307 | CLA | O2A-CGA | 4.36 | 1.46 | 1.33 |
| 48 | 41 | 215 | A86 | C21-C20 | 4.36 | 1.58 | 1.51 |
| 37 | B | 508 | CLA | C1B-NB | -4.36 | 1.32 | 1.37 |
| 47 | 15 | 304 | KC1 | CHB-C1B | 4.35 | 1.46 | 1.38 |
| 47 | 16 | 308 | KC1 | CHC-C4B | 4.35 | 1.46 | 1.38 |
| 37 | 37 | 308 | CLA | CHD-C1D | 4.35 | 1.46 | 1.38 |
| 37 | b | 502 | CLA | CHC-C1C | 4.35 | 1.47 | 1.38 |
| 48 | 20 | 311 | A86 | O4-C38 | 4.35 | 1.44 | 1.35 |
| 47 | 37 | 307 | KC1 | C1A-CHA | 4.35 | 1.51 | 1.40 |
| 37 | C | 512 | CLA | CHC-C1C | 4.35 | 1.47 | 1.38 |
| 37 | b | 514 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 47 | 14 | 309 | KC1 | C1A-NA | -4.35 | 1.28 | 1.38 |
| 47 | 34 | 309 | KC1 | C1A-NA | -4.35 | 1.28 | 1.38 |
| 37 | 14 | 310 | CLA | CHC-C1C | 4.35 | 1.47 | 1.38 |
| 37 | 12 | 204 | CLA | C1B-NB | -4.35 | 1.32 | 1.37 |
| 37 | d | 401 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 47 | 13 | 309 | KC1 | CHC-C4B | 4.35 | 1.46 | 1.38 |
| 47 | 37 | 307 | KC1 | CHC-C4B | 4.35 | 1.46 | 1.38 |
| 37 | A | 405 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 48 | 15 | 316 | A86 | C17-C18 | -4.35 | 1.46 | 1.52 |
| 47 | 11 | 309 | KC1 | C1A-NA | -4.35 | 1.28 | 1.38 |
| 37 | b | 501 | CLA | CHC-C1C | 4.35 | 1.47 | 1.38 |
| 47 | 32 | 209 | KC1 | CHD-C4C | 4.35 | 1.47 | 1.38 |
| 37 | 39 | 303 | CLA | O2D-CGD | 4.35 | 1.43 | 1.33 |
| 48 | 17 | 320 | A86 | O4-C38 | 4.35 | 1.44 | 1.35 |
| 48 | 37 | 311 | A86 | C7-C6 | 4.35 | 1.59 | 1.50 |
| 48 | 35 | 312 | A86 | C17-C18 | -4.35 | 1.46 | 1.52 |
| 48 | 17 | 313 | A86 | O4-C38 | 4.35 | 1.44 | 1.35 |
| 48 | 32 | 221 | A86 | C17-C18 | -4.35 | 1.46 | 1.52 |
| 37 | b | 509 | CLA | C1B-NB | -4.35 | 1.32 | 1.37 |
| 48 | 40 | 213 | A86 | C10-C11 | 4.34 | 1.46 | 1.34 |
| 48 | 15 | 312 | A86 | C7-C6 | 4.34 | 1.59 | 1.50 |
| 47 | 15 | 306 | KC1 | C1A-NA | -4.34 | 1.28 | 1.38 |
| 48 | 20 | 311 | A86 | C10-C11 | 4.34 | 1.46 | 1.34 |
| 48 | 17 | 311 | A86 | C7-C6 | 4.34 | 1.59 | 1.50 |
| 48 | 13 | 312 | A86 | O4-C38 | 4.34 | 1.44 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 38 | 203 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 37 | z | 101 | CLA | CHC-C1C | 4.34 | 1.47 | 1.38 |
| 37 | 12 | 204 | CLA | CHC-C1C | 4.34 | 1.47 | 1.38 |
| 37 | 32 | 205 | CLA | CHC-C1C | 4.34 | 1.47 | 1.38 |
| 47 | 40 | 207 | KC1 | CHC-C4B | 4.34 | 1.46 | 1.38 |
| 48 | 13 | 311 | A86 | O4-C38 | 4.34 | 1.44 | 1.35 |
| 47 | 20 | 305 | KC1 | CHC-C4B | 4.34 | 1.46 | 1.38 |
| 37 | C | 505 | CLA | C1B-NB | -4.34 | 1.32 | 1.37 |
| 37 | a | 407 | CLA | O2A-CGA | 4.34 | 1.46 | 1.33 |
| 47 | 41 | 203 | KC1 | CHC-C4B | 4.34 | 1.46 | 1.38 |
| 37 | B | 516 | CLA | C1B-NB | -4.34 | 1.32 | 1.37 |
| 48 | 40 | 211 | A86 | C7-C6 | 4.34 | 1.59 | 1.50 |
| 48 | 12 | 213 | A86 | O4-C38 | 4.34 | 1.44 | 1.35 |
| 48 | 32 | 214 | A86 | O4-C38 | 4.34 | 1.44 | 1.35 |
| 48 | 37 | 319 | A86 | O4-C38 | 4.34 | 1.44 | 1.35 |
| 47 | 20 | 304 | KC1 | C1A-CHA | 4.34 | 1.51 | 1.40 |
| 48 | 11 | 314 | A86 | C9-C8 | 4.34 | 1.46 | 1.34 |
| 47 | 12 | 208 | KC1 | CHD-C4C | 4.34 | 1.47 | 1.38 |
| 48 | 33 | 311 | A86 | C17-C18 | -4.34 | 1.46 | 1.52 |
| 37 | 12 | 203 | CLA | C1D-ND | 4.34 | 1.43 | 1.37 |
| 37 | 31 | 308 | CLA | CHC-C1C | 4.34 | 1.47 | 1.38 |
| 48 | 36 | 311 | A86 | C17-C18 | -4.34 | 1.46 | 1.52 |
| 37 | 13 | 303 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 47 | 31 | 309 | KC1 | C1A-NA | -4.33 | 1.28 | 1.38 |
| 37 | D | 406 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 48 | 15 | 314 | A86 | O4-C38 | 4.33 | 1.44 | 1.35 |
| 37 | A | 405 | CLA | CHC-C1C | 4.33 | 1.47 | 1.38 |
| 48 | 32 | 217 | A86 | O4-C38 | 4.33 | 1.44 | 1.35 |
| 37 | B | 501 | CLA | CHC-C1C | 4.33 | 1.47 | 1.38 |
| 47 | 40 | 206 | KC1 | C1A-CHA | 4.33 | 1.51 | 1.40 |
| 47 | 12 | 211 | KC1 | C1B-NB | -4.33 | 1.32 | 1.37 |
| 47 | 35 | 302 | KC1 | C1A-NA | -4.33 | 1.28 | 1.38 |
| 37 | Z | 101 | CLA | CHC-C1C | 4.33 | 1.47 | 1.38 |
| 48 | 21 | 211 | A86 | C21-C20 | 4.33 | 1.58 | 1.51 |
| 47 | 14 | 309 | KC1 | C1B-NB | -4.33 | 1.32 | 1.37 |
| 37 | w | 101 | CLA | CHC-C1C | 4.33 | 1.47 | 1.38 |
| 48 | 37 | 313 | A86 | C7-C6 | 4.33 | 1.59 | 1.50 |
| 37 | 39 | 307 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 48 | 37 | 310 | A86 | C7-C6 | 4.33 | 1.59 | 1.50 |
| 47 | 11 | 302 | KC1 | C1B-NB | -4.33 | 1.32 | 1.37 |
| 47 | 31 | 309 | KC1 | C1B-NB | -4.33 | 1.32 | 1.37 |
| 48 | 36 | 310 | A86 | C7-C6 | 4.33 | 1.59 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 33 | 304 | KC1 | CHB-C1B | 4.33 | 1.46 | 1.38 |
| 48 | 39 | 313 | A86 | C9-C10 | 4.33 | 1.56 | 1.43 |
| 48 | 17 | 320 | A86 | C17-C18 | -4.33 | 1.46 | 1.52 |
| 48 | 38 | 214 | A86 | C7-C6 | 4.33 | 1.59 | 1.50 |
| 47 | 11 | 306 | KC1 | C1D-ND | 4.33 | 1.43 | 1.37 |
| 37 | 40 | 210 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 37 | B | 514 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 48 | 18 | 214 | A86 | O4-C38 | 4.33 | 1.44 | 1.35 |
| 48 | 21 | 215 | A86 | C21-C20 | 4.33 | 1.58 | 1.51 |
| 48 | 38 | 212 | A86 | C21-C20 | 4.33 | 1.58 | 1.51 |
| 37 | 12 | 207 | CLA | C1D-ND | 4.33 | 1.43 | 1.37 |
| 37 | 18 | 208 | CLA | C1D-ND | 4.33 | 1.43 | 1.37 |
| 37 | 38 | 208 | CLA | C1D-ND | 4.33 | 1.43 | 1.37 |
| 37 | 41 | 202 | CLA | CHD-C1D | 4.33 | 1.46 | 1.38 |
| 48 | 35 | 313 | A86 | C21-C20 | 4.33 | 1.58 | 1.51 |
| 37 | 16 | 303 | CLA | CHD-C1D | 4.33 | 1.46 | 1.38 |
| 37 | 21 | 210 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |
| 47 | 40 | 206 | KC1 | C1A-NA | -4.32 | 1.29 | 1.38 |
| 37 | 21 | 208 | CLA | O2A-CGA | 4.32 | 1.46 | 1.33 |
| 47 | 32 | 212 | KC1 | C1B-NB | -4.32 | 1.32 | 1.37 |
| 37 | b | 515 | CLA | CHC-C1C | 4.32 | 1.47 | 1.38 |
| 47 | 33 | 306 | KC1 | C1D-ND | 4.32 | 1.43 | 1.37 |
| 48 | 15 | 313 | A86 | C21-C20 | 4.32 | 1.58 | 1.51 |
| 37 | 12 | 210 | CLA | C1D-ND | 4.32 | 1.43 | 1.37 |
| 37 | 32 | 211 | CLA | C1D-ND | 4.32 | 1.43 | 1.37 |
| 47 | 41 | 207 | KC1 | C1A-NA | -4.32 | 1.29 | 1.38 |
| 48 | 33 | 313 | A86 | C7-C6 | 4.32 | 1.59 | 1.50 |
| 48 | 35 | 311 | A86 | C21-C20 | 4.32 | 1.58 | 1.51 |
| 48 | 15 | 313 | A86 | C7-C6 | 4.32 | 1.59 | 1.50 |
| 47 | 35 | 306 | KC1 | CHB-C1B | 4.32 | 1.46 | 1.38 |
| 37 | 15 | 307 | CLA | C1D-ND | 4.32 | 1.43 | 1.37 |
| 37 | 33 | 307 | CLA | C1B-NB | -4.32 | 1.32 | 1.37 |
| 47 | 12 | 211 | KC1 | CHC-C4B | 4.32 | 1.46 | 1.38 |
| 47 | 32 | 212 | KC1 | CHC-C4B | 4.32 | 1.46 | 1.38 |
| 47 | 12 | 208 | KC1 | C1A-NA | -4.32 | 1.29 | 1.38 |
| 47 | 32 | 209 | KC1 | C1A-NA | -4.32 | 1.29 | 1.38 |
| 37 | 13 | 308 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |
| 48 | 18 | 213 | A86 | C21-C20 | 4.32 | 1.58 | 1.51 |
| 37 | 35 | 303 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |
| 47 | 31 | 305 | KC1 | C1D-ND | 4.32 | 1.43 | 1.37 |
| 48 | 19 | 313 | A86 | C7-C6 | 4.32 | 1.59 | 1.50 |
| 37 | 41 | 209 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 18 | 214 | A86 | C21-C20 | 4.32 | 1.58 | 1.51 |
| 48 | 17 | 314 | A86 | O4-C38 | 4.32 | 1.44 | 1.35 |
| 48 | 18 | 215 | A86 | O4-C38 | 4.32 | 1.44 | 1.35 |
| 37 | 19 | 310 | CLA | C1D-ND | 4.32 | 1.43 | 1.37 |
| 47 | 12 | 211 | KC1 | C1D-ND | 4.32 | 1.43 | 1.37 |
| 48 | 15 | 312 | A86 | C17-C18 | -4.32 | 1.46 | 1.52 |
| 47 | 31 | 307 | KC1 | C1A-CHA | 4.32 | 1.51 | 1.40 |
| 37 | 13 | 303 | CLA | C1D-ND | 4.32 | 1.43 | 1.37 |
| 37 | w | 101 | CLA | O2D-CGD | 4.32 | 1.43 | 1.33 |
| 37 | 18 | 203 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 37 | 11 | 307 | CLA | CHC-C1C | 4.31 | 1.47 | 1.38 |
| 37 | W | 101 | CLA | O2D-CGD | 4.31 | 1.43 | 1.33 |
| 48 | 31 | 314 | A86 | C9-C8 | 4.31 | 1.45 | 1.34 |
| 37 | a | 403 | CLA | O2D-CGD | 4.31 | 1.43 | 1.33 |
| 37 | 32 | 208 | CLA | C1D-ND | 4.31 | 1.43 | 1.37 |
| 37 | b | 504 | CLA | C3C-C2C | 4.31 | 1.46 | 1.36 |
| 37 | D | 401 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 37 | 39 | 302 | CLA | CHC-C1C | 4.31 | 1.47 | 1.38 |
| 48 | 19 | 311 | A86 | C17-C18 | -4.31 | 1.46 | 1.52 |
| 48 | 39 | 311 | A86 | C17-C18 | -4.31 | 1.46 | 1.52 |
| 37 | 14 | 302 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 37 | 41 | 208 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 47 | 11 | 309 | KC1 | C1D-ND | 4.31 | 1.43 | 1.37 |
| 37 | A | 403 | CLA | O2D-CGD | 4.31 | 1.43 | 1.33 |
| 48 | 33 | 311 | A86 | O4-C38 | 4.31 | 1.44 | 1.35 |
| 47 | 13 | 306 | KC1 | C1A-NA | -4.31 | 1.29 | 1.38 |
| 47 | 20 | 304 | KC1 | C1A-NA | -4.31 | 1.29 | 1.38 |
| 48 | 16 | 310 | A86 | C7-C6 | 4.31 | 1.59 | 1.50 |
| 48 | 14 | 312 | A86 | O4-C38 | 4.31 | 1.44 | 1.35 |
| 37 | c | 511 | CLA | C1D-ND | 4.31 | 1.43 | 1.37 |
| 37 | B | 509 | CLA | C1B-NB | -4.31 | 1.32 | 1.37 |
| 47 | 12 | 206 | KC1 | C1B-NB | -4.31 | 1.32 | 1.37 |
| 47 | 17 | 306 | KC1 | CHB-C1B | 4.31 | 1.46 | 1.38 |
| 37 | 20 | 308 | CLA | CHC-C1C | 4.31 | 1.47 | 1.38 |
| 37 | 15 | 301 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 37 | c | 503 | CLA | C1D-ND | 4.31 | 1.43 | 1.37 |
| 48 | 18 | 215 | A86 | C21-C20 | 4.31 | 1.58 | 1.51 |
| 37 | 32 | 205 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 37 | 38 | 209 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 37 | 38 | 206 | CLA | CHD-C1D | 4.31 | 1.46 | 1.38 |
| 47 | 21 | 207 | KC1 | C1A-NA | -4.31 | 1.29 | 1.38 |
| 48 | 11 | 313 | A86 | C7-C6 | 4.31 | 1.59 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | A | 403 | CLA | C1B-NB | -4.31 | 1.32 | 1.37 |
| 37 | 13 | 307 | CLA | C1B-NB | -4.31 | 1.32 | 1.37 |
| 48 | 35 | 319 | A86 | O4-C38 | 4.31 | 1.44 | 1.35 |
| 48 | 14 | 315 | A86 | C17-C18 | -4.30 | 1.46 | 1.52 |
| 48 | 31 | 314 | A86 | O4-C38 | 4.30 | 1.44 | 1.35 |
| 37 | W | 101 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 37 | Z | 102 | CLA | CHD-C1D | 4.30 | 1.46 | 1.38 |
| 37 | C | 503 | CLA | C1D-ND | 4.30 | 1.43 | 1.37 |
| 37 | c | 505 | CLA | CHC-C1C | 4.30 | 1.47 | 1.38 |
| 47 | 33 | 309 | KC1 | CHC-C4B | 4.30 | 1.46 | 1.38 |
| 37 | 15 | 303 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 48 | 18 | 212 | A86 | C7-C6 | 4.30 | 1.59 | 1.50 |
| 48 | 33 | 312 | A86 | C7-C6 | 4.30 | 1.59 | 1.50 |
| 37 | W | 101 | CLA | CHC-C1C | 4.30 | 1.47 | 1.38 |
| 37 | 20 | 308 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 37 | 18 | 203 | CLA | CHD-C1D | 4.30 | 1.46 | 1.38 |
| 37 | D | 406 | CLA | CHC-C1C | 4.30 | 1.47 | 1.38 |
| 47 | 32 | 207 | KC1 | C1B-NB | -4.30 | 1.32 | 1.37 |
| 37 | B | 504 | CLA | C3C-C2C | 4.30 | 1.46 | 1.36 |
| 48 | 39 | 311 | A86 | C7-C6 | 4.30 | 1.59 | 1.50 |
| 48 | 38 | 212 | A86 | C10-C11 | 4.30 | 1.46 | 1.34 |
| 47 | 21 | 203 | KC1 | C1A-NA | -4.30 | 1.29 | 1.38 |
| 48 | 31 | 319 | A86 | C9-C8 | 4.30 | 1.45 | 1.34 |
| 37 | 18 | 206 | CLA | CHD-C1D | 4.30 | 1.46 | 1.38 |
| 47 | 31 | 309 | KC1 | C1D-ND | 4.30 | 1.43 | 1.37 |
| 48 | 41 | 211 | A86 | C21-C20 | 4.30 | 1.58 | 1.51 |
| 37 | d | 404 | CLA | CHC-C1C | 4.30 | 1.47 | 1.38 |
| 48 | 12 | 214 | A86 | O4-C38 | 4.30 | 1.44 | 1.35 |
| 48 | 32 | 215 | A86 | O4-C38 | 4.30 | 1.44 | 1.35 |
| 37 | a | 404 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 48 | 34 | 315 | A86 | C17-C18 | -4.29 | 1.46 | 1.52 |
| 48 | 38 | 214 | A86 | C21-C20 | 4.29 | 1.58 | 1.51 |
| 47 | 16 | 308 | KC1 | C1A-CHA | 4.29 | 1.51 | 1.40 |
| 37 | 39 | 302 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 37 | Z | 102 | CLA | O2A-CGA | 4.29 | 1.45 | 1.30 |
| 37 | z | 102 | CLA | CHD-C1D | 4.29 | 1.46 | 1.38 |
| 37 | C | 511 | CLA | CHC-C1C | 4.29 | 1.47 | 1.38 |
| 48 | 11 | 319 | A86 | C9-C8 | 4.29 | 1.45 | 1.34 |
| 47 | 41 | 203 | KC1 | C1A-NA | -4.29 | 1.29 | 1.38 |
| 47 | 31 | 307 | KC1 | C1D-ND | 4.29 | 1.43 | 1.37 |
| 48 | 17 | 310 | A86 | C7-C6 | 4.29 | 1.59 | 1.50 |
| 48 | 39 | 313 | A86 | C7-C6 | 4.29 | 1.59 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 36 | 303 | CLA | CHD-C1D | 4.29 | 1.46 | 1.38 |
| 47 | 11 | 302 | KC1 | C1A-CHA | 4.29 | 1.51 | 1.40 |
| 47 | 12 | 206 | KC1 | C1A-CHA | 4.29 | 1.51 | 1.40 |
| 48 | 11 | 315 | A86 | C9-C8 | 4.29 | 1.45 | 1.34 |
| 37 | 40 | 208 | CLA | C1D-ND | 4.29 | 1.43 | 1.37 |
| 37 | b | 516 | CLA | C1B-NB | -4.29 | 1.32 | 1.37 |
| 37 | 33 | 303 | CLA | CHD-C1D | 4.29 | 1.46 | 1.38 |
| 48 | 34 | 316 | A86 | C17-C18 | -4.29 | 1.46 | 1.52 |
| 37 | 34 | 302 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 37 | B | 524 | CLA | C1B-NB | -4.29 | 1.32 | 1.37 |
| 48 | 39 | 311 | A86 | C21-C20 | 4.29 | 1.58 | 1.51 |
| 48 | 13 | 312 | A86 | C7-C6 | 4.29 | 1.59 | 1.50 |
| 48 | 21 | 213 | A86 | C17-C18 | -4.29 | 1.46 | 1.52 |
| 48 | 35 | 314 | A86 | O4-C38 | 4.29 | 1.44 | 1.35 |
| 37 | 21 | 209 | CLA | CHD-C1D | 4.29 | 1.46 | 1.38 |
| 37 | 34 | 310 | CLA | CHC-C1C | 4.29 | 1.47 | 1.38 |
| 47 | 31 | 303 | KC1 | C1A-CHA | 4.29 | 1.51 | 1.40 |
| 37 | B | 515 | CLA | CHC-C1C | 4.29 | 1.47 | 1.38 |
| 47 | 37 | 305 | KC1 | CHB-C1B | 4.29 | 1.46 | 1.38 |
| 48 | 12 | 213 | A86 | C21-C20 | 4.29 | 1.58 | 1.51 |
| 48 | 32 | 214 | A86 | C21-C20 | 4.29 | 1.58 | 1.51 |
| 37 | w | 101 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 47 | 36 | 308 | KC1 | C1A-CHA | 4.29 | 1.51 | 1.40 |
| 47 | 33 | 306 | KC1 | C1A-NA | -4.28 | 1.29 | 1.38 |
| 37 | 34 | 305 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 48 | 41 | 211 | A86 | C7-C6 | 4.28 | 1.59 | 1.50 |
| 47 | 13 | 306 | KC1 | C1D-ND | 4.28 | 1.43 | 1.37 |
| 48 | 14 | 316 | A86 | C17-C18 | -4.28 | 1.46 | 1.52 |
| 47 | 13 | 304 | KC1 | CHB-C1B | 4.28 | 1.46 | 1.38 |
| 37 | 12 | 204 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 37 | 41 | 208 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 47 | 16 | 302 | KC1 | CHC-C4B | 4.28 | 1.46 | 1.38 |
| 47 | 13 | 306 | KC1 | C1A-CHA | 4.28 | 1.51 | 1.40 |
| 37 | c | 506 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 48 | 31 | 315 | A86 | C9-C8 | 4.28 | 1.45 | 1.34 |
| 48 | 16 | 310 | A86 | C21-C20 | 4.28 | 1.58 | 1.51 |
| 37 | C | 513 | CLA | C1D-ND | 4.28 | 1.43 | 1.37 |
| 37 | 11 | 308 | CLA | C1D-ND | 4.28 | 1.43 | 1.37 |
| 37 | 32 | 202 | CLA | C1D-ND | 4.28 | 1.43 | 1.37 |
| 37 | 20 | 306 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 47 | 11 | 306 | KC1 | C1A-CHA | 4.28 | 1.51 | 1.40 |
| 48 | 33 | 312 | A86 | O4-C38 | 4.28 | 1.44 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 40 | 208 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 47 | 36 | 302 | KC1 | CHC-C4B | 4.28 | 1.46 | 1.38 |
| 37 | B | 508 | CLA | CHC-C1C | 4.28 | 1.47 | 1.38 |
| 37 | 15 | 308 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 48 | 38 | 215 | A86 | C21-C20 | 4.28 | 1.58 | 1.51 |
| 48 | 21 | 211 | A86 | C7-C6 | 4.28 | 1.59 | 1.50 |
| 48 | 12 | 216 | A86 | C7-C6 | 4.28 | 1.59 | 1.50 |
| 47 | 12 | 208 | KC1 | C1B-NB | -4.28 | 1.32 | 1.37 |
| 47 | 32 | 209 | KC1 | C1B-NB | -4.28 | 1.32 | 1.37 |
| 48 | 33 | 311 | A86 | C7-C6 | 4.28 | 1.59 | 1.50 |
| 37 | 35 | 307 | CLA | C1D-ND | 4.28 | 1.43 | 1.37 |
| 37 | 39 | 310 | CLA | C1D-ND | 4.28 | 1.43 | 1.37 |
| 37 | 41 | 210 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 37 | B | 516 | CLA | C1D-ND | 4.27 | 1.43 | 1.37 |
| 37 | 39 | 303 | CLA | C1D-ND | 4.27 | 1.43 | 1.37 |
| 47 | 13 | 309 | KC1 | C1D-ND | 4.27 | 1.43 | 1.37 |
| 47 | 33 | 309 | KC1 | C1D-ND | 4.27 | 1.43 | 1.37 |
| 48 | 11 | 314 | A86 | C7-C6 | 4.27 | 1.59 | 1.50 |
| 47 | 13 | 309 | KC1 | C1A-NA | -4.27 | 1.29 | 1.38 |
| 37 | 36 | 303 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 37 | 21 | 208 | CLA | CHD-C1D | 4.27 | 1.46 | 1.38 |
| 47 | 39 | 308 | KC1 | CHB-C1B | 4.27 | 1.46 | 1.38 |
| 37 | C | 505 | CLA | CHC-C1C | 4.27 | 1.47 | 1.38 |
| 37 | 40 | 210 | CLA | CHC-C1C | 4.27 | 1.47 | 1.38 |
| 48 | 35 | 311 | A86 | C7-C6 | 4.27 | 1.59 | 1.50 |
| 37 | 31 | 308 | CLA | C1B-NB | -4.27 | 1.32 | 1.37 |
| 47 | 40 | 207 | KC1 | CHB-C1B | 4.27 | 1.46 | 1.38 |
| 37 | 35 | 303 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 48 | 12 | 220 | A86 | C7-C6 | 4.27 | 1.59 | 1.50 |
| 48 | 36 | 310 | A86 | C21-C20 | 4.27 | 1.58 | 1.51 |
| 37 | 16 | 306 | CLA | C1B-NB | -4.27 | 1.32 | 1.37 |
| 37 | c | 511 | CLA | CHC-C1C | 4.27 | 1.47 | 1.38 |
| 37 | 35 | 301 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 47 | 15 | 306 | KC1 | CHB-C1B | 4.27 | 1.46 | 1.38 |
| 48 | 32 | 217 | A86 | C21-C20 | 4.27 | 1.58 | 1.51 |
| 48 | 11 | 315 | A86 | C7-C6 | 4.26 | 1.59 | 1.50 |
| 47 | 33 | 306 | KC1 | C1A-CHA | 4.26 | 1.51 | 1.40 |
| 48 | 13 | 315 | A86 | C21-C20 | 4.26 | 1.58 | 1.51 |
| 37 | 17 | 302 | CLA | CHD-C1D | 4.26 | 1.46 | 1.38 |
| 47 | 38 | 205 | KC1 | C1A-CHA | 4.26 | 1.51 | 1.40 |
| 37 | 39 | 303 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 48 | 31 | 313 | A86 | C7-C6 | 4.26 | 1.59 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 11 | 301 | CLA | C1D-ND | 4.26 | 1.43 | 1.37 |
| 37 | 31 | 302 | CLA | C1D-ND | 4.26 | 1.43 | 1.37 |
| 37 | 18 | 202 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 47 | 33 | 306 | KC1 | CHB-C1B | 4.26 | 1.46 | 1.38 |
| 37 | z | 102 | CLA | O2A-CGA | 4.26 | 1.44 | 1.30 |
| 47 | 36 | 305 | KC1 | CHB-C1B | 4.26 | 1.46 | 1.38 |
| 48 | 34 | 315 | A86 | C7-C6 | 4.26 | 1.59 | 1.50 |
| 37 | b | 508 | CLA | CHC-C1C | 4.26 | 1.47 | 1.38 |
| 37 | 19 | 302 | CLA | CHC-C1C | 4.26 | 1.47 | 1.38 |
| 48 | 37 | 309 | A86 | C7-C6 | 4.26 | 1.59 | 1.50 |
| 37 | a | 403 | CLA | C1B-NB | -4.26 | 1.32 | 1.37 |
| 47 | 33 | 309 | KC1 | C1A-NA | -4.26 | 1.29 | 1.38 |
| 37 | 20 | 301 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 48 | 32 | 221 | A86 | C7-C6 | 4.26 | 1.59 | 1.50 |
| 48 | 34 | 313 | A86 | C10-C11 | 4.26 | 1.46 | 1.34 |
| 47 | 18 | 205 | KC1 | C1A-CHA | 4.26 | 1.51 | 1.40 |
| 37 | 34 | 308 | CLA | CHC-C1C | 4.26 | 1.47 | 1.38 |
| 47 | 11 | 304 | KC1 | CHC-C4B | 4.26 | 1.46 | 1.38 |
| 47 | 20 | 305 | KC1 | C1A-CHA | 4.26 | 1.51 | 1.40 |
| 37 | 19 | 303 | CLA | C1D-ND | 4.26 | 1.43 | 1.37 |
| 47 | 32 | 207 | KC1 | C1A-CHA | 4.26 | 1.51 | 1.40 |
| 48 | 16 | 313 | A86 | C9-C10 | 4.26 | 1.56 | 1.43 |
| 37 | 40 | 203 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 37 | 18 | 209 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 48 | 13 | 311 | A86 | C7-C6 | 4.25 | 1.59 | 1.50 |
| 48 | 19 | 311 | A86 | C7-C6 | 4.25 | 1.59 | 1.50 |
| 48 | 15 | 319 | A86 | O4-C38 | 4.25 | 1.44 | 1.35 |
| 37 | 15 | 308 | CLA | CHC-C1C | 4.25 | 1.47 | 1.38 |
| 48 | 19 | 311 | A86 | C21-C20 | 4.25 | 1.58 | 1.51 |
| 37 | B | 501 | CLA | C1D-ND | 4.25 | 1.43 | 1.37 |
| 37 | 13 | 305 | CLA | CHD-C1D | 4.25 | 1.46 | 1.38 |
| 47 | 19 | 308 | KC1 | CHB-C1B | 4.25 | 1.46 | 1.38 |
| 37 | 16 | 303 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 37 | 33 | 307 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 47 | 20 | 305 | KC1 | CHB-C1B | 4.25 | 1.46 | 1.38 |
| 37 | c | 513 | CLA | C1D-ND | 4.25 | 1.43 | 1.37 |
| 37 | C | 506 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 47 | 21 | 207 | KC1 | C1A-CHA | 4.25 | 1.51 | 1.40 |
| 47 | 40 | 207 | KC1 | C1A-CHA | 4.25 | 1.51 | 1.40 |
| 48 | 14 | 315 | A86 | C7-C6 | 4.25 | 1.59 | 1.50 |
| 47 | 11 | 306 | KC1 | C1A-NA | -4.25 | 1.29 | 1.38 |
| 48 | 34 | 312 | A86 | O4-C38 | 4.25 | 1.44 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 35 | 313 | A86 | C10-C11 | 4.25 | 1.46 | 1.34 |
| 37 | 14 | 305 | CLA | CHD-C1D | 4.25 | 1.46 | 1.38 |
| 37 | a | 404 | CLA | C1D-ND | 4.25 | 1.43 | 1.37 |
| 37 | 11 | 307 | CLA | C1B-NB | -4.25 | 1.32 | 1.37 |
| 37 | 34 | 310 | CLA | CHD-C1D | 4.25 | 1.46 | 1.38 |
| 48 | 19 | 313 | A86 | C9-C10 | 4.25 | 1.56 | 1.43 |
| 48 | 13 | 312 | A86 | C21-C20 | 4.25 | 1.58 | 1.51 |
| 48 | 33 | 312 | A86 | C21-C20 | 4.25 | 1.58 | 1.51 |
| 37 | b | 523 | CLA | C1B-NB | -4.25 | 1.32 | 1.37 |
| 37 | 33 | 305 | CLA | CHD-C1D | 4.25 | 1.46 | 1.38 |
| 48 | 31 | 311 | A86 | C9-C8 | 4.25 | 1.45 | 1.34 |
| 37 | b | 501 | CLA | C1D-ND | 4.24 | 1.43 | 1.37 |
| 48 | 11 | 311 | A86 | C9-C8 | 4.24 | 1.45 | 1.34 |
| 37 | 34 | 303 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 48 | 31 | 314 | A86 | C17-C18 | -4.24 | 1.46 | 1.52 |
| 37 | 11 | 310 | CLA | C1B-NB | -4.24 | 1.32 | 1.37 |
| 37 | 31 | 310 | CLA | C1B-NB | -4.24 | 1.32 | 1.37 |
| 48 | 15 | 314 | A86 | C21-C20 | 4.24 | 1.58 | 1.51 |
| 48 | 38 | 213 | A86 | C21-C20 | 4.24 | 1.58 | 1.51 |
| 47 | 16 | 305 | KC1 | CHB-C1B | 4.24 | 1.46 | 1.38 |
| 37 | 13 | 301 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 48 | 21 | 214 | A86 | C21-C20 | 4.24 | 1.58 | 1.51 |
| 37 | 14 | 303 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 48 | 14 | 313 | A86 | C10-C11 | 4.24 | 1.46 | 1.34 |
| 37 | 12 | 212 | CLA | CHD-C1D | 4.24 | 1.46 | 1.38 |
| 37 | 16 | 307 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 48 | 41 | 213 | A86 | C17-C18 | -4.24 | 1.46 | 1.52 |
| 37 | 11 | 308 | CLA | C1B-NB | -4.24 | 1.32 | 1.37 |
| 37 | 35 | 308 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 48 | 18 | 212 | A86 | C10-C11 | 4.24 | 1.46 | 1.34 |
| 47 | 15 | 302 | KC1 | C1A-CHA | 4.24 | 1.51 | 1.40 |
| 47 | 31 | 305 | KC1 | CHC-C4B | 4.24 | 1.46 | 1.38 |
| 48 | 17 | 320 | A86 | C7-C6 | 4.24 | 1.59 | 1.50 |
| 37 | C | 511 | CLA | C1D-ND | 4.24 | 1.43 | 1.37 |
| 37 | 40 | 203 | CLA | CHD-C1D | 4.24 | 1.46 | 1.38 |
| 47 | 35 | 302 | KC1 | C1A-CHA | 4.24 | 1.51 | 1.40 |
| 37 | 33 | 301 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 48 | 31 | 314 | A86 | C7-C6 | 4.24 | 1.59 | 1.50 |
| 48 | 12 | 214 | A86 | C9-C8 | 4.23 | 1.45 | 1.34 |
| 37 | 36 | 307 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 48 | 15 | 311 | A86 | C21-C20 | 4.23 | 1.58 | 1.51 |
| 37 | 32 | 206 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 13 | 315 | A86 | C10-C11 | 4.23 | 1.46 | 1.34 |
| 48 | 15 | 313 | A86 | C10-C11 | 4.23 | 1.46 | 1.34 |
| 48 | 17 | 315 | A86 | C10-C11 | 4.23 | 1.46 | 1.34 |
| 48 | 37 | 314 | A86 | C10-C11 | 4.23 | 1.46 | 1.34 |
| 37 | 31 | 301 | CLA | CHD-C1D | 4.23 | 1.46 | 1.38 |
| 37 | 33 | 308 | CLA | CHC-C1C | 4.23 | 1.47 | 1.38 |
| 37 | 12 | 205 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 37 | 19 | 303 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 37 | 20 | 301 | CLA | CHD-C1D | 4.23 | 1.46 | 1.38 |
| 37 | b | 516 | CLA | C1D-ND | 4.23 | 1.43 | 1.37 |
| 48 | 18 | 215 | A86 | C7-C6 | 4.23 | 1.59 | 1.50 |
| 37 | 13 | 307 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 37 | 11 | 303 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 37 | 31 | 304 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 47 | 14 | 306 | KC1 | CHB-C1B | 4.23 | 1.46 | 1.38 |
| 48 | 32 | 217 | A86 | C7-C6 | 4.23 | 1.59 | 1.50 |
| 48 | 14 | 315 | A86 | C21-C20 | 4.23 | 1.58 | 1.51 |
| 37 | 38 | 201 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 48 | 17 | 310 | A86 | C10-C11 | 4.23 | 1.46 | 1.34 |
| 48 | 33 | 315 | A86 | C10-C11 | 4.23 | 1.46 | 1.34 |
| 48 | 12 | 220 | A86 | C21-C20 | 4.23 | 1.58 | 1.51 |
| 48 | 32 | 221 | A86 | C21-C20 | 4.23 | 1.58 | 1.51 |
| 48 | 12 | 214 | A86 | C7-C6 | 4.23 | 1.59 | 1.50 |
| 48 | 14 | 312 | A86 | C7-C6 | 4.23 | 1.59 | 1.50 |
| 47 | 31 | 303 | KC1 | C1D-ND | 4.22 | 1.43 | 1.37 |
| 37 | 11 | 308 | CLA | CHC-C1C | 4.22 | 1.46 | 1.38 |
| 37 | 14 | 303 | CLA | CHD-C1D | 4.22 | 1.46 | 1.38 |
| 48 | 41 | 214 | A86 | C21-C20 | 4.22 | 1.58 | 1.51 |
| 47 | 41 | 207 | KC1 | C1A-CHA | 4.22 | 1.51 | 1.40 |
| 37 | c | 502 | CLA | C1D-ND | 4.22 | 1.43 | 1.37 |
| 48 | 40 | 201 | A86 | C9-C10 | 4.22 | 1.56 | 1.43 |
| 37 | C | 507 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 48 | 36 | 313 | A86 | C21-C20 | 4.22 | 1.58 | 1.51 |
| 37 | 14 | 308 | CLA | CHC-C1C | 4.22 | 1.46 | 1.38 |
| 48 | 11 | 312 | A86 | C9-C8 | 4.22 | 1.45 | 1.34 |
| 48 | 11 | 314 | A86 | C17-C18 | -4.22 | 1.46 | 1.52 |
| 37 | B | 501 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 37 | 20 | 307 | CLA | CHD-C1D | 4.22 | 1.46 | 1.38 |
| 47 | 17 | 303 | KC1 | CHB-C1B | 4.22 | 1.46 | 1.38 |
| 48 | 37 | 319 | A86 | C7-C6 | 4.22 | 1.59 | 1.50 |
| 37 | 34 | 303 | CLA | CHD-C1D | 4.22 | 1.46 | 1.38 |
| 47 | 19 | 308 | KC1 | C1D-ND | 4.22 | 1.43 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | b | 512 | CLA | CHC-C1C | 4.22 | 1.46 | 1.38 |
| 37 | b | 501 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 47 | 32 | 207 | KC1 | CHD-C4C | 4.22 | 1.46 | 1.38 |
| 47 | 12 | 208 | KC1 | C1D-ND | 4.22 | 1.43 | 1.37 |
| 37 | 36 | 301 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 48 | 12 | 202 | A86 | C7-C6 | 4.21 | 1.59 | 1.50 |
| 48 | 32 | 203 | A86 | C7-C6 | 4.21 | 1.59 | 1.50 |
| 48 | 32 | 216 | A86 | C7-C6 | 4.21 | 1.59 | 1.50 |
| 48 | 16 | 310 | A86 | O4-C38 | 4.21 | 1.44 | 1.35 |
| 47 | 13 | 306 | KC1 | CHB-C1B | 4.21 | 1.46 | 1.38 |
| 37 | 39 | 301 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 48 | 35 | 314 | A86 | C10-C11 | 4.21 | 1.46 | 1.34 |
| 48 | 14 | 312 | A86 | C21-C20 | 4.21 | 1.58 | 1.51 |
| 48 | 34 | 312 | A86 | C21-C20 | 4.21 | 1.58 | 1.51 |
| 47 | 39 | 308 | KC1 | C1D-ND | 4.21 | 1.43 | 1.37 |
| 48 | 12 | 215 | A86 | C7-C6 | 4.21 | 1.59 | 1.50 |
| 47 | 33 | 304 | KC1 | C1A-CHA | 4.21 | 1.51 | 1.40 |
| 37 | 13 | 308 | CLA | CHC-C1C | 4.21 | 1.46 | 1.38 |
| 48 | 21 | 213 | A86 | C7-C6 | 4.21 | 1.59 | 1.50 |
| 48 | 12 | 216 | A86 | C21-C20 | 4.21 | 1.58 | 1.51 |
| 47 | 13 | 304 | KC1 | C1A-CHA | 4.21 | 1.51 | 1.40 |
| 37 | c | 507 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 37 | 15 | 307 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 37 | 14 | 310 | CLA | CHD-C1D | 4.21 | 1.46 | 1.38 |
| 37 | 37 | 306 | CLA | C1D-ND | 4.21 | 1.43 | 1.37 |
| 48 | 38 | 215 | A86 | C7-C6 | 4.21 | 1.59 | 1.50 |
| 37 | 38 | 201 | CLA | CHD-C1D | 4.21 | 1.46 | 1.38 |
| 47 | 31 | 307 | KC1 | C1A-NA | -4.21 | 1.29 | 1.38 |
| 48 | 35 | 312 | A86 | C21-C20 | 4.21 | 1.58 | 1.51 |
| 48 | 32 | 215 | A86 | C7-C6 | 4.21 | 1.59 | 1.50 |
| 48 | 33 | 315 | A86 | C21-C20 | 4.21 | 1.58 | 1.51 |
| 48 | 16 | 311 | A86 | C7-C6 | 4.21 | 1.59 | 1.50 |
| 37 | 34 | 302 | CLA | CHD-C1D | 4.21 | 1.46 | 1.38 |
| 37 | 38 | 204 | CLA | CHD-C1D | 4.21 | 1.46 | 1.38 |
| 48 | 15 | 311 | A86 | C7-C6 | 4.21 | 1.59 | 1.50 |
| 37 | C | 510 | CLA | C1B-NB | -4.21 | 1.32 | 1.37 |
| 48 | 37 | 311 | A86 | C10-C11 | 4.21 | 1.46 | 1.34 |
| 48 | 21 | 213 | A86 | C21-C20 | 4.20 | 1.58 | 1.51 |
| 48 | 34 | 312 | A86 | C7-C6 | 4.20 | 1.59 | 1.50 |
| 37 | 40 | 209 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 48 | 32 | 215 | A86 | C9-C8 | 4.20 | 1.45 | 1.34 |
| 48 | 15 | 316 | A86 | C7-C6 | 4.20 | 1.59 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 36 | 306 | CLA | C1B-NB | -4.20 | 1.32 | 1.37 |
| 48 | 11 | 312 | A86 | C7-C6 | 4.20 | 1.59 | 1.50 |
| 47 | 34 | 306 | KC1 | C1A-NA | -4.20 | 1.29 | 1.38 |
| 37 | C | 501 | CLA | CHC-C1C | 4.20 | 1.46 | 1.38 |
| 37 | 37 | 303 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 48 | 31 | 312 | A86 | C9-C8 | 4.20 | 1.45 | 1.34 |
| 48 | 36 | 310 | A86 | O4-C38 | 4.20 | 1.44 | 1.35 |
| 47 | 11 | 302 | KC1 | C1D-ND | 4.20 | 1.43 | 1.37 |
| 37 | B | 507 | CLA | CHC-C1C | 4.20 | 1.46 | 1.38 |
| 37 | 35 | 307 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 37 | 39 | 309 | CLA | C1D-ND | 4.20 | 1.43 | 1.37 |
| 48 | 14 | 311 | A86 | C17-C18 | -4.20 | 1.46 | 1.52 |
| 37 | c | 513 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 47 | 36 | 304 | KC1 | CHB-C1B | 4.20 | 1.46 | 1.38 |
| 48 | 16 | 314 | A86 | C21-C20 | 4.20 | 1.58 | 1.51 |
| 47 | 34 | 306 | KC1 | CHB-C1B | 4.20 | 1.46 | 1.38 |
| 48 | 37 | 309 | A86 | C10-C11 | 4.20 | 1.46 | 1.34 |
| 37 | 37 | 301 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 48 | 15 | 312 | A86 | O4-C38 | 4.20 | 1.44 | 1.35 |
| 37 | D | 401 | CLA | C1D-ND | 4.20 | 1.43 | 1.37 |
| 37 | 33 | 303 | CLA | CHC-C1C | 4.20 | 1.46 | 1.38 |
| 47 | 35 | 302 | KC1 | CHB-C1B | 4.20 | 1.46 | 1.38 |
| 47 | 40 | 206 | KC1 | CHC-C4B | 4.20 | 1.46 | 1.38 |
| 37 | B | 512 | CLA | CHC-C1C | 4.20 | 1.46 | 1.38 |
| 37 | 12 | 210 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 48 | 31 | 315 | A86 | C7-C6 | 4.20 | 1.59 | 1.50 |
| 37 | 32 | 202 | CLA | C1B-NB | -4.20 | 1.32 | 1.37 |
| 37 | 14 | 307 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 37 | 19 | 301 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 37 | c | 501 | CLA | CHC-C1C | 4.20 | 1.46 | 1.38 |
| 37 | 17 | 309 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 37 | 18 | 201 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 47 | 40 | 207 | KC1 | C1A-NA | -4.20 | 1.29 | 1.38 |
| 37 | 19 | 302 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 37 | 34 | 307 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 48 | 33 | 314 | A86 | C10-C11 | 4.19 | 1.46 | 1.34 |
| 37 | 21 | 206 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 47 | 11 | 304 | KC1 | C1A-CHA | 4.19 | 1.51 | 1.40 |
| 37 | 38 | 203 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 47 | 31 | 309 | KC1 | C1A-CHA | 4.19 | 1.51 | 1.40 |
| 37 | 41 | 206 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 37 | B | 502 | CLA | C1D-ND | 4.19 | 1.43 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 18 | 205 | KC1 | CHB-C1B | 4.19 | 1.46 | 1.38 |
| 47 | 38 | 205 | KC1 | CHB-C1B | 4.19 | 1.46 | 1.38 |
| 48 | 35 | 316 | A86 | C7-C6 | 4.19 | 1.59 | 1.50 |
| 37 | C | 513 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 48 | 15 | 314 | A86 | C10-C11 | 4.19 | 1.46 | 1.34 |
| 37 | W | 102 | CLA | CHD-C1D | 4.19 | 1.46 | 1.38 |
| 48 | 32 | 214 | A86 | C7-C6 | 4.19 | 1.59 | 1.50 |
| 37 | 31 | 301 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 48 | 12 | 213 | A86 | C7-C6 | 4.19 | 1.59 | 1.50 |
| 37 | c | 510 | CLA | C1B-NB | -4.19 | 1.32 | 1.37 |
| 47 | 17 | 303 | KC1 | C1A-NA | -4.19 | 1.29 | 1.38 |
| 37 | C | 502 | CLA | C1D-ND | 4.19 | 1.43 | 1.37 |
| 48 | 14 | 312 | A86 | C19-C18 | 4.19 | 1.58 | 1.52 |
| 47 | 31 | 309 | KC1 | CHC-C4B | 4.19 | 1.46 | 1.38 |
| 47 | 11 | 309 | KC1 | C1A-CHA | 4.19 | 1.51 | 1.40 |
| 47 | 12 | 206 | KC1 | CHD-C4C | 4.19 | 1.46 | 1.38 |
| 37 | 17 | 302 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 48 | 17 | 310 | A86 | C21-C20 | 4.19 | 1.58 | 1.51 |
| 37 | W | 102 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 48 | 34 | 311 | A86 | C7-C6 | 4.18 | 1.59 | 1.50 |
| 47 | 16 | 304 | KC1 | C1A-CHA | 4.18 | 1.51 | 1.40 |
| 47 | 36 | 304 | KC1 | C1A-CHA | 4.18 | 1.51 | 1.40 |
| 37 | 14 | 302 | CLA | CHD-C1D | 4.18 | 1.46 | 1.38 |
| 47 | 17 | 308 | KC1 | C1A-NA | -4.18 | 1.29 | 1.38 |
| 48 | 41 | 213 | A86 | C7-C6 | 4.18 | 1.59 | 1.50 |
| 37 | 12 | 207 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 48 | 14 | 311 | A86 | C21-C20 | 4.18 | 1.58 | 1.51 |
| 48 | 34 | 311 | A86 | C21-C20 | 4.18 | 1.58 | 1.51 |
| 48 | 31 | 312 | A86 | C7-C6 | 4.18 | 1.59 | 1.50 |
| 37 | c | 512 | CLA | C1B-NB | -4.18 | 1.32 | 1.37 |
| 37 | 16 | 301 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 47 | 14 | 306 | KC1 | C1A-NA | -4.18 | 1.29 | 1.38 |
| 48 | 36 | 311 | A86 | C7-C6 | 4.18 | 1.59 | 1.50 |
| 47 | 41 | 203 | KC1 | C1A-CHA | 4.18 | 1.51 | 1.40 |
| 37 | 13 | 307 | CLA | C1D-ND | 4.18 | 1.43 | 1.37 |
| 37 | 33 | 307 | CLA | C1D-ND | 4.18 | 1.43 | 1.37 |
| 37 | 39 | 305 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 48 | 34 | 315 | A86 | C21-C20 | 4.18 | 1.58 | 1.51 |
| 37 | 33 | 307 | CLA | CHC-C1C | 4.18 | 1.46 | 1.38 |
| 37 | b | 510 | CLA | C1B-NB | -4.18 | 1.32 | 1.37 |
| 37 | 21 | 204 | CLA | CHD-C4C | 4.18 | 1.48 | 1.39 |
| 48 | 31 | 315 | A86 | O4-C38 | 4.18 | 1.44 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 14 | 308 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 37 | 34 | 308 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 47 | 16 | 304 | KC1 | CHB-C1B | 4.18 | 1.46 | 1.38 |
| 48 | 11 | 315 | A86 | O4-C38 | 4.18 | 1.44 | 1.35 |
| 47 | 20 | 305 | KC1 | C1A-NA | -4.18 | 1.29 | 1.38 |
| 47 | 16 | 302 | KC1 | CHB-C1B | 4.18 | 1.46 | 1.38 |
| 37 | 38 | 202 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 37 | 17 | 307 | CLA | C1D-ND | 4.18 | 1.43 | 1.37 |
| 37 | b | 507 | CLA | C1D-ND | 4.18 | 1.43 | 1.37 |
| 48 | 13 | 314 | A86 | C10-C11 | 4.18 | 1.45 | 1.34 |
| 37 | 19 | 307 | CLA | CHC-C1C | 4.18 | 1.46 | 1.38 |
| 37 | B | 507 | CLA | C1D-ND | 4.17 | 1.43 | 1.37 |
| 37 | 36 | 306 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 37 | 18 | 204 | CLA | CHD-C1D | 4.17 | 1.46 | 1.38 |
| 48 | 37 | 312 | A86 | C7-C6 | 4.17 | 1.59 | 1.50 |
| 37 | C | 501 | CLA | C1D-ND | 4.17 | 1.43 | 1.37 |
| 37 | a | 404 | CLA | C1B-NB | -4.17 | 1.32 | 1.37 |
| 48 | 37 | 309 | A86 | C21-C20 | 4.17 | 1.58 | 1.51 |
| 37 | C | 502 | CLA | CHC-C1C | 4.17 | 1.46 | 1.38 |
| 37 | 19 | 305 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 48 | 35 | 312 | A86 | O4-C38 | 4.17 | 1.44 | 1.35 |
| 37 | 17 | 304 | CLA | CHD-C1D | 4.17 | 1.46 | 1.38 |
| 48 | 15 | 312 | A86 | C21-C20 | 4.17 | 1.58 | 1.51 |
| 37 | 19 | 309 | CLA | C1D-ND | 4.17 | 1.43 | 1.37 |
| 37 | 32 | 213 | CLA | CHD-C1D | 4.17 | 1.46 | 1.38 |
| 37 | 13 | 307 | CLA | CHC-C1C | 4.17 | 1.46 | 1.38 |
| 37 | C | 507 | CLA | C4B-NB | -4.17 | 1.32 | 1.37 |
| 47 | 37 | 302 | KC1 | CHB-C1B | 4.17 | 1.46 | 1.38 |
| 48 | 21 | 213 | A86 | C10-C11 | 4.17 | 1.45 | 1.34 |
| 37 | 32 | 211 | CLA | CHD-C1D | 4.17 | 1.46 | 1.38 |
| 48 | 38 | 213 | A86 | C10-C11 | 4.17 | 1.45 | 1.34 |
| 37 | 19 | 304 | CLA | C1D-ND | 4.17 | 1.43 | 1.37 |
| 37 | 39 | 304 | CLA | C1D-ND | 4.17 | 1.43 | 1.37 |
| 37 | B | 510 | CLA | C1B-NB | -4.17 | 1.32 | 1.37 |
| 48 | 19 | 313 | A86 | C19-C18 | 4.17 | 1.58 | 1.52 |
| 47 | 21 | 203 | KC1 | C1A-CHA | 4.17 | 1.51 | 1.40 |
| 37 | 21 | 202 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 37 | 11 | 303 | CLA | CHC-C1C | 4.16 | 1.46 | 1.38 |
| 48 | 20 | 309 | A86 | C10-C11 | 4.16 | 1.45 | 1.34 |
| 37 | 32 | 211 | CLA | CHC-C1C | 4.16 | 1.46 | 1.38 |
| 48 | 41 | 213 | A86 | C10-C11 | 4.16 | 1.45 | 1.34 |
| 47 | 17 | 305 | KC1 | CHB-C1B | 4.16 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 12 | 208 | KC1 | CHC-C4B | 4.16 | 1.46 | 1.38 |
| 48 | 17 | 312 | A86 | C10-C11 | 4.16 | 1.45 | 1.34 |
| 37 | B | 513 | CLA | C1B-NB | -4.16 | 1.32 | 1.37 |
| 37 | C | 512 | CLA | C1B-NB | -4.16 | 1.32 | 1.37 |
| 48 | 35 | 319 | A86 | C21-C20 | 4.16 | 1.58 | 1.51 |
| 37 | 32 | 208 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 37 | b | 502 | CLA | C1D-ND | 4.16 | 1.43 | 1.37 |
| 48 | 34 | 311 | A86 | C17-C18 | -4.16 | 1.46 | 1.52 |
| 37 | 32 | 202 | CLA | CHC-C1C | 4.16 | 1.46 | 1.38 |
| 37 | 37 | 308 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 47 | 34 | 309 | KC1 | C1A-CHA | 4.16 | 1.51 | 1.40 |
| 37 | 16 | 306 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 48 | 38 | 214 | A86 | C17-C18 | -4.16 | 1.46 | 1.52 |
| 37 | 15 | 307 | CLA | C1B-NB | -4.16 | 1.32 | 1.37 |
| 37 | 41 | 204 | CLA | CHD-C4C | 4.16 | 1.48 | 1.39 |
| 37 | 41 | 202 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 47 | 20 | 304 | KC1 | CHC-C4B | 4.16 | 1.46 | 1.38 |
| 47 | 32 | 212 | KC1 | C1A-CHA | 4.15 | 1.51 | 1.40 |
| 37 | 13 | 301 | CLA | CHD-C1D | 4.15 | 1.46 | 1.38 |
| 37 | 39 | 302 | CLA | CHD-C1D | 4.15 | 1.46 | 1.38 |
| 47 | 20 | 302 | KC1 | C1A-CHA | 4.15 | 1.51 | 1.40 |
| 48 | 34 | 311 | A86 | O4-C38 | 4.15 | 1.44 | 1.35 |
| 37 | 33 | 301 | CLA | CHD-C1D | 4.15 | 1.46 | 1.38 |
| 47 | 36 | 302 | KC1 | CHB-C1B | 4.15 | 1.46 | 1.38 |
| 48 | 15 | 319 | A86 | C21-C20 | 4.15 | 1.58 | 1.51 |
| 37 | 31 | 308 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 37 | 32 | 208 | CLA | CHD-C1D | 4.15 | 1.46 | 1.38 |
| 37 | b | 507 | CLA | CHC-C1C | 4.15 | 1.46 | 1.38 |
| 37 | 12 | 210 | CLA | CHC-C1C | 4.15 | 1.46 | 1.38 |
| 48 | 35 | 315 | A86 | C21-C20 | 4.15 | 1.58 | 1.51 |
| 48 | 21 | 211 | A86 | C9-C10 | 4.15 | 1.56 | 1.43 |
| 37 | 11 | 310 | CLA | CHC-C1C | 4.15 | 1.46 | 1.38 |
| 37 | 31 | 310 | CLA | CHC-C1C | 4.15 | 1.46 | 1.38 |
| 37 | 19 | 306 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 37 | 32 | 206 | CLA | C1D-ND | 4.15 | 1.43 | 1.37 |
| 48 | 13 | 314 | A86 | C17-C18 | -4.15 | 1.46 | 1.52 |
| 48 | 35 | 314 | A86 | C17-C18 | -4.15 | 1.46 | 1.52 |
| 48 | 38 | 214 | A86 | C10-C11 | 4.15 | 1.45 | 1.34 |
| 47 | 41 | 203 | KC1 | CHB-C1B | 4.15 | 1.46 | 1.38 |
| 37 | b | 504 | CLA | C1B-NB | -4.15 | 1.32 | 1.37 |
| 37 | b | 512 | CLA | C4B-NB | -4.15 | 1.32 | 1.37 |
| 47 | 37 | 302 | KC1 | C1A-NA | -4.15 | 1.29 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | D | 401 | CLA | C1B-NB | -4.14 | 1.32 | 1.37 |
| 47 | 37 | 307 | KC1 | C1A-NA | -4.14 | 1.29 | 1.38 |
| 48 | 34 | 312 | A86 | C19-C18 | 4.14 | 1.58 | 1.52 |
| 47 | 16 | 305 | KC1 | C1A-NA | -4.14 | 1.29 | 1.38 |
| 47 | 13 | 309 | KC1 | C1A-CHA | 4.14 | 1.51 | 1.40 |
| 47 | 33 | 309 | KC1 | C1A-CHA | 4.14 | 1.51 | 1.40 |
| 37 | b | 507 | CLA | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 48 | 18 | 214 | A86 | C17-C18 | -4.14 | 1.46 | 1.52 |
| 48 | 41 | 213 | A86 | C21-C20 | 4.14 | 1.58 | 1.51 |
| 47 | 31 | 305 | KC1 | C1A-CHA | 4.14 | 1.51 | 1.40 |
| 37 | B | 524 | CLA | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 47 | 34 | 304 | KC1 | CHB-C1B | 4.14 | 1.46 | 1.38 |
| 48 | 33 | 311 | A86 | C21-C20 | 4.14 | 1.58 | 1.51 |
| 37 | c | 507 | CLA | C1B-NB | -4.14 | 1.32 | 1.37 |
| 47 | 40 | 204 | KC1 | C1A-CHA | 4.14 | 1.51 | 1.40 |
| 48 | 12 | 217 | A86 | C7-C6 | 4.14 | 1.59 | 1.50 |
| 47 | 37 | 304 | KC1 | CHB-C1B | 4.14 | 1.46 | 1.38 |
| 48 | 13 | 313 | A86 | C10-C11 | 4.14 | 1.45 | 1.34 |
| 48 | 33 | 313 | A86 | C10-C11 | 4.14 | 1.45 | 1.34 |
| 37 | D | 406 | CLA | C1D-ND | 4.14 | 1.43 | 1.37 |
| 47 | 14 | 309 | KC1 | C1A-CHA | 4.14 | 1.50 | 1.40 |
| 37 | B | 503 | CLA | CHC-C1C | 4.14 | 1.46 | 1.38 |
| 37 | b | 503 | CLA | CHC-C1C | 4.14 | 1.46 | 1.38 |
| 48 | 14 | 311 | A86 | O4-C38 | 4.14 | 1.44 | 1.35 |
| 48 | 40 | 211 | A86 | C10-C11 | 4.14 | 1.45 | 1.34 |
| 37 | B | 504 | CLA | C1B-NB | -4.14 | 1.32 | 1.37 |
| 37 | d | 401 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 37 | 17 | 307 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 37 | 37 | 306 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 45 | D | 404 | PL9 | C7-C3 | -4.13 | 1.45 | 1.51 |
| 37 | 11 | 303 | CLA | CHD-C1D | 4.13 | 1.46 | 1.38 |
| 47 | 32 | 209 | KC1 | CHC-C4B | 4.13 | 1.46 | 1.38 |
| 37 | 39 | 306 | CLA | O2A-CGA | 4.13 | 1.45 | 1.33 |
| 37 | C | 508 | CLA | CHC-C1C | 4.13 | 1.46 | 1.38 |
| 47 | 11 | 304 | KC1 | CHB-C1B | 4.13 | 1.46 | 1.38 |
| 47 | 11 | 309 | KC1 | CHC-C4B | 4.13 | 1.46 | 1.38 |
| 48 | 33 | 314 | A86 | C21-C20 | 4.13 | 1.58 | 1.51 |
| 37 | 11 | 305 | CLA | C1D-ND | 4.13 | 1.43 | 1.37 |
| 37 | 18 | 201 | CLA | CHD-C1D | 4.13 | 1.46 | 1.38 |
| 37 | 19 | 302 | CLA | CHD-C1D | 4.13 | 1.46 | 1.38 |
| 37 | 19 | 303 | CLA | CHD-C1D | 4.13 | 1.46 | 1.38 |
| 37 | 39 | 303 | CLA | CHD-C1D | 4.13 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 31 | 305 | KC1 | CHB-C1B | 4.13 | 1.46 | 1.38 |
| 48 | 17 | 311 | A86 | C21-C20 | 4.13 | 1.58 | 1.51 |
| 48 | 41 | 211 | A86 | C9-C10 | 4.13 | 1.56 | 1.43 |
| 37 | 38 | 211 | CLA | CHD-C4C | 4.13 | 1.48 | 1.39 |
| 37 | 17 | 307 | CLA | C1B-NB | -4.13 | 1.32 | 1.37 |
| 37 | 33 | 310 | CLA | CHD-C4C | 4.13 | 1.48 | 1.39 |
| 48 | 40 | 213 | A86 | C17-C18 | -4.13 | 1.46 | 1.52 |
| 37 | c | 507 | CLA | C4B-NB | -4.13 | 1.32 | 1.37 |
| 37 | 15 | 303 | CLA | CHD-C4C | 4.12 | 1.48 | 1.39 |
| 48 | 21 | 214 | A86 | C17-C18 | -4.12 | 1.46 | 1.52 |
| 37 | B | 507 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 48 | 33 | 315 | A86 | C9-C10 | 4.12 | 1.56 | 1.43 |
| 47 | 37 | 302 | KC1 | CHC-C4B | 4.12 | 1.46 | 1.38 |
| 37 | B | 514 | CLA | C1B-NB | -4.12 | 1.32 | 1.37 |
| 47 | 32 | 207 | KC1 | CHB-C1B | 4.12 | 1.46 | 1.38 |
| 37 | 11 | 307 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 37 | b | 523 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 37 | c | 501 | CLA | C1D-ND | 4.12 | 1.43 | 1.37 |
| 37 | 31 | 306 | CLA | C1D-ND | 4.12 | 1.43 | 1.37 |
| 48 | 14 | 311 | A86 | C7-C6 | 4.12 | 1.59 | 1.50 |
| 37 | 39 | 310 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 37 | c | 504 | CLA | C1D-ND | 4.12 | 1.43 | 1.37 |
| 48 | 12 | 216 | A86 | C17-C18 | -4.12 | 1.46 | 1.52 |
| 37 | b | 501 | CLA | CHD-C1D | 4.12 | 1.46 | 1.38 |
| 37 | 12 | 205 | CLA | C1B-NB | -4.12 | 1.32 | 1.37 |
| 37 | 39 | 307 | CLA | CHD-C1D | 4.11 | 1.46 | 1.38 |
| 48 | 11 | 312 | A86 | O4-C38 | 4.11 | 1.44 | 1.35 |
| 48 | 14 | 316 | A86 | C7-C6 | 4.11 | 1.59 | 1.50 |
| 48 | 34 | 316 | A86 | C21-C20 | 4.11 | 1.57 | 1.51 |
| 47 | 33 | 309 | KC1 | C1B-NB | -4.11 | 1.32 | 1.37 |
| 37 | b | 513 | CLA | C1B-NB | -4.11 | 1.32 | 1.37 |
| 37 | Z | 101 | CLA | CHD-C1D | 4.11 | 1.46 | 1.38 |
| 37 | c | 502 | CLA | CHC-C1C | 4.11 | 1.46 | 1.38 |
| 37 | D | 402 | CLA | CHD-C1D | 4.11 | 1.46 | 1.38 |
| 37 | 32 | 206 | CLA | C1B-NB | -4.11 | 1.32 | 1.37 |
| 37 | 13 | 303 | CLA | CHC-C1C | 4.11 | 1.46 | 1.38 |
| 37 | 35 | 308 | CLA | CHD-C1D | 4.11 | 1.46 | 1.38 |
| 48 | 17 | 313 | A86 | C21-C20 | 4.11 | 1.57 | 1.51 |
| 37 | 39 | 307 | CLA | CHC-C1C | 4.11 | 1.46 | 1.38 |
| 37 | 12 | 207 | CLA | CHD-C1D | 4.11 | 1.46 | 1.38 |
| 47 | 17 | 303 | KC1 | CHC-C4B | 4.11 | 1.46 | 1.38 |
| 48 | 12 | 202 | A86 | C21-C20 | 4.11 | 1.57 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 31 | 319 | A86 | C21-C20 | 4.11 | 1.57 | 1.51 |
| 37 | 17 | 302 | CLA | C1D-ND | 4.11 | 1.43 | 1.37 |
| 47 | 21 | 203 | KC1 | CHB-C1B | 4.11 | 1.46 | 1.38 |
| 47 | 12 | 211 | KC1 | C1A-CHA | 4.11 | 1.50 | 1.40 |
| 37 | 35 | 303 | CLA | CHD-C4C | 4.11 | 1.48 | 1.39 |
| 37 | a | 404 | CLA | CHC-C1C | 4.11 | 1.46 | 1.38 |
| 37 | 34 | 301 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 47 | 14 | 304 | KC1 | CHB-C1B | 4.11 | 1.46 | 1.38 |
| 37 | z | 101 | CLA | CHD-C1D | 4.11 | 1.46 | 1.38 |
| 37 | 37 | 306 | CLA | C1B-NB | -4.11 | 1.32 | 1.37 |
| 37 | b | 509 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 37 | 32 | 210 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 45 | d | 402 | PL9 | C7-C3 | -4.11 | 1.45 | 1.51 |
| 48 | 34 | 316 | A86 | C7-C6 | 4.11 | 1.59 | 1.50 |
| 37 | 35 | 307 | CLA | C1B-NB | -4.11 | 1.32 | 1.37 |
| 37 | 19 | 307 | CLA | CHD-C1D | 4.10 | 1.46 | 1.38 |
| 47 | 13 | 302 | KC1 | C1A-CHA | 4.10 | 1.50 | 1.40 |
| 47 | 33 | 302 | KC1 | C1A-CHA | 4.10 | 1.50 | 1.40 |
| 48 | 40 | 201 | A86 | C21-C20 | 4.10 | 1.57 | 1.51 |
| 48 | 13 | 315 | A86 | C9-C10 | 4.10 | 1.55 | 1.43 |
| 37 | 19 | 310 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 37 | 31 | 304 | CLA | CHC-C1C | 4.10 | 1.46 | 1.38 |
| 48 | 15 | 311 | A86 | C10-C11 | 4.10 | 1.45 | 1.34 |
| 37 | 36 | 306 | CLA | CHD-C1D | 4.10 | 1.46 | 1.38 |
| 37 | C | 504 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 37 | B | 512 | CLA | C4B-NB | -4.10 | 1.32 | 1.37 |
| 37 | 38 | 204 | CLA | CHD-C4C | 4.10 | 1.48 | 1.39 |
| 37 | 18 | 204 | CLA | CHD-C4C | 4.10 | 1.48 | 1.39 |
| 37 | c | 508 | CLA | CHC-C1C | 4.10 | 1.46 | 1.38 |
| 37 | c | 504 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 37 | d | 401 | CLA | C1D-ND | 4.10 | 1.43 | 1.37 |
| 37 | B | 501 | CLA | CHD-C1D | 4.10 | 1.46 | 1.38 |
| 37 | C | 510 | CLA | CHC-C1C | 4.10 | 1.46 | 1.38 |
| 37 | 31 | 304 | CLA | CHD-C1D | 4.10 | 1.46 | 1.38 |
| 47 | 12 | 206 | KC1 | CHB-C1B | 4.10 | 1.46 | 1.38 |
| 37 | 12 | 209 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 48 | 35 | 311 | A86 | C10-C11 | 4.10 | 1.45 | 1.34 |
| 37 | 34 | 307 | CLA | C1D-ND | 4.10 | 1.43 | 1.37 |
| 48 | 32 | 218 | A86 | C7-C6 | 4.10 | 1.59 | 1.50 |
| 48 | 37 | 312 | A86 | C17-C18 | -4.10 | 1.46 | 1.52 |
| 48 | 17 | 311 | A86 | O4-C38 | 4.10 | 1.44 | 1.35 |
| 37 | 21 | 209 | CLA | CHD-C4C | 4.10 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 15 | 304 | KC1 | C1A-CHA | 4.10 | 1.50 | 1.40 |
| 48 | 11 | 319 | A86 | C7-C6 | 4.10 | 1.59 | 1.50 |
| 48 | 18 | 213 | A86 | C17-C18 | -4.10 | 1.46 | 1.52 |
| 37 | 12 | 205 | CLA | C1D-ND | 4.10 | 1.43 | 1.37 |
| 37 | a | 403 | CLA | CHC-C1C | 4.10 | 1.46 | 1.38 |
| 37 | 12 | 210 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 37 | D | 401 | CLA | CHC-C1C | 4.10 | 1.46 | 1.38 |
| 47 | 32 | 209 | KC1 | C1D-ND | 4.10 | 1.43 | 1.37 |
| 37 | 20 | 308 | CLA | CHD-C1D | 4.09 | 1.46 | 1.38 |
| 37 | B | 516 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 47 | 36 | 305 | KC1 | C1A-NA | -4.09 | 1.29 | 1.38 |
| 37 | B | 508 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 37 | 14 | 301 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 37 | d | 404 | CLA | C1D-ND | 4.09 | 1.43 | 1.37 |
| 37 | 16 | 309 | CLA | CHD-C1D | 4.09 | 1.46 | 1.38 |
| 37 | b | 515 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 47 | 17 | 303 | KC1 | C1B-NB | -4.09 | 1.32 | 1.37 |
| 48 | 13 | 311 | A86 | C21-C20 | 4.09 | 1.57 | 1.51 |
| 37 | B | 502 | CLA | CHD-C1D | 4.09 | 1.46 | 1.38 |
| 37 | b | 508 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 37 | 41 | 209 | CLA | CHD-C4C | 4.09 | 1.48 | 1.39 |
| 48 | 16 | 313 | A86 | C19-C18 | 4.09 | 1.58 | 1.52 |
| 48 | 41 | 214 | A86 | C17-C18 | -4.09 | 1.46 | 1.52 |
| 37 | B | 502 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 37 | c | 509 | CLA | CHC-C1C | 4.09 | 1.46 | 1.38 |
| 37 | 39 | 310 | CLA | CHD-C1D | 4.08 | 1.46 | 1.38 |
| 37 | 17 | 309 | CLA | CHD-C4C | 4.08 | 1.48 | 1.39 |
| 37 | B | 515 | CLA | O2A-CGA | 4.08 | 1.45 | 1.33 |
| 48 | 32 | 217 | A86 | C17-C18 | -4.08 | 1.46 | 1.52 |
| 37 | C | 509 | CLA | CHC-C1C | 4.08 | 1.46 | 1.38 |
| 37 | c | 507 | CLA | CHC-C1C | 4.08 | 1.46 | 1.38 |
| 47 | 15 | 302 | KC1 | CHB-C1B | 4.08 | 1.46 | 1.38 |
| 37 | b | 516 | CLA | O2A-CGA | 4.08 | 1.45 | 1.33 |
| 37 | c | 510 | CLA | CHC-C1C | 4.08 | 1.46 | 1.38 |
| 37 | C | 504 | CLA | C1D-ND | 4.08 | 1.43 | 1.37 |
| 37 | b | 505 | CLA | C1D-ND | 4.08 | 1.43 | 1.37 |
| 37 | B | 513 | CLA | CHC-C1C | 4.08 | 1.46 | 1.38 |
| 47 | 35 | 304 | KC1 | C1A-CHA | 4.08 | 1.50 | 1.40 |
| 37 | B | 503 | CLA | O2A-CGA | 4.08 | 1.45 | 1.33 |
| 37 | B | 515 | CLA | C1D-ND | 4.08 | 1.43 | 1.37 |
| 47 | 11 | 304 | KC1 | C1B-NB | -4.08 | 1.32 | 1.37 |
| 37 | 34 | 308 | CLA | CHD-C1D | 4.08 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | C | 507 | CLA | CHC-C1C | 4.08 | 1.46 | 1.38 |
| 48 | 37 | 312 | A86 | C21-C20 | 4.08 | 1.57 | 1.51 |
| 37 | 21 | 210 | CLA | CHD-C4C | 4.08 | 1.48 | 1.39 |
| 37 | B | 509 | CLA | O2A-CGA | 4.08 | 1.45 | 1.33 |
| 37 | B | 505 | CLA | C1D-ND | 4.08 | 1.43 | 1.37 |
| 37 | 19 | 306 | CLA | C1D-ND | 4.08 | 1.43 | 1.37 |
| 37 | 39 | 306 | CLA | C1D-ND | 4.08 | 1.43 | 1.37 |
| 48 | 15 | 314 | A86 | C9-C10 | 4.08 | 1.55 | 1.43 |
| 48 | 31 | 312 | A86 | O4-C38 | 4.08 | 1.44 | 1.35 |
| 37 | 14 | 308 | CLA | CHD-C1D | 4.08 | 1.46 | 1.38 |
| 48 | 13 | 313 | A86 | C9-C10 | 4.07 | 1.55 | 1.43 |
| 48 | 33 | 313 | A86 | C9-C10 | 4.07 | 1.55 | 1.43 |
| 48 | 14 | 316 | A86 | C21-C20 | 4.07 | 1.57 | 1.51 |
| 48 | 31 | 319 | A86 | C7-C6 | 4.07 | 1.59 | 1.50 |
| 37 | c | 509 | CLA | C1D-ND | 4.07 | 1.43 | 1.37 |
| 48 | 14 | 315 | A86 | O4-C38 | 4.07 | 1.44 | 1.35 |
| 48 | 34 | 315 | A86 | O4-C38 | 4.07 | 1.44 | 1.35 |
| 37 | b | 514 | CLA | C1B-NB | -4.07 | 1.32 | 1.37 |
| 37 | A | 403 | CLA | CHC-C1C | 4.07 | 1.46 | 1.38 |
| 48 | 40 | 211 | A86 | C9-C10 | 4.07 | 1.55 | 1.43 |
| 48 | 40 | 213 | A86 | C9-C10 | 4.07 | 1.55 | 1.43 |
| 37 | W | 101 | CLA | C1D-ND | 4.07 | 1.43 | 1.37 |
| 37 | 33 | 307 | CLA | CHD-C1D | 4.07 | 1.46 | 1.38 |
| 37 | b | 502 | CLA | O2A-CGA | 4.07 | 1.45 | 1.33 |
| 48 | 15 | 314 | A86 | C17-C18 | -4.07 | 1.46 | 1.52 |
| 37 | 32 | 211 | CLA | O2A-CGA | 4.07 | 1.45 | 1.33 |
| 37 | 14 | 307 | CLA | CHD-C1D | 4.07 | 1.46 | 1.38 |
| 37 | 40 | 210 | CLA | CHD-C1D | 4.07 | 1.46 | 1.38 |
| 37 | 41 | 208 | CLA | CHD-C4C | 4.06 | 1.48 | 1.39 |
| 37 | 36 | 309 | CLA | CHD-C1D | 4.06 | 1.46 | 1.38 |
| 37 | 35 | 310 | CLA | CHD-C4C | 4.06 | 1.48 | 1.39 |
| 48 | 11 | 319 | A86 | C21-C20 | 4.06 | 1.57 | 1.51 |
| 47 | 14 | 304 | KC1 | C1A-CHA | 4.06 | 1.50 | 1.40 |
| 47 | 34 | 304 | KC1 | C1A-CHA | 4.06 | 1.50 | 1.40 |
| 37 | 40 | 208 | CLA | CHD-C1D | 4.06 | 1.46 | 1.38 |
| 37 | C | 508 | CLA | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 37 | 19 | 310 | CLA | CHD-C1D | 4.06 | 1.46 | 1.38 |
| 47 | 37 | 302 | KC1 | C1B-NB | -4.06 | 1.32 | 1.37 |
| 48 | 20 | 311 | A86 | C9-C10 | 4.06 | 1.55 | 1.43 |
| 37 | b | 513 | CLA | CHC-C1C | 4.06 | 1.46 | 1.38 |
| 37 | 14 | 307 | CLA | C1D-ND | 4.06 | 1.43 | 1.37 |
| 37 | w | 101 | CLA | C1D-ND | 4.06 | 1.43 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 11 | 303 | CLA | C1D-ND | 4.06 | 1.43 | 1.37 |
| 37 | 41 | 202 | CLA | CHD-C4C | 4.06 | 1.48 | 1.39 |
| 48 | 12 | 202 | A86 | C10-C11 | 4.05 | 1.45 | 1.34 |
| 48 | 20 | 309 | A86 | C9-C10 | 4.05 | 1.55 | 1.43 |
| 37 | 21 | 208 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 48 | 12 | 217 | A86 | C21-C20 | 4.05 | 1.57 | 1.51 |
| 37 | 15 | 301 | CLA | CHD-C1D | 4.05 | 1.46 | 1.38 |
| 37 | 16 | 306 | CLA | CHD-C1D | 4.05 | 1.46 | 1.38 |
| 37 | 35 | 301 | CLA | CHD-C1D | 4.05 | 1.46 | 1.38 |
| 37 | c | 508 | CLA | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 37 | C | 507 | CLA | C1B-NB | -4.05 | 1.32 | 1.37 |
| 37 | 13 | 310 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 37 | b | 503 | CLA | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 48 | 32 | 203 | A86 | C10-C11 | 4.05 | 1.45 | 1.34 |
| 48 | 17 | 314 | A86 | C10-C11 | 4.05 | 1.45 | 1.34 |
| 37 | 41 | 210 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 48 | 12 | 215 | A86 | C10-C11 | 4.05 | 1.45 | 1.34 |
| 37 | 20 | 306 | CLA | CHD-C1D | 4.05 | 1.46 | 1.38 |
| 37 | B | 513 | CLA | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 48 | 35 | 314 | A86 | C9-C10 | 4.05 | 1.55 | 1.43 |
| 37 | 15 | 308 | CLA | CHD-C1D | 4.05 | 1.46 | 1.38 |
| 48 | 38 | 214 | A86 | C9-C10 | 4.05 | 1.55 | 1.43 |
| 48 | 32 | 203 | A86 | C21-C20 | 4.05 | 1.57 | 1.51 |
| 47 | 13 | 309 | KC1 | C1B-NB | -4.05 | 1.32 | 1.37 |
| 37 | 38 | 208 | CLA | CHD-C1D | 4.05 | 1.46 | 1.38 |
| 37 | 38 | 201 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 37 | 18 | 209 | CLA | CHD-C1D | 4.04 | 1.46 | 1.38 |
| 37 | 38 | 209 | CLA | CHD-C1D | 4.04 | 1.46 | 1.38 |
| 48 | 37 | 313 | A86 | C10-C11 | 4.04 | 1.45 | 1.34 |
| 37 | b | 502 | CLA | CHD-C1D | 4.04 | 1.46 | 1.38 |
| 37 | 19 | 304 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 48 | 15 | 315 | A86 | C21-C20 | 4.04 | 1.57 | 1.51 |
| 48 | 11 | 311 | A86 | C7-C6 | 4.04 | 1.59 | 1.50 |
| 48 | 31 | 311 | A86 | C7-C6 | 4.04 | 1.59 | 1.50 |
| 37 | b | 513 | CLA | O2A-CGA | 4.04 | 1.45 | 1.33 |
| 37 | c | 503 | CLA | O2A-CGA | 4.04 | 1.45 | 1.33 |
| 37 | b | 506 | CLA | CHC-C1C | 4.04 | 1.46 | 1.38 |
| 37 | 38 | 206 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 37 | 13 | 307 | CLA | CHD-C1D | 4.04 | 1.46 | 1.38 |
| 48 | 38 | 215 | A86 | C9-C10 | 4.04 | 1.55 | 1.43 |
| 48 | 40 | 201 | A86 | C19-C18 | 4.04 | 1.58 | 1.52 |
| 48 | 20 | 311 | A86 | C17-C18 | -4.04 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 33 | 314 | A86 | C17-C18 | -4.04 | 1.46 | 1.52 |
| 37 | b | 515 | CLA | C1D-ND | 4.04 | 1.43 | 1.37 |
| 37 | C | 511 | CLA | O2A-CGA | 4.04 | 1.45 | 1.33 |
| 47 | 16 | 308 | KC1 | C1A-NA | -4.04 | 1.29 | 1.38 |
| 37 | 35 | 305 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 37 | 13 | 303 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 37 | 37 | 301 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 48 | 16 | 313 | A86 | C21-C20 | 4.04 | 1.57 | 1.51 |
| 37 | a | 407 | CLA | C1B-NB | -4.04 | 1.32 | 1.37 |
| 37 | 19 | 305 | CLA | CHD-C1D | 4.04 | 1.46 | 1.38 |
| 37 | 31 | 306 | CLA | CHD-C1D | 4.04 | 1.46 | 1.38 |
| 37 | 39 | 309 | CLA | CHD-C1D | 4.04 | 1.46 | 1.38 |
| 37 | 37 | 308 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 48 | 21 | 213 | A86 | C9-C10 | 4.03 | 1.55 | 1.43 |
| 37 | A | 403 | CLA | CHD-C1D | 4.03 | 1.46 | 1.38 |
| 37 | D | 402 | CLA | C1D-ND | 4.03 | 1.43 | 1.37 |
| 37 | C | 509 | CLA | C1D-ND | 4.03 | 1.43 | 1.37 |
| 37 | b | 509 | CLA | C1D-ND | 4.03 | 1.43 | 1.37 |
| 37 | c | 502 | CLA | C1B-NB | -4.03 | 1.32 | 1.37 |
| 48 | 11 | 312 | A86 | C21-C20 | 4.03 | 1.57 | 1.51 |
| 37 | b | 516 | CLA | CHC-C1C | 4.03 | 1.46 | 1.38 |
| 37 | 18 | 203 | CLA | CHD-C4C | 4.03 | 1.48 | 1.39 |
| 37 | b | 511 | CLA | CHC-C1C | 4.03 | 1.46 | 1.38 |
| 48 | 35 | 312 | A86 | C10-C11 | 4.03 | 1.45 | 1.34 |
| 37 | C | 511 | CLA | C1B-NB | -4.03 | 1.32 | 1.37 |
| 37 | 12 | 205 | CLA | CHD-C1D | 4.03 | 1.46 | 1.38 |
| 37 | c | 509 | CLA | C4B-NB | -4.02 | 1.32 | 1.37 |
| 48 | 31 | 313 | A86 | O4-C38 | 4.02 | 1.44 | 1.35 |
| 48 | 17 | 313 | A86 | C17-C18 | -4.02 | 1.46 | 1.52 |
| 37 | 15 | 305 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 48 | 32 | 216 | A86 | C21-C20 | 4.02 | 1.57 | 1.51 |
| 48 | 11 | 314 | A86 | C21-C20 | 4.02 | 1.57 | 1.51 |
| 47 | 37 | 305 | KC1 | C1A-NA | -4.02 | 1.29 | 1.38 |
| 37 | 21 | 202 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 37 | B | 511 | CLA | C1D-ND | 4.02 | 1.43 | 1.37 |
| 47 | 31 | 303 | KC1 | CHC-C4B | 4.02 | 1.46 | 1.38 |
| 48 | 41 | 211 | A86 | C17-C18 | -4.02 | 1.46 | 1.52 |
| 37 | B | 506 | CLA | CHC-C1C | 4.02 | 1.46 | 1.38 |
| 37 | 11 | 305 | CLA | CHD-C1D | 4.02 | 1.46 | 1.38 |
| 37 | B | 516 | CLA | CHC-C1C | 4.02 | 1.46 | 1.38 |
| 48 | 37 | 310 | A86 | O4-C38 | 4.02 | 1.44 | 1.35 |
| 37 | 34 | 307 | CLA | CHD-C1D | 4.02 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | C | 503 | CLA | O2A-CGA | 4.02 | 1.45 | 1.33 |
| 37 | 21 | 205 | CLA | CHD-C1D | 4.02 | 1.46 | 1.38 |
| 37 | 41 | 205 | CLA | CHD-C1D | 4.02 | 1.46 | 1.38 |
| 37 | 39 | 305 | CLA | CHD-C1D | 4.02 | 1.46 | 1.38 |
| 37 | 33 | 305 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 48 | 15 | 312 | A86 | C10-C11 | 4.02 | 1.45 | 1.34 |
| 37 | 34 | 310 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 37 | 39 | 304 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 48 | 14 | 314 | A86 | C21-C20 | 4.01 | 1.57 | 1.51 |
| 48 | 31 | 314 | A86 | C21-C20 | 4.01 | 1.57 | 1.51 |
| 37 | 12 | 209 | CLA | C1D-ND | 4.01 | 1.43 | 1.37 |
| 48 | 33 | 314 | A86 | C9-C10 | 4.01 | 1.55 | 1.43 |
| 48 | 37 | 311 | A86 | C21-C20 | 4.01 | 1.57 | 1.51 |
| 47 | 36 | 308 | KC1 | C1A-NA | -4.01 | 1.29 | 1.38 |
| 37 | 15 | 310 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 48 | 32 | 216 | A86 | C10-C11 | 4.01 | 1.45 | 1.34 |
| 37 | 11 | 308 | CLA | CHD-C1D | 4.01 | 1.46 | 1.38 |
| 37 | 32 | 202 | CLA | CHD-C1D | 4.01 | 1.46 | 1.38 |
| 37 | B | 502 | CLA | C1B-NB | -4.01 | 1.32 | 1.37 |
| 37 | b | 511 | CLA | C1D-ND | 4.01 | 1.43 | 1.37 |
| 37 | D | 405 | CLA | C1B-NB | -4.01 | 1.32 | 1.37 |
| 48 | 21 | 211 | A86 | C17-C18 | -4.01 | 1.46 | 1.52 |
| 37 | D | 402 | CLA | C1B-NB | -4.01 | 1.32 | 1.37 |
| 37 | D | 406 | CLA | C1B-NB | -4.01 | 1.32 | 1.37 |
| 37 | a | 403 | CLA | CHD-C1D | 4.01 | 1.46 | 1.38 |
| 37 | 16 | 303 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 48 | 17 | 315 | A86 | C9-C10 | 4.01 | 1.55 | 1.43 |
| 37 | 14 | 310 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 37 | c | 511 | CLA | O2A-CGA | 4.01 | 1.45 | 1.33 |
| 37 | d | 401 | CLA | C1B-NB | -4.01 | 1.32 | 1.37 |
| 37 | 18 | 206 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 37 | 14 | 305 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 37 | 11 | 307 | CLA | C1D-ND | 4.01 | 1.43 | 1.37 |
| 37 | c | 501 | CLA | CHD-C1D | 4.01 | 1.46 | 1.38 |
| 48 | 41 | 213 | A86 | C9-C10 | 4.00 | 1.55 | 1.43 |
| 37 | 31 | 308 | CLA | C1D-ND | 4.00 | 1.43 | 1.37 |
| 37 | 18 | 208 | CLA | CHD-C1D | 4.00 | 1.46 | 1.38 |
| 48 | 37 | 314 | A86 | C9-C10 | 4.00 | 1.55 | 1.43 |
| 48 | 18 | 213 | A86 | C10-C11 | 4.00 | 1.45 | 1.34 |
| 48 | 33 | 311 | A86 | C10-C11 | 4.00 | 1.45 | 1.34 |
| 48 | 18 | 214 | A86 | C10-C11 | 4.00 | 1.45 | 1.34 |
| 47 | 18 | 210 | KC1 | C1A-NA | -4.00 | 1.29 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 38 | 215 | A86 | C10-C11 | 4.00 | 1.45 | 1.34 |
| 48 | 13 | 314 | A86 | C21-C20 | 4.00 | 1.57 | 1.51 |
| 37 | 19 | 309 | CLA | CHD-C1D | 4.00 | 1.46 | 1.38 |
| 37 | B | 509 | CLA | C1D-ND | 4.00 | 1.43 | 1.37 |
| 37 | a | 403 | CLA | C4B-NB | -4.00 | 1.32 | 1.37 |
| 37 | B | 507 | CLA | CHD-C1D | 4.00 | 1.46 | 1.38 |
| 37 | C | 510 | CLA | O2A-CGA | 4.00 | 1.45 | 1.33 |
| 48 | 12 | 215 | A86 | C21-C20 | 4.00 | 1.57 | 1.51 |
| 47 | 16 | 308 | KC1 | CHB-C1B | 4.00 | 1.46 | 1.38 |
| 37 | c | 510 | CLA | C1D-ND | 4.00 | 1.43 | 1.37 |
| 37 | 33 | 303 | CLA | CHD-C4C | 4.00 | 1.48 | 1.39 |
| 47 | 35 | 309 | KC1 | CHB-C1B | 4.00 | 1.46 | 1.38 |
| 37 | 31 | 304 | CLA | C1D-ND | 4.00 | 1.43 | 1.37 |
| 37 | 11 | 310 | CLA | O2A-CGA | 4.00 | 1.45 | 1.33 |
| 47 | 38 | 210 | KC1 | C1A-NA | -4.00 | 1.29 | 1.38 |
| 47 | 18 | 210 | KC1 | CHB-C1B | 4.00 | 1.46 | 1.38 |
| 47 | 17 | 306 | KC1 | C1A-NA | -4.00 | 1.29 | 1.38 |
| 48 | 18 | 214 | A86 | C9-C10 | 4.00 | 1.55 | 1.43 |
| 47 | 38 | 210 | KC1 | CHB-C1B | 4.00 | 1.46 | 1.38 |
| 37 | C | 501 | CLA | CHD-C1D | 3.99 | 1.46 | 1.38 |
| 47 | 17 | 305 | KC1 | C1A-CHA | 3.99 | 1.50 | 1.40 |
| 48 | 13 | 314 | A86 | C9-C10 | 3.99 | 1.55 | 1.43 |
| 37 | A | 405 | CLA | C1B-NB | -3.99 | 1.32 | 1.37 |
| 47 | 11 | 302 | KC1 | CHB-C1B | 3.99 | 1.46 | 1.38 |
| 37 | 16 | 306 | CLA | C1D-ND | 3.99 | 1.43 | 1.37 |
| 48 | 18 | 215 | A86 | C9-C10 | 3.99 | 1.55 | 1.43 |
| 47 | 36 | 308 | KC1 | C1B-NB | -3.99 | 1.32 | 1.37 |
| 37 | B | 511 | CLA | O2A-CGA | 3.99 | 1.45 | 1.33 |
| 37 | 36 | 306 | CLA | C1D-ND | 3.99 | 1.43 | 1.37 |
| 37 | 36 | 303 | CLA | CHD-C4C | 3.99 | 1.48 | 1.39 |
| 48 | 13 | 312 | A86 | C10-C11 | 3.99 | 1.45 | 1.34 |
| 48 | 33 | 312 | A86 | C10-C11 | 3.99 | 1.45 | 1.34 |
| 37 | C | 502 | CLA | C1B-NB | -3.99 | 1.32 | 1.37 |
| 37 | C | 510 | CLA | C1D-ND | 3.99 | 1.43 | 1.37 |
| 48 | 13 | 311 | A86 | C10-C11 | 3.99 | 1.45 | 1.34 |
| 47 | 11 | 302 | KC1 | CHC-C4B | 3.99 | 1.46 | 1.38 |
| 47 | 41 | 207 | KC1 | CHC-C1C | 3.99 | 1.48 | 1.39 |
| 48 | 12 | 217 | A86 | C9-C10 | 3.99 | 1.55 | 1.43 |
| 37 | b | 507 | CLA | CHD-C1D | 3.99 | 1.46 | 1.38 |
| 47 | 18 | 207 | KC1 | C1A-NA | -3.99 | 1.29 | 1.38 |
| 37 | 21 | 206 | CLA | CHD-C1D | 3.99 | 1.46 | 1.38 |
| 47 | 31 | 303 | KC1 | CHB-C1B | 3.99 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 31 | 312 | A86 | C21-C20 | 3.99 | 1.57 | 1.51 |
| 37 | C | 509 | CLA | C4B-NB | -3.99 | 1.32 | 1.37 |
| 37 | B | 511 | CLA | CHC-C1C | 3.99 | 1.46 | 1.38 |
| 37 | 36 | 307 | CLA | CHD-C1D | 3.99 | 1.46 | 1.38 |
| 48 | 37 | 319 | A86 | C10-C11 | 3.98 | 1.45 | 1.34 |
| 37 | 13 | 305 | CLA | CHD-C4C | 3.98 | 1.48 | 1.39 |
| 37 | d | 404 | CLA | C1B-NB | -3.98 | 1.32 | 1.37 |
| 37 | c | 510 | CLA | O2A-CGA | 3.98 | 1.45 | 1.33 |
| 37 | d | 403 | CLA | C1B-NB | -3.98 | 1.32 | 1.37 |
| 37 | 12 | 203 | CLA | O2A-CGA | 3.98 | 1.45 | 1.33 |
| 37 | 31 | 310 | CLA | O2A-CGA | 3.98 | 1.45 | 1.33 |
| 47 | 12 | 208 | KC1 | CHB-C1B | 3.98 | 1.46 | 1.38 |
| 47 | 32 | 209 | KC1 | CHB-C1B | 3.98 | 1.46 | 1.38 |
| 37 | 38 | 202 | CLA | CHD-C1D | 3.98 | 1.46 | 1.38 |
| 37 | 34 | 305 | CLA | CHD-C4C | 3.98 | 1.48 | 1.39 |
| 48 | 34 | 314 | A86 | C19-C18 | 3.98 | 1.57 | 1.52 |
| 37 | b | 511 | CLA | O2A-CGA | 3.98 | 1.44 | 1.33 |
| 48 | 20 | 309 | A86 | C17-C18 | -3.98 | 1.46 | 1.52 |
| 37 | 18 | 206 | CLA | C1B-NB | -3.98 | 1.32 | 1.37 |
| 48 | 40 | 213 | A86 | C19-C18 | 3.98 | 1.57 | 1.52 |
| 47 | 37 | 304 | KC1 | C1A-CHA | 3.98 | 1.50 | 1.40 |
| 48 | 31 | 312 | A86 | C17-C18 | -3.97 | 1.46 | 1.52 |
| 47 | 21 | 207 | KC1 | CHC-C1C | 3.97 | 1.48 | 1.39 |
| 37 | 37 | 303 | CLA | CHD-C4C | 3.97 | 1.48 | 1.39 |
| 37 | b | 501 | CLA | C1B-NB | -3.97 | 1.32 | 1.37 |
| 37 | c | 511 | CLA | C1B-NB | -3.97 | 1.32 | 1.37 |
| 48 | 11 | 312 | A86 | C17-C18 | -3.97 | 1.46 | 1.52 |
| 37 | b | 502 | CLA | C1B-NB | -3.97 | 1.32 | 1.37 |
| 47 | 38 | 207 | KC1 | C1A-NA | -3.97 | 1.29 | 1.38 |
| 48 | 14 | 313 | A86 | C9-C10 | 3.97 | 1.55 | 1.43 |
| 37 | 17 | 304 | CLA | CHD-C4C | 3.97 | 1.48 | 1.39 |
| 48 | 17 | 312 | A86 | C21-C20 | 3.97 | 1.57 | 1.51 |
| 48 | 14 | 314 | A86 | C19-C18 | 3.97 | 1.57 | 1.52 |
| 47 | 15 | 309 | KC1 | C1A-NA | -3.97 | 1.29 | 1.38 |
| 37 | 15 | 307 | CLA | CHD-C1D | 3.97 | 1.46 | 1.38 |
| 37 | 40 | 209 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 48 | 38 | 212 | A86 | O4-C38 | 3.96 | 1.44 | 1.35 |
| 47 | 17 | 308 | KC1 | C1B-NB | -3.96 | 1.32 | 1.37 |
| 37 | c | 510 | CLA | CHD-C1D | 3.96 | 1.46 | 1.38 |
| 47 | 16 | 308 | KC1 | C1B-NB | -3.96 | 1.32 | 1.37 |
| 48 | 32 | 218 | A86 | C21-C20 | 3.96 | 1.57 | 1.51 |
| 37 | 38 | 203 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | W | 101 | CLA | C1B-NB | -3.96 | 1.32 | 1.37 |
| 37 | 32 | 206 | CLA | CHD-C1D | 3.96 | 1.46 | 1.38 |
| 48 | 35 | 319 | A86 | C17-C18 | -3.96 | 1.46 | 1.52 |
| 37 | A | 403 | CLA | C4B-NB | -3.96 | 1.32 | 1.37 |
| 37 | b | 504 | CLA | CHD-C1D | 3.96 | 1.46 | 1.38 |
| 48 | 32 | 218 | A86 | C9-C10 | 3.96 | 1.55 | 1.43 |
| 37 | 16 | 309 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 47 | 36 | 308 | KC1 | CHB-C1B | 3.96 | 1.46 | 1.38 |
| 48 | 14 | 316 | A86 | C9-C10 | 3.96 | 1.55 | 1.43 |
| 48 | 34 | 316 | A86 | C9-C10 | 3.96 | 1.55 | 1.43 |
| 37 | 35 | 307 | CLA | CHD-C1D | 3.96 | 1.46 | 1.38 |
| 37 | 18 | 211 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 48 | 34 | 314 | A86 | C21-C20 | 3.96 | 1.57 | 1.51 |
| 48 | 14 | 314 | A86 | C10-C11 | 3.96 | 1.45 | 1.34 |
| 37 | b | 511 | CLA | C4B-NB | -3.96 | 1.32 | 1.37 |
| 47 | 17 | 306 | KC1 | C1B-NB | -3.96 | 1.32 | 1.37 |
| 37 | 36 | 309 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 48 | 37 | 310 | A86 | C21-C20 | 3.95 | 1.57 | 1.51 |
| 48 | 34 | 313 | A86 | C9-C10 | 3.95 | 1.55 | 1.43 |
| 37 | 17 | 304 | CLA | C1B-NB | -3.95 | 1.32 | 1.37 |
| 37 | c | 503 | CLA | C1B-NB | -3.95 | 1.32 | 1.37 |
| 47 | 35 | 309 | KC1 | C1A-NA | -3.95 | 1.29 | 1.38 |
| 37 | B | 504 | CLA | CHD-C1D | 3.95 | 1.46 | 1.38 |
| 37 | 16 | 307 | CLA | CHD-C1D | 3.95 | 1.46 | 1.38 |
| 37 | 11 | 310 | CLA | C1D-ND | 3.95 | 1.43 | 1.37 |
| 37 | B | 515 | CLA | C1B-NB | -3.95 | 1.32 | 1.37 |
| 37 | C | 501 | CLA | C1B-NB | -3.95 | 1.32 | 1.37 |
| 48 | 11 | 313 | A86 | O4-C38 | 3.95 | 1.43 | 1.35 |
| 48 | 13 | 313 | A86 | C21-C20 | 3.95 | 1.57 | 1.51 |
| 37 | 14 | 303 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 48 | 38 | 212 | A86 | C9-C10 | 3.95 | 1.55 | 1.43 |
| 47 | 31 | 305 | KC1 | C1B-NB | -3.95 | 1.32 | 1.37 |
| 48 | 18 | 215 | A86 | C10-C11 | 3.95 | 1.45 | 1.34 |
| 47 | 39 | 308 | KC1 | C1A-CHA | 3.95 | 1.50 | 1.40 |
| 37 | 32 | 210 | CLA | C1D-ND | 3.95 | 1.43 | 1.37 |
| 48 | 32 | 216 | A86 | C9-C10 | 3.95 | 1.55 | 1.43 |
| 37 | 20 | 307 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 37 | C | 503 | CLA | C1B-NB | -3.95 | 1.32 | 1.37 |
| 48 | 40 | 211 | A86 | C17-C18 | -3.95 | 1.46 | 1.52 |
| 37 | C | 510 | CLA | CHD-C1D | 3.95 | 1.46 | 1.38 |
| 37 | 31 | 310 | CLA | C1D-ND | 3.94 | 1.43 | 1.37 |
| 37 | B | 501 | CLA | C1B-NB | -3.94 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 37 | 303 | CLA | C1B-NB | -3.94 | 1.32 | 1.37 |
| 37 | 41 | 206 | CLA | CHD-C1D | 3.94 | 1.46 | 1.38 |
| 37 | 13 | 308 | CLA | CHD-C4C | 3.94 | 1.48 | 1.39 |
| 37 | 32 | 204 | CLA | O2A-CGA | 3.94 | 1.44 | 1.33 |
| 47 | 37 | 307 | KC1 | C1B-NB | -3.94 | 1.32 | 1.37 |
| 37 | B | 510 | CLA | CHC-C1C | 3.94 | 1.46 | 1.38 |
| 37 | 12 | 209 | CLA | CHD-C1D | 3.94 | 1.46 | 1.38 |
| 37 | 32 | 210 | CLA | CHD-C1D | 3.94 | 1.46 | 1.38 |
| 48 | 12 | 215 | A86 | C9-C10 | 3.94 | 1.55 | 1.43 |
| 37 | c | 506 | CLA | CHD-C1D | 3.94 | 1.46 | 1.38 |
| 47 | 15 | 309 | KC1 | CHB-C1B | 3.94 | 1.46 | 1.38 |
| 48 | 14 | 315 | A86 | C9-C10 | 3.94 | 1.55 | 1.43 |
| 48 | 34 | 315 | A86 | C9-C10 | 3.94 | 1.55 | 1.43 |
| 37 | 41 | 205 | CLA | CHD-C4C | 3.94 | 1.48 | 1.39 |
| 48 | 11 | 315 | A86 | C21-C20 | 3.94 | 1.57 | 1.51 |
| 48 | 31 | 315 | A86 | C21-C20 | 3.94 | 1.57 | 1.51 |
| 48 | 41 | 214 | A86 | C10-C11 | 3.94 | 1.45 | 1.34 |
| 37 | b | 510 | CLA | CHC-C1C | 3.94 | 1.46 | 1.38 |
| 37 | 11 | 303 | CLA | C4B-NB | -3.94 | 1.32 | 1.37 |
| 37 | 31 | 304 | CLA | C4B-NB | -3.94 | 1.32 | 1.37 |
| 48 | 21 | 215 | A86 | C10-C11 | 3.94 | 1.45 | 1.34 |
| 48 | 34 | 314 | A86 | C10-C11 | 3.94 | 1.45 | 1.34 |
| 48 | 37 | 309 | A86 | C9-C10 | 3.93 | 1.55 | 1.43 |
| 48 | 16 | 311 | A86 | O4-C38 | 3.93 | 1.43 | 1.35 |
| 37 | C | 501 | CLA | O2A-CGA | 3.93 | 1.44 | 1.33 |
| 37 | 35 | 308 | CLA | CHD-C4C | 3.93 | 1.48 | 1.39 |
| 47 | 19 | 308 | KC1 | C1A-CHA | 3.93 | 1.50 | 1.40 |
| 47 | 17 | 306 | KC1 | CHC-C4B | 3.93 | 1.46 | 1.38 |
| 47 | 37 | 305 | KC1 | CHC-C4B | 3.93 | 1.46 | 1.38 |
| 48 | 39 | 311 | A86 | C10-C11 | 3.93 | 1.45 | 1.34 |
| 37 | 11 | 308 | CLA | O2A-CGA | 3.93 | 1.44 | 1.33 |
| 48 | 18 | 212 | A86 | O4-C38 | 3.93 | 1.43 | 1.35 |
| 37 | 33 | 310 | CLA | C3D-C2D | 3.93 | 1.49 | 1.39 |
| 48 | 21 | 214 | A86 | C10-C11 | 3.92 | 1.45 | 1.34 |
| 48 | 36 | 311 | A86 | O4-C38 | 3.92 | 1.43 | 1.35 |
| 37 | A | 403 | CLA | C1D-ND | 3.92 | 1.43 | 1.37 |
| 37 | 31 | 304 | CLA | C1B-NB | -3.92 | 1.32 | 1.37 |
| 37 | a | 403 | CLA | C1D-ND | 3.92 | 1.43 | 1.37 |
| 48 | 18 | 212 | A86 | C9-C10 | 3.92 | 1.55 | 1.43 |
| 37 | C | 503 | CLA | CHD-C1D | 3.92 | 1.46 | 1.38 |
| 37 | c | 503 | CLA | CHD-C1D | 3.92 | 1.46 | 1.38 |
| 37 | 19 | 302 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | w | 101 | CLA | C1B-NB | -3.92 | 1.32 | 1.37 |
| 48 | 37 | 309 | A86 | C19-C18 | 3.92 | 1.57 | 1.52 |
| 48 | 19 | 311 | A86 | C10-C11 | 3.92 | 1.45 | 1.34 |
| 48 | 17 | 310 | A86 | C9-C10 | 3.92 | 1.55 | 1.43 |
| 37 | 32 | 204 | CLA | CHD-C1D | 3.92 | 1.46 | 1.38 |
| 37 | 19 | 309 | CLA | C1B-NB | -3.92 | 1.32 | 1.37 |
| 48 | 15 | 313 | A86 | C9-C10 | 3.92 | 1.55 | 1.43 |
| 37 | D | 401 | CLA | CHD-C1D | 3.91 | 1.46 | 1.38 |
| 37 | a | 404 | CLA | CHD-C1D | 3.91 | 1.46 | 1.38 |
| 37 | 33 | 308 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 37 | 12 | 203 | CLA | CHD-C1D | 3.91 | 1.46 | 1.38 |
| 48 | 17 | 310 | A86 | C17-C18 | -3.91 | 1.46 | 1.52 |
| 48 | 20 | 311 | A86 | C19-C18 | 3.91 | 1.57 | 1.52 |
| 47 | 21 | 207 | KC1 | OBD-CAD | 3.91 | 1.29 | 1.22 |
| 37 | 32 | 202 | CLA | O2A-CGA | 3.91 | 1.44 | 1.33 |
| 37 | d | 403 | CLA | O2A-CGA | 3.91 | 1.44 | 1.33 |
| 37 | b | 515 | CLA | C1B-NB | -3.91 | 1.32 | 1.37 |
| 37 | C | 506 | CLA | CHD-C1D | 3.91 | 1.46 | 1.38 |
| 37 | 39 | 302 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 37 | D | 406 | CLA | CHD-C1D | 3.91 | 1.46 | 1.38 |
| 37 | 19 | 301 | CLA | CHD-C1D | 3.91 | 1.46 | 1.38 |
| 37 | 39 | 301 | CLA | CHD-C1D | 3.91 | 1.46 | 1.38 |
| 37 | c | 501 | CLA | O2A-CGA | 3.90 | 1.44 | 1.33 |
| 48 | 15 | 319 | A86 | C17-C18 | -3.90 | 1.46 | 1.52 |
| 47 | 37 | 305 | KC1 | C1B-NB | -3.90 | 1.32 | 1.37 |
| 37 | c | 501 | CLA | C1B-NB | -3.90 | 1.32 | 1.37 |
| 48 | 41 | 215 | A86 | C10-C11 | 3.90 | 1.45 | 1.34 |
| 37 | 21 | 205 | CLA | CHD-C4C | 3.90 | 1.48 | 1.39 |
| 48 | 37 | 309 | A86 | C17-C18 | -3.90 | 1.46 | 1.52 |
| 37 | B | 511 | CLA | C4B-NB | -3.90 | 1.32 | 1.37 |
| 37 | 39 | 309 | CLA | C1B-NB | -3.90 | 1.32 | 1.37 |
| 37 | 12 | 207 | CLA | CHD-C4C | 3.90 | 1.48 | 1.39 |
| 48 | 14 | 314 | A86 | C17-C18 | -3.90 | 1.46 | 1.52 |
| 48 | 34 | 314 | A86 | C17-C18 | -3.90 | 1.46 | 1.52 |
| 37 | a | 407 | CLA | CHD-C1D | 3.90 | 1.46 | 1.38 |
| 47 | 17 | 305 | KC1 | C1B-NB | -3.90 | 1.32 | 1.37 |
| 48 | 11 | 311 | A86 | C21-C20 | 3.90 | 1.57 | 1.51 |
| 47 | 36 | 302 | KC1 | C1A-NA | -3.90 | 1.29 | 1.38 |
| 37 | A | 405 | CLA | CHD-C1D | 3.90 | 1.46 | 1.38 |
| 37 | B | 510 | CLA | O2A-CGA | 3.90 | 1.44 | 1.33 |
| 48 | 33 | 313 | A86 | C21-C20 | 3.90 | 1.57 | 1.51 |
| 37 | b | 505 | CLA | C1B-NB | -3.89 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | D | 405 | CLA | O2A-CGA | 3.89 | 1.44 | 1.33 |
| 37 | B | 515 | CLA | CHD-C1D | 3.89 | 1.46 | 1.38 |
| 37 | B | 513 | CLA | C1D-ND | 3.89 | 1.43 | 1.37 |
| 47 | 17 | 308 | KC1 | CHB-C1B | 3.89 | 1.46 | 1.38 |
| 48 | 21 | 214 | A86 | C19-C18 | 3.89 | 1.57 | 1.52 |
| 47 | 16 | 302 | KC1 | C1A-NA | -3.89 | 1.29 | 1.38 |
| 48 | 35 | 316 | A86 | C10-C11 | 3.89 | 1.45 | 1.34 |
| 37 | b | 510 | CLA | O2A-CGA | 3.89 | 1.44 | 1.33 |
| 48 | 17 | 314 | A86 | C9-C10 | 3.89 | 1.55 | 1.43 |
| 48 | 37 | 313 | A86 | C9-C10 | 3.89 | 1.55 | 1.43 |
| 47 | 41 | 207 | KC1 | OBD-CAD | 3.89 | 1.29 | 1.22 |
| 48 | 15 | 316 | A86 | C10-C11 | 3.89 | 1.45 | 1.34 |
| 37 | 37 | 306 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 37 | 31 | 306 | CLA | C1B-NB | -3.89 | 1.32 | 1.37 |
| 48 | 14 | 314 | A86 | C9-C10 | 3.89 | 1.55 | 1.43 |
| 48 | 35 | 313 | A86 | C9-C10 | 3.89 | 1.55 | 1.43 |
| 37 | 34 | 303 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 37 | b | 512 | CLA | O2A-CGA | 3.89 | 1.44 | 1.33 |
| 48 | 31 | 311 | A86 | C21-C20 | 3.88 | 1.57 | 1.51 |
| 37 | 39 | 310 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 37 | c | 504 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 37 | B | 509 | CLA | CHC-C1C | 3.88 | 1.46 | 1.38 |
| 37 | 15 | 308 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 48 | 12 | 217 | A86 | C10-C11 | 3.88 | 1.45 | 1.34 |
| 37 | B | 512 | CLA | O2A-CGA | 3.88 | 1.44 | 1.33 |
| 37 | 19 | 303 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 48 | 37 | 312 | A86 | C10-C11 | 3.88 | 1.45 | 1.34 |
| 37 | 17 | 307 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 48 | 17 | 320 | A86 | C10-C11 | 3.88 | 1.45 | 1.34 |
| 48 | 16 | 311 | A86 | C10-C11 | 3.88 | 1.45 | 1.34 |
| 37 | 19 | 310 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 37 | 34 | 301 | CLA | CHD-C1D | 3.88 | 1.46 | 1.38 |
| 37 | 12 | 210 | CLA | C1B-NB | -3.88 | 1.32 | 1.37 |
| 37 | 15 | 301 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 47 | 33 | 309 | KC1 | CHB-C1B | 3.87 | 1.46 | 1.38 |
| 37 | 39 | 303 | CLA | CHD-C4C | 3.87 | 1.48 | 1.39 |
| 37 | d | 404 | CLA | CHD-C1D | 3.87 | 1.46 | 1.38 |
| 37 | 41 | 210 | CLA | C3D-C2D | 3.87 | 1.49 | 1.39 |
| 37 | C | 513 | CLA | CHD-C1D | 3.87 | 1.46 | 1.38 |
| 48 | 14 | 316 | A86 | C10-C11 | 3.87 | 1.45 | 1.34 |
| 37 | 13 | 301 | CLA | CHD-C4C | 3.87 | 1.48 | 1.39 |
| 48 | 33 | 314 | A86 | C19-C18 | 3.87 | 1.57 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 34 | 314 | A86 | C9-C10 | 3.87 | 1.55 | 1.43 |
| 48 | 18 | 213 | A86 | C19-C18 | 3.87 | 1.57 | 1.52 |
| 48 | 15 | 312 | A86 | C9-C10 | 3.86 | 1.55 | 1.43 |
| 37 | C | 510 | CLA | C4B-NB | -3.86 | 1.32 | 1.37 |
| 37 | C | 504 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 37 | 38 | 209 | CLA | C3D-C2D | 3.86 | 1.49 | 1.39 |
| 37 | z | 102 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 37 | B | 505 | CLA | C1B-NB | -3.86 | 1.32 | 1.37 |
| 48 | 13 | 312 | A86 | C9-C10 | 3.86 | 1.55 | 1.43 |
| 48 | 12 | 214 | A86 | C21-C20 | 3.86 | 1.57 | 1.51 |
| 48 | 32 | 215 | A86 | C21-C20 | 3.86 | 1.57 | 1.51 |
| 48 | 14 | 311 | A86 | C10-C11 | 3.86 | 1.45 | 1.34 |
| 48 | 34 | 311 | A86 | C10-C11 | 3.86 | 1.45 | 1.34 |
| 37 | b | 509 | CLA | CHC-C1C | 3.86 | 1.46 | 1.38 |
| 37 | 35 | 301 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 37 | a | 404 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 37 | 11 | 303 | CLA | C1B-NB | -3.86 | 1.32 | 1.37 |
| 47 | 13 | 306 | KC1 | C1B-NB | -3.86 | 1.32 | 1.37 |
| 47 | 33 | 306 | KC1 | C1B-NB | -3.86 | 1.32 | 1.37 |
| 37 | W | 101 | CLA | CHD-C1D | 3.86 | 1.45 | 1.38 |
| 48 | 31 | 313 | A86 | C10-C11 | 3.86 | 1.45 | 1.34 |
| 48 | 34 | 316 | A86 | C10-C11 | 3.86 | 1.45 | 1.34 |
| 37 | D | 402 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 37 | Z | 102 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 48 | 17 | 313 | A86 | C10-C11 | 3.86 | 1.45 | 1.34 |
| 48 | 38 | 214 | A86 | C19-C18 | 3.86 | 1.57 | 1.52 |
| 47 | 41 | 203 | KC1 | C1B-NB | -3.86 | 1.32 | 1.37 |
| 37 | 32 | 208 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 48 | 17 | 310 | A86 | C19-C18 | 3.86 | 1.57 | 1.52 |
| 37 | 13 | 308 | CLA | C1B-NB | -3.86 | 1.32 | 1.37 |
| 47 | 20 | 305 | KC1 | C1B-NB | -3.86 | 1.32 | 1.37 |
| 47 | 20 | 302 | KC1 | C1B-NB | -3.86 | 1.32 | 1.37 |
| 37 | 17 | 302 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 37 | c | 505 | CLA | O2A-CGA | 3.85 | 1.44 | 1.33 |
| 48 | 15 | 314 | A86 | C19-C18 | 3.85 | 1.57 | 1.52 |
| 47 | 40 | 207 | KC1 | C1B-NB | -3.85 | 1.32 | 1.37 |
| 47 | 12 | 206 | KC1 | C1D-ND | 3.85 | 1.42 | 1.37 |
| 48 | 32 | 218 | A86 | C10-C11 | 3.85 | 1.45 | 1.34 |
| 37 | 20 | 303 | CLA | C1B-NB | -3.85 | 1.32 | 1.37 |
| 37 | b | 515 | CLA | CHD-C1D | 3.85 | 1.45 | 1.38 |
| 47 | 40 | 204 | KC1 | C1B-NB | -3.85 | 1.32 | 1.37 |
| 48 | 17 | 312 | A86 | C9-C10 | 3.85 | 1.55 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 12 | 202 | A86 | C9-C10 | 3.85 | 1.55 | 1.43 |
| 37 | 21 | 206 | CLA | CHD-C4C | 3.85 | 1.48 | 1.39 |
| 48 | 36 | 311 | A86 | C10-C11 | 3.85 | 1.45 | 1.34 |
| 37 | c | 506 | CLA | C1D-ND | 3.85 | 1.42 | 1.37 |
| 37 | 16 | 301 | CLA | CHD-C1D | 3.85 | 1.45 | 1.38 |
| 48 | 12 | 213 | A86 | C10-C11 | 3.85 | 1.45 | 1.34 |
| 48 | 14 | 313 | A86 | C21-C20 | 3.85 | 1.57 | 1.51 |
| 47 | 41 | 207 | KC1 | CHB-C1B | 3.85 | 1.45 | 1.38 |
| 48 | 37 | 311 | A86 | C9-C10 | 3.85 | 1.55 | 1.43 |
| 47 | 37 | 307 | KC1 | CHB-C1B | 3.84 | 1.45 | 1.38 |
| 37 | 21 | 210 | CLA | C3D-C2D | 3.84 | 1.49 | 1.39 |
| 37 | 18 | 209 | CLA | C3D-C2D | 3.84 | 1.49 | 1.39 |
| 37 | D | 401 | CLA | C4B-NB | -3.84 | 1.32 | 1.37 |
| 47 | 13 | 309 | KC1 | CHB-C1B | 3.84 | 1.45 | 1.38 |
| 37 | C | 504 | CLA | C1B-NB | -3.84 | 1.32 | 1.37 |
| 37 | c | 504 | CLA | C1B-NB | -3.84 | 1.32 | 1.37 |
| 48 | 33 | 312 | A86 | C9-C10 | 3.84 | 1.55 | 1.43 |
| 37 | w | 101 | CLA | CHD-C1D | 3.84 | 1.45 | 1.38 |
| 37 | 34 | 302 | CLA | CHD-C4C | 3.84 | 1.47 | 1.39 |
| 47 | 16 | 302 | KC1 | C1B-NB | -3.84 | 1.32 | 1.37 |
| 37 | C | 505 | CLA | O2A-CGA | 3.84 | 1.44 | 1.33 |
| 48 | 32 | 203 | A86 | C9-C10 | 3.84 | 1.55 | 1.43 |
| 48 | 13 | 314 | A86 | C19-C18 | 3.84 | 1.57 | 1.52 |
| 37 | 33 | 301 | CLA | CHD-C4C | 3.84 | 1.47 | 1.39 |
| 37 | c | 510 | CLA | C4B-NB | -3.84 | 1.32 | 1.37 |
| 47 | 21 | 203 | KC1 | C1B-NB | -3.84 | 1.32 | 1.37 |
| 37 | C | 509 | CLA | CHD-C1D | 3.84 | 1.45 | 1.38 |
| 37 | 31 | 310 | CLA | CHD-C1D | 3.84 | 1.45 | 1.38 |
| 37 | 19 | 306 | CLA | C1B-NB | -3.84 | 1.32 | 1.37 |
| 37 | 14 | 308 | CLA | CHD-C4C | 3.84 | 1.47 | 1.39 |
| 37 | 18 | 201 | CLA | CHD-C4C | 3.84 | 1.47 | 1.39 |
| 37 | b | 508 | CLA | CHD-C1D | 3.84 | 1.45 | 1.38 |
| 37 | 36 | 301 | CLA | CHD-C1D | 3.84 | 1.45 | 1.38 |
| 48 | 36 | 310 | A86 | C10-C11 | 3.83 | 1.45 | 1.34 |
| 48 | 32 | 214 | A86 | C10-C11 | 3.83 | 1.45 | 1.34 |
| 50 | 40 | 212 | DD6 | C35-C34 | 3.83 | 1.58 | 1.52 |
| 37 | 40 | 203 | CLA | CHD-C4C | 3.83 | 1.47 | 1.39 |
| 48 | 41 | 214 | A86 | C19-C18 | 3.83 | 1.57 | 1.52 |
| 37 | c | 509 | CLA | CHD-C1D | 3.83 | 1.45 | 1.38 |
| 37 | 38 | 202 | CLA | CHC-C4B | 3.83 | 1.48 | 1.39 |
| 48 | 11 | 311 | A86 | C10-C11 | 3.83 | 1.45 | 1.34 |
| 37 | C | 502 | CLA | O2A-CGA | 3.83 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 39 | 309 | CLA | CHD-C4C | 3.83 | 1.47 | 1.39 |
| 37 | c | 513 | CLA | CHD-C1D | 3.83 | 1.45 | 1.38 |
| 37 | 36 | 307 | CLA | C1B-NB | -3.83 | 1.32 | 1.37 |
| 48 | 11 | 313 | A86 | C10-C11 | 3.83 | 1.45 | 1.34 |
| 47 | 35 | 309 | KC1 | C1B-NB | -3.83 | 1.32 | 1.37 |
| 48 | 35 | 312 | A86 | C9-C10 | 3.83 | 1.55 | 1.43 |
| 48 | 13 | 311 | A86 | C9-C10 | 3.83 | 1.55 | 1.43 |
| 48 | 33 | 311 | A86 | C9-C10 | 3.83 | 1.55 | 1.43 |
| 37 | B | 513 | CLA | C4B-NB | -3.83 | 1.32 | 1.37 |
| 37 | 15 | 303 | CLA | C3D-C2D | 3.83 | 1.49 | 1.39 |
| 37 | 15 | 307 | CLA | C3D-C2D | 3.83 | 1.49 | 1.39 |
| 37 | 40 | 210 | CLA | CHD-C4C | 3.83 | 1.47 | 1.39 |
| 37 | b | 513 | CLA | C1D-ND | 3.83 | 1.42 | 1.37 |
| 37 | a | 404 | CLA | C4B-NB | -3.83 | 1.32 | 1.37 |
| 48 | 21 | 211 | A86 | C19-C18 | 3.83 | 1.57 | 1.52 |
| 37 | 18 | 202 | CLA | CHD-C4C | 3.83 | 1.47 | 1.39 |
| 48 | 17 | 311 | A86 | C10-C11 | 3.83 | 1.45 | 1.34 |
| 48 | 35 | 316 | A86 | C9-C10 | 3.83 | 1.55 | 1.43 |
| 47 | 14 | 306 | KC1 | C1B-NB | -3.83 | 1.32 | 1.37 |
| 47 | 34 | 306 | KC1 | C1B-NB | -3.83 | 1.32 | 1.37 |
| 48 | 39 | 311 | A86 | C9-C10 | 3.82 | 1.55 | 1.43 |
| 37 | 41 | 206 | CLA | CHD-C4C | 3.82 | 1.47 | 1.39 |
| 37 | 11 | 305 | CLA | C1B-NB | -3.82 | 1.32 | 1.37 |
| 48 | 35 | 319 | A86 | C10-C11 | 3.82 | 1.45 | 1.34 |
| 37 | 14 | 301 | CLA | CHD-C1D | 3.82 | 1.45 | 1.38 |
| 50 | 20 | 310 | DD6 | C35-C34 | 3.82 | 1.58 | 1.52 |
| 37 | D | 401 | CLA | CHD-C4C | 3.82 | 1.47 | 1.39 |
| 37 | 40 | 208 | CLA | C1B-NB | -3.82 | 1.32 | 1.37 |
| 48 | 35 | 311 | A86 | C9-C10 | 3.82 | 1.55 | 1.43 |
| 37 | 15 | 308 | CLA | C3D-C2D | 3.82 | 1.49 | 1.39 |
| 48 | 35 | 315 | A86 | C9-C10 | 3.82 | 1.55 | 1.43 |
| 37 | z | 102 | CLA | OBD-CAD | 3.82 | 1.29 | 1.22 |
| 47 | 11 | 302 | KC1 | C4B-NB | -3.82 | 1.32 | 1.37 |
| 47 | 31 | 303 | KC1 | C4B-NB | -3.82 | 1.32 | 1.37 |
| 37 | 12 | 210 | CLA | CHD-C4C | 3.82 | 1.47 | 1.39 |
| 48 | 40 | 211 | A86 | C19-C18 | 3.82 | 1.57 | 1.52 |
| 37 | 15 | 305 | CLA | C3D-C2D | 3.82 | 1.49 | 1.39 |
| 37 | C | 506 | CLA | C1D-ND | 3.82 | 1.42 | 1.37 |
| 37 | 13 | 303 | CLA | C1B-NB | -3.82 | 1.32 | 1.37 |
| 37 | 14 | 302 | CLA | CHD-C4C | 3.82 | 1.47 | 1.39 |
| 37 | 38 | 211 | CLA | C3D-C2D | 3.82 | 1.49 | 1.39 |
| 37 | c | 502 | CLA | O2A-CGA | 3.82 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | z | 101 | CLA | CHD-C4C | 3.82 | 1.47 | 1.39 |
| 37 | 39 | 306 | CLA | C1B-NB | -3.82 | 1.32 | 1.37 |
| 37 | 20 | 306 | CLA | C1B-NB | -3.81 | 1.32 | 1.37 |
| 37 | 35 | 305 | CLA | C3D-C2D | 3.81 | 1.49 | 1.39 |
| 37 | 13 | 303 | CLA | C3D-C2D | 3.81 | 1.49 | 1.39 |
| 37 | 32 | 213 | CLA | CHD-C4C | 3.81 | 1.47 | 1.39 |
| 37 | 40 | 208 | CLA | CHD-C4C | 3.81 | 1.47 | 1.39 |
| 48 | 41 | 214 | A86 | C9-C10 | 3.81 | 1.55 | 1.43 |
| 48 | 17 | 313 | A86 | C9-C10 | 3.81 | 1.55 | 1.43 |
| 37 | 32 | 211 | CLA | C1B-NB | -3.81 | 1.32 | 1.37 |
| 47 | 15 | 309 | KC1 | C1B-NB | -3.81 | 1.32 | 1.37 |
| 37 | 35 | 307 | CLA | C3D-C2D | 3.81 | 1.49 | 1.39 |
| 37 | 11 | 301 | CLA | O2A-CGA | 3.81 | 1.44 | 1.33 |
| 37 | 16 | 306 | CLA | CHD-C4C | 3.81 | 1.47 | 1.39 |
| 37 | b | 513 | CLA | C4B-NB | -3.81 | 1.32 | 1.37 |
| 37 | W | 102 | CLA | CHD-C4C | 3.81 | 1.47 | 1.39 |
| 37 | 31 | 304 | CLA | CHD-C4C | 3.81 | 1.47 | 1.39 |
| 48 | 31 | 311 | A86 | C10-C11 | 3.81 | 1.45 | 1.34 |
| 37 | 41 | 204 | CLA | C3D-C2D | 3.81 | 1.49 | 1.39 |
| 37 | b | 504 | CLA | O2A-CGA | 3.81 | 1.44 | 1.33 |
| 37 | B | 504 | CLA | O2A-CGA | 3.81 | 1.44 | 1.33 |
| 48 | 19 | 311 | A86 | C9-C10 | 3.81 | 1.55 | 1.43 |
| 37 | b | 502 | CLA | CHD-C4C | 3.81 | 1.47 | 1.39 |
| 37 | 12 | 203 | CLA | C1B-NB | -3.80 | 1.32 | 1.37 |
| 37 | d | 401 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 48 | 15 | 319 | A86 | C10-C11 | 3.80 | 1.44 | 1.34 |
| 48 | 18 | 215 | A86 | C17-C18 | -3.80 | 1.46 | 1.52 |
| 37 | 11 | 307 | CLA | C4B-NB | -3.80 | 1.32 | 1.37 |
| 48 | 41 | 211 | A86 | C19-C18 | 3.80 | 1.57 | 1.52 |
| 37 | 40 | 209 | CLA | C3D-C2D | 3.80 | 1.49 | 1.39 |
| 37 | 20 | 307 | CLA | C3D-C2D | 3.80 | 1.49 | 1.39 |
| 37 | 33 | 303 | CLA | C3D-C2D | 3.80 | 1.49 | 1.39 |
| 48 | 14 | 315 | A86 | C10-C11 | 3.80 | 1.44 | 1.34 |
| 37 | 12 | 212 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 37 | 20 | 308 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 48 | 35 | 315 | A86 | C10-C11 | 3.80 | 1.44 | 1.34 |
| 37 | 38 | 202 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 37 | 33 | 308 | CLA | C1B-NB | -3.80 | 1.32 | 1.37 |
| 37 | a | 407 | CLA | C1D-ND | 3.80 | 1.42 | 1.37 |
| 37 | A | 405 | CLA | C1D-ND | 3.80 | 1.42 | 1.37 |
| 47 | 20 | 302 | KC1 | CHB-C1B | 3.80 | 1.45 | 1.38 |
| 37 | 31 | 302 | CLA | O2A-CGA | 3.80 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 15 | 307 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 37 | 19 | 309 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 48 | 15 | 319 | A86 | C9-C10 | 3.80 | 1.55 | 1.43 |
| 47 | 32 | 207 | KC1 | C1D-ND | 3.80 | 1.42 | 1.37 |
| 37 | b | 504 | CLA | C1D-ND | 3.80 | 1.42 | 1.37 |
| 37 | 20 | 301 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 37 | 36 | 306 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 48 | 37 | 312 | A86 | C9-C10 | 3.79 | 1.54 | 1.43 |
| 37 | 11 | 310 | CLA | CHD-C1D | 3.79 | 1.45 | 1.38 |
| 48 | 34 | 313 | A86 | C21-C20 | 3.79 | 1.57 | 1.51 |
| 37 | B | 501 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 48 | 16 | 310 | A86 | C10-C11 | 3.79 | 1.44 | 1.34 |
| 48 | 34 | 315 | A86 | C10-C11 | 3.79 | 1.44 | 1.34 |
| 37 | b | 505 | CLA | CHD-C1D | 3.79 | 1.45 | 1.38 |
| 37 | 17 | 309 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 37 | 21 | 204 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 47 | 21 | 207 | KC1 | CHB-C1B | 3.79 | 1.45 | 1.38 |
| 37 | 40 | 205 | CLA | C1B-NB | -3.79 | 1.32 | 1.37 |
| 37 | c | 508 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 37 | C | 508 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 37 | b | 501 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 37 | B | 514 | CLA | CHD-C1D | 3.79 | 1.45 | 1.38 |
| 37 | 39 | 301 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 37 | b | 508 | CLA | C1D-ND | 3.79 | 1.42 | 1.37 |
| 37 | B | 508 | CLA | CHD-C1D | 3.79 | 1.45 | 1.38 |
| 37 | c | 512 | CLA | C1D-ND | 3.79 | 1.42 | 1.37 |
| 37 | 32 | 211 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 37 | 20 | 306 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 37 | B | 502 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 37 | 20 | 306 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 48 | 12 | 216 | A86 | C10-C11 | 3.79 | 1.44 | 1.34 |
| 37 | 14 | 301 | CLA | CHC-C4B | 3.79 | 1.47 | 1.39 |
| 37 | 35 | 303 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 37 | B | 504 | CLA | C1D-ND | 3.78 | 1.42 | 1.37 |
| 37 | C | 502 | CLA | CHD-C1D | 3.78 | 1.45 | 1.38 |
| 37 | 11 | 303 | CLA | CHD-C4C | 3.78 | 1.47 | 1.39 |
| 47 | 36 | 302 | KC1 | C1B-NB | -3.78 | 1.32 | 1.37 |
| 47 | 40 | 204 | KC1 | CHB-C1B | 3.78 | 1.45 | 1.38 |
| 47 | 35 | 304 | KC1 | OBD-CAD | 3.78 | 1.29 | 1.22 |
| 37 | 18 | 211 | CLA | C3D-C2D | 3.78 | 1.49 | 1.39 |
| 48 | 15 | 315 | A86 | C9-C10 | 3.78 | 1.54 | 1.43 |
| 48 | 38 | 213 | A86 | C9-C10 | 3.78 | 1.54 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | B | 505 | CLA | CHD-C1D | 3.78 | 1.45 | 1.38 |
| 48 | 20 | 309 | A86 | C19-C18 | 3.78 | 1.57 | 1.52 |
| 37 | 37 | 308 | CLA | OBD-CAD | 3.78 | 1.29 | 1.22 |
| 37 | 21 | 209 | CLA | C3D-C2D | 3.78 | 1.49 | 1.39 |
| 48 | 37 | 310 | A86 | C10-C11 | 3.78 | 1.44 | 1.34 |
| 37 | 39 | 302 | CLA | C3D-C2D | 3.78 | 1.49 | 1.39 |
| 37 | Z | 102 | CLA | OBD-CAD | 3.78 | 1.29 | 1.22 |
| 37 | 16 | 307 | CLA | C1B-NB | -3.78 | 1.32 | 1.37 |
| 37 | Z | 101 | CLA | CHD-C4C | 3.78 | 1.47 | 1.39 |
| 37 | C | 504 | CLA | CHD-C1D | 3.78 | 1.45 | 1.38 |
| 37 | c | 504 | CLA | CHD-C1D | 3.78 | 1.45 | 1.38 |
| 48 | 15 | 311 | A86 | C9-C10 | 3.78 | 1.54 | 1.43 |
| 37 | 33 | 303 | CLA | C1B-NB | -3.78 | 1.32 | 1.37 |
| 37 | 35 | 301 | CLA | CHC-C4B | 3.78 | 1.47 | 1.39 |
| 37 | 34 | 308 | CLA | CHD-C4C | 3.77 | 1.47 | 1.39 |
| 37 | 35 | 308 | CLA | C3D-C2D | 3.77 | 1.49 | 1.39 |
| 37 | C | 512 | CLA | C1D-ND | 3.77 | 1.42 | 1.37 |
| 37 | 19 | 307 | CLA | C1B-NB | -3.77 | 1.32 | 1.37 |
| 37 | C | 503 | CLA | CHD-C4C | 3.77 | 1.47 | 1.39 |
| 37 | 31 | 308 | CLA | C4B-NB | -3.77 | 1.32 | 1.37 |
| 37 | 13 | 303 | CLA | C4B-NB | -3.77 | 1.32 | 1.37 |
| 37 | 12 | 212 | CLA | C1B-NB | -3.77 | 1.32 | 1.37 |
| 37 | 32 | 213 | CLA | C1B-NB | -3.77 | 1.32 | 1.37 |
| 37 | C | 511 | CLA | CHD-C1D | 3.77 | 1.45 | 1.38 |
| 37 | c | 503 | CLA | CHD-C4C | 3.77 | 1.47 | 1.39 |
| 37 | B | 511 | CLA | CHD-C1D | 3.77 | 1.45 | 1.38 |
| 47 | 12 | 211 | KC1 | CHB-C1B | 3.77 | 1.45 | 1.38 |
| 48 | 38 | 213 | A86 | C19-C18 | 3.77 | 1.57 | 1.52 |
| 48 | 12 | 216 | A86 | C9-C10 | 3.77 | 1.54 | 1.43 |
| 48 | 32 | 217 | A86 | C9-C10 | 3.77 | 1.54 | 1.43 |
| 37 | 37 | 308 | CLA | C3D-C2D | 3.77 | 1.49 | 1.39 |
| 47 | 32 | 212 | KC1 | CHB-C1B | 3.77 | 1.45 | 1.38 |
| 37 | 40 | 208 | CLA | C3D-C2D | 3.77 | 1.49 | 1.39 |
| 37 | 41 | 209 | CLA | C3D-C2D | 3.77 | 1.49 | 1.39 |
| 37 | 20 | 307 | CLA | OBD-CAD | 3.77 | 1.29 | 1.22 |
| 48 | 35 | 319 | A86 | C9-C10 | 3.77 | 1.54 | 1.43 |
| 37 | A | 403 | CLA | O2A-CGA | 3.77 | 1.44 | 1.33 |
| 37 | 31 | 301 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 37 | 38 | 203 | CLA | C3D-C2D | 3.76 | 1.49 | 1.39 |
| 37 | c | 502 | CLA | CHD-C1D | 3.76 | 1.45 | 1.38 |
| 37 | 17 | 309 | CLA | OBD-CAD | 3.76 | 1.29 | 1.22 |
| 37 | 38 | 203 | CLA | OBD-CAD | 3.76 | 1.29 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 15 | 316 | A86 | C9-C10 | 3.76 | 1.54 | 1.43 |
| 37 | b | 507 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 37 | 35 | 307 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 48 | 32 | 214 | A86 | C9-C10 | 3.76 | 1.54 | 1.43 |
| 37 | c | 511 | CLA | CHD-C1D | 3.76 | 1.45 | 1.38 |
| 48 | 11 | 312 | A86 | C19-C18 | 3.76 | 1.57 | 1.52 |
| 48 | 21 | 214 | A86 | C9-C10 | 3.76 | 1.54 | 1.43 |
| 37 | 17 | 304 | CLA | C3D-C2D | 3.76 | 1.49 | 1.39 |
| 37 | 19 | 301 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 37 | 19 | 307 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 48 | 15 | 315 | A86 | C10-C11 | 3.76 | 1.44 | 1.34 |
| 37 | B | 515 | CLA | C4B-NB | -3.76 | 1.32 | 1.37 |
| 37 | 38 | 204 | CLA | C1B-NB | -3.76 | 1.32 | 1.37 |
| 37 | a | 403 | CLA | O2A-CGA | 3.76 | 1.44 | 1.33 |
| 48 | 33 | 313 | A86 | C19-C18 | 3.76 | 1.57 | 1.52 |
| 37 | 33 | 303 | CLA | C4B-NB | -3.76 | 1.32 | 1.37 |
| 37 | c | 502 | CLA | C4B-NB | -3.76 | 1.32 | 1.37 |
| 37 | 18 | 208 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 37 | 39 | 307 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 37 | 34 | 301 | CLA | CHC-C4B | 3.76 | 1.47 | 1.39 |
| 48 | 32 | 217 | A86 | C10-C11 | 3.76 | 1.44 | 1.34 |
| 37 | W | 101 | CLA | C4B-NB | -3.75 | 1.32 | 1.37 |
| 37 | 40 | 209 | CLA | OBD-CAD | 3.75 | 1.28 | 1.22 |
| 37 | B | 507 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 37 | 41 | 202 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 37 | 21 | 202 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 37 | c | 508 | CLA | C4B-NB | -3.75 | 1.32 | 1.37 |
| 37 | B | 508 | CLA | C1D-ND | 3.75 | 1.42 | 1.37 |
| 37 | b | 515 | CLA | C4B-NB | -3.75 | 1.32 | 1.37 |
| 48 | 21 | 215 | A86 | C9-C10 | 3.75 | 1.54 | 1.43 |
| 37 | 19 | 305 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 37 | c | 508 | CLA | C1D-ND | 3.75 | 1.42 | 1.37 |
| 37 | 12 | 207 | CLA | C1B-NB | -3.75 | 1.32 | 1.37 |
| 37 | 32 | 208 | CLA | C1B-NB | -3.75 | 1.32 | 1.37 |
| 37 | 13 | 310 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 48 | 35 | 314 | A86 | C19-C18 | 3.75 | 1.57 | 1.52 |
| 47 | 13 | 304 | KC1 | C1B-NB | -3.75 | 1.32 | 1.37 |
| 37 | 18 | 206 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 37 | 37 | 303 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 37 | 11 | 305 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 47 | 33 | 302 | KC1 | C4B-NB | -3.75 | 1.32 | 1.37 |
| 39 | y | 101 | BCR | C1-C6 | -3.75 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 14 | 303 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 37 | 34 | 303 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 37 | b | 514 | CLA | CHD-C1D | 3.74 | 1.45 | 1.38 |
| 37 | 19 | 302 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 48 | 18 | 214 | A86 | C19-C18 | 3.74 | 1.57 | 1.52 |
| 37 | 16 | 307 | CLA | CHD-C4C | 3.74 | 1.47 | 1.39 |
| 37 | 39 | 306 | CLA | CHC-C4B | 3.74 | 1.47 | 1.39 |
| 37 | b | 503 | CLA | CHD-C1D | 3.74 | 1.45 | 1.38 |
| 37 | b | 511 | CLA | CHD-C1D | 3.74 | 1.45 | 1.38 |
| 37 | 36 | 307 | CLA | CHD-C4C | 3.74 | 1.47 | 1.39 |
| 37 | C | 502 | CLA | C4B-NB | -3.74 | 1.32 | 1.37 |
| 47 | 19 | 308 | KC1 | C1B-NB | -3.74 | 1.32 | 1.37 |
| 37 | B | 503 | CLA | CHD-C1D | 3.74 | 1.45 | 1.38 |
| 47 | 20 | 304 | KC1 | C1B-NB | -3.74 | 1.32 | 1.37 |
| 47 | 33 | 304 | KC1 | C1B-NB | -3.74 | 1.32 | 1.37 |
| 37 | 36 | 303 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 37 | 15 | 310 | CLA | OBD-CAD | 3.74 | 1.28 | 1.22 |
| 48 | 13 | 313 | A86 | C19-C18 | 3.74 | 1.57 | 1.52 |
| 37 | b | 503 | CLA | C1D-ND | 3.74 | 1.42 | 1.37 |
| 48 | 12 | 213 | A86 | C9-C10 | 3.74 | 1.54 | 1.43 |
| 37 | 16 | 303 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 37 | 32 | 204 | CLA | C1B-NB | -3.74 | 1.33 | 1.37 |
| 48 | 14 | 312 | A86 | C10-C11 | 3.74 | 1.44 | 1.34 |
| 48 | 41 | 215 | A86 | C9-C10 | 3.74 | 1.54 | 1.43 |
| 37 | B | 507 | CLA | C4B-NB | -3.73 | 1.33 | 1.37 |
| 37 | 39 | 305 | CLA | CHD-C4C | 3.73 | 1.47 | 1.39 |
| 48 | 34 | 311 | A86 | C9-C10 | 3.73 | 1.54 | 1.43 |
| 37 | C | 508 | CLA | C4B-NB | -3.73 | 1.33 | 1.37 |
| 37 | 31 | 306 | CLA | CHD-C4C | 3.73 | 1.47 | 1.39 |
| 37 | C | 505 | CLA | C1D-ND | 3.73 | 1.42 | 1.37 |
| 37 | 35 | 303 | CLA | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 48 | 39 | 313 | A86 | C21-C20 | 3.73 | 1.57 | 1.51 |
| 48 | 34 | 312 | A86 | C10-C11 | 3.73 | 1.44 | 1.34 |
| 37 | 14 | 302 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 37 | 34 | 302 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 37 | 39 | 307 | CLA | C1B-NB | -3.73 | 1.33 | 1.37 |
| 37 | 15 | 303 | CLA | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 37 | 21 | 208 | CLA | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 48 | 14 | 311 | A86 | C9-C10 | 3.73 | 1.54 | 1.43 |
| 37 | C | 508 | CLA | C1D-ND | 3.73 | 1.42 | 1.37 |
| 37 | 16 | 301 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 37 | 39 | 301 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 41 | 208 | CLA | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 47 | 35 | 302 | KC1 | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 39 | K | 101 | BCR | C1-C6 | -3.73 | 1.49 | 1.53 |
| 37 | 39 | 310 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 37 | 15 | 301 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 37 | 35 | 301 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 37 | d | 404 | CLA | CHD-C4C | 3.73 | 1.47 | 1.39 |
| 37 | 41 | 208 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 37 | b | 510 | CLA | C1D-ND | 3.73 | 1.42 | 1.37 |
| 47 | 34 | 304 | KC1 | C1B-NB | -3.73 | 1.33 | 1.37 |
| 48 | 38 | 215 | A86 | C17-C18 | -3.73 | 1.47 | 1.52 |
| 37 | 20 | 303 | CLA | CHD-C1D | 3.73 | 1.45 | 1.38 |
| 37 | c | 501 | CLA | CHD-C4C | 3.73 | 1.47 | 1.39 |
| 37 | 18 | 203 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 37 | 35 | 301 | CLA | OBD-CAD | 3.72 | 1.28 | 1.22 |
| 50 | 21 | 216 | DD6 | C35-C34 | 3.72 | 1.58 | 1.52 |
| 37 | B | 504 | CLA | CHC-C1C | 3.72 | 1.45 | 1.38 |
| 37 | 15 | 310 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 48 | 37 | 319 | A86 | C9-C10 | 3.72 | 1.54 | 1.43 |
| 47 | 13 | 302 | KC1 | C1B-NB | -3.72 | 1.33 | 1.37 |
| 47 | 33 | 302 | KC1 | C1B-NB | -3.72 | 1.33 | 1.37 |
| 37 | b | 516 | CLA | CHD-C1D | 3.72 | 1.45 | 1.38 |
| 37 | 38 | 206 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 37 | 19 | 301 | CLA | C1B-NB | -3.72 | 1.33 | 1.37 |
| 37 | 14 | 310 | CLA | OBD-CAD | 3.72 | 1.28 | 1.22 |
| 37 | 21 | 209 | CLA | OBD-CAD | 3.72 | 1.28 | 1.22 |
| 37 | 34 | 310 | CLA | OBD-CAD | 3.72 | 1.28 | 1.22 |
| 50 | 41 | 212 | DD6 | C35-C34 | 3.72 | 1.58 | 1.52 |
| 37 | 35 | 310 | CLA | OBD-CAD | 3.72 | 1.28 | 1.22 |
| 37 | D | 406 | CLA | CHD-C4C | 3.72 | 1.47 | 1.39 |
| 37 | b | 515 | CLA | CHD-C4C | 3.72 | 1.47 | 1.39 |
| 37 | B | 505 | CLA | O2A-CGA | 3.72 | 1.44 | 1.33 |
| 37 | 39 | 301 | CLA | C1B-NB | -3.72 | 1.33 | 1.37 |
| 37 | 18 | 203 | CLA | OBD-CAD | 3.72 | 1.28 | 1.22 |
| 37 | w | 101 | CLA | C4B-NB | -3.72 | 1.33 | 1.37 |
| 37 | 11 | 301 | CLA | C1B-NB | -3.72 | 1.33 | 1.37 |
| 37 | 31 | 302 | CLA | C1B-NB | -3.72 | 1.33 | 1.37 |
| 48 | 31 | 315 | A86 | C10-C11 | 3.72 | 1.44 | 1.34 |
| 37 | B | 516 | CLA | CHD-C1D | 3.72 | 1.45 | 1.38 |
| 37 | C | 501 | CLA | CHD-C4C | 3.72 | 1.47 | 1.39 |
| 37 | 15 | 301 | CLA | CHC-C4B | 3.72 | 1.47 | 1.39 |
| 37 | 33 | 301 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | c | 510 | CLA | CHD-C4C | 3.72 | 1.47 | 1.39 |
| 47 | 36 | 305 | KC1 | CHC-C1C | 3.72 | 1.47 | 1.39 |
| 47 | 13 | 302 | KC1 | CHB-C1B | 3.72 | 1.45 | 1.38 |
| 37 | a | 403 | CLA | CHD-C4C | 3.72 | 1.47 | 1.39 |
| 37 | 36 | 303 | CLA | C1B-NB | -3.71 | 1.33 | 1.37 |
| 47 | 16 | 305 | KC1 | CHC-C1C | 3.71 | 1.47 | 1.39 |
| 47 | 38 | 207 | KC1 | OBD-CAD | 3.71 | 1.28 | 1.22 |
| 37 | B | 505 | CLA | CHD-C4C | 3.71 | 1.47 | 1.39 |
| 37 | 38 | 208 | CLA | CHD-C4C | 3.71 | 1.47 | 1.39 |
| 37 | 38 | 208 | CLA | C1B-NB | -3.71 | 1.33 | 1.37 |
| 37 | B | 506 | CLA | O2A-CGA | 3.71 | 1.44 | 1.33 |
| 48 | 18 | 213 | A86 | C9-C10 | 3.71 | 1.54 | 1.43 |
| 37 | 35 | 307 | CLA | CHC-C4B | 3.71 | 1.47 | 1.39 |
| 47 | 41 | 207 | KC1 | C1B-NB | -3.71 | 1.33 | 1.37 |
| 48 | 31 | 312 | A86 | C19-C18 | 3.71 | 1.57 | 1.52 |
| 37 | 40 | 203 | CLA | CHC-C4B | 3.71 | 1.47 | 1.39 |
| 37 | 36 | 301 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 37 | 18 | 211 | CLA | OBD-CAD | 3.71 | 1.28 | 1.22 |
| 37 | z | 102 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 37 | 11 | 305 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 37 | 31 | 308 | CLA | CHD-C1D | 3.71 | 1.45 | 1.38 |
| 48 | 11 | 315 | A86 | C10-C11 | 3.71 | 1.44 | 1.34 |
| 37 | b | 505 | CLA | CHD-C4C | 3.71 | 1.47 | 1.39 |
| 37 | 34 | 307 | CLA | CHD-C4C | 3.71 | 1.47 | 1.39 |
| 37 | 19 | 306 | CLA | CHC-C4B | 3.71 | 1.47 | 1.39 |
| 37 | 13 | 301 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 50 | 41 | 216 | DD6 | C35-C34 | 3.70 | 1.58 | 1.52 |
| 37 | 11 | 307 | CLA | CHD-C1D | 3.70 | 1.45 | 1.38 |
| 37 | 13 | 307 | CLA | C4B-NB | -3.70 | 1.33 | 1.37 |
| 37 | 18 | 208 | CLA | C1B-NB | -3.70 | 1.33 | 1.37 |
| 37 | 37 | 306 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 47 | 18 | 210 | KC1 | CHC-C1C | 3.70 | 1.47 | 1.39 |
| 37 | c | 508 | CLA | CHD-C1D | 3.70 | 1.45 | 1.38 |
| 37 | b | 505 | CLA | O2A-CGA | 3.70 | 1.44 | 1.33 |
| 37 | 20 | 301 | CLA | CHC-C4B | 3.70 | 1.47 | 1.39 |
| 37 | 40 | 205 | CLA | CHD-C1D | 3.70 | 1.45 | 1.38 |
| 47 | 14 | 304 | KC1 | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 47 | 34 | 304 | KC1 | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 37 | 11 | 308 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 37 | 32 | 202 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 37 | 18 | 204 | CLA | C1B-NB | -3.70 | 1.33 | 1.37 |
| 37 | 34 | 302 | CLA | C1B-NB | -3.70 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 34 | 308 | CLA | C1B-NB | -3.70 | 1.33 | 1.37 |
| 37 | 40 | 210 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 48 | 36 | 311 | A86 | C9-C10 | 3.70 | 1.54 | 1.43 |
| 47 | 39 | 308 | KC1 | C1B-NB | -3.70 | 1.33 | 1.37 |
| 37 | 36 | 306 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 37 | C | 512 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 37 | 12 | 205 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 37 | 15 | 307 | CLA | CHC-C4B | 3.70 | 1.47 | 1.39 |
| 37 | 11 | 301 | CLA | CHD-C1D | 3.70 | 1.45 | 1.38 |
| 37 | 31 | 302 | CLA | CHD-C1D | 3.70 | 1.45 | 1.38 |
| 37 | B | 503 | CLA | C1D-ND | 3.70 | 1.42 | 1.37 |
| 37 | 12 | 203 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 48 | 35 | 315 | A86 | C19-C18 | 3.70 | 1.57 | 1.52 |
| 37 | 19 | 310 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 37 | 18 | 202 | CLA | CHC-C4B | 3.70 | 1.47 | 1.39 |
| 37 | 32 | 206 | CLA | C4B-NB | -3.70 | 1.33 | 1.37 |
| 37 | b | 506 | CLA | O2A-CGA | 3.70 | 1.44 | 1.33 |
| 37 | b | 504 | CLA | CHC-C1C | 3.70 | 1.45 | 1.38 |
| 37 | 41 | 209 | CLA | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 37 | C | 510 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 37 | 16 | 303 | CLA | C1B-NB | -3.70 | 1.33 | 1.37 |
| 37 | Z | 101 | CLA | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 37 | 18 | 206 | CLA | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 37 | 18 | 209 | CLA | CHD-C4C | 3.69 | 1.47 | 1.39 |
| 37 | B | 509 | CLA | CHD-C1D | 3.69 | 1.45 | 1.38 |
| 48 | 36 | 313 | A86 | C10-C11 | 3.69 | 1.44 | 1.34 |
| 37 | 15 | 301 | CLA | OBD-CAD | 3.69 | 1.28 | 1.22 |
| 37 | b | 510 | CLA | CHD-C1D | 3.69 | 1.45 | 1.38 |
| 37 | B | 510 | CLA | C1D-ND | 3.69 | 1.42 | 1.37 |
| 47 | 40 | 206 | KC1 | C1B-NB | -3.69 | 1.33 | 1.37 |
| 47 | 15 | 306 | KC1 | CHC-C1C | 3.69 | 1.47 | 1.39 |
| 37 | 20 | 301 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 37 | 41 | 210 | CLA | OBD-CAD | 3.69 | 1.28 | 1.22 |
| 47 | 13 | 302 | KC1 | C4B-NB | -3.69 | 1.33 | 1.37 |
| 37 | 14 | 307 | CLA | CHD-C4C | 3.69 | 1.47 | 1.39 |
| 37 | 13 | 301 | CLA | C1B-NB | -3.69 | 1.33 | 1.37 |
| 37 | 14 | 303 | CLA | C1B-NB | -3.69 | 1.33 | 1.37 |
| 37 | 33 | 301 | CLA | C1B-NB | -3.69 | 1.33 | 1.37 |
| 37 | 34 | 303 | CLA | C1B-NB | -3.69 | 1.33 | 1.37 |
| 37 | B | 510 | CLA | CHD-C1D | 3.69 | 1.45 | 1.38 |
| 48 | 14 | 312 | A86 | C9-C10 | 3.69 | 1.54 | 1.43 |
| 37 | 13 | 305 | CLA | OBD-CAD | 3.69 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 33 | 305 | CLA | OBD-CAD | 3.69 | 1.28 | 1.22 |
| 47 | 36 | 305 | KC1 | C1B-NB | -3.69 | 1.33 | 1.37 |
| 37 | Z | 102 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 37 | 38 | 211 | CLA | OBD-CAD | 3.68 | 1.28 | 1.22 |
| 47 | 31 | 309 | KC1 | C4B-NB | -3.68 | 1.33 | 1.37 |
| 37 | 31 | 306 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 47 | 14 | 304 | KC1 | CHC-C1C | 3.68 | 1.47 | 1.39 |
| 37 | 38 | 201 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 37 | B | 515 | CLA | CHD-C4C | 3.68 | 1.47 | 1.39 |
| 37 | 12 | 209 | CLA | CHD-C4C | 3.68 | 1.47 | 1.39 |
| 37 | 14 | 305 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 37 | 34 | 305 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 37 | A | 403 | CLA | CHD-C4C | 3.68 | 1.47 | 1.39 |
| 47 | 14 | 304 | KC1 | C1B-NB | -3.68 | 1.33 | 1.37 |
| 37 | 40 | 203 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 48 | 19 | 313 | A86 | C21-C20 | 3.68 | 1.57 | 1.51 |
| 48 | 16 | 311 | A86 | C9-C10 | 3.68 | 1.54 | 1.43 |
| 37 | 33 | 307 | CLA | C4B-NB | -3.68 | 1.33 | 1.37 |
| 47 | 37 | 304 | KC1 | C1B-NB | -3.68 | 1.33 | 1.37 |
| 37 | z | 101 | CLA | OBD-CAD | 3.68 | 1.28 | 1.22 |
| 37 | 19 | 307 | CLA | CHC-C4B | 3.68 | 1.47 | 1.39 |
| 37 | 36 | 309 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 37 | C | 512 | CLA | CHD-C1D | 3.68 | 1.45 | 1.38 |
| 37 | 12 | 204 | CLA | CHD-C1D | 3.68 | 1.45 | 1.38 |
| 48 | 12 | 216 | A86 | C19-C18 | 3.68 | 1.57 | 1.52 |
| 37 | 21 | 208 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 37 | B | 514 | CLA | C4B-NB | -3.68 | 1.33 | 1.37 |
| 37 | b | 507 | CLA | C4B-NB | -3.68 | 1.33 | 1.37 |
| 37 | c | 512 | CLA | CHD-C1D | 3.68 | 1.45 | 1.38 |
| 47 | 21 | 207 | KC1 | C1B-NB | -3.68 | 1.33 | 1.37 |
| 37 | 17 | 307 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 37 | 32 | 204 | CLA | CHD-C4C | 3.68 | 1.47 | 1.39 |
| 37 | 41 | 204 | CLA | C1B-NB | -3.67 | 1.33 | 1.37 |
| 37 | 16 | 306 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 37 | 20 | 308 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 48 | 17 | 311 | A86 | C9-C10 | 3.67 | 1.54 | 1.43 |
| 37 | 16 | 309 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 48 | 34 | 312 | A86 | C9-C10 | 3.67 | 1.54 | 1.43 |
| 37 | 32 | 213 | CLA | OBD-CAD | 3.67 | 1.28 | 1.22 |
| 37 | C | 508 | CLA | CHD-C1D | 3.67 | 1.45 | 1.38 |
| 37 | c | 505 | CLA | C1D-ND | 3.67 | 1.42 | 1.37 |
| 48 | 16 | 314 | A86 | C10-C11 | 3.67 | 1.44 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | Z | 101 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 47 | 33 | 302 | KC1 | CHB-C1B | 3.67 | 1.45 | 1.38 |
| 37 | 18 | 201 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 37 | 32 | 213 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 37 | 18 | 208 | CLA | OBD-CAD | 3.67 | 1.28 | 1.22 |
| 37 | b | 509 | CLA | CHD-C1D | 3.67 | 1.45 | 1.38 |
| 37 | 19 | 301 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 37 | 19 | 305 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 37 | 38 | 201 | CLA | C1B-NB | -3.67 | 1.33 | 1.37 |
| 37 | 21 | 205 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 47 | 38 | 210 | KC1 | CHC-C1C | 3.67 | 1.47 | 1.39 |
| 37 | 38 | 209 | CLA | CHD-C4C | 3.67 | 1.47 | 1.39 |
| 39 | B | 517 | BCR | C1-C6 | -3.67 | 1.49 | 1.53 |
| 39 | b | 517 | BCR | C1-C6 | -3.67 | 1.49 | 1.53 |
| 37 | B | 502 | CLA | C4B-NB | -3.66 | 1.33 | 1.37 |
| 37 | 33 | 310 | CLA | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 37 | 19 | 306 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 37 | 35 | 310 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 37 | 17 | 302 | CLA | C1B-NB | -3.66 | 1.33 | 1.37 |
| 47 | 15 | 302 | KC1 | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 37 | A | 405 | CLA | CHD-C4C | 3.66 | 1.47 | 1.39 |
| 37 | 32 | 210 | CLA | CHD-C4C | 3.66 | 1.47 | 1.39 |
| 37 | 14 | 302 | CLA | C1B-NB | -3.66 | 1.33 | 1.37 |
| 50 | 21 | 212 | DD6 | C35-C34 | 3.66 | 1.58 | 1.52 |
| 47 | 34 | 304 | KC1 | CHC-C1C | 3.66 | 1.47 | 1.39 |
| 37 | c | 509 | CLA | CHD-C4C | 3.66 | 1.47 | 1.39 |
| 47 | 18 | 207 | KC1 | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 37 | 20 | 307 | CLA | CHC-C4B | 3.66 | 1.47 | 1.39 |
| 37 | 33 | 305 | CLA | CHC-C4B | 3.66 | 1.47 | 1.39 |
| 48 | 36 | 310 | A86 | C9-C10 | 3.66 | 1.54 | 1.43 |
| 37 | z | 101 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 37 | 19 | 304 | CLA | CHD-C1D | 3.66 | 1.45 | 1.38 |
| 48 | 11 | 319 | A86 | C10-C11 | 3.66 | 1.44 | 1.34 |
| 47 | 40 | 204 | KC1 | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 37 | 19 | 301 | CLA | CHC-C4B | 3.66 | 1.47 | 1.39 |
| 48 | 32 | 217 | A86 | C19-C18 | 3.66 | 1.57 | 1.52 |
| 37 | 39 | 304 | CLA | CHD-C1D | 3.66 | 1.45 | 1.38 |
| 37 | 32 | 206 | CLA | CHD-C4C | 3.66 | 1.47 | 1.39 |
| 37 | 41 | 205 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 37 | 15 | 305 | CLA | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 37 | c | 513 | CLA | CHD-C4C | 3.66 | 1.47 | 1.39 |
| 47 | 36 | 304 | KC1 | CHC-C1C | 3.66 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 19 | 310 | CLA | C1B-NB | -3.66 | 1.33 | 1.37 |
| 47 | 18 | 210 | KC1 | C1B-NB | -3.66 | 1.33 | 1.37 |
| 37 | 39 | 306 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 47 | 16 | 304 | KC1 | CHC-C1C | 3.66 | 1.47 | 1.39 |
| 37 | 20 | 306 | CLA | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 37 | 36 | 301 | CLA | CHC-C4B | 3.66 | 1.47 | 1.39 |
| 37 | 14 | 303 | CLA | C4B-NB | -3.65 | 1.33 | 1.37 |
| 37 | 34 | 303 | CLA | C4B-NB | -3.65 | 1.33 | 1.37 |
| 48 | 15 | 315 | A86 | C19-C18 | 3.65 | 1.57 | 1.52 |
| 37 | c | 512 | CLA | CHD-C4C | 3.65 | 1.47 | 1.39 |
| 37 | 35 | 305 | CLA | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 37 | 14 | 305 | CLA | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 37 | 34 | 305 | CLA | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 37 | 39 | 307 | CLA | C3D-C2D | 3.65 | 1.49 | 1.39 |
| 37 | C | 506 | CLA | CHD-C4C | 3.65 | 1.47 | 1.39 |
| 48 | 31 | 313 | A86 | C9-C10 | 3.65 | 1.54 | 1.43 |
| 37 | a | 407 | CLA | CHD-C4C | 3.65 | 1.47 | 1.39 |
| 37 | 12 | 212 | CLA | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 37 | 12 | 212 | CLA | C3D-C2D | 3.65 | 1.49 | 1.39 |
| 37 | 13 | 305 | CLA | C3D-C2D | 3.65 | 1.48 | 1.39 |
| 37 | 33 | 305 | CLA | C3D-C2D | 3.65 | 1.48 | 1.39 |
| 37 | 13 | 305 | CLA | CHC-C4B | 3.65 | 1.47 | 1.39 |
| 37 | z | 101 | CLA | C1B-NB | -3.65 | 1.33 | 1.37 |
| 37 | 36 | 307 | CLA | C3D-C2D | 3.65 | 1.48 | 1.39 |
| 37 | 38 | 209 | CLA | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 37 | 16 | 309 | CLA | C1B-NB | -3.65 | 1.33 | 1.37 |
| 37 | 21 | 209 | CLA | CHC-C4B | 3.65 | 1.47 | 1.39 |
| 37 | 19 | 307 | CLA | C3D-C2D | 3.65 | 1.48 | 1.39 |
| 47 | 41 | 203 | KC1 | CHC-C1C | 3.65 | 1.47 | 1.39 |
| 37 | 40 | 205 | CLA | CHD-C4C | 3.64 | 1.47 | 1.39 |
| 37 | 11 | 301 | CLA | CHC-C4B | 3.64 | 1.47 | 1.39 |
| 37 | 31 | 302 | CLA | CHC-C4B | 3.64 | 1.47 | 1.39 |
| 37 | 36 | 309 | CLA | CHC-C4B | 3.64 | 1.47 | 1.39 |
| 37 | 38 | 208 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 47 | 16 | 305 | KC1 | C1B-NB | -3.64 | 1.33 | 1.37 |
| 37 | 12 | 209 | CLA | C3D-C2D | 3.64 | 1.48 | 1.39 |
| 48 | 18 | 213 | A86 | C7-C6 | 3.64 | 1.58 | 1.50 |
| 37 | 14 | 308 | CLA | C1B-NB | -3.64 | 1.33 | 1.37 |
| 37 | 39 | 305 | CLA | C3D-C2D | 3.64 | 1.48 | 1.39 |
| 37 | 14 | 310 | CLA | C1B-NB | -3.64 | 1.33 | 1.37 |
| 47 | 16 | 304 | KC1 | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 37 | 13 | 307 | CLA | CHD-C4C | 3.64 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 33 | 307 | CLA | CHD-C4C | 3.64 | 1.47 | 1.39 |
| 37 | B | 510 | CLA | C4B-NB | -3.64 | 1.33 | 1.37 |
| 37 | 21 | 210 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 37 | c | 506 | CLA | CHD-C4C | 3.64 | 1.47 | 1.39 |
| 37 | 40 | 208 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 37 | 36 | 309 | CLA | C1B-NB | -3.64 | 1.33 | 1.37 |
| 48 | 35 | 314 | A86 | C21-C20 | 3.64 | 1.57 | 1.51 |
| 50 | 20 | 312 | DD6 | C-C1 | 3.64 | 1.58 | 1.50 |
| 47 | 37 | 302 | KC1 | OBD-CAD | 3.63 | 1.28 | 1.22 |
| 47 | 31 | 309 | KC1 | CHB-C1B | 3.63 | 1.45 | 1.38 |
| 37 | 40 | 209 | CLA | CHC-C4B | 3.63 | 1.47 | 1.39 |
| 37 | c | 507 | CLA | C1D-ND | 3.63 | 1.42 | 1.37 |
| 48 | 16 | 310 | A86 | C9-C10 | 3.63 | 1.54 | 1.43 |
| 48 | 21 | 213 | A86 | C19-C18 | 3.63 | 1.57 | 1.52 |
| 47 | 37 | 304 | KC1 | CHC-C1C | 3.63 | 1.47 | 1.39 |
| 47 | 11 | 309 | KC1 | CHB-C1B | 3.63 | 1.45 | 1.38 |
| 37 | C | 506 | CLA | CHC-C1C | 3.63 | 1.45 | 1.38 |
| 37 | 18 | 209 | CLA | OBD-CAD | 3.63 | 1.28 | 1.22 |
| 47 | 20 | 302 | KC1 | OBD-CAD | 3.63 | 1.28 | 1.22 |
| 37 | C | 512 | CLA | C3D-C2D | 3.63 | 1.48 | 1.39 |
| 37 | 39 | 304 | CLA | C1B-NB | -3.63 | 1.33 | 1.37 |
| 48 | 11 | 314 | A86 | C9-C10 | 3.63 | 1.54 | 1.43 |
| 48 | 31 | 314 | A86 | C9-C10 | 3.63 | 1.54 | 1.43 |
| 37 | Z | 101 | CLA | C1B-NB | -3.63 | 1.33 | 1.37 |
| 48 | 11 | 313 | A86 | C9-C10 | 3.63 | 1.54 | 1.43 |
| 48 | 17 | 320 | A86 | C9-C10 | 3.63 | 1.54 | 1.43 |
| 47 | 14 | 309 | KC1 | CHC-C1C | 3.63 | 1.47 | 1.39 |
| 37 | b | 502 | CLA | C4B-NB | -3.63 | 1.33 | 1.37 |
| 48 | 31 | 319 | A86 | C10-C11 | 3.63 | 1.44 | 1.34 |
| 48 | 11 | 314 | A86 | C19-C18 | 3.63 | 1.57 | 1.52 |
| 48 | 31 | 314 | A86 | C19-C18 | 3.63 | 1.57 | 1.52 |
| 37 | W | 102 | CLA | C3D-C2D | 3.63 | 1.48 | 1.39 |
| 37 | 19 | 301 | CLA | OBD-CAD | 3.63 | 1.28 | 1.22 |
| 47 | 16 | 304 | KC1 | C1B-NB | -3.63 | 1.33 | 1.37 |
| 37 | C | 513 | CLA | CHD-C4C | 3.63 | 1.47 | 1.39 |
| 37 | c | 506 | CLA | CHC-C1C | 3.63 | 1.45 | 1.38 |
| 37 | C | 507 | CLA | C1D-ND | 3.63 | 1.42 | 1.37 |
| 37 | 12 | 205 | CLA | C4B-NB | -3.63 | 1.33 | 1.37 |
| 47 | 34 | 309 | KC1 | CHC-C1C | 3.62 | 1.47 | 1.39 |
| 47 | 15 | 304 | KC1 | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 47 | 36 | 304 | KC1 | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 37 | 39 | 301 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 18 | 205 | KC1 | CHC-C1C | 3.62 | 1.47 | 1.39 |
| 37 | 16 | 309 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |
| 37 | 39 | 307 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |
| 47 | 37 | 307 | KC1 | CHC-C1C | 3.62 | 1.47 | 1.39 |
| 37 | C | 509 | CLA | CHD-C4C | 3.62 | 1.47 | 1.39 |
| 37 | 17 | 302 | CLA | C3D-C2D | 3.62 | 1.48 | 1.39 |
| 37 | 31 | 304 | CLA | C3D-C2D | 3.62 | 1.48 | 1.39 |
| 48 | 32 | 221 | A86 | C10-C11 | 3.62 | 1.44 | 1.34 |
| 37 | 39 | 304 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |
| 47 | 14 | 309 | KC1 | CHB-C1B | 3.62 | 1.45 | 1.38 |
| 37 | 12 | 205 | CLA | C3D-C2D | 3.62 | 1.48 | 1.39 |
| 37 | 12 | 210 | CLA | C3D-C2D | 3.62 | 1.48 | 1.39 |
| 37 | 12 | 209 | CLA | C4B-NB | -3.62 | 1.33 | 1.37 |
| 48 | 13 | 313 | A86 | C17-C18 | -3.62 | 1.47 | 1.52 |
| 37 | 38 | 209 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |
| 47 | 35 | 306 | KC1 | CHC-C1C | 3.62 | 1.47 | 1.39 |
| 37 | 31 | 301 | CLA | C3D-C2D | 3.62 | 1.48 | 1.39 |
| 37 | 32 | 206 | CLA | C3D-C2D | 3.62 | 1.48 | 1.39 |
| 48 | 18 | 212 | A86 | C19-C18 | 3.62 | 1.57 | 1.52 |
| 37 | 13 | 310 | CLA | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 37 | 41 | 209 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |
| 37 | C | 502 | CLA | C3D-C2D | 3.62 | 1.48 | 1.39 |
| 48 | 37 | 310 | A86 | C9-C10 | 3.62 | 1.54 | 1.43 |
| 37 | 13 | 310 | CLA | C1B-NB | -3.62 | 1.33 | 1.37 |
| 37 | 39 | 310 | CLA | C1B-NB | -3.62 | 1.33 | 1.37 |
| 37 | 16 | 301 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |
| 37 | 41 | 206 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |
| 47 | 18 | 205 | KC1 | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 37 | 38 | 202 | CLA | C3D-C2D | 3.62 | 1.48 | 1.39 |
| 37 | 21 | 206 | CLA | CHC-C4B | 3.62 | 1.47 | 1.39 |
| 37 | 38 | 206 | CLA | C1B-NB | -3.62 | 1.33 | 1.37 |
| 37 | 18 | 204 | CLA | CHC-C4B | 3.61 | 1.47 | 1.39 |
| 37 | c | 507 | CLA | CHD-C1D | 3.61 | 1.45 | 1.38 |
| 37 | 32 | 205 | CLA | CHD-C1D | 3.61 | 1.45 | 1.38 |
| 37 | 14 | 301 | CLA | CHD-C4C | 3.61 | 1.47 | 1.39 |
| 37 | 31 | 301 | CLA | CHC-C4B | 3.61 | 1.47 | 1.39 |
| 37 | c | 505 | CLA | CHD-C1D | 3.61 | 1.45 | 1.38 |
| 47 | 40 | 206 | KC1 | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 37 | 38 | 201 | CLA | CHC-C4B | 3.61 | 1.47 | 1.39 |
| 37 | 21 | 204 | CLA | C1B-NB | -3.61 | 1.33 | 1.37 |
| 47 | 18 | 207 | KC1 | C1B-NB | -3.61 | 1.33 | 1.37 |
| 37 | 41 | 206 | CLA | C3D-C2D | 3.61 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 19 | 303 | CLA | C3D-C2D | 3.61 | 1.48 | 1.39 |
| 37 | 39 | 303 | CLA | C3D-C2D | 3.61 | 1.48 | 1.39 |
| 48 | 12 | 220 | A86 | C10-C11 | 3.61 | 1.44 | 1.34 |
| 37 | 38 | 206 | CLA | CHC-C4B | 3.61 | 1.47 | 1.39 |
| 48 | 16 | 314 | A86 | C9-C10 | 3.61 | 1.54 | 1.43 |
| 48 | 11 | 314 | A86 | C10-C11 | 3.61 | 1.44 | 1.34 |
| 50 | 40 | 214 | DD6 | C-C1 | 3.61 | 1.58 | 1.50 |
| 37 | 32 | 210 | CLA | C3D-C2D | 3.61 | 1.48 | 1.39 |
| 47 | 36 | 305 | KC1 | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 37 | 14 | 307 | CLA | C3D-C2D | 3.61 | 1.48 | 1.39 |
| 37 | 34 | 301 | CLA | CHD-C4C | 3.61 | 1.47 | 1.39 |
| 50 | 41 | 216 | DD6 | O2-C18 | 3.61 | 1.53 | 1.43 |
| 37 | 39 | 301 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 37 | B | 513 | CLA | CHD-C1D | 3.61 | 1.45 | 1.38 |
| 50 | 36 | 312 | DD6 | C35-C34 | 3.60 | 1.58 | 1.52 |
| 37 | 31 | 308 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 48 | 31 | 314 | A86 | C10-C11 | 3.60 | 1.44 | 1.34 |
| 37 | 20 | 303 | CLA | CHD-C4C | 3.60 | 1.47 | 1.39 |
| 47 | 35 | 309 | KC1 | CHC-C1C | 3.60 | 1.47 | 1.39 |
| 37 | 41 | 208 | CLA | CHC-C4B | 3.60 | 1.47 | 1.39 |
| 37 | c | 502 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 48 | 33 | 313 | A86 | C17-C18 | -3.60 | 1.47 | 1.52 |
| 37 | 39 | 307 | CLA | MG-ND | -3.60 | 1.98 | 2.05 |
| 37 | 14 | 301 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 37 | 34 | 301 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 37 | C | 506 | CLA | C4B-NB | -3.60 | 1.33 | 1.37 |
| 47 | 38 | 205 | KC1 | OBD-CAD | 3.60 | 1.28 | 1.22 |
| 37 | 32 | 211 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 47 | 35 | 304 | KC1 | CHC-C1C | 3.60 | 1.47 | 1.39 |
| 37 | c | 512 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 47 | 17 | 305 | KC1 | CHC-C1C | 3.60 | 1.47 | 1.39 |
| 37 | W | 102 | CLA | CHC-C4B | 3.60 | 1.47 | 1.39 |
| 47 | 16 | 305 | KC1 | OBD-CAD | 3.60 | 1.28 | 1.22 |
| 47 | 12 | 211 | KC1 | CHC-C1C | 3.60 | 1.47 | 1.39 |
| 37 | b | 501 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 37 | 38 | 202 | CLA | OBD-CAD | 3.60 | 1.28 | 1.22 |
| 47 | 21 | 203 | KC1 | CHC-C1C | 3.60 | 1.47 | 1.39 |
| 37 | 34 | 307 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 37 | B | 514 | CLA | C1D-ND | 3.60 | 1.42 | 1.37 |
| 37 | b | 506 | CLA | CHD-C1D | 3.60 | 1.45 | 1.38 |
| 37 | B | 508 | CLA | CHD-C4C | 3.60 | 1.47 | 1.39 |
| 37 | 11 | 303 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 37 | 301 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 37 | 11 | 307 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 37 | 16 | 307 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 47 | 17 | 308 | KC1 | CHC-C1C | 3.60 | 1.47 | 1.39 |
| 37 | C | 505 | CLA | CHD-C1D | 3.60 | 1.45 | 1.38 |
| 37 | 12 | 212 | CLA | CHC-C4B | 3.59 | 1.47 | 1.39 |
| 37 | 32 | 213 | CLA | CHC-C4B | 3.59 | 1.47 | 1.39 |
| 47 | 31 | 307 | KC1 | CHC-C1C | 3.59 | 1.47 | 1.39 |
| 37 | 21 | 206 | CLA | C3D-C2D | 3.59 | 1.48 | 1.39 |
| 37 | b | 510 | CLA | C4B-NB | -3.59 | 1.33 | 1.37 |
| 37 | b | 514 | CLA | C4B-NB | -3.59 | 1.33 | 1.37 |
| 37 | B | 506 | CLA | CHD-C1D | 3.59 | 1.45 | 1.38 |
| 37 | 35 | 307 | CLA | OBD-CAD | 3.59 | 1.28 | 1.22 |
| 37 | 19 | 304 | CLA | CHC-C4B | 3.59 | 1.47 | 1.39 |
| 37 | 19 | 304 | CLA | C1B-NB | -3.59 | 1.33 | 1.37 |
| 48 | 12 | 214 | A86 | C10-C11 | 3.59 | 1.44 | 1.34 |
| 47 | 13 | 304 | KC1 | CHC-C1C | 3.59 | 1.47 | 1.39 |
| 48 | 17 | 313 | A86 | C19-C18 | 3.59 | 1.57 | 1.52 |
| 48 | 37 | 312 | A86 | C19-C18 | 3.59 | 1.57 | 1.52 |
| 47 | 15 | 302 | KC1 | CHC-C1C | 3.59 | 1.47 | 1.39 |
| 37 | b | 508 | CLA | CHD-C4C | 3.59 | 1.47 | 1.39 |
| 37 | B | 501 | CLA | C3D-C2D | 3.59 | 1.48 | 1.39 |
| 37 | 32 | 210 | CLA | C4B-NB | -3.59 | 1.33 | 1.37 |
| 37 | 32 | 208 | CLA | C3D-C2D | 3.59 | 1.48 | 1.39 |
| 47 | 36 | 302 | KC1 | OBD-CAD | 3.59 | 1.28 | 1.22 |
| 48 | 31 | 312 | A86 | C10-C11 | 3.59 | 1.44 | 1.34 |
| 37 | 34 | 301 | CLA | OBD-CAD | 3.59 | 1.28 | 1.22 |
| 37 | 18 | 209 | CLA | CHC-C4B | 3.59 | 1.47 | 1.39 |
| 37 | c | 513 | CLA | C1B-NB | -3.59 | 1.33 | 1.37 |
| 37 | 17 | 302 | CLA | C4B-NB | -3.59 | 1.33 | 1.37 |
| 37 | 19 | 302 | CLA | C1B-NB | -3.58 | 1.33 | 1.37 |
| 37 | 39 | 302 | CLA | C1B-NB | -3.58 | 1.33 | 1.37 |
| 37 | 36 | 301 | CLA | CHD-C4C | 3.58 | 1.47 | 1.39 |
| 37 | 32 | 205 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 48 | 11 | 312 | A86 | C10-C11 | 3.58 | 1.44 | 1.34 |
| 37 | 17 | 309 | CLA | CHC-C4B | 3.58 | 1.47 | 1.39 |
| 47 | 34 | 309 | KC1 | CHB-C1B | 3.58 | 1.45 | 1.38 |
| 37 | 14 | 305 | CLA | CHC-C4B | 3.58 | 1.47 | 1.39 |
| 37 | 37 | 308 | CLA | CHC-C4B | 3.58 | 1.47 | 1.39 |
| 37 | 18 | 202 | CLA | C1B-NB | -3.58 | 1.33 | 1.37 |
| 47 | 11 | 309 | KC1 | C4B-NB | -3.58 | 1.33 | 1.37 |
| 47 | 15 | 302 | KC1 | C1B-NB | -3.58 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 50 | 21 | 216 | DD6 | O2-C18 | 3.58 | 1.53 | 1.43 |
| 47 | 38 | 205 | KC1 | CHC-C1C | 3.58 | 1.47 | 1.39 |
| 37 | 19 | 306 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 37 | 34 | 305 | CLA | CHC-C4B | 3.58 | 1.47 | 1.39 |
| 37 | 31 | 302 | CLA | CHD-C4C | 3.58 | 1.47 | 1.39 |
| 37 | 12 | 207 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 37 | b | 503 | CLA | C4B-NB | -3.58 | 1.33 | 1.37 |
| 37 | 33 | 310 | CLA | C1B-NB | -3.58 | 1.33 | 1.37 |
| 47 | 35 | 309 | KC1 | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 37 | b | 509 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 37 | 14 | 303 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 37 | c | 503 | CLA | C4B-NB | -3.58 | 1.33 | 1.37 |
| 37 | b | 514 | CLA | C1D-ND | 3.58 | 1.42 | 1.37 |
| 47 | 18 | 205 | KC1 | C1B-NB | -3.58 | 1.33 | 1.37 |
| 47 | 15 | 304 | KC1 | CHC-C1C | 3.58 | 1.47 | 1.39 |
| 37 | 19 | 306 | CLA | CHD-C1D | 3.58 | 1.45 | 1.38 |
| 37 | 34 | 310 | CLA | C1B-NB | -3.58 | 1.33 | 1.37 |
| 47 | 36 | 304 | KC1 | C1B-NB | -3.58 | 1.33 | 1.37 |
| 37 | 32 | 204 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 47 | 35 | 302 | KC1 | C1B-NB | -3.58 | 1.33 | 1.37 |
| 47 | 15 | 309 | KC1 | CHC-C1C | 3.58 | 1.47 | 1.39 |
| 37 | 18 | 201 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 37 | b | 523 | CLA | CHC-C4B | 3.58 | 1.47 | 1.39 |
| 37 | 38 | 206 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 37 | 34 | 302 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 37 | 11 | 301 | CLA | CHD-C4C | 3.57 | 1.47 | 1.39 |
| 48 | 11 | 319 | A86 | C9-C10 | 3.57 | 1.54 | 1.43 |
| 48 | 31 | 319 | A86 | C9-C10 | 3.57 | 1.54 | 1.43 |
| 37 | C | 507 | CLA | CHD-C1D | 3.57 | 1.45 | 1.38 |
| 37 | 12 | 204 | CLA | C3D-C2D | 3.57 | 1.48 | 1.39 |
| 47 | 33 | 304 | KC1 | CHC-C1C | 3.57 | 1.47 | 1.39 |
| 37 | c | 506 | CLA | C4B-NB | -3.57 | 1.33 | 1.37 |
| 50 | 16 | 312 | DD6 | C35-C34 | 3.57 | 1.58 | 1.52 |
| 48 | 41 | 213 | A86 | C19-C18 | 3.57 | 1.57 | 1.52 |
| 37 | D | 405 | CLA | CHD-C4C | 3.57 | 1.47 | 1.39 |
| 37 | b | 513 | CLA | CHD-C1D | 3.57 | 1.45 | 1.38 |
| 37 | 18 | 201 | CLA | CHC-C4B | 3.57 | 1.47 | 1.39 |
| 47 | 16 | 302 | KC1 | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 37 | B | 524 | CLA | CHC-C4B | 3.57 | 1.47 | 1.39 |
| 37 | B | 509 | CLA | C3D-C2D | 3.57 | 1.48 | 1.39 |
| 37 | 33 | 301 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 37 | 41 | 205 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 13 | 301 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 47 | 33 | 309 | KC1 | CHC-C1C | 3.57 | 1.47 | 1.39 |
| 37 | 18 | 209 | CLA | CHB-C1B | 3.57 | 1.47 | 1.39 |
| 47 | 12 | 206 | KC1 | CHC-C1C | 3.57 | 1.47 | 1.39 |
| 37 | 21 | 205 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 37 | C | 513 | CLA | C1B-NB | -3.57 | 1.33 | 1.37 |
| 37 | 36 | 309 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 47 | 17 | 303 | KC1 | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 37 | 17 | 304 | CLA | C4B-NB | -3.57 | 1.33 | 1.37 |
| 47 | 38 | 210 | KC1 | C1B-NB | -3.56 | 1.33 | 1.37 |
| 47 | 20 | 302 | KC1 | CHC-C1C | 3.56 | 1.47 | 1.39 |
| 37 | b | 511 | CLA | CHD-C4C | 3.56 | 1.47 | 1.39 |
| 37 | 38 | 204 | CLA | CHC-C4B | 3.56 | 1.47 | 1.39 |
| 48 | 17 | 314 | A86 | C19-C18 | 3.56 | 1.57 | 1.52 |
| 47 | 39 | 308 | KC1 | CHC-C1C | 3.56 | 1.47 | 1.39 |
| 37 | b | 508 | CLA | C3D-C2D | 3.56 | 1.48 | 1.39 |
| 37 | B | 508 | CLA | C3D-C2D | 3.56 | 1.48 | 1.39 |
| 37 | 20 | 306 | CLA | CHC-C4B | 3.56 | 1.47 | 1.39 |
| 48 | 32 | 215 | A86 | C10-C11 | 3.56 | 1.44 | 1.34 |
| 37 | 19 | 304 | CLA | C3D-C2D | 3.56 | 1.48 | 1.39 |
| 37 | 39 | 304 | CLA | C3D-C2D | 3.56 | 1.48 | 1.39 |
| 37 | 38 | 202 | CLA | C1B-NB | -3.56 | 1.33 | 1.37 |
| 48 | 38 | 212 | A86 | C19-C18 | 3.56 | 1.57 | 1.52 |
| 48 | 36 | 313 | A86 | C9-C10 | 3.56 | 1.54 | 1.43 |
| 37 | 21 | 204 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 37 | 19 | 309 | CLA | C3D-C2D | 3.56 | 1.48 | 1.39 |
| 48 | 11 | 315 | A86 | C9-C10 | 3.56 | 1.54 | 1.43 |
| 37 | 21 | 208 | CLA | CHC-C4B | 3.56 | 1.47 | 1.39 |
| 37 | 14 | 301 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 37 | B | 503 | CLA | CHD-C4C | 3.55 | 1.47 | 1.39 |
| 47 | 20 | 304 | KC1 | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 47 | 40 | 204 | KC1 | CHC-C1C | 3.55 | 1.47 | 1.39 |
| 37 | d | 403 | CLA | CHD-C4C | 3.55 | 1.47 | 1.39 |
| 37 | 17 | 302 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 37 | 39 | 306 | CLA | CHD-C1D | 3.55 | 1.45 | 1.38 |
| 37 | c | 511 | CLA | C4B-NB | -3.55 | 1.33 | 1.37 |
| 37 | 18 | 203 | CLA | C1B-NB | -3.55 | 1.33 | 1.37 |
| 37 | 34 | 303 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 37 | 18 | 201 | CLA | C1B-NB | -3.55 | 1.33 | 1.37 |
| 37 | 38 | 203 | CLA | C1B-NB | -3.55 | 1.33 | 1.37 |
| 47 | 18 | 210 | KC1 | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 48 | 31 | 315 | A86 | C9-C10 | 3.55 | 1.54 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | W | 101 | CLA | CHC-C4B | 3.55 | 1.47 | 1.39 |
| 37 | 40 | 208 | CLA | CHC-C4B | 3.55 | 1.47 | 1.39 |
| 37 | 31 | 308 | CLA | CHD-C4C | 3.55 | 1.47 | 1.39 |
| 37 | 38 | 201 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 48 | 36 | 313 | A86 | C17-C18 | -3.55 | 1.47 | 1.52 |
| 37 | b | 503 | CLA | CHD-C4C | 3.55 | 1.47 | 1.39 |
| 37 | C | 503 | CLA | C4B-NB | -3.55 | 1.33 | 1.37 |
| 47 | 11 | 306 | KC1 | C1B-NB | -3.55 | 1.33 | 1.37 |
| 37 | b | 506 | CLA | C1D-ND | 3.54 | 1.42 | 1.37 |
| 47 | 15 | 309 | KC1 | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 37 | c | 511 | CLA | CHD-C4C | 3.54 | 1.47 | 1.39 |
| 37 | 34 | 308 | CLA | CHB-C1B | 3.54 | 1.47 | 1.39 |
| 37 | 12 | 203 | CLA | C3D-C2D | 3.54 | 1.48 | 1.39 |
| 37 | 12 | 204 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 37 | 32 | 205 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 37 | C | 511 | CLA | C4B-NB | -3.54 | 1.33 | 1.37 |
| 37 | 16 | 301 | CLA | CHD-C4C | 3.54 | 1.47 | 1.39 |
| 37 | c | 506 | CLA | C3D-C2D | 3.54 | 1.48 | 1.39 |
| 37 | 16 | 309 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 39 | H | 101 | BCR | C1-C6 | -3.54 | 1.49 | 1.53 |
| 37 | 15 | 307 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 47 | 11 | 306 | KC1 | CHC-C1C | 3.54 | 1.47 | 1.39 |
| 37 | 41 | 204 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 47 | 38 | 210 | KC1 | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 37 | C | 506 | CLA | C3D-C2D | 3.53 | 1.48 | 1.39 |
| 37 | C | 504 | CLA | C4B-NB | -3.53 | 1.33 | 1.37 |
| 37 | B | 511 | CLA | CHD-C4C | 3.53 | 1.47 | 1.39 |
| 47 | 35 | 306 | KC1 | OBD-CAD | 3.53 | 1.28 | 1.22 |
| 37 | W | 101 | CLA | CHD-C4C | 3.53 | 1.47 | 1.39 |
| 37 | C | 511 | CLA | CHD-C4C | 3.53 | 1.47 | 1.39 |
| 37 | 36 | 306 | CLA | CHC-C4B | 3.53 | 1.47 | 1.39 |
| 37 | 14 | 302 | CLA | OBD-CAD | 3.53 | 1.28 | 1.22 |
| 37 | Z | 102 | CLA | CHC-C4B | 3.53 | 1.47 | 1.39 |
| 37 | w | 101 | CLA | CHC-C4B | 3.53 | 1.47 | 1.39 |
| 37 | A | 405 | CLA | C4B-NB | -3.53 | 1.33 | 1.37 |
| 37 | d | 401 | CLA | C4B-NB | -3.53 | 1.33 | 1.37 |
| 47 | 38 | 205 | KC1 | C1B-NB | -3.53 | 1.33 | 1.37 |
| 37 | 11 | 307 | CLA | CHD-C4C | 3.53 | 1.47 | 1.39 |
| 37 | 39 | 306 | CLA | CHD-C4C | 3.53 | 1.47 | 1.39 |
| 37 | 36 | 307 | CLA | OBD-CAD | 3.53 | 1.28 | 1.22 |
| 47 | 16 | 308 | KC1 | CHC-C1C | 3.53 | 1.47 | 1.39 |
| 47 | 32 | 207 | KC1 | CHC-C1C | 3.53 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 13 | 308 | CLA | C3D-C2D | 3.53 | 1.48 | 1.39 |
| 37 | 31 | 310 | CLA | C3D-C2D | 3.53 | 1.48 | 1.39 |
| 37 | 16 | 306 | CLA | CHC-C4B | 3.53 | 1.47 | 1.39 |
| 48 | 11 | 311 | A86 | C9-C10 | 3.53 | 1.54 | 1.43 |
| 48 | 31 | 311 | A86 | C9-C10 | 3.53 | 1.54 | 1.43 |
| 37 | 14 | 308 | CLA | OBD-CAD | 3.53 | 1.28 | 1.22 |
| 37 | 34 | 308 | CLA | OBD-CAD | 3.53 | 1.28 | 1.22 |
| 37 | 31 | 301 | CLA | CHB-C1B | 3.53 | 1.47 | 1.39 |
| 47 | 19 | 308 | KC1 | CHC-C1C | 3.52 | 1.47 | 1.39 |
| 37 | z | 102 | CLA | CHC-C4B | 3.52 | 1.47 | 1.39 |
| 37 | B | 506 | CLA | C1D-ND | 3.52 | 1.42 | 1.37 |
| 37 | B | 513 | CLA | CHD-C4C | 3.52 | 1.47 | 1.39 |
| 37 | 11 | 305 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 37 | 37 | 301 | CLA | C1B-NB | -3.52 | 1.33 | 1.37 |
| 47 | 15 | 306 | KC1 | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 48 | 12 | 214 | A86 | C9-C10 | 3.52 | 1.54 | 1.43 |
| 48 | 32 | 215 | A86 | C9-C10 | 3.52 | 1.54 | 1.43 |
| 47 | 34 | 306 | KC1 | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 37 | b | 513 | CLA | CHD-C4C | 3.52 | 1.47 | 1.39 |
| 37 | w | 101 | CLA | CHD-C4C | 3.52 | 1.47 | 1.39 |
| 47 | 13 | 309 | KC1 | CHC-C1C | 3.52 | 1.47 | 1.39 |
| 48 | 12 | 220 | A86 | C9-C10 | 3.52 | 1.54 | 1.43 |
| 48 | 32 | 221 | A86 | C9-C10 | 3.52 | 1.54 | 1.43 |
| 48 | 16 | 313 | A86 | C17-C18 | -3.52 | 1.47 | 1.52 |
| 37 | 12 | 210 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 37 | 31 | 306 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 47 | 36 | 308 | KC1 | CHC-C1C | 3.52 | 1.47 | 1.39 |
| 37 | 18 | 202 | CLA | C3D-C2D | 3.52 | 1.48 | 1.39 |
| 37 | 19 | 306 | CLA | CHD-C4C | 3.52 | 1.47 | 1.39 |
| 47 | 35 | 304 | KC1 | C1B-NB | -3.51 | 1.33 | 1.37 |
| 37 | D | 406 | CLA | C3D-C2D | 3.51 | 1.48 | 1.39 |
| 37 | 39 | 309 | CLA | C3D-C2D | 3.51 | 1.48 | 1.39 |
| 48 | 37 | 313 | A86 | C19-C18 | 3.51 | 1.57 | 1.52 |
| 37 | 18 | 208 | CLA | C3D-C2D | 3.51 | 1.48 | 1.39 |
| 48 | 16 | 314 | A86 | C17-C18 | -3.51 | 1.47 | 1.52 |
| 37 | B | 503 | CLA | C4B-NB | -3.51 | 1.33 | 1.37 |
| 37 | 32 | 211 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 37 | D | 402 | CLA | C4B-NB | -3.51 | 1.33 | 1.37 |
| 37 | 32 | 202 | CLA | C3D-C2D | 3.51 | 1.48 | 1.39 |
| 37 | 21 | 205 | CLA | CHC-C4B | 3.51 | 1.47 | 1.39 |
| 47 | 31 | 307 | KC1 | C1B-NB | -3.51 | 1.33 | 1.37 |
| 37 | 40 | 210 | CLA | CHC-C4B | 3.51 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 20 | 308 | CLA | CHC-C4B | 3.51 | 1.47 | 1.39 |
| 37 | B | 501 | CLA | C4B-NB | -3.51 | 1.33 | 1.37 |
| 37 | 34 | 302 | CLA | C4B-NB | -3.51 | 1.33 | 1.37 |
| 37 | 11 | 308 | CLA | C3D-C2D | 3.51 | 1.48 | 1.39 |
| 37 | 21 | 210 | CLA | CHC-C4B | 3.51 | 1.47 | 1.39 |
| 48 | 40 | 201 | A86 | C17-C18 | -3.50 | 1.47 | 1.52 |
| 37 | 41 | 210 | CLA | CHC-C4B | 3.50 | 1.47 | 1.39 |
| 37 | 37 | 308 | CLA | C1B-NB | -3.50 | 1.33 | 1.37 |
| 37 | 39 | 306 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 37 | 38 | 208 | CLA | C3D-C2D | 3.50 | 1.48 | 1.39 |
| 37 | 11 | 310 | CLA | C3D-C2D | 3.50 | 1.48 | 1.39 |
| 37 | 35 | 303 | CLA | CHC-C4B | 3.50 | 1.47 | 1.39 |
| 37 | 14 | 310 | CLA | C3D-C2D | 3.50 | 1.48 | 1.39 |
| 37 | 34 | 310 | CLA | C3D-C2D | 3.50 | 1.48 | 1.39 |
| 37 | 37 | 303 | CLA | C4B-NB | -3.50 | 1.33 | 1.37 |
| 37 | 41 | 202 | CLA | C1B-NB | -3.50 | 1.33 | 1.37 |
| 37 | W | 102 | CLA | CHB-C1B | 3.50 | 1.47 | 1.39 |
| 37 | b | 515 | CLA | C3D-C2D | 3.50 | 1.48 | 1.39 |
| 37 | 20 | 308 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 37 | b | 507 | CLA | C3D-C2D | 3.50 | 1.48 | 1.39 |
| 37 | 41 | 206 | CLA | C1B-NB | -3.50 | 1.33 | 1.37 |
| 48 | 31 | 312 | A86 | C9-C10 | 3.50 | 1.54 | 1.43 |
| 37 | 37 | 301 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 47 | 14 | 306 | KC1 | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 37 | 13 | 310 | CLA | CHC-C4B | 3.50 | 1.47 | 1.39 |
| 37 | 16 | 307 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 37 | 40 | 210 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 50 | 16 | 312 | DD6 | C-C1 | 3.50 | 1.57 | 1.50 |
| 47 | 35 | 302 | KC1 | CHC-C1C | 3.49 | 1.47 | 1.39 |
| 37 | 34 | 302 | CLA | CHC-C4B | 3.49 | 1.47 | 1.39 |
| 37 | 39 | 303 | CLA | CHC-C4B | 3.49 | 1.47 | 1.39 |
| 37 | c | 504 | CLA | C4B-NB | -3.49 | 1.33 | 1.37 |
| 47 | 18 | 207 | KC1 | CHC-C1C | 3.49 | 1.47 | 1.39 |
| 37 | 35 | 310 | CLA | CHC-C4B | 3.49 | 1.47 | 1.39 |
| 47 | 20 | 305 | KC1 | OBD-CAD | 3.49 | 1.28 | 1.22 |
| 37 | 17 | 309 | CLA | C1B-NB | -3.49 | 1.33 | 1.37 |
| 37 | a | 407 | CLA | C3D-C2D | 3.49 | 1.48 | 1.39 |
| 37 | 14 | 308 | CLA | C3D-C2D | 3.49 | 1.48 | 1.39 |
| 37 | 38 | 209 | CLA | CHB-C1B | 3.49 | 1.47 | 1.39 |
| 37 | 11 | 310 | CLA | CHC-C4B | 3.49 | 1.47 | 1.39 |
| 37 | 11 | 310 | CLA | CHD-C4C | 3.49 | 1.47 | 1.39 |
| 37 | B | 504 | CLA | CHD-C4C | 3.49 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 15 | 305 | CLA | CHC-C4B | 3.49 | 1.47 | 1.39 |
| 50 | 36 | 312 | DD6 | C-C1 | 3.49 | 1.57 | 1.50 |
| 37 | 35 | 305 | CLA | CHC-C4B | 3.49 | 1.47 | 1.39 |
| 37 | 38 | 203 | CLA | CHC-C4B | 3.49 | 1.47 | 1.39 |
| 37 | b | 516 | CLA | C3D-C2D | 3.49 | 1.48 | 1.39 |
| 37 | 18 | 202 | CLA | OBD-CAD | 3.49 | 1.28 | 1.22 |
| 37 | 11 | 310 | CLA | C4B-NB | -3.49 | 1.33 | 1.37 |
| 37 | B | 507 | CLA | C3D-C2D | 3.49 | 1.48 | 1.39 |
| 37 | C | 503 | CLA | C3D-C2D | 3.49 | 1.48 | 1.39 |
| 37 | 41 | 205 | CLA | CHC-C4B | 3.49 | 1.47 | 1.39 |
| 37 | 37 | 306 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 37 | 21 | 202 | CLA | C4B-NB | -3.48 | 1.33 | 1.37 |
| 37 | 36 | 307 | CLA | CHC-C4B | 3.48 | 1.47 | 1.39 |
| 48 | 13 | 312 | A86 | C19-C18 | 3.48 | 1.57 | 1.52 |
| 37 | 21 | 202 | CLA | C1B-NB | -3.48 | 1.33 | 1.37 |
| 48 | 33 | 312 | A86 | C19-C18 | 3.48 | 1.57 | 1.52 |
| 37 | D | 401 | CLA | C3D-C2D | 3.48 | 1.48 | 1.39 |
| 47 | 38 | 207 | KC1 | CHC-C1C | 3.48 | 1.47 | 1.39 |
| 37 | A | 405 | CLA | C3D-C2D | 3.48 | 1.48 | 1.39 |
| 37 | 14 | 308 | CLA | CHB-C1B | 3.48 | 1.47 | 1.39 |
| 37 | 14 | 302 | CLA | C4B-NB | -3.48 | 1.33 | 1.37 |
| 37 | d | 404 | CLA | C3D-C2D | 3.48 | 1.48 | 1.39 |
| 48 | 39 | 313 | A86 | C14-C15 | 3.48 | 1.59 | 1.52 |
| 37 | 19 | 303 | CLA | CHC-C4B | 3.48 | 1.47 | 1.39 |
| 39 | c | 514 | BCR | C30-C25 | -3.48 | 1.49 | 1.53 |
| 37 | 33 | 308 | CLA | C3D-C2D | 3.48 | 1.48 | 1.39 |
| 37 | 14 | 302 | CLA | CHC-C4B | 3.48 | 1.47 | 1.39 |
| 50 | 41 | 212 | DD6 | O2-C18 | 3.48 | 1.53 | 1.43 |
| 37 | c | 503 | CLA | C3D-C2D | 3.48 | 1.48 | 1.39 |
| 37 | 16 | 307 | CLA | CHC-C4B | 3.48 | 1.47 | 1.39 |
| 37 | 35 | 303 | CLA | C1B-NB | -3.47 | 1.33 | 1.37 |
| 37 | a | 404 | CLA | C3D-C2D | 3.47 | 1.48 | 1.39 |
| 48 | 11 | 312 | A86 | C9-C10 | 3.47 | 1.54 | 1.43 |
| 37 | b | 514 | CLA | CHD-C4C | 3.47 | 1.47 | 1.39 |
| 48 | 11 | 313 | A86 | C21-C20 | 3.47 | 1.57 | 1.51 |
| 48 | 15 | 315 | A86 | C17-C18 | -3.47 | 1.47 | 1.52 |
| 47 | 36 | 302 | KC1 | CHC-C1C | 3.47 | 1.47 | 1.39 |
| 48 | 14 | 311 | A86 | C19-C18 | 3.47 | 1.57 | 1.52 |
| 37 | 20 | 308 | CLA | CHB-C1B | 3.47 | 1.47 | 1.39 |
| 37 | 18 | 203 | CLA | CHC-C4B | 3.47 | 1.47 | 1.39 |
| 48 | 37 | 319 | A86 | C19-C18 | 3.47 | 1.57 | 1.52 |
| 37 | 18 | 202 | CLA | CHD-C1D | 3.47 | 1.45 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | b | 501 | CLA | C4B-NB | -3.47 | 1.33 | 1.37 |
| 37 | B | 515 | CLA | C3D-C2D | 3.47 | 1.48 | 1.39 |
| 50 | 20 | 310 | DD6 | O2-C18 | 3.47 | 1.53 | 1.43 |
| 37 | 15 | 308 | CLA | C1B-NB | -3.47 | 1.33 | 1.37 |
| 37 | B | 516 | CLA | C3D-C2D | 3.47 | 1.48 | 1.39 |
| 37 | C | 513 | CLA | C3D-C2D | 3.47 | 1.48 | 1.39 |
| 37 | 15 | 303 | CLA | CHC-C4B | 3.47 | 1.47 | 1.39 |
| 37 | 31 | 310 | CLA | CHC-C4B | 3.47 | 1.47 | 1.39 |
| 37 | 39 | 310 | CLA | CHC-C4B | 3.47 | 1.47 | 1.39 |
| 50 | 21 | 212 | DD6 | O2-C18 | 3.47 | 1.53 | 1.43 |
| 47 | 32 | 212 | KC1 | CHC-C1C | 3.47 | 1.47 | 1.39 |
| 37 | 39 | 309 | CLA | OBD-CAD | 3.47 | 1.28 | 1.22 |
| 47 | 13 | 302 | KC1 | OBD-CAD | 3.47 | 1.28 | 1.22 |
| 37 | 11 | 301 | CLA | C3D-C2D | 3.46 | 1.48 | 1.39 |
| 37 | b | 510 | CLA | CHD-C4C | 3.46 | 1.47 | 1.39 |
| 37 | 15 | 310 | CLA | CHC-C4B | 3.46 | 1.47 | 1.39 |
| 48 | 31 | 313 | A86 | C21-C20 | 3.46 | 1.57 | 1.51 |
| 37 | 17 | 307 | CLA | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 47 | 15 | 306 | KC1 | C1B-NB | -3.46 | 1.33 | 1.37 |
| 37 | b | 504 | CLA | CHD-C4C | 3.46 | 1.47 | 1.39 |
| 37 | 34 | 305 | CLA | C1B-NB | -3.46 | 1.33 | 1.37 |
| 47 | 40 | 207 | KC1 | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 47 | 14 | 306 | KC1 | CHC-C1C | 3.46 | 1.47 | 1.39 |
| 37 | 41 | 202 | CLA | C4B-NB | -3.46 | 1.33 | 1.37 |
| 37 | 33 | 310 | CLA | CHC-C4B | 3.46 | 1.47 | 1.39 |
| 47 | 37 | 304 | KC1 | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 37 | 31 | 302 | CLA | C3D-C2D | 3.46 | 1.48 | 1.39 |
| 37 | z | 102 | CLA | C1B-NB | -3.46 | 1.33 | 1.37 |
| 37 | 31 | 310 | CLA | CHD-C4C | 3.46 | 1.47 | 1.39 |
| 48 | 12 | 213 | A86 | C19-C18 | 3.46 | 1.57 | 1.52 |
| 48 | 32 | 214 | A86 | C19-C18 | 3.46 | 1.57 | 1.52 |
| 37 | 19 | 310 | CLA | CHC-C4B | 3.46 | 1.47 | 1.39 |
| 47 | 13 | 302 | KC1 | CHC-C1C | 3.46 | 1.47 | 1.39 |
| 47 | 16 | 302 | KC1 | CHC-C1C | 3.46 | 1.47 | 1.39 |
| 37 | b | 516 | CLA | C4B-NB | -3.46 | 1.33 | 1.37 |
| 37 | b | 510 | CLA | C3D-C2D | 3.46 | 1.48 | 1.39 |
| 47 | 36 | 308 | KC1 | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 37 | c | 513 | CLA | C3D-C2D | 3.45 | 1.48 | 1.39 |
| 37 | 18 | 206 | CLA | CHC-C4B | 3.45 | 1.47 | 1.39 |
| 37 | C | 504 | CLA | C3D-C2D | 3.45 | 1.48 | 1.39 |
| 37 | b | 516 | CLA | CHD-C4C | 3.45 | 1.47 | 1.39 |
| 47 | 33 | 302 | KC1 | CHC-C1C | 3.45 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | b | 514 | CLA | C3D-C2D | 3.45 | 1.48 | 1.39 |
| 39 | C | 514 | BCR | C30-C25 | -3.45 | 1.49 | 1.53 |
| 37 | B | 524 | CLA | CHD-C1D | 3.45 | 1.45 | 1.38 |
| 47 | 32 | 209 | KC1 | CHC-C1C | 3.45 | 1.47 | 1.39 |
| 48 | 12 | 215 | A86 | C19-C18 | 3.45 | 1.57 | 1.52 |
| 37 | B | 510 | CLA | CHD-C4C | 3.45 | 1.47 | 1.39 |
| 39 | b | 517 | BCR | C30-C25 | -3.45 | 1.49 | 1.53 |
| 48 | 32 | 216 | A86 | C19-C18 | 3.45 | 1.57 | 1.52 |
| 50 | 40 | 212 | DD6 | O2-C18 | 3.45 | 1.53 | 1.43 |
| 37 | 12 | 207 | CLA | C4B-NB | -3.45 | 1.33 | 1.37 |
| 37 | 32 | 208 | CLA | C4B-NB | -3.45 | 1.33 | 1.37 |
| 37 | 40 | 209 | CLA | CHB-C1B | 3.45 | 1.47 | 1.39 |
| 37 | C | 502 | CLA | CHD-C4C | 3.45 | 1.47 | 1.39 |
| 37 | 13 | 301 | CLA | C4B-NB | -3.45 | 1.33 | 1.37 |
| 47 | 15 | 304 | KC1 | C1B-NB | -3.45 | 1.33 | 1.37 |
| 37 | B | 514 | CLA | CHD-C4C | 3.45 | 1.47 | 1.39 |
| 37 | 33 | 305 | CLA | C1B-NB | -3.44 | 1.33 | 1.37 |
| 37 | 40 | 210 | CLA | CHB-C1B | 3.44 | 1.47 | 1.39 |
| 37 | 34 | 308 | CLA | C3D-C2D | 3.44 | 1.48 | 1.39 |
| 37 | B | 514 | CLA | C3D-C2D | 3.44 | 1.48 | 1.39 |
| 37 | c | 510 | CLA | CHB-C1B | 3.44 | 1.47 | 1.39 |
| 37 | Z | 102 | CLA | C1B-NB | -3.44 | 1.33 | 1.37 |
| 37 | 38 | 208 | CLA | CHC-C4B | 3.44 | 1.47 | 1.39 |
| 47 | 31 | 305 | KC1 | CHC-C1C | 3.44 | 1.47 | 1.39 |
| 37 | 37 | 301 | CLA | CHC-C4B | 3.44 | 1.47 | 1.39 |
| 37 | 14 | 301 | CLA | C1B-NB | -3.44 | 1.33 | 1.37 |
| 37 | 34 | 301 | CLA | C1B-NB | -3.44 | 1.33 | 1.37 |
| 37 | c | 508 | CLA | CHD-C4C | 3.44 | 1.47 | 1.39 |
| 39 | h | 101 | BCR | C1-C6 | -3.44 | 1.49 | 1.53 |
| 37 | 35 | 308 | CLA | CHC-C4B | 3.44 | 1.47 | 1.39 |
| 37 | 38 | 211 | CLA | CHC-C4B | 3.44 | 1.47 | 1.39 |
| 47 | 35 | 304 | KC1 | CHD-C1D | 3.44 | 1.47 | 1.39 |
| 37 | b | 502 | CLA | C3D-C2D | 3.44 | 1.48 | 1.39 |
| 37 | 39 | 303 | CLA | OBD-CAD | 3.44 | 1.28 | 1.22 |
| 37 | B | 504 | CLA | CHB-C1B | 3.44 | 1.47 | 1.39 |
| 37 | c | 502 | CLA | CHD-C4C | 3.43 | 1.47 | 1.39 |
| 37 | B | 502 | CLA | C3D-C2D | 3.43 | 1.48 | 1.39 |
| 37 | 18 | 211 | CLA | CHC-C4B | 3.43 | 1.47 | 1.39 |
| 37 | a | 407 | CLA | C4B-NB | -3.43 | 1.33 | 1.37 |
| 37 | 20 | 307 | CLA | CHB-C1B | 3.43 | 1.47 | 1.39 |
| 37 | b | 523 | CLA | CHD-C1D | 3.43 | 1.45 | 1.38 |
| 37 | 37 | 301 | CLA | C4B-NB | -3.43 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 36 | 306 | CLA | OBD-CAD | 3.43 | 1.28 | 1.22 |
| 37 | B | 508 | CLA | CHC-C4B | 3.43 | 1.47 | 1.39 |
| 37 | 19 | 305 | CLA | OBD-CAD | 3.43 | 1.28 | 1.22 |
| 37 | b | 504 | CLA | CHB-C1B | 3.43 | 1.47 | 1.39 |
| 37 | c | 511 | CLA | CHB-C1B | 3.43 | 1.47 | 1.39 |
| 47 | 40 | 207 | KC1 | CHC-C1C | 3.43 | 1.47 | 1.39 |
| 37 | W | 102 | CLA | OBD-CAD | 3.43 | 1.28 | 1.22 |
| 37 | C | 513 | CLA | CHC-C4B | 3.43 | 1.47 | 1.39 |
| 37 | 12 | 203 | CLA | C4B-NB | -3.43 | 1.33 | 1.37 |
| 37 | 20 | 301 | CLA | OBD-CAD | 3.43 | 1.28 | 1.22 |
| 47 | 15 | 304 | KC1 | CHD-C1D | 3.43 | 1.47 | 1.39 |
| 37 | 33 | 301 | CLA | C4B-NB | -3.43 | 1.33 | 1.37 |
| 37 | B | 510 | CLA | C3D-C2D | 3.43 | 1.48 | 1.39 |
| 37 | 39 | 310 | CLA | OBD-CAD | 3.43 | 1.28 | 1.22 |
| 47 | 16 | 308 | KC1 | OBD-CAD | 3.43 | 1.28 | 1.22 |
| 37 | 19 | 310 | CLA | OBD-CAD | 3.43 | 1.28 | 1.22 |
| 47 | 35 | 306 | KC1 | C1B-NB | -3.43 | 1.33 | 1.37 |
| 50 | 20 | 312 | DD6 | O2-C18 | 3.43 | 1.53 | 1.43 |
| 50 | 40 | 214 | DD6 | O2-C18 | 3.43 | 1.53 | 1.43 |
| 37 | 12 | 207 | CLA | CHC-C4B | 3.43 | 1.47 | 1.39 |
| 37 | 21 | 206 | CLA | C1B-NB | -3.43 | 1.33 | 1.37 |
| 47 | 34 | 306 | KC1 | CHC-C1C | 3.42 | 1.47 | 1.39 |
| 37 | 37 | 306 | CLA | CHC-C4B | 3.42 | 1.47 | 1.39 |
| 48 | 17 | 320 | A86 | C19-C18 | 3.42 | 1.57 | 1.52 |
| 37 | 15 | 303 | CLA | C1B-NB | -3.42 | 1.33 | 1.37 |
| 37 | 20 | 303 | CLA | CHC-C4B | 3.42 | 1.47 | 1.39 |
| 37 | 13 | 307 | CLA | C3D-C2D | 3.42 | 1.48 | 1.39 |
| 37 | 33 | 307 | CLA | C3D-C2D | 3.42 | 1.48 | 1.39 |
| 37 | C | 510 | CLA | CHB-C1B | 3.42 | 1.47 | 1.39 |
| 37 | 12 | 204 | CLA | CHC-C4B | 3.42 | 1.47 | 1.39 |
| 37 | 32 | 205 | CLA | CHC-C4B | 3.42 | 1.47 | 1.39 |
| 37 | 19 | 309 | CLA | OBD-CAD | 3.42 | 1.28 | 1.22 |
| 37 | 39 | 305 | CLA | OBD-CAD | 3.42 | 1.28 | 1.22 |
| 47 | 11 | 304 | KC1 | OBD-CAD | 3.42 | 1.28 | 1.22 |
| 37 | 41 | 202 | CLA | OBD-CAD | 3.42 | 1.28 | 1.22 |
| 37 | 16 | 306 | CLA | OBD-CAD | 3.42 | 1.28 | 1.22 |
| 37 | c | 513 | CLA | CHC-C4B | 3.42 | 1.47 | 1.39 |
| 37 | 13 | 308 | CLA | CHB-C1B | 3.42 | 1.47 | 1.39 |
| 37 | 40 | 203 | CLA | OBD-CAD | 3.42 | 1.28 | 1.22 |
| 37 | B | 516 | CLA | CHD-C4C | 3.42 | 1.47 | 1.39 |
| 37 | C | 508 | CLA | CHD-C4C | 3.42 | 1.47 | 1.39 |
| 37 | c | 507 | CLA | C3D-C2D | 3.42 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | b | 508 | CLA | CHC-C4B | 3.42 | 1.47 | 1.39 |
| 37 | B | 516 | CLA | C4B-NB | -3.42 | 1.33 | 1.37 |
| 37 | 31 | 310 | CLA | C4B-NB | -3.42 | 1.33 | 1.37 |
| 37 | 21 | 202 | CLA | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 48 | 19 | 311 | A86 | C19-C18 | 3.41 | 1.57 | 1.52 |
| 48 | 39 | 311 | A86 | C19-C18 | 3.41 | 1.57 | 1.52 |
| 37 | c | 505 | CLA | CHC-C4B | 3.41 | 1.47 | 1.39 |
| 37 | 19 | 303 | CLA | CHB-C1B | 3.41 | 1.47 | 1.39 |
| 37 | B | 504 | CLA | C4B-NB | -3.41 | 1.33 | 1.37 |
| 37 | 39 | 303 | CLA | C1B-NB | -3.41 | 1.33 | 1.37 |
| 37 | c | 505 | CLA | CHD-C4C | 3.41 | 1.47 | 1.39 |
| 37 | 21 | 208 | CLA | CHB-C1B | 3.41 | 1.47 | 1.39 |
| 37 | 15 | 308 | CLA | CHC-C4B | 3.41 | 1.47 | 1.39 |
| 39 | B | 517 | BCR | C30-C25 | -3.41 | 1.49 | 1.53 |
| 37 | B | 511 | CLA | C3D-C2D | 3.41 | 1.48 | 1.39 |
| 37 | c | 507 | CLA | CHD-C4C | 3.41 | 1.47 | 1.39 |
| 37 | 12 | 210 | CLA | C4B-NB | -3.41 | 1.33 | 1.37 |
| 37 | c | 504 | CLA | C3D-C2D | 3.41 | 1.48 | 1.39 |
| 37 | 19 | 305 | CLA | CHC-C4B | 3.41 | 1.47 | 1.39 |
| 37 | 39 | 305 | CLA | CHC-C4B | 3.41 | 1.47 | 1.39 |
| 37 | B | 510 | CLA | CHC-C4B | 3.41 | 1.47 | 1.39 |
| 37 | 15 | 308 | CLA | CHB-C1B | 3.41 | 1.47 | 1.39 |
| 37 | 32 | 204 | CLA | C4B-NB | -3.41 | 1.33 | 1.37 |
| 37 | C | 507 | CLA | C3D-C2D | 3.41 | 1.48 | 1.39 |
| 37 | 14 | 307 | CLA | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 37 | 34 | 307 | CLA | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 37 | b | 510 | CLA | CHC-C4B | 3.41 | 1.47 | 1.39 |
| 37 | 17 | 307 | CLA | CHC-C4B | 3.41 | 1.47 | 1.39 |
| 37 | 18 | 209 | CLA | C1B-NB | -3.41 | 1.33 | 1.37 |
| 50 | 36 | 312 | DD6 | O2-C18 | 3.41 | 1.53 | 1.43 |
| 37 | 18 | 208 | CLA | CHC-C4B | 3.41 | 1.47 | 1.39 |
| 47 | 20 | 305 | KC1 | CHC-C1C | 3.40 | 1.47 | 1.39 |
| 47 | 31 | 305 | KC1 | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 37 | 19 | 309 | CLA | CHC-C4B | 3.40 | 1.47 | 1.39 |
| 37 | 39 | 309 | CLA | CHC-C4B | 3.40 | 1.47 | 1.39 |
| 47 | 38 | 207 | KC1 | C1B-NB | -3.40 | 1.33 | 1.37 |
| 47 | 33 | 304 | KC1 | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 37 | C | 507 | CLA | CHD-C4C | 3.40 | 1.46 | 1.39 |
| 37 | 14 | 307 | CLA | C4B-NB | -3.40 | 1.33 | 1.37 |
| 47 | 19 | 308 | KC1 | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 37 | 13 | 308 | CLA | CHC-C4B | 3.40 | 1.47 | 1.39 |
| 37 | 33 | 308 | CLA | CHC-C4B | 3.40 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 301 | CLA | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 37 | 13 | 308 | CLA | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 47 | 37 | 305 | KC1 | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 37 | d | 404 | CLA | C4B-NB | -3.40 | 1.33 | 1.37 |
| 37 | 32 | 208 | CLA | CHC-C4B | 3.40 | 1.47 | 1.39 |
| 48 | 35 | 311 | A86 | C19-C18 | 3.40 | 1.57 | 1.52 |
| 37 | 17 | 302 | CLA | CHC-C4B | 3.40 | 1.47 | 1.39 |
| 37 | 21 | 205 | CLA | CHB-C1B | 3.40 | 1.47 | 1.39 |
| 37 | 32 | 210 | CLA | CHC-C4B | 3.40 | 1.47 | 1.39 |
| 37 | 39 | 303 | CLA | CHB-C1B | 3.40 | 1.47 | 1.39 |
| 37 | C | 512 | CLA | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 37 | 33 | 308 | CLA | CHB-C1B | 3.40 | 1.47 | 1.39 |
| 37 | w | 101 | CLA | C3D-C2D | 3.39 | 1.48 | 1.39 |
| 37 | 16 | 301 | CLA | C1B-NB | -3.39 | 1.33 | 1.37 |
| 47 | 33 | 302 | KC1 | OBD-CAD | 3.39 | 1.28 | 1.22 |
| 37 | 11 | 307 | CLA | CHC-C4B | 3.39 | 1.47 | 1.39 |
| 48 | 34 | 311 | A86 | C19-C18 | 3.39 | 1.57 | 1.52 |
| 39 | D | 407 | BCR | C1-C6 | -3.39 | 1.49 | 1.53 |
| 50 | 16 | 312 | DD6 | O2-C18 | 3.39 | 1.53 | 1.43 |
| 37 | 19 | 303 | CLA | C1B-NB | -3.39 | 1.33 | 1.37 |
| 47 | 12 | 208 | KC1 | CHC-C1C | 3.39 | 1.46 | 1.39 |
| 37 | b | 504 | CLA | C4B-NB | -3.39 | 1.33 | 1.37 |
| 38 | A | 404 | PHO | C4D-CHA | 3.39 | 1.44 | 1.39 |
| 37 | 12 | 209 | CLA | CHC-C4B | 3.39 | 1.47 | 1.39 |
| 37 | 40 | 205 | CLA | CHC-C4B | 3.39 | 1.47 | 1.39 |
| 47 | 13 | 306 | KC1 | OBD-CAD | 3.39 | 1.28 | 1.22 |
| 47 | 17 | 306 | KC1 | OBD-CAD | 3.39 | 1.28 | 1.22 |
| 47 | 33 | 306 | KC1 | OBD-CAD | 3.39 | 1.28 | 1.22 |
| 37 | 38 | 211 | CLA | CHB-C1B | 3.39 | 1.47 | 1.39 |
| 47 | 13 | 304 | KC1 | OBD-CAD | 3.39 | 1.28 | 1.22 |
| 48 | 18 | 215 | A86 | C19-C18 | 3.39 | 1.57 | 1.52 |
| 39 | C | 519 | BCR | C30-C25 | -3.38 | 1.49 | 1.53 |
| 37 | C | 511 | CLA | CHB-C1B | 3.38 | 1.47 | 1.39 |
| 37 | b | 511 | CLA | C3D-C2D | 3.38 | 1.48 | 1.39 |
| 37 | 14 | 308 | CLA | CHC-C4B | 3.38 | 1.47 | 1.39 |
| 37 | 41 | 204 | CLA | CHC-C4B | 3.38 | 1.47 | 1.39 |
| 37 | 11 | 305 | CLA | C4B-NB | -3.38 | 1.33 | 1.37 |
| 37 | 13 | 305 | CLA | C1B-NB | -3.38 | 1.33 | 1.37 |
| 37 | 31 | 306 | CLA | C4B-NB | -3.38 | 1.33 | 1.37 |
| 37 | C | 505 | CLA | CHD-C4C | 3.38 | 1.46 | 1.39 |
| 37 | 21 | 204 | CLA | CHC-C4B | 3.38 | 1.47 | 1.39 |
| 37 | b | 523 | CLA | C4B-NB | -3.38 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 15 | 310 | CLA | C1B-NB | -3.38 | 1.33 | 1.37 |
| 37 | 20 | 303 | CLA | CHB-C1B | 3.38 | 1.47 | 1.39 |
| 48 | 33 | 311 | A86 | C19-C18 | 3.38 | 1.57 | 1.52 |
| 37 | C | 501 | CLA | C3D-C2D | 3.38 | 1.48 | 1.39 |
| 48 | 35 | 313 | A86 | C19-C18 | 3.38 | 1.57 | 1.52 |
| 37 | W | 101 | CLA | C3D-C2D | 3.38 | 1.48 | 1.39 |
| 47 | 13 | 306 | KC1 | CHC-C1C | 3.38 | 1.46 | 1.39 |
| 37 | 38 | 204 | CLA | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 47 | 37 | 304 | KC1 | CHD-C1D | 3.38 | 1.47 | 1.39 |
| 47 | 11 | 304 | KC1 | CHC-C1C | 3.38 | 1.46 | 1.39 |
| 37 | 36 | 301 | CLA | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 47 | 33 | 309 | KC1 | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 37 | 35 | 308 | CLA | CHB-C1B | 3.38 | 1.47 | 1.39 |
| 37 | 32 | 204 | CLA | CHC-C4B | 3.38 | 1.47 | 1.39 |
| 48 | 37 | 310 | A86 | C19-C18 | 3.38 | 1.57 | 1.52 |
| 37 | C | 513 | CLA | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 37 | 19 | 307 | CLA | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 37 | 39 | 307 | CLA | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 37 | C | 505 | CLA | CHC-C4B | 3.38 | 1.47 | 1.39 |
| 37 | 12 | 203 | CLA | CHC-C4B | 3.38 | 1.47 | 1.39 |
| 37 | 33 | 301 | CLA | CHC-C4B | 3.38 | 1.47 | 1.39 |
| 37 | D | 406 | CLA | C4B-NB | -3.38 | 1.33 | 1.37 |
| 37 | b | 505 | CLA | C4B-NB | -3.38 | 1.33 | 1.37 |
| 37 | 20 | 308 | CLA | C1B-NB | -3.38 | 1.33 | 1.37 |
| 37 | C | 501 | CLA | CHB-C1B | 3.38 | 1.47 | 1.39 |
| 37 | 38 | 209 | CLA | C1B-NB | -3.38 | 1.33 | 1.37 |
| 37 | 14 | 307 | CLA | CHC-C4B | 3.37 | 1.47 | 1.39 |
| 37 | 34 | 307 | CLA | C4B-NB | -3.37 | 1.33 | 1.37 |
| 37 | 31 | 308 | CLA | CHC-C4B | 3.37 | 1.47 | 1.39 |
| 45 | D | 408 | PL9 | C52-C5 | -3.37 | 1.43 | 1.50 |
| 48 | 17 | 311 | A86 | C19-C18 | 3.37 | 1.57 | 1.52 |
| 37 | c | 512 | CLA | OBD-CAD | 3.37 | 1.28 | 1.22 |
| 37 | B | 505 | CLA | C4B-NB | -3.37 | 1.33 | 1.37 |
| 37 | 33 | 308 | CLA | OBD-CAD | 3.37 | 1.28 | 1.22 |
| 47 | 39 | 308 | KC1 | OBD-CAD | 3.37 | 1.28 | 1.22 |
| 37 | 36 | 301 | CLA | C1B-NB | -3.37 | 1.33 | 1.37 |
| 39 | B | 525 | BCR | C1-C6 | -3.37 | 1.49 | 1.53 |
| 37 | d | 401 | CLA | C3D-C2D | 3.37 | 1.48 | 1.39 |
| 37 | 15 | 303 | CLA | CHB-C1B | 3.37 | 1.47 | 1.39 |
| 37 | 35 | 303 | CLA | CHB-C1B | 3.37 | 1.47 | 1.39 |
| 37 | 38 | 206 | CLA | CHB-C1B | 3.37 | 1.47 | 1.39 |
| 37 | 34 | 310 | CLA | CHC-C4B | 3.37 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 31 | 303 | KC1 | CHC-C1C | 3.37 | 1.46 | 1.39 |
| 37 | B | 506 | CLA | CHC-C4B | 3.37 | 1.47 | 1.39 |
| 37 | 34 | 308 | CLA | CHC-C4B | 3.37 | 1.47 | 1.39 |
| 37 | c | 513 | CLA | OBD-CAD | 3.37 | 1.28 | 1.22 |
| 39 | c | 519 | BCR | C30-C25 | -3.37 | 1.49 | 1.53 |
| 37 | 41 | 205 | CLA | CHB-C1B | 3.36 | 1.47 | 1.39 |
| 37 | C | 501 | CLA | C4B-NB | -3.36 | 1.33 | 1.37 |
| 47 | 17 | 305 | KC1 | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 37 | 34 | 307 | CLA | CHC-C4B | 3.36 | 1.47 | 1.39 |
| 37 | 19 | 305 | CLA | C1B-NB | -3.36 | 1.33 | 1.37 |
| 37 | b | 513 | CLA | C3D-C2D | 3.36 | 1.48 | 1.39 |
| 38 | D | 403 | PHO | C1D-C2D | 3.36 | 1.43 | 1.39 |
| 37 | d | 401 | CLA | CHC-C4B | 3.36 | 1.47 | 1.39 |
| 37 | 41 | 208 | CLA | CHB-C1B | 3.36 | 1.47 | 1.39 |
| 37 | 32 | 211 | CLA | C4B-NB | -3.36 | 1.33 | 1.37 |
| 37 | 35 | 310 | CLA | C1B-NB | -3.36 | 1.33 | 1.37 |
| 37 | b | 506 | CLA | CHC-C4B | 3.36 | 1.47 | 1.39 |
| 38 | a | 405 | PHO | C1D-C2D | 3.36 | 1.43 | 1.39 |
| 47 | 36 | 302 | KC1 | CHD-C1D | 3.36 | 1.47 | 1.39 |
| 37 | 19 | 303 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 37 | d | 403 | CLA | C4B-NB | -3.36 | 1.33 | 1.37 |
| 37 | 21 | 209 | CLA | CHB-C1B | 3.36 | 1.47 | 1.39 |
| 37 | 18 | 204 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 37 | B | 501 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 47 | 31 | 309 | KC1 | CHC-C1C | 3.36 | 1.46 | 1.39 |
| 37 | b | 501 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 37 | C | 509 | CLA | C3D-C2D | 3.36 | 1.48 | 1.39 |
| 47 | 20 | 304 | KC1 | CHC-C1C | 3.36 | 1.46 | 1.39 |
| 39 | c | 515 | BCR | C1-C6 | -3.36 | 1.49 | 1.53 |
| 37 | 12 | 207 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 47 | 40 | 206 | KC1 | CHD-C1D | 3.35 | 1.46 | 1.39 |
| 50 | 20 | 312 | DD6 | C35-C34 | 3.35 | 1.58 | 1.52 |
| 37 | c | 512 | CLA | CHC-C4B | 3.35 | 1.46 | 1.39 |
| 48 | 15 | 311 | A86 | C19-C18 | 3.35 | 1.57 | 1.52 |
| 48 | 35 | 319 | A86 | C19-C18 | 3.35 | 1.57 | 1.52 |
| 37 | 18 | 211 | CLA | CHB-C1B | 3.35 | 1.46 | 1.39 |
| 37 | 40 | 210 | CLA | C1B-NB | -3.35 | 1.33 | 1.37 |
| 37 | 35 | 301 | CLA | CHB-C1B | 3.35 | 1.46 | 1.39 |
| 47 | 16 | 302 | KC1 | CHD-C1D | 3.35 | 1.46 | 1.39 |
| 37 | C | 512 | CLA | CHC-C4B | 3.35 | 1.46 | 1.39 |
| 37 | 32 | 210 | CLA | OBD-CAD | 3.35 | 1.28 | 1.22 |
| 48 | 13 | 311 | A86 | C19-C18 | 3.35 | 1.57 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 15 | 301 | CLA | CHB-C1B | 3.35 | 1.46 | 1.39 |
| 37 | 14 | 310 | CLA | CHC-C4B | 3.35 | 1.46 | 1.39 |
| 37 | 13 | 301 | CLA | CHC-C4B | 3.35 | 1.46 | 1.39 |
| 37 | 40 | 205 | CLA | CHB-C1B | 3.35 | 1.46 | 1.39 |
| 47 | 12 | 206 | KC1 | OBD-CAD | 3.35 | 1.28 | 1.22 |
| 37 | 41 | 210 | CLA | CHB-C1B | 3.35 | 1.46 | 1.39 |
| 37 | 16 | 301 | CLA | OBD-CAD | 3.35 | 1.28 | 1.22 |
| 37 | c | 501 | CLA | C3D-C2D | 3.34 | 1.48 | 1.39 |
| 37 | b | 509 | CLA | CHD-C4C | 3.34 | 1.46 | 1.39 |
| 37 | D | 402 | CLA | C3D-C2D | 3.34 | 1.48 | 1.39 |
| 37 | C | 503 | CLA | OBD-CAD | 3.34 | 1.28 | 1.22 |
| 47 | 20 | 304 | KC1 | CHD-C1D | 3.34 | 1.46 | 1.39 |
| 37 | 21 | 205 | CLA | C1B-NB | -3.34 | 1.33 | 1.37 |
| 37 | 18 | 201 | CLA | CHB-C1B | 3.34 | 1.46 | 1.39 |
| 39 | b | 524 | BCR | C1-C6 | -3.34 | 1.49 | 1.53 |
| 37 | B | 506 | CLA | C3D-C2D | 3.34 | 1.48 | 1.39 |
| 37 | D | 402 | CLA | CHC-C4B | 3.34 | 1.46 | 1.39 |
| 37 | 35 | 310 | CLA | CHB-C1B | 3.34 | 1.46 | 1.39 |
| 50 | 40 | 214 | DD6 | C35-C34 | 3.34 | 1.58 | 1.52 |
| 37 | D | 405 | CLA | CHC-C4B | 3.34 | 1.46 | 1.39 |
| 37 | 14 | 305 | CLA | C1B-NB | -3.34 | 1.33 | 1.37 |
| 37 | 36 | 301 | CLA | C4B-NB | -3.34 | 1.33 | 1.37 |
| 48 | 38 | 215 | A86 | C19-C18 | 3.34 | 1.57 | 1.52 |
| 47 | 33 | 306 | KC1 | CHC-C1C | 3.34 | 1.46 | 1.39 |
| 47 | 38 | 205 | KC1 | CHD-C1D | 3.34 | 1.46 | 1.39 |
| 47 | 21 | 203 | KC1 | OBD-CAD | 3.34 | 1.28 | 1.22 |
| 37 | 14 | 310 | CLA | CHB-C1B | 3.34 | 1.46 | 1.39 |
| 45 | d | 406 | PL9 | C52-C5 | -3.34 | 1.43 | 1.50 |
| 37 | 32 | 202 | CLA | C4B-NB | -3.34 | 1.33 | 1.37 |
| 37 | Z | 101 | CLA | CHC-C4B | 3.34 | 1.46 | 1.39 |
| 37 | 32 | 208 | CLA | OBD-CAD | 3.34 | 1.28 | 1.22 |
| 37 | 39 | 304 | CLA | OBD-CAD | 3.34 | 1.28 | 1.22 |
| 47 | 40 | 206 | KC1 | CHC-C1C | 3.34 | 1.46 | 1.39 |
| 51 | 39 | 315 | LMU | O5B-C1B | 3.33 | 1.50 | 1.41 |
| 47 | 32 | 207 | KC1 | OBD-CAD | 3.33 | 1.28 | 1.22 |
| 37 | z | 101 | CLA | CHC-C4B | 3.33 | 1.46 | 1.39 |
| 37 | c | 509 | CLA | C3D-C2D | 3.33 | 1.48 | 1.39 |
| 47 | 11 | 302 | KC1 | CHC-C1C | 3.33 | 1.46 | 1.39 |
| 37 | 19 | 302 | CLA | CHC-C4B | 3.33 | 1.46 | 1.39 |
| 47 | 11 | 309 | KC1 | CHC-C1C | 3.33 | 1.46 | 1.39 |
| 51 | 19 | 315 | LMU | O5B-C1B | 3.33 | 1.50 | 1.41 |
| 47 | 41 | 203 | KC1 | OBD-CAD | 3.33 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 32 | 202 | CLA | CHC-C4B | 3.33 | 1.46 | 1.39 |
| 37 | 37 | 306 | CLA | C4B-NB | -3.33 | 1.33 | 1.37 |
| 37 | 21 | 210 | CLA | C1B-NB | -3.33 | 1.33 | 1.37 |
| 37 | b | 506 | CLA | C3D-C2D | 3.33 | 1.48 | 1.39 |
| 37 | B | 509 | CLA | CHD-C4C | 3.33 | 1.46 | 1.39 |
| 37 | 41 | 205 | CLA | C1B-NB | -3.33 | 1.33 | 1.37 |
| 37 | 12 | 209 | CLA | OBD-CAD | 3.33 | 1.28 | 1.22 |
| 37 | B | 513 | CLA | C3D-C2D | 3.33 | 1.48 | 1.39 |
| 37 | 31 | 308 | CLA | OBD-CAD | 3.33 | 1.28 | 1.22 |
| 37 | B | 505 | CLA | CHC-C4B | 3.33 | 1.46 | 1.39 |
| 37 | b | 505 | CLA | CHC-C4B | 3.33 | 1.46 | 1.39 |
| 37 | D | 405 | CLA | C4B-NB | -3.33 | 1.33 | 1.37 |
| 47 | 14 | 309 | KC1 | C4B-NB | -3.33 | 1.33 | 1.37 |
| 37 | 41 | 209 | CLA | CHB-C1B | 3.33 | 1.46 | 1.39 |
| 47 | 37 | 302 | KC1 | CHC-C1C | 3.33 | 1.46 | 1.39 |
| 38 | a | 406 | PHO | C4D-CHA | 3.33 | 1.44 | 1.39 |
| 37 | c | 501 | CLA | C4B-NB | -3.32 | 1.33 | 1.37 |
| 37 | 15 | 305 | CLA | C1B-NB | -3.32 | 1.33 | 1.37 |
| 37 | b | 505 | CLA | C3D-C2D | 3.32 | 1.48 | 1.39 |
| 39 | d | 405 | BCR | C1-C6 | -3.32 | 1.49 | 1.53 |
| 48 | 15 | 319 | A86 | C19-C18 | 3.32 | 1.57 | 1.52 |
| 47 | 17 | 305 | KC1 | C4B-NB | -3.32 | 1.33 | 1.37 |
| 37 | c | 501 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 37 | 11 | 301 | CLA | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 37 | 31 | 302 | CLA | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 37 | 32 | 204 | CLA | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 37 | 12 | 203 | CLA | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 37 | 21 | 210 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 47 | 31 | 305 | KC1 | C4B-NB | -3.32 | 1.33 | 1.37 |
| 37 | d | 403 | CLA | CHC-C4B | 3.32 | 1.46 | 1.39 |
| 37 | 36 | 303 | CLA | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 47 | 11 | 302 | KC1 | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 37 | 15 | 310 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 47 | 37 | 307 | KC1 | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 37 | 20 | 301 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 37 | 34 | 310 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 47 | 18 | 205 | KC1 | CHD-C1D | 3.32 | 1.46 | 1.39 |
| 37 | C | 511 | CLA | C3D-C2D | 3.32 | 1.48 | 1.39 |
| 39 | a | 408 | BCR | C30-C25 | -3.32 | 1.49 | 1.53 |
| 37 | 19 | 302 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 47 | 11 | 304 | KC1 | C4B-NB | -3.31 | 1.33 | 1.37 |
| 37 | 15 | 305 | CLA | CHB-C1B | 3.31 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 18 | 202 | CLA | CHB-C1B | 3.31 | 1.46 | 1.39 |
| 37 | 34 | 305 | CLA | CHB-C1B | 3.31 | 1.46 | 1.39 |
| 37 | c | 503 | CLA | OBD-CAD | 3.31 | 1.28 | 1.22 |
| 37 | b | 501 | CLA | CHC-C4B | 3.31 | 1.46 | 1.39 |
| 37 | 11 | 308 | CLA | CHC-C4B | 3.31 | 1.46 | 1.39 |
| 37 | 40 | 203 | CLA | CHB-C1B | 3.31 | 1.46 | 1.39 |
| 39 | A | 406 | BCR | C30-C25 | -3.31 | 1.49 | 1.53 |
| 37 | 12 | 210 | CLA | CHC-C4B | 3.31 | 1.46 | 1.39 |
| 37 | B | 515 | CLA | OBD-CAD | 3.31 | 1.28 | 1.22 |
| 37 | 33 | 303 | CLA | OBD-CAD | 3.31 | 1.28 | 1.22 |
| 37 | b | 503 | CLA | C3D-C2D | 3.31 | 1.48 | 1.39 |
| 48 | 15 | 313 | A86 | C19-C18 | 3.31 | 1.57 | 1.52 |
| 37 | 11 | 307 | CLA | OBD-CAD | 3.31 | 1.28 | 1.22 |
| 37 | 16 | 301 | CLA | C4B-NB | -3.30 | 1.33 | 1.37 |
| 37 | 21 | 209 | CLA | C1B-NB | -3.30 | 1.33 | 1.37 |
| 37 | 39 | 302 | CLA | CHC-C4B | 3.30 | 1.46 | 1.39 |
| 37 | c | 511 | CLA | C3D-C2D | 3.30 | 1.48 | 1.39 |
| 37 | 21 | 208 | CLA | C1B-NB | -3.30 | 1.33 | 1.37 |
| 37 | B | 503 | CLA | C3D-C2D | 3.30 | 1.48 | 1.39 |
| 37 | 20 | 303 | CLA | C3D-C2D | 3.30 | 1.48 | 1.39 |
| 37 | 40 | 205 | CLA | C3D-C2D | 3.30 | 1.48 | 1.39 |
| 37 | A | 405 | CLA | CHC-C4B | 3.30 | 1.46 | 1.39 |
| 50 | 41 | 216 | DD6 | C-C1 | 3.30 | 1.57 | 1.50 |
| 37 | 19 | 304 | CLA | OBD-CAD | 3.30 | 1.28 | 1.22 |
| 37 | B | 501 | CLA | CHC-C4B | 3.30 | 1.46 | 1.39 |
| 50 | 20 | 310 | DD6 | C-C1 | 3.30 | 1.57 | 1.50 |
| 47 | 17 | 308 | KC1 | OBD-CAD | 3.30 | 1.28 | 1.22 |
| 37 | B | 505 | CLA | C3D-C2D | 3.30 | 1.48 | 1.39 |
| 37 | 19 | 309 | CLA | C4B-NB | -3.30 | 1.33 | 1.37 |
| 37 | 39 | 305 | CLA | C1B-NB | -3.30 | 1.33 | 1.37 |
| 37 | 40 | 210 | CLA | C4B-NB | -3.30 | 1.33 | 1.37 |
| 48 | 14 | 312 | A86 | C17-C18 | -3.30 | 1.47 | 1.52 |
| 37 | 41 | 204 | CLA | C4B-NB | -3.29 | 1.33 | 1.37 |
| 37 | 41 | 210 | CLA | C1B-NB | -3.29 | 1.33 | 1.37 |
| 50 | 19 | 312 | DD6 | C-C1 | 3.29 | 1.57 | 1.50 |
| 47 | 13 | 309 | KC1 | OBD-CAD | 3.29 | 1.28 | 1.22 |
| 37 | 33 | 310 | CLA | CHB-C1B | 3.29 | 1.46 | 1.39 |
| 47 | 31 | 303 | KC1 | OBD-CAD | 3.29 | 1.28 | 1.22 |
| 37 | 41 | 202 | CLA | CHB-C1B | 3.29 | 1.46 | 1.39 |
| 37 | 11 | 308 | CLA | C4B-NB | -3.29 | 1.33 | 1.37 |
| 37 | 21 | 204 | CLA | C4B-NB | -3.29 | 1.33 | 1.37 |
| 48 | 15 | 316 | A86 | C19-C18 | 3.29 | 1.57 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | c | 510 | CLA | OBD-CAD | 3.29 | 1.28 | 1.22 |
| 37 | 39 | 307 | CLA | C4B-NB | -3.29 | 1.33 | 1.37 |
| 37 | 17 | 307 | CLA | C4B-NB | -3.29 | 1.33 | 1.37 |
| 47 | 34 | 309 | KC1 | C4B-NB | -3.29 | 1.33 | 1.37 |
| 39 | C | 515 | BCR | C1-C6 | -3.29 | 1.49 | 1.53 |
| 37 | 14 | 305 | CLA | CHB-C1B | 3.28 | 1.46 | 1.39 |
| 37 | 31 | 306 | CLA | CHC-C4B | 3.28 | 1.46 | 1.39 |
| 37 | 35 | 305 | CLA | C1B-NB | -3.28 | 1.33 | 1.37 |
| 37 | d | 403 | CLA | C3D-C2D | 3.28 | 1.47 | 1.39 |
| 37 | 19 | 305 | CLA | C4B-NB | -3.28 | 1.33 | 1.37 |
| 37 | 35 | 308 | CLA | C1B-NB | -3.28 | 1.33 | 1.37 |
| 37 | 15 | 301 | CLA | C1B-NB | -3.28 | 1.33 | 1.37 |
| 37 | 35 | 301 | CLA | C1B-NB | -3.28 | 1.33 | 1.37 |
| 37 | B | 513 | CLA | CHB-C1B | 3.28 | 1.46 | 1.39 |
| 48 | 16 | 311 | A86 | C19-C18 | 3.28 | 1.57 | 1.52 |
| 37 | 12 | 204 | CLA | CHD-C4C | 3.28 | 1.46 | 1.39 |
| 37 | 32 | 205 | CLA | CHD-C4C | 3.28 | 1.46 | 1.39 |
| 37 | 11 | 310 | CLA | OBD-CAD | 3.28 | 1.28 | 1.22 |
| 47 | 20 | 305 | KC1 | CHD-C1D | 3.28 | 1.46 | 1.39 |
| 37 | D | 401 | CLA | OBD-CAD | 3.28 | 1.28 | 1.22 |
| 37 | a | 404 | CLA | OBD-CAD | 3.28 | 1.28 | 1.22 |
| 47 | 17 | 303 | KC1 | CHC-C1C | 3.28 | 1.46 | 1.39 |
| 48 | 18 | 213 | A86 | O-C13 | -3.28 | 1.16 | 1.23 |
| 37 | 39 | 302 | CLA | CHB-C1B | 3.28 | 1.46 | 1.39 |
| 47 | 15 | 302 | KC1 | CHD-C1D | 3.28 | 1.46 | 1.39 |
| 37 | 16 | 303 | CLA | CHC-C4B | 3.28 | 1.46 | 1.39 |
| 37 | D | 402 | CLA | OBD-CAD | 3.28 | 1.28 | 1.22 |
| 37 | 19 | 310 | CLA | C4B-NB | -3.28 | 1.33 | 1.37 |
| 37 | 39 | 310 | CLA | C4B-NB | -3.28 | 1.33 | 1.37 |
| 37 | 19 | 305 | CLA | CHB-C1B | 3.28 | 1.46 | 1.39 |
| 37 | 35 | 305 | CLA | CHB-C1B | 3.28 | 1.46 | 1.39 |
| 47 | 35 | 302 | KC1 | CHD-C1D | 3.28 | 1.46 | 1.39 |
| 48 | 34 | 312 | A86 | C17-C18 | -3.28 | 1.47 | 1.52 |
| 37 | 16 | 303 | CLA | C4B-NB | -3.27 | 1.33 | 1.37 |
| 37 | 19 | 307 | CLA | C4B-NB | -3.27 | 1.33 | 1.37 |
| 37 | b | 512 | CLA | CHC-C4B | 3.27 | 1.46 | 1.39 |
| 37 | 39 | 305 | CLA | C4B-NB | -3.27 | 1.33 | 1.37 |
| 37 | 11 | 305 | CLA | CHC-C4B | 3.27 | 1.46 | 1.39 |
| 37 | 32 | 202 | CLA | OBD-CAD | 3.27 | 1.28 | 1.22 |
| 37 | 39 | 304 | CLA | CHB-C1B | 3.27 | 1.46 | 1.39 |
| 37 | 19 | 304 | CLA | C4B-NB | -3.27 | 1.33 | 1.37 |
| 37 | 20 | 308 | CLA | C4B-NB | -3.27 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 39 | 304 | CLA | C4B-NB | -3.27 | 1.33 | 1.37 |
| 50 | 39 | 312 | DD6 | C-C1 | 3.27 | 1.57 | 1.50 |
| 37 | b | 513 | CLA | CHB-C1B | 3.27 | 1.46 | 1.39 |
| 37 | a | 407 | CLA | CHC-C4B | 3.27 | 1.46 | 1.39 |
| 37 | 13 | 310 | CLA | CHB-C1B | 3.27 | 1.46 | 1.39 |
| 37 | B | 524 | CLA | CHB-C1B | 3.27 | 1.46 | 1.39 |
| 37 | 19 | 304 | CLA | CHB-C1B | 3.27 | 1.46 | 1.39 |
| 37 | d | 403 | CLA | CHB-C1B | 3.27 | 1.46 | 1.39 |
| 37 | 12 | 210 | CLA | CHB-C1B | 3.27 | 1.46 | 1.39 |
| 37 | 38 | 211 | CLA | C1B-NB | -3.27 | 1.33 | 1.37 |
| 37 | 36 | 301 | CLA | CHB-C1B | 3.26 | 1.46 | 1.39 |
| 37 | 31 | 301 | CLA | C1B-NB | -3.26 | 1.33 | 1.37 |
| 37 | B | 512 | CLA | CHC-C4B | 3.26 | 1.46 | 1.39 |
| 37 | 21 | 202 | CLA | CHB-C1B | 3.26 | 1.46 | 1.39 |
| 37 | B | 524 | CLA | C4B-NB | -3.26 | 1.33 | 1.37 |
| 37 | D | 405 | CLA | CHB-C1B | 3.26 | 1.46 | 1.39 |
| 47 | 17 | 306 | KC1 | CHD-C1D | 3.26 | 1.46 | 1.39 |
| 44 | c | 517 | DGD | O1G-C1G | -3.26 | 1.37 | 1.45 |
| 48 | 34 | 315 | A86 | C19-C18 | 3.26 | 1.56 | 1.52 |
| 37 | D | 405 | CLA | C3D-C2D | 3.26 | 1.47 | 1.39 |
| 37 | 11 | 301 | CLA | C4B-NB | -3.26 | 1.33 | 1.37 |
| 37 | 31 | 302 | CLA | C4B-NB | -3.26 | 1.33 | 1.37 |
| 50 | 21 | 216 | DD6 | C-C1 | 3.26 | 1.57 | 1.50 |
| 48 | 38 | 213 | A86 | O-C13 | -3.26 | 1.16 | 1.23 |
| 44 | C | 517 | DGD | O1G-C1G | -3.26 | 1.37 | 1.45 |
| 47 | 37 | 305 | KC1 | CHD-C1D | 3.26 | 1.46 | 1.39 |
| 37 | 32 | 211 | CLA | CHC-C4B | 3.26 | 1.46 | 1.39 |
| 37 | 39 | 305 | CLA | CHB-C1B | 3.26 | 1.46 | 1.39 |
| 48 | 36 | 311 | A86 | C19-C18 | 3.25 | 1.56 | 1.52 |
| 37 | 16 | 303 | CLA | OBD-CAD | 3.25 | 1.28 | 1.22 |
| 37 | 18 | 208 | CLA | CHB-C1B | 3.25 | 1.46 | 1.39 |
| 48 | 14 | 315 | A86 | C19-C18 | 3.25 | 1.56 | 1.52 |
| 37 | D | 406 | CLA | OBD-CAD | 3.25 | 1.28 | 1.22 |
| 37 | 32 | 211 | CLA | CHB-C1B | 3.25 | 1.46 | 1.39 |
| 37 | B | 502 | CLA | OBD-CAD | 3.25 | 1.28 | 1.22 |
| 37 | 33 | 305 | CLA | CHB-C1B | 3.25 | 1.46 | 1.39 |
| 37 | 36 | 303 | CLA | CHC-C4B | 3.25 | 1.46 | 1.39 |
| 47 | 13 | 302 | KC1 | CHD-C1D | 3.25 | 1.46 | 1.39 |
| 47 | 31 | 307 | KC1 | OBD-CAD | 3.25 | 1.28 | 1.22 |
| 37 | 20 | 307 | CLA | C1B-NB | -3.25 | 1.33 | 1.37 |
| 37 | W | 102 | CLA | C1B-NB | -3.25 | 1.33 | 1.37 |
| 47 | 41 | 207 | KC1 | CHD-C1D | 3.25 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 14 | 301 | CLA | CHB-C1B | 3.25 | 1.46 | 1.39 |
| 37 | 34 | 301 | CLA | CHB-C1B | 3.25 | 1.46 | 1.39 |
| 37 | 36 | 303 | CLA | C4B-NB | -3.25 | 1.33 | 1.37 |
| 37 | b | 515 | CLA | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 37 | 38 | 208 | CLA | CHB-C1B | 3.24 | 1.46 | 1.39 |
| 37 | 16 | 301 | CLA | CHB-C1B | 3.24 | 1.46 | 1.39 |
| 48 | 12 | 214 | A86 | C19-C18 | 3.24 | 1.56 | 1.52 |
| 37 | d | 404 | CLA | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 48 | 14 | 313 | A86 | C25-C24 | 3.24 | 1.43 | 1.34 |
| 37 | z | 101 | CLA | CHB-C1B | 3.24 | 1.46 | 1.39 |
| 37 | 31 | 310 | CLA | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 37 | 41 | 208 | CLA | C1B-NB | -3.24 | 1.33 | 1.37 |
| 50 | 40 | 212 | DD6 | C-C1 | 3.24 | 1.57 | 1.50 |
| 37 | b | 523 | CLA | CHB-C1B | 3.24 | 1.46 | 1.39 |
| 37 | 21 | 206 | CLA | CHB-C1B | 3.24 | 1.46 | 1.39 |
| 37 | 41 | 209 | CLA | C1B-NB | -3.24 | 1.33 | 1.37 |
| 37 | b | 502 | CLA | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 37 | B | 524 | CLA | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 37 | C | 510 | CLA | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 37 | d | 401 | CLA | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 37 | 18 | 211 | CLA | C1B-NB | -3.24 | 1.33 | 1.37 |
| 47 | 15 | 302 | KC1 | C4B-NB | -3.24 | 1.33 | 1.37 |
| 37 | 18 | 206 | CLA | CHB-C1B | 3.23 | 1.46 | 1.39 |
| 47 | 18 | 210 | KC1 | CHD-C1D | 3.23 | 1.46 | 1.39 |
| 37 | C | 513 | CLA | C4B-NB | -3.23 | 1.33 | 1.37 |
| 47 | 21 | 207 | KC1 | CHD-C1D | 3.23 | 1.46 | 1.39 |
| 37 | B | 509 | CLA | C4B-NB | -3.23 | 1.33 | 1.37 |
| 37 | C | 511 | CLA | CHC-C4B | 3.23 | 1.46 | 1.39 |
| 37 | A | 405 | CLA | OBD-CAD | 3.23 | 1.28 | 1.22 |
| 37 | b | 523 | CLA | OBD-CAD | 3.23 | 1.28 | 1.22 |
| 37 | C | 504 | CLA | OBD-CAD | 3.23 | 1.28 | 1.22 |
| 37 | a | 407 | CLA | OBD-CAD | 3.23 | 1.28 | 1.22 |
| 37 | c | 512 | CLA | C4B-NB | -3.23 | 1.33 | 1.37 |
| 48 | 35 | 312 | A86 | C26-C27 | 3.23 | 1.43 | 1.35 |
| 47 | 37 | 304 | KC1 | C4B-NB | -3.23 | 1.33 | 1.37 |
| 37 | Z | 101 | CLA | CHB-C1B | 3.23 | 1.46 | 1.39 |
| 48 | 34 | 313 | A86 | C25-C24 | 3.23 | 1.43 | 1.34 |
| 37 | C | 501 | CLA | CHC-C4B | 3.23 | 1.46 | 1.39 |
| 47 | 40 | 207 | KC1 | CHD-C1D | 3.23 | 1.46 | 1.39 |
| 37 | 39 | 309 | CLA | C4B-NB | -3.23 | 1.33 | 1.37 |
| 47 | 12 | 208 | KC1 | OBD-CAD | 3.23 | 1.28 | 1.22 |
| 47 | 17 | 305 | KC1 | CHD-C1D | 3.23 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 15 | 312 | A86 | C26-C27 | 3.22 | 1.43 | 1.35 |
| 37 | c | 501 | CLA | CHC-C4B | 3.22 | 1.46 | 1.39 |
| 37 | 20 | 303 | CLA | C4B-NB | -3.22 | 1.33 | 1.37 |
| 37 | d | 404 | CLA | CHC-C4B | 3.22 | 1.46 | 1.39 |
| 37 | B | 507 | CLA | OBD-CAD | 3.22 | 1.28 | 1.22 |
| 37 | c | 511 | CLA | CHC-C4B | 3.22 | 1.46 | 1.39 |
| 48 | 36 | 310 | A86 | C19-C18 | 3.22 | 1.56 | 1.52 |
| 37 | 40 | 205 | CLA | C4B-NB | -3.22 | 1.33 | 1.37 |
| 37 | 13 | 305 | CLA | CHB-C1B | 3.22 | 1.46 | 1.39 |
| 37 | b | 507 | CLA | OBD-CAD | 3.22 | 1.28 | 1.22 |
| 37 | W | 101 | CLA | OBD-CAD | 3.22 | 1.28 | 1.22 |
| 47 | 41 | 203 | KC1 | CHD-C1D | 3.22 | 1.46 | 1.39 |
| 47 | 15 | 306 | KC1 | CHD-C1D | 3.22 | 1.46 | 1.39 |
| 37 | c | 504 | CLA | OBD-CAD | 3.22 | 1.28 | 1.22 |
| 37 | D | 406 | CLA | CHC-C4B | 3.22 | 1.46 | 1.39 |
| 48 | 35 | 316 | A86 | C19-C18 | 3.22 | 1.56 | 1.52 |
| 47 | 33 | 309 | KC1 | CHD-C1D | 3.22 | 1.46 | 1.39 |
| 37 | 41 | 206 | CLA | CHB-C1B | 3.21 | 1.46 | 1.39 |
| 37 | w | 101 | CLA | OBD-CAD | 3.21 | 1.28 | 1.22 |
| 48 | 21 | 215 | A86 | C19-C18 | 3.21 | 1.56 | 1.52 |
| 47 | 32 | 209 | KC1 | C4B-NB | -3.21 | 1.33 | 1.37 |
| 37 | B | 514 | CLA | CHB-C1B | 3.21 | 1.46 | 1.39 |
| 47 | 36 | 304 | KC1 | CHD-C1D | 3.21 | 1.46 | 1.39 |
| 37 | 36 | 303 | CLA | CHB-C1B | 3.21 | 1.46 | 1.39 |
| 47 | 33 | 302 | KC1 | CHD-C1D | 3.21 | 1.46 | 1.39 |
| 37 | 11 | 308 | CLA | OBD-CAD | 3.21 | 1.28 | 1.22 |
| 37 | 17 | 304 | CLA | CHC-C4B | 3.21 | 1.46 | 1.39 |
| 37 | C | 512 | CLA | C4B-NB | -3.20 | 1.33 | 1.37 |
| 37 | B | 512 | CLA | CHD-C1D | 3.20 | 1.44 | 1.38 |
| 37 | b | 512 | CLA | CHB-C1B | 3.20 | 1.46 | 1.39 |
| 37 | 36 | 307 | CLA | CHB-C1B | 3.20 | 1.46 | 1.39 |
| 37 | c | 513 | CLA | C4B-NB | -3.20 | 1.33 | 1.37 |
| 37 | c | 504 | CLA | CHC-C4B | 3.20 | 1.46 | 1.39 |
| 47 | 21 | 203 | KC1 | CHD-C1D | 3.20 | 1.46 | 1.39 |
| 48 | 35 | 312 | A86 | C19-C18 | 3.20 | 1.56 | 1.52 |
| 37 | b | 504 | CLA | C3D-C2D | 3.20 | 1.47 | 1.39 |
| 37 | 13 | 303 | CLA | OBD-CAD | 3.20 | 1.28 | 1.22 |
| 47 | 16 | 308 | KC1 | C4B-NB | -3.20 | 1.33 | 1.37 |
| 37 | 16 | 307 | CLA | CHB-C1B | 3.20 | 1.46 | 1.39 |
| 47 | 36 | 308 | KC1 | C4B-NB | -3.20 | 1.33 | 1.37 |
| 37 | b | 523 | CLA | CHD-C4C | 3.19 | 1.46 | 1.39 |
| 48 | 15 | 312 | A86 | C19-C18 | 3.19 | 1.56 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | C | 504 | CLA | CHC-C4B | 3.19 | 1.46 | 1.39 |
| 40 | 40 | 202 | SQD | O48-C23 | 3.19 | 1.42 | 1.33 |
| 37 | 38 | 203 | CLA | CHB-C1B | 3.19 | 1.46 | 1.39 |
| 37 | b | 506 | CLA | OBD-CAD | 3.19 | 1.28 | 1.22 |
| 37 | 14 | 308 | CLA | C4B-NB | -3.19 | 1.33 | 1.37 |
| 37 | 34 | 308 | CLA | C4B-NB | -3.19 | 1.33 | 1.37 |
| 47 | 17 | 303 | KC1 | CHD-C1D | 3.19 | 1.46 | 1.39 |
| 47 | 32 | 209 | KC1 | OBD-CAD | 3.19 | 1.28 | 1.22 |
| 47 | 32 | 212 | KC1 | C4B-NB | -3.19 | 1.33 | 1.37 |
| 37 | 41 | 206 | CLA | OBD-CAD | 3.19 | 1.28 | 1.22 |
| 37 | B | 524 | CLA | C3D-C2D | 3.19 | 1.47 | 1.39 |
| 37 | 19 | 310 | CLA | CHB-C1B | 3.19 | 1.46 | 1.39 |
| 37 | B | 506 | CLA | OBD-CAD | 3.19 | 1.28 | 1.22 |
| 47 | 11 | 306 | KC1 | OBD-CAD | 3.19 | 1.28 | 1.22 |
| 37 | B | 509 | CLA | OBD-CAD | 3.19 | 1.28 | 1.22 |
| 47 | 35 | 306 | KC1 | CHD-C1D | 3.18 | 1.46 | 1.39 |
| 37 | B | 510 | CLA | OBD-CAD | 3.18 | 1.28 | 1.22 |
| 48 | 40 | 213 | A86 | C25-C24 | 3.18 | 1.43 | 1.34 |
| 47 | 13 | 309 | KC1 | CHD-C1D | 3.18 | 1.46 | 1.39 |
| 40 | 16 | 315 | SQD | O48-C23 | 3.18 | 1.42 | 1.33 |
| 48 | 35 | 313 | A86 | C25-C24 | 3.18 | 1.43 | 1.34 |
| 39 | A | 406 | BCR | C1-C6 | -3.18 | 1.49 | 1.53 |
| 37 | b | 523 | CLA | C3D-C2D | 3.18 | 1.47 | 1.39 |
| 37 | 19 | 303 | CLA | C4B-NB | -3.18 | 1.33 | 1.37 |
| 37 | B | 524 | CLA | CHD-C4C | 3.18 | 1.46 | 1.39 |
| 37 | 21 | 206 | CLA | OBD-CAD | 3.18 | 1.28 | 1.22 |
| 48 | 20 | 311 | A86 | C25-C24 | 3.18 | 1.43 | 1.34 |
| 48 | 13 | 313 | A86 | C25-C24 | 3.18 | 1.43 | 1.34 |
| 48 | 33 | 313 | A86 | C25-C24 | 3.18 | 1.43 | 1.34 |
| 37 | B | 504 | CLA | C3D-C2D | 3.18 | 1.47 | 1.39 |
| 47 | 16 | 304 | KC1 | CHD-C1D | 3.18 | 1.46 | 1.39 |
| 37 | B | 514 | CLA | CHC-C4B | 3.18 | 1.46 | 1.39 |
| 37 | 16 | 303 | CLA | CHB-C1B | 3.18 | 1.46 | 1.39 |
| 48 | 15 | 313 | A86 | C25-C24 | 3.18 | 1.43 | 1.34 |
| 37 | 37 | 301 | CLA | CHB-C1B | 3.18 | 1.46 | 1.39 |
| 47 | 17 | 306 | KC1 | CHC-C1C | 3.18 | 1.46 | 1.39 |
| 47 | 37 | 305 | KC1 | CHC-C1C | 3.18 | 1.46 | 1.39 |
| 47 | 36 | 305 | KC1 | CHD-C1D | 3.17 | 1.46 | 1.39 |
| 37 | 19 | 302 | CLA | C4B-NB | -3.17 | 1.33 | 1.37 |
| 47 | 16 | 305 | KC1 | CHD-C1D | 3.17 | 1.46 | 1.39 |
| 37 | 40 | 209 | CLA | C1B-NB | -3.17 | 1.33 | 1.37 |
| 37 | c | 507 | CLA | OBD-CAD | 3.17 | 1.27 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | b | 509 | CLA | C4B-NB | -3.17 | 1.33 | 1.37 |
| 47 | 12 | 211 | KC1 | C4B-NB | -3.17 | 1.33 | 1.37 |
| 37 | 38 | 202 | CLA | CHB-C1B | 3.17 | 1.46 | 1.39 |
| 37 | B | 512 | CLA | CHB-C1B | 3.17 | 1.46 | 1.39 |
| 48 | 32 | 215 | A86 | C19-C18 | 3.17 | 1.56 | 1.52 |
| 37 | b | 505 | CLA | OBD-CAD | 3.17 | 1.27 | 1.22 |
| 37 | 18 | 203 | CLA | CHB-C1B | 3.17 | 1.46 | 1.39 |
| 37 | 39 | 310 | CLA | CHB-C1B | 3.17 | 1.46 | 1.39 |
| 37 | 34 | 303 | CLA | CHC-C4B | 3.17 | 1.46 | 1.39 |
| 47 | 16 | 302 | KC1 | C2A-C1A | 3.16 | 1.54 | 1.44 |
| 51 | 19 | 315 | LMU | O5'-C1' | 3.16 | 1.50 | 1.41 |
| 37 | b | 514 | CLA | CHB-C1B | 3.16 | 1.46 | 1.39 |
| 37 | 32 | 205 | CLA | CHB-C1B | 3.16 | 1.46 | 1.39 |
| 47 | 37 | 302 | KC1 | C4B-NB | -3.16 | 1.33 | 1.37 |
| 37 | 39 | 301 | CLA | CHB-C1B | 3.16 | 1.46 | 1.39 |
| 37 | 36 | 306 | CLA | C4B-NB | -3.16 | 1.33 | 1.37 |
| 37 | 21 | 204 | CLA | CHB-C1B | 3.16 | 1.46 | 1.39 |
| 47 | 38 | 210 | KC1 | CHD-C1D | 3.16 | 1.46 | 1.39 |
| 47 | 15 | 309 | KC1 | CHD-C1D | 3.16 | 1.46 | 1.39 |
| 37 | 37 | 303 | CLA | CHC-C4B | 3.16 | 1.46 | 1.39 |
| 43 | d | 408 | LHG | O7-C5 | -3.16 | 1.39 | 1.46 |
| 47 | 37 | 302 | KC1 | CHD-C1D | 3.16 | 1.46 | 1.39 |
| 48 | 41 | 215 | A86 | C19-C18 | 3.16 | 1.56 | 1.52 |
| 37 | A | 403 | CLA | OBD-CAD | 3.16 | 1.27 | 1.22 |
| 37 | b | 512 | CLA | CHD-C1D | 3.16 | 1.44 | 1.38 |
| 37 | 40 | 208 | CLA | C4B-NB | -3.16 | 1.33 | 1.37 |
| 37 | 39 | 303 | CLA | C4B-NB | -3.16 | 1.33 | 1.37 |
| 37 | B | 510 | CLA | CHB-C1B | 3.15 | 1.46 | 1.39 |
| 47 | 38 | 207 | KC1 | CHD-C1D | 3.15 | 1.46 | 1.39 |
| 37 | b | 510 | CLA | OBD-CAD | 3.15 | 1.27 | 1.22 |
| 37 | c | 506 | CLA | OBD-CAD | 3.15 | 1.27 | 1.22 |
| 47 | 35 | 309 | KC1 | CHD-C1D | 3.15 | 1.46 | 1.39 |
| 47 | 17 | 308 | KC1 | C4B-NB | -3.15 | 1.33 | 1.37 |
| 40 | 17 | 301 | SQD | O48-C23 | 3.15 | 1.42 | 1.33 |
| 37 | C | 507 | CLA | OBD-CAD | 3.15 | 1.27 | 1.22 |
| 48 | 21 | 213 | A86 | C25-C24 | 3.15 | 1.42 | 1.34 |
| 37 | b | 514 | CLA | CHC-C4B | 3.15 | 1.46 | 1.39 |
| 37 | C | 509 | CLA | CHB-C1B | 3.15 | 1.46 | 1.39 |
| 38 | a | 406 | PHO | C1D-C2D | 3.15 | 1.43 | 1.39 |
| 37 | B | 515 | CLA | CHC-C4B | 3.15 | 1.46 | 1.39 |
| 37 | 18 | 204 | CLA | CHB-C1B | 3.15 | 1.46 | 1.39 |
| 37 | a | 403 | CLA | OBD-CAD | 3.15 | 1.27 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | C | 505 | CLA | C4B-NB | -3.15 | 1.33 | 1.37 |
| 37 | c | 505 | CLA | C4B-NB | -3.15 | 1.33 | 1.37 |
| 38 | a | 405 | PHO | C4D-ND | -3.15 | 1.33 | 1.38 |
| 37 | B | 508 | CLA | C4B-NB | -3.14 | 1.33 | 1.37 |
| 37 | 19 | 301 | CLA | C4B-NB | -3.14 | 1.33 | 1.37 |
| 47 | 14 | 304 | KC1 | C4B-NB | -3.14 | 1.33 | 1.37 |
| 37 | B | 508 | CLA | OBD-CAD | 3.14 | 1.27 | 1.22 |
| 37 | 38 | 201 | CLA | CHB-C1B | 3.14 | 1.46 | 1.39 |
| 37 | 17 | 302 | CLA | CHB-C1B | 3.14 | 1.46 | 1.39 |
| 47 | 14 | 304 | KC1 | CHD-C1D | 3.14 | 1.46 | 1.39 |
| 37 | 39 | 306 | CLA | C4B-NB | -3.14 | 1.33 | 1.37 |
| 40 | 36 | 315 | SQD | O48-C23 | 3.14 | 1.42 | 1.33 |
| 37 | 37 | 308 | CLA | CHB-C1B | 3.14 | 1.46 | 1.39 |
| 37 | 41 | 204 | CLA | CHB-C1B | 3.14 | 1.46 | 1.39 |
| 37 | 31 | 301 | CLA | C4B-NB | -3.14 | 1.33 | 1.37 |
| 37 | c | 509 | CLA | CHB-C1B | 3.14 | 1.46 | 1.39 |
| 43 | D | 410 | LHG | O7-C5 | -3.14 | 1.39 | 1.46 |
| 37 | 38 | 204 | CLA | C3D-C2D | 3.14 | 1.47 | 1.39 |
| 37 | 13 | 303 | CLA | CHC-C4B | 3.14 | 1.46 | 1.39 |
| 48 | 16 | 310 | A86 | C19-C18 | 3.14 | 1.56 | 1.52 |
| 39 | C | 519 | BCR | C1-C6 | -3.14 | 1.49 | 1.53 |
| 37 | C | 506 | CLA | CHB-C1B | 3.14 | 1.46 | 1.39 |
| 48 | 15 | 312 | A86 | C25-C24 | 3.14 | 1.42 | 1.34 |
| 37 | B | 516 | CLA | C1C-NC | -3.14 | 1.32 | 1.37 |
| 37 | b | 509 | CLA | OBD-CAD | 3.14 | 1.27 | 1.22 |
| 47 | 40 | 204 | KC1 | CHD-C1D | 3.13 | 1.46 | 1.39 |
| 37 | b | 509 | CLA | CHB-C1B | 3.13 | 1.46 | 1.39 |
| 44 | c | 517 | DGD | O6D-C5D | -3.13 | 1.36 | 1.44 |
| 38 | D | 403 | PHO | C4D-ND | -3.13 | 1.33 | 1.38 |
| 37 | 18 | 204 | CLA | C3D-C2D | 3.13 | 1.47 | 1.39 |
| 37 | B | 505 | CLA | OBD-CAD | 3.13 | 1.27 | 1.22 |
| 37 | 17 | 304 | CLA | OBD-CAD | 3.13 | 1.27 | 1.22 |
| 47 | 36 | 302 | KC1 | C2A-C1A | 3.13 | 1.54 | 1.44 |
| 37 | 32 | 205 | CLA | C1D-ND | 3.13 | 1.42 | 1.37 |
| 37 | 19 | 301 | CLA | CHB-C1B | 3.13 | 1.46 | 1.39 |
| 47 | 20 | 305 | KC1 | C4B-NB | -3.13 | 1.33 | 1.37 |
| 37 | B | 511 | CLA | OBD-CAD | 3.13 | 1.27 | 1.22 |
| 37 | b | 508 | CLA | OBD-CAD | 3.13 | 1.27 | 1.22 |
| 37 | 14 | 303 | CLA | CHC-C4B | 3.13 | 1.46 | 1.39 |
| 44 | C | 517 | DGD | O6D-C5D | -3.13 | 1.36 | 1.44 |
| 37 | 39 | 309 | CLA | CHB-C1B | 3.13 | 1.46 | 1.39 |
| 47 | 34 | 304 | KC1 | CHD-C1D | 3.13 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 12 | 214 | A86 | C25-C24 | 3.13 | 1.42 | 1.34 |
| 47 | 12 | 208 | KC1 | C4B-NB | -3.13 | 1.33 | 1.37 |
| 37 | B | 516 | CLA | CHC-C4B | 3.13 | 1.46 | 1.39 |
| 48 | 35 | 315 | A86 | C17-C18 | -3.13 | 1.47 | 1.52 |
| 38 | A | 404 | PHO | C1D-C2D | 3.13 | 1.43 | 1.39 |
| 48 | 17 | 312 | A86 | C19-C18 | 3.13 | 1.56 | 1.52 |
| 47 | 17 | 306 | KC1 | C4B-NB | -3.13 | 1.33 | 1.37 |
| 47 | 37 | 305 | KC1 | C4B-NB | -3.13 | 1.33 | 1.37 |
| 48 | 36 | 313 | A86 | C19-C18 | 3.12 | 1.56 | 1.52 |
| 37 | C | 506 | CLA | OBD-CAD | 3.12 | 1.27 | 1.22 |
| 47 | 40 | 206 | KC1 | C4B-NB | -3.12 | 1.33 | 1.37 |
| 37 | 11 | 310 | CLA | CHB-C1B | 3.12 | 1.46 | 1.39 |
| 37 | 35 | 307 | CLA | C4B-NB | -3.12 | 1.33 | 1.37 |
| 39 | a | 413 | BCR | C1-C6 | -3.12 | 1.49 | 1.53 |
| 48 | 41 | 213 | A86 | C25-C24 | 3.12 | 1.42 | 1.34 |
| 47 | 20 | 302 | KC1 | CHD-C1D | 3.12 | 1.46 | 1.39 |
| 48 | 35 | 314 | A86 | C25-C24 | 3.12 | 1.42 | 1.34 |
| 37 | 12 | 204 | CLA | CHB-C1B | 3.12 | 1.46 | 1.39 |
| 37 | B | 504 | CLA | OBD-CAD | 3.12 | 1.27 | 1.22 |
| 37 | d | 403 | CLA | CHD-C1D | 3.12 | 1.44 | 1.38 |
| 37 | 33 | 308 | CLA | C4B-NB | -3.12 | 1.33 | 1.37 |
| 37 | C | 501 | CLA | OBD-CAD | 3.12 | 1.27 | 1.22 |
| 46 | f | 101 | HEM | CAC-C3C | 3.12 | 1.55 | 1.47 |
| 37 | 20 | 301 | CLA | C1B-NB | -3.12 | 1.33 | 1.37 |
| 37 | b | 511 | CLA | OBD-CAD | 3.12 | 1.27 | 1.22 |
| 37 | b | 511 | CLA | CHB-C1B | 3.12 | 1.46 | 1.39 |
| 37 | 19 | 306 | CLA | CHB-C1B | 3.12 | 1.46 | 1.39 |
| 37 | D | 405 | CLA | CHD-C1D | 3.12 | 1.44 | 1.38 |
| 48 | 35 | 312 | A86 | C25-C24 | 3.12 | 1.42 | 1.34 |
| 37 | 20 | 306 | CLA | C4B-NB | -3.11 | 1.33 | 1.37 |
| 37 | B | 502 | CLA | CHC-C4B | 3.11 | 1.46 | 1.39 |
| 37 | 37 | 303 | CLA | OBD-CAD | 3.11 | 1.27 | 1.22 |
| 38 | D | 403 | PHO | C4D-CHA | 3.11 | 1.44 | 1.39 |
| 39 | A | 410 | BCR | C1-C6 | -3.11 | 1.49 | 1.53 |
| 47 | 41 | 203 | KC1 | C4B-NB | -3.11 | 1.33 | 1.37 |
| 48 | 32 | 215 | A86 | C25-C24 | 3.11 | 1.42 | 1.34 |
| 48 | 37 | 311 | A86 | C19-C18 | 3.11 | 1.56 | 1.52 |
| 47 | 17 | 308 | KC1 | CHD-C1D | 3.11 | 1.46 | 1.39 |
| 47 | 37 | 307 | KC1 | CHD-C1D | 3.11 | 1.46 | 1.39 |
| 37 | 15 | 308 | CLA | OBD-CAD | 3.11 | 1.27 | 1.22 |
| 37 | 11 | 301 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |
| 37 | 16 | 309 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 20 | 306 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |
| 47 | 18 | 207 | KC1 | CHD-C1D | 3.11 | 1.46 | 1.39 |
| 37 | Z | 102 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |
| 37 | c | 506 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |
| 37 | b | 504 | CLA | OBD-CAD | 3.11 | 1.27 | 1.22 |
| 37 | 31 | 302 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |
| 37 | c | 501 | CLA | OBD-CAD | 3.11 | 1.27 | 1.22 |
| 37 | b | 515 | CLA | CHC-C4B | 3.11 | 1.46 | 1.39 |
| 37 | 19 | 309 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |
| 37 | 40 | 208 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |
| 47 | 36 | 304 | KC1 | C4B-NB | -3.11 | 1.33 | 1.37 |
| 37 | D | 405 | CLA | C1D-ND | 3.11 | 1.41 | 1.37 |
| 37 | a | 403 | CLA | C3D-C2D | 3.11 | 1.47 | 1.39 |
| 37 | 17 | 309 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |
| 37 | 36 | 309 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |
| 48 | 16 | 314 | A86 | C19-C18 | 3.10 | 1.56 | 1.52 |
| 37 | 33 | 303 | CLA | CHC-C4B | 3.10 | 1.46 | 1.39 |
| 48 | 13 | 314 | A86 | C25-C24 | 3.10 | 1.42 | 1.34 |
| 39 | C | 514 | BCR | C1-C6 | -3.10 | 1.49 | 1.53 |
| 37 | 35 | 301 | CLA | C4B-NB | -3.10 | 1.33 | 1.37 |
| 37 | D | 401 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 37 | C | 509 | CLA | OBD-CAD | 3.10 | 1.27 | 1.22 |
| 37 | b | 516 | CLA | C1C-NC | -3.10 | 1.33 | 1.37 |
| 39 | B | 518 | BCR | C1-C6 | -3.10 | 1.49 | 1.53 |
| 37 | C | 510 | CLA | C3D-C4D | -3.10 | 1.37 | 1.44 |
| 37 | 16 | 306 | CLA | C4B-NB | -3.10 | 1.33 | 1.37 |
| 37 | 35 | 308 | CLA | OBD-CAD | 3.10 | 1.27 | 1.22 |
| 37 | A | 403 | CLA | C3D-C2D | 3.10 | 1.47 | 1.39 |
| 37 | 11 | 308 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 47 | 17 | 303 | KC1 | C4B-NB | -3.10 | 1.33 | 1.37 |
| 37 | 12 | 204 | CLA | C1D-ND | 3.10 | 1.41 | 1.37 |
| 37 | W | 102 | CLA | C4B-NB | -3.10 | 1.33 | 1.37 |
| 46 | F | 101 | HEM | CAC-C3C | 3.10 | 1.55 | 1.47 |
| 37 | B | 511 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 37 | d | 403 | CLA | C1D-ND | 3.10 | 1.41 | 1.37 |
| 47 | 14 | 306 | KC1 | C4B-NB | -3.10 | 1.33 | 1.37 |
| 37 | a | 404 | CLA | CHC-C4B | 3.10 | 1.46 | 1.39 |
| 51 | 39 | 315 | LMU | O5'-C1' | 3.10 | 1.49 | 1.41 |
| 38 | a | 405 | PHO | C4D-CHA | 3.10 | 1.44 | 1.39 |
| 37 | 36 | 306 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 48 | 13 | 315 | A86 | C19-C18 | 3.10 | 1.56 | 1.52 |
| 37 | 32 | 213 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | b | 502 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 37 | z | 102 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 37 | 38 | 204 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 37 | 13 | 308 | CLA | C4B-NB | -3.10 | 1.33 | 1.37 |
| 48 | 15 | 314 | A86 | C25-C24 | 3.10 | 1.42 | 1.34 |
| 37 | c | 510 | CLA | C3D-C4D | -3.09 | 1.37 | 1.44 |
| 37 | 12 | 205 | CLA | CHC-C4B | 3.09 | 1.46 | 1.39 |
| 37 | C | 503 | CLA | CHC-C4B | 3.09 | 1.46 | 1.39 |
| 37 | 12 | 203 | CLA | CHB-C1B | 3.09 | 1.46 | 1.39 |
| 39 | b | 518 | BCR | C1-C6 | -3.09 | 1.49 | 1.53 |
| 47 | 35 | 302 | KC1 | C4B-NB | -3.09 | 1.33 | 1.37 |
| 48 | 34 | 316 | A86 | C19-C18 | 3.09 | 1.56 | 1.52 |
| 37 | 16 | 306 | CLA | CHB-C1B | 3.09 | 1.46 | 1.39 |
| 47 | 20 | 304 | KC1 | C4B-NB | -3.09 | 1.33 | 1.37 |
| 37 | a | 404 | CLA | CHB-C1B | 3.09 | 1.46 | 1.39 |
| 37 | b | 502 | CLA | CHC-C4B | 3.09 | 1.46 | 1.39 |
| 48 | 32 | 221 | A86 | C19-C18 | 3.09 | 1.56 | 1.52 |
| 37 | B | 509 | CLA | CHB-C1B | 3.09 | 1.46 | 1.39 |
| 37 | 32 | 206 | CLA | OBD-CAD | 3.09 | 1.27 | 1.22 |
| 37 | 33 | 307 | CLA | CHC-C4B | 3.09 | 1.46 | 1.39 |
| 37 | 40 | 203 | CLA | C1B-NB | -3.09 | 1.33 | 1.37 |
| 37 | 38 | 211 | CLA | C4B-NB | -3.08 | 1.33 | 1.37 |
| 47 | 37 | 307 | KC1 | C4B-NB | -3.08 | 1.33 | 1.37 |
| 37 | b | 510 | CLA | CHB-C1B | 3.08 | 1.46 | 1.39 |
| 37 | 31 | 310 | CLA | CHB-C1B | 3.08 | 1.46 | 1.39 |
| 47 | 32 | 212 | KC1 | OBD-CAD | 3.08 | 1.27 | 1.22 |
| 37 | b | 516 | CLA | CHC-C4B | 3.08 | 1.46 | 1.39 |
| 37 | 12 | 205 | CLA | OBD-CAD | 3.08 | 1.27 | 1.22 |
| 37 | c | 505 | CLA | OBD-CAD | 3.08 | 1.27 | 1.22 |
| 37 | c | 504 | CLA | CHB-C1B | 3.08 | 1.46 | 1.39 |
| 37 | D | 401 | CLA | CHC-C4B | 3.08 | 1.46 | 1.39 |
| 37 | 19 | 306 | CLA | C4B-NB | -3.08 | 1.33 | 1.37 |
| 47 | 21 | 203 | KC1 | C4B-NB | -3.08 | 1.33 | 1.37 |
| 47 | 16 | 308 | KC1 | CHD-C1D | 3.08 | 1.46 | 1.39 |
| 37 | 39 | 301 | CLA | C4B-NB | -3.08 | 1.33 | 1.37 |
| 37 | c | 503 | CLA | CHC-C4B | 3.08 | 1.46 | 1.39 |
| 37 | 18 | 211 | CLA | C4B-NB | -3.08 | 1.33 | 1.37 |
| 37 | 12 | 212 | CLA | CHB-C1B | 3.08 | 1.46 | 1.39 |
| 37 | 13 | 307 | CLA | CHC-C4B | 3.07 | 1.46 | 1.39 |
| 48 | 33 | 314 | A86 | C25-C24 | 3.07 | 1.42 | 1.34 |
| 39 | a | 408 | BCR | C1-C6 | -3.07 | 1.49 | 1.53 |
| 37 | 39 | 302 | CLA | C4B-NB | -3.07 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 14 | 309 | KC1 | OBD-CAD | 3.07 | 1.27 | 1.22 |
| 37 | 32 | 206 | CLA | CHB-C1B | 3.07 | 1.46 | 1.39 |
| 47 | 31 | 305 | KC1 | CHD-C1D | 3.07 | 1.46 | 1.39 |
| 37 | 32 | 206 | CLA | CHC-C4B | 3.07 | 1.46 | 1.39 |
| 37 | c | 509 | CLA | OBD-CAD | 3.07 | 1.27 | 1.22 |
| 48 | 19 | 313 | A86 | C14-C15 | 3.07 | 1.58 | 1.52 |
| 48 | 14 | 316 | A86 | C19-C18 | 3.07 | 1.56 | 1.52 |
| 37 | 14 | 310 | CLA | C4B-NB | -3.07 | 1.33 | 1.37 |
| 37 | 34 | 310 | CLA | C4B-NB | -3.07 | 1.33 | 1.37 |
| 47 | 16 | 304 | KC1 | C4B-NB | -3.07 | 1.33 | 1.37 |
| 47 | 40 | 207 | KC1 | C4B-NB | -3.07 | 1.33 | 1.37 |
| 48 | 18 | 215 | A86 | C25-C24 | 3.07 | 1.42 | 1.34 |
| 37 | 39 | 306 | CLA | CHB-C1B | 3.07 | 1.46 | 1.39 |
| 37 | B | 506 | CLA | C4B-NB | -3.07 | 1.33 | 1.37 |
| 37 | Z | 101 | CLA | C4B-NB | -3.07 | 1.33 | 1.37 |
| 37 | 36 | 309 | CLA | C4B-NB | -3.07 | 1.33 | 1.37 |
| 47 | 35 | 309 | KC1 | C4B-NB | -3.07 | 1.33 | 1.37 |
| 47 | 34 | 309 | KC1 | OBD-CAD | 3.07 | 1.27 | 1.22 |
| 37 | b | 508 | CLA | C4B-NB | -3.07 | 1.33 | 1.37 |
| 47 | 34 | 304 | KC1 | C4B-NB | -3.07 | 1.33 | 1.37 |
| 37 | b | 512 | CLA | OBD-CAD | 3.07 | 1.27 | 1.22 |
| 48 | 12 | 215 | A86 | C25-C24 | 3.07 | 1.42 | 1.34 |
| 37 | b | 503 | CLA | CHC-C4B | 3.07 | 1.46 | 1.39 |
| 37 | B | 502 | CLA | CHB-C1B | 3.06 | 1.46 | 1.39 |
| 47 | 32 | 212 | KC1 | CHD-C1D | 3.06 | 1.46 | 1.39 |
| 39 | B | 525 | BCR | C30-C25 | -3.06 | 1.49 | 1.53 |
| 47 | 15 | 309 | KC1 | C4B-NB | -3.06 | 1.33 | 1.37 |
| 37 | 11 | 303 | CLA | OBD-CAD | 3.06 | 1.27 | 1.22 |
| 37 | c | 510 | CLA | CHC-C4B | 3.06 | 1.46 | 1.39 |
| 37 | C | 504 | CLA | CHB-C1B | 3.06 | 1.46 | 1.39 |
| 47 | 12 | 211 | KC1 | CHD-C1D | 3.06 | 1.46 | 1.39 |
| 50 | 19 | 312 | DD6 | O2-C18 | 3.06 | 1.52 | 1.43 |
| 50 | 39 | 312 | DD6 | O2-C18 | 3.06 | 1.52 | 1.43 |
| 46 | f | 101 | HEM | CAB-C3B | 3.06 | 1.55 | 1.47 |
| 47 | 11 | 304 | KC1 | CHD-C1D | 3.06 | 1.46 | 1.39 |
| 37 | 31 | 304 | CLA | CHC-C4B | 3.06 | 1.46 | 1.39 |
| 48 | 21 | 214 | A86 | C25-C24 | 3.06 | 1.42 | 1.34 |
| 37 | B | 512 | CLA | OBD-CAD | 3.05 | 1.27 | 1.22 |
| 37 | b | 506 | CLA | C4B-NB | -3.05 | 1.33 | 1.37 |
| 37 | 18 | 208 | CLA | C4B-NB | -3.05 | 1.33 | 1.37 |
| 39 | b | 524 | BCR | C30-C25 | -3.05 | 1.49 | 1.53 |
| 48 | 37 | 311 | A86 | C25-C24 | 3.05 | 1.42 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 13 | 301 | CLA | CHB-C1B | 3.05 | 1.46 | 1.39 |
| 37 | 33 | 301 | CLA | CHB-C1B | 3.05 | 1.46 | 1.39 |
| 48 | 41 | 214 | A86 | C25-C24 | 3.05 | 1.42 | 1.34 |
| 48 | 31 | 312 | A86 | O-C13 | -3.05 | 1.16 | 1.23 |
| 44 | c | 516 | DGD | O1G-C1G | -3.05 | 1.38 | 1.45 |
| 48 | 11 | 311 | A86 | O-C13 | -3.05 | 1.16 | 1.23 |
| 48 | 31 | 311 | A86 | O-C13 | -3.05 | 1.16 | 1.23 |
| 44 | C | 516 | DGD | O1G-C1G | -3.05 | 1.38 | 1.45 |
| 37 | 14 | 303 | CLA | CHB-C1B | 3.05 | 1.46 | 1.39 |
| 37 | C | 502 | CLA | CHB-C1B | 3.05 | 1.46 | 1.39 |
| 37 | C | 513 | CLA | CHB-C1B | 3.05 | 1.46 | 1.39 |
| 37 | 15 | 307 | CLA | C4B-NB | -3.05 | 1.33 | 1.37 |
| 37 | C | 505 | CLA | OBD-CAD | 3.05 | 1.27 | 1.22 |
| 37 | 31 | 304 | CLA | OBD-CAD | 3.05 | 1.27 | 1.22 |
| 37 | B | 512 | CLA | C3D-C2D | 3.05 | 1.47 | 1.39 |
| 39 | c | 514 | BCR | C1-C6 | -3.05 | 1.49 | 1.53 |
| 37 | 32 | 204 | CLA | CHB-C1B | 3.05 | 1.46 | 1.39 |
| 47 | 38 | 205 | KC1 | C4B-NB | -3.05 | 1.33 | 1.37 |
| 37 | c | 502 | CLA | CHB-C1B | 3.05 | 1.46 | 1.39 |
| 50 | 21 | 212 | DD6 | C-C1 | 3.05 | 1.57 | 1.50 |
| 48 | 37 | 314 | A86 | C19-C18 | 3.04 | 1.56 | 1.52 |
| 37 | c | 508 | CLA | CHC-C4B | 3.04 | 1.46 | 1.39 |
| 37 | 32 | 202 | CLA | CHB-C1B | 3.04 | 1.46 | 1.39 |
| 37 | 38 | 208 | CLA | C4B-NB | -3.04 | 1.33 | 1.37 |
| 37 | B | 503 | CLA | CHC-C4B | 3.04 | 1.46 | 1.39 |
| 47 | 33 | 306 | KC1 | C4B-NB | -3.04 | 1.33 | 1.37 |
| 47 | 15 | 306 | KC1 | C4B-NB | -3.04 | 1.33 | 1.37 |
| 47 | 39 | 308 | KC1 | C4B-NB | -3.04 | 1.33 | 1.37 |
| 47 | 12 | 206 | KC1 | C4B-NB | -3.04 | 1.33 | 1.37 |
| 47 | 32 | 207 | KC1 | C4B-NB | -3.04 | 1.33 | 1.37 |
| 48 | 37 | 310 | A86 | C26-C27 | 3.04 | 1.42 | 1.35 |
| 48 | 33 | 315 | A86 | C19-C18 | 3.04 | 1.56 | 1.52 |
| 37 | 12 | 205 | CLA | CHB-C1B | 3.04 | 1.46 | 1.39 |
| 39 | c | 519 | BCR | C1-C6 | -3.04 | 1.49 | 1.53 |
| 46 | F | 101 | HEM | CAB-C3B | 3.04 | 1.55 | 1.47 |
| 48 | 34 | 313 | A86 | C19-C18 | 3.04 | 1.56 | 1.52 |
| 50 | 41 | 212 | DD6 | C-C1 | 3.04 | 1.57 | 1.50 |
| 47 | 31 | 309 | KC1 | CHB-C4A | -3.03 | 1.32 | 1.39 |
| 47 | 19 | 308 | KC1 | CHD-C1D | 3.03 | 1.46 | 1.39 |
| 47 | 36 | 308 | KC1 | CHD-C1D | 3.03 | 1.46 | 1.39 |
| 48 | 41 | 215 | A86 | C25-C24 | 3.03 | 1.42 | 1.34 |
| 47 | 34 | 306 | KC1 | C4B-NB | -3.03 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | c | 508 | CLA | OBD-CAD | 3.03 | 1.27 | 1.22 |
| 47 | 39 | 308 | KC1 | CHD-C1D | 3.03 | 1.46 | 1.39 |
| 37 | 34 | 301 | CLA | C4B-NB | -3.03 | 1.33 | 1.37 |
| 37 | c | 505 | CLA | CHB-C1B | 3.03 | 1.46 | 1.39 |
| 37 | b | 515 | CLA | CHB-C1B | 3.03 | 1.46 | 1.39 |
| 48 | 32 | 216 | A86 | C25-C24 | 3.03 | 1.42 | 1.34 |
| 48 | 38 | 215 | A86 | C25-C24 | 3.03 | 1.42 | 1.34 |
| 48 | 41 | 213 | A86 | C14-C15 | 3.03 | 1.58 | 1.52 |
| 37 | B | 513 | CLA | CHC-C4B | 3.03 | 1.46 | 1.39 |
| 37 | 34 | 303 | CLA | CHB-C1B | 3.03 | 1.46 | 1.39 |
| 37 | 38 | 204 | CLA | C4B-NB | -3.03 | 1.33 | 1.37 |
| 48 | 18 | 214 | A86 | C25-C24 | 3.03 | 1.42 | 1.34 |
| 37 | 15 | 301 | CLA | C4B-NB | -3.03 | 1.33 | 1.37 |
| 37 | 12 | 204 | CLA | C4B-NB | -3.02 | 1.33 | 1.37 |
| 37 | 32 | 205 | CLA | C4B-NB | -3.02 | 1.33 | 1.37 |
| 44 | J | 101 | DGD | O2G-C2G | -3.02 | 1.39 | 1.46 |
| 37 | C | 505 | CLA | CHB-C1B | 3.02 | 1.46 | 1.39 |
| 37 | C | 510 | CLA | CHC-C4B | 3.02 | 1.46 | 1.39 |
| 47 | 13 | 306 | KC1 | C4B-NB | -3.02 | 1.33 | 1.37 |
| 37 | 12 | 207 | CLA | CHB-C1B | 3.02 | 1.46 | 1.39 |
| 37 | 32 | 208 | CLA | CHB-C1B | 3.02 | 1.46 | 1.39 |
| 37 | B | 515 | CLA | CHB-C1B | 3.02 | 1.46 | 1.39 |
| 37 | c | 513 | CLA | CHB-C1B | 3.02 | 1.46 | 1.39 |
| 37 | 11 | 303 | CLA | CHC-C4B | 3.02 | 1.46 | 1.39 |
| 37 | 31 | 304 | CLA | CHB-C1B | 3.02 | 1.46 | 1.39 |
| 37 | 33 | 303 | CLA | CHB-C1B | 3.02 | 1.46 | 1.39 |
| 37 | C | 505 | CLA | C3D-C2D | 3.02 | 1.47 | 1.39 |
| 47 | 18 | 205 | KC1 | C4B-NB | -3.02 | 1.33 | 1.37 |
| 47 | 13 | 302 | KC1 | CHB-C4A | -3.02 | 1.32 | 1.39 |
| 37 | 14 | 301 | CLA | C4B-NB | -3.02 | 1.33 | 1.37 |
| 37 | C | 508 | CLA | CHC-C4B | 3.02 | 1.46 | 1.39 |
| 37 | C | 508 | CLA | OBD-CAD | 3.02 | 1.27 | 1.22 |
| 37 | 16 | 309 | CLA | C4B-NB | -3.02 | 1.33 | 1.37 |
| 48 | 17 | 315 | A86 | C19-C18 | 3.02 | 1.56 | 1.52 |
| 37 | 21 | 210 | CLA | C4B-NB | -3.02 | 1.33 | 1.37 |
| 44 | j | 101 | DGD | O2G-C2G | -3.02 | 1.39 | 1.46 |
| 48 | 17 | 311 | A86 | C26-C27 | 3.02 | 1.42 | 1.35 |
| 37 | 21 | 206 | CLA | C4B-NB | -3.02 | 1.33 | 1.37 |
| 48 | 14 | 314 | A86 | C25-C24 | 3.02 | 1.42 | 1.34 |
| 37 | 18 | 206 | CLA | C4B-NB | -3.02 | 1.33 | 1.37 |
| 47 | 34 | 309 | KC1 | CHD-C1D | 3.02 | 1.46 | 1.39 |
| 48 | 38 | 214 | A86 | C25-C24 | 3.02 | 1.42 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | b | 513 | CLA | CHC-C4B | 3.01 | 1.46 | 1.39 |
| 48 | 21 | 215 | A86 | C25-C24 | 3.01 | 1.42 | 1.34 |
| 48 | 17 | 320 | A86 | O-C13 | -3.01 | 1.17 | 1.23 |
| 48 | 21 | 213 | A86 | C14-C15 | 3.01 | 1.58 | 1.52 |
| 37 | B | 511 | CLA | CHC-C4B | 3.01 | 1.46 | 1.39 |
| 48 | 17 | 312 | A86 | C25-C24 | 3.01 | 1.42 | 1.34 |
| 48 | 34 | 314 | A86 | C25-C24 | 3.01 | 1.42 | 1.34 |
| 37 | b | 511 | CLA | CHC-C4B | 3.01 | 1.46 | 1.39 |
| 48 | 15 | 319 | A86 | C14-C15 | 3.01 | 1.58 | 1.52 |
| 37 | B | 524 | CLA | C1D-ND | 3.01 | 1.41 | 1.37 |
| 48 | 14 | 313 | A86 | C19-C18 | 3.01 | 1.56 | 1.52 |
| 37 | b | 509 | CLA | CHC-C4B | 3.01 | 1.46 | 1.39 |
| 47 | 11 | 309 | KC1 | CHD-C1D | 3.01 | 1.46 | 1.39 |
| 47 | 31 | 309 | KC1 | CHD-C1D | 3.01 | 1.46 | 1.39 |
| 37 | b | 512 | CLA | C3D-C2D | 3.00 | 1.47 | 1.39 |
| 37 | C | 509 | CLA | CHC-C4B | 3.00 | 1.46 | 1.39 |
| 37 | 16 | 307 | CLA | C4B-NB | -3.00 | 1.33 | 1.37 |
| 37 | 17 | 309 | CLA | C4B-NB | -3.00 | 1.33 | 1.37 |
| 47 | 12 | 211 | KC1 | OBD-CAD | 3.00 | 1.27 | 1.22 |
| 37 | B | 501 | CLA | CHB-C1B | 3.00 | 1.46 | 1.39 |
| 48 | 33 | 312 | A86 | C25-C24 | 3.00 | 1.42 | 1.34 |
| 37 | 15 | 310 | CLA | C4B-NB | -3.00 | 1.33 | 1.37 |
| 37 | 35 | 310 | CLA | C4B-NB | -3.00 | 1.33 | 1.37 |
| 46 | V | 201 | HEM | CAB-C3B | 3.00 | 1.55 | 1.47 |
| 46 | v | 201 | HEM | CAB-C3B | 3.00 | 1.55 | 1.47 |
| 47 | 13 | 304 | KC1 | CHD-C1D | 3.00 | 1.46 | 1.39 |
| 48 | 35 | 319 | A86 | C14-C15 | 3.00 | 1.58 | 1.52 |
| 37 | 11 | 303 | CLA | CHB-C1B | 3.00 | 1.46 | 1.39 |
| 37 | 13 | 307 | CLA | OBD-CAD | 3.00 | 1.27 | 1.22 |
| 37 | A | 403 | CLA | CHB-C1B | 3.00 | 1.46 | 1.39 |
| 37 | 38 | 202 | CLA | C4B-NB | -3.00 | 1.33 | 1.37 |
| 37 | c | 509 | CLA | CHC-C4B | 3.00 | 1.46 | 1.39 |
| 47 | 11 | 309 | KC1 | CHB-C4A | -3.00 | 1.32 | 1.39 |
| 47 | 14 | 309 | KC1 | CHB-C4A | -3.00 | 1.32 | 1.39 |
| 47 | 35 | 306 | KC1 | C4B-NB | -2.99 | 1.33 | 1.37 |
| 37 | c | 505 | CLA | C3D-C2D | 2.99 | 1.47 | 1.39 |
| 47 | 33 | 302 | KC1 | CHB-C4A | -2.99 | 1.32 | 1.39 |
| 37 | z | 101 | CLA | C4B-NB | -2.99 | 1.33 | 1.37 |
| 37 | 33 | 307 | CLA | OBD-CAD | 2.99 | 1.27 | 1.22 |
| 47 | 34 | 306 | KC1 | CHD-C1D | 2.99 | 1.46 | 1.39 |
| 37 | d | 401 | CLA | CHB-C1B | 2.99 | 1.46 | 1.39 |
| 37 | W | 101 | CLA | CHB-C1B | 2.99 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 17 | 304 | CLA | CHB-C1B | 2.99 | 1.46 | 1.39 |
| 37 | 13 | 305 | CLA | C4B-NB | -2.99 | 1.33 | 1.37 |
| 37 | 33 | 305 | CLA | C4B-NB | -2.99 | 1.33 | 1.37 |
| 37 | 13 | 307 | CLA | CHB-C1B | 2.99 | 1.46 | 1.39 |
| 37 | 33 | 307 | CLA | CHB-C1B | 2.99 | 1.46 | 1.39 |
| 37 | 20 | 301 | CLA | C4B-NB | -2.99 | 1.33 | 1.37 |
| 48 | 12 | 220 | A86 | C19-C18 | 2.99 | 1.56 | 1.52 |
| 37 | c | 511 | CLA | OBD-CAD | 2.99 | 1.27 | 1.22 |
| 37 | 41 | 206 | CLA | C4B-NB | -2.99 | 1.33 | 1.37 |
| 37 | a | 403 | CLA | CHB-C1B | 2.99 | 1.46 | 1.39 |
| 37 | B | 512 | CLA | CHD-C4C | 2.99 | 1.46 | 1.39 |
| 37 | b | 503 | CLA | OBD-CAD | 2.99 | 1.27 | 1.22 |
| 47 | 14 | 309 | KC1 | CHD-C1D | 2.99 | 1.46 | 1.39 |
| 47 | 14 | 306 | KC1 | CHD-C1D | 2.99 | 1.46 | 1.39 |
| 37 | w | 101 | CLA | CHB-C1B | 2.99 | 1.46 | 1.39 |
| 37 | B | 506 | CLA | CHD-C4C | 2.98 | 1.46 | 1.39 |
| 47 | 33 | 304 | KC1 | CHD-C1D | 2.98 | 1.46 | 1.39 |
| 37 | 37 | 308 | CLA | C4B-NB | -2.98 | 1.33 | 1.37 |
| 37 | B | 509 | CLA | CHC-C4B | 2.98 | 1.46 | 1.39 |
| 37 | 14 | 302 | CLA | CHB-C1B | 2.98 | 1.46 | 1.39 |
| 48 | 35 | 312 | A86 | O-C13 | -2.98 | 1.17 | 1.23 |
| 47 | 20 | 302 | KC1 | C4B-NB | -2.98 | 1.33 | 1.37 |
| 37 | 13 | 303 | CLA | CHB-C1B | 2.98 | 1.46 | 1.39 |
| 50 | 39 | 312 | DD6 | C26-C27 | -2.98 | 1.30 | 1.37 |
| 37 | 36 | 307 | CLA | C4B-NB | -2.98 | 1.33 | 1.37 |
| 37 | 40 | 203 | CLA | C4B-NB | -2.98 | 1.33 | 1.37 |
| 47 | 34 | 309 | KC1 | CHB-C4A | -2.98 | 1.32 | 1.39 |
| 37 | C | 507 | CLA | CHC-C4B | 2.98 | 1.46 | 1.39 |
| 37 | c | 507 | CLA | CHC-C4B | 2.98 | 1.46 | 1.39 |
| 37 | 15 | 305 | CLA | C4B-NB | -2.98 | 1.33 | 1.37 |
| 40 | L | 101 | SQD | O48-C23 | 2.98 | 1.42 | 1.33 |
| 37 | 41 | 210 | CLA | C4B-NB | -2.98 | 1.34 | 1.37 |
| 48 | 11 | 312 | A86 | O-C13 | -2.98 | 1.17 | 1.23 |
| 37 | b | 501 | CLA | CHB-C1B | 2.98 | 1.46 | 1.39 |
| 37 | 37 | 303 | CLA | CHB-C1B | 2.98 | 1.46 | 1.39 |
| 50 | 19 | 312 | DD6 | C26-C27 | -2.97 | 1.30 | 1.37 |
| 37 | b | 512 | CLA | CHD-C4C | 2.97 | 1.46 | 1.39 |
| 37 | D | 402 | CLA | CHB-C1B | 2.97 | 1.46 | 1.39 |
| 47 | 31 | 307 | KC1 | C4B-NB | -2.97 | 1.34 | 1.37 |
| 48 | 15 | 316 | A86 | C14-C15 | 2.97 | 1.58 | 1.52 |
| 37 | 13 | 310 | CLA | C4B-NB | -2.97 | 1.34 | 1.37 |
| 37 | b | 512 | CLA | C3D-C4D | -2.97 | 1.37 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | b | 506 | CLA | CHD-C4C | 2.97 | 1.46 | 1.39 |
| 48 | 13 | 312 | A86 | C25-C24 | 2.97 | 1.42 | 1.34 |
| 37 | z | 102 | CLA | C4B-NB | -2.97 | 1.34 | 1.37 |
| 40 | B | 519 | SQD | O48-C23 | 2.97 | 1.42 | 1.33 |
| 37 | 35 | 305 | CLA | C4B-NB | -2.96 | 1.34 | 1.37 |
| 47 | 19 | 308 | KC1 | C4B-NB | -2.96 | 1.34 | 1.37 |
| 41 | c | 518 | LMG | O1-C7 | -2.96 | 1.38 | 1.43 |
| 37 | a | 407 | CLA | CHB-C1B | 2.96 | 1.46 | 1.39 |
| 48 | 31 | 313 | A86 | C19-C18 | 2.96 | 1.56 | 1.52 |
| 47 | 13 | 304 | KC1 | C4B-NB | -2.96 | 1.34 | 1.37 |
| 37 | B | 512 | CLA | C3D-C4D | -2.96 | 1.37 | 1.44 |
| 48 | 17 | 314 | A86 | O-C13 | -2.96 | 1.17 | 1.23 |
| 37 | a | 407 | CLA | C3D-C4D | -2.96 | 1.37 | 1.44 |
| 37 | A | 403 | CLA | CHC-C4B | 2.96 | 1.46 | 1.39 |
| 37 | a | 403 | CLA | CHC-C4B | 2.96 | 1.46 | 1.39 |
| 37 | B | 507 | CLA | CHC-C4B | 2.95 | 1.46 | 1.39 |
| 41 | a | 410 | LMG | O7-C8 | -2.95 | 1.39 | 1.46 |
| 48 | 18 | 214 | A86 | C14-C15 | 2.95 | 1.58 | 1.52 |
| 37 | A | 405 | CLA | CHB-C1B | 2.95 | 1.46 | 1.39 |
| 37 | C | 507 | CLA | CHB-C1B | 2.95 | 1.46 | 1.39 |
| 41 | A | 408 | LMG | O7-C8 | -2.95 | 1.39 | 1.46 |
| 37 | c | 507 | CLA | CHB-C1B | 2.95 | 1.46 | 1.39 |
| 48 | 12 | 215 | A86 | O-C13 | -2.95 | 1.17 | 1.23 |
| 37 | b | 523 | CLA | C1D-ND | 2.95 | 1.41 | 1.37 |
| 37 | 18 | 203 | CLA | C4B-NB | -2.95 | 1.34 | 1.37 |
| 37 | 31 | 306 | CLA | CHB-C1B | 2.95 | 1.46 | 1.39 |
| 48 | 32 | 215 | A86 | O-C13 | -2.95 | 1.17 | 1.23 |
| 37 | b | 507 | CLA | CHC-C4B | 2.95 | 1.46 | 1.39 |
| 47 | 41 | 207 | KC1 | CHB-C4A | -2.95 | 1.32 | 1.39 |
| 38 | A | 404 | PHO | CMC-C2C | -2.94 | 1.46 | 1.50 |
| 48 | 40 | 213 | A86 | C14-C15 | 2.94 | 1.58 | 1.52 |
| 47 | 11 | 306 | KC1 | C4B-NB | -2.94 | 1.34 | 1.37 |
| 37 | 34 | 302 | CLA | CHB-C1B | 2.94 | 1.46 | 1.39 |
| 37 | B | 503 | CLA | OBD-CAD | 2.94 | 1.27 | 1.22 |
| 37 | 38 | 211 | CLA | C4C-C3C | 2.94 | 1.50 | 1.45 |
| 37 | A | 403 | CLA | C3D-C4D | -2.94 | 1.37 | 1.44 |
| 37 | 38 | 203 | CLA | C4B-NB | -2.94 | 1.34 | 1.37 |
| 37 | d | 403 | CLA | OBD-CAD | 2.94 | 1.27 | 1.22 |
| 39 | 5 | 101 | BCR | C30-C25 | -2.94 | 1.50 | 1.53 |
| 48 | 11 | 313 | A86 | C19-C18 | 2.94 | 1.56 | 1.52 |
| 37 | D | 405 | CLA | OBD-CAD | 2.94 | 1.27 | 1.22 |
| 50 | 21 | 216 | DD6 | C9-C8 | 2.94 | 1.42 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | C | 511 | CLA | OBD-CAD | 2.94 | 1.27 | 1.22 |
| 47 | 35 | 304 | KC1 | C4B-NB | -2.94 | 1.34 | 1.37 |
| 48 | 13 | 312 | A86 | C26-C27 | 2.93 | 1.42 | 1.35 |
| 48 | 35 | 313 | A86 | C26-C27 | 2.93 | 1.42 | 1.35 |
| 48 | 35 | 313 | A86 | C24-C1 | 2.93 | 1.52 | 1.46 |
| 37 | a | 403 | CLA | C3D-C4D | -2.93 | 1.37 | 1.44 |
| 48 | 40 | 201 | A86 | C25-C24 | 2.93 | 1.42 | 1.34 |
| 48 | 15 | 312 | A86 | O-C13 | -2.93 | 1.17 | 1.23 |
| 47 | 11 | 302 | KC1 | CHD-C1D | 2.93 | 1.46 | 1.39 |
| 48 | 12 | 214 | A86 | O-C13 | -2.93 | 1.17 | 1.23 |
| 48 | 18 | 212 | A86 | C25-C24 | 2.93 | 1.42 | 1.34 |
| 48 | 16 | 313 | A86 | C25-C24 | 2.93 | 1.42 | 1.34 |
| 48 | 35 | 316 | A86 | C25-C24 | 2.93 | 1.42 | 1.34 |
| 48 | 37 | 311 | A86 | C14-C15 | 2.93 | 1.58 | 1.52 |
| 48 | 15 | 313 | A86 | C26-C27 | 2.93 | 1.42 | 1.35 |
| 37 | 33 | 310 | CLA | C4B-NB | -2.93 | 1.34 | 1.37 |
| 39 | 0 | 101 | BCR | C1-C6 | -2.93 | 1.50 | 1.53 |
| 38 | a | 406 | PHO | CMC-C2C | -2.93 | 1.46 | 1.50 |
| 47 | 31 | 303 | KC1 | CHD-C1D | 2.93 | 1.46 | 1.39 |
| 48 | 20 | 311 | A86 | C14-C15 | 2.93 | 1.58 | 1.52 |
| 50 | 41 | 216 | DD6 | C9-C8 | 2.92 | 1.42 | 1.34 |
| 41 | C | 518 | LMG | O1-C7 | -2.92 | 1.38 | 1.43 |
| 37 | 11 | 305 | CLA | CHB-C1B | 2.92 | 1.46 | 1.39 |
| 47 | 33 | 304 | KC1 | C4B-NB | -2.92 | 1.34 | 1.37 |
| 48 | 37 | 313 | A86 | O-C13 | -2.92 | 1.17 | 1.23 |
| 48 | 15 | 313 | A86 | C24-C1 | 2.92 | 1.52 | 1.46 |
| 37 | C | 510 | CLA | C3D-C2D | 2.92 | 1.47 | 1.39 |
| 47 | 13 | 309 | KC1 | C4B-NB | -2.92 | 1.34 | 1.37 |
| 47 | 16 | 305 | KC1 | C4B-NB | -2.92 | 1.34 | 1.37 |
| 37 | B | 506 | CLA | CHB-C1B | 2.92 | 1.46 | 1.39 |
| 37 | 18 | 201 | CLA | C4B-NB | -2.92 | 1.34 | 1.37 |
| 47 | 21 | 207 | KC1 | CHB-C4A | -2.92 | 1.32 | 1.39 |
| 37 | d | 404 | CLA | CHB-C1B | 2.92 | 1.46 | 1.39 |
| 47 | 40 | 204 | KC1 | C4B-NB | -2.92 | 1.34 | 1.37 |
| 48 | 33 | 314 | A86 | C-C1 | 2.92 | 1.56 | 1.50 |
| 48 | 35 | 314 | A86 | C14-C15 | 2.92 | 1.58 | 1.52 |
| 40 | B | 522 | SQD | O48-C23 | 2.92 | 1.41 | 1.33 |
| 37 | Z | 102 | CLA | C4B-NB | -2.92 | 1.34 | 1.37 |
| 37 | 18 | 204 | CLA | C4B-NB | -2.91 | 1.34 | 1.37 |
| 48 | 38 | 212 | A86 | C25-C24 | 2.91 | 1.42 | 1.34 |
| 38 | a | 406 | PHO | C4D-ND | -2.91 | 1.34 | 1.38 |
| 37 | c | 502 | CLA | CHC-C4B | 2.91 | 1.45 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 205 | CLA | C4B-NB | -2.91 | 1.34 | 1.37 |
| 47 | 36 | 305 | KC1 | C4B-NB | -2.91 | 1.34 | 1.37 |
| 46 | v | 201 | HEM | CAC-C3C | 2.91 | 1.55 | 1.47 |
| 48 | 32 | 216 | A86 | C26-C27 | 2.91 | 1.42 | 1.35 |
| 48 | 33 | 313 | A86 | C24-C1 | 2.91 | 1.52 | 1.46 |
| 50 | 40 | 214 | DD6 | C9-C8 | 2.90 | 1.42 | 1.34 |
| 37 | B | 513 | CLA | OBD-CAD | 2.90 | 1.27 | 1.22 |
| 38 | A | 404 | PHO | C4D-ND | -2.90 | 1.34 | 1.38 |
| 48 | 17 | 310 | A86 | C25-C24 | 2.90 | 1.42 | 1.34 |
| 37 | c | 510 | CLA | C3D-C2D | 2.90 | 1.46 | 1.39 |
| 38 | D | 403 | PHO | CMC-C2C | -2.90 | 1.46 | 1.50 |
| 48 | 41 | 211 | A86 | C14-C15 | 2.90 | 1.58 | 1.52 |
| 48 | 31 | 319 | A86 | C19-C18 | 2.90 | 1.56 | 1.52 |
| 37 | C | 508 | CLA | CHB-C1B | 2.90 | 1.45 | 1.39 |
| 48 | 31 | 313 | A86 | C25-C24 | 2.90 | 1.42 | 1.34 |
| 37 | 41 | 205 | CLA | C4B-NB | -2.90 | 1.34 | 1.37 |
| 48 | 21 | 213 | A86 | C26-C27 | 2.90 | 1.42 | 1.35 |
| 48 | 37 | 311 | A86 | C26-C27 | 2.90 | 1.42 | 1.35 |
| 48 | 38 | 214 | A86 | C14-C15 | 2.90 | 1.58 | 1.52 |
| 37 | 38 | 201 | CLA | C4B-NB | -2.90 | 1.34 | 1.37 |
| 48 | 21 | 213 | A86 | C24-C1 | 2.90 | 1.52 | 1.46 |
| 39 | 0 | 101 | BCR | C30-C25 | -2.90 | 1.50 | 1.53 |
| 50 | 21 | 212 | DD6 | C9-C8 | 2.90 | 1.42 | 1.34 |
| 48 | 11 | 319 | A86 | C19-C18 | 2.90 | 1.56 | 1.52 |
| 46 | V | 201 | HEM | CAC-C3C | 2.90 | 1.55 | 1.47 |
| 40 | b | 521 | SQD | O48-C23 | 2.89 | 1.41 | 1.33 |
| 48 | 41 | 213 | A86 | C24-C1 | 2.89 | 1.52 | 1.46 |
| 48 | 40 | 211 | A86 | C25-C24 | 2.89 | 1.42 | 1.34 |
| 48 | 17 | 312 | A86 | C14-C15 | 2.89 | 1.58 | 1.52 |
| 37 | c | 508 | CLA | CHB-C1B | 2.89 | 1.45 | 1.39 |
| 48 | 13 | 315 | A86 | C25-C24 | 2.89 | 1.42 | 1.34 |
| 48 | 37 | 309 | A86 | C25-C24 | 2.89 | 1.42 | 1.34 |
| 37 | b | 516 | CLA | CHB-C1B | 2.89 | 1.45 | 1.39 |
| 37 | b | 506 | CLA | CHB-C1B | 2.89 | 1.45 | 1.39 |
| 37 | A | 405 | CLA | C3D-C4D | -2.89 | 1.37 | 1.44 |
| 48 | 12 | 217 | A86 | C25-C24 | 2.89 | 1.42 | 1.34 |
| 48 | 32 | 218 | A86 | C25-C24 | 2.89 | 1.42 | 1.34 |
| 48 | 13 | 313 | A86 | C24-C1 | 2.89 | 1.52 | 1.46 |
| 39 | 5 | 101 | BCR | C1-C6 | -2.89 | 1.50 | 1.53 |
| 37 | 32 | 213 | CLA | C4B-NB | -2.89 | 1.34 | 1.37 |
| 37 | c | 509 | CLA | C3D-C4D | -2.89 | 1.37 | 1.44 |
| 50 | 20 | 312 | DD6 | C9-C8 | 2.89 | 1.42 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 14 | 313 | A86 | C14-C15 | 2.89 | 1.58 | 1.52 |
| 48 | 34 | 313 | A86 | C14-C15 | 2.89 | 1.58 | 1.52 |
| 48 | 17 | 313 | A86 | C25-C24 | 2.89 | 1.42 | 1.34 |
| 48 | 37 | 312 | A86 | C25-C24 | 2.89 | 1.42 | 1.34 |
| 47 | 12 | 206 | KC1 | CHB-C4A | -2.89 | 1.32 | 1.39 |
| 47 | 32 | 207 | KC1 | CHB-C4A | -2.89 | 1.32 | 1.39 |
| 48 | 15 | 316 | A86 | C25-C24 | 2.88 | 1.42 | 1.34 |
| 48 | 41 | 213 | A86 | C26-C27 | 2.88 | 1.42 | 1.35 |
| 48 | 14 | 313 | A86 | C24-C1 | 2.88 | 1.52 | 1.46 |
| 37 | 15 | 308 | CLA | C4B-NB | -2.88 | 1.34 | 1.37 |
| 48 | 32 | 216 | A86 | O-C13 | -2.88 | 1.17 | 1.23 |
| 47 | 31 | 309 | KC1 | OBD-CAD | 2.88 | 1.27 | 1.22 |
| 45 | d | 402 | PL9 | C3-C4 | -2.88 | 1.45 | 1.49 |
| 48 | 13 | 314 | A86 | C-C1 | 2.88 | 1.56 | 1.50 |
| 48 | 37 | 314 | A86 | C25-C24 | 2.88 | 1.42 | 1.34 |
| 48 | 19 | 313 | A86 | C17-C18 | -2.88 | 1.48 | 1.52 |
| 37 | B | 516 | CLA | CHB-C1B | 2.88 | 1.45 | 1.39 |
| 47 | 15 | 304 | KC1 | C4B-NB | -2.88 | 1.34 | 1.37 |
| 50 | 41 | 212 | DD6 | C9-C8 | 2.88 | 1.42 | 1.34 |
| 37 | 14 | 305 | CLA | C4B-NB | -2.88 | 1.34 | 1.37 |
| 47 | 16 | 302 | KC1 | C4B-NB | -2.88 | 1.34 | 1.37 |
| 48 | 17 | 312 | A86 | C26-C27 | 2.88 | 1.42 | 1.35 |
| 48 | 33 | 312 | A86 | C26-C27 | 2.88 | 1.42 | 1.35 |
| 38 | a | 405 | PHO | CMC-C2C | -2.88 | 1.46 | 1.50 |
| 37 | 38 | 203 | CLA | C4D-CHA | 2.88 | 1.48 | 1.38 |
| 47 | 32 | 209 | KC1 | CHD-C1D | 2.87 | 1.45 | 1.39 |
| 37 | b | 504 | CLA | C3D-C4D | -2.87 | 1.37 | 1.44 |
| 40 | a | 409 | SQD | O48-C23 | 2.87 | 1.41 | 1.33 |
| 37 | B | 504 | CLA | C3D-C4D | -2.87 | 1.37 | 1.44 |
| 47 | 17 | 303 | KC1 | C2A-C1A | 2.87 | 1.53 | 1.44 |
| 37 | D | 406 | CLA | CHB-C1B | 2.87 | 1.45 | 1.39 |
| 48 | 11 | 314 | A86 | C25-C24 | 2.87 | 1.42 | 1.34 |
| 48 | 21 | 211 | A86 | C14-C15 | 2.87 | 1.58 | 1.52 |
| 48 | 12 | 215 | A86 | C26-C27 | 2.87 | 1.42 | 1.35 |
| 48 | 14 | 314 | A86 | C14-C15 | 2.87 | 1.58 | 1.52 |
| 48 | 34 | 314 | A86 | C14-C15 | 2.87 | 1.58 | 1.52 |
| 37 | 18 | 203 | CLA | C4D-CHA | 2.87 | 1.48 | 1.38 |
| 41 | D | 412 | LMG | O7-C8 | -2.87 | 1.39 | 1.46 |
| 44 | c | 517 | DGD | O5D-C6D | -2.87 | 1.38 | 1.43 |
| 48 | 33 | 315 | A86 | C25-C24 | 2.87 | 1.42 | 1.34 |
| 37 | b | 513 | CLA | OBD-CAD | 2.87 | 1.27 | 1.22 |
| 50 | 41 | 216 | DD6 | C26-C27 | -2.87 | 1.31 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | C | 502 | CLA | CHC-C4B | 2.87 | 1.45 | 1.39 |
| 50 | 21 | 216 | DD6 | C26-C27 | -2.86 | 1.31 | 1.37 |
| 40 | A | 407 | SQD | O48-C23 | 2.86 | 1.41 | 1.33 |
| 48 | 16 | 311 | A86 | C25-C24 | 2.86 | 1.42 | 1.34 |
| 47 | 33 | 309 | KC1 | C4B-NB | -2.86 | 1.34 | 1.37 |
| 37 | B | 502 | CLA | C3D-C4D | -2.86 | 1.37 | 1.44 |
| 37 | 12 | 212 | CLA | C4B-NB | -2.86 | 1.34 | 1.37 |
| 50 | 21 | 216 | DD6 | C35-C36 | 2.86 | 1.55 | 1.51 |
| 45 | D | 404 | PL9 | C3-C4 | -2.86 | 1.45 | 1.49 |
| 37 | C | 509 | CLA | C3D-C4D | -2.86 | 1.37 | 1.44 |
| 48 | 15 | 312 | A86 | C24-C1 | 2.86 | 1.52 | 1.46 |
| 48 | 20 | 309 | A86 | C25-C24 | 2.86 | 1.42 | 1.34 |
| 48 | 17 | 315 | A86 | C25-C24 | 2.86 | 1.42 | 1.34 |
| 44 | C | 517 | DGD | O2G-C2G | -2.85 | 1.39 | 1.46 |
| 44 | c | 517 | DGD | O2G-C2G | -2.85 | 1.39 | 1.46 |
| 48 | 35 | 316 | A86 | C14-C15 | 2.85 | 1.58 | 1.52 |
| 48 | 35 | 315 | A86 | C25-C24 | 2.85 | 1.42 | 1.34 |
| 48 | 35 | 319 | A86 | C25-C24 | 2.85 | 1.42 | 1.34 |
| 50 | 41 | 216 | DD6 | C35-C36 | 2.85 | 1.55 | 1.51 |
| 37 | c | 511 | CLA | C3D-C4D | -2.85 | 1.37 | 1.44 |
| 43 | a | 412 | LHG | O8-C6 | -2.85 | 1.38 | 1.45 |
| 48 | 34 | 313 | A86 | C-C1 | 2.85 | 1.56 | 1.50 |
| 47 | 37 | 302 | KC1 | C2A-C1A | 2.85 | 1.53 | 1.44 |
| 48 | 35 | 312 | A86 | C-C1 | 2.85 | 1.56 | 1.50 |
| 37 | b | 508 | CLA | CHB-C1B | 2.85 | 1.45 | 1.39 |
| 41 | d | 409 | LMG | O7-C8 | -2.85 | 1.39 | 1.46 |
| 43 | D | 411 | LHG | O8-C6 | -2.85 | 1.38 | 1.45 |
| 44 | C | 517 | DGD | O5D-C6D | -2.85 | 1.38 | 1.43 |
| 47 | 32 | 212 | KC1 | CHB-C4A | -2.85 | 1.32 | 1.39 |
| 48 | 31 | 314 | A86 | C25-C24 | 2.85 | 1.42 | 1.34 |
| 40 | L | 101 | SQD | O47-C7 | 2.85 | 1.42 | 1.34 |
| 47 | 41 | 207 | KC1 | C4B-NB | -2.85 | 1.34 | 1.37 |
| 47 | 12 | 211 | KC1 | CHB-C4A | -2.85 | 1.32 | 1.39 |
| 48 | 15 | 315 | A86 | C25-C24 | 2.85 | 1.42 | 1.34 |
| 48 | 33 | 313 | A86 | C-C1 | 2.85 | 1.56 | 1.50 |
| 48 | 15 | 314 | A86 | C14-C15 | 2.85 | 1.58 | 1.52 |
| 37 | 34 | 305 | CLA | C4B-NB | -2.84 | 1.34 | 1.37 |
| 48 | 15 | 319 | A86 | C25-C24 | 2.84 | 1.42 | 1.34 |
| 37 | B | 503 | CLA | CHB-C1B | 2.84 | 1.45 | 1.39 |
| 48 | 34 | 313 | A86 | C24-C1 | 2.84 | 1.52 | 1.46 |
| 47 | 12 | 208 | KC1 | CHD-C1D | 2.84 | 1.45 | 1.39 |
| 48 | 37 | 310 | A86 | O-C13 | -2.84 | 1.17 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 11 | 306 | KC1 | CHD-C1D | 2.84 | 1.45 | 1.39 |
| 47 | 31 | 307 | KC1 | CHD-C1D | 2.84 | 1.45 | 1.39 |
| 48 | 35 | 314 | A86 | C26-C27 | 2.84 | 1.42 | 1.35 |
| 48 | 15 | 315 | A86 | C14-C15 | 2.84 | 1.58 | 1.52 |
| 40 | B | 519 | SQD | O47-C7 | 2.84 | 1.42 | 1.34 |
| 48 | 15 | 314 | A86 | C-C1 | 2.84 | 1.56 | 1.50 |
| 47 | 36 | 302 | KC1 | C4B-NB | -2.84 | 1.34 | 1.37 |
| 47 | 38 | 207 | KC1 | C4B-NB | -2.84 | 1.34 | 1.37 |
| 37 | b | 502 | CLA | C3D-C4D | -2.84 | 1.37 | 1.44 |
| 37 | C | 511 | CLA | C3D-C4D | -2.83 | 1.37 | 1.44 |
| 37 | D | 402 | CLA | C3D-C4D | -2.83 | 1.37 | 1.44 |
| 48 | 37 | 312 | A86 | C-C1 | 2.83 | 1.56 | 1.50 |
| 48 | 13 | 313 | A86 | C26-C27 | 2.83 | 1.42 | 1.35 |
| 47 | 11 | 309 | KC1 | OBD-CAD | 2.83 | 1.27 | 1.22 |
| 48 | 32 | 215 | A86 | C26-C27 | 2.83 | 1.42 | 1.35 |
| 48 | 12 | 216 | A86 | C25-C24 | 2.83 | 1.42 | 1.34 |
| 48 | 11 | 319 | A86 | O-C13 | -2.83 | 1.17 | 1.23 |
| 37 | b | 503 | CLA | CHB-C1B | 2.83 | 1.45 | 1.39 |
| 48 | 15 | 319 | A86 | C-C1 | 2.83 | 1.56 | 1.50 |
| 48 | 12 | 214 | A86 | C26-C27 | 2.83 | 1.42 | 1.35 |
| 37 | 41 | 202 | CLA | CHC-C4B | 2.83 | 1.45 | 1.39 |
| 48 | 17 | 313 | A86 | C-C1 | 2.83 | 1.56 | 1.50 |
| 48 | 36 | 311 | A86 | C25-C24 | 2.83 | 1.42 | 1.34 |
| 48 | 17 | 311 | A86 | O-C13 | -2.83 | 1.17 | 1.23 |
| 39 | C | 515 | BCR | C30-C25 | -2.83 | 1.50 | 1.53 |
| 48 | 32 | 217 | A86 | C25-C24 | 2.83 | 1.42 | 1.34 |
| 48 | 38 | 214 | A86 | C-C1 | 2.83 | 1.56 | 1.50 |
| 48 | 35 | 315 | A86 | O-C13 | -2.82 | 1.17 | 1.23 |
| 43 | D | 411 | LHG | O7-C5 | -2.82 | 1.40 | 1.46 |
| 37 | 38 | 209 | CLA | C4B-NB | -2.82 | 1.34 | 1.37 |
| 48 | 17 | 312 | A86 | C-C1 | 2.82 | 1.56 | 1.50 |
| 48 | 17 | 311 | A86 | C25-C24 | 2.82 | 1.42 | 1.34 |
| 48 | 33 | 313 | A86 | C26-C27 | 2.82 | 1.42 | 1.35 |
| 48 | 31 | 313 | A86 | O-C13 | -2.82 | 1.17 | 1.23 |
| 48 | 35 | 314 | A86 | C-C1 | 2.82 | 1.56 | 1.50 |
| 48 | 34 | 313 | A86 | C26-C27 | 2.82 | 1.42 | 1.35 |
| 37 | B | 508 | CLA | CHB-C1B | 2.82 | 1.45 | 1.39 |
| 37 | 21 | 202 | CLA | CHC-C4B | 2.82 | 1.45 | 1.39 |
| 48 | 21 | 214 | A86 | C14-C15 | 2.82 | 1.58 | 1.52 |
| 43 | a | 412 | LHG | O7-C5 | -2.82 | 1.40 | 1.46 |
| 48 | 35 | 312 | A86 | C24-C1 | 2.82 | 1.52 | 1.46 |
| 37 | 17 | 307 | CLA | CHB-C1B | 2.82 | 1.45 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 31 | 314 | A86 | O-C13 | -2.82 | 1.17 | 1.23 |
| 37 | B | 503 | CLA | C3D-C4D | -2.81 | 1.37 | 1.44 |
| 48 | 14 | 313 | A86 | C26-C27 | 2.81 | 1.42 | 1.35 |
| 50 | 20 | 310 | DD6 | O1-C20 | 2.81 | 1.49 | 1.46 |
| 48 | 15 | 312 | A86 | C-C1 | 2.81 | 1.56 | 1.50 |
| 39 | c | 515 | BCR | C30-C25 | -2.81 | 1.50 | 1.53 |
| 48 | 33 | 314 | A86 | C24-C1 | 2.81 | 1.52 | 1.46 |
| 48 | 14 | 314 | A86 | C-C1 | 2.81 | 1.56 | 1.50 |
| 48 | 34 | 314 | A86 | C-C1 | 2.81 | 1.56 | 1.50 |
| 48 | 31 | 319 | A86 | O-C13 | -2.81 | 1.17 | 1.23 |
| 47 | 13 | 306 | KC1 | CHD-C1D | 2.81 | 1.45 | 1.39 |
| 48 | 18 | 214 | A86 | C-C1 | 2.81 | 1.56 | 1.50 |
| 37 | C | 502 | CLA | C1C-NC | -2.81 | 1.33 | 1.37 |
| 50 | 36 | 312 | DD6 | C35-C36 | 2.81 | 1.55 | 1.51 |
| 48 | 41 | 211 | A86 | C25-C24 | 2.80 | 1.42 | 1.34 |
| 50 | 40 | 212 | DD6 | O1-C20 | 2.80 | 1.49 | 1.46 |
| 37 | b | 510 | CLA | C3D-C4D | -2.80 | 1.37 | 1.44 |
| 48 | 11 | 314 | A86 | O-C13 | -2.80 | 1.17 | 1.23 |
| 48 | 15 | 315 | A86 | O-C13 | -2.80 | 1.17 | 1.23 |
| 47 | 18 | 207 | KC1 | C4B-NB | -2.80 | 1.34 | 1.37 |
| 37 | C | 507 | CLA | C3D-C4D | -2.80 | 1.37 | 1.44 |
| 48 | 40 | 213 | A86 | C24-C1 | 2.80 | 1.51 | 1.46 |
| 48 | 15 | 314 | A86 | C26-C27 | 2.80 | 1.42 | 1.35 |
| 37 | d | 401 | CLA | C3D-C4D | -2.80 | 1.37 | 1.44 |
| 48 | 12 | 215 | A86 | C-C1 | 2.80 | 1.56 | 1.50 |
| 48 | 21 | 215 | A86 | C24-C1 | 2.80 | 1.51 | 1.46 |
| 48 | 37 | 311 | A86 | C-C1 | 2.80 | 1.56 | 1.50 |
| 48 | 41 | 214 | A86 | C14-C15 | 2.80 | 1.58 | 1.52 |
| 48 | 15 | 311 | A86 | C26-C27 | 2.80 | 1.42 | 1.35 |
| 48 | 35 | 319 | A86 | C-C1 | 2.80 | 1.56 | 1.50 |
| 47 | 16 | 308 | KC1 | C2A-C1A | 2.80 | 1.53 | 1.44 |
| 37 | 41 | 208 | CLA | C4B-NB | -2.80 | 1.34 | 1.37 |
| 37 | c | 507 | CLA | C3D-C4D | -2.80 | 1.37 | 1.44 |
| 37 | b | 515 | CLA | C3D-C4D | -2.80 | 1.37 | 1.44 |
| 37 | B | 504 | CLA | CHC-C4B | 2.79 | 1.45 | 1.39 |
| 37 | b | 505 | CLA | CHB-C1B | 2.79 | 1.45 | 1.39 |
| 48 | 32 | 203 | A86 | C19-C18 | 2.79 | 1.56 | 1.52 |
| 48 | 13 | 314 | A86 | C24-C1 | 2.79 | 1.51 | 1.46 |
| 37 | 12 | 212 | CLA | C4D-CHA | 2.79 | 1.48 | 1.38 |
| 37 | 18 | 209 | CLA | C4D-CHA | 2.79 | 1.48 | 1.38 |
| 37 | 21 | 208 | CLA | C4B-NB | -2.79 | 1.34 | 1.37 |
| 48 | 12 | 217 | A86 | C19-C18 | 2.79 | 1.56 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | B | 514 | CLA | C3D-C4D | -2.79 | 1.37 | 1.44 |
| 37 | 32 | 213 | CLA | C4D-CHA | 2.79 | 1.48 | 1.38 |
| 48 | 11 | 312 | A86 | C25-C24 | 2.79 | 1.42 | 1.34 |
| 37 | 40 | 209 | CLA | C4B-NB | -2.79 | 1.34 | 1.37 |
| 47 | 15 | 309 | KC1 | C2A-C1A | 2.79 | 1.53 | 1.44 |
| 37 | B | 510 | CLA | C3D-C4D | -2.79 | 1.37 | 1.44 |
| 48 | 14 | 312 | A86 | O-C13 | -2.79 | 1.17 | 1.23 |
| 48 | 34 | 312 | A86 | O-C13 | -2.79 | 1.17 | 1.23 |
| 48 | 11 | 315 | A86 | O-C13 | -2.79 | 1.17 | 1.23 |
| 37 | 15 | 305 | CLA | C4D-CHA | 2.79 | 1.47 | 1.38 |
| 48 | 14 | 312 | A86 | C14-C15 | 2.79 | 1.58 | 1.52 |
| 48 | 11 | 313 | A86 | O-C13 | -2.79 | 1.17 | 1.23 |
| 47 | 17 | 306 | KC1 | C2A-C1A | 2.79 | 1.53 | 1.44 |
| 47 | 37 | 305 | KC1 | C2A-C1A | 2.79 | 1.53 | 1.44 |
| 47 | 40 | 204 | KC1 | CHB-C4A | -2.78 | 1.32 | 1.39 |
| 48 | 14 | 313 | A86 | C-C1 | 2.78 | 1.56 | 1.50 |
| 48 | 41 | 215 | A86 | C-C1 | 2.78 | 1.56 | 1.50 |
| 48 | 34 | 312 | A86 | C14-C15 | 2.78 | 1.58 | 1.52 |
| 48 | 33 | 312 | A86 | C24-C1 | 2.78 | 1.51 | 1.46 |
| 37 | 35 | 305 | CLA | C4D-CHA | 2.78 | 1.47 | 1.38 |
| 37 | b | 504 | CLA | CHC-C4B | 2.78 | 1.45 | 1.39 |
| 43 | B | 523 | LHG | O7-C5 | -2.78 | 1.40 | 1.46 |
| 48 | 13 | 313 | A86 | C-C1 | 2.78 | 1.56 | 1.50 |
| 37 | b | 508 | CLA | C3D-C4D | -2.78 | 1.37 | 1.44 |
| 37 | 41 | 208 | CLA | C4D-CHA | 2.78 | 1.47 | 1.38 |
| 37 | 38 | 209 | CLA | C4D-CHA | 2.78 | 1.47 | 1.38 |
| 48 | 18 | 213 | A86 | C-C1 | 2.78 | 1.56 | 1.50 |
| 48 | 35 | 315 | A86 | C14-C15 | 2.78 | 1.58 | 1.52 |
| 37 | 14 | 302 | CLA | C4D-CHA | 2.78 | 1.47 | 1.38 |
| 40 | 17 | 301 | SQD | O47-C7 | 2.78 | 1.42 | 1.34 |
| 48 | 36 | 310 | A86 | O-C13 | -2.78 | 1.17 | 1.23 |
| 48 | 13 | 312 | A86 | C24-C1 | 2.78 | 1.51 | 1.46 |
| 48 | 15 | 313 | A86 | C-C1 | 2.78 | 1.56 | 1.50 |
| 48 | 35 | 313 | A86 | C-C1 | 2.78 | 1.56 | 1.50 |
| 43 | b | 522 | LHG | O7-C5 | -2.78 | 1.40 | 1.46 |
| 48 | 13 | 314 | A86 | C26-C27 | 2.77 | 1.42 | 1.35 |
| 37 | 19 | 307 | CLA | CHB-C1B | 2.77 | 1.45 | 1.39 |
| 37 | 37 | 306 | CLA | CHB-C1B | 2.77 | 1.45 | 1.39 |
| 48 | 37 | 314 | A86 | C-C1 | 2.77 | 1.56 | 1.50 |
| 47 | 12 | 208 | KC1 | C2A-C1A | 2.77 | 1.53 | 1.44 |
| 48 | 16 | 311 | A86 | C14-C15 | 2.77 | 1.58 | 1.52 |
| 47 | 36 | 308 | KC1 | C2A-C1A | 2.77 | 1.53 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 35 | 311 | A86 | C26-C27 | 2.77 | 1.42 | 1.35 |
| 48 | 21 | 214 | A86 | C-C1 | 2.77 | 1.56 | 1.50 |
| 37 | B | 505 | CLA | CHB-C1B | 2.77 | 1.45 | 1.39 |
| 48 | 34 | 314 | A86 | C26-C27 | 2.77 | 1.42 | 1.35 |
| 48 | 16 | 310 | A86 | O-C13 | -2.77 | 1.17 | 1.23 |
| 48 | 37 | 312 | A86 | C14-C15 | 2.77 | 1.58 | 1.52 |
| 37 | B | 508 | CLA | C3D-C4D | -2.77 | 1.38 | 1.44 |
| 37 | 15 | 303 | CLA | C4B-NB | -2.77 | 1.34 | 1.37 |
| 48 | 21 | 215 | A86 | C-C1 | 2.77 | 1.56 | 1.50 |
| 37 | 18 | 211 | CLA | C4D-CHA | 2.77 | 1.47 | 1.38 |
| 47 | 35 | 309 | KC1 | C2A-C1A | 2.77 | 1.53 | 1.44 |
| 41 | c | 518 | LMG | O8-C9 | -2.77 | 1.39 | 1.45 |
| 47 | 33 | 306 | KC1 | CHD-C1D | 2.77 | 1.45 | 1.39 |
| 41 | C | 518 | LMG | O7-C8 | -2.77 | 1.40 | 1.46 |
| 37 | b | 516 | CLA | C3D-C4D | -2.77 | 1.38 | 1.44 |
| 37 | 38 | 211 | CLA | C4D-CHA | 2.77 | 1.47 | 1.38 |
| 48 | 32 | 216 | A86 | C14-C15 | 2.77 | 1.58 | 1.52 |
| 47 | 20 | 302 | KC1 | CHB-C4A | -2.76 | 1.32 | 1.39 |
| 48 | 12 | 202 | A86 | C19-C18 | 2.76 | 1.56 | 1.52 |
| 37 | D | 405 | CLA | C3D-C4D | -2.76 | 1.38 | 1.44 |
| 47 | 41 | 203 | KC1 | C2A-C1A | 2.76 | 1.53 | 1.44 |
| 37 | b | 503 | CLA | C3D-C4D | -2.76 | 1.38 | 1.44 |
| 37 | 19 | 304 | CLA | C4C-C3C | 2.76 | 1.49 | 1.45 |
| 37 | c | 506 | CLA | C3D-C4D | -2.76 | 1.38 | 1.44 |
| 48 | 18 | 215 | A86 | C-C1 | 2.76 | 1.56 | 1.50 |
| 48 | 35 | 316 | A86 | C-C1 | 2.76 | 1.56 | 1.50 |
| 47 | 16 | 308 | KC1 | C4A-C3A | 2.76 | 1.50 | 1.44 |
| 47 | 34 | 304 | KC1 | CHB-C4A | -2.76 | 1.32 | 1.39 |
| 37 | b | 505 | CLA | C3D-C4D | -2.76 | 1.38 | 1.44 |
| 37 | B | 515 | CLA | C3D-C4D | -2.76 | 1.38 | 1.44 |
| 37 | 13 | 307 | CLA | C4D-CHA | 2.76 | 1.47 | 1.38 |
| 48 | 20 | 311 | A86 | C24-C1 | 2.76 | 1.51 | 1.46 |
| 48 | 32 | 216 | A86 | C-C1 | 2.76 | 1.56 | 1.50 |
| 37 | 15 | 307 | CLA | CHB-C1B | 2.76 | 1.45 | 1.39 |
| 48 | 21 | 211 | A86 | C25-C24 | 2.75 | 1.41 | 1.34 |
| 37 | 34 | 302 | CLA | C4D-CHA | 2.75 | 1.47 | 1.38 |
| 48 | 31 | 312 | A86 | C25-C24 | 2.75 | 1.41 | 1.34 |
| 50 | 16 | 312 | DD6 | C35-C36 | 2.75 | 1.55 | 1.51 |
| 37 | 18 | 209 | CLA | C4B-NB | -2.75 | 1.34 | 1.37 |
| 47 | 21 | 207 | KC1 | C4B-NB | -2.75 | 1.34 | 1.37 |
| 37 | 33 | 307 | CLA | C3D-C4D | -2.75 | 1.38 | 1.44 |
| 37 | 33 | 307 | CLA | C4D-CHA | 2.75 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 35 | 303 | CLA | C4B-NB | -2.75 | 1.34 | 1.37 |
| 48 | 31 | 315 | A86 | O-C13 | -2.75 | 1.17 | 1.23 |
| 37 | 21 | 208 | CLA | C4D-CHA | 2.75 | 1.47 | 1.38 |
| 47 | 21 | 203 | KC1 | C2A-C1A | 2.75 | 1.53 | 1.44 |
| 37 | B | 516 | CLA | C3D-C4D | -2.75 | 1.38 | 1.44 |
| 48 | 38 | 215 | A86 | C-C1 | 2.75 | 1.56 | 1.50 |
| 37 | B | 512 | CLA | C1D-ND | 2.75 | 1.41 | 1.37 |
| 48 | 15 | 316 | A86 | C-C1 | 2.75 | 1.56 | 1.50 |
| 48 | 18 | 214 | A86 | C26-C27 | 2.75 | 1.42 | 1.35 |
| 37 | 38 | 202 | CLA | C4D-CHA | 2.75 | 1.47 | 1.38 |
| 37 | 39 | 304 | CLA | C4C-C3C | 2.75 | 1.49 | 1.45 |
| 37 | d | 403 | CLA | C3D-C4D | -2.75 | 1.38 | 1.44 |
| 37 | C | 506 | CLA | C3D-C4D | -2.75 | 1.38 | 1.44 |
| 37 | d | 404 | CLA | C3D-C4D | -2.75 | 1.38 | 1.44 |
| 47 | 36 | 308 | KC1 | C4A-C3A | 2.75 | 1.50 | 1.44 |
| 37 | b | 514 | CLA | C3D-C4D | -2.75 | 1.38 | 1.44 |
| 48 | 15 | 311 | A86 | C25-C24 | 2.75 | 1.41 | 1.34 |
| 41 | c | 518 | LMG | O7-C8 | -2.74 | 1.40 | 1.46 |
| 48 | 39 | 313 | A86 | C25-C24 | 2.74 | 1.41 | 1.34 |
| 37 | c | 502 | CLA | C1C-NC | -2.74 | 1.33 | 1.37 |
| 37 | 39 | 307 | CLA | CHB-C1B | 2.74 | 1.45 | 1.39 |
| 48 | 41 | 214 | A86 | C-C1 | 2.74 | 1.56 | 1.50 |
| 48 | 32 | 217 | A86 | C-C1 | 2.74 | 1.56 | 1.50 |
| 37 | B | 507 | CLA | C3D-C4D | -2.74 | 1.38 | 1.44 |
| 37 | C | 501 | CLA | C3D-C4D | -2.74 | 1.38 | 1.44 |
| 48 | 13 | 315 | A86 | C-C1 | 2.74 | 1.56 | 1.50 |
| 48 | 36 | 313 | A86 | C-C1 | 2.74 | 1.56 | 1.50 |
| 47 | 32 | 209 | KC1 | C2A-C1A | 2.74 | 1.53 | 1.44 |
| 37 | 13 | 307 | CLA | C3D-C4D | -2.74 | 1.38 | 1.44 |
| 48 | 14 | 314 | A86 | C26-C27 | 2.74 | 1.42 | 1.35 |
| 37 | B | 505 | CLA | C3D-C4D | -2.74 | 1.38 | 1.44 |
| 41 | d | 409 | LMG | O1-C7 | -2.74 | 1.39 | 1.43 |
| 48 | 13 | 311 | A86 | C25-C24 | 2.74 | 1.41 | 1.34 |
| 47 | 40 | 206 | KC1 | C4A-C3A | 2.74 | 1.50 | 1.44 |
| 41 | C | 518 | LMG | O8-C9 | -2.74 | 1.39 | 1.45 |
| 37 | 20 | 307 | CLA | C4D-CHA | 2.74 | 1.47 | 1.38 |
| 37 | b | 512 | CLA | C1D-ND | 2.74 | 1.41 | 1.37 |
| 37 | c | 505 | CLA | C3D-C4D | -2.74 | 1.38 | 1.44 |
| 48 | 17 | 313 | A86 | O-C13 | -2.74 | 1.17 | 1.23 |
| 48 | 41 | 213 | A86 | C-C1 | 2.74 | 1.56 | 1.50 |
| 48 | 17 | 313 | A86 | C14-C15 | 2.74 | 1.58 | 1.52 |
| 37 | 40 | 205 | CLA | C4D-CHA | 2.74 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 12 | 216 | A86 | O-C13 | -2.74 | 1.17 | 1.23 |
| 37 | B | 511 | CLA | C3D-C4D | -2.74 | 1.38 | 1.44 |
| 48 | 21 | 213 | A86 | C-C1 | 2.74 | 1.56 | 1.50 |
| 37 | 41 | 205 | CLA | C4D-CHA | 2.73 | 1.47 | 1.38 |
| 50 | 19 | 312 | DD6 | C35-C34 | 2.73 | 1.57 | 1.52 |
| 48 | 19 | 313 | A86 | C25-C24 | 2.73 | 1.41 | 1.34 |
| 47 | 11 | 304 | KC1 | CHB-C4A | -2.73 | 1.33 | 1.39 |
| 47 | 17 | 308 | KC1 | CHB-C4A | -2.73 | 1.33 | 1.39 |
| 47 | 31 | 305 | KC1 | CHB-C4A | -2.73 | 1.33 | 1.39 |
| 47 | 37 | 307 | KC1 | CHB-C4A | -2.73 | 1.33 | 1.39 |
| 37 | B | 510 | CLA | C1C-NC | -2.73 | 1.33 | 1.37 |
| 48 | 38 | 213 | A86 | C-C1 | 2.73 | 1.56 | 1.50 |
| 37 | D | 406 | CLA | C3D-C4D | -2.73 | 1.38 | 1.44 |
| 37 | 38 | 206 | CLA | C4B-NB | -2.73 | 1.34 | 1.37 |
| 48 | 12 | 215 | A86 | C14-C15 | 2.73 | 1.58 | 1.52 |
| 48 | 41 | 215 | A86 | C24-C1 | 2.73 | 1.51 | 1.46 |
| 44 | J | 101 | DGD | O1G-C1G | -2.73 | 1.39 | 1.45 |
| 47 | 16 | 302 | KC1 | C4A-C3A | 2.73 | 1.50 | 1.44 |
| 48 | 18 | 213 | A86 | C25-C24 | 2.73 | 1.41 | 1.34 |
| 48 | 41 | 211 | A86 | C26-C27 | 2.73 | 1.42 | 1.35 |
| 37 | 35 | 308 | CLA | C4B-NB | -2.73 | 1.34 | 1.37 |
| 37 | c | 501 | CLA | C3D-C4D | -2.73 | 1.38 | 1.44 |
| 48 | 21 | 215 | A86 | C26-C27 | 2.73 | 1.42 | 1.35 |
| 48 | 32 | 216 | A86 | C24-C1 | 2.73 | 1.51 | 1.46 |
| 47 | 12 | 208 | KC1 | CHB-C4A | -2.73 | 1.33 | 1.39 |
| 37 | 20 | 303 | CLA | C4D-CHA | 2.73 | 1.47 | 1.38 |
| 47 | 40 | 207 | KC1 | C4C-C3C | 2.73 | 1.49 | 1.45 |
| 40 | 36 | 315 | SQD | O47-C7 | 2.73 | 1.42 | 1.34 |
| 47 | 20 | 304 | KC1 | C4A-C3A | 2.73 | 1.50 | 1.44 |
| 48 | 33 | 312 | A86 | O-C13 | -2.73 | 1.17 | 1.23 |
| 48 | 32 | 218 | A86 | C19-C18 | 2.73 | 1.56 | 1.52 |
| 48 | 20 | 311 | A86 | C-C1 | 2.73 | 1.56 | 1.50 |
| 37 | 17 | 309 | CLA | C4C-C3C | 2.72 | 1.49 | 1.45 |
| 37 | 21 | 205 | CLA | C4D-CHA | 2.72 | 1.47 | 1.38 |
| 37 | 33 | 310 | CLA | C4D-CHA | 2.72 | 1.47 | 1.38 |
| 48 | 38 | 213 | A86 | C25-C24 | 2.72 | 1.41 | 1.34 |
| 48 | 37 | 319 | A86 | C25-C24 | 2.72 | 1.41 | 1.34 |
| 47 | 37 | 307 | KC1 | C2A-C1A | 2.72 | 1.53 | 1.44 |
| 48 | 14 | 316 | A86 | C25-C24 | 2.72 | 1.41 | 1.34 |
| 48 | 34 | 316 | A86 | C25-C24 | 2.72 | 1.41 | 1.34 |
| 48 | 12 | 216 | A86 | C-C1 | 2.72 | 1.56 | 1.50 |
| 37 | b | 510 | CLA | C1C-NC | -2.72 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 32 | 209 | KC1 | CHB-C4A | -2.72 | 1.33 | 1.39 |
| 47 | 33 | 304 | KC1 | CHB-C4A | -2.72 | 1.33 | 1.39 |
| 38 | D | 403 | PHO | CMD-C2D | -2.72 | 1.46 | 1.51 |
| 37 | 20 | 308 | CLA | C4D-CHA | 2.72 | 1.47 | 1.38 |
| 48 | 39 | 313 | A86 | C-C1 | 2.72 | 1.56 | 1.50 |
| 50 | 39 | 312 | DD6 | C35-C34 | 2.72 | 1.57 | 1.52 |
| 48 | 38 | 215 | A86 | C26-C27 | 2.72 | 1.42 | 1.35 |
| 38 | a | 405 | PHO | CMD-C2D | -2.72 | 1.46 | 1.51 |
| 48 | 35 | 313 | A86 | O-C13 | -2.72 | 1.17 | 1.23 |
| 48 | 40 | 213 | A86 | C-C1 | 2.72 | 1.56 | 1.50 |
| 48 | 14 | 315 | A86 | O-C13 | -2.72 | 1.17 | 1.23 |
| 37 | 33 | 305 | CLA | C4D-CHA | 2.72 | 1.47 | 1.38 |
| 37 | 20 | 307 | CLA | C4B-NB | -2.72 | 1.34 | 1.37 |
| 48 | 17 | 315 | A86 | C-C1 | 2.72 | 1.56 | 1.50 |
| 47 | 36 | 302 | KC1 | C4A-C3A | 2.72 | 1.50 | 1.44 |
| 44 | j | 101 | DGD | O1G-C1G | -2.71 | 1.39 | 1.45 |
| 37 | 15 | 307 | CLA | C4D-CHA | 2.71 | 1.47 | 1.38 |
| 37 | 35 | 307 | CLA | C4D-CHA | 2.71 | 1.47 | 1.38 |
| 48 | 33 | 314 | A86 | C26-C27 | 2.71 | 1.42 | 1.35 |
| 48 | 17 | 320 | A86 | C25-C24 | 2.71 | 1.41 | 1.34 |
| 37 | 18 | 202 | CLA | C4B-NB | -2.71 | 1.34 | 1.37 |
| 48 | 37 | 314 | A86 | O-C13 | -2.71 | 1.17 | 1.23 |
| 47 | 14 | 304 | KC1 | CHB-C4A | -2.71 | 1.33 | 1.39 |
| 37 | 39 | 307 | CLA | C4D-CHA | 2.71 | 1.47 | 1.38 |
| 48 | 41 | 215 | A86 | C26-C27 | 2.71 | 1.42 | 1.35 |
| 47 | 17 | 308 | KC1 | C2A-C1A | 2.71 | 1.53 | 1.44 |
| 48 | 33 | 311 | A86 | C25-C24 | 2.71 | 1.41 | 1.34 |
| 48 | 18 | 215 | A86 | C26-C27 | 2.71 | 1.42 | 1.35 |
| 41 | D | 412 | LMG | O1-C7 | -2.71 | 1.39 | 1.43 |
| 37 | D | 401 | CLA | C3D-C4D | -2.71 | 1.38 | 1.44 |
| 37 | 35 | 307 | CLA | CHB-C1B | 2.71 | 1.45 | 1.39 |
| 39 | D | 407 | BCR | C30-C25 | -2.71 | 1.50 | 1.53 |
| 48 | 16 | 310 | A86 | C14-C15 | 2.71 | 1.58 | 1.52 |
| 37 | 13 | 301 | CLA | C4D-CHA | 2.71 | 1.47 | 1.38 |
| 37 | 33 | 301 | CLA | C4D-CHA | 2.71 | 1.47 | 1.38 |
| 47 | 18 | 210 | KC1 | C4B-NB | -2.71 | 1.34 | 1.37 |
| 37 | 38 | 204 | CLA | C3D-C4D | -2.71 | 1.38 | 1.44 |
| 39 | K | 101 | BCR | C30-C25 | -2.71 | 1.50 | 1.53 |
| 47 | 20 | 305 | KC1 | C4C-C3C | 2.71 | 1.49 | 1.45 |
| 48 | 37 | 313 | A86 | C25-C24 | 2.71 | 1.41 | 1.34 |
| 37 | B | 507 | CLA | CHB-C1B | 2.71 | 1.45 | 1.39 |
| 37 | 40 | 205 | CLA | C3D-C4D | -2.71 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 18 | 210 | KC1 | C2A-C1A | 2.71 | 1.53 | 1.44 |
| 39 | y | 101 | BCR | C30-C25 | -2.71 | 1.50 | 1.53 |
| 48 | 32 | 218 | A86 | C-C1 | 2.71 | 1.56 | 1.50 |
| 47 | 38 | 210 | KC1 | C4B-NB | -2.70 | 1.34 | 1.37 |
| 48 | 38 | 214 | A86 | C26-C27 | 2.70 | 1.42 | 1.35 |
| 48 | 32 | 203 | A86 | O-C13 | -2.70 | 1.17 | 1.23 |
| 37 | B | 524 | CLA | C3D-C4D | -2.70 | 1.38 | 1.44 |
| 48 | 16 | 314 | A86 | C-C1 | 2.70 | 1.56 | 1.50 |
| 37 | B | 516 | CLA | OBD-CAD | 2.70 | 1.27 | 1.22 |
| 37 | 18 | 206 | CLA | C4D-CHA | 2.70 | 1.47 | 1.38 |
| 48 | 12 | 217 | A86 | C-C1 | 2.70 | 1.56 | 1.50 |
| 37 | 18 | 204 | CLA | C3D-C4D | -2.70 | 1.38 | 1.44 |
| 48 | 19 | 311 | A86 | C14-C15 | 2.70 | 1.58 | 1.52 |
| 48 | 36 | 310 | A86 | C14-C15 | 2.70 | 1.58 | 1.52 |
| 48 | 37 | 309 | A86 | C14-C15 | 2.70 | 1.58 | 1.52 |
| 48 | 39 | 311 | A86 | C14-C15 | 2.70 | 1.58 | 1.52 |
| 37 | 15 | 308 | CLA | C4D-CHA | 2.70 | 1.47 | 1.38 |
| 37 | 37 | 306 | CLA | C4D-CHA | 2.70 | 1.47 | 1.38 |
| 48 | 31 | 315 | A86 | C19-C18 | 2.70 | 1.56 | 1.52 |
| 48 | 11 | 315 | A86 | C25-C24 | 2.70 | 1.41 | 1.34 |
| 48 | 19 | 313 | A86 | C-C1 | 2.70 | 1.56 | 1.50 |
| 37 | b | 507 | CLA | CHB-C1B | 2.70 | 1.45 | 1.39 |
| 37 | 40 | 210 | CLA | C4D-CHA | 2.70 | 1.47 | 1.38 |
| 48 | 17 | 310 | A86 | C14-C15 | 2.70 | 1.58 | 1.52 |
| 47 | 38 | 207 | KC1 | C2A-C1A | 2.70 | 1.53 | 1.44 |
| 37 | 13 | 305 | CLA | C4D-CHA | 2.70 | 1.47 | 1.38 |
| 37 | C | 505 | CLA | C3D-C4D | -2.70 | 1.38 | 1.44 |
| 37 | b | 513 | CLA | C3D-C4D | -2.70 | 1.38 | 1.44 |
| 47 | 16 | 304 | KC1 | CHB-C4A | -2.70 | 1.33 | 1.39 |
| 48 | 40 | 211 | A86 | C14-C15 | 2.70 | 1.58 | 1.52 |
| 47 | 36 | 304 | KC1 | CHB-C4A | -2.70 | 1.33 | 1.39 |
| 37 | 31 | 301 | CLA | C4D-CHA | 2.70 | 1.47 | 1.38 |
| 48 | 36 | 311 | A86 | C14-C15 | 2.70 | 1.58 | 1.52 |
| 37 | 40 | 209 | CLA | C4D-CHA | 2.70 | 1.47 | 1.38 |
| 37 | 20 | 303 | CLA | C3D-C4D | -2.70 | 1.38 | 1.44 |
| 48 | 14 | 316 | A86 | C-C1 | 2.70 | 1.56 | 1.50 |
| 48 | 34 | 316 | A86 | C-C1 | 2.70 | 1.56 | 1.50 |
| 48 | 11 | 319 | A86 | C26-C27 | 2.70 | 1.42 | 1.35 |
| 48 | 31 | 319 | A86 | C26-C27 | 2.70 | 1.42 | 1.35 |
| 37 | 35 | 310 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 37 | 16 | 307 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 37 | 41 | 209 | CLA | C3B-C4B | 2.69 | 1.50 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 50 | 19 | 312 | DD6 | C9-C8 | 2.69 | 1.41 | 1.34 |
| 37 | B | 501 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 37 | 19 | 310 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 37 | 39 | 310 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 37 | b | 511 | CLA | C3D-C4D | -2.69 | 1.38 | 1.44 |
| 48 | 19 | 311 | A86 | O-C13 | -2.69 | 1.17 | 1.23 |
| 37 | 11 | 307 | CLA | CHB-C1B | 2.69 | 1.45 | 1.39 |
| 39 | h | 101 | BCR | C30-C25 | -2.69 | 1.50 | 1.53 |
| 47 | 38 | 210 | KC1 | C2A-C1A | 2.69 | 1.53 | 1.44 |
| 48 | 35 | 311 | A86 | C25-C24 | 2.69 | 1.41 | 1.34 |
| 48 | 15 | 313 | A86 | O-C13 | -2.69 | 1.17 | 1.23 |
| 48 | 20 | 309 | A86 | C14-C15 | 2.69 | 1.58 | 1.52 |
| 38 | a | 406 | PHO | CMD-C2D | -2.69 | 1.46 | 1.51 |
| 48 | 32 | 214 | A86 | O-C13 | -2.69 | 1.17 | 1.23 |
| 48 | 34 | 315 | A86 | C26-C27 | 2.69 | 1.42 | 1.35 |
| 37 | 19 | 307 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 48 | 33 | 315 | A86 | C-C1 | 2.69 | 1.56 | 1.50 |
| 37 | 15 | 310 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 48 | 32 | 217 | A86 | O-C13 | -2.69 | 1.17 | 1.23 |
| 37 | b | 516 | CLA | OBD-CAD | 2.69 | 1.27 | 1.22 |
| 48 | 39 | 313 | A86 | O-C13 | -2.69 | 1.17 | 1.23 |
| 37 | b | 523 | CLA | C3D-C4D | -2.69 | 1.38 | 1.44 |
| 50 | 20 | 310 | DD6 | C9-C8 | 2.69 | 1.41 | 1.34 |
| 48 | 35 | 315 | A86 | C-C1 | 2.69 | 1.56 | 1.50 |
| 37 | b | 501 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 47 | 33 | 306 | KC1 | CHB-C4A | -2.69 | 1.33 | 1.39 |
| 48 | 35 | 316 | A86 | C24-C1 | 2.68 | 1.51 | 1.46 |
| 47 | 13 | 304 | KC1 | CHB-C4A | -2.68 | 1.33 | 1.39 |
| 48 | 36 | 311 | A86 | O-C13 | -2.68 | 1.17 | 1.23 |
| 48 | 37 | 310 | A86 | C25-C24 | 2.68 | 1.41 | 1.34 |
| 48 | 16 | 313 | A86 | C26-C27 | 2.68 | 1.42 | 1.35 |
| 50 | 39 | 312 | DD6 | C9-C8 | 2.68 | 1.41 | 1.34 |
| 37 | b | 506 | CLA | C3D-C4D | -2.68 | 1.38 | 1.44 |
| 48 | 32 | 218 | A86 | O-C13 | -2.68 | 1.17 | 1.23 |
| 48 | 17 | 320 | A86 | C-C1 | 2.68 | 1.56 | 1.50 |
| 47 | 11 | 302 | KC1 | C2A-C1A | 2.68 | 1.53 | 1.44 |
| 48 | 18 | 215 | A86 | C24-C1 | 2.68 | 1.51 | 1.46 |
| 48 | 34 | 315 | A86 | O-C13 | -2.68 | 1.17 | 1.23 |
| 48 | 41 | 214 | A86 | C24-C1 | 2.68 | 1.51 | 1.46 |
| 37 | z | 102 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 39 | d | 405 | BCR | C30-C25 | -2.68 | 1.50 | 1.53 |
| 37 | B | 506 | CLA | C3D-C4D | -2.68 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 34 | 313 | A86 | O-C13 | -2.68 | 1.17 | 1.23 |
| 37 | C | 503 | CLA | CHB-C1B | 2.68 | 1.45 | 1.39 |
| 37 | c | 503 | CLA | CHB-C1B | 2.68 | 1.45 | 1.39 |
| 37 | 38 | 206 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 48 | 37 | 319 | A86 | C-C1 | 2.68 | 1.56 | 1.50 |
| 37 | 41 | 209 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 37 | W | 102 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 48 | 11 | 314 | A86 | C-C1 | 2.68 | 1.56 | 1.50 |
| 37 | 36 | 307 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 37 | 15 | 303 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 37 | b | 507 | CLA | C3D-C4D | -2.67 | 1.38 | 1.44 |
| 50 | 36 | 312 | DD6 | C9-C8 | 2.67 | 1.41 | 1.34 |
| 37 | 37 | 308 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 37 | 21 | 209 | CLA | C3B-C4B | 2.67 | 1.50 | 1.42 |
| 37 | 13 | 310 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 38 | A | 404 | PHO | CMD-C2D | -2.67 | 1.46 | 1.51 |
| 48 | 37 | 319 | A86 | C14-C15 | 2.67 | 1.57 | 1.52 |
| 37 | B | 507 | CLA | C1C-NC | -2.67 | 1.33 | 1.37 |
| 50 | 16 | 312 | DD6 | C9-C8 | 2.67 | 1.41 | 1.34 |
| 37 | B | 513 | CLA | C3D-C4D | -2.67 | 1.38 | 1.44 |
| 47 | 17 | 306 | KC1 | C4C-C3C | 2.67 | 1.49 | 1.45 |
| 47 | 41 | 203 | KC1 | C4A-C3A | 2.67 | 1.49 | 1.44 |
| 48 | 14 | 315 | A86 | C26-C27 | 2.67 | 1.42 | 1.35 |
| 37 | 31 | 308 | CLA | CHB-C1B | 2.67 | 1.45 | 1.39 |
| 37 | a | 404 | CLA | C3D-C4D | -2.67 | 1.38 | 1.44 |
| 47 | 37 | 305 | KC1 | C4C-C3C | 2.67 | 1.49 | 1.45 |
| 37 | Z | 102 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 37 | 18 | 202 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 48 | 11 | 313 | A86 | C25-C24 | 2.67 | 1.41 | 1.34 |
| 37 | 17 | 307 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 37 | 21 | 202 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 48 | 15 | 312 | A86 | C14-C15 | 2.67 | 1.57 | 1.52 |
| 48 | 21 | 214 | A86 | C24-C1 | 2.67 | 1.51 | 1.46 |
| 48 | 38 | 212 | A86 | C26-C27 | 2.67 | 1.42 | 1.35 |
| 44 | j | 101 | DGD | O5D-C6D | -2.67 | 1.39 | 1.43 |
| 37 | b | 507 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 37 | 21 | 209 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 47 | 31 | 303 | KC1 | C2A-C1A | 2.67 | 1.52 | 1.44 |
| 47 | 35 | 309 | KC1 | C4A-C3A | 2.67 | 1.49 | 1.44 |
| 48 | 12 | 215 | A86 | C24-C1 | 2.67 | 1.51 | 1.46 |
| 37 | 41 | 209 | CLA | C4B-NB | -2.66 | 1.34 | 1.37 |
| 47 | 38 | 210 | KC1 | C4A-C3A | 2.66 | 1.49 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 203 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 37 | 32 | 204 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 48 | 31 | 313 | A86 | C-C1 | 2.66 | 1.56 | 1.50 |
| 48 | 35 | 314 | A86 | C24-C1 | 2.66 | 1.51 | 1.46 |
| 47 | 21 | 203 | KC1 | C4A-C3A | 2.66 | 1.49 | 1.44 |
| 48 | 35 | 313 | A86 | C14-C15 | 2.66 | 1.57 | 1.52 |
| 37 | 35 | 308 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 48 | 35 | 312 | A86 | C14-C15 | 2.66 | 1.57 | 1.52 |
| 48 | 40 | 201 | A86 | C26-C27 | 2.66 | 1.42 | 1.35 |
| 47 | 15 | 302 | KC1 | CHB-C4A | -2.66 | 1.33 | 1.39 |
| 48 | 17 | 311 | A86 | C14-C15 | 2.66 | 1.57 | 1.52 |
| 37 | 14 | 307 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 50 | 40 | 212 | DD6 | C9-C8 | 2.66 | 1.41 | 1.34 |
| 48 | 12 | 213 | A86 | O-C13 | -2.66 | 1.17 | 1.23 |
| 37 | 14 | 305 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 37 | 17 | 309 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 37 | 34 | 305 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 48 | 17 | 315 | A86 | O-C13 | -2.66 | 1.17 | 1.23 |
| 48 | 38 | 215 | A86 | C24-C1 | 2.66 | 1.51 | 1.46 |
| 48 | 12 | 202 | A86 | O-C13 | -2.66 | 1.17 | 1.23 |
| 48 | 21 | 211 | A86 | C26-C27 | 2.66 | 1.42 | 1.35 |
| 48 | 17 | 314 | A86 | C25-C24 | 2.66 | 1.41 | 1.34 |
| 37 | 16 | 306 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 48 | 31 | 315 | A86 | C25-C24 | 2.66 | 1.41 | 1.34 |
| 47 | 15 | 309 | KC1 | C4A-C3A | 2.66 | 1.49 | 1.44 |
| 48 | 13 | 312 | A86 | C-C1 | 2.66 | 1.56 | 1.50 |
| 47 | 21 | 203 | KC1 | CHB-C4A | -2.66 | 1.33 | 1.39 |
| 48 | 37 | 310 | A86 | C14-C15 | 2.66 | 1.57 | 1.52 |
| 48 | 17 | 310 | A86 | C-C1 | 2.66 | 1.56 | 1.50 |
| 37 | 31 | 306 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 37 | 41 | 204 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 50 | 20 | 310 | DD6 | C35-C36 | 2.66 | 1.55 | 1.51 |
| 37 | 34 | 307 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 47 | 41 | 203 | KC1 | CHB-C4A | -2.66 | 1.33 | 1.39 |
| 48 | 18 | 215 | A86 | O-C13 | -2.66 | 1.17 | 1.23 |
| 37 | 31 | 304 | CLA | C3D-C4D | -2.65 | 1.38 | 1.44 |
| 37 | 41 | 205 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |
| 48 | 11 | 315 | A86 | C19-C18 | 2.65 | 1.56 | 1.52 |
| 48 | 38 | 212 | A86 | C-C1 | 2.65 | 1.56 | 1.50 |
| 48 | 37 | 312 | A86 | O-C13 | -2.65 | 1.17 | 1.23 |
| 37 | 38 | 201 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 47 | 13 | 304 | KC1 | C2A-C1A | 2.65 | 1.52 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | B | 507 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 37 | 21 | 204 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 37 | 32 | 211 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 48 | 31 | 314 | A86 | C-C1 | 2.65 | 1.56 | 1.50 |
| 47 | 16 | 305 | KC1 | C2A-C1A | 2.65 | 1.52 | 1.44 |
| 47 | 13 | 309 | KC1 | CHB-C4A | -2.65 | 1.33 | 1.39 |
| 47 | 33 | 309 | KC1 | CHB-C4A | -2.65 | 1.33 | 1.39 |
| 47 | 16 | 305 | KC1 | C4A-C3A | 2.65 | 1.49 | 1.44 |
| 37 | 39 | 302 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 48 | 15 | 315 | A86 | C-C1 | 2.65 | 1.56 | 1.50 |
| 47 | 35 | 304 | KC1 | C1D-C2D | 2.65 | 1.49 | 1.43 |
| 48 | 16 | 311 | A86 | O4-C34 | -2.65 | 1.40 | 1.46 |
| 48 | 37 | 309 | A86 | C-C1 | 2.65 | 1.56 | 1.50 |
| 47 | 12 | 206 | KC1 | C2A-C1A | 2.65 | 1.52 | 1.44 |
| 47 | 32 | 207 | KC1 | C2A-C1A | 2.65 | 1.52 | 1.44 |
| 37 | 35 | 308 | CLA | C1B-C2B | 2.65 | 1.49 | 1.43 |
| 37 | 18 | 201 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 48 | 17 | 320 | A86 | C14-C15 | 2.65 | 1.57 | 1.52 |
| 48 | 15 | 314 | A86 | C24-C1 | 2.65 | 1.51 | 1.46 |
| 48 | 33 | 312 | A86 | C-C1 | 2.65 | 1.56 | 1.50 |
| 37 | 36 | 306 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 47 | 18 | 207 | KC1 | C2A-C1A | 2.65 | 1.52 | 1.44 |
| 37 | c | 508 | CLA | C3D-C4D | -2.65 | 1.38 | 1.44 |
| 48 | 12 | 217 | A86 | O-C13 | -2.65 | 1.17 | 1.23 |
| 37 | 12 | 204 | CLA | C3D-C4D | -2.65 | 1.38 | 1.44 |
| 37 | 32 | 205 | CLA | C3D-C4D | -2.65 | 1.38 | 1.44 |
| 48 | 33 | 311 | A86 | C14-C15 | 2.65 | 1.57 | 1.52 |
| 50 | 40 | 212 | DD6 | C26-C27 | -2.65 | 1.31 | 1.37 |
| 48 | 13 | 312 | A86 | O-C13 | -2.65 | 1.17 | 1.23 |
| 47 | 33 | 304 | KC1 | C2A-C1A | 2.65 | 1.52 | 1.44 |
| 37 | 40 | 208 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 48 | 13 | 311 | A86 | C14-C15 | 2.65 | 1.57 | 1.52 |
| 48 | 39 | 311 | A86 | O-C13 | -2.65 | 1.17 | 1.23 |
| 37 | C | 502 | CLA | C3D-C4D | -2.65 | 1.38 | 1.44 |
| 47 | 17 | 303 | KC1 | CHB-C4A | -2.65 | 1.33 | 1.39 |
| 47 | 35 | 302 | KC1 | C2A-C1A | 2.64 | 1.52 | 1.44 |
| 48 | 19 | 313 | A86 | O-C13 | -2.64 | 1.17 | 1.23 |
| 37 | C | 506 | CLA | CHC-C4B | 2.64 | 1.45 | 1.39 |
| 37 | 14 | 308 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 37 | 21 | 202 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 48 | 34 | 314 | A86 | O-C13 | -2.64 | 1.17 | 1.23 |
| 37 | 21 | 206 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 11 | 301 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 37 | 37 | 308 | CLA | C4C-C3C | 2.64 | 1.49 | 1.45 |
| 37 | 41 | 206 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 37 | C | 508 | CLA | C3D-C4D | -2.64 | 1.38 | 1.44 |
| 48 | 31 | 314 | A86 | C14-C15 | 2.64 | 1.57 | 1.52 |
| 37 | 32 | 210 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 47 | 36 | 305 | KC1 | C2A-C1A | 2.64 | 1.52 | 1.44 |
| 47 | 35 | 309 | KC1 | CHB-C4A | -2.64 | 1.33 | 1.39 |
| 44 | H | 102 | DGD | O2G-C2G | -2.64 | 1.40 | 1.46 |
| 37 | 33 | 308 | CLA | C4C-C3C | 2.64 | 1.49 | 1.45 |
| 37 | 35 | 303 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 37 | 21 | 205 | CLA | C1B-C2B | 2.64 | 1.49 | 1.43 |
| 48 | 14 | 314 | A86 | O-C13 | -2.64 | 1.17 | 1.23 |
| 37 | 31 | 302 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 39 | H | 101 | BCR | C30-C25 | -2.64 | 1.50 | 1.53 |
| 48 | 41 | 214 | A86 | C26-C27 | 2.64 | 1.41 | 1.35 |
| 48 | 15 | 316 | A86 | C24-C1 | 2.63 | 1.51 | 1.46 |
| 37 | 18 | 211 | CLA | C4C-C3C | 2.63 | 1.49 | 1.45 |
| 47 | 13 | 306 | KC1 | CHB-C4A | -2.63 | 1.33 | 1.39 |
| 47 | 19 | 308 | KC1 | CHB-C4A | -2.63 | 1.33 | 1.39 |
| 37 | 31 | 304 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 48 | 13 | 312 | A86 | C2-C1 | 2.63 | 1.41 | 1.35 |
| 37 | c | 506 | CLA | CHC-C4B | 2.63 | 1.45 | 1.39 |
| 37 | 11 | 305 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 37 | 34 | 308 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 50 | 40 | 212 | DD6 | C35-C36 | 2.63 | 1.55 | 1.51 |
| 48 | 17 | 312 | A86 | O-C13 | -2.63 | 1.17 | 1.23 |
| 47 | 38 | 205 | KC1 | CHB-C4A | -2.63 | 1.33 | 1.39 |
| 47 | 18 | 210 | KC1 | C4A-C3A | 2.63 | 1.49 | 1.44 |
| 37 | 19 | 302 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 47 | 37 | 304 | KC1 | C1D-C2D | 2.63 | 1.49 | 1.43 |
| 37 | 17 | 304 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 37 | 37 | 303 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 37 | 12 | 210 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 37 | 34 | 301 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 37 | 34 | 310 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 48 | 11 | 314 | A86 | C14-C15 | 2.63 | 1.57 | 1.52 |
| 37 | 12 | 209 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 37 | 41 | 202 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 47 | 36 | 305 | KC1 | C4A-C3A | 2.63 | 1.49 | 1.44 |
| 48 | 15 | 312 | A86 | C2-C1 | 2.63 | 1.41 | 1.35 |
| 47 | 11 | 309 | KC1 | C2A-C1A | 2.63 | 1.52 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 31 | 309 | KC1 | C2A-C1A | 2.63 | 1.52 | 1.44 |
| 48 | 18 | 212 | A86 | C26-C27 | 2.63 | 1.41 | 1.35 |
| 37 | 11 | 307 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 47 | 39 | 308 | KC1 | CHB-C4A | -2.63 | 1.33 | 1.39 |
| 37 | 18 | 208 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 37 | 38 | 208 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 47 | 14 | 309 | KC1 | C2A-C1A | 2.62 | 1.52 | 1.44 |
| 47 | 34 | 309 | KC1 | C2A-C1A | 2.62 | 1.52 | 1.44 |
| 37 | 15 | 308 | CLA | C1B-C2B | 2.62 | 1.49 | 1.43 |
| 37 | c | 502 | CLA | C3D-C4D | -2.62 | 1.38 | 1.44 |
| 37 | 37 | 301 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 37 | c | 502 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 37 | w | 101 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 47 | 37 | 302 | KC1 | CHB-C4A | -2.62 | 1.33 | 1.39 |
| 48 | 16 | 311 | A86 | O-C13 | -2.62 | 1.17 | 1.23 |
| 44 | h | 102 | DGD | O2G-C2G | -2.62 | 1.40 | 1.46 |
| 48 | 37 | 311 | A86 | O-C13 | -2.62 | 1.17 | 1.23 |
| 37 | 41 | 210 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 47 | 40 | 207 | KC1 | C2A-C1A | 2.62 | 1.52 | 1.44 |
| 47 | 15 | 309 | KC1 | CHB-C4A | -2.62 | 1.33 | 1.39 |
| 48 | 33 | 312 | A86 | C2-C1 | 2.62 | 1.41 | 1.35 |
| 37 | 14 | 303 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 37 | 34 | 303 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 37 | B | 515 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 48 | 11 | 311 | A86 | C26-C27 | 2.62 | 1.41 | 1.35 |
| 47 | 20 | 304 | KC1 | C2A-C1A | 2.62 | 1.52 | 1.44 |
| 47 | 20 | 305 | KC1 | C2A-C1A | 2.62 | 1.52 | 1.44 |
| 48 | 38 | 212 | A86 | C14-C15 | 2.62 | 1.57 | 1.52 |
| 37 | b | 515 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 37 | 20 | 306 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 47 | 15 | 302 | KC1 | C2A-C1A | 2.62 | 1.52 | 1.44 |
| 48 | 36 | 311 | A86 | O4-C34 | -2.62 | 1.40 | 1.46 |
| 37 | 35 | 301 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 40 | a | 409 | SQD | O47-C7 | 2.62 | 1.41 | 1.34 |
| 48 | 11 | 313 | A86 | C-C1 | 2.62 | 1.56 | 1.50 |
| 37 | 32 | 206 | CLA | C3D-C4D | -2.62 | 1.38 | 1.44 |
| 37 | b | 504 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 50 | 20 | 310 | DD6 | C26-C27 | -2.62 | 1.31 | 1.37 |
| 48 | 13 | 312 | A86 | C14-C15 | 2.62 | 1.57 | 1.52 |
| 47 | 12 | 211 | KC1 | C2A-C1A | 2.62 | 1.52 | 1.44 |
| 37 | 35 | 308 | CLA | C4C-C3C | 2.62 | 1.49 | 1.45 |
| 37 | 14 | 310 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 15 | 313 | A86 | C2-C1 | 2.61 | 1.41 | 1.35 |
| 48 | 35 | 312 | A86 | C2-C1 | 2.61 | 1.41 | 1.35 |
| 48 | 32 | 203 | A86 | C-C1 | 2.61 | 1.56 | 1.50 |
| 48 | 11 | 315 | A86 | C14-C15 | 2.61 | 1.57 | 1.52 |
| 47 | 16 | 308 | KC1 | CHB-C4A | -2.61 | 1.33 | 1.39 |
| 37 | B | 509 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 41 | 11 | 316 | LMG | C4-C5 | 2.61 | 1.58 | 1.53 |
| 50 | 21 | 216 | DD6 | C4-C5 | 2.61 | 1.51 | 1.43 |
| 37 | 11 | 303 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 37 | 14 | 301 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 37 | b | 509 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 47 | 31 | 307 | KC1 | CHB-C4A | -2.61 | 1.33 | 1.39 |
| 48 | 11 | 315 | A86 | C26-C27 | 2.61 | 1.41 | 1.35 |
| 48 | 12 | 216 | A86 | C14-C15 | 2.61 | 1.57 | 1.52 |
| 37 | 11 | 303 | CLA | C3D-C4D | -2.61 | 1.38 | 1.44 |
| 48 | 14 | 313 | A86 | O-C13 | -2.61 | 1.17 | 1.23 |
| 37 | 38 | 202 | CLA | C3B-C4B | 2.61 | 1.50 | 1.42 |
| 37 | 41 | 202 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 40 | A | 407 | SQD | O47-C7 | 2.61 | 1.41 | 1.34 |
| 48 | 37 | 319 | A86 | O-C13 | -2.61 | 1.17 | 1.23 |
| 48 | 15 | 313 | A86 | C14-C15 | 2.61 | 1.57 | 1.52 |
| 37 | 21 | 210 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 37 | 19 | 309 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 44 | C | 516 | DGD | O5D-C6D | -2.61 | 1.39 | 1.43 |
| 48 | 21 | 213 | A86 | C2-C1 | 2.61 | 1.41 | 1.35 |
| 37 | c | 511 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 47 | 17 | 306 | KC1 | C4A-C3A | 2.61 | 1.49 | 1.44 |
| 48 | 21 | 215 | A86 | O1-C20 | 2.61 | 1.49 | 1.46 |
| 48 | 31 | 315 | A86 | C14-C15 | 2.61 | 1.57 | 1.52 |
| 48 | 21 | 214 | A86 | C26-C27 | 2.61 | 1.41 | 1.35 |
| 37 | 31 | 308 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 47 | 20 | 304 | KC1 | CHB-C4A | -2.61 | 1.33 | 1.39 |
| 37 | C | 502 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 44 | J | 101 | DGD | O5D-C6D | -2.61 | 1.39 | 1.43 |
| 37 | 21 | 209 | CLA | C4B-NB | -2.61 | 1.34 | 1.37 |
| 37 | 39 | 309 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 47 | 32 | 212 | KC1 | C2A-C1A | 2.61 | 1.52 | 1.44 |
| 48 | 34 | 315 | A86 | C25-C24 | 2.61 | 1.41 | 1.34 |
| 47 | 37 | 305 | KC1 | C4A-C3A | 2.61 | 1.49 | 1.44 |
| 37 | 18 | 211 | CLA | C1B-C2B | 2.61 | 1.49 | 1.43 |
| 37 | 15 | 308 | CLA | C4C-C3C | 2.61 | 1.49 | 1.45 |
| 48 | 39 | 311 | A86 | C26-C27 | 2.60 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 18 | 214 | A86 | C24-C1 | 2.60 | 1.51 | 1.46 |
| 48 | 14 | 312 | A86 | C-C1 | 2.60 | 1.56 | 1.50 |
| 48 | 13 | 313 | A86 | C2-C1 | 2.60 | 1.41 | 1.35 |
| 48 | 12 | 202 | A86 | C-C1 | 2.60 | 1.56 | 1.50 |
| 37 | W | 101 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 48 | 17 | 311 | A86 | C-C1 | 2.60 | 1.56 | 1.50 |
| 37 | 18 | 209 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 41 | 11 | 316 | LMG | C3-C2 | 2.60 | 1.59 | 1.52 |
| 45 | d | 406 | PL9 | C7-C8 | -2.60 | 1.46 | 1.50 |
| 47 | 18 | 205 | KC1 | CHB-C4A | -2.60 | 1.33 | 1.39 |
| 37 | 12 | 204 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 37 | 32 | 205 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 37 | C | 511 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 48 | 38 | 213 | A86 | C14-C15 | 2.60 | 1.57 | 1.52 |
| 48 | 41 | 215 | A86 | O1-C20 | 2.60 | 1.49 | 1.46 |
| 37 | 13 | 308 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 48 | 33 | 311 | A86 | O-C13 | -2.60 | 1.17 | 1.23 |
| 37 | C | 502 | CLA | OBD-CAD | 2.60 | 1.27 | 1.22 |
| 47 | 40 | 206 | KC1 | C2A-C1A | 2.60 | 1.52 | 1.44 |
| 37 | 19 | 307 | CLA | C3B-C4B | 2.60 | 1.50 | 1.42 |
| 37 | B | 509 | CLA | C3D-C4D | -2.60 | 1.38 | 1.44 |
| 50 | 41 | 216 | DD6 | C4-C5 | 2.60 | 1.51 | 1.43 |
| 47 | 14 | 306 | KC1 | C2A-C1A | 2.60 | 1.52 | 1.44 |
| 37 | 38 | 209 | CLA | C1B-C2B | 2.60 | 1.49 | 1.43 |
| 39 | a | 413 | BCR | C30-C25 | -2.60 | 1.50 | 1.53 |
| 48 | 13 | 314 | A86 | C2-C1 | 2.60 | 1.41 | 1.35 |
| 48 | 33 | 314 | A86 | C2-C1 | 2.60 | 1.41 | 1.35 |
| 47 | 17 | 305 | KC1 | CHB-C4A | -2.60 | 1.33 | 1.39 |
| 48 | 34 | 312 | A86 | C-C1 | 2.60 | 1.56 | 1.50 |
| 37 | 33 | 308 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 48 | 18 | 212 | A86 | O-C13 | -2.60 | 1.17 | 1.23 |
| 37 | 13 | 308 | CLA | C4C-C3C | 2.59 | 1.49 | 1.45 |
| 47 | 13 | 309 | KC1 | C2A-C1A | 2.59 | 1.52 | 1.44 |
| 47 | 33 | 309 | KC1 | C2A-C1A | 2.59 | 1.52 | 1.44 |
| 47 | 40 | 206 | KC1 | CHB-C4A | -2.59 | 1.33 | 1.39 |
| 48 | 37 | 311 | A86 | C24-C1 | 2.59 | 1.51 | 1.46 |
| 48 | 17 | 313 | A86 | C26-C27 | 2.59 | 1.41 | 1.35 |
| 37 | 15 | 307 | CLA | C3B-C4B | 2.59 | 1.50 | 1.42 |
| 47 | 37 | 302 | KC1 | C4A-C3A | 2.59 | 1.49 | 1.44 |
| 37 | C | 512 | CLA | CHB-C1B | 2.59 | 1.45 | 1.39 |
| 43 | D | 409 | LHG | O7-C5 | -2.59 | 1.40 | 1.46 |
| 48 | 39 | 313 | A86 | C17-C18 | -2.59 | 1.48 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 15 | 316 | A86 | C26-C27 | 2.59 | 1.41 | 1.35 |
| 37 | c | 502 | CLA | OBD-CAD | 2.59 | 1.26 | 1.22 |
| 37 | 15 | 301 | CLA | C4D-CHA | 2.59 | 1.47 | 1.38 |
| 37 | 35 | 307 | CLA | C3B-C4B | 2.59 | 1.50 | 1.42 |
| 37 | B | 504 | CLA | C4D-CHA | 2.59 | 1.47 | 1.38 |
| 47 | 14 | 306 | KC1 | CHB-C4A | -2.59 | 1.33 | 1.39 |
| 48 | 41 | 213 | A86 | C2-C1 | 2.59 | 1.41 | 1.35 |
| 48 | 31 | 311 | A86 | C26-C27 | 2.59 | 1.41 | 1.35 |
| 48 | 32 | 217 | A86 | C14-C15 | 2.59 | 1.57 | 1.52 |
| 47 | 33 | 302 | KC1 | C2A-C1A | 2.59 | 1.52 | 1.44 |
| 41 | 31 | 316 | LMG | C3-C2 | 2.58 | 1.59 | 1.52 |
| 37 | 32 | 208 | CLA | C3D-C4D | -2.58 | 1.38 | 1.44 |
| 37 | 16 | 303 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 48 | 41 | 214 | A86 | O-C13 | -2.58 | 1.17 | 1.23 |
| 37 | 11 | 308 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 37 | b | 507 | CLA | C1C-NC | -2.58 | 1.33 | 1.37 |
| 48 | 13 | 311 | A86 | O-C13 | -2.58 | 1.17 | 1.23 |
| 48 | 14 | 315 | A86 | C25-C24 | 2.58 | 1.41 | 1.34 |
| 37 | 40 | 210 | CLA | C1B-C2B | 2.58 | 1.49 | 1.43 |
| 48 | 40 | 211 | A86 | C-C1 | 2.58 | 1.56 | 1.50 |
| 37 | 20 | 308 | CLA | C1B-C2B | 2.58 | 1.49 | 1.43 |
| 50 | 40 | 214 | DD6 | C35-C36 | 2.58 | 1.55 | 1.51 |
| 37 | C | 508 | CLA | C1C-NC | -2.58 | 1.33 | 1.37 |
| 39 | A | 410 | BCR | C30-C25 | -2.58 | 1.50 | 1.53 |
| 48 | 12 | 216 | A86 | C26-C27 | 2.58 | 1.41 | 1.35 |
| 37 | C | 506 | CLA | C1C-NC | -2.58 | 1.33 | 1.37 |
| 39 | B | 518 | BCR | C30-C25 | -2.58 | 1.50 | 1.53 |
| 39 | b | 518 | BCR | C30-C25 | -2.58 | 1.50 | 1.53 |
| 37 | C | 504 | CLA | C3D-C4D | -2.58 | 1.38 | 1.44 |
| 47 | 13 | 302 | KC1 | C2A-C1A | 2.58 | 1.52 | 1.44 |
| 37 | 19 | 305 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 48 | 17 | 315 | A86 | C24-C1 | 2.58 | 1.51 | 1.46 |
| 37 | c | 512 | CLA | CHB-C1B | 2.58 | 1.45 | 1.39 |
| 37 | B | 514 | CLA | OBD-CAD | 2.58 | 1.26 | 1.22 |
| 48 | 14 | 315 | A86 | O4-C34 | -2.58 | 1.40 | 1.46 |
| 48 | 34 | 315 | A86 | O4-C34 | -2.58 | 1.40 | 1.46 |
| 47 | 35 | 304 | KC1 | CHB-C4A | -2.58 | 1.33 | 1.39 |
| 37 | 16 | 309 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 43 | d | 407 | LHG | O7-C5 | -2.58 | 1.40 | 1.46 |
| 48 | 31 | 313 | A86 | C26-C27 | 2.58 | 1.41 | 1.35 |
| 37 | b | 509 | CLA | C3D-C4D | -2.58 | 1.38 | 1.44 |
| 37 | 12 | 205 | CLA | C3D-C4D | -2.58 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 38 | 211 | CLA | C1B-C2B | 2.57 | 1.49 | 1.43 |
| 37 | c | 508 | CLA | C1C-NC | -2.57 | 1.33 | 1.37 |
| 48 | 18 | 214 | A86 | O-C13 | -2.57 | 1.17 | 1.23 |
| 48 | 21 | 213 | A86 | O-C13 | -2.57 | 1.17 | 1.23 |
| 48 | 31 | 315 | A86 | C26-C27 | 2.57 | 1.41 | 1.35 |
| 37 | 32 | 206 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 37 | C | 507 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 37 | c | 507 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 37 | b | 514 | CLA | OBD-CAD | 2.57 | 1.26 | 1.22 |
| 48 | 35 | 313 | A86 | C2-C1 | 2.57 | 1.41 | 1.35 |
| 37 | 36 | 303 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 47 | 36 | 308 | KC1 | CHB-C4A | -2.57 | 1.33 | 1.39 |
| 37 | 39 | 302 | CLA | C3D-C4D | -2.57 | 1.38 | 1.44 |
| 37 | 39 | 305 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 48 | 32 | 214 | A86 | C-C1 | 2.57 | 1.56 | 1.50 |
| 37 | C | 503 | CLA | C3D-C4D | -2.57 | 1.38 | 1.44 |
| 37 | 18 | 206 | CLA | C1B-C2B | 2.57 | 1.49 | 1.43 |
| 48 | 17 | 311 | A86 | C2-C1 | 2.57 | 1.41 | 1.35 |
| 47 | 34 | 306 | KC1 | C2A-C1A | 2.57 | 1.52 | 1.44 |
| 48 | 17 | 312 | A86 | C24-C1 | 2.57 | 1.51 | 1.46 |
| 48 | 38 | 214 | A86 | C24-C1 | 2.57 | 1.51 | 1.46 |
| 47 | 37 | 304 | KC1 | C4A-C3A | 2.57 | 1.49 | 1.44 |
| 48 | 37 | 314 | A86 | C26-C27 | 2.57 | 1.41 | 1.35 |
| 37 | c | 504 | CLA | C3D-C4D | -2.57 | 1.38 | 1.44 |
| 50 | 20 | 312 | DD6 | C4-C5 | 2.57 | 1.51 | 1.43 |
| 48 | 37 | 312 | A86 | C26-C27 | 2.57 | 1.41 | 1.35 |
| 50 | 40 | 214 | DD6 | C4-C5 | 2.57 | 1.51 | 1.43 |
| 37 | 13 | 303 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 48 | 33 | 313 | A86 | C2-C1 | 2.57 | 1.41 | 1.35 |
| 41 | 31 | 316 | LMG | C4-C5 | 2.57 | 1.58 | 1.53 |
| 48 | 17 | 310 | A86 | O-C13 | -2.57 | 1.17 | 1.23 |
| 48 | 37 | 309 | A86 | O-C13 | -2.57 | 1.17 | 1.23 |
| 47 | 11 | 302 | KC1 | CHB-C4A | -2.57 | 1.33 | 1.39 |
| 47 | 31 | 303 | KC1 | CHB-C4A | -2.57 | 1.33 | 1.39 |
| 40 | B | 522 | SQD | O47-C7 | 2.57 | 1.41 | 1.34 |
| 48 | 33 | 315 | A86 | C24-C1 | 2.57 | 1.51 | 1.46 |
| 37 | 38 | 201 | CLA | C3B-C4B | 2.57 | 1.50 | 1.42 |
| 47 | 15 | 304 | KC1 | C1D-C2D | 2.57 | 1.49 | 1.43 |
| 37 | B | 514 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 48 | 14 | 312 | A86 | C25-C24 | 2.57 | 1.41 | 1.34 |
| 37 | 41 | 205 | CLA | C4C-C3C | 2.57 | 1.49 | 1.45 |
| 37 | 21 | 208 | CLA | C4C-C3C | 2.57 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 13 | 303 | CLA | C3D-C4D | -2.57 | 1.38 | 1.44 |
| 37 | 32 | 202 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 47 | 11 | 306 | KC1 | CHB-C4A | -2.57 | 1.33 | 1.39 |
| 37 | 15 | 303 | CLA | C3B-C4B | 2.57 | 1.50 | 1.42 |
| 37 | 39 | 303 | CLA | C3D-C4D | -2.57 | 1.38 | 1.44 |
| 37 | 33 | 303 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 37 | b | 512 | CLA | C1C-NC | -2.57 | 1.33 | 1.37 |
| 48 | 14 | 315 | A86 | C14-C15 | 2.57 | 1.57 | 1.52 |
| 48 | 34 | 315 | A86 | C14-C15 | 2.57 | 1.57 | 1.52 |
| 48 | 33 | 312 | A86 | C14-C15 | 2.56 | 1.57 | 1.52 |
| 37 | c | 503 | CLA | C3D-C4D | -2.56 | 1.38 | 1.44 |
| 47 | 37 | 304 | KC1 | CHB-C4A | -2.56 | 1.33 | 1.39 |
| 37 | C | 503 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 47 | 15 | 306 | KC1 | C4A-C3A | 2.56 | 1.49 | 1.44 |
| 48 | 34 | 315 | A86 | C-C1 | 2.56 | 1.56 | 1.50 |
| 48 | 37 | 313 | A86 | C-C1 | 2.56 | 1.56 | 1.50 |
| 48 | 41 | 215 | A86 | O-C13 | -2.56 | 1.17 | 1.23 |
| 48 | 11 | 312 | A86 | C14-C15 | 2.56 | 1.57 | 1.52 |
| 37 | 32 | 213 | CLA | C3B-C4B | 2.56 | 1.50 | 1.42 |
| 48 | 19 | 311 | A86 | C26-C27 | 2.56 | 1.41 | 1.35 |
| 48 | 14 | 316 | A86 | O-C13 | -2.56 | 1.17 | 1.23 |
| 47 | 15 | 304 | KC1 | CHB-C4A | -2.56 | 1.33 | 1.39 |
| 37 | 11 | 310 | CLA | C3D-C4D | -2.56 | 1.38 | 1.44 |
| 48 | 13 | 315 | A86 | C24-C1 | 2.56 | 1.51 | 1.46 |
| 48 | 34 | 316 | A86 | O-C13 | -2.56 | 1.17 | 1.23 |
| 37 | 16 | 301 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 48 | 14 | 313 | A86 | C2-C1 | 2.56 | 1.41 | 1.35 |
| 37 | 36 | 309 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 44 | j | 101 | DGD | O3D-C3D | -2.56 | 1.36 | 1.43 |
| 37 | b | 513 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 37 | 12 | 207 | CLA | C3D-C4D | -2.56 | 1.38 | 1.44 |
| 47 | 17 | 303 | KC1 | C4A-C3A | 2.56 | 1.49 | 1.44 |
| 37 | 12 | 205 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 48 | 41 | 213 | A86 | O-C13 | -2.56 | 1.17 | 1.23 |
| 50 | 20 | 312 | DD6 | C35-C36 | 2.56 | 1.55 | 1.51 |
| 37 | 35 | 303 | CLA | C3B-C4B | 2.56 | 1.50 | 1.42 |
| 47 | 35 | 306 | KC1 | C4A-C3A | 2.56 | 1.49 | 1.44 |
| 37 | c | 503 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 47 | 15 | 306 | KC1 | CHB-C4A | -2.56 | 1.33 | 1.39 |
| 48 | 21 | 214 | A86 | O-C13 | -2.56 | 1.17 | 1.23 |
| 48 | 15 | 311 | A86 | C-C1 | 2.56 | 1.56 | 1.50 |
| 48 | 13 | 313 | A86 | O-C13 | -2.56 | 1.17 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 36 | 302 | KC1 | CAA-C2A | 2.55 | 1.54 | 1.46 |
| 47 | 33 | 306 | KC1 | C4A-C3A | 2.55 | 1.49 | 1.44 |
| 48 | 20 | 309 | A86 | C-C1 | 2.55 | 1.56 | 1.50 |
| 47 | 35 | 302 | KC1 | CHB-C4A | -2.55 | 1.33 | 1.39 |
| 47 | 18 | 207 | KC1 | C4A-C3A | 2.55 | 1.49 | 1.44 |
| 37 | 39 | 307 | CLA | C3B-C4B | 2.55 | 1.50 | 1.42 |
| 37 | 18 | 204 | CLA | C3B-C4B | 2.55 | 1.50 | 1.42 |
| 37 | 38 | 204 | CLA | C3B-C4B | 2.55 | 1.50 | 1.42 |
| 37 | z | 101 | CLA | C3D-C4D | -2.55 | 1.38 | 1.44 |
| 48 | 34 | 311 | A86 | C25-C24 | 2.55 | 1.41 | 1.34 |
| 48 | 34 | 312 | A86 | C25-C24 | 2.55 | 1.41 | 1.34 |
| 37 | 20 | 301 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 48 | 14 | 311 | A86 | O-C13 | -2.55 | 1.17 | 1.23 |
| 48 | 34 | 311 | A86 | O-C13 | -2.55 | 1.17 | 1.23 |
| 48 | 17 | 315 | A86 | C26-C27 | 2.55 | 1.41 | 1.35 |
| 48 | 33 | 313 | A86 | O-C13 | -2.55 | 1.17 | 1.23 |
| 47 | 16 | 302 | KC1 | CAA-C2A | 2.55 | 1.54 | 1.46 |
| 48 | 35 | 316 | A86 | C26-C27 | 2.55 | 1.41 | 1.35 |
| 37 | 17 | 309 | CLA | C3B-C4B | 2.55 | 1.50 | 1.42 |
| 37 | B | 510 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 40 | b | 521 | SQD | O47-C7 | 2.55 | 1.41 | 1.34 |
| 45 | D | 408 | PL9 | C7-C8 | -2.55 | 1.46 | 1.50 |
| 37 | C | 504 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 48 | 36 | 313 | A86 | C25-C24 | 2.55 | 1.41 | 1.34 |
| 48 | 12 | 220 | A86 | C25-C24 | 2.55 | 1.41 | 1.34 |
| 40 | 16 | 315 | SQD | O47-C7 | 2.55 | 1.41 | 1.34 |
| 37 | 21 | 202 | CLA | C4C-C3C | 2.55 | 1.49 | 1.45 |
| 48 | 17 | 314 | A86 | C-C1 | 2.55 | 1.56 | 1.50 |
| 48 | 32 | 217 | A86 | C26-C27 | 2.55 | 1.41 | 1.35 |
| 37 | c | 506 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 37 | c | 513 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 40 | 40 | 202 | SQD | O47-C7 | 2.54 | 1.41 | 1.34 |
| 48 | 12 | 202 | A86 | C25-C24 | 2.54 | 1.41 | 1.34 |
| 37 | 15 | 310 | CLA | C4C-C3C | 2.54 | 1.49 | 1.45 |
| 47 | 38 | 210 | KC1 | CHB-C4A | -2.54 | 1.33 | 1.39 |
| 48 | 32 | 221 | A86 | C25-C24 | 2.54 | 1.41 | 1.34 |
| 37 | b | 514 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 50 | 21 | 212 | DD6 | O1-C20 | 2.54 | 1.49 | 1.46 |
| 41 | l | 101 | LMG | O8-C9 | -2.54 | 1.39 | 1.45 |
| 47 | 20 | 302 | KC1 | C2A-C1A | 2.54 | 1.52 | 1.44 |
| 44 | c | 516 | DGD | O5D-C6D | -2.54 | 1.39 | 1.43 |
| 37 | 15 | 303 | CLA | C4C-C3C | 2.54 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | b | 510 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 48 | 13 | 315 | A86 | C26-C27 | 2.54 | 1.41 | 1.35 |
| 37 | 17 | 302 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 37 | 21 | 205 | CLA | C4C-C3C | 2.54 | 1.49 | 1.45 |
| 47 | 15 | 304 | KC1 | C4A-C3A | 2.54 | 1.49 | 1.44 |
| 37 | 32 | 202 | CLA | C3D-C4D | -2.54 | 1.38 | 1.44 |
| 37 | c | 504 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 37 | 19 | 303 | CLA | C3D-C4D | -2.54 | 1.38 | 1.44 |
| 37 | 12 | 212 | CLA | C3B-C4B | 2.54 | 1.50 | 1.42 |
| 48 | 37 | 314 | A86 | C24-C1 | 2.54 | 1.51 | 1.46 |
| 37 | 40 | 203 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 48 | 21 | 215 | A86 | O-C13 | -2.54 | 1.18 | 1.23 |
| 38 | a | 405 | PHO | CAC-C3C | -2.54 | 1.47 | 1.51 |
| 48 | 34 | 313 | A86 | C2-C1 | 2.54 | 1.41 | 1.35 |
| 47 | 35 | 304 | KC1 | C4C-C3C | 2.54 | 1.49 | 1.45 |
| 37 | 15 | 301 | CLA | C1C-C2C | 2.54 | 1.49 | 1.44 |
| 37 | 34 | 307 | CLA | CHB-C1B | 2.54 | 1.45 | 1.39 |
| 47 | 15 | 304 | KC1 | C4C-C3C | 2.54 | 1.49 | 1.45 |
| 44 | J | 101 | DGD | O3D-C3D | -2.53 | 1.36 | 1.43 |
| 37 | 39 | 301 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 47 | 34 | 306 | KC1 | CHB-C4A | -2.53 | 1.33 | 1.39 |
| 48 | 37 | 310 | A86 | C2-C1 | 2.53 | 1.41 | 1.35 |
| 48 | 40 | 213 | A86 | C2-C1 | 2.53 | 1.41 | 1.35 |
| 48 | 16 | 314 | A86 | C25-C24 | 2.53 | 1.41 | 1.34 |
| 48 | 14 | 315 | A86 | C-C1 | 2.53 | 1.56 | 1.50 |
| 37 | 15 | 301 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 37 | 15 | 305 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 37 | B | 513 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 48 | 32 | 203 | A86 | C25-C24 | 2.53 | 1.41 | 1.34 |
| 37 | 13 | 310 | CLA | C4C-C3C | 2.53 | 1.49 | 1.45 |
| 37 | 36 | 301 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 47 | 12 | 206 | KC1 | CHD-C1D | 2.53 | 1.45 | 1.39 |
| 48 | 14 | 311 | A86 | C25-C24 | 2.53 | 1.41 | 1.34 |
| 37 | 36 | 303 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 37 | 19 | 302 | CLA | C3D-C4D | -2.53 | 1.38 | 1.44 |
| 47 | 40 | 207 | KC1 | CHB-C4A | -2.53 | 1.33 | 1.39 |
| 38 | D | 403 | PHO | CAC-C3C | -2.53 | 1.47 | 1.51 |
| 37 | 16 | 303 | CLA | C1B-C2B | 2.53 | 1.49 | 1.43 |
| 37 | c | 506 | CLA | C1C-NC | -2.53 | 1.33 | 1.37 |
| 48 | 32 | 216 | A86 | C2-C1 | 2.53 | 1.41 | 1.35 |
| 50 | 16 | 312 | DD6 | C26-C27 | -2.53 | 1.31 | 1.37 |
| 37 | Z | 101 | CLA | C3D-C4D | -2.53 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 39 | 302 | CLA | OBD-CAD | 2.53 | 1.26 | 1.22 |
| 48 | 32 | 221 | A86 | O-C13 | -2.53 | 1.18 | 1.23 |
| 48 | 12 | 215 | A86 | C2-C1 | 2.53 | 1.41 | 1.35 |
| 37 | 13 | 303 | CLA | C4C-C3C | 2.53 | 1.49 | 1.45 |
| 38 | a | 405 | PHO | CMB-C2B | -2.53 | 1.46 | 1.51 |
| 50 | 36 | 312 | DD6 | C26-C27 | -2.53 | 1.31 | 1.37 |
| 47 | 31 | 305 | KC1 | C2A-C1A | 2.53 | 1.52 | 1.44 |
| 37 | 19 | 301 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 47 | 40 | 204 | KC1 | C2A-C1A | 2.53 | 1.52 | 1.44 |
| 37 | b | 516 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 50 | 41 | 212 | DD6 | O1-C20 | 2.53 | 1.49 | 1.46 |
| 48 | 38 | 212 | A86 | C2-C1 | 2.52 | 1.41 | 1.35 |
| 37 | C | 513 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 37 | 19 | 302 | CLA | OBD-CAD | 2.52 | 1.26 | 1.22 |
| 37 | 35 | 301 | CLA | C1B-C2B | 2.52 | 1.49 | 1.43 |
| 48 | 11 | 312 | A86 | O4-C34 | -2.52 | 1.40 | 1.46 |
| 37 | C | 506 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 48 | 31 | 313 | A86 | C24-C1 | 2.52 | 1.51 | 1.46 |
| 37 | 37 | 308 | CLA | C3B-C4B | 2.52 | 1.50 | 1.42 |
| 48 | 33 | 315 | A86 | C26-C27 | 2.52 | 1.41 | 1.35 |
| 48 | 16 | 311 | A86 | C-C1 | 2.52 | 1.55 | 1.50 |
| 37 | 14 | 307 | CLA | CHB-C1B | 2.52 | 1.45 | 1.39 |
| 37 | 32 | 210 | CLA | CHB-C1B | 2.52 | 1.45 | 1.39 |
| 48 | 13 | 311 | A86 | C-C1 | 2.52 | 1.55 | 1.50 |
| 48 | 18 | 212 | A86 | C14-C15 | 2.52 | 1.57 | 1.52 |
| 37 | 12 | 209 | CLA | CHB-C1B | 2.52 | 1.45 | 1.39 |
| 47 | 18 | 205 | KC1 | C1D-C2D | 2.52 | 1.49 | 1.43 |
| 37 | 19 | 309 | CLA | C3D-C4D | -2.52 | 1.38 | 1.44 |
| 37 | 39 | 304 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 48 | 33 | 311 | A86 | C-C1 | 2.52 | 1.55 | 1.50 |
| 47 | 11 | 306 | KC1 | C2A-C1A | 2.52 | 1.52 | 1.44 |
| 48 | 38 | 212 | A86 | O-C13 | -2.52 | 1.18 | 1.23 |
| 47 | 37 | 307 | KC1 | C4A-C3A | 2.52 | 1.49 | 1.44 |
| 38 | D | 403 | PHO | CMB-C2B | -2.52 | 1.46 | 1.51 |
| 48 | 20 | 311 | A86 | C2-C1 | 2.52 | 1.41 | 1.35 |
| 47 | 13 | 306 | KC1 | C4A-C3A | 2.52 | 1.49 | 1.44 |
| 47 | 35 | 304 | KC1 | C4A-C3A | 2.52 | 1.49 | 1.44 |
| 37 | C | 509 | CLA | C1C-NC | -2.52 | 1.33 | 1.37 |
| 47 | 11 | 304 | KC1 | C2A-C1A | 2.52 | 1.52 | 1.44 |
| 47 | 18 | 210 | KC1 | CHB-C4A | -2.52 | 1.33 | 1.39 |
| 37 | 14 | 310 | CLA | C3D-C4D | -2.52 | 1.38 | 1.44 |
| 48 | 12 | 220 | A86 | O-C13 | -2.52 | 1.18 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 35 | 311 | A86 | C-C1 | 2.52 | 1.55 | 1.50 |
| 48 | 40 | 213 | A86 | C26-C27 | 2.52 | 1.41 | 1.35 |
| 37 | d | 404 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 47 | 35 | 302 | KC1 | C4C-C3C | 2.51 | 1.49 | 1.45 |
| 37 | 16 | 306 | CLA | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 37 | 36 | 306 | CLA | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 37 | 15 | 310 | CLA | C1B-C2B | 2.51 | 1.49 | 1.43 |
| 37 | 20 | 303 | CLA | C1B-C2B | 2.51 | 1.49 | 1.43 |
| 37 | 35 | 310 | CLA | C1B-C2B | 2.51 | 1.49 | 1.43 |
| 41 | L | 102 | LMG | O8-C9 | -2.51 | 1.39 | 1.45 |
| 47 | 38 | 205 | KC1 | C1D-C2D | 2.51 | 1.49 | 1.43 |
| 47 | 16 | 302 | KC1 | CHB-C4A | -2.51 | 1.33 | 1.39 |
| 37 | c | 512 | CLA | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 37 | c | 512 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 37 | C | 512 | CLA | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 47 | 17 | 305 | KC1 | C4A-C3A | 2.51 | 1.49 | 1.44 |
| 37 | 11 | 310 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 37 | D | 406 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 37 | 31 | 310 | CLA | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 48 | 11 | 313 | A86 | O4-C34 | -2.51 | 1.40 | 1.46 |
| 48 | 37 | 310 | A86 | O4-C34 | -2.51 | 1.40 | 1.46 |
| 48 | 18 | 212 | A86 | C2-C1 | 2.51 | 1.41 | 1.35 |
| 37 | 20 | 307 | CLA | C1B-C2B | 2.51 | 1.49 | 1.43 |
| 47 | 15 | 302 | KC1 | C4C-C3C | 2.51 | 1.49 | 1.45 |
| 48 | 34 | 316 | A86 | C26-C27 | 2.51 | 1.41 | 1.35 |
| 37 | 41 | 202 | CLA | C4C-C3C | 2.51 | 1.49 | 1.45 |
| 47 | 16 | 305 | KC1 | CHB-C4A | -2.51 | 1.33 | 1.39 |
| 48 | 18 | 212 | A86 | C-C1 | 2.51 | 1.55 | 1.50 |
| 37 | 40 | 203 | CLA | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 48 | 18 | 212 | A86 | C24-C1 | 2.51 | 1.51 | 1.46 |
| 37 | B | 506 | CLA | C1C-NC | -2.51 | 1.34 | 1.37 |
| 37 | C | 512 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 48 | 38 | 212 | A86 | C24-C1 | 2.51 | 1.51 | 1.46 |
| 47 | 36 | 302 | KC1 | CHB-C4A | -2.51 | 1.33 | 1.39 |
| 37 | B | 516 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 37 | 35 | 303 | CLA | C4C-C3C | 2.51 | 1.49 | 1.45 |
| 37 | 13 | 305 | CLA | C1B-C2B | 2.50 | 1.49 | 1.43 |
| 48 | 36 | 313 | A86 | O-C13 | -2.50 | 1.18 | 1.23 |
| 37 | 20 | 301 | CLA | C3D-C4D | -2.50 | 1.38 | 1.44 |
| 47 | 40 | 207 | KC1 | C4A-C3A | 2.50 | 1.49 | 1.44 |
| 37 | 39 | 309 | CLA | C3D-C4D | -2.50 | 1.38 | 1.44 |
| 48 | 41 | 211 | A86 | C2-C1 | 2.50 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 19 | 304 | CLA | C4D-CHA | 2.50 | 1.47 | 1.38 |
| 37 | 35 | 305 | CLA | C1B-C2B | 2.50 | 1.49 | 1.43 |
| 37 | 39 | 303 | CLA | C4D-CHA | 2.50 | 1.47 | 1.38 |
| 37 | a | 404 | CLA | C1C-NC | -2.50 | 1.34 | 1.37 |
| 37 | 19 | 306 | CLA | C4D-CHA | 2.50 | 1.47 | 1.38 |
| 37 | 40 | 205 | CLA | C1B-C2B | 2.50 | 1.49 | 1.43 |
| 47 | 14 | 306 | KC1 | C4A-C3A | 2.50 | 1.49 | 1.44 |
| 37 | 12 | 210 | CLA | C4C-C3C | 2.50 | 1.49 | 1.45 |
| 48 | 16 | 313 | A86 | C24-C1 | 2.50 | 1.51 | 1.46 |
| 47 | 13 | 304 | KC1 | C4A-C3A | 2.50 | 1.49 | 1.44 |
| 47 | 17 | 308 | KC1 | C4A-C3A | 2.50 | 1.49 | 1.44 |
| 47 | 33 | 304 | KC1 | C4A-C3A | 2.50 | 1.49 | 1.44 |
| 47 | 35 | 306 | KC1 | CHB-C4A | -2.50 | 1.33 | 1.39 |
| 48 | 31 | 312 | A86 | C14-C15 | 2.50 | 1.57 | 1.52 |
| 37 | B | 511 | CLA | C4D-CHA | 2.50 | 1.47 | 1.38 |
| 47 | 18 | 205 | KC1 | C2A-C1A | 2.50 | 1.52 | 1.44 |
| 48 | 31 | 312 | A86 | O4-C34 | -2.50 | 1.40 | 1.46 |
| 37 | 19 | 305 | CLA | C1B-C2B | 2.50 | 1.49 | 1.43 |
| 37 | 33 | 305 | CLA | C1B-C2B | 2.50 | 1.49 | 1.43 |
| 37 | w | 101 | CLA | C1C-NC | -2.50 | 1.34 | 1.37 |
| 45 | d | 402 | PL9 | C53-C6 | -2.50 | 1.45 | 1.50 |
| 47 | 20 | 304 | KC1 | C4C-C3C | 2.50 | 1.49 | 1.45 |
| 37 | b | 506 | CLA | C1C-NC | -2.50 | 1.34 | 1.37 |
| 37 | 32 | 211 | CLA | C4C-C3C | 2.50 | 1.49 | 1.45 |
| 37 | 41 | 208 | CLA | C4C-C3C | 2.50 | 1.49 | 1.45 |
| 38 | a | 406 | PHO | CMB-C2B | -2.50 | 1.46 | 1.51 |
| 37 | 36 | 309 | CLA | C3B-C4B | 2.50 | 1.50 | 1.42 |
| 37 | 19 | 306 | CLA | C3B-C4B | 2.50 | 1.50 | 1.42 |
| 48 | 35 | 314 | A86 | C2-C1 | 2.50 | 1.41 | 1.35 |
| 37 | 41 | 210 | CLA | C1B-C2B | 2.50 | 1.49 | 1.43 |
| 37 | B | 512 | CLA | C1C-NC | -2.49 | 1.34 | 1.37 |
| 48 | 41 | 214 | A86 | C2-C1 | 2.49 | 1.41 | 1.35 |
| 47 | 31 | 307 | KC1 | C2A-C1A | 2.49 | 1.52 | 1.44 |
| 48 | 13 | 314 | A86 | C14-C15 | 2.49 | 1.57 | 1.52 |
| 48 | 21 | 214 | A86 | C2-C1 | 2.49 | 1.41 | 1.35 |
| 47 | 38 | 207 | KC1 | C4A-C3A | 2.49 | 1.49 | 1.44 |
| 48 | 16 | 314 | A86 | O-C13 | -2.49 | 1.18 | 1.23 |
| 37 | 34 | 310 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 37 | 35 | 301 | CLA | C1C-C2C | 2.49 | 1.49 | 1.44 |
| 48 | 35 | 315 | A86 | C26-C27 | 2.49 | 1.41 | 1.35 |
| 48 | 12 | 214 | A86 | C-C1 | 2.49 | 1.55 | 1.50 |
| 37 | 18 | 202 | CLA | C3B-C4B | 2.49 | 1.50 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | B | 501 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 47 | 38 | 205 | KC1 | C4A-C3A | 2.49 | 1.49 | 1.44 |
| 37 | a | 404 | CLA | C4D-CHA | 2.49 | 1.46 | 1.38 |
| 37 | b | 506 | CLA | C4D-CHA | 2.49 | 1.46 | 1.38 |
| 37 | 19 | 303 | CLA | C4D-CHA | 2.49 | 1.46 | 1.38 |
| 37 | 39 | 306 | CLA | C4D-CHA | 2.49 | 1.46 | 1.38 |
| 47 | 40 | 206 | KC1 | C4C-C3C | 2.49 | 1.49 | 1.45 |
| 37 | 14 | 310 | CLA | C1B-C2B | 2.49 | 1.49 | 1.43 |
| 37 | 11 | 305 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 37 | 39 | 305 | CLA | C1B-C2B | 2.49 | 1.49 | 1.43 |
| 37 | 31 | 310 | CLA | C4D-CHA | 2.49 | 1.46 | 1.38 |
| 37 | 20 | 308 | CLA | C4C-C3C | 2.49 | 1.49 | 1.45 |
| 48 | 36 | 311 | A86 | C-C1 | 2.49 | 1.55 | 1.50 |
| 37 | 17 | 309 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 37 | 37 | 308 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 48 | 32 | 215 | A86 | C-C1 | 2.49 | 1.55 | 1.50 |
| 47 | 20 | 305 | KC1 | C4A-C3A | 2.49 | 1.49 | 1.44 |
| 48 | 40 | 201 | A86 | C24-C1 | 2.49 | 1.51 | 1.46 |
| 37 | 11 | 308 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 48 | 14 | 316 | A86 | C26-C27 | 2.49 | 1.41 | 1.35 |
| 48 | 20 | 311 | A86 | C26-C27 | 2.49 | 1.41 | 1.35 |
| 48 | 13 | 315 | A86 | O-C13 | -2.49 | 1.18 | 1.23 |
| 37 | 12 | 209 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 37 | 32 | 210 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 48 | 17 | 311 | A86 | O4-C34 | -2.49 | 1.40 | 1.46 |
| 37 | 20 | 307 | CLA | C4C-C3C | 2.49 | 1.49 | 1.45 |
| 47 | 36 | 305 | KC1 | C4C-C3C | 2.49 | 1.49 | 1.45 |
| 48 | 20 | 309 | A86 | C24-C1 | 2.49 | 1.51 | 1.46 |
| 50 | 40 | 212 | DD6 | C4-C5 | 2.48 | 1.50 | 1.43 |
| 48 | 33 | 314 | A86 | C14-C15 | 2.48 | 1.57 | 1.52 |
| 37 | 35 | 310 | CLA | C4C-C3C | 2.48 | 1.49 | 1.45 |
| 48 | 21 | 211 | A86 | C24-C1 | 2.48 | 1.51 | 1.46 |
| 47 | 18 | 205 | KC1 | C4A-C3A | 2.48 | 1.49 | 1.44 |
| 48 | 32 | 218 | A86 | C26-C27 | 2.48 | 1.41 | 1.35 |
| 37 | D | 401 | CLA | C4D-CHA | 2.48 | 1.46 | 1.38 |
| 48 | 40 | 211 | A86 | C24-C1 | 2.48 | 1.51 | 1.46 |
| 37 | 16 | 309 | CLA | C3B-C4B | 2.48 | 1.50 | 1.42 |
| 44 | j | 101 | DGD | O3G-C3G | -2.48 | 1.39 | 1.43 |
| 48 | 39 | 311 | A86 | C25-C24 | 2.48 | 1.41 | 1.34 |
| 48 | 12 | 217 | A86 | C26-C27 | 2.48 | 1.41 | 1.35 |
| 48 | 17 | 310 | A86 | C26-C27 | 2.48 | 1.41 | 1.35 |
| 48 | 37 | 309 | A86 | C26-C27 | 2.48 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 32 | 214 | A86 | C25-C24 | 2.48 | 1.41 | 1.34 |
| 48 | 17 | 312 | A86 | C2-C1 | 2.48 | 1.41 | 1.35 |
| 37 | C | 511 | CLA | C1B-C2B | 2.48 | 1.49 | 1.43 |
| 37 | b | 511 | CLA | C4D-CHA | 2.48 | 1.46 | 1.38 |
| 37 | 21 | 208 | CLA | C1B-C2B | 2.48 | 1.48 | 1.43 |
| 37 | c | 512 | CLA | C3B-C4B | 2.48 | 1.50 | 1.42 |
| 37 | B | 506 | CLA | C4D-CHA | 2.48 | 1.46 | 1.38 |
| 48 | 14 | 315 | A86 | C2-C1 | 2.48 | 1.41 | 1.35 |
| 48 | 12 | 213 | A86 | C14-C15 | 2.48 | 1.57 | 1.52 |
| 37 | D | 401 | CLA | C1C-NC | -2.48 | 1.34 | 1.37 |
| 47 | 36 | 305 | KC1 | CHB-C4A | -2.48 | 1.33 | 1.39 |
| 47 | 38 | 205 | KC1 | C2A-C1A | 2.48 | 1.52 | 1.44 |
| 37 | 11 | 307 | CLA | C3D-C4D | -2.48 | 1.38 | 1.44 |
| 37 | 31 | 308 | CLA | C3D-C4D | -2.48 | 1.38 | 1.44 |
| 37 | c | 509 | CLA | C1C-NC | -2.48 | 1.34 | 1.37 |
| 45 | D | 404 | PL9 | C53-C6 | -2.48 | 1.45 | 1.50 |
| 48 | 18 | 215 | A86 | C2-C1 | 2.48 | 1.41 | 1.35 |
| 48 | 38 | 214 | A86 | O-C13 | -2.48 | 1.18 | 1.23 |
| 48 | 38 | 215 | A86 | C2-C1 | 2.48 | 1.41 | 1.35 |
| 37 | 36 | 303 | CLA | C3D-C4D | -2.48 | 1.38 | 1.44 |
| 48 | 17 | 314 | A86 | C14-C15 | 2.48 | 1.57 | 1.52 |
| 48 | 21 | 211 | A86 | C2-C1 | 2.48 | 1.41 | 1.35 |
| 48 | 34 | 314 | A86 | C24-C1 | 2.48 | 1.51 | 1.46 |
| 37 | 32 | 202 | CLA | C3B-C4B | 2.48 | 1.49 | 1.42 |
| 48 | 31 | 315 | A86 | O4-C34 | -2.48 | 1.40 | 1.46 |
| 50 | 21 | 212 | DD6 | C4-C5 | 2.48 | 1.50 | 1.43 |
| 50 | 41 | 212 | DD6 | C4-C5 | 2.48 | 1.50 | 1.43 |
| 37 | b | 502 | CLA | C4D-CHA | 2.48 | 1.46 | 1.38 |
| 37 | 31 | 306 | CLA | C3D-C4D | -2.48 | 1.38 | 1.44 |
| 37 | b | 501 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 37 | 40 | 209 | CLA | C4C-C3C | 2.47 | 1.49 | 1.45 |
| 47 | 15 | 306 | KC1 | C2A-C1A | 2.47 | 1.52 | 1.44 |
| 41 | 11 | 316 | LMG | O7-C8 | -2.47 | 1.40 | 1.46 |
| 41 | 31 | 316 | LMG | O7-C8 | -2.47 | 1.40 | 1.46 |
| 37 | W | 101 | CLA | C1C-NC | -2.47 | 1.34 | 1.37 |
| 37 | 38 | 204 | CLA | C4D-CHA | 2.47 | 1.46 | 1.38 |
| 48 | 15 | 314 | A86 | C2-C1 | 2.47 | 1.41 | 1.35 |
| 48 | 41 | 215 | A86 | C2-C1 | 2.47 | 1.41 | 1.35 |
| 37 | 33 | 310 | CLA | C4C-C3C | 2.47 | 1.49 | 1.45 |
| 47 | 32 | 207 | KC1 | CHD-C1D | 2.47 | 1.45 | 1.39 |
| 37 | B | 505 | CLA | C4D-CHA | 2.47 | 1.46 | 1.38 |
| 47 | 20 | 304 | KC1 | C1D-C2D | 2.47 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 31 | 319 | A86 | O4-C34 | -2.47 | 1.40 | 1.46 |
| 48 | 33 | 315 | A86 | O-C13 | -2.47 | 1.18 | 1.23 |
| 37 | 17 | 302 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 37 | 39 | 303 | CLA | C1B-C2B | 2.47 | 1.48 | 1.43 |
| 39 | y | 101 | BCR | C33-C5 | -2.47 | 1.47 | 1.50 |
| 43 | 41 | 201 | LHG | O7-C5 | -2.47 | 1.40 | 1.46 |
| 48 | 40 | 211 | A86 | C26-C27 | 2.47 | 1.41 | 1.35 |
| 47 | 34 | 306 | KC1 | C4A-C3A | 2.47 | 1.49 | 1.44 |
| 48 | 37 | 313 | A86 | C14-C15 | 2.47 | 1.57 | 1.52 |
| 37 | B | 502 | CLA | C4D-CHA | 2.47 | 1.46 | 1.38 |
| 37 | A | 405 | CLA | C4D-CHA | 2.47 | 1.46 | 1.38 |
| 37 | 21 | 210 | CLA | C1B-C2B | 2.46 | 1.48 | 1.43 |
| 47 | 35 | 306 | KC1 | C2A-C1A | 2.46 | 1.52 | 1.44 |
| 37 | 32 | 208 | CLA | C4D-CHA | 2.46 | 1.46 | 1.38 |
| 37 | c | 513 | CLA | C3D-C4D | -2.46 | 1.38 | 1.44 |
| 47 | 11 | 304 | KC1 | C4A-C3A | 2.46 | 1.49 | 1.44 |
| 47 | 17 | 305 | KC1 | C4C-C3C | 2.46 | 1.49 | 1.45 |
| 37 | C | 512 | CLA | C3B-C4B | 2.46 | 1.49 | 1.42 |
| 37 | B | 508 | CLA | C3B-C4B | 2.46 | 1.49 | 1.42 |
| 47 | 33 | 306 | KC1 | C2A-C1A | 2.46 | 1.52 | 1.44 |
| 48 | 15 | 311 | A86 | C2-C1 | 2.46 | 1.41 | 1.35 |
| 48 | 35 | 316 | A86 | C2-C1 | 2.46 | 1.41 | 1.35 |
| 37 | 38 | 206 | CLA | C3B-C4B | 2.46 | 1.49 | 1.42 |
| 37 | 41 | 208 | CLA | C1B-C2B | 2.46 | 1.48 | 1.43 |
| 48 | 15 | 319 | A86 | O-C13 | -2.46 | 1.18 | 1.23 |
| 48 | 31 | 311 | A86 | C25-C24 | 2.46 | 1.41 | 1.34 |
| 48 | 37 | 311 | A86 | C2-C1 | 2.46 | 1.41 | 1.35 |
| 37 | 33 | 303 | CLA | C3D-C4D | -2.46 | 1.38 | 1.44 |
| 48 | 12 | 220 | A86 | C-C1 | 2.46 | 1.55 | 1.50 |
| 48 | 15 | 315 | A86 | C26-C27 | 2.46 | 1.41 | 1.35 |
| 37 | 34 | 310 | CLA | C1B-C2B | 2.46 | 1.48 | 1.43 |
| 48 | 11 | 315 | A86 | O4-C34 | -2.46 | 1.40 | 1.46 |
| 50 | 20 | 310 | DD6 | C4-C5 | 2.46 | 1.50 | 1.43 |
| 48 | 19 | 311 | A86 | C25-C24 | 2.46 | 1.41 | 1.34 |
| 37 | c | 507 | CLA | C1C-NC | -2.46 | 1.34 | 1.37 |
| 37 | z | 102 | CLA | C3B-C4B | 2.46 | 1.49 | 1.42 |
| 47 | 15 | 304 | KC1 | C2A-C1A | 2.46 | 1.52 | 1.44 |
| 38 | A | 404 | PHO | CMB-C2B | -2.46 | 1.46 | 1.51 |
| 48 | 13 | 312 | A86 | O4-C34 | -2.46 | 1.40 | 1.46 |
| 37 | b | 511 | CLA | C1C-NC | -2.46 | 1.34 | 1.37 |
| 37 | 40 | 209 | CLA | C1B-C2B | 2.46 | 1.48 | 1.43 |
| 37 | 39 | 307 | CLA | C3D-C4D | -2.45 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 37 | 304 | KC1 | C4C-C3C | 2.45 | 1.49 | 1.45 |
| 37 | 41 | 209 | CLA | C1B-C2B | 2.45 | 1.48 | 1.43 |
| 37 | b | 505 | CLA | C4D-CHA | 2.45 | 1.46 | 1.38 |
| 37 | a | 407 | CLA | C4D-CHA | 2.45 | 1.46 | 1.38 |
| 37 | 36 | 309 | CLA | C4C-C3C | 2.45 | 1.49 | 1.45 |
| 37 | c | 511 | CLA | C1B-C2B | 2.45 | 1.48 | 1.43 |
| 48 | 32 | 214 | A86 | C14-C15 | 2.45 | 1.57 | 1.52 |
| 37 | d | 401 | CLA | C4D-CHA | 2.45 | 1.46 | 1.38 |
| 37 | a | 403 | CLA | C1C-NC | -2.45 | 1.34 | 1.37 |
| 48 | 15 | 316 | A86 | C2-C1 | 2.45 | 1.41 | 1.35 |
| 48 | 35 | 311 | A86 | C2-C1 | 2.45 | 1.41 | 1.35 |
| 48 | 38 | 214 | A86 | C2-C1 | 2.45 | 1.41 | 1.35 |
| 37 | 38 | 206 | CLA | C1B-C2B | 2.45 | 1.48 | 1.43 |
| 47 | 13 | 306 | KC1 | C2A-C1A | 2.45 | 1.52 | 1.44 |
| 47 | 20 | 305 | KC1 | CHB-C4A | -2.45 | 1.33 | 1.39 |
| 37 | 35 | 308 | CLA | C3B-C4B | 2.45 | 1.49 | 1.42 |
| 37 | b | 508 | CLA | C4D-CHA | 2.45 | 1.46 | 1.38 |
| 48 | 15 | 311 | A86 | O-C13 | -2.45 | 1.18 | 1.23 |
| 37 | b | 508 | CLA | C3B-C4B | 2.45 | 1.49 | 1.42 |
| 45 | d | 406 | PL9 | C53-C6 | -2.45 | 1.45 | 1.50 |
| 37 | 21 | 209 | CLA | C1B-C2B | 2.45 | 1.48 | 1.43 |
| 37 | C | 513 | CLA | C3D-C4D | -2.45 | 1.38 | 1.44 |
| 37 | 39 | 306 | CLA | C3B-C4B | 2.45 | 1.49 | 1.42 |
| 48 | 20 | 309 | A86 | O-C13 | -2.45 | 1.18 | 1.23 |
| 47 | 17 | 305 | KC1 | C2A-C1A | 2.45 | 1.52 | 1.44 |
| 47 | 37 | 304 | KC1 | C2A-C1A | 2.45 | 1.52 | 1.44 |
| 37 | 31 | 302 | CLA | C3D-C4D | -2.45 | 1.38 | 1.44 |
| 37 | 12 | 207 | CLA | C4D-CHA | 2.45 | 1.46 | 1.38 |
| 48 | 14 | 314 | A86 | C2-C1 | 2.45 | 1.41 | 1.35 |
| 48 | 31 | 314 | A86 | C26-C27 | 2.45 | 1.41 | 1.35 |
| 47 | 38 | 207 | KC1 | CHB-C4A | -2.44 | 1.33 | 1.39 |
| 37 | a | 403 | CLA | C4D-CHA | 2.44 | 1.46 | 1.38 |
| 47 | 31 | 305 | KC1 | C4A-C3A | 2.44 | 1.49 | 1.44 |
| 37 | 32 | 211 | CLA | C1B-C2B | 2.44 | 1.48 | 1.43 |
| 48 | 21 | 215 | A86 | C2-C1 | 2.44 | 1.41 | 1.35 |
| 48 | 38 | 213 | A86 | C26-C27 | 2.44 | 1.41 | 1.35 |
| 37 | C | 508 | CLA | C4D-CHA | 2.44 | 1.46 | 1.38 |
| 45 | D | 408 | PL9 | C53-C6 | -2.44 | 1.45 | 1.50 |
| 48 | 19 | 313 | A86 | C2-C1 | 2.44 | 1.41 | 1.35 |
| 37 | 33 | 310 | CLA | C3B-C4B | 2.44 | 1.49 | 1.42 |
| 37 | c | 508 | CLA | C4D-CHA | 2.44 | 1.46 | 1.38 |
| 37 | 11 | 308 | CLA | C3B-C4B | 2.44 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 13 | 315 | A86 | C14-C15 | 2.44 | 1.57 | 1.52 |
| 37 | A | 403 | CLA | C1C-NC | -2.44 | 1.34 | 1.37 |
| 37 | 16 | 309 | CLA | C3D-C4D | -2.44 | 1.38 | 1.44 |
| 37 | Z | 102 | CLA | C3B-C4B | 2.44 | 1.49 | 1.42 |
| 48 | 12 | 213 | A86 | O4-C34 | -2.44 | 1.40 | 1.46 |
| 48 | 35 | 311 | A86 | O-C13 | -2.44 | 1.18 | 1.23 |
| 39 | K | 101 | BCR | C33-C5 | -2.44 | 1.47 | 1.50 |
| 48 | 32 | 218 | A86 | C24-C1 | 2.44 | 1.51 | 1.46 |
| 48 | 15 | 319 | A86 | C26-C27 | 2.44 | 1.41 | 1.35 |
| 48 | 11 | 319 | A86 | C-C1 | 2.44 | 1.55 | 1.50 |
| 44 | J | 101 | DGD | O3G-C3G | -2.44 | 1.39 | 1.43 |
| 37 | 41 | 209 | CLA | C4C-C3C | 2.44 | 1.49 | 1.45 |
| 48 | 32 | 221 | A86 | C-C1 | 2.44 | 1.55 | 1.50 |
| 47 | 36 | 304 | KC1 | C1D-C2D | 2.44 | 1.48 | 1.43 |
| 48 | 20 | 309 | A86 | C26-C27 | 2.44 | 1.41 | 1.35 |
| 37 | 18 | 204 | CLA | C4D-CHA | 2.44 | 1.46 | 1.38 |
| 37 | 14 | 307 | CLA | C3D-C4D | -2.44 | 1.38 | 1.44 |
| 37 | 16 | 303 | CLA | C3D-C4D | -2.44 | 1.38 | 1.44 |
| 37 | 34 | 307 | CLA | C3D-C4D | -2.44 | 1.38 | 1.44 |
| 48 | 34 | 315 | A86 | C2-C1 | 2.44 | 1.41 | 1.35 |
| 37 | 21 | 206 | CLA | C1B-C2B | 2.44 | 1.48 | 1.43 |
| 37 | 13 | 305 | CLA | C3B-C4B | 2.44 | 1.49 | 1.42 |
| 48 | 11 | 314 | A86 | C26-C27 | 2.44 | 1.41 | 1.35 |
| 37 | 15 | 305 | CLA | C3B-C4B | 2.44 | 1.49 | 1.42 |
| 37 | B | 508 | CLA | C4D-CHA | 2.44 | 1.46 | 1.38 |
| 37 | 15 | 305 | CLA | C4C-C3C | 2.44 | 1.49 | 1.45 |
| 37 | 40 | 210 | CLA | C4C-C3C | 2.44 | 1.49 | 1.45 |
| 48 | 37 | 309 | A86 | C24-C1 | 2.44 | 1.51 | 1.46 |
| 37 | A | 403 | CLA | C4D-CHA | 2.44 | 1.46 | 1.38 |
| 47 | 16 | 305 | KC1 | C4C-C3C | 2.44 | 1.49 | 1.45 |
| 48 | 33 | 315 | A86 | C14-C15 | 2.43 | 1.57 | 1.52 |
| 48 | 14 | 314 | A86 | C24-C1 | 2.43 | 1.51 | 1.46 |
| 37 | 33 | 303 | CLA | C4C-C3C | 2.43 | 1.49 | 1.45 |
| 37 | 41 | 206 | CLA | C1B-C2B | 2.43 | 1.48 | 1.43 |
| 37 | C | 507 | CLA | C1C-NC | -2.43 | 1.34 | 1.37 |
| 37 | 21 | 204 | CLA | C4C-C3C | 2.43 | 1.49 | 1.45 |
| 37 | D | 402 | CLA | C4D-CHA | 2.43 | 1.46 | 1.38 |
| 47 | 12 | 211 | KC1 | C4A-C3A | 2.43 | 1.49 | 1.44 |
| 47 | 32 | 212 | KC1 | C4A-C3A | 2.43 | 1.49 | 1.44 |
| 37 | C | 510 | CLA | C1B-C2B | 2.43 | 1.48 | 1.43 |
| 48 | 11 | 319 | A86 | O4-C34 | -2.43 | 1.40 | 1.46 |
| 47 | 31 | 307 | KC1 | C4A-C3A | 2.43 | 1.49 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 18 | 214 | A86 | C2-C1 | 2.43 | 1.41 | 1.35 |
| 37 | 19 | 303 | CLA | C1B-C2B | 2.43 | 1.48 | 1.43 |
| 48 | 40 | 211 | A86 | O-C13 | -2.43 | 1.18 | 1.23 |
| 37 | 33 | 308 | CLA | C3D-C4D | -2.43 | 1.38 | 1.44 |
| 37 | c | 505 | CLA | C1C-NC | -2.43 | 1.34 | 1.37 |
| 50 | 39 | 312 | DD6 | C22-C16 | -2.43 | 1.49 | 1.53 |
| 37 | 19 | 307 | CLA | C3D-C4D | -2.43 | 1.38 | 1.44 |
| 48 | 12 | 217 | A86 | C24-C1 | 2.43 | 1.51 | 1.46 |
| 37 | 33 | 305 | CLA | C3B-C4B | 2.43 | 1.49 | 1.42 |
| 37 | z | 101 | CLA | C4D-CHA | 2.43 | 1.46 | 1.38 |
| 50 | 21 | 212 | DD6 | C35-C36 | 2.43 | 1.54 | 1.51 |
| 48 | 40 | 213 | A86 | C5-C6 | 2.43 | 1.41 | 1.35 |
| 37 | 33 | 307 | CLA | O1D-CGD | 2.43 | 1.27 | 1.21 |
| 48 | 20 | 311 | A86 | C5-C6 | 2.43 | 1.41 | 1.35 |
| 48 | 12 | 220 | A86 | C14-C15 | 2.43 | 1.57 | 1.52 |
| 41 | A | 408 | LMG | O8-C9 | -2.43 | 1.39 | 1.45 |
| 48 | 18 | 213 | A86 | C26-C27 | 2.43 | 1.41 | 1.35 |
| 50 | 19 | 312 | DD6 | C22-C16 | -2.43 | 1.49 | 1.53 |
| 48 | 11 | 311 | A86 | C25-C24 | 2.43 | 1.41 | 1.34 |
| 37 | 41 | 204 | CLA | C4C-C3C | 2.43 | 1.49 | 1.45 |
| 37 | C | 509 | CLA | C4D-CHA | 2.43 | 1.46 | 1.38 |
| 48 | 17 | 310 | A86 | C24-C1 | 2.43 | 1.51 | 1.46 |
| 48 | 21 | 211 | A86 | C-C1 | 2.43 | 1.55 | 1.50 |
| 37 | 32 | 211 | CLA | C3D-C4D | -2.43 | 1.38 | 1.44 |
| 37 | c | 510 | CLA | C1B-C2B | 2.43 | 1.48 | 1.43 |
| 44 | H | 102 | DGD | O5D-C6D | -2.43 | 1.39 | 1.43 |
| 37 | 12 | 210 | CLA | C1B-C2B | 2.42 | 1.48 | 1.43 |
| 48 | 33 | 312 | A86 | O4-C34 | -2.42 | 1.40 | 1.46 |
| 48 | 14 | 311 | A86 | C-C1 | 2.42 | 1.55 | 1.50 |
| 48 | 34 | 311 | A86 | C-C1 | 2.42 | 1.55 | 1.50 |
| 37 | 12 | 210 | CLA | C3D-C4D | -2.42 | 1.38 | 1.44 |
| 48 | 32 | 221 | A86 | C14-C15 | 2.42 | 1.57 | 1.52 |
| 37 | b | 502 | CLA | C1C-NC | -2.42 | 1.34 | 1.37 |
| 37 | 14 | 305 | CLA | C3B-C4B | 2.42 | 1.49 | 1.42 |
| 37 | 21 | 208 | CLA | C3B-C4B | 2.42 | 1.49 | 1.42 |
| 37 | 19 | 310 | CLA | C3D-C4D | -2.42 | 1.38 | 1.44 |
| 48 | 11 | 319 | A86 | C14-C15 | 2.42 | 1.57 | 1.52 |
| 48 | 18 | 213 | A86 | C14-C15 | 2.42 | 1.57 | 1.52 |
| 48 | 31 | 319 | A86 | C14-C15 | 2.42 | 1.57 | 1.52 |
| 48 | 32 | 214 | A86 | O4-C34 | -2.42 | 1.40 | 1.46 |
| 37 | 40 | 205 | CLA | OBD-CAD | 2.42 | 1.26 | 1.22 |
| 37 | 37 | 301 | CLA | C3D-C4D | -2.42 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | z | 102 | CLA | C3D-C4D | -2.42 | 1.38 | 1.44 |
| 37 | B | 508 | CLA | C1C-NC | -2.42 | 1.34 | 1.37 |
| 47 | 35 | 304 | KC1 | C2A-C1A | 2.42 | 1.52 | 1.44 |
| 44 | H | 102 | DGD | O1G-C1G | -2.42 | 1.39 | 1.45 |
| 37 | c | 505 | CLA | C3B-C4B | 2.42 | 1.49 | 1.42 |
| 37 | B | 511 | CLA | C1C-NC | -2.42 | 1.34 | 1.37 |
| 37 | b | 508 | CLA | C1C-NC | -2.42 | 1.34 | 1.37 |
| 48 | 37 | 312 | A86 | C24-C1 | 2.42 | 1.51 | 1.46 |
| 37 | Z | 101 | CLA | C4D-CHA | 2.42 | 1.46 | 1.38 |
| 44 | C | 517 | DGD | O4E-C4E | -2.42 | 1.37 | 1.43 |
| 44 | h | 102 | DGD | O1G-C1G | -2.42 | 1.39 | 1.45 |
| 37 | 14 | 303 | CLA | C3D-C4D | -2.42 | 1.38 | 1.44 |
| 41 | 17 | 317 | LMG | O8-C9 | -2.42 | 1.39 | 1.45 |
| 37 | 16 | 309 | CLA | C4C-C3C | 2.42 | 1.49 | 1.45 |
| 37 | 20 | 303 | CLA | OBD-CAD | 2.42 | 1.26 | 1.22 |
| 48 | 41 | 211 | A86 | C24-C1 | 2.42 | 1.51 | 1.46 |
| 48 | 41 | 211 | A86 | C-C1 | 2.42 | 1.55 | 1.50 |
| 48 | 35 | 319 | A86 | O-C13 | -2.42 | 1.18 | 1.23 |
| 47 | 38 | 205 | KC1 | C4C-C3C | 2.42 | 1.49 | 1.45 |
| 37 | 41 | 208 | CLA | C3B-C4B | 2.42 | 1.49 | 1.42 |
| 37 | 39 | 310 | CLA | C3D-C4D | -2.42 | 1.38 | 1.44 |
| 37 | 13 | 310 | CLA | C1B-C2B | 2.41 | 1.48 | 1.43 |
| 37 | 21 | 204 | CLA | C1B-C2B | 2.41 | 1.48 | 1.43 |
| 37 | 41 | 204 | CLA | C1B-C2B | 2.41 | 1.48 | 1.43 |
| 47 | 40 | 206 | KC1 | C1D-C2D | 2.41 | 1.48 | 1.43 |
| 48 | 15 | 312 | A86 | O4-C34 | -2.41 | 1.40 | 1.46 |
| 47 | 12 | 206 | KC1 | C4A-C3A | 2.41 | 1.49 | 1.44 |
| 47 | 32 | 207 | KC1 | C4A-C3A | 2.41 | 1.49 | 1.44 |
| 44 | c | 517 | DGD | O4E-C4E | -2.41 | 1.37 | 1.43 |
| 37 | C | 505 | CLA | C3B-C4B | 2.41 | 1.49 | 1.42 |
| 37 | 13 | 310 | CLA | C3B-C4B | 2.41 | 1.49 | 1.42 |
| 37 | 35 | 305 | CLA | C3B-C4B | 2.41 | 1.49 | 1.42 |
| 41 | a | 410 | LMG | O8-C9 | -2.41 | 1.39 | 1.45 |
| 48 | 12 | 213 | A86 | C25-C24 | 2.41 | 1.41 | 1.34 |
| 37 | B | 503 | CLA | C4D-CHA | 2.41 | 1.46 | 1.38 |
| 48 | 35 | 319 | A86 | C26-C27 | 2.41 | 1.41 | 1.35 |
| 37 | b | 516 | CLA | C3B-C4B | 2.41 | 1.49 | 1.42 |
| 41 | 16 | 316 | LMG | C4-C5 | 2.41 | 1.58 | 1.53 |
| 47 | 16 | 304 | KC1 | C1D-C2D | 2.41 | 1.48 | 1.43 |
| 48 | 34 | 314 | A86 | C2-C1 | 2.41 | 1.41 | 1.35 |
| 48 | 31 | 313 | A86 | O4-C34 | -2.41 | 1.40 | 1.46 |
| 37 | Z | 102 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 39 | 302 | CLA | C3B-C4B | 2.41 | 1.49 | 1.42 |
| 37 | b | 523 | CLA | C4D-CHA | 2.41 | 1.46 | 1.38 |
| 48 | 11 | 311 | A86 | O4-C34 | -2.41 | 1.40 | 1.46 |
| 37 | C | 505 | CLA | C1C-NC | -2.41 | 1.34 | 1.37 |
| 37 | 19 | 302 | CLA | C3B-C4B | 2.41 | 1.49 | 1.42 |
| 37 | 36 | 309 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |
| 37 | 38 | 203 | CLA | C4C-C3C | 2.41 | 1.49 | 1.45 |
| 43 | 21 | 201 | LHG | O7-C5 | -2.41 | 1.40 | 1.46 |
| 48 | 35 | 315 | A86 | C24-C1 | 2.41 | 1.51 | 1.46 |
| 37 | 21 | 209 | CLA | C4C-C3C | 2.41 | 1.49 | 1.45 |
| 37 | 19 | 306 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |
| 37 | 40 | 209 | CLA | C3B-C4B | 2.41 | 1.49 | 1.42 |
| 37 | c | 509 | CLA | C4D-CHA | 2.41 | 1.46 | 1.38 |
| 48 | 35 | 319 | A86 | C24-C1 | 2.41 | 1.51 | 1.46 |
| 37 | c | 505 | CLA | CBD-CAD | -2.41 | 1.45 | 1.56 |
| 48 | 39 | 313 | A86 | C2-C1 | 2.41 | 1.41 | 1.35 |
| 37 | 21 | 205 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 48 | 31 | 311 | A86 | O4-C34 | -2.40 | 1.40 | 1.46 |
| 37 | 34 | 305 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 37 | 35 | 310 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 37 | 18 | 201 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 37 | 34 | 310 | CLA | C4C-C3C | 2.40 | 1.49 | 1.45 |
| 48 | 31 | 319 | A86 | C-C1 | 2.40 | 1.55 | 1.50 |
| 37 | 34 | 303 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 37 | 16 | 303 | CLA | C4C-C3C | 2.40 | 1.49 | 1.45 |
| 37 | 34 | 301 | CLA | C1B-C2B | 2.40 | 1.48 | 1.43 |
| 37 | 41 | 205 | CLA | C3B-C4B | 2.40 | 1.49 | 1.42 |
| 47 | 16 | 302 | KC1 | C4C-C3C | 2.40 | 1.49 | 1.45 |
| 48 | 17 | 313 | A86 | C24-C1 | 2.40 | 1.51 | 1.46 |
| 37 | c | 501 | CLA | C4D-CHA | 2.40 | 1.46 | 1.38 |
| 47 | 16 | 304 | KC1 | C4A-C3A | 2.40 | 1.49 | 1.44 |
| 41 | 37 | 316 | LMG | O8-C9 | -2.40 | 1.39 | 1.45 |
| 48 | 12 | 216 | A86 | C24-C1 | 2.40 | 1.51 | 1.46 |
| 48 | 32 | 217 | A86 | C24-C1 | 2.40 | 1.51 | 1.46 |
| 44 | h | 102 | DGD | O5D-C6D | -2.40 | 1.39 | 1.43 |
| 37 | 41 | 204 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 48 | 38 | 215 | A86 | C14-C15 | 2.40 | 1.57 | 1.52 |
| 47 | 21 | 207 | KC1 | C1C-C2C | 2.40 | 1.49 | 1.44 |
| 37 | c | 510 | CLA | C4D-CHA | 2.40 | 1.46 | 1.38 |
| 37 | C | 505 | CLA | C4D-CHA | 2.40 | 1.46 | 1.38 |
| 37 | 19 | 304 | CLA | C1B-C2B | 2.39 | 1.48 | 1.43 |
| 37 | 39 | 304 | CLA | C1B-C2B | 2.39 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 11 | 301 | CLA | C3D-C4D | -2.39 | 1.38 | 1.44 |
| 47 | 41 | 207 | KC1 | C1C-C2C | 2.39 | 1.49 | 1.44 |
| 48 | 15 | 315 | A86 | C24-C1 | 2.39 | 1.51 | 1.46 |
| 47 | 18 | 207 | KC1 | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 37 | 14 | 301 | CLA | C1B-C2B | 2.39 | 1.48 | 1.43 |
| 37 | 31 | 301 | CLA | C3D-C4D | -2.39 | 1.38 | 1.44 |
| 37 | 21 | 206 | CLA | C3B-C4B | 2.39 | 1.49 | 1.42 |
| 47 | 35 | 302 | KC1 | C4A-C3A | 2.39 | 1.49 | 1.44 |
| 37 | b | 503 | CLA | C4D-CHA | 2.39 | 1.46 | 1.38 |
| 48 | 39 | 313 | A86 | C24-C1 | 2.39 | 1.51 | 1.46 |
| 47 | 13 | 309 | KC1 | C4A-C3A | 2.39 | 1.49 | 1.44 |
| 37 | B | 516 | CLA | C3B-C4B | 2.39 | 1.49 | 1.42 |
| 37 | 16 | 301 | CLA | C1B-C2B | 2.39 | 1.48 | 1.43 |
| 37 | 41 | 210 | CLA | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 37 | B | 524 | CLA | C4D-CHA | 2.39 | 1.46 | 1.38 |
| 48 | 19 | 313 | A86 | C22-C16 | 2.39 | 1.58 | 1.53 |
| 47 | 36 | 302 | KC1 | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 48 | 17 | 311 | A86 | C24-C1 | 2.39 | 1.51 | 1.46 |
| 37 | 33 | 310 | CLA | C1B-C2B | 2.39 | 1.48 | 1.43 |
| 48 | 15 | 319 | A86 | C24-C1 | 2.39 | 1.51 | 1.46 |
| 37 | C | 510 | CLA | C4D-CHA | 2.39 | 1.46 | 1.38 |
| 37 | 15 | 310 | CLA | C3B-C4B | 2.39 | 1.49 | 1.42 |
| 48 | 41 | 211 | A86 | C5-C6 | 2.39 | 1.41 | 1.35 |
| 50 | 41 | 212 | DD6 | C35-C36 | 2.39 | 1.54 | 1.51 |
| 37 | C | 505 | CLA | CBD-CAD | -2.39 | 1.45 | 1.56 |
| 47 | 15 | 306 | KC1 | C1D-C2D | 2.39 | 1.48 | 1.43 |
| 37 | B | 506 | CLA | C3B-C4B | 2.39 | 1.49 | 1.42 |
| 37 | 19 | 304 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 41 | 36 | 314 | LMG | C4-C5 | 2.38 | 1.58 | 1.53 |
| 48 | 12 | 213 | A86 | C-C1 | 2.38 | 1.55 | 1.50 |
| 48 | 39 | 313 | A86 | C22-C16 | 2.38 | 1.58 | 1.53 |
| 50 | 36 | 312 | DD6 | O1-C20 | 2.38 | 1.49 | 1.46 |
| 37 | 13 | 307 | CLA | O1D-CGD | 2.38 | 1.27 | 1.21 |
| 37 | B | 502 | CLA | C1C-NC | -2.38 | 1.34 | 1.37 |
| 48 | 16 | 310 | A86 | O4-C34 | -2.38 | 1.41 | 1.46 |
| 48 | 40 | 201 | A86 | C2-C1 | 2.38 | 1.41 | 1.35 |
| 50 | 36 | 312 | DD6 | C4-C5 | 2.38 | 1.50 | 1.43 |
| 37 | b | 506 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 37 | 39 | 306 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 37 | B | 515 | CLA | C1B-C2B | 2.38 | 1.48 | 1.43 |
| 37 | 11 | 308 | CLA | C1C-NC | -2.38 | 1.34 | 1.37 |
| 48 | 16 | 313 | A86 | C2-C1 | 2.38 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 17 | 304 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 37 | 37 | 303 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 37 | 13 | 303 | CLA | C1B-C2B | 2.38 | 1.48 | 1.43 |
| 37 | 36 | 307 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 37 | 35 | 305 | CLA | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 48 | 13 | 314 | A86 | C5-C6 | 2.38 | 1.41 | 1.35 |
| 37 | 36 | 303 | CLA | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 47 | 36 | 304 | KC1 | C4A-C3A | 2.38 | 1.49 | 1.44 |
| 48 | 31 | 311 | A86 | C14-C15 | 2.38 | 1.57 | 1.52 |
| 47 | 39 | 308 | KC1 | C4A-C3A | 2.38 | 1.49 | 1.44 |
| 37 | W | 102 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 37 | Z | 102 | CLA | C1B-C2B | 2.38 | 1.48 | 1.43 |
| 37 | 13 | 308 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 37 | 12 | 204 | CLA | C3B-C4B | 2.38 | 1.49 | 1.42 |
| 48 | 33 | 311 | A86 | C26-C27 | 2.38 | 1.41 | 1.35 |
| 47 | 11 | 306 | KC1 | C4A-C3A | 2.38 | 1.49 | 1.44 |
| 37 | z | 102 | CLA | C1B-C2B | 2.37 | 1.48 | 1.43 |
| 48 | 35 | 312 | A86 | O4-C34 | -2.37 | 1.41 | 1.46 |
| 47 | 32 | 209 | KC1 | C4A-C3A | 2.37 | 1.49 | 1.44 |
| 48 | 17 | 313 | A86 | C2-C1 | 2.37 | 1.41 | 1.35 |
| 37 | 34 | 302 | CLA | C3D-C4D | -2.37 | 1.38 | 1.44 |
| 37 | 37 | 301 | CLA | C1B-C2B | 2.37 | 1.48 | 1.43 |
| 37 | 21 | 204 | CLA | C3D-C4D | -2.37 | 1.38 | 1.44 |
| 37 | 32 | 205 | CLA | C3B-C4B | 2.37 | 1.49 | 1.42 |
| 47 | 37 | 305 | KC1 | CHB-C4A | -2.37 | 1.33 | 1.39 |
| 44 | c | 516 | DGD | O2G-C2G | -2.37 | 1.41 | 1.46 |
| 37 | c | 501 | CLA | C1B-C2B | 2.37 | 1.48 | 1.43 |
| 47 | 11 | 309 | KC1 | C4A-C3A | 2.37 | 1.49 | 1.44 |
| 37 | 38 | 208 | CLA | C3D-C4D | -2.37 | 1.38 | 1.44 |
| 47 | 18 | 207 | KC1 | CHB-C4A | -2.37 | 1.33 | 1.39 |
| 48 | 15 | 314 | A86 | O-C13 | -2.37 | 1.18 | 1.23 |
| 37 | 20 | 307 | CLA | C3B-C4B | 2.37 | 1.49 | 1.42 |
| 37 | 18 | 202 | CLA | C1B-C2B | 2.37 | 1.48 | 1.43 |
| 47 | 41 | 207 | KC1 | C3B-C4B | 2.36 | 1.50 | 1.46 |
| 37 | 21 | 210 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 37 | 39 | 301 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 48 | 31 | 315 | A86 | C-C1 | 2.36 | 1.55 | 1.50 |
| 37 | c | 505 | CLA | C4D-CHA | 2.36 | 1.46 | 1.38 |
| 48 | 33 | 315 | A86 | C2-C1 | 2.36 | 1.41 | 1.35 |
| 37 | 14 | 308 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 37 | 39 | 304 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 37 | b | 503 | CLA | C1C-NC | -2.36 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 36 | 310 | A86 | O4-C34 | -2.36 | 1.41 | 1.46 |
| 37 | C | 501 | CLA | C4D-CHA | 2.36 | 1.46 | 1.38 |
| 37 | 41 | 206 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 48 | 20 | 309 | A86 | C2-C1 | 2.36 | 1.41 | 1.35 |
| 37 | 33 | 303 | CLA | C1B-C2B | 2.36 | 1.48 | 1.43 |
| 37 | 14 | 302 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 48 | 34 | 316 | A86 | C14-C15 | 2.36 | 1.57 | 1.52 |
| 37 | 34 | 305 | CLA | C1B-C2B | 2.36 | 1.48 | 1.43 |
| 50 | 16 | 312 | DD6 | C4-C5 | 2.36 | 1.50 | 1.43 |
| 47 | 33 | 309 | KC1 | C4A-C3A | 2.36 | 1.49 | 1.44 |
| 37 | 41 | 210 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 48 | 36 | 310 | A86 | C26-C27 | 2.36 | 1.41 | 1.35 |
| 48 | 37 | 309 | A86 | C2-C1 | 2.36 | 1.41 | 1.35 |
| 47 | 31 | 309 | KC1 | C4A-C3A | 2.36 | 1.49 | 1.44 |
| 48 | 11 | 313 | A86 | C24-C1 | 2.36 | 1.51 | 1.46 |
| 37 | 35 | 301 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 48 | 14 | 316 | A86 | C14-C15 | 2.36 | 1.57 | 1.52 |
| 48 | 17 | 310 | A86 | C2-C1 | 2.36 | 1.41 | 1.35 |
| 48 | 34 | 311 | A86 | O4-C34 | -2.36 | 1.41 | 1.46 |
| 48 | 13 | 315 | A86 | C2-C1 | 2.36 | 1.41 | 1.35 |
| 48 | 21 | 211 | A86 | C5-C6 | 2.36 | 1.41 | 1.35 |
| 37 | D | 405 | CLA | C1B-C2B | 2.36 | 1.48 | 1.43 |
| 44 | c | 516 | DGD | O3G-C3G | -2.36 | 1.39 | 1.43 |
| 37 | 34 | 308 | CLA | C1B-C2B | 2.36 | 1.48 | 1.43 |
| 48 | 37 | 312 | A86 | C2-C1 | 2.36 | 1.41 | 1.35 |
| 37 | 18 | 206 | CLA | C3B-C4B | 2.36 | 1.49 | 1.42 |
| 37 | 21 | 210 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 47 | 18 | 205 | KC1 | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 48 | 37 | 313 | A86 | O4-C34 | -2.36 | 1.41 | 1.46 |
| 37 | b | 504 | CLA | C1C-NC | -2.36 | 1.34 | 1.37 |
| 44 | C | 516 | DGD | O3G-C3G | -2.36 | 1.39 | 1.43 |
| 37 | 32 | 204 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 48 | 13 | 311 | A86 | C26-C27 | 2.36 | 1.41 | 1.35 |
| 48 | 33 | 314 | A86 | C5-C6 | 2.36 | 1.41 | 1.35 |
| 47 | 35 | 306 | KC1 | C1D-C2D | 2.35 | 1.48 | 1.43 |
| 37 | 12 | 203 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 48 | 14 | 312 | A86 | O4-C34 | -2.35 | 1.41 | 1.46 |
| 37 | 18 | 208 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 47 | 15 | 304 | KC1 | CAA-C2A | 2.35 | 1.53 | 1.46 |
| 37 | B | 505 | CLA | C1C-NC | -2.35 | 1.34 | 1.37 |
| 37 | 18 | 206 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 48 | 34 | 312 | A86 | O4-C34 | -2.35 | 1.41 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 17 | 302 | CLA | C1B-C2B | 2.35 | 1.48 | 1.43 |
| 48 | 31 | 311 | A86 | C19-C18 | 2.35 | 1.55 | 1.52 |
| 44 | C | 516 | DGD | O2G-C2G | -2.35 | 1.41 | 1.46 |
| 37 | 31 | 301 | CLA | C1B-C2B | 2.35 | 1.48 | 1.43 |
| 37 | 14 | 308 | CLA | C1B-C2B | 2.35 | 1.48 | 1.43 |
| 47 | 21 | 207 | KC1 | C2A-C1A | 2.35 | 1.51 | 1.44 |
| 50 | 39 | 312 | DD6 | C4-C5 | 2.35 | 1.50 | 1.43 |
| 40 | A | 407 | SQD | O2-C2 | -2.35 | 1.37 | 1.43 |
| 37 | 19 | 301 | CLA | C3B-C4B | 2.35 | 1.49 | 1.42 |
| 37 | 40 | 208 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 47 | 15 | 302 | KC1 | C4A-C3A | 2.35 | 1.49 | 1.44 |
| 48 | 40 | 211 | A86 | C2-C1 | 2.35 | 1.41 | 1.35 |
| 46 | V | 201 | HEM | C2A-C3A | -2.35 | 1.32 | 1.38 |
| 37 | B | 503 | CLA | C1C-NC | -2.35 | 1.34 | 1.37 |
| 48 | 19 | 313 | A86 | C24-C1 | 2.35 | 1.51 | 1.46 |
| 47 | 14 | 309 | KC1 | C4A-C3A | 2.35 | 1.49 | 1.44 |
| 37 | 36 | 306 | CLA | C3B-C4B | 2.35 | 1.49 | 1.42 |
| 37 | B | 504 | CLA | C1C-NC | -2.34 | 1.34 | 1.37 |
| 47 | 19 | 308 | KC1 | C4A-C3A | 2.34 | 1.49 | 1.44 |
| 47 | 17 | 306 | KC1 | CHB-C4A | -2.34 | 1.33 | 1.39 |
| 48 | 17 | 315 | A86 | C2-C1 | 2.34 | 1.41 | 1.35 |
| 37 | 34 | 308 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 47 | 36 | 304 | KC1 | C2A-C1A | 2.34 | 1.51 | 1.44 |
| 47 | 41 | 207 | KC1 | C2A-C1A | 2.34 | 1.51 | 1.44 |
| 37 | 20 | 306 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 37 | b | 515 | CLA | C1B-C2B | 2.34 | 1.48 | 1.43 |
| 37 | 18 | 201 | CLA | C1B-C2B | 2.34 | 1.48 | 1.43 |
| 47 | 39 | 308 | KC1 | CAA-C2A | 2.34 | 1.53 | 1.46 |
| 48 | 39 | 313 | A86 | C26-C27 | 2.34 | 1.41 | 1.35 |
| 37 | 16 | 307 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 48 | 40 | 201 | A86 | O-C13 | -2.34 | 1.18 | 1.23 |
| 37 | 35 | 303 | CLA | C1B-C2B | 2.34 | 1.48 | 1.43 |
| 37 | 32 | 202 | CLA | C1C-NC | -2.34 | 1.34 | 1.37 |
| 47 | 16 | 304 | KC1 | C2A-C1A | 2.34 | 1.51 | 1.44 |
| 48 | 14 | 311 | A86 | O4-C34 | -2.34 | 1.41 | 1.46 |
| 50 | 21 | 212 | DD6 | C26-C27 | -2.34 | 1.32 | 1.37 |
| 50 | 41 | 212 | DD6 | C26-C27 | -2.34 | 1.32 | 1.37 |
| 37 | 13 | 308 | CLA | C1B-C2B | 2.34 | 1.48 | 1.43 |
| 48 | 40 | 201 | A86 | C14-C15 | 2.34 | 1.57 | 1.52 |
| 37 | 11 | 310 | CLA | C3B-C4B | 2.34 | 1.49 | 1.42 |
| 47 | 13 | 302 | KC1 | C4A-C3A | 2.34 | 1.49 | 1.44 |
| 37 | C | 501 | CLA | C1B-C2B | 2.34 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 36 | 301 | CLA | C1B-C2B | 2.34 | 1.48 | 1.43 |
| 48 | 16 | 310 | A86 | C26-C27 | 2.34 | 1.41 | 1.35 |
| 48 | 41 | 213 | A86 | C5-C6 | 2.34 | 1.41 | 1.35 |
| 48 | 38 | 215 | A86 | O-C13 | -2.34 | 1.18 | 1.23 |
| 48 | 11 | 319 | A86 | C39-C38 | 2.34 | 1.57 | 1.49 |
| 37 | 17 | 309 | CLA | C1B-C2B | 2.33 | 1.48 | 1.43 |
| 48 | 37 | 314 | A86 | C2-C1 | 2.33 | 1.41 | 1.35 |
| 37 | 17 | 307 | CLA | C3D-C4D | -2.33 | 1.38 | 1.44 |
| 37 | 37 | 306 | CLA | C3D-C4D | -2.33 | 1.38 | 1.44 |
| 48 | 11 | 315 | A86 | C-C1 | 2.33 | 1.55 | 1.50 |
| 47 | 11 | 302 | KC1 | C4A-C3A | 2.33 | 1.49 | 1.44 |
| 47 | 21 | 207 | KC1 | C3B-C4B | 2.33 | 1.50 | 1.46 |
| 48 | 41 | 215 | A86 | C5-C6 | 2.33 | 1.41 | 1.35 |
| 37 | 14 | 310 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 50 | 16 | 312 | DD6 | O1-C20 | 2.33 | 1.49 | 1.46 |
| 48 | 38 | 213 | A86 | C15-C16 | -2.33 | 1.51 | 1.55 |
| 46 | v | 201 | HEM | C2A-C3A | -2.33 | 1.32 | 1.38 |
| 37 | b | 505 | CLA | C1C-NC | -2.33 | 1.34 | 1.37 |
| 48 | 13 | 314 | A86 | O4-C34 | -2.33 | 1.41 | 1.46 |
| 48 | 33 | 314 | A86 | O4-C34 | -2.33 | 1.41 | 1.46 |
| 48 | 11 | 311 | A86 | C19-C18 | 2.33 | 1.55 | 1.52 |
| 40 | a | 409 | SQD | O2-C2 | -2.33 | 1.37 | 1.43 |
| 48 | 15 | 311 | A86 | C24-C1 | 2.33 | 1.50 | 1.46 |
| 47 | 18 | 207 | KC1 | CAA-C2A | 2.33 | 1.53 | 1.46 |
| 37 | 15 | 303 | CLA | C1B-C2B | 2.33 | 1.48 | 1.43 |
| 37 | 19 | 304 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 48 | 31 | 319 | A86 | C39-C38 | 2.33 | 1.57 | 1.49 |
| 37 | B | 513 | CLA | C1C-NC | -2.33 | 1.34 | 1.37 |
| 37 | 15 | 301 | CLA | C3D-C4D | -2.33 | 1.38 | 1.44 |
| 50 | 40 | 214 | DD6 | C22-C16 | -2.33 | 1.49 | 1.53 |
| 48 | 11 | 313 | A86 | C26-C27 | 2.33 | 1.41 | 1.35 |
| 48 | 11 | 311 | A86 | C14-C15 | 2.33 | 1.57 | 1.52 |
| 37 | W | 102 | CLA | C1B-C2B | 2.33 | 1.48 | 1.43 |
| 37 | 16 | 306 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 37 | 38 | 203 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 37 | 39 | 304 | CLA | C3B-C4B | 2.33 | 1.49 | 1.42 |
| 37 | 18 | 203 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 37 | Z | 101 | CLA | C3B-C2B | 2.33 | 1.49 | 1.41 |
| 50 | 19 | 312 | DD6 | C4-C5 | 2.33 | 1.50 | 1.43 |
| 48 | 37 | 319 | A86 | C26-C27 | 2.33 | 1.41 | 1.35 |
| 47 | 12 | 208 | KC1 | C4A-C3A | 2.33 | 1.49 | 1.44 |
| 50 | 20 | 312 | DD6 | C22-C16 | -2.33 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | B | 513 | CLA | C1B-C2B | 2.33 | 1.48 | 1.43 |
| 48 | 20 | 311 | A86 | O-C13 | -2.32 | 1.18 | 1.23 |
| 48 | 35 | 315 | A86 | C2-C1 | 2.32 | 1.41 | 1.35 |
| 37 | d | 403 | CLA | C1B-C2B | 2.32 | 1.48 | 1.43 |
| 48 | 15 | 319 | A86 | C2-C1 | 2.32 | 1.41 | 1.35 |
| 48 | 19 | 313 | A86 | C26-C27 | 2.32 | 1.41 | 1.35 |
| 37 | 18 | 211 | CLA | C3B-C4B | 2.32 | 1.49 | 1.42 |
| 48 | 32 | 215 | A86 | O4-C34 | -2.32 | 1.41 | 1.46 |
| 44 | h | 102 | DGD | O3G-C3G | -2.32 | 1.39 | 1.43 |
| 37 | 14 | 303 | CLA | C1B-C2B | 2.32 | 1.48 | 1.43 |
| 37 | 14 | 305 | CLA | C1B-C2B | 2.32 | 1.48 | 1.43 |
| 46 | V | 201 | HEM | FE-NC | 2.32 | 2.02 | 1.95 |
| 37 | 18 | 203 | CLA | C1B-C2B | 2.32 | 1.48 | 1.43 |
| 48 | 17 | 314 | A86 | O4-C34 | -2.32 | 1.41 | 1.46 |
| 37 | 18 | 203 | CLA | C3B-C4B | 2.32 | 1.49 | 1.42 |
| 48 | 37 | 319 | A86 | C24-C1 | 2.32 | 1.50 | 1.46 |
| 37 | 40 | 203 | CLA | C1B-C2B | 2.32 | 1.48 | 1.43 |
| 48 | 13 | 311 | A86 | O4-C34 | -2.32 | 1.41 | 1.46 |
| 37 | Z | 102 | CLA | CAA-C2A | -2.32 | 1.49 | 1.54 |
| 37 | z | 101 | CLA | C3B-C2B | 2.32 | 1.49 | 1.41 |
| 37 | b | 513 | CLA | C1B-C2B | 2.32 | 1.48 | 1.43 |
| 37 | A | 403 | CLA | CBD-CAD | -2.31 | 1.46 | 1.56 |
| 37 | 31 | 310 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 48 | 35 | 314 | A86 | O-C13 | -2.31 | 1.18 | 1.23 |
| 37 | 14 | 305 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 37 | 34 | 305 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 47 | 17 | 305 | KC1 | C1D-C2D | 2.31 | 1.48 | 1.43 |
| 47 | 16 | 305 | KC1 | CAA-C2A | 2.31 | 1.53 | 1.46 |
| 47 | 19 | 308 | KC1 | CAA-C2A | 2.31 | 1.53 | 1.46 |
| 37 | 17 | 307 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 37 | 37 | 306 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 37 | 41 | 210 | CLA | C1C-C2C | 2.31 | 1.49 | 1.44 |
| 48 | 32 | 217 | A86 | C2-C1 | 2.31 | 1.41 | 1.35 |
| 48 | 14 | 314 | A86 | O4-C34 | -2.31 | 1.41 | 1.46 |
| 37 | 13 | 305 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 37 | 33 | 305 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 37 | 34 | 301 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 37 | 38 | 209 | CLA | C3B-C4B | 2.31 | 1.49 | 1.42 |
| 47 | 15 | 302 | KC1 | C1D-C2D | 2.31 | 1.48 | 1.43 |
| 48 | 17 | 320 | A86 | C26-C27 | 2.31 | 1.41 | 1.35 |
| 37 | 33 | 308 | CLA | C1B-C2B | 2.31 | 1.48 | 1.43 |
| 48 | 16 | 313 | A86 | O-C13 | -2.31 | 1.18 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 32 | 221 | A86 | O4-C34 | -2.31 | 1.41 | 1.46 |
| 47 | 17 | 303 | KC1 | C1D-C2D | 2.31 | 1.48 | 1.43 |
| 47 | 34 | 309 | KC1 | C4A-C3A | 2.31 | 1.49 | 1.44 |
| 47 | 40 | 204 | KC1 | C4A-C3A | 2.31 | 1.49 | 1.44 |
| 48 | 40 | 213 | A86 | O-C13 | -2.31 | 1.18 | 1.23 |
| 44 | H | 102 | DGD | O3G-C3G | -2.31 | 1.39 | 1.43 |
| 48 | 34 | 316 | A86 | C2-C1 | 2.31 | 1.41 | 1.35 |
| 47 | 31 | 303 | KC1 | C4A-C3A | 2.31 | 1.49 | 1.44 |
| 48 | 15 | 315 | A86 | C2-C1 | 2.31 | 1.41 | 1.35 |
| 48 | 33 | 311 | A86 | O4-C34 | -2.31 | 1.41 | 1.46 |
| 48 | 33 | 313 | A86 | C14-C15 | 2.30 | 1.57 | 1.52 |
| 37 | B | 524 | CLA | C1C-C2C | 2.30 | 1.49 | 1.44 |
| 37 | 38 | 206 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 37 | 31 | 301 | CLA | C3B-C2B | 2.30 | 1.48 | 1.41 |
| 37 | 34 | 303 | CLA | C4C-C3C | 2.30 | 1.48 | 1.45 |
| 47 | 37 | 304 | KC1 | CAA-C2A | 2.30 | 1.53 | 1.46 |
| 41 | 32 | 201 | LMG | O8-C9 | -2.30 | 1.40 | 1.45 |
| 37 | W | 102 | CLA | C3B-C2B | 2.30 | 1.48 | 1.41 |
| 47 | 35 | 304 | KC1 | CAA-C2A | 2.30 | 1.53 | 1.46 |
| 48 | 18 | 212 | A86 | O4-C34 | -2.30 | 1.41 | 1.46 |
| 48 | 12 | 216 | A86 | C2-C1 | 2.30 | 1.41 | 1.35 |
| 47 | 36 | 305 | KC1 | CAA-C2A | 2.30 | 1.53 | 1.46 |
| 46 | v | 201 | HEM | FE-NC | 2.30 | 2.02 | 1.95 |
| 37 | d | 404 | CLA | C1C-NC | -2.30 | 1.34 | 1.37 |
| 37 | 38 | 202 | CLA | C1B-C2B | 2.30 | 1.48 | 1.43 |
| 47 | 18 | 210 | KC1 | C1D-C2D | 2.30 | 1.48 | 1.43 |
| 48 | 39 | 313 | A86 | O1-C20 | 2.30 | 1.49 | 1.46 |
| 48 | 35 | 319 | A86 | C2-C1 | 2.30 | 1.41 | 1.35 |
| 37 | 13 | 310 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 37 | 39 | 302 | CLA | C4C-C3C | 2.30 | 1.48 | 1.45 |
| 37 | a | 403 | CLA | CBD-CAD | -2.30 | 1.46 | 1.56 |
| 48 | 15 | 313 | A86 | C5-C6 | 2.30 | 1.41 | 1.35 |
| 48 | 35 | 313 | A86 | C5-C6 | 2.30 | 1.41 | 1.35 |
| 37 | 38 | 203 | CLA | C1B-C2B | 2.30 | 1.48 | 1.43 |
| 48 | 12 | 214 | A86 | O4-C34 | -2.30 | 1.41 | 1.46 |
| 41 | b | 519 | LMG | O7-C8 | -2.30 | 1.41 | 1.46 |
| 48 | 12 | 217 | A86 | C14-C15 | 2.30 | 1.57 | 1.52 |
| 47 | 37 | 302 | KC1 | C1D-C2D | 2.30 | 1.48 | 1.43 |
| 48 | 34 | 316 | A86 | C24-C1 | 2.30 | 1.50 | 1.46 |
| 37 | c | 506 | CLA | C4C-C3C | 2.30 | 1.48 | 1.45 |
| 48 | 12 | 220 | A86 | O4-C34 | -2.30 | 1.41 | 1.46 |
| 40 | 40 | 202 | SQD | O47-C45 | -2.30 | 1.41 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 17 | 303 | KC1 | CAA-C2A | 2.30 | 1.53 | 1.46 |
| 37 | 36 | 306 | CLA | C1C-C2C | 2.30 | 1.49 | 1.44 |
| 48 | 41 | 211 | A86 | O-C13 | -2.30 | 1.18 | 1.23 |
| 37 | 14 | 301 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 37 | 34 | 301 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 37 | 34 | 308 | CLA | C3B-C4B | 2.30 | 1.49 | 1.42 |
| 37 | b | 508 | CLA | CHB-C4A | -2.30 | 1.31 | 1.37 |
| 48 | 39 | 311 | A86 | C2-C1 | 2.30 | 1.41 | 1.35 |
| 48 | 16 | 313 | A86 | C14-C15 | 2.29 | 1.57 | 1.52 |
| 47 | 35 | 302 | KC1 | C1D-C2D | 2.29 | 1.48 | 1.43 |
| 47 | 41 | 207 | KC1 | CAA-C2A | 2.29 | 1.53 | 1.46 |
| 37 | 37 | 308 | CLA | C1B-C2B | 2.29 | 1.48 | 1.43 |
| 40 | 16 | 315 | SQD | O47-C45 | -2.29 | 1.41 | 1.46 |
| 48 | 15 | 314 | A86 | O4-C34 | -2.29 | 1.41 | 1.46 |
| 48 | 40 | 213 | A86 | O4-C34 | -2.29 | 1.41 | 1.46 |
| 37 | 12 | 210 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 37 | 18 | 209 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 37 | 39 | 307 | CLA | C1C-NC | -2.29 | 1.34 | 1.37 |
| 47 | 33 | 302 | KC1 | C4A-C3A | 2.29 | 1.49 | 1.44 |
| 48 | 21 | 215 | A86 | C5-C6 | 2.29 | 1.41 | 1.35 |
| 48 | 18 | 213 | A86 | C15-C16 | -2.29 | 1.51 | 1.55 |
| 47 | 19 | 308 | KC1 | C2A-C1A | 2.29 | 1.51 | 1.44 |
| 47 | 39 | 308 | KC1 | C2A-C1A | 2.29 | 1.51 | 1.44 |
| 37 | 20 | 301 | CLA | C1B-C2B | 2.29 | 1.48 | 1.43 |
| 47 | 37 | 307 | KC1 | C1D-C2D | 2.29 | 1.48 | 1.43 |
| 47 | 38 | 210 | KC1 | C1D-C2D | 2.29 | 1.48 | 1.43 |
| 37 | 15 | 301 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 48 | 35 | 311 | A86 | C14-C15 | 2.29 | 1.57 | 1.52 |
| 48 | 17 | 310 | A86 | C15-C16 | -2.29 | 1.51 | 1.55 |
| 47 | 14 | 304 | KC1 | C2A-C1A | 2.29 | 1.51 | 1.44 |
| 47 | 34 | 304 | KC1 | C2A-C1A | 2.29 | 1.51 | 1.44 |
| 37 | 38 | 211 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 37 | 19 | 305 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |
| 47 | 21 | 207 | KC1 | CAA-C2A | 2.29 | 1.53 | 1.46 |
| 48 | 16 | 310 | A86 | C25-C24 | 2.29 | 1.40 | 1.34 |
| 37 | 38 | 206 | CLA | C4C-C3C | 2.29 | 1.48 | 1.45 |
| 37 | 15 | 303 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |
| 37 | 34 | 310 | CLA | C3B-C4B | 2.29 | 1.49 | 1.42 |
| 37 | 38 | 201 | CLA | C1C-C2C | 2.28 | 1.49 | 1.44 |
| 47 | 38 | 207 | KC1 | C4C-C3C | 2.28 | 1.48 | 1.45 |
| 37 | D | 405 | CLA | C4D-CHA | 2.28 | 1.46 | 1.38 |
| 37 | 19 | 310 | CLA | C1B-C2B | 2.28 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 35 | 314 | A86 | O4-C34 | -2.28 | 1.41 | 1.46 |
| 37 | B | 503 | CLA | CBD-CAD | -2.28 | 1.46 | 1.56 |
| 37 | 34 | 303 | CLA | C1B-C2B | 2.28 | 1.48 | 1.43 |
| 48 | 14 | 316 | A86 | C2-C1 | 2.28 | 1.41 | 1.35 |
| 48 | 18 | 215 | A86 | C14-C15 | 2.28 | 1.57 | 1.52 |
| 48 | 38 | 212 | A86 | O4-C34 | -2.28 | 1.41 | 1.46 |
| 48 | 13 | 313 | A86 | C5-C6 | 2.28 | 1.41 | 1.35 |
| 48 | 33 | 313 | A86 | C5-C6 | 2.28 | 1.41 | 1.35 |
| 48 | 14 | 316 | A86 | C24-C1 | 2.28 | 1.50 | 1.46 |
| 37 | 16 | 306 | CLA | C1C-C2C | 2.28 | 1.49 | 1.44 |
| 37 | 21 | 210 | CLA | C1C-C2C | 2.28 | 1.49 | 1.44 |
| 37 | 17 | 304 | CLA | C4C-C3C | 2.28 | 1.48 | 1.45 |
| 37 | 37 | 303 | CLA | C4C-C3C | 2.28 | 1.48 | 1.45 |
| 47 | 13 | 302 | KC1 | C4C-C3C | 2.28 | 1.48 | 1.45 |
| 47 | 33 | 302 | KC1 | C4C-C3C | 2.28 | 1.48 | 1.45 |
| 37 | 32 | 211 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 37 | D | 402 | CLA | C1C-NC | -2.28 | 1.34 | 1.37 |
| 37 | 19 | 302 | CLA | C4C-C3C | 2.28 | 1.48 | 1.45 |
| 47 | 13 | 302 | KC1 | C1D-C2D | 2.28 | 1.48 | 1.43 |
| 47 | 33 | 302 | KC1 | C1D-C2D | 2.28 | 1.48 | 1.43 |
| 47 | 38 | 207 | KC1 | C3B-C4B | 2.28 | 1.50 | 1.46 |
| 40 | 16 | 315 | SQD | O2-C2 | -2.28 | 1.37 | 1.43 |
| 37 | 20 | 306 | CLA | C1B-C2B | 2.28 | 1.48 | 1.43 |
| 45 | D | 408 | PL9 | C46-C44 | -2.28 | 1.46 | 1.51 |
| 37 | 35 | 301 | CLA | C3B-C4B | 2.28 | 1.49 | 1.42 |
| 37 | 39 | 310 | CLA | C1B-C2B | 2.28 | 1.48 | 1.43 |
| 48 | 36 | 310 | A86 | C25-C24 | 2.28 | 1.40 | 1.34 |
| 37 | C | 501 | CLA | C1C-NC | -2.28 | 1.34 | 1.37 |
| 47 | 21 | 207 | KC1 | C1D-C2D | 2.28 | 1.48 | 1.43 |
| 48 | 34 | 312 | A86 | C26-C27 | 2.28 | 1.41 | 1.35 |
| 37 | 19 | 307 | CLA | C1C-NC | -2.28 | 1.34 | 1.37 |
| 48 | 12 | 217 | A86 | C2-C1 | 2.28 | 1.41 | 1.35 |
| 48 | 17 | 320 | A86 | C24-C1 | 2.27 | 1.50 | 1.46 |
| 48 | 35 | 315 | A86 | O4-C34 | -2.27 | 1.41 | 1.46 |
| 37 | w | 101 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 37 | B | 514 | CLA | CBD-CAD | -2.27 | 1.46 | 1.56 |
| 47 | 37 | 302 | KC1 | CAA-C2A | 2.27 | 1.53 | 1.46 |
| 48 | 31 | 319 | A86 | C25-C24 | 2.27 | 1.40 | 1.34 |
| 48 | 34 | 314 | A86 | O4-C34 | -2.27 | 1.41 | 1.46 |
| 47 | 21 | 203 | KC1 | C4C-C3C | 2.27 | 1.48 | 1.45 |
| 37 | d | 401 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |
| 37 | b | 503 | CLA | CBD-CAD | -2.27 | 1.46 | 1.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 50 | 20 | 312 | DD6 | C26-C27 | -2.27 | 1.32 | 1.37 |
| 37 | 11 | 307 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |
| 48 | 37 | 309 | A86 | C15-C16 | -2.27 | 1.51 | 1.55 |
| 37 | 12 | 212 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 37 | 32 | 213 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 37 | 35 | 303 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 37 | B | 508 | CLA | CHB-C4A | -2.27 | 1.32 | 1.37 |
| 37 | 35 | 310 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 40 | 40 | 202 | SQD | O2-C2 | -2.27 | 1.37 | 1.43 |
| 37 | 11 | 305 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 48 | 39 | 313 | A86 | C15-C16 | -2.27 | 1.51 | 1.55 |
| 37 | 35 | 307 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 37 | 34 | 305 | CLA | C4C-C3C | 2.27 | 1.48 | 1.45 |
| 37 | D | 406 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |
| 37 | 14 | 301 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 37 | 15 | 308 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 48 | 20 | 311 | A86 | O4-C34 | -2.27 | 1.41 | 1.46 |
| 47 | 17 | 308 | KC1 | C1D-C2D | 2.27 | 1.48 | 1.43 |
| 37 | B | 509 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |
| 37 | 33 | 301 | CLA | C1B-C2B | 2.27 | 1.48 | 1.43 |
| 37 | b | 501 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |
| 37 | 14 | 310 | CLA | C3B-C4B | 2.27 | 1.49 | 1.42 |
| 48 | 16 | 314 | A86 | C14-C15 | 2.27 | 1.57 | 1.52 |
| 37 | b | 513 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |
| 48 | 12 | 202 | A86 | C26-C27 | 2.27 | 1.41 | 1.35 |
| 37 | 14 | 308 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 48 | 21 | 213 | A86 | C5-C6 | 2.26 | 1.41 | 1.35 |
| 37 | 41 | 202 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 48 | 35 | 311 | A86 | C24-C1 | 2.26 | 1.50 | 1.46 |
| 37 | 36 | 309 | CLA | C1B-C2B | 2.26 | 1.48 | 1.43 |
| 37 | 40 | 208 | CLA | C1B-C2B | 2.26 | 1.48 | 1.43 |
| 37 | b | 509 | CLA | C1C-NC | -2.26 | 1.34 | 1.37 |
| 37 | d | 404 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 37 | 41 | 206 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 37 | b | 523 | CLA | C1C-C2C | 2.26 | 1.49 | 1.44 |
| 37 | 20 | 308 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 48 | 32 | 218 | A86 | C2-C1 | 2.26 | 1.41 | 1.35 |
| 37 | b | 516 | CLA | CHB-C4A | -2.26 | 1.32 | 1.37 |
| 47 | 34 | 304 | KC1 | CAA-C2A | 2.26 | 1.53 | 1.46 |
| 37 | 17 | 309 | CLA | C1C-NC | -2.26 | 1.34 | 1.37 |
| 48 | 21 | 211 | A86 | O-C13 | -2.26 | 1.18 | 1.23 |
| 48 | 34 | 313 | A86 | C5-C6 | 2.26 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 16 | 309 | CLA | C1B-C2B | 2.26 | 1.48 | 1.43 |
| 47 | 38 | 210 | KC1 | C3B-C4B | 2.26 | 1.50 | 1.46 |
| 41 | B | 520 | LMG | O7-C8 | -2.26 | 1.41 | 1.46 |
| 48 | 38 | 215 | A86 | C5-C6 | 2.26 | 1.41 | 1.35 |
| 48 | 35 | 319 | A86 | O4-C34 | -2.26 | 1.41 | 1.46 |
| 37 | b | 514 | CLA | CBD-CAD | -2.26 | 1.46 | 1.56 |
| 48 | 15 | 315 | A86 | O4-C34 | -2.26 | 1.41 | 1.46 |
| 47 | 41 | 203 | KC1 | C4C-C3C | 2.26 | 1.48 | 1.45 |
| 37 | W | 101 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 47 | 18 | 210 | KC1 | C4C-C3C | 2.26 | 1.48 | 1.45 |
| 37 | 38 | 202 | CLA | C1C-C2C | 2.26 | 1.49 | 1.44 |
| 47 | 20 | 302 | KC1 | C4A-C3A | 2.26 | 1.49 | 1.44 |
| 48 | 16 | 314 | A86 | O4-C34 | -2.26 | 1.41 | 1.46 |
| 48 | 37 | 312 | A86 | O4-C34 | -2.26 | 1.41 | 1.46 |
| 48 | 11 | 319 | A86 | C25-C24 | 2.26 | 1.40 | 1.34 |
| 37 | b | 510 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 48 | 11 | 313 | A86 | C2-C1 | 2.26 | 1.41 | 1.35 |
| 37 | 39 | 301 | CLA | C1B-C2B | 2.26 | 1.48 | 1.43 |
| 37 | 14 | 305 | CLA | C4C-C3C | 2.26 | 1.48 | 1.45 |
| 37 | 21 | 206 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 37 | 13 | 310 | CLA | C3B-C2B | 2.26 | 1.48 | 1.41 |
| 37 | 14 | 303 | CLA | C4C-C3C | 2.26 | 1.48 | 1.45 |
| 38 | a | 406 | PHO | CAC-C3C | -2.26 | 1.47 | 1.51 |
| 47 | 38 | 207 | KC1 | CAA-C2A | 2.26 | 1.53 | 1.46 |
| 37 | W | 102 | CLA | C3B-C4B | 2.26 | 1.49 | 1.42 |
| 48 | 32 | 218 | A86 | C14-C15 | 2.26 | 1.57 | 1.52 |
| 37 | 18 | 208 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 47 | 12 | 211 | KC1 | CBD-CAD | -2.25 | 1.46 | 1.56 |
| 47 | 32 | 212 | KC1 | CBD-CAD | -2.25 | 1.46 | 1.56 |
| 48 | 12 | 216 | A86 | O4-C34 | -2.25 | 1.41 | 1.46 |
| 37 | d | 403 | CLA | C4D-CHA | 2.25 | 1.46 | 1.38 |
| 48 | 20 | 309 | A86 | C5-C6 | 2.25 | 1.41 | 1.35 |
| 48 | 37 | 313 | A86 | C24-C1 | 2.25 | 1.50 | 1.46 |
| 50 | 40 | 214 | DD6 | C26-C27 | -2.25 | 1.32 | 1.37 |
| 37 | 38 | 208 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 37 | z | 102 | CLA | CAA-C2A | -2.25 | 1.50 | 1.54 |
| 48 | 31 | 312 | A86 | C26-C27 | 2.25 | 1.41 | 1.35 |
| 45 | d | 406 | PL9 | C46-C44 | -2.25 | 1.46 | 1.51 |
| 37 | 16 | 301 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 37 | 41 | 209 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 37 | B | 512 | CLA | C4D-CHA | 2.25 | 1.46 | 1.38 |
| 48 | 40 | 211 | A86 | C5-C6 | 2.25 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 306 | KC1 | CAA-C2A | 2.25 | 1.53 | 1.46 |
| 37 | B | 502 | CLA | C1B-C2B | 2.25 | 1.48 | 1.43 |
| 37 | c | 501 | CLA | C1C-NC | -2.25 | 1.34 | 1.37 |
| 47 | 13 | 304 | KC1 | CAA-C2A | 2.25 | 1.53 | 1.46 |
| 47 | 33 | 304 | KC1 | CAA-C2A | 2.25 | 1.53 | 1.46 |
| 48 | 19 | 311 | A86 | C2-C1 | 2.25 | 1.41 | 1.35 |
| 37 | 40 | 210 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 37 | 13 | 308 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 37 | 33 | 308 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 48 | 14 | 313 | A86 | C5-C6 | 2.25 | 1.41 | 1.35 |
| 37 | 38 | 203 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 37 | 21 | 209 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 39 | d | 405 | BCR | C33-C5 | -2.25 | 1.47 | 1.50 |
| 37 | D | 406 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 47 | 31 | 309 | KC1 | CBD-CAD | -2.25 | 1.46 | 1.56 |
| 48 | 11 | 312 | A86 | C-C1 | 2.25 | 1.55 | 1.50 |
| 41 | 32 | 201 | LMG | O4-C4 | -2.25 | 1.37 | 1.43 |
| 47 | 17 | 305 | KC1 | CAA-C2A | 2.25 | 1.53 | 1.46 |
| 37 | 39 | 310 | CLA | C3B-C4B | 2.25 | 1.49 | 1.42 |
| 37 | C | 506 | CLA | C4C-C3C | 2.25 | 1.48 | 1.45 |
| 37 | 15 | 307 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 47 | 18 | 210 | KC1 | C3B-C4B | 2.25 | 1.49 | 1.46 |
| 48 | 15 | 311 | A86 | C14-C15 | 2.24 | 1.57 | 1.52 |
| 37 | B | 501 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 48 | 36 | 311 | A86 | C2-C1 | 2.24 | 1.41 | 1.35 |
| 41 | 12 | 201 | LMG | O8-C9 | -2.24 | 1.40 | 1.45 |
| 37 | 31 | 301 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 37 | B | 514 | CLA | C1B-C2B | 2.24 | 1.48 | 1.43 |
| 37 | 13 | 301 | CLA | C1B-C2B | 2.24 | 1.48 | 1.43 |
| 37 | 19 | 301 | CLA | C1B-C2B | 2.24 | 1.48 | 1.43 |
| 37 | c | 511 | CLA | C1C-NC | -2.24 | 1.34 | 1.37 |
| 37 | B | 510 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 37 | 31 | 306 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 37 | 12 | 209 | CLA | CHB-C4A | -2.24 | 1.32 | 1.37 |
| 37 | 32 | 210 | CLA | CHB-C4A | -2.24 | 1.32 | 1.37 |
| 37 | C | 507 | CLA | C1B-C2B | 2.24 | 1.48 | 1.43 |
| 48 | 17 | 313 | A86 | O4-C34 | -2.24 | 1.41 | 1.46 |
| 37 | 13 | 305 | CLA | C4C-C3C | 2.24 | 1.48 | 1.45 |
| 37 | 33 | 305 | CLA | C4C-C3C | 2.24 | 1.48 | 1.45 |
| 37 | 11 | 303 | CLA | C1C-NC | -2.24 | 1.34 | 1.37 |
| 47 | 41 | 207 | KC1 | C1D-C2D | 2.24 | 1.48 | 1.43 |
| 37 | 33 | 310 | CLA | C3B-C2B | 2.24 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 38 | 210 | KC1 | C4C-C3C | 2.24 | 1.48 | 1.45 |
| 37 | B | 516 | CLA | CHB-C4A | -2.24 | 1.32 | 1.37 |
| 48 | 14 | 312 | A86 | C26-C27 | 2.24 | 1.41 | 1.35 |
| 37 | c | 513 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 37 | 15 | 308 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |
| 48 | 36 | 313 | A86 | O4-C34 | -2.24 | 1.41 | 1.46 |
| 37 | 20 | 307 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |
| 47 | 15 | 306 | KC1 | CAA-C2A | 2.24 | 1.53 | 1.46 |
| 37 | 20 | 301 | CLA | C1C-C2C | 2.24 | 1.49 | 1.44 |
| 48 | 13 | 313 | A86 | C14-C15 | 2.24 | 1.57 | 1.52 |
| 37 | b | 513 | CLA | CBD-CAD | -2.24 | 1.46 | 1.56 |
| 48 | 11 | 314 | A86 | C24-C1 | 2.24 | 1.50 | 1.46 |
| 37 | b | 501 | CLA | C3B-C4B | 2.24 | 1.49 | 1.42 |
| 47 | 21 | 203 | KC1 | C1D-C2D | 2.24 | 1.48 | 1.43 |
| 37 | C | 511 | CLA | C1C-NC | -2.24 | 1.34 | 1.37 |
| 37 | 39 | 305 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |
| 37 | 15 | 310 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |
| 47 | 20 | 302 | KC1 | C3B-C4B | 2.24 | 1.49 | 1.46 |
| 48 | 11 | 314 | A86 | C2-C1 | 2.24 | 1.41 | 1.35 |
| 37 | 36 | 307 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |
| 37 | 12 | 207 | CLA | C1C-NC | -2.24 | 1.34 | 1.37 |
| 37 | 32 | 208 | CLA | C1C-NC | -2.24 | 1.34 | 1.37 |
| 37 | c | 507 | CLA | C1B-C2B | 2.24 | 1.48 | 1.43 |
| 37 | b | 512 | CLA | C4D-CHA | 2.24 | 1.46 | 1.38 |
| 37 | 40 | 203 | CLA | C1C-C2C | 2.24 | 1.49 | 1.44 |
| 37 | b | 514 | CLA | C1B-C2B | 2.24 | 1.48 | 1.43 |
| 37 | 11 | 310 | CLA | C1C-NC | -2.24 | 1.34 | 1.37 |
| 37 | 31 | 310 | CLA | C1C-NC | -2.24 | 1.34 | 1.37 |
| 47 | 14 | 304 | KC1 | CAA-C2A | 2.24 | 1.53 | 1.46 |
| 37 | 18 | 209 | CLA | C4C-C3C | 2.24 | 1.48 | 1.45 |
| 38 | A | 404 | PHO | CAC-C3C | -2.24 | 1.47 | 1.51 |
| 48 | 37 | 313 | A86 | C2-C1 | 2.23 | 1.41 | 1.35 |
| 37 | B | 505 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 37 | 38 | 209 | CLA | C1C-C2C | 2.23 | 1.49 | 1.44 |
| 48 | 14 | 316 | A86 | O4-C34 | -2.23 | 1.41 | 1.46 |
| 48 | 34 | 316 | A86 | O4-C34 | -2.23 | 1.41 | 1.46 |
| 37 | 21 | 205 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 37 | 41 | 205 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 37 | b | 513 | CLA | C3B-C2B | 2.23 | 1.48 | 1.41 |
| 37 | W | 101 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 37 | w | 101 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 37 | 19 | 309 | CLA | C1B-C2B | 2.23 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 40 | 209 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 37 | 40 | 203 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 37 | 39 | 302 | CLA | C1B-C2B | 2.23 | 1.48 | 1.43 |
| 37 | 18 | 203 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 47 | 37 | 305 | KC1 | CAA-C2A | 2.23 | 1.53 | 1.46 |
| 48 | 38 | 214 | A86 | O4-C34 | -2.23 | 1.41 | 1.46 |
| 37 | 38 | 211 | CLA | C3B-C2B | 2.23 | 1.48 | 1.41 |
| 37 | 18 | 211 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 37 | b | 502 | CLA | C1B-C2B | 2.23 | 1.48 | 1.43 |
| 37 | 14 | 301 | CLA | C1C-C2C | 2.23 | 1.49 | 1.44 |
| 47 | 14 | 304 | KC1 | C4A-C3A | 2.23 | 1.49 | 1.44 |
| 37 | 18 | 211 | CLA | C3B-C2B | 2.23 | 1.48 | 1.41 |
| 37 | 21 | 202 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 47 | 38 | 210 | KC1 | CAA-C2A | 2.23 | 1.53 | 1.46 |
| 37 | 15 | 307 | CLA | C1C-C2C | 2.23 | 1.49 | 1.44 |
| 37 | 18 | 209 | CLA | C1C-C2C | 2.23 | 1.49 | 1.44 |
| 37 | 35 | 307 | CLA | C1C-C2C | 2.23 | 1.49 | 1.44 |
| 48 | 32 | 215 | A86 | C24-C1 | 2.23 | 1.50 | 1.46 |
| 37 | 19 | 301 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 38 | A | 404 | PHO | CBD-CGD | -2.23 | 1.49 | 1.52 |
| 37 | 13 | 301 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 47 | 11 | 309 | KC1 | CBD-CAD | -2.23 | 1.46 | 1.56 |
| 47 | 15 | 302 | KC1 | CAA-C2A | 2.23 | 1.53 | 1.46 |
| 48 | 33 | 311 | A86 | C2-C1 | 2.23 | 1.41 | 1.35 |
| 37 | w | 101 | CLA | CBD-CAD | -2.23 | 1.46 | 1.56 |
| 48 | 38 | 213 | A86 | C24-C1 | 2.23 | 1.50 | 1.46 |
| 48 | 32 | 218 | A86 | O4-C34 | -2.23 | 1.41 | 1.46 |
| 37 | 33 | 301 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 48 | 32 | 203 | A86 | C26-C27 | 2.23 | 1.40 | 1.35 |
| 47 | 17 | 306 | KC1 | CAA-C2A | 2.23 | 1.53 | 1.46 |
| 37 | 31 | 308 | CLA | C1C-NC | -2.23 | 1.34 | 1.37 |
| 37 | Z | 102 | CLA | C3B-C2B | 2.23 | 1.48 | 1.41 |
| 37 | 15 | 305 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 37 | 33 | 305 | CLA | C1C-C2C | 2.23 | 1.49 | 1.44 |
| 37 | b | 505 | CLA | C3B-C4B | 2.23 | 1.49 | 1.42 |
| 48 | 17 | 320 | A86 | O4-C34 | -2.23 | 1.41 | 1.46 |
| 48 | 31 | 314 | A86 | C2-C1 | 2.23 | 1.40 | 1.35 |
| 48 | 37 | 319 | A86 | O4-C34 | -2.23 | 1.41 | 1.46 |
| 37 | B | 512 | CLA | C3B-C2B | 2.23 | 1.48 | 1.41 |
| 48 | 16 | 311 | A86 | C2-C1 | 2.22 | 1.40 | 1.35 |
| 48 | 31 | 314 | A86 | C24-C1 | 2.22 | 1.50 | 1.46 |
| 37 | 34 | 302 | CLA | C1B-C2B | 2.22 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 41 | 12 | 201 | LMG | O4-C4 | -2.22 | 1.37 | 1.43 |
| 47 | 41 | 203 | KC1 | C1D-C2D | 2.22 | 1.48 | 1.43 |
| 37 | C | 513 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 47 | 35 | 302 | KC1 | CAA-C2A | 2.22 | 1.53 | 1.46 |
| 37 | z | 102 | CLA | C3B-C2B | 2.22 | 1.48 | 1.41 |
| 37 | 11 | 301 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 37 | 31 | 302 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 37 | 18 | 206 | CLA | C3D-C4D | -2.22 | 1.39 | 1.44 |
| 37 | 19 | 310 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 37 | 18 | 204 | CLA | C1C-C2C | 2.22 | 1.49 | 1.44 |
| 37 | 16 | 307 | CLA | C3D-C4D | -2.22 | 1.39 | 1.44 |
| 47 | 11 | 304 | KC1 | CAA-C2A | 2.22 | 1.53 | 1.46 |
| 48 | 36 | 313 | A86 | C14-C15 | 2.22 | 1.57 | 1.52 |
| 47 | 35 | 309 | KC1 | C4C-C3C | 2.22 | 1.48 | 1.45 |
| 37 | 38 | 206 | CLA | C3B-C2B | 2.22 | 1.48 | 1.41 |
| 47 | 31 | 305 | KC1 | CAA-C2A | 2.22 | 1.53 | 1.46 |
| 37 | 18 | 208 | CLA | C3B-C2B | 2.22 | 1.48 | 1.41 |
| 37 | 20 | 306 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 37 | b | 505 | CLA | CHB-C4A | -2.22 | 1.32 | 1.37 |
| 40 | B | 522 | SQD | O47-C45 | -2.22 | 1.41 | 1.46 |
| 48 | 32 | 217 | A86 | O4-C34 | -2.22 | 1.41 | 1.46 |
| 37 | b | 512 | CLA | C3B-C2B | 2.22 | 1.48 | 1.41 |
| 37 | B | 513 | CLA | CBD-CAD | -2.22 | 1.46 | 1.56 |
| 37 | 33 | 307 | CLA | C1B-C2B | 2.22 | 1.48 | 1.43 |
| 48 | 11 | 312 | A86 | C26-C27 | 2.22 | 1.40 | 1.35 |
| 47 | 37 | 307 | KC1 | C4C-C3C | 2.22 | 1.48 | 1.45 |
| 48 | 13 | 311 | A86 | C2-C1 | 2.22 | 1.40 | 1.35 |
| 37 | 39 | 309 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 48 | 21 | 215 | A86 | O4-C34 | -2.22 | 1.41 | 1.46 |
| 37 | z | 101 | CLA | C1B-C2B | 2.22 | 1.48 | 1.43 |
| 48 | 33 | 315 | A86 | O4-C34 | -2.22 | 1.41 | 1.46 |
| 48 | 31 | 312 | A86 | C-C1 | 2.22 | 1.55 | 1.50 |
| 37 | 13 | 301 | CLA | C3B-C4B | 2.22 | 1.49 | 1.42 |
| 37 | Z | 101 | CLA | C1B-C2B | 2.22 | 1.48 | 1.43 |
| 39 | D | 407 | BCR | C33-C5 | -2.22 | 1.47 | 1.50 |
| 48 | 11 | 312 | A86 | C2-C1 | 2.22 | 1.40 | 1.35 |
| 37 | 36 | 301 | CLA | C3D-C4D | -2.22 | 1.39 | 1.44 |
| 37 | 40 | 208 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 37 | 39 | 301 | CLA | C3D-C4D | -2.21 | 1.39 | 1.44 |
| 40 | b | 521 | SQD | O47-C45 | -2.21 | 1.41 | 1.46 |
| 37 | B | 505 | CLA | CHB-C4A | -2.21 | 1.32 | 1.37 |
| 37 | 19 | 302 | CLA | C1B-C2B | 2.21 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 36 | 302 | KC1 | C1D-C2D | 2.21 | 1.48 | 1.43 |
| 37 | W | 101 | CLA | CBD-CAD | -2.21 | 1.46 | 1.56 |
| 48 | 12 | 214 | A86 | C24-C1 | 2.21 | 1.50 | 1.46 |
| 37 | 38 | 208 | CLA | C3B-C2B | 2.21 | 1.48 | 1.41 |
| 37 | 32 | 206 | CLA | C1C-NC | -2.21 | 1.34 | 1.37 |
| 37 | b | 501 | CLA | C1B-C2B | 2.21 | 1.48 | 1.43 |
| 37 | 39 | 307 | CLA | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 47 | 17 | 306 | KC1 | C1D-C2D | 2.21 | 1.48 | 1.43 |
| 48 | 18 | 214 | A86 | O4-C34 | -2.21 | 1.41 | 1.46 |
| 37 | 19 | 303 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 37 | 39 | 303 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 47 | 37 | 302 | KC1 | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 48 | 32 | 215 | A86 | C15-C16 | -2.21 | 1.52 | 1.55 |
| 37 | B | 513 | CLA | C3B-C2B | 2.21 | 1.48 | 1.41 |
| 48 | 34 | 315 | A86 | C24-C1 | 2.21 | 1.50 | 1.46 |
| 37 | 35 | 308 | CLA | CBD-CAD | -2.21 | 1.46 | 1.56 |
| 37 | 37 | 308 | CLA | C1C-NC | -2.21 | 1.34 | 1.37 |
| 48 | 15 | 319 | A86 | O4-C34 | -2.21 | 1.41 | 1.46 |
| 47 | 36 | 304 | KC1 | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 47 | 21 | 207 | KC1 | C4A-C3A | 2.21 | 1.49 | 1.44 |
| 37 | a | 407 | CLA | C1C-NC | -2.21 | 1.34 | 1.37 |
| 37 | 20 | 301 | CLA | C3B-C4B | 2.21 | 1.49 | 1.42 |
| 47 | 20 | 305 | KC1 | CAA-C2A | 2.21 | 1.53 | 1.46 |
| 37 | 39 | 309 | CLA | C1B-C2B | 2.21 | 1.48 | 1.43 |
| 37 | 33 | 310 | CLA | C3D-C4D | -2.21 | 1.39 | 1.44 |
| 37 | 38 | 211 | CLA | C3D-C4D | -2.21 | 1.39 | 1.44 |
| 48 | 12 | 214 | A86 | C15-C16 | -2.21 | 1.52 | 1.55 |
| 47 | 13 | 309 | KC1 | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 37 | 35 | 310 | CLA | C3B-C2B | 2.21 | 1.48 | 1.41 |
| 37 | 21 | 210 | CLA | C3D-C4D | -2.21 | 1.39 | 1.44 |
| 37 | B | 501 | CLA | C1C-NC | -2.21 | 1.34 | 1.37 |
| 47 | 15 | 309 | KC1 | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 47 | 16 | 304 | KC1 | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 37 | B | 524 | CLA | CBD-CAD | -2.21 | 1.46 | 1.56 |
| 37 | 41 | 210 | CLA | C3D-C4D | -2.21 | 1.39 | 1.44 |
| 37 | 19 | 309 | CLA | C3B-C4B | 2.20 | 1.49 | 1.42 |
| 37 | 35 | 305 | CLA | C3D-C4D | -2.20 | 1.39 | 1.44 |
| 48 | 12 | 217 | A86 | O4-C34 | -2.20 | 1.41 | 1.46 |
| 37 | C | 510 | CLA | CBD-CAD | -2.20 | 1.46 | 1.56 |
| 37 | 32 | 204 | CLA | C1B-C2B | 2.20 | 1.48 | 1.43 |
| 37 | 19 | 307 | CLA | C4C-C3C | 2.20 | 1.48 | 1.45 |
| 47 | 41 | 203 | KC1 | C1C-C2C | 2.20 | 1.49 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 17 | 315 | A86 | O4-C34 | -2.20 | 1.41 | 1.46 |
| 48 | 37 | 314 | A86 | O4-C34 | -2.20 | 1.41 | 1.46 |
| 48 | 31 | 311 | A86 | C-C1 | 2.20 | 1.55 | 1.50 |
| 48 | 16 | 310 | A86 | C2-C1 | 2.20 | 1.40 | 1.35 |
| 47 | 14 | 304 | KC1 | C1D-C2D | 2.20 | 1.48 | 1.43 |
| 37 | 13 | 307 | CLA | C1B-C2B | 2.20 | 1.48 | 1.43 |
| 37 | 14 | 302 | CLA | C1B-C2B | 2.20 | 1.48 | 1.43 |
| 37 | 15 | 310 | CLA | C3B-C2B | 2.20 | 1.48 | 1.41 |
| 37 | 12 | 203 | CLA | C1B-C2B | 2.20 | 1.48 | 1.43 |
| 37 | 37 | 308 | CLA | C3B-C2B | 2.20 | 1.48 | 1.41 |
| 37 | b | 504 | CLA | CBD-CAD | -2.20 | 1.46 | 1.56 |
| 37 | C | 504 | CLA | C1B-C2B | 2.20 | 1.48 | 1.43 |
| 37 | 38 | 201 | CLA | C4C-C3C | 2.20 | 1.48 | 1.45 |
| 47 | 11 | 304 | KC1 | C1D-C2D | 2.20 | 1.48 | 1.43 |
| 47 | 31 | 305 | KC1 | C1D-C2D | 2.20 | 1.48 | 1.43 |
| 37 | 38 | 204 | CLA | C3B-C2B | 2.20 | 1.48 | 1.41 |
| 37 | B | 504 | CLA | CBD-CAD | -2.20 | 1.46 | 1.56 |
| 37 | 12 | 212 | CLA | C1B-C2B | 2.20 | 1.48 | 1.43 |
| 37 | 32 | 213 | CLA | C1B-C2B | 2.20 | 1.48 | 1.43 |
| 37 | 13 | 305 | CLA | C1C-C2C | 2.20 | 1.49 | 1.44 |
| 48 | 38 | 215 | A86 | O4-C34 | -2.20 | 1.41 | 1.46 |
| 37 | 38 | 209 | CLA | C4C-C3C | 2.20 | 1.48 | 1.45 |
| 47 | 40 | 204 | KC1 | C3B-C4B | 2.20 | 1.49 | 1.46 |
| 48 | 16 | 314 | A86 | C26-C27 | 2.20 | 1.40 | 1.35 |
| 37 | 40 | 210 | CLA | C3B-C2B | 2.20 | 1.48 | 1.41 |
| 47 | 40 | 207 | KC1 | CAA-C2A | 2.20 | 1.53 | 1.46 |
| 37 | 38 | 208 | CLA | C1B-C2B | 2.19 | 1.48 | 1.43 |
| 37 | 35 | 305 | CLA | C1C-C2C | 2.19 | 1.49 | 1.44 |
| 37 | 15 | 308 | CLA | CBD-CAD | -2.19 | 1.46 | 1.56 |
| 37 | 21 | 205 | CLA | C3B-C2B | 2.19 | 1.48 | 1.41 |
| 37 | C | 510 | CLA | C1C-NC | -2.19 | 1.34 | 1.37 |
| 47 | 41 | 207 | KC1 | C4A-C3A | 2.19 | 1.49 | 1.44 |
| 48 | 36 | 310 | A86 | C2-C1 | 2.19 | 1.40 | 1.35 |
| 37 | b | 523 | CLA | CBD-CAD | -2.19 | 1.46 | 1.56 |
| 48 | 11 | 311 | A86 | C-C1 | 2.19 | 1.55 | 1.50 |
| 37 | 18 | 201 | CLA | C1C-C2C | 2.19 | 1.49 | 1.44 |
| 46 | v | 201 | HEM | C3C-C2C | -2.19 | 1.32 | 1.37 |
| 47 | 15 | 306 | KC1 | C4C-C3C | 2.19 | 1.48 | 1.45 |
| 37 | 20 | 308 | CLA | C3B-C2B | 2.19 | 1.48 | 1.41 |
| 37 | 13 | 307 | CLA | C1C-NC | -2.19 | 1.34 | 1.37 |
| 37 | 33 | 307 | CLA | C1C-NC | -2.19 | 1.34 | 1.37 |
| 47 | 20 | 302 | KC1 | C1D-C2D | 2.19 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 18 | 204 | CLA | C3B-C2B | 2.19 | 1.48 | 1.41 |
| 48 | 37 | 310 | A86 | C-C1 | 2.19 | 1.55 | 1.50 |
| 37 | 41 | 208 | CLA | C3B-C2B | 2.19 | 1.48 | 1.41 |
| 47 | 17 | 308 | KC1 | CAA-C2A | 2.19 | 1.53 | 1.46 |
| 47 | 18 | 210 | KC1 | CAA-C2A | 2.19 | 1.53 | 1.46 |
| 47 | 39 | 308 | KC1 | C3B-C4B | 2.19 | 1.49 | 1.46 |
| 47 | 21 | 203 | KC1 | CAA-C2A | 2.19 | 1.53 | 1.46 |
| 37 | 21 | 202 | CLA | C1C-NC | -2.19 | 1.34 | 1.37 |
| 47 | 18 | 205 | KC1 | CAA-C2A | 2.19 | 1.53 | 1.46 |
| 37 | 12 | 207 | CLA | C1B-C2B | 2.19 | 1.48 | 1.43 |
| 37 | 32 | 208 | CLA | C1B-C2B | 2.19 | 1.48 | 1.43 |
| 37 | 12 | 207 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 37 | 32 | 208 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 37 | 14 | 308 | CLA | C3B-C2B | 2.19 | 1.48 | 1.41 |
| 37 | c | 510 | CLA | CBD-CAD | -2.19 | 1.46 | 1.56 |
| 37 | 33 | 301 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 37 | 12 | 209 | CLA | C3B-C4B | 2.19 | 1.49 | 1.42 |
| 47 | 34 | 304 | KC1 | C4A-C3A | 2.19 | 1.49 | 1.44 |
| 47 | 35 | 306 | KC1 | C1C-C2C | 2.18 | 1.49 | 1.44 |
| 48 | 31 | 319 | A86 | C2-C1 | 2.18 | 1.40 | 1.35 |
| 48 | 19 | 311 | A86 | O4-C34 | -2.18 | 1.41 | 1.46 |
| 37 | 41 | 209 | CLA | C3B-C2B | 2.18 | 1.48 | 1.41 |
| 37 | 32 | 210 | CLA | C3B-C4B | 2.18 | 1.49 | 1.42 |
| 37 | a | 407 | CLA | C1B-C2B | 2.18 | 1.48 | 1.43 |
| 41 | 11 | 317 | LMG | O7-C8 | -2.18 | 1.41 | 1.46 |
| 48 | 31 | 314 | A86 | O4-C34 | -2.18 | 1.41 | 1.46 |
| 37 | 38 | 204 | CLA | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 37 | A | 405 | CLA | C1C-NC | -2.18 | 1.34 | 1.37 |
| 37 | C | 503 | CLA | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 47 | 16 | 308 | KC1 | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 47 | 21 | 203 | KC1 | C1C-C2C | 2.18 | 1.49 | 1.44 |
| 47 | 34 | 304 | KC1 | C1D-C2D | 2.18 | 1.48 | 1.43 |
| 48 | 41 | 215 | A86 | O4-C34 | -2.18 | 1.41 | 1.46 |
| 37 | 36 | 307 | CLA | C1B-C2B | 2.18 | 1.48 | 1.43 |
| 37 | 34 | 308 | CLA | C3B-C2B | 2.18 | 1.48 | 1.41 |
| 37 | c | 502 | CLA | CBD-CAD | -2.18 | 1.46 | 1.56 |
| 48 | 17 | 320 | A86 | C2-C1 | 2.18 | 1.40 | 1.35 |
| 37 | 20 | 307 | CLA | C3B-C2B | 2.18 | 1.48 | 1.41 |
| 37 | 40 | 209 | CLA | C3B-C2B | 2.18 | 1.48 | 1.41 |
| 47 | 14 | 309 | KC1 | CBD-CAD | -2.18 | 1.46 | 1.56 |
| 47 | 34 | 309 | KC1 | CBD-CAD | -2.18 | 1.46 | 1.56 |
| 37 | 18 | 204 | CLA | C4C-C3C | 2.18 | 1.48 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 41 | 205 | CLA | C3B-C2B | 2.18 | 1.48 | 1.41 |
| 37 | 31 | 301 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 37 | 17 | 307 | CLA | C3B-C2B | 2.18 | 1.48 | 1.41 |
| 37 | C | 502 | CLA | CBD-CAD | -2.18 | 1.46 | 1.56 |
| 37 | 15 | 305 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 37 | 21 | 206 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 37 | 35 | 308 | CLA | C3D-C4D | -2.18 | 1.39 | 1.44 |
| 41 | l | 101 | LMG | O2-C2 | -2.18 | 1.37 | 1.43 |
| 47 | 36 | 308 | KC1 | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 48 | 35 | 316 | A86 | O-C13 | -2.18 | 1.18 | 1.23 |
| 47 | 41 | 203 | KC1 | CAA-C2A | 2.18 | 1.53 | 1.46 |
| 37 | 37 | 306 | CLA | C3B-C2B | 2.18 | 1.48 | 1.41 |
| 37 | 19 | 309 | CLA | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 37 | c | 512 | CLA | C1C-NC | -2.18 | 1.34 | 1.37 |
| 47 | 36 | 302 | KC1 | C3B-C4B | 2.18 | 1.49 | 1.46 |
| 48 | 14 | 315 | A86 | C24-C1 | 2.18 | 1.50 | 1.46 |
| 41 | L | 102 | LMG | O2-C2 | -2.18 | 1.37 | 1.43 |
| 37 | C | 502 | CLA | C1B-C2B | 2.18 | 1.48 | 1.43 |
| 37 | 20 | 307 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 48 | 11 | 319 | A86 | C2-C1 | 2.17 | 1.40 | 1.35 |
| 48 | 36 | 311 | A86 | C26-C27 | 2.17 | 1.40 | 1.35 |
| 37 | c | 504 | CLA | C1B-C2B | 2.17 | 1.48 | 1.43 |
| 48 | 32 | 215 | A86 | C14-C15 | 2.17 | 1.57 | 1.52 |
| 37 | A | 403 | CLA | C3B-C2B | 2.17 | 1.48 | 1.41 |
| 37 | 40 | 205 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 48 | 35 | 316 | A86 | C5-C6 | 2.17 | 1.40 | 1.35 |
| 48 | 11 | 311 | A86 | C2-C1 | 2.17 | 1.40 | 1.35 |
| 48 | 37 | 319 | A86 | C2-C1 | 2.17 | 1.40 | 1.35 |
| 47 | 17 | 303 | KC1 | C4C-C3C | 2.17 | 1.48 | 1.45 |
| 46 | V | 201 | HEM | C3C-C2C | -2.17 | 1.32 | 1.37 |
| 40 | a | 409 | SQD | O47-C45 | -2.17 | 1.41 | 1.46 |
| 37 | B | 514 | CLA | C1C-NC | -2.17 | 1.34 | 1.37 |
| 37 | C | 503 | CLA | C1B-C2B | 2.17 | 1.48 | 1.43 |
| 37 | W | 102 | CLA | C4C-C3C | 2.17 | 1.48 | 1.45 |
| 37 | 19 | 307 | CLA | CHB-C4A | -2.17 | 1.32 | 1.37 |
| 37 | 40 | 210 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 47 | 37 | 305 | KC1 | C1D-C2D | 2.17 | 1.48 | 1.43 |
| 37 | C | 512 | CLA | C1C-NC | -2.17 | 1.34 | 1.37 |
| 37 | 32 | 205 | CLA | C1B-C2B | 2.17 | 1.48 | 1.43 |
| 47 | 16 | 302 | KC1 | C1D-C2D | 2.17 | 1.48 | 1.43 |
| 37 | 39 | 307 | CLA | CHB-C4A | -2.17 | 1.32 | 1.37 |
| 47 | 16 | 302 | KC1 | C3B-C4B | 2.17 | 1.49 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | A | 405 | CLA | C1B-C2B | 2.17 | 1.48 | 1.43 |
| 37 | 35 | 303 | CLA | C3B-C2B | 2.17 | 1.48 | 1.41 |
| 47 | 36 | 304 | KC1 | CAA-C2A | 2.17 | 1.52 | 1.46 |
| 37 | 15 | 305 | CLA | C3B-C2B | 2.17 | 1.48 | 1.41 |
| 37 | 21 | 208 | CLA | C3B-C2B | 2.17 | 1.48 | 1.41 |
| 37 | 18 | 208 | CLA | C1B-C2B | 2.17 | 1.48 | 1.43 |
| 37 | C | 504 | CLA | C1C-NC | -2.17 | 1.34 | 1.37 |
| 37 | b | 514 | CLA | C1C-NC | -2.17 | 1.34 | 1.37 |
| 37 | 35 | 308 | CLA | C3B-C2B | 2.17 | 1.48 | 1.41 |
| 37 | b | 504 | CLA | C1B-C2B | 2.17 | 1.48 | 1.43 |
| 47 | 40 | 204 | KC1 | C1D-C2D | 2.17 | 1.48 | 1.43 |
| 37 | 15 | 303 | CLA | C3B-C2B | 2.17 | 1.48 | 1.41 |
| 48 | 36 | 310 | A86 | C-C1 | 2.17 | 1.55 | 1.50 |
| 47 | 33 | 309 | KC1 | C4C-C3C | 2.17 | 1.48 | 1.45 |
| 37 | W | 102 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 37 | 17 | 302 | CLA | C1C-NC | -2.17 | 1.34 | 1.37 |
| 48 | 21 | 214 | A86 | O4-C34 | -2.16 | 1.41 | 1.46 |
| 37 | B | 506 | CLA | CHB-C4A | -2.16 | 1.32 | 1.37 |
| 48 | 17 | 314 | A86 | C2-C1 | 2.16 | 1.40 | 1.35 |
| 37 | 34 | 301 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 37 | 13 | 305 | CLA | C3B-C2B | 2.16 | 1.48 | 1.41 |
| 37 | 33 | 305 | CLA | C3B-C2B | 2.16 | 1.48 | 1.41 |
| 47 | 12 | 211 | KC1 | C1D-C2D | 2.16 | 1.48 | 1.43 |
| 48 | 16 | 310 | A86 | C-C1 | 2.16 | 1.55 | 1.50 |
| 37 | B | 501 | CLA | C1B-C2B | 2.16 | 1.48 | 1.43 |
| 48 | 36 | 313 | A86 | C26-C27 | 2.16 | 1.40 | 1.35 |
| 37 | 34 | 302 | CLA | C3B-C4B | 2.16 | 1.49 | 1.42 |
| 47 | 38 | 205 | KC1 | CAA-C2A | 2.16 | 1.52 | 1.46 |
| 47 | 17 | 308 | KC1 | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 37 | 41 | 202 | CLA | C1C-NC | -2.16 | 1.34 | 1.37 |
| 37 | 21 | 208 | CLA | C3D-C4D | -2.16 | 1.39 | 1.44 |
| 37 | 34 | 305 | CLA | C3B-C2B | 2.16 | 1.48 | 1.41 |
| 48 | 37 | 313 | A86 | C26-C27 | 2.16 | 1.40 | 1.35 |
| 44 | J | 101 | DGD | O2E-C2E | -2.16 | 1.37 | 1.43 |
| 37 | 15 | 308 | CLA | C3B-C2B | 2.16 | 1.48 | 1.41 |
| 48 | 37 | 314 | A86 | C14-C15 | 2.16 | 1.57 | 1.52 |
| 48 | 13 | 315 | A86 | O4-C34 | -2.16 | 1.41 | 1.46 |
| 37 | c | 504 | CLA | C1C-NC | -2.16 | 1.34 | 1.37 |
| 37 | d | 403 | CLA | C1C-NC | -2.16 | 1.34 | 1.37 |
| 37 | 12 | 203 | CLA | C3B-C4B | 2.16 | 1.49 | 1.42 |
| 47 | 19 | 308 | KC1 | C3B-C4B | 2.16 | 1.49 | 1.46 |
| 43 | 37 | 321 | LHG | O7-C5 | -2.16 | 1.41 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 41 | 214 | A86 | O4-C34 | -2.16 | 1.41 | 1.46 |
| 37 | c | 502 | CLA | C1B-C2B | 2.16 | 1.48 | 1.43 |
| 48 | 34 | 311 | A86 | C26-C27 | 2.16 | 1.40 | 1.35 |
| 47 | 37 | 307 | KC1 | CAA-C2A | 2.16 | 1.52 | 1.46 |
| 37 | 11 | 307 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 37 | 18 | 206 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 48 | 17 | 314 | A86 | C24-C1 | 2.16 | 1.50 | 1.46 |
| 37 | B | 511 | CLA | CBD-CAD | -2.16 | 1.46 | 1.56 |
| 37 | 21 | 209 | CLA | C3B-C2B | 2.16 | 1.48 | 1.41 |
| 48 | 32 | 214 | A86 | C24-C1 | 2.16 | 1.50 | 1.46 |
| 37 | 14 | 302 | CLA | C3B-C4B | 2.16 | 1.49 | 1.42 |
| 37 | 31 | 301 | CLA | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 37 | 36 | 306 | CLA | CHB-C4A | -2.16 | 1.32 | 1.37 |
| 37 | a | 403 | CLA | C3B-C2B | 2.16 | 1.48 | 1.41 |
| 37 | B | 511 | CLA | C3B-C2B | 2.16 | 1.48 | 1.41 |
| 37 | b | 511 | CLA | C3B-C2B | 2.16 | 1.48 | 1.41 |
| 37 | B | 504 | CLA | C1B-C2B | 2.16 | 1.48 | 1.43 |
| 37 | 17 | 309 | CLA | C3B-C2B | 2.15 | 1.48 | 1.41 |
| 37 | 20 | 306 | CLA | C4C-C3C | 2.15 | 1.48 | 1.45 |
| 47 | 12 | 206 | KC1 | CBD-CAD | -2.15 | 1.46 | 1.56 |
| 47 | 32 | 207 | KC1 | CBD-CAD | -2.15 | 1.46 | 1.56 |
| 37 | 39 | 306 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 47 | 36 | 308 | KC1 | C1D-C2D | 2.15 | 1.48 | 1.43 |
| 48 | 18 | 215 | A86 | O4-C34 | -2.15 | 1.41 | 1.46 |
| 48 | 14 | 312 | A86 | C2-C1 | 2.15 | 1.40 | 1.35 |
| 48 | 31 | 312 | A86 | C2-C1 | 2.15 | 1.40 | 1.35 |
| 44 | H | 102 | DGD | O2D-C2D | -2.15 | 1.37 | 1.43 |
| 48 | 38 | 213 | A86 | O4-C34 | -2.15 | 1.41 | 1.46 |
| 37 | 20 | 303 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 37 | 14 | 302 | CLA | C4C-C3C | 2.15 | 1.48 | 1.45 |
| 44 | h | 102 | DGD | O2D-C2D | -2.15 | 1.37 | 1.43 |
| 45 | D | 408 | PL9 | C26-C24 | -2.15 | 1.46 | 1.51 |
| 37 | 31 | 304 | CLA | C1C-NC | -2.15 | 1.34 | 1.37 |
| 37 | 31 | 306 | CLA | C1C-NC | -2.15 | 1.34 | 1.37 |
| 47 | 12 | 211 | KC1 | C3B-C4B | 2.15 | 1.49 | 1.46 |
| 37 | b | 511 | CLA | CBD-CAD | -2.15 | 1.46 | 1.56 |
| 44 | j | 101 | DGD | O2E-C2E | -2.15 | 1.37 | 1.43 |
| 48 | 16 | 311 | A86 | C26-C27 | 2.15 | 1.40 | 1.35 |
| 37 | D | 405 | CLA | C1C-NC | -2.15 | 1.34 | 1.37 |
| 37 | c | 513 | CLA | C1B-C2B | 2.15 | 1.48 | 1.43 |
| 37 | 11 | 305 | CLA | C1C-NC | -2.15 | 1.34 | 1.37 |
| 39 | H | 101 | BCR | C33-C5 | -2.15 | 1.47 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 36 | 301 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 37 | 37 | 303 | CLA | C3B-C2B | 2.15 | 1.48 | 1.41 |
| 45 | d | 402 | PL9 | C6-C1 | -2.15 | 1.45 | 1.48 |
| 48 | 39 | 311 | A86 | O4-C34 | -2.15 | 1.41 | 1.46 |
| 37 | 41 | 206 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 37 | b | 516 | CLA | CBD-CAD | -2.15 | 1.46 | 1.56 |
| 47 | 16 | 304 | KC1 | CAA-C2A | 2.15 | 1.52 | 1.46 |
| 47 | 40 | 207 | KC1 | C1D-C2D | 2.15 | 1.48 | 1.43 |
| 37 | 34 | 302 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 47 | 12 | 208 | KC1 | CAA-C2A | 2.15 | 1.52 | 1.46 |
| 37 | 19 | 309 | CLA | C1C-NC | -2.15 | 1.34 | 1.37 |
| 37 | c | 510 | CLA | C3B-C2B | 2.15 | 1.48 | 1.41 |
| 37 | B | 516 | CLA | CBD-CAD | -2.14 | 1.46 | 1.56 |
| 37 | C | 501 | CLA | CBD-CAD | -2.14 | 1.46 | 1.56 |
| 37 | 41 | 208 | CLA | C3D-C4D | -2.14 | 1.39 | 1.44 |
| 37 | 14 | 302 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 37 | b | 506 | CLA | CHB-C4A | -2.14 | 1.32 | 1.37 |
| 41 | 37 | 316 | LMG | C4-C5 | 2.14 | 1.57 | 1.53 |
| 48 | 14 | 314 | A86 | C5-C6 | 2.14 | 1.40 | 1.35 |
| 48 | 34 | 314 | A86 | C5-C6 | 2.14 | 1.40 | 1.35 |
| 37 | C | 513 | CLA | C1B-C2B | 2.14 | 1.48 | 1.43 |
| 37 | 12 | 204 | CLA | C1B-C2B | 2.14 | 1.48 | 1.43 |
| 47 | 12 | 208 | KC1 | CBD-CAD | -2.14 | 1.46 | 1.56 |
| 37 | 12 | 210 | CLA | C1C-NC | -2.14 | 1.34 | 1.37 |
| 45 | d | 406 | PL9 | C26-C24 | -2.14 | 1.46 | 1.51 |
| 37 | 19 | 306 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 37 | c | 512 | CLA | CHB-C4A | -2.14 | 1.32 | 1.37 |
| 47 | 16 | 305 | KC1 | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 48 | 39 | 313 | A86 | O4-C34 | -2.14 | 1.41 | 1.46 |
| 41 | 31 | 317 | LMG | O7-C8 | -2.14 | 1.41 | 1.46 |
| 37 | 17 | 304 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 37 | 18 | 204 | CLA | C1B-C2B | 2.14 | 1.48 | 1.43 |
| 47 | 13 | 306 | KC1 | CAA-C2A | 2.14 | 1.52 | 1.46 |
| 40 | B | 522 | SQD | O2-C2 | -2.14 | 1.37 | 1.43 |
| 37 | b | 505 | CLA | CBD-CAD | -2.14 | 1.46 | 1.56 |
| 37 | c | 501 | CLA | CBD-CAD | -2.14 | 1.46 | 1.56 |
| 47 | 16 | 308 | KC1 | C1D-C2D | 2.14 | 1.48 | 1.43 |
| 37 | 16 | 307 | CLA | C1B-C2B | 2.14 | 1.48 | 1.43 |
| 37 | C | 510 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 48 | 14 | 311 | A86 | C14-C15 | 2.14 | 1.56 | 1.52 |
| 37 | 39 | 309 | CLA | C4C-C3C | 2.14 | 1.48 | 1.45 |
| 37 | b | 523 | CLA | C3B-C4B | 2.14 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 204 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 48 | 13 | 311 | A86 | C24-C1 | 2.14 | 1.50 | 1.46 |
| 37 | c | 510 | CLA | C1C-NC | -2.14 | 1.34 | 1.37 |
| 40 | b | 521 | SQD | O2-C2 | -2.14 | 1.37 | 1.43 |
| 47 | 32 | 209 | KC1 | CBD-CAD | -2.14 | 1.46 | 1.56 |
| 37 | c | 507 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 37 | 14 | 305 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 37 | 32 | 213 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 48 | 31 | 311 | A86 | C2-C1 | 2.14 | 1.40 | 1.35 |
| 37 | 11 | 307 | CLA | C3B-C4B | 2.14 | 1.49 | 1.42 |
| 37 | 31 | 308 | CLA | C3B-C4B | 2.14 | 1.49 | 1.42 |
| 48 | 18 | 215 | A86 | C5-C6 | 2.14 | 1.40 | 1.35 |
| 37 | 35 | 307 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 37 | 38 | 202 | CLA | C3B-C2B | 2.14 | 1.48 | 1.41 |
| 47 | 20 | 305 | KC1 | C1D-C2D | 2.13 | 1.48 | 1.43 |
| 37 | 38 | 206 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 43 | 21 | 217 | LHG | O7-C5 | -2.13 | 1.41 | 1.46 |
| 37 | c | 503 | CLA | C1B-C2B | 2.13 | 1.48 | 1.43 |
| 47 | 36 | 305 | KC1 | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 47 | 32 | 209 | KC1 | CAA-C2A | 2.13 | 1.52 | 1.46 |
| 48 | 15 | 316 | A86 | C5-C6 | 2.13 | 1.40 | 1.35 |
| 37 | b | 503 | CLA | CHB-C4A | -2.13 | 1.32 | 1.37 |
| 37 | b | 515 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |
| 47 | 32 | 212 | KC1 | C3B-C4B | 2.13 | 1.49 | 1.46 |
| 47 | 40 | 204 | KC1 | CAA-C2A | 2.13 | 1.52 | 1.46 |
| 47 | 36 | 308 | KC1 | CAA-C2A | 2.13 | 1.52 | 1.46 |
| 37 | c | 505 | CLA | CHB-C4A | -2.13 | 1.32 | 1.37 |
| 37 | 33 | 308 | CLA | C3B-C2B | 2.13 | 1.48 | 1.41 |
| 40 | A | 407 | SQD | O47-C45 | -2.13 | 1.41 | 1.46 |
| 48 | 19 | 313 | A86 | O4-C34 | -2.13 | 1.41 | 1.46 |
| 38 | a | 406 | PHO | CBD-CGD | -2.13 | 1.49 | 1.52 |
| 37 | B | 524 | CLA | C3B-C4B | 2.13 | 1.48 | 1.42 |
| 47 | 36 | 305 | KC1 | C1D-C2D | 2.13 | 1.48 | 1.43 |
| 37 | 41 | 204 | CLA | C3B-C2B | 2.13 | 1.48 | 1.41 |
| 47 | 33 | 306 | KC1 | CAA-C2A | 2.13 | 1.52 | 1.46 |
| 37 | B | 503 | CLA | CHB-C4A | -2.13 | 1.32 | 1.37 |
| 37 | 21 | 202 | CLA | C3B-C4B | 2.13 | 1.48 | 1.42 |
| 47 | 32 | 212 | KC1 | C1D-C2D | 2.13 | 1.48 | 1.43 |
| 40 | a | 409 | SQD | O4-C4 | -2.13 | 1.37 | 1.43 |
| 37 | C | 507 | CLA | C3B-C2B | 2.13 | 1.48 | 1.41 |
| 37 | B | 505 | CLA | CBD-CAD | -2.13 | 1.47 | 1.56 |
| 48 | 34 | 312 | A86 | C2-C1 | 2.13 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 18 | 213 | A86 | O4-C34 | -2.13 | 1.41 | 1.46 |
| 47 | 16 | 305 | KC1 | C1D-C2D | 2.13 | 1.48 | 1.43 |
| 37 | 32 | 204 | CLA | C3B-C4B | 2.13 | 1.48 | 1.42 |
| 37 | 32 | 206 | CLA | CBD-CAD | -2.13 | 1.47 | 1.56 |
| 37 | 15 | 307 | CLA | C3B-C2B | 2.13 | 1.48 | 1.41 |
| 37 | 16 | 307 | CLA | C3B-C2B | 2.13 | 1.48 | 1.41 |
| 40 | B | 519 | SQD | O2-C2 | -2.13 | 1.37 | 1.43 |
| 46 | f | 101 | HEM | C2A-C3A | -2.13 | 1.33 | 1.38 |
| 37 | 12 | 205 | CLA | CBD-CAD | -2.12 | 1.47 | 1.56 |
| 37 | 17 | 304 | CLA | C1B-C2B | 2.12 | 1.48 | 1.43 |
| 47 | 35 | 306 | KC1 | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 37 | 39 | 309 | CLA | C1C-NC | -2.12 | 1.34 | 1.37 |
| 37 | 16 | 306 | CLA | CHB-C4A | -2.12 | 1.32 | 1.37 |
| 37 | 31 | 304 | CLA | C1B-C2B | 2.12 | 1.48 | 1.43 |
| 37 | 12 | 212 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 48 | 16 | 313 | A86 | C5-C6 | 2.12 | 1.40 | 1.35 |
| 37 | C | 512 | CLA | CHB-C4A | -2.12 | 1.32 | 1.37 |
| 37 | 14 | 307 | CLA | CHB-C4A | -2.12 | 1.32 | 1.37 |
| 48 | 12 | 214 | A86 | C14-C15 | 2.12 | 1.56 | 1.52 |
| 37 | 16 | 301 | CLA | C3B-C4B | 2.12 | 1.48 | 1.42 |
| 47 | 13 | 302 | KC1 | C3B-C4B | 2.12 | 1.49 | 1.46 |
| 37 | c | 503 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 46 | F | 101 | HEM | C2A-C3A | -2.12 | 1.33 | 1.38 |
| 37 | 36 | 307 | CLA | C3B-C2B | 2.12 | 1.48 | 1.41 |
| 37 | 40 | 205 | CLA | C3B-C2B | 2.12 | 1.48 | 1.41 |
| 37 | 18 | 201 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 50 | 21 | 216 | DD6 | O1-C20 | 2.12 | 1.49 | 1.46 |
| 37 | 16 | 301 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 48 | 40 | 201 | A86 | C5-C6 | 2.12 | 1.40 | 1.35 |
| 37 | 38 | 203 | CLA | C3B-C2B | 2.12 | 1.48 | 1.41 |
| 37 | c | 508 | CLA | CBD-CAD | -2.12 | 1.47 | 1.56 |
| 45 | D | 404 | PL9 | C10-C9 | -2.12 | 1.45 | 1.50 |
| 37 | 19 | 302 | CLA | C3B-C2B | 2.12 | 1.48 | 1.41 |
| 37 | 31 | 310 | CLA | C3B-C2B | 2.12 | 1.48 | 1.41 |
| 37 | 39 | 302 | CLA | C3B-C2B | 2.12 | 1.48 | 1.41 |
| 41 | 17 | 317 | LMG | C4-C5 | 2.12 | 1.57 | 1.53 |
| 37 | B | 515 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 37 | 38 | 204 | CLA | C1B-C2B | 2.12 | 1.48 | 1.43 |
| 47 | 13 | 302 | KC1 | CAA-C2A | 2.12 | 1.52 | 1.46 |
| 47 | 33 | 302 | KC1 | CAA-C2A | 2.12 | 1.52 | 1.46 |
| 37 | 38 | 201 | CLA | C3D-C4D | -2.12 | 1.39 | 1.44 |
| 37 | C | 503 | CLA | CHB-C4A | -2.12 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 12 | 214 | A86 | C2-C1 | 2.12 | 1.40 | 1.35 |
| 47 | 16 | 304 | KC1 | C3B-C4B | 2.12 | 1.49 | 1.46 |
| 48 | 17 | 315 | A86 | C14-C15 | 2.12 | 1.56 | 1.52 |
| 50 | 36 | 312 | DD6 | C22-C16 | -2.12 | 1.49 | 1.53 |
| 37 | 40 | 209 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 37 | B | 510 | CLA | CBD-CAD | -2.11 | 1.47 | 1.56 |
| 45 | D | 404 | PL9 | C6-C1 | -2.11 | 1.45 | 1.48 |
| 37 | A | 403 | CLA | C1B-C2B | 2.11 | 1.48 | 1.43 |
| 37 | 37 | 303 | CLA | C1B-C2B | 2.11 | 1.48 | 1.43 |
| 37 | 32 | 205 | CLA | MG-ND | -2.11 | 2.01 | 2.05 |
| 37 | c | 503 | CLA | CHB-C4A | -2.11 | 1.32 | 1.37 |
| 37 | b | 512 | CLA | CBD-CAD | -2.11 | 1.47 | 1.56 |
| 37 | 14 | 307 | CLA | C3B-C4B | 2.11 | 1.48 | 1.42 |
| 37 | C | 509 | CLA | C3B-C2B | 2.11 | 1.48 | 1.41 |
| 47 | 33 | 302 | KC1 | C3B-C4B | 2.11 | 1.49 | 1.46 |
| 40 | A | 407 | SQD | O4-C4 | -2.11 | 1.37 | 1.43 |
| 37 | c | 509 | CLA | CBD-CAD | -2.11 | 1.47 | 1.56 |
| 37 | 11 | 303 | CLA | C1B-C2B | 2.11 | 1.48 | 1.43 |
| 37 | 11 | 310 | CLA | C3B-C2B | 2.11 | 1.48 | 1.41 |
| 48 | 11 | 315 | A86 | C24-C1 | 2.11 | 1.50 | 1.46 |
| 48 | 31 | 315 | A86 | C24-C1 | 2.11 | 1.50 | 1.46 |
| 48 | 38 | 213 | A86 | C2-C1 | 2.11 | 1.40 | 1.35 |
| 37 | 41 | 202 | CLA | C3B-C4B | 2.11 | 1.48 | 1.42 |
| 47 | 36 | 304 | KC1 | C3B-C4B | 2.11 | 1.49 | 1.46 |
| 37 | C | 508 | CLA | CBD-CAD | -2.11 | 1.47 | 1.56 |
| 48 | 15 | 314 | A86 | C5-C6 | 2.11 | 1.40 | 1.35 |
| 37 | 18 | 211 | CLA | C1C-NC | -2.11 | 1.34 | 1.37 |
| 37 | 13 | 308 | CLA | C3B-C2B | 2.11 | 1.48 | 1.41 |
| 37 | 20 | 308 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 37 | W | 101 | CLA | C1B-C2B | 2.11 | 1.48 | 1.43 |
| 37 | w | 101 | CLA | C1B-C2B | 2.11 | 1.48 | 1.43 |
| 47 | 14 | 309 | KC1 | C1D-C2D | 2.11 | 1.48 | 1.43 |
| 47 | 13 | 309 | KC1 | C3B-C4B | 2.11 | 1.49 | 1.46 |
| 37 | 16 | 309 | CLA | C3B-C2B | 2.11 | 1.48 | 1.41 |
| 37 | 19 | 304 | CLA | C3B-C2B | 2.11 | 1.48 | 1.41 |
| 37 | C | 509 | CLA | CBD-CAD | -2.11 | 1.47 | 1.56 |
| 47 | 11 | 306 | KC1 | CAA-C2A | 2.11 | 1.52 | 1.46 |
| 37 | D | 402 | CLA | C3B-C4B | 2.11 | 1.48 | 1.42 |
| 37 | 32 | 205 | CLA | C4C-C3C | 2.11 | 1.48 | 1.45 |
| 37 | 31 | 308 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 37 | 19 | 302 | CLA | CBD-CAD | -2.11 | 1.47 | 1.56 |
| 48 | 39 | 311 | A86 | C39-C38 | 2.11 | 1.56 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 31 | 305 | KC1 | C4C-C3C | 2.11 | 1.48 | 1.45 |
| 40 | B | 522 | SQD | O4-C4 | -2.11 | 1.37 | 1.43 |
| 48 | 14 | 311 | A86 | C26-C27 | 2.11 | 1.40 | 1.35 |
| 37 | a | 403 | CLA | C1B-C2B | 2.11 | 1.48 | 1.43 |
| 37 | z | 101 | CLA | C1C-NC | -2.11 | 1.34 | 1.37 |
| 37 | 35 | 305 | CLA | C3B-C2B | 2.11 | 1.48 | 1.41 |
| 48 | 34 | 312 | A86 | C24-C1 | 2.11 | 1.50 | 1.46 |
| 37 | 34 | 307 | CLA | CHB-C4A | -2.11 | 1.32 | 1.37 |
| 47 | 15 | 302 | KC1 | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 48 | 12 | 213 | A86 | C26-C27 | 2.10 | 1.40 | 1.35 |
| 48 | 12 | 202 | A86 | O4-C34 | -2.10 | 1.41 | 1.46 |
| 48 | 32 | 203 | A86 | O4-C34 | -2.10 | 1.41 | 1.46 |
| 47 | 20 | 302 | KC1 | CAA-C2A | 2.10 | 1.52 | 1.46 |
| 37 | C | 504 | CLA | C3B-C4B | 2.10 | 1.48 | 1.42 |
| 37 | b | 510 | CLA | CBD-CAD | -2.10 | 1.47 | 1.56 |
| 37 | 13 | 307 | CLA | C3B-C2B | 2.10 | 1.48 | 1.41 |
| 40 | b | 521 | SQD | O3-C3 | -2.10 | 1.37 | 1.43 |
| 48 | 34 | 311 | A86 | C14-C15 | 2.10 | 1.56 | 1.52 |
| 37 | C | 503 | CLA | CBD-CAD | -2.10 | 1.47 | 1.56 |
| 37 | 18 | 202 | CLA | C3D-C4D | -2.10 | 1.39 | 1.44 |
| 48 | 11 | 315 | A86 | C2-C1 | 2.10 | 1.40 | 1.35 |
| 37 | c | 504 | CLA | C3B-C4B | 2.10 | 1.48 | 1.42 |
| 37 | 39 | 306 | CLA | C1B-C2B | 2.10 | 1.48 | 1.43 |
| 37 | 39 | 302 | CLA | CBD-CAD | -2.10 | 1.47 | 1.56 |
| 37 | 33 | 308 | CLA | C1C-NC | -2.10 | 1.34 | 1.37 |
| 37 | B | 512 | CLA | CBD-CAD | -2.10 | 1.47 | 1.56 |
| 37 | 41 | 202 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 47 | 15 | 306 | KC1 | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 47 | 33 | 309 | KC1 | C3B-C4B | 2.10 | 1.49 | 1.46 |
| 37 | 33 | 303 | CLA | C1C-NC | -2.10 | 1.34 | 1.37 |
| 37 | 36 | 309 | CLA | C3B-C2B | 2.10 | 1.48 | 1.41 |
| 37 | 31 | 306 | CLA | C4C-C3C | 2.10 | 1.48 | 1.45 |
| 37 | 31 | 304 | CLA | CBD-CAD | -2.10 | 1.47 | 1.56 |
| 37 | d | 403 | CLA | CBD-CAD | -2.10 | 1.47 | 1.56 |
| 37 | 18 | 202 | CLA | C3B-C2B | 2.10 | 1.48 | 1.41 |
| 37 | 20 | 303 | CLA | C3B-C2B | 2.10 | 1.48 | 1.41 |
| 37 | 35 | 301 | CLA | C3B-C2B | 2.10 | 1.48 | 1.41 |
| 37 | 35 | 310 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 37 | 39 | 301 | CLA | C1C-NC | -2.10 | 1.34 | 1.37 |
| 48 | 17 | 314 | A86 | C26-C27 | 2.10 | 1.40 | 1.35 |
| 37 | c | 507 | CLA | CBD-CAD | -2.10 | 1.47 | 1.56 |
| 41 | B | 521 | LMG | C4-C5 | 2.10 | 1.57 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 47 | 16 | 308 | KC1 | CAA-C2A | 2.10 | 1.52 | 1.46 |
| 37 | 21 | 206 | CLA | C3B-C2B | 2.10 | 1.48 | 1.41 |
| 37 | 19 | 303 | CLA | C3B-C2B | 2.10 | 1.48 | 1.41 |
| 37 | b | 523 | CLA | C1B-C2B | 2.10 | 1.48 | 1.43 |
| 37 | d | 401 | CLA | C3B-C4B | 2.10 | 1.48 | 1.42 |
| 37 | b | 523 | CLA | C1C-NC | -2.09 | 1.34 | 1.37 |
| 48 | 41 | 211 | A86 | O4-C34 | -2.09 | 1.41 | 1.46 |
| 47 | 14 | 306 | KC1 | CAA-C2A | 2.09 | 1.52 | 1.46 |
| 40 | A | 407 | SQD | O3-C3 | -2.09 | 1.37 | 1.43 |
| 37 | 32 | 211 | CLA | C1C-NC | -2.09 | 1.34 | 1.37 |
| 47 | 17 | 308 | KC1 | C3B-C4B | 2.09 | 1.49 | 1.46 |
| 40 | L | 101 | SQD | O2-C2 | -2.09 | 1.37 | 1.43 |
| 47 | 21 | 207 | KC1 | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 37 | 36 | 301 | CLA | C3B-C4B | 2.09 | 1.48 | 1.42 |
| 40 | B | 522 | SQD | O3-C3 | -2.09 | 1.37 | 1.43 |
| 50 | 41 | 216 | DD6 | O1-C20 | 2.09 | 1.49 | 1.46 |
| 48 | 31 | 311 | A86 | C20-C15 | 2.09 | 1.50 | 1.48 |
| 37 | C | 507 | CLA | CBD-CAD | -2.09 | 1.47 | 1.56 |
| 48 | 11 | 314 | A86 | O4-C34 | -2.09 | 1.41 | 1.46 |
| 37 | 11 | 301 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 39 | h | 101 | BCR | C33-C5 | -2.09 | 1.47 | 1.50 |
| 37 | 18 | 206 | CLA | C3B-C2B | 2.09 | 1.48 | 1.41 |
| 40 | b | 521 | SQD | O4-C4 | -2.09 | 1.37 | 1.43 |
| 37 | 19 | 306 | CLA | C1B-C2B | 2.09 | 1.48 | 1.43 |
| 37 | 36 | 301 | CLA | C1C-NC | -2.09 | 1.34 | 1.37 |
| 37 | 40 | 208 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 40 | 17 | 301 | SQD | O47-C45 | -2.09 | 1.41 | 1.46 |
| 37 | 38 | 204 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 37 | 18 | 201 | CLA | C3D-C4D | -2.09 | 1.39 | 1.44 |
| 37 | z | 101 | CLA | C3B-C4B | 2.09 | 1.48 | 1.42 |
| 48 | 14 | 312 | A86 | C24-C1 | 2.09 | 1.50 | 1.46 |
| 40 | 17 | 301 | SQD | O2-C2 | -2.09 | 1.37 | 1.43 |
| 37 | 39 | 305 | CLA | C1C-NC | -2.09 | 1.34 | 1.37 |
| 37 | 12 | 204 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 37 | 12 | 204 | CLA | MG-ND | -2.09 | 2.01 | 2.05 |
| 47 | 37 | 307 | KC1 | C3B-C4B | 2.09 | 1.49 | 1.46 |
| 48 | 18 | 213 | A86 | C24-C1 | 2.09 | 1.50 | 1.46 |
| 37 | B | 524 | CLA | C1C-NC | -2.09 | 1.34 | 1.37 |
| 37 | c | 511 | CLA | C3B-C2B | 2.09 | 1.48 | 1.41 |
| 37 | 38 | 201 | CLA | C1B-C2B | 2.09 | 1.48 | 1.43 |
| 44 | C | 516 | DGD | O3G-C1D | -2.09 | 1.36 | 1.40 |
| 44 | c | 516 | DGD | O3G-C1D | -2.09 | 1.36 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 14 | 313 | A86 | C39-C38 | 2.09 | 1.56 | 1.49 |
| 37 | Z | 101 | CLA | C1C-NC | -2.09 | 1.34 | 1.37 |
| 37 | c | 509 | CLA | C3B-C2B | 2.09 | 1.48 | 1.41 |
| 47 | 11 | 304 | KC1 | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 48 | 15 | 315 | A86 | C39-C38 | 2.09 | 1.56 | 1.49 |
| 37 | 34 | 310 | CLA | C3B-C2B | 2.09 | 1.48 | 1.41 |
| 37 | 17 | 304 | CLA | CBD-CAD | -2.09 | 1.47 | 1.56 |
| 37 | 37 | 303 | CLA | CBD-CAD | -2.09 | 1.47 | 1.56 |
| 45 | d | 402 | PL9 | C10-C9 | -2.09 | 1.45 | 1.50 |
| 37 | 12 | 205 | CLA | C3B-C2B | 2.09 | 1.48 | 1.41 |
| 37 | C | 505 | CLA | CHB-C4A | -2.09 | 1.32 | 1.37 |
| 50 | 16 | 312 | DD6 | C22-C16 | -2.09 | 1.49 | 1.53 |
| 37 | B | 501 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 37 | 11 | 303 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 37 | 31 | 304 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 47 | 18 | 205 | KC1 | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 37 | 39 | 304 | CLA | C3B-C2B | 2.08 | 1.48 | 1.41 |
| 37 | D | 401 | CLA | C3B-C2B | 2.08 | 1.48 | 1.41 |
| 37 | 15 | 308 | CLA | C1C-NC | -2.08 | 1.34 | 1.37 |
| 48 | 35 | 314 | A86 | C5-C6 | 2.08 | 1.40 | 1.35 |
| 37 | 21 | 202 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 37 | 11 | 305 | CLA | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 47 | 37 | 304 | KC1 | CBD-CAD | -2.08 | 1.47 | 1.56 |
| 37 | 32 | 205 | CLA | C1C-NC | -2.08 | 1.34 | 1.37 |
| 37 | B | 524 | CLA | MG-ND | -2.08 | 2.01 | 2.05 |
| 47 | 34 | 306 | KC1 | CAA-C2A | 2.08 | 1.52 | 1.46 |
| 47 | 35 | 309 | KC1 | CAA-C2A | 2.08 | 1.52 | 1.46 |
| 37 | 16 | 303 | CLA | C3B-C2B | 2.08 | 1.48 | 1.41 |
| 41 | b | 520 | LMG | C4-C5 | 2.08 | 1.57 | 1.53 |
| 37 | 32 | 206 | CLA | C3B-C2B | 2.08 | 1.48 | 1.41 |
| 46 | F | 101 | HEM | CMB-C2B | 2.08 | 1.55 | 1.50 |
| 37 | D | 405 | CLA | CBD-CAD | -2.08 | 1.47 | 1.56 |
| 37 | 13 | 303 | CLA | C1C-NC | -2.08 | 1.34 | 1.37 |
| 37 | 18 | 209 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 37 | b | 501 | CLA | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 47 | 33 | 306 | KC1 | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 48 | 19 | 311 | A86 | C39-C38 | 2.08 | 1.56 | 1.49 |
| 37 | 34 | 307 | CLA | C3B-C4B | 2.08 | 1.48 | 1.42 |
| 48 | 35 | 315 | A86 | C39-C38 | 2.08 | 1.56 | 1.49 |
| 48 | 15 | 316 | A86 | O4-C34 | -2.08 | 1.41 | 1.46 |
| 37 | 20 | 301 | CLA | C3B-C2B | 2.08 | 1.48 | 1.41 |
| 37 | 41 | 208 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 36 | 303 | CLA | C3B-C2B | 2.08 | 1.48 | 1.41 |
| 47 | 14 | 309 | KC1 | C3B-C4B | 2.08 | 1.49 | 1.46 |
| 47 | 34 | 309 | KC1 | C3B-C4B | 2.08 | 1.49 | 1.46 |
| 47 | 15 | 309 | KC1 | CAA-C2A | 2.08 | 1.52 | 1.46 |
| 37 | 18 | 203 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 37 | 32 | 206 | CLA | C1B-C2B | 2.08 | 1.48 | 1.43 |
| 37 | 19 | 303 | CLA | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 37 | 39 | 303 | CLA | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 48 | 17 | 312 | A86 | C5-C6 | 2.08 | 1.40 | 1.35 |
| 37 | 17 | 302 | CLA | C3B-C2B | 2.08 | 1.48 | 1.41 |
| 37 | 31 | 302 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 48 | 33 | 314 | A86 | O-C13 | -2.08 | 1.18 | 1.23 |
| 37 | b | 508 | CLA | CBD-CAD | -2.08 | 1.47 | 1.56 |
| 37 | 19 | 305 | CLA | C3B-C4B | 2.08 | 1.48 | 1.42 |
| 37 | 39 | 305 | CLA | C3B-C4B | 2.08 | 1.48 | 1.42 |
| 37 | 39 | 303 | CLA | C3B-C2B | 2.08 | 1.48 | 1.41 |
| 37 | B | 524 | CLA | C1B-C2B | 2.08 | 1.48 | 1.43 |
| 47 | 13 | 304 | KC1 | C1D-C2D | 2.08 | 1.48 | 1.43 |
| 48 | 19 | 311 | A86 | C-C1 | 2.08 | 1.55 | 1.50 |
| 37 | B | 508 | CLA | CBD-CAD | -2.08 | 1.47 | 1.56 |
| 37 | c | 503 | CLA | CBD-CAD | -2.08 | 1.47 | 1.56 |
| 37 | 11 | 305 | CLA | C1B-C2B | 2.07 | 1.48 | 1.43 |
| 37 | 34 | 308 | CLA | C4C-C3C | 2.07 | 1.48 | 1.45 |
| 47 | 34 | 306 | KC1 | C4C-C3C | 2.07 | 1.48 | 1.45 |
| 37 | C | 508 | CLA | CHB-C4A | -2.07 | 1.32 | 1.37 |
| 48 | 33 | 311 | A86 | C24-C1 | 2.07 | 1.50 | 1.46 |
| 37 | d | 404 | CLA | CHB-C4A | -2.07 | 1.32 | 1.37 |
| 37 | 12 | 204 | CLA | C1C-NC | -2.07 | 1.34 | 1.37 |
| 48 | 16 | 314 | A86 | C24-C1 | 2.07 | 1.50 | 1.46 |
| 47 | 31 | 307 | KC1 | CAA-C2A | 2.07 | 1.52 | 1.46 |
| 37 | 38 | 209 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 48 | 37 | 311 | A86 | C5-C6 | 2.07 | 1.40 | 1.35 |
| 37 | Z | 101 | CLA | C3B-C4B | 2.07 | 1.48 | 1.42 |
| 37 | 15 | 301 | CLA | C3B-C2B | 2.07 | 1.48 | 1.41 |
| 37 | 38 | 202 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 37 | d | 401 | CLA | CHB-C4A | -2.07 | 1.32 | 1.37 |
| 47 | 16 | 308 | KC1 | CBD-CAD | -2.07 | 1.47 | 1.56 |
| 47 | 38 | 207 | KC1 | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 37 | 38 | 208 | CLA | C4C-C3C | 2.07 | 1.48 | 1.45 |
| 37 | b | 512 | CLA | MG-ND | -2.07 | 2.01 | 2.05 |
| 37 | C | 501 | CLA | C3B-C4B | 2.07 | 1.48 | 1.42 |
| 37 | 40 | 203 | CLA | C4C-C3C | 2.07 | 1.48 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | B | 507 | CLA | CHB-C4A | -2.07 | 1.32 | 1.37 |
| 37 | 20 | 308 | CLA | C3B-C4B | 2.07 | 1.48 | 1.42 |
| 37 | 12 | 205 | CLA | C1B-C2B | 2.07 | 1.48 | 1.43 |
| 40 | 36 | 315 | SQD | O2-C2 | -2.07 | 1.37 | 1.43 |
| 37 | 11 | 310 | CLA | CBD-CAD | -2.07 | 1.47 | 1.56 |
| 37 | 31 | 310 | CLA | CBD-CAD | -2.07 | 1.47 | 1.56 |
| 48 | 34 | 313 | A86 | C39-C38 | 2.07 | 1.56 | 1.49 |
| 37 | 36 | 306 | CLA | C4C-C3C | 2.07 | 1.48 | 1.45 |
| 46 | F | 101 | HEM | FE-NA | 2.07 | 2.02 | 1.95 |
| 47 | 17 | 308 | KC1 | CBD-CAD | -2.07 | 1.47 | 1.56 |
| 47 | 37 | 307 | KC1 | CBD-CAD | -2.07 | 1.47 | 1.56 |
| 48 | 32 | 214 | A86 | C26-C27 | 2.07 | 1.40 | 1.35 |
| 37 | c | 508 | CLA | CHB-C4A | -2.07 | 1.32 | 1.37 |
| 37 | 41 | 210 | CLA | C3B-C2B | 2.07 | 1.48 | 1.41 |
| 40 | a | 409 | SQD | O3-C3 | -2.07 | 1.37 | 1.43 |
| 37 | c | 513 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 37 | 33 | 307 | CLA | C3B-C2B | 2.07 | 1.48 | 1.41 |
| 37 | D | 402 | CLA | CHB-C4A | -2.07 | 1.32 | 1.37 |
| 37 | 11 | 307 | CLA | CHB-C4A | -2.07 | 1.32 | 1.37 |
| 47 | 36 | 308 | KC1 | CBD-CAD | -2.07 | 1.47 | 1.56 |
| 40 | 36 | 315 | SQD | O47-C45 | -2.07 | 1.41 | 1.46 |
| 37 | 34 | 302 | CLA | C4C-C3C | 2.07 | 1.48 | 1.45 |
| 37 | 14 | 310 | CLA | C3B-C2B | 2.07 | 1.48 | 1.41 |
| 48 | 12 | 213 | A86 | C2-C1 | 2.07 | 1.40 | 1.35 |
| 37 | 12 | 209 | CLA | C1C-NC | -2.07 | 1.34 | 1.37 |
| 47 | 31 | 307 | KC1 | CBD-CAD | -2.07 | 1.47 | 1.56 |
| 48 | 39 | 311 | A86 | C-C1 | 2.07 | 1.55 | 1.50 |
| 37 | b | 507 | CLA | CHB-C4A | -2.07 | 1.32 | 1.37 |
| 37 | 15 | 303 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 37 | 38 | 211 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 37 | a | 404 | CLA | C1B-C2B | 2.07 | 1.48 | 1.43 |
| 48 | 31 | 315 | A86 | C2-C1 | 2.07 | 1.40 | 1.35 |
| 37 | 15 | 310 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 37 | 31 | 310 | CLA | C1B-C2B | 2.07 | 1.48 | 1.43 |
| 47 | 39 | 308 | KC1 | C1D-C2D | 2.07 | 1.48 | 1.43 |
| 37 | 11 | 303 | CLA | CBD-CAD | -2.06 | 1.47 | 1.56 |
| 37 | 16 | 301 | CLA | C1C-NC | -2.06 | 1.34 | 1.37 |
| 48 | 37 | 310 | A86 | C24-C1 | 2.06 | 1.50 | 1.46 |
| 37 | 37 | 301 | CLA | C3B-C2B | 2.06 | 1.48 | 1.41 |
| 48 | 15 | 312 | A86 | C5-C6 | 2.06 | 1.40 | 1.35 |
| 48 | 31 | 313 | A86 | C2-C1 | 2.06 | 1.40 | 1.35 |
| 37 | 20 | 301 | CLA | C4C-C3C | 2.06 | 1.48 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 32 | 214 | A86 | C2-C1 | 2.06 | 1.40 | 1.35 |
| 47 | 13 | 306 | KC1 | C4C-C3C | 2.06 | 1.48 | 1.45 |
| 48 | 11 | 311 | A86 | C20-C15 | 2.06 | 1.50 | 1.48 |
| 37 | 18 | 203 | CLA | C3B-C2B | 2.06 | 1.48 | 1.41 |
| 47 | 31 | 303 | KC1 | CAA-C2A | 2.06 | 1.52 | 1.46 |
| 37 | 38 | 203 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 37 | 41 | 208 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 37 | 21 | 208 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 37 | C | 513 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 40 | 40 | 202 | SQD | O4-C4 | -2.06 | 1.37 | 1.43 |
| 37 | 17 | 307 | CLA | C4C-C3C | 2.06 | 1.48 | 1.45 |
| 37 | 37 | 306 | CLA | C4C-C3C | 2.06 | 1.48 | 1.45 |
| 47 | 41 | 207 | KC1 | C4C-C3C | 2.06 | 1.48 | 1.45 |
| 37 | 41 | 206 | CLA | C3B-C2B | 2.06 | 1.48 | 1.41 |
| 37 | 37 | 301 | CLA | C4C-C3C | 2.06 | 1.48 | 1.45 |
| 45 | d | 402 | PL9 | C36-C34 | -2.06 | 1.47 | 1.51 |
| 37 | b | 515 | CLA | C1C-NC | -2.06 | 1.34 | 1.37 |
| 41 | l | 101 | LMG | O4-C4 | -2.06 | 1.37 | 1.43 |
| 48 | 21 | 211 | A86 | O4-C34 | -2.06 | 1.41 | 1.46 |
| 37 | 11 | 301 | CLA | CBD-CAD | -2.06 | 1.47 | 1.56 |
| 37 | a | 404 | CLA | C3B-C2B | 2.06 | 1.48 | 1.41 |
| 37 | 19 | 309 | CLA | C3B-C2B | 2.06 | 1.48 | 1.41 |
| 37 | 39 | 309 | CLA | C3B-C2B | 2.06 | 1.48 | 1.41 |
| 37 | B | 515 | CLA | C1C-NC | -2.06 | 1.34 | 1.37 |
| 48 | 32 | 215 | A86 | C2-C1 | 2.06 | 1.40 | 1.35 |
| 37 | C | 511 | CLA | C3B-C2B | 2.06 | 1.48 | 1.41 |
| 48 | 16 | 314 | A86 | C2-C1 | 2.06 | 1.40 | 1.35 |
| 47 | 20 | 304 | KC1 | CAA-C2A | 2.06 | 1.52 | 1.46 |
| 37 | 41 | 204 | CLA | C3B-C4B | 2.06 | 1.48 | 1.42 |
| 37 | 21 | 204 | CLA | C3B-C4B | 2.06 | 1.48 | 1.42 |
| 47 | 15 | 309 | KC1 | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 37 | 12 | 212 | CLA | C3B-C2B | 2.05 | 1.48 | 1.41 |
| 41 | L | 102 | LMG | O4-C4 | -2.05 | 1.37 | 1.43 |
| 37 | 40 | 210 | CLA | C3B-C4B | 2.05 | 1.48 | 1.42 |
| 48 | 32 | 203 | A86 | C2-C1 | 2.05 | 1.40 | 1.35 |
| 40 | 16 | 315 | SQD | O4-C4 | -2.05 | 1.37 | 1.43 |
| 37 | 39 | 310 | CLA | C4C-C3C | 2.05 | 1.48 | 1.45 |
| 37 | 33 | 303 | CLA | C3B-C2B | 2.05 | 1.48 | 1.41 |
| 37 | 19 | 301 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 37 | 11 | 308 | CLA | CBD-CAD | -2.05 | 1.47 | 1.56 |
| 37 | 32 | 202 | CLA | CBD-CAD | -2.05 | 1.47 | 1.56 |
| 37 | D | 406 | CLA | CHB-C4A | -2.05 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 36 | 313 | A86 | C2-C1 | 2.05 | 1.40 | 1.35 |
| 37 | 32 | 208 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 37 | B | 515 | CLA | CBD-CAD | -2.05 | 1.47 | 1.56 |
| 37 | 31 | 302 | CLA | CBD-CAD | -2.05 | 1.47 | 1.56 |
| 37 | 31 | 308 | CLA | CHB-C4A | -2.05 | 1.32 | 1.37 |
| 41 | D | 412 | LMG | O4-C4 | -2.05 | 1.37 | 1.43 |
| 37 | 40 | 203 | CLA | C3B-C2B | 2.05 | 1.48 | 1.41 |
| 48 | 40 | 201 | A86 | C-C1 | 2.05 | 1.55 | 1.50 |
| 37 | b | 523 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 37 | c | 501 | CLA | C3B-C4B | 2.05 | 1.48 | 1.42 |
| 47 | 35 | 309 | KC1 | C1D-C2D | 2.05 | 1.47 | 1.43 |
| 47 | 34 | 309 | KC1 | C1D-C2D | 2.05 | 1.47 | 1.43 |
| 37 | 34 | 303 | CLA | C3B-C2B | 2.05 | 1.48 | 1.41 |
| 37 | 31 | 302 | CLA | C1B-C2B | 2.05 | 1.47 | 1.43 |
| 48 | 21 | 214 | A86 | C5-C6 | 2.05 | 1.40 | 1.35 |
| 48 | 32 | 216 | A86 | C5-C6 | 2.05 | 1.40 | 1.35 |
| 37 | 11 | 301 | CLA | C1B-C2B | 2.05 | 1.47 | 1.43 |
| 39 | a | 408 | BCR | C33-C5 | -2.05 | 1.47 | 1.50 |
| 37 | C | 504 | CLA | CBD-CAD | -2.05 | 1.47 | 1.56 |
| 37 | 12 | 210 | CLA | C3B-C2B | 2.05 | 1.48 | 1.41 |
| 47 | 35 | 309 | KC1 | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 47 | 15 | 309 | KC1 | C1D-C2D | 2.05 | 1.47 | 1.43 |
| 48 | 15 | 311 | A86 | C5-C6 | 2.05 | 1.40 | 1.35 |
| 37 | D | 406 | CLA | C1B-C2B | 2.05 | 1.47 | 1.43 |
| 47 | 11 | 306 | KC1 | CBD-CAD | -2.05 | 1.47 | 1.56 |
| 48 | 12 | 215 | A86 | C39-C38 | 2.05 | 1.56 | 1.49 |
| 47 | 38 | 207 | KC1 | C1D-C2D | 2.05 | 1.47 | 1.43 |
| 41 | b | 520 | LMG | O4-C4 | -2.05 | 1.37 | 1.43 |
| 37 | 18 | 208 | CLA | C4C-C3C | 2.05 | 1.48 | 1.45 |
| 37 | b | 515 | CLA | CBD-CAD | -2.05 | 1.47 | 1.56 |
| 37 | B | 512 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 48 | 12 | 215 | A86 | C5-C6 | 2.05 | 1.40 | 1.35 |
| 37 | 14 | 307 | CLA | CBD-CAD | -2.04 | 1.47 | 1.56 |
| 37 | 34 | 307 | CLA | CBD-CAD | -2.04 | 1.47 | 1.56 |
| 41 | d | 409 | LMG | O4-C4 | -2.04 | 1.37 | 1.43 |
| 37 | 21 | 210 | CLA | C3B-C2B | 2.04 | 1.48 | 1.41 |
| 37 | 20 | 308 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 37 | 17 | 302 | CLA | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 47 | 14 | 304 | KC1 | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 47 | 34 | 304 | KC1 | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 41 | B | 521 | LMG | C7-C8 | 2.04 | 1.57 | 1.50 |
| 37 | 40 | 210 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 44 | C | 517 | DGD | O3D-C3D | -2.04 | 1.37 | 1.43 |
| 37 | c | 505 | CLA | C1B-C2B | 2.04 | 1.47 | 1.43 |
| 47 | 19 | 308 | KC1 | C1D-C2D | 2.04 | 1.47 | 1.43 |
| 37 | C | 512 | CLA | CBD-CAD | -2.04 | 1.47 | 1.56 |
| 48 | 36 | 313 | A86 | C24-C1 | 2.04 | 1.50 | 1.46 |
| 37 | 19 | 305 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |
| 47 | 11 | 302 | KC1 | CAA-C2A | 2.04 | 1.52 | 1.46 |
| 48 | 34 | 316 | A86 | C5-C6 | 2.04 | 1.40 | 1.35 |
| 37 | 19 | 301 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |
| 47 | 13 | 302 | KC1 | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 37 | 31 | 306 | CLA | C1B-C2B | 2.04 | 1.47 | 1.43 |
| 41 | b | 520 | LMG | C7-C8 | 2.04 | 1.57 | 1.50 |
| 46 | f | 101 | HEM | FE-NA | 2.04 | 2.01 | 1.95 |
| 37 | 20 | 301 | CLA | C1D-C2D | 2.04 | 1.49 | 1.45 |
| 37 | 11 | 303 | CLA | C3B-C2B | 2.04 | 1.48 | 1.41 |
| 37 | 31 | 304 | CLA | C3B-C2B | 2.04 | 1.48 | 1.41 |
| 48 | 12 | 220 | A86 | C39-C38 | 2.04 | 1.56 | 1.49 |
| 47 | 38 | 205 | KC1 | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 47 | 13 | 309 | KC1 | CAA-C2A | 2.04 | 1.52 | 1.46 |
| 37 | 11 | 308 | CLA | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 48 | 35 | 311 | A86 | C5-C6 | 2.04 | 1.40 | 1.35 |
| 37 | 38 | 209 | CLA | C3B-C2B | 2.04 | 1.48 | 1.41 |
| 37 | 12 | 205 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |
| 37 | 13 | 308 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |
| 48 | 13 | 314 | A86 | O-C13 | -2.04 | 1.19 | 1.23 |
| 37 | c | 504 | CLA | CBD-CAD | -2.04 | 1.47 | 1.56 |
| 46 | V | 201 | HEM | FE-NA | 2.04 | 2.01 | 1.95 |
| 48 | 18 | 212 | A86 | C5-C6 | 2.04 | 1.40 | 1.35 |
| 48 | 32 | 221 | A86 | C39-C38 | 2.04 | 1.56 | 1.49 |
| 50 | 41 | 216 | DD6 | C15-C14 | 2.04 | 1.54 | 1.50 |
| 37 | 19 | 310 | CLA | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 39 | 5 | 101 | BCR | C33-C5 | -2.04 | 1.47 | 1.50 |
| 37 | 32 | 213 | CLA | C3B-C2B | 2.04 | 1.48 | 1.41 |
| 48 | 32 | 216 | A86 | C39-C38 | 2.04 | 1.56 | 1.49 |
| 47 | 40 | 206 | KC1 | CAA-C2A | 2.04 | 1.52 | 1.46 |
| 37 | 11 | 307 | CLA | CBD-CAD | -2.04 | 1.47 | 1.56 |
| 47 | 15 | 304 | KC1 | C3B-C4B | 2.04 | 1.49 | 1.46 |
| 48 | 41 | 213 | A86 | C39-C38 | 2.04 | 1.56 | 1.49 |
| 37 | B | 506 | CLA | CBD-CAD | -2.04 | 1.47 | 1.56 |
| 37 | 32 | 202 | CLA | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 37 | 18 | 209 | CLA | C3B-C2B | 2.03 | 1.48 | 1.41 |
| 37 | c | 508 | CLA | C3B-C2B | 2.03 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 41 | 214 | A86 | C5-C6 | 2.03 | 1.40 | 1.35 |
| 48 | 37 | 311 | A86 | C39-C38 | 2.03 | 1.56 | 1.49 |
| 37 | B | 507 | CLA | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 46 | f | 101 | HEM | CMB-C2B | 2.03 | 1.54 | 1.50 |
| 37 | 11 | 310 | CLA | C1B-C2B | 2.03 | 1.47 | 1.43 |
| 37 | 34 | 303 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 37 | b | 507 | CLA | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 37 | 12 | 203 | CLA | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 48 | 18 | 213 | A86 | C2-C1 | 2.03 | 1.40 | 1.35 |
| 37 | 31 | 310 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 37 | 18 | 204 | CLA | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 47 | 33 | 304 | KC1 | C1D-C2D | 2.03 | 1.47 | 1.43 |
| 37 | 35 | 303 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 37 | 32 | 204 | CLA | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 37 | 32 | 202 | CLA | CHB-C4A | -2.03 | 1.32 | 1.37 |
| 47 | 40 | 204 | KC1 | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 37 | 16 | 306 | CLA | C3B-C2B | 2.03 | 1.48 | 1.41 |
| 48 | 35 | 312 | A86 | C5-C6 | 2.03 | 1.40 | 1.35 |
| 37 | c | 512 | CLA | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 37 | 13 | 301 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 37 | 37 | 303 | CLA | C3B-C4B | 2.03 | 1.48 | 1.42 |
| 37 | 37 | 301 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 37 | B | 502 | CLA | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 47 | 33 | 302 | KC1 | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 45 | d | 406 | PL9 | C31-C29 | -2.03 | 1.47 | 1.51 |
| 47 | 41 | 203 | KC1 | C3D-C2D | 2.03 | 1.49 | 1.42 |
| 48 | 19 | 313 | A86 | C5-C6 | 2.03 | 1.40 | 1.35 |
| 37 | b | 506 | CLA | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 37 | 21 | 209 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 37 | 41 | 209 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 47 | 18 | 207 | KC1 | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 47 | 17 | 305 | KC1 | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 37 | 32 | 210 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 37 | 39 | 301 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 48 | 38 | 212 | A86 | C5-C6 | 2.03 | 1.40 | 1.35 |
| 37 | 14 | 305 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 48 | 38 | 214 | A86 | C5-C6 | 2.03 | 1.40 | 1.35 |
| 50 | 40 | 212 | DD6 | C22-C16 | -2.03 | 1.49 | 1.53 |
| 37 | B | 510 | CLA | CHB-C4A | -2.03 | 1.32 | 1.37 |
| 37 | 32 | 211 | CLA | C3B-C2B | 2.03 | 1.48 | 1.41 |
| 48 | 38 | 213 | A86 | C23-C16 | -2.03 | 1.49 | 1.53 |
| 48 | 17 | 312 | A86 | C39-C38 | 2.03 | 1.56 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | z | 102 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 48 | 12 | 202 | A86 | C24-C1 | 2.03 | 1.50 | 1.46 |
| 37 | 13 | 303 | CLA | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 47 | 35 | 304 | KC1 | C3D-C2D | 2.03 | 1.49 | 1.42 |
| 37 | b | 502 | CLA | CBD-CAD | -2.03 | 1.47 | 1.56 |
| 39 | A | 406 | BCR | C33-C5 | -2.03 | 1.47 | 1.50 |
| 48 | 13 | 313 | A86 | C39-C38 | 2.02 | 1.56 | 1.49 |
| 37 | 16 | 306 | CLA | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 37 | C | 513 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 37 | 39 | 302 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 47 | 12 | 211 | KC1 | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 47 | 32 | 212 | KC1 | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 46 | f | 101 | HEM | CMC-C2C | 2.02 | 1.54 | 1.50 |
| 37 | 36 | 309 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 37 | 12 | 212 | CLA | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 48 | 12 | 220 | A86 | C26-C27 | 2.02 | 1.40 | 1.35 |
| 48 | 32 | 221 | A86 | C26-C27 | 2.02 | 1.40 | 1.35 |
| 37 | 12 | 203 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 37 | C | 504 | CLA | CHB-C4A | -2.02 | 1.32 | 1.37 |
| 48 | 16 | 313 | A86 | O4-C34 | -2.02 | 1.41 | 1.46 |
| 37 | D | 401 | CLA | C1B-C2B | 2.02 | 1.47 | 1.43 |
| 50 | 20 | 312 | DD6 | O1-C20 | 2.02 | 1.48 | 1.46 |
| 37 | 14 | 303 | CLA | C3B-C2B | 2.02 | 1.48 | 1.41 |
| 47 | 14 | 306 | KC1 | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 47 | 18 | 207 | KC1 | C1B-C2B | 2.02 | 1.49 | 1.45 |
| 47 | 13 | 309 | KC1 | C1D-C2D | 2.02 | 1.47 | 1.43 |
| 47 | 33 | 309 | KC1 | C1D-C2D | 2.02 | 1.47 | 1.43 |
| 37 | B | 509 | CLA | C3B-C4B | 2.02 | 1.48 | 1.42 |
| 48 | 34 | 311 | A86 | C2-C1 | 2.02 | 1.40 | 1.35 |
| 37 | 11 | 305 | CLA | CHB-C4A | -2.02 | 1.32 | 1.37 |
| 37 | 15 | 307 | CLA | CHB-C4A | -2.02 | 1.32 | 1.37 |
| 48 | 18 | 214 | A86 | C5-C6 | 2.02 | 1.40 | 1.35 |
| 48 | 15 | 313 | A86 | C39-C38 | 2.02 | 1.56 | 1.49 |
| 48 | 19 | 311 | A86 | C24-C1 | 2.02 | 1.50 | 1.46 |
| 37 | 37 | 301 | CLA | C3B-C4B | 2.02 | 1.48 | 1.42 |
| 37 | B | 507 | CLA | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 37 | 11 | 310 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 37 | 21 | 204 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 37 | 39 | 304 | CLA | CBD-CAD | -2.02 | 1.47 | 1.56 |
| 37 | a | 403 | CLA | O2D-CED | -2.02 | 1.40 | 1.45 |
| 37 | c | 503 | CLA | C3B-C4B | 2.02 | 1.48 | 1.42 |
| 37 | 34 | 305 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 48 | 36 | 310 | A86 | C24-C1 | 2.02 | 1.50 | 1.46 |
| 37 | 21 | 208 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 41 | B | 521 | LMG | O4-C4 | -2.02 | 1.38 | 1.43 |
| 37 | 31 | 308 | CLA | CBD-CAD | -2.02 | 1.47 | 1.56 |
| 37 | 17 | 302 | CLA | C3B-C4B | 2.02 | 1.48 | 1.42 |
| 47 | 35 | 304 | KC1 | C3B-C4B | 2.02 | 1.49 | 1.46 |
| 37 | w | 101 | CLA | CHB-C4A | -2.02 | 1.32 | 1.37 |
| 48 | 21 | 215 | A86 | C39-C38 | 2.02 | 1.56 | 1.49 |
| 47 | 20 | 302 | KC1 | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 48 | 12 | 213 | A86 | C24-C1 | 2.02 | 1.50 | 1.46 |
| 50 | 40 | 214 | DD6 | O1-C20 | 2.02 | 1.48 | 1.46 |
| 48 | 41 | 215 | A86 | C39-C38 | 2.02 | 1.56 | 1.49 |
| 47 | 40 | 207 | KC1 | C3B-C4B | 2.02 | 1.49 | 1.46 |
| 37 | 41 | 204 | CLA | C1D-C2D | 2.01 | 1.49 | 1.45 |
| 37 | b | 510 | CLA | CHB-C4A | -2.01 | 1.32 | 1.37 |
| 37 | 38 | 204 | CLA | CBD-CAD | -2.01 | 1.47 | 1.56 |
| 47 | 13 | 309 | KC1 | C3D-C2D | 2.01 | 1.49 | 1.42 |
| 37 | 12 | 207 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 37 | 34 | 308 | CLA | CBD-CAD | -2.01 | 1.47 | 1.56 |
| 40 | 17 | 301 | SQD | O4-C4 | -2.01 | 1.38 | 1.43 |
| 37 | 11 | 308 | CLA | C1B-C2B | 2.01 | 1.47 | 1.43 |
| 47 | 32 | 207 | KC1 | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 37 | B | 509 | CLA | CHB-C4A | -2.01 | 1.32 | 1.37 |
| 37 | W | 101 | CLA | CHB-C4A | -2.01 | 1.32 | 1.37 |
| 37 | c | 513 | CLA | C1C-NC | -2.01 | 1.34 | 1.37 |
| 37 | 36 | 306 | CLA | C3B-C2B | 2.01 | 1.48 | 1.41 |
| 48 | 35 | 313 | A86 | C39-C38 | 2.01 | 1.56 | 1.49 |
| 37 | C | 505 | CLA | C1B-C2B | 2.01 | 1.47 | 1.43 |
| 47 | 21 | 203 | KC1 | C3D-C2D | 2.01 | 1.49 | 1.42 |
| 47 | 20 | 305 | KC1 | C3B-C4B | 2.01 | 1.49 | 1.46 |
| 48 | 33 | 314 | A86 | C39-C38 | 2.01 | 1.56 | 1.49 |
| 48 | 37 | 309 | A86 | C39-C38 | 2.01 | 1.56 | 1.49 |
| 48 | 35 | 316 | A86 | O4-C34 | -2.01 | 1.41 | 1.46 |
| 37 | 19 | 304 | CLA | CBD-CAD | -2.01 | 1.47 | 1.56 |
| 37 | z | 102 | CLA | C4C-C3C | 2.01 | 1.48 | 1.45 |
| 37 | b | 505 | CLA | C1B-C2B | 2.01 | 1.47 | 1.43 |
| 37 | z | 102 | CLA | CHB-C4A | -2.01 | 1.32 | 1.37 |
| 37 | 16 | 309 | CLA | C1C-NC | -2.01 | 1.34 | 1.37 |
| 46 | v | 201 | HEM | FE-NA | 2.01 | 2.01 | 1.95 |
| 37 | 31 | 306 | CLA | CHB-C4A | -2.01 | 1.32 | 1.37 |
| 37 | 19 | 303 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 37 | 35 | 308 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 37 | 39 | 303 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 39 | H | 101 | BCR | C38-C26 | -2.01 | 1.47 | 1.50 |
| 47 | 33 | 309 | KC1 | CAA-C2A | 2.01 | 1.52 | 1.46 |
| 37 | 40 | 208 | CLA | C3B-C2B | 2.01 | 1.47 | 1.41 |
| 37 | 14 | 303 | CLA | C1C-NC | -2.01 | 1.34 | 1.37 |
| 37 | 13 | 303 | CLA | C3B-C2B | 2.01 | 1.47 | 1.41 |
| 45 | D | 408 | PL9 | C31-C29 | -2.01 | 1.47 | 1.51 |
| 37 | 35 | 307 | CLA | CHB-C4A | -2.01 | 1.32 | 1.37 |
| 37 | 19 | 303 | CLA | C1C-NC | -2.01 | 1.34 | 1.37 |
| 37 | C | 508 | CLA | C3B-C2B | 2.01 | 1.47 | 1.41 |
| 37 | 32 | 204 | CLA | C3B-C2B | 2.01 | 1.47 | 1.41 |
| 40 | B | 519 | SQD | O3-C3 | -2.01 | 1.38 | 1.43 |
| 47 | 16 | 308 | KC1 | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 44 | c | 517 | DGD | O3D-C3D | -2.01 | 1.38 | 1.43 |
| 37 | c | 504 | CLA | CHB-C4A | -2.01 | 1.32 | 1.37 |
| 37 | d | 401 | CLA | CBD-CAD | -2.01 | 1.47 | 1.56 |
| 50 | 21 | 216 | DD6 | C15-C14 | 2.01 | 1.54 | 1.50 |
| 37 | 16 | 307 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 37 | 18 | 201 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 37 | C | 506 | CLA | CBD-CAD | -2.01 | 1.47 | 1.56 |
| 48 | 33 | 315 | A86 | C39-C38 | 2.00 | 1.56 | 1.49 |
| 37 | 17 | 304 | CLA | C3B-C4B | 2.00 | 1.48 | 1.42 |
| 37 | Z | 102 | CLA | CHB-C4A | -2.00 | 1.32 | 1.37 |
| 43 | d | 408 | LHG | C8-C7 | -2.00 | 1.44 | 1.50 |
| 38 | A | 404 | PHO | C3D-CAD | -2.00 | 1.43 | 1.47 |
| 37 | 33 | 301 | CLA | C1C-C2C | 2.00 | 1.48 | 1.44 |
| 37 | 19 | 305 | CLA | CBD-CAD | -2.00 | 1.47 | 1.56 |
| 48 | 33 | 313 | A86 | C39-C38 | 2.00 | 1.56 | 1.49 |
| 37 | C | 513 | CLA | CBD-CAD | -2.00 | 1.47 | 1.56 |
| 47 | 33 | 309 | KC1 | C3D-C2D | 2.00 | 1.49 | 1.42 |
| 43 | 21 | 201 | LHG | P-O6 | 2.00 | 1.67 | 1.59 |
| 37 | B | 509 | CLA | C1B-C2B | 2.00 | 1.47 | 1.43 |
| 37 | 40 | 203 | CLA | C1D-C2D | 2.00 | 1.49 | 1.45 |
| 48 | 21 | 213 | A86 | C39-C38 | 2.00 | 1.56 | 1.49 |
| 48 | 14 | 316 | A86 | C5-C6 | 2.00 | 1.40 | 1.35 |
| 37 | 41 | 202 | CLA | C3B-C2B | 2.00 | 1.47 | 1.41 |
| 37 | 36 | 309 | CLA | C1C-C2C | 2.00 | 1.48 | 1.44 |
| 44 | J | 101 | DGD | O2D-C2D | -2.00 | 1.38 | 1.43 |
| 37 | b | 509 | CLA | CHB-C4A | -2.00 | 1.32 | 1.37 |
| 47 | 11 | 309 | KC1 | C4C-C3C | 2.00 | 1.48 | 1.45 |
| 37 | D | 402 | CLA | CBD-CAD | -2.00 | 1.47 | 1.56 |

All (12213) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 17 | 314 | A86 | O1-C20-C19 | 46.24 | 156.82 | 113.49 |
| 48 | 37 | 313 | A86 | O1-C20-C19 | 46.19 | 156.78 | 113.49 |
| 48 | 39 | 313 | A86 | O1-C20-C19 | 46.06 | 156.66 | 113.49 |
| 48 | 40 | 213 | A86 | O1-C20-C19 | 45.80 | 156.42 | 113.49 |
| 48 | 20 | 311 | A86 | O1-C20-C19 | 45.78 | 156.40 | 113.49 |
| 48 | 19 | 313 | A86 | O1-C20-C19 | 45.77 | 156.39 | 113.49 |
| 48 | 13 | 313 | A86 | O1-C20-C19 | 45.41 | 156.05 | 113.49 |
| 48 | 33 | 313 | A86 | O1-C20-C19 | 45.38 | 156.03 | 113.49 |
| 48 | 40 | 211 | A86 | O1-C20-C19 | 45.36 | 156.00 | 113.49 |
| 48 | 20 | 309 | A86 | O1-C20-C19 | 45.33 | 155.98 | 113.49 |
| 48 | 33 | 314 | A86 | O1-C20-C19 | 45.07 | 155.73 | 113.49 |
| 48 | 13 | 314 | A86 | O1-C20-C19 | 45.03 | 155.69 | 113.49 |
| 48 | 35 | 314 | A86 | O1-C20-C19 | 44.59 | 155.28 | 113.49 |
| 48 | 14 | 314 | A86 | O1-C20-C19 | 44.54 | 155.24 | 113.49 |
| 48 | 34 | 314 | A86 | O1-C20-C19 | 44.48 | 155.18 | 113.49 |
| 48 | 17 | 310 | A86 | O1-C20-C19 | 44.35 | 155.06 | 113.49 |
| 48 | 37 | 309 | A86 | O1-C20-C19 | 44.27 | 154.98 | 113.49 |
| 48 | 21 | 214 | A86 | O1-C20-C19 | 44.21 | 154.93 | 113.49 |
| 48 | 41 | 214 | A86 | O1-C20-C19 | 44.18 | 154.90 | 113.49 |
| 48 | 15 | 314 | A86 | O1-C20-C19 | 44.11 | 154.83 | 113.49 |
| 48 | 37 | 312 | A86 | O1-C20-C19 | 44.08 | 154.80 | 113.49 |
| 48 | 34 | 311 | A86 | O1-C20-C19 | 43.98 | 154.71 | 113.49 |
| 48 | 17 | 313 | A86 | O1-C20-C19 | 43.97 | 154.70 | 113.49 |
| 48 | 14 | 311 | A86 | O1-C20-C19 | 43.96 | 154.69 | 113.49 |
| 48 | 41 | 215 | A86 | O1-C20-C19 | 43.91 | 154.64 | 113.49 |
| 48 | 21 | 215 | A86 | O1-C20-C19 | 43.83 | 154.57 | 113.49 |
| 48 | 40 | 201 | A86 | O1-C20-C19 | 43.50 | 154.26 | 113.49 |
| 48 | 16 | 313 | A86 | O1-C20-C19 | 43.46 | 154.22 | 113.49 |
| 48 | 31 | 314 | A86 | O1-C20-C19 | 43.46 | 154.22 | 113.49 |
| 48 | 11 | 314 | A86 | O1-C20-C19 | 43.43 | 154.19 | 113.49 |
| 48 | 41 | 211 | A86 | O1-C20-C19 | 43.37 | 154.13 | 113.49 |
| 48 | 21 | 211 | A86 | O1-C20-C19 | 43.36 | 154.13 | 113.49 |
| 48 | 12 | 215 | A86 | O1-C20-C19 | 43.28 | 154.06 | 113.49 |
| 48 | 32 | 216 | A86 | O1-C20-C19 | 43.23 | 154.01 | 113.49 |
| 48 | 38 | 214 | A86 | O1-C20-C19 | 43.15 | 153.93 | 113.49 |
| 48 | 21 | 213 | A86 | O1-C20-C19 | 43.14 | 153.92 | 113.49 |
| 48 | 18 | 212 | A86 | O1-C20-C19 | 43.12 | 153.90 | 113.49 |
| 48 | 38 | 212 | A86 | O1-C20-C19 | 43.10 | 153.89 | 113.49 |
| 48 | 41 | 213 | A86 | O1-C20-C19 | 43.09 | 153.88 | 113.49 |
| 48 | 32 | 217 | A86 | O1-C20-C19 | 42.99 | 153.79 | 113.49 |
| 48 | 12 | 216 | A86 | O1-C20-C19 | 42.97 | 153.77 | 113.49 |
| 48 | 18 | 214 | A86 | O1-C20-C19 | 42.81 | 153.61 | 113.49 |
| 48 | 14 | 315 | A86 | O1-C20-C19 | 42.69 | 153.50 | 113.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 34 | 315 | A86 | O1-C20-C19 | 42.65 | 153.47 | 113.49 |
| 48 | 32 | 214 | A86 | O1-C20-C19 | 42.56 | 153.38 | 113.49 |
| 48 | 12 | 213 | A86 | O1-C20-C19 | 42.51 | 153.33 | 113.49 |
| 48 | 18 | 213 | A86 | O1-C20-C19 | 41.99 | 152.85 | 113.49 |
| 48 | 33 | 311 | A86 | O1-C20-C19 | 41.92 | 152.78 | 113.49 |
| 48 | 13 | 311 | A86 | O1-C20-C19 | 41.90 | 152.76 | 113.49 |
| 48 | 13 | 312 | A86 | O1-C20-C19 | 41.82 | 152.68 | 113.49 |
| 48 | 33 | 312 | A86 | O1-C20-C19 | 41.77 | 152.64 | 113.49 |
| 48 | 32 | 221 | A86 | O1-C20-C19 | 41.69 | 152.57 | 113.49 |
| 48 | 38 | 213 | A86 | O1-C20-C19 | 41.67 | 152.54 | 113.49 |
| 48 | 12 | 220 | A86 | O1-C20-C19 | 41.65 | 152.53 | 113.49 |
| 48 | 15 | 311 | A86 | O1-C20-C19 | 41.60 | 152.48 | 113.49 |
| 48 | 35 | 311 | A86 | O1-C20-C19 | 41.57 | 152.46 | 113.49 |
| 48 | 34 | 312 | A86 | O1-C20-C19 | 41.35 | 152.25 | 113.49 |
| 48 | 14 | 312 | A86 | O1-C20-C19 | 41.33 | 152.23 | 113.49 |
| 48 | 15 | 312 | A86 | O1-C20-C19 | 41.09 | 152.00 | 113.49 |
| 48 | 35 | 312 | A86 | O1-C20-C19 | 41.08 | 151.99 | 113.49 |
| 48 | 32 | 215 | A86 | O1-C20-C19 | 41.06 | 151.97 | 113.49 |
| 48 | 12 | 214 | A86 | O1-C20-C19 | 41.05 | 151.96 | 113.49 |
| 48 | 39 | 311 | A86 | O1-C20-C19 | 41.00 | 151.91 | 113.49 |
| 48 | 19 | 311 | A86 | O1-C20-C19 | 40.98 | 151.89 | 113.49 |
| 48 | 15 | 315 | A86 | O1-C20-C19 | 40.97 | 151.89 | 113.49 |
| 48 | 18 | 215 | A86 | O1-C20-C19 | 40.84 | 151.77 | 113.49 |
| 48 | 35 | 315 | A86 | O1-C20-C19 | 40.81 | 151.74 | 113.49 |
| 48 | 17 | 320 | A86 | O1-C20-C19 | 40.80 | 151.72 | 113.49 |
| 48 | 38 | 215 | A86 | O1-C20-C19 | 40.68 | 151.62 | 113.49 |
| 48 | 17 | 315 | A86 | O1-C20-C19 | 40.68 | 151.62 | 113.49 |
| 48 | 37 | 314 | A86 | O1-C20-C19 | 40.65 | 151.59 | 113.49 |
| 48 | 37 | 319 | A86 | O1-C20-C19 | 40.63 | 151.57 | 113.49 |
| 48 | 11 | 312 | A86 | O1-C20-C19 | 40.56 | 151.50 | 113.49 |
| 48 | 11 | 315 | A86 | O1-C20-C19 | 40.55 | 151.50 | 113.49 |
| 48 | 31 | 315 | A86 | O1-C20-C19 | 40.55 | 151.49 | 113.49 |
| 48 | 31 | 312 | A86 | O1-C20-C19 | 40.53 | 151.48 | 113.49 |
| 48 | 35 | 316 | A86 | O1-C20-C19 | 40.17 | 151.14 | 113.49 |
| 48 | 15 | 316 | A86 | O1-C20-C19 | 40.10 | 151.07 | 113.49 |
| 48 | 12 | 202 | A86 | O1-C20-C19 | 39.98 | 150.96 | 113.49 |
| 48 | 32 | 203 | A86 | O1-C20-C19 | 39.94 | 150.93 | 113.49 |
| 48 | 37 | 310 | A86 | O1-C20-C19 | 39.68 | 150.68 | 113.49 |
| 48 | 13 | 315 | A86 | O1-C20-C19 | 39.62 | 150.62 | 113.49 |
| 48 | 36 | 313 | A86 | O1-C20-C19 | 39.57 | 150.58 | 113.49 |
| 48 | 36 | 310 | A86 | O1-C20-C19 | 39.57 | 150.58 | 113.49 |
| 48 | 33 | 315 | A86 | O1-C20-C19 | 39.55 | 150.56 | 113.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 16 | 310 | A86 | O1-C20-C19 | 39.53 | 150.54 | 113.49 |
| 48 | 16 | 314 | A86 | O1-C20-C19 | 39.52 | 150.53 | 113.49 |
| 48 | 17 | 311 | A86 | O1-C20-C19 | 39.52 | 150.53 | 113.49 |
| 48 | 15 | 313 | A86 | O1-C20-C19 | 39.31 | 150.33 | 113.49 |
| 48 | 35 | 313 | A86 | O1-C20-C19 | 39.30 | 150.33 | 113.49 |
| 48 | 31 | 319 | A86 | O1-C20-C19 | 39.28 | 150.31 | 113.49 |
| 48 | 14 | 313 | A86 | O1-C20-C19 | 39.25 | 150.27 | 113.49 |
| 48 | 11 | 319 | A86 | O1-C20-C19 | 39.22 | 150.25 | 113.49 |
| 48 | 34 | 313 | A86 | O1-C20-C19 | 39.20 | 150.23 | 113.49 |
| 48 | 36 | 311 | A86 | O1-C20-C19 | 39.19 | 150.22 | 113.49 |
| 48 | 16 | 311 | A86 | O1-C20-C19 | 39.15 | 150.18 | 113.49 |
| 48 | 11 | 311 | A86 | O1-C20-C19 | 38.91 | 149.95 | 113.49 |
| 48 | 31 | 311 | A86 | O1-C20-C19 | 38.87 | 149.93 | 113.49 |
| 48 | 32 | 218 | A86 | O1-C20-C19 | 38.60 | 149.67 | 113.49 |
| 48 | 12 | 217 | A86 | O1-C20-C19 | 38.56 | 149.63 | 113.49 |
| 48 | 17 | 312 | A86 | O1-C20-C19 | 38.55 | 149.62 | 113.49 |
| 48 | 37 | 311 | A86 | O1-C20-C19 | 38.47 | 149.54 | 113.49 |
| 48 | 34 | 316 | A86 | O1-C20-C19 | 38.23 | 149.32 | 113.49 |
| 48 | 14 | 316 | A86 | O1-C20-C19 | 38.20 | 149.29 | 113.49 |
| 48 | 15 | 319 | A86 | O1-C20-C19 | 38.05 | 149.15 | 113.49 |
| 48 | 35 | 319 | A86 | O1-C20-C19 | 38.03 | 149.14 | 113.49 |
| 48 | 31 | 313 | A86 | O1-C20-C19 | 36.34 | 147.55 | 113.49 |
| 48 | 11 | 313 | A86 | O1-C20-C19 | 36.28 | 147.50 | 113.49 |
| 50 | 20 | 310 | DD6 | O1-C20-C19 | 25.22 | 137.13 | 113.49 |
| 50 | 40 | 212 | DD6 | O1-C20-C19 | 25.14 | 137.05 | 113.49 |
| 50 | 41 | 212 | DD6 | O1-C20-C19 | 25.06 | 136.97 | 113.49 |
| 50 | 21 | 212 | DD6 | O1-C20-C19 | 25.01 | 136.93 | 113.49 |
| 50 | 21 | 216 | DD6 | O1-C20-C19 | 24.76 | 136.69 | 113.49 |
| 50 | 41 | 216 | DD6 | O1-C20-C19 | 24.72 | 136.66 | 113.49 |
| 50 | 40 | 214 | DD6 | O1-C20-C19 | 24.01 | 135.99 | 113.49 |
| 50 | 20 | 312 | DD6 | O1-C20-C19 | 23.98 | 135.97 | 113.49 |
| 50 | 16 | 312 | DD6 | O1-C20-C19 | 21.60 | 133.74 | 113.49 |
| 50 | 36 | 312 | DD6 | O1-C20-C19 | 21.51 | 133.65 | 113.49 |
| 50 | 19 | 312 | DD6 | O1-C20-C19 | 19.42 | 131.69 | 113.49 |
| 50 | 39 | 312 | DD6 | O1-C20-C19 | 19.40 | 131.67 | 113.49 |
| 50 | 20 | 310 | DD6 | C29-C30-C31 | -17.76 | 134.13 | 175.48 |
| 50 | 40 | 212 | DD6 | C29-C30-C31 | -17.74 | 134.17 | 175.48 |
| 50 | 39 | 312 | DD6 | C29-C30-C31 | -16.25 | 137.63 | 175.48 |
| 50 | 19 | 312 | DD6 | C29-C30-C31 | -16.23 | 137.69 | 175.48 |
| 50 | 21 | 212 | DD6 | C29-C30-C31 | -16.18 | 137.80 | 175.48 |
| 50 | 41 | 212 | DD6 | C29-C30-C31 | -16.18 | 137.80 | 175.48 |
| 50 | 40 | 214 | DD6 | C29-C30-C31 | -16.01 | 138.20 | 175.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 20 | 312 | DD6 | C29-C30-C31 | -16.00 | 138.23 | 175.48 |
| 50 | 36 | 312 | DD6 | C29-C30-C31 | -15.02 | 140.51 | 175.48 |
| 50 | 16 | 312 | DD6 | C29-C30-C31 | -15.02 | 140.52 | 175.48 |
| 48 | 20 | 311 | A86 | O1-C20-C21 | -14.39 | 98.97 | 115.05 |
| 48 | 40 | 213 | A86 | O1-C20-C21 | -14.34 | 99.02 | 115.05 |
| 50 | 21 | 216 | DD6 | C29-C30-C31 | -13.58 | 143.85 | 175.48 |
| 50 | 41 | 216 | DD6 | C29-C30-C31 | -13.57 | 143.89 | 175.48 |
| 48 | 19 | 313 | A86 | O1-C20-C21 | -13.28 | 100.21 | 115.05 |
| 48 | 40 | 211 | A86 | O1-C20-C21 | -12.94 | 100.58 | 115.05 |
| 48 | 20 | 309 | A86 | O1-C20-C21 | -12.93 | 100.59 | 115.05 |
| 48 | 14 | 314 | A86 | O1-C20-C21 | -12.79 | 100.75 | 115.05 |
| 48 | 34 | 314 | A86 | O1-C20-C21 | -12.72 | 100.83 | 115.05 |
| 48 | 41 | 215 | A86 | O1-C20-C21 | -12.56 | 101.01 | 115.05 |
| 48 | 21 | 215 | A86 | O1-C20-C21 | -12.50 | 101.08 | 115.05 |
| 50 | 20 | 310 | DD6 | C3-C2-C1 | -12.45 | 109.81 | 127.28 |
| 50 | 40 | 212 | DD6 | C3-C2-C1 | -12.45 | 109.82 | 127.28 |
| 48 | 31 | 314 | A86 | O1-C20-C21 | -12.40 | 101.19 | 115.05 |
| 48 | 11 | 314 | A86 | O1-C20-C21 | -12.38 | 101.22 | 115.05 |
| 48 | 39 | 313 | A86 | O1-C20-C21 | -12.37 | 101.23 | 115.05 |
| 48 | 13 | 313 | A86 | C21-C20-C19 | -12.32 | 100.40 | 114.24 |
| 48 | 41 | 214 | A86 | O1-C20-C21 | -12.30 | 101.30 | 115.05 |
| 48 | 21 | 214 | A86 | O1-C20-C21 | -12.29 | 101.31 | 115.05 |
| 48 | 33 | 313 | A86 | C21-C20-C19 | -12.29 | 100.43 | 114.24 |
| 48 | 17 | 314 | A86 | C21-C20-C19 | -12.23 | 100.50 | 114.24 |
| 48 | 18 | 214 | A86 | O1-C20-C21 | -12.22 | 101.39 | 115.05 |
| 48 | 38 | 214 | A86 | O1-C20-C21 | -12.21 | 101.40 | 115.05 |
| 48 | 37 | 313 | A86 | C21-C20-C19 | -12.07 | 100.69 | 114.24 |
| 48 | 41 | 211 | A86 | O1-C20-C21 | -11.96 | 101.69 | 115.05 |
| 48 | 17 | 310 | A86 | O1-C20-C21 | -11.94 | 101.71 | 115.05 |
| 48 | 21 | 211 | A86 | O1-C20-C21 | -11.93 | 101.71 | 115.05 |
| 48 | 15 | 314 | A86 | O1-C20-C21 | -11.88 | 101.77 | 115.05 |
| 48 | 37 | 309 | A86 | O1-C20-C21 | -11.84 | 101.82 | 115.05 |
| 48 | 33 | 314 | A86 | C21-C20-C19 | -11.82 | 100.97 | 114.24 |
| 48 | 37 | 312 | A86 | O1-C20-C21 | -11.80 | 101.86 | 115.05 |
| 48 | 37 | 313 | A86 | O1-C20-C21 | -11.75 | 101.91 | 115.05 |
| 48 | 13 | 314 | A86 | C21-C20-C19 | -11.75 | 101.05 | 114.24 |
| 48 | 17 | 313 | A86 | O1-C20-C21 | -11.73 | 101.93 | 115.05 |
| 47 | 40 | 204 | KC1 | CMA-C3A-C4A | -11.71 | 106.73 | 125.03 |
| 48 | 32 | 216 | A86 | O1-C20-C21 | -11.68 | 101.99 | 115.05 |
| 47 | 20 | 302 | KC1 | CMA-C3A-C4A | -11.67 | 106.80 | 125.03 |
| 48 | 12 | 215 | A86 | O1-C20-C21 | -11.63 | 102.06 | 115.05 |
| 48 | 17 | 314 | A86 | O1-C20-C21 | -11.63 | 102.06 | 115.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 14 | 309 | KC1 | C2A-C3A-C4A | -11.61 | 97.70 | 106.41 |
| 47 | 34 | 309 | KC1 | C2A-C3A-C4A | -11.55 | 97.74 | 106.41 |
| 48 | 35 | 314 | A86 | O1-C20-C21 | -11.54 | 102.15 | 115.05 |
| 48 | 11 | 311 | A86 | C21-C20-C19 | -11.50 | 101.32 | 114.24 |
| 48 | 13 | 314 | A86 | O1-C20-C21 | -11.50 | 102.20 | 115.05 |
| 48 | 31 | 311 | A86 | C21-C20-C19 | -11.49 | 101.34 | 114.24 |
| 48 | 33 | 314 | A86 | O1-C20-C21 | -11.48 | 102.21 | 115.05 |
| 48 | 12 | 216 | A86 | O1-C20-C21 | -11.47 | 102.22 | 115.05 |
| 48 | 32 | 217 | A86 | O1-C20-C21 | -11.47 | 102.23 | 115.05 |
| 48 | 32 | 214 | A86 | O1-C20-C21 | -11.45 | 102.26 | 115.05 |
| 48 | 12 | 213 | A86 | O1-C20-C21 | -11.43 | 102.27 | 115.05 |
| 48 | 18 | 212 | A86 | O1-C20-C21 | -11.42 | 102.29 | 115.05 |
| 50 | 20 | 312 | DD6 | C3-C2-C1 | -11.38 | 111.31 | 127.28 |
| 50 | 40 | 214 | DD6 | C3-C2-C1 | -11.38 | 111.32 | 127.28 |
| 48 | 35 | 314 | A86 | C21-C20-C19 | -11.38 | 101.46 | 114.24 |
| 48 | 34 | 311 | A86 | O1-C20-C21 | -11.37 | 102.34 | 115.05 |
| 48 | 38 | 212 | A86 | O1-C20-C21 | -11.36 | 102.36 | 115.05 |
| 48 | 15 | 315 | A86 | O1-C20-C21 | -11.35 | 102.36 | 115.05 |
| 47 | 14 | 304 | KC1 | CMA-C3A-C4A | -11.35 | 107.30 | 125.03 |
| 48 | 14 | 311 | A86 | O1-C20-C21 | -11.34 | 102.37 | 115.05 |
| 47 | 34 | 304 | KC1 | CMA-C3A-C4A | -11.31 | 107.36 | 125.03 |
| 50 | 20 | 310 | DD6 | C9-C10-C11 | -11.31 | 111.41 | 127.28 |
| 50 | 40 | 212 | DD6 | C9-C10-C11 | -11.28 | 111.45 | 127.28 |
| 47 | 41 | 207 | KC1 | CMA-C3A-C4A | -11.28 | 107.40 | 125.03 |
| 47 | 21 | 207 | KC1 | CMA-C3A-C4A | -11.28 | 107.41 | 125.03 |
| 48 | 21 | 213 | A86 | O1-C20-C21 | -11.23 | 102.50 | 115.05 |
| 48 | 41 | 213 | A86 | O1-C20-C21 | -11.22 | 102.51 | 115.05 |
| 48 | 32 | 215 | A86 | O1-C20-C21 | -11.21 | 102.52 | 115.05 |
| 48 | 12 | 214 | A86 | O1-C20-C21 | -11.19 | 102.55 | 115.05 |
| 48 | 35 | 315 | A86 | O1-C20-C21 | -11.15 | 102.58 | 115.05 |
| 48 | 40 | 201 | A86 | C33-C32-C31 | 11.12 | 120.02 | 109.21 |
| 48 | 39 | 313 | A86 | C21-C20-C19 | -11.11 | 101.77 | 114.24 |
| 48 | 13 | 313 | A86 | O1-C20-C21 | -11.10 | 102.64 | 115.05 |
| 48 | 33 | 313 | A86 | O1-C20-C21 | -11.09 | 102.65 | 115.05 |
| 48 | 16 | 313 | A86 | C33-C32-C31 | 11.09 | 119.99 | 109.21 |
| 50 | 20 | 310 | DD6 | C4-C5-C6 | -11.08 | 111.74 | 127.28 |
| 50 | 40 | 212 | DD6 | C4-C5-C6 | -11.06 | 111.77 | 127.28 |
| 48 | 40 | 201 | A86 | O1-C20-C21 | -11.02 | 102.73 | 115.05 |
| 50 | 21 | 216 | DD6 | C9-C10-C11 | -11.00 | 111.85 | 127.28 |
| 50 | 41 | 216 | DD6 | C9-C10-C11 | -11.00 | 111.85 | 127.28 |
| 48 | 18 | 213 | A86 | O1-C20-C21 | -11.00 | 102.76 | 115.05 |
| 48 | 16 | 313 | A86 | O1-C20-C21 | -10.98 | 102.77 | 115.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 14 | 315 | A86 | O1-C20-C21 | -10.97 | 102.79 | 115.05 |
| 47 | 15 | 309 | KC1 | C2A-C3A-C4A | -10.96 | 98.18 | 106.41 |
| 47 | 38 | 210 | KC1 | C2A-C3A-C4A | -10.95 | 98.19 | 106.41 |
| 48 | 32 | 203 | A86 | C21-C20-C19 | -10.95 | 101.94 | 114.24 |
| 47 | 18 | 210 | KC1 | C2A-C3A-C4A | -10.94 | 98.19 | 106.41 |
| 48 | 12 | 202 | A86 | C21-C20-C19 | -10.94 | 101.95 | 114.24 |
| 48 | 34 | 312 | A86 | O1-C20-C21 | -10.93 | 102.83 | 115.05 |
| 48 | 14 | 312 | A86 | O1-C20-C21 | -10.93 | 102.83 | 115.05 |
| 37 | 18 | 202 | CLA | C1D-ND-C4D | -10.92 | 98.65 | 106.31 |
| 48 | 38 | 213 | A86 | O1-C20-C21 | -10.92 | 102.84 | 115.05 |
| 47 | 11 | 309 | KC1 | C2A-C3A-C4A | -10.91 | 98.22 | 106.41 |
| 48 | 34 | 315 | A86 | O1-C20-C21 | -10.91 | 102.86 | 115.05 |
| 47 | 35 | 309 | KC1 | C2A-C3A-C4A | -10.90 | 98.23 | 106.41 |
| 47 | 17 | 308 | KC1 | C2A-C3A-C4A | -10.90 | 98.23 | 106.41 |
| 47 | 37 | 307 | KC1 | C2A-C3A-C4A | -10.88 | 98.24 | 106.41 |
| 48 | 14 | 311 | A86 | C21-C20-C19 | -10.87 | 102.03 | 114.24 |
| 48 | 34 | 311 | A86 | C21-C20-C19 | -10.87 | 102.03 | 114.24 |
| 47 | 31 | 309 | KC1 | C2A-C3A-C4A | -10.85 | 98.26 | 106.41 |
| 47 | 15 | 304 | KC1 | CMA-C3A-C4A | -10.84 | 108.10 | 125.03 |
| 48 | 13 | 312 | A86 | O1-C20-C21 | -10.83 | 102.95 | 115.05 |
| 48 | 17 | 315 | A86 | C21-C20-C19 | -10.82 | 102.08 | 114.24 |
| 48 | 37 | 309 | A86 | C21-C20-C19 | -10.79 | 102.12 | 114.24 |
| 48 | 37 | 314 | A86 | C21-C20-C19 | -10.79 | 102.12 | 114.24 |
| 48 | 35 | 311 | A86 | O1-C20-C21 | -10.79 | 102.99 | 115.05 |
| 48 | 15 | 311 | A86 | O1-C20-C21 | -10.78 | 103.00 | 115.05 |
| 48 | 33 | 312 | A86 | O1-C20-C21 | -10.76 | 103.02 | 115.05 |
| 48 | 17 | 310 | A86 | C21-C20-C19 | -10.76 | 102.15 | 114.24 |
| 48 | 13 | 315 | A86 | C21-C20-C19 | -10.76 | 102.16 | 114.24 |
| 47 | 39 | 308 | KC1 | CMA-C3A-C4A | -10.75 | 108.23 | 125.03 |
| 47 | 19 | 308 | KC1 | CMA-C3A-C4A | -10.75 | 108.24 | 125.03 |
| 48 | 13 | 311 | A86 | O1-C20-C21 | -10.74 | 103.05 | 115.05 |
| 48 | 33 | 311 | A86 | O1-C20-C21 | -10.74 | 103.05 | 115.05 |
| 48 | 33 | 315 | A86 | C21-C20-C19 | -10.73 | 102.19 | 114.24 |
| 48 | 16 | 313 | A86 | C21-C20-C19 | -10.69 | 102.23 | 114.24 |
| 47 | 35 | 304 | KC1 | CMA-C3A-C4A | -10.69 | 108.33 | 125.03 |
| 48 | 40 | 201 | A86 | C21-C20-C19 | -10.69 | 102.23 | 114.24 |
| 48 | 17 | 313 | A86 | C21-C20-C19 | -10.67 | 102.26 | 114.24 |
| 48 | 37 | 312 | A86 | C21-C20-C19 | -10.67 | 102.26 | 114.24 |
| 48 | 15 | 314 | A86 | C21-C20-C19 | -10.65 | 102.28 | 114.24 |
| 48 | 19 | 313 | A86 | C21-C20-C19 | -10.58 | 102.36 | 114.24 |
| 37 | D | 405 | CLA | C1D-ND-C4D | -10.55 | 98.91 | 106.31 |
| 47 | 16 | 304 | KC1 | CMA-C3A-C4A | -10.54 | 108.57 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 36 | 304 | KC1 | CMA-C3A-C4A | -10.52 | 108.59 | 125.03 |
| 48 | 17 | 311 | A86 | O1-C20-C21 | -10.48 | 103.33 | 115.05 |
| 48 | 17 | 320 | A86 | O1-C20-C21 | -10.48 | 103.33 | 115.05 |
| 48 | 21 | 213 | A86 | C21-C20-C19 | -10.48 | 102.47 | 114.24 |
| 48 | 38 | 215 | A86 | C21-C20-C19 | -10.47 | 102.48 | 114.24 |
| 47 | 15 | 302 | KC1 | CMA-C3A-C4A | -10.46 | 108.69 | 125.03 |
| 37 | d | 403 | CLA | C1D-ND-C4D | -10.45 | 98.98 | 106.31 |
| 48 | 34 | 315 | A86 | C21-C20-C19 | -10.44 | 102.51 | 114.24 |
| 48 | 41 | 213 | A86 | C21-C20-C19 | -10.44 | 102.52 | 114.24 |
| 48 | 14 | 315 | A86 | C21-C20-C19 | -10.42 | 102.54 | 114.24 |
| 47 | 35 | 302 | KC1 | CMA-C3A-C4A | -10.39 | 108.80 | 125.03 |
| 48 | 17 | 313 | A86 | C33-C32-C31 | 10.38 | 119.30 | 109.21 |
| 48 | 32 | 221 | A86 | O1-C20-C21 | -10.34 | 103.49 | 115.05 |
| 48 | 37 | 312 | A86 | C33-C32-C31 | 10.33 | 119.25 | 109.21 |
| 48 | 37 | 319 | A86 | O1-C20-C21 | -10.33 | 103.51 | 115.05 |
| 48 | 12 | 220 | A86 | O1-C20-C21 | -10.32 | 103.51 | 115.05 |
| 48 | 19 | 311 | A86 | O1-C20-C21 | -10.32 | 103.52 | 115.05 |
| 47 | 40 | 204 | KC1 | C2A-C3A-C4A | -10.31 | 98.67 | 106.41 |
| 48 | 11 | 315 | A86 | O1-C20-C21 | -10.30 | 103.54 | 115.05 |
| 47 | 20 | 302 | KC1 | C2A-C3A-C4A | -10.29 | 98.68 | 106.41 |
| 48 | 38 | 212 | A86 | C21-C20-C19 | -10.29 | 102.68 | 114.24 |
| 48 | 31 | 315 | A86 | O1-C20-C21 | -10.29 | 103.55 | 115.05 |
| 48 | 39 | 311 | A86 | O1-C20-C21 | -10.29 | 103.55 | 115.05 |
| 48 | 12 | 215 | A86 | C21-C20-C19 | -10.28 | 102.69 | 114.24 |
| 50 | 19 | 312 | DD6 | C9-C10-C11 | -10.27 | 112.88 | 127.28 |
| 48 | 32 | 221 | A86 | C21-C20-C19 | -10.27 | 102.71 | 114.24 |
| 50 | 20 | 312 | DD6 | C9-C10-C11 | -10.25 | 112.90 | 127.28 |
| 48 | 12 | 220 | A86 | C21-C20-C19 | -10.24 | 102.74 | 114.24 |
| 50 | 40 | 214 | DD6 | C9-C10-C11 | -10.24 | 112.92 | 127.28 |
| 48 | 21 | 214 | A86 | C21-C20-C19 | -10.23 | 102.75 | 114.24 |
| 48 | 40 | 211 | A86 | C21-C20-C19 | -10.22 | 102.76 | 114.24 |
| 48 | 20 | 309 | A86 | C21-C20-C19 | -10.22 | 102.76 | 114.24 |
| 50 | 39 | 312 | DD6 | C9-C10-C11 | -10.22 | 112.94 | 127.28 |
| 50 | 36 | 312 | DD6 | C3-C2-C1 | -10.21 | 112.96 | 127.28 |
| 48 | 15 | 312 | A86 | C21-C20-C19 | -10.21 | 102.77 | 114.24 |
| 48 | 35 | 312 | A86 | C21-C20-C19 | -10.20 | 102.78 | 114.24 |
| 48 | 41 | 214 | A86 | C21-C20-C19 | -10.20 | 102.78 | 114.24 |
| 48 | 18 | 213 | A86 | C21-C20-C19 | -10.20 | 102.78 | 114.24 |
| 48 | 32 | 216 | A86 | C21-C20-C19 | -10.20 | 102.79 | 114.24 |
| 50 | 16 | 312 | DD6 | C3-C2-C1 | -10.19 | 112.99 | 127.28 |
| 48 | 37 | 310 | A86 | O1-C20-C21 | -10.19 | 103.66 | 115.05 |
| 48 | 15 | 316 | A86 | C21-C20-C19 | -10.19 | 102.80 | 114.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 35 | 316 | A86 | C21-C20-C19 | -10.19 | 102.80 | 114.24 |
| 48 | 18 | 212 | A86 | C21-C20-C19 | -10.14 | 102.85 | 114.24 |
| 48 | 34 | 314 | A86 | C21-C20-C19 | -10.14 | 102.85 | 114.24 |
| 48 | 32 | 217 | A86 | C21-C20-C19 | -10.13 | 102.86 | 114.24 |
| 37 | 16 | 301 | CLA | C1D-ND-C4D | -10.13 | 99.21 | 106.31 |
| 48 | 14 | 314 | A86 | C21-C20-C19 | -10.13 | 102.87 | 114.24 |
| 48 | 39 | 311 | A86 | C21-C20-C19 | -10.12 | 102.87 | 114.24 |
| 48 | 12 | 216 | A86 | C21-C20-C19 | -10.12 | 102.88 | 114.24 |
| 48 | 33 | 311 | A86 | C21-C20-C19 | -10.10 | 102.90 | 114.24 |
| 48 | 19 | 311 | A86 | C21-C20-C19 | -10.10 | 102.90 | 114.24 |
| 47 | 33 | 302 | KC1 | C2A-C3A-C4A | -10.09 | 98.83 | 106.41 |
| 47 | 13 | 302 | KC1 | C2A-C3A-C4A | -10.08 | 98.84 | 106.41 |
| 48 | 13 | 311 | A86 | C21-C20-C19 | -10.08 | 102.92 | 114.24 |
| 48 | 15 | 312 | A86 | O1-C20-C21 | -10.05 | 103.81 | 115.05 |
| 37 | 15 | 301 | CLA | C1D-ND-C4D | -10.05 | 99.26 | 106.31 |
| 37 | 35 | 301 | CLA | C1D-ND-C4D | -10.05 | 99.26 | 106.31 |
| 37 | 36 | 301 | CLA | C1D-ND-C4D | -10.05 | 99.26 | 106.31 |
| 48 | 18 | 215 | A86 | C21-C20-C19 | -10.04 | 102.96 | 114.24 |
| 48 | 38 | 213 | A86 | C21-C20-C19 | -10.04 | 102.97 | 114.24 |
| 48 | 35 | 312 | A86 | O1-C20-C21 | -10.03 | 103.84 | 115.05 |
| 47 | 36 | 304 | KC1 | C2A-C3A-C4A | -10.01 | 98.89 | 106.41 |
| 47 | 16 | 304 | KC1 | C2A-C3A-C4A | -9.99 | 98.91 | 106.41 |
| 47 | 33 | 309 | KC1 | C2A-C3A-C4A | -9.99 | 98.91 | 106.41 |
| 48 | 33 | 312 | A86 | C21-C20-C19 | -9.99 | 103.02 | 114.24 |
| 47 | 13 | 309 | KC1 | C2A-C3A-C4A | -9.99 | 98.91 | 106.41 |
| 37 | 38 | 202 | CLA | C1D-ND-C4D | -9.98 | 99.31 | 106.31 |
| 47 | 13 | 304 | KC1 | C2A-C3A-C4A | -9.97 | 98.92 | 106.41 |
| 47 | 31 | 305 | KC1 | C2A-C3A-C4A | -9.97 | 98.93 | 106.41 |
| 48 | 13 | 312 | A86 | C21-C20-C19 | -9.97 | 103.05 | 114.24 |
| 48 | 12 | 217 | A86 | C21-C20-C19 | -9.97 | 103.05 | 114.24 |
| 48 | 21 | 215 | A86 | C21-C20-C19 | -9.95 | 103.06 | 114.24 |
| 48 | 41 | 215 | A86 | C21-C20-C19 | -9.95 | 103.06 | 114.24 |
| 47 | 11 | 304 | KC1 | C2A-C3A-C4A | -9.95 | 98.94 | 106.41 |
| 47 | 18 | 205 | KC1 | C2A-C3A-C4A | -9.95 | 98.94 | 106.41 |
| 47 | 38 | 205 | KC1 | C2A-C3A-C4A | -9.94 | 98.95 | 106.41 |
| 47 | 33 | 304 | KC1 | C2A-C3A-C4A | -9.93 | 98.96 | 106.41 |
| 48 | 11 | 312 | A86 | C21-C20-C19 | -9.92 | 103.09 | 114.24 |
| 48 | 14 | 313 | A86 | C21-C20-C19 | -9.92 | 103.10 | 114.24 |
| 48 | 32 | 218 | A86 | C21-C20-C19 | -9.92 | 103.10 | 114.24 |
| 48 | 31 | 312 | A86 | C21-C20-C19 | -9.92 | 103.10 | 114.24 |
| 37 | 19 | 304 | CLA | C1D-ND-C4D | -9.91 | 99.36 | 106.31 |
| 37 | 39 | 304 | CLA | C1D-ND-C4D | -9.90 | 99.36 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 34 | 313 | A86 | C21-C20-C19 | -9.90 | 103.12 | 114.24 |
| 47 | 21 | 203 | KC1 | C2A-C3A-C4A | -9.89 | 98.98 | 106.41 |
| 47 | 37 | 304 | KC1 | CMD-C2D-C1D | 9.89 | 140.48 | 125.42 |
| 47 | 12 | 211 | KC1 | C2A-C3A-C4A | -9.89 | 98.99 | 106.41 |
| 47 | 34 | 304 | KC1 | C2A-C3A-C4A | -9.88 | 98.99 | 106.41 |
| 48 | 15 | 311 | A86 | C21-C20-C19 | -9.88 | 103.15 | 114.24 |
| 47 | 14 | 304 | KC1 | C2A-C3A-C4A | -9.87 | 99.00 | 106.41 |
| 37 | 40 | 203 | CLA | C1D-ND-C4D | -9.87 | 99.39 | 106.31 |
| 47 | 32 | 209 | KC1 | C2A-C3A-C4A | -9.86 | 99.00 | 106.41 |
| 47 | 32 | 212 | KC1 | C2A-C3A-C4A | -9.86 | 99.01 | 106.41 |
| 47 | 40 | 206 | KC1 | C2A-C3A-C4A | -9.85 | 99.01 | 106.41 |
| 47 | 12 | 208 | KC1 | C2A-C3A-C4A | -9.85 | 99.01 | 106.41 |
| 48 | 11 | 312 | A86 | O1-C20-C21 | -9.85 | 104.04 | 115.05 |
| 47 | 41 | 203 | KC1 | C2A-C3A-C4A | -9.85 | 99.02 | 106.41 |
| 48 | 32 | 214 | A86 | C21-C20-C19 | -9.84 | 103.18 | 114.24 |
| 48 | 31 | 312 | A86 | O1-C20-C21 | -9.84 | 104.05 | 115.05 |
| 48 | 21 | 211 | A86 | C21-C20-C19 | -9.84 | 103.19 | 114.24 |
| 48 | 12 | 213 | A86 | C21-C20-C19 | -9.83 | 103.19 | 114.24 |
| 48 | 41 | 211 | A86 | C21-C20-C19 | -9.83 | 103.20 | 114.24 |
| 47 | 36 | 308 | KC1 | C2A-C3A-C4A | -9.82 | 99.04 | 106.41 |
| 37 | 19 | 305 | CLA | C1D-ND-C4D | -9.82 | 99.42 | 106.31 |
| 48 | 16 | 311 | A86 | O1-C20-C21 | -9.82 | 104.08 | 115.05 |
| 47 | 15 | 306 | KC1 | C2A-C3A-C4A | -9.81 | 99.04 | 106.41 |
| 48 | 34 | 316 | A86 | C21-C20-C19 | -9.81 | 103.22 | 114.24 |
| 48 | 35 | 311 | A86 | C21-C20-C19 | -9.81 | 103.22 | 114.24 |
| 50 | 20 | 310 | DD6 | C12-C11-C10 | -9.80 | 106.94 | 122.82 |
| 48 | 36 | 311 | A86 | O1-C20-C21 | -9.80 | 104.10 | 115.05 |
| 37 | 41 | 210 | CLA | C1D-ND-C4D | -9.80 | 99.44 | 106.31 |
| 48 | 35 | 315 | A86 | C21-C20-C19 | -9.79 | 103.24 | 114.24 |
| 50 | 40 | 212 | DD6 | C12-C11-C10 | -9.79 | 106.96 | 122.82 |
| 37 | 20 | 301 | CLA | C1D-ND-C4D | -9.79 | 99.45 | 106.31 |
| 48 | 14 | 316 | A86 | C21-C20-C19 | -9.78 | 103.25 | 114.24 |
| 48 | 16 | 314 | A86 | C21-C20-C19 | -9.77 | 103.27 | 114.24 |
| 50 | 21 | 216 | DD6 | C4-C5-C6 | -9.76 | 113.59 | 127.28 |
| 50 | 20 | 312 | DD6 | C4-C5-C6 | -9.75 | 113.60 | 127.28 |
| 47 | 16 | 308 | KC1 | C2A-C3A-C4A | -9.75 | 99.09 | 106.41 |
| 37 | 21 | 210 | CLA | C1D-ND-C4D | -9.75 | 99.47 | 106.31 |
| 37 | 39 | 305 | CLA | C1D-ND-C4D | -9.75 | 99.47 | 106.31 |
| 50 | 41 | 216 | DD6 | C4-C5-C6 | -9.74 | 113.62 | 127.28 |
| 47 | 32 | 207 | KC1 | C2A-C3A-C4A | -9.74 | 99.10 | 106.41 |
| 50 | 41 | 212 | DD6 | C9-C10-C11 | -9.73 | 113.63 | 127.28 |
| 50 | 40 | 214 | DD6 | C4-C5-C6 | -9.73 | 113.63 | 127.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 36 | 313 | A86 | C21-C20-C19 | -9.73 | 103.31 | 114.24 |
| 48 | 15 | 315 | A86 | C21-C20-C19 | -9.72 | 103.32 | 114.24 |
| 50 | 21 | 212 | DD6 | C9-C10-C11 | -9.72 | 113.64 | 127.28 |
| 47 | 20 | 304 | KC1 | C2A-C3A-C4A | -9.72 | 99.11 | 106.41 |
| 47 | 12 | 206 | KC1 | C2A-C3A-C4A | -9.72 | 99.12 | 106.41 |
| 37 | 34 | 301 | CLA | C1D-ND-C4D | -9.71 | 99.50 | 106.31 |
| 37 | C | 513 | CLA | C1D-ND-C4D | -9.71 | 99.50 | 106.31 |
| 48 | 36 | 310 | A86 | C21-C20-C19 | -9.69 | 103.36 | 114.24 |
| 47 | 35 | 306 | KC1 | C2A-C3A-C4A | -9.69 | 99.14 | 106.41 |
| 47 | 31 | 307 | KC1 | CMA-C3A-C4A | -9.69 | 109.89 | 125.03 |
| 37 | c | 513 | CLA | C1D-ND-C4D | -9.69 | 99.52 | 106.31 |
| 37 | 18 | 201 | CLA | C1D-ND-C4D | -9.68 | 99.52 | 106.31 |
| 48 | 38 | 214 | A86 | C21-C20-C19 | -9.67 | 103.38 | 114.24 |
| 47 | 11 | 306 | KC1 | CMA-C3A-C4A | -9.67 | 109.92 | 125.03 |
| 47 | 13 | 302 | KC1 | CMA-C3A-C4A | -9.67 | 109.92 | 125.03 |
| 37 | 19 | 306 | CLA | C1D-ND-C4D | -9.67 | 99.53 | 106.31 |
| 37 | 39 | 306 | CLA | C1D-ND-C4D | -9.66 | 99.53 | 106.31 |
| 50 | 36 | 312 | DD6 | C13-C11-C10 | -9.66 | 103.82 | 119.01 |
| 47 | 33 | 302 | KC1 | CMA-C3A-C4A | -9.66 | 109.94 | 125.03 |
| 48 | 31 | 314 | A86 | C33-C32-C31 | 9.65 | 118.59 | 109.21 |
| 50 | 16 | 312 | DD6 | C13-C11-C10 | -9.65 | 103.83 | 119.01 |
| 37 | 16 | 309 | CLA | C1D-ND-C4D | -9.64 | 99.55 | 106.31 |
| 37 | 14 | 301 | CLA | C1D-ND-C4D | -9.64 | 99.55 | 106.31 |
| 48 | 16 | 310 | A86 | C21-C20-C19 | -9.63 | 103.42 | 114.24 |
| 48 | 11 | 314 | A86 | C21-C20-C19 | -9.63 | 103.42 | 114.24 |
| 48 | 31 | 314 | A86 | C21-C20-C19 | -9.62 | 103.44 | 114.24 |
| 48 | 17 | 312 | A86 | C21-C20-C19 | -9.61 | 103.44 | 114.24 |
| 47 | 15 | 302 | KC1 | C2A-C3A-C4A | -9.61 | 99.19 | 106.41 |
| 37 | 39 | 301 | CLA | C1D-ND-C4D | -9.61 | 99.57 | 106.31 |
| 50 | 21 | 216 | DD6 | C3-C2-C1 | -9.61 | 113.81 | 127.28 |
| 37 | 36 | 309 | CLA | C1D-ND-C4D | -9.60 | 99.57 | 106.31 |
| 47 | 31 | 303 | KC1 | C2A-C3A-C4A | -9.60 | 99.20 | 106.41 |
| 48 | 35 | 313 | A86 | C21-C20-C19 | -9.60 | 103.46 | 114.24 |
| 37 | a | 404 | CLA | C1D-ND-C4D | -9.60 | 99.58 | 106.31 |
| 37 | D | 401 | CLA | C1D-ND-C4D | -9.59 | 99.58 | 106.31 |
| 37 | b | 506 | CLA | C1D-ND-C4D | -9.58 | 99.59 | 106.31 |
| 50 | 41 | 216 | DD6 | C3-C2-C1 | -9.58 | 113.84 | 127.28 |
| 37 | 19 | 301 | CLA | C1D-ND-C4D | -9.57 | 99.60 | 106.31 |
| 48 | 15 | 319 | A86 | O1-C20-C21 | -9.57 | 104.36 | 115.05 |
| 48 | 35 | 319 | A86 | O1-C20-C21 | -9.57 | 104.36 | 115.05 |
| 37 | D | 406 | CLA | C1D-ND-C4D | -9.57 | 99.60 | 106.31 |
| 48 | 15 | 313 | A86 | C21-C20-C19 | -9.56 | 103.50 | 114.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 11 | 302 | KC1 | C2A-C3A-C4A | -9.56 | 99.23 | 106.41 |
| 48 | 37 | 319 | A86 | C21-C20-C19 | -9.55 | 103.51 | 114.24 |
| 47 | 16 | 302 | KC1 | C2A-C3A-C4A | -9.55 | 99.24 | 106.41 |
| 47 | 37 | 304 | KC1 | C2A-C3A-C4A | -9.55 | 99.24 | 106.41 |
| 37 | B | 506 | CLA | C1D-ND-C4D | -9.55 | 99.61 | 106.31 |
| 37 | A | 405 | CLA | C1D-ND-C4D | -9.54 | 99.62 | 106.31 |
| 37 | c | 504 | CLA | C1D-ND-C4D | -9.54 | 99.62 | 106.31 |
| 48 | 17 | 320 | A86 | C21-C20-C19 | -9.54 | 103.53 | 114.24 |
| 37 | a | 407 | CLA | C1D-ND-C4D | -9.53 | 99.62 | 106.31 |
| 47 | 36 | 302 | KC1 | C2A-C3A-C4A | -9.52 | 99.26 | 106.41 |
| 48 | 18 | 214 | A86 | C21-C20-C19 | -9.52 | 103.55 | 114.24 |
| 47 | 18 | 207 | KC1 | CMA-C3A-C4A | -9.51 | 110.17 | 125.03 |
| 48 | 18 | 215 | A86 | O1-C20-C21 | -9.51 | 104.42 | 115.05 |
| 50 | 41 | 212 | DD6 | C13-C11-C10 | -9.49 | 104.08 | 119.01 |
| 37 | d | 404 | CLA | C1D-ND-C4D | -9.49 | 99.65 | 106.31 |
| 47 | 34 | 306 | KC1 | CMA-C3A-C4A | -9.49 | 110.21 | 125.03 |
| 48 | 37 | 311 | A86 | C21-C20-C19 | -9.48 | 103.59 | 114.24 |
| 37 | D | 402 | CLA | C1D-ND-C4D | -9.48 | 99.66 | 106.31 |
| 47 | 14 | 306 | KC1 | CMA-C3A-C4A | -9.48 | 110.21 | 125.03 |
| 48 | 31 | 319 | A86 | C21-C20-C19 | -9.48 | 103.59 | 114.24 |
| 37 | d | 401 | CLA | C1D-ND-C4D | -9.48 | 99.66 | 106.31 |
| 37 | C | 504 | CLA | C1D-ND-C4D | -9.48 | 99.66 | 106.31 |
| 50 | 41 | 216 | DD6 | C12-C11-C10 | -9.47 | 107.47 | 122.82 |
| 37 | b | 505 | CLA | C1D-ND-C4D | -9.47 | 99.67 | 106.31 |
| 50 | 21 | 212 | DD6 | C13-C11-C10 | -9.47 | 104.11 | 119.01 |
| 48 | 11 | 319 | A86 | C21-C20-C19 | -9.47 | 103.60 | 114.24 |
| 37 | B | 505 | CLA | C1D-ND-C4D | -9.47 | 99.67 | 106.31 |
| 47 | 38 | 207 | KC1 | CMA-C3A-C4A | -9.47 | 110.24 | 125.03 |
| 47 | 20 | 305 | KC1 | C2A-C3A-C4A | -9.46 | 99.31 | 106.41 |
| 37 | 21 | 206 | CLA | C1D-ND-C4D | -9.46 | 99.68 | 106.31 |
| 50 | 21 | 216 | DD6 | C12-C11-C10 | -9.45 | 107.50 | 122.82 |
| 48 | 16 | 310 | A86 | O1-C20-C21 | -9.44 | 104.49 | 115.05 |
| 48 | 31 | 319 | A86 | O1-C20-C21 | -9.44 | 104.49 | 115.05 |
| 37 | 41 | 206 | CLA | C1D-ND-C4D | -9.44 | 99.69 | 106.31 |
| 47 | 17 | 305 | KC1 | C2A-C3A-C4A | -9.43 | 99.33 | 106.41 |
| 37 | b | 508 | CLA | C1D-ND-C4D | -9.43 | 99.69 | 106.31 |
| 37 | 32 | 208 | CLA | C1D-ND-C4D | -9.43 | 99.69 | 106.31 |
| 37 | 12 | 207 | CLA | C1D-ND-C4D | -9.43 | 99.69 | 106.31 |
| 48 | 36 | 310 | A86 | O1-C20-C21 | -9.43 | 104.51 | 115.05 |
| 37 | 38 | 201 | CLA | C1D-ND-C4D | -9.42 | 99.70 | 106.31 |
| 47 | 35 | 304 | KC1 | C2A-C3A-C4A | -9.42 | 99.34 | 106.41 |
| 47 | 15 | 304 | KC1 | C2A-C3A-C4A | -9.41 | 99.34 | 106.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 11 | 319 | A86 | O1-C20-C21 | -9.41 | 104.53 | 115.05 |
| 37 | c | 501 | CLA | C1D-ND-C4D | -9.41 | 99.71 | 106.31 |
| 37 | C | 501 | CLA | C1D-ND-C4D | -9.41 | 99.71 | 106.31 |
| 47 | 40 | 207 | KC1 | C2A-C3A-C4A | -9.40 | 99.35 | 106.41 |
| 48 | 12 | 216 | A86 | C33-C32-C31 | 9.40 | 118.34 | 109.21 |
| 48 | 32 | 217 | A86 | C33-C32-C31 | 9.40 | 118.34 | 109.21 |
| 50 | 16 | 312 | DD6 | C9-C10-C11 | -9.39 | 114.11 | 127.28 |
| 50 | 36 | 312 | DD6 | C9-C10-C11 | -9.39 | 114.11 | 127.28 |
| 37 | 39 | 303 | CLA | C1D-ND-C4D | -9.39 | 99.73 | 106.31 |
| 37 | B | 508 | CLA | C1D-ND-C4D | -9.39 | 99.73 | 106.31 |
| 37 | 37 | 301 | CLA | C1D-ND-C4D | -9.38 | 99.73 | 106.31 |
| 37 | 18 | 204 | CLA | C1D-ND-C4D | -9.38 | 99.73 | 106.31 |
| 48 | 11 | 314 | A86 | C33-C32-C31 | 9.38 | 118.32 | 109.21 |
| 47 | 35 | 302 | KC1 | C2A-C3A-C4A | -9.37 | 99.37 | 106.41 |
| 47 | 11 | 306 | KC1 | C2A-C3A-C4A | -9.37 | 99.38 | 106.41 |
| 47 | 36 | 305 | KC1 | CMA-C3A-C4A | -9.36 | 110.40 | 125.03 |
| 47 | 31 | 307 | KC1 | C2A-C3A-C4A | -9.36 | 99.38 | 106.41 |
| 37 | W | 101 | CLA | C1D-ND-C4D | -9.36 | 99.75 | 106.31 |
| 47 | 16 | 305 | KC1 | CMA-C3A-C4A | -9.35 | 110.42 | 125.03 |
| 37 | 38 | 204 | CLA | C1D-ND-C4D | -9.35 | 99.75 | 106.31 |
| 48 | 14 | 312 | A86 | C21-C20-C19 | -9.35 | 103.74 | 114.24 |
| 48 | 34 | 312 | A86 | C21-C20-C19 | -9.35 | 103.74 | 114.24 |
| 37 | 19 | 303 | CLA | C1D-ND-C4D | -9.35 | 99.75 | 106.31 |
| 37 | 41 | 208 | CLA | C1D-ND-C4D | -9.34 | 99.76 | 106.31 |
| 48 | 15 | 313 | A86 | O1-C20-C21 | -9.34 | 104.61 | 115.05 |
| 37 | 31 | 302 | CLA | C1D-ND-C4D | -9.34 | 99.76 | 106.31 |
| 47 | 21 | 207 | KC1 | C2A-C3A-C4A | -9.33 | 99.40 | 106.41 |
| 47 | 38 | 205 | KC1 | CMA-C3A-C4A | -9.33 | 110.45 | 125.03 |
| 47 | 13 | 306 | KC1 | C1D-ND-C4D | -9.33 | 99.77 | 106.31 |
| 48 | 12 | 217 | A86 | C4-C5-C6 | -9.32 | 114.20 | 127.28 |
| 47 | 18 | 205 | KC1 | CMA-C3A-C4A | -9.32 | 110.47 | 125.03 |
| 37 | C | 512 | CLA | C1D-ND-C4D | -9.32 | 99.78 | 106.31 |
| 47 | 40 | 207 | KC1 | CMA-C3A-C4A | -9.32 | 110.48 | 125.03 |
| 37 | 38 | 206 | CLA | C1D-ND-C4D | -9.31 | 99.78 | 106.31 |
| 37 | 36 | 307 | CLA | C1D-ND-C4D | -9.31 | 99.78 | 106.31 |
| 47 | 20 | 305 | KC1 | CMA-C3A-C4A | -9.31 | 110.49 | 125.03 |
| 47 | 38 | 207 | KC1 | C2A-C3A-C4A | -9.31 | 99.42 | 106.41 |
| 37 | 11 | 310 | CLA | C1D-ND-C4D | -9.31 | 99.78 | 106.31 |
| 48 | 32 | 218 | A86 | C4-C5-C6 | -9.31 | 114.23 | 127.28 |
| 47 | 41 | 207 | KC1 | C2A-C3A-C4A | -9.30 | 99.43 | 106.41 |
| 50 | 39 | 312 | DD6 | C3-C2-C1 | -9.30 | 114.24 | 127.28 |
| 37 | 16 | 307 | CLA | C1D-ND-C4D | -9.30 | 99.79 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 35 | 313 | A86 | O1-C20-C21 | -9.30 | 104.66 | 115.05 |
| 50 | 41 | 212 | DD6 | C12-C11-C10 | -9.28 | 107.78 | 122.82 |
| 37 | 11 | 301 | CLA | C1D-ND-C4D | -9.28 | 99.80 | 106.31 |
| 47 | 33 | 306 | KC1 | C1D-ND-C4D | -9.28 | 99.80 | 106.31 |
| 48 | 37 | 310 | A86 | C21-C20-C19 | -9.28 | 103.82 | 114.24 |
| 37 | 31 | 310 | CLA | C1D-ND-C4D | -9.27 | 99.80 | 106.31 |
| 50 | 21 | 212 | DD6 | C12-C11-C10 | -9.27 | 107.79 | 122.82 |
| 50 | 19 | 312 | DD6 | C3-C2-C1 | -9.27 | 114.28 | 127.28 |
| 47 | 18 | 207 | KC1 | C2A-C3A-C4A | -9.26 | 99.46 | 106.41 |
| 47 | 34 | 306 | KC1 | C2A-C3A-C4A | -9.26 | 99.46 | 106.41 |
| 37 | B | 513 | CLA | C1D-ND-C4D | -9.25 | 99.82 | 106.31 |
| 47 | 36 | 305 | KC1 | C2A-C3A-C4A | -9.25 | 99.47 | 106.41 |
| 47 | 16 | 305 | KC1 | C2A-C3A-C4A | -9.25 | 99.47 | 106.41 |
| 37 | 33 | 305 | CLA | C1D-ND-C4D | -9.24 | 99.83 | 106.31 |
| 37 | 21 | 208 | CLA | C1D-ND-C4D | -9.24 | 99.83 | 106.31 |
| 37 | C | 505 | CLA | C1D-ND-C4D | -9.24 | 99.83 | 106.31 |
| 48 | 12 | 214 | A86 | C21-C20-C19 | -9.23 | 103.87 | 114.24 |
| 37 | 18 | 211 | CLA | C1D-ND-C4D | -9.23 | 99.84 | 106.31 |
| 47 | 13 | 306 | KC1 | CMA-C3A-C4A | -9.23 | 110.62 | 125.03 |
| 47 | 18 | 205 | KC1 | C1D-ND-C4D | -9.22 | 99.84 | 106.31 |
| 47 | 33 | 306 | KC1 | CMA-C3A-C4A | -9.22 | 110.62 | 125.03 |
| 47 | 11 | 304 | KC1 | CMA-C3A-C4A | -9.22 | 110.62 | 125.03 |
| 37 | 41 | 205 | CLA | C1D-ND-C4D | -9.22 | 99.84 | 106.31 |
| 47 | 13 | 306 | KC1 | C2A-C3A-C4A | -9.22 | 99.49 | 106.41 |
| 47 | 31 | 305 | KC1 | CMA-C3A-C4A | -9.22 | 110.63 | 125.03 |
| 37 | c | 512 | CLA | C1D-ND-C4D | -9.21 | 99.85 | 106.31 |
| 37 | w | 101 | CLA | C1D-ND-C4D | -9.21 | 99.85 | 106.31 |
| 47 | 41 | 203 | KC1 | CMA-C3A-C4A | -9.21 | 110.64 | 125.03 |
| 48 | 32 | 215 | A86 | C21-C20-C19 | -9.21 | 103.90 | 114.24 |
| 47 | 14 | 306 | KC1 | C2A-C3A-C4A | -9.21 | 99.50 | 106.41 |
| 47 | 17 | 306 | KC1 | C2A-C3A-C4A | -9.20 | 99.51 | 106.41 |
| 37 | C | 503 | CLA | C1D-ND-C4D | -9.19 | 99.86 | 106.31 |
| 47 | 32 | 209 | KC1 | CMA-C3A-C4A | -9.19 | 110.67 | 125.03 |
| 37 | 21 | 205 | CLA | C1D-ND-C4D | -9.19 | 99.86 | 106.31 |
| 37 | 33 | 308 | CLA | C1D-ND-C4D | -9.19 | 99.86 | 106.31 |
| 37 | c | 503 | CLA | C1D-ND-C4D | -9.18 | 99.87 | 106.31 |
| 37 | c | 505 | CLA | C1D-ND-C4D | -9.18 | 99.87 | 106.31 |
| 47 | 21 | 203 | KC1 | CMA-C3A-C4A | -9.17 | 110.70 | 125.03 |
| 48 | 14 | 313 | A86 | O1-C20-C21 | -9.17 | 104.80 | 115.05 |
| 37 | B | 515 | CLA | C1D-ND-C4D | -9.17 | 99.88 | 106.31 |
| 47 | 33 | 306 | KC1 | C2A-C3A-C4A | -9.17 | 99.53 | 106.41 |
| 47 | 17 | 303 | KC1 | C2A-C3A-C4A | -9.17 | 99.53 | 106.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 513 | CLA | C1D-ND-C4D | -9.17 | 99.88 | 106.31 |
| 47 | 12 | 208 | KC1 | CMA-C3A-C4A | -9.16 | 110.72 | 125.03 |
| 37 | 34 | 310 | CLA | C1D-ND-C4D | -9.16 | 99.89 | 106.31 |
| 37 | B | 502 | CLA | C1D-ND-C4D | -9.16 | 99.89 | 106.31 |
| 47 | 38 | 205 | KC1 | C1D-ND-C4D | -9.16 | 99.89 | 106.31 |
| 37 | 13 | 305 | CLA | C1D-ND-C4D | -9.15 | 99.89 | 106.31 |
| 37 | 35 | 303 | CLA | C1D-ND-C4D | -9.15 | 99.89 | 106.31 |
| 37 | b | 515 | CLA | C1D-ND-C4D | -9.15 | 99.89 | 106.31 |
| 37 | 35 | 310 | CLA | C1D-ND-C4D | -9.14 | 99.90 | 106.31 |
| 37 | 14 | 310 | CLA | C1D-ND-C4D | -9.14 | 99.90 | 106.31 |
| 48 | 34 | 313 | A86 | O1-C20-C21 | -9.14 | 104.84 | 115.05 |
| 47 | 37 | 305 | KC1 | CMA-C3A-C4A | -9.14 | 110.76 | 125.03 |
| 47 | 11 | 302 | KC1 | CMA-C3A-C4A | -9.13 | 110.76 | 125.03 |
| 50 | 41 | 212 | DD6 | C4-C5-C6 | -9.13 | 114.47 | 127.28 |
| 50 | 21 | 212 | DD6 | C4-C5-C6 | -9.13 | 114.47 | 127.28 |
| 47 | 17 | 305 | KC1 | C1D-ND-C4D | -9.13 | 99.91 | 106.31 |
| 47 | 17 | 306 | KC1 | CMA-C3A-C4A | -9.13 | 110.77 | 125.03 |
| 47 | 37 | 305 | KC1 | C2A-C3A-C4A | -9.12 | 99.56 | 106.41 |
| 50 | 39 | 312 | DD6 | C4-C5-C6 | -9.12 | 114.48 | 127.28 |
| 37 | 21 | 204 | CLA | C1D-ND-C4D | -9.12 | 99.91 | 106.31 |
| 37 | 15 | 308 | CLA | C1D-ND-C4D | -9.12 | 99.91 | 106.31 |
| 48 | 35 | 316 | A86 | O1-C20-C21 | -9.12 | 104.86 | 115.05 |
| 37 | 41 | 204 | CLA | C1D-ND-C4D | -9.12 | 99.92 | 106.31 |
| 37 | 35 | 308 | CLA | C1D-ND-C4D | -9.11 | 99.92 | 106.31 |
| 37 | 13 | 308 | CLA | C1D-ND-C4D | -9.11 | 99.92 | 106.31 |
| 47 | 31 | 303 | KC1 | CMA-C3A-C4A | -9.10 | 110.81 | 125.03 |
| 37 | b | 502 | CLA | C1D-ND-C4D | -9.10 | 99.93 | 106.31 |
| 37 | 15 | 310 | CLA | C1D-ND-C4D | -9.10 | 99.93 | 106.31 |
| 37 | 41 | 209 | CLA | C1D-ND-C4D | -9.10 | 99.93 | 106.31 |
| 50 | 19 | 312 | DD6 | C4-C5-C6 | -9.10 | 114.52 | 127.28 |
| 37 | B | 511 | CLA | C1D-ND-C4D | -9.10 | 99.93 | 106.31 |
| 47 | 37 | 302 | KC1 | C2A-C3A-C4A | -9.09 | 99.58 | 106.41 |
| 37 | 15 | 303 | CLA | C1D-ND-C4D | -9.09 | 99.93 | 106.31 |
| 48 | 11 | 315 | A86 | C21-C20-C19 | -9.09 | 104.03 | 114.24 |
| 48 | 31 | 315 | A86 | C21-C20-C19 | -9.09 | 104.03 | 114.24 |
| 48 | 18 | 213 | A86 | C33-C32-C31 | 9.09 | 118.04 | 109.21 |
| 37 | 18 | 209 | CLA | C1D-ND-C4D | -9.09 | 99.94 | 106.31 |
| 47 | 12 | 206 | KC1 | C1D-ND-C4D | -9.08 | 99.94 | 106.31 |
| 48 | 15 | 316 | A86 | O1-C20-C21 | -9.08 | 104.91 | 115.05 |
| 37 | 21 | 209 | CLA | C1D-ND-C4D | -9.07 | 99.95 | 106.31 |
| 48 | 17 | 311 | A86 | C21-C20-C19 | -9.07 | 104.06 | 114.24 |
| 48 | 38 | 213 | A86 | C33-C32-C31 | 9.06 | 118.02 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 33 | 310 | CLA | C1D-ND-C4D | -9.06 | 99.96 | 106.31 |
| 37 | b | 511 | CLA | C1D-ND-C4D | -9.04 | 99.97 | 106.31 |
| 48 | 40 | 213 | A86 | C21-C20-C19 | -9.04 | 104.08 | 114.24 |
| 37 | 15 | 305 | CLA | C1D-ND-C4D | -9.03 | 99.97 | 106.31 |
| 37 | 14 | 305 | CLA | C1D-ND-C4D | -9.03 | 99.98 | 106.31 |
| 37 | 34 | 305 | CLA | C1D-ND-C4D | -9.03 | 99.98 | 106.31 |
| 48 | 34 | 316 | A86 | C4-C5-C6 | -9.03 | 114.62 | 127.28 |
| 37 | 14 | 308 | CLA | C1D-ND-C4D | -9.01 | 99.99 | 106.31 |
| 37 | 21 | 202 | CLA | C1D-ND-C4D | -9.01 | 99.99 | 106.31 |
| 37 | 38 | 209 | CLA | C1D-ND-C4D | -9.01 | 99.99 | 106.31 |
| 37 | 32 | 202 | CLA | C1D-ND-C4D | -9.01 | 99.99 | 106.31 |
| 37 | 13 | 310 | CLA | C1D-ND-C4D | -9.01 | 99.99 | 106.31 |
| 37 | 11 | 308 | CLA | C1D-ND-C4D | -9.01 | 99.99 | 106.31 |
| 47 | 32 | 207 | KC1 | C1D-ND-C4D | -9.00 | 100.00 | 106.31 |
| 37 | 11 | 307 | CLA | C1D-ND-C4D | -9.00 | 100.00 | 106.31 |
| 47 | 19 | 308 | KC1 | C2A-C3A-C4A | -9.00 | 99.65 | 106.41 |
| 48 | 20 | 311 | A86 | C21-C20-C19 | -9.00 | 104.13 | 114.24 |
| 48 | 14 | 316 | A86 | C4-C5-C6 | -9.00 | 114.66 | 127.28 |
| 47 | 39 | 308 | KC1 | C2A-C3A-C4A | -9.00 | 99.66 | 106.41 |
| 37 | 18 | 206 | CLA | C1D-ND-C4D | -8.99 | 100.00 | 106.31 |
| 37 | 16 | 303 | CLA | C1D-ND-C4D | -8.99 | 100.00 | 106.31 |
| 48 | 37 | 314 | A86 | O1-C20-C21 | -8.99 | 105.00 | 115.05 |
| 48 | 19 | 313 | A86 | C33-C32-C31 | 8.99 | 117.95 | 109.21 |
| 37 | 17 | 302 | CLA | C1D-ND-C4D | -8.99 | 100.00 | 106.31 |
| 48 | 38 | 215 | A86 | O1-C20-C21 | -8.99 | 105.00 | 115.05 |
| 48 | 39 | 313 | A86 | C33-C32-C31 | 8.99 | 117.95 | 109.21 |
| 48 | 17 | 315 | A86 | O1-C20-C21 | -8.98 | 105.01 | 115.05 |
| 47 | 35 | 306 | KC1 | C1D-ND-C4D | -8.97 | 100.02 | 106.31 |
| 37 | 34 | 308 | CLA | C1D-ND-C4D | -8.97 | 100.02 | 106.31 |
| 37 | 36 | 303 | CLA | C1D-ND-C4D | -8.97 | 100.02 | 106.31 |
| 37 | B | 516 | CLA | C1D-ND-C4D | -8.96 | 100.02 | 106.31 |
| 37 | b | 516 | CLA | C1D-ND-C4D | -8.96 | 100.02 | 106.31 |
| 37 | 12 | 210 | CLA | C1D-ND-C4D | -8.96 | 100.03 | 106.31 |
| 37 | 32 | 211 | CLA | C1D-ND-C4D | -8.96 | 100.03 | 106.31 |
| 37 | 13 | 301 | CLA | C1D-ND-C4D | -8.95 | 100.03 | 106.31 |
| 37 | 31 | 308 | CLA | C1D-ND-C4D | -8.95 | 100.03 | 106.31 |
| 37 | 33 | 301 | CLA | C1D-ND-C4D | -8.95 | 100.03 | 106.31 |
| 47 | 13 | 304 | KC1 | CMA-C3A-C4A | -8.95 | 111.05 | 125.03 |
| 47 | 14 | 304 | KC1 | C1D-ND-C4D | -8.95 | 100.03 | 106.31 |
| 47 | 31 | 307 | KC1 | C1D-ND-C4D | -8.93 | 100.04 | 106.31 |
| 47 | 34 | 304 | KC1 | C1D-ND-C4D | -8.93 | 100.05 | 106.31 |
| 47 | 33 | 304 | KC1 | CMA-C3A-C4A | -8.93 | 111.08 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 20 | 307 | CLA | C1D-ND-C4D | -8.92 | 100.05 | 106.31 |
| 37 | 41 | 202 | CLA | C1D-ND-C4D | -8.92 | 100.05 | 106.31 |
| 47 | 11 | 306 | KC1 | C1D-ND-C4D | -8.89 | 100.07 | 106.31 |
| 48 | 36 | 311 | A86 | C21-C20-C19 | -8.89 | 104.26 | 114.24 |
| 37 | b | 510 | CLA | C1D-ND-C4D | -8.88 | 100.08 | 106.31 |
| 47 | 15 | 306 | KC1 | C1D-ND-C4D | -8.88 | 100.08 | 106.31 |
| 50 | 41 | 216 | DD6 | C37-C36-C31 | -8.88 | 107.55 | 124.16 |
| 37 | 40 | 209 | CLA | C1D-ND-C4D | -8.88 | 100.08 | 106.31 |
| 50 | 36 | 312 | DD6 | C4-C5-C6 | -8.88 | 114.82 | 127.28 |
| 50 | 21 | 216 | DD6 | C37-C36-C31 | -8.87 | 107.57 | 124.16 |
| 47 | 37 | 304 | KC1 | C1D-ND-C4D | -8.87 | 100.09 | 106.31 |
| 47 | 19 | 308 | KC1 | C1D-ND-C4D | -8.87 | 100.09 | 106.31 |
| 50 | 16 | 312 | DD6 | C4-C5-C6 | -8.87 | 114.84 | 127.28 |
| 47 | 35 | 306 | KC1 | CMA-C3A-C4A | -8.86 | 111.20 | 125.03 |
| 37 | 14 | 303 | CLA | C1D-ND-C4D | -8.85 | 100.10 | 106.31 |
| 37 | b | 512 | CLA | C1D-ND-C4D | -8.84 | 100.11 | 106.31 |
| 47 | 39 | 308 | KC1 | C1D-ND-C4D | -8.84 | 100.11 | 106.31 |
| 37 | 38 | 211 | CLA | C1D-ND-C4D | -8.84 | 100.11 | 106.31 |
| 37 | 39 | 302 | CLA | C1D-ND-C4D | -8.84 | 100.11 | 106.31 |
| 47 | 20 | 302 | KC1 | C1D-ND-C4D | -8.84 | 100.11 | 106.31 |
| 37 | B | 510 | CLA | C1D-ND-C4D | -8.83 | 100.11 | 106.31 |
| 37 | B | 512 | CLA | C1D-ND-C4D | -8.83 | 100.11 | 106.31 |
| 47 | 40 | 204 | KC1 | C1D-ND-C4D | -8.83 | 100.11 | 106.31 |
| 37 | 37 | 303 | CLA | C1D-ND-C4D | -8.83 | 100.12 | 106.31 |
| 48 | 15 | 316 | A86 | C4-C5-C6 | -8.83 | 114.90 | 127.28 |
| 47 | 13 | 304 | KC1 | C1D-ND-C4D | -8.82 | 100.12 | 106.31 |
| 47 | 13 | 309 | KC1 | CMA-C3A-C4A | -8.82 | 111.25 | 125.03 |
| 48 | 16 | 311 | A86 | C21-C20-C19 | -8.82 | 104.34 | 114.24 |
| 48 | 36 | 313 | A86 | O1-C20-C21 | -8.81 | 105.20 | 115.05 |
| 47 | 34 | 306 | KC1 | C1D-ND-C4D | -8.81 | 100.13 | 106.31 |
| 37 | 19 | 302 | CLA | C1D-ND-C4D | -8.81 | 100.13 | 106.31 |
| 47 | 33 | 304 | KC1 | C1D-ND-C4D | -8.81 | 100.13 | 106.31 |
| 48 | 37 | 311 | A86 | O1-C20-C21 | -8.80 | 105.21 | 115.05 |
| 50 | 40 | 214 | DD6 | C37-C36-C31 | -8.80 | 107.70 | 124.16 |
| 47 | 33 | 309 | KC1 | CMA-C3A-C4A | -8.80 | 111.28 | 125.03 |
| 37 | 35 | 305 | CLA | C1D-ND-C4D | -8.80 | 100.14 | 106.31 |
| 47 | 17 | 305 | KC1 | CMA-C3A-C4A | -8.80 | 111.28 | 125.03 |
| 50 | 40 | 214 | DD6 | C12-C11-C10 | -8.80 | 108.56 | 122.82 |
| 47 | 15 | 306 | KC1 | CMA-C3A-C4A | -8.80 | 111.29 | 125.03 |
| 50 | 20 | 312 | DD6 | C37-C36-C31 | -8.79 | 107.72 | 124.16 |
| 50 | 20 | 312 | DD6 | C12-C11-C10 | -8.79 | 108.58 | 122.82 |
| 37 | 17 | 304 | CLA | C1D-ND-C4D | -8.79 | 100.15 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 20 | 306 | CLA | C1D-ND-C4D | -8.79 | 100.15 | 106.31 |
| 48 | 16 | 311 | A86 | C33-C32-C31 | 8.79 | 117.75 | 109.21 |
| 37 | 40 | 208 | CLA | C1D-ND-C4D | -8.78 | 100.15 | 106.31 |
| 37 | 34 | 303 | CLA | C1D-ND-C4D | -8.78 | 100.15 | 106.31 |
| 37 | 39 | 307 | CLA | C1D-ND-C4D | -8.78 | 100.15 | 106.31 |
| 47 | 37 | 304 | KC1 | CMA-C3A-C4A | -8.77 | 111.33 | 125.03 |
| 37 | 37 | 308 | CLA | C1D-ND-C4D | -8.77 | 100.16 | 106.31 |
| 47 | 14 | 306 | KC1 | C1D-ND-C4D | -8.77 | 100.16 | 106.31 |
| 37 | 17 | 307 | CLA | C1D-ND-C4D | -8.76 | 100.16 | 106.31 |
| 48 | 17 | 312 | A86 | O1-C20-C21 | -8.76 | 105.25 | 115.05 |
| 47 | 16 | 304 | KC1 | C1D-ND-C4D | -8.76 | 100.16 | 106.31 |
| 37 | c | 508 | CLA | C1D-ND-C4D | -8.76 | 100.17 | 106.31 |
| 48 | 36 | 311 | A86 | C33-C32-C31 | 8.76 | 117.72 | 109.21 |
| 48 | 33 | 314 | A86 | C33-C32-C31 | 8.75 | 117.72 | 109.21 |
| 47 | 38 | 210 | KC1 | C1D-ND-C4D | -8.75 | 100.17 | 106.31 |
| 47 | 40 | 206 | KC1 | C1D-ND-C4D | -8.74 | 100.18 | 106.31 |
| 37 | 32 | 213 | CLA | C1D-ND-C4D | -8.74 | 100.18 | 106.31 |
| 48 | 35 | 316 | A86 | C4-C5-C6 | -8.74 | 115.02 | 127.28 |
| 37 | 17 | 309 | CLA | C1D-ND-C4D | -8.74 | 100.18 | 106.31 |
| 48 | 20 | 311 | A86 | C33-C32-C31 | 8.73 | 117.70 | 109.21 |
| 48 | 40 | 213 | A86 | C33-C32-C31 | 8.73 | 117.70 | 109.21 |
| 37 | 38 | 204 | CLA | CMD-C2D-C1D | 8.73 | 140.11 | 124.73 |
| 48 | 13 | 314 | A86 | C33-C32-C31 | 8.73 | 117.70 | 109.21 |
| 48 | 16 | 314 | A86 | O1-C20-C21 | -8.73 | 105.29 | 115.05 |
| 37 | 18 | 204 | CLA | CMD-C2D-C1D | 8.72 | 140.08 | 124.73 |
| 47 | 35 | 302 | KC1 | C1D-ND-C4D | -8.71 | 100.20 | 106.31 |
| 37 | 19 | 309 | CLA | C1D-ND-C4D | -8.71 | 100.20 | 106.31 |
| 47 | 41 | 207 | KC1 | C1D-ND-C4D | -8.71 | 100.20 | 106.31 |
| 47 | 20 | 304 | KC1 | C1D-ND-C4D | -8.71 | 100.20 | 106.31 |
| 47 | 36 | 304 | KC1 | C1D-ND-C4D | -8.71 | 100.20 | 106.31 |
| 50 | 39 | 312 | DD6 | C37-C36-C31 | -8.70 | 107.89 | 124.16 |
| 37 | C | 508 | CLA | C1D-ND-C4D | -8.70 | 100.21 | 106.31 |
| 48 | 35 | 311 | A86 | C33-C32-C31 | 8.69 | 117.66 | 109.21 |
| 37 | 19 | 307 | CLA | C1D-ND-C4D | -8.69 | 100.21 | 106.31 |
| 47 | 17 | 308 | KC1 | C1D-ND-C4D | -8.69 | 100.21 | 106.31 |
| 37 | 31 | 306 | CLA | C1D-ND-C4D | -8.69 | 100.22 | 106.31 |
| 37 | 39 | 309 | CLA | C1D-ND-C4D | -8.69 | 100.22 | 106.31 |
| 37 | 12 | 212 | CLA | C1D-ND-C4D | -8.68 | 100.22 | 106.31 |
| 37 | 37 | 306 | CLA | C1D-ND-C4D | -8.68 | 100.22 | 106.31 |
| 47 | 21 | 207 | KC1 | C1D-ND-C4D | -8.68 | 100.22 | 106.31 |
| 37 | B | 514 | CLA | C1D-ND-C4D | -8.68 | 100.22 | 106.31 |
| 37 | 20 | 308 | CLA | C1D-ND-C4D | -8.68 | 100.22 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 19 | 312 | DD6 | C37-C36-C31 | -8.67 | 107.94 | 124.16 |
| 50 | 16 | 312 | DD6 | C12-C11-C10 | -8.66 | 108.78 | 122.82 |
| 50 | 21 | 212 | DD6 | C7-C6-C5 | -8.66 | 108.78 | 122.82 |
| 50 | 41 | 212 | DD6 | C7-C6-C5 | -8.66 | 108.78 | 122.82 |
| 50 | 36 | 312 | DD6 | C12-C11-C10 | -8.66 | 108.78 | 122.82 |
| 37 | 38 | 208 | CLA | C1D-ND-C4D | -8.65 | 100.24 | 106.31 |
| 37 | 32 | 204 | CLA | C1D-ND-C4D | -8.64 | 100.25 | 106.31 |
| 47 | 37 | 307 | KC1 | C1D-ND-C4D | -8.64 | 100.25 | 106.31 |
| 50 | 16 | 312 | DD6 | C37-C36-C31 | -8.64 | 108.00 | 124.16 |
| 37 | 12 | 203 | CLA | C1D-ND-C4D | -8.64 | 100.25 | 106.31 |
| 37 | 15 | 307 | CLA | C1D-ND-C4D | -8.64 | 100.25 | 106.31 |
| 37 | 40 | 210 | CLA | C1D-ND-C4D | -8.63 | 100.26 | 106.31 |
| 37 | 11 | 305 | CLA | C1D-ND-C4D | -8.63 | 100.26 | 106.31 |
| 37 | b | 514 | CLA | C1D-ND-C4D | -8.62 | 100.26 | 106.31 |
| 48 | 16 | 314 | A86 | C4-C5-C6 | -8.62 | 115.19 | 127.28 |
| 37 | c | 511 | CLA | C1D-ND-C4D | -8.62 | 100.26 | 106.31 |
| 48 | 33 | 313 | A86 | C33-C32-C31 | 8.62 | 117.58 | 109.21 |
| 37 | a | 403 | CLA | C1D-ND-C4D | -8.62 | 100.27 | 106.31 |
| 50 | 36 | 312 | DD6 | C37-C36-C31 | -8.61 | 108.06 | 124.16 |
| 37 | 18 | 208 | CLA | C1D-ND-C4D | -8.61 | 100.27 | 106.31 |
| 47 | 31 | 303 | KC1 | C1D-ND-C4D | -8.61 | 100.27 | 106.31 |
| 47 | 14 | 309 | KC1 | C1D-ND-C4D | -8.61 | 100.27 | 106.31 |
| 37 | Z | 101 | CLA | C1D-ND-C4D | -8.61 | 100.27 | 106.31 |
| 48 | 36 | 313 | A86 | C4-C5-C6 | -8.61 | 115.21 | 127.28 |
| 37 | C | 511 | CLA | C1D-ND-C4D | -8.60 | 100.28 | 106.31 |
| 47 | 18 | 210 | KC1 | C1D-ND-C4D | -8.60 | 100.28 | 106.31 |
| 37 | c | 502 | CLA | C1D-ND-C4D | -8.60 | 100.28 | 106.31 |
| 47 | 34 | 309 | KC1 | C1D-ND-C4D | -8.59 | 100.28 | 106.31 |
| 47 | 17 | 305 | KC1 | CMD-C2D-C1D | 8.59 | 138.50 | 125.42 |
| 37 | 32 | 206 | CLA | C1D-ND-C4D | -8.59 | 100.28 | 106.31 |
| 37 | b | 509 | CLA | C1D-ND-C4D | -8.59 | 100.29 | 106.31 |
| 47 | 12 | 208 | KC1 | C1D-ND-C4D | -8.59 | 100.29 | 106.31 |
| 37 | A | 403 | CLA | C1D-ND-C4D | -8.58 | 100.29 | 106.31 |
| 37 | B | 509 | CLA | C1D-ND-C4D | -8.58 | 100.29 | 106.31 |
| 37 | 35 | 307 | CLA | C1D-ND-C4D | -8.57 | 100.30 | 106.31 |
| 47 | 16 | 308 | KC1 | C1D-ND-C4D | -8.57 | 100.30 | 106.31 |
| 48 | 13 | 313 | A86 | C33-C32-C31 | 8.56 | 117.53 | 109.21 |
| 50 | 41 | 216 | DD6 | C7-C6-C5 | -8.56 | 108.95 | 122.82 |
| 37 | 20 | 303 | CLA | C1D-ND-C4D | -8.56 | 100.31 | 106.31 |
| 37 | c | 509 | CLA | C1D-ND-C4D | -8.56 | 100.31 | 106.31 |
| 37 | z | 101 | CLA | C1D-ND-C4D | -8.55 | 100.31 | 106.31 |
| 50 | 21 | 216 | DD6 | C7-C6-C5 | -8.55 | 108.96 | 122.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 502 | CLA | C1D-ND-C4D | -8.55 | 100.31 | 106.31 |
| 37 | 40 | 205 | CLA | C1D-ND-C4D | -8.55 | 100.31 | 106.31 |
| 37 | B | 501 | CLA | C1D-ND-C4D | -8.53 | 100.32 | 106.31 |
| 37 | C | 509 | CLA | C1D-ND-C4D | -8.53 | 100.32 | 106.31 |
| 47 | 11 | 302 | KC1 | C1D-ND-C4D | -8.53 | 100.33 | 106.31 |
| 47 | 32 | 212 | KC1 | C1D-ND-C4D | -8.53 | 100.33 | 106.31 |
| 48 | 12 | 213 | A86 | C33-C32-C31 | 8.52 | 117.49 | 109.21 |
| 37 | b | 501 | CLA | C1D-ND-C4D | -8.51 | 100.34 | 106.31 |
| 37 | 12 | 205 | CLA | C1D-ND-C4D | -8.51 | 100.34 | 106.31 |
| 47 | 35 | 304 | KC1 | C1D-ND-C4D | -8.50 | 100.35 | 106.31 |
| 47 | 15 | 302 | KC1 | C1D-ND-C4D | -8.49 | 100.35 | 106.31 |
| 47 | 32 | 209 | KC1 | C1D-ND-C4D | -8.49 | 100.36 | 106.31 |
| 47 | 38 | 207 | KC1 | C1D-ND-C4D | -8.48 | 100.36 | 106.31 |
| 47 | 12 | 211 | KC1 | C1D-ND-C4D | -8.47 | 100.37 | 106.31 |
| 47 | 18 | 207 | KC1 | C1D-ND-C4D | -8.47 | 100.37 | 106.31 |
| 48 | 18 | 215 | A86 | C4-C5-C6 | -8.47 | 115.40 | 127.28 |
| 48 | 32 | 214 | A86 | C33-C32-C31 | 8.47 | 117.44 | 109.21 |
| 37 | z | 102 | CLA | C1D-ND-C4D | -8.47 | 100.37 | 106.31 |
| 47 | 36 | 308 | KC1 | C1D-ND-C4D | -8.47 | 100.37 | 106.31 |
| 37 | B | 507 | CLA | C1D-ND-C4D | -8.46 | 100.37 | 106.31 |
| 37 | 33 | 303 | CLA | C1D-ND-C4D | -8.46 | 100.38 | 106.31 |
| 37 | B | 503 | CLA | C1D-ND-C4D | -8.46 | 100.38 | 106.31 |
| 50 | 40 | 212 | DD6 | C-C1-C2 | -8.45 | 109.12 | 122.82 |
| 37 | 38 | 203 | CLA | C1D-ND-C4D | -8.45 | 100.38 | 106.31 |
| 48 | 12 | 202 | A86 | O1-C20-C21 | -8.45 | 105.60 | 115.05 |
| 50 | 20 | 310 | DD6 | C-C1-C2 | -8.45 | 109.13 | 122.82 |
| 37 | 39 | 310 | CLA | C1D-ND-C4D | -8.44 | 100.39 | 106.31 |
| 37 | 34 | 302 | CLA | C1D-ND-C4D | -8.44 | 100.39 | 106.31 |
| 50 | 20 | 310 | DD6 | C13-C11-C10 | -8.43 | 105.75 | 119.01 |
| 37 | 19 | 310 | CLA | C1D-ND-C4D | -8.43 | 100.40 | 106.31 |
| 48 | 13 | 315 | A86 | O1-C20-C21 | -8.42 | 105.63 | 115.05 |
| 48 | 16 | 313 | A86 | C4-C5-C6 | -8.42 | 115.47 | 127.28 |
| 48 | 32 | 203 | A86 | O1-C20-C21 | -8.42 | 105.64 | 115.05 |
| 37 | C | 510 | CLA | C1D-ND-C4D | -8.42 | 100.40 | 106.31 |
| 48 | 17 | 310 | A86 | C33-C32-C31 | 8.42 | 117.39 | 109.21 |
| 48 | 32 | 218 | A86 | O1-C20-C21 | -8.41 | 105.65 | 115.05 |
| 50 | 40 | 212 | DD6 | C13-C11-C10 | -8.40 | 105.79 | 119.01 |
| 48 | 38 | 215 | A86 | C4-C5-C6 | -8.40 | 115.49 | 127.28 |
| 37 | b | 507 | CLA | C1D-ND-C4D | -8.40 | 100.42 | 106.31 |
| 37 | Z | 102 | CLA | C1D-ND-C4D | -8.40 | 100.42 | 106.31 |
| 48 | 33 | 315 | A86 | O1-C20-C21 | -8.40 | 105.66 | 115.05 |
| 37 | 14 | 302 | CLA | C1D-ND-C4D | -8.40 | 100.42 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 36 | 306 | CLA | C1D-ND-C4D | -8.40 | 100.42 | 106.31 |
| 37 | b | 503 | CLA | C1D-ND-C4D | -8.40 | 100.42 | 106.31 |
| 48 | 37 | 309 | A86 | C33-C32-C31 | 8.39 | 117.36 | 109.21 |
| 47 | 15 | 304 | KC1 | C1D-ND-C4D | -8.39 | 100.43 | 106.31 |
| 50 | 21 | 212 | DD6 | C3-C2-C1 | -8.39 | 115.52 | 127.28 |
| 37 | 11 | 303 | CLA | C1D-ND-C4D | -8.38 | 100.43 | 106.31 |
| 48 | 40 | 201 | A86 | C4-C5-C6 | -8.38 | 115.53 | 127.28 |
| 37 | c | 510 | CLA | C1D-ND-C4D | -8.38 | 100.43 | 106.31 |
| 47 | 37 | 302 | KC1 | CMA-C3A-C4A | -8.38 | 111.95 | 125.03 |
| 37 | 16 | 306 | CLA | C1D-ND-C4D | -8.36 | 100.45 | 106.31 |
| 48 | 12 | 217 | A86 | O1-C20-C21 | -8.36 | 105.71 | 115.05 |
| 48 | 18 | 213 | A86 | C4-C5-C6 | -8.36 | 115.56 | 127.28 |
| 48 | 34 | 311 | A86 | C33-C32-C31 | 8.35 | 117.33 | 109.21 |
| 50 | 41 | 212 | DD6 | C3-C2-C1 | -8.35 | 115.57 | 127.28 |
| 37 | 18 | 203 | CLA | C1D-ND-C4D | -8.35 | 100.45 | 106.31 |
| 47 | 11 | 309 | KC1 | C1D-ND-C4D | -8.34 | 100.46 | 106.31 |
| 47 | 13 | 302 | KC1 | C1D-ND-C4D | -8.34 | 100.46 | 106.31 |
| 47 | 33 | 302 | KC1 | C1D-ND-C4D | -8.34 | 100.46 | 106.31 |
| 47 | 17 | 303 | KC1 | CMA-C3A-C4A | -8.33 | 112.01 | 125.03 |
| 47 | 36 | 305 | KC1 | C1D-ND-C4D | -8.33 | 100.47 | 106.31 |
| 48 | 14 | 311 | A86 | C33-C32-C31 | 8.33 | 117.31 | 109.21 |
| 37 | 13 | 303 | CLA | C1D-ND-C4D | -8.32 | 100.47 | 106.31 |
| 37 | c | 506 | CLA | C1D-ND-C4D | -8.31 | 100.48 | 106.31 |
| 37 | 31 | 304 | CLA | C1D-ND-C4D | -8.31 | 100.48 | 106.31 |
| 47 | 16 | 305 | KC1 | C1D-ND-C4D | -8.31 | 100.48 | 106.31 |
| 47 | 35 | 309 | KC1 | C1D-ND-C4D | -8.31 | 100.48 | 106.31 |
| 37 | B | 524 | CLA | C1D-ND-C4D | -8.30 | 100.49 | 106.31 |
| 47 | 15 | 309 | KC1 | C1D-ND-C4D | -8.29 | 100.50 | 106.31 |
| 37 | c | 510 | CLA | CMD-C2D-C1D | 8.28 | 139.31 | 124.73 |
| 37 | C | 510 | CLA | CMD-C2D-C1D | 8.28 | 139.31 | 124.73 |
| 47 | 31 | 309 | KC1 | C1D-ND-C4D | -8.28 | 100.50 | 106.31 |
| 50 | 41 | 216 | DD6 | C28-C27-C26 | -8.28 | 108.10 | 124.18 |
| 37 | 32 | 210 | CLA | C1D-ND-C4D | -8.27 | 100.51 | 106.31 |
| 48 | 15 | 319 | A86 | C21-C20-C19 | -8.27 | 104.95 | 114.24 |
| 48 | 11 | 313 | A86 | C21-C20-C19 | -8.27 | 104.95 | 114.24 |
| 48 | 35 | 319 | A86 | C21-C20-C19 | -8.27 | 104.95 | 114.24 |
| 37 | b | 523 | CLA | C1D-ND-C4D | -8.26 | 100.52 | 106.31 |
| 48 | 31 | 313 | A86 | C21-C20-C19 | -8.26 | 104.97 | 114.24 |
| 50 | 39 | 312 | DD6 | C12-C11-C10 | -8.25 | 109.44 | 122.82 |
| 50 | 41 | 216 | DD6 | C-C1-C24 | -8.25 | 105.49 | 118.09 |
| 50 | 19 | 312 | DD6 | C12-C11-C10 | -8.25 | 109.46 | 122.82 |
| 37 | C | 506 | CLA | C1D-ND-C4D | -8.24 | 100.53 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 209 | CLA | C1D-ND-C4D | -8.24 | 100.53 | 106.31 |
| 50 | 21 | 216 | DD6 | C28-C27-C26 | -8.23 | 108.19 | 124.18 |
| 50 | 21 | 216 | DD6 | C-C1-C24 | -8.22 | 105.54 | 118.09 |
| 47 | 13 | 309 | KC1 | C1D-ND-C4D | -8.22 | 100.55 | 106.31 |
| 47 | 33 | 309 | KC1 | C1D-ND-C4D | -8.22 | 100.55 | 106.31 |
| 48 | 31 | 312 | A86 | C3-C2-C1 | -8.17 | 115.82 | 127.28 |
| 37 | 31 | 301 | CLA | C1D-ND-C4D | -8.17 | 100.58 | 106.31 |
| 48 | 11 | 312 | A86 | C3-C2-C1 | -8.16 | 115.83 | 127.28 |
| 48 | 39 | 313 | A86 | C4-C5-C6 | -8.16 | 115.83 | 127.28 |
| 47 | 16 | 302 | KC1 | C1D-ND-C4D | -8.14 | 100.60 | 106.31 |
| 50 | 16 | 312 | DD6 | C8-C6-C5 | -8.11 | 106.25 | 119.01 |
| 37 | W | 102 | CLA | C1D-ND-C4D | -8.11 | 100.62 | 106.31 |
| 37 | c | 507 | CLA | C1D-ND-C4D | -8.10 | 100.63 | 106.31 |
| 50 | 36 | 312 | DD6 | C8-C6-C5 | -8.10 | 106.27 | 119.01 |
| 47 | 41 | 203 | KC1 | C1D-ND-C4D | -8.10 | 100.63 | 106.31 |
| 48 | 16 | 310 | A86 | C33-C32-C31 | 8.09 | 117.08 | 109.21 |
| 47 | 18 | 210 | KC1 | CMA-C3A-C4A | -8.09 | 112.40 | 125.03 |
| 47 | 34 | 304 | KC1 | CMA-C3A-C2A | -8.07 | 108.89 | 128.43 |
| 47 | 14 | 304 | KC1 | CMA-C3A-C2A | -8.07 | 108.90 | 128.43 |
| 48 | 36 | 310 | A86 | C33-C32-C31 | 8.06 | 117.04 | 109.21 |
| 47 | 37 | 302 | KC1 | C1D-ND-C4D | -8.06 | 100.66 | 106.31 |
| 50 | 20 | 310 | DD6 | C7-C6-C5 | -8.05 | 109.77 | 122.82 |
| 50 | 20 | 310 | DD6 | C37-C36-C31 | -8.05 | 109.11 | 124.16 |
| 47 | 36 | 302 | KC1 | C1D-ND-C4D | -8.05 | 100.67 | 106.31 |
| 50 | 40 | 212 | DD6 | C37-C36-C31 | -8.04 | 109.14 | 124.16 |
| 47 | 38 | 210 | KC1 | CMA-C3A-C4A | -8.04 | 112.48 | 125.03 |
| 50 | 40 | 212 | DD6 | C7-C6-C5 | -8.03 | 109.80 | 122.82 |
| 37 | C | 507 | CLA | C1D-ND-C4D | -8.03 | 100.68 | 106.31 |
| 47 | 11 | 304 | KC1 | C1D-ND-C4D | -8.02 | 100.69 | 106.31 |
| 47 | 21 | 203 | KC1 | C1D-ND-C4D | -8.02 | 100.69 | 106.31 |
| 48 | 14 | 312 | A86 | C33-C32-C31 | 8.01 | 117.00 | 109.21 |
| 47 | 17 | 303 | KC1 | C1D-ND-C4D | -8.00 | 100.70 | 106.31 |
| 48 | 14 | 316 | A86 | O1-C20-C21 | -8.00 | 106.11 | 115.05 |
| 37 | 14 | 303 | CLA | CAA-C2A-C3A | -7.99 | 91.40 | 113.00 |
| 37 | 34 | 303 | CLA | CAA-C2A-C3A | -7.99 | 91.40 | 113.00 |
| 47 | 31 | 305 | KC1 | C1D-ND-C4D | -7.99 | 100.70 | 106.31 |
| 37 | 14 | 307 | CLA | C1D-ND-C4D | -7.99 | 100.71 | 106.31 |
| 50 | 19 | 312 | DD6 | C8-C6-C5 | -7.98 | 106.45 | 119.01 |
| 50 | 39 | 312 | DD6 | C8-C6-C5 | -7.98 | 106.45 | 119.01 |
| 37 | 34 | 307 | CLA | C1D-ND-C4D | -7.98 | 100.72 | 106.31 |
| 48 | 34 | 312 | A86 | C33-C32-C31 | 7.97 | 116.96 | 109.21 |
| 38 | A | 404 | PHO | C4D-CHA-CBD | -7.97 | 104.63 | 108.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 34 | 316 | A86 | O1-C20-C21 | -7.96 | 106.15 | 115.05 |
| 38 | a | 406 | PHO | C4D-CHA-CBD | -7.95 | 104.64 | 108.45 |
| 48 | 19 | 313 | A86 | C4-C5-C6 | -7.94 | 116.14 | 127.28 |
| 50 | 20 | 312 | DD6 | C7-C6-C5 | -7.93 | 109.98 | 122.82 |
| 50 | 40 | 214 | DD6 | C7-C6-C5 | -7.90 | 110.01 | 122.82 |
| 48 | 15 | 311 | A86 | C33-C32-C31 | 7.90 | 116.89 | 109.21 |
| 48 | 11 | 319 | A86 | C3-C2-C1 | -7.88 | 116.23 | 127.28 |
| 48 | 12 | 202 | A86 | C4-C5-C6 | -7.87 | 116.25 | 127.28 |
| 48 | 32 | 203 | A86 | C4-C5-C6 | -7.86 | 116.25 | 127.28 |
| 48 | 31 | 319 | A86 | C3-C2-C1 | -7.84 | 116.28 | 127.28 |
| 50 | 16 | 312 | DD6 | C7-C6-C5 | -7.83 | 110.12 | 122.82 |
| 50 | 36 | 312 | DD6 | C7-C6-C5 | -7.82 | 110.14 | 122.82 |
| 48 | 18 | 212 | A86 | C33-C32-C31 | 7.81 | 116.81 | 109.21 |
| 48 | 18 | 214 | A86 | C33-C32-C31 | 7.80 | 116.79 | 109.21 |
| 48 | 31 | 313 | A86 | O1-C20-C21 | -7.80 | 106.33 | 115.05 |
| 48 | 38 | 212 | A86 | C33-C32-C31 | 7.79 | 116.78 | 109.21 |
| 48 | 38 | 214 | A86 | C33-C32-C31 | 7.78 | 116.78 | 109.21 |
| 50 | 19 | 312 | DD6 | C7-C6-C5 | -7.78 | 110.20 | 122.82 |
| 50 | 21 | 212 | DD6 | C-C1-C2 | -7.78 | 110.22 | 122.82 |
| 50 | 39 | 312 | DD6 | C7-C6-C5 | -7.77 | 110.22 | 122.82 |
| 48 | 11 | 313 | A86 | O1-C20-C21 | -7.76 | 106.37 | 115.05 |
| 50 | 19 | 312 | DD6 | O1-C15-C14 | -7.76 | 94.64 | 116.88 |
| 50 | 41 | 212 | DD6 | C-C1-C2 | -7.76 | 110.25 | 122.82 |
| 50 | 41 | 212 | DD6 | C37-C36-C31 | -7.75 | 109.67 | 124.16 |
| 50 | 21 | 212 | DD6 | C37-C36-C31 | -7.74 | 109.69 | 124.16 |
| 50 | 39 | 312 | DD6 | O1-C15-C14 | -7.74 | 94.70 | 116.88 |
| 48 | 13 | 315 | A86 | C4-C5-C6 | -7.72 | 116.44 | 127.28 |
| 47 | 16 | 308 | KC1 | CMD-C2D-C1D | 7.72 | 137.18 | 125.42 |
| 48 | 33 | 315 | A86 | C4-C5-C6 | -7.72 | 116.45 | 127.28 |
| 37 | W | 101 | CLA | O2D-CGD-CBD | 7.70 | 124.69 | 111.23 |
| 37 | 13 | 307 | CLA | C1D-ND-C4D | -7.69 | 100.91 | 106.31 |
| 37 | 33 | 307 | CLA | C1D-ND-C4D | -7.69 | 100.91 | 106.31 |
| 47 | 36 | 308 | KC1 | CMD-C2D-C1D | 7.69 | 137.13 | 125.42 |
| 47 | 40 | 207 | KC1 | C1D-ND-C4D | -7.68 | 100.92 | 106.31 |
| 37 | 12 | 204 | CLA | C1D-ND-C4D | -7.67 | 100.93 | 106.31 |
| 37 | w | 101 | CLA | O2D-CGD-CBD | 7.67 | 124.64 | 111.23 |
| 37 | 32 | 205 | CLA | C1D-ND-C4D | -7.67 | 100.93 | 106.31 |
| 48 | 31 | 313 | A86 | C36-C31-C32 | -7.67 | 112.09 | 119.70 |
| 48 | 37 | 314 | A86 | C4-C5-C6 | -7.66 | 116.54 | 127.28 |
| 47 | 15 | 304 | KC1 | CMA-C3A-C2A | -7.65 | 109.92 | 128.43 |
| 47 | 20 | 305 | KC1 | C1D-ND-C4D | -7.65 | 100.95 | 106.31 |
| 48 | 17 | 315 | A86 | C4-C5-C6 | -7.64 | 116.57 | 127.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 37 | 305 | KC1 | C1D-ND-C4D | -7.62 | 100.96 | 106.31 |
| 47 | 17 | 306 | KC1 | C1D-ND-C4D | -7.62 | 100.97 | 106.31 |
| 47 | 38 | 205 | KC1 | CMD-C2D-C1D | 7.60 | 136.99 | 125.42 |
| 50 | 20 | 312 | DD6 | C28-C27-C26 | -7.59 | 109.44 | 124.18 |
| 50 | 40 | 214 | DD6 | C28-C27-C26 | -7.58 | 109.45 | 124.18 |
| 37 | a | 403 | CLA | CMD-C2D-C1D | 7.58 | 138.07 | 124.73 |
| 37 | A | 403 | CLA | CMD-C2D-C1D | 7.56 | 138.04 | 124.73 |
| 47 | 35 | 304 | KC1 | CMA-C3A-C2A | -7.56 | 110.14 | 128.43 |
| 48 | 34 | 313 | A86 | C33-C32-C31 | 7.53 | 116.53 | 109.21 |
| 48 | 17 | 311 | A86 | C33-C32-C31 | 7.53 | 116.53 | 109.21 |
| 37 | b | 504 | CLA | C1D-ND-C4D | -7.52 | 101.04 | 106.31 |
| 48 | 14 | 313 | A86 | C33-C32-C31 | 7.51 | 116.51 | 109.21 |
| 48 | 37 | 310 | A86 | C33-C32-C31 | 7.51 | 116.51 | 109.21 |
| 47 | 40 | 206 | KC1 | CMD-C2D-C1D | 7.50 | 136.85 | 125.42 |
| 48 | 14 | 314 | A86 | C33-C32-C31 | 7.49 | 116.49 | 109.21 |
| 47 | 14 | 309 | KC1 | CHB-C4A-C3A | -7.49 | 113.20 | 125.03 |
| 37 | B | 504 | CLA | C1D-ND-C4D | -7.49 | 101.06 | 106.31 |
| 47 | 20 | 304 | KC1 | CMD-C2D-C1D | 7.48 | 136.81 | 125.42 |
| 47 | 18 | 205 | KC1 | CMD-C2D-C1D | 7.48 | 136.81 | 125.42 |
| 48 | 11 | 311 | A86 | O1-C20-C21 | -7.47 | 106.70 | 115.05 |
| 47 | 15 | 304 | KC1 | CMD-C2D-C1D | 7.47 | 136.79 | 125.42 |
| 48 | 34 | 314 | A86 | C33-C32-C31 | 7.46 | 116.47 | 109.21 |
| 47 | 34 | 309 | KC1 | CHB-C4A-C3A | -7.46 | 113.25 | 125.03 |
| 50 | 16 | 312 | DD6 | C28-C27-C26 | -7.46 | 109.69 | 124.18 |
| 50 | 36 | 312 | DD6 | C28-C27-C26 | -7.46 | 109.69 | 124.18 |
| 37 | 18 | 202 | CLA | C2D-C1D-ND | 7.46 | 117.51 | 110.13 |
| 37 | 40 | 205 | CLA | CMD-C2D-C1D | 7.45 | 137.84 | 124.73 |
| 37 | 20 | 303 | CLA | CMD-C2D-C1D | 7.43 | 137.82 | 124.73 |
| 47 | 16 | 304 | KC1 | CMD-C2D-C1D | 7.43 | 136.74 | 125.42 |
| 48 | 31 | 311 | A86 | O1-C20-C21 | -7.43 | 106.74 | 115.05 |
| 48 | 11 | 312 | A86 | C33-C32-C31 | 7.43 | 116.43 | 109.21 |
| 50 | 21 | 216 | DD6 | C-C1-C2 | -7.42 | 110.80 | 122.82 |
| 50 | 41 | 216 | DD6 | C-C1-C2 | -7.41 | 110.81 | 122.82 |
| 47 | 36 | 304 | KC1 | CMD-C2D-C1D | 7.41 | 136.70 | 125.42 |
| 47 | 34 | 309 | KC1 | CMD-C2D-C1D | 7.40 | 136.69 | 125.42 |
| 48 | 33 | 311 | A86 | C33-C32-C31 | 7.40 | 116.40 | 109.21 |
| 48 | 21 | 213 | A86 | C33-C32-C31 | 7.39 | 116.40 | 109.21 |
| 48 | 31 | 312 | A86 | C33-C32-C31 | 7.39 | 116.39 | 109.21 |
| 48 | 41 | 213 | A86 | C33-C32-C31 | 7.39 | 116.39 | 109.21 |
| 48 | 36 | 311 | A86 | C3-C2-C1 | -7.38 | 116.93 | 127.28 |
| 47 | 13 | 302 | KC1 | CHB-C4A-C3A | -7.37 | 113.39 | 125.03 |
| 47 | 33 | 302 | KC1 | CHB-C4A-C3A | -7.36 | 113.41 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 19 | 312 | DD6 | C28-C27-C26 | -7.36 | 109.88 | 124.18 |
| 48 | 13 | 311 | A86 | C33-C32-C31 | 7.35 | 116.36 | 109.21 |
| 47 | 14 | 309 | KC1 | CMD-C2D-C1D | 7.35 | 136.61 | 125.42 |
| 48 | 16 | 311 | A86 | C3-C2-C1 | -7.35 | 116.97 | 127.28 |
| 37 | b | 505 | CLA | CMD-C2D-C1D | 7.34 | 137.65 | 124.73 |
| 47 | 18 | 210 | KC1 | CHB-C4A-C3A | -7.33 | 113.45 | 125.03 |
| 47 | 17 | 308 | KC1 | CMA-C3A-C4A | -7.32 | 113.59 | 125.03 |
| 37 | B | 505 | CLA | CMD-C2D-C1D | 7.32 | 137.62 | 124.73 |
| 50 | 39 | 312 | DD6 | C28-C27-C26 | -7.32 | 109.97 | 124.18 |
| 47 | 35 | 304 | KC1 | CMD-C2D-C1D | 7.31 | 136.56 | 125.42 |
| 47 | 37 | 307 | KC1 | CMA-C3A-C4A | -7.31 | 113.60 | 125.03 |
| 50 | 36 | 312 | DD6 | C-C1-C24 | -7.31 | 106.92 | 118.09 |
| 47 | 38 | 210 | KC1 | CHB-C4A-C3A | -7.30 | 113.50 | 125.03 |
| 47 | 19 | 308 | KC1 | CMA-C3A-C2A | -7.30 | 110.76 | 128.43 |
| 47 | 31 | 305 | KC1 | CMD-C2D-C1D | 7.30 | 136.54 | 125.42 |
| 47 | 20 | 302 | KC1 | CMD-C2D-C1D | 7.30 | 136.53 | 125.42 |
| 50 | 16 | 312 | DD6 | C-C1-C24 | -7.30 | 106.94 | 118.09 |
| 47 | 39 | 308 | KC1 | CMA-C3A-C2A | -7.30 | 110.77 | 128.43 |
| 50 | 39 | 312 | DD6 | C13-C11-C10 | -7.29 | 107.53 | 119.01 |
| 47 | 11 | 309 | KC1 | CHB-C4A-C3A | -7.29 | 113.52 | 125.03 |
| 48 | 35 | 314 | A86 | C33-C32-C31 | 7.29 | 116.30 | 109.21 |
| 47 | 11 | 304 | KC1 | CMD-C2D-C1D | 7.29 | 136.51 | 125.42 |
| 37 | C | 503 | CLA | CMD-C2D-C1D | 7.29 | 137.56 | 124.73 |
| 37 | c | 503 | CLA | CMD-C2D-C1D | 7.29 | 137.56 | 124.73 |
| 47 | 40 | 204 | KC1 | CMD-C2D-C1D | 7.29 | 136.51 | 125.42 |
| 50 | 19 | 312 | DD6 | C13-C11-C10 | -7.28 | 107.56 | 119.01 |
| 47 | 15 | 309 | KC1 | CHB-C4A-C3A | -7.27 | 113.55 | 125.03 |
| 48 | 15 | 314 | A86 | C33-C32-C31 | 7.27 | 116.28 | 109.21 |
| 38 | a | 405 | PHO | C4D-CHA-CBD | -7.26 | 104.97 | 108.45 |
| 47 | 35 | 309 | KC1 | CHB-C4A-C3A | -7.26 | 113.57 | 125.03 |
| 37 | D | 402 | CLA | CMD-C2D-C1D | 7.25 | 137.50 | 124.73 |
| 47 | 31 | 309 | KC1 | CHB-C4A-C3A | -7.25 | 113.58 | 125.03 |
| 47 | 17 | 308 | KC1 | CHB-C4A-C3A | -7.25 | 113.58 | 125.03 |
| 48 | 40 | 211 | A86 | C33-C32-C31 | 7.24 | 116.25 | 109.21 |
| 47 | 16 | 304 | KC1 | CMA-C3A-C2A | -7.24 | 110.90 | 128.43 |
| 47 | 37 | 307 | KC1 | CHB-C4A-C3A | -7.24 | 113.60 | 125.03 |
| 37 | d | 401 | CLA | CMD-C2D-C1D | 7.24 | 137.47 | 124.73 |
| 47 | 36 | 304 | KC1 | CMA-C3A-C2A | -7.23 | 110.94 | 128.43 |
| 48 | 35 | 312 | A86 | C3-C2-C1 | -7.22 | 117.16 | 127.28 |
| 48 | 21 | 211 | A86 | C33-C32-C31 | 7.22 | 116.22 | 109.21 |
| 38 | D | 403 | PHO | C4D-CHA-CBD | -7.22 | 104.99 | 108.45 |
| 50 | 40 | 212 | DD6 | C28-C27-C26 | -7.22 | 110.17 | 124.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 20 | 310 | DD6 | C28-C27-C26 | -7.21 | 110.17 | 124.18 |
| 47 | 38 | 207 | KC1 | O2D-CGD-CBD | 7.21 | 123.84 | 111.23 |
| 48 | 20 | 309 | A86 | C33-C32-C31 | 7.21 | 116.22 | 109.21 |
| 47 | 33 | 302 | KC1 | CMD-C2D-C1D | 7.21 | 136.40 | 125.42 |
| 47 | 33 | 304 | KC1 | CMA-C3A-C2A | -7.20 | 111.01 | 128.43 |
| 47 | 13 | 304 | KC1 | CMA-C3A-C2A | -7.19 | 111.02 | 128.43 |
| 37 | 19 | 302 | CLA | O2D-CGD-CBD | 7.19 | 123.80 | 111.23 |
| 47 | 13 | 302 | KC1 | CMD-C2D-C1D | 7.18 | 136.36 | 125.42 |
| 37 | D | 405 | CLA | C2D-C1D-ND | 7.18 | 117.23 | 110.13 |
| 37 | 40 | 203 | CLA | CMD-C2D-C1D | 7.18 | 137.37 | 124.73 |
| 47 | 12 | 211 | KC1 | CMD-C2D-C1D | 7.18 | 136.35 | 125.42 |
| 48 | 13 | 313 | A86 | C4-C5-C6 | -7.18 | 117.21 | 127.28 |
| 48 | 31 | 311 | A86 | C33-C32-C31 | 7.18 | 116.19 | 109.21 |
| 37 | C | 505 | CLA | O2D-CGD-CBD | 7.17 | 123.77 | 111.23 |
| 50 | 16 | 312 | DD6 | C-C1-C2 | -7.17 | 111.19 | 122.82 |
| 48 | 11 | 311 | A86 | C33-C32-C31 | 7.17 | 116.18 | 109.21 |
| 47 | 20 | 302 | KC1 | CMA-C3A-C2A | -7.17 | 111.08 | 128.43 |
| 47 | 40 | 204 | KC1 | CMA-C3A-C2A | -7.17 | 111.08 | 128.43 |
| 37 | c | 505 | CLA | O2D-CGD-CBD | 7.17 | 123.76 | 111.23 |
| 37 | d | 403 | CLA | C2D-C1D-ND | 7.17 | 117.22 | 110.13 |
| 47 | 40 | 207 | KC1 | O2D-CGD-CBD | 7.17 | 123.76 | 111.23 |
| 37 | 20 | 301 | CLA | CMD-C2D-C1D | 7.16 | 137.34 | 124.73 |
| 48 | 41 | 211 | A86 | C33-C32-C31 | 7.16 | 116.17 | 109.21 |
| 47 | 20 | 305 | KC1 | O2D-CGD-CBD | 7.16 | 123.75 | 111.23 |
| 47 | 16 | 308 | KC1 | CMA-C3A-C4A | -7.16 | 113.84 | 125.03 |
| 48 | 33 | 313 | A86 | C4-C5-C6 | -7.16 | 117.24 | 127.28 |
| 47 | 20 | 302 | KC1 | CHB-C4A-C3A | -7.16 | 113.73 | 125.03 |
| 50 | 36 | 312 | DD6 | C-C1-C2 | -7.15 | 111.23 | 122.82 |
| 37 | 39 | 302 | CLA | O2D-CGD-CBD | 7.15 | 123.73 | 111.23 |
| 47 | 32 | 212 | KC1 | CMD-C2D-C1D | 7.14 | 136.29 | 125.42 |
| 47 | 40 | 204 | KC1 | CHB-C4A-C3A | -7.14 | 113.76 | 125.03 |
| 47 | 36 | 308 | KC1 | CMA-C3A-C4A | -7.14 | 113.88 | 125.03 |
| 37 | C | 511 | CLA | CMD-C2D-C1D | 7.14 | 137.30 | 124.73 |
| 47 | 18 | 207 | KC1 | O2D-CGD-CBD | 7.13 | 123.70 | 111.23 |
| 50 | 40 | 214 | DD6 | C-C1-C2 | -7.13 | 111.27 | 122.82 |
| 50 | 20 | 312 | DD6 | C-C1-C24 | -7.13 | 107.20 | 118.09 |
| 50 | 20 | 312 | DD6 | C-C1-C2 | -7.12 | 111.28 | 122.82 |
| 47 | 31 | 309 | KC1 | CMD-C2D-C1D | 7.12 | 136.26 | 125.42 |
| 37 | c | 511 | CLA | CMD-C2D-C1D | 7.11 | 137.26 | 124.73 |
| 50 | 40 | 214 | DD6 | C-C1-C24 | -7.11 | 107.23 | 118.09 |
| 47 | 11 | 309 | KC1 | CMD-C2D-C1D | 7.10 | 136.24 | 125.42 |
| 47 | 15 | 302 | KC1 | CHB-C4A-C3A | -7.10 | 113.81 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 32 | 212 | KC1 | CMA-C3A-C4A | -7.10 | 113.93 | 125.03 |
| 47 | 12 | 211 | KC1 | CMA-C3A-C4A | -7.10 | 113.94 | 125.03 |
| 37 | b | 503 | CLA | O2D-CGD-CBD | 7.09 | 123.63 | 111.23 |
| 37 | b | 506 | CLA | CMD-C2D-C1D | 7.09 | 137.21 | 124.73 |
| 37 | C | 501 | CLA | CMD-C2D-C1D | 7.09 | 137.21 | 124.73 |
| 37 | b | 502 | CLA | CMD-C2D-C1D | 7.09 | 137.21 | 124.73 |
| 47 | 35 | 302 | KC1 | CMD-C2D-C1D | 7.08 | 136.21 | 125.42 |
| 37 | B | 503 | CLA | O2D-CGD-CBD | 7.08 | 123.61 | 111.23 |
| 48 | 15 | 312 | A86 | C3-C2-C1 | -7.08 | 117.35 | 127.28 |
| 37 | B | 502 | CLA | CMD-C2D-C1D | 7.08 | 137.19 | 124.73 |
| 37 | B | 506 | CLA | CMD-C2D-C1D | 7.07 | 137.17 | 124.73 |
| 37 | c | 501 | CLA | CMD-C2D-C1D | 7.07 | 137.17 | 124.73 |
| 47 | 21 | 207 | KC1 | CMA-C3A-C2A | -7.07 | 111.33 | 128.43 |
| 47 | 41 | 207 | KC1 | CMA-C3A-C2A | -7.06 | 111.33 | 128.43 |
| 37 | Z | 101 | CLA | CMD-C2D-C1D | 7.04 | 137.12 | 124.73 |
| 47 | 37 | 302 | KC1 | CMD-C2D-C1D | 7.03 | 136.12 | 125.42 |
| 37 | 14 | 310 | CLA | CMD-C2D-C1D | 7.03 | 137.10 | 124.73 |
| 37 | z | 101 | CLA | CMD-C2D-C1D | 7.02 | 137.10 | 124.73 |
| 37 | 34 | 310 | CLA | CMD-C2D-C1D | 7.02 | 137.10 | 124.73 |
| 47 | 15 | 302 | KC1 | CMD-C2D-C1D | 7.02 | 136.11 | 125.42 |
| 47 | 33 | 309 | KC1 | CHB-C4A-C3A | -7.02 | 113.94 | 125.03 |
| 47 | 35 | 306 | KC1 | CMD-C2D-C1D | 7.02 | 136.10 | 125.42 |
| 48 | 35 | 314 | A86 | C25-C26-C27 | -7.02 | 117.44 | 127.28 |
| 47 | 12 | 211 | KC1 | CHB-C4A-C3A | -7.01 | 113.95 | 125.03 |
| 47 | 17 | 303 | KC1 | CMD-C2D-C1D | 7.01 | 136.09 | 125.42 |
| 47 | 13 | 309 | KC1 | CHB-C4A-C3A | -7.00 | 113.97 | 125.03 |
| 47 | 16 | 302 | KC1 | CHB-C4A-C3A | -7.00 | 113.97 | 125.03 |
| 47 | 15 | 306 | KC1 | CMD-C2D-C1D | 7.00 | 136.08 | 125.42 |
| 37 | b | 507 | CLA | CMD-C2D-C1D | 6.99 | 137.04 | 124.73 |
| 37 | 33 | 301 | CLA | CMD-C2D-C1D | 6.99 | 137.04 | 124.73 |
| 47 | 32 | 212 | KC1 | CHB-C4A-C3A | -6.99 | 113.99 | 125.03 |
| 37 | 13 | 301 | CLA | CMD-C2D-C1D | 6.99 | 137.04 | 124.73 |
| 48 | 15 | 314 | A86 | C25-C26-C27 | -6.99 | 117.48 | 127.28 |
| 50 | 20 | 310 | DD6 | C8-C6-C5 | -6.98 | 108.02 | 119.01 |
| 50 | 40 | 212 | DD6 | C8-C6-C5 | -6.98 | 108.03 | 119.01 |
| 47 | 36 | 302 | KC1 | CHB-C4A-C3A | -6.98 | 114.01 | 125.03 |
| 47 | 21 | 207 | KC1 | CHB-C4A-C3A | -6.97 | 114.02 | 125.03 |
| 47 | 18 | 210 | KC1 | CMD-C2D-C1D | 6.97 | 136.04 | 125.42 |
| 37 | B | 507 | CLA | CMD-C2D-C1D | 6.97 | 137.00 | 124.73 |
| 47 | 33 | 302 | KC1 | C3B-C2B-C1B | -6.96 | 100.46 | 107.05 |
| 50 | 21 | 216 | DD6 | C13-C11-C10 | -6.96 | 108.06 | 119.01 |
| 48 | 11 | 313 | A86 | C36-C31-C32 | -6.96 | 112.79 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 41 | 207 | KC1 | CHB-C4A-C3A | -6.96 | 114.05 | 125.03 |
| 47 | 41 | 207 | KC1 | CMD-C2D-C1D | 6.95 | 136.01 | 125.42 |
| 37 | C | 504 | CLA | CMD-C2D-C1D | 6.95 | 136.97 | 124.73 |
| 37 | 37 | 301 | CLA | CMD-C2D-C1D | 6.95 | 136.97 | 124.73 |
| 47 | 21 | 207 | KC1 | CMD-C2D-C1D | 6.95 | 136.00 | 125.42 |
| 37 | 39 | 304 | CLA | CMD-C2D-C1D | 6.94 | 136.96 | 124.73 |
| 50 | 41 | 216 | DD6 | C13-C11-C10 | -6.94 | 108.09 | 119.01 |
| 48 | 11 | 314 | A86 | C40-C32-C31 | -6.94 | 104.26 | 110.47 |
| 47 | 37 | 307 | KC1 | CMD-C2D-C1D | 6.94 | 135.99 | 125.42 |
| 37 | 33 | 305 | CLA | CMD-C2D-C1D | 6.94 | 136.95 | 124.73 |
| 37 | B | 511 | CLA | CMD-C2D-C1D | 6.93 | 136.94 | 124.73 |
| 37 | 41 | 208 | CLA | CMD-C2D-C1D | 6.93 | 136.94 | 124.73 |
| 37 | 13 | 305 | CLA | CMD-C2D-C1D | 6.93 | 136.93 | 124.73 |
| 37 | c | 504 | CLA | CMD-C2D-C1D | 6.93 | 136.92 | 124.73 |
| 47 | 32 | 209 | KC1 | CHB-C4A-C3A | -6.92 | 114.10 | 125.03 |
| 37 | 41 | 206 | CLA | CMD-C2D-C1D | 6.92 | 136.92 | 124.73 |
| 37 | 21 | 206 | CLA | CMD-C2D-C1D | 6.92 | 136.92 | 124.73 |
| 47 | 35 | 302 | KC1 | CHB-C4A-C3A | -6.92 | 114.10 | 125.03 |
| 37 | 18 | 201 | CLA | CMD-C2D-C1D | 6.92 | 136.91 | 124.73 |
| 37 | 14 | 308 | CLA | CMD-C2D-C1D | 6.91 | 136.91 | 124.73 |
| 37 | 19 | 304 | CLA | CMD-C2D-C1D | 6.91 | 136.91 | 124.73 |
| 47 | 12 | 206 | KC1 | CMD-C2D-C1D | 6.91 | 135.94 | 125.42 |
| 47 | 12 | 208 | KC1 | CHB-C4A-C3A | -6.91 | 114.12 | 125.03 |
| 37 | C | 509 | CLA | CMD-C2D-C1D | 6.91 | 136.89 | 124.73 |
| 37 | 21 | 209 | CLA | CMD-C2D-C1D | 6.90 | 136.89 | 124.73 |
| 37 | W | 101 | CLA | CMD-C2D-C1D | 6.90 | 136.88 | 124.73 |
| 47 | 13 | 304 | KC1 | CMD-C2D-C1D | 6.90 | 135.93 | 125.42 |
| 47 | 14 | 304 | KC1 | CMD-C2D-C1D | 6.90 | 135.93 | 125.42 |
| 37 | 21 | 208 | CLA | CMD-C2D-C1D | 6.90 | 136.88 | 124.73 |
| 37 | b | 511 | CLA | CMD-C2D-C1D | 6.90 | 136.88 | 124.73 |
| 47 | 17 | 308 | KC1 | CMD-C2D-C1D | 6.89 | 135.91 | 125.42 |
| 47 | 32 | 207 | KC1 | CMD-C2D-C1D | 6.89 | 135.91 | 125.42 |
| 37 | w | 101 | CLA | CMD-C2D-C1D | 6.89 | 136.86 | 124.73 |
| 37 | 34 | 308 | CLA | CMD-C2D-C1D | 6.89 | 136.86 | 124.73 |
| 37 | c | 509 | CLA | CMD-C2D-C1D | 6.89 | 136.85 | 124.73 |
| 37 | 41 | 209 | CLA | CMD-C2D-C1D | 6.88 | 136.85 | 124.73 |
| 47 | 33 | 304 | KC1 | CMD-C2D-C1D | 6.88 | 135.90 | 125.42 |
| 37 | 38 | 201 | CLA | CMD-C2D-C1D | 6.88 | 136.84 | 124.73 |
| 48 | 13 | 312 | A86 | C3-C2-C1 | -6.87 | 117.64 | 127.28 |
| 50 | 20 | 312 | DD6 | C13-C11-C10 | -6.87 | 108.20 | 119.01 |
| 47 | 13 | 304 | KC1 | CHB-C4A-C3A | -6.87 | 114.18 | 125.03 |
| 37 | 37 | 308 | CLA | O2D-CGD-CBD | 6.86 | 123.23 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 33 | 304 | KC1 | CHB-C4A-C3A | -6.86 | 114.20 | 125.03 |
| 47 | 31 | 303 | KC1 | CHB-C4A-C3A | -6.86 | 114.20 | 125.03 |
| 47 | 38 | 210 | KC1 | CMD-C2D-C1D | 6.86 | 135.86 | 125.42 |
| 50 | 40 | 214 | DD6 | C13-C11-C10 | -6.86 | 108.22 | 119.01 |
| 47 | 20 | 305 | KC1 | CHB-C4A-C3A | -6.86 | 114.20 | 125.03 |
| 47 | 34 | 304 | KC1 | CMD-C2D-C1D | 6.85 | 135.85 | 125.42 |
| 47 | 13 | 302 | KC1 | C3B-C2B-C1B | -6.85 | 100.57 | 107.05 |
| 48 | 31 | 314 | A86 | C40-C32-C31 | -6.85 | 104.34 | 110.47 |
| 37 | 18 | 202 | CLA | CMD-C2D-C1D | 6.84 | 136.78 | 124.73 |
| 48 | 41 | 214 | A86 | C33-C32-C31 | 6.84 | 115.86 | 109.21 |
| 47 | 11 | 302 | KC1 | CHB-C4A-C3A | -6.84 | 114.23 | 125.03 |
| 47 | 38 | 207 | KC1 | CHB-C4A-C3A | -6.84 | 114.23 | 125.03 |
| 48 | 37 | 313 | A86 | C4-C5-C6 | -6.84 | 117.69 | 127.28 |
| 48 | 21 | 214 | A86 | C33-C32-C31 | 6.84 | 115.86 | 109.21 |
| 50 | 16 | 312 | DD6 | C12-C11-C13 | -6.84 | 107.64 | 118.09 |
| 37 | 17 | 309 | CLA | O2D-CGD-CBD | 6.83 | 123.17 | 111.23 |
| 37 | 21 | 202 | CLA | CMD-C2D-C1D | 6.83 | 136.75 | 124.73 |
| 50 | 36 | 312 | DD6 | C12-C11-C13 | -6.82 | 107.66 | 118.09 |
| 37 | b | 513 | CLA | CMD-C2D-C1D | 6.82 | 136.74 | 124.73 |
| 50 | 39 | 312 | DD6 | C-C1-C2 | -6.82 | 111.77 | 122.82 |
| 50 | 19 | 312 | DD6 | C-C1-C2 | -6.82 | 111.77 | 122.82 |
| 47 | 37 | 305 | KC1 | CMD-C2D-C1D | 6.82 | 135.80 | 125.42 |
| 37 | 38 | 203 | CLA | CMD-C2D-C1D | 6.82 | 136.73 | 124.73 |
| 47 | 40 | 207 | KC1 | CHB-C4A-C3A | -6.81 | 114.27 | 125.03 |
| 37 | z | 102 | CLA | CMD-C2D-C1D | 6.81 | 136.72 | 124.73 |
| 47 | 14 | 304 | KC1 | CHB-C4A-C3A | -6.81 | 114.27 | 125.03 |
| 37 | 41 | 202 | CLA | CMD-C2D-C1D | 6.81 | 136.72 | 124.73 |
| 47 | 17 | 306 | KC1 | CMD-C2D-C1D | 6.81 | 135.79 | 125.42 |
| 37 | B | 513 | CLA | CMD-C2D-C1D | 6.80 | 136.71 | 124.73 |
| 47 | 36 | 308 | KC1 | CHB-C4A-C3A | -6.80 | 114.29 | 125.03 |
| 47 | 38 | 205 | KC1 | CHB-C4A-C3A | -6.80 | 114.29 | 125.03 |
| 37 | Z | 102 | CLA | CMD-C2D-C1D | 6.80 | 136.70 | 124.73 |
| 47 | 16 | 304 | KC1 | CHB-C4A-C3A | -6.80 | 114.29 | 125.03 |
| 47 | 36 | 304 | KC1 | CHB-C4A-C3A | -6.80 | 114.30 | 125.03 |
| 47 | 16 | 308 | KC1 | CHB-C4A-C3A | -6.79 | 114.30 | 125.03 |
| 47 | 34 | 304 | KC1 | CHB-C4A-C3A | -6.79 | 114.31 | 125.03 |
| 47 | 17 | 303 | KC1 | CHB-C4A-C3A | -6.79 | 114.31 | 125.03 |
| 47 | 15 | 306 | KC1 | CHB-C4A-C3A | -6.79 | 114.31 | 125.03 |
| 47 | 18 | 205 | KC1 | CHB-C4A-C3A | -6.79 | 114.31 | 125.03 |
| 47 | 37 | 304 | KC1 | CHB-C4A-C3A | -6.78 | 114.32 | 125.03 |
| 47 | 17 | 305 | KC1 | CHB-C4A-C3A | -6.78 | 114.32 | 125.03 |
| 47 | 11 | 306 | KC1 | CMD-C2D-C1D | 6.78 | 135.75 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 20 | 305 | KC1 | CMD-C2D-C1D | 6.78 | 135.74 | 125.42 |
| 47 | 20 | 304 | KC1 | CMA-C3A-C4A | -6.78 | 114.44 | 125.03 |
| 47 | 40 | 207 | KC1 | CMD-C2D-C1D | 6.78 | 135.74 | 125.42 |
| 48 | 33 | 312 | A86 | C3-C2-C1 | -6.77 | 117.78 | 127.28 |
| 50 | 20 | 312 | DD6 | O1-C15-C14 | -6.77 | 97.49 | 116.88 |
| 47 | 31 | 307 | KC1 | CMD-C2D-C1D | 6.77 | 135.72 | 125.42 |
| 37 | 16 | 303 | CLA | CMD-C2D-C1D | 6.76 | 136.64 | 124.73 |
| 48 | 38 | 215 | A86 | C33-C32-C31 | 6.76 | 115.78 | 109.21 |
| 47 | 17 | 306 | KC1 | CHB-C4A-C3A | -6.76 | 114.35 | 125.03 |
| 37 | 18 | 203 | CLA | CMD-C2D-C1D | 6.76 | 136.63 | 124.73 |
| 50 | 40 | 214 | DD6 | O1-C15-C14 | -6.76 | 97.52 | 116.88 |
| 37 | 37 | 308 | CLA | CMD-C2D-C1D | 6.76 | 136.62 | 124.73 |
| 47 | 16 | 302 | KC1 | CMA-C3A-C4A | -6.75 | 114.48 | 125.03 |
| 47 | 40 | 206 | KC1 | CMA-C3A-C4A | -6.75 | 114.49 | 125.03 |
| 47 | 31 | 303 | KC1 | C3B-C2B-C1B | -6.75 | 100.66 | 107.05 |
| 48 | 18 | 215 | A86 | C33-C32-C31 | 6.75 | 115.77 | 109.21 |
| 37 | 40 | 209 | CLA | CMD-C2D-C1D | 6.75 | 136.61 | 124.73 |
| 37 | 41 | 204 | CLA | CMD-C2D-C1D | 6.74 | 136.60 | 124.73 |
| 37 | 38 | 202 | CLA | CMD-C2D-C1D | 6.74 | 136.60 | 124.73 |
| 47 | 17 | 306 | KC1 | O2D-CGD-CBD | 6.74 | 123.02 | 111.23 |
| 47 | 11 | 302 | KC1 | C3B-C2B-C1B | -6.74 | 100.67 | 107.05 |
| 37 | 36 | 303 | CLA | CMD-C2D-C1D | 6.74 | 136.59 | 124.73 |
| 37 | 38 | 206 | CLA | CMD-C2D-C1D | 6.74 | 136.59 | 124.73 |
| 47 | 36 | 302 | KC1 | CMA-C3A-C4A | -6.74 | 114.50 | 125.03 |
| 47 | 37 | 302 | KC1 | CHB-C4A-C3A | -6.74 | 114.39 | 125.03 |
| 37 | 21 | 204 | CLA | CMD-C2D-C1D | 6.74 | 136.59 | 124.73 |
| 47 | 37 | 305 | KC1 | CHB-C4A-C3A | -6.73 | 114.40 | 125.03 |
| 37 | 13 | 308 | CLA | CMD-C2D-C1D | 6.73 | 136.58 | 124.73 |
| 37 | 33 | 308 | CLA | CMD-C2D-C1D | 6.73 | 136.58 | 124.73 |
| 37 | 39 | 309 | CLA | CMD-C2D-C1D | 6.72 | 136.57 | 124.73 |
| 37 | c | 513 | CLA | CMD-C2D-C1D | 6.72 | 136.57 | 124.73 |
| 37 | 20 | 307 | CLA | CMD-C2D-C1D | 6.72 | 136.57 | 124.73 |
| 37 | 14 | 305 | CLA | CMD-C2D-C1D | 6.72 | 136.56 | 124.73 |
| 37 | 34 | 305 | CLA | CMD-C2D-C1D | 6.72 | 136.56 | 124.73 |
| 37 | 32 | 204 | CLA | CMD-C2D-C1D | 6.72 | 136.56 | 124.73 |
| 37 | 35 | 310 | CLA | CMD-C2D-C1D | 6.72 | 136.56 | 124.73 |
| 48 | 31 | 313 | A86 | C4-C5-C6 | -6.72 | 117.86 | 127.28 |
| 37 | C | 513 | CLA | CMD-C2D-C1D | 6.72 | 136.56 | 124.73 |
| 50 | 40 | 214 | DD6 | C8-C6-C5 | -6.72 | 108.44 | 119.01 |
| 47 | 41 | 203 | KC1 | CMD-C2D-C1D | 6.72 | 135.64 | 125.42 |
| 50 | 20 | 312 | DD6 | C8-C6-C5 | -6.71 | 108.45 | 119.01 |
| 37 | 18 | 206 | CLA | CMD-C2D-C1D | 6.71 | 136.55 | 124.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 35 | 303 | CLA | CMD-C2D-C1D | 6.71 | 136.55 | 124.73 |
| 47 | 11 | 304 | KC1 | CHB-C4A-C3A | -6.71 | 114.43 | 125.03 |
| 47 | 12 | 206 | KC1 | CMA-C3A-C4A | -6.71 | 114.55 | 125.03 |
| 48 | 13 | 312 | A86 | C33-C32-C31 | 6.71 | 115.73 | 109.21 |
| 37 | 12 | 203 | CLA | CMD-C2D-C1D | 6.71 | 136.54 | 124.73 |
| 37 | 21 | 205 | CLA | CMD-C2D-C1D | 6.71 | 136.54 | 124.73 |
| 47 | 21 | 203 | KC1 | CMD-C2D-C1D | 6.71 | 135.63 | 125.42 |
| 47 | 32 | 207 | KC1 | CMA-C3A-C4A | -6.71 | 114.56 | 125.03 |
| 47 | 34 | 306 | KC1 | CHB-C4A-C3A | -6.70 | 114.44 | 125.03 |
| 37 | 16 | 301 | CLA | C2D-C1D-ND | 6.70 | 116.76 | 110.13 |
| 47 | 31 | 305 | KC1 | CHB-C4A-C3A | -6.70 | 114.45 | 125.03 |
| 37 | 12 | 207 | CLA | CMD-C2D-C1D | 6.70 | 136.53 | 124.73 |
| 37 | 36 | 301 | CLA | C2D-C1D-ND | 6.70 | 116.76 | 110.13 |
| 37 | 18 | 211 | CLA | CMD-C2D-C1D | 6.70 | 136.53 | 124.73 |
| 37 | 37 | 303 | CLA | CMD-C2D-C1D | 6.69 | 136.52 | 124.73 |
| 47 | 37 | 305 | KC1 | O2D-CGD-CBD | 6.69 | 122.93 | 111.23 |
| 47 | 36 | 302 | KC1 | CMD-C2D-C1D | 6.69 | 135.61 | 125.42 |
| 37 | 41 | 205 | CLA | CMD-C2D-C1D | 6.69 | 136.51 | 124.73 |
| 37 | 32 | 208 | CLA | CMD-C2D-C1D | 6.69 | 136.51 | 124.73 |
| 47 | 14 | 306 | KC1 | CHB-C4A-C3A | -6.68 | 114.47 | 125.03 |
| 37 | 17 | 309 | CLA | CMD-C2D-C1D | 6.68 | 136.50 | 124.73 |
| 47 | 35 | 306 | KC1 | CHB-C4A-C3A | -6.68 | 114.48 | 125.03 |
| 37 | 15 | 303 | CLA | CMD-C2D-C1D | 6.68 | 136.49 | 124.73 |
| 47 | 16 | 302 | KC1 | CMD-C2D-C1D | 6.68 | 135.58 | 125.42 |
| 37 | 32 | 213 | CLA | O2D-CGD-CBD | 6.67 | 122.89 | 111.23 |
| 37 | 17 | 304 | CLA | CMD-C2D-C1D | 6.67 | 136.47 | 124.73 |
| 37 | 31 | 302 | CLA | CMD-C2D-C1D | 6.66 | 136.47 | 124.73 |
| 37 | a | 404 | CLA | CMD-C2D-C1D | 6.66 | 136.46 | 124.73 |
| 47 | 12 | 206 | KC1 | CHB-C4A-C3A | -6.66 | 114.52 | 125.03 |
| 47 | 32 | 207 | KC1 | CHB-C4A-C3A | -6.66 | 114.52 | 125.03 |
| 37 | D | 401 | CLA | CMD-C2D-C1D | 6.65 | 136.44 | 124.73 |
| 47 | 31 | 307 | KC1 | CHB-C4A-C3A | -6.65 | 114.53 | 125.03 |
| 47 | 14 | 309 | KC1 | CMA-C3A-C4A | -6.65 | 114.65 | 125.03 |
| 47 | 34 | 309 | KC1 | CMA-C3A-C4A | -6.64 | 114.65 | 125.03 |
| 47 | 11 | 306 | KC1 | CHB-C4A-C3A | -6.64 | 114.54 | 125.03 |
| 37 | 11 | 301 | CLA | CMD-C2D-C1D | 6.63 | 136.40 | 124.73 |
| 50 | 21 | 216 | DD6 | C8-C6-C5 | -6.63 | 108.58 | 119.01 |
| 37 | 38 | 211 | CLA | CMD-C2D-C1D | 6.63 | 136.40 | 124.73 |
| 37 | 38 | 202 | CLA | C2D-C1D-ND | 6.63 | 116.68 | 110.13 |
| 47 | 15 | 304 | KC1 | CHB-C4A-C3A | -6.62 | 114.57 | 125.03 |
| 37 | D | 406 | CLA | CMD-C2D-C1D | 6.62 | 136.39 | 124.73 |
| 37 | 12 | 212 | CLA | O2D-CGD-CBD | 6.62 | 122.81 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 41 | 216 | DD6 | C8-C6-C5 | -6.62 | 108.60 | 119.01 |
| 48 | 33 | 312 | A86 | C33-C32-C31 | 6.62 | 115.64 | 109.21 |
| 47 | 16 | 305 | KC1 | CHB-C4A-C3A | -6.62 | 114.58 | 125.03 |
| 37 | d | 404 | CLA | CMD-C2D-C1D | 6.61 | 136.37 | 124.73 |
| 47 | 35 | 304 | KC1 | CHB-C4A-C3A | -6.61 | 114.60 | 125.03 |
| 37 | 12 | 209 | CLA | O2D-CGD-CBD | 6.61 | 122.78 | 111.23 |
| 47 | 36 | 305 | KC1 | CHB-C4A-C3A | -6.61 | 114.60 | 125.03 |
| 37 | B | 512 | CLA | CHD-C4C-C3C | -6.60 | 115.15 | 124.77 |
| 47 | 16 | 308 | KC1 | O2D-CGD-CBD | 6.60 | 122.77 | 111.23 |
| 37 | 39 | 305 | CLA | CMD-C2D-C1D | 6.60 | 136.34 | 124.73 |
| 47 | 18 | 210 | KC1 | O2D-CGD-CBD | 6.59 | 122.76 | 111.23 |
| 47 | 32 | 209 | KC1 | CMD-C2D-C1D | 6.58 | 135.44 | 125.42 |
| 37 | 12 | 205 | CLA | CMD-C2D-C1D | 6.58 | 136.32 | 124.73 |
| 37 | 15 | 301 | CLA | CMD-C2D-C1D | 6.58 | 136.32 | 124.73 |
| 47 | 36 | 308 | KC1 | O2D-CGD-CBD | 6.58 | 122.74 | 111.23 |
| 47 | 34 | 306 | KC1 | CMD-C2D-C1D | 6.58 | 135.44 | 125.42 |
| 37 | 32 | 202 | CLA | CMD-C2D-C1D | 6.58 | 136.31 | 124.73 |
| 37 | 32 | 206 | CLA | CMD-C2D-C1D | 6.58 | 136.31 | 124.73 |
| 37 | 35 | 301 | CLA | CMD-C2D-C1D | 6.58 | 136.31 | 124.73 |
| 47 | 20 | 302 | KC1 | C3A-C4A-NA | 6.57 | 118.59 | 110.45 |
| 37 | 11 | 308 | CLA | CMD-C2D-C1D | 6.57 | 136.30 | 124.73 |
| 37 | 15 | 305 | CLA | CMD-C2D-C1D | 6.57 | 136.30 | 124.73 |
| 47 | 18 | 207 | KC1 | CHB-C4A-C3A | -6.57 | 114.66 | 125.03 |
| 47 | 33 | 302 | KC1 | C3A-C4A-NA | 6.57 | 118.58 | 110.45 |
| 47 | 13 | 306 | KC1 | CHB-C4A-C3A | -6.57 | 114.66 | 125.03 |
| 47 | 40 | 206 | KC1 | CHB-C4A-C3A | -6.57 | 114.66 | 125.03 |
| 37 | b | 512 | CLA | CHD-C4C-C3C | -6.57 | 115.20 | 124.77 |
| 47 | 14 | 306 | KC1 | CMD-C2D-C1D | 6.56 | 135.41 | 125.42 |
| 47 | 12 | 208 | KC1 | CMD-C2D-C1D | 6.56 | 135.40 | 125.42 |
| 47 | 33 | 306 | KC1 | CMD-C2D-C1D | 6.55 | 135.40 | 125.42 |
| 47 | 21 | 203 | KC1 | CHB-C4A-C3A | -6.55 | 114.68 | 125.03 |
| 47 | 33 | 306 | KC1 | CHB-C4A-C3A | -6.55 | 114.68 | 125.03 |
| 37 | 15 | 308 | CLA | CMD-C2D-C1D | 6.55 | 136.26 | 124.73 |
| 47 | 41 | 203 | KC1 | CHB-C4A-C3A | -6.55 | 114.69 | 125.03 |
| 37 | 33 | 303 | CLA | CMD-C2D-C1D | 6.55 | 136.26 | 124.73 |
| 37 | 19 | 304 | CLA | C2D-C1D-ND | 6.55 | 116.61 | 110.13 |
| 50 | 21 | 212 | DD6 | C8-C6-C5 | -6.55 | 108.71 | 119.01 |
| 50 | 41 | 212 | DD6 | C8-C6-C5 | -6.54 | 108.72 | 119.01 |
| 48 | 17 | 314 | A86 | C4-C5-C6 | -6.54 | 118.10 | 127.28 |
| 47 | 13 | 306 | KC1 | CMD-C2D-C1D | 6.54 | 135.38 | 125.42 |
| 47 | 40 | 204 | KC1 | C3A-C4A-NA | 6.54 | 118.55 | 110.45 |
| 47 | 20 | 304 | KC1 | CHB-C4A-C3A | -6.54 | 114.71 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 308 | CLA | CHD-C4C-C3C | -6.53 | 115.25 | 124.77 |
| 48 | 16 | 310 | A86 | C3-C2-C1 | -6.53 | 118.12 | 127.28 |
| 47 | 13 | 302 | KC1 | C3A-C4A-NA | 6.53 | 118.53 | 110.45 |
| 48 | 15 | 314 | A86 | C3-C2-C1 | -6.53 | 118.12 | 127.28 |
| 37 | 35 | 305 | CLA | CMD-C2D-C1D | 6.53 | 136.22 | 124.73 |
| 37 | 40 | 210 | CLA | CMD-C2D-C1D | 6.52 | 136.22 | 124.73 |
| 37 | 39 | 304 | CLA | C2D-C1D-ND | 6.52 | 116.58 | 110.13 |
| 47 | 35 | 309 | KC1 | CMA-C3A-C4A | -6.52 | 114.84 | 125.03 |
| 37 | B | 513 | CLA | C2D-C1D-ND | 6.52 | 116.58 | 110.13 |
| 37 | 13 | 310 | CLA | CMD-C2D-C1D | 6.52 | 136.21 | 124.73 |
| 37 | 11 | 307 | CLA | CHD-C4C-C3C | -6.51 | 115.27 | 124.77 |
| 37 | B | 501 | CLA | CMD-C2D-C1D | 6.51 | 136.19 | 124.73 |
| 48 | 36 | 310 | A86 | C3-C2-C1 | -6.51 | 118.15 | 127.28 |
| 37 | 31 | 302 | CLA | CHD-C4C-C3C | -6.51 | 115.28 | 124.77 |
| 47 | 36 | 305 | KC1 | CMD-C2D-C1D | 6.51 | 135.33 | 125.42 |
| 37 | C | 505 | CLA | CMD-C2D-C1D | 6.51 | 136.19 | 124.73 |
| 37 | 36 | 309 | CLA | CMD-C2D-C1D | 6.50 | 136.18 | 124.73 |
| 37 | 20 | 308 | CLA | CMD-C2D-C1D | 6.50 | 136.18 | 124.73 |
| 47 | 39 | 308 | KC1 | CMD-C2D-C1D | 6.50 | 135.32 | 125.42 |
| 37 | b | 501 | CLA | CMD-C2D-C1D | 6.50 | 136.18 | 124.73 |
| 47 | 19 | 308 | KC1 | CMD-C2D-C1D | 6.50 | 135.31 | 125.42 |
| 37 | 16 | 309 | CLA | CMD-C2D-C1D | 6.50 | 136.17 | 124.73 |
| 47 | 15 | 309 | KC1 | CMA-C3A-C4A | -6.50 | 114.88 | 125.03 |
| 37 | 32 | 210 | CLA | O2D-CGD-CBD | 6.50 | 122.59 | 111.23 |
| 47 | 38 | 205 | KC1 | CMA-C3A-C2A | -6.50 | 112.71 | 128.43 |
| 37 | 12 | 212 | CLA | CMD-C2D-C1D | 6.50 | 136.17 | 124.73 |
| 37 | 39 | 301 | CLA | C2D-C1D-ND | 6.49 | 116.55 | 110.13 |
| 48 | 33 | 315 | A86 | C33-C32-C31 | 6.49 | 115.52 | 109.21 |
| 48 | 13 | 315 | A86 | C33-C32-C31 | 6.49 | 115.52 | 109.21 |
| 47 | 34 | 306 | KC1 | O2D-CGD-CBD | 6.49 | 122.58 | 111.23 |
| 47 | 16 | 305 | KC1 | CMD-C2D-C1D | 6.49 | 135.30 | 125.42 |
| 47 | 18 | 205 | KC1 | CMA-C3A-C2A | -6.49 | 112.72 | 128.43 |
| 37 | 32 | 213 | CLA | CMD-C2D-C1D | 6.49 | 136.15 | 124.73 |
| 37 | 19 | 305 | CLA | CMD-C2D-C1D | 6.49 | 136.15 | 124.73 |
| 47 | 38 | 210 | KC1 | O2D-CGD-CBD | 6.48 | 122.56 | 111.23 |
| 37 | c | 505 | CLA | CMD-C2D-C1D | 6.48 | 136.15 | 124.73 |
| 37 | c | 507 | CLA | O2D-CGD-CBD | 6.48 | 122.56 | 111.23 |
| 37 | b | 513 | CLA | C2D-C1D-ND | 6.48 | 116.54 | 110.13 |
| 37 | 14 | 303 | CLA | CMD-C2D-C1D | 6.48 | 136.14 | 124.73 |
| 37 | 34 | 303 | CLA | CMD-C2D-C1D | 6.48 | 136.14 | 124.73 |
| 37 | 11 | 301 | CLA | CHD-C4C-C3C | -6.48 | 115.33 | 124.77 |
| 37 | b | 516 | CLA | O2D-CGD-CBD | 6.47 | 122.55 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 34 | 301 | CLA | CMD-C2D-C1D | 6.47 | 136.12 | 124.73 |
| 47 | 14 | 306 | KC1 | O2D-CGD-CBD | 6.47 | 122.54 | 111.23 |
| 48 | 39 | 313 | A86 | O4-C38-C39 | 6.47 | 122.62 | 111.09 |
| 37 | 39 | 302 | CLA | CMD-C2D-C1D | 6.47 | 136.12 | 124.73 |
| 48 | 13 | 314 | A86 | C3-C2-C1 | -6.47 | 118.21 | 127.28 |
| 47 | 39 | 308 | KC1 | CHB-C4A-C3A | -6.47 | 114.82 | 125.03 |
| 37 | b | 512 | CLA | O2D-CGD-CBD | 6.46 | 122.53 | 111.23 |
| 37 | C | 507 | CLA | O2D-CGD-CBD | 6.46 | 122.53 | 111.23 |
| 47 | 19 | 308 | KC1 | CHB-C4A-C3A | -6.45 | 114.85 | 125.03 |
| 48 | 33 | 314 | A86 | C3-C2-C1 | -6.45 | 118.24 | 127.28 |
| 37 | b | 504 | CLA | CMD-C2D-C1D | 6.45 | 136.08 | 124.73 |
| 37 | B | 516 | CLA | O2D-CGD-CBD | 6.44 | 122.50 | 111.23 |
| 47 | 14 | 309 | KC1 | C3A-C4A-NA | 6.44 | 118.42 | 110.45 |
| 37 | b | 523 | CLA | CHD-C4C-C3C | -6.44 | 115.38 | 124.77 |
| 47 | 11 | 309 | KC1 | C3B-C2B-C1B | -6.44 | 100.95 | 107.05 |
| 48 | 11 | 319 | A86 | O4-C38-C39 | 6.44 | 122.57 | 111.09 |
| 37 | B | 512 | CLA | O2D-CGD-CBD | 6.44 | 122.48 | 111.23 |
| 48 | 15 | 313 | A86 | C33-C32-C31 | 6.43 | 115.47 | 109.21 |
| 50 | 39 | 312 | DD6 | C24-C1-C2 | -6.43 | 108.89 | 119.01 |
| 37 | c | 506 | CLA | CMD-C2D-C1D | 6.43 | 136.05 | 124.73 |
| 37 | 14 | 301 | CLA | CMD-C2D-C1D | 6.43 | 136.05 | 124.73 |
| 47 | 34 | 309 | KC1 | C3A-C4A-NA | 6.43 | 118.41 | 110.45 |
| 37 | B | 524 | CLA | CHD-C4C-C3C | -6.43 | 115.40 | 124.77 |
| 48 | 19 | 313 | A86 | O4-C38-C39 | 6.43 | 122.55 | 111.09 |
| 37 | C | 506 | CLA | CMD-C2D-C1D | 6.42 | 136.04 | 124.73 |
| 48 | 37 | 319 | A86 | C4-C5-C6 | -6.42 | 118.27 | 127.28 |
| 37 | 19 | 302 | CLA | CMD-C2D-C1D | 6.42 | 136.04 | 124.73 |
| 37 | 31 | 306 | CLA | CMD-C2D-C1D | 6.42 | 136.03 | 124.73 |
| 48 | 35 | 314 | A86 | C3-C2-C1 | -6.42 | 118.28 | 127.28 |
| 37 | 31 | 304 | CLA | CMD-C2D-C1D | 6.41 | 136.02 | 124.73 |
| 37 | 15 | 310 | CLA | CMD-C2D-C1D | 6.41 | 136.02 | 124.73 |
| 50 | 19 | 312 | DD6 | C24-C1-C2 | -6.41 | 108.93 | 119.01 |
| 37 | 19 | 301 | CLA | C2D-C1D-ND | 6.41 | 116.47 | 110.13 |
| 48 | 31 | 319 | A86 | O4-C38-C39 | 6.41 | 122.52 | 111.09 |
| 37 | B | 504 | CLA | CMD-C2D-C1D | 6.41 | 136.01 | 124.73 |
| 37 | 36 | 307 | CLA | CMD-C2D-C1D | 6.41 | 136.01 | 124.73 |
| 48 | 17 | 312 | A86 | C33-C32-C31 | 6.40 | 115.43 | 109.21 |
| 37 | 34 | 301 | CLA | C2D-C1D-ND | 6.40 | 116.46 | 110.13 |
| 37 | 11 | 303 | CLA | CMD-C2D-C1D | 6.40 | 136.00 | 124.73 |
| 37 | 31 | 304 | CLA | O2D-CGD-CBD | 6.40 | 122.42 | 111.23 |
| 37 | 11 | 305 | CLA | CMD-C2D-C1D | 6.40 | 136.00 | 124.73 |
| 48 | 17 | 311 | A86 | C3-C2-C1 | -6.39 | 118.31 | 127.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 11 | 303 | CLA | O2D-CGD-CBD | 6.39 | 122.41 | 111.23 |
| 37 | 21 | 210 | CLA | CMD-C2D-C1D | 6.39 | 135.99 | 124.73 |
| 37 | 39 | 306 | CLA | C2D-C1D-ND | 6.39 | 116.45 | 110.13 |
| 37 | 16 | 307 | CLA | CMD-C2D-C1D | 6.38 | 135.97 | 124.73 |
| 37 | 41 | 210 | CLA | CMD-C2D-C1D | 6.38 | 135.97 | 124.73 |
| 37 | 19 | 307 | CLA | CMD-C2D-C1D | 6.38 | 135.97 | 124.73 |
| 37 | 39 | 307 | CLA | CMD-C2D-C1D | 6.38 | 135.97 | 124.73 |
| 37 | 21 | 206 | CLA | CHD-C4C-C3C | -6.38 | 115.47 | 124.77 |
| 37 | 41 | 206 | CLA | CHD-C4C-C3C | -6.38 | 115.47 | 124.77 |
| 37 | B | 503 | CLA | CMD-C2D-C1D | 6.38 | 135.96 | 124.73 |
| 37 | 18 | 209 | CLA | C2D-C1D-ND | 6.38 | 116.44 | 110.13 |
| 37 | 19 | 303 | CLA | CMD-C2D-C1D | 6.38 | 135.96 | 124.73 |
| 37 | 39 | 303 | CLA | CMD-C2D-C1D | 6.38 | 135.96 | 124.73 |
| 47 | 21 | 203 | KC1 | C3A-C4A-NA | 6.38 | 118.34 | 110.45 |
| 47 | 31 | 303 | KC1 | CMD-C2D-C1D | 6.38 | 135.13 | 125.42 |
| 47 | 41 | 203 | KC1 | C3A-C4A-NA | 6.37 | 118.34 | 110.45 |
| 47 | 19 | 308 | KC1 | C1A-C2A-C3A | -6.37 | 101.42 | 107.28 |
| 37 | 19 | 306 | CLA | CHD-C4C-C3C | -6.37 | 115.48 | 124.77 |
| 37 | 14 | 301 | CLA | C2D-C1D-ND | 6.37 | 116.43 | 110.13 |
| 37 | 19 | 306 | CLA | C2D-C1D-ND | 6.37 | 116.43 | 110.13 |
| 37 | 34 | 302 | CLA | CMD-C2D-C1D | 6.37 | 135.94 | 124.73 |
| 37 | 13 | 303 | CLA | CMD-C2D-C1D | 6.36 | 135.94 | 124.73 |
| 37 | b | 503 | CLA | CMD-C2D-C1D | 6.36 | 135.93 | 124.73 |
| 47 | 31 | 309 | KC1 | C3B-C2B-C1B | -6.36 | 101.03 | 107.05 |
| 37 | b | 515 | CLA | CMD-C2D-C1D | 6.36 | 135.93 | 124.73 |
| 37 | 18 | 202 | CLA | CHD-C4C-C3C | -6.36 | 115.50 | 124.77 |
| 37 | 14 | 302 | CLA | CMD-C2D-C1D | 6.35 | 135.92 | 124.73 |
| 37 | 39 | 306 | CLA | CHD-C4C-C3C | -6.35 | 115.51 | 124.77 |
| 47 | 34 | 309 | KC1 | C3B-C2B-C1B | -6.35 | 101.04 | 107.05 |
| 47 | 35 | 302 | KC1 | CMA-C3A-C2A | -6.35 | 113.06 | 128.43 |
| 47 | 39 | 308 | KC1 | C1A-C2A-C3A | -6.35 | 101.44 | 107.28 |
| 37 | 38 | 209 | CLA | C2D-C1D-ND | 6.35 | 116.41 | 110.13 |
| 47 | 34 | 309 | KC1 | C2B-C1B-NB | 6.35 | 116.41 | 110.13 |
| 37 | B | 515 | CLA | CMD-C2D-C1D | 6.35 | 135.90 | 124.73 |
| 47 | 11 | 302 | KC1 | CMD-C2D-C1D | 6.34 | 135.08 | 125.42 |
| 48 | 40 | 213 | A86 | C4-C5-C6 | -6.34 | 118.38 | 127.28 |
| 37 | 39 | 305 | CLA | C2D-C1D-ND | 6.34 | 116.40 | 110.13 |
| 48 | 35 | 315 | A86 | C33-C32-C31 | 6.34 | 115.37 | 109.21 |
| 37 | 15 | 301 | CLA | C2D-C1D-ND | 6.34 | 116.40 | 110.13 |
| 37 | 38 | 202 | CLA | CHD-C4C-C3C | -6.34 | 115.53 | 124.77 |
| 37 | 16 | 301 | CLA | CMD-C2D-C1D | 6.33 | 135.88 | 124.73 |
| 37 | 40 | 205 | CLA | CHD-C4C-C3C | -6.33 | 115.54 | 124.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 14 | 309 | KC1 | C2B-C1B-NB | 6.33 | 116.39 | 110.13 |
| 48 | 35 | 313 | A86 | C33-C32-C31 | 6.33 | 115.36 | 109.21 |
| 37 | 34 | 301 | CLA | CHD-C4C-C3C | -6.33 | 115.55 | 124.77 |
| 48 | 20 | 311 | A86 | C4-C5-C6 | -6.33 | 118.41 | 127.28 |
| 48 | 32 | 221 | A86 | C4-C5-C6 | -6.33 | 118.41 | 127.28 |
| 37 | 14 | 301 | CLA | CHD-C4C-C3C | -6.32 | 115.55 | 124.77 |
| 37 | 19 | 309 | CLA | CMD-C2D-C1D | 6.32 | 135.86 | 124.73 |
| 50 | 20 | 310 | DD6 | C7-C6-C8 | -6.32 | 108.43 | 118.09 |
| 37 | 19 | 305 | CLA | C2D-C1D-ND | 6.32 | 116.38 | 110.13 |
| 48 | 12 | 220 | A86 | C4-C5-C6 | -6.32 | 118.42 | 127.28 |
| 48 | 31 | 315 | A86 | C3-C2-C1 | -6.32 | 118.42 | 127.28 |
| 37 | 35 | 301 | CLA | C2D-C1D-ND | 6.32 | 116.38 | 110.13 |
| 37 | 36 | 301 | CLA | CMD-C2D-C1D | 6.32 | 135.85 | 124.73 |
| 48 | 17 | 320 | A86 | C33-C32-C31 | 6.32 | 115.35 | 109.21 |
| 48 | 11 | 315 | A86 | C3-C2-C1 | -6.32 | 118.42 | 127.28 |
| 37 | C | 513 | CLA | C2D-C1D-ND | 6.32 | 116.38 | 110.13 |
| 47 | 41 | 203 | KC1 | C2B-C1B-NB | 6.32 | 116.38 | 110.13 |
| 50 | 40 | 212 | DD6 | C7-C6-C8 | -6.32 | 108.44 | 118.09 |
| 47 | 12 | 208 | KC1 | C3A-C4A-NA | 6.31 | 118.26 | 110.45 |
| 47 | 37 | 302 | KC1 | C1A-C2A-C3A | -6.31 | 101.48 | 107.28 |
| 50 | 41 | 216 | DD6 | O1-C15-C14 | -6.31 | 98.81 | 116.88 |
| 47 | 14 | 309 | KC1 | C3B-C2B-C1B | -6.30 | 101.08 | 107.05 |
| 47 | 34 | 304 | KC1 | C3B-C2B-C1B | -6.30 | 101.08 | 107.05 |
| 37 | 31 | 302 | CLA | C2D-C1D-ND | 6.30 | 116.36 | 110.13 |
| 47 | 35 | 309 | KC1 | C3B-C2B-C1B | -6.30 | 101.09 | 107.05 |
| 48 | 40 | 211 | A86 | C4-C5-C6 | -6.30 | 118.45 | 127.28 |
| 48 | 35 | 313 | A86 | C4-C5-C6 | -6.30 | 118.45 | 127.28 |
| 37 | 20 | 303 | CLA | CHD-C4C-C3C | -6.30 | 115.59 | 124.77 |
| 48 | 15 | 313 | A86 | C4-C5-C6 | -6.29 | 118.45 | 127.28 |
| 37 | 39 | 310 | CLA | CMD-C2D-C1D | 6.29 | 135.81 | 124.73 |
| 37 | c | 513 | CLA | C2D-C1D-ND | 6.29 | 116.35 | 110.13 |
| 47 | 21 | 203 | KC1 | C2B-C1B-NB | 6.29 | 116.35 | 110.13 |
| 48 | 37 | 319 | A86 | C33-C32-C31 | 6.29 | 115.33 | 109.21 |
| 48 | 15 | 312 | A86 | C33-C32-C31 | 6.29 | 115.33 | 109.21 |
| 37 | 39 | 301 | CLA | CMD-C2D-C1D | 6.29 | 135.80 | 124.73 |
| 48 | 35 | 312 | A86 | C33-C32-C31 | 6.29 | 115.32 | 109.21 |
| 47 | 15 | 309 | KC1 | C3B-C2B-C1B | -6.29 | 101.10 | 107.05 |
| 47 | 32 | 209 | KC1 | C3A-C4A-NA | 6.29 | 118.23 | 110.45 |
| 47 | 15 | 302 | KC1 | CMA-C3A-C2A | -6.28 | 113.22 | 128.43 |
| 37 | b | 506 | CLA | C2D-C1D-ND | 6.28 | 116.34 | 110.13 |
| 47 | 17 | 303 | KC1 | C1A-C2A-C3A | -6.28 | 101.51 | 107.28 |
| 50 | 21 | 216 | DD6 | O1-C15-C14 | -6.28 | 98.89 | 116.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 506 | CLA | C2D-C1D-ND | 6.28 | 116.34 | 110.13 |
| 47 | 20 | 302 | KC1 | C2B-C1B-NB | 6.28 | 116.34 | 110.13 |
| 50 | 41 | 216 | DD6 | C12-C11-C13 | -6.28 | 108.50 | 118.09 |
| 37 | C | 512 | CLA | C2D-C1D-ND | 6.28 | 116.34 | 110.13 |
| 37 | B | 504 | CLA | O2D-CGD-CBD | 6.28 | 122.20 | 111.23 |
| 47 | 11 | 309 | KC1 | C2B-C1B-NB | 6.27 | 116.34 | 110.13 |
| 37 | C | 507 | CLA | CHD-C4C-C3C | -6.27 | 115.62 | 124.77 |
| 48 | 15 | 315 | A86 | C33-C32-C31 | 6.27 | 115.31 | 109.21 |
| 37 | 11 | 301 | CLA | C2D-C1D-ND | 6.27 | 116.33 | 110.13 |
| 47 | 41 | 207 | KC1 | C3B-C2B-C1B | -6.27 | 101.12 | 107.05 |
| 47 | 15 | 306 | KC1 | C3B-C2B-C1B | -6.27 | 101.12 | 107.05 |
| 37 | c | 507 | CLA | CHD-C4C-C3C | -6.26 | 115.64 | 124.77 |
| 47 | 21 | 207 | KC1 | C3B-C2B-C1B | -6.26 | 101.12 | 107.05 |
| 47 | 40 | 204 | KC1 | C2B-C1B-NB | 6.26 | 116.33 | 110.13 |
| 37 | A | 405 | CLA | CMD-C2D-C1D | 6.26 | 135.75 | 124.73 |
| 50 | 21 | 216 | DD6 | C12-C11-C13 | -6.26 | 108.53 | 118.09 |
| 37 | b | 504 | CLA | O2D-CGD-CBD | 6.25 | 122.16 | 111.23 |
| 47 | 17 | 308 | KC1 | C3B-C2B-C1B | -6.25 | 101.13 | 107.05 |
| 47 | 13 | 306 | KC1 | C2D-C1D-ND | 6.25 | 116.81 | 110.33 |
| 47 | 33 | 302 | KC1 | C2B-C1B-NB | 6.25 | 116.31 | 110.13 |
| 47 | 35 | 309 | KC1 | CMD-C2D-C1D | 6.25 | 134.93 | 125.42 |
| 47 | 18 | 210 | KC1 | C3A-C4A-NA | 6.25 | 118.18 | 110.45 |
| 47 | 31 | 309 | KC1 | C2B-C1B-NB | 6.25 | 116.31 | 110.13 |
| 47 | 15 | 302 | KC1 | C3A-C4A-NA | 6.25 | 118.18 | 110.45 |
| 47 | 13 | 302 | KC1 | CMA-C3A-C2A | -6.24 | 113.32 | 128.43 |
| 37 | 19 | 301 | CLA | CMD-C2D-C1D | 6.24 | 135.72 | 124.73 |
| 47 | 38 | 207 | KC1 | CMD-C2D-C1D | 6.24 | 134.92 | 125.42 |
| 37 | 19 | 310 | CLA | CMD-C2D-C1D | 6.24 | 135.72 | 124.73 |
| 50 | 41 | 212 | DD6 | C7-C6-C8 | -6.24 | 108.56 | 118.09 |
| 47 | 14 | 304 | KC1 | C3B-C2B-C1B | -6.24 | 101.14 | 107.05 |
| 37 | 33 | 310 | CLA | CMD-C2D-C1D | 6.24 | 135.72 | 124.73 |
| 48 | 20 | 309 | A86 | C4-C5-C6 | -6.24 | 118.53 | 127.28 |
| 50 | 21 | 212 | DD6 | C7-C6-C8 | -6.23 | 108.56 | 118.09 |
| 48 | 18 | 213 | A86 | C3-C2-C1 | -6.23 | 118.54 | 127.28 |
| 47 | 18 | 207 | KC1 | CMD-C2D-C1D | 6.23 | 134.91 | 125.42 |
| 37 | c | 512 | CLA | O2D-CGD-CBD | 6.23 | 122.12 | 111.23 |
| 37 | 11 | 307 | CLA | C2D-C1D-ND | 6.23 | 116.29 | 110.13 |
| 37 | a | 407 | CLA | CMD-C2D-C1D | 6.23 | 135.70 | 124.73 |
| 47 | 13 | 302 | KC1 | C2B-C1B-NB | 6.23 | 116.29 | 110.13 |
| 47 | 15 | 302 | KC1 | C3B-C2B-C1B | -6.23 | 101.15 | 107.05 |
| 37 | 31 | 301 | CLA | CMD-C2D-C1D | 6.23 | 135.70 | 124.73 |
| 37 | d | 403 | CLA | CMD-C2D-C1D | 6.23 | 135.69 | 124.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 11 | 307 | CLA | O2D-CGD-CBD | 6.23 | 122.11 | 111.23 |
| 37 | c | 507 | CLA | CMD-C2D-C1D | 6.22 | 135.69 | 124.73 |
| 37 | 18 | 201 | CLA | C2D-C1D-ND | 6.22 | 116.29 | 110.13 |
| 47 | 11 | 309 | KC1 | O2D-CGD-CBD | 6.22 | 122.11 | 111.23 |
| 47 | 33 | 302 | KC1 | CMA-C3A-C2A | -6.22 | 113.37 | 128.43 |
| 37 | c | 508 | CLA | C2D-C1D-ND | 6.22 | 116.28 | 110.13 |
| 47 | 33 | 306 | KC1 | C2D-C1D-ND | 6.22 | 116.77 | 110.33 |
| 37 | c | 505 | CLA | CHD-C4C-C3C | -6.22 | 115.71 | 124.77 |
| 47 | 31 | 305 | KC1 | C3A-C4A-NA | 6.22 | 118.14 | 110.45 |
| 37 | C | 512 | CLA | O2D-CGD-CBD | 6.22 | 122.10 | 111.23 |
| 37 | 35 | 308 | CLA | CMD-C2D-C1D | 6.21 | 135.67 | 124.73 |
| 37 | D | 405 | CLA | CMD-C2D-C1D | 6.21 | 135.67 | 124.73 |
| 48 | 13 | 314 | A86 | C25-C26-C27 | -6.21 | 118.56 | 127.28 |
| 37 | 31 | 308 | CLA | O2D-CGD-CBD | 6.21 | 122.09 | 111.23 |
| 48 | 31 | 311 | A86 | O4-C38-C39 | 6.21 | 122.16 | 111.09 |
| 37 | C | 505 | CLA | CHD-C4C-C3C | -6.21 | 115.72 | 124.77 |
| 37 | c | 513 | CLA | CHD-C4C-C3C | -6.21 | 115.72 | 124.77 |
| 47 | 12 | 211 | KC1 | C2B-C1B-NB | 6.21 | 116.27 | 110.13 |
| 48 | 12 | 202 | A86 | C3-C2-C1 | -6.20 | 118.58 | 127.28 |
| 48 | 37 | 311 | A86 | C33-C32-C31 | 6.20 | 115.24 | 109.21 |
| 37 | c | 512 | CLA | C2D-C1D-ND | 6.20 | 116.27 | 110.13 |
| 37 | W | 102 | CLA | CMD-C2D-C1D | 6.20 | 135.65 | 124.73 |
| 37 | C | 507 | CLA | CMD-C2D-C1D | 6.20 | 135.65 | 124.73 |
| 37 | W | 101 | CLA | C2D-C1D-ND | 6.20 | 116.26 | 110.13 |
| 47 | 11 | 304 | KC1 | C3A-C4A-NA | 6.20 | 118.12 | 110.45 |
| 47 | 38 | 210 | KC1 | C3A-C4A-NA | 6.20 | 118.12 | 110.45 |
| 37 | C | 508 | CLA | C2D-C1D-ND | 6.20 | 116.26 | 110.13 |
| 50 | 41 | 212 | DD6 | C28-C27-C26 | -6.19 | 112.15 | 124.18 |
| 37 | C | 513 | CLA | CHD-C4C-C3C | -6.19 | 115.74 | 124.77 |
| 37 | 36 | 301 | CLA | CHD-C4C-C3C | -6.19 | 115.74 | 124.77 |
| 37 | 16 | 301 | CLA | CHD-C4C-C3C | -6.19 | 115.75 | 124.77 |
| 37 | 31 | 308 | CLA | C2D-C1D-ND | 6.19 | 116.25 | 110.13 |
| 48 | 32 | 203 | A86 | C3-C2-C1 | -6.19 | 118.60 | 127.28 |
| 47 | 32 | 212 | KC1 | C2B-C1B-NB | 6.19 | 116.25 | 110.13 |
| 48 | 11 | 311 | A86 | O4-C38-C39 | 6.19 | 122.12 | 111.09 |
| 47 | 15 | 309 | KC1 | C3A-C4A-NA | 6.19 | 118.11 | 110.45 |
| 37 | B | 513 | CLA | CHD-C4C-C3C | -6.19 | 115.75 | 124.77 |
| 48 | 33 | 314 | A86 | C25-C26-C27 | -6.18 | 118.60 | 127.28 |
| 47 | 13 | 304 | KC1 | C3A-C4A-NA | 6.18 | 118.10 | 110.45 |
| 37 | b | 509 | CLA | CHD-C4C-C3C | -6.18 | 115.76 | 124.77 |
| 37 | b | 514 | CLA | O2D-CGD-CBD | 6.18 | 122.04 | 111.23 |
| 47 | 21 | 207 | KC1 | C2B-C1B-NB | 6.18 | 116.24 | 110.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 17 | 308 | KC1 | C2B-C1B-NB | 6.18 | 116.24 | 110.13 |
| 47 | 31 | 309 | KC1 | O2D-CGD-CBD | 6.18 | 122.03 | 111.23 |
| 37 | 40 | 203 | CLA | CHD-C4C-C3C | -6.18 | 115.77 | 124.77 |
| 47 | 15 | 309 | KC1 | CMD-C2D-C1D | 6.18 | 134.82 | 125.42 |
| 47 | 37 | 307 | KC1 | C3B-C2B-C1B | -6.17 | 101.20 | 107.05 |
| 47 | 41 | 207 | KC1 | C2B-C1B-NB | 6.17 | 116.24 | 110.13 |
| 48 | 39 | 311 | A86 | C3-C2-C1 | -6.17 | 118.62 | 127.28 |
| 37 | b | 516 | CLA | CMD-C2D-C1D | 6.17 | 135.60 | 124.73 |
| 37 | B | 514 | CLA | O2D-CGD-CBD | 6.17 | 122.02 | 111.23 |
| 47 | 35 | 309 | KC1 | C3A-C4A-NA | 6.17 | 118.09 | 110.45 |
| 47 | 35 | 306 | KC1 | C3B-C2B-C1B | -6.17 | 101.21 | 107.05 |
| 48 | 37 | 309 | A86 | O4-C38-C39 | 6.17 | 122.09 | 111.09 |
| 47 | 37 | 307 | KC1 | C3A-C4A-NA | 6.17 | 118.09 | 110.45 |
| 47 | 33 | 304 | KC1 | C3A-C4A-NA | 6.17 | 118.08 | 110.45 |
| 37 | B | 509 | CLA | CHD-C4C-C3C | -6.17 | 115.78 | 124.77 |
| 37 | 20 | 301 | CLA | CHD-C4C-C3C | -6.16 | 115.79 | 124.77 |
| 37 | b | 513 | CLA | CHD-C4C-C3C | -6.16 | 115.79 | 124.77 |
| 50 | 21 | 212 | DD6 | C28-C27-C26 | -6.16 | 112.22 | 124.18 |
| 48 | 34 | 316 | A86 | O4-C38-C39 | 6.16 | 122.07 | 111.09 |
| 48 | 14 | 316 | A86 | O4-C38-C39 | 6.16 | 122.07 | 111.09 |
| 37 | B | 516 | CLA | CMD-C2D-C1D | 6.15 | 135.56 | 124.73 |
| 47 | 33 | 309 | KC1 | C3A-C4A-NA | 6.15 | 118.06 | 110.45 |
| 47 | 17 | 308 | KC1 | C3A-C4A-NA | 6.15 | 118.06 | 110.45 |
| 37 | b | 510 | CLA | CMD-C2D-C1D | 6.15 | 135.56 | 124.73 |
| 37 | C | 512 | CLA | C2B-C1B-NB | 6.14 | 116.70 | 110.33 |
| 47 | 33 | 306 | KC1 | C1A-C2A-C3A | -6.14 | 101.63 | 107.28 |
| 47 | 11 | 306 | KC1 | C3B-C2B-C1B | -6.14 | 101.23 | 107.05 |
| 47 | 34 | 304 | KC1 | C3A-C4A-NA | 6.14 | 118.05 | 110.45 |
| 48 | 19 | 311 | A86 | C3-C2-C1 | -6.14 | 118.67 | 127.28 |
| 47 | 37 | 307 | KC1 | C2B-C1B-NB | 6.14 | 116.20 | 110.13 |
| 37 | C | 506 | CLA | C2C-C1C-NC | 6.14 | 116.43 | 109.98 |
| 48 | 17 | 310 | A86 | O4-C38-C39 | 6.14 | 122.03 | 111.09 |
| 48 | 12 | 214 | A86 | C33-C32-C31 | 6.13 | 115.17 | 109.21 |
| 48 | 17 | 320 | A86 | C4-C5-C6 | -6.13 | 118.68 | 127.28 |
| 37 | 35 | 303 | CLA | O2D-CGD-CBD | 6.13 | 121.95 | 111.23 |
| 37 | B | 510 | CLA | CMD-C2D-C1D | 6.13 | 135.52 | 124.73 |
| 37 | 15 | 307 | CLA | C2B-C1B-NB | 6.13 | 116.68 | 110.33 |
| 37 | c | 512 | CLA | C2B-C1B-NB | 6.13 | 116.68 | 110.33 |
| 37 | 39 | 301 | CLA | CHD-C4C-C3C | -6.13 | 115.84 | 124.77 |
| 37 | 19 | 301 | CLA | CHD-C4C-C3C | -6.13 | 115.84 | 124.77 |
| 37 | 36 | 309 | CLA | C2D-C1D-ND | 6.12 | 116.19 | 110.13 |
| 37 | 38 | 208 | CLA | CMD-C2D-C1D | 6.12 | 135.51 | 124.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 13 | 309 | KC1 | C3A-C4A-NA | 6.12 | 118.03 | 110.45 |
| 37 | 31 | 310 | CLA | C2D-C1D-ND | 6.12 | 116.19 | 110.13 |
| 37 | c | 506 | CLA | C2C-C1C-NC | 6.12 | 116.41 | 109.98 |
| 47 | 37 | 304 | KC1 | C1A-C2A-C3A | -6.12 | 101.66 | 107.28 |
| 37 | 16 | 309 | CLA | C2D-C1D-ND | 6.12 | 116.18 | 110.13 |
| 47 | 20 | 302 | KC1 | C3B-C2B-C1B | -6.12 | 101.26 | 107.05 |
| 47 | 13 | 306 | KC1 | C1A-C2A-C3A | -6.12 | 101.66 | 107.28 |
| 37 | w | 101 | CLA | C2D-C1D-ND | 6.11 | 116.18 | 110.13 |
| 47 | 13 | 309 | KC1 | CMD-C2D-C1D | 6.11 | 134.73 | 125.42 |
| 47 | 35 | 302 | KC1 | C3B-C2B-C1B | -6.11 | 101.26 | 107.05 |
| 48 | 32 | 215 | A86 | C33-C32-C31 | 6.11 | 115.15 | 109.21 |
| 47 | 37 | 304 | KC1 | C3B-C2B-C1B | -6.11 | 101.27 | 107.05 |
| 47 | 32 | 207 | KC1 | C3C-C4C-NC | 6.11 | 116.44 | 109.90 |
| 37 | c | 504 | CLA | C2D-C1D-ND | 6.11 | 116.17 | 110.13 |
| 47 | 11 | 302 | KC1 | C2B-C1B-NB | 6.11 | 116.17 | 110.13 |
| 48 | 12 | 216 | A86 | C3-C2-C1 | -6.11 | 118.72 | 127.28 |
| 47 | 31 | 307 | KC1 | C3B-C2B-C1B | -6.10 | 101.27 | 107.05 |
| 37 | 21 | 206 | CLA | C2D-C1D-ND | 6.10 | 116.17 | 110.13 |
| 47 | 14 | 304 | KC1 | C3A-C4A-NA | 6.10 | 118.00 | 110.45 |
| 37 | 19 | 303 | CLA | CAA-C2A-C3A | -6.10 | 96.51 | 113.00 |
| 48 | 34 | 314 | A86 | C3-C2-C1 | -6.10 | 118.72 | 127.28 |
| 47 | 33 | 309 | KC1 | CMD-C2D-C1D | 6.10 | 134.70 | 125.42 |
| 37 | C | 504 | CLA | C2D-C1D-ND | 6.10 | 116.16 | 110.13 |
| 37 | 11 | 310 | CLA | C2D-C1D-ND | 6.10 | 116.16 | 110.13 |
| 47 | 31 | 303 | KC1 | C2B-C1B-NB | 6.10 | 116.16 | 110.13 |
| 47 | 40 | 204 | KC1 | C3B-C2B-C1B | -6.10 | 101.28 | 107.05 |
| 47 | 35 | 306 | KC1 | CMA-C3A-C2A | -6.09 | 113.68 | 128.43 |
| 48 | 14 | 314 | A86 | C3-C2-C1 | -6.09 | 118.73 | 127.28 |
| 47 | 12 | 206 | KC1 | C3C-C4C-NC | 6.09 | 116.43 | 109.90 |
| 37 | 35 | 307 | CLA | CHD-C4C-C3C | -6.09 | 115.89 | 124.77 |
| 47 | 11 | 309 | KC1 | C3A-C4A-NA | 6.09 | 117.99 | 110.45 |
| 37 | 36 | 307 | CLA | C2D-C1D-ND | 6.09 | 116.15 | 110.13 |
| 37 | 35 | 307 | CLA | C2B-C1B-NB | 6.08 | 116.64 | 110.33 |
| 37 | 21 | 210 | CLA | C2D-C1D-ND | 6.08 | 116.15 | 110.13 |
| 47 | 35 | 302 | KC1 | C3A-C4A-NA | 6.08 | 117.98 | 110.45 |
| 37 | 41 | 210 | CLA | C2D-C1D-ND | 6.08 | 116.15 | 110.13 |
| 37 | 39 | 303 | CLA | CAA-C2A-C3A | -6.08 | 96.57 | 113.00 |
| 37 | 32 | 211 | CLA | CMD-C2D-C1D | 6.08 | 135.44 | 124.73 |
| 37 | b | 508 | CLA | CMD-C2D-C1D | 6.08 | 135.44 | 124.73 |
| 37 | 12 | 210 | CLA | CMD-C2D-C1D | 6.08 | 135.43 | 124.73 |
| 37 | B | 508 | CLA | CMD-C2D-C1D | 6.08 | 135.43 | 124.73 |
| 37 | 41 | 206 | CLA | C2D-C1D-ND | 6.08 | 116.14 | 110.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 21 | 203 | KC1 | C3B-C2B-C1B | -6.06 | 101.31 | 107.05 |
| 37 | C | 503 | CLA | C2B-C1B-NB | 6.06 | 116.61 | 110.33 |
| 47 | 12 | 211 | KC1 | C3B-C2B-C1B | -6.06 | 101.31 | 107.05 |
| 37 | 21 | 205 | CLA | C2D-C1D-ND | 6.06 | 116.12 | 110.13 |
| 48 | 12 | 217 | A86 | O4-C38-C39 | 6.06 | 121.90 | 111.09 |
| 37 | 31 | 310 | CLA | CMD-C2D-C1D | 6.06 | 135.39 | 124.73 |
| 47 | 31 | 309 | KC1 | C3A-C4A-NA | 6.06 | 117.94 | 110.45 |
| 48 | 38 | 214 | A86 | C3-C2-C1 | -6.06 | 118.79 | 127.28 |
| 37 | 15 | 307 | CLA | CHD-C4C-C3C | -6.05 | 115.94 | 124.77 |
| 37 | 16 | 309 | CLA | CAA-C2A-C3A | -6.05 | 96.64 | 113.00 |
| 37 | 11 | 310 | CLA | CMD-C2D-C1D | 6.05 | 135.39 | 124.73 |
| 48 | 32 | 218 | A86 | O4-C38-C39 | 6.05 | 121.89 | 111.09 |
| 37 | D | 406 | CLA | C2D-C1D-ND | 6.05 | 116.12 | 110.13 |
| 37 | c | 509 | CLA | O2D-CGD-CBD | 6.05 | 121.81 | 111.23 |
| 48 | 31 | 313 | A86 | C25-C26-C27 | -6.05 | 118.79 | 127.28 |
| 37 | a | 404 | CLA | C2D-C1D-ND | 6.05 | 116.11 | 110.13 |
| 47 | 18 | 205 | KC1 | C3A-C4A-NA | 6.05 | 117.94 | 110.45 |
| 37 | c | 503 | CLA | C2B-C1B-NB | 6.05 | 116.60 | 110.33 |
| 37 | b | 505 | CLA | C2D-C1D-ND | 6.05 | 116.11 | 110.13 |
| 47 | 32 | 212 | KC1 | C3B-C2B-C1B | -6.05 | 101.32 | 107.05 |
| 47 | 38 | 205 | KC1 | C3A-C4A-NA | 6.05 | 117.93 | 110.45 |
| 37 | C | 509 | CLA | O2D-CGD-CBD | 6.04 | 121.80 | 111.23 |
| 48 | 32 | 217 | A86 | C3-C2-C1 | -6.04 | 118.80 | 127.28 |
| 37 | D | 401 | CLA | C2D-C1D-ND | 6.04 | 116.11 | 110.13 |
| 37 | 41 | 205 | CLA | C2D-C1D-ND | 6.04 | 116.11 | 110.13 |
| 48 | 12 | 214 | A86 | C3-C2-C1 | -6.04 | 118.80 | 127.28 |
| 37 | c | 508 | CLA | CHD-C4C-C3C | -6.04 | 115.96 | 124.77 |
| 47 | 32 | 207 | KC1 | C3A-C4A-NA | 6.04 | 117.93 | 110.45 |
| 37 | 35 | 301 | CLA | CHD-C4C-C3C | -6.04 | 115.97 | 124.77 |
| 37 | 36 | 309 | CLA | CAA-C2A-C3A | -6.04 | 96.68 | 113.00 |
| 47 | 38 | 210 | KC1 | CBA-CAA-C2A | -6.04 | 101.22 | 125.45 |
| 48 | 15 | 311 | A86 | O4-C38-C39 | 6.04 | 121.85 | 111.09 |
| 37 | 21 | 204 | CLA | O2D-CGD-CBD | 6.04 | 121.78 | 111.23 |
| 47 | 12 | 206 | KC1 | C3A-C4A-NA | 6.03 | 117.92 | 110.45 |
| 47 | 41 | 203 | KC1 | C3B-C2B-C1B | -6.03 | 101.34 | 107.05 |
| 47 | 18 | 210 | KC1 | CBA-CAA-C2A | -6.03 | 101.24 | 125.45 |
| 37 | A | 405 | CLA | C2D-C1D-ND | 6.03 | 116.10 | 110.13 |
| 37 | 16 | 307 | CLA | C2D-C1D-ND | 6.03 | 116.10 | 110.13 |
| 48 | 12 | 215 | A86 | C33-C32-C31 | 6.03 | 115.07 | 109.21 |
| 47 | 41 | 207 | KC1 | O2D-CGD-CBD | 6.03 | 121.77 | 111.23 |
| 37 | d | 404 | CLA | C2D-C1D-ND | 6.03 | 116.09 | 110.13 |
| 47 | 21 | 207 | KC1 | C3A-C4A-NA | 6.02 | 117.91 | 110.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 209 | CLA | C2B-C1B-NB | 6.02 | 116.57 | 110.33 |
| 37 | B | 506 | CLA | CHD-C4C-C3C | -6.02 | 116.00 | 124.77 |
| 37 | 20 | 303 | CLA | C2D-C1D-ND | 6.02 | 116.08 | 110.13 |
| 47 | 12 | 211 | KC1 | C3A-C4A-NA | 6.02 | 117.90 | 110.45 |
| 48 | 39 | 311 | A86 | O4-C38-C39 | 6.02 | 121.82 | 111.09 |
| 47 | 13 | 306 | KC1 | CMA-C3A-C2A | -6.02 | 113.87 | 128.43 |
| 47 | 33 | 306 | KC1 | CMA-C3A-C2A | -6.02 | 113.87 | 128.43 |
| 47 | 17 | 305 | KC1 | C1A-C2A-C3A | -6.02 | 101.75 | 107.28 |
| 37 | 18 | 208 | CLA | CMD-C2D-C1D | 6.02 | 135.32 | 124.73 |
| 47 | 20 | 305 | KC1 | C3A-C4A-NA | 6.01 | 117.89 | 110.45 |
| 37 | 15 | 301 | CLA | CHD-C4C-C3C | -6.01 | 116.01 | 124.77 |
| 48 | 19 | 311 | A86 | O4-C38-C39 | 6.01 | 121.81 | 111.09 |
| 48 | 32 | 215 | A86 | C3-C2-C1 | -6.01 | 118.85 | 127.28 |
| 37 | 41 | 204 | CLA | O2D-CGD-CBD | 6.01 | 121.73 | 111.23 |
| 37 | c | 511 | CLA | CHD-C4C-C3C | -6.01 | 116.01 | 124.77 |
| 47 | 21 | 207 | KC1 | O2D-CGD-CBD | 6.01 | 121.73 | 111.23 |
| 37 | b | 506 | CLA | CHD-C4C-C3C | -6.01 | 116.02 | 124.77 |
| 47 | 18 | 207 | KC1 | CMA-C3A-C2A | -6.01 | 113.89 | 128.43 |
| 37 | B | 501 | CLA | O2D-CGD-CBD | 6.01 | 121.73 | 111.23 |
| 48 | 32 | 216 | A86 | C33-C32-C31 | 6.00 | 115.05 | 109.21 |
| 37 | B | 510 | CLA | O2D-CGD-CBD | 6.00 | 121.72 | 111.23 |
| 37 | a | 407 | CLA | C2D-C1D-ND | 6.00 | 116.07 | 110.13 |
| 37 | C | 508 | CLA | CHD-C4C-C3C | -6.00 | 116.03 | 124.77 |
| 37 | B | 516 | CLA | C2D-C1D-ND | 6.00 | 116.06 | 110.13 |
| 37 | 31 | 310 | CLA | CHD-C4C-C3C | -6.00 | 116.03 | 124.77 |
| 47 | 41 | 207 | KC1 | C3A-C4A-NA | 5.99 | 117.87 | 110.45 |
| 37 | B | 505 | CLA | C2D-C1D-ND | 5.99 | 116.06 | 110.13 |
| 37 | b | 510 | CLA | O2D-CGD-CBD | 5.99 | 121.70 | 111.23 |
| 47 | 32 | 212 | KC1 | C3A-C4A-NA | 5.99 | 117.86 | 110.45 |
| 37 | b | 501 | CLA | O2D-CGD-CBD | 5.99 | 121.70 | 111.23 |
| 37 | B | 509 | CLA | C2D-C1D-ND | 5.99 | 116.05 | 110.13 |
| 48 | 16 | 314 | A86 | C3-C2-C1 | -5.99 | 118.88 | 127.28 |
| 37 | 40 | 205 | CLA | C2D-C1D-ND | 5.99 | 116.05 | 110.13 |
| 37 | C | 511 | CLA | CHD-C4C-C3C | -5.99 | 116.04 | 124.77 |
| 37 | 12 | 212 | CLA | CHD-C4C-C3C | -5.99 | 116.05 | 124.77 |
| 37 | b | 516 | CLA | C2D-C1D-ND | 5.98 | 116.05 | 110.13 |
| 47 | 37 | 304 | KC1 | C3A-C4A-NA | 5.98 | 117.85 | 110.45 |
| 37 | b | 509 | CLA | C2D-C1D-ND | 5.98 | 116.04 | 110.13 |
| 37 | 11 | 310 | CLA | CHD-C4C-C3C | -5.98 | 116.06 | 124.77 |
| 37 | 36 | 306 | CLA | CHD-C4C-C3C | -5.97 | 116.06 | 124.77 |
| 37 | 32 | 210 | CLA | C2B-C1B-NB | 5.97 | 116.52 | 110.33 |
| 37 | B | 516 | CLA | C4A-NA-C1A | -5.97 | 103.95 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 15 | 306 | KC1 | C3A-C4A-NA | 5.97 | 117.84 | 110.45 |
| 50 | 20 | 310 | DD6 | C-C1-C24 | -5.97 | 108.97 | 118.09 |
| 47 | 15 | 306 | KC1 | CMA-C3A-C2A | -5.97 | 113.98 | 128.43 |
| 47 | 12 | 206 | KC1 | CHD-C4C-C3C | -5.96 | 114.23 | 125.23 |
| 37 | b | 510 | CLA | CHD-C4C-C3C | -5.96 | 116.08 | 124.77 |
| 37 | c | 502 | CLA | C2D-C1D-ND | 5.96 | 116.03 | 110.13 |
| 47 | 12 | 206 | KC1 | C2D-C1D-ND | 5.96 | 116.51 | 110.33 |
| 47 | 32 | 207 | KC1 | CHD-C4C-C3C | -5.96 | 114.23 | 125.23 |
| 47 | 17 | 303 | KC1 | C3A-C4A-NA | 5.96 | 117.83 | 110.45 |
| 37 | 32 | 204 | CLA | CHD-C4C-C3C | -5.96 | 116.08 | 124.77 |
| 37 | C | 502 | CLA | C2D-C1D-ND | 5.96 | 116.02 | 110.13 |
| 47 | 38 | 207 | KC1 | C3A-C4A-NA | 5.96 | 117.83 | 110.45 |
| 48 | 36 | 313 | A86 | C3-C2-C1 | -5.96 | 118.92 | 127.28 |
| 37 | B | 515 | CLA | C2D-C1D-ND | 5.96 | 116.02 | 110.13 |
| 37 | B | 510 | CLA | CHD-C4C-C3C | -5.96 | 116.09 | 124.77 |
| 47 | 35 | 304 | KC1 | C3A-C4A-NA | 5.96 | 117.82 | 110.45 |
| 37 | 16 | 306 | CLA | CHD-C4C-C3C | -5.95 | 116.09 | 124.77 |
| 37 | w | 101 | CLA | CHD-C4C-C3C | -5.95 | 116.09 | 124.77 |
| 50 | 40 | 212 | DD6 | C-C1-C24 | -5.95 | 109.00 | 118.09 |
| 47 | 36 | 304 | KC1 | C3A-C4A-NA | 5.95 | 117.81 | 110.45 |
| 47 | 40 | 207 | KC1 | C3A-C4A-NA | 5.95 | 117.81 | 110.45 |
| 47 | 32 | 212 | KC1 | O2D-CGD-CBD | 5.95 | 121.62 | 111.23 |
| 47 | 32 | 212 | KC1 | C1A-C2A-C3A | -5.95 | 101.81 | 107.28 |
| 37 | C | 502 | CLA | CHD-C4C-C3C | -5.94 | 116.11 | 124.77 |
| 37 | 32 | 205 | CLA | CHD-C4C-C3C | -5.94 | 116.11 | 124.77 |
| 48 | 34 | 312 | A86 | C25-C26-C27 | -5.94 | 118.94 | 127.28 |
| 37 | d | 403 | CLA | CHD-C4C-C3C | -5.94 | 116.11 | 124.77 |
| 37 | b | 515 | CLA | C2D-C1D-ND | 5.94 | 116.00 | 110.13 |
| 37 | 40 | 205 | CLA | CAA-C2A-C3A | -5.94 | 96.95 | 113.00 |
| 47 | 16 | 304 | KC1 | C3A-C4A-NA | 5.94 | 117.80 | 110.45 |
| 37 | 12 | 203 | CLA | CHD-C4C-C3C | -5.94 | 116.12 | 124.77 |
| 37 | 32 | 213 | CLA | CHD-C4C-C3C | -5.93 | 116.12 | 124.77 |
| 37 | 40 | 208 | CLA | CMD-C2D-C1D | 5.93 | 135.18 | 124.73 |
| 47 | 12 | 211 | KC1 | O2D-CGD-CBD | 5.93 | 121.60 | 111.23 |
| 37 | z | 102 | CLA | CHD-C4C-C3C | -5.93 | 116.12 | 124.77 |
| 47 | 20 | 305 | KC1 | CMA-C3A-C2A | -5.93 | 114.07 | 128.43 |
| 48 | 13 | 315 | A86 | O4-C38-C39 | 5.93 | 121.67 | 111.09 |
| 37 | W | 101 | CLA | CHD-C4C-C3C | -5.93 | 116.13 | 124.77 |
| 47 | 11 | 306 | KC1 | C3A-C4A-NA | 5.93 | 117.79 | 110.45 |
| 37 | z | 101 | CLA | CHD-C4C-C3C | -5.93 | 116.13 | 124.77 |
| 47 | 11 | 306 | KC1 | O2D-CGD-CBD | 5.93 | 121.59 | 111.23 |
| 48 | 14 | 312 | A86 | C25-C26-C27 | -5.93 | 118.96 | 127.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 20 | 306 | CLA | CMD-C2D-C1D | 5.93 | 135.17 | 124.73 |
| 37 | 38 | 208 | CLA | CHD-C4C-C3C | -5.93 | 116.13 | 124.77 |
| 37 | c | 502 | CLA | CHD-C4C-C3C | -5.93 | 116.13 | 124.77 |
| 37 | 12 | 204 | CLA | CHD-C4C-C3C | -5.93 | 116.13 | 124.77 |
| 37 | Z | 102 | CLA | CHD-C4C-C3C | -5.93 | 116.13 | 124.77 |
| 37 | 20 | 303 | CLA | CAA-C2A-C3A | -5.92 | 96.99 | 113.00 |
| 37 | D | 405 | CLA | CHD-C4C-C3C | -5.92 | 116.14 | 124.77 |
| 37 | C | 503 | CLA | C2D-C1D-ND | 5.92 | 115.99 | 110.13 |
| 47 | 35 | 302 | KC1 | C1A-C2A-C3A | -5.92 | 101.84 | 107.28 |
| 37 | 33 | 301 | CLA | C2D-C1D-ND | 5.92 | 115.99 | 110.13 |
| 37 | 39 | 303 | CLA | CHD-C4C-C3C | -5.92 | 116.14 | 124.77 |
| 37 | c | 503 | CLA | C2D-C1D-ND | 5.92 | 115.98 | 110.13 |
| 47 | 38 | 210 | KC1 | C2B-C1B-NB | 5.92 | 115.98 | 110.13 |
| 48 | 38 | 213 | A86 | C4-C5-C6 | -5.92 | 118.98 | 127.28 |
| 37 | 13 | 301 | CLA | C2D-C1D-ND | 5.92 | 115.98 | 110.13 |
| 37 | B | 511 | CLA | C2D-C1D-ND | 5.91 | 115.98 | 110.13 |
| 37 | 19 | 303 | CLA | CHD-C4C-C3C | -5.91 | 116.15 | 124.77 |
| 47 | 32 | 207 | KC1 | C2D-C1D-ND | 5.91 | 116.46 | 110.33 |
| 48 | 33 | 315 | A86 | O4-C38-C39 | 5.91 | 121.63 | 111.09 |
| 47 | 34 | 309 | KC1 | CBA-CAA-C2A | -5.91 | 101.72 | 125.45 |
| 48 | 35 | 316 | A86 | O4-C38-C39 | 5.91 | 121.63 | 111.09 |
| 47 | 37 | 302 | KC1 | C3A-C4A-NA | 5.91 | 117.77 | 110.45 |
| 48 | 19 | 311 | A86 | C33-C32-C31 | 5.91 | 114.96 | 109.21 |
| 37 | 40 | 203 | CLA | C2D-C1D-ND | 5.91 | 115.98 | 110.13 |
| 47 | 31 | 307 | KC1 | C3A-C4A-NA | 5.91 | 117.77 | 110.45 |
| 37 | 34 | 307 | CLA | C2B-C1B-NB | 5.91 | 116.45 | 110.33 |
| 37 | 13 | 307 | CLA | CMD-C2D-C1D | 5.91 | 135.13 | 124.73 |
| 48 | 18 | 214 | A86 | C3-C2-C1 | -5.91 | 118.99 | 127.28 |
| 47 | 36 | 308 | KC1 | C3A-C4A-NA | 5.91 | 117.76 | 110.45 |
| 37 | 14 | 302 | CLA | CHD-C4C-C3C | -5.91 | 116.16 | 124.77 |
| 37 | b | 511 | CLA | C2D-C1D-ND | 5.91 | 115.97 | 110.13 |
| 37 | 38 | 201 | CLA | C2D-C1D-ND | 5.91 | 115.97 | 110.13 |
| 47 | 31 | 307 | KC1 | O2D-CGD-CBD | 5.91 | 121.56 | 111.23 |
| 47 | 14 | 309 | KC1 | CBA-CAA-C2A | -5.91 | 101.75 | 125.45 |
| 37 | 18 | 201 | CLA | CHD-C4C-C3C | -5.91 | 116.16 | 124.77 |
| 47 | 40 | 207 | KC1 | CMA-C3A-C2A | -5.90 | 114.14 | 128.43 |
| 37 | 39 | 307 | CLA | C2D-C1D-ND | 5.90 | 115.97 | 110.13 |
| 50 | 40 | 214 | DD6 | C12-C11-C13 | -5.90 | 109.07 | 118.09 |
| 37 | 18 | 208 | CLA | CHD-C4C-C3C | -5.90 | 116.17 | 124.77 |
| 47 | 31 | 303 | KC1 | C3A-C4A-NA | 5.90 | 117.75 | 110.45 |
| 47 | 17 | 303 | KC1 | C3B-C2B-C1B | -5.90 | 101.46 | 107.05 |
| 48 | 39 | 311 | A86 | C33-C32-C31 | 5.90 | 114.94 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 209 | CLA | CMD-C2D-C1D | 5.90 | 135.12 | 124.73 |
| 37 | 38 | 211 | CLA | O2D-CGD-CBD | 5.90 | 121.54 | 111.23 |
| 37 | 34 | 302 | CLA | CHD-C4C-C3C | -5.89 | 116.18 | 124.77 |
| 50 | 20 | 312 | DD6 | C12-C11-C13 | -5.89 | 109.08 | 118.09 |
| 47 | 16 | 302 | KC1 | C3A-C4A-NA | 5.89 | 117.74 | 110.45 |
| 37 | 38 | 204 | CLA | O2D-CGD-CBD | 5.89 | 121.53 | 111.23 |
| 47 | 12 | 211 | KC1 | C1A-C2A-C3A | -5.89 | 101.86 | 107.28 |
| 37 | 37 | 306 | CLA | CMD-C2D-C1D | 5.89 | 135.10 | 124.73 |
| 37 | 14 | 307 | CLA | CMD-C2D-C1D | 5.89 | 135.09 | 124.73 |
| 47 | 36 | 305 | KC1 | C3A-C4A-NA | 5.89 | 117.73 | 110.45 |
| 47 | 11 | 302 | KC1 | C3A-C4A-NA | 5.88 | 117.73 | 110.45 |
| 37 | 33 | 307 | CLA | CMD-C2D-C1D | 5.88 | 135.09 | 124.73 |
| 47 | 32 | 209 | KC1 | C1A-C2A-C3A | -5.88 | 101.87 | 107.28 |
| 37 | 36 | 307 | CLA | CHD-C4C-C3C | -5.88 | 116.20 | 124.77 |
| 37 | Z | 101 | CLA | CHD-C4C-C3C | -5.88 | 116.20 | 124.77 |
| 47 | 41 | 203 | KC1 | C1A-C2A-C3A | -5.88 | 101.87 | 107.28 |
| 37 | 14 | 307 | CLA | C2B-C1B-NB | 5.88 | 116.42 | 110.33 |
| 37 | 18 | 209 | CLA | CMD-C2D-C1D | 5.88 | 135.08 | 124.73 |
| 47 | 18 | 210 | KC1 | C2B-C1B-NB | 5.88 | 115.94 | 110.13 |
| 47 | 37 | 302 | KC1 | C3B-C2B-C1B | -5.87 | 101.49 | 107.05 |
| 37 | 17 | 307 | CLA | CMD-C2D-C1D | 5.87 | 135.07 | 124.73 |
| 37 | 15 | 308 | CLA | C2D-C1D-ND | 5.87 | 115.94 | 110.13 |
| 37 | 19 | 305 | CLA | CHD-C4C-C3C | -5.87 | 116.21 | 124.77 |
| 47 | 35 | 306 | KC1 | C3A-C4A-NA | 5.87 | 117.72 | 110.45 |
| 37 | 39 | 305 | CLA | CHD-C4C-C3C | -5.87 | 116.21 | 124.77 |
| 37 | B | 514 | CLA | C2D-C1D-ND | 5.87 | 115.93 | 110.13 |
| 37 | 34 | 307 | CLA | CMD-C2D-C1D | 5.87 | 135.06 | 124.73 |
| 37 | a | 404 | CLA | CHD-C4C-C3C | -5.87 | 116.22 | 124.77 |
| 37 | 20 | 301 | CLA | C2D-C1D-ND | 5.87 | 115.93 | 110.13 |
| 47 | 18 | 205 | KC1 | C3B-C2B-C1B | -5.87 | 101.50 | 107.05 |
| 47 | 36 | 302 | KC1 | C1A-C2A-C3A | -5.86 | 101.89 | 107.28 |
| 37 | 38 | 209 | CLA | CMD-C2D-C1D | 5.86 | 135.05 | 124.73 |
| 47 | 38 | 207 | KC1 | CMA-C3A-C2A | -5.86 | 114.24 | 128.43 |
| 37 | 18 | 204 | CLA | CHD-C4C-C3C | -5.86 | 116.22 | 124.77 |
| 47 | 40 | 206 | KC1 | CMA-C3A-C2A | -5.86 | 114.24 | 128.43 |
| 47 | 18 | 207 | KC1 | C3A-C4A-NA | 5.86 | 117.71 | 110.45 |
| 37 | b | 514 | CLA | C2D-C1D-ND | 5.86 | 115.93 | 110.13 |
| 47 | 36 | 304 | KC1 | C3B-C2B-C1B | -5.86 | 101.50 | 107.05 |
| 47 | 20 | 304 | KC1 | CMA-C3A-C2A | -5.86 | 114.25 | 128.43 |
| 48 | 15 | 316 | A86 | O4-C38-C39 | 5.86 | 121.53 | 111.09 |
| 47 | 15 | 304 | KC1 | C3A-C4A-NA | 5.86 | 117.70 | 110.45 |
| 37 | 37 | 306 | CLA | C2B-C1B-NB | 5.86 | 116.40 | 110.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 13 | 306 | KC1 | C3A-C4A-NA | 5.85 | 117.70 | 110.45 |
| 37 | B | 503 | CLA | CHD-C4C-C3C | -5.85 | 116.24 | 124.77 |
| 47 | 16 | 308 | KC1 | C3A-C4A-NA | 5.85 | 117.69 | 110.45 |
| 37 | 16 | 307 | CLA | CHD-C4C-C3C | -5.85 | 116.24 | 124.77 |
| 47 | 35 | 309 | KC1 | C2B-C1B-NB | 5.85 | 115.92 | 110.13 |
| 47 | 17 | 305 | KC1 | C3A-C4A-NA | 5.85 | 117.69 | 110.45 |
| 37 | 11 | 307 | CLA | CMD-C2D-C1D | 5.85 | 135.03 | 124.73 |
| 47 | 36 | 302 | KC1 | C3A-C4A-NA | 5.85 | 117.69 | 110.45 |
| 37 | 35 | 310 | CLA | O2D-CGD-CBD | 5.85 | 121.45 | 111.23 |
| 47 | 16 | 302 | KC1 | C1A-C2A-C3A | -5.85 | 101.90 | 107.28 |
| 37 | D | 401 | CLA | CHD-C4C-C3C | -5.85 | 116.25 | 124.77 |
| 37 | b | 516 | CLA | CHD-C4C-C3C | -5.85 | 116.25 | 124.77 |
| 37 | B | 508 | CLA | C2D-C1D-ND | 5.85 | 115.91 | 110.13 |
| 37 | B | 505 | CLA | CHD-C4C-C3C | -5.85 | 116.25 | 124.77 |
| 47 | 40 | 206 | KC1 | C3A-C4A-NA | 5.85 | 117.69 | 110.45 |
| 47 | 37 | 305 | KC1 | C1A-C2A-C3A | -5.84 | 101.91 | 107.28 |
| 37 | 19 | 307 | CLA | C2D-C1D-ND | 5.84 | 115.91 | 110.13 |
| 37 | b | 503 | CLA | CHD-C4C-C3C | -5.84 | 116.25 | 124.77 |
| 37 | 38 | 204 | CLA | C2B-C1B-NB | 5.84 | 116.39 | 110.33 |
| 47 | 16 | 305 | KC1 | C3A-C4A-NA | 5.84 | 117.68 | 110.45 |
| 47 | 17 | 306 | KC1 | C1A-C2A-C3A | -5.84 | 101.91 | 107.28 |
| 47 | 12 | 208 | KC1 | C1A-C2A-C3A | -5.84 | 101.91 | 107.28 |
| 47 | 21 | 203 | KC1 | C1A-C2A-C3A | -5.84 | 101.91 | 107.28 |
| 37 | 17 | 307 | CLA | C2B-C1B-NB | 5.84 | 116.38 | 110.33 |
| 37 | A | 405 | CLA | CHD-C4C-C3C | -5.84 | 116.26 | 124.77 |
| 37 | b | 510 | CLA | C2D-C1D-ND | 5.84 | 115.90 | 110.13 |
| 37 | b | 508 | CLA | C2D-C1D-ND | 5.84 | 115.90 | 110.13 |
| 37 | 32 | 206 | CLA | CHD-C4C-C3C | -5.83 | 116.27 | 124.77 |
| 37 | 41 | 208 | CLA | C2D-C1D-ND | 5.83 | 115.90 | 110.13 |
| 47 | 16 | 308 | KC1 | C1A-C2A-C3A | -5.83 | 101.92 | 107.28 |
| 47 | 15 | 309 | KC1 | C2B-C1B-NB | 5.83 | 115.90 | 110.13 |
| 37 | B | 514 | CLA | CMD-C2D-C1D | 5.83 | 135.00 | 124.73 |
| 37 | 18 | 204 | CLA | C2B-C1B-NB | 5.83 | 116.37 | 110.33 |
| 37 | b | 505 | CLA | CHD-C4C-C3C | -5.83 | 116.27 | 124.77 |
| 37 | 31 | 308 | CLA | CMD-C2D-C1D | 5.83 | 134.99 | 124.73 |
| 37 | 32 | 210 | CLA | CMD-C2D-C1D | 5.83 | 134.99 | 124.73 |
| 47 | 35 | 306 | KC1 | O2D-CGD-CBD | 5.83 | 121.42 | 111.23 |
| 37 | 18 | 204 | CLA | O2D-CGD-CBD | 5.83 | 121.42 | 111.23 |
| 47 | 20 | 305 | KC1 | C3B-C2B-C1B | -5.83 | 101.53 | 107.05 |
| 37 | a | 407 | CLA | CHD-C4C-C3C | -5.83 | 116.28 | 124.77 |
| 47 | 36 | 308 | KC1 | C1A-C2A-C3A | -5.83 | 101.92 | 107.28 |
| 47 | 33 | 306 | KC1 | C3A-C4A-NA | 5.83 | 117.66 | 110.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 308 | CLA | C2B-C1B-NB | 5.83 | 116.37 | 110.33 |
| 37 | 32 | 210 | CLA | CHD-C4C-C3C | -5.82 | 116.28 | 124.77 |
| 47 | 17 | 306 | KC1 | C3A-C4A-NA | 5.82 | 117.66 | 110.45 |
| 48 | 12 | 220 | A86 | C3-C2-C1 | -5.82 | 119.11 | 127.28 |
| 37 | b | 514 | CLA | CMD-C2D-C1D | 5.82 | 134.98 | 124.73 |
| 37 | 38 | 209 | CLA | CHD-C4C-C3C | -5.82 | 116.28 | 124.77 |
| 47 | 38 | 205 | KC1 | C3B-C2B-C1B | -5.82 | 101.54 | 107.05 |
| 37 | 12 | 212 | CLA | C2D-C1D-ND | 5.82 | 115.88 | 110.13 |
| 37 | 12 | 209 | CLA | CHD-C4C-C3C | -5.82 | 116.29 | 124.77 |
| 47 | 16 | 308 | KC1 | C3B-C2B-C1B | -5.82 | 101.54 | 107.05 |
| 37 | 15 | 303 | CLA | O2D-CGD-CBD | 5.82 | 121.40 | 111.23 |
| 47 | 15 | 302 | KC1 | C1A-C2A-C3A | -5.82 | 101.93 | 107.28 |
| 47 | 16 | 305 | KC1 | C1A-C2A-C3A | -5.82 | 101.93 | 107.28 |
| 47 | 35 | 304 | KC1 | C1A-C2A-C3A | -5.82 | 101.93 | 107.28 |
| 37 | B | 510 | CLA | C2D-C1D-ND | 5.81 | 115.88 | 110.13 |
| 37 | 15 | 310 | CLA | O2D-CGD-CBD | 5.81 | 121.39 | 111.23 |
| 47 | 16 | 304 | KC1 | C3B-C2B-C1B | -5.81 | 101.55 | 107.05 |
| 37 | B | 516 | CLA | CHD-C4C-C3C | -5.81 | 116.30 | 124.77 |
| 50 | 21 | 216 | DD6 | C7-C6-C8 | -5.81 | 109.21 | 118.09 |
| 37 | 33 | 305 | CLA | C2D-C1D-ND | 5.81 | 115.88 | 110.13 |
| 48 | 35 | 311 | A86 | C41-C32-C31 | -5.81 | 105.27 | 110.47 |
| 48 | 37 | 310 | A86 | C3-C2-C1 | -5.81 | 119.13 | 127.28 |
| 47 | 38 | 210 | KC1 | C3B-C2B-C1B | -5.81 | 101.55 | 107.05 |
| 37 | 11 | 307 | CLA | C2B-C1B-NB | 5.81 | 116.35 | 110.33 |
| 50 | 41 | 216 | DD6 | C7-C6-C8 | -5.80 | 109.22 | 118.09 |
| 37 | b | 516 | CLA | C4A-NA-C1A | -5.80 | 104.03 | 106.68 |
| 37 | 32 | 206 | CLA | O2D-CGD-CBD | 5.80 | 121.37 | 111.23 |
| 48 | 32 | 221 | A86 | C3-C2-C1 | -5.80 | 119.14 | 127.28 |
| 37 | 32 | 208 | CLA | C2D-C1D-ND | 5.80 | 115.87 | 110.13 |
| 37 | 18 | 209 | CLA | CHD-C4C-C3C | -5.80 | 116.32 | 124.77 |
| 47 | 15 | 306 | KC1 | O2D-CGD-CBD | 5.80 | 121.36 | 111.23 |
| 47 | 20 | 305 | KC1 | C3C-C4C-NC | 5.80 | 116.11 | 109.90 |
| 47 | 15 | 304 | KC1 | C3B-C2B-C1B | -5.80 | 101.56 | 107.05 |
| 47 | 40 | 207 | KC1 | C3B-C2B-C1B | -5.80 | 101.56 | 107.05 |
| 47 | 34 | 306 | KC1 | C2D-C1D-ND | 5.80 | 116.34 | 110.33 |
| 47 | 31 | 309 | KC1 | CMA-C3A-C4A | -5.79 | 115.98 | 125.03 |
| 37 | 12 | 203 | CLA | C2D-C1D-ND | 5.79 | 115.86 | 110.13 |
| 47 | 19 | 308 | KC1 | C3A-C4A-NA | 5.79 | 117.62 | 110.45 |
| 47 | 11 | 309 | KC1 | CMA-C3A-C4A | -5.79 | 115.99 | 125.03 |
| 37 | 12 | 207 | CLA | C2D-C1D-ND | 5.79 | 115.86 | 110.13 |
| 47 | 20 | 304 | KC1 | C3A-C4A-NA | 5.79 | 117.61 | 110.45 |
| 37 | 32 | 213 | CLA | C2D-C1D-ND | 5.78 | 115.85 | 110.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 205 | CLA | O2D-CGD-CBD | 5.78 | 121.34 | 111.23 |
| 37 | 19 | 307 | CLA | C2B-C1B-NB | 5.78 | 116.32 | 110.33 |
| 47 | 36 | 308 | KC1 | C3B-C2B-C1B | -5.78 | 101.58 | 107.05 |
| 47 | 34 | 304 | KC1 | C2B-C1B-NB | 5.78 | 115.84 | 110.13 |
| 47 | 33 | 309 | KC1 | C2B-C1B-NB | 5.78 | 115.84 | 110.13 |
| 47 | 36 | 305 | KC1 | C1A-C2A-C3A | -5.78 | 101.97 | 107.28 |
| 37 | 32 | 204 | CLA | C2D-C1D-ND | 5.78 | 115.84 | 110.13 |
| 47 | 39 | 308 | KC1 | C3A-C4A-NA | 5.77 | 117.59 | 110.45 |
| 47 | 12 | 206 | KC1 | C1A-C2A-C3A | -5.77 | 101.98 | 107.28 |
| 47 | 40 | 207 | KC1 | C3C-C4C-NC | 5.77 | 116.08 | 109.90 |
| 48 | 14 | 313 | A86 | C4-C5-C6 | -5.77 | 119.19 | 127.28 |
| 47 | 37 | 305 | KC1 | C3A-C4A-NA | 5.77 | 117.59 | 110.45 |
| 37 | C | 504 | CLA | O2D-CGD-CBD | 5.77 | 121.31 | 111.23 |
| 47 | 16 | 305 | KC1 | CMA-C3A-C2A | -5.76 | 114.48 | 128.43 |
| 47 | 11 | 302 | KC1 | C1A-C2A-C3A | -5.76 | 101.98 | 107.28 |
| 37 | 33 | 305 | CLA | CHD-C4C-C3C | -5.76 | 116.37 | 124.77 |
| 47 | 18 | 210 | KC1 | C3B-C2B-C1B | -5.76 | 101.59 | 107.05 |
| 48 | 34 | 313 | A86 | C4-C5-C6 | -5.76 | 119.20 | 127.28 |
| 47 | 34 | 306 | KC1 | C3B-C2B-C1B | -5.76 | 101.59 | 107.05 |
| 37 | c | 502 | CLA | CMD-C2D-C1D | 5.76 | 134.87 | 124.73 |
| 37 | 36 | 306 | CLA | CMD-C2D-C1D | 5.76 | 134.87 | 124.73 |
| 48 | 36 | 310 | A86 | C41-C32-C31 | -5.76 | 105.32 | 110.47 |
| 37 | 13 | 305 | CLA | CHD-C4C-C3C | -5.76 | 116.38 | 124.77 |
| 37 | 35 | 308 | CLA | C2D-C1D-ND | 5.76 | 115.82 | 110.13 |
| 47 | 31 | 305 | KC1 | CMA-C3A-C2A | -5.76 | 114.50 | 128.43 |
| 37 | C | 502 | CLA | CMD-C2D-C1D | 5.76 | 134.87 | 124.73 |
| 47 | 14 | 306 | KC1 | C1A-C2A-C3A | -5.76 | 101.99 | 107.28 |
| 37 | 38 | 203 | CLA | CHD-C4C-C3C | -5.76 | 116.38 | 124.77 |
| 48 | 16 | 310 | A86 | C41-C32-C31 | -5.76 | 105.32 | 110.47 |
| 37 | 14 | 307 | CLA | CHD-C4C-C3C | -5.75 | 116.38 | 124.77 |
| 37 | 34 | 302 | CLA | C2D-C1D-ND | 5.75 | 115.82 | 110.13 |
| 47 | 32 | 207 | KC1 | C1A-C2A-C3A | -5.75 | 101.99 | 107.28 |
| 47 | 31 | 307 | KC1 | C2D-C1D-ND | 5.75 | 116.29 | 110.33 |
| 37 | c | 504 | CLA | O2D-CGD-CBD | 5.75 | 121.28 | 111.23 |
| 37 | 21 | 208 | CLA | C2D-C1D-ND | 5.75 | 115.81 | 110.13 |
| 47 | 11 | 306 | KC1 | C1A-C2A-C3A | -5.75 | 102.00 | 107.28 |
| 37 | 18 | 203 | CLA | CHD-C4C-C3C | -5.74 | 116.40 | 124.77 |
| 37 | 20 | 306 | CLA | CHD-C4C-C3C | -5.74 | 116.40 | 124.77 |
| 47 | 11 | 306 | KC1 | C2D-C1D-ND | 5.74 | 116.28 | 110.33 |
| 47 | 36 | 305 | KC1 | CMA-C3A-C2A | -5.74 | 114.53 | 128.43 |
| 37 | 19 | 310 | CLA | CHD-C4C-C3C | -5.74 | 116.40 | 124.77 |
| 50 | 16 | 312 | DD6 | C24-C1-C2 | -5.74 | 109.98 | 119.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 13 | 305 | CLA | C2D-C1D-ND | 5.74 | 115.81 | 110.13 |
| 37 | 15 | 307 | CLA | C2D-C1D-ND | 5.74 | 115.81 | 110.13 |
| 37 | 11 | 308 | CLA | C2D-C1D-ND | 5.74 | 115.81 | 110.13 |
| 37 | 32 | 202 | CLA | C2D-C1D-ND | 5.74 | 115.81 | 110.13 |
| 37 | 14 | 305 | CLA | O2D-CGD-CBD | 5.74 | 121.26 | 111.23 |
| 47 | 21 | 203 | KC1 | O2D-CGD-CBD | 5.74 | 121.26 | 111.23 |
| 47 | 34 | 306 | KC1 | C1A-C2A-C3A | -5.74 | 102.01 | 107.28 |
| 37 | 39 | 310 | CLA | CHD-C4C-C3C | -5.74 | 116.41 | 124.77 |
| 37 | 16 | 306 | CLA | CMD-C2D-C1D | 5.74 | 134.83 | 124.73 |
| 47 | 13 | 309 | KC1 | C2B-C1B-NB | 5.74 | 115.80 | 110.13 |
| 47 | 14 | 304 | KC1 | C2B-C1B-NB | 5.74 | 115.80 | 110.13 |
| 37 | 32 | 208 | CLA | CHD-C4C-C3C | -5.73 | 116.41 | 124.77 |
| 37 | 12 | 209 | CLA | C2D-C1D-ND | 5.73 | 115.80 | 110.13 |
| 47 | 16 | 308 | KC1 | C2B-C1B-NB | 5.73 | 115.80 | 110.13 |
| 37 | B | 514 | CLA | CHD-C4C-C3C | -5.73 | 116.42 | 124.77 |
| 37 | 37 | 301 | CLA | C2D-C1D-ND | 5.73 | 115.80 | 110.13 |
| 47 | 11 | 304 | KC1 | CMA-C3A-C2A | -5.73 | 114.57 | 128.43 |
| 37 | 35 | 307 | CLA | C2D-C1D-ND | 5.73 | 115.79 | 110.13 |
| 37 | 34 | 307 | CLA | CHD-C4C-C3C | -5.72 | 116.43 | 124.77 |
| 47 | 14 | 306 | KC1 | C2D-C1D-ND | 5.72 | 116.26 | 110.33 |
| 37 | 13 | 301 | CLA | CHD-C4C-C3C | -5.72 | 116.43 | 124.77 |
| 37 | 34 | 305 | CLA | O2D-CGD-CBD | 5.72 | 121.23 | 111.23 |
| 37 | B | 511 | CLA | CHD-C4C-C3C | -5.72 | 116.43 | 124.77 |
| 37 | C | 509 | CLA | CHD-C4C-C3C | -5.72 | 116.43 | 124.77 |
| 37 | b | 511 | CLA | CHD-C4C-C3C | -5.72 | 116.44 | 124.77 |
| 37 | 38 | 204 | CLA | CHD-C4C-C3C | -5.72 | 116.44 | 124.77 |
| 47 | 14 | 306 | KC1 | C3B-C2B-C1B | -5.72 | 101.64 | 107.05 |
| 37 | 17 | 307 | CLA | C2D-C1D-ND | 5.72 | 115.78 | 110.13 |
| 37 | 32 | 210 | CLA | C2D-C1D-ND | 5.72 | 115.78 | 110.13 |
| 47 | 33 | 309 | KC1 | C3B-C2B-C1B | -5.72 | 101.64 | 107.05 |
| 48 | 35 | 315 | A86 | C4-C5-C6 | -5.71 | 119.27 | 127.28 |
| 37 | 39 | 303 | CLA | C2D-C1D-ND | 5.71 | 115.78 | 110.13 |
| 47 | 36 | 308 | KC1 | C2B-C1B-NB | 5.71 | 115.78 | 110.13 |
| 47 | 31 | 303 | KC1 | C1A-C2A-C3A | -5.71 | 102.03 | 107.28 |
| 37 | c | 509 | CLA | CHD-C4C-C3C | -5.71 | 116.45 | 124.77 |
| 37 | c | 507 | CLA | C2D-C1D-ND | 5.71 | 115.78 | 110.13 |
| 37 | d | 404 | CLA | CHD-C4C-C3C | -5.71 | 116.45 | 124.77 |
| 37 | b | 514 | CLA | CHD-C4C-C3C | -5.71 | 116.45 | 124.77 |
| 37 | 12 | 205 | CLA | CHD-C4C-C3C | -5.71 | 116.45 | 124.77 |
| 37 | 40 | 208 | CLA | CHD-C4C-C3C | -5.71 | 116.45 | 124.77 |
| 47 | 17 | 306 | KC1 | CHC-C1C-C2C | -5.71 | 116.02 | 125.03 |
| 47 | 37 | 305 | KC1 | CHC-C1C-C2C | -5.71 | 116.02 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 36 | 312 | DD6 | C24-C1-C2 | -5.71 | 110.03 | 119.01 |
| 48 | 41 | 213 | A86 | C25-C26-C27 | -5.71 | 119.27 | 127.28 |
| 37 | 18 | 211 | CLA | O2D-CGD-CBD | 5.71 | 121.21 | 111.23 |
| 37 | B | 509 | CLA | CMD-C2D-C1D | 5.71 | 134.78 | 124.73 |
| 47 | 41 | 203 | KC1 | O2D-CGD-CBD | 5.71 | 121.21 | 111.23 |
| 37 | W | 102 | CLA | CHD-C4C-C3C | -5.71 | 116.45 | 124.77 |
| 47 | 13 | 302 | KC1 | C1A-C2A-C3A | -5.71 | 102.03 | 107.28 |
| 47 | 31 | 307 | KC1 | C1A-C2A-C3A | -5.71 | 102.03 | 107.28 |
| 37 | 40 | 210 | CLA | C2D-C1D-ND | 5.70 | 115.77 | 110.13 |
| 37 | D | 406 | CLA | O2D-CGD-CBD | 5.70 | 121.20 | 111.23 |
| 37 | c | 508 | CLA | O2D-CGD-CBD | 5.70 | 121.20 | 111.23 |
| 47 | 35 | 304 | KC1 | C3B-C2B-C1B | -5.70 | 101.65 | 107.05 |
| 40 | a | 409 | SQD | O6-C1-C2 | 5.70 | 116.93 | 108.27 |
| 37 | 12 | 207 | CLA | CHD-C4C-C3C | -5.70 | 116.46 | 124.77 |
| 37 | 37 | 303 | CLA | C2D-C1D-ND | 5.70 | 115.77 | 110.13 |
| 37 | b | 507 | CLA | O2D-CGD-CBD | 5.70 | 121.19 | 111.23 |
| 47 | 15 | 304 | KC1 | C1A-C2A-C3A | -5.70 | 102.04 | 107.28 |
| 37 | C | 512 | CLA | CHD-C4C-C3C | -5.70 | 116.47 | 124.77 |
| 47 | 34 | 306 | KC1 | C3A-C4A-NA | 5.69 | 117.50 | 110.45 |
| 37 | B | 507 | CLA | O2D-CGD-CBD | 5.69 | 121.19 | 111.23 |
| 37 | 35 | 308 | CLA | CED-O2D-CGD | 5.69 | 128.83 | 115.92 |
| 47 | 20 | 305 | KC1 | C1A-C2A-C3A | -5.69 | 102.05 | 107.28 |
| 37 | C | 511 | CLA | C2D-C1D-ND | 5.69 | 115.76 | 110.13 |
| 37 | 14 | 308 | CLA | CHD-C4C-C3C | -5.69 | 116.47 | 124.77 |
| 37 | 20 | 308 | CLA | C2D-C1D-ND | 5.69 | 115.76 | 110.13 |
| 48 | 21 | 213 | A86 | C25-C26-C27 | -5.69 | 119.30 | 127.28 |
| 37 | 15 | 305 | CLA | C2D-C1D-ND | 5.69 | 115.76 | 110.13 |
| 37 | 19 | 303 | CLA | C2D-C1D-ND | 5.69 | 115.76 | 110.13 |
| 37 | 20 | 308 | CLA | CHD-C4C-C3C | -5.69 | 116.48 | 124.77 |
| 37 | 13 | 303 | CLA | C3B-C2B-C1B | -5.69 | 100.46 | 107.17 |
| 37 | 14 | 302 | CLA | C2D-C1D-ND | 5.69 | 115.76 | 110.13 |
| 37 | d | 404 | CLA | O2D-CGD-CBD | 5.69 | 121.17 | 111.23 |
| 47 | 11 | 304 | KC1 | C3B-C2B-C1B | -5.69 | 101.66 | 107.05 |
| 37 | D | 406 | CLA | CHD-C4C-C3C | -5.69 | 116.48 | 124.77 |
| 40 | A | 407 | SQD | O6-C1-C2 | 5.69 | 116.91 | 108.27 |
| 37 | C | 508 | CLA | O2D-CGD-CBD | 5.68 | 121.17 | 111.23 |
| 37 | 33 | 301 | CLA | CHD-C4C-C3C | -5.68 | 116.49 | 124.77 |
| 37 | 31 | 301 | CLA | CHD-C4C-C3C | -5.68 | 116.49 | 124.77 |
| 37 | 31 | 306 | CLA | C2D-C1D-ND | 5.68 | 115.75 | 110.13 |
| 37 | 34 | 308 | CLA | CHD-C4C-C3C | -5.68 | 116.49 | 124.77 |
| 47 | 33 | 302 | KC1 | C1A-C2A-C3A | -5.68 | 102.06 | 107.28 |
| 47 | 41 | 207 | KC1 | C1A-C2A-C3A | -5.68 | 102.06 | 107.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 13 | 309 | KC1 | C3B-C2B-C1B | -5.68 | 101.67 | 107.05 |
| 37 | 12 | 210 | CLA | C2D-C1D-ND | 5.68 | 115.74 | 110.13 |
| 37 | b | 509 | CLA | CMD-C2D-C1D | 5.68 | 134.72 | 124.73 |
| 37 | 39 | 302 | CLA | C2D-C1D-ND | 5.68 | 115.74 | 110.13 |
| 37 | B | 524 | CLA | O2D-CGD-CBD | 5.67 | 121.15 | 111.23 |
| 37 | 14 | 308 | CLA | C2C-C1C-NC | 5.67 | 115.94 | 109.98 |
| 37 | 34 | 308 | CLA | C2C-C1C-NC | 5.67 | 115.94 | 109.98 |
| 47 | 40 | 207 | KC1 | C1A-C2A-C3A | -5.67 | 102.07 | 107.28 |
| 37 | 40 | 208 | CLA | C2D-C1D-ND | 5.67 | 115.74 | 110.13 |
| 37 | 38 | 206 | CLA | C2D-C1D-ND | 5.67 | 115.74 | 110.13 |
| 48 | 15 | 315 | A86 | C4-C5-C6 | -5.67 | 119.33 | 127.28 |
| 37 | c | 512 | CLA | CHD-C4C-C3C | -5.67 | 116.51 | 124.77 |
| 37 | 40 | 210 | CLA | CHD-C4C-C3C | -5.67 | 116.51 | 124.77 |
| 37 | D | 402 | CLA | C2D-C1D-ND | 5.67 | 115.73 | 110.13 |
| 47 | 21 | 207 | KC1 | C1A-C2A-C3A | -5.67 | 102.07 | 107.28 |
| 48 | 11 | 314 | A86 | O4-C38-C39 | 5.67 | 121.19 | 111.09 |
| 37 | 20 | 306 | CLA | C2D-C1D-ND | 5.66 | 115.73 | 110.13 |
| 47 | 14 | 306 | KC1 | C3A-C4A-NA | 5.66 | 117.46 | 110.45 |
| 48 | 21 | 215 | A86 | O4-C38-C39 | 5.66 | 121.19 | 111.09 |
| 37 | 32 | 211 | CLA | C2D-C1D-ND | 5.66 | 115.73 | 110.13 |
| 47 | 20 | 305 | KC1 | C2B-C1B-NB | 5.66 | 115.73 | 110.13 |
| 47 | 31 | 305 | KC1 | C3B-C2B-C1B | -5.66 | 101.69 | 107.05 |
| 37 | c | 507 | CLA | C3B-C2B-C1B | -5.66 | 100.50 | 107.17 |
| 37 | B | 509 | CLA | C2C-C1C-NC | 5.66 | 115.93 | 109.98 |
| 47 | 13 | 309 | KC1 | O2D-CGD-CBD | 5.66 | 121.12 | 111.23 |
| 37 | 37 | 306 | CLA | C2D-C1D-ND | 5.66 | 115.73 | 110.13 |
| 37 | 33 | 310 | CLA | O2D-CGD-CBD | 5.66 | 121.12 | 111.23 |
| 48 | 17 | 315 | A86 | C3-C2-C1 | -5.66 | 119.34 | 127.28 |
| 47 | 15 | 306 | KC1 | C2B-C1B-NB | 5.66 | 115.73 | 110.13 |
| 37 | b | 502 | CLA | O2D-CGD-CBD | 5.66 | 121.12 | 111.23 |
| 47 | 33 | 309 | KC1 | O2D-CGD-CBD | 5.66 | 121.12 | 111.23 |
| 37 | 13 | 307 | CLA | CHD-C4C-C3C | -5.66 | 116.53 | 124.77 |
| 47 | 16 | 305 | KC1 | C3B-C2B-C1B | -5.65 | 101.70 | 107.05 |
| 37 | b | 509 | CLA | C2C-C1C-NC | 5.65 | 115.92 | 109.98 |
| 48 | 41 | 215 | A86 | O4-C38-C39 | 5.65 | 121.17 | 111.09 |
| 48 | 31 | 314 | A86 | C3-C2-C1 | -5.65 | 119.36 | 127.28 |
| 37 | 33 | 307 | CLA | CHD-C4C-C3C | -5.65 | 116.54 | 124.77 |
| 47 | 36 | 305 | KC1 | C3B-C2B-C1B | -5.65 | 101.70 | 107.05 |
| 47 | 14 | 306 | KC1 | CMA-C3A-C2A | -5.65 | 114.76 | 128.43 |
| 47 | 34 | 306 | KC1 | CMA-C3A-C2A | -5.65 | 114.76 | 128.43 |
| 37 | B | 502 | CLA | CHD-C4C-C3C | -5.65 | 116.54 | 124.77 |
| 37 | 14 | 308 | CLA | C2D-C1D-ND | 5.65 | 115.71 | 110.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 502 | CLA | C2D-C1D-ND | 5.64 | 115.71 | 110.13 |
| 37 | d | 401 | CLA | C2D-C1D-ND | 5.64 | 115.71 | 110.13 |
| 47 | 36 | 304 | KC1 | C2B-C1B-NB | 5.64 | 115.71 | 110.13 |
| 47 | 11 | 304 | KC1 | C1A-C2A-C3A | -5.64 | 102.09 | 107.28 |
| 47 | 15 | 302 | KC1 | C2B-C1B-NB | 5.64 | 115.71 | 110.13 |
| 37 | 17 | 304 | CLA | C2D-C1D-ND | 5.64 | 115.71 | 110.13 |
| 47 | 40 | 207 | KC1 | C2B-C1B-NB | 5.64 | 115.71 | 110.13 |
| 37 | C | 507 | CLA | C2D-C1D-ND | 5.64 | 115.70 | 110.13 |
| 37 | b | 523 | CLA | O2D-CGD-CBD | 5.64 | 121.08 | 111.23 |
| 37 | 36 | 306 | CLA | C4A-NA-C1A | -5.63 | 104.11 | 106.68 |
| 37 | c | 511 | CLA | C2D-C1D-ND | 5.63 | 115.70 | 110.13 |
| 37 | 33 | 310 | CLA | C2D-C1D-ND | 5.63 | 115.70 | 110.13 |
| 37 | C | 513 | CLA | C2B-C1B-NB | 5.63 | 116.17 | 110.33 |
| 48 | 11 | 314 | A86 | C3-C2-C1 | -5.63 | 119.38 | 127.28 |
| 37 | b | 502 | CLA | CHD-C4C-C3C | -5.63 | 116.56 | 124.77 |
| 37 | 38 | 206 | CLA | CHD-C4C-C3C | -5.63 | 116.56 | 124.77 |
| 37 | b | 502 | CLA | C2D-C1D-ND | 5.63 | 115.70 | 110.13 |
| 48 | 34 | 313 | A86 | O4-C38-C39 | 5.63 | 121.13 | 111.09 |
| 37 | b | 508 | CLA | CHD-C4C-C3C | -5.63 | 116.56 | 124.77 |
| 37 | C | 501 | CLA | C2D-C1D-ND | 5.63 | 115.70 | 110.13 |
| 37 | 21 | 210 | CLA | O2D-CGD-CBD | 5.63 | 121.07 | 111.23 |
| 37 | C | 507 | CLA | C3B-C2B-C1B | -5.63 | 100.53 | 107.17 |
| 37 | 19 | 302 | CLA | C2D-C1D-ND | 5.63 | 115.70 | 110.13 |
| 37 | 37 | 308 | CLA | CAA-C2A-C3A | -5.63 | 97.79 | 113.00 |
| 37 | 14 | 303 | CLA | C2D-C1D-ND | 5.63 | 115.69 | 110.13 |
| 37 | 35 | 303 | CLA | C2D-C1D-ND | 5.63 | 115.69 | 110.13 |
| 37 | B | 508 | CLA | CHD-C4C-C3C | -5.63 | 116.57 | 124.77 |
| 37 | c | 501 | CLA | C2D-C1D-ND | 5.62 | 115.69 | 110.13 |
| 37 | 21 | 209 | CLA | C2D-C1D-ND | 5.62 | 115.69 | 110.13 |
| 47 | 18 | 207 | KC1 | C1A-C2A-C3A | -5.62 | 102.11 | 107.28 |
| 37 | 18 | 211 | CLA | C2D-C1D-ND | 5.62 | 115.69 | 110.13 |
| 37 | 41 | 210 | CLA | O2D-CGD-CBD | 5.62 | 121.06 | 111.23 |
| 37 | B | 502 | CLA | O2D-CGD-CBD | 5.62 | 121.05 | 111.23 |
| 37 | c | 510 | CLA | CHD-C4C-C3C | -5.61 | 116.59 | 124.77 |
| 37 | 11 | 305 | CLA | C2D-C1D-ND | 5.61 | 115.68 | 110.13 |
| 48 | 37 | 314 | A86 | C3-C2-C1 | -5.61 | 119.41 | 127.28 |
| 37 | 18 | 206 | CLA | CHD-C4C-C3C | -5.61 | 116.59 | 124.77 |
| 37 | 16 | 306 | CLA | C4A-NA-C1A | -5.61 | 104.12 | 106.68 |
| 37 | 40 | 209 | CLA | C2D-C1D-ND | 5.61 | 115.68 | 110.13 |
| 37 | 41 | 209 | CLA | C2D-C1D-ND | 5.61 | 115.68 | 110.13 |
| 50 | 21 | 212 | DD6 | C12-C11-C13 | -5.61 | 109.52 | 118.09 |
| 37 | 20 | 307 | CLA | C2D-C1D-ND | 5.60 | 115.67 | 110.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 14 | 313 | A86 | O4-C38-C39 | 5.60 | 121.08 | 111.09 |
| 37 | 13 | 308 | CLA | C2D-C1D-ND | 5.60 | 115.67 | 110.13 |
| 37 | 33 | 308 | CLA | C2D-C1D-ND | 5.60 | 115.67 | 110.13 |
| 37 | d | 404 | CLA | C2B-C1B-NB | 5.60 | 116.13 | 110.33 |
| 37 | 19 | 307 | CLA | CHD-C4C-C3C | -5.60 | 116.61 | 124.77 |
| 37 | 14 | 305 | CLA | C2D-C1D-ND | 5.60 | 115.67 | 110.13 |
| 37 | 34 | 305 | CLA | C2D-C1D-ND | 5.60 | 115.67 | 110.13 |
| 50 | 41 | 212 | DD6 | C12-C11-C13 | -5.60 | 109.54 | 118.09 |
| 37 | 15 | 303 | CLA | C2D-C1D-ND | 5.60 | 115.66 | 110.13 |
| 37 | 34 | 308 | CLA | C2D-C1D-ND | 5.60 | 115.66 | 110.13 |
| 37 | 33 | 303 | CLA | C3B-C2B-C1B | -5.60 | 100.57 | 107.17 |
| 47 | 38 | 207 | KC1 | C1A-C2A-C3A | -5.60 | 102.14 | 107.28 |
| 47 | 16 | 304 | KC1 | C2B-C1B-NB | 5.59 | 115.66 | 110.13 |
| 37 | c | 506 | CLA | C2D-C1D-ND | 5.59 | 115.66 | 110.13 |
| 47 | 37 | 304 | KC1 | C2B-C1B-NB | 5.59 | 115.66 | 110.13 |
| 47 | 17 | 305 | KC1 | C3B-C2B-C1B | -5.59 | 101.76 | 107.05 |
| 37 | D | 406 | CLA | C2B-C1B-NB | 5.59 | 116.12 | 110.33 |
| 47 | 15 | 309 | KC1 | O2D-CGD-CBD | 5.58 | 120.99 | 111.23 |
| 47 | 37 | 307 | KC1 | O2D-CGD-CBD | 5.58 | 120.99 | 111.23 |
| 48 | 35 | 315 | A86 | O4-C38-C39 | 5.58 | 121.04 | 111.09 |
| 37 | C | 510 | CLA | CHD-C4C-C3C | -5.58 | 116.64 | 124.77 |
| 48 | 40 | 211 | A86 | C25-C26-C27 | -5.58 | 119.45 | 127.28 |
| 37 | 34 | 303 | CLA | C2D-C1D-ND | 5.58 | 115.65 | 110.13 |
| 37 | 35 | 305 | CLA | C2D-C1D-ND | 5.58 | 115.65 | 110.13 |
| 47 | 35 | 302 | KC1 | C2B-C1B-NB | 5.58 | 115.65 | 110.13 |
| 47 | 17 | 308 | KC1 | O2D-CGD-CBD | 5.58 | 120.98 | 111.23 |
| 48 | 15 | 315 | A86 | O4-C38-C39 | 5.58 | 121.04 | 111.09 |
| 37 | C | 503 | CLA | C3B-C2B-C1B | -5.58 | 100.59 | 107.17 |
| 37 | 12 | 204 | CLA | O2D-CGD-CBD | 5.58 | 120.98 | 111.23 |
| 37 | 40 | 209 | CLA | CHD-C4C-C3C | -5.58 | 116.64 | 124.77 |
| 37 | c | 513 | CLA | C2B-C1B-NB | 5.57 | 116.11 | 110.33 |
| 47 | 31 | 305 | KC1 | C1A-C2A-C3A | -5.57 | 102.16 | 107.28 |
| 37 | 14 | 305 | CLA | CHD-C4C-C3C | -5.57 | 116.65 | 124.77 |
| 48 | 38 | 213 | A86 | C3-C2-C1 | -5.57 | 119.47 | 127.28 |
| 48 | 31 | 315 | A86 | O4-C38-C39 | 5.57 | 121.02 | 111.09 |
| 48 | 33 | 313 | A86 | O4-C38-C39 | 5.57 | 121.02 | 111.09 |
| 48 | 20 | 309 | A86 | C25-C26-C27 | -5.57 | 119.47 | 127.28 |
| 37 | 12 | 212 | CLA | C2B-C1B-NB | 5.56 | 116.10 | 110.33 |
| 37 | 32 | 213 | CLA | C2B-C1B-NB | 5.56 | 116.10 | 110.33 |
| 37 | 34 | 305 | CLA | CHD-C4C-C3C | -5.56 | 116.66 | 124.77 |
| 37 | B | 501 | CLA | C2D-C1D-ND | 5.56 | 115.63 | 110.13 |
| 47 | 31 | 303 | KC1 | C2D-C1D-ND | 5.56 | 116.09 | 110.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 17 | 309 | CLA | CAA-C2A-C3A | -5.56 | 97.98 | 113.00 |
| 47 | 36 | 304 | KC1 | O2D-CGD-CBD | 5.55 | 120.94 | 111.23 |
| 37 | C | 506 | CLA | C2D-C1D-ND | 5.55 | 115.62 | 110.13 |
| 37 | 20 | 307 | CLA | CHD-C4C-C3C | -5.55 | 116.68 | 124.77 |
| 37 | 32 | 205 | CLA | O2D-CGD-CBD | 5.55 | 120.94 | 111.23 |
| 48 | 17 | 310 | A86 | C4-C5-C6 | -5.55 | 119.49 | 127.28 |
| 37 | 39 | 307 | CLA | C2B-C1B-NB | 5.55 | 116.08 | 110.33 |
| 47 | 14 | 309 | KC1 | O2D-CGD-CBD | 5.55 | 120.93 | 111.23 |
| 47 | 16 | 304 | KC1 | O2D-CGD-CBD | 5.55 | 120.93 | 111.23 |
| 37 | B | 512 | CLA | C2D-C1D-ND | 5.55 | 115.62 | 110.13 |
| 37 | 11 | 305 | CLA | CHD-C4C-C3C | -5.55 | 116.69 | 124.77 |
| 37 | 13 | 310 | CLA | O2D-CGD-CBD | 5.55 | 120.92 | 111.23 |
| 37 | 39 | 307 | CLA | CHD-C4C-C3C | -5.55 | 116.69 | 124.77 |
| 47 | 19 | 308 | KC1 | C3B-C2B-C1B | -5.54 | 101.80 | 107.05 |
| 37 | b | 501 | CLA | C2D-C1D-ND | 5.54 | 115.61 | 110.13 |
| 48 | 37 | 309 | A86 | C4-C5-C6 | -5.54 | 119.50 | 127.28 |
| 37 | B | 507 | CLA | C2D-C1D-ND | 5.54 | 115.61 | 110.13 |
| 48 | 11 | 315 | A86 | O4-C38-C39 | 5.54 | 120.97 | 111.09 |
| 37 | 21 | 210 | CLA | CHD-C4C-C3C | -5.54 | 116.69 | 124.77 |
| 48 | 36 | 313 | A86 | O4-C38-C39 | 5.54 | 120.97 | 111.09 |
| 48 | 13 | 313 | A86 | O4-C38-C39 | 5.53 | 120.96 | 111.09 |
| 47 | 15 | 304 | KC1 | C2B-C1B-NB | 5.53 | 115.60 | 110.13 |
| 50 | 41 | 212 | DD6 | C26-C25-C24 | 5.53 | 139.23 | 123.20 |
| 47 | 13 | 306 | KC1 | C3B-C2B-C1B | -5.53 | 101.81 | 107.05 |
| 37 | b | 523 | CLA | CAA-C2A-C3A | -5.53 | 98.05 | 113.00 |
| 50 | 21 | 212 | DD6 | C26-C25-C24 | 5.53 | 139.22 | 123.20 |
| 37 | 32 | 206 | CLA | C2D-C1D-ND | 5.53 | 115.60 | 110.13 |
| 37 | C | 501 | CLA | O2D-CGD-CBD | 5.53 | 120.89 | 111.23 |
| 37 | b | 507 | CLA | C2D-C1D-ND | 5.52 | 115.59 | 110.13 |
| 37 | 21 | 202 | CLA | C2D-C1D-ND | 5.52 | 115.59 | 110.13 |
| 47 | 35 | 306 | KC1 | C2D-C1D-ND | 5.52 | 116.05 | 110.33 |
| 37 | c | 503 | CLA | C3B-C2B-C1B | -5.52 | 100.66 | 107.17 |
| 47 | 34 | 309 | KC1 | O2D-CGD-CBD | 5.52 | 120.88 | 111.23 |
| 47 | 17 | 308 | KC1 | CBA-CAA-C2A | -5.52 | 103.30 | 125.45 |
| 47 | 37 | 307 | KC1 | CBA-CAA-C2A | -5.52 | 103.30 | 125.45 |
| 47 | 11 | 302 | KC1 | C2D-C1D-ND | 5.52 | 116.05 | 110.33 |
| 37 | 34 | 303 | CLA | O2D-CGD-CBD | 5.52 | 120.88 | 111.23 |
| 47 | 11 | 302 | KC1 | O2D-CGD-CBD | 5.52 | 120.88 | 111.23 |
| 37 | 18 | 206 | CLA | O2D-CGD-CBD | 5.52 | 120.87 | 111.23 |
| 37 | 41 | 210 | CLA | CHD-C4C-C3C | -5.52 | 116.73 | 124.77 |
| 50 | 16 | 312 | DD6 | O1-C15-C14 | -5.52 | 101.08 | 116.88 |
| 47 | 39 | 308 | KC1 | C3B-C2B-C1B | -5.52 | 101.83 | 107.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 309 | KC1 | O2D-CGD-CBD | 5.51 | 120.87 | 111.23 |
| 37 | 13 | 301 | CLA | C2B-C1B-NB | 5.51 | 116.04 | 110.33 |
| 47 | 32 | 209 | KC1 | O2D-CGD-CBD | 5.51 | 120.87 | 111.23 |
| 50 | 39 | 312 | DD6 | C12-C11-C13 | -5.51 | 109.67 | 118.09 |
| 50 | 36 | 312 | DD6 | O1-C15-C14 | -5.51 | 101.09 | 116.88 |
| 37 | 38 | 206 | CLA | O2D-CGD-CBD | 5.51 | 120.86 | 111.23 |
| 47 | 35 | 306 | KC1 | C2B-C1B-NB | 5.51 | 115.58 | 110.13 |
| 48 | 16 | 314 | A86 | O4-C38-C39 | 5.51 | 120.91 | 111.09 |
| 37 | b | 515 | CLA | C2B-C1B-NB | 5.51 | 116.04 | 110.33 |
| 47 | 33 | 306 | KC1 | C3B-C2B-C1B | -5.51 | 101.83 | 107.05 |
| 37 | 12 | 205 | CLA | C2D-C1D-ND | 5.51 | 115.58 | 110.13 |
| 47 | 41 | 203 | KC1 | CMA-C3A-C2A | -5.50 | 115.11 | 128.43 |
| 47 | 12 | 208 | KC1 | O2D-CGD-CBD | 5.50 | 120.85 | 111.23 |
| 37 | 31 | 306 | CLA | CHD-C4C-C3C | -5.50 | 116.75 | 124.77 |
| 37 | C | 503 | CLA | CHD-C4C-C3C | -5.50 | 116.75 | 124.77 |
| 37 | B | 501 | CLA | C2B-C1B-NB | 5.50 | 116.03 | 110.33 |
| 47 | 11 | 306 | KC1 | CMA-C3A-C2A | -5.50 | 115.12 | 128.43 |
| 37 | 38 | 203 | CLA | C2D-C1D-ND | 5.50 | 115.57 | 110.13 |
| 37 | b | 512 | CLA | C2D-C1D-ND | 5.50 | 115.56 | 110.13 |
| 47 | 32 | 209 | KC1 | C2D-C1D-ND | 5.50 | 116.03 | 110.33 |
| 47 | 14 | 306 | KC1 | C2B-C1B-NB | 5.49 | 115.56 | 110.13 |
| 37 | 14 | 303 | CLA | O2D-CGD-CBD | 5.49 | 120.83 | 111.23 |
| 37 | 16 | 303 | CLA | C2D-C1D-ND | 5.49 | 115.56 | 110.13 |
| 47 | 34 | 306 | KC1 | C2B-C1B-NB | 5.49 | 115.56 | 110.13 |
| 37 | 37 | 306 | CLA | CHD-C4C-C3C | -5.49 | 116.77 | 124.77 |
| 37 | 13 | 303 | CLA | C2B-C1B-NB | 5.49 | 116.02 | 110.33 |
| 37 | c | 503 | CLA | CHD-C4C-C3C | -5.49 | 116.77 | 124.77 |
| 37 | 39 | 310 | CLA | C2D-C1D-ND | 5.49 | 115.56 | 110.13 |
| 48 | 11 | 311 | A86 | C3-C4-C5 | -5.48 | 112.30 | 123.52 |
| 47 | 31 | 303 | KC1 | O2D-CGD-CBD | 5.48 | 120.82 | 111.23 |
| 47 | 31 | 307 | KC1 | CMA-C3A-C2A | -5.48 | 115.16 | 128.43 |
| 37 | c | 501 | CLA | O2D-CGD-CBD | 5.48 | 120.82 | 111.23 |
| 37 | b | 501 | CLA | C2B-C1B-NB | 5.48 | 116.01 | 110.33 |
| 37 | 33 | 301 | CLA | C2B-C1B-NB | 5.48 | 116.01 | 110.33 |
| 47 | 21 | 203 | KC1 | CMA-C3A-C2A | -5.48 | 115.17 | 128.43 |
| 37 | 12 | 210 | CLA | C2C-C1C-NC | 5.48 | 115.74 | 109.98 |
| 37 | 15 | 310 | CLA | C2D-C1D-ND | 5.48 | 115.55 | 110.13 |
| 50 | 19 | 312 | DD6 | C12-C11-C13 | -5.48 | 109.72 | 118.09 |
| 47 | 12 | 208 | KC1 | C2D-C1D-ND | 5.48 | 116.00 | 110.33 |
| 48 | 32 | 216 | A86 | C3-C2-C1 | -5.48 | 119.60 | 127.28 |
| 37 | 38 | 201 | CLA | CHD-C4C-C3C | -5.47 | 116.79 | 124.77 |
| 37 | 37 | 303 | CLA | C2B-C1B-NB | 5.47 | 116.00 | 110.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 19 | 309 | CLA | CHD-C4C-C3C | -5.47 | 116.80 | 124.77 |
| 37 | B | 515 | CLA | C2B-C1B-NB | 5.47 | 116.00 | 110.33 |
| 37 | A | 403 | CLA | CHD-C4C-C3C | -5.47 | 116.80 | 124.77 |
| 37 | 35 | 310 | CLA | C2D-C1D-ND | 5.47 | 115.54 | 110.13 |
| 48 | 12 | 215 | A86 | C3-C2-C1 | -5.46 | 119.61 | 127.28 |
| 37 | b | 515 | CLA | CHD-C4C-C3C | -5.46 | 116.81 | 124.77 |
| 37 | 32 | 211 | CLA | C2C-C1C-NC | 5.46 | 115.72 | 109.98 |
| 37 | B | 505 | CLA | O2D-CGD-CBD | 5.46 | 120.78 | 111.23 |
| 37 | 17 | 307 | CLA | CHD-C4C-C3C | -5.46 | 116.81 | 124.77 |
| 37 | 38 | 202 | CLA | C2B-C1B-NB | 5.46 | 115.99 | 110.33 |
| 37 | 15 | 305 | CLA | CHD-C4C-C3C | -5.46 | 116.82 | 124.77 |
| 48 | 15 | 311 | A86 | C41-C32-C31 | -5.46 | 105.59 | 110.47 |
| 37 | 41 | 202 | CLA | C2D-C1D-ND | 5.46 | 115.53 | 110.13 |
| 37 | a | 403 | CLA | CHD-C4C-C3C | -5.46 | 116.82 | 124.77 |
| 47 | 13 | 304 | KC1 | C2D-C1D-ND | 5.45 | 115.98 | 110.33 |
| 47 | 15 | 306 | KC1 | C2D-C1D-ND | 5.45 | 115.98 | 110.33 |
| 37 | z | 101 | CLA | C4A-NA-C1A | -5.45 | 104.19 | 106.68 |
| 37 | 35 | 305 | CLA | CHD-C4C-C3C | -5.45 | 116.83 | 124.77 |
| 37 | 31 | 308 | CLA | C3B-C2B-C1B | -5.45 | 100.75 | 107.17 |
| 47 | 12 | 206 | KC1 | O2D-CGD-CBD | 5.45 | 120.75 | 111.23 |
| 48 | 41 | 211 | A86 | O4-C38-C39 | 5.45 | 120.80 | 111.09 |
| 48 | 31 | 311 | A86 | C3-C4-C5 | -5.45 | 112.38 | 123.52 |
| 48 | 21 | 211 | A86 | O4-C38-C39 | 5.45 | 120.80 | 111.09 |
| 37 | 19 | 309 | CLA | C2D-C1D-ND | 5.44 | 115.51 | 110.13 |
| 37 | 11 | 303 | CLA | C2D-C1D-ND | 5.44 | 115.51 | 110.13 |
| 37 | Z | 101 | CLA | C4A-NA-C1A | -5.44 | 104.20 | 106.68 |
| 37 | b | 515 | CLA | C3B-C2B-C1B | -5.44 | 100.75 | 107.17 |
| 47 | 33 | 304 | KC1 | C3B-C2B-C1B | -5.44 | 101.90 | 107.05 |
| 37 | B | 515 | CLA | CHD-C4C-C3C | -5.44 | 116.84 | 124.77 |
| 37 | 17 | 304 | CLA | C2B-C1B-NB | 5.44 | 115.97 | 110.33 |
| 37 | B | 515 | CLA | C3B-C2B-C1B | -5.44 | 100.76 | 107.17 |
| 47 | 35 | 306 | KC1 | C1A-C2A-C3A | -5.44 | 102.28 | 107.28 |
| 37 | 18 | 206 | CLA | C2D-C1D-ND | 5.43 | 115.50 | 110.13 |
| 37 | b | 505 | CLA | O2D-CGD-CBD | 5.43 | 120.73 | 111.23 |
| 37 | b | 508 | CLA | C2B-C1B-NB | 5.43 | 115.96 | 110.33 |
| 37 | c | 504 | CLA | C2B-C1B-NB | 5.43 | 115.96 | 110.33 |
| 37 | 19 | 310 | CLA | C2D-C1D-ND | 5.43 | 115.50 | 110.13 |
| 47 | 18 | 205 | KC1 | C2B-C1B-NB | 5.43 | 115.50 | 110.13 |
| 37 | 36 | 303 | CLA | C2D-C1D-ND | 5.43 | 115.50 | 110.13 |
| 37 | C | 512 | CLA | CMD-C2D-C1D | 5.42 | 134.28 | 124.73 |
| 37 | 20 | 308 | CLA | C2C-C1C-NC | 5.42 | 115.68 | 109.98 |
| 37 | 39 | 309 | CLA | C2D-C1D-ND | 5.42 | 115.49 | 110.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 41 | 210 | CLA | C2B-C1B-NB | 5.42 | 115.95 | 110.33 |
| 37 | 14 | 302 | CLA | C3B-C2B-C1B | -5.42 | 100.78 | 107.17 |
| 47 | 33 | 309 | KC1 | C1A-C2A-C3A | -5.42 | 102.30 | 107.28 |
| 37 | 17 | 304 | CLA | CHD-C4C-C3C | -5.42 | 116.87 | 124.77 |
| 37 | c | 512 | CLA | CMD-C2D-C1D | 5.42 | 134.27 | 124.73 |
| 37 | 39 | 309 | CLA | CHD-C4C-C3C | -5.42 | 116.87 | 124.77 |
| 37 | 41 | 204 | CLA | C2D-C1D-ND | 5.42 | 115.49 | 110.13 |
| 48 | 35 | 311 | A86 | O4-C38-C39 | 5.42 | 120.75 | 111.09 |
| 37 | 31 | 304 | CLA | C2D-C1D-ND | 5.42 | 115.49 | 110.13 |
| 37 | 34 | 302 | CLA | C3B-C2B-C1B | -5.42 | 100.78 | 107.17 |
| 47 | 33 | 304 | KC1 | C2D-C1D-ND | 5.42 | 115.94 | 110.33 |
| 37 | 18 | 211 | CLA | CHD-C4C-C3C | -5.41 | 116.88 | 124.77 |
| 37 | C | 504 | CLA | C2B-C1B-NB | 5.41 | 115.94 | 110.33 |
| 37 | z | 102 | CLA | C4A-NA-C1A | -5.41 | 104.21 | 106.68 |
| 37 | 38 | 201 | CLA | C2B-C1B-NB | 5.41 | 115.94 | 110.33 |
| 37 | 18 | 202 | CLA | C3D-C2D-C1D | -5.41 | 98.45 | 105.83 |
| 37 | 38 | 211 | CLA | C2C-C1C-NC | 5.41 | 115.66 | 109.98 |
| 37 | 39 | 307 | CLA | C2C-C1C-NC | 5.41 | 115.66 | 109.98 |
| 37 | 11 | 307 | CLA | C3B-C2B-C1B | -5.41 | 100.80 | 107.17 |
| 37 | 14 | 302 | CLA | C2B-C1B-NB | 5.41 | 115.93 | 110.33 |
| 37 | 21 | 204 | CLA | C2D-C1D-ND | 5.41 | 115.48 | 110.13 |
| 47 | 35 | 304 | KC1 | C2B-C1B-NB | 5.40 | 115.47 | 110.13 |
| 37 | D | 402 | CLA | CHD-C4C-C3C | -5.40 | 116.89 | 124.77 |
| 47 | 13 | 309 | KC1 | C1A-C2A-C3A | -5.40 | 102.31 | 107.28 |
| 37 | 33 | 303 | CLA | O2D-CGD-CBD | 5.40 | 120.67 | 111.23 |
| 37 | 21 | 210 | CLA | C2B-C1B-NB | 5.40 | 115.93 | 110.33 |
| 37 | 41 | 209 | CLA | CHD-C4C-C3C | -5.40 | 116.90 | 124.77 |
| 37 | 19 | 306 | CLA | CMD-C2D-C1D | 5.40 | 134.24 | 124.73 |
| 37 | B | 524 | CLA | CAA-C2A-C3A | -5.40 | 98.41 | 113.00 |
| 37 | b | 504 | CLA | C2C-C1C-NC | 5.40 | 115.65 | 109.98 |
| 48 | 21 | 213 | A86 | C3-C2-C1 | -5.40 | 119.71 | 127.28 |
| 47 | 39 | 308 | KC1 | O2D-CGD-CBD | 5.40 | 120.66 | 111.23 |
| 47 | 18 | 205 | KC1 | C2D-C1D-ND | 5.39 | 115.92 | 110.33 |
| 37 | 37 | 303 | CLA | CHD-C4C-C3C | -5.39 | 116.91 | 124.77 |
| 37 | 14 | 310 | CLA | C2D-C1D-ND | 5.39 | 115.46 | 110.13 |
| 37 | 20 | 303 | CLA | C3D-C2D-C1D | -5.39 | 98.47 | 105.83 |
| 37 | 21 | 209 | CLA | CHD-C4C-C3C | -5.39 | 116.91 | 124.77 |
| 37 | 36 | 306 | CLA | C2D-C1D-ND | 5.39 | 115.46 | 110.13 |
| 37 | 35 | 307 | CLA | O2D-CGD-CBD | 5.39 | 120.65 | 111.23 |
| 37 | B | 504 | CLA | C2C-C1C-NC | 5.39 | 115.64 | 109.98 |
| 47 | 19 | 308 | KC1 | O2D-CGD-CBD | 5.39 | 120.64 | 111.23 |
| 48 | 32 | 221 | A86 | O4-C38-C39 | 5.38 | 120.69 | 111.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 41 | 213 | A86 | C3-C2-C1 | -5.38 | 119.73 | 127.28 |
| 37 | d | 401 | CLA | CHD-C4C-C3C | -5.38 | 116.93 | 124.77 |
| 37 | 34 | 310 | CLA | C2D-C1D-ND | 5.38 | 115.45 | 110.13 |
| 47 | 38 | 205 | KC1 | C2B-C1B-NB | 5.38 | 115.45 | 110.13 |
| 37 | 39 | 306 | CLA | CMD-C2D-C1D | 5.38 | 134.20 | 124.73 |
| 47 | 36 | 302 | KC1 | C2B-C1B-NB | 5.38 | 115.45 | 110.13 |
| 47 | 17 | 303 | KC1 | C2B-C1B-NB | 5.38 | 115.45 | 110.13 |
| 47 | 32 | 207 | KC1 | O2D-CGD-CBD | 5.38 | 120.63 | 111.23 |
| 37 | 37 | 308 | CLA | C2B-C1B-NB | 5.38 | 115.90 | 110.33 |
| 37 | 13 | 301 | CLA | C3B-C2B-C1B | -5.38 | 100.83 | 107.17 |
| 37 | 15 | 308 | CLA | C2C-C1C-NC | 5.38 | 115.63 | 109.98 |
| 37 | 37 | 308 | CLA | C2D-C1D-ND | 5.37 | 115.44 | 110.13 |
| 37 | W | 101 | CLA | C2B-C1B-NB | 5.37 | 115.90 | 110.33 |
| 37 | 14 | 303 | CLA | C4A-NA-C1A | -5.37 | 104.23 | 106.68 |
| 37 | 13 | 310 | CLA | C2D-C1D-ND | 5.37 | 115.44 | 110.13 |
| 47 | 16 | 302 | KC1 | C2B-C1B-NB | 5.37 | 115.44 | 110.13 |
| 47 | 34 | 309 | KC1 | C2D-C1D-ND | 5.37 | 115.90 | 110.33 |
| 37 | 18 | 203 | CLA | C2D-C1D-ND | 5.37 | 115.44 | 110.13 |
| 37 | 40 | 210 | CLA | C2C-C1C-NC | 5.37 | 115.62 | 109.98 |
| 47 | 11 | 309 | KC1 | CBA-CAA-C2A | -5.37 | 103.90 | 125.45 |
| 47 | 14 | 304 | KC1 | C1A-C2A-C3A | -5.37 | 102.35 | 107.28 |
| 47 | 34 | 304 | KC1 | C1A-C2A-C3A | -5.37 | 102.35 | 107.28 |
| 37 | w | 101 | CLA | C2B-C1B-NB | 5.37 | 115.89 | 110.33 |
| 37 | C | 505 | CLA | C2D-C1D-ND | 5.37 | 115.44 | 110.13 |
| 47 | 19 | 308 | KC1 | C2D-C1D-ND | 5.37 | 115.89 | 110.33 |
| 37 | C | 509 | CLA | C2D-C1D-ND | 5.36 | 115.44 | 110.13 |
| 47 | 37 | 302 | KC1 | C2B-C1B-NB | 5.36 | 115.43 | 110.13 |
| 37 | b | 512 | CLA | C3B-C2B-C1B | -5.36 | 100.85 | 107.17 |
| 37 | 19 | 307 | CLA | C2C-C1C-NC | 5.36 | 115.61 | 109.98 |
| 47 | 31 | 309 | KC1 | CBA-CAA-C2A | -5.36 | 103.94 | 125.45 |
| 47 | 11 | 306 | KC1 | C2B-C1B-NB | 5.36 | 115.43 | 110.13 |
| 37 | 34 | 310 | CLA | CHD-C4C-C3C | -5.36 | 116.96 | 124.77 |
| 37 | 32 | 204 | CLA | C2B-C1B-NB | 5.36 | 115.88 | 110.33 |
| 37 | 13 | 303 | CLA | C2C-C1C-NC | 5.36 | 115.61 | 109.98 |
| 37 | B | 508 | CLA | C2B-C1B-NB | 5.36 | 115.88 | 110.33 |
| 37 | 34 | 302 | CLA | C2B-C1B-NB | 5.36 | 115.88 | 110.33 |
| 37 | c | 509 | CLA | C2D-C1D-ND | 5.35 | 115.42 | 110.13 |
| 47 | 14 | 304 | KC1 | C2D-C1D-ND | 5.35 | 115.88 | 110.33 |
| 37 | B | 512 | CLA | C3B-C2B-C1B | -5.35 | 100.86 | 107.17 |
| 37 | 40 | 205 | CLA | C3D-C2D-C1D | -5.35 | 98.53 | 105.83 |
| 37 | 33 | 301 | CLA | C3B-C2B-C1B | -5.35 | 100.86 | 107.17 |
| 37 | C | 510 | CLA | C2C-C1C-NC | 5.35 | 115.60 | 109.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 508 | CLA | CMD-C2D-C1D | 5.35 | 134.15 | 124.73 |
| 42 | A | 409 | BCT | O2-C-O1 | 5.35 | 133.35 | 119.68 |
| 47 | 14 | 309 | KC1 | C2D-C1D-ND | 5.35 | 115.87 | 110.33 |
| 37 | 19 | 310 | CLA | C2C-C1C-NC | 5.35 | 115.60 | 109.98 |
| 47 | 13 | 304 | KC1 | C3B-C2B-C1B | -5.34 | 101.99 | 107.05 |
| 37 | 34 | 303 | CLA | C3B-C2B-C1B | -5.34 | 100.87 | 107.17 |
| 37 | C | 508 | CLA | CMD-C2D-C1D | 5.34 | 134.14 | 124.73 |
| 37 | c | 505 | CLA | C2D-C1D-ND | 5.34 | 115.41 | 110.13 |
| 37 | 37 | 301 | CLA | C3B-C2B-C1B | -5.34 | 100.87 | 107.17 |
| 37 | Z | 102 | CLA | C2B-C1B-NB | 5.34 | 115.86 | 110.33 |
| 47 | 15 | 306 | KC1 | C1A-C2A-C3A | -5.34 | 102.37 | 107.28 |
| 42 | a | 411 | BCT | O2-C-O1 | 5.34 | 133.34 | 119.68 |
| 37 | 14 | 310 | CLA | C2C-C1C-NC | 5.34 | 115.59 | 109.98 |
| 47 | 35 | 309 | KC1 | CBA-CAA-C2A | -5.34 | 104.02 | 125.45 |
| 37 | 39 | 302 | CLA | CHD-C4C-C3C | -5.34 | 116.99 | 124.77 |
| 37 | 14 | 303 | CLA | C3B-C2B-C1B | -5.34 | 100.88 | 107.17 |
| 47 | 16 | 305 | KC1 | C2B-C1B-NB | 5.34 | 115.41 | 110.13 |
| 47 | 36 | 305 | KC1 | C2B-C1B-NB | 5.34 | 115.41 | 110.13 |
| 48 | 11 | 313 | A86 | C3-C2-C1 | -5.34 | 119.79 | 127.28 |
| 37 | 17 | 302 | CLA | C3B-C2B-C1B | -5.34 | 100.88 | 107.17 |
| 37 | 39 | 301 | CLA | C2B-C1B-NB | 5.34 | 115.86 | 110.33 |
| 47 | 39 | 308 | KC1 | C2D-C1D-ND | 5.34 | 115.86 | 110.33 |
| 47 | 38 | 205 | KC1 | C2D-C1D-ND | 5.33 | 115.86 | 110.33 |
| 37 | c | 510 | CLA | O2D-CGD-CBD | 5.33 | 120.56 | 111.23 |
| 37 | b | 516 | CLA | C2B-C1B-NB | 5.33 | 115.86 | 110.33 |
| 47 | 20 | 302 | KC1 | C1A-C2A-C3A | -5.33 | 102.38 | 107.28 |
| 37 | 12 | 203 | CLA | C2B-C1B-NB | 5.33 | 115.86 | 110.33 |
| 37 | Z | 101 | CLA | C2D-C1D-ND | 5.33 | 115.40 | 110.13 |
| 37 | 34 | 307 | CLA | C3B-C2B-C1B | -5.33 | 100.89 | 107.17 |
| 37 | 12 | 209 | CLA | C3B-C2B-C1B | -5.33 | 100.89 | 107.17 |
| 37 | 34 | 310 | CLA | C2C-C1C-NC | 5.33 | 115.58 | 109.98 |
| 37 | 19 | 302 | CLA | CHD-C4C-C3C | -5.33 | 117.00 | 124.77 |
| 37 | 16 | 309 | CLA | C4A-NA-C1A | -5.33 | 104.25 | 106.68 |
| 37 | 37 | 303 | CLA | O2D-CGD-CBD | 5.33 | 120.54 | 111.23 |
| 47 | 16 | 305 | KC1 | C3C-C4C-NC | 5.33 | 115.61 | 109.90 |
| 47 | 40 | 204 | KC1 | C2D-C1D-ND | 5.32 | 115.85 | 110.33 |
| 37 | 16 | 306 | CLA | C2D-C1D-ND | 5.32 | 115.40 | 110.13 |
| 47 | 15 | 309 | KC1 | CBA-CAA-C2A | -5.32 | 104.08 | 125.45 |
| 37 | 13 | 308 | CLA | C2C-C1C-NC | 5.32 | 115.57 | 109.98 |
| 37 | 20 | 301 | CLA | C3B-C2B-C1B | -5.32 | 100.89 | 107.17 |
| 37 | C | 501 | CLA | CHD-C4C-C3C | -5.32 | 117.01 | 124.77 |
| 37 | 15 | 307 | CLA | O2D-CGD-CBD | 5.32 | 120.53 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 40 | 203 | CLA | C3B-C2B-C1B | -5.32 | 100.90 | 107.17 |
| 37 | 17 | 309 | CLA | C2B-C1B-NB | 5.32 | 115.84 | 110.33 |
| 37 | 31 | 304 | CLA | CHD-C4C-C3C | -5.32 | 117.02 | 124.77 |
| 37 | 33 | 310 | CLA | C2B-C1B-NB | 5.32 | 115.84 | 110.33 |
| 47 | 20 | 302 | KC1 | C2D-C1D-ND | 5.32 | 115.84 | 110.33 |
| 47 | 12 | 208 | KC1 | C3B-C2B-C1B | -5.32 | 102.02 | 107.05 |
| 48 | 31 | 313 | A86 | C3-C2-C1 | -5.32 | 119.82 | 127.28 |
| 37 | 31 | 304 | CLA | C3B-C2B-C1B | -5.31 | 100.91 | 107.17 |
| 37 | 33 | 310 | CLA | C4A-NA-C1A | -5.31 | 104.25 | 106.68 |
| 48 | 32 | 217 | A86 | C25-C26-C27 | -5.31 | 119.83 | 127.28 |
| 48 | 33 | 312 | A86 | O4-C38-C39 | 5.31 | 120.56 | 111.09 |
| 37 | c | 510 | CLA | C2C-C1C-NC | 5.31 | 115.56 | 109.98 |
| 37 | z | 101 | CLA | C2D-C1D-ND | 5.31 | 115.38 | 110.13 |
| 37 | 11 | 305 | CLA | O2D-CGD-CBD | 5.31 | 120.51 | 111.23 |
| 37 | C | 513 | CLA | C3B-C2B-C1B | -5.31 | 100.91 | 107.17 |
| 37 | 17 | 309 | CLA | C2D-C1D-ND | 5.31 | 115.38 | 110.13 |
| 47 | 36 | 305 | KC1 | C3C-C4C-NC | 5.31 | 115.59 | 109.90 |
| 37 | 21 | 209 | CLA | C2B-C1B-NB | 5.31 | 115.83 | 110.33 |
| 37 | 39 | 310 | CLA | C2C-C1C-NC | 5.31 | 115.56 | 109.98 |
| 48 | 13 | 312 | A86 | O4-C38-C39 | 5.31 | 120.56 | 111.09 |
| 37 | 32 | 210 | CLA | C3B-C2B-C1B | -5.31 | 100.91 | 107.17 |
| 48 | 12 | 216 | A86 | C25-C26-C27 | -5.31 | 119.83 | 127.28 |
| 37 | c | 501 | CLA | CHD-C4C-C3C | -5.31 | 117.04 | 124.77 |
| 37 | 11 | 303 | CLA | CHD-C4C-C3C | -5.31 | 117.04 | 124.77 |
| 37 | 13 | 310 | CLA | C2B-C1B-NB | 5.30 | 115.83 | 110.33 |
| 48 | 12 | 220 | A86 | O4-C38-C39 | 5.30 | 120.55 | 111.09 |
| 37 | B | 507 | CLA | CHD-C4C-C3C | -5.30 | 117.04 | 124.77 |
| 37 | 34 | 303 | CLA | C4A-NA-C1A | -5.30 | 104.26 | 106.68 |
| 37 | 33 | 308 | CLA | C2C-C1C-NC | 5.30 | 115.55 | 109.98 |
| 37 | 35 | 310 | CLA | CHD-C4C-C3C | -5.30 | 117.04 | 124.77 |
| 47 | 31 | 307 | KC1 | CHD-C4C-C3C | -5.30 | 115.45 | 125.23 |
| 50 | 41 | 212 | DD6 | C21-C20-C19 | -5.30 | 108.29 | 114.24 |
| 37 | 17 | 304 | CLA | O2D-CGD-CBD | 5.30 | 120.50 | 111.23 |
| 37 | 41 | 204 | CLA | C2B-C1B-NB | 5.30 | 115.82 | 110.33 |
| 37 | 32 | 205 | CLA | C2C-C1C-NC | 5.30 | 115.55 | 109.98 |
| 37 | B | 506 | CLA | C2B-C1B-NB | 5.30 | 115.82 | 110.33 |
| 37 | 33 | 305 | CLA | C2B-C1B-NB | 5.30 | 115.82 | 110.33 |
| 37 | 38 | 211 | CLA | C2D-C1D-ND | 5.30 | 115.37 | 110.13 |
| 47 | 37 | 305 | KC1 | C3B-C2B-C1B | -5.30 | 102.03 | 107.05 |
| 47 | 33 | 306 | KC1 | C2B-C1B-NB | 5.30 | 115.37 | 110.13 |
| 37 | C | 510 | CLA | O2D-CGD-CBD | 5.30 | 120.49 | 111.23 |
| 37 | 15 | 310 | CLA | CHD-C4C-C3C | -5.30 | 117.05 | 124.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 202 | CLA | CHD-C4C-C3C | -5.30 | 117.05 | 124.77 |
| 37 | 41 | 205 | CLA | CHD-C4C-C3C | -5.30 | 117.05 | 124.77 |
| 48 | 31 | 314 | A86 | O4-C38-C39 | 5.29 | 120.53 | 111.09 |
| 37 | B | 503 | CLA | C2D-C1D-ND | 5.29 | 115.36 | 110.13 |
| 47 | 13 | 306 | KC1 | C2B-C1B-NB | 5.29 | 115.36 | 110.13 |
| 37 | 19 | 301 | CLA | C2B-C1B-NB | 5.29 | 115.81 | 110.33 |
| 37 | 14 | 307 | CLA | C3B-C2B-C1B | -5.29 | 100.93 | 107.17 |
| 37 | 11 | 305 | CLA | C2B-C1B-NB | 5.29 | 115.81 | 110.33 |
| 37 | Z | 102 | CLA | C4A-NA-C1A | -5.29 | 104.27 | 106.68 |
| 37 | 31 | 306 | CLA | O2D-CGD-CBD | 5.29 | 120.48 | 111.23 |
| 37 | z | 102 | CLA | C2B-C1B-NB | 5.29 | 115.81 | 110.33 |
| 50 | 21 | 212 | DD6 | C21-C20-C19 | -5.29 | 108.30 | 114.24 |
| 37 | 31 | 306 | CLA | C2B-C1B-NB | 5.29 | 115.81 | 110.33 |
| 47 | 17 | 308 | KC1 | C2D-C1D-ND | 5.29 | 115.81 | 110.33 |
| 37 | b | 507 | CLA | CHD-C4C-C3C | -5.29 | 117.06 | 124.77 |
| 37 | 41 | 202 | CLA | CHD-C4C-C3C | -5.29 | 117.06 | 124.77 |
| 37 | 15 | 305 | CLA | O2D-CGD-CBD | 5.29 | 120.48 | 111.23 |
| 47 | 18 | 207 | KC1 | C2D-C1D-ND | 5.29 | 115.81 | 110.33 |
| 47 | 11 | 309 | KC1 | C2D-C1D-ND | 5.29 | 115.81 | 110.33 |
| 37 | 11 | 303 | CLA | C3B-C2B-C1B | -5.29 | 100.94 | 107.17 |
| 48 | 12 | 220 | A86 | C12-C11-C13 | 5.29 | 124.57 | 116.00 |
| 37 | 13 | 310 | CLA | C4A-NA-C1A | -5.29 | 104.27 | 106.68 |
| 47 | 37 | 305 | KC1 | CMA-C3A-C2A | -5.29 | 115.63 | 128.43 |
| 37 | B | 516 | CLA | C2B-C1B-NB | 5.29 | 115.81 | 110.33 |
| 47 | 40 | 204 | KC1 | C1A-C2A-C3A | -5.29 | 102.42 | 107.28 |
| 37 | b | 506 | CLA | C2B-C1B-NB | 5.29 | 115.81 | 110.33 |
| 48 | 32 | 215 | A86 | C4-C5-C6 | -5.29 | 119.87 | 127.28 |
| 37 | 18 | 203 | CLA | C2B-C1B-NB | 5.28 | 115.81 | 110.33 |
| 37 | 14 | 303 | CLA | CHD-C4C-C3C | -5.28 | 117.07 | 124.77 |
| 37 | 35 | 305 | CLA | O2D-CGD-CBD | 5.28 | 120.46 | 111.23 |
| 47 | 17 | 306 | KC1 | CMA-C3A-C2A | -5.28 | 115.65 | 128.43 |
| 47 | 32 | 209 | KC1 | C3B-C2B-C1B | -5.28 | 102.05 | 107.05 |
| 47 | 11 | 306 | KC1 | CHD-C4C-C3C | -5.28 | 115.49 | 125.23 |
| 37 | 40 | 205 | CLA | O2D-CGD-CBD | 5.28 | 120.46 | 111.23 |
| 47 | 34 | 304 | KC1 | C2D-C1D-ND | 5.28 | 115.80 | 110.33 |
| 37 | 21 | 205 | CLA | CHD-C4C-C3C | -5.28 | 117.08 | 124.77 |
| 37 | b | 503 | CLA | C2D-C1D-ND | 5.28 | 115.35 | 110.13 |
| 50 | 20 | 312 | DD6 | C7-C6-C8 | -5.28 | 110.03 | 118.09 |
| 37 | 13 | 303 | CLA | CHD-C4C-C3C | -5.27 | 117.08 | 124.77 |
| 37 | 36 | 309 | CLA | C4A-NA-C1A | -5.27 | 104.27 | 106.68 |
| 47 | 38 | 207 | KC1 | C3B-C2B-C1B | -5.27 | 102.06 | 107.05 |
| 47 | 19 | 308 | KC1 | C2B-C1B-NB | 5.27 | 115.34 | 110.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 507 | CLA | C2C-C1C-NC | 5.27 | 115.52 | 109.98 |
| 37 | 34 | 303 | CLA | CHD-C4C-C3C | -5.27 | 117.09 | 124.77 |
| 47 | 31 | 307 | KC1 | C2B-C1B-NB | 5.27 | 115.34 | 110.13 |
| 37 | 19 | 307 | CLA | C3B-C2B-C1B | -5.27 | 100.96 | 107.17 |
| 37 | 21 | 204 | CLA | C2B-C1B-NB | 5.27 | 115.79 | 110.33 |
| 47 | 13 | 304 | KC1 | O2D-CGD-CBD | 5.27 | 120.44 | 111.23 |
| 37 | 13 | 303 | CLA | O2D-CGD-CBD | 5.27 | 120.44 | 111.23 |
| 37 | 38 | 208 | CLA | C2D-C1D-ND | 5.27 | 115.34 | 110.13 |
| 37 | 32 | 204 | CLA | C3B-C2B-C1B | -5.27 | 100.96 | 107.17 |
| 37 | 12 | 204 | CLA | C2C-C1C-NC | 5.27 | 115.52 | 109.98 |
| 37 | B | 505 | CLA | C2B-C1B-NB | 5.27 | 115.79 | 110.33 |
| 48 | 15 | 319 | A86 | O4-C38-C39 | 5.27 | 120.48 | 111.09 |
| 37 | 14 | 310 | CLA | CHD-C4C-C3C | -5.27 | 117.09 | 124.77 |
| 37 | 37 | 301 | CLA | CHD-C4C-C3C | -5.27 | 117.09 | 124.77 |
| 37 | A | 405 | CLA | O2D-CGD-CBD | 5.26 | 120.43 | 111.23 |
| 47 | 38 | 210 | KC1 | CMA-C3A-C2A | -5.26 | 115.69 | 128.43 |
| 37 | 11 | 308 | CLA | C2B-C1B-NB | 5.26 | 115.78 | 110.33 |
| 47 | 18 | 210 | KC1 | CMA-C3A-C2A | -5.26 | 115.70 | 128.43 |
| 48 | 32 | 221 | A86 | C12-C11-C13 | 5.26 | 124.53 | 116.00 |
| 47 | 20 | 304 | KC1 | C1A-C2A-C3A | -5.26 | 102.45 | 107.28 |
| 37 | b | 505 | CLA | C2B-C1B-NB | 5.26 | 115.78 | 110.33 |
| 47 | 31 | 309 | KC1 | C2D-C1D-ND | 5.26 | 115.78 | 110.33 |
| 47 | 37 | 307 | KC1 | C2D-C1D-ND | 5.26 | 115.78 | 110.33 |
| 47 | 17 | 306 | KC1 | C3B-C2B-C1B | -5.26 | 102.07 | 107.05 |
| 48 | 12 | 214 | A86 | C4-C5-C6 | -5.26 | 119.91 | 127.28 |
| 47 | 33 | 304 | KC1 | O2D-CGD-CBD | 5.26 | 120.42 | 111.23 |
| 37 | 33 | 303 | CLA | C2C-C1C-NC | 5.26 | 115.50 | 109.98 |
| 37 | 39 | 302 | CLA | C4A-NA-C1A | -5.25 | 104.28 | 106.68 |
| 37 | 16 | 309 | CLA | C2B-C1B-NB | 5.25 | 115.77 | 110.33 |
| 37 | a | 407 | CLA | O2D-CGD-CBD | 5.25 | 120.41 | 111.23 |
| 47 | 39 | 308 | KC1 | C2B-C1B-NB | 5.25 | 115.32 | 110.13 |
| 48 | 35 | 319 | A86 | O4-C38-C39 | 5.25 | 120.45 | 111.09 |
| 37 | c | 502 | CLA | O2D-CGD-CBD | 5.25 | 120.41 | 111.23 |
| 37 | 13 | 305 | CLA | C2B-C1B-NB | 5.25 | 115.77 | 110.33 |
| 37 | 41 | 209 | CLA | C2B-C1B-NB | 5.25 | 115.77 | 110.33 |
| 37 | B | 513 | CLA | C3D-C2D-C1D | -5.25 | 98.67 | 105.83 |
| 50 | 40 | 214 | DD6 | C7-C6-C8 | -5.25 | 110.07 | 118.09 |
| 37 | c | 507 | CLA | C2C-C1C-NC | 5.25 | 115.49 | 109.98 |
| 37 | 20 | 303 | CLA | O2D-CGD-CBD | 5.24 | 120.40 | 111.23 |
| 48 | 37 | 313 | A86 | C25-C26-C27 | -5.24 | 119.92 | 127.28 |
| 37 | c | 512 | CLA | C4A-NA-C1A | -5.24 | 104.29 | 106.68 |
| 37 | 17 | 302 | CLA | CHD-C4C-C3C | -5.24 | 117.13 | 124.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 502 | CLA | O2D-CGD-CBD | 5.24 | 120.39 | 111.23 |
| 37 | b | 513 | CLA | C3D-C2D-C1D | -5.24 | 98.68 | 105.83 |
| 37 | 32 | 202 | CLA | C2B-C1B-NB | 5.24 | 115.76 | 110.33 |
| 47 | 38 | 207 | KC1 | C2B-C1B-NB | 5.24 | 115.31 | 110.13 |
| 47 | 37 | 302 | KC1 | CHC-C1C-C2C | -5.24 | 116.75 | 125.03 |
| 37 | 33 | 303 | CLA | C2B-C1B-NB | 5.24 | 115.76 | 110.33 |
| 47 | 15 | 309 | KC1 | C2D-C1D-ND | 5.24 | 115.76 | 110.33 |
| 47 | 38 | 205 | KC1 | C1A-C2A-C3A | -5.24 | 102.46 | 107.28 |
| 37 | 16 | 303 | CLA | CHD-C4C-C3C | -5.24 | 117.14 | 124.77 |
| 37 | 34 | 303 | CLA | C2B-C1B-NB | 5.24 | 115.75 | 110.33 |
| 37 | 12 | 203 | CLA | C3B-C2B-C1B | -5.23 | 101.00 | 107.17 |
| 37 | 33 | 303 | CLA | C2D-C1D-ND | 5.23 | 115.31 | 110.13 |
| 37 | B | 504 | CLA | CHD-C4C-C3C | -5.23 | 117.14 | 124.77 |
| 37 | c | 513 | CLA | C3B-C2B-C1B | -5.23 | 101.00 | 107.17 |
| 37 | 13 | 307 | CLA | C3B-C2B-C1B | -5.23 | 101.00 | 107.17 |
| 37 | 12 | 207 | CLA | C2B-C1B-NB | 5.23 | 115.75 | 110.33 |
| 37 | 32 | 208 | CLA | C2B-C1B-NB | 5.23 | 115.75 | 110.33 |
| 37 | C | 512 | CLA | C4A-NA-C1A | -5.23 | 104.29 | 106.68 |
| 37 | D | 401 | CLA | C2B-C1B-NB | 5.23 | 115.75 | 110.33 |
| 37 | 18 | 211 | CLA | C2B-C1B-NB | 5.22 | 115.74 | 110.33 |
| 37 | 11 | 303 | CLA | C2C-C1C-NC | 5.22 | 115.47 | 109.98 |
| 37 | 15 | 303 | CLA | CHD-C4C-C3C | -5.22 | 117.16 | 124.77 |
| 37 | 14 | 307 | CLA | C2D-C1D-ND | 5.22 | 115.30 | 110.13 |
| 37 | b | 502 | CLA | C2B-C1B-NB | 5.22 | 115.74 | 110.33 |
| 37 | 38 | 211 | CLA | C2B-C1B-NB | 5.22 | 115.74 | 110.33 |
| 47 | 40 | 206 | KC1 | C1A-C2A-C3A | -5.22 | 102.48 | 107.28 |
| 48 | 16 | 313 | A86 | C26-C25-C24 | -5.22 | 108.07 | 123.20 |
| 47 | 16 | 305 | KC1 | C2D-C1D-ND | 5.22 | 115.74 | 110.33 |
| 37 | 21 | 208 | CLA | CHD-C4C-C3C | -5.22 | 117.16 | 124.77 |
| 37 | 33 | 307 | CLA | C3B-C2B-C1B | -5.22 | 101.02 | 107.17 |
| 37 | 36 | 309 | CLA | C2B-C1B-NB | 5.22 | 115.74 | 110.33 |
| 47 | 35 | 304 | KC1 | O2D-CGD-CBD | 5.22 | 120.35 | 111.23 |
| 47 | 36 | 305 | KC1 | C2D-C1D-ND | 5.22 | 115.74 | 110.33 |
| 47 | 38 | 207 | KC1 | C2D-C1D-ND | 5.22 | 115.74 | 110.33 |
| 37 | 14 | 303 | CLA | C2B-C1B-NB | 5.22 | 115.74 | 110.33 |
| 47 | 18 | 205 | KC1 | C1A-C2A-C3A | -5.22 | 102.49 | 107.28 |
| 47 | 38 | 210 | KC1 | C2D-C1D-ND | 5.21 | 115.73 | 110.33 |
| 37 | 36 | 303 | CLA | CHD-C4C-C3C | -5.21 | 117.17 | 124.77 |
| 47 | 33 | 304 | KC1 | C1A-C2A-C3A | -5.21 | 102.49 | 107.28 |
| 37 | 41 | 208 | CLA | C2B-C1B-NB | 5.21 | 115.73 | 110.33 |
| 37 | b | 504 | CLA | CHD-C4C-C3C | -5.21 | 117.17 | 124.77 |
| 47 | 16 | 305 | KC1 | O2D-CGD-CBD | 5.21 | 120.34 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 40 | 201 | A86 | C26-C25-C24 | -5.21 | 108.10 | 123.20 |
| 37 | 17 | 309 | CLA | C4A-NA-C1A | -5.21 | 104.30 | 106.68 |
| 37 | 37 | 306 | CLA | O2D-CGD-CBD | 5.21 | 120.34 | 111.23 |
| 37 | 15 | 305 | CLA | C2B-C1B-NB | 5.21 | 115.73 | 110.33 |
| 37 | 21 | 208 | CLA | C2B-C1B-NB | 5.21 | 115.73 | 110.33 |
| 37 | 35 | 303 | CLA | CHD-C4C-C3C | -5.21 | 117.18 | 124.77 |
| 37 | 18 | 208 | CLA | C2D-C1D-ND | 5.21 | 115.28 | 110.13 |
| 48 | 34 | 311 | A86 | C41-C32-C31 | -5.21 | 105.81 | 110.47 |
| 47 | 13 | 304 | KC1 | C1A-C2A-C3A | -5.21 | 102.50 | 107.28 |
| 48 | 14 | 311 | A86 | C41-C32-C31 | -5.20 | 105.82 | 110.47 |
| 47 | 35 | 302 | KC1 | C2D-C1D-ND | 5.20 | 115.72 | 110.33 |
| 47 | 16 | 308 | KC1 | C2D-C1D-ND | 5.20 | 115.72 | 110.33 |
| 37 | 38 | 203 | CLA | C2B-C1B-NB | 5.20 | 115.72 | 110.33 |
| 37 | 31 | 301 | CLA | O2D-CGD-CBD | 5.20 | 120.32 | 111.23 |
| 37 | B | 502 | CLA | C2B-C1B-NB | 5.20 | 115.72 | 110.33 |
| 37 | 33 | 303 | CLA | CHD-C4C-C3C | -5.19 | 117.20 | 124.77 |
| 48 | 13 | 311 | A86 | O4-C38-C39 | 5.19 | 120.35 | 111.09 |
| 37 | 41 | 204 | CLA | C3B-C2B-C1B | -5.19 | 101.05 | 107.17 |
| 37 | 41 | 208 | CLA | CHD-C4C-C3C | -5.19 | 117.21 | 124.77 |
| 37 | a | 404 | CLA | C2B-C1B-NB | 5.19 | 115.71 | 110.33 |
| 37 | 11 | 301 | CLA | C3B-C2B-C1B | -5.19 | 101.05 | 107.17 |
| 37 | 31 | 302 | CLA | C3B-C2B-C1B | -5.19 | 101.05 | 107.17 |
| 47 | 32 | 209 | KC1 | C2B-C1B-NB | 5.19 | 115.26 | 110.13 |
| 48 | 12 | 216 | A86 | O4-C38-C39 | 5.19 | 120.34 | 111.09 |
| 37 | 15 | 310 | CLA | C2C-C1C-NC | 5.19 | 115.43 | 109.98 |
| 47 | 35 | 309 | KC1 | C2D-C1D-ND | 5.19 | 115.71 | 110.33 |
| 48 | 36 | 313 | A86 | C33-C32-C31 | 5.19 | 114.25 | 109.21 |
| 37 | 17 | 302 | CLA | C2D-C1D-ND | 5.19 | 115.26 | 110.13 |
| 37 | 13 | 310 | CLA | CHD-C4C-C3C | -5.19 | 117.21 | 124.77 |
| 37 | D | 405 | CLA | CAA-C2A-C3A | -5.19 | 98.98 | 113.00 |
| 37 | b | 501 | CLA | CHD-C4C-C3C | -5.19 | 117.21 | 124.77 |
| 37 | d | 403 | CLA | CAA-C2A-C3A | -5.19 | 98.99 | 113.00 |
| 37 | 15 | 308 | CLA | CED-O2D-CGD | 5.18 | 127.68 | 115.92 |
| 37 | 21 | 204 | CLA | C3B-C2B-C1B | -5.18 | 101.06 | 107.17 |
| 37 | W | 102 | CLA | O2D-CGD-CBD | 5.18 | 120.29 | 111.23 |
| 37 | B | 510 | CLA | C2B-C1B-NB | 5.18 | 115.70 | 110.33 |
| 37 | z | 102 | CLA | CAA-C2A-C3A | -5.18 | 98.99 | 113.00 |
| 37 | z | 102 | CLA | C2D-C1D-ND | 5.18 | 115.25 | 110.13 |
| 37 | 19 | 306 | CLA | C2B-C1B-NB | 5.18 | 115.70 | 110.33 |
| 37 | 34 | 307 | CLA | C2D-C1D-ND | 5.18 | 115.25 | 110.13 |
| 37 | w | 101 | CLA | C3B-C2B-C1B | -5.18 | 101.06 | 107.17 |
| 47 | 12 | 208 | KC1 | C2B-C1B-NB | 5.18 | 115.25 | 110.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 205 | CLA | C2B-C1B-NB | 5.18 | 115.70 | 110.33 |
| 47 | 38 | 205 | KC1 | O2D-CGD-CBD | 5.18 | 120.28 | 111.23 |
| 37 | Z | 102 | CLA | C2D-C1D-ND | 5.18 | 115.25 | 110.13 |
| 47 | 40 | 206 | KC1 | C3B-C2B-C1B | -5.18 | 102.15 | 107.05 |
| 47 | 18 | 205 | KC1 | O2D-CGD-CBD | 5.18 | 120.28 | 111.23 |
| 37 | 31 | 304 | CLA | C2C-C1C-NC | 5.18 | 115.42 | 109.98 |
| 37 | 16 | 309 | CLA | CHD-C4C-C3C | -5.17 | 117.23 | 124.77 |
| 37 | W | 101 | CLA | C3B-C2B-C1B | -5.17 | 101.07 | 107.17 |
| 47 | 17 | 303 | KC1 | CHC-C1C-C2C | -5.17 | 116.86 | 125.03 |
| 47 | 36 | 305 | KC1 | O2D-CGD-CBD | 5.17 | 120.28 | 111.23 |
| 48 | 32 | 203 | A86 | C33-C32-C31 | 5.17 | 114.24 | 109.21 |
| 37 | 17 | 302 | CLA | CMD-C2D-C1D | 5.17 | 133.84 | 124.73 |
| 37 | 17 | 307 | CLA | O2D-CGD-CBD | 5.17 | 120.27 | 111.23 |
| 47 | 13 | 304 | KC1 | CHD-C4C-C3C | -5.17 | 115.69 | 125.23 |
| 37 | 34 | 305 | CLA | C2B-C1B-NB | 5.17 | 115.69 | 110.33 |
| 37 | B | 501 | CLA | C3B-C2B-C1B | -5.17 | 101.08 | 107.17 |
| 48 | 33 | 311 | A86 | O4-C38-C39 | 5.17 | 120.30 | 111.09 |
| 37 | Z | 102 | CLA | CAA-C2A-C3A | -5.16 | 99.04 | 113.00 |
| 48 | 37 | 311 | A86 | C4-C5-C6 | -5.16 | 120.04 | 127.28 |
| 48 | 16 | 314 | A86 | C33-C32-C31 | 5.16 | 114.23 | 109.21 |
| 50 | 36 | 312 | DD6 | C7-C6-C8 | -5.16 | 110.20 | 118.09 |
| 37 | 36 | 301 | CLA | C3B-C2B-C1B | -5.16 | 101.08 | 107.17 |
| 48 | 32 | 217 | A86 | O4-C38-C39 | 5.16 | 120.29 | 111.09 |
| 47 | 11 | 304 | KC1 | C2B-C1B-NB | 5.16 | 115.23 | 110.13 |
| 48 | 20 | 311 | A86 | C25-C26-C27 | -5.16 | 120.04 | 127.28 |
| 37 | 38 | 203 | CLA | C2C-C1C-NC | 5.16 | 115.40 | 109.98 |
| 37 | 38 | 202 | CLA | C3B-C2B-C1B | -5.16 | 101.09 | 107.17 |
| 37 | 20 | 301 | CLA | C2B-C1B-NB | 5.16 | 115.68 | 110.33 |
| 47 | 33 | 304 | KC1 | CHD-C4C-C3C | -5.16 | 115.72 | 125.23 |
| 47 | 20 | 304 | KC1 | C3B-C2B-C1B | -5.16 | 102.17 | 107.05 |
| 37 | 31 | 302 | CLA | C2B-C1B-NB | 5.16 | 115.67 | 110.33 |
| 37 | 11 | 301 | CLA | C2B-C1B-NB | 5.16 | 115.67 | 110.33 |
| 37 | 11 | 310 | CLA | C2B-C1B-NB | 5.16 | 115.67 | 110.33 |
| 37 | 40 | 210 | CLA | C3B-C2B-C1B | -5.15 | 101.09 | 107.17 |
| 37 | B | 506 | CLA | O2D-CGD-CBD | 5.15 | 120.24 | 111.23 |
| 37 | b | 506 | CLA | O2D-CGD-CBD | 5.15 | 120.24 | 111.23 |
| 37 | b | 501 | CLA | C3B-C2B-C1B | -5.15 | 101.10 | 107.17 |
| 37 | Z | 101 | CLA | O2D-CGD-CBD | 5.15 | 120.23 | 111.23 |
| 48 | 33 | 315 | A86 | C3-C2-C1 | -5.15 | 120.05 | 127.28 |
| 37 | 36 | 309 | CLA | CHD-C4C-C3C | -5.15 | 117.27 | 124.77 |
| 37 | 19 | 302 | CLA | C4A-NA-C1A | -5.15 | 104.33 | 106.68 |
| 37 | 35 | 305 | CLA | C2B-C1B-NB | 5.15 | 115.66 | 110.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 16 | 301 | CLA | C3B-C2B-C1B | -5.15 | 101.10 | 107.17 |
| 37 | 11 | 307 | CLA | C2C-C1C-NC | 5.15 | 115.39 | 109.98 |
| 37 | B | 501 | CLA | CHD-C4C-C3C | -5.15 | 117.27 | 124.77 |
| 37 | 40 | 208 | CLA | O2D-CGD-CBD | 5.15 | 120.22 | 111.23 |
| 37 | d | 403 | CLA | C3D-C2D-C1D | -5.14 | 98.81 | 105.83 |
| 37 | 40 | 208 | CLA | C2B-C1B-NB | 5.14 | 115.66 | 110.33 |
| 37 | 31 | 308 | CLA | C2C-C1C-NC | 5.14 | 115.38 | 109.98 |
| 37 | 41 | 204 | CLA | CHD-C4C-C3C | -5.14 | 117.28 | 124.77 |
| 37 | 21 | 204 | CLA | CHD-C4C-C3C | -5.14 | 117.28 | 124.77 |
| 48 | 40 | 213 | A86 | C25-C26-C27 | -5.14 | 120.07 | 127.28 |
| 37 | 20 | 306 | CLA | O2D-CGD-CBD | 5.14 | 120.22 | 111.23 |
| 37 | B | 512 | CLA | C2B-C1B-NB | 5.14 | 115.66 | 110.33 |
| 37 | 20 | 306 | CLA | C2B-C1B-NB | 5.14 | 115.66 | 110.33 |
| 37 | 41 | 205 | CLA | C2B-C1B-NB | 5.14 | 115.66 | 110.33 |
| 47 | 18 | 210 | KC1 | C2D-C1D-ND | 5.14 | 115.66 | 110.33 |
| 37 | 40 | 203 | CLA | C2B-C1B-NB | 5.14 | 115.65 | 110.33 |
| 37 | 18 | 203 | CLA | C2C-C1C-NC | 5.14 | 115.38 | 109.98 |
| 37 | 35 | 310 | CLA | C2C-C1C-NC | 5.14 | 115.38 | 109.98 |
| 37 | z | 101 | CLA | O2D-CGD-CBD | 5.14 | 120.21 | 111.23 |
| 37 | 33 | 310 | CLA | CHD-C4C-C3C | -5.14 | 117.28 | 124.77 |
| 48 | 12 | 202 | A86 | C33-C32-C31 | 5.14 | 114.20 | 109.21 |
| 37 | D | 405 | CLA | C3D-C2D-C1D | -5.13 | 98.82 | 105.83 |
| 48 | 14 | 315 | A86 | C3-C2-C1 | -5.13 | 120.08 | 127.28 |
| 37 | 31 | 310 | CLA | C2B-C1B-NB | 5.13 | 115.65 | 110.33 |
| 47 | 31 | 305 | KC1 | C2B-C1B-NB | 5.13 | 115.21 | 110.13 |
| 48 | 40 | 211 | A86 | O4-C38-C39 | 5.13 | 120.24 | 111.09 |
| 47 | 33 | 302 | KC1 | C1A-NA-C4A | -5.13 | 104.34 | 106.68 |
| 48 | 40 | 201 | A86 | C3-C2-C1 | -5.13 | 120.08 | 127.28 |
| 50 | 16 | 312 | DD6 | C7-C6-C8 | -5.13 | 110.25 | 118.09 |
| 48 | 34 | 312 | A86 | O4-C38-C39 | 5.13 | 120.24 | 111.09 |
| 47 | 36 | 302 | KC1 | C3B-C2B-C1B | -5.13 | 102.19 | 107.05 |
| 50 | 19 | 312 | DD6 | C-C1-C24 | -5.13 | 110.25 | 118.09 |
| 37 | b | 510 | CLA | C2B-C1B-NB | 5.13 | 115.64 | 110.33 |
| 37 | 32 | 206 | CLA | C3B-C2B-C1B | -5.13 | 101.12 | 107.17 |
| 37 | 31 | 301 | CLA | C2D-C1D-ND | 5.13 | 115.20 | 110.13 |
| 50 | 16 | 312 | DD6 | C21-C20-C15 | -5.12 | 113.87 | 122.30 |
| 37 | b | 512 | CLA | C2B-C1B-NB | 5.12 | 115.64 | 110.33 |
| 48 | 14 | 313 | A86 | C41-C32-C31 | -5.12 | 105.89 | 110.47 |
| 47 | 17 | 305 | KC1 | CMA-C3A-C2A | -5.12 | 116.03 | 128.43 |
| 47 | 16 | 302 | KC1 | C3B-C2B-C1B | -5.12 | 102.20 | 107.05 |
| 48 | 20 | 309 | A86 | O4-C38-C39 | 5.12 | 120.22 | 111.09 |
| 37 | 38 | 201 | CLA | C4A-NA-C1A | -5.12 | 104.34 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 41 | 208 | CLA | O2D-CGD-CBD | 5.12 | 120.18 | 111.23 |
| 50 | 36 | 312 | DD6 | C21-C20-C15 | -5.12 | 113.88 | 122.30 |
| 37 | 12 | 205 | CLA | C3B-C2B-C1B | -5.12 | 101.14 | 107.17 |
| 37 | 18 | 206 | CLA | C2B-C1B-NB | 5.12 | 115.63 | 110.33 |
| 48 | 34 | 315 | A86 | C3-C2-C1 | -5.12 | 120.10 | 127.28 |
| 37 | 20 | 308 | CLA | C3B-C2B-C1B | -5.12 | 101.14 | 107.17 |
| 47 | 17 | 305 | KC1 | C2B-C1B-NB | 5.12 | 115.19 | 110.13 |
| 37 | 14 | 305 | CLA | C2B-C1B-NB | 5.12 | 115.63 | 110.33 |
| 48 | 16 | 313 | A86 | C3-C2-C1 | -5.11 | 120.11 | 127.28 |
| 37 | 12 | 204 | CLA | C2D-C1D-ND | 5.11 | 115.19 | 110.13 |
| 37 | B | 502 | CLA | CAA-C2A-C3A | -5.11 | 99.18 | 113.00 |
| 37 | b | 502 | CLA | CAA-C2A-C3A | -5.11 | 99.18 | 113.00 |
| 37 | 37 | 303 | CLA | C3B-C2B-C1B | -5.11 | 101.14 | 107.17 |
| 37 | 11 | 308 | CLA | CHD-C4C-C3C | -5.11 | 117.32 | 124.77 |
| 37 | 21 | 206 | CLA | C2B-C1B-NB | 5.11 | 115.63 | 110.33 |
| 37 | 17 | 304 | CLA | C3B-C2B-C1B | -5.11 | 101.14 | 107.17 |
| 37 | 39 | 306 | CLA | C2B-C1B-NB | 5.11 | 115.63 | 110.33 |
| 37 | c | 506 | CLA | CHD-C4C-C3C | -5.11 | 117.32 | 124.77 |
| 48 | 13 | 315 | A86 | C3-C2-C1 | -5.11 | 120.11 | 127.28 |
| 37 | 32 | 202 | CLA | CHD-C4C-C3C | -5.11 | 117.33 | 124.77 |
| 47 | 20 | 304 | KC1 | O2D-CGD-CBD | 5.11 | 120.16 | 111.23 |
| 47 | 40 | 206 | KC1 | O2D-CGD-CBD | 5.11 | 120.16 | 111.23 |
| 47 | 36 | 304 | KC1 | C2D-C1D-ND | 5.11 | 115.62 | 110.33 |
| 37 | C | 512 | CLA | C3B-C2B-C1B | -5.11 | 101.15 | 107.17 |
| 37 | 39 | 307 | CLA | C3B-C2B-C1B | -5.11 | 101.15 | 107.17 |
| 37 | 20 | 301 | CLA | O2D-CGD-CBD | 5.11 | 120.16 | 111.23 |
| 48 | 34 | 314 | A86 | C25-C26-C27 | -5.11 | 120.12 | 127.28 |
| 37 | A | 403 | CLA | C2B-C1B-NB | 5.11 | 115.62 | 110.33 |
| 47 | 16 | 304 | KC1 | C2D-C1D-ND | 5.11 | 115.62 | 110.33 |
| 37 | 12 | 207 | CLA | C3B-C2B-C1B | -5.11 | 101.15 | 107.17 |
| 37 | 32 | 208 | CLA | C3B-C2B-C1B | -5.11 | 101.15 | 107.17 |
| 37 | 35 | 308 | CLA | CHD-C4C-C3C | -5.10 | 117.33 | 124.77 |
| 37 | 33 | 305 | CLA | C3B-C2B-C1B | -5.10 | 101.15 | 107.17 |
| 47 | 21 | 207 | KC1 | CHD-C4C-C3C | -5.10 | 115.82 | 125.23 |
| 37 | 13 | 307 | CLA | C2B-C1B-NB | 5.10 | 115.62 | 110.33 |
| 48 | 14 | 312 | A86 | O4-C38-C39 | 5.10 | 120.19 | 111.09 |
| 47 | 31 | 305 | KC1 | O2D-CGD-CBD | 5.10 | 120.15 | 111.23 |
| 37 | 37 | 308 | CLA | CHD-C4C-C3C | -5.10 | 117.34 | 124.77 |
| 47 | 36 | 308 | KC1 | C2D-C1D-ND | 5.10 | 115.61 | 110.33 |
| 48 | 18 | 213 | A86 | C23-C16-C22 | -5.10 | 99.96 | 107.37 |
| 47 | 40 | 206 | KC1 | CHC-C1C-C2C | -5.10 | 116.98 | 125.03 |
| 37 | 18 | 202 | CLA | C2B-C1B-NB | 5.10 | 115.61 | 110.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 208 | CLA | O2D-CGD-CBD | 5.10 | 120.14 | 111.23 |
| 47 | 38 | 207 | KC1 | C3C-C4C-NC | 5.10 | 115.36 | 109.90 |
| 37 | c | 512 | CLA | C3B-C2B-C1B | -5.10 | 101.16 | 107.17 |
| 48 | 14 | 314 | A86 | C25-C26-C27 | -5.09 | 120.13 | 127.28 |
| 37 | C | 506 | CLA | CHD-C4C-C3C | -5.09 | 117.34 | 124.77 |
| 47 | 41 | 207 | KC1 | CHD-C4C-C3C | -5.09 | 115.83 | 125.23 |
| 37 | 41 | 202 | CLA | O2D-CGD-CBD | 5.09 | 120.14 | 111.23 |
| 37 | 34 | 301 | CLA | C3B-C2B-C1B | -5.09 | 101.17 | 107.17 |
| 37 | d | 401 | CLA | C2B-C1B-NB | 5.09 | 115.61 | 110.33 |
| 48 | 34 | 313 | A86 | C41-C32-C31 | -5.09 | 105.91 | 110.47 |
| 47 | 32 | 212 | KC1 | C2D-C1D-ND | 5.09 | 115.61 | 110.33 |
| 37 | W | 102 | CLA | C2D-C1D-ND | 5.09 | 115.16 | 110.13 |
| 37 | 41 | 209 | CLA | O2D-CGD-CBD | 5.09 | 120.13 | 111.23 |
| 37 | 41 | 210 | CLA | C3B-C2B-C1B | -5.09 | 101.17 | 107.17 |
| 37 | 15 | 303 | CLA | C2C-C1C-NC | 5.09 | 115.33 | 109.98 |
| 37 | D | 402 | CLA | C2B-C1B-NB | 5.09 | 115.60 | 110.33 |
| 47 | 36 | 302 | KC1 | CHC-C1C-C2C | -5.09 | 117.00 | 125.03 |
| 47 | 32 | 209 | KC1 | CHD-C4C-C3C | -5.09 | 115.85 | 125.23 |
| 37 | 18 | 209 | CLA | C2C-C1C-NC | 5.09 | 115.32 | 109.98 |
| 37 | 33 | 307 | CLA | C2B-C1B-NB | 5.09 | 115.60 | 110.33 |
| 37 | C | 504 | CLA | C3B-C2B-C1B | -5.09 | 101.17 | 107.17 |
| 47 | 40 | 207 | KC1 | CHC-C1C-C2C | -5.08 | 117.00 | 125.03 |
| 37 | 37 | 306 | CLA | C3B-C2B-C1B | -5.08 | 101.18 | 107.17 |
| 37 | 13 | 303 | CLA | C2D-C1D-ND | 5.08 | 115.16 | 110.13 |
| 37 | 37 | 308 | CLA | C4A-NA-C1A | -5.08 | 104.36 | 106.68 |
| 37 | a | 403 | CLA | C2B-C1B-NB | 5.08 | 115.60 | 110.33 |
| 47 | 15 | 302 | KC1 | C2D-C1D-ND | 5.08 | 115.60 | 110.33 |
| 37 | 37 | 303 | CLA | CAA-C2A-C3A | -5.08 | 99.27 | 113.00 |
| 47 | 37 | 304 | KC1 | CMA-C3A-C2A | -5.08 | 116.13 | 128.43 |
| 37 | Z | 102 | CLA | C3B-C2B-C1B | -5.08 | 101.18 | 107.17 |
| 37 | 32 | 205 | CLA | C2D-C1D-ND | 5.08 | 115.15 | 110.13 |
| 50 | 39 | 312 | DD6 | C-C1-C24 | -5.08 | 110.33 | 118.09 |
| 37 | c | 503 | CLA | O2D-CGD-CBD | 5.08 | 120.11 | 111.23 |
| 48 | 17 | 312 | A86 | O4-C38-C39 | 5.08 | 120.14 | 111.09 |
| 48 | 17 | 314 | A86 | C25-C26-C27 | -5.08 | 120.16 | 127.28 |
| 37 | 18 | 208 | CLA | C2B-C1B-NB | 5.08 | 115.59 | 110.33 |
| 37 | 17 | 307 | CLA | C3B-C2B-C1B | -5.08 | 101.19 | 107.17 |
| 37 | 35 | 307 | CLA | C3B-C2B-C1B | -5.07 | 101.19 | 107.17 |
| 47 | 20 | 305 | KC1 | CHC-C1C-C2C | -5.07 | 117.02 | 125.03 |
| 47 | 11 | 304 | KC1 | O2D-CGD-CBD | 5.07 | 120.10 | 111.23 |
| 48 | 41 | 211 | A86 | C41-C32-C31 | -5.07 | 105.93 | 110.47 |
| 48 | 14 | 311 | A86 | O4-C38-C39 | 5.07 | 120.14 | 111.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 37 | 301 | CLA | C2B-C1B-NB | 5.07 | 115.59 | 110.33 |
| 47 | 12 | 211 | KC1 | C2D-C1D-ND | 5.07 | 115.59 | 110.33 |
| 37 | 21 | 210 | CLA | C3B-C2B-C1B | -5.07 | 101.19 | 107.17 |
| 47 | 12 | 208 | KC1 | CHD-C4C-C3C | -5.07 | 115.88 | 125.23 |
| 47 | 20 | 304 | KC1 | CHC-C1C-C2C | -5.07 | 117.02 | 125.03 |
| 37 | c | 508 | CLA | C2B-C1B-NB | 5.07 | 115.58 | 110.33 |
| 47 | 34 | 304 | KC1 | O2D-CGD-CBD | 5.07 | 120.09 | 111.23 |
| 37 | 17 | 309 | CLA | C2C-C1C-NC | 5.07 | 115.31 | 109.98 |
| 37 | 21 | 202 | CLA | O2D-CGD-CBD | 5.07 | 120.09 | 111.23 |
| 37 | 41 | 206 | CLA | C2B-C1B-NB | 5.07 | 115.58 | 110.33 |
| 37 | 15 | 308 | CLA | CHD-C4C-C3C | -5.07 | 117.38 | 124.77 |
| 37 | 15 | 307 | CLA | C3B-C2B-C1B | -5.07 | 101.20 | 107.17 |
| 48 | 21 | 211 | A86 | C41-C32-C31 | -5.07 | 105.94 | 110.47 |
| 37 | c | 504 | CLA | C3B-C2B-C1B | -5.07 | 101.20 | 107.17 |
| 37 | 17 | 309 | CLA | CHD-C4C-C3C | -5.07 | 117.39 | 124.77 |
| 37 | z | 102 | CLA | C3B-C2B-C1B | -5.06 | 101.20 | 107.17 |
| 37 | 38 | 211 | CLA | C3B-C2B-C1B | -5.06 | 101.20 | 107.17 |
| 37 | 13 | 305 | CLA | C3B-C2B-C1B | -5.06 | 101.20 | 107.17 |
| 37 | 14 | 301 | CLA | C3B-C2B-C1B | -5.06 | 101.20 | 107.17 |
| 48 | 17 | 313 | A86 | O4-C38-C39 | 5.06 | 120.11 | 111.09 |
| 37 | D | 406 | CLA | C3B-C2B-C1B | -5.06 | 101.20 | 107.17 |
| 37 | b | 523 | CLA | C2D-C1D-ND | 5.06 | 115.14 | 110.13 |
| 37 | 20 | 306 | CLA | C3B-C2B-C1B | -5.06 | 101.20 | 107.17 |
| 37 | 40 | 208 | CLA | C3B-C2B-C1B | -5.06 | 101.20 | 107.17 |
| 47 | 40 | 206 | KC1 | C2D-C1D-ND | 5.06 | 115.57 | 110.33 |
| 37 | B | 524 | CLA | C2D-C1D-ND | 5.06 | 115.13 | 110.13 |
| 37 | 36 | 303 | CLA | O2D-CGD-CBD | 5.06 | 120.08 | 111.23 |
| 37 | c | 509 | CLA | C2C-C1C-NC | 5.06 | 115.30 | 109.98 |
| 37 | 40 | 203 | CLA | O2D-CGD-CBD | 5.06 | 120.07 | 111.23 |
| 37 | 35 | 301 | CLA | C3B-C2B-C1B | -5.06 | 101.21 | 107.17 |
| 48 | 34 | 311 | A86 | O4-C38-C39 | 5.06 | 120.11 | 111.09 |
| 37 | C | 501 | CLA | C2C-C1C-NC | 5.06 | 115.29 | 109.98 |
| 37 | C | 503 | CLA | O2D-CGD-CBD | 5.06 | 120.07 | 111.23 |
| 48 | 37 | 311 | A86 | O4-C38-C39 | 5.05 | 120.10 | 111.09 |
| 48 | 37 | 312 | A86 | O4-C38-C39 | 5.05 | 120.10 | 111.09 |
| 37 | 39 | 302 | CLA | C2C-C1C-NC | 5.05 | 115.29 | 109.98 |
| 48 | 13 | 314 | A86 | O4-C38-C39 | 5.05 | 120.10 | 111.09 |
| 47 | 41 | 203 | KC1 | C1A-NA-C4A | -5.05 | 104.38 | 106.68 |
| 47 | 39 | 308 | KC1 | CHD-C4C-C3C | -5.05 | 115.92 | 125.23 |
| 37 | a | 404 | CLA | C2C-C1C-NC | 5.05 | 115.29 | 109.98 |
| 48 | 33 | 314 | A86 | O4-C38-C39 | 5.05 | 120.09 | 111.09 |
| 37 | c | 501 | CLA | C2C-C1C-NC | 5.05 | 115.28 | 109.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 13 | 307 | CLA | C2C-C1C-NC | 5.05 | 115.28 | 109.98 |
| 37 | 33 | 307 | CLA | C2C-C1C-NC | 5.05 | 115.28 | 109.98 |
| 48 | 41 | 211 | A86 | C25-C26-C27 | -5.05 | 120.20 | 127.28 |
| 37 | 38 | 208 | CLA | C2B-C1B-NB | 5.05 | 115.56 | 110.33 |
| 37 | 32 | 206 | CLA | C2B-C1B-NB | 5.05 | 115.56 | 110.33 |
| 37 | 13 | 305 | CLA | O2D-CGD-CBD | 5.05 | 120.05 | 111.23 |
| 47 | 13 | 302 | KC1 | C1A-NA-C4A | -5.05 | 104.38 | 106.68 |
| 37 | 18 | 211 | CLA | C3B-C2B-C1B | -5.04 | 101.22 | 107.17 |
| 37 | 16 | 303 | CLA | O2D-CGD-CBD | 5.04 | 120.05 | 111.23 |
| 47 | 19 | 308 | KC1 | CHD-C4C-C3C | -5.04 | 115.93 | 125.23 |
| 37 | 13 | 308 | CLA | C4A-NA-C1A | -5.04 | 104.38 | 106.68 |
| 37 | 35 | 303 | CLA | C2C-C1C-NC | 5.04 | 115.28 | 109.98 |
| 37 | 39 | 304 | CLA | C2B-C1B-NB | 5.04 | 115.55 | 110.33 |
| 37 | D | 401 | CLA | O2D-CGD-CBD | 5.04 | 120.04 | 111.23 |
| 37 | d | 404 | CLA | C3B-C2B-C1B | -5.04 | 101.23 | 107.17 |
| 37 | 41 | 204 | CLA | CAA-C2A-C3A | -5.04 | 99.38 | 113.00 |
| 47 | 21 | 207 | KC1 | C3D-C4D-ND | 5.04 | 117.22 | 110.20 |
| 37 | 21 | 209 | CLA | O2D-CGD-CBD | 5.04 | 120.04 | 111.23 |
| 47 | 14 | 304 | KC1 | O2D-CGD-CBD | 5.04 | 120.04 | 111.23 |
| 37 | 39 | 304 | CLA | C3B-C2B-C1B | -5.04 | 101.23 | 107.17 |
| 47 | 33 | 304 | KC1 | C3C-C4C-NC | 5.04 | 115.30 | 109.90 |
| 37 | C | 509 | CLA | C2C-C1C-NC | 5.04 | 115.27 | 109.98 |
| 37 | B | 507 | CLA | C2B-C1B-NB | 5.04 | 115.55 | 110.33 |
| 37 | 39 | 310 | CLA | C2B-C1B-NB | 5.04 | 115.55 | 110.33 |
| 47 | 13 | 309 | KC1 | C2D-C1D-ND | 5.04 | 115.55 | 110.33 |
| 47 | 33 | 309 | KC1 | C2D-C1D-ND | 5.04 | 115.55 | 110.33 |
| 37 | 33 | 308 | CLA | CHD-C4C-C3C | -5.04 | 117.43 | 124.77 |
| 37 | a | 404 | CLA | O2D-CGD-CBD | 5.04 | 120.03 | 111.23 |
| 37 | 19 | 302 | CLA | C2C-C1C-NC | 5.04 | 115.27 | 109.98 |
| 37 | 38 | 209 | CLA | C2C-C1C-NC | 5.04 | 115.27 | 109.98 |
| 37 | C | 508 | CLA | C2B-C1B-NB | 5.04 | 115.55 | 110.33 |
| 47 | 17 | 305 | KC1 | C2D-C1D-ND | 5.04 | 115.55 | 110.33 |
| 37 | c | 504 | CLA | CHD-C4C-C3C | -5.03 | 117.43 | 124.77 |
| 47 | 16 | 302 | KC1 | CHC-C1C-C2C | -5.03 | 117.08 | 125.03 |
| 48 | 17 | 312 | A86 | C4-C5-C6 | -5.03 | 120.22 | 127.28 |
| 47 | 37 | 304 | KC1 | O2D-CGD-CBD | 5.03 | 120.03 | 111.23 |
| 37 | 15 | 301 | CLA | C3B-C2B-C1B | -5.03 | 101.24 | 107.17 |
| 37 | C | 504 | CLA | CHD-C4C-C3C | -5.03 | 117.44 | 124.77 |
| 47 | 18 | 207 | KC1 | C3C-C4C-NC | 5.03 | 115.29 | 109.90 |
| 37 | 17 | 304 | CLA | CAA-C2A-C3A | -5.03 | 99.40 | 113.00 |
| 37 | B | 502 | CLA | C3B-C2B-C1B | -5.03 | 101.24 | 107.17 |
| 47 | 20 | 304 | KC1 | C2D-C1D-ND | 5.03 | 115.54 | 110.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 13 | 304 | KC1 | C3C-C4C-NC | 5.03 | 115.29 | 109.90 |
| 48 | 40 | 211 | A86 | C3-C2-C1 | -5.03 | 120.22 | 127.28 |
| 47 | 15 | 304 | KC1 | O2D-CGD-CBD | 5.03 | 120.02 | 111.23 |
| 37 | b | 502 | CLA | C3B-C2B-C1B | -5.03 | 101.24 | 107.17 |
| 37 | 35 | 310 | CLA | C2B-C1B-NB | 5.03 | 115.54 | 110.33 |
| 48 | 20 | 309 | A86 | C3-C2-C1 | -5.03 | 120.23 | 127.28 |
| 37 | 33 | 305 | CLA | O2D-CGD-CBD | 5.03 | 120.02 | 111.23 |
| 48 | 38 | 214 | A86 | O4-C38-C39 | 5.03 | 120.06 | 111.09 |
| 37 | 16 | 303 | CLA | C3B-C2B-C1B | -5.03 | 101.24 | 107.17 |
| 37 | b | 507 | CLA | C2B-C1B-NB | 5.03 | 115.54 | 110.33 |
| 37 | 19 | 310 | CLA | C2B-C1B-NB | 5.03 | 115.54 | 110.33 |
| 37 | 36 | 303 | CLA | C2B-C1B-NB | 5.03 | 115.54 | 110.33 |
| 47 | 41 | 203 | KC1 | C2D-C1D-ND | 5.03 | 115.54 | 110.33 |
| 48 | 18 | 215 | A86 | O4-C38-C39 | 5.03 | 120.05 | 111.09 |
| 37 | 39 | 301 | CLA | C3B-C2B-C1B | -5.03 | 101.25 | 107.17 |
| 37 | 31 | 304 | CLA | C2B-C1B-NB | 5.02 | 115.54 | 110.33 |
| 37 | 38 | 206 | CLA | C2B-C1B-NB | 5.02 | 115.54 | 110.33 |
| 47 | 16 | 302 | KC1 | C2D-C1D-ND | 5.02 | 115.54 | 110.33 |
| 37 | 36 | 306 | CLA | O2D-CGD-CBD | 5.02 | 120.01 | 111.23 |
| 48 | 21 | 211 | A86 | C25-C26-C27 | -5.02 | 120.23 | 127.28 |
| 37 | C | 505 | CLA | C2B-C1B-NB | 5.02 | 115.53 | 110.33 |
| 48 | 37 | 319 | A86 | O4-C38-C39 | 5.02 | 120.05 | 111.09 |
| 37 | 19 | 304 | CLA | C3B-C2B-C1B | -5.02 | 101.25 | 107.17 |
| 37 | 36 | 303 | CLA | C3B-C2B-C1B | -5.02 | 101.25 | 107.17 |
| 37 | 36 | 309 | CLA | O2D-CGD-CBD | 5.02 | 120.01 | 111.23 |
| 37 | 12 | 205 | CLA | C2B-C1B-NB | 5.02 | 115.53 | 110.33 |
| 37 | 19 | 301 | CLA | C3B-C2B-C1B | -5.02 | 101.25 | 107.17 |
| 37 | 16 | 301 | CLA | C3D-C2D-C1D | -5.02 | 98.98 | 105.83 |
| 37 | 12 | 210 | CLA | CHD-C4C-C3C | -5.02 | 117.45 | 124.77 |
| 48 | 17 | 320 | A86 | O4-C38-C39 | 5.02 | 120.04 | 111.09 |
| 47 | 41 | 207 | KC1 | C3D-C4D-ND | 5.02 | 117.20 | 110.20 |
| 37 | a | 404 | CLA | C3B-C2B-C1B | -5.02 | 101.25 | 107.17 |
| 37 | 16 | 303 | CLA | C2B-C1B-NB | 5.02 | 115.53 | 110.33 |
| 37 | 21 | 204 | CLA | CAA-C2A-C3A | -5.02 | 99.44 | 113.00 |
| 48 | 38 | 215 | A86 | O4-C38-C39 | 5.02 | 120.03 | 111.09 |
| 37 | D | 401 | CLA | C3B-C2B-C1B | -5.01 | 101.26 | 107.17 |
| 37 | 39 | 309 | CLA | C2B-C1B-NB | 5.01 | 115.53 | 110.33 |
| 37 | 41 | 205 | CLA | C3B-C2B-C1B | -5.01 | 101.26 | 107.17 |
| 37 | A | 403 | CLA | C3B-C2B-C1B | -5.01 | 101.26 | 107.17 |
| 37 | B | 513 | CLA | C2C-C1C-NC | 5.01 | 115.25 | 109.98 |
| 37 | 13 | 308 | CLA | CHD-C4C-C3C | -5.01 | 117.47 | 124.77 |
| 47 | 17 | 303 | KC1 | O2D-CGD-CBD | 5.01 | 119.99 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 38 | 202 | CLA | C3D-C2D-C1D | -5.01 | 98.99 | 105.83 |
| 37 | b | 506 | CLA | C2C-C1C-NC | 5.01 | 115.25 | 109.98 |
| 37 | 18 | 204 | CLA | C3B-C2B-C1B | -5.01 | 101.26 | 107.17 |
| 48 | 14 | 314 | A86 | O4-C38-C39 | 5.01 | 120.02 | 111.09 |
| 37 | 16 | 309 | CLA | O2D-CGD-CBD | 5.01 | 119.99 | 111.23 |
| 47 | 32 | 209 | KC1 | C3C-C4C-NC | 5.01 | 115.27 | 109.90 |
| 48 | 34 | 314 | A86 | O4-C38-C39 | 5.01 | 120.02 | 111.09 |
| 37 | 16 | 306 | CLA | O2D-CGD-CBD | 5.01 | 119.98 | 111.23 |
| 47 | 37 | 302 | KC1 | O2D-CGD-CBD | 5.01 | 119.98 | 111.23 |
| 48 | 18 | 214 | A86 | O4-C38-C39 | 5.01 | 120.02 | 111.09 |
| 37 | b | 515 | CLA | C2C-C1C-NC | 5.01 | 115.24 | 109.98 |
| 37 | 19 | 310 | CLA | C3B-C2B-C1B | -5.00 | 101.27 | 107.17 |
| 37 | D | 401 | CLA | C2C-C1C-NC | 5.00 | 115.24 | 109.98 |
| 37 | a | 403 | CLA | C3B-C2B-C1B | -5.00 | 101.27 | 107.17 |
| 37 | 19 | 304 | CLA | C2B-C1B-NB | 5.00 | 115.52 | 110.33 |
| 47 | 33 | 304 | KC1 | C2B-C1B-NB | 5.00 | 115.08 | 110.13 |
| 47 | 21 | 203 | KC1 | C1A-NA-C4A | -5.00 | 104.40 | 106.68 |
| 37 | b | 511 | CLA | C2B-C1B-NB | 5.00 | 115.51 | 110.33 |
| 37 | b | 513 | CLA | C2B-C1B-NB | 5.00 | 115.51 | 110.33 |
| 47 | 11 | 304 | KC1 | C2D-C1D-ND | 5.00 | 115.51 | 110.33 |
| 37 | 36 | 301 | CLA | C3D-C2D-C1D | -5.00 | 99.01 | 105.83 |
| 48 | 32 | 216 | A86 | O4-C38-C39 | 5.00 | 120.00 | 111.09 |
| 37 | 36 | 307 | CLA | C2B-C1B-NB | 5.00 | 115.51 | 110.33 |
| 47 | 12 | 208 | KC1 | C3C-C4C-NC | 4.99 | 115.25 | 109.90 |
| 47 | 36 | 302 | KC1 | C2D-C1D-ND | 4.99 | 115.50 | 110.33 |
| 37 | 21 | 205 | CLA | C3B-C2B-C1B | -4.99 | 101.28 | 107.17 |
| 47 | 21 | 203 | KC1 | C2D-C1D-ND | 4.99 | 115.50 | 110.33 |
| 37 | 11 | 303 | CLA | C2B-C1B-NB | 4.99 | 115.50 | 110.33 |
| 37 | 39 | 310 | CLA | C3B-C2B-C1B | -4.99 | 101.28 | 107.17 |
| 37 | 32 | 211 | CLA | CHD-C4C-C3C | -4.99 | 117.50 | 124.77 |
| 37 | 15 | 305 | CLA | C2C-C1C-NC | 4.99 | 115.22 | 109.98 |
| 37 | 17 | 302 | CLA | C2B-C1B-NB | 4.99 | 115.50 | 110.33 |
| 48 | 31 | 313 | A86 | O4-C38-C39 | 4.99 | 119.99 | 111.09 |
| 37 | 14 | 302 | CLA | C2C-C1C-NC | 4.99 | 115.22 | 109.98 |
| 47 | 35 | 302 | KC1 | O2D-CGD-CBD | 4.99 | 119.95 | 111.23 |
| 37 | b | 513 | CLA | C2C-C1C-NC | 4.99 | 115.22 | 109.98 |
| 37 | 39 | 305 | CLA | C2C-C1C-NC | 4.99 | 115.22 | 109.98 |
| 37 | 41 | 202 | CLA | C2B-C1B-NB | 4.99 | 115.50 | 110.33 |
| 37 | c | 505 | CLA | C2B-C1B-NB | 4.98 | 115.50 | 110.33 |
| 48 | 12 | 216 | A86 | C40-C32-C31 | -4.98 | 106.01 | 110.47 |
| 48 | 32 | 217 | A86 | C40-C32-C31 | -4.98 | 106.01 | 110.47 |
| 37 | 37 | 308 | CLA | C2C-C1C-NC | 4.98 | 115.22 | 109.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 17 | 305 | KC1 | O2D-CGD-CBD | 4.98 | 119.94 | 111.23 |
| 37 | 33 | 303 | CLA | C4A-NA-C1A | -4.98 | 104.41 | 106.68 |
| 48 | 11 | 313 | A86 | C4-C5-C6 | -4.98 | 120.29 | 127.28 |
| 48 | 12 | 215 | A86 | O4-C38-C39 | 4.98 | 119.97 | 111.09 |
| 47 | 31 | 305 | KC1 | C2D-C1D-ND | 4.98 | 115.49 | 110.33 |
| 37 | b | 513 | CLA | C3B-C2B-C1B | -4.98 | 101.30 | 107.17 |
| 37 | B | 511 | CLA | C2B-C1B-NB | 4.98 | 115.49 | 110.33 |
| 37 | 41 | 202 | CLA | C2C-C1C-NC | 4.98 | 115.21 | 109.98 |
| 37 | c | 508 | CLA | C3D-C2D-C1D | -4.98 | 99.04 | 105.83 |
| 37 | b | 509 | CLA | C4A-NA-C1A | -4.98 | 104.41 | 106.68 |
| 48 | 15 | 312 | A86 | O4-C38-C39 | 4.98 | 119.96 | 111.09 |
| 37 | 34 | 307 | CLA | O2D-CGD-CBD | 4.97 | 119.93 | 111.23 |
| 37 | B | 504 | CLA | CMB-C2B-C1B | 4.97 | 132.99 | 125.42 |
| 37 | 21 | 202 | CLA | C2C-C1C-NC | 4.97 | 115.21 | 109.98 |
| 47 | 16 | 304 | KC1 | C1A-C2A-C3A | -4.97 | 102.71 | 107.28 |
| 47 | 13 | 302 | KC1 | C2D-C1D-ND | 4.97 | 115.48 | 110.33 |
| 47 | 33 | 302 | KC1 | C2D-C1D-ND | 4.97 | 115.48 | 110.33 |
| 37 | 32 | 213 | CLA | C3B-C2B-C1B | -4.97 | 101.31 | 107.17 |
| 37 | 39 | 309 | CLA | C2C-C1C-NC | 4.97 | 115.20 | 109.98 |
| 47 | 36 | 304 | KC1 | C1A-C2A-C3A | -4.97 | 102.71 | 107.28 |
| 47 | 35 | 306 | KC1 | CHD-C4C-C3C | -4.97 | 116.06 | 125.23 |
| 37 | c | 503 | CLA | C4A-NA-C1A | -4.97 | 104.41 | 106.68 |
| 37 | 19 | 304 | CLA | C3D-C2D-C1D | -4.97 | 99.05 | 105.83 |
| 37 | 12 | 212 | CLA | C3B-C2B-C1B | -4.97 | 101.31 | 107.17 |
| 47 | 37 | 302 | KC1 | C2D-C1D-ND | 4.97 | 115.48 | 110.33 |
| 48 | 35 | 311 | A86 | C3-C4-C5 | -4.97 | 113.36 | 123.52 |
| 47 | 33 | 309 | KC1 | CHC-C1C-C2C | -4.97 | 117.19 | 125.03 |
| 37 | B | 513 | CLA | C2B-C1B-NB | 4.97 | 115.47 | 110.33 |
| 37 | 15 | 310 | CLA | C2B-C1B-NB | 4.97 | 115.47 | 110.33 |
| 37 | B | 509 | CLA | O2D-CGD-CBD | 4.97 | 119.91 | 111.23 |
| 37 | a | 407 | CLA | C2B-C1B-NB | 4.96 | 115.47 | 110.33 |
| 47 | 18 | 207 | KC1 | C3B-C2B-C1B | -4.96 | 102.35 | 107.05 |
| 48 | 41 | 211 | A86 | C3-C2-C1 | -4.96 | 120.32 | 127.28 |
| 37 | b | 503 | CLA | C2C-C1C-NC | 4.96 | 115.19 | 109.98 |
| 37 | 34 | 301 | CLA | C2B-C1B-NB | 4.96 | 115.47 | 110.33 |
| 37 | 14 | 301 | CLA | C2B-C1B-NB | 4.96 | 115.47 | 110.33 |
| 48 | 15 | 311 | A86 | C3-C4-C5 | -4.96 | 113.37 | 123.52 |
| 37 | 18 | 204 | CLA | C2D-C1D-ND | 4.96 | 115.03 | 110.13 |
| 37 | 18 | 203 | CLA | C3B-C2B-C1B | -4.96 | 101.32 | 107.17 |
| 48 | 35 | 312 | A86 | O4-C38-C39 | 4.96 | 119.93 | 111.09 |
| 37 | 35 | 307 | CLA | CMD-C2D-C1D | 4.96 | 133.46 | 124.73 |
| 37 | 39 | 305 | CLA | C3B-C2B-C1B | -4.96 | 101.32 | 107.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 16 | 307 | CLA | C2B-C1B-NB | 4.96 | 115.47 | 110.33 |
| 37 | 19 | 309 | CLA | C2B-C1B-NB | 4.96 | 115.47 | 110.33 |
| 47 | 13 | 309 | KC1 | CHC-C1C-C2C | -4.96 | 117.20 | 125.03 |
| 37 | B | 506 | CLA | C2C-C1C-NC | 4.96 | 115.19 | 109.98 |
| 37 | 14 | 307 | CLA | O2D-CGD-CBD | 4.96 | 119.89 | 111.23 |
| 37 | B | 515 | CLA | C2C-C1C-NC | 4.96 | 115.19 | 109.98 |
| 47 | 15 | 302 | KC1 | O2D-CGD-CBD | 4.95 | 119.89 | 111.23 |
| 37 | C | 508 | CLA | C3D-C2D-C1D | -4.95 | 99.07 | 105.83 |
| 37 | 33 | 308 | CLA | C4A-NA-C1A | -4.95 | 104.42 | 106.68 |
| 48 | 35 | 314 | A86 | O4-C38-C39 | 4.95 | 119.92 | 111.09 |
| 37 | 12 | 205 | CLA | C4A-NA-C1A | -4.95 | 104.42 | 106.68 |
| 48 | 21 | 211 | A86 | C3-C2-C1 | -4.95 | 120.33 | 127.28 |
| 37 | 31 | 301 | CLA | C3B-C2B-C1B | -4.95 | 101.33 | 107.17 |
| 47 | 13 | 309 | KC1 | CMA-C3A-C2A | -4.95 | 116.45 | 128.43 |
| 37 | 39 | 304 | CLA | C3D-C2D-C1D | -4.95 | 99.08 | 105.83 |
| 37 | A | 403 | CLA | C2C-C1C-NC | 4.95 | 115.18 | 109.98 |
| 37 | 37 | 303 | CLA | C2C-C1C-NC | 4.95 | 115.18 | 109.98 |
| 37 | B | 516 | CLA | C3D-C2D-C1D | -4.95 | 99.08 | 105.83 |
| 47 | 33 | 309 | KC1 | CMA-C3A-C2A | -4.95 | 116.45 | 128.43 |
| 37 | C | 502 | CLA | C3D-C2D-C1D | -4.95 | 99.08 | 105.83 |
| 37 | a | 403 | CLA | C2C-C1C-NC | 4.95 | 115.18 | 109.98 |
| 47 | 34 | 309 | KC1 | CHD-C4C-C3C | -4.95 | 116.11 | 125.23 |
| 37 | b | 509 | CLA | O2D-CGD-CBD | 4.95 | 119.88 | 111.23 |
| 37 | 37 | 303 | CLA | C4A-NA-C1A | -4.94 | 104.42 | 106.68 |
| 47 | 14 | 309 | KC1 | CHD-C4C-C3C | -4.94 | 116.11 | 125.23 |
| 37 | 38 | 204 | CLA | C3B-C2B-C1B | -4.94 | 101.34 | 107.17 |
| 37 | 39 | 306 | CLA | C3B-C2B-C1B | -4.94 | 101.34 | 107.17 |
| 48 | 12 | 213 | A86 | C25-C26-C27 | -4.94 | 120.35 | 127.28 |
| 37 | B | 510 | CLA | C2C-C1C-NC | 4.94 | 115.17 | 109.98 |
| 37 | 19 | 309 | CLA | C2C-C1C-NC | 4.94 | 115.17 | 109.98 |
| 48 | 15 | 314 | A86 | O4-C38-C39 | 4.94 | 119.90 | 111.09 |
| 37 | z | 101 | CLA | C2C-C1C-NC | 4.94 | 115.17 | 109.98 |
| 48 | 37 | 314 | A86 | O4-C38-C39 | 4.94 | 119.90 | 111.09 |
| 37 | 39 | 301 | CLA | C3D-C2D-C1D | -4.94 | 99.09 | 105.83 |
| 48 | 16 | 313 | A86 | O4-C38-C39 | 4.94 | 119.89 | 111.09 |
| 37 | 21 | 202 | CLA | C2B-C1B-NB | 4.94 | 115.45 | 110.33 |
| 37 | B | 513 | CLA | C3B-C2B-C1B | -4.94 | 101.35 | 107.17 |
| 37 | W | 102 | CLA | C3B-C2B-C1B | -4.94 | 101.35 | 107.17 |
| 47 | 17 | 306 | KC1 | C2B-C1B-NB | 4.93 | 115.01 | 110.13 |
| 48 | 21 | 214 | A86 | O4-C38-C39 | 4.93 | 119.89 | 111.09 |
| 37 | 19 | 305 | CLA | C3B-C2B-C1B | -4.93 | 101.36 | 107.17 |
| 37 | B | 503 | CLA | C2C-C1C-NC | 4.93 | 115.16 | 109.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 16 | 309 | CLA | C3B-C2B-C1B | -4.93 | 101.36 | 107.17 |
| 48 | 40 | 201 | A86 | O4-C38-C39 | 4.93 | 119.88 | 111.09 |
| 37 | 33 | 307 | CLA | C2D-C1D-ND | 4.93 | 115.00 | 110.13 |
| 37 | 19 | 306 | CLA | C3B-C2B-C1B | -4.93 | 101.36 | 107.17 |
| 47 | 37 | 305 | KC1 | C2B-C1B-NB | 4.93 | 115.00 | 110.13 |
| 48 | 17 | 315 | A86 | O4-C38-C39 | 4.93 | 119.88 | 111.09 |
| 37 | 32 | 208 | CLA | O2D-CGD-CBD | 4.92 | 119.84 | 111.23 |
| 37 | 13 | 307 | CLA | C2D-C1D-ND | 4.92 | 115.00 | 110.13 |
| 47 | 38 | 207 | KC1 | CHD-C4C-C3C | -4.92 | 116.15 | 125.23 |
| 48 | 17 | 314 | A86 | O4-C38-C39 | 4.92 | 119.86 | 111.09 |
| 48 | 32 | 214 | A86 | O4-C38-C39 | 4.92 | 119.86 | 111.09 |
| 37 | a | 407 | CLA | C3B-C2B-C1B | -4.92 | 101.37 | 107.17 |
| 37 | b | 516 | CLA | C3D-C2D-C1D | -4.92 | 99.12 | 105.83 |
| 37 | c | 503 | CLA | C2C-C1C-NC | 4.92 | 115.15 | 109.98 |
| 47 | 31 | 303 | KC1 | CMA-C3A-C2A | -4.92 | 116.53 | 128.43 |
| 47 | 17 | 303 | KC1 | C2D-C1D-ND | 4.92 | 115.43 | 110.33 |
| 47 | 35 | 304 | KC1 | C2D-C1D-ND | 4.92 | 115.43 | 110.33 |
| 47 | 11 | 302 | KC1 | CMA-C3A-C2A | -4.92 | 116.53 | 128.43 |
| 37 | 12 | 207 | CLA | O2D-CGD-CBD | 4.92 | 119.83 | 111.23 |
| 37 | 35 | 305 | CLA | C3B-C2B-C1B | -4.92 | 101.37 | 107.17 |
| 48 | 21 | 213 | A86 | O4-C38-C39 | 4.92 | 119.86 | 111.09 |
| 37 | 13 | 310 | CLA | C3B-C2B-C1B | -4.91 | 101.38 | 107.17 |
| 47 | 15 | 306 | KC1 | CHD-C4C-C3C | -4.91 | 116.17 | 125.23 |
| 48 | 41 | 214 | A86 | O4-C38-C39 | 4.91 | 119.85 | 111.09 |
| 37 | 17 | 304 | CLA | C2C-C1C-NC | 4.91 | 115.14 | 109.98 |
| 37 | b | 504 | CLA | CMB-C2B-C1B | 4.91 | 132.90 | 125.42 |
| 37 | 34 | 303 | CLA | C2C-C1C-NC | 4.91 | 115.14 | 109.98 |
| 37 | 35 | 305 | CLA | C2C-C1C-NC | 4.91 | 115.14 | 109.98 |
| 37 | b | 505 | CLA | C3D-C2D-C1D | -4.91 | 99.13 | 105.83 |
| 45 | D | 404 | PL9 | C7-C3-C4 | 4.91 | 120.95 | 116.91 |
| 37 | 14 | 303 | CLA | C2C-C1C-NC | 4.91 | 115.14 | 109.98 |
| 37 | 20 | 306 | CLA | C4A-NA-C1A | -4.91 | 104.44 | 106.68 |
| 37 | 15 | 305 | CLA | C3B-C2B-C1B | -4.91 | 101.38 | 107.17 |
| 37 | 11 | 305 | CLA | C3B-C2B-C1B | -4.91 | 101.39 | 107.17 |
| 47 | 41 | 203 | KC1 | C3C-C4C-NC | 4.91 | 115.16 | 109.90 |
| 37 | c | 502 | CLA | C3D-C2D-C1D | -4.91 | 99.13 | 105.83 |
| 37 | 15 | 307 | CLA | CMD-C2D-C1D | 4.90 | 133.37 | 124.73 |
| 47 | 32 | 207 | KC1 | C3B-C2B-C1B | -4.90 | 102.41 | 107.05 |
| 37 | Z | 101 | CLA | C2C-C1C-NC | 4.90 | 115.13 | 109.98 |
| 48 | 41 | 213 | A86 | O4-C38-C39 | 4.90 | 119.83 | 111.09 |
| 37 | b | 511 | CLA | C2C-C1C-NC | 4.90 | 115.13 | 109.98 |
| 47 | 12 | 206 | KC1 | C3B-C2B-C1B | -4.90 | 102.41 | 107.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 21 | 216 | DD6 | C24-C1-C2 | -4.90 | 111.30 | 119.01 |
| 48 | 38 | 213 | A86 | O4-C38-C39 | 4.90 | 119.83 | 111.09 |
| 47 | 13 | 304 | KC1 | C2B-C1B-NB | 4.90 | 114.97 | 110.13 |
| 47 | 41 | 203 | KC1 | CHD-C4C-C3C | -4.90 | 116.20 | 125.23 |
| 50 | 41 | 216 | DD6 | C24-C1-C2 | -4.90 | 111.31 | 119.01 |
| 37 | 36 | 309 | CLA | C3B-C2B-C1B | -4.90 | 101.40 | 107.17 |
| 37 | 19 | 309 | CLA | O2D-CGD-CBD | 4.90 | 119.79 | 111.23 |
| 37 | 21 | 208 | CLA | C3B-C2B-C1B | -4.90 | 101.40 | 107.17 |
| 37 | 34 | 302 | CLA | C2C-C1C-NC | 4.90 | 115.12 | 109.98 |
| 47 | 21 | 203 | KC1 | CHD-C4C-C3C | -4.89 | 116.20 | 125.23 |
| 37 | 31 | 304 | CLA | C4A-NA-C1A | -4.89 | 104.45 | 106.68 |
| 37 | 38 | 206 | CLA | C4A-NA-C1A | -4.89 | 104.45 | 106.68 |
| 37 | 39 | 309 | CLA | O2D-CGD-CBD | 4.89 | 119.79 | 111.23 |
| 37 | 37 | 308 | CLA | C3B-C2B-C1B | -4.89 | 101.40 | 107.17 |
| 48 | 12 | 213 | A86 | O4-C38-C39 | 4.89 | 119.81 | 111.09 |
| 37 | 19 | 301 | CLA | C3D-C2D-C1D | -4.89 | 99.16 | 105.83 |
| 37 | 34 | 310 | CLA | C2B-C1B-NB | 4.89 | 115.40 | 110.33 |
| 37 | 38 | 204 | CLA | C2D-C1D-ND | 4.89 | 114.97 | 110.13 |
| 37 | b | 523 | CLA | C4A-NA-C1A | -4.89 | 104.45 | 106.68 |
| 37 | A | 405 | CLA | C2B-C1B-NB | 4.89 | 115.40 | 110.33 |
| 37 | 31 | 306 | CLA | C3B-C2B-C1B | -4.89 | 101.41 | 107.17 |
| 48 | 13 | 312 | A86 | C36-C31-C32 | -4.89 | 114.85 | 119.70 |
| 37 | 35 | 308 | CLA | C4A-NA-C1A | -4.89 | 104.45 | 106.68 |
| 37 | 16 | 303 | CLA | CAA-C2A-C3A | -4.89 | 99.80 | 113.00 |
| 37 | 36 | 303 | CLA | CAA-C2A-C3A | -4.89 | 99.80 | 113.00 |
| 37 | 21 | 206 | CLA | C3B-C2B-C1B | -4.89 | 101.41 | 107.17 |
| 48 | 33 | 312 | A86 | C36-C31-C32 | -4.88 | 114.85 | 119.70 |
| 48 | 17 | 315 | A86 | C25-C26-C27 | -4.88 | 120.43 | 127.28 |
| 37 | 41 | 208 | CLA | C3B-C2B-C1B | -4.88 | 101.41 | 107.17 |
| 37 | b | 505 | CLA | C3B-C2B-C1B | -4.88 | 101.41 | 107.17 |
| 37 | C | 503 | CLA | C4A-NA-C1A | -4.88 | 104.45 | 106.68 |
| 37 | d | 403 | CLA | C3B-C2B-C1B | -4.88 | 101.42 | 107.17 |
| 47 | 17 | 306 | KC1 | C2D-C1D-ND | 4.88 | 115.39 | 110.33 |
| 37 | 38 | 211 | CLA | CHD-C4C-C3C | -4.88 | 117.66 | 124.77 |
| 37 | B | 511 | CLA | C2C-C1C-NC | 4.88 | 115.11 | 109.98 |
| 37 | 31 | 302 | CLA | C3D-C2D-C1D | -4.88 | 99.17 | 105.83 |
| 37 | 14 | 310 | CLA | C2B-C1B-NB | 4.88 | 115.39 | 110.33 |
| 37 | D | 405 | CLA | C3B-C2B-C1B | -4.88 | 101.42 | 107.17 |
| 45 | d | 402 | PL9 | C7-C3-C4 | 4.88 | 120.93 | 116.91 |
| 47 | 31 | 309 | KC1 | C1A-C2A-C3A | -4.88 | 102.80 | 107.28 |
| 47 | 21 | 203 | KC1 | C3C-C4C-NC | 4.88 | 115.12 | 109.90 |
| 37 | 19 | 305 | CLA | C2C-C1C-NC | 4.88 | 115.10 | 109.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | A | 405 | CLA | C3B-C2B-C1B | -4.87 | 101.42 | 107.17 |
| 37 | 38 | 201 | CLA | C3B-C2B-C1B | -4.87 | 101.42 | 107.17 |
| 37 | B | 524 | CLA | C4A-NA-C1A | -4.87 | 104.45 | 106.68 |
| 37 | 31 | 301 | CLA | C2B-C1B-NB | 4.87 | 115.38 | 110.33 |
| 37 | C | 503 | CLA | C3D-C2D-C1D | -4.87 | 99.18 | 105.83 |
| 37 | W | 102 | CLA | C2B-C1B-NB | 4.87 | 115.38 | 110.33 |
| 48 | 18 | 214 | A86 | C25-C26-C27 | -4.87 | 120.44 | 127.28 |
| 37 | w | 101 | CLA | C2C-C1C-NC | 4.87 | 115.10 | 109.98 |
| 37 | d | 401 | CLA | O2D-CGD-CBD | 4.87 | 119.75 | 111.23 |
| 47 | 11 | 309 | KC1 | C1A-C2A-C3A | -4.87 | 102.80 | 107.28 |
| 37 | 41 | 206 | CLA | C3B-C2B-C1B | -4.87 | 101.43 | 107.17 |
| 37 | B | 505 | CLA | C3D-C2D-C1D | -4.87 | 99.19 | 105.83 |
| 37 | a | 403 | CLA | C2D-C1D-ND | 4.87 | 114.94 | 110.13 |
| 48 | 31 | 312 | A86 | O4-C38-C39 | 4.87 | 119.77 | 111.09 |
| 37 | b | 510 | CLA | C2C-C1C-NC | 4.87 | 115.09 | 109.98 |
| 37 | 17 | 304 | CLA | C4A-NA-C1A | -4.87 | 104.46 | 106.68 |
| 37 | D | 401 | CLA | C3D-C2D-C1D | -4.87 | 99.19 | 105.83 |
| 48 | 16 | 310 | A86 | O4-C38-C39 | 4.87 | 119.77 | 111.09 |
| 48 | 37 | 314 | A86 | C25-C26-C27 | -4.86 | 120.46 | 127.28 |
| 37 | b | 503 | CLA | C4A-NA-C1A | -4.86 | 104.46 | 106.68 |
| 47 | 17 | 306 | KC1 | C3C-C4C-NC | 4.86 | 115.11 | 109.90 |
| 37 | 17 | 309 | CLA | C3B-C2B-C1B | -4.86 | 101.44 | 107.17 |
| 47 | 31 | 305 | KC1 | CHC-C1C-C2C | -4.86 | 117.35 | 125.03 |
| 47 | 16 | 305 | KC1 | CHD-C4C-C3C | -4.86 | 116.26 | 125.23 |
| 37 | B | 503 | CLA | C4A-NA-C1A | -4.86 | 104.46 | 106.68 |
| 37 | 11 | 303 | CLA | C4A-NA-C1A | -4.86 | 104.46 | 106.68 |
| 37 | 33 | 310 | CLA | C3B-C2B-C1B | -4.86 | 101.44 | 107.17 |
| 44 | c | 516 | DGD | O3G-C3G-C2G | -4.86 | 98.99 | 110.82 |
| 37 | B | 510 | CLA | C3B-C2B-C1B | -4.86 | 101.44 | 107.17 |
| 47 | 32 | 207 | KC1 | C2B-C1B-NB | 4.86 | 114.94 | 110.13 |
| 37 | 11 | 301 | CLA | C3D-C2D-C1D | -4.86 | 99.20 | 105.83 |
| 37 | B | 505 | CLA | C3B-C2B-C1B | -4.86 | 101.44 | 107.17 |
| 37 | 13 | 301 | CLA | C3D-C2D-C1D | -4.86 | 99.20 | 105.83 |
| 47 | 15 | 309 | KC1 | C3C-C4C-NC | 4.86 | 115.11 | 109.90 |
| 37 | 18 | 202 | CLA | C3B-C2B-C1B | -4.86 | 101.44 | 107.17 |
| 37 | b | 508 | CLA | O2D-CGD-CBD | 4.86 | 119.72 | 111.23 |
| 48 | 12 | 214 | A86 | O4-C38-C39 | 4.86 | 119.75 | 111.09 |
| 48 | 32 | 215 | A86 | O4-C38-C39 | 4.86 | 119.75 | 111.09 |
| 48 | 40 | 213 | A86 | O4-C38-C39 | 4.85 | 119.75 | 111.09 |
| 37 | d | 401 | CLA | C3B-C2B-C1B | -4.85 | 101.45 | 107.17 |
| 47 | 36 | 305 | KC1 | CHD-C4C-C3C | -4.85 | 116.28 | 125.23 |
| 48 | 18 | 213 | A86 | O4-C38-C39 | 4.85 | 119.74 | 111.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 310 | CLA | C2C-C1C-NC | 4.85 | 115.08 | 109.98 |
| 37 | 34 | 305 | CLA | C2C-C1C-NC | 4.85 | 115.08 | 109.98 |
| 37 | 34 | 301 | CLA | C3D-C2D-C1D | -4.85 | 99.21 | 105.83 |
| 37 | C | 513 | CLA | O2D-CGD-CBD | 4.85 | 119.71 | 111.23 |
| 44 | C | 516 | DGD | O3G-C3G-C2G | -4.85 | 99.02 | 110.82 |
| 37 | c | 503 | CLA | C3D-C2D-C1D | -4.85 | 99.21 | 105.83 |
| 47 | 11 | 304 | KC1 | CHC-C1C-C2C | -4.85 | 117.37 | 125.03 |
| 37 | 11 | 308 | CLA | C2C-C1C-NC | 4.85 | 115.08 | 109.98 |
| 37 | 21 | 205 | CLA | C2C-C1C-NC | 4.85 | 115.08 | 109.98 |
| 37 | 21 | 206 | CLA | C3D-C2D-C1D | -4.85 | 99.21 | 105.83 |
| 37 | 18 | 206 | CLA | C4A-NA-C1A | -4.85 | 104.47 | 106.68 |
| 37 | 41 | 206 | CLA | C3D-C2D-C1D | -4.85 | 99.22 | 105.83 |
| 50 | 41 | 216 | DD6 | C21-C20-C19 | -4.85 | 108.80 | 114.24 |
| 37 | 34 | 310 | CLA | O2D-CGD-CBD | 4.85 | 119.70 | 111.23 |
| 37 | c | 510 | CLA | C3B-C2B-C1B | -4.85 | 101.46 | 107.17 |
| 48 | 20 | 311 | A86 | O4-C38-C39 | 4.85 | 119.73 | 111.09 |
| 48 | 11 | 312 | A86 | O4-C38-C39 | 4.84 | 119.73 | 111.09 |
| 47 | 37 | 305 | KC1 | C3C-C4C-NC | 4.84 | 115.09 | 109.90 |
| 37 | 32 | 206 | CLA | C4A-NA-C1A | -4.84 | 104.47 | 106.68 |
| 37 | B | 508 | CLA | O2D-CGD-CBD | 4.84 | 119.70 | 111.23 |
| 37 | B | 507 | CLA | C2C-C1C-NC | 4.84 | 115.07 | 109.98 |
| 37 | 19 | 304 | CLA | O2D-CGD-CBD | 4.84 | 119.69 | 111.23 |
| 47 | 35 | 304 | KC1 | CHC-C1C-C2C | -4.84 | 117.38 | 125.03 |
| 47 | 14 | 306 | KC1 | C3C-C4C-NC | 4.84 | 115.09 | 109.90 |
| 37 | 18 | 208 | CLA | C3B-C2B-C1B | -4.84 | 101.46 | 107.17 |
| 37 | 18 | 206 | CLA | C2C-C1C-NC | 4.84 | 115.06 | 109.98 |
| 37 | 31 | 301 | CLA | C2C-C1C-NC | 4.84 | 115.06 | 109.98 |
| 37 | 39 | 307 | CLA | C3D-C2D-C1D | -4.84 | 99.23 | 105.83 |
| 47 | 37 | 305 | KC1 | C2D-C1D-ND | 4.84 | 115.34 | 110.33 |
| 37 | c | 513 | CLA | O2D-CGD-CBD | 4.84 | 119.69 | 111.23 |
| 37 | 34 | 305 | CLA | C3B-C2B-C1B | -4.84 | 101.47 | 107.17 |
| 37 | 12 | 210 | CLA | C2B-C1B-NB | 4.84 | 115.34 | 110.33 |
| 47 | 13 | 306 | KC1 | C3C-C4C-NC | 4.84 | 115.08 | 109.90 |
| 48 | 36 | 310 | A86 | O4-C38-C39 | 4.84 | 119.71 | 111.09 |
| 37 | 11 | 310 | CLA | C2C-C1C-NC | 4.84 | 115.06 | 109.98 |
| 37 | C | 511 | CLA | C3D-C2D-C1D | -4.84 | 99.23 | 105.83 |
| 37 | b | 506 | CLA | C4A-NA-C1A | -4.84 | 104.47 | 106.68 |
| 47 | 35 | 304 | KC1 | C1A-NA-C4A | -4.84 | 104.47 | 106.68 |
| 37 | 38 | 208 | CLA | C3B-C2B-C1B | -4.83 | 101.47 | 107.17 |
| 37 | 41 | 205 | CLA | C2C-C1C-NC | 4.83 | 115.06 | 109.98 |
| 37 | a | 404 | CLA | C3D-C2D-C1D | -4.83 | 99.23 | 105.83 |
| 37 | B | 506 | CLA | C4A-NA-C1A | -4.83 | 104.47 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 21 | 216 | DD6 | C21-C20-C19 | -4.83 | 108.81 | 114.24 |
| 47 | 15 | 304 | KC1 | CHC-C1C-C2C | -4.83 | 117.40 | 125.03 |
| 47 | 20 | 305 | KC1 | C2D-C1D-ND | 4.83 | 115.34 | 110.33 |
| 37 | c | 511 | CLA | C3B-C2B-C1B | -4.83 | 101.47 | 107.17 |
| 48 | 36 | 313 | A86 | C12-C11-C13 | 4.83 | 123.83 | 116.00 |
| 47 | 16 | 308 | KC1 | C3C-C4C-NC | 4.83 | 115.07 | 109.90 |
| 37 | C | 503 | CLA | C2C-C1C-NC | 4.83 | 115.05 | 109.98 |
| 47 | 14 | 306 | KC1 | CHD-C4C-C3C | -4.83 | 116.32 | 125.23 |
| 47 | 19 | 308 | KC1 | C3C-C4C-NC | 4.83 | 115.07 | 109.90 |
| 37 | b | 511 | CLA | C3D-C2D-C1D | -4.83 | 99.24 | 105.83 |
| 37 | B | 511 | CLA | C3D-C2D-C1D | -4.83 | 99.24 | 105.83 |
| 37 | 14 | 301 | CLA | C3D-C2D-C1D | -4.83 | 99.24 | 105.83 |
| 37 | D | 402 | CLA | C3B-C2B-C1B | -4.83 | 101.48 | 107.17 |
| 47 | 20 | 304 | KC1 | C2B-C1B-NB | 4.83 | 114.90 | 110.13 |
| 47 | 20 | 302 | KC1 | C1A-NA-C4A | -4.83 | 104.48 | 106.68 |
| 47 | 17 | 306 | KC1 | C2C-C1C-NC | 4.83 | 116.42 | 110.45 |
| 47 | 37 | 305 | KC1 | C2C-C1C-NC | 4.83 | 116.42 | 110.45 |
| 37 | C | 510 | CLA | C3B-C2B-C1B | -4.83 | 101.48 | 107.17 |
| 37 | D | 402 | CLA | O2D-CGD-CBD | 4.82 | 119.66 | 111.23 |
| 37 | b | 507 | CLA | C2C-C1C-NC | 4.82 | 115.05 | 109.98 |
| 37 | 33 | 301 | CLA | C3D-C2D-C1D | -4.82 | 99.25 | 105.83 |
| 48 | 38 | 214 | A86 | C25-C26-C27 | -4.82 | 120.51 | 127.28 |
| 37 | B | 514 | CLA | C3B-C2B-C1B | -4.82 | 101.48 | 107.17 |
| 47 | 37 | 304 | KC1 | C3D-C4D-ND | 4.82 | 116.92 | 110.20 |
| 37 | C | 511 | CLA | O2D-CGD-CBD | 4.82 | 119.66 | 111.23 |
| 37 | 32 | 202 | CLA | C2C-C1C-NC | 4.82 | 115.05 | 109.98 |
| 37 | C | 513 | CLA | C3D-C2D-C1D | -4.82 | 99.25 | 105.83 |
| 47 | 34 | 306 | KC1 | C3C-C4C-NC | 4.82 | 115.06 | 109.90 |
| 37 | 39 | 309 | CLA | C4A-NA-C1A | -4.82 | 104.48 | 106.68 |
| 37 | 16 | 303 | CLA | C2C-C1C-NC | 4.82 | 115.04 | 109.98 |
| 47 | 34 | 306 | KC1 | CHD-C4C-C3C | -4.82 | 116.34 | 125.23 |
| 37 | c | 513 | CLA | C3D-C2D-C1D | -4.82 | 99.25 | 105.83 |
| 47 | 16 | 308 | KC1 | CHD-C4C-C3C | -4.82 | 116.34 | 125.23 |
| 37 | 14 | 310 | CLA | O2D-CGD-CBD | 4.82 | 119.65 | 111.23 |
| 47 | 15 | 304 | KC1 | C2D-C1D-ND | 4.82 | 115.32 | 110.33 |
| 37 | W | 102 | CLA | C2C-C1C-NC | 4.82 | 115.04 | 109.98 |
| 37 | 40 | 210 | CLA | C2B-C1B-NB | 4.82 | 115.32 | 110.33 |
| 37 | 20 | 307 | CLA | C2B-C1B-NB | 4.82 | 115.32 | 110.33 |
| 37 | 40 | 209 | CLA | C2B-C1B-NB | 4.82 | 115.32 | 110.33 |
| 47 | 36 | 308 | KC1 | C3C-C4C-NC | 4.81 | 115.06 | 109.90 |
| 47 | 18 | 205 | KC1 | C3D-C4D-ND | 4.81 | 116.91 | 110.20 |
| 37 | 38 | 209 | CLA | C3D-C2D-C1D | -4.81 | 99.26 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | W | 101 | CLA | C2C-C1C-NC | 4.81 | 115.04 | 109.98 |
| 37 | 11 | 307 | CLA | C3D-C2D-C1D | -4.81 | 99.26 | 105.83 |
| 47 | 38 | 205 | KC1 | C3D-C4D-ND | 4.81 | 116.91 | 110.20 |
| 47 | 35 | 309 | KC1 | C3C-C4C-NC | 4.81 | 115.06 | 109.90 |
| 37 | A | 403 | CLA | C2D-C1D-ND | 4.81 | 114.89 | 110.13 |
| 37 | b | 510 | CLA | C3B-C2B-C1B | -4.81 | 101.50 | 107.17 |
| 37 | 38 | 203 | CLA | C3B-C2B-C1B | -4.81 | 101.50 | 107.17 |
| 37 | 36 | 301 | CLA | C2B-C1B-NB | 4.81 | 115.31 | 110.33 |
| 47 | 40 | 207 | KC1 | C2D-C1D-ND | 4.81 | 115.31 | 110.33 |
| 47 | 17 | 305 | KC1 | C3D-C4D-ND | 4.81 | 116.91 | 110.20 |
| 37 | c | 511 | CLA | O2D-CGD-CBD | 4.81 | 119.64 | 111.23 |
| 37 | 19 | 307 | CLA | C3D-C2D-C1D | -4.81 | 99.27 | 105.83 |
| 37 | B | 509 | CLA | C4A-NA-C1A | -4.81 | 104.49 | 106.68 |
| 37 | 40 | 208 | CLA | C4A-NA-C1A | -4.81 | 104.49 | 106.68 |
| 37 | b | 514 | CLA | C3B-C2B-C1B | -4.81 | 101.50 | 107.17 |
| 37 | A | 403 | CLA | C4A-NA-C1A | -4.80 | 104.49 | 106.68 |
| 37 | 15 | 303 | CLA | C2B-C1B-NB | 4.80 | 115.31 | 110.33 |
| 37 | Z | 102 | CLA | C2C-C1C-NC | 4.80 | 115.02 | 109.98 |
| 47 | 15 | 309 | KC1 | CHD-C4C-C3C | -4.80 | 116.38 | 125.23 |
| 37 | 35 | 310 | CLA | C3B-C2B-C1B | -4.80 | 101.51 | 107.17 |
| 47 | 31 | 303 | KC1 | CHC-C1C-C2C | -4.80 | 117.45 | 125.03 |
| 48 | 16 | 314 | A86 | C12-C11-C13 | 4.80 | 123.78 | 116.00 |
| 47 | 33 | 306 | KC1 | O2D-CGD-CBD | 4.80 | 119.62 | 111.23 |
| 37 | 18 | 209 | CLA | C3D-C2D-C1D | -4.80 | 99.28 | 105.83 |
| 47 | 37 | 307 | KC1 | CHD-C4C-C3C | -4.80 | 116.38 | 125.23 |
| 37 | 39 | 303 | CLA | C3B-C2B-C1B | -4.80 | 101.52 | 107.17 |
| 37 | 14 | 305 | CLA | C2C-C1C-NC | 4.80 | 115.02 | 109.98 |
| 47 | 13 | 306 | KC1 | CHD-C4C-C3C | -4.80 | 116.39 | 125.23 |
| 47 | 12 | 206 | KC1 | C2B-C1B-NB | 4.80 | 114.87 | 110.13 |
| 37 | 20 | 308 | CLA | O2D-CGD-CBD | 4.80 | 119.61 | 111.23 |
| 37 | c | 511 | CLA | C3D-C2D-C1D | -4.80 | 99.29 | 105.83 |
| 47 | 13 | 306 | KC1 | O2D-CGD-CBD | 4.79 | 119.61 | 111.23 |
| 37 | 39 | 305 | CLA | C3D-C2D-C1D | -4.79 | 99.29 | 105.83 |
| 47 | 36 | 308 | KC1 | CHD-C4C-C3C | -4.79 | 116.39 | 125.23 |
| 37 | 36 | 303 | CLA | C2C-C1C-NC | 4.79 | 115.02 | 109.98 |
| 37 | 40 | 210 | CLA | O2D-CGD-CBD | 4.79 | 119.61 | 111.23 |
| 37 | 20 | 308 | CLA | C2B-C1B-NB | 4.79 | 115.30 | 110.33 |
| 37 | B | 509 | CLA | C3D-C2D-C1D | -4.79 | 99.29 | 105.83 |
| 37 | 15 | 301 | CLA | C3D-C2D-C1D | -4.79 | 99.29 | 105.83 |
| 37 | 19 | 303 | CLA | C4A-NA-C1A | -4.79 | 104.49 | 106.68 |
| 37 | 39 | 303 | CLA | C4A-NA-C1A | -4.79 | 104.49 | 106.68 |
| 50 | 16 | 312 | DD6 | C15-C14-C13 | -4.79 | 115.87 | 125.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 19 | 303 | CLA | C3B-C2B-C1B | -4.79 | 101.52 | 107.17 |
| 47 | 35 | 309 | KC1 | CHD-C4C-C3C | -4.79 | 116.40 | 125.23 |
| 37 | 16 | 306 | CLA | C2B-C1B-NB | 4.79 | 115.29 | 110.33 |
| 37 | 35 | 301 | CLA | C2B-C1B-NB | 4.79 | 115.29 | 110.33 |
| 47 | 40 | 206 | KC1 | C2B-C1B-NB | 4.79 | 114.86 | 110.13 |
| 37 | B | 506 | CLA | C3D-C2D-C1D | -4.79 | 99.30 | 105.83 |
| 37 | c | 506 | CLA | C3D-C2D-C1D | -4.79 | 99.30 | 105.83 |
| 37 | 39 | 304 | CLA | O2D-CGD-CBD | 4.79 | 119.60 | 111.23 |
| 37 | 41 | 202 | CLA | C3B-C4B-NB | 4.79 | 114.80 | 110.53 |
| 37 | 31 | 308 | CLA | C3D-C2D-C1D | -4.79 | 99.30 | 105.83 |
| 47 | 21 | 207 | KC1 | C3C-C4C-NC | 4.79 | 115.03 | 109.90 |
| 37 | 16 | 301 | CLA | C2B-C1B-NB | 4.78 | 115.29 | 110.33 |
| 47 | 33 | 306 | KC1 | CHD-C4C-C3C | -4.78 | 116.41 | 125.23 |
| 47 | 33 | 306 | KC1 | C3C-C4C-NC | 4.78 | 115.03 | 109.90 |
| 37 | z | 102 | CLA | C2C-C1C-NC | 4.78 | 115.01 | 109.98 |
| 47 | 17 | 308 | KC1 | CHD-C4C-C3C | -4.78 | 116.41 | 125.23 |
| 37 | 19 | 309 | CLA | C3B-C2B-C1B | -4.78 | 101.53 | 107.17 |
| 47 | 14 | 304 | KC1 | C3D-C4D-ND | 4.78 | 116.87 | 110.20 |
| 37 | 21 | 208 | CLA | C2C-C1C-NC | 4.78 | 115.01 | 109.98 |
| 37 | 39 | 309 | CLA | C3B-C2B-C1B | -4.78 | 101.53 | 107.17 |
| 47 | 20 | 304 | KC1 | CBA-CAA-C2A | -4.78 | 106.26 | 125.45 |
| 47 | 31 | 309 | KC1 | CHC-C1C-C2C | -4.78 | 117.48 | 125.03 |
| 37 | 20 | 301 | CLA | C3D-C2D-C1D | -4.78 | 99.31 | 105.83 |
| 37 | 13 | 310 | CLA | C2C-C1C-NC | 4.78 | 115.00 | 109.98 |
| 47 | 41 | 207 | KC1 | C3C-C4C-NC | 4.78 | 115.02 | 109.90 |
| 37 | 35 | 303 | CLA | C4A-NA-C1A | -4.78 | 104.50 | 106.68 |
| 50 | 36 | 312 | DD6 | C15-C14-C13 | -4.78 | 115.89 | 125.99 |
| 50 | 39 | 312 | DD6 | C21-C20-C15 | -4.78 | 114.44 | 122.30 |
| 47 | 11 | 302 | KC1 | CHD-C4C-C3C | -4.78 | 116.42 | 125.23 |
| 37 | 21 | 205 | CLA | C3D-C2D-C1D | -4.78 | 99.31 | 105.83 |
| 37 | b | 506 | CLA | C3D-C2D-C1D | -4.78 | 99.31 | 105.83 |
| 37 | 35 | 301 | CLA | C3D-C2D-C1D | -4.78 | 99.31 | 105.83 |
| 37 | b | 509 | CLA | C3D-C2D-C1D | -4.78 | 99.31 | 105.83 |
| 37 | d | 404 | CLA | C3D-C2D-C1D | -4.78 | 99.31 | 105.83 |
| 47 | 40 | 206 | KC1 | CBA-CAA-C2A | -4.77 | 106.29 | 125.45 |
| 37 | C | 511 | CLA | C3B-C2B-C1B | -4.77 | 101.54 | 107.17 |
| 47 | 14 | 304 | KC1 | CHD-C4C-C3C | -4.77 | 116.42 | 125.23 |
| 47 | 34 | 304 | KC1 | CHD-C4C-C3C | -4.77 | 116.42 | 125.23 |
| 37 | 13 | 307 | CLA | CED-O2D-CGD | 4.77 | 126.74 | 115.92 |
| 37 | 32 | 211 | CLA | C2B-C1B-NB | 4.77 | 115.28 | 110.33 |
| 37 | 14 | 310 | CLA | C3B-C2B-C1B | -4.77 | 101.54 | 107.17 |
| 47 | 34 | 304 | KC1 | C3D-C4D-ND | 4.77 | 116.86 | 110.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 19 | 305 | CLA | C3D-C2D-C1D | -4.77 | 99.32 | 105.83 |
| 48 | 12 | 215 | A86 | C25-C26-C27 | -4.77 | 120.59 | 127.28 |
| 47 | 18 | 207 | KC1 | CHD-C4C-C3C | -4.77 | 116.43 | 125.23 |
| 37 | C | 501 | CLA | C2B-C1B-NB | 4.77 | 115.27 | 110.33 |
| 37 | 21 | 202 | CLA | C3B-C4B-NB | 4.77 | 114.79 | 110.53 |
| 37 | w | 101 | CLA | C3D-C2D-C1D | -4.77 | 99.32 | 105.83 |
| 48 | 11 | 315 | A86 | C33-C32-C31 | 4.77 | 113.85 | 109.21 |
| 37 | b | 512 | CLA | C1D-CHD-C4C | -4.77 | 115.88 | 126.02 |
| 37 | 34 | 310 | CLA | C3B-C2B-C1B | -4.77 | 101.55 | 107.17 |
| 37 | 14 | 305 | CLA | C3B-C2B-C1B | -4.77 | 101.55 | 107.17 |
| 37 | 15 | 310 | CLA | C3B-C2B-C1B | -4.77 | 101.55 | 107.17 |
| 37 | B | 512 | CLA | C1D-CHD-C4C | -4.77 | 115.89 | 126.02 |
| 47 | 31 | 303 | KC1 | CHD-C4C-C3C | -4.76 | 116.44 | 125.23 |
| 37 | 34 | 302 | CLA | C3D-C2D-C1D | -4.76 | 99.33 | 105.83 |
| 37 | 40 | 203 | CLA | C3D-C2D-C1D | -4.76 | 99.33 | 105.83 |
| 48 | 32 | 216 | A86 | C25-C26-C27 | -4.76 | 120.60 | 127.28 |
| 50 | 19 | 312 | DD6 | C21-C20-C15 | -4.76 | 114.47 | 122.30 |
| 47 | 39 | 308 | KC1 | C3C-C4C-NC | 4.76 | 115.00 | 109.90 |
| 37 | C | 506 | CLA | C3D-C2D-C1D | -4.76 | 99.33 | 105.83 |
| 37 | 12 | 205 | CLA | CAA-C2A-C3A | -4.76 | 100.13 | 113.00 |
| 47 | 41 | 203 | KC1 | C4B-C3B-C2B | -4.76 | 102.69 | 106.81 |
| 37 | b | 501 | CLA | C2C-C1C-NC | 4.76 | 114.98 | 109.98 |
| 37 | 38 | 206 | CLA | C2C-C1C-NC | 4.76 | 114.98 | 109.98 |
| 47 | 35 | 306 | KC1 | C3C-C4C-NC | 4.76 | 115.00 | 109.90 |
| 37 | 33 | 303 | CLA | CAA-C2A-C3A | -4.76 | 100.14 | 113.00 |
| 37 | 39 | 304 | CLA | C4A-NA-C1A | -4.76 | 104.51 | 106.68 |
| 37 | W | 101 | CLA | C3D-C2D-C1D | -4.76 | 99.34 | 105.83 |
| 37 | 36 | 306 | CLA | C2B-C1B-NB | 4.76 | 115.26 | 110.33 |
| 47 | 11 | 302 | KC1 | CHC-C1C-C2C | -4.76 | 117.52 | 125.03 |
| 37 | 33 | 307 | CLA | CED-O2D-CGD | 4.76 | 126.70 | 115.92 |
| 37 | 31 | 310 | CLA | C3B-C2B-C1B | -4.76 | 101.56 | 107.17 |
| 37 | 21 | 210 | CLA | C2C-C1C-NC | 4.75 | 114.98 | 109.98 |
| 37 | 41 | 210 | CLA | C2C-C1C-NC | 4.75 | 114.98 | 109.98 |
| 48 | 13 | 313 | A86 | C25-C26-C27 | -4.75 | 120.61 | 127.28 |
| 37 | 19 | 302 | CLA | C2B-C1B-NB | 4.75 | 115.26 | 110.33 |
| 37 | 33 | 310 | CLA | C2C-C1C-NC | 4.75 | 114.97 | 109.98 |
| 47 | 11 | 306 | KC1 | C3C-C4C-NC | 4.75 | 114.99 | 109.90 |
| 37 | 11 | 310 | CLA | C3B-C2B-C1B | -4.75 | 101.57 | 107.17 |
| 37 | D | 406 | CLA | C3D-C2D-C1D | -4.75 | 99.35 | 105.83 |
| 37 | 19 | 309 | CLA | C4A-NA-C1A | -4.75 | 104.51 | 106.68 |
| 37 | 41 | 205 | CLA | C3D-C2D-C1D | -4.75 | 99.35 | 105.83 |
| 37 | 32 | 206 | CLA | CAA-C2A-C3A | -4.75 | 100.16 | 113.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 507 | CLA | C3D-C2D-C1D | -4.75 | 99.35 | 105.83 |
| 37 | 19 | 307 | CLA | C4A-NA-C1A | -4.75 | 104.51 | 106.68 |
| 48 | 32 | 216 | A86 | C4-C5-C6 | -4.75 | 120.62 | 127.28 |
| 37 | 19 | 310 | CLA | O2D-CGD-CBD | 4.75 | 119.53 | 111.23 |
| 37 | b | 514 | CLA | C2C-C1C-NC | 4.75 | 114.97 | 109.98 |
| 37 | 41 | 208 | CLA | C2C-C1C-NC | 4.75 | 114.97 | 109.98 |
| 48 | 33 | 313 | A86 | C25-C26-C27 | -4.75 | 120.62 | 127.28 |
| 47 | 18 | 207 | KC1 | C2B-C1B-NB | 4.75 | 114.83 | 110.13 |
| 37 | B | 514 | CLA | C2C-C1C-NC | 4.75 | 114.97 | 109.98 |
| 48 | 37 | 309 | A86 | C25-C26-C27 | -4.74 | 120.62 | 127.28 |
| 47 | 31 | 307 | KC1 | C3C-C4C-NC | 4.74 | 114.98 | 109.90 |
| 37 | c | 507 | CLA | C2B-C1B-NB | 4.74 | 115.25 | 110.33 |
| 37 | C | 511 | CLA | C2C-C1C-NC | 4.74 | 114.96 | 109.98 |
| 37 | 21 | 209 | CLA | C4A-NA-C1A | -4.74 | 104.52 | 106.68 |
| 37 | c | 507 | CLA | C3D-C2D-C1D | -4.74 | 99.36 | 105.83 |
| 37 | 39 | 310 | CLA | O2D-CGD-CBD | 4.74 | 119.52 | 111.23 |
| 47 | 11 | 309 | KC1 | CHC-C1C-C2C | -4.74 | 117.54 | 125.03 |
| 37 | 38 | 208 | CLA | O2D-CGD-CBD | 4.74 | 119.52 | 111.23 |
| 48 | 14 | 313 | A86 | C3-C2-C1 | -4.74 | 120.63 | 127.28 |
| 37 | 14 | 302 | CLA | C3D-C2D-C1D | -4.74 | 99.36 | 105.83 |
| 48 | 37 | 312 | A86 | C3-C2-C1 | -4.74 | 120.63 | 127.28 |
| 37 | 20 | 307 | CLA | C3B-C2B-C1B | -4.74 | 101.58 | 107.17 |
| 37 | 15 | 301 | CLA | C2B-C1B-NB | 4.74 | 115.24 | 110.33 |
| 37 | B | 515 | CLA | C3D-C2D-C1D | -4.74 | 99.36 | 105.83 |
| 37 | b | 523 | CLA | C2C-C1C-NC | 4.74 | 114.96 | 109.98 |
| 37 | 12 | 212 | CLA | C3D-C2D-C1D | -4.74 | 99.36 | 105.83 |
| 48 | 33 | 311 | A86 | C25-C26-C27 | -4.74 | 120.63 | 127.28 |
| 37 | 18 | 201 | CLA | C3D-C2D-C1D | -4.74 | 99.37 | 105.83 |
| 37 | D | 405 | CLA | C2B-C1B-NB | 4.74 | 115.24 | 110.33 |
| 37 | C | 504 | CLA | C3D-C2D-C1D | -4.74 | 99.37 | 105.83 |
| 37 | B | 501 | CLA | C2C-C1C-NC | 4.73 | 114.95 | 109.98 |
| 37 | 11 | 305 | CLA | C2C-C1C-NC | 4.73 | 114.95 | 109.98 |
| 37 | 35 | 308 | CLA | C2C-C1C-NC | 4.73 | 114.95 | 109.98 |
| 48 | 15 | 313 | A86 | O4-C38-C39 | 4.73 | 119.53 | 111.09 |
| 37 | c | 505 | CLA | C2C-C1C-NC | 4.73 | 114.95 | 109.98 |
| 37 | c | 504 | CLA | C3D-C2D-C1D | -4.73 | 99.37 | 105.83 |
| 47 | 40 | 204 | KC1 | C1A-NA-C4A | -4.73 | 104.52 | 106.68 |
| 48 | 35 | 313 | A86 | O4-C38-C39 | 4.73 | 119.52 | 111.09 |
| 37 | 39 | 302 | CLA | C2B-C1B-NB | 4.73 | 115.23 | 110.33 |
| 37 | 35 | 303 | CLA | C2B-C1B-NB | 4.73 | 115.23 | 110.33 |
| 37 | b | 515 | CLA | C3D-C2D-C1D | -4.73 | 99.38 | 105.83 |
| 37 | 36 | 309 | CLA | C3D-C2D-C1D | -4.72 | 99.38 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 306 | CLA | C2C-C1C-NC | 4.72 | 114.94 | 109.98 |
| 37 | c | 501 | CLA | C2B-C1B-NB | 4.72 | 115.22 | 110.33 |
| 37 | d | 403 | CLA | C2B-C1B-NB | 4.72 | 115.22 | 110.33 |
| 37 | b | 514 | CLA | C1-O2A-CGA | 4.72 | 128.09 | 116.65 |
| 37 | 13 | 303 | CLA | CAA-C2A-C3A | -4.72 | 100.23 | 113.00 |
| 37 | B | 524 | CLA | C2C-C1C-NC | 4.72 | 114.94 | 109.98 |
| 37 | 16 | 309 | CLA | C3D-C2D-C1D | -4.72 | 99.39 | 105.83 |
| 48 | 17 | 310 | A86 | C25-C26-C27 | -4.72 | 120.65 | 127.28 |
| 37 | 17 | 302 | CLA | C2C-C1C-NC | 4.72 | 114.94 | 109.98 |
| 37 | B | 506 | CLA | CHD-C1D-ND | -4.72 | 118.16 | 124.80 |
| 37 | 20 | 301 | CLA | C3D-C4D-ND | 4.72 | 117.66 | 109.99 |
| 37 | C | 506 | CLA | C3B-C4B-NB | 4.72 | 114.74 | 110.53 |
| 48 | 15 | 319 | A86 | C4-C5-C6 | -4.72 | 120.66 | 127.28 |
| 37 | 40 | 203 | CLA | C3D-C4D-ND | 4.72 | 117.66 | 109.99 |
| 48 | 12 | 215 | A86 | C4-C5-C6 | -4.72 | 120.66 | 127.28 |
| 37 | b | 506 | CLA | CHD-C1D-ND | -4.72 | 118.16 | 124.80 |
| 47 | 15 | 306 | KC1 | C3C-C4C-NC | 4.72 | 114.95 | 109.90 |
| 47 | 39 | 308 | KC1 | C3D-C4D-ND | 4.72 | 116.78 | 110.20 |
| 37 | b | 507 | CLA | C3D-C2D-C1D | -4.72 | 99.40 | 105.83 |
| 37 | b | 511 | CLA | C3B-C2B-C1B | -4.72 | 101.61 | 107.17 |
| 47 | 38 | 210 | KC1 | CHD-C4C-C3C | -4.71 | 116.54 | 125.23 |
| 37 | C | 507 | CLA | C3D-C2D-C1D | -4.71 | 99.40 | 105.83 |
| 47 | 12 | 211 | KC1 | CHD-C4C-C3C | -4.71 | 116.54 | 125.23 |
| 37 | 20 | 307 | CLA | C2C-C1C-NC | 4.71 | 114.93 | 109.98 |
| 37 | B | 514 | CLA | C1-O2A-CGA | 4.71 | 128.06 | 116.65 |
| 37 | 39 | 302 | CLA | C3D-C2D-C1D | -4.71 | 99.40 | 105.83 |
| 48 | 41 | 215 | A86 | C4-C5-C6 | -4.71 | 120.67 | 127.28 |
| 48 | 37 | 313 | A86 | O4-C38-C39 | 4.71 | 119.49 | 111.09 |
| 37 | B | 508 | CLA | C2C-C1C-NC | 4.71 | 114.93 | 109.98 |
| 48 | 35 | 319 | A86 | C4-C5-C6 | -4.71 | 120.67 | 127.28 |
| 37 | B | 515 | CLA | O2D-CGD-CBD | 4.71 | 119.46 | 111.23 |
| 37 | 40 | 209 | CLA | C3B-C2B-C1B | -4.71 | 101.62 | 107.17 |
| 37 | c | 511 | CLA | C2C-C1C-NC | 4.71 | 114.92 | 109.98 |
| 37 | 15 | 303 | CLA | C4A-NA-C1A | -4.71 | 104.53 | 106.68 |
| 48 | 34 | 313 | A86 | C3-C2-C1 | -4.71 | 120.68 | 127.28 |
| 48 | 31 | 315 | A86 | C33-C32-C31 | 4.71 | 113.78 | 109.21 |
| 37 | 40 | 203 | CLA | CHD-C1D-ND | -4.70 | 118.18 | 124.80 |
| 47 | 19 | 308 | KC1 | C3D-C4D-ND | 4.70 | 116.76 | 110.20 |
| 37 | 40 | 209 | CLA | C2C-C1C-NC | 4.70 | 114.92 | 109.98 |
| 37 | 32 | 204 | CLA | C3D-C2D-C1D | -4.70 | 99.41 | 105.83 |
| 37 | 12 | 203 | CLA | C3D-C2D-C1D | -4.70 | 99.42 | 105.83 |
| 37 | b | 515 | CLA | O2D-CGD-CBD | 4.70 | 119.45 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 512 | CLA | C2C-C1C-NC | 4.70 | 114.92 | 109.98 |
| 37 | c | 512 | CLA | C2C-C1C-NC | 4.70 | 114.92 | 109.98 |
| 37 | 37 | 303 | CLA | C3D-C2D-C1D | -4.70 | 99.42 | 105.83 |
| 37 | 21 | 204 | CLA | C2C-C1C-NC | 4.70 | 114.92 | 109.98 |
| 47 | 18 | 210 | KC1 | CHC-C1C-C2C | -4.70 | 117.61 | 125.03 |
| 47 | 21 | 203 | KC1 | C4B-C3B-C2B | -4.70 | 102.74 | 106.81 |
| 47 | 38 | 210 | KC1 | CHC-C1C-C2C | -4.70 | 117.61 | 125.03 |
| 37 | a | 407 | CLA | C2C-C1C-NC | 4.69 | 114.91 | 109.98 |
| 37 | 15 | 307 | CLA | C4A-NA-C1A | -4.69 | 104.54 | 106.68 |
| 37 | 20 | 301 | CLA | CHD-C1D-ND | -4.69 | 118.20 | 124.80 |
| 37 | Z | 101 | CLA | C3B-C2B-C1B | -4.69 | 101.64 | 107.17 |
| 37 | C | 507 | CLA | C2B-C1B-NB | 4.69 | 115.19 | 110.33 |
| 37 | 32 | 213 | CLA | C3D-C2D-C1D | -4.69 | 99.43 | 105.83 |
| 48 | 18 | 213 | A86 | C40-C32-C31 | -4.69 | 106.27 | 110.47 |
| 47 | 35 | 302 | KC1 | CHC-C1C-C2C | -4.69 | 117.62 | 125.03 |
| 47 | 16 | 304 | KC1 | C3D-C4D-ND | 4.69 | 116.74 | 110.20 |
| 37 | D | 406 | CLA | C2C-C1C-NC | 4.69 | 114.91 | 109.98 |
| 47 | 35 | 304 | KC1 | C3D-C4D-ND | 4.69 | 116.74 | 110.20 |
| 37 | 12 | 210 | CLA | C3B-C2B-C1B | -4.69 | 101.64 | 107.17 |
| 37 | 41 | 204 | CLA | C2C-C1C-NC | 4.69 | 114.91 | 109.98 |
| 37 | z | 101 | CLA | C2B-C1B-NB | 4.69 | 115.19 | 110.33 |
| 47 | 18 | 210 | KC1 | CHD-C4C-C3C | -4.69 | 116.59 | 125.23 |
| 37 | c | 508 | CLA | C2C-C1C-NC | 4.69 | 114.90 | 109.98 |
| 37 | 19 | 302 | CLA | C3D-C2D-C1D | -4.68 | 99.44 | 105.83 |
| 37 | C | 508 | CLA | C2C-C1C-NC | 4.68 | 114.90 | 109.98 |
| 47 | 32 | 212 | KC1 | CHD-C4C-C3C | -4.68 | 116.60 | 125.23 |
| 48 | 21 | 214 | A86 | C3-C2-C1 | -4.68 | 120.71 | 127.28 |
| 47 | 37 | 307 | KC1 | C1A-C2A-C3A | -4.68 | 102.98 | 107.28 |
| 48 | 38 | 213 | A86 | C40-C32-C31 | -4.68 | 106.28 | 110.47 |
| 47 | 14 | 304 | KC1 | CHC-C1C-C2C | -4.68 | 117.64 | 125.03 |
| 37 | C | 509 | CLA | C3B-C2B-C1B | -4.68 | 101.65 | 107.17 |
| 48 | 11 | 313 | A86 | C25-C24-C1 | -4.68 | 113.53 | 126.36 |
| 37 | 17 | 304 | CLA | C3D-C2D-C1D | -4.68 | 99.45 | 105.83 |
| 37 | a | 404 | CLA | C1C-C2C-C3C | -4.68 | 102.06 | 106.98 |
| 37 | A | 405 | CLA | C2C-C1C-NC | 4.68 | 114.89 | 109.98 |
| 37 | z | 101 | CLA | C3B-C2B-C1B | -4.68 | 101.66 | 107.17 |
| 37 | C | 505 | CLA | C2C-C1C-NC | 4.68 | 114.89 | 109.98 |
| 37 | 41 | 209 | CLA | C2C-C1C-NC | 4.67 | 114.89 | 109.98 |
| 37 | b | 502 | CLA | C3D-C2D-C1D | -4.67 | 99.45 | 105.83 |
| 37 | C | 501 | CLA | C3B-C2B-C1B | -4.67 | 101.66 | 107.17 |
| 37 | a | 407 | CLA | C3D-C2D-C1D | -4.67 | 99.46 | 105.83 |
| 48 | 35 | 315 | A86 | C25-C26-C27 | -4.67 | 120.73 | 127.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 209 | CLA | C2C-C1C-NC | 4.67 | 114.89 | 109.98 |
| 48 | 21 | 215 | A86 | C4-C5-C6 | -4.67 | 120.73 | 127.28 |
| 47 | 18 | 207 | KC1 | CHC-C1C-C2C | -4.67 | 117.66 | 125.03 |
| 37 | a | 403 | CLA | C4A-NA-C1A | -4.67 | 104.55 | 106.68 |
| 37 | 19 | 304 | CLA | C4A-NA-C1A | -4.67 | 104.55 | 106.68 |
| 37 | B | 511 | CLA | C3B-C2B-C1B | -4.67 | 101.67 | 107.17 |
| 37 | 18 | 201 | CLA | C2B-C1B-NB | 4.67 | 115.17 | 110.33 |
| 37 | d | 404 | CLA | C2C-C1C-NC | 4.67 | 114.89 | 109.98 |
| 37 | 37 | 301 | CLA | C2C-C1C-NC | 4.67 | 114.88 | 109.98 |
| 50 | 19 | 312 | DD6 | C21-C20-C19 | -4.67 | 109.00 | 114.24 |
| 37 | 32 | 211 | CLA | C3B-C2B-C1B | -4.66 | 101.67 | 107.17 |
| 37 | 14 | 307 | CLA | C4A-NA-C1A | -4.66 | 104.55 | 106.68 |
| 37 | 40 | 205 | CLA | C3B-C2B-C1B | -4.66 | 101.67 | 107.17 |
| 37 | 38 | 203 | CLA | O2D-CGD-CBD | 4.66 | 119.38 | 111.23 |
| 50 | 39 | 312 | DD6 | C7-C6-C8 | -4.66 | 110.97 | 118.09 |
| 37 | 19 | 304 | CLA | C2C-C1C-NC | 4.66 | 114.88 | 109.98 |
| 47 | 33 | 302 | KC1 | O2D-CGD-CBD | 4.66 | 119.38 | 111.23 |
| 47 | 13 | 302 | KC1 | C3C-C4C-NC | 4.66 | 114.89 | 109.90 |
| 47 | 33 | 302 | KC1 | C3C-C4C-NC | 4.66 | 114.89 | 109.90 |
| 37 | c | 506 | CLA | C3B-C4B-NB | 4.66 | 114.69 | 110.53 |
| 37 | 33 | 305 | CLA | C3D-C2D-C1D | -4.66 | 99.47 | 105.83 |
| 47 | 17 | 308 | KC1 | C1A-C2A-C3A | -4.66 | 103.00 | 107.28 |
| 37 | A | 405 | CLA | C3D-C2D-C1D | -4.66 | 99.47 | 105.83 |
| 37 | 39 | 304 | CLA | C2C-C1C-NC | 4.66 | 114.87 | 109.98 |
| 47 | 15 | 304 | KC1 | C3D-C4D-ND | 4.66 | 116.69 | 110.20 |
| 37 | b | 509 | CLA | C2B-C1B-NB | 4.66 | 115.15 | 110.33 |
| 47 | 34 | 304 | KC1 | CHC-C1C-C2C | -4.65 | 117.68 | 125.03 |
| 37 | Z | 101 | CLA | C2B-C1B-NB | 4.65 | 115.15 | 110.33 |
| 47 | 36 | 304 | KC1 | C3D-C4D-ND | 4.65 | 116.69 | 110.20 |
| 48 | 41 | 214 | A86 | C3-C2-C1 | -4.65 | 120.75 | 127.28 |
| 47 | 17 | 308 | KC1 | CHC-C1C-C2C | -4.65 | 117.68 | 125.03 |
| 37 | c | 501 | CLA | C3B-C2B-C1B | -4.65 | 101.69 | 107.17 |
| 50 | 19 | 312 | DD6 | C7-C6-C8 | -4.65 | 110.98 | 118.09 |
| 47 | 20 | 304 | KC1 | C3D-C4D-ND | 4.65 | 116.69 | 110.20 |
| 47 | 40 | 206 | KC1 | C3D-C4D-ND | 4.65 | 116.68 | 110.20 |
| 37 | 36 | 307 | CLA | C3D-C2D-C1D | -4.65 | 99.49 | 105.83 |
| 37 | 18 | 203 | CLA | O2D-CGD-CBD | 4.65 | 119.36 | 111.23 |
| 37 | 15 | 308 | CLA | C3D-C2D-C1D | -4.65 | 99.49 | 105.83 |
| 37 | D | 401 | CLA | C1C-C2C-C3C | -4.65 | 102.09 | 106.98 |
| 37 | d | 403 | CLA | C4A-NA-C1A | -4.65 | 104.56 | 106.68 |
| 37 | 16 | 307 | CLA | C2C-C1C-NC | 4.65 | 114.86 | 109.98 |
| 37 | B | 524 | CLA | C1D-CHD-C4C | -4.64 | 116.15 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 41 | 210 | CLA | C3D-C2D-C1D | -4.64 | 99.49 | 105.83 |
| 37 | b | 523 | CLA | C1D-CHD-C4C | -4.64 | 116.15 | 126.02 |
| 37 | 41 | 202 | CLA | C3B-C2B-C1B | -4.64 | 101.70 | 107.17 |
| 47 | 37 | 302 | KC1 | C1C-C2C-C3C | -4.64 | 102.10 | 106.98 |
| 37 | 39 | 307 | CLA | C4A-NA-C1A | -4.64 | 104.56 | 106.68 |
| 37 | 36 | 307 | CLA | C2C-C1C-NC | 4.64 | 114.86 | 109.98 |
| 48 | 39 | 313 | A86 | C36-C31-C32 | -4.64 | 115.09 | 119.70 |
| 37 | b | 508 | CLA | C2C-C1C-NC | 4.64 | 114.86 | 109.98 |
| 37 | 12 | 209 | CLA | C3D-C2D-C1D | -4.64 | 99.50 | 105.83 |
| 37 | 34 | 308 | CLA | C2B-C1B-NB | 4.64 | 115.14 | 110.33 |
| 50 | 40 | 212 | DD6 | C25-C24-C1 | -4.64 | 113.65 | 126.36 |
| 37 | 21 | 210 | CLA | C3D-C2D-C1D | -4.64 | 99.50 | 105.83 |
| 48 | 21 | 215 | A86 | C36-C31-C32 | -4.64 | 115.09 | 119.70 |
| 37 | 21 | 209 | CLA | C3B-C2B-C1B | -4.64 | 101.70 | 107.17 |
| 47 | 14 | 306 | KC1 | CHC-C1C-C2C | -4.64 | 117.71 | 125.03 |
| 50 | 20 | 310 | DD6 | C25-C24-C1 | -4.64 | 113.65 | 126.36 |
| 37 | 41 | 210 | CLA | C3D-C4D-ND | 4.64 | 117.52 | 109.99 |
| 37 | 13 | 305 | CLA | C3D-C2D-C1D | -4.64 | 99.50 | 105.83 |
| 37 | B | 502 | CLA | C3D-C2D-C1D | -4.63 | 99.51 | 105.83 |
| 37 | B | 510 | CLA | C4A-NA-C1A | -4.63 | 104.56 | 106.68 |
| 47 | 36 | 304 | KC1 | CHD-C4C-C3C | -4.63 | 116.68 | 125.23 |
| 37 | 18 | 209 | CLA | C2B-C1B-NB | 4.63 | 115.13 | 110.33 |
| 37 | 32 | 208 | CLA | C3D-C2D-C1D | -4.63 | 99.51 | 105.83 |
| 50 | 39 | 312 | DD6 | C21-C20-C19 | -4.63 | 109.04 | 114.24 |
| 37 | 16 | 307 | CLA | C3D-C2D-C1D | -4.63 | 99.51 | 105.83 |
| 48 | 16 | 314 | A86 | C25-C26-C27 | -4.63 | 120.78 | 127.28 |
| 48 | 34 | 311 | A86 | C25-C26-C27 | -4.63 | 120.78 | 127.28 |
| 37 | 41 | 209 | CLA | C4A-NA-C1A | -4.63 | 104.57 | 106.68 |
| 48 | 41 | 215 | A86 | C36-C31-C32 | -4.63 | 115.10 | 119.70 |
| 48 | 36 | 313 | A86 | C25-C26-C27 | -4.63 | 120.78 | 127.28 |
| 48 | 11 | 313 | A86 | O4-C38-C39 | 4.63 | 119.35 | 111.09 |
| 37 | 20 | 303 | CLA | C2C-C1C-NC | 4.63 | 114.84 | 109.98 |
| 37 | 20 | 303 | CLA | C3B-C2B-C1B | -4.63 | 101.71 | 107.17 |
| 48 | 13 | 311 | A86 | C25-C26-C27 | -4.63 | 120.79 | 127.28 |
| 37 | B | 506 | CLA | C3C-C4C-NC | 4.63 | 116.36 | 110.43 |
| 37 | 21 | 202 | CLA | C3B-C2B-C1B | -4.63 | 101.71 | 107.17 |
| 37 | b | 502 | CLA | C2C-C1C-NC | 4.63 | 114.84 | 109.98 |
| 37 | B | 514 | CLA | C4A-NA-C1A | -4.63 | 104.57 | 106.68 |
| 37 | 34 | 307 | CLA | C4A-NA-C1A | -4.63 | 104.57 | 106.68 |
| 37 | 35 | 301 | CLA | C3D-C4D-ND | 4.63 | 117.51 | 109.99 |
| 47 | 31 | 305 | KC1 | CHD-C4C-C3C | -4.63 | 116.70 | 125.23 |
| 37 | b | 514 | CLA | C3D-C2D-C1D | -4.63 | 99.52 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 17 | 313 | A86 | C3-C2-C1 | -4.62 | 120.79 | 127.28 |
| 47 | 16 | 304 | KC1 | CHD-C4C-C3C | -4.62 | 116.70 | 125.23 |
| 37 | 18 | 204 | CLA | C4A-NA-C1A | -4.62 | 104.57 | 106.68 |
| 47 | 37 | 302 | KC1 | CMA-C3A-C2A | -4.62 | 117.24 | 128.43 |
| 37 | z | 101 | CLA | C3D-C2D-C1D | -4.62 | 99.52 | 105.83 |
| 37 | B | 514 | CLA | C3D-C2D-C1D | -4.62 | 99.52 | 105.83 |
| 37 | b | 513 | CLA | C3B-C4B-NB | 4.62 | 114.66 | 110.53 |
| 37 | D | 405 | CLA | C3D-C4D-ND | 4.62 | 117.50 | 109.99 |
| 37 | 15 | 301 | CLA | C3D-C4D-ND | 4.62 | 117.50 | 109.99 |
| 47 | 34 | 306 | KC1 | CHC-C1C-C2C | -4.62 | 117.74 | 125.03 |
| 37 | 38 | 206 | CLA | C3B-C2B-C1B | -4.62 | 101.73 | 107.17 |
| 37 | b | 510 | CLA | C3D-C2D-C1D | -4.62 | 99.53 | 105.83 |
| 37 | 21 | 210 | CLA | C3D-C4D-ND | 4.62 | 117.49 | 109.99 |
| 47 | 17 | 306 | KC1 | C4B-C3B-C2B | -4.62 | 102.81 | 106.81 |
| 47 | 17 | 303 | KC1 | CBC-CAC-C3C | -4.62 | 99.91 | 112.42 |
| 48 | 15 | 315 | A86 | C25-C26-C27 | -4.62 | 120.80 | 127.28 |
| 47 | 32 | 207 | KC1 | CAC-C3C-C2C | 4.62 | 136.04 | 127.56 |
| 37 | 11 | 310 | CLA | C3D-C2D-C1D | -4.62 | 99.53 | 105.83 |
| 47 | 13 | 302 | KC1 | O2D-CGD-CBD | 4.61 | 119.30 | 111.23 |
| 37 | c | 509 | CLA | C3B-C2B-C1B | -4.61 | 101.73 | 107.17 |
| 47 | 17 | 303 | KC1 | C1C-C2C-C3C | -4.61 | 102.13 | 106.98 |
| 48 | 14 | 311 | A86 | C25-C26-C27 | -4.61 | 120.81 | 127.28 |
| 37 | 38 | 208 | CLA | C4A-NA-C1A | -4.61 | 104.58 | 106.68 |
| 47 | 11 | 304 | KC1 | CHD-C4C-C3C | -4.61 | 116.73 | 125.23 |
| 47 | 12 | 206 | KC1 | CAC-C3C-C2C | 4.61 | 136.03 | 127.56 |
| 37 | 38 | 204 | CLA | C3D-C4D-ND | 4.61 | 117.48 | 109.99 |
| 37 | 14 | 302 | CLA | O2D-CGD-CBD | 4.61 | 119.29 | 111.23 |
| 47 | 37 | 302 | KC1 | CBC-CAC-C3C | -4.61 | 99.93 | 112.42 |
| 37 | 19 | 303 | CLA | C2B-C1B-NB | 4.61 | 115.10 | 110.33 |
| 37 | 18 | 208 | CLA | C4A-NA-C1A | -4.61 | 104.58 | 106.68 |
| 47 | 40 | 204 | KC1 | CHC-C1C-C2C | -4.61 | 117.75 | 125.03 |
| 37 | 18 | 204 | CLA | C3D-C4D-ND | 4.61 | 117.48 | 109.99 |
| 47 | 16 | 305 | KC1 | CHC-C1C-C2C | -4.60 | 117.76 | 125.03 |
| 48 | 13 | 313 | A86 | C3-C2-C1 | -4.60 | 120.82 | 127.28 |
| 47 | 17 | 303 | KC1 | CMA-C3A-C2A | -4.60 | 117.29 | 128.43 |
| 37 | B | 510 | CLA | C3D-C2D-C1D | -4.60 | 99.55 | 105.83 |
| 37 | 36 | 307 | CLA | C3B-C2B-C1B | -4.60 | 101.74 | 107.17 |
| 37 | 38 | 204 | CLA | C4A-NA-C1A | -4.60 | 104.58 | 106.68 |
| 47 | 20 | 302 | KC1 | CHC-C1C-C2C | -4.60 | 117.76 | 125.03 |
| 37 | C | 502 | CLA | C2C-C1C-NC | 4.60 | 114.82 | 109.98 |
| 37 | 16 | 309 | CLA | C2C-C1C-NC | 4.60 | 114.82 | 109.98 |
| 47 | 14 | 309 | KC1 | C3C-C4C-NC | 4.60 | 114.83 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 19 | 313 | A86 | C36-C31-C32 | -4.60 | 115.13 | 119.70 |
| 48 | 33 | 313 | A86 | C3-C2-C1 | -4.60 | 120.82 | 127.28 |
| 37 | 12 | 207 | CLA | C3D-C2D-C1D | -4.60 | 99.55 | 105.83 |
| 48 | 21 | 213 | A86 | C41-C32-C31 | -4.60 | 106.36 | 110.47 |
| 37 | 18 | 208 | CLA | O2D-CGD-CBD | 4.60 | 119.27 | 111.23 |
| 37 | 18 | 206 | CLA | C3B-C2B-C1B | -4.60 | 101.75 | 107.17 |
| 47 | 11 | 309 | KC1 | CHD-C4C-C3C | -4.60 | 116.75 | 125.23 |
| 37 | B | 502 | CLA | C2C-C1C-NC | 4.60 | 114.81 | 109.98 |
| 47 | 13 | 302 | KC1 | CHD-C4C-C3C | -4.60 | 116.75 | 125.23 |
| 47 | 31 | 309 | KC1 | CHD-C4C-C3C | -4.60 | 116.75 | 125.23 |
| 47 | 37 | 307 | KC1 | CHC-C1C-C2C | -4.60 | 117.77 | 125.03 |
| 37 | 14 | 308 | CLA | C2B-C1B-NB | 4.60 | 115.09 | 110.33 |
| 47 | 35 | 302 | KC1 | C3D-C4D-ND | 4.60 | 116.61 | 110.20 |
| 37 | 39 | 303 | CLA | C2B-C1B-NB | 4.60 | 115.09 | 110.33 |
| 37 | 34 | 302 | CLA | O2D-CGD-CBD | 4.60 | 119.27 | 111.23 |
| 37 | 18 | 208 | CLA | C2C-C1C-NC | 4.60 | 114.81 | 109.98 |
| 37 | 38 | 203 | CLA | C3D-C2D-C1D | -4.60 | 99.56 | 105.83 |
| 37 | 19 | 303 | CLA | C3D-C4D-ND | 4.60 | 117.46 | 109.99 |
| 47 | 19 | 308 | KC1 | C2A-C1A-NA | 4.60 | 116.71 | 109.34 |
| 47 | 39 | 308 | KC1 | C2A-C1A-NA | 4.60 | 116.71 | 109.34 |
| 47 | 34 | 304 | KC1 | C1A-NA-C4A | -4.60 | 104.58 | 106.68 |
| 47 | 20 | 302 | KC1 | O2D-CGD-CBD | 4.60 | 119.26 | 111.23 |
| 37 | 32 | 210 | CLA | C3D-C2D-C1D | -4.59 | 99.56 | 105.83 |
| 37 | B | 503 | CLA | C2B-C1B-NB | 4.59 | 115.09 | 110.33 |
| 37 | c | 502 | CLA | C2C-C1C-NC | 4.59 | 114.81 | 109.98 |
| 37 | 41 | 208 | CLA | C3D-C2D-C1D | -4.59 | 99.56 | 105.83 |
| 37 | 41 | 209 | CLA | C3B-C2B-C1B | -4.59 | 101.76 | 107.17 |
| 37 | Z | 101 | CLA | C3D-C2D-C1D | -4.59 | 99.57 | 105.83 |
| 48 | 35 | 319 | A86 | C3-C2-C1 | -4.59 | 120.84 | 127.28 |
| 37 | 31 | 310 | CLA | C3D-C2D-C1D | -4.59 | 99.57 | 105.83 |
| 37 | b | 514 | CLA | C4A-NA-C1A | -4.59 | 104.59 | 106.68 |
| 37 | c | 505 | CLA | C4A-NA-C1A | -4.59 | 104.59 | 106.68 |
| 37 | 37 | 301 | CLA | C3D-C2D-C1D | -4.59 | 99.57 | 105.83 |
| 37 | 39 | 305 | CLA | C2B-C1B-NB | 4.59 | 115.08 | 110.33 |
| 37 | 33 | 305 | CLA | C2C-C1C-NC | 4.59 | 114.80 | 109.98 |
| 37 | c | 511 | CLA | C2B-C1B-NB | 4.59 | 115.08 | 110.33 |
| 50 | 41 | 212 | DD6 | C24-C1-C2 | -4.59 | 111.80 | 119.01 |
| 37 | B | 509 | CLA | C2B-C1B-NB | 4.58 | 115.08 | 110.33 |
| 37 | 39 | 303 | CLA | C3D-C4D-ND | 4.58 | 117.44 | 109.99 |
| 37 | B | 513 | CLA | C3B-C4B-NB | 4.58 | 114.62 | 110.53 |
| 37 | 20 | 308 | CLA | C3D-C2D-C1D | -4.58 | 99.58 | 105.83 |
| 37 | 32 | 206 | CLA | C3D-C2D-C1D | -4.58 | 99.58 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 512 | CLA | C3D-C2D-C1D | -4.58 | 99.58 | 105.83 |
| 37 | d | 401 | CLA | C3D-C4D-ND | 4.58 | 117.43 | 109.99 |
| 37 | d | 403 | CLA | C3D-C4D-ND | 4.58 | 117.43 | 109.99 |
| 37 | 16 | 307 | CLA | C3B-C2B-C1B | -4.58 | 101.77 | 107.17 |
| 37 | C | 512 | CLA | C3D-C2D-C1D | -4.58 | 99.58 | 105.83 |
| 37 | 39 | 306 | CLA | C3D-C2D-C1D | -4.58 | 99.58 | 105.83 |
| 47 | 19 | 308 | KC1 | C1A-NA-C4A | -4.58 | 104.59 | 106.68 |
| 47 | 39 | 308 | KC1 | C1A-NA-C4A | -4.58 | 104.59 | 106.68 |
| 48 | 15 | 319 | A86 | C3-C2-C1 | -4.58 | 120.86 | 127.28 |
| 37 | W | 102 | CLA | C1D-CHD-C4C | -4.58 | 116.29 | 126.02 |
| 47 | 35 | 306 | KC1 | C3D-C4D-ND | 4.58 | 116.58 | 110.20 |
| 37 | 40 | 210 | CLA | C3D-C2D-C1D | -4.58 | 99.58 | 105.83 |
| 48 | 13 | 311 | A86 | C41-C32-C31 | -4.58 | 106.38 | 110.47 |
| 47 | 40 | 204 | KC1 | O2D-CGD-CBD | 4.58 | 119.23 | 111.23 |
| 37 | 36 | 309 | CLA | C2C-C1C-NC | 4.58 | 114.79 | 109.98 |
| 37 | 21 | 210 | CLA | C4A-NA-C1A | -4.58 | 104.59 | 106.68 |
| 50 | 21 | 212 | DD6 | C24-C1-C2 | -4.58 | 111.81 | 119.01 |
| 47 | 38 | 210 | KC1 | C3C-C4C-NC | 4.58 | 114.80 | 109.90 |
| 37 | 31 | 304 | CLA | C3D-C2D-C1D | -4.57 | 99.59 | 105.83 |
| 37 | 16 | 301 | CLA | C3D-C4D-ND | 4.57 | 117.42 | 109.99 |
| 37 | b | 506 | CLA | C3C-C4C-NC | 4.57 | 116.29 | 110.43 |
| 37 | b | 508 | CLA | C3D-C4D-ND | 4.57 | 117.42 | 109.99 |
| 37 | a | 404 | CLA | CHD-C1D-ND | -4.57 | 118.37 | 124.80 |
| 47 | 33 | 302 | KC1 | CHD-C4C-C3C | -4.57 | 116.80 | 125.23 |
| 47 | 38 | 207 | KC1 | CHC-C1C-C2C | -4.57 | 117.81 | 125.03 |
| 37 | 40 | 205 | CLA | C2C-C1C-NC | 4.57 | 114.78 | 109.98 |
| 47 | 38 | 205 | KC1 | CHC-C1C-C2C | -4.57 | 117.81 | 125.03 |
| 48 | 17 | 311 | A86 | O4-C38-C39 | 4.57 | 119.23 | 111.09 |
| 47 | 15 | 306 | KC1 | C3D-C4D-ND | 4.57 | 116.57 | 110.20 |
| 37 | 21 | 208 | CLA | C3D-C2D-C1D | -4.57 | 99.60 | 105.83 |
| 47 | 18 | 210 | KC1 | C3C-C4C-NC | 4.57 | 114.79 | 109.90 |
| 37 | 21 | 204 | CLA | C3D-C4D-ND | 4.57 | 117.41 | 109.99 |
| 37 | 41 | 204 | CLA | C3D-C4D-ND | 4.57 | 117.41 | 109.99 |
| 37 | 12 | 205 | CLA | C3D-C2D-C1D | -4.57 | 99.60 | 105.83 |
| 37 | 14 | 308 | CLA | C3B-C2B-C1B | -4.57 | 101.79 | 107.17 |
| 37 | 34 | 308 | CLA | C3B-C2B-C1B | -4.57 | 101.79 | 107.17 |
| 37 | 20 | 307 | CLA | C3D-C2D-C1D | -4.56 | 99.60 | 105.83 |
| 37 | D | 402 | CLA | C3D-C2D-C1D | -4.56 | 99.60 | 105.83 |
| 47 | 37 | 305 | KC1 | C4B-C3B-C2B | -4.56 | 102.86 | 106.81 |
| 48 | 41 | 214 | A86 | C4-C5-C6 | -4.56 | 120.88 | 127.28 |
| 47 | 20 | 302 | KC1 | CHD-C4C-C3C | -4.56 | 116.81 | 125.23 |
| 37 | 21 | 209 | CLA | C3D-C2D-C1D | -4.56 | 99.60 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 13 | 305 | CLA | C2C-C1C-NC | 4.56 | 114.77 | 109.98 |
| 47 | 38 | 210 | KC1 | C3D-C4D-ND | 4.56 | 116.56 | 110.20 |
| 47 | 40 | 204 | KC1 | CHD-C4C-C3C | -4.56 | 116.82 | 125.23 |
| 37 | c | 504 | CLA | C2C-C1C-NC | 4.56 | 114.77 | 109.98 |
| 37 | 19 | 306 | CLA | C3D-C2D-C1D | -4.56 | 99.61 | 105.83 |
| 37 | 31 | 301 | CLA | C1D-CHD-C4C | -4.56 | 116.33 | 126.02 |
| 47 | 36 | 304 | KC1 | CHC-C1C-C2C | -4.56 | 117.83 | 125.03 |
| 37 | 38 | 201 | CLA | C3D-C2D-C1D | -4.56 | 99.61 | 105.83 |
| 37 | c | 501 | CLA | C3D-C4D-ND | 4.56 | 117.39 | 109.99 |
| 37 | 19 | 305 | CLA | CHD-C1D-ND | -4.56 | 118.39 | 124.80 |
| 37 | 32 | 202 | CLA | C3D-C2D-C1D | -4.56 | 99.61 | 105.83 |
| 47 | 16 | 308 | KC1 | CHC-C1C-C2C | -4.56 | 117.84 | 125.03 |
| 37 | 35 | 303 | CLA | C3D-C2D-C1D | -4.56 | 99.61 | 105.83 |
| 37 | 11 | 303 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 37 | b | 503 | CLA | C2B-C1B-NB | 4.55 | 115.05 | 110.33 |
| 37 | c | 502 | CLA | C2B-C1B-NB | 4.55 | 115.05 | 110.33 |
| 48 | 20 | 311 | A86 | C40-C32-C31 | -4.55 | 106.40 | 110.47 |
| 37 | B | 501 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 48 | 35 | 316 | A86 | C41-C32-C31 | -4.55 | 106.40 | 110.47 |
| 37 | 31 | 306 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 47 | 36 | 305 | KC1 | CHC-C1C-C2C | -4.55 | 117.84 | 125.03 |
| 37 | 40 | 209 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 37 | d | 401 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 47 | 34 | 309 | KC1 | C3C-C4C-NC | 4.55 | 114.78 | 109.90 |
| 37 | 18 | 209 | CLA | C3B-C2B-C1B | -4.55 | 101.81 | 107.17 |
| 48 | 21 | 214 | A86 | C4-C5-C6 | -4.55 | 120.90 | 127.28 |
| 37 | C | 504 | CLA | C2C-C1C-NC | 4.55 | 114.76 | 109.98 |
| 37 | 12 | 207 | CLA | C3D-C4D-ND | 4.55 | 117.38 | 109.99 |
| 47 | 16 | 302 | KC1 | C4B-C3B-C2B | -4.55 | 102.87 | 106.81 |
| 37 | 15 | 310 | CLA | C4A-NA-C1A | -4.55 | 104.61 | 106.68 |
| 37 | D | 401 | CLA | CHD-C1D-ND | -4.55 | 118.41 | 124.80 |
| 37 | B | 524 | CLA | CBA-CAA-C2A | 4.54 | 127.31 | 113.79 |
| 47 | 37 | 307 | KC1 | C3D-C4D-ND | 4.54 | 116.54 | 110.20 |
| 47 | 35 | 302 | KC1 | CHD-C4C-C3C | -4.54 | 116.85 | 125.23 |
| 37 | D | 402 | CLA | C3D-C4D-ND | 4.54 | 117.37 | 109.99 |
| 47 | 13 | 304 | KC1 | C3D-C4D-ND | 4.54 | 116.53 | 110.20 |
| 48 | 41 | 213 | A86 | C41-C32-C31 | -4.54 | 106.41 | 110.47 |
| 47 | 32 | 212 | KC1 | CHC-C1C-C2C | -4.54 | 117.86 | 125.03 |
| 47 | 15 | 302 | KC1 | C3D-C4D-ND | 4.54 | 116.53 | 110.20 |
| 37 | 35 | 307 | CLA | C4A-NA-C1A | -4.54 | 104.61 | 106.68 |
| 37 | 32 | 208 | CLA | C3D-C4D-ND | 4.54 | 117.37 | 109.99 |
| 48 | 37 | 312 | A86 | C40-C32-C31 | -4.54 | 106.41 | 110.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 309 | KC1 | C1A-C2A-C3A | -4.54 | 103.11 | 107.28 |
| 47 | 16 | 304 | KC1 | CHC-C1C-C2C | -4.54 | 117.86 | 125.03 |
| 37 | C | 510 | CLA | C2D-C1D-ND | 4.54 | 114.62 | 110.13 |
| 37 | C | 501 | CLA | C3D-C4D-ND | 4.54 | 117.37 | 109.99 |
| 37 | 11 | 307 | CLA | C1C-C2C-C3C | -4.54 | 102.20 | 106.98 |
| 37 | 19 | 305 | CLA | C2B-C1B-NB | 4.54 | 115.03 | 110.33 |
| 48 | 40 | 201 | A86 | C24-C1-C2 | 4.54 | 126.15 | 119.01 |
| 37 | b | 504 | CLA | C2D-C1D-ND | 4.54 | 114.62 | 110.13 |
| 37 | 14 | 303 | CLA | C3D-C2D-C1D | -4.54 | 99.64 | 105.83 |
| 37 | 34 | 303 | CLA | C3D-C2D-C1D | -4.54 | 99.64 | 105.83 |
| 47 | 18 | 205 | KC1 | CHD-C4C-C3C | -4.54 | 116.86 | 125.23 |
| 37 | C | 502 | CLA | C2B-C1B-NB | 4.54 | 115.03 | 110.33 |
| 37 | 19 | 304 | CLA | CHD-C4C-C3C | -4.54 | 118.16 | 124.77 |
| 37 | 41 | 204 | CLA | C4A-NA-C1A | -4.54 | 104.61 | 106.68 |
| 37 | 12 | 209 | CLA | C4A-NA-C1A | -4.54 | 104.61 | 106.68 |
| 47 | 33 | 304 | KC1 | C3D-C4D-ND | 4.53 | 116.52 | 110.20 |
| 37 | c | 509 | CLA | C3D-C2D-C1D | -4.53 | 99.64 | 105.83 |
| 37 | B | 508 | CLA | C3D-C4D-ND | 4.53 | 117.36 | 109.99 |
| 37 | 17 | 302 | CLA | C3D-C4D-ND | 4.53 | 117.36 | 109.99 |
| 50 | 40 | 214 | DD6 | C15-C14-C13 | 4.53 | 135.58 | 125.99 |
| 37 | C | 505 | CLA | C4A-NA-C1A | -4.53 | 104.61 | 106.68 |
| 37 | D | 405 | CLA | C4A-NA-C1A | -4.53 | 104.61 | 106.68 |
| 37 | b | 510 | CLA | C4A-NA-C1A | -4.53 | 104.61 | 106.68 |
| 37 | 41 | 210 | CLA | C4A-NA-C1A | -4.53 | 104.61 | 106.68 |
| 47 | 17 | 308 | KC1 | C3D-C4D-ND | 4.53 | 116.52 | 110.20 |
| 37 | 19 | 304 | CLA | CHD-C1D-ND | -4.53 | 118.42 | 124.80 |
| 37 | 11 | 308 | CLA | C3D-C2D-C1D | -4.53 | 99.65 | 105.83 |
| 37 | 39 | 305 | CLA | CHD-C1D-ND | -4.53 | 118.42 | 124.80 |
| 37 | 39 | 304 | CLA | CHD-C1D-ND | -4.53 | 118.43 | 124.80 |
| 37 | 34 | 307 | CLA | C2C-C1C-NC | 4.53 | 114.74 | 109.98 |
| 37 | 18 | 202 | CLA | CHD-C1D-ND | -4.53 | 118.43 | 124.80 |
| 48 | 16 | 313 | A86 | C24-C1-C2 | 4.53 | 126.13 | 119.01 |
| 48 | 33 | 311 | A86 | C41-C32-C31 | -4.53 | 106.42 | 110.47 |
| 47 | 36 | 308 | KC1 | CHC-C1C-C2C | -4.53 | 117.88 | 125.03 |
| 37 | C | 502 | CLA | C3B-C2B-C1B | -4.53 | 101.83 | 107.17 |
| 37 | 12 | 204 | CLA | C1D-CHD-C4C | -4.53 | 116.40 | 126.02 |
| 47 | 15 | 302 | KC1 | CHD-C4C-C3C | -4.52 | 116.88 | 125.23 |
| 37 | c | 510 | CLA | C2D-C1D-ND | 4.52 | 114.60 | 110.13 |
| 37 | 17 | 307 | CLA | C2C-C1C-NC | 4.52 | 114.73 | 109.98 |
| 37 | b | 508 | CLA | C4A-NA-C1A | -4.52 | 104.61 | 106.68 |
| 37 | c | 502 | CLA | C3B-C2B-C1B | -4.52 | 101.84 | 107.17 |
| 37 | C | 508 | CLA | C3B-C4B-NB | 4.52 | 114.57 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 38 | 209 | CLA | C2B-C1B-NB | 4.52 | 115.02 | 110.33 |
| 47 | 12 | 211 | KC1 | CHC-C1C-C2C | -4.52 | 117.89 | 125.03 |
| 37 | 15 | 303 | CLA | C3D-C2D-C1D | -4.52 | 99.66 | 105.83 |
| 48 | 18 | 213 | A86 | C36-C31-C32 | -4.52 | 115.21 | 119.70 |
| 37 | b | 501 | CLA | C3D-C2D-C1D | -4.52 | 99.66 | 105.83 |
| 43 | d | 408 | LHG | O4-P-O5 | 4.52 | 133.47 | 112.44 |
| 37 | 37 | 303 | CLA | CHD-C1D-ND | -4.52 | 118.44 | 124.80 |
| 48 | 17 | 313 | A86 | C40-C32-C31 | -4.52 | 106.43 | 110.47 |
| 37 | C | 509 | CLA | C3D-C2D-C1D | -4.52 | 99.66 | 105.83 |
| 37 | 41 | 209 | CLA | C3D-C2D-C1D | -4.52 | 99.67 | 105.83 |
| 50 | 20 | 312 | DD6 | C15-C14-C13 | 4.52 | 135.55 | 125.99 |
| 47 | 15 | 302 | KC1 | C1A-NA-C4A | -4.52 | 104.62 | 106.68 |
| 37 | C | 509 | CLA | C2B-C1B-NB | 4.52 | 115.01 | 110.33 |
| 48 | 32 | 214 | A86 | C25-C26-C27 | -4.52 | 120.94 | 127.28 |
| 37 | A | 405 | CLA | C3D-C4D-ND | 4.52 | 117.33 | 109.99 |
| 37 | c | 508 | CLA | C3B-C4B-NB | 4.52 | 114.56 | 110.53 |
| 37 | 32 | 205 | CLA | C1D-CHD-C4C | -4.52 | 116.42 | 126.02 |
| 48 | 31 | 313 | A86 | C21-C20-C15 | -4.51 | 108.78 | 123.35 |
| 37 | B | 504 | CLA | C2D-C1D-ND | 4.51 | 114.59 | 110.13 |
| 47 | 15 | 302 | KC1 | CHC-C1C-C2C | -4.51 | 117.90 | 125.03 |
| 37 | a | 407 | CLA | C3D-C4D-ND | 4.51 | 117.32 | 109.99 |
| 37 | 18 | 201 | CLA | C3B-C2B-C1B | -4.51 | 101.85 | 107.17 |
| 37 | 19 | 302 | CLA | O2D-CGD-O1D | -4.51 | 115.06 | 123.85 |
| 37 | 35 | 305 | CLA | C3D-C2D-C1D | -4.51 | 99.67 | 105.83 |
| 37 | 15 | 305 | CLA | C3D-C2D-C1D | -4.51 | 99.67 | 105.83 |
| 37 | 11 | 305 | CLA | C3D-C2D-C1D | -4.51 | 99.67 | 105.83 |
| 43 | D | 410 | LHG | O4-P-O5 | 4.51 | 133.43 | 112.44 |
| 43 | d | 407 | LHG | O4-P-O5 | 4.51 | 133.42 | 112.44 |
| 47 | 15 | 309 | KC1 | C1A-C2A-C3A | -4.51 | 103.14 | 107.28 |
| 37 | 18 | 211 | CLA | C2C-C1C-NC | 4.51 | 114.72 | 109.98 |
| 37 | 36 | 301 | CLA | C3D-C4D-ND | 4.51 | 117.31 | 109.99 |
| 48 | 38 | 213 | A86 | C36-C31-C32 | -4.51 | 115.22 | 119.70 |
| 37 | B | 524 | CLA | C3B-C2B-C1B | -4.51 | 101.86 | 107.17 |
| 48 | 40 | 213 | A86 | C40-C32-C31 | -4.51 | 106.44 | 110.47 |
| 37 | b | 511 | CLA | C3B-C4B-NB | 4.51 | 114.55 | 110.53 |
| 37 | C | 511 | CLA | C2B-C1B-NB | 4.51 | 115.00 | 110.33 |
| 43 | b | 522 | LHG | O4-P-O5 | 4.50 | 133.40 | 112.44 |
| 37 | 21 | 204 | CLA | C4A-NA-C1A | -4.50 | 104.62 | 106.68 |
| 37 | 37 | 306 | CLA | C2C-C1C-NC | 4.50 | 114.71 | 109.98 |
| 48 | 17 | 310 | A86 | C41-C32-C31 | -4.50 | 106.44 | 110.47 |
| 47 | 13 | 309 | KC1 | C3D-C4D-ND | 4.50 | 116.48 | 110.20 |
| 37 | c | 510 | CLA | C2B-C1B-NB | 4.50 | 114.99 | 110.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 32 | 209 | KC1 | CMA-C3A-C2A | -4.50 | 117.53 | 128.43 |
| 43 | D | 409 | LHG | O4-P-O5 | 4.50 | 133.38 | 112.44 |
| 48 | 15 | 313 | A86 | C3-C2-C1 | -4.50 | 120.97 | 127.28 |
| 37 | 17 | 304 | CLA | CHD-C1D-ND | -4.50 | 118.47 | 124.80 |
| 37 | C | 506 | CLA | C4B-C3B-C2B | -4.50 | 101.71 | 107.30 |
| 48 | 35 | 311 | A86 | C3-C2-C1 | -4.50 | 120.97 | 127.28 |
| 37 | 14 | 305 | CLA | C3D-C2D-C1D | -4.50 | 99.69 | 105.83 |
| 37 | 34 | 305 | CLA | C3D-C2D-C1D | -4.50 | 99.69 | 105.83 |
| 37 | b | 523 | CLA | C3B-C2B-C1B | -4.50 | 101.87 | 107.17 |
| 43 | B | 523 | LHG | O4-P-O5 | 4.50 | 133.37 | 112.44 |
| 47 | 18 | 205 | KC1 | CHC-C1C-C2C | -4.50 | 117.93 | 125.03 |
| 47 | 12 | 208 | KC1 | CMA-C3A-C2A | -4.50 | 117.55 | 128.43 |
| 47 | 31 | 309 | KC1 | C3C-C4C-NC | 4.50 | 114.72 | 109.90 |
| 47 | 36 | 302 | KC1 | C3C-C4C-NC | 4.50 | 114.72 | 109.90 |
| 37 | 37 | 301 | CLA | CHD-C1D-ND | -4.50 | 118.47 | 124.80 |
| 37 | 11 | 301 | CLA | O2D-CGD-CBD | 4.50 | 119.09 | 111.23 |
| 47 | 33 | 306 | KC1 | CHC-C1C-C2C | -4.50 | 117.93 | 125.03 |
| 37 | B | 511 | CLA | C3B-C4B-NB | 4.50 | 114.54 | 110.53 |
| 47 | 12 | 208 | KC1 | CHC-C1C-C2C | -4.50 | 117.93 | 125.03 |
| 47 | 20 | 302 | KC1 | C3D-C4D-ND | 4.50 | 116.47 | 110.20 |
| 37 | C | 501 | CLA | C3D-C2D-C1D | -4.49 | 99.70 | 105.83 |
| 37 | c | 501 | CLA | C3D-C2D-C1D | -4.49 | 99.70 | 105.83 |
| 47 | 38 | 205 | KC1 | CHD-C4C-C3C | -4.49 | 116.94 | 125.23 |
| 37 | b | 523 | CLA | CBA-CAA-C2A | 4.49 | 127.16 | 113.79 |
| 48 | 31 | 315 | A86 | C4-C5-C6 | -4.49 | 120.98 | 127.28 |
| 37 | 39 | 304 | CLA | CHD-C4C-C3C | -4.49 | 118.22 | 124.77 |
| 47 | 36 | 302 | KC1 | CHD-C4C-C3C | -4.49 | 116.95 | 125.23 |
| 47 | 32 | 212 | KC1 | C3D-C4D-ND | 4.49 | 116.46 | 110.20 |
| 37 | 18 | 203 | CLA | C3D-C2D-C1D | -4.49 | 99.70 | 105.83 |
| 37 | 12 | 203 | CLA | O2D-CGD-CBD | 4.49 | 119.08 | 111.23 |
| 37 | c | 506 | CLA | C4B-C3B-C2B | -4.49 | 101.72 | 107.30 |
| 37 | c | 510 | CLA | C3B-C4B-NB | 4.49 | 114.53 | 110.53 |
| 47 | 33 | 309 | KC1 | C3D-C4D-ND | 4.49 | 116.45 | 110.20 |
| 37 | 33 | 308 | CLA | C2B-C1B-NB | 4.48 | 114.98 | 110.33 |
| 37 | 40 | 209 | CLA | C4A-NA-C1A | -4.48 | 104.63 | 106.68 |
| 47 | 32 | 209 | KC1 | CHC-C1C-C2C | -4.48 | 117.95 | 125.03 |
| 47 | 37 | 302 | KC1 | CHD-C4C-C3C | -4.48 | 116.96 | 125.23 |
| 47 | 11 | 304 | KC1 | C3C-C4C-NC | 4.48 | 114.70 | 109.90 |
| 48 | 37 | 319 | A86 | C3-C2-C1 | -4.48 | 120.99 | 127.28 |
| 37 | d | 401 | CLA | C2C-C1C-NC | 4.48 | 114.69 | 109.98 |
| 37 | D | 401 | CLA | C3D-C4D-ND | 4.48 | 117.28 | 109.99 |
| 37 | B | 512 | CLA | C3C-C4C-NC | 4.48 | 116.17 | 110.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 308 | CLA | C1C-C2C-C3C | -4.48 | 102.27 | 106.98 |
| 37 | 16 | 309 | CLA | C3D-C4D-ND | 4.48 | 117.27 | 109.99 |
| 47 | 37 | 304 | KC1 | C2A-C1A-NA | 4.48 | 116.52 | 109.34 |
| 37 | D | 402 | CLA | CHD-C1D-ND | -4.48 | 118.50 | 124.80 |
| 37 | d | 401 | CLA | CHD-C1D-ND | -4.48 | 118.50 | 124.80 |
| 37 | C | 510 | CLA | C4A-NA-C1A | -4.48 | 104.64 | 106.68 |
| 37 | 18 | 202 | CLA | C3D-C4D-ND | 4.48 | 117.27 | 109.99 |
| 37 | 19 | 305 | CLA | C3D-C4D-ND | 4.48 | 117.27 | 109.99 |
| 48 | 11 | 313 | A86 | C21-C20-C15 | -4.48 | 108.89 | 123.35 |
| 37 | a | 404 | CLA | C3D-C4D-ND | 4.48 | 117.27 | 109.99 |
| 37 | 33 | 310 | CLA | C3D-C2D-C1D | -4.48 | 99.72 | 105.83 |
| 47 | 31 | 305 | KC1 | C3C-C4C-NC | 4.48 | 114.70 | 109.90 |
| 37 | 32 | 213 | CLA | C2C-C1C-NC | 4.47 | 114.68 | 109.98 |
| 47 | 37 | 302 | KC1 | C2C-C1C-NC | 4.47 | 115.99 | 110.45 |
| 37 | c | 503 | CLA | CHD-C1D-ND | -4.47 | 118.51 | 124.80 |
| 37 | a | 403 | CLA | CAA-C2A-C3A | -4.47 | 100.91 | 113.00 |
| 37 | 15 | 308 | CLA | C2B-C1B-NB | 4.47 | 114.97 | 110.33 |
| 37 | 12 | 212 | CLA | C2C-C1C-NC | 4.47 | 114.68 | 109.98 |
| 47 | 41 | 207 | KC1 | C2D-C1D-ND | 4.47 | 114.96 | 110.33 |
| 37 | 33 | 301 | CLA | C2C-C1C-NC | 4.47 | 114.68 | 109.98 |
| 47 | 21 | 207 | KC1 | C2D-C1D-ND | 4.47 | 114.96 | 110.33 |
| 47 | 20 | 305 | KC1 | CHD-C4C-C3C | -4.47 | 116.98 | 125.23 |
| 37 | c | 509 | CLA | C2B-C1B-NB | 4.47 | 114.96 | 110.33 |
| 37 | 39 | 303 | CLA | C3D-C2D-C1D | -4.47 | 99.73 | 105.83 |
| 37 | 13 | 308 | CLA | C2B-C1B-NB | 4.47 | 114.96 | 110.33 |
| 37 | C | 503 | CLA | CHD-C1D-ND | -4.47 | 118.52 | 124.80 |
| 47 | 17 | 303 | KC1 | CHD-C4C-C3C | -4.47 | 116.99 | 125.23 |
| 37 | b | 523 | CLA | C3C-C4C-NC | 4.47 | 116.15 | 110.43 |
| 47 | 18 | 210 | KC1 | C3D-C4D-ND | 4.47 | 116.43 | 110.20 |
| 37 | C | 510 | CLA | C3B-C4B-NB | 4.47 | 114.52 | 110.53 |
| 37 | 38 | 206 | CLA | C3D-C4D-ND | 4.47 | 117.25 | 109.99 |
| 47 | 40 | 204 | KC1 | C3D-C4D-ND | 4.47 | 116.43 | 110.20 |
| 37 | 41 | 204 | CLA | C3D-C2D-C1D | -4.47 | 99.74 | 105.83 |
| 47 | 13 | 306 | KC1 | CHC-C1C-C2C | -4.46 | 117.98 | 125.03 |
| 37 | 38 | 209 | CLA | C3B-C2B-C1B | -4.46 | 101.91 | 107.17 |
| 37 | 33 | 308 | CLA | C3D-C2D-C1D | -4.46 | 99.74 | 105.83 |
| 47 | 36 | 302 | KC1 | C4B-C3B-C2B | -4.46 | 102.94 | 106.81 |
| 37 | 36 | 303 | CLA | C3D-C4D-ND | 4.46 | 117.24 | 109.99 |
| 37 | 36 | 309 | CLA | C3D-C4D-ND | 4.46 | 117.24 | 109.99 |
| 37 | 15 | 301 | CLA | CHD-C1D-ND | -4.46 | 118.52 | 124.80 |
| 37 | 35 | 301 | CLA | CHD-C1D-ND | -4.46 | 118.52 | 124.80 |
| 47 | 18 | 207 | KC1 | C4B-C3B-C2B | -4.46 | 102.95 | 106.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 38 | 206 | CLA | C3D-C2D-C1D | -4.46 | 99.74 | 105.83 |
| 37 | 15 | 310 | CLA | C3D-C4D-ND | 4.46 | 117.24 | 109.99 |
| 37 | 16 | 303 | CLA | C3D-C4D-ND | 4.46 | 117.24 | 109.99 |
| 47 | 12 | 211 | KC1 | C3D-C4D-ND | 4.46 | 116.42 | 110.20 |
| 37 | A | 403 | CLA | CAA-C2A-C3A | -4.46 | 100.95 | 113.00 |
| 48 | 35 | 313 | A86 | C3-C2-C1 | -4.46 | 121.03 | 127.28 |
| 37 | B | 524 | CLA | C3C-C4C-NC | 4.46 | 116.14 | 110.43 |
| 48 | 11 | 315 | A86 | C4-C5-C6 | -4.46 | 121.03 | 127.28 |
| 37 | b | 514 | CLA | C2B-C1B-NB | 4.46 | 114.95 | 110.33 |
| 37 | 14 | 307 | CLA | C2C-C1C-NC | 4.46 | 114.66 | 109.98 |
| 37 | 14 | 308 | CLA | C3D-C2D-C1D | -4.46 | 99.75 | 105.83 |
| 37 | C | 510 | CLA | C2B-C1B-NB | 4.45 | 114.94 | 110.33 |
| 37 | d | 401 | CLA | C4A-NA-C1A | -4.45 | 104.65 | 106.68 |
| 37 | D | 402 | CLA | C2C-C1C-NC | 4.45 | 114.66 | 109.98 |
| 37 | 31 | 302 | CLA | O2D-CGD-CBD | 4.45 | 119.01 | 111.23 |
| 47 | 13 | 302 | KC1 | C3D-C4D-ND | 4.45 | 116.41 | 110.20 |
| 37 | 38 | 208 | CLA | C2C-C1C-NC | 4.45 | 114.66 | 109.98 |
| 37 | 32 | 210 | CLA | C4A-NA-C1A | -4.45 | 104.65 | 106.68 |
| 47 | 21 | 207 | KC1 | C1A-NA-C4A | -4.45 | 104.65 | 106.68 |
| 47 | 33 | 302 | KC1 | C3D-C4D-ND | 4.45 | 116.41 | 110.20 |
| 47 | 16 | 302 | KC1 | C3C-C4C-NC | 4.45 | 114.67 | 109.90 |
| 37 | D | 406 | CLA | C3D-C4D-ND | 4.45 | 117.22 | 109.99 |
| 37 | B | 508 | CLA | C4A-NA-C1A | -4.45 | 104.65 | 106.68 |
| 37 | 20 | 307 | CLA | C4A-NA-C1A | -4.45 | 104.65 | 106.68 |
| 47 | 18 | 205 | KC1 | C3C-C4C-NC | 4.45 | 114.67 | 109.90 |
| 37 | 32 | 204 | CLA | O2D-CGD-CBD | 4.45 | 119.01 | 111.23 |
| 37 | 13 | 308 | CLA | C3D-C2D-C1D | -4.45 | 99.76 | 105.83 |
| 37 | 21 | 202 | CLA | C3D-C2D-C1D | -4.45 | 99.76 | 105.83 |
| 37 | 39 | 302 | CLA | O2D-CGD-O1D | -4.45 | 115.19 | 123.85 |
| 37 | 39 | 304 | CLA | C3D-C4D-ND | 4.45 | 117.22 | 109.99 |
| 37 | 15 | 308 | CLA | C3B-C2B-C1B | -4.45 | 101.93 | 107.17 |
| 37 | 12 | 207 | CLA | C2C-C1C-NC | 4.45 | 114.65 | 109.98 |
| 37 | 32 | 208 | CLA | C2C-C1C-NC | 4.45 | 114.65 | 109.98 |
| 37 | 36 | 303 | CLA | C3D-C2D-C1D | -4.45 | 99.76 | 105.83 |
| 37 | 19 | 303 | CLA | C3D-C2D-C1D | -4.45 | 99.76 | 105.83 |
| 47 | 37 | 304 | KC1 | CHC-C1C-C2C | -4.45 | 118.01 | 125.03 |
| 47 | 11 | 309 | KC1 | C3C-C4C-NC | 4.44 | 114.66 | 109.90 |
| 37 | 32 | 211 | CLA | C4A-NA-C1A | -4.44 | 104.65 | 106.68 |
| 47 | 14 | 304 | KC1 | C1A-NA-C4A | -4.44 | 104.65 | 106.68 |
| 37 | 19 | 306 | CLA | C3D-C4D-ND | 4.44 | 117.21 | 109.99 |
| 37 | 37 | 308 | CLA | C3D-C2D-C1D | -4.44 | 99.77 | 105.83 |
| 47 | 40 | 207 | KC1 | C2C-C1C-NC | 4.44 | 115.95 | 110.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 16 | 302 | KC1 | CHD-C4C-C3C | -4.44 | 117.04 | 125.23 |
| 48 | 37 | 309 | A86 | C41-C32-C31 | -4.44 | 106.50 | 110.47 |
| 47 | 18 | 207 | KC1 | C2C-C1C-NC | 4.44 | 115.95 | 110.45 |
| 37 | 20 | 307 | CLA | O2D-CGD-CBD | 4.44 | 118.99 | 111.23 |
| 43 | 37 | 315 | LHG | O4-P-O5 | 4.44 | 133.10 | 112.44 |
| 37 | 39 | 305 | CLA | C3D-C4D-ND | 4.44 | 117.20 | 109.99 |
| 50 | 41 | 212 | DD6 | C-C1-C24 | -4.44 | 111.31 | 118.09 |
| 47 | 20 | 305 | KC1 | C2C-C1C-NC | 4.44 | 115.94 | 110.45 |
| 47 | 40 | 207 | KC1 | CHD-C4C-C3C | -4.44 | 117.05 | 125.23 |
| 37 | 40 | 209 | CLA | O2D-CGD-CBD | 4.44 | 118.99 | 111.23 |
| 37 | 39 | 306 | CLA | C3D-C4D-ND | 4.44 | 117.20 | 109.99 |
| 37 | 16 | 303 | CLA | C4A-NA-C1A | -4.44 | 104.66 | 106.68 |
| 37 | D | 402 | CLA | C4A-NA-C1A | -4.43 | 104.66 | 106.68 |
| 37 | 12 | 212 | CLA | C4A-NA-C1A | -4.43 | 104.66 | 106.68 |
| 37 | 32 | 213 | CLA | C4A-NA-C1A | -4.43 | 104.66 | 106.68 |
| 37 | B | 514 | CLA | C2B-C1B-NB | 4.43 | 114.92 | 110.33 |
| 37 | 11 | 303 | CLA | CAA-C2A-C3A | -4.43 | 101.02 | 113.00 |
| 37 | 31 | 304 | CLA | CAA-C2A-C3A | -4.43 | 101.02 | 113.00 |
| 37 | 15 | 303 | CLA | C3D-C4D-ND | 4.43 | 117.19 | 109.99 |
| 37 | 35 | 310 | CLA | C3D-C4D-ND | 4.43 | 117.19 | 109.99 |
| 37 | 34 | 308 | CLA | C3D-C2D-C1D | -4.43 | 99.78 | 105.83 |
| 37 | 36 | 303 | CLA | C4A-NA-C1A | -4.43 | 104.66 | 106.68 |
| 37 | 38 | 201 | CLA | CHD-C1D-ND | -4.43 | 118.56 | 124.80 |
| 47 | 20 | 304 | KC1 | C4B-C3B-C2B | -4.43 | 102.97 | 106.81 |
| 37 | b | 512 | CLA | C3C-C4C-NC | 4.43 | 116.11 | 110.43 |
| 47 | 17 | 303 | KC1 | C2C-C1C-NC | 4.43 | 115.94 | 110.45 |
| 47 | 17 | 308 | KC1 | C3C-C4C-NC | 4.43 | 114.65 | 109.90 |
| 37 | 16 | 303 | CLA | C3D-C2D-C1D | -4.43 | 99.79 | 105.83 |
| 37 | B | 502 | CLA | C4A-NA-C1A | -4.43 | 104.66 | 106.68 |
| 37 | 35 | 308 | CLA | C3D-C2D-C1D | -4.43 | 99.79 | 105.83 |
| 48 | 15 | 311 | A86 | C3-C2-C1 | -4.43 | 121.07 | 127.28 |
| 47 | 37 | 307 | KC1 | C3C-C4C-NC | 4.43 | 114.64 | 109.90 |
| 37 | 18 | 211 | CLA | C3D-C2D-C1D | -4.43 | 99.79 | 105.83 |
| 37 | 21 | 204 | CLA | C3D-C2D-C1D | -4.43 | 99.79 | 105.83 |
| 47 | 37 | 304 | KC1 | C2D-C1D-ND | 4.43 | 114.92 | 110.33 |
| 48 | 16 | 313 | A86 | C28-C27-C26 | -4.43 | 115.64 | 122.82 |
| 37 | 19 | 304 | CLA | C3D-C4D-ND | 4.43 | 117.18 | 109.99 |
| 47 | 40 | 206 | KC1 | C2C-C1C-NC | 4.42 | 115.93 | 110.45 |
| 37 | 41 | 202 | CLA | C3D-C2D-C1D | -4.42 | 99.79 | 105.83 |
| 37 | 33 | 303 | CLA | C3D-C2D-C1D | -4.42 | 99.80 | 105.83 |
| 47 | 13 | 306 | KC1 | C3D-C4D-ND | 4.42 | 116.36 | 110.20 |
| 48 | 16 | 311 | A86 | O4-C38-C39 | 4.42 | 118.97 | 111.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 502 | CLA | C4A-NA-C1A | -4.42 | 104.66 | 106.68 |
| 43 | 37 | 321 | LHG | O4-P-O5 | 4.42 | 133.00 | 112.44 |
| 37 | 35 | 303 | CLA | C3D-C4D-ND | 4.42 | 117.17 | 109.99 |
| 43 | 17 | 316 | LHG | O4-P-O5 | 4.42 | 133.00 | 112.44 |
| 47 | 20 | 304 | KC1 | C2C-C1C-NC | 4.42 | 115.92 | 110.45 |
| 48 | 18 | 213 | A86 | C25-C26-C27 | -4.42 | 121.08 | 127.28 |
| 37 | 38 | 201 | CLA | C3D-C4D-ND | 4.42 | 117.17 | 109.99 |
| 48 | 20 | 311 | A86 | C3-C2-C1 | -4.42 | 121.08 | 127.28 |
| 47 | 40 | 206 | KC1 | C4B-C3B-C2B | -4.42 | 102.98 | 106.81 |
| 47 | 33 | 306 | KC1 | C3D-C4D-ND | 4.41 | 116.36 | 110.20 |
| 37 | 12 | 205 | CLA | C2C-C1C-NC | 4.41 | 114.62 | 109.98 |
| 48 | 40 | 213 | A86 | C3-C2-C1 | -4.41 | 121.09 | 127.28 |
| 37 | b | 512 | CLA | C2C-C1C-NC | 4.41 | 114.62 | 109.98 |
| 37 | 13 | 301 | CLA | C2C-C1C-NC | 4.41 | 114.61 | 109.98 |
| 38 | D | 403 | PHO | C2B-C1B-NB | -4.41 | 106.24 | 109.43 |
| 43 | 21 | 217 | LHG | O4-P-O5 | 4.41 | 132.96 | 112.44 |
| 47 | 16 | 302 | KC1 | O2D-CGD-CBD | 4.41 | 118.94 | 111.23 |
| 37 | Z | 102 | CLA | C3D-C2D-C1D | -4.41 | 99.81 | 105.83 |
| 50 | 21 | 212 | DD6 | C-C1-C24 | -4.41 | 111.35 | 118.09 |
| 47 | 35 | 304 | KC1 | C2A-C1A-NA | 4.41 | 116.41 | 109.34 |
| 37 | 35 | 301 | CLA | O2D-CGD-CBD | 4.41 | 118.94 | 111.23 |
| 37 | z | 102 | CLA | C3D-C2D-C1D | -4.41 | 99.82 | 105.83 |
| 37 | 15 | 301 | CLA | O2D-CGD-CBD | 4.41 | 118.94 | 111.23 |
| 37 | B | 512 | CLA | C2C-C1C-NC | 4.41 | 114.61 | 109.98 |
| 47 | 35 | 309 | KC1 | CHC-C1C-C2C | -4.41 | 118.07 | 125.03 |
| 37 | 34 | 310 | CLA | C3D-C4D-ND | 4.41 | 117.15 | 109.99 |
| 37 | 35 | 310 | CLA | C4A-NA-C1A | -4.41 | 104.67 | 106.68 |
| 47 | 15 | 304 | KC1 | C1A-NA-C4A | -4.41 | 104.67 | 106.68 |
| 43 | 41 | 201 | LHG | O4-P-O5 | 4.41 | 132.94 | 112.44 |
| 37 | 14 | 310 | CLA | C1C-C2C-C3C | -4.40 | 102.35 | 106.98 |
| 37 | 11 | 308 | CLA | C3B-C2B-C1B | -4.40 | 101.98 | 107.17 |
| 43 | a | 412 | LHG | O4-P-O5 | 4.40 | 132.93 | 112.44 |
| 37 | 18 | 211 | CLA | C3D-C4D-ND | 4.40 | 117.14 | 109.99 |
| 37 | 37 | 301 | CLA | C3D-C4D-ND | 4.40 | 117.14 | 109.99 |
| 47 | 36 | 302 | KC1 | O2D-CGD-CBD | 4.40 | 118.93 | 111.23 |
| 37 | C | 510 | CLA | C1C-C2C-C3C | -4.40 | 102.35 | 106.98 |
| 47 | 13 | 309 | KC1 | CHD-C4C-C3C | -4.40 | 117.11 | 125.23 |
| 43 | D | 411 | LHG | O4-P-O5 | 4.40 | 132.93 | 112.44 |
| 37 | 19 | 303 | CLA | C2C-C1C-NC | 4.40 | 114.61 | 109.98 |
| 48 | 36 | 310 | A86 | C12-C11-C13 | 4.40 | 123.14 | 116.00 |
| 37 | 17 | 307 | CLA | C3D-C2D-C1D | -4.40 | 99.82 | 105.83 |
| 38 | a | 405 | PHO | C2B-C1B-NB | -4.40 | 106.25 | 109.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 15 | 302 | KC1 | C3C-C4C-NC | 4.40 | 114.61 | 109.90 |
| 37 | C | 505 | CLA | C3B-C2B-C1B | -4.40 | 101.98 | 107.17 |
| 47 | 12 | 206 | KC1 | C3D-C4D-ND | 4.40 | 116.34 | 110.20 |
| 37 | 18 | 201 | CLA | C4A-NA-C1A | -4.40 | 104.67 | 106.68 |
| 37 | d | 404 | CLA | C3D-C4D-ND | 4.40 | 117.14 | 109.99 |
| 48 | 36 | 311 | A86 | O4-C38-C39 | 4.40 | 118.93 | 111.09 |
| 48 | 16 | 313 | A86 | C10-C9-C8 | -4.40 | 110.46 | 123.20 |
| 37 | 19 | 302 | CLA | C3B-C2B-C1B | -4.40 | 101.98 | 107.17 |
| 37 | c | 504 | CLA | CHD-C1D-ND | -4.40 | 118.61 | 124.80 |
| 47 | 14 | 309 | KC1 | CHC-C1C-C2C | -4.40 | 118.09 | 125.03 |
| 50 | 20 | 310 | DD6 | C21-C20-C19 | -4.40 | 109.30 | 114.24 |
| 48 | 11 | 315 | A86 | C12-C11-C13 | 4.40 | 123.13 | 116.00 |
| 37 | 17 | 309 | CLA | C3D-C2D-C1D | -4.40 | 99.83 | 105.83 |
| 47 | 11 | 302 | KC1 | C3C-C4C-NC | 4.39 | 114.61 | 109.90 |
| 37 | B | 502 | CLA | CHD-C1D-ND | -4.39 | 118.62 | 124.80 |
| 37 | c | 510 | CLA | C4A-NA-C1A | -4.39 | 104.67 | 106.68 |
| 37 | 12 | 207 | CLA | C4A-NA-C1A | -4.39 | 104.67 | 106.68 |
| 48 | 31 | 315 | A86 | C12-C11-C13 | 4.39 | 123.12 | 116.00 |
| 37 | 18 | 201 | CLA | C3D-C4D-ND | 4.39 | 117.13 | 109.99 |
| 47 | 33 | 309 | KC1 | CHD-C4C-C3C | -4.39 | 117.13 | 125.23 |
| 37 | 18 | 206 | CLA | C3D-C4D-ND | 4.39 | 117.12 | 109.99 |
| 37 | 35 | 308 | CLA | C3B-C4B-NB | 4.39 | 114.45 | 110.53 |
| 37 | 34 | 310 | CLA | C1C-C2C-C3C | -4.39 | 102.36 | 106.98 |
| 47 | 38 | 207 | KC1 | C2C-C1C-NC | 4.39 | 115.88 | 110.45 |
| 37 | 37 | 306 | CLA | C3D-C2D-C1D | -4.39 | 99.84 | 105.83 |
| 37 | 13 | 310 | CLA | C3D-C4D-ND | 4.39 | 117.12 | 109.99 |
| 47 | 32 | 212 | KC1 | C3C-C4C-NC | 4.39 | 114.60 | 109.90 |
| 37 | 32 | 208 | CLA | C4A-NA-C1A | -4.39 | 104.68 | 106.68 |
| 37 | 39 | 310 | CLA | C3D-C2D-C1D | -4.39 | 99.85 | 105.83 |
| 37 | 38 | 204 | CLA | CAA-C2A-C3A | -4.39 | 101.15 | 113.00 |
| 48 | 40 | 201 | A86 | C10-C9-C8 | -4.39 | 110.49 | 123.20 |
| 37 | 32 | 211 | CLA | C3D-C2D-C1D | -4.38 | 99.85 | 105.83 |
| 37 | B | 506 | CLA | C3B-C2B-C1B | -4.38 | 102.00 | 107.17 |
| 37 | b | 508 | CLA | C3B-C2B-C1B | -4.38 | 102.00 | 107.17 |
| 37 | D | 405 | CLA | CHD-C1D-ND | -4.38 | 118.64 | 124.80 |
| 43 | 21 | 201 | LHG | O4-P-O5 | 4.38 | 132.82 | 112.44 |
| 37 | 12 | 204 | CLA | C2B-C1B-NB | 4.38 | 114.87 | 110.33 |
| 37 | 13 | 303 | CLA | C3D-C4D-ND | 4.38 | 117.10 | 109.99 |
| 37 | 35 | 308 | CLA | CHD-C1D-ND | -4.38 | 118.64 | 124.80 |
| 37 | 19 | 306 | CLA | C4A-NA-C1A | -4.38 | 104.68 | 106.68 |
| 37 | B | 508 | CLA | C3D-C2D-C1D | -4.38 | 99.86 | 105.83 |
| 37 | 38 | 204 | CLA | CBA-CAA-C2A | 4.38 | 126.81 | 113.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 32 | 207 | KC1 | C3D-C4D-ND | 4.38 | 116.30 | 110.20 |
| 37 | 39 | 304 | CLA | CAC-C3C-C4C | 4.38 | 130.48 | 124.79 |
| 37 | 32 | 205 | CLA | C2B-C1B-NB | 4.38 | 114.86 | 110.33 |
| 37 | D | 405 | CLA | C2C-C1C-NC | 4.38 | 114.58 | 109.98 |
| 37 | 39 | 302 | CLA | C3B-C2B-C1B | -4.38 | 102.01 | 107.17 |
| 37 | 21 | 202 | CLA | CHD-C1D-ND | -4.38 | 118.64 | 124.80 |
| 37 | 18 | 211 | CLA | C4A-NA-C1A | -4.38 | 104.68 | 106.68 |
| 47 | 41 | 207 | KC1 | C1A-NA-C4A | -4.38 | 104.68 | 106.68 |
| 48 | 40 | 201 | A86 | C28-C27-C26 | -4.38 | 115.73 | 122.82 |
| 37 | 32 | 210 | CLA | C2C-C1C-NC | 4.37 | 114.58 | 109.98 |
| 37 | c | 505 | CLA | C3B-C2B-C1B | -4.37 | 102.01 | 107.17 |
| 47 | 33 | 304 | KC1 | CHC-C1C-C2C | -4.37 | 118.12 | 125.03 |
| 37 | 14 | 310 | CLA | C3D-C4D-ND | 4.37 | 117.10 | 109.99 |
| 37 | 12 | 210 | CLA | C3D-C2D-C1D | -4.37 | 99.86 | 105.83 |
| 48 | 16 | 310 | A86 | C12-C11-C13 | 4.37 | 123.09 | 116.00 |
| 37 | b | 516 | CLA | C1D-CHD-C4C | -4.37 | 116.73 | 126.02 |
| 37 | b | 506 | CLA | C3B-C2B-C1B | -4.37 | 102.02 | 107.17 |
| 37 | d | 403 | CLA | CHD-C1D-ND | -4.37 | 118.65 | 124.80 |
| 47 | 36 | 302 | KC1 | C2C-C1C-NC | 4.37 | 115.86 | 110.45 |
| 37 | c | 508 | CLA | C3B-C2B-C1B | -4.37 | 102.02 | 107.17 |
| 37 | c | 505 | CLA | C1D-CHD-C4C | -4.37 | 116.73 | 126.02 |
| 37 | 41 | 208 | CLA | C3D-C4D-ND | 4.37 | 117.09 | 109.99 |
| 37 | 19 | 310 | CLA | C3D-C2D-C1D | -4.37 | 99.87 | 105.83 |
| 37 | 19 | 304 | CLA | CAC-C3C-C4C | 4.37 | 130.48 | 124.79 |
| 37 | 39 | 303 | CLA | C2C-C1C-NC | 4.37 | 114.57 | 109.98 |
| 47 | 37 | 304 | KC1 | C1A-NA-C4A | -4.37 | 104.69 | 106.68 |
| 37 | C | 504 | CLA | CHD-C1D-ND | -4.37 | 118.66 | 124.80 |
| 47 | 36 | 304 | KC1 | C3C-C4C-NC | 4.37 | 114.58 | 109.90 |
| 37 | C | 507 | CLA | C1D-CHD-C4C | -4.37 | 116.74 | 126.02 |
| 37 | 38 | 211 | CLA | C4A-NA-C1A | -4.37 | 104.69 | 106.68 |
| 37 | 38 | 211 | CLA | C3D-C4D-ND | 4.37 | 117.08 | 109.99 |
| 37 | 40 | 205 | CLA | C2B-C1B-NB | 4.36 | 114.85 | 110.33 |
| 37 | c | 510 | CLA | C1C-C2C-C3C | -4.36 | 102.39 | 106.98 |
| 37 | 34 | 301 | CLA | O2D-CGD-CBD | 4.36 | 118.86 | 111.23 |
| 37 | 40 | 208 | CLA | C3D-C2D-C1D | -4.36 | 99.88 | 105.83 |
| 37 | 32 | 205 | CLA | C3C-C4C-NC | 4.36 | 116.02 | 110.43 |
| 37 | b | 509 | CLA | C1C-C2C-C3C | -4.36 | 102.39 | 106.98 |
| 37 | 20 | 306 | CLA | C3D-C2D-C1D | -4.36 | 99.88 | 105.83 |
| 37 | 40 | 205 | CLA | C1D-CHD-C4C | -4.36 | 116.75 | 126.02 |
| 37 | d | 404 | CLA | C4A-NA-C1A | -4.36 | 104.69 | 106.68 |
| 37 | b | 508 | CLA | C3D-C2D-C1D | -4.36 | 99.88 | 105.83 |
| 37 | 20 | 303 | CLA | C1D-CHD-C4C | -4.36 | 116.76 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | d | 403 | CLA | C2C-C1C-NC | 4.36 | 114.56 | 109.98 |
| 37 | c | 513 | CLA | C4A-NA-C1A | -4.36 | 104.69 | 106.68 |
| 37 | 13 | 303 | CLA | C4A-NA-C1A | -4.36 | 104.69 | 106.68 |
| 47 | 15 | 309 | KC1 | CHC-C1C-C2C | -4.36 | 118.15 | 125.03 |
| 48 | 14 | 312 | A86 | C3-C2-C1 | -4.36 | 121.17 | 127.28 |
| 47 | 16 | 304 | KC1 | C3C-C4C-NC | 4.36 | 114.57 | 109.90 |
| 37 | 32 | 202 | CLA | C3B-C2B-C1B | -4.36 | 102.03 | 107.17 |
| 48 | 11 | 311 | A86 | C41-C32-C31 | -4.36 | 106.57 | 110.47 |
| 47 | 31 | 303 | KC1 | C3C-C4C-NC | 4.35 | 114.57 | 109.90 |
| 37 | 14 | 310 | CLA | C3D-C2D-C1D | -4.35 | 99.89 | 105.83 |
| 37 | 34 | 310 | CLA | C3D-C2D-C1D | -4.35 | 99.89 | 105.83 |
| 37 | 19 | 306 | CLA | C1D-CHD-C4C | -4.35 | 116.77 | 126.02 |
| 37 | B | 505 | CLA | C3D-C4D-ND | 4.35 | 117.06 | 109.99 |
| 37 | 36 | 309 | CLA | CHD-C1D-ND | -4.35 | 118.68 | 124.80 |
| 37 | B | 507 | CLA | C3B-C2B-C1B | -4.35 | 102.04 | 107.17 |
| 37 | 16 | 309 | CLA | CHD-C1D-ND | -4.35 | 118.68 | 124.80 |
| 37 | 32 | 208 | CLA | CHD-C1D-ND | -4.35 | 118.68 | 124.80 |
| 37 | 20 | 303 | CLA | C2B-C1B-NB | 4.35 | 114.84 | 110.33 |
| 48 | 34 | 312 | A86 | C3-C2-C1 | -4.35 | 121.18 | 127.28 |
| 37 | 21 | 202 | CLA | C3D-C4D-ND | 4.35 | 117.06 | 109.99 |
| 37 | c | 507 | CLA | C1D-CHD-C4C | -4.35 | 116.78 | 126.02 |
| 37 | C | 505 | CLA | C1D-CHD-C4C | -4.35 | 116.78 | 126.02 |
| 47 | 13 | 304 | KC1 | CHC-C1C-C2C | -4.35 | 118.17 | 125.03 |
| 37 | 41 | 209 | CLA | C3D-C4D-ND | 4.35 | 117.05 | 109.99 |
| 48 | 31 | 311 | A86 | C41-C32-C31 | -4.35 | 106.58 | 110.47 |
| 37 | 39 | 309 | CLA | C3D-C2D-C1D | -4.35 | 99.90 | 105.83 |
| 37 | 39 | 306 | CLA | C4A-NA-C1A | -4.35 | 104.70 | 106.68 |
| 47 | 20 | 302 | KC1 | C1C-C2C-C3C | -4.35 | 102.41 | 106.98 |
| 47 | 35 | 302 | KC1 | C3C-C4C-NC | 4.35 | 114.56 | 109.90 |
| 37 | B | 524 | CLA | C2B-C1B-NB | 4.35 | 114.83 | 110.33 |
| 37 | B | 516 | CLA | C1D-CHD-C4C | -4.34 | 116.79 | 126.02 |
| 37 | C | 513 | CLA | C3D-C4D-ND | 4.34 | 117.05 | 109.99 |
| 50 | 40 | 212 | DD6 | C21-C20-C19 | -4.34 | 109.36 | 114.24 |
| 37 | 33 | 310 | CLA | C3D-C4D-ND | 4.34 | 117.05 | 109.99 |
| 37 | B | 508 | CLA | C3B-C2B-C1B | -4.34 | 102.05 | 107.17 |
| 37 | 14 | 301 | CLA | O2D-CGD-CBD | 4.34 | 118.82 | 111.23 |
| 47 | 34 | 309 | KC1 | CHC-C1C-C2C | -4.34 | 118.17 | 125.03 |
| 37 | b | 507 | CLA | C3B-C2B-C1B | -4.34 | 102.05 | 107.17 |
| 37 | 12 | 204 | CLA | C3C-C4C-NC | 4.34 | 115.99 | 110.43 |
| 37 | b | 502 | CLA | C3D-C4D-ND | 4.34 | 117.04 | 109.99 |
| 47 | 38 | 207 | KC1 | C4B-C3B-C2B | -4.34 | 103.05 | 106.81 |
| 47 | 33 | 306 | KC1 | C2A-C1A-NA | 4.34 | 116.29 | 109.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 502 | CLA | CHD-C1D-ND | -4.34 | 118.70 | 124.80 |
| 37 | C | 504 | CLA | C3D-C4D-ND | 4.34 | 117.04 | 109.99 |
| 37 | b | 503 | CLA | C3B-C2B-C1B | -4.34 | 102.06 | 107.17 |
| 37 | B | 502 | CLA | C3D-C4D-ND | 4.34 | 117.03 | 109.99 |
| 37 | B | 509 | CLA | C1C-C2C-C3C | -4.33 | 102.42 | 106.98 |
| 37 | b | 516 | CLA | C3B-C2B-C1B | -4.33 | 102.06 | 107.17 |
| 37 | 40 | 203 | CLA | C4A-NA-C1A | -4.33 | 104.70 | 106.68 |
| 37 | 33 | 303 | CLA | C3D-C4D-ND | 4.33 | 117.03 | 109.99 |
| 37 | 17 | 304 | CLA | C3D-C4D-ND | 4.33 | 117.03 | 109.99 |
| 37 | 12 | 209 | CLA | C2C-C1C-NC | 4.33 | 114.53 | 109.98 |
| 37 | C | 506 | CLA | C4A-NA-C1A | -4.33 | 104.70 | 106.68 |
| 37 | 40 | 205 | CLA | C4A-NA-C1A | -4.33 | 104.70 | 106.68 |
| 37 | B | 503 | CLA | C3B-C2B-C1B | -4.33 | 102.06 | 107.17 |
| 47 | 34 | 309 | KC1 | C3D-C4D-ND | 4.33 | 116.24 | 110.20 |
| 37 | c | 513 | CLA | C3D-C4D-ND | 4.33 | 117.03 | 109.99 |
| 37 | 39 | 306 | CLA | C1D-CHD-C4C | -4.33 | 116.81 | 126.02 |
| 47 | 13 | 306 | KC1 | C2A-C1A-NA | 4.33 | 116.28 | 109.34 |
| 37 | 35 | 307 | CLA | C3D-C2D-C1D | -4.33 | 99.92 | 105.83 |
| 47 | 32 | 207 | KC1 | CMA-C3A-C2A | -4.33 | 117.95 | 128.43 |
| 37 | c | 506 | CLA | C4A-NA-C1A | -4.33 | 104.70 | 106.68 |
| 37 | 14 | 303 | CLA | C3D-C4D-ND | 4.33 | 117.02 | 109.99 |
| 37 | 21 | 204 | CLA | CHD-C1D-ND | -4.33 | 118.71 | 124.80 |
| 37 | 35 | 308 | CLA | C3D-C4D-ND | 4.33 | 117.02 | 109.99 |
| 37 | 41 | 202 | CLA | C3D-C4D-ND | 4.33 | 117.02 | 109.99 |
| 37 | 16 | 301 | CLA | O2D-CGD-CBD | 4.33 | 118.80 | 111.23 |
| 37 | C | 505 | CLA | C3D-C4D-ND | 4.33 | 117.02 | 109.99 |
| 47 | 31 | 307 | KC1 | C3D-C4D-ND | 4.33 | 116.23 | 110.20 |
| 37 | b | 505 | CLA | CHD-C1D-ND | -4.33 | 118.71 | 124.80 |
| 37 | 21 | 209 | CLA | C3D-C4D-ND | 4.33 | 117.02 | 109.99 |
| 37 | 34 | 301 | CLA | C3D-C4D-ND | 4.32 | 117.02 | 109.99 |
| 37 | 38 | 202 | CLA | C3D-C4D-ND | 4.32 | 117.02 | 109.99 |
| 47 | 11 | 302 | KC1 | C3D-C4D-ND | 4.32 | 116.23 | 110.20 |
| 37 | B | 506 | CLA | C3D-C4D-ND | 4.32 | 117.01 | 109.99 |
| 37 | c | 504 | CLA | C3D-C4D-ND | 4.32 | 117.01 | 109.99 |
| 48 | 14 | 316 | A86 | C25-C26-C27 | -4.32 | 121.22 | 127.28 |
| 37 | 13 | 308 | CLA | C3B-C2B-C1B | -4.32 | 102.08 | 107.17 |
| 37 | 36 | 301 | CLA | O2D-CGD-CBD | 4.32 | 118.78 | 111.23 |
| 37 | b | 506 | CLA | C3D-C4D-ND | 4.32 | 117.01 | 109.99 |
| 37 | 33 | 308 | CLA | C3B-C2B-C1B | -4.32 | 102.08 | 107.17 |
| 47 | 31 | 303 | KC1 | C3D-C4D-ND | 4.32 | 116.22 | 110.20 |
| 47 | 37 | 305 | KC1 | CHD-C4C-C3C | -4.32 | 117.26 | 125.23 |
| 37 | 41 | 202 | CLA | CHD-C1D-ND | -4.32 | 118.72 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 508 | CLA | C3B-C2B-C1B | -4.32 | 102.08 | 107.17 |
| 37 | 12 | 207 | CLA | CHD-C1D-ND | -4.32 | 118.72 | 124.80 |
| 47 | 40 | 204 | KC1 | C1C-C2C-C3C | -4.32 | 102.44 | 106.98 |
| 47 | 13 | 309 | KC1 | C3C-C4C-NC | 4.32 | 114.53 | 109.90 |
| 37 | b | 510 | CLA | CAA-C2A-C3A | -4.32 | 101.33 | 113.00 |
| 37 | 41 | 204 | CLA | CHD-C1D-ND | -4.32 | 118.73 | 124.80 |
| 37 | 15 | 308 | CLA | C3D-C4D-ND | 4.32 | 117.00 | 109.99 |
| 47 | 33 | 309 | KC1 | C3C-C4C-NC | 4.32 | 114.53 | 109.90 |
| 47 | 13 | 309 | KC1 | CBA-CAA-C2A | -4.32 | 108.13 | 125.45 |
| 47 | 40 | 206 | KC1 | C1C-C2C-C3C | -4.32 | 102.44 | 106.98 |
| 37 | W | 101 | CLA | CHD-C1D-ND | -4.32 | 118.73 | 124.80 |
| 47 | 15 | 304 | KC1 | CHD-C4C-C3C | -4.32 | 117.27 | 125.23 |
| 47 | 12 | 206 | KC1 | CMA-C3A-C2A | -4.32 | 117.98 | 128.43 |
| 37 | B | 510 | CLA | CAA-C2A-C3A | -4.32 | 101.34 | 113.00 |
| 37 | b | 505 | CLA | C3D-C4D-ND | 4.32 | 117.00 | 109.99 |
| 47 | 33 | 309 | KC1 | CBA-CAA-C2A | -4.32 | 108.13 | 125.45 |
| 47 | 17 | 305 | KC1 | C2A-C1A-NA | 4.31 | 116.25 | 109.34 |
| 37 | 21 | 208 | CLA | C3D-C4D-ND | 4.31 | 117.00 | 109.99 |
| 37 | 37 | 303 | CLA | C3D-C4D-ND | 4.31 | 117.00 | 109.99 |
| 37 | 20 | 307 | CLA | C3D-C4D-ND | 4.31 | 117.00 | 109.99 |
| 47 | 17 | 306 | KC1 | CHD-C4C-C3C | -4.31 | 117.28 | 125.23 |
| 37 | B | 516 | CLA | C3B-C2B-C1B | -4.31 | 102.09 | 107.17 |
| 37 | 15 | 301 | CLA | C2C-C1C-NC | 4.31 | 114.51 | 109.98 |
| 37 | 21 | 206 | CLA | C2C-C1C-NC | 4.31 | 114.51 | 109.98 |
| 37 | 34 | 303 | CLA | C3D-C4D-ND | 4.31 | 116.99 | 109.99 |
| 47 | 11 | 306 | KC1 | C3D-C4D-ND | 4.31 | 116.21 | 110.20 |
| 47 | 12 | 211 | KC1 | C3C-C4C-NC | 4.31 | 114.52 | 109.90 |
| 37 | 41 | 206 | CLA | C2C-C1C-NC | 4.31 | 114.50 | 109.98 |
| 37 | 13 | 310 | CLA | C3D-C2D-C1D | -4.31 | 99.95 | 105.83 |
| 47 | 41 | 203 | KC1 | C2A-C1A-NA | 4.30 | 116.24 | 109.34 |
| 37 | 39 | 301 | CLA | C3D-C4D-ND | 4.30 | 116.98 | 109.99 |
| 37 | 21 | 206 | CLA | CHD-C1D-ND | -4.30 | 118.75 | 124.80 |
| 37 | 16 | 303 | CLA | CHD-C1D-ND | -4.30 | 118.75 | 124.80 |
| 37 | 41 | 206 | CLA | C3D-C4D-ND | 4.30 | 116.98 | 109.99 |
| 37 | 35 | 305 | CLA | C4A-NA-C1A | -4.30 | 104.72 | 106.68 |
| 47 | 40 | 204 | KC1 | CBC-CAC-C3C | -4.30 | 100.76 | 112.42 |
| 47 | 41 | 203 | KC1 | C3D-C4D-ND | 4.30 | 116.19 | 110.20 |
| 48 | 14 | 315 | A86 | O4-C38-C39 | 4.30 | 118.75 | 111.09 |
| 48 | 34 | 315 | A86 | O4-C38-C39 | 4.30 | 118.75 | 111.09 |
| 47 | 14 | 309 | KC1 | C3D-C4D-ND | 4.30 | 116.19 | 110.20 |
| 37 | C | 513 | CLA | C4A-NA-C1A | -4.30 | 104.72 | 106.68 |
| 47 | 38 | 205 | KC1 | C3C-C4C-NC | 4.30 | 114.50 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 41 | 210 | CLA | CHD-C1D-ND | -4.30 | 118.76 | 124.80 |
| 37 | c | 505 | CLA | C3D-C4D-ND | 4.30 | 116.97 | 109.99 |
| 48 | 37 | 310 | A86 | O4-C38-C39 | 4.29 | 118.75 | 111.09 |
| 50 | 39 | 312 | DD6 | C23-C16-C22 | -4.29 | 101.13 | 107.37 |
| 47 | 15 | 304 | KC1 | C2A-C1A-NA | 4.29 | 116.22 | 109.34 |
| 47 | 16 | 302 | KC1 | C2C-C1C-NC | 4.29 | 115.76 | 110.45 |
| 47 | 36 | 305 | KC1 | C3D-C4D-ND | 4.29 | 116.19 | 110.20 |
| 37 | 18 | 204 | CLA | CBA-CAA-C2A | 4.29 | 126.56 | 113.79 |
| 37 | 33 | 308 | CLA | C3D-C4D-ND | 4.29 | 116.96 | 109.99 |
| 47 | 21 | 203 | KC1 | C2A-C1A-NA | 4.29 | 116.22 | 109.34 |
| 37 | 18 | 206 | CLA | C3D-C2D-C1D | -4.29 | 99.98 | 105.83 |
| 48 | 13 | 313 | A86 | C41-C32-C31 | -4.29 | 106.63 | 110.47 |
| 37 | C | 509 | CLA | C4A-NA-C1A | -4.29 | 104.72 | 106.68 |
| 37 | B | 505 | CLA | CHD-C1D-ND | -4.29 | 118.77 | 124.80 |
| 37 | 19 | 309 | CLA | C3D-C2D-C1D | -4.29 | 99.98 | 105.83 |
| 47 | 33 | 302 | KC1 | CHC-C1C-C2C | -4.29 | 118.26 | 125.03 |
| 48 | 33 | 313 | A86 | C41-C32-C31 | -4.29 | 106.63 | 110.47 |
| 50 | 19 | 312 | DD6 | C23-C16-C22 | -4.29 | 101.14 | 107.37 |
| 50 | 21 | 216 | DD6 | C15-C14-C13 | 4.29 | 135.06 | 125.99 |
| 37 | a | 403 | CLA | C3B-C4B-NB | 4.29 | 114.36 | 110.53 |
| 37 | 14 | 305 | CLA | C3D-C4D-ND | 4.29 | 116.96 | 109.99 |
| 37 | 34 | 305 | CLA | C3D-C4D-ND | 4.29 | 116.96 | 109.99 |
| 48 | 17 | 311 | A86 | C3-C4-C5 | -4.29 | 114.75 | 123.52 |
| 37 | 35 | 310 | CLA | C3D-C2D-C1D | -4.29 | 99.98 | 105.83 |
| 37 | 35 | 301 | CLA | C2C-C1C-NC | 4.29 | 114.48 | 109.98 |
| 37 | 14 | 301 | CLA | C3D-C4D-ND | 4.29 | 116.95 | 109.99 |
| 37 | 19 | 301 | CLA | C3D-C4D-ND | 4.29 | 116.95 | 109.99 |
| 37 | 35 | 308 | CLA | CAC-C3C-C4C | 4.29 | 130.37 | 124.79 |
| 37 | 20 | 303 | CLA | C4A-NA-C1A | -4.29 | 104.72 | 106.68 |
| 37 | 36 | 303 | CLA | CHD-C1D-ND | -4.28 | 118.77 | 124.80 |
| 37 | 15 | 307 | CLA | C1D-CHD-C4C | -4.28 | 116.92 | 126.02 |
| 37 | 12 | 210 | CLA | C4A-NA-C1A | -4.28 | 104.72 | 106.68 |
| 37 | b | 523 | CLA | C2B-C1B-NB | 4.28 | 114.77 | 110.33 |
| 37 | 15 | 303 | CLA | C3B-C2B-C1B | -4.28 | 102.12 | 107.17 |
| 37 | A | 403 | CLA | C3D-C4D-ND | 4.28 | 116.95 | 109.99 |
| 37 | 35 | 307 | CLA | C1D-CHD-C4C | -4.28 | 116.92 | 126.02 |
| 50 | 41 | 216 | DD6 | C15-C14-C13 | 4.28 | 135.04 | 125.99 |
| 37 | 39 | 301 | CLA | C1-C2-C3 | -4.28 | 119.18 | 126.20 |
| 47 | 14 | 304 | KC1 | C3C-C4C-NC | 4.28 | 114.49 | 109.90 |
| 47 | 34 | 304 | KC1 | C3C-C4C-NC | 4.28 | 114.49 | 109.90 |
| 37 | 20 | 301 | CLA | C4A-NA-C1A | -4.28 | 104.73 | 106.68 |
| 37 | b | 511 | CLA | CHD-C1D-ND | -4.28 | 118.78 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 18 | 201 | CLA | CHD-C1D-ND | -4.28 | 118.78 | 124.80 |
| 47 | 14 | 304 | KC1 | C1C-C2C-C3C | -4.28 | 102.48 | 106.98 |
| 37 | 21 | 206 | CLA | C3D-C4D-ND | 4.28 | 116.94 | 109.99 |
| 37 | B | 504 | CLA | CAC-C3C-C4C | 4.28 | 130.35 | 124.79 |
| 37 | 21 | 210 | CLA | CHD-C1D-ND | -4.28 | 118.78 | 124.80 |
| 47 | 13 | 306 | KC1 | C2C-C1C-NC | 4.28 | 115.74 | 110.45 |
| 37 | 38 | 208 | CLA | C1D-CHD-C4C | -4.28 | 116.93 | 126.02 |
| 37 | Z | 101 | CLA | C3D-C4D-ND | 4.27 | 116.94 | 109.99 |
| 47 | 16 | 305 | KC1 | C3D-C4D-ND | 4.27 | 116.16 | 110.20 |
| 47 | 16 | 308 | KC1 | C3D-C4D-ND | 4.27 | 116.16 | 110.20 |
| 47 | 13 | 302 | KC1 | C2A-C1A-NA | 4.27 | 116.19 | 109.34 |
| 37 | 13 | 303 | CLA | C3D-C2D-C1D | -4.27 | 100.00 | 105.83 |
| 37 | 40 | 209 | CLA | C3D-C4D-ND | 4.27 | 116.93 | 109.99 |
| 37 | 41 | 206 | CLA | CHD-C1D-ND | -4.27 | 118.79 | 124.80 |
| 48 | 34 | 316 | A86 | C25-C26-C27 | -4.27 | 121.29 | 127.28 |
| 37 | 13 | 308 | CLA | C3D-C4D-ND | 4.27 | 116.93 | 109.99 |
| 47 | 21 | 203 | KC1 | C3D-C4D-ND | 4.27 | 116.16 | 110.20 |
| 37 | B | 511 | CLA | CHD-C1D-ND | -4.27 | 118.79 | 124.80 |
| 37 | 38 | 204 | CLA | CHD-C1D-ND | -4.27 | 118.79 | 124.80 |
| 47 | 20 | 302 | KC1 | CBC-CAC-C3C | -4.27 | 100.85 | 112.42 |
| 47 | 35 | 309 | KC1 | C3D-C4D-ND | 4.27 | 116.15 | 110.20 |
| 37 | 15 | 307 | CLA | C3D-C2D-C1D | -4.27 | 100.01 | 105.83 |
| 37 | 19 | 301 | CLA | C1-C2-C3 | -4.27 | 119.21 | 126.20 |
| 48 | 18 | 213 | A86 | C7-C6-C8 | 4.27 | 124.61 | 118.09 |
| 37 | d | 403 | CLA | O2D-CGD-CBD | 4.27 | 118.69 | 111.23 |
| 47 | 38 | 207 | KC1 | C3D-C4D-ND | 4.27 | 116.15 | 110.20 |
| 37 | 37 | 308 | CLA | C3D-C4D-ND | 4.27 | 116.92 | 109.99 |
| 37 | a | 403 | CLA | C3D-C4D-ND | 4.27 | 116.92 | 109.99 |
| 37 | C | 512 | CLA | C3D-C4D-ND | 4.26 | 116.92 | 109.99 |
| 37 | 17 | 309 | CLA | C3D-C4D-ND | 4.26 | 116.92 | 109.99 |
| 47 | 33 | 306 | KC1 | C1C-C2C-C3C | -4.26 | 102.50 | 106.98 |
| 47 | 31 | 307 | KC1 | CHC-C1C-C2C | -4.26 | 118.30 | 125.03 |
| 50 | 21 | 216 | DD6 | O1-C20-C21 | -4.26 | 110.29 | 115.05 |
| 47 | 15 | 306 | KC1 | CHC-C1C-C2C | -4.26 | 118.30 | 125.03 |
| 37 | 18 | 208 | CLA | C1D-CHD-C4C | -4.26 | 116.96 | 126.02 |
| 37 | 20 | 306 | CLA | C3D-C4D-ND | 4.26 | 116.91 | 109.99 |
| 47 | 36 | 308 | KC1 | C3D-C4D-ND | 4.26 | 116.14 | 110.20 |
| 37 | z | 101 | CLA | C3D-C4D-ND | 4.26 | 116.91 | 109.99 |
| 48 | 17 | 320 | A86 | C25-C26-C27 | -4.26 | 121.31 | 127.28 |
| 37 | B | 516 | CLA | C2C-C1C-NC | 4.26 | 114.45 | 109.98 |
| 47 | 18 | 207 | KC1 | C3D-C4D-ND | 4.26 | 116.14 | 110.20 |
| 37 | b | 504 | CLA | CAC-C3C-C4C | 4.26 | 130.33 | 124.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 40 | 208 | CLA | C3D-C4D-ND | 4.26 | 116.91 | 109.99 |
| 47 | 33 | 302 | KC1 | C2A-C1A-NA | 4.26 | 116.16 | 109.34 |
| 37 | 16 | 306 | CLA | C2C-C1C-NC | 4.26 | 114.45 | 109.98 |
| 47 | 17 | 305 | KC1 | CHC-C1C-C2C | -4.26 | 118.31 | 125.03 |
| 37 | 21 | 209 | CLA | CHD-C1D-ND | -4.25 | 118.81 | 124.80 |
| 37 | 41 | 208 | CLA | CHD-C1D-ND | -4.25 | 118.81 | 124.80 |
| 37 | 11 | 310 | CLA | C3D-C4D-ND | 4.25 | 116.90 | 109.99 |
| 37 | w | 101 | CLA | CHD-C1D-ND | -4.25 | 118.82 | 124.80 |
| 37 | A | 403 | CLA | C3B-C4B-NB | 4.25 | 114.33 | 110.53 |
| 37 | 12 | 210 | CLA | C3D-C4D-ND | 4.25 | 116.90 | 109.99 |
| 47 | 13 | 302 | KC1 | CHC-C1C-C2C | -4.25 | 118.31 | 125.03 |
| 47 | 35 | 306 | KC1 | CHC-C1C-C2C | -4.25 | 118.31 | 125.03 |
| 37 | 41 | 209 | CLA | CHD-C1D-ND | -4.25 | 118.82 | 124.80 |
| 48 | 14 | 316 | A86 | C4-C3-C2 | -4.25 | 114.82 | 123.52 |
| 47 | 35 | 304 | KC1 | CHD-C4C-C3C | -4.25 | 117.39 | 125.23 |
| 37 | C | 501 | CLA | CHD-C1D-ND | -4.25 | 118.82 | 124.80 |
| 37 | 18 | 204 | CLA | CHD-C1D-ND | -4.25 | 118.82 | 124.80 |
| 37 | C | 503 | CLA | C3D-C4D-ND | 4.25 | 116.89 | 109.99 |
| 37 | 32 | 211 | CLA | C3D-C4D-ND | 4.25 | 116.89 | 109.99 |
| 37 | D | 405 | CLA | O2D-CGD-CBD | 4.25 | 118.66 | 111.23 |
| 37 | 36 | 307 | CLA | C3D-C4D-ND | 4.25 | 116.89 | 109.99 |
| 48 | 34 | 316 | A86 | C4-C3-C2 | -4.25 | 114.83 | 123.52 |
| 47 | 17 | 303 | KC1 | C3D-C4D-ND | 4.25 | 116.12 | 110.20 |
| 48 | 34 | 316 | A86 | C35-C34-C33 | 4.24 | 117.51 | 109.89 |
| 37 | c | 501 | CLA | CHD-C1D-ND | -4.24 | 118.83 | 124.80 |
| 47 | 17 | 306 | KC1 | C1C-C2C-C3C | -4.24 | 102.52 | 106.98 |
| 47 | 37 | 305 | KC1 | C1C-C2C-C3C | -4.24 | 102.52 | 106.98 |
| 37 | 35 | 308 | CLA | C2B-C1B-NB | 4.24 | 114.73 | 110.33 |
| 37 | C | 506 | CLA | CAA-C2A-C3A | -4.24 | 101.53 | 113.00 |
| 37 | 33 | 305 | CLA | C3D-C4D-ND | 4.24 | 116.88 | 109.99 |
| 47 | 12 | 208 | KC1 | C3D-C4D-ND | 4.24 | 116.11 | 110.20 |
| 37 | 15 | 308 | CLA | CHD-C1D-ND | -4.24 | 118.83 | 124.80 |
| 37 | 15 | 305 | CLA | C3D-C4D-ND | 4.24 | 116.88 | 109.99 |
| 47 | 31 | 305 | KC1 | C3D-C4D-ND | 4.24 | 116.11 | 110.20 |
| 37 | c | 506 | CLA | C1C-C2C-C3C | -4.24 | 102.52 | 106.98 |
| 47 | 20 | 304 | KC1 | C1C-C2C-C3C | -4.24 | 102.52 | 106.98 |
| 37 | B | 511 | CLA | C3D-C4D-ND | 4.24 | 116.88 | 109.99 |
| 40 | L | 101 | SQD | O7-S-C6 | 4.24 | 113.08 | 106.76 |
| 37 | 39 | 303 | CLA | CBA-CAA-C2A | 4.24 | 126.40 | 113.79 |
| 37 | 32 | 206 | CLA | C2C-C1C-NC | 4.24 | 114.43 | 109.98 |
| 47 | 13 | 306 | KC1 | C1C-C2C-C3C | -4.24 | 102.53 | 106.98 |
| 37 | 31 | 310 | CLA | C3D-C4D-ND | 4.24 | 116.87 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 20 | 310 | DD6 | O1-C20-C21 | -4.24 | 110.31 | 115.05 |
| 37 | 16 | 307 | CLA | C3D-C4D-ND | 4.23 | 116.87 | 109.99 |
| 37 | c | 512 | CLA | C3D-C4D-ND | 4.23 | 116.87 | 109.99 |
| 37 | 14 | 308 | CLA | C3D-C4D-ND | 4.23 | 116.87 | 109.99 |
| 37 | C | 513 | CLA | CHD-C1D-ND | -4.23 | 118.84 | 124.80 |
| 37 | 33 | 303 | CLA | CHD-C1D-ND | -4.23 | 118.85 | 124.80 |
| 47 | 37 | 302 | KC1 | C3D-C4D-ND | 4.23 | 116.10 | 110.20 |
| 37 | 36 | 306 | CLA | C2C-C1C-NC | 4.23 | 114.43 | 109.98 |
| 37 | 38 | 211 | CLA | C3D-C2D-C1D | -4.23 | 100.06 | 105.83 |
| 47 | 33 | 306 | KC1 | C2C-C1C-NC | 4.23 | 115.69 | 110.45 |
| 37 | 35 | 303 | CLA | C3B-C2B-C1B | -4.23 | 102.18 | 107.17 |
| 50 | 40 | 212 | DD6 | O1-C20-C21 | -4.23 | 110.32 | 115.05 |
| 37 | 19 | 302 | CLA | C3D-C4D-ND | 4.23 | 116.86 | 109.99 |
| 47 | 14 | 306 | KC1 | C3D-C4D-ND | 4.23 | 116.10 | 110.20 |
| 37 | 39 | 302 | CLA | C3D-C4D-ND | 4.23 | 116.86 | 109.99 |
| 47 | 34 | 304 | KC1 | C1C-C2C-C3C | -4.23 | 102.53 | 106.98 |
| 37 | c | 506 | CLA | CAA-C2A-C3A | -4.23 | 101.57 | 113.00 |
| 47 | 11 | 304 | KC1 | C3D-C4D-ND | 4.23 | 116.10 | 110.20 |
| 40 | B | 519 | SQD | O7-S-C6 | 4.23 | 113.07 | 106.76 |
| 47 | 33 | 304 | KC1 | CBA-CAA-C2A | -4.23 | 108.48 | 125.45 |
| 37 | 35 | 307 | CLA | C2C-C1C-NC | 4.23 | 114.42 | 109.98 |
| 48 | 11 | 319 | A86 | C12-C11-C13 | 4.23 | 122.85 | 116.00 |
| 37 | 13 | 305 | CLA | C3D-C4D-ND | 4.23 | 116.86 | 109.99 |
| 47 | 11 | 306 | KC1 | CHC-C1C-C2C | -4.23 | 118.36 | 125.03 |
| 37 | 19 | 303 | CLA | CBA-CAA-C2A | 4.22 | 126.36 | 113.79 |
| 37 | b | 516 | CLA | C2C-C1C-NC | 4.22 | 114.42 | 109.98 |
| 48 | 14 | 316 | A86 | C35-C34-C33 | 4.22 | 117.47 | 109.89 |
| 37 | 38 | 202 | CLA | C1D-CHD-C4C | -4.22 | 117.05 | 126.02 |
| 48 | 13 | 311 | A86 | C4-C5-C6 | -4.22 | 121.36 | 127.28 |
| 47 | 13 | 304 | KC1 | CBA-CAA-C2A | -4.22 | 108.51 | 125.45 |
| 47 | 17 | 305 | KC1 | C3C-C4C-NC | 4.22 | 114.42 | 109.90 |
| 37 | b | 503 | CLA | C3D-C2D-C1D | -4.22 | 100.07 | 105.83 |
| 50 | 41 | 216 | DD6 | O1-C20-C21 | -4.22 | 110.33 | 115.05 |
| 37 | c | 513 | CLA | CHD-C1D-ND | -4.22 | 118.86 | 124.80 |
| 48 | 35 | 316 | A86 | C4-C3-C2 | -4.22 | 114.89 | 123.52 |
| 37 | C | 506 | CLA | C1C-C2C-C3C | -4.22 | 102.54 | 106.98 |
| 40 | B | 519 | SQD | O9-S-C6 | 4.22 | 113.05 | 106.76 |
| 37 | B | 503 | CLA | C3D-C2D-C1D | -4.22 | 100.08 | 105.83 |
| 37 | 40 | 203 | CLA | C2C-C1C-NC | 4.22 | 114.41 | 109.98 |
| 37 | c | 503 | CLA | C3D-C4D-ND | 4.22 | 116.84 | 109.99 |
| 37 | 35 | 303 | CLA | CAA-C2A-C3A | -4.22 | 101.61 | 113.00 |
| 48 | 15 | 315 | A86 | C12-C11-C13 | 4.22 | 122.84 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 502 | CLA | C1D-CHD-C4C | -4.22 | 117.06 | 126.02 |
| 37 | 20 | 301 | CLA | C2C-C1C-NC | 4.21 | 114.41 | 109.98 |
| 37 | c | 502 | CLA | C1D-CHD-C4C | -4.21 | 117.06 | 126.02 |
| 48 | 41 | 214 | A86 | C36-C31-C32 | -4.21 | 115.51 | 119.70 |
| 48 | 33 | 311 | A86 | C4-C5-C6 | -4.21 | 121.37 | 127.28 |
| 48 | 33 | 314 | A86 | C41-C32-C31 | -4.21 | 106.70 | 110.47 |
| 37 | 21 | 208 | CLA | CHD-C1D-ND | -4.21 | 118.88 | 124.80 |
| 48 | 21 | 214 | A86 | C36-C31-C32 | -4.21 | 115.52 | 119.70 |
| 37 | 31 | 301 | CLA | C3D-C2D-C1D | -4.21 | 100.09 | 105.83 |
| 47 | 15 | 309 | KC1 | C3D-C4D-ND | 4.21 | 116.07 | 110.20 |
| 37 | 39 | 306 | CLA | O2D-CGD-CBD | 4.21 | 118.59 | 111.23 |
| 37 | 19 | 309 | CLA | C3D-C4D-ND | 4.21 | 116.83 | 109.99 |
| 37 | C | 513 | CLA | C2C-C1C-NC | 4.21 | 114.40 | 109.98 |
| 48 | 31 | 319 | A86 | C12-C11-C13 | 4.21 | 122.82 | 116.00 |
| 37 | W | 101 | CLA | C3D-C4D-ND | 4.20 | 116.82 | 109.99 |
| 37 | D | 406 | CLA | C4A-NA-C1A | -4.20 | 104.76 | 106.68 |
| 37 | Z | 102 | CLA | C1D-CHD-C4C | -4.20 | 117.09 | 126.02 |
| 48 | 15 | 316 | A86 | C4-C3-C2 | -4.20 | 114.92 | 123.52 |
| 37 | c | 501 | CLA | C4A-NA-C1A | -4.20 | 104.76 | 106.68 |
| 37 | b | 510 | CLA | C3D-C4D-ND | 4.20 | 116.82 | 109.99 |
| 48 | 31 | 312 | A86 | C3-C4-C5 | -4.20 | 114.93 | 123.52 |
| 37 | 14 | 308 | CLA | C1C-C2C-C3C | -4.20 | 102.56 | 106.98 |
| 37 | 34 | 308 | CLA | C3D-C4D-ND | 4.20 | 116.81 | 109.99 |
| 40 | L | 101 | SQD | O9-S-C6 | 4.20 | 113.02 | 106.76 |
| 47 | 16 | 302 | KC1 | C3D-C4D-ND | 4.20 | 116.05 | 110.20 |
| 37 | 11 | 308 | CLA | C3D-C4D-ND | 4.20 | 116.81 | 109.99 |
| 37 | 16 | 301 | CLA | CHD-C1D-ND | -4.20 | 118.90 | 124.80 |
| 37 | 15 | 308 | CLA | C4A-NA-C1A | -4.20 | 104.77 | 106.68 |
| 37 | B | 505 | CLA | C2C-C1C-NC | 4.19 | 114.39 | 109.98 |
| 37 | 19 | 306 | CLA | O2D-CGD-CBD | 4.19 | 118.56 | 111.23 |
| 37 | D | 406 | CLA | CHD-C1D-ND | -4.19 | 118.90 | 124.80 |
| 37 | 36 | 301 | CLA | CHD-C1D-ND | -4.19 | 118.90 | 124.80 |
| 37 | 32 | 205 | CLA | C3B-C2B-C1B | -4.19 | 102.23 | 107.17 |
| 48 | 38 | 213 | A86 | C25-C26-C27 | -4.19 | 121.40 | 127.28 |
| 37 | 15 | 310 | CLA | C3D-C2D-C1D | -4.19 | 100.11 | 105.83 |
| 37 | z | 102 | CLA | C1D-CHD-C4C | -4.19 | 117.11 | 126.02 |
| 47 | 34 | 306 | KC1 | C3D-C4D-ND | 4.19 | 116.05 | 110.20 |
| 47 | 18 | 210 | KC1 | C1A-C2A-C3A | -4.19 | 103.43 | 107.28 |
| 37 | b | 511 | CLA | C3D-C4D-ND | 4.19 | 116.80 | 109.99 |
| 37 | c | 508 | CLA | C1D-CHD-C4C | -4.19 | 117.11 | 126.02 |
| 37 | z | 101 | CLA | C1D-CHD-C4C | -4.19 | 117.11 | 126.02 |
| 37 | B | 505 | CLA | C4A-NA-C1A | -4.19 | 104.77 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 31 | 305 | KC1 | C1A-NA-C4A | -4.19 | 104.77 | 106.68 |
| 37 | b | 509 | CLA | C1D-CHD-C4C | -4.19 | 117.11 | 126.02 |
| 37 | 36 | 306 | CLA | C3D-C2D-C1D | -4.19 | 100.11 | 105.83 |
| 47 | 11 | 309 | KC1 | C3D-C4D-ND | 4.19 | 116.04 | 110.20 |
| 48 | 37 | 319 | A86 | C25-C26-C27 | -4.19 | 121.40 | 127.28 |
| 47 | 32 | 209 | KC1 | C3D-C4D-ND | 4.19 | 116.04 | 110.20 |
| 48 | 32 | 203 | A86 | O4-C38-C39 | 4.19 | 118.56 | 111.09 |
| 37 | 35 | 303 | CLA | CHD-C1D-ND | -4.19 | 118.91 | 124.80 |
| 48 | 11 | 312 | A86 | C3-C4-C5 | -4.19 | 114.95 | 123.52 |
| 47 | 37 | 302 | KC1 | C3C-C4C-NC | 4.19 | 114.39 | 109.90 |
| 47 | 11 | 304 | KC1 | C2A-C1A-NA | 4.19 | 116.05 | 109.34 |
| 37 | C | 508 | CLA | C1D-CHD-C4C | -4.18 | 117.12 | 126.02 |
| 37 | d | 404 | CLA | CHD-C1D-ND | -4.18 | 118.91 | 124.80 |
| 37 | 19 | 303 | CLA | CHD-C1D-ND | -4.18 | 118.91 | 124.80 |
| 48 | 16 | 310 | A86 | C34-O4-C38 | -4.18 | 110.46 | 117.85 |
| 37 | 32 | 204 | CLA | C1D-CHD-C4C | -4.18 | 117.13 | 126.02 |
| 37 | 32 | 206 | CLA | C3D-C4D-ND | 4.18 | 116.79 | 109.99 |
| 37 | 38 | 202 | CLA | CHD-C1D-ND | -4.18 | 118.92 | 124.80 |
| 37 | b | 515 | CLA | C3D-C4D-ND | 4.18 | 116.78 | 109.99 |
| 48 | 15 | 315 | A86 | C3-C2-C1 | -4.18 | 121.41 | 127.28 |
| 47 | 31 | 305 | KC1 | C2C-C1C-NC | 4.18 | 115.62 | 110.45 |
| 37 | B | 509 | CLA | C1D-CHD-C4C | -4.18 | 117.13 | 126.02 |
| 48 | 37 | 313 | A86 | C9-C10-C11 | -4.18 | 114.83 | 126.64 |
| 48 | 36 | 310 | A86 | C34-O4-C38 | -4.18 | 110.46 | 117.85 |
| 37 | 32 | 202 | CLA | C3D-C4D-ND | 4.18 | 116.78 | 109.99 |
| 47 | 36 | 302 | KC1 | C3D-C4D-ND | 4.18 | 116.03 | 110.20 |
| 37 | 11 | 308 | CLA | C4A-NA-C1A | -4.18 | 104.77 | 106.68 |
| 37 | 34 | 308 | CLA | C1C-C2C-C3C | -4.18 | 102.59 | 106.98 |
| 37 | z | 102 | CLA | C3D-C4D-ND | 4.18 | 116.78 | 109.99 |
| 37 | 39 | 309 | CLA | C3D-C4D-ND | 4.18 | 116.78 | 109.99 |
| 37 | 39 | 303 | CLA | CHD-C1D-ND | -4.18 | 118.93 | 124.80 |
| 48 | 12 | 202 | A86 | O4-C38-C39 | 4.18 | 118.53 | 111.09 |
| 37 | w | 101 | CLA | C3D-C4D-ND | 4.17 | 116.77 | 109.99 |
| 47 | 15 | 302 | KC1 | C2A-C1A-NA | 4.17 | 116.03 | 109.34 |
| 47 | 20 | 304 | KC1 | CHD-C4C-C3C | -4.17 | 117.53 | 125.23 |
| 37 | 12 | 204 | CLA | C3B-C2B-C1B | -4.17 | 102.25 | 107.17 |
| 47 | 40 | 206 | KC1 | CHD-C4C-C3C | -4.17 | 117.53 | 125.23 |
| 37 | W | 102 | CLA | C3D-C2D-C1D | -4.17 | 100.14 | 105.83 |
| 47 | 38 | 210 | KC1 | C1A-C2A-C3A | -4.17 | 103.45 | 107.28 |
| 47 | 17 | 303 | KC1 | C3C-C4C-NC | 4.17 | 114.37 | 109.90 |
| 37 | b | 512 | CLA | C3D-C4D-ND | 4.17 | 116.77 | 109.99 |
| 37 | 13 | 301 | CLA | O2D-CGD-CBD | 4.17 | 118.52 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 33 | 301 | CLA | O2D-CGD-CBD | 4.17 | 118.52 | 111.23 |
| 37 | b | 515 | CLA | C4A-NA-C1A | -4.17 | 104.78 | 106.68 |
| 37 | w | 101 | CLA | C4A-NA-C1A | -4.17 | 104.78 | 106.68 |
| 37 | B | 512 | CLA | C3D-C4D-ND | 4.17 | 116.76 | 109.99 |
| 37 | B | 510 | CLA | C3D-C4D-ND | 4.17 | 116.76 | 109.99 |
| 37 | B | 504 | CLA | C1D-CHD-C4C | -4.17 | 117.17 | 126.02 |
| 47 | 19 | 308 | KC1 | CHC-C1C-C2C | -4.17 | 118.45 | 125.03 |
| 37 | 16 | 306 | CLA | C3D-C2D-C1D | -4.17 | 100.15 | 105.83 |
| 40 | 40 | 202 | SQD | O7-S-C6 | 4.16 | 112.97 | 106.76 |
| 48 | 35 | 315 | A86 | C3-C2-C1 | -4.16 | 121.44 | 127.28 |
| 47 | 16 | 305 | KC1 | C2C-C1C-NC | 4.16 | 115.60 | 110.45 |
| 37 | b | 505 | CLA | C2C-C1C-NC | 4.16 | 114.35 | 109.98 |
| 48 | 16 | 311 | A86 | C12-C11-C13 | 4.16 | 122.75 | 116.00 |
| 37 | Z | 101 | CLA | C1D-CHD-C4C | -4.16 | 117.17 | 126.02 |
| 37 | 11 | 305 | CLA | C3D-C4D-ND | 4.16 | 116.75 | 109.99 |
| 47 | 39 | 308 | KC1 | CHC-C1C-C2C | -4.16 | 118.46 | 125.03 |
| 37 | a | 403 | CLA | CHD-C1D-ND | -4.16 | 118.95 | 124.80 |
| 37 | B | 511 | CLA | C4A-NA-C1A | -4.16 | 104.78 | 106.68 |
| 47 | 11 | 304 | KC1 | C1A-NA-C4A | -4.16 | 104.78 | 106.68 |
| 48 | 21 | 215 | A86 | C3-C2-C1 | -4.16 | 121.44 | 127.28 |
| 37 | B | 515 | CLA | C3D-C4D-ND | 4.16 | 116.75 | 109.99 |
| 37 | c | 508 | CLA | C3D-C4D-ND | 4.16 | 116.75 | 109.99 |
| 37 | C | 507 | CLA | C1C-C2C-C3C | -4.16 | 102.61 | 106.98 |
| 37 | 16 | 306 | CLA | C3D-C4D-ND | 4.16 | 116.75 | 109.99 |
| 37 | 15 | 307 | CLA | C2C-C1C-NC | 4.16 | 114.35 | 109.98 |
| 37 | 35 | 305 | CLA | C3D-C4D-ND | 4.16 | 116.75 | 109.99 |
| 50 | 21 | 212 | DD6 | O1-C20-C21 | -4.16 | 110.40 | 115.05 |
| 50 | 41 | 212 | DD6 | O1-C20-C21 | -4.16 | 110.40 | 115.05 |
| 37 | 12 | 205 | CLA | CHD-C1D-ND | -4.16 | 118.95 | 124.80 |
| 37 | C | 510 | CLA | C3D-C4D-ND | 4.15 | 116.74 | 109.99 |
| 37 | 18 | 208 | CLA | C3D-C4D-ND | 4.15 | 116.74 | 109.99 |
| 37 | b | 504 | CLA | C1D-CHD-C4C | -4.15 | 117.19 | 126.02 |
| 47 | 31 | 309 | KC1 | C3D-C4D-ND | 4.15 | 115.99 | 110.20 |
| 37 | 41 | 206 | CLA | C1D-CHD-C4C | -4.15 | 117.19 | 126.02 |
| 48 | 41 | 215 | A86 | C3-C2-C1 | -4.15 | 121.45 | 127.28 |
| 40 | 16 | 315 | SQD | O7-S-C6 | 4.15 | 112.96 | 106.76 |
| 37 | 12 | 205 | CLA | C3D-C4D-ND | 4.15 | 116.73 | 109.99 |
| 37 | 12 | 203 | CLA | C1D-CHD-C4C | -4.15 | 117.20 | 126.02 |
| 47 | 31 | 305 | KC1 | C2A-C1A-NA | 4.15 | 115.99 | 109.34 |
| 37 | b | 510 | CLA | C1D-CHD-C4C | -4.15 | 117.20 | 126.02 |
| 37 | 31 | 306 | CLA | C3D-C4D-ND | 4.15 | 116.73 | 109.99 |
| 47 | 34 | 304 | KC1 | C2A-C1A-NA | 4.15 | 115.99 | 109.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 523 | CLA | CMD-C2D-C1D | 4.15 | 132.03 | 124.73 |
| 47 | 13 | 306 | KC1 | C4B-C3B-C2B | -4.15 | 103.22 | 106.81 |
| 37 | 21 | 206 | CLA | C1D-CHD-C4C | -4.15 | 117.21 | 126.02 |
| 48 | 13 | 314 | A86 | C41-C32-C31 | -4.15 | 106.76 | 110.47 |
| 37 | 33 | 307 | CLA | C1D-CHD-C4C | -4.15 | 117.21 | 126.02 |
| 48 | 31 | 314 | A86 | C3-C4-C5 | -4.15 | 115.04 | 123.52 |
| 37 | 36 | 306 | CLA | C3D-C4D-ND | 4.15 | 116.72 | 109.99 |
| 37 | 31 | 308 | CLA | C1D-CHD-C4C | -4.14 | 117.21 | 126.02 |
| 37 | W | 101 | CLA | C4A-NA-C1A | -4.14 | 104.79 | 106.68 |
| 37 | b | 511 | CLA | C4A-NA-C1A | -4.14 | 104.79 | 106.68 |
| 47 | 40 | 207 | KC1 | C4B-C3B-C2B | -4.14 | 103.22 | 106.81 |
| 47 | 35 | 304 | KC1 | C1C-C2C-C3C | -4.14 | 102.62 | 106.98 |
| 37 | 15 | 303 | CLA | CHD-C1D-ND | -4.14 | 118.97 | 124.80 |
| 37 | B | 510 | CLA | C1D-CHD-C4C | -4.14 | 117.21 | 126.02 |
| 48 | 38 | 215 | A86 | C3-C2-C1 | -4.14 | 121.47 | 127.28 |
| 48 | 41 | 215 | A86 | C25-C26-C27 | -4.14 | 121.47 | 127.28 |
| 37 | b | 511 | CLA | C1D-CHD-C4C | -4.14 | 117.21 | 126.02 |
| 37 | Z | 101 | CLA | CHD-C1D-ND | -4.14 | 118.97 | 124.80 |
| 37 | B | 511 | CLA | C1D-CHD-C4C | -4.14 | 117.22 | 126.02 |
| 37 | 17 | 307 | CLA | C3D-C4D-ND | 4.14 | 116.72 | 109.99 |
| 37 | 37 | 306 | CLA | C3D-C4D-ND | 4.14 | 116.72 | 109.99 |
| 47 | 20 | 305 | KC1 | C4B-C3B-C2B | -4.14 | 103.22 | 106.81 |
| 37 | 41 | 205 | CLA | C3D-C4D-ND | 4.14 | 116.72 | 109.99 |
| 37 | 33 | 308 | CLA | O2D-CGD-CBD | 4.14 | 118.47 | 111.23 |
| 37 | 40 | 208 | CLA | C2C-C1C-NC | 4.14 | 114.33 | 109.98 |
| 37 | 13 | 307 | CLA | C1D-CHD-C4C | -4.14 | 117.22 | 126.02 |
| 47 | 11 | 304 | KC1 | C2C-C1C-NC | 4.14 | 115.57 | 110.45 |
| 47 | 14 | 306 | KC1 | C2C-C1C-NC | 4.14 | 115.57 | 110.45 |
| 37 | 20 | 308 | CLA | C1D-CHD-C4C | -4.14 | 117.22 | 126.02 |
| 37 | 38 | 208 | CLA | C3D-C4D-ND | 4.14 | 116.71 | 109.99 |
| 37 | 40 | 203 | CLA | C1D-CHD-C4C | -4.14 | 117.23 | 126.02 |
| 37 | B | 524 | CLA | CMD-C2D-C1D | 4.14 | 132.01 | 124.73 |
| 47 | 32 | 209 | KC1 | C4B-C3B-C2B | -4.14 | 103.23 | 106.81 |
| 37 | B | 513 | CLA | CHD-C1D-ND | -4.14 | 118.98 | 124.80 |
| 48 | 21 | 215 | A86 | C25-C26-C27 | -4.14 | 121.48 | 127.28 |
| 37 | 13 | 308 | CLA | O2D-CGD-CBD | 4.14 | 118.46 | 111.23 |
| 37 | 32 | 202 | CLA | C4A-NA-C1A | -4.14 | 104.79 | 106.68 |
| 37 | C | 508 | CLA | C3D-C4D-ND | 4.13 | 116.71 | 109.99 |
| 47 | 21 | 207 | KC1 | C2A-C1A-NA | 4.13 | 115.96 | 109.34 |
| 48 | 18 | 212 | A86 | C41-C32-C31 | -4.13 | 106.77 | 110.47 |
| 37 | 20 | 306 | CLA | C2C-C1C-NC | 4.13 | 114.32 | 109.98 |
| 37 | c | 513 | CLA | C2C-C1C-NC | 4.13 | 114.32 | 109.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 509 | CLA | C4A-NA-C1A | -4.13 | 104.79 | 106.68 |
| 37 | c | 507 | CLA | C1C-C2C-C3C | -4.13 | 102.64 | 106.98 |
| 37 | 17 | 302 | CLA | C1D-CHD-C4C | -4.13 | 117.24 | 126.02 |
| 47 | 14 | 304 | KC1 | C2A-C1A-NA | 4.13 | 115.96 | 109.34 |
| 47 | 35 | 302 | KC1 | C2A-C1A-NA | 4.13 | 115.96 | 109.34 |
| 37 | 11 | 307 | CLA | C1D-CHD-C4C | -4.13 | 117.24 | 126.02 |
| 37 | Z | 102 | CLA | C3D-C4D-ND | 4.13 | 116.70 | 109.99 |
| 48 | 19 | 311 | A86 | C3-C4-C5 | -4.13 | 115.07 | 123.52 |
| 37 | c | 510 | CLA | C3D-C4D-ND | 4.13 | 116.70 | 109.99 |
| 37 | C | 513 | CLA | C1D-CHD-C4C | -4.13 | 117.25 | 126.02 |
| 47 | 41 | 207 | KC1 | C2A-C1A-NA | 4.13 | 115.95 | 109.34 |
| 37 | c | 513 | CLA | C1D-CHD-C4C | -4.13 | 117.25 | 126.02 |
| 48 | 17 | 313 | A86 | C41-C32-C31 | -4.13 | 106.78 | 110.47 |
| 47 | 33 | 306 | KC1 | C4B-C3B-C2B | -4.13 | 103.24 | 106.81 |
| 37 | B | 503 | CLA | C1D-CHD-C4C | -4.12 | 117.25 | 126.02 |
| 47 | 15 | 304 | KC1 | C3C-C4C-NC | 4.12 | 114.32 | 109.90 |
| 37 | 33 | 305 | CLA | CHD-C1D-ND | -4.12 | 119.00 | 124.80 |
| 47 | 31 | 303 | KC1 | C1C-C2C-C3C | -4.12 | 102.64 | 106.98 |
| 47 | 36 | 305 | KC1 | C2C-C1C-NC | 4.12 | 115.55 | 110.45 |
| 37 | B | 515 | CLA | C4A-NA-C1A | -4.12 | 104.80 | 106.68 |
| 37 | 15 | 307 | CLA | C3D-C4D-ND | 4.12 | 116.69 | 109.99 |
| 37 | 21 | 205 | CLA | C3D-C4D-ND | 4.12 | 116.69 | 109.99 |
| 48 | 11 | 314 | A86 | C3-C4-C5 | -4.12 | 115.08 | 123.52 |
| 37 | 39 | 301 | CLA | CHD-C1D-ND | -4.12 | 119.00 | 124.80 |
| 37 | 18 | 204 | CLA | C2C-C1C-NC | 4.12 | 114.31 | 109.98 |
| 37 | 20 | 301 | CLA | C1D-CHD-C4C | -4.12 | 117.26 | 126.02 |
| 37 | 31 | 308 | CLA | C4A-NA-C1A | -4.12 | 104.80 | 106.68 |
| 37 | A | 403 | CLA | CHD-C1D-ND | -4.12 | 119.00 | 124.80 |
| 37 | 35 | 301 | CLA | C1D-CHD-C4C | -4.12 | 117.26 | 126.02 |
| 37 | 14 | 307 | CLA | C3D-C2D-C1D | -4.12 | 100.21 | 105.83 |
| 37 | 13 | 305 | CLA | CHD-C1D-ND | -4.12 | 119.00 | 124.80 |
| 47 | 34 | 309 | KC1 | C1A-C2A-C3A | -4.12 | 103.49 | 107.28 |
| 37 | 11 | 307 | CLA | C4A-NA-C1A | -4.12 | 104.80 | 106.68 |
| 37 | b | 515 | CLA | C1D-CHD-C4C | -4.12 | 117.27 | 126.02 |
| 37 | 38 | 204 | CLA | C2C-C1C-NC | 4.12 | 114.31 | 109.98 |
| 37 | B | 515 | CLA | C1D-CHD-C4C | -4.12 | 117.27 | 126.02 |
| 40 | 40 | 202 | SQD | O6-C1-C2 | 4.12 | 114.53 | 108.27 |
| 48 | 37 | 312 | A86 | C41-C32-C31 | -4.12 | 106.79 | 110.47 |
| 37 | B | 507 | CLA | C3B-C4B-NB | 4.12 | 114.20 | 110.53 |
| 37 | 12 | 210 | CLA | C1D-CHD-C4C | -4.12 | 117.27 | 126.02 |
| 37 | 11 | 303 | CLA | C3D-C4D-ND | 4.11 | 116.68 | 109.99 |
| 47 | 16 | 305 | KC1 | C2A-C1A-NA | 4.11 | 115.93 | 109.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 40 | 210 | CLA | C1D-CHD-C4C | -4.11 | 117.28 | 126.02 |
| 50 | 39 | 312 | DD6 | C15-C14-C13 | 4.11 | 134.69 | 125.99 |
| 37 | 31 | 304 | CLA | C3D-C4D-ND | 4.11 | 116.67 | 109.99 |
| 37 | 14 | 308 | CLA | C1D-CHD-C4C | -4.11 | 117.28 | 126.02 |
| 37 | 39 | 302 | CLA | CHD-C1D-ND | -4.11 | 119.02 | 124.80 |
| 40 | A | 407 | SQD | O9-S-O7 | -4.11 | 100.45 | 113.82 |
| 40 | a | 409 | SQD | O9-S-O7 | -4.11 | 100.45 | 113.82 |
| 37 | b | 503 | CLA | C1D-CHD-C4C | -4.11 | 117.28 | 126.02 |
| 47 | 31 | 305 | KC1 | C1C-C2C-C3C | -4.11 | 102.66 | 106.98 |
| 37 | 34 | 307 | CLA | C3D-C2D-C1D | -4.11 | 100.22 | 105.83 |
| 37 | 18 | 202 | CLA | C1D-CHD-C4C | -4.11 | 117.28 | 126.02 |
| 48 | 15 | 319 | A86 | C33-C32-C31 | 4.11 | 113.20 | 109.21 |
| 37 | c | 502 | CLA | CMB-C2B-C1B | 4.11 | 131.67 | 125.42 |
| 48 | 35 | 315 | A86 | C12-C11-C13 | 4.11 | 122.66 | 116.00 |
| 37 | 18 | 209 | CLA | C1D-CHD-C4C | -4.11 | 117.29 | 126.02 |
| 48 | 32 | 221 | A86 | C10-C9-C8 | -4.11 | 111.31 | 123.20 |
| 47 | 36 | 305 | KC1 | C2A-C1A-NA | 4.10 | 115.92 | 109.34 |
| 37 | 40 | 205 | CLA | CBA-CAA-C2A | 4.10 | 126.00 | 113.79 |
| 37 | 34 | 308 | CLA | C1D-CHD-C4C | -4.10 | 117.30 | 126.02 |
| 37 | B | 507 | CLA | CHD-C1D-ND | -4.10 | 119.03 | 124.80 |
| 48 | 17 | 314 | A86 | C9-C10-C11 | -4.10 | 115.05 | 126.64 |
| 47 | 15 | 306 | KC1 | C1C-C2C-C3C | -4.10 | 102.67 | 106.98 |
| 37 | 20 | 303 | CLA | CBA-CAA-C2A | 4.10 | 126.00 | 113.79 |
| 47 | 35 | 302 | KC1 | C1A-NA-C4A | -4.10 | 104.81 | 106.68 |
| 47 | 32 | 207 | KC1 | C4B-C3B-C2B | -4.10 | 103.26 | 106.81 |
| 37 | 38 | 202 | CLA | O2D-CGD-CBD | 4.10 | 118.40 | 111.23 |
| 37 | 15 | 301 | CLA | C1D-CHD-C4C | -4.10 | 117.30 | 126.02 |
| 37 | 38 | 209 | CLA | C1D-CHD-C4C | -4.10 | 117.31 | 126.02 |
| 37 | 19 | 307 | CLA | C1D-CHD-C4C | -4.10 | 117.31 | 126.02 |
| 48 | 15 | 316 | A86 | C41-C32-C31 | -4.10 | 106.80 | 110.47 |
| 39 | 0 | 101 | BCR | C2-C1-C6 | 4.10 | 116.39 | 110.44 |
| 48 | 39 | 311 | A86 | C3-C4-C5 | -4.10 | 115.13 | 123.52 |
| 37 | 38 | 211 | CLA | CHD-C1D-ND | -4.10 | 119.03 | 124.80 |
| 48 | 35 | 319 | A86 | C33-C32-C31 | 4.10 | 113.19 | 109.21 |
| 47 | 20 | 302 | KC1 | C3C-C4C-NC | 4.10 | 114.29 | 109.90 |
| 37 | A | 405 | CLA | C4A-NA-C1A | -4.10 | 104.81 | 106.68 |
| 37 | C | 501 | CLA | C4A-NA-C1A | -4.10 | 104.81 | 106.68 |
| 47 | 35 | 306 | KC1 | C1C-C2C-C3C | -4.10 | 102.67 | 106.98 |
| 37 | b | 509 | CLA | C3B-C2B-C1B | -4.10 | 102.34 | 107.17 |
| 37 | 13 | 303 | CLA | CHD-C1D-ND | -4.10 | 119.04 | 124.80 |
| 50 | 19 | 312 | DD6 | C15-C14-C13 | 4.10 | 134.66 | 125.99 |
| 37 | 39 | 307 | CLA | C1D-CHD-C4C | -4.10 | 117.31 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | z | 101 | CLA | CHD-C1D-ND | -4.10 | 119.04 | 124.80 |
| 37 | 33 | 301 | CLA | CHD-C1D-ND | -4.10 | 119.04 | 124.80 |
| 48 | 36 | 311 | A86 | C12-C11-C13 | 4.10 | 122.64 | 116.00 |
| 47 | 18 | 210 | KC1 | C4B-C3B-C2B | -4.10 | 103.26 | 106.81 |
| 37 | 19 | 301 | CLA | CHD-C1D-ND | -4.10 | 119.04 | 124.80 |
| 48 | 11 | 312 | A86 | C26-C25-C24 | -4.09 | 111.33 | 123.20 |
| 37 | 32 | 206 | CLA | CHD-C1D-ND | -4.09 | 119.04 | 124.80 |
| 47 | 40 | 204 | KC1 | C3C-C4C-NC | 4.09 | 114.29 | 109.90 |
| 37 | 32 | 204 | CLA | C2C-C1C-NC | 4.09 | 114.28 | 109.98 |
| 48 | 17 | 320 | A86 | C12-C11-C13 | 4.09 | 122.64 | 116.00 |
| 37 | 12 | 203 | CLA | C2C-C1C-NC | 4.09 | 114.28 | 109.98 |
| 37 | 31 | 302 | CLA | C1D-CHD-C4C | -4.09 | 117.32 | 126.02 |
| 48 | 31 | 312 | A86 | C26-C25-C24 | -4.09 | 111.34 | 123.20 |
| 50 | 21 | 212 | DD6 | C35-C36-C31 | -4.09 | 111.99 | 120.50 |
| 47 | 35 | 304 | KC1 | C2C-C1C-NC | 4.09 | 115.51 | 110.45 |
| 47 | 14 | 306 | KC1 | C1C-C2C-C3C | -4.09 | 102.68 | 106.98 |
| 37 | 19 | 301 | CLA | C2C-C1C-NC | 4.09 | 114.28 | 109.98 |
| 37 | B | 524 | CLA | C3D-C4D-ND | 4.09 | 116.63 | 109.99 |
| 37 | b | 513 | CLA | CHD-C1D-ND | -4.09 | 119.05 | 124.80 |
| 37 | 11 | 301 | CLA | C1D-CHD-C4C | -4.09 | 117.33 | 126.02 |
| 37 | b | 516 | CLA | C3D-C4D-ND | 4.09 | 116.63 | 109.99 |
| 37 | a | 403 | CLA | C3D-C2D-C1D | -4.09 | 100.25 | 105.83 |
| 48 | 37 | 310 | A86 | C3-C4-C5 | -4.09 | 115.16 | 123.52 |
| 47 | 40 | 207 | KC1 | C3D-C4D-ND | 4.09 | 115.90 | 110.20 |
| 47 | 35 | 302 | KC1 | C2C-C1C-NC | 4.09 | 115.51 | 110.45 |
| 47 | 12 | 206 | KC1 | CHC-C1C-C2C | -4.09 | 118.58 | 125.03 |
| 37 | 19 | 307 | CLA | O2D-CGD-CBD | 4.09 | 118.37 | 111.23 |
| 37 | 32 | 211 | CLA | C1D-CHD-C4C | -4.09 | 117.34 | 126.02 |
| 47 | 17 | 305 | KC1 | CHD-C4C-C3C | -4.09 | 117.69 | 125.23 |
| 37 | A | 403 | CLA | C1D-CHD-C4C | -4.08 | 117.34 | 126.02 |
| 47 | 15 | 302 | KC1 | C1C-C2C-C3C | -4.08 | 102.68 | 106.98 |
| 37 | 39 | 301 | CLA | C2C-C1C-NC | 4.08 | 114.27 | 109.98 |
| 37 | 34 | 301 | CLA | C1D-CHD-C4C | -4.08 | 117.34 | 126.02 |
| 37 | C | 503 | CLA | C1D-CHD-C4C | -4.08 | 117.34 | 126.02 |
| 47 | 34 | 306 | KC1 | C2C-C1C-NC | 4.08 | 115.50 | 110.45 |
| 47 | 14 | 309 | KC1 | C1A-C2A-C3A | -4.08 | 103.53 | 107.28 |
| 47 | 15 | 304 | KC1 | C1C-C2C-C3C | -4.08 | 102.69 | 106.98 |
| 37 | A | 403 | CLA | C3D-C2D-C1D | -4.08 | 100.26 | 105.83 |
| 37 | A | 405 | CLA | CHD-C1D-ND | -4.08 | 119.06 | 124.80 |
| 37 | c | 503 | CLA | C1D-CHD-C4C | -4.08 | 117.35 | 126.02 |
| 37 | 19 | 310 | CLA | C3D-C4D-ND | 4.08 | 116.62 | 109.99 |
| 37 | 39 | 310 | CLA | C3D-C4D-ND | 4.08 | 116.62 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 18 | 207 | KC1 | C1C-C2C-C3C | -4.08 | 102.69 | 106.98 |
| 37 | 15 | 305 | CLA | C4A-NA-C1A | -4.08 | 104.82 | 106.68 |
| 47 | 33 | 309 | KC1 | C1C-C2C-C3C | -4.08 | 102.69 | 106.98 |
| 47 | 36 | 302 | KC1 | C1C-C2C-C3C | -4.08 | 102.69 | 106.98 |
| 39 | 5 | 101 | BCR | C2-C1-C6 | 4.08 | 116.36 | 110.44 |
| 37 | B | 513 | CLA | C1C-C2C-C3C | -4.08 | 102.69 | 106.98 |
| 37 | c | 501 | CLA | C1C-C2C-C3C | -4.08 | 102.69 | 106.98 |
| 37 | 35 | 307 | CLA | C3D-C4D-ND | 4.08 | 116.61 | 109.99 |
| 40 | 16 | 315 | SQD | O6-C1-C2 | 4.08 | 114.46 | 108.27 |
| 48 | 12 | 220 | A86 | C10-C9-C8 | -4.08 | 111.39 | 123.20 |
| 47 | 35 | 304 | KC1 | C3C-C4C-NC | 4.08 | 114.27 | 109.90 |
| 37 | 41 | 205 | CLA | O2D-CGD-CBD | 4.08 | 118.36 | 111.23 |
| 37 | b | 507 | CLA | C3B-C4B-NB | 4.08 | 114.17 | 110.53 |
| 37 | b | 523 | CLA | C3D-C4D-ND | 4.07 | 116.61 | 109.99 |
| 37 | 14 | 301 | CLA | C1D-CHD-C4C | -4.07 | 117.36 | 126.02 |
| 47 | 20 | 304 | KC1 | C3C-C4C-NC | 4.07 | 114.27 | 109.90 |
| 37 | C | 502 | CLA | CMB-C2B-C1B | 4.07 | 131.62 | 125.42 |
| 50 | 41 | 212 | DD6 | C35-C36-C31 | -4.07 | 112.02 | 120.50 |
| 37 | 31 | 302 | CLA | C3D-C4D-ND | 4.07 | 116.61 | 109.99 |
| 37 | 11 | 301 | CLA | C3D-C4D-ND | 4.07 | 116.61 | 109.99 |
| 47 | 12 | 206 | KC1 | C4B-C3B-C2B | -4.07 | 103.28 | 106.81 |
| 47 | 17 | 305 | KC1 | CAC-C3C-C4C | 4.07 | 130.09 | 124.79 |
| 37 | 21 | 205 | CLA | O2D-CGD-CBD | 4.07 | 118.35 | 111.23 |
| 37 | b | 507 | CLA | CHD-C1D-ND | -4.07 | 119.07 | 124.80 |
| 37 | 13 | 301 | CLA | CHD-C1D-ND | -4.07 | 119.07 | 124.80 |
| 37 | 14 | 303 | CLA | CHD-C1D-ND | -4.07 | 119.07 | 124.80 |
| 37 | 34 | 308 | CLA | CHD-C1D-ND | -4.07 | 119.07 | 124.80 |
| 37 | a | 403 | CLA | C1D-CHD-C4C | -4.07 | 117.37 | 126.02 |
| 37 | a | 407 | CLA | CHD-C1D-ND | -4.07 | 119.08 | 124.80 |
| 47 | 11 | 304 | KC1 | C1C-C2C-C3C | -4.07 | 102.70 | 106.98 |
| 37 | 13 | 308 | CLA | CHD-C1D-ND | -4.07 | 119.08 | 124.80 |
| 37 | 11 | 307 | CLA | C3D-C4D-ND | 4.07 | 116.60 | 109.99 |
| 47 | 33 | 302 | KC1 | C2C-C1C-NC | 4.07 | 115.48 | 110.45 |
| 37 | 15 | 303 | CLA | CAA-C2A-C3A | -4.07 | 102.01 | 113.00 |
| 47 | 11 | 302 | KC1 | C1C-C2C-C3C | -4.07 | 102.70 | 106.98 |
| 47 | 15 | 304 | KC1 | C2C-C1C-NC | 4.07 | 115.48 | 110.45 |
| 48 | 38 | 212 | A86 | C41-C32-C31 | -4.07 | 106.83 | 110.47 |
| 47 | 35 | 302 | KC1 | C1C-C2C-C3C | -4.07 | 102.70 | 106.98 |
| 37 | 38 | 202 | CLA | C2C-C1C-NC | 4.07 | 114.25 | 109.98 |
| 37 | 13 | 301 | CLA | C3D-C4D-ND | 4.07 | 116.59 | 109.99 |
| 37 | C | 501 | CLA | C1C-C2C-C3C | -4.06 | 102.70 | 106.98 |
| 37 | b | 513 | CLA | C1C-C2C-C3C | -4.06 | 102.70 | 106.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 32 | 207 | KC1 | CHC-C1C-C2C | -4.06 | 118.61 | 125.03 |
| 37 | 33 | 301 | CLA | C3D-C4D-ND | 4.06 | 116.59 | 109.99 |
| 37 | 19 | 302 | CLA | CHD-C1D-ND | -4.06 | 119.09 | 124.80 |
| 37 | 38 | 206 | CLA | CHD-C1D-ND | -4.06 | 119.09 | 124.80 |
| 37 | 39 | 302 | CLA | C1C-C2C-C3C | -4.06 | 102.71 | 106.98 |
| 37 | 18 | 206 | CLA | C3B-C4B-NB | 4.06 | 114.15 | 110.53 |
| 37 | b | 505 | CLA | C4A-NA-C1A | -4.06 | 104.83 | 106.68 |
| 37 | C | 509 | CLA | C3D-C4D-ND | 4.06 | 116.58 | 109.99 |
| 47 | 40 | 206 | KC1 | C3C-C4C-NC | 4.06 | 114.25 | 109.90 |
| 48 | 36 | 310 | A86 | C4-C5-C6 | -4.06 | 121.59 | 127.28 |
| 37 | 17 | 309 | CLA | O2D-CGD-O1D | -4.06 | 115.95 | 123.85 |
| 37 | 33 | 310 | CLA | CHD-C1D-ND | -4.06 | 119.09 | 124.80 |
| 37 | B | 516 | CLA | C3D-C4D-ND | 4.06 | 116.58 | 109.99 |
| 37 | 34 | 303 | CLA | CHD-C1D-ND | -4.06 | 119.09 | 124.80 |
| 37 | 31 | 308 | CLA | C3D-C4D-ND | 4.06 | 116.58 | 109.99 |
| 48 | 16 | 310 | A86 | C4-C5-C6 | -4.06 | 121.59 | 127.28 |
| 47 | 34 | 306 | KC1 | C1C-C2C-C3C | -4.06 | 102.71 | 106.98 |
| 37 | 33 | 308 | CLA | CHD-C1D-ND | -4.06 | 119.09 | 124.80 |
| 37 | 12 | 210 | CLA | CAC-C3C-C4C | 4.05 | 130.07 | 124.79 |
| 47 | 20 | 305 | KC1 | C3D-C4D-ND | 4.05 | 115.85 | 110.20 |
| 48 | 35 | 319 | A86 | C12-C11-C13 | 4.05 | 122.58 | 116.00 |
| 47 | 18 | 205 | KC1 | CBA-CAA-C2A | -4.05 | 109.18 | 125.45 |
| 37 | 35 | 310 | CLA | CHD-C1D-ND | -4.05 | 119.10 | 124.80 |
| 47 | 38 | 207 | KC1 | C1C-C2C-C3C | -4.05 | 102.72 | 106.98 |
| 48 | 33 | 314 | A86 | C36-C31-C32 | -4.05 | 115.67 | 119.70 |
| 47 | 38 | 205 | KC1 | CBA-CAA-C2A | -4.05 | 109.19 | 125.45 |
| 37 | 39 | 307 | CLA | O2D-CGD-CBD | 4.05 | 118.31 | 111.23 |
| 37 | 40 | 209 | CLA | C1D-CHD-C4C | -4.05 | 117.41 | 126.02 |
| 37 | 19 | 310 | CLA | C1C-C2C-C3C | -4.05 | 102.72 | 106.98 |
| 47 | 12 | 208 | KC1 | C4B-C3B-C2B | -4.05 | 103.30 | 106.81 |
| 37 | 34 | 310 | CLA | CHD-C1D-ND | -4.05 | 119.10 | 124.80 |
| 37 | c | 509 | CLA | C3D-C4D-ND | 4.05 | 116.57 | 109.99 |
| 37 | 14 | 308 | CLA | CHD-C1D-ND | -4.05 | 119.10 | 124.80 |
| 37 | 14 | 310 | CLA | CHD-C1D-ND | -4.05 | 119.11 | 124.80 |
| 47 | 37 | 302 | KC1 | C2A-C1A-NA | 4.05 | 115.83 | 109.34 |
| 37 | 39 | 310 | CLA | C1D-CHD-C4C | -4.05 | 117.42 | 126.02 |
| 47 | 31 | 307 | KC1 | C2A-C1A-NA | 4.05 | 115.82 | 109.34 |
| 48 | 31 | 319 | A86 | C25-C26-C27 | 4.05 | 132.95 | 127.28 |
| 38 | a | 406 | PHO | CMB-C2B-C3B | 4.04 | 132.77 | 124.68 |
| 48 | 15 | 319 | A86 | C12-C11-C13 | 4.04 | 122.56 | 116.00 |
| 37 | 20 | 307 | CLA | CHD-C1D-ND | -4.04 | 119.11 | 124.80 |
| 37 | 35 | 310 | CLA | C1C-C2C-C3C | -4.04 | 102.73 | 106.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 16 | 312 | DD6 | C21-C20-C19 | -4.04 | 109.70 | 114.24 |
| 48 | 11 | 314 | A86 | C10-C9-C8 | -4.04 | 111.49 | 123.20 |
| 37 | C | 509 | CLA | C1D-CHD-C4C | -4.04 | 117.43 | 126.02 |
| 47 | 13 | 309 | KC1 | C1C-C2C-C3C | -4.04 | 102.73 | 106.98 |
| 37 | 37 | 308 | CLA | O2D-CGD-O1D | -4.04 | 115.98 | 123.85 |
| 37 | B | 502 | CLA | C3B-C4B-NB | 4.04 | 114.14 | 110.53 |
| 37 | c | 509 | CLA | C1D-CHD-C4C | -4.04 | 117.43 | 126.02 |
| 47 | 20 | 302 | KC1 | C2A-C1A-NA | 4.04 | 115.81 | 109.34 |
| 40 | 40 | 202 | SQD | O9-S-O7 | -4.04 | 100.68 | 113.82 |
| 48 | 31 | 314 | A86 | C10-C9-C8 | -4.04 | 111.49 | 123.20 |
| 37 | 41 | 209 | CLA | C1D-CHD-C4C | -4.04 | 117.43 | 126.02 |
| 37 | 19 | 310 | CLA | C1D-CHD-C4C | -4.04 | 117.44 | 126.02 |
| 48 | 11 | 319 | A86 | C25-C26-C27 | 4.04 | 132.94 | 127.28 |
| 47 | 38 | 210 | KC1 | C4B-C3B-C2B | -4.04 | 103.31 | 106.81 |
| 40 | 16 | 315 | SQD | O9-S-O7 | -4.04 | 100.70 | 113.82 |
| 37 | 11 | 303 | CLA | C1C-C2C-C3C | -4.03 | 102.74 | 106.98 |
| 47 | 40 | 204 | KC1 | C2C-C1C-NC | 4.03 | 115.44 | 110.45 |
| 48 | 18 | 215 | A86 | C3-C2-C1 | -4.03 | 121.62 | 127.28 |
| 47 | 35 | 306 | KC1 | C2A-C1A-NA | 4.03 | 115.80 | 109.34 |
| 47 | 37 | 304 | KC1 | CHD-C4C-C3C | -4.03 | 117.79 | 125.23 |
| 37 | B | 524 | CLA | CAA-C2A-C1A | 4.03 | 125.19 | 111.97 |
| 37 | D | 401 | CLA | C3B-C4B-NB | 4.03 | 114.13 | 110.53 |
| 37 | 19 | 302 | CLA | C1C-C2C-C3C | -4.03 | 102.74 | 106.98 |
| 47 | 15 | 302 | KC1 | C2C-C1C-NC | 4.03 | 115.44 | 110.45 |
| 37 | 38 | 204 | CLA | C3D-C2D-C1D | -4.03 | 100.33 | 105.83 |
| 48 | 41 | 213 | A86 | C4-C5-C6 | -4.03 | 121.63 | 127.28 |
| 47 | 35 | 304 | KC1 | C4B-C3B-C2B | -4.03 | 103.32 | 106.81 |
| 37 | 40 | 209 | CLA | CHD-C1D-ND | -4.03 | 119.13 | 124.80 |
| 50 | 40 | 214 | DD6 | O1-C20-C21 | -4.03 | 110.55 | 115.05 |
| 37 | B | 509 | CLA | C3B-C2B-C1B | -4.03 | 102.42 | 107.17 |
| 37 | 14 | 302 | CLA | C1D-CHD-C4C | -4.03 | 117.46 | 126.02 |
| 37 | 14 | 305 | CLA | CHD-C1D-ND | -4.02 | 119.14 | 124.80 |
| 47 | 11 | 306 | KC1 | C2A-C1A-NA | 4.02 | 115.79 | 109.34 |
| 37 | b | 501 | CLA | C3D-C4D-ND | 4.02 | 116.53 | 109.99 |
| 37 | 37 | 301 | CLA | O2D-CGD-CBD | 4.02 | 118.27 | 111.23 |
| 37 | 31 | 308 | CLA | C3C-C4C-NC | 4.02 | 115.58 | 110.43 |
| 47 | 13 | 309 | KC1 | C4B-C3B-C2B | -4.02 | 103.33 | 106.81 |
| 38 | A | 404 | PHO | CMB-C2B-C3B | 4.02 | 132.72 | 124.68 |
| 37 | a | 407 | CLA | C4A-NA-C1A | -4.02 | 104.84 | 106.68 |
| 37 | 20 | 307 | CLA | C1D-CHD-C4C | -4.02 | 117.47 | 126.02 |
| 37 | 21 | 209 | CLA | C1D-CHD-C4C | -4.02 | 117.47 | 126.02 |
| 48 | 17 | 311 | A86 | C36-C31-C32 | -4.02 | 115.71 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 501 | CLA | C3D-C4D-ND | 4.02 | 116.52 | 109.99 |
| 37 | 39 | 307 | CLA | C3D-C4D-ND | 4.02 | 116.52 | 109.99 |
| 47 | 17 | 303 | KC1 | C2A-C1A-NA | 4.02 | 115.78 | 109.34 |
| 47 | 40 | 204 | KC1 | C2A-C1A-NA | 4.02 | 115.78 | 109.34 |
| 47 | 20 | 302 | KC1 | C2C-C1C-NC | 4.02 | 115.42 | 110.45 |
| 37 | B | 503 | CLA | C3D-C4D-ND | 4.02 | 116.52 | 109.99 |
| 37 | 16 | 306 | CLA | C3B-C2B-C1B | -4.02 | 102.43 | 107.17 |
| 50 | 19 | 312 | DD6 | C35-C36-C31 | -4.02 | 112.14 | 120.50 |
| 47 | 20 | 305 | KC1 | C2A-C1A-NA | 4.02 | 115.78 | 109.34 |
| 48 | 12 | 217 | A86 | C3-C2-C1 | -4.02 | 121.64 | 127.28 |
| 37 | 37 | 308 | CLA | CHD-C1D-ND | -4.02 | 119.15 | 124.80 |
| 37 | 39 | 310 | CLA | C1C-C2C-C3C | -4.02 | 102.75 | 106.98 |
| 37 | 18 | 211 | CLA | CHD-C1D-ND | -4.02 | 119.15 | 124.80 |
| 37 | 31 | 302 | CLA | CAA-CBA-CGA | -4.02 | 101.80 | 113.21 |
| 37 | 35 | 305 | CLA | C1D-CHD-C4C | -4.02 | 117.48 | 126.02 |
| 47 | 33 | 309 | KC1 | C2C-C1C-NC | 4.02 | 115.42 | 110.45 |
| 37 | 11 | 303 | CLA | CHD-C1D-ND | -4.01 | 119.15 | 124.80 |
| 47 | 36 | 308 | KC1 | C4B-C3B-C2B | -4.01 | 103.33 | 106.81 |
| 37 | 34 | 305 | CLA | CHD-C1D-ND | -4.01 | 119.16 | 124.80 |
| 47 | 16 | 302 | KC1 | C1C-C2C-C3C | -4.01 | 102.76 | 106.98 |
| 50 | 39 | 312 | DD6 | C35-C36-C31 | -4.01 | 112.15 | 120.50 |
| 37 | 12 | 207 | CLA | CAA-C2A-C3A | -4.01 | 102.16 | 113.00 |
| 37 | 17 | 309 | CLA | CHD-C1D-ND | -4.01 | 119.16 | 124.80 |
| 48 | 16 | 314 | A86 | C9-C8-C6 | -4.01 | 115.37 | 126.36 |
| 37 | 36 | 306 | CLA | C1D-CHD-C4C | -4.01 | 117.50 | 126.02 |
| 48 | 21 | 213 | A86 | C4-C5-C6 | -4.01 | 121.66 | 127.28 |
| 37 | 34 | 302 | CLA | C1D-CHD-C4C | -4.01 | 117.50 | 126.02 |
| 37 | 18 | 204 | CLA | C3D-C2D-C1D | -4.01 | 100.36 | 105.83 |
| 37 | 15 | 308 | CLA | CAC-C3C-C4C | 4.01 | 130.00 | 124.79 |
| 37 | 40 | 208 | CLA | C1D-CHD-C4C | -4.01 | 117.50 | 126.02 |
| 48 | 37 | 319 | A86 | C12-C11-C13 | 4.01 | 122.50 | 116.00 |
| 47 | 15 | 306 | KC1 | C2C-C1C-NC | 4.01 | 115.41 | 110.45 |
| 47 | 13 | 309 | KC1 | C2C-C1C-NC | 4.01 | 115.41 | 110.45 |
| 47 | 40 | 207 | KC1 | C2A-C1A-NA | 4.01 | 115.76 | 109.34 |
| 37 | 38 | 208 | CLA | C3D-C2D-C1D | -4.00 | 100.37 | 105.83 |
| 48 | 32 | 218 | A86 | C3-C2-C1 | -4.00 | 121.66 | 127.28 |
| 37 | 39 | 307 | CLA | CHD-C1D-ND | -4.00 | 119.17 | 124.80 |
| 37 | 32 | 211 | CLA | CAC-C3C-C4C | 4.00 | 130.00 | 124.79 |
| 37 | 20 | 306 | CLA | C1D-CHD-C4C | -4.00 | 117.51 | 126.02 |
| 48 | 14 | 312 | A86 | C4-C5-C6 | -4.00 | 121.67 | 127.28 |
| 37 | 11 | 301 | CLA | CAA-CBA-CGA | -4.00 | 101.84 | 113.21 |
| 48 | 34 | 312 | A86 | C4-C5-C6 | -4.00 | 121.67 | 127.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 501 | CLA | C1D-CHD-C4C | -4.00 | 117.52 | 126.02 |
| 47 | 13 | 306 | KC1 | C1A-NA-C4A | -4.00 | 104.85 | 106.68 |
| 37 | c | 501 | CLA | C1D-CHD-C4C | -4.00 | 117.52 | 126.02 |
| 37 | 11 | 307 | CLA | C3C-C4C-NC | 4.00 | 115.55 | 110.43 |
| 50 | 20 | 312 | DD6 | O1-C20-C21 | -4.00 | 110.58 | 115.05 |
| 37 | 36 | 307 | CLA | O2D-CGD-CBD | 4.00 | 118.22 | 111.23 |
| 48 | 37 | 311 | A86 | C3-C2-C1 | -4.00 | 121.67 | 127.28 |
| 37 | 13 | 310 | CLA | CHD-C1D-ND | -4.00 | 119.17 | 124.80 |
| 37 | 36 | 307 | CLA | CHD-C1D-ND | -4.00 | 119.17 | 124.80 |
| 48 | 19 | 313 | A86 | C40-C32-C31 | -4.00 | 106.89 | 110.47 |
| 37 | 33 | 307 | CLA | C3D-C2D-C1D | -4.00 | 100.38 | 105.83 |
| 47 | 15 | 306 | KC1 | C2A-C1A-NA | 4.00 | 115.75 | 109.34 |
| 37 | 19 | 307 | CLA | CHD-C1D-ND | -4.00 | 119.18 | 124.80 |
| 37 | 18 | 203 | CLA | C1D-CHD-C4C | -4.00 | 117.53 | 126.02 |
| 37 | c | 506 | CLA | C3D-C4D-ND | 4.00 | 116.48 | 109.99 |
| 37 | 31 | 304 | CLA | C1C-C2C-C3C | -4.00 | 102.78 | 106.98 |
| 37 | 11 | 308 | CLA | CHD-C1D-ND | -3.99 | 119.18 | 124.80 |
| 37 | 32 | 202 | CLA | CHD-C1D-ND | -3.99 | 119.18 | 124.80 |
| 37 | b | 523 | CLA | CAA-C2A-C1A | 3.99 | 125.07 | 111.97 |
| 37 | 17 | 304 | CLA | C1C-C2C-C3C | -3.99 | 102.78 | 106.98 |
| 37 | 16 | 306 | CLA | C1D-CHD-C4C | -3.99 | 117.53 | 126.02 |
| 37 | B | 512 | CLA | C4A-NA-C1A | -3.99 | 104.86 | 106.68 |
| 48 | 13 | 314 | A86 | C36-C31-C32 | -3.99 | 115.73 | 119.70 |
| 37 | b | 503 | CLA | C3D-C4D-ND | 3.99 | 116.48 | 109.99 |
| 37 | 13 | 307 | CLA | C3D-C2D-C1D | -3.99 | 100.38 | 105.83 |
| 37 | 38 | 203 | CLA | C1D-CHD-C4C | -3.99 | 117.53 | 126.02 |
| 48 | 36 | 313 | A86 | C9-C8-C6 | -3.99 | 115.42 | 126.36 |
| 37 | 15 | 305 | CLA | CHD-C1D-ND | -3.99 | 119.18 | 124.80 |
| 47 | 38 | 205 | KC1 | C2A-C1A-NA | 3.99 | 115.74 | 109.34 |
| 37 | 31 | 301 | CLA | C4A-NA-C1A | -3.99 | 104.86 | 106.68 |
| 37 | 13 | 301 | CLA | C1D-CHD-C4C | -3.99 | 117.54 | 126.02 |
| 37 | 31 | 310 | CLA | C4A-NA-C1A | -3.99 | 104.86 | 106.68 |
| 37 | 32 | 208 | CLA | CAA-C2A-C3A | -3.99 | 102.22 | 113.00 |
| 37 | a | 404 | CLA | C3B-C4B-NB | 3.99 | 114.09 | 110.53 |
| 47 | 33 | 309 | KC1 | C4B-C3B-C2B | -3.99 | 103.36 | 106.81 |
| 44 | c | 517 | DGD | O3G-C3G-C2G | -3.99 | 101.12 | 110.82 |
| 37 | 20 | 308 | CLA | C3D-C4D-ND | 3.99 | 116.47 | 109.99 |
| 37 | 19 | 307 | CLA | C3D-C4D-ND | 3.99 | 116.47 | 109.99 |
| 45 | D | 404 | PL9 | C7-C3-C2 | -3.99 | 118.69 | 123.39 |
| 47 | 16 | 308 | KC1 | C4B-C3B-C2B | -3.99 | 103.36 | 106.81 |
| 45 | d | 402 | PL9 | C7-C3-C2 | -3.98 | 118.69 | 123.39 |
| 37 | 16 | 307 | CLA | O2D-CGD-CBD | 3.98 | 118.20 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | C | 517 | DGD | O3G-C3G-C2G | -3.98 | 101.13 | 110.82 |
| 50 | 36 | 312 | DD6 | C21-C20-C19 | -3.98 | 109.77 | 114.24 |
| 47 | 31 | 309 | KC1 | C2C-C1C-NC | 3.98 | 115.38 | 110.45 |
| 37 | 36 | 306 | CLA | C3B-C2B-C1B | -3.98 | 102.47 | 107.17 |
| 37 | 16 | 307 | CLA | CHD-C1D-ND | -3.98 | 119.20 | 124.80 |
| 37 | b | 512 | CLA | C4A-NA-C1A | -3.98 | 104.86 | 106.68 |
| 47 | 33 | 306 | KC1 | C1A-NA-C4A | -3.98 | 104.86 | 106.68 |
| 37 | 15 | 305 | CLA | C1D-CHD-C4C | -3.98 | 117.56 | 126.02 |
| 37 | b | 502 | CLA | C3B-C4B-NB | 3.98 | 114.08 | 110.53 |
| 47 | 32 | 212 | KC1 | C4B-C3B-C2B | -3.98 | 103.36 | 106.81 |
| 47 | 31 | 303 | KC1 | CBC-CAC-C3C | -3.98 | 101.64 | 112.42 |
| 47 | 13 | 304 | KC1 | C4B-C3B-C2B | -3.98 | 103.37 | 106.81 |
| 37 | W | 102 | CLA | C4A-NA-C1A | -3.98 | 104.86 | 106.68 |
| 47 | 18 | 205 | KC1 | C2A-C1A-NA | 3.97 | 115.71 | 109.34 |
| 37 | B | 508 | CLA | CHD-C1D-ND | -3.97 | 119.21 | 124.80 |
| 37 | c | 506 | CLA | CHD-C1D-ND | -3.97 | 119.21 | 124.80 |
| 47 | 11 | 302 | KC1 | CBC-CAC-C3C | -3.97 | 101.65 | 112.42 |
| 48 | 17 | 312 | A86 | C12-C11-C13 | 3.97 | 122.44 | 116.00 |
| 37 | c | 507 | CLA | C3C-C4C-NC | 3.97 | 115.52 | 110.43 |
| 37 | 31 | 306 | CLA | CHD-C1D-ND | -3.97 | 119.21 | 124.80 |
| 37 | 19 | 305 | CLA | O2D-CGD-CBD | 3.97 | 118.17 | 111.23 |
| 47 | 32 | 209 | KC1 | C2C-C1C-NC | 3.97 | 115.37 | 110.45 |
| 37 | 14 | 301 | CLA | CHD-C1D-ND | -3.97 | 119.21 | 124.80 |
| 37 | 15 | 310 | CLA | C1C-C2C-C3C | -3.97 | 102.80 | 106.98 |
| 47 | 32 | 207 | KC1 | CBA-CAA-C2A | -3.97 | 109.52 | 125.45 |
| 37 | 12 | 203 | CLA | CHD-C1D-ND | -3.97 | 119.22 | 124.80 |
| 48 | 34 | 315 | A86 | C3-C4-C5 | -3.97 | 115.40 | 123.52 |
| 37 | 33 | 301 | CLA | C1D-CHD-C4C | -3.97 | 117.58 | 126.02 |
| 37 | C | 507 | CLA | C3C-C4C-NC | 3.97 | 115.52 | 110.43 |
| 47 | 12 | 206 | KC1 | CBA-CAA-C2A | -3.97 | 109.52 | 125.45 |
| 37 | 33 | 303 | CLA | C1C-C2C-C3C | -3.97 | 102.81 | 106.98 |
| 37 | 18 | 201 | CLA | C2C-C1C-NC | 3.97 | 114.15 | 109.98 |
| 37 | 32 | 204 | CLA | C3D-C4D-ND | 3.97 | 116.44 | 109.99 |
| 37 | 38 | 209 | CLA | C1C-C2C-C3C | -3.97 | 102.81 | 106.98 |
| 47 | 41 | 203 | KC1 | CHC-C1C-C2C | -3.97 | 118.76 | 125.03 |
| 47 | 13 | 302 | KC1 | C2C-C1C-NC | 3.97 | 115.36 | 110.45 |
| 37 | C | 506 | CLA | C3D-C4D-ND | 3.97 | 116.44 | 109.99 |
| 37 | 18 | 209 | CLA | C1C-C2C-C3C | -3.97 | 102.81 | 106.98 |
| 47 | 33 | 302 | KC1 | C1C-C2C-C3C | -3.97 | 102.81 | 106.98 |
| 47 | 35 | 306 | KC1 | C2C-C1C-NC | 3.97 | 115.36 | 110.45 |
| 37 | 40 | 210 | CLA | C3D-C4D-ND | 3.96 | 116.43 | 109.99 |
| 37 | 37 | 303 | CLA | C1C-C2C-C3C | -3.96 | 102.81 | 106.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 39 | 312 | DD6 | C19-C18-C17 | 3.96 | 118.20 | 110.79 |
| 37 | C | 509 | CLA | C3B-C4B-NB | 3.96 | 114.07 | 110.53 |
| 47 | 21 | 203 | KC1 | CHC-C1C-C2C | -3.96 | 118.77 | 125.03 |
| 37 | 35 | 308 | CLA | C4B-C3B-C2B | -3.96 | 102.38 | 107.30 |
| 37 | c | 509 | CLA | C3B-C4B-NB | 3.96 | 114.07 | 110.53 |
| 37 | 12 | 212 | CLA | C1D-CHD-C4C | -3.96 | 117.60 | 126.02 |
| 37 | B | 514 | CLA | C3D-C4D-ND | 3.96 | 116.42 | 109.99 |
| 47 | 16 | 304 | KC1 | C4B-C3B-C2B | -3.96 | 103.38 | 106.81 |
| 50 | 21 | 212 | DD6 | C37-C36-C35 | -3.96 | 107.14 | 114.42 |
| 47 | 14 | 306 | KC1 | CBA-CAA-C2A | -3.96 | 109.57 | 125.45 |
| 47 | 34 | 306 | KC1 | CBA-CAA-C2A | -3.96 | 109.57 | 125.45 |
| 37 | b | 508 | CLA | CHD-C1D-ND | -3.96 | 119.24 | 124.80 |
| 37 | z | 102 | CLA | CHD-C1D-ND | -3.96 | 119.24 | 124.80 |
| 50 | 19 | 312 | DD6 | C19-C18-C17 | 3.95 | 118.19 | 110.79 |
| 37 | 36 | 301 | CLA | C1D-CHD-C4C | -3.95 | 117.61 | 126.02 |
| 50 | 20 | 310 | DD6 | C35-C36-C31 | -3.95 | 112.27 | 120.50 |
| 37 | 39 | 305 | CLA | O2D-CGD-CBD | 3.95 | 118.14 | 111.23 |
| 47 | 13 | 304 | KC1 | C2C-C1C-NC | 3.95 | 115.34 | 110.45 |
| 48 | 14 | 315 | A86 | C3-C4-C5 | -3.95 | 115.43 | 123.52 |
| 37 | 39 | 310 | CLA | CHD-C1D-ND | -3.95 | 119.24 | 124.80 |
| 37 | 35 | 305 | CLA | CHD-C1D-ND | -3.95 | 119.24 | 124.80 |
| 37 | z | 102 | CLA | O2D-CGD-CBD | 3.95 | 118.13 | 111.23 |
| 37 | 31 | 301 | CLA | C3D-C4D-ND | 3.95 | 116.41 | 109.99 |
| 37 | C | 506 | CLA | CHD-C1D-ND | -3.95 | 119.25 | 124.80 |
| 37 | 15 | 303 | CLA | C1C-C2C-C3C | -3.95 | 102.83 | 106.98 |
| 37 | B | 514 | CLA | C1D-CHD-C4C | -3.95 | 117.63 | 126.02 |
| 37 | 34 | 301 | CLA | CHD-C1D-ND | -3.95 | 119.25 | 124.80 |
| 48 | 18 | 215 | A86 | C41-C32-C31 | -3.95 | 106.94 | 110.47 |
| 37 | 31 | 304 | CLA | CHD-C1D-ND | -3.95 | 119.25 | 124.80 |
| 37 | b | 514 | CLA | C3D-C4D-ND | 3.95 | 116.40 | 109.99 |
| 47 | 31 | 307 | KC1 | C1C-C2C-C3C | -3.95 | 102.83 | 106.98 |
| 47 | 32 | 212 | KC1 | C1C-C2C-C3C | -3.95 | 102.83 | 106.98 |
| 37 | 15 | 310 | CLA | CAA-C2A-C3A | -3.95 | 102.33 | 113.00 |
| 48 | 15 | 316 | A86 | C35-C34-C33 | 3.95 | 116.97 | 109.89 |
| 37 | 18 | 206 | CLA | CHD-C1D-ND | -3.95 | 119.25 | 124.80 |
| 37 | 18 | 209 | CLA | C3D-C4D-ND | 3.95 | 116.40 | 109.99 |
| 37 | 38 | 209 | CLA | C3D-C4D-ND | 3.95 | 116.40 | 109.99 |
| 37 | 35 | 310 | CLA | CAA-C2A-C3A | -3.95 | 102.34 | 113.00 |
| 47 | 33 | 304 | KC1 | C2C-C1C-NC | 3.94 | 115.33 | 110.45 |
| 37 | Z | 102 | CLA | O2D-CGD-CBD | 3.94 | 118.12 | 111.23 |
| 37 | 11 | 301 | CLA | CHD-C1D-ND | -3.94 | 119.25 | 124.80 |
| 37 | 31 | 302 | CLA | CHD-C1D-ND | -3.94 | 119.25 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 514 | CLA | C1D-CHD-C4C | -3.94 | 117.64 | 126.02 |
| 47 | 31 | 303 | KC1 | C2C-C1C-NC | 3.94 | 115.33 | 110.45 |
| 37 | 16 | 301 | CLA | C1D-CHD-C4C | -3.94 | 117.64 | 126.02 |
| 37 | 34 | 310 | CLA | C1D-CHD-C4C | -3.94 | 117.64 | 126.02 |
| 37 | 18 | 204 | CLA | CAA-C2A-C3A | -3.94 | 102.35 | 113.00 |
| 37 | c | 508 | CLA | C3C-C4C-NC | 3.94 | 115.48 | 110.43 |
| 37 | 21 | 210 | CLA | C1D-CHD-C4C | -3.94 | 117.64 | 126.02 |
| 37 | B | 515 | CLA | CHD-C1D-ND | -3.94 | 119.26 | 124.80 |
| 37 | C | 504 | CLA | C1D-CHD-C4C | -3.94 | 117.64 | 126.02 |
| 37 | 12 | 203 | CLA | C3D-C4D-ND | 3.94 | 116.39 | 109.99 |
| 50 | 41 | 212 | DD6 | C37-C36-C35 | -3.94 | 107.18 | 114.42 |
| 48 | 38 | 215 | A86 | C41-C32-C31 | -3.94 | 106.95 | 110.47 |
| 37 | 14 | 302 | CLA | C3D-C4D-ND | 3.94 | 116.39 | 109.99 |
| 37 | 35 | 305 | CLA | C1C-C2C-C3C | -3.94 | 102.84 | 106.98 |
| 37 | Z | 102 | CLA | CHD-C1D-ND | -3.94 | 119.26 | 124.80 |
| 48 | 34 | 315 | A86 | C41-C32-C31 | -3.94 | 106.95 | 110.47 |
| 47 | 15 | 304 | KC1 | C4B-C3B-C2B | -3.94 | 103.40 | 106.81 |
| 47 | 33 | 304 | KC1 | C4B-C3B-C2B | -3.94 | 103.40 | 106.81 |
| 47 | 16 | 308 | KC1 | C2C-C1C-NC | 3.94 | 115.32 | 110.45 |
| 37 | 19 | 310 | CLA | CHD-C1D-ND | -3.94 | 119.26 | 124.80 |
| 37 | 38 | 202 | CLA | C4A-NA-C1A | -3.94 | 104.88 | 106.68 |
| 50 | 20 | 312 | DD6 | C23-C16-C15 | 3.94 | 120.67 | 110.05 |
| 47 | 38 | 205 | KC1 | C1C-C2C-C3C | -3.94 | 102.84 | 106.98 |
| 37 | c | 510 | CLA | C3D-C2D-C1D | -3.93 | 100.46 | 105.83 |
| 48 | 12 | 217 | A86 | C12-C11-C13 | 3.93 | 122.38 | 116.00 |
| 47 | 39 | 308 | KC1 | C4B-C3B-C2B | -3.93 | 103.40 | 106.81 |
| 37 | 40 | 210 | CLA | C1C-C2C-C3C | -3.93 | 102.84 | 106.98 |
| 37 | C | 508 | CLA | C4B-C3B-C2B | -3.93 | 102.41 | 107.30 |
| 50 | 40 | 214 | DD6 | C23-C16-C15 | 3.93 | 120.66 | 110.05 |
| 50 | 40 | 212 | DD6 | C35-C36-C31 | -3.93 | 112.32 | 120.50 |
| 37 | c | 510 | CLA | C1D-CHD-C4C | -3.93 | 117.67 | 126.02 |
| 47 | 17 | 303 | KC1 | C4B-C3B-C2B | -3.93 | 103.41 | 106.81 |
| 48 | 14 | 315 | A86 | C41-C32-C31 | -3.93 | 106.95 | 110.47 |
| 37 | W | 101 | CLA | C3C-C4C-NC | 3.93 | 115.46 | 110.43 |
| 37 | 32 | 213 | CLA | C1D-CHD-C4C | -3.93 | 117.67 | 126.02 |
| 47 | 41 | 203 | KC1 | C2C-C1C-NC | 3.93 | 115.31 | 110.45 |
| 37 | W | 102 | CLA | C3D-C4D-ND | 3.93 | 116.37 | 109.99 |
| 37 | 32 | 213 | CLA | C3D-C4D-ND | 3.93 | 116.37 | 109.99 |
| 37 | 39 | 306 | CLA | C1-C2-C3 | -3.93 | 119.76 | 126.20 |
| 40 | 17 | 301 | SQD | O9-S-O7 | -3.93 | 101.05 | 113.82 |
| 37 | 13 | 303 | CLA | C1C-C2C-C3C | -3.93 | 102.85 | 106.98 |
| 37 | 18 | 203 | CLA | C3D-C4D-ND | 3.93 | 116.37 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 504 | CLA | C1D-CHD-C4C | -3.93 | 117.67 | 126.02 |
| 37 | C | 506 | CLA | O2D-CGD-CBD | 3.93 | 118.09 | 111.23 |
| 37 | 38 | 203 | CLA | C3D-C4D-ND | 3.93 | 116.37 | 109.99 |
| 37 | 14 | 307 | CLA | C1D-CHD-C4C | -3.93 | 117.67 | 126.02 |
| 47 | 11 | 309 | KC1 | C2C-C1C-NC | 3.93 | 115.31 | 110.45 |
| 37 | b | 515 | CLA | CHD-C1D-ND | -3.93 | 119.28 | 124.80 |
| 37 | 35 | 303 | CLA | C1C-C2C-C3C | -3.92 | 102.85 | 106.98 |
| 40 | 36 | 315 | SQD | O9-S-O7 | -3.92 | 101.06 | 113.82 |
| 37 | C | 510 | CLA | C1D-CHD-C4C | -3.92 | 117.68 | 126.02 |
| 37 | 17 | 302 | CLA | O2D-CGD-CBD | 3.92 | 118.09 | 111.23 |
| 37 | 13 | 310 | CLA | C1D-CHD-C4C | -3.92 | 117.68 | 126.02 |
| 37 | 38 | 211 | CLA | C1C-C2C-C3C | -3.92 | 102.86 | 106.98 |
| 37 | 14 | 310 | CLA | C1D-CHD-C4C | -3.92 | 117.69 | 126.02 |
| 37 | 11 | 305 | CLA | CHD-C1D-ND | -3.92 | 119.28 | 124.80 |
| 37 | 21 | 205 | CLA | CHD-C1D-ND | -3.92 | 119.28 | 124.80 |
| 47 | 36 | 304 | KC1 | C4B-C3B-C2B | -3.92 | 103.42 | 106.81 |
| 37 | 31 | 310 | CLA | CHD-C1D-ND | -3.92 | 119.29 | 124.80 |
| 37 | b | 507 | CLA | C3D-C4D-ND | 3.92 | 116.36 | 109.99 |
| 37 | 15 | 310 | CLA | CHD-C1D-ND | -3.92 | 119.29 | 124.80 |
| 47 | 32 | 212 | KC1 | C2A-C1A-NA | 3.92 | 115.62 | 109.34 |
| 37 | c | 508 | CLA | C4B-C3B-C2B | -3.92 | 102.43 | 107.30 |
| 48 | 40 | 211 | A86 | C41-C32-C31 | -3.92 | 106.97 | 110.47 |
| 47 | 12 | 208 | KC1 | C2C-C1C-NC | 3.92 | 115.30 | 110.45 |
| 47 | 12 | 206 | KC1 | C2A-C1A-NA | 3.92 | 115.62 | 109.34 |
| 47 | 32 | 207 | KC1 | C2A-C1A-NA | 3.92 | 115.62 | 109.34 |
| 37 | c | 508 | CLA | C4A-NA-C1A | -3.92 | 104.89 | 106.68 |
| 37 | B | 507 | CLA | C3D-C4D-ND | 3.92 | 116.35 | 109.99 |
| 37 | 36 | 307 | CLA | C1D-CHD-C4C | -3.92 | 117.70 | 126.02 |
| 37 | 39 | 309 | CLA | CHD-C1D-ND | -3.92 | 119.29 | 124.80 |
| 47 | 36 | 308 | KC1 | C2C-C1C-NC | 3.92 | 115.30 | 110.45 |
| 37 | 13 | 301 | CLA | C4A-NA-C1A | -3.91 | 104.89 | 106.68 |
| 37 | 33 | 301 | CLA | C4A-NA-C1A | -3.91 | 104.89 | 106.68 |
| 37 | 32 | 204 | CLA | CHD-C1D-ND | -3.91 | 119.29 | 124.80 |
| 37 | 20 | 308 | CLA | C1C-C2C-C3C | -3.91 | 102.86 | 106.98 |
| 37 | 18 | 208 | CLA | C3D-C2D-C1D | -3.91 | 100.49 | 105.83 |
| 37 | 19 | 306 | CLA | C1-C2-C3 | -3.91 | 119.78 | 126.20 |
| 37 | 12 | 210 | CLA | C1C-C2C-C3C | -3.91 | 102.86 | 106.98 |
| 50 | 40 | 212 | DD6 | C24-C1-C2 | -3.91 | 112.85 | 119.01 |
| 37 | 41 | 210 | CLA | C1D-CHD-C4C | -3.91 | 117.70 | 126.02 |
| 37 | w | 101 | CLA | C3C-C4C-NC | 3.91 | 115.44 | 110.43 |
| 37 | 33 | 308 | CLA | CAC-C3C-C4C | 3.91 | 129.88 | 124.79 |
| 37 | 11 | 310 | CLA | C3C-C4C-NC | 3.91 | 115.44 | 110.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 35 | 308 | CLA | C1-C2-C3 | -3.91 | 119.79 | 126.20 |
| 37 | 34 | 302 | CLA | C3D-C4D-ND | 3.91 | 116.34 | 109.99 |
| 37 | 33 | 310 | CLA | C1D-CHD-C4C | -3.91 | 117.71 | 126.02 |
| 37 | 34 | 307 | CLA | C1D-CHD-C4C | -3.91 | 117.71 | 126.02 |
| 37 | 38 | 209 | CLA | C4A-NA-C1A | -3.91 | 104.89 | 106.68 |
| 47 | 38 | 207 | KC1 | C1D-CHD-C4C | -3.91 | 117.05 | 126.25 |
| 37 | 15 | 310 | CLA | C1D-CHD-C4C | -3.91 | 117.71 | 126.02 |
| 37 | 15 | 305 | CLA | C1C-C2C-C3C | -3.91 | 102.87 | 106.98 |
| 47 | 18 | 205 | KC1 | C1C-C2C-C3C | -3.91 | 102.87 | 106.98 |
| 37 | C | 510 | CLA | C3D-C2D-C1D | -3.91 | 100.50 | 105.83 |
| 37 | 39 | 303 | CLA | C1D-CHD-C4C | -3.91 | 117.71 | 126.02 |
| 50 | 20 | 310 | DD6 | C24-C1-C2 | -3.91 | 112.86 | 119.01 |
| 37 | 41 | 205 | CLA | CHD-C1D-ND | -3.91 | 119.30 | 124.80 |
| 37 | 11 | 310 | CLA | C4A-NA-C1A | -3.91 | 104.90 | 106.68 |
| 37 | 18 | 206 | CLA | C1D-CHD-C4C | -3.91 | 117.72 | 126.02 |
| 47 | 16 | 304 | KC1 | C2A-C1A-NA | 3.91 | 115.60 | 109.34 |
| 37 | A | 405 | CLA | CAA-C2A-C3A | -3.91 | 102.44 | 113.00 |
| 48 | 39 | 313 | A86 | C19-C18-C17 | 3.91 | 118.09 | 110.79 |
| 48 | 18 | 212 | A86 | C4-C5-C6 | -3.90 | 121.81 | 127.28 |
| 37 | 19 | 303 | CLA | C1D-CHD-C4C | -3.90 | 117.73 | 126.02 |
| 37 | 34 | 310 | CLA | C4A-NA-C1A | -3.90 | 104.90 | 106.68 |
| 47 | 11 | 304 | KC1 | C4B-C3B-C2B | -3.90 | 103.43 | 106.81 |
| 37 | c | 511 | CLA | C1D-CHD-C4C | -3.90 | 117.73 | 126.02 |
| 50 | 40 | 214 | DD6 | C33-C32-C31 | 3.90 | 117.17 | 109.49 |
| 37 | 18 | 203 | CLA | CHD-C1D-ND | -3.90 | 119.31 | 124.80 |
| 37 | 38 | 203 | CLA | CHD-C1D-ND | -3.90 | 119.31 | 124.80 |
| 37 | c | 504 | CLA | C1C-C2C-C3C | -3.90 | 102.88 | 106.98 |
| 37 | 16 | 307 | CLA | C1D-CHD-C4C | -3.90 | 117.73 | 126.02 |
| 48 | 36 | 311 | A86 | C40-C32-C31 | -3.90 | 106.98 | 110.47 |
| 37 | c | 502 | CLA | C3D-C4D-ND | 3.90 | 116.32 | 109.99 |
| 37 | 34 | 301 | CLA | C2C-C1C-NC | 3.90 | 114.08 | 109.98 |
| 47 | 36 | 305 | KC1 | C1A-NA-C4A | -3.90 | 104.90 | 106.68 |
| 37 | b | 501 | CLA | CHD-C1D-ND | -3.90 | 119.32 | 124.80 |
| 48 | 17 | 312 | A86 | C3-C2-C1 | -3.90 | 121.81 | 127.28 |
| 37 | 18 | 211 | CLA | C1D-CHD-C4C | -3.90 | 117.74 | 126.02 |
| 48 | 35 | 313 | A86 | C41-C32-C31 | -3.90 | 106.99 | 110.47 |
| 37 | 14 | 301 | CLA | C2C-C1C-NC | 3.90 | 114.07 | 109.98 |
| 37 | 13 | 308 | CLA | CAC-C3C-C4C | 3.89 | 129.86 | 124.79 |
| 48 | 32 | 218 | A86 | C12-C11-C13 | 3.89 | 122.32 | 116.00 |
| 48 | 37 | 311 | A86 | C12-C11-C13 | 3.89 | 122.31 | 116.00 |
| 47 | 14 | 304 | KC1 | C2C-C1C-NC | 3.89 | 115.27 | 110.45 |
| 48 | 19 | 311 | A86 | C25-C24-C1 | -3.89 | 115.69 | 126.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 310 | CLA | C1C-C2C-C3C | -3.89 | 102.89 | 106.98 |
| 47 | 21 | 203 | KC1 | C2C-C1C-NC | 3.89 | 115.27 | 110.45 |
| 48 | 20 | 309 | A86 | C41-C32-C31 | -3.89 | 106.99 | 110.47 |
| 48 | 39 | 313 | A86 | C40-C32-C31 | -3.89 | 106.99 | 110.47 |
| 37 | 12 | 212 | CLA | C3D-C4D-ND | 3.89 | 116.31 | 109.99 |
| 37 | 39 | 301 | CLA | C4A-NA-C1A | -3.89 | 104.90 | 106.68 |
| 47 | 16 | 302 | KC1 | CBA-CAA-C2A | -3.89 | 109.83 | 125.45 |
| 48 | 14 | 315 | A86 | C4-C5-C6 | -3.89 | 121.82 | 127.28 |
| 47 | 32 | 209 | KC1 | C1C-C2C-C3C | -3.89 | 102.89 | 106.98 |
| 47 | 36 | 302 | KC1 | CBA-CAA-C2A | -3.89 | 109.83 | 125.45 |
| 37 | 38 | 201 | CLA | C2C-C1C-NC | 3.89 | 114.07 | 109.98 |
| 47 | 12 | 211 | KC1 | C4B-C3B-C2B | -3.89 | 103.44 | 106.81 |
| 47 | 37 | 305 | KC1 | C2A-C1A-NA | 3.89 | 115.58 | 109.34 |
| 37 | c | 506 | CLA | O2D-CGD-CBD | 3.89 | 118.03 | 111.23 |
| 47 | 38 | 205 | KC1 | C2C-C1C-NC | 3.89 | 115.27 | 110.45 |
| 37 | C | 511 | CLA | C1D-CHD-C4C | -3.89 | 117.75 | 126.02 |
| 47 | 37 | 302 | KC1 | C4B-C3B-C2B | -3.89 | 103.44 | 106.81 |
| 37 | 39 | 309 | CLA | C1C-C2C-C3C | -3.89 | 102.89 | 106.98 |
| 47 | 13 | 304 | KC1 | C1C-C2C-C3C | -3.89 | 102.89 | 106.98 |
| 48 | 18 | 212 | A86 | O4-C38-C39 | 3.89 | 118.02 | 111.09 |
| 48 | 34 | 315 | A86 | C4-C5-C6 | -3.89 | 121.82 | 127.28 |
| 47 | 12 | 206 | KC1 | C1C-C2C-C3C | -3.89 | 102.89 | 106.98 |
| 37 | B | 509 | CLA | C3C-C4C-NC | 3.89 | 115.41 | 110.43 |
| 37 | b | 509 | CLA | C3C-C4C-NC | 3.89 | 115.41 | 110.43 |
| 48 | 38 | 212 | A86 | O4-C38-C39 | 3.89 | 118.02 | 111.09 |
| 37 | 34 | 305 | CLA | C1D-CHD-C4C | -3.89 | 117.76 | 126.02 |
| 37 | b | 513 | CLA | C3D-C4D-ND | 3.89 | 116.31 | 109.99 |
| 37 | a | 407 | CLA | CAA-C2A-C3A | -3.89 | 102.49 | 113.00 |
| 37 | 36 | 307 | CLA | C1C-C2C-C3C | -3.89 | 102.89 | 106.98 |
| 47 | 31 | 305 | KC1 | C4B-C3B-C2B | -3.89 | 103.44 | 106.81 |
| 37 | 38 | 209 | CLA | O2D-CGD-CBD | 3.89 | 118.03 | 111.23 |
| 47 | 18 | 207 | KC1 | C2A-C1A-NA | 3.89 | 115.57 | 109.34 |
| 37 | 11 | 310 | CLA | C1C-C2C-C3C | -3.89 | 102.89 | 106.98 |
| 37 | 38 | 201 | CLA | O2D-CGD-CBD | 3.89 | 118.02 | 111.23 |
| 48 | 34 | 315 | A86 | C25-C24-C1 | -3.89 | 115.71 | 126.36 |
| 37 | 32 | 210 | CLA | C3D-C4D-ND | 3.89 | 116.30 | 109.99 |
| 37 | 31 | 310 | CLA | C3C-C4C-NC | 3.89 | 115.41 | 110.43 |
| 47 | 37 | 305 | KC1 | C3D-C4D-ND | 3.89 | 115.62 | 110.20 |
| 47 | 36 | 304 | KC1 | C2A-C1A-NA | 3.89 | 115.57 | 109.34 |
| 37 | 11 | 310 | CLA | CHD-C1D-ND | -3.88 | 119.34 | 124.80 |
| 47 | 12 | 208 | KC1 | C1C-C2C-C3C | -3.88 | 102.89 | 106.98 |
| 37 | C | 504 | CLA | C1C-C2C-C3C | -3.88 | 102.90 | 106.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 501 | CLA | CHD-C1D-ND | -3.88 | 119.34 | 124.80 |
| 37 | C | 511 | CLA | C3C-C4C-NC | 3.88 | 115.40 | 110.43 |
| 47 | 38 | 205 | KC1 | C1A-NA-C4A | -3.88 | 104.91 | 106.68 |
| 47 | 17 | 306 | KC1 | C2A-C1A-NA | 3.88 | 115.56 | 109.34 |
| 37 | 14 | 307 | CLA | C3D-C4D-ND | 3.88 | 116.30 | 109.99 |
| 37 | 34 | 307 | CLA | C3D-C4D-ND | 3.88 | 116.30 | 109.99 |
| 37 | 40 | 205 | CLA | C3C-C4C-NC | 3.88 | 115.40 | 110.43 |
| 47 | 34 | 304 | KC1 | C2C-C1C-NC | 3.88 | 115.25 | 110.45 |
| 37 | C | 502 | CLA | C3D-C4D-ND | 3.88 | 116.29 | 109.99 |
| 48 | 14 | 315 | A86 | C25-C24-C1 | -3.88 | 115.72 | 126.36 |
| 37 | Z | 102 | CLA | C1C-C2C-C3C | -3.88 | 102.90 | 106.98 |
| 47 | 13 | 302 | KC1 | C1C-C2C-C3C | -3.88 | 102.90 | 106.98 |
| 47 | 12 | 211 | KC1 | C2A-C1A-NA | 3.88 | 115.56 | 109.34 |
| 37 | 16 | 306 | CLA | C3C-C4C-NC | 3.88 | 115.40 | 110.43 |
| 37 | d | 404 | CLA | C1D-CHD-C4C | -3.88 | 117.78 | 126.02 |
| 37 | 33 | 305 | CLA | C1D-CHD-C4C | -3.88 | 117.78 | 126.02 |
| 37 | 38 | 206 | CLA | C1D-CHD-C4C | -3.88 | 117.78 | 126.02 |
| 37 | c | 511 | CLA | C3C-C4C-NC | 3.88 | 115.40 | 110.43 |
| 37 | 14 | 310 | CLA | C4A-NA-C1A | -3.88 | 104.91 | 106.68 |
| 37 | 16 | 307 | CLA | C1C-C2C-C3C | -3.88 | 102.90 | 106.98 |
| 37 | 18 | 201 | CLA | O2D-CGD-CBD | 3.88 | 118.01 | 111.23 |
| 37 | D | 406 | CLA | C1D-CHD-C4C | -3.88 | 117.78 | 126.02 |
| 37 | C | 505 | CLA | C3C-C4C-NC | 3.88 | 115.40 | 110.43 |
| 48 | 16 | 311 | A86 | C40-C32-C31 | -3.88 | 107.00 | 110.47 |
| 48 | 35 | 312 | A86 | C3-C4-C5 | -3.88 | 115.59 | 123.52 |
| 48 | 39 | 311 | A86 | C25-C24-C1 | -3.87 | 115.74 | 126.36 |
| 37 | B | 513 | CLA | C3D-C4D-ND | 3.87 | 116.28 | 109.99 |
| 37 | c | 509 | CLA | CHD-C1D-ND | -3.87 | 119.35 | 124.80 |
| 37 | C | 509 | CLA | CHD-C1D-ND | -3.87 | 119.35 | 124.80 |
| 37 | b | 504 | CLA | C1C-C2C-C3C | -3.87 | 102.91 | 106.98 |
| 47 | 20 | 305 | KC1 | C4C-C3C-C2C | -3.87 | 101.25 | 106.89 |
| 37 | c | 505 | CLA | C3C-C4C-NC | 3.87 | 115.39 | 110.43 |
| 47 | 18 | 205 | KC1 | C2C-C1C-NC | 3.87 | 115.24 | 110.45 |
| 48 | 17 | 314 | A86 | C4-C3-C2 | -3.87 | 115.60 | 123.52 |
| 37 | 17 | 302 | CLA | C4A-NA-C1A | -3.87 | 104.91 | 106.68 |
| 37 | 34 | 302 | CLA | C4A-NA-C1A | -3.87 | 104.91 | 106.68 |
| 47 | 18 | 205 | KC1 | C1A-NA-C4A | -3.87 | 104.91 | 106.68 |
| 37 | 16 | 303 | CLA | C1C-C2C-C3C | -3.87 | 102.91 | 106.98 |
| 37 | 21 | 204 | CLA | C1C-C2C-C3C | -3.87 | 102.91 | 106.98 |
| 50 | 20 | 312 | DD6 | C33-C32-C31 | 3.87 | 117.11 | 109.49 |
| 48 | 15 | 312 | A86 | C3-C4-C5 | -3.87 | 115.60 | 123.52 |
| 37 | 14 | 305 | CLA | C1D-CHD-C4C | -3.87 | 117.80 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 14 | 306 | KC1 | C4B-C3B-C2B | -3.87 | 103.46 | 106.81 |
| 37 | B | 513 | CLA | C4A-NA-C1A | -3.87 | 104.91 | 106.68 |
| 37 | 12 | 209 | CLA | C1D-CHD-C4C | -3.87 | 117.80 | 126.02 |
| 37 | 16 | 303 | CLA | C3B-C4B-NB | 3.87 | 113.98 | 110.53 |
| 37 | 36 | 303 | CLA | C3B-C4B-NB | 3.87 | 113.98 | 110.53 |
| 37 | z | 102 | CLA | C1C-C2C-C3C | -3.87 | 102.91 | 106.98 |
| 47 | 40 | 206 | KC1 | C2A-C1A-NA | 3.87 | 115.54 | 109.34 |
| 37 | C | 508 | CLA | C3C-C4C-NC | 3.87 | 115.38 | 110.43 |
| 48 | 18 | 213 | A86 | C3-C4-C5 | -3.87 | 115.61 | 123.52 |
| 47 | 32 | 209 | KC1 | C1D-CHD-C4C | -3.87 | 117.16 | 126.25 |
| 47 | 32 | 207 | KC1 | C1C-C2C-C3C | -3.86 | 102.92 | 106.98 |
| 37 | c | 506 | CLA | CHC-C1C-C2C | -3.86 | 115.97 | 126.95 |
| 48 | 13 | 315 | A86 | C25-C26-C27 | -3.86 | 121.86 | 127.28 |
| 37 | B | 514 | CLA | O2D-CGD-O1D | -3.86 | 116.33 | 123.85 |
| 37 | 12 | 209 | CLA | C3D-C4D-ND | 3.86 | 116.27 | 109.99 |
| 37 | 32 | 211 | CLA | C1C-C2C-C3C | -3.86 | 102.92 | 106.98 |
| 37 | 32 | 202 | CLA | O2D-CGD-CBD | 3.86 | 117.98 | 111.23 |
| 37 | 13 | 305 | CLA | C1D-CHD-C4C | -3.86 | 117.81 | 126.02 |
| 37 | 14 | 308 | CLA | O2D-CGD-CBD | 3.86 | 117.98 | 111.23 |
| 47 | 36 | 302 | KC1 | C1D-CHD-C4C | -3.86 | 117.17 | 126.25 |
| 47 | 39 | 308 | KC1 | C1C-C2C-C3C | -3.86 | 102.92 | 106.98 |
| 37 | 37 | 301 | CLA | C4A-NA-C1A | -3.86 | 104.92 | 106.68 |
| 47 | 12 | 206 | KC1 | C2C-C1C-NC | 3.86 | 115.23 | 110.45 |
| 37 | b | 507 | CLA | C1D-CHD-C4C | -3.86 | 117.82 | 126.02 |
| 47 | 11 | 306 | KC1 | C1C-C2C-C3C | -3.86 | 102.92 | 106.98 |
| 47 | 17 | 306 | KC1 | C3D-C4D-ND | 3.86 | 115.58 | 110.20 |
| 37 | 19 | 305 | CLA | C1D-CHD-C4C | -3.86 | 117.82 | 126.02 |
| 37 | b | 513 | CLA | C4A-NA-C1A | -3.86 | 104.92 | 106.68 |
| 37 | 34 | 308 | CLA | O2D-CGD-CBD | 3.86 | 117.97 | 111.23 |
| 47 | 20 | 302 | KC1 | C1D-CHD-C4C | -3.86 | 117.18 | 126.25 |
| 48 | 17 | 320 | A86 | C3-C2-C1 | -3.86 | 121.87 | 127.28 |
| 37 | C | 506 | CLA | CHC-C1C-C2C | -3.86 | 115.99 | 126.95 |
| 37 | 35 | 310 | CLA | C1D-CHD-C4C | -3.86 | 117.82 | 126.02 |
| 47 | 20 | 304 | KC1 | C2A-C1A-NA | 3.86 | 115.52 | 109.34 |
| 37 | b | 514 | CLA | O2D-CGD-O1D | -3.86 | 116.34 | 123.85 |
| 47 | 13 | 304 | KC1 | C1D-CHD-C4C | -3.85 | 117.18 | 126.25 |
| 47 | 35 | 309 | KC1 | C1D-CHD-C4C | -3.85 | 117.18 | 126.25 |
| 37 | 11 | 308 | CLA | O2D-CGD-CBD | 3.85 | 117.97 | 111.23 |
| 47 | 31 | 309 | KC1 | C1C-C2C-C3C | -3.85 | 102.93 | 106.98 |
| 47 | 32 | 209 | KC1 | C2A-C1A-NA | 3.85 | 115.52 | 109.34 |
| 37 | 14 | 303 | CLA | C1D-CHD-C4C | -3.85 | 117.83 | 126.02 |
| 37 | 32 | 210 | CLA | C1D-CHD-C4C | -3.85 | 117.83 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 11 | 302 | KC1 | C4B-C3B-C2B | -3.85 | 103.47 | 106.81 |
| 47 | 31 | 303 | KC1 | C4B-C3B-C2B | -3.85 | 103.47 | 106.81 |
| 48 | 12 | 214 | A86 | C12-C11-C13 | 3.85 | 122.25 | 116.00 |
| 47 | 40 | 207 | KC1 | C4C-C3C-C2C | -3.85 | 101.28 | 106.89 |
| 47 | 18 | 207 | KC1 | C1D-CHD-C4C | -3.85 | 117.19 | 126.25 |
| 47 | 12 | 211 | KC1 | C1C-C2C-C3C | -3.85 | 102.93 | 106.98 |
| 48 | 31 | 319 | A86 | C28-C27-C26 | 3.85 | 129.06 | 122.82 |
| 47 | 13 | 302 | KC1 | CBA-CAA-C2A | -3.85 | 109.99 | 125.45 |
| 47 | 33 | 302 | KC1 | CBA-CAA-C2A | -3.85 | 109.99 | 125.45 |
| 37 | 19 | 309 | CLA | C1D-CHD-C4C | -3.85 | 117.83 | 126.02 |
| 47 | 11 | 302 | KC1 | C2C-C1C-NC | 3.85 | 115.22 | 110.45 |
| 47 | 17 | 305 | KC1 | C1A-NA-C4A | -3.85 | 104.92 | 106.68 |
| 47 | 33 | 304 | KC1 | C1C-C2C-C3C | -3.85 | 102.93 | 106.98 |
| 47 | 32 | 212 | KC1 | C2C-C1C-NC | 3.85 | 115.22 | 110.45 |
| 37 | B | 507 | CLA | C1D-CHD-C4C | -3.85 | 117.84 | 126.02 |
| 37 | c | 506 | CLA | C1D-CHD-C4C | -3.85 | 117.84 | 126.02 |
| 48 | 32 | 215 | A86 | C12-C11-C13 | 3.85 | 122.24 | 116.00 |
| 47 | 33 | 304 | KC1 | C2A-C1A-NA | 3.85 | 115.51 | 109.34 |
| 37 | 16 | 301 | CLA | C2C-C1C-NC | 3.85 | 114.02 | 109.98 |
| 37 | B | 504 | CLA | C1C-C2C-C3C | -3.85 | 102.93 | 106.98 |
| 47 | 38 | 207 | KC1 | C2A-C1A-NA | 3.85 | 115.50 | 109.34 |
| 37 | 15 | 308 | CLA | C1C-C2C-C3C | -3.85 | 102.94 | 106.98 |
| 47 | 36 | 304 | KC1 | C1C-C2C-C3C | -3.85 | 102.94 | 106.98 |
| 37 | 36 | 301 | CLA | C2C-C1C-NC | 3.85 | 114.02 | 109.98 |
| 48 | 33 | 313 | A86 | C36-C31-C32 | -3.85 | 115.88 | 119.70 |
| 37 | 36 | 306 | CLA | C3C-C4C-NC | 3.85 | 115.36 | 110.43 |
| 47 | 19 | 308 | KC1 | C4B-C3B-C2B | -3.84 | 103.48 | 106.81 |
| 37 | 39 | 305 | CLA | C1D-CHD-C4C | -3.84 | 117.85 | 126.02 |
| 48 | 12 | 217 | A86 | C35-C34-C33 | 3.84 | 116.79 | 109.89 |
| 37 | 41 | 204 | CLA | C1C-C2C-C3C | -3.84 | 102.94 | 106.98 |
| 37 | 13 | 305 | CLA | C4A-NA-C1A | -3.84 | 104.93 | 106.68 |
| 47 | 16 | 304 | KC1 | C1C-C2C-C3C | -3.84 | 102.94 | 106.98 |
| 47 | 33 | 304 | KC1 | C1D-CHD-C4C | -3.84 | 117.21 | 126.25 |
| 47 | 40 | 204 | KC1 | C1D-CHD-C4C | -3.84 | 117.22 | 126.25 |
| 37 | 34 | 303 | CLA | C1D-CHD-C4C | -3.84 | 117.86 | 126.02 |
| 48 | 37 | 310 | A86 | C36-C31-C32 | -3.84 | 115.89 | 119.70 |
| 48 | 34 | 314 | A86 | C41-C32-C31 | -3.84 | 107.04 | 110.47 |
| 37 | 19 | 309 | CLA | C1C-C2C-C3C | -3.84 | 102.94 | 106.98 |
| 50 | 21 | 212 | DD6 | O1-C15-C14 | -3.84 | 105.88 | 116.88 |
| 48 | 33 | 315 | A86 | C25-C26-C27 | -3.84 | 121.90 | 127.28 |
| 47 | 35 | 306 | KC1 | CBA-CAA-C2A | -3.84 | 110.06 | 125.45 |
| 37 | C | 506 | CLA | C1D-CHD-C4C | -3.84 | 117.87 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 516 | CLA | C4C-C3C-C2C | -3.83 | 101.31 | 106.89 |
| 47 | 13 | 304 | KC1 | C2A-C1A-NA | 3.83 | 115.48 | 109.34 |
| 37 | 41 | 202 | CLA | C1D-CHD-C4C | -3.83 | 117.88 | 126.02 |
| 47 | 21 | 207 | KC1 | C1D-CHD-C4C | -3.83 | 117.24 | 126.25 |
| 37 | c | 508 | CLA | CHD-C1D-ND | -3.83 | 119.41 | 124.80 |
| 37 | c | 511 | CLA | C3B-C4B-NB | 3.83 | 113.95 | 110.53 |
| 37 | 14 | 302 | CLA | C1C-C2C-C3C | -3.83 | 102.95 | 106.98 |
| 47 | 12 | 208 | KC1 | C1D-CHD-C4C | -3.83 | 117.24 | 126.25 |
| 37 | 36 | 303 | CLA | C1C-C2C-C3C | -3.83 | 102.95 | 106.98 |
| 37 | 32 | 206 | CLA | CBA-CAA-C2A | 3.83 | 125.19 | 113.79 |
| 48 | 12 | 217 | A86 | C25-C26-C27 | -3.83 | 121.91 | 127.28 |
| 47 | 15 | 309 | KC1 | C1D-CHD-C4C | -3.83 | 117.25 | 126.25 |
| 47 | 34 | 306 | KC1 | C2A-C1A-NA | 3.83 | 115.47 | 109.34 |
| 37 | 11 | 303 | CLA | CBA-CAA-C2A | 3.83 | 125.18 | 113.79 |
| 37 | 38 | 204 | CLA | C1D-CHD-C4C | -3.83 | 117.89 | 126.02 |
| 37 | 41 | 204 | CLA | C1D-CHD-C4C | -3.83 | 117.89 | 126.02 |
| 37 | C | 508 | CLA | CHD-C1D-ND | -3.83 | 119.42 | 124.80 |
| 48 | 36 | 310 | A86 | C26-C25-C24 | -3.83 | 112.12 | 123.20 |
| 37 | 34 | 305 | CLA | C1C-C2C-C3C | -3.82 | 102.96 | 106.98 |
| 47 | 19 | 308 | KC1 | C1C-C2C-C3C | -3.82 | 102.96 | 106.98 |
| 47 | 41 | 203 | KC1 | C1C-C2C-C3C | -3.82 | 102.96 | 106.98 |
| 37 | 18 | 209 | CLA | C4A-NA-C1A | -3.82 | 104.93 | 106.68 |
| 37 | 19 | 301 | CLA | C4A-NA-C1A | -3.82 | 104.93 | 106.68 |
| 37 | 33 | 305 | CLA | C4A-NA-C1A | -3.82 | 104.93 | 106.68 |
| 47 | 15 | 306 | KC1 | CBA-CAA-C2A | -3.82 | 110.10 | 125.45 |
| 37 | 33 | 308 | CLA | C1D-CHD-C4C | -3.82 | 117.89 | 126.02 |
| 48 | 32 | 218 | A86 | C35-C34-C33 | 3.82 | 116.75 | 109.89 |
| 47 | 35 | 309 | KC1 | C2C-C1C-NC | 3.82 | 115.18 | 110.45 |
| 37 | B | 516 | CLA | C4C-C3C-C2C | -3.82 | 101.33 | 106.89 |
| 47 | 41 | 207 | KC1 | C1D-CHD-C4C | -3.82 | 117.26 | 126.25 |
| 47 | 16 | 302 | KC1 | C1D-CHD-C4C | -3.82 | 117.26 | 126.25 |
| 48 | 11 | 319 | A86 | C28-C27-C26 | 3.82 | 129.01 | 122.82 |
| 47 | 12 | 208 | KC1 | C2A-C1A-NA | 3.82 | 115.46 | 109.34 |
| 47 | 31 | 307 | KC1 | CBA-CAA-C2A | -3.82 | 110.12 | 125.45 |
| 48 | 32 | 218 | A86 | C25-C26-C27 | -3.82 | 121.92 | 127.28 |
| 37 | 18 | 209 | CLA | O2D-CGD-CBD | 3.82 | 117.91 | 111.23 |
| 37 | 17 | 304 | CLA | C3B-C4B-NB | 3.82 | 113.94 | 110.53 |
| 47 | 33 | 304 | KC1 | C1A-NA-C4A | -3.82 | 104.94 | 106.68 |
| 48 | 16 | 310 | A86 | C26-C25-C24 | -3.82 | 112.14 | 123.20 |
| 50 | 20 | 310 | DD6 | O1-C15-C14 | -3.82 | 105.94 | 116.88 |
| 37 | 31 | 302 | CLA | C3C-C4C-NC | 3.82 | 115.32 | 110.43 |
| 50 | 41 | 212 | DD6 | O1-C15-C14 | -3.82 | 105.94 | 116.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 205 | CLA | CBA-CAA-C2A | 3.82 | 125.15 | 113.79 |
| 47 | 14 | 306 | KC1 | C2A-C1A-NA | 3.82 | 115.46 | 109.34 |
| 37 | c | 510 | CLA | CHD-C1D-ND | -3.82 | 119.43 | 124.80 |
| 37 | b | 514 | CLA | C3C-C4C-NC | 3.82 | 115.32 | 110.43 |
| 47 | 14 | 309 | KC1 | C1D-CHD-C4C | -3.81 | 117.28 | 126.25 |
| 44 | j | 101 | DGD | O3G-C3G-C2G | -3.81 | 101.54 | 110.82 |
| 37 | C | 508 | CLA | C4A-NA-C1A | -3.81 | 104.94 | 106.68 |
| 48 | 14 | 314 | A86 | C41-C32-C31 | -3.81 | 107.06 | 110.47 |
| 37 | 21 | 202 | CLA | C1D-CHD-C4C | -3.81 | 117.92 | 126.02 |
| 37 | 21 | 204 | CLA | C1D-CHD-C4C | -3.81 | 117.92 | 126.02 |
| 47 | 34 | 309 | KC1 | C1D-CHD-C4C | -3.81 | 117.28 | 126.25 |
| 37 | 17 | 307 | CLA | CHD-C1D-ND | -3.81 | 119.44 | 124.80 |
| 37 | 31 | 304 | CLA | CBA-CAA-C2A | 3.81 | 125.13 | 113.79 |
| 47 | 16 | 305 | KC1 | C4B-C3B-C2B | -3.81 | 103.51 | 106.81 |
| 37 | C | 510 | CLA | CHD-C1D-ND | -3.81 | 119.44 | 124.80 |
| 47 | 32 | 207 | KC1 | C2C-C1C-NC | 3.81 | 115.17 | 110.45 |
| 37 | B | 509 | CLA | C3D-C4D-ND | 3.81 | 116.18 | 109.99 |
| 48 | 11 | 314 | A86 | C12-C11-C13 | 3.81 | 122.17 | 116.00 |
| 37 | 11 | 305 | CLA | C1D-CHD-C4C | -3.81 | 117.93 | 126.02 |
| 47 | 15 | 309 | KC1 | C2C-C1C-NC | 3.81 | 115.16 | 110.45 |
| 47 | 20 | 304 | KC1 | CAC-C3C-C4C | 3.81 | 129.74 | 124.79 |
| 37 | 13 | 308 | CLA | C1D-CHD-C4C | -3.81 | 117.93 | 126.02 |
| 50 | 41 | 212 | DD6 | C25-C26-C27 | 3.81 | 137.27 | 126.61 |
| 37 | a | 407 | CLA | C1D-CHD-C4C | -3.81 | 117.93 | 126.02 |
| 47 | 21 | 203 | KC1 | C1C-C2C-C3C | -3.81 | 102.98 | 106.98 |
| 48 | 17 | 320 | A86 | C10-C9-C8 | -3.80 | 112.17 | 123.20 |
| 37 | b | 509 | CLA | C3D-C4D-ND | 3.80 | 116.17 | 109.99 |
| 48 | 21 | 214 | A86 | C25-C26-C27 | -3.80 | 121.94 | 127.28 |
| 37 | B | 513 | CLA | C1D-CHD-C4C | -3.80 | 117.93 | 126.02 |
| 37 | 16 | 307 | CLA | C4A-NA-C1A | -3.80 | 104.94 | 106.68 |
| 37 | b | 513 | CLA | C1D-CHD-C4C | -3.80 | 117.94 | 126.02 |
| 37 | 20 | 303 | CLA | C3C-C4C-NC | 3.80 | 115.30 | 110.43 |
| 47 | 36 | 305 | KC1 | C4B-C3B-C2B | -3.80 | 103.52 | 106.81 |
| 47 | 16 | 308 | KC1 | C1C-C2C-C3C | -3.80 | 102.98 | 106.98 |
| 50 | 21 | 216 | DD6 | C35-C36-C31 | -3.80 | 112.59 | 120.50 |
| 37 | A | 405 | CLA | C1D-CHD-C4C | -3.80 | 117.94 | 126.02 |
| 37 | D | 401 | CLA | C1D-CHD-C4C | -3.80 | 117.94 | 126.02 |
| 37 | 32 | 206 | CLA | C1D-CHD-C4C | -3.80 | 117.94 | 126.02 |
| 37 | C | 511 | CLA | C3B-C4B-NB | 3.80 | 113.92 | 110.53 |
| 37 | B | 514 | CLA | C3C-C4C-NC | 3.80 | 115.30 | 110.43 |
| 37 | 18 | 204 | CLA | C1D-CHD-C4C | -3.80 | 117.94 | 126.02 |
| 37 | 39 | 309 | CLA | C1D-CHD-C4C | -3.80 | 117.94 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | J | 101 | DGD | O3G-C3G-C2G | -3.80 | 101.58 | 110.82 |
| 37 | b | 504 | CLA | C4A-NA-C1A | -3.80 | 104.95 | 106.68 |
| 37 | 36 | 307 | CLA | C4A-NA-C1A | -3.80 | 104.95 | 106.68 |
| 50 | 40 | 212 | DD6 | O1-C15-C14 | -3.80 | 106.00 | 116.88 |
| 47 | 40 | 206 | KC1 | CAC-C3C-C4C | 3.80 | 129.73 | 124.79 |
| 37 | 34 | 302 | CLA | CHD-C1D-ND | -3.80 | 119.46 | 124.80 |
| 37 | B | 508 | CLA | C1C-C2C-C3C | -3.80 | 102.99 | 106.98 |
| 47 | 11 | 309 | KC1 | C1C-C2C-C3C | -3.80 | 102.99 | 106.98 |
| 48 | 11 | 314 | A86 | C25-C26-C27 | -3.80 | 121.95 | 127.28 |
| 37 | C | 502 | CLA | C3C-C4C-NC | 3.80 | 115.29 | 110.43 |
| 48 | 17 | 315 | A86 | C35-C34-C33 | 3.80 | 116.70 | 109.89 |
| 47 | 11 | 306 | KC1 | CBA-CAA-C2A | -3.80 | 110.22 | 125.45 |
| 47 | 14 | 304 | KC1 | CBA-CAA-C2A | -3.79 | 110.22 | 125.45 |
| 37 | 39 | 305 | CLA | CMB-C2B-C1B | 3.79 | 131.20 | 125.42 |
| 37 | 32 | 205 | CLA | C3D-C4D-ND | 3.79 | 116.15 | 109.99 |
| 47 | 18 | 207 | KC1 | O2D-CGD-O1D | -3.79 | 116.47 | 123.85 |
| 37 | B | 516 | CLA | CHD-C1D-ND | -3.79 | 119.47 | 124.80 |
| 37 | 14 | 305 | CLA | C1C-C2C-C3C | -3.79 | 102.99 | 106.98 |
| 47 | 34 | 304 | KC1 | CBA-CAA-C2A | -3.79 | 110.23 | 125.45 |
| 37 | a | 404 | CLA | C1D-CHD-C4C | -3.79 | 117.96 | 126.02 |
| 37 | 13 | 303 | CLA | C3B-C4B-NB | 3.79 | 113.91 | 110.53 |
| 47 | 37 | 307 | KC1 | C4B-C3B-C2B | -3.79 | 103.53 | 106.81 |
| 48 | 37 | 314 | A86 | C35-C34-C33 | 3.79 | 116.69 | 109.89 |
| 37 | c | 505 | CLA | C3D-C2D-C1D | -3.79 | 100.66 | 105.83 |
| 47 | 32 | 212 | KC1 | CBA-CAA-C2A | -3.79 | 110.25 | 125.45 |
| 50 | 41 | 216 | DD6 | C35-C36-C31 | -3.79 | 112.62 | 120.50 |
| 37 | 34 | 302 | CLA | C1C-C2C-C3C | -3.79 | 103.00 | 106.98 |
| 37 | 35 | 308 | CLA | C3B-C2B-C1B | -3.79 | 102.71 | 107.17 |
| 48 | 37 | 313 | A86 | C4-C3-C2 | -3.79 | 115.77 | 123.52 |
| 47 | 37 | 304 | KC1 | C3C-C4C-NC | 3.79 | 113.96 | 109.90 |
| 48 | 13 | 313 | A86 | C36-C31-C32 | -3.78 | 115.94 | 119.70 |
| 47 | 14 | 304 | KC1 | C1D-CHD-C4C | -3.78 | 117.35 | 126.25 |
| 47 | 12 | 211 | KC1 | CBA-CAA-C2A | -3.78 | 110.26 | 125.45 |
| 47 | 18 | 207 | KC1 | CBA-CAA-C2A | -3.78 | 110.27 | 125.45 |
| 37 | 19 | 305 | CLA | C3C-C4C-NC | 3.78 | 115.28 | 110.43 |
| 37 | b | 508 | CLA | C1C-C2C-C3C | -3.78 | 103.00 | 106.98 |
| 48 | 31 | 314 | A86 | C12-C11-C13 | 3.78 | 122.13 | 116.00 |
| 50 | 21 | 212 | DD6 | C25-C26-C27 | 3.78 | 137.19 | 126.61 |
| 48 | 31 | 314 | A86 | C25-C26-C27 | -3.78 | 121.97 | 127.28 |
| 37 | C | 505 | CLA | C3D-C2D-C1D | -3.78 | 100.67 | 105.83 |
| 48 | 15 | 314 | A86 | C36-C31-C32 | -3.78 | 115.94 | 119.70 |
| 47 | 41 | 207 | KC1 | CHC-C1C-C2C | -3.78 | 119.06 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 512 | CLA | CMD-C2D-C1D | 3.78 | 131.39 | 124.73 |
| 37 | 11 | 301 | CLA | C3C-C4C-NC | 3.78 | 115.27 | 110.43 |
| 48 | 38 | 215 | A86 | C25-C26-C27 | -3.78 | 121.98 | 127.28 |
| 37 | b | 504 | CLA | C3D-C2D-C1D | -3.78 | 100.67 | 105.83 |
| 50 | 20 | 312 | DD6 | C21-C20-C19 | -3.78 | 110.00 | 114.24 |
| 37 | 39 | 307 | CLA | C1C-C2C-C3C | -3.78 | 103.01 | 106.98 |
| 47 | 17 | 308 | KC1 | C4B-C3B-C2B | -3.78 | 103.54 | 106.81 |
| 37 | a | 407 | CLA | C1C-C2C-C3C | -3.78 | 103.01 | 106.98 |
| 37 | 31 | 306 | CLA | C1D-CHD-C4C | -3.78 | 117.99 | 126.02 |
| 37 | c | 509 | CLA | CAA-C2A-C3A | -3.78 | 102.79 | 113.00 |
| 47 | 34 | 304 | KC1 | C1D-CHD-C4C | -3.78 | 117.36 | 126.25 |
| 47 | 20 | 305 | KC1 | C1A-NA-C4A | -3.78 | 104.96 | 106.68 |
| 37 | 38 | 202 | CLA | C3C-C4C-NC | 3.78 | 115.27 | 110.43 |
| 37 | 12 | 204 | CLA | C3D-C4D-ND | 3.78 | 116.12 | 109.99 |
| 48 | 15 | 313 | A86 | C41-C32-C31 | -3.77 | 107.09 | 110.47 |
| 47 | 38 | 207 | KC1 | CBA-CAA-C2A | -3.77 | 110.30 | 125.45 |
| 37 | 17 | 307 | CLA | C4A-NA-C1A | -3.77 | 104.96 | 106.68 |
| 47 | 36 | 304 | KC1 | C2C-C1C-NC | 3.77 | 115.12 | 110.45 |
| 37 | C | 512 | CLA | CHD-C1D-ND | -3.77 | 119.49 | 124.80 |
| 47 | 16 | 304 | KC1 | C2C-C1C-NC | 3.77 | 115.12 | 110.45 |
| 47 | 12 | 211 | KC1 | C1D-CHD-C4C | -3.77 | 117.38 | 126.25 |
| 47 | 13 | 302 | KC1 | C1D-CHD-C4C | -3.77 | 117.38 | 126.25 |
| 37 | 19 | 305 | CLA | CMB-C2B-C1B | 3.77 | 131.16 | 125.42 |
| 37 | 37 | 306 | CLA | CHD-C1D-ND | -3.77 | 119.49 | 124.80 |
| 47 | 37 | 304 | KC1 | C1C-C2C-C3C | -3.77 | 103.01 | 106.98 |
| 37 | b | 515 | CLA | C3C-C4C-NC | 3.77 | 115.26 | 110.43 |
| 37 | c | 511 | CLA | C3D-C4D-ND | 3.77 | 116.12 | 109.99 |
| 37 | 19 | 301 | CLA | C1D-CHD-C4C | -3.77 | 118.00 | 126.02 |
| 37 | B | 504 | CLA | C3D-C2D-C1D | -3.77 | 100.69 | 105.83 |
| 37 | 34 | 303 | CLA | C3B-C4B-NB | 3.77 | 113.90 | 110.53 |
| 48 | 11 | 311 | A86 | C3-C2-C1 | -3.77 | 121.99 | 127.28 |
| 37 | 31 | 306 | CLA | C4A-NA-C1A | -3.77 | 104.96 | 106.68 |
| 37 | 19 | 309 | CLA | CHD-C1D-ND | -3.77 | 119.50 | 124.80 |
| 37 | 14 | 302 | CLA | CHD-C1D-ND | -3.77 | 119.50 | 124.80 |
| 47 | 35 | 304 | KC1 | CBA-CAA-C2A | -3.77 | 110.33 | 125.45 |
| 37 | 31 | 304 | CLA | C1D-CHD-C4C | -3.77 | 118.01 | 126.02 |
| 37 | b | 515 | CLA | CAC-C3C-C4C | 3.77 | 129.69 | 124.79 |
| 47 | 32 | 212 | KC1 | C1D-CHD-C4C | -3.77 | 117.39 | 126.25 |
| 47 | 37 | 304 | KC1 | CAC-C3C-C4C | 3.77 | 129.69 | 124.79 |
| 48 | 37 | 319 | A86 | C10-C9-C8 | -3.77 | 112.28 | 123.20 |
| 48 | 41 | 214 | A86 | C25-C26-C27 | -3.77 | 122.00 | 127.28 |
| 47 | 36 | 308 | KC1 | C1C-C2C-C3C | -3.77 | 103.02 | 106.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 40 | 205 | CLA | CHD-C1D-ND | -3.77 | 119.50 | 124.80 |
| 37 | 20 | 303 | CLA | CHD-C1D-ND | -3.76 | 119.50 | 124.80 |
| 47 | 36 | 308 | KC1 | C2A-C1A-NA | 3.76 | 115.37 | 109.34 |
| 47 | 31 | 309 | KC1 | C4B-C3B-C2B | -3.76 | 103.55 | 106.81 |
| 37 | C | 509 | CLA | C1C-C2C-C3C | -3.76 | 103.02 | 106.98 |
| 37 | 14 | 303 | CLA | C3B-C4B-NB | 3.76 | 113.89 | 110.53 |
| 37 | b | 504 | CLA | O2A-CGA-CBA | 3.76 | 123.31 | 111.83 |
| 37 | d | 403 | CLA | C3C-C4C-NC | 3.76 | 115.25 | 110.43 |
| 37 | c | 509 | CLA | C1C-C2C-C3C | -3.76 | 103.02 | 106.98 |
| 47 | 34 | 306 | KC1 | C4B-C3B-C2B | -3.76 | 103.55 | 106.81 |
| 39 | C | 519 | BCR | C24-C23-C22 | -3.76 | 120.67 | 126.23 |
| 37 | C | 509 | CLA | CAA-C2A-C3A | -3.76 | 102.83 | 113.00 |
| 37 | 19 | 302 | CLA | C1D-CHD-C4C | -3.76 | 118.03 | 126.02 |
| 47 | 17 | 308 | KC1 | C1D-CHD-C4C | -3.76 | 117.40 | 126.25 |
| 47 | 37 | 307 | KC1 | C1D-CHD-C4C | -3.76 | 117.40 | 126.25 |
| 48 | 11 | 312 | A86 | C25-C26-C27 | -3.76 | 122.00 | 127.28 |
| 37 | c | 502 | CLA | C3C-C4C-NC | 3.76 | 115.25 | 110.43 |
| 48 | 33 | 311 | A86 | C12-C11-C13 | 3.76 | 122.10 | 116.00 |
| 50 | 40 | 214 | DD6 | C21-C20-C19 | -3.76 | 110.02 | 114.24 |
| 47 | 16 | 308 | KC1 | C2A-C1A-NA | 3.76 | 115.37 | 109.34 |
| 39 | c | 519 | BCR | C24-C23-C22 | -3.76 | 120.67 | 126.23 |
| 37 | 18 | 211 | CLA | C3B-C4B-NB | 3.76 | 113.89 | 110.53 |
| 37 | 37 | 303 | CLA | C3B-C4B-NB | 3.76 | 113.89 | 110.53 |
| 37 | b | 516 | CLA | CHD-C1D-ND | -3.76 | 119.51 | 124.80 |
| 37 | 18 | 209 | CLA | C3C-C4C-NC | 3.76 | 115.25 | 110.43 |
| 37 | 39 | 305 | CLA | C3C-C4C-NC | 3.76 | 115.25 | 110.43 |
| 37 | b | 512 | CLA | CMD-C2D-C1D | 3.76 | 131.35 | 124.73 |
| 47 | 21 | 207 | KC1 | CHC-C1C-C2C | -3.76 | 119.09 | 125.03 |
| 37 | 39 | 301 | CLA | C1D-CHD-C4C | -3.76 | 118.03 | 126.02 |
| 47 | 15 | 304 | KC1 | CBA-CAA-C2A | -3.76 | 110.37 | 125.45 |
| 37 | 14 | 303 | CLA | C1C-C2C-C3C | -3.76 | 103.03 | 106.98 |
| 37 | 14 | 302 | CLA | C4A-NA-C1A | -3.76 | 104.97 | 106.68 |
| 37 | C | 512 | CLA | C1D-CHD-C4C | -3.76 | 118.04 | 126.02 |
| 37 | 13 | 303 | CLA | C1D-CHD-C4C | -3.76 | 118.04 | 126.02 |
| 47 | 13 | 304 | KC1 | C1A-NA-C4A | -3.75 | 104.97 | 106.68 |
| 48 | 18 | 215 | A86 | C25-C26-C27 | -3.75 | 122.01 | 127.28 |
| 37 | c | 512 | CLA | C1D-CHD-C4C | -3.75 | 118.04 | 126.02 |
| 37 | 20 | 306 | CLA | CAC-C3C-C4C | 3.75 | 129.67 | 124.79 |
| 48 | 35 | 314 | A86 | C36-C31-C32 | -3.75 | 115.97 | 119.70 |
| 37 | B | 501 | CLA | C1D-CHD-C4C | -3.75 | 118.04 | 126.02 |
| 37 | 32 | 202 | CLA | CAC-C3C-C4C | 3.75 | 129.67 | 124.79 |
| 37 | 15 | 301 | CLA | C1C-C2C-C3C | -3.75 | 103.03 | 106.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 35 | 301 | CLA | C1C-C2C-C3C | -3.75 | 103.03 | 106.98 |
| 47 | 33 | 302 | KC1 | C1D-CHD-C4C | -3.75 | 117.42 | 126.25 |
| 37 | B | 502 | CLA | C1D-CHD-C4C | -3.75 | 118.05 | 126.02 |
| 37 | b | 501 | CLA | C1D-CHD-C4C | -3.75 | 118.05 | 126.02 |
| 37 | B | 504 | CLA | O2A-CGA-CBA | 3.75 | 123.27 | 111.83 |
| 48 | 14 | 314 | A86 | C3-C4-C5 | -3.75 | 115.84 | 123.52 |
| 37 | 39 | 302 | CLA | C1D-CHD-C4C | -3.75 | 118.05 | 126.02 |
| 47 | 41 | 203 | KC1 | CBA-CAA-C2A | -3.75 | 110.40 | 125.45 |
| 37 | 11 | 308 | CLA | C1D-CHD-C4C | -3.75 | 118.05 | 126.02 |
| 37 | 32 | 202 | CLA | C1D-CHD-C4C | -3.75 | 118.05 | 126.02 |
| 40 | L | 101 | SQD | C1-O5-C5 | 3.75 | 121.04 | 113.72 |
| 37 | B | 515 | CLA | C3B-C4B-NB | 3.75 | 113.88 | 110.53 |
| 47 | 21 | 203 | KC1 | CBA-CAA-C2A | -3.75 | 110.41 | 125.45 |
| 37 | C | 511 | CLA | C3D-C4D-ND | 3.75 | 116.08 | 109.99 |
| 37 | 13 | 307 | CLA | C1C-C2C-C3C | -3.75 | 103.04 | 106.98 |
| 37 | 33 | 307 | CLA | C1C-C2C-C3C | -3.75 | 103.04 | 106.98 |
| 37 | 37 | 301 | CLA | C1C-C2C-C3C | -3.75 | 103.04 | 106.98 |
| 47 | 11 | 309 | KC1 | C1D-CHD-C4C | -3.75 | 117.43 | 126.25 |
| 47 | 31 | 309 | KC1 | C1D-CHD-C4C | -3.75 | 117.43 | 126.25 |
| 37 | 17 | 304 | CLA | CBA-CAA-C2A | 3.75 | 124.95 | 113.79 |
| 37 | 38 | 209 | CLA | C3C-C4C-NC | 3.75 | 115.23 | 110.43 |
| 37 | 12 | 204 | CLA | C4A-NA-C1A | -3.75 | 104.97 | 106.68 |
| 37 | 41 | 208 | CLA | C4A-NA-C1A | -3.75 | 104.97 | 106.68 |
| 37 | 38 | 206 | CLA | C1C-C2C-C3C | -3.75 | 103.04 | 106.98 |
| 37 | b | 502 | CLA | C1D-CHD-C4C | -3.74 | 118.06 | 126.02 |
| 48 | 34 | 314 | A86 | C3-C4-C5 | -3.74 | 115.86 | 123.52 |
| 37 | A | 405 | CLA | C1C-C2C-C3C | -3.74 | 103.04 | 106.98 |
| 37 | 11 | 308 | CLA | C1C-C2C-C3C | -3.74 | 103.04 | 106.98 |
| 37 | 39 | 305 | CLA | C1C-C2C-C3C | -3.74 | 103.04 | 106.98 |
| 37 | B | 515 | CLA | CAC-C3C-C4C | 3.74 | 129.66 | 124.79 |
| 47 | 17 | 305 | KC1 | C4B-C3B-C2B | -3.74 | 103.57 | 106.81 |
| 37 | 32 | 202 | CLA | C1C-C2C-C3C | -3.74 | 103.04 | 106.98 |
| 37 | C | 502 | CLA | C3B-C4B-NB | 3.74 | 113.87 | 110.53 |
| 37 | D | 405 | CLA | C3C-C4C-NC | 3.74 | 115.22 | 110.43 |
| 37 | 12 | 212 | CLA | CHD-C1D-ND | -3.74 | 119.54 | 124.80 |
| 37 | 40 | 208 | CLA | CAC-C3C-C4C | 3.74 | 129.66 | 124.79 |
| 47 | 36 | 304 | KC1 | C1D-CHD-C4C | -3.74 | 117.45 | 126.25 |
| 37 | 11 | 308 | CLA | CAC-C3C-C4C | 3.74 | 129.66 | 124.79 |
| 48 | 37 | 312 | A86 | C3-C4-C5 | -3.74 | 115.86 | 123.52 |
| 37 | 40 | 203 | CLA | C3C-C4C-NC | 3.74 | 115.22 | 110.43 |
| 37 | b | 515 | CLA | C3B-C4B-NB | 3.74 | 113.87 | 110.53 |
| 37 | 39 | 306 | CLA | C3C-C4C-NC | 3.74 | 115.22 | 110.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 503 | CLA | C1C-C2C-C3C | -3.74 | 103.05 | 106.98 |
| 37 | 15 | 303 | CLA | C1D-CHD-C4C | -3.74 | 118.07 | 126.02 |
| 37 | 41 | 205 | CLA | C1D-CHD-C4C | -3.74 | 118.07 | 126.02 |
| 37 | 32 | 213 | CLA | CHD-C1D-ND | -3.74 | 119.54 | 124.80 |
| 48 | 15 | 316 | A86 | C25-C26-C27 | -3.74 | 122.04 | 127.28 |
| 48 | 36 | 311 | A86 | C35-C34-C33 | 3.74 | 116.60 | 109.89 |
| 37 | 19 | 306 | CLA | C3C-C4C-NC | 3.74 | 115.22 | 110.43 |
| 37 | 33 | 307 | CLA | C4A-NA-C1A | -3.74 | 104.97 | 106.68 |
| 47 | 33 | 309 | KC1 | C1D-CHD-C4C | -3.74 | 117.46 | 126.25 |
| 37 | 41 | 204 | CLA | CBA-CAA-C2A | 3.74 | 124.91 | 113.79 |
| 37 | 11 | 303 | CLA | C1D-CHD-C4C | -3.74 | 118.08 | 126.02 |
| 48 | 18 | 214 | A86 | C3-C4-C5 | -3.74 | 115.87 | 123.52 |
| 37 | b | 508 | CLA | C1D-CHD-C4C | -3.74 | 118.08 | 126.02 |
| 37 | 21 | 204 | CLA | CBA-CAA-C2A | 3.73 | 124.91 | 113.79 |
| 48 | 16 | 311 | A86 | C35-C34-C33 | 3.73 | 116.59 | 109.89 |
| 37 | B | 502 | CLA | C1C-C2C-C3C | -3.73 | 103.05 | 106.98 |
| 47 | 16 | 304 | KC1 | C1D-CHD-C4C | -3.73 | 117.47 | 126.25 |
| 37 | b | 502 | CLA | C1C-C2C-C3C | -3.73 | 103.05 | 106.98 |
| 47 | 36 | 304 | KC1 | CBA-CAA-C2A | -3.73 | 110.47 | 125.45 |
| 37 | 37 | 303 | CLA | CBA-CAA-C2A | 3.73 | 124.90 | 113.79 |
| 47 | 38 | 205 | KC1 | C4B-C3B-C2B | -3.73 | 103.58 | 106.81 |
| 47 | 16 | 305 | KC1 | C1A-NA-C4A | -3.73 | 104.98 | 106.68 |
| 37 | 38 | 203 | CLA | C1C-C2C-C3C | -3.73 | 103.05 | 106.98 |
| 47 | 35 | 309 | KC1 | C1C-C2C-C3C | -3.73 | 103.05 | 106.98 |
| 48 | 31 | 311 | A86 | C3-C2-C1 | -3.73 | 122.04 | 127.28 |
| 47 | 21 | 207 | KC1 | CAA-CBA-CGA | -3.73 | 108.07 | 127.05 |
| 48 | 35 | 313 | A86 | C25-C26-C27 | -3.73 | 122.05 | 127.28 |
| 37 | b | 501 | CLA | CAC-C3C-C4C | 3.73 | 129.65 | 124.79 |
| 47 | 38 | 207 | KC1 | O2D-CGD-O1D | -3.73 | 116.59 | 123.85 |
| 47 | 16 | 304 | KC1 | CBA-CAA-C2A | -3.73 | 110.48 | 125.45 |
| 47 | 16 | 304 | KC1 | C1A-NA-C4A | -3.73 | 104.98 | 106.68 |
| 47 | 41 | 207 | KC1 | CAA-CBA-CGA | -3.73 | 108.08 | 127.05 |
| 47 | 14 | 306 | KC1 | C1D-CHD-C4C | -3.73 | 117.48 | 126.25 |
| 37 | 18 | 211 | CLA | C3C-C4C-NC | 3.73 | 115.21 | 110.43 |
| 37 | 18 | 211 | CLA | CAC-C3C-C4C | 3.73 | 129.64 | 124.79 |
| 37 | 40 | 210 | CLA | C3C-C4C-NC | 3.73 | 115.21 | 110.43 |
| 37 | 41 | 208 | CLA | C1C-C2C-C3C | -3.73 | 103.06 | 106.98 |
| 37 | 37 | 306 | CLA | C1D-CHD-C4C | -3.73 | 118.10 | 126.02 |
| 37 | z | 101 | CLA | C1C-C2C-C3C | -3.73 | 103.06 | 106.98 |
| 47 | 13 | 309 | KC1 | C1D-CHD-C4C | -3.73 | 117.48 | 126.25 |
| 37 | 21 | 204 | CLA | CAC-C3C-C4C | 3.73 | 129.64 | 124.79 |
| 37 | 15 | 308 | CLA | C1D-CHD-C4C | -3.73 | 118.10 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 503 | CLA | C1C-C2C-C3C | -3.73 | 103.06 | 106.98 |
| 37 | b | 501 | CLA | C1C-C2C-C3C | -3.73 | 103.06 | 106.98 |
| 47 | 32 | 207 | KC1 | C1D-CHD-C4C | -3.73 | 117.48 | 126.25 |
| 37 | 18 | 201 | CLA | C1D-CHD-C4C | -3.73 | 118.10 | 126.02 |
| 37 | 11 | 307 | CLA | CHD-C1D-ND | -3.73 | 119.56 | 124.80 |
| 37 | c | 502 | CLA | C3B-C4B-NB | 3.73 | 113.86 | 110.53 |
| 48 | 13 | 311 | A86 | C12-C11-C13 | 3.73 | 122.04 | 116.00 |
| 47 | 39 | 308 | KC1 | C2C-C1C-NC | 3.73 | 115.06 | 110.45 |
| 47 | 38 | 210 | KC1 | C1D-CHD-C4C | -3.72 | 117.49 | 126.25 |
| 37 | 20 | 301 | CLA | C3C-C4C-NC | 3.72 | 115.20 | 110.43 |
| 48 | 12 | 213 | A86 | C4-C5-C6 | -3.72 | 122.06 | 127.28 |
| 37 | 21 | 210 | CLA | C1C-C2C-C3C | -3.72 | 103.06 | 106.98 |
| 37 | 37 | 306 | CLA | C4A-NA-C1A | -3.72 | 104.98 | 106.68 |
| 37 | 32 | 211 | CLA | CHD-C1D-ND | -3.72 | 119.56 | 124.80 |
| 40 | a | 409 | SQD | O47-C7-C8 | 3.72 | 119.54 | 111.48 |
| 40 | B | 519 | SQD | C1-O5-C5 | 3.72 | 120.99 | 113.72 |
| 37 | 35 | 303 | CLA | C1D-CHD-C4C | -3.72 | 118.11 | 126.02 |
| 48 | 32 | 214 | A86 | C4-C5-C6 | -3.72 | 122.06 | 127.28 |
| 37 | B | 515 | CLA | C3C-C4C-NC | 3.72 | 115.20 | 110.43 |
| 37 | b | 511 | CLA | O2D-CGD-CBD | 3.72 | 117.74 | 111.23 |
| 37 | b | 503 | CLA | C3C-C4C-NC | 3.72 | 115.20 | 110.43 |
| 37 | w | 101 | CLA | C1D-CHD-C4C | -3.72 | 118.11 | 126.02 |
| 47 | 12 | 206 | KC1 | C1D-CHD-C4C | -3.72 | 117.50 | 126.25 |
| 47 | 33 | 306 | KC1 | CBA-CAA-C2A | -3.72 | 110.52 | 125.45 |
| 37 | b | 513 | CLA | C3C-C4C-NC | 3.72 | 115.20 | 110.43 |
| 37 | b | 516 | CLA | CAC-C3C-C4C | 3.72 | 129.63 | 124.79 |
| 37 | 21 | 205 | CLA | C1D-CHD-C4C | -3.72 | 118.11 | 126.02 |
| 37 | 17 | 302 | CLA | C1C-C2C-C3C | -3.72 | 103.07 | 106.98 |
| 37 | 20 | 306 | CLA | CHD-C1D-ND | -3.72 | 119.57 | 124.80 |
| 37 | B | 501 | CLA | C1C-C2C-C3C | -3.72 | 103.07 | 106.98 |
| 37 | c | 512 | CLA | CHD-C1D-ND | -3.72 | 119.57 | 124.80 |
| 37 | 41 | 210 | CLA | C1C-C2C-C3C | -3.72 | 103.07 | 106.98 |
| 47 | 31 | 303 | KC1 | C1D-CHD-C4C | -3.72 | 117.50 | 126.25 |
| 47 | 39 | 308 | KC1 | C1D-CHD-C4C | -3.72 | 117.50 | 126.25 |
| 37 | 41 | 204 | CLA | CAC-C3C-C4C | 3.72 | 129.63 | 124.79 |
| 37 | B | 508 | CLA | C1D-CHD-C4C | -3.72 | 118.12 | 126.02 |
| 37 | 18 | 203 | CLA | C1C-C2C-C3C | -3.72 | 103.07 | 106.98 |
| 37 | 33 | 305 | CLA | C1C-C2C-C3C | -3.72 | 103.07 | 106.98 |
| 37 | A | 403 | CLA | C1C-C2C-C3C | -3.72 | 103.07 | 106.98 |
| 37 | B | 503 | CLA | C3C-C4C-NC | 3.72 | 115.19 | 110.43 |
| 48 | 31 | 312 | A86 | C25-C26-C27 | -3.72 | 122.07 | 127.28 |
| 47 | 13 | 309 | KC1 | C2A-C1A-NA | 3.72 | 115.30 | 109.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 38 | 211 | CLA | C3B-C4B-NB | 3.72 | 113.85 | 110.53 |
| 37 | 41 | 205 | CLA | C4A-NA-C1A | -3.72 | 104.98 | 106.68 |
| 37 | 19 | 307 | CLA | C1C-C2C-C3C | -3.71 | 103.07 | 106.98 |
| 37 | 21 | 208 | CLA | C1C-C2C-C3C | -3.71 | 103.07 | 106.98 |
| 47 | 18 | 205 | KC1 | C4B-C3B-C2B | -3.71 | 103.59 | 106.81 |
| 47 | 18 | 210 | KC1 | C1D-CHD-C4C | -3.71 | 117.52 | 126.25 |
| 47 | 16 | 305 | KC1 | C1C-C2C-C3C | -3.71 | 103.08 | 106.98 |
| 48 | 18 | 214 | A86 | C41-C32-C31 | -3.71 | 107.15 | 110.47 |
| 37 | 18 | 206 | CLA | C1C-C2C-C3C | -3.71 | 103.08 | 106.98 |
| 37 | b | 510 | CLA | C3C-C4C-NC | 3.71 | 115.19 | 110.43 |
| 37 | 20 | 308 | CLA | C3C-C4C-NC | 3.71 | 115.19 | 110.43 |
| 40 | A | 407 | SQD | O47-C7-C8 | 3.71 | 119.51 | 111.48 |
| 37 | B | 505 | CLA | C1D-CHD-C4C | -3.71 | 118.13 | 126.02 |
| 37 | 14 | 308 | CLA | C3C-C4C-NC | 3.71 | 115.18 | 110.43 |
| 47 | 16 | 305 | KC1 | C1D-CHD-C4C | -3.71 | 117.52 | 126.25 |
| 37 | B | 510 | CLA | C3C-C4C-NC | 3.71 | 115.18 | 110.43 |
| 37 | 17 | 307 | CLA | C1D-CHD-C4C | -3.71 | 118.14 | 126.02 |
| 47 | 36 | 308 | KC1 | C1D-CHD-C4C | -3.71 | 117.52 | 126.25 |
| 47 | 13 | 306 | KC1 | CBA-CAA-C2A | -3.71 | 110.56 | 125.45 |
| 37 | 18 | 209 | CLA | CHD-C1D-ND | -3.71 | 119.58 | 124.80 |
| 37 | 37 | 308 | CLA | C1D-CHD-C4C | -3.71 | 118.14 | 126.02 |
| 37 | b | 504 | CLA | C3D-C4D-ND | 3.71 | 116.02 | 109.99 |
| 47 | 36 | 305 | KC1 | C1D-CHD-C4C | -3.71 | 117.53 | 126.25 |
| 37 | 11 | 301 | CLA | C4A-NA-C1A | -3.71 | 104.99 | 106.68 |
| 47 | 31 | 307 | KC1 | C1A-NA-C4A | -3.71 | 104.99 | 106.68 |
| 37 | B | 513 | CLA | C3C-C4C-NC | 3.71 | 115.18 | 110.43 |
| 47 | 11 | 302 | KC1 | C1D-CHD-C4C | -3.71 | 117.53 | 126.25 |
| 47 | 21 | 203 | KC1 | C1D-CHD-C4C | -3.71 | 117.53 | 126.25 |
| 37 | Z | 101 | CLA | C1C-C2C-C3C | -3.71 | 103.08 | 106.98 |
| 48 | 38 | 212 | A86 | C4-C5-C6 | -3.70 | 122.08 | 127.28 |
| 37 | c | 507 | CLA | C3D-C4D-ND | 3.70 | 116.01 | 109.99 |
| 37 | 34 | 303 | CLA | C1C-C2C-C3C | -3.70 | 103.08 | 106.98 |
| 50 | 41 | 212 | DD6 | C21-C20-C15 | -3.70 | 116.21 | 122.30 |
| 47 | 33 | 309 | KC1 | C2A-C1A-NA | 3.70 | 115.27 | 109.34 |
| 47 | 18 | 210 | KC1 | C2C-C1C-NC | 3.70 | 115.03 | 110.45 |
| 48 | 15 | 313 | A86 | C25-C26-C27 | -3.70 | 122.09 | 127.28 |
| 37 | a | 403 | CLA | C1C-C2C-C3C | -3.70 | 103.09 | 106.98 |
| 37 | 37 | 301 | CLA | C1D-CHD-C4C | -3.70 | 118.16 | 126.02 |
| 47 | 34 | 306 | KC1 | C1D-CHD-C4C | -3.70 | 117.55 | 126.25 |
| 37 | 34 | 302 | CLA | C3C-C4C-NC | 3.70 | 115.17 | 110.43 |
| 48 | 38 | 214 | A86 | C41-C32-C31 | -3.70 | 107.16 | 110.47 |
| 37 | 11 | 305 | CLA | C4A-NA-C1A | -3.70 | 104.99 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 16 | 308 | KC1 | C1D-CHD-C4C | -3.70 | 117.55 | 126.25 |
| 37 | c | 513 | CLA | C3C-C4C-NC | 3.70 | 115.17 | 110.43 |
| 37 | 34 | 301 | CLA | C3C-C4C-NC | 3.70 | 115.17 | 110.43 |
| 37 | B | 513 | CLA | O2D-CGD-CBD | 3.70 | 117.69 | 111.23 |
| 37 | d | 401 | CLA | C1C-C2C-C3C | -3.70 | 103.09 | 106.98 |
| 37 | 14 | 301 | CLA | C3C-C4C-NC | 3.70 | 115.16 | 110.43 |
| 37 | W | 101 | CLA | C1D-CHD-C4C | -3.69 | 118.17 | 126.02 |
| 37 | b | 505 | CLA | C1D-CHD-C4C | -3.69 | 118.17 | 126.02 |
| 37 | B | 516 | CLA | CAC-C3C-C4C | 3.69 | 129.60 | 124.79 |
| 37 | 32 | 208 | CLA | C1D-CHD-C4C | -3.69 | 118.17 | 126.02 |
| 37 | 41 | 205 | CLA | CAC-C3C-C4C | 3.69 | 129.60 | 124.79 |
| 37 | B | 504 | CLA | C3D-C4D-ND | 3.69 | 115.99 | 109.99 |
| 47 | 15 | 306 | KC1 | C1A-NA-C4A | -3.69 | 104.99 | 106.68 |
| 37 | C | 503 | CLA | C3B-C4B-NB | 3.69 | 113.83 | 110.53 |
| 47 | 11 | 302 | KC1 | C2A-C1A-NA | 3.69 | 115.26 | 109.34 |
| 37 | B | 511 | CLA | O2D-CGD-CBD | 3.69 | 117.68 | 111.23 |
| 37 | c | 511 | CLA | CHD-C1D-ND | -3.69 | 119.61 | 124.80 |
| 37 | 13 | 307 | CLA | C3C-C4C-NC | 3.69 | 115.16 | 110.43 |
| 37 | 39 | 306 | CLA | C2C-C1C-NC | 3.69 | 113.86 | 109.98 |
| 37 | C | 511 | CLA | CHD-C1D-ND | -3.69 | 119.61 | 124.80 |
| 38 | A | 404 | PHO | C2B-C1B-NB | -3.69 | 106.76 | 109.43 |
| 37 | d | 404 | CLA | C1C-C2C-C3C | -3.69 | 103.10 | 106.98 |
| 37 | b | 513 | CLA | O2D-CGD-CBD | 3.69 | 117.68 | 111.23 |
| 37 | C | 507 | CLA | C3D-C4D-ND | 3.69 | 115.98 | 109.99 |
| 37 | 31 | 308 | CLA | CHD-C1D-ND | -3.69 | 119.61 | 124.80 |
| 37 | 12 | 210 | CLA | CHD-C1D-ND | -3.69 | 119.61 | 124.80 |
| 47 | 38 | 210 | KC1 | C2C-C1C-NC | 3.69 | 115.01 | 110.45 |
| 37 | b | 507 | CLA | C4B-C3B-C2B | -3.69 | 102.72 | 107.30 |
| 40 | B | 519 | SQD | O47-C7-C8 | 3.69 | 119.46 | 111.48 |
| 37 | B | 504 | CLA | C4A-NA-C1A | -3.69 | 105.00 | 106.68 |
| 37 | 18 | 202 | CLA | O2D-CGD-CBD | 3.69 | 117.67 | 111.23 |
| 37 | 40 | 208 | CLA | CHD-C1D-ND | -3.69 | 119.61 | 124.80 |
| 47 | 41 | 203 | KC1 | C1D-CHD-C4C | -3.69 | 117.58 | 126.25 |
| 37 | 21 | 205 | CLA | CAC-C3C-C4C | 3.69 | 129.59 | 124.79 |
| 47 | 40 | 207 | KC1 | C1A-NA-C4A | -3.68 | 105.00 | 106.68 |
| 47 | 15 | 309 | KC1 | C1C-C2C-C3C | -3.68 | 103.11 | 106.98 |
| 47 | 31 | 303 | KC1 | C2A-C1A-NA | 3.68 | 115.24 | 109.34 |
| 37 | 36 | 301 | CLA | CAC-C3C-C4C | 3.68 | 129.58 | 124.79 |
| 47 | 19 | 308 | KC1 | C1D-CHD-C4C | -3.68 | 117.58 | 126.25 |
| 47 | 12 | 211 | KC1 | C2C-C1C-NC | 3.68 | 115.01 | 110.45 |
| 37 | B | 511 | CLA | C4B-C3B-C2B | -3.68 | 102.72 | 107.30 |
| 48 | 32 | 221 | A86 | C7-C6-C8 | 3.68 | 123.71 | 118.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 38 | 213 | A86 | C23-C16-C22 | -3.68 | 102.02 | 107.37 |
| 37 | 21 | 208 | CLA | C4A-NA-C1A | -3.68 | 105.00 | 106.68 |
| 37 | 31 | 302 | CLA | C4A-NA-C1A | -3.68 | 105.00 | 106.68 |
| 37 | 12 | 205 | CLA | C1D-CHD-C4C | -3.68 | 118.19 | 126.02 |
| 37 | D | 402 | CLA | C1C-C2C-C3C | -3.68 | 103.11 | 106.98 |
| 37 | D | 402 | CLA | C1D-CHD-C4C | -3.68 | 118.20 | 126.02 |
| 37 | 33 | 303 | CLA | C3B-C4B-NB | 3.68 | 113.81 | 110.53 |
| 48 | 12 | 220 | A86 | C7-C6-C8 | 3.68 | 123.71 | 118.09 |
| 38 | a | 406 | PHO | C2B-C1B-NB | -3.68 | 106.77 | 109.43 |
| 37 | 31 | 301 | CLA | C1C-C2C-C3C | -3.68 | 103.11 | 106.98 |
| 37 | B | 507 | CLA | C4B-C3B-C2B | -3.68 | 102.73 | 107.30 |
| 37 | b | 511 | CLA | C4B-C3B-C2B | -3.68 | 102.73 | 107.30 |
| 37 | B | 501 | CLA | CAC-C3C-C4C | 3.68 | 129.57 | 124.79 |
| 37 | 19 | 307 | CLA | C3C-C4C-NC | 3.68 | 115.14 | 110.43 |
| 50 | 36 | 312 | DD6 | C37-C36-C35 | -3.68 | 107.66 | 114.42 |
| 37 | 12 | 207 | CLA | C1D-CHD-C4C | -3.68 | 118.21 | 126.02 |
| 37 | b | 505 | CLA | C4-C3-C5 | 3.68 | 121.61 | 115.23 |
| 37 | d | 401 | CLA | C1D-CHD-C4C | -3.68 | 118.21 | 126.02 |
| 48 | 34 | 314 | A86 | C36-C31-C32 | -3.68 | 116.05 | 119.70 |
| 37 | 19 | 305 | CLA | C1C-C2C-C3C | -3.67 | 103.11 | 106.98 |
| 37 | 41 | 204 | CLA | C3B-C4B-NB | 3.67 | 113.81 | 110.53 |
| 37 | 38 | 209 | CLA | CHD-C1D-ND | -3.67 | 119.63 | 124.80 |
| 47 | 37 | 304 | KC1 | CHD-C1D-ND | -3.67 | 118.54 | 124.05 |
| 37 | D | 406 | CLA | C1C-C2C-C3C | -3.67 | 103.12 | 106.98 |
| 37 | 38 | 211 | CLA | C1D-CHD-C4C | -3.67 | 118.22 | 126.02 |
| 37 | 31 | 306 | CLA | C1C-C2C-C3C | -3.67 | 103.12 | 106.98 |
| 37 | 16 | 301 | CLA | CAC-C3C-C4C | 3.67 | 129.57 | 124.79 |
| 48 | 35 | 316 | A86 | C33-C32-C31 | 3.67 | 112.78 | 109.21 |
| 48 | 12 | 220 | A86 | C25-C26-C27 | -3.67 | 122.13 | 127.28 |
| 37 | 33 | 307 | CLA | C3C-C4C-NC | 3.67 | 115.13 | 110.43 |
| 48 | 12 | 213 | A86 | C25-C24-C1 | -3.67 | 116.30 | 126.36 |
| 48 | 31 | 311 | A86 | C35-C34-C33 | 3.67 | 116.48 | 109.89 |
| 37 | C | 506 | CLA | C2B-C1B-NB | 3.67 | 114.13 | 110.33 |
| 37 | 39 | 309 | CLA | CAA-C2A-C3A | -3.67 | 103.08 | 113.00 |
| 37 | c | 512 | CLA | C1C-C2C-C3C | -3.67 | 103.12 | 106.98 |
| 37 | c | 509 | CLA | C3C-C4C-NC | 3.67 | 115.13 | 110.43 |
| 37 | 17 | 309 | CLA | C1D-CHD-C4C | -3.67 | 118.22 | 126.02 |
| 37 | 13 | 305 | CLA | C1C-C2C-C3C | -3.67 | 103.12 | 106.98 |
| 47 | 19 | 308 | KC1 | C2C-C1C-NC | 3.67 | 114.99 | 110.45 |
| 37 | 14 | 310 | CLA | CAA-C2A-C3A | -3.67 | 103.09 | 113.00 |
| 37 | c | 503 | CLA | C3B-C4B-NB | 3.67 | 113.80 | 110.53 |
| 37 | B | 505 | CLA | C4-C3-C5 | 3.67 | 121.59 | 115.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 512 | CLA | C1C-C2C-C3C | -3.67 | 103.12 | 106.98 |
| 48 | 11 | 311 | A86 | C35-C34-C33 | 3.67 | 116.47 | 109.89 |
| 47 | 11 | 309 | KC1 | C4B-C3B-C2B | -3.66 | 103.64 | 106.81 |
| 37 | 39 | 307 | CLA | C3C-C4C-NC | 3.66 | 115.12 | 110.43 |
| 37 | C | 502 | CLA | C4C-C3C-C2C | -3.66 | 101.56 | 106.89 |
| 37 | c | 502 | CLA | C4C-C3C-C2C | -3.66 | 101.56 | 106.89 |
| 48 | 19 | 313 | A86 | C19-C18-C17 | 3.66 | 117.64 | 110.79 |
| 37 | 12 | 209 | CLA | CHD-C1D-ND | -3.66 | 119.65 | 124.80 |
| 48 | 14 | 311 | A86 | C12-C11-C13 | 3.66 | 121.94 | 116.00 |
| 37 | 18 | 211 | CLA | C4C-C3C-C2C | -3.66 | 101.56 | 106.89 |
| 37 | 34 | 308 | CLA | C3C-C4C-NC | 3.66 | 115.12 | 110.43 |
| 47 | 34 | 309 | KC1 | CMA-C3A-C2A | -3.66 | 119.57 | 128.43 |
| 37 | a | 404 | CLA | CAA-C2A-C3A | -3.66 | 103.11 | 113.00 |
| 37 | w | 101 | CLA | C1C-C2C-C3C | -3.66 | 103.13 | 106.98 |
| 47 | 36 | 304 | KC1 | C1A-NA-C4A | -3.66 | 105.01 | 106.68 |
| 47 | 18 | 207 | KC1 | CMB-C2B-C1B | 3.66 | 131.17 | 124.73 |
| 37 | C | 509 | CLA | C3C-C4C-NC | 3.66 | 115.12 | 110.43 |
| 48 | 11 | 315 | A86 | C10-C9-C8 | -3.66 | 112.59 | 123.20 |
| 50 | 21 | 212 | DD6 | C21-C20-C15 | -3.66 | 116.28 | 122.30 |
| 48 | 31 | 315 | A86 | C10-C9-C8 | -3.66 | 112.60 | 123.20 |
| 37 | 21 | 204 | CLA | C3B-C4B-NB | 3.66 | 113.80 | 110.53 |
| 37 | 34 | 310 | CLA | CAA-C2A-C3A | -3.66 | 103.12 | 113.00 |
| 47 | 31 | 305 | KC1 | C1D-CHD-C4C | -3.66 | 117.65 | 126.25 |
| 37 | 21 | 208 | CLA | C1D-CHD-C4C | -3.66 | 118.25 | 126.02 |
| 48 | 14 | 314 | A86 | C36-C31-C32 | -3.66 | 116.07 | 119.70 |
| 37 | 13 | 308 | CLA | C3C-C4C-NC | 3.66 | 115.11 | 110.43 |
| 47 | 35 | 306 | KC1 | C1D-CHD-C4C | -3.66 | 117.65 | 126.25 |
| 47 | 14 | 309 | KC1 | CMA-C3A-C2A | -3.66 | 119.58 | 128.43 |
| 48 | 13 | 311 | A86 | C3-C2-C1 | -3.66 | 122.15 | 127.28 |
| 37 | C | 513 | CLA | C3C-C4C-NC | 3.65 | 115.11 | 110.43 |
| 48 | 32 | 218 | A86 | C41-C32-C31 | -3.65 | 107.20 | 110.47 |
| 37 | 34 | 305 | CLA | C4A-NA-C1A | -3.65 | 105.01 | 106.68 |
| 37 | 32 | 210 | CLA | CHD-C1D-ND | -3.65 | 119.66 | 124.80 |
| 48 | 40 | 201 | A86 | C8-C6-C5 | 3.65 | 124.75 | 119.01 |
| 48 | 11 | 311 | A86 | C36-C31-C32 | -3.65 | 116.07 | 119.70 |
| 48 | 31 | 311 | A86 | C36-C31-C32 | -3.65 | 116.07 | 119.70 |
| 37 | 33 | 303 | CLA | C1D-CHD-C4C | -3.65 | 118.26 | 126.02 |
| 37 | 35 | 308 | CLA | C1D-CHD-C4C | -3.65 | 118.26 | 126.02 |
| 37 | b | 509 | CLA | C3B-C4B-NB | 3.65 | 113.79 | 110.53 |
| 37 | 32 | 205 | CLA | C4A-NA-C1A | -3.65 | 105.01 | 106.68 |
| 37 | 11 | 305 | CLA | C1C-C2C-C3C | -3.65 | 103.14 | 106.98 |
| 37 | 18 | 201 | CLA | CMB-C2B-C1B | 3.65 | 130.97 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 504 | CLA | C3B-C4B-NB | 3.65 | 113.79 | 110.53 |
| 37 | 41 | 202 | CLA | C1C-C2C-C3C | -3.65 | 103.14 | 106.98 |
| 37 | C | 512 | CLA | C3C-C4C-NC | 3.65 | 115.10 | 110.43 |
| 37 | 14 | 302 | CLA | C3C-C4C-NC | 3.65 | 115.10 | 110.43 |
| 37 | D | 401 | CLA | CAA-C2A-C3A | -3.65 | 103.14 | 113.00 |
| 37 | 32 | 208 | CLA | C1C-C2C-C3C | -3.65 | 103.14 | 106.98 |
| 37 | 19 | 302 | CLA | CAA-C2A-C3A | -3.65 | 103.15 | 113.00 |
| 50 | 16 | 312 | DD6 | C37-C36-C35 | -3.65 | 107.72 | 114.42 |
| 37 | B | 509 | CLA | C3B-C4B-NB | 3.65 | 113.78 | 110.53 |
| 40 | B | 519 | SQD | O9-S-O7 | -3.64 | 101.97 | 113.82 |
| 47 | 11 | 304 | KC1 | C1D-CHD-C4C | -3.64 | 117.68 | 126.25 |
| 48 | 34 | 311 | A86 | C12-C11-C13 | 3.64 | 121.91 | 116.00 |
| 37 | 15 | 301 | CLA | C3C-C4C-NC | 3.64 | 115.10 | 110.43 |
| 40 | L | 101 | SQD | O9-S-O7 | -3.64 | 101.97 | 113.82 |
| 40 | L | 101 | SQD | O47-C7-C8 | 3.64 | 119.36 | 111.48 |
| 37 | 36 | 301 | CLA | C3C-C4C-NC | 3.64 | 115.10 | 110.43 |
| 48 | 35 | 316 | A86 | C25-C26-C27 | -3.64 | 122.17 | 127.28 |
| 48 | 32 | 221 | A86 | C4-C3-C2 | -3.64 | 116.07 | 123.52 |
| 37 | B | 503 | CLA | CHD-C1D-ND | -3.64 | 119.68 | 124.80 |
| 47 | 35 | 302 | KC1 | C1D-CHD-C4C | -3.64 | 117.69 | 126.25 |
| 37 | b | 503 | CLA | CHD-C1D-ND | -3.64 | 119.68 | 124.80 |
| 37 | C | 501 | CLA | C1-C2-C3 | -3.64 | 120.23 | 126.20 |
| 48 | 35 | 316 | A86 | C35-C34-C33 | 3.64 | 116.42 | 109.89 |
| 37 | 33 | 308 | CLA | C1C-C2C-C3C | -3.64 | 103.15 | 106.98 |
| 48 | 12 | 220 | A86 | C4-C3-C2 | -3.64 | 116.08 | 123.52 |
| 40 | B | 522 | SQD | O7-S-C6 | 3.64 | 112.19 | 106.76 |
| 37 | 16 | 301 | CLA | C3C-C4C-NC | 3.64 | 115.09 | 110.43 |
| 37 | 41 | 208 | CLA | C1D-CHD-C4C | -3.64 | 118.29 | 126.02 |
| 37 | 39 | 310 | CLA | C3C-C4C-NC | 3.64 | 115.09 | 110.43 |
| 48 | 12 | 216 | A86 | C12-C11-C13 | 3.63 | 121.89 | 116.00 |
| 37 | 17 | 302 | CLA | C3D-C2D-C1D | -3.63 | 100.87 | 105.83 |
| 48 | 34 | 315 | A86 | C12-C11-C13 | 3.63 | 121.89 | 116.00 |
| 37 | B | 514 | CLA | C1C-C2C-C3C | -3.63 | 103.16 | 106.98 |
| 37 | W | 102 | CLA | C1C-C2C-C3C | -3.63 | 103.16 | 106.98 |
| 47 | 15 | 306 | KC1 | C1D-CHD-C4C | -3.63 | 117.70 | 126.25 |
| 47 | 40 | 206 | KC1 | C1D-CHD-C4C | -3.63 | 117.70 | 126.25 |
| 37 | 19 | 310 | CLA | C3C-C4C-NC | 3.63 | 115.08 | 110.43 |
| 37 | 33 | 308 | CLA | C3C-C4C-NC | 3.63 | 115.08 | 110.43 |
| 40 | b | 521 | SQD | O7-S-C6 | 3.63 | 112.18 | 106.76 |
| 37 | 13 | 307 | CLA | C4A-NA-C1A | -3.63 | 105.02 | 106.68 |
| 37 | 17 | 304 | CLA | C1D-CHD-C4C | -3.63 | 118.30 | 126.02 |
| 37 | 31 | 310 | CLA | C1D-CHD-C4C | -3.63 | 118.30 | 126.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 32 | 221 | A86 | C25-C26-C27 | -3.63 | 122.19 | 127.28 |
| 37 | 21 | 209 | CLA | C1C-C2C-C3C | -3.63 | 103.16 | 106.98 |
| 37 | c | 512 | CLA | C3C-C4C-NC | 3.63 | 115.08 | 110.43 |
| 37 | B | 524 | CLA | C1C-C2C-C3C | -3.63 | 103.16 | 106.98 |
| 37 | 21 | 202 | CLA | C1C-C2C-C3C | -3.63 | 103.16 | 106.98 |
| 37 | 19 | 309 | CLA | CAA-C2A-C3A | -3.63 | 103.19 | 113.00 |
| 37 | 12 | 203 | CLA | C4A-NA-C1A | -3.63 | 105.02 | 106.68 |
| 37 | 37 | 303 | CLA | C1D-CHD-C4C | -3.63 | 118.31 | 126.02 |
| 37 | 39 | 301 | CLA | C3C-C4C-NC | 3.63 | 115.08 | 110.43 |
| 37 | 11 | 310 | CLA | C1D-CHD-C4C | -3.63 | 118.31 | 126.02 |
| 37 | D | 405 | CLA | C1C-C2C-C3C | -3.63 | 103.17 | 106.98 |
| 47 | 20 | 304 | KC1 | C1D-CHD-C4C | -3.63 | 117.72 | 126.25 |
| 37 | W | 101 | CLA | C1C-C2C-C3C | -3.63 | 103.17 | 106.98 |
| 47 | 36 | 305 | KC1 | C1C-C2C-C3C | -3.62 | 103.17 | 106.98 |
| 37 | 19 | 310 | CLA | C4A-NA-C1A | -3.62 | 105.03 | 106.68 |
| 37 | b | 523 | CLA | O2A-CGA-CBA | 3.62 | 122.88 | 111.83 |
| 48 | 12 | 217 | A86 | C4-C3-C2 | -3.62 | 116.11 | 123.52 |
| 47 | 31 | 307 | KC1 | C1D-CHD-C4C | -3.62 | 117.73 | 126.25 |
| 37 | 12 | 207 | CLA | C1C-C2C-C3C | -3.62 | 103.17 | 106.98 |
| 37 | 13 | 308 | CLA | C1C-C2C-C3C | -3.62 | 103.17 | 106.98 |
| 37 | 16 | 309 | CLA | C1D-CHD-C4C | -3.62 | 118.33 | 126.02 |
| 37 | c | 506 | CLA | C2B-C1B-NB | 3.62 | 114.08 | 110.33 |
| 37 | c | 503 | CLA | C1C-C2C-C3C | -3.62 | 103.17 | 106.98 |
| 37 | b | 504 | CLA | C3B-C4B-NB | 3.62 | 113.76 | 110.53 |
| 37 | b | 516 | CLA | C3C-C4C-NC | 3.62 | 115.06 | 110.43 |
| 37 | 41 | 206 | CLA | O2D-CGD-CBD | 3.62 | 117.55 | 111.23 |
| 50 | 40 | 214 | DD6 | C21-C20-C15 | -3.62 | 116.35 | 122.30 |
| 37 | 34 | 301 | CLA | C4A-NA-C1A | -3.61 | 105.03 | 106.68 |
| 37 | 19 | 306 | CLA | C2C-C1C-NC | 3.61 | 113.78 | 109.98 |
| 47 | 14 | 309 | KC1 | C4B-C3B-C2B | -3.61 | 103.68 | 106.81 |
| 37 | 15 | 308 | CLA | C3B-C4B-NB | 3.61 | 113.75 | 110.53 |
| 37 | 39 | 302 | CLA | CAA-C2A-C3A | -3.61 | 103.24 | 113.00 |
| 37 | B | 514 | CLA | CHD-C1D-ND | -3.61 | 119.72 | 124.80 |
| 47 | 11 | 306 | KC1 | C1D-CHD-C4C | -3.61 | 117.75 | 126.25 |
| 37 | b | 503 | CLA | CAA-C2A-C3A | -3.61 | 103.24 | 113.00 |
| 37 | c | 501 | CLA | C1-C2-C3 | -3.61 | 120.28 | 126.20 |
| 48 | 32 | 217 | A86 | C12-C11-C13 | 3.61 | 121.86 | 116.00 |
| 48 | 16 | 311 | A86 | C34-O4-C38 | -3.61 | 111.47 | 117.85 |
| 37 | 35 | 301 | CLA | C3C-C4C-NC | 3.61 | 115.05 | 110.43 |
| 37 | 38 | 208 | CLA | C3C-C4C-NC | 3.61 | 115.05 | 110.43 |
| 48 | 36 | 311 | A86 | C34-O4-C38 | -3.61 | 111.47 | 117.85 |
| 37 | 41 | 202 | CLA | C4A-NA-C1A | -3.61 | 105.03 | 106.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 206 | CLA | O2D-CGD-CBD | 3.61 | 117.54 | 111.23 |
| 37 | 36 | 309 | CLA | C1D-CHD-C4C | -3.61 | 118.35 | 126.02 |
| 37 | 18 | 202 | CLA | C2C-C1C-NC | 3.61 | 113.77 | 109.98 |
| 37 | 19 | 301 | CLA | C3C-C4C-NC | 3.61 | 115.05 | 110.43 |
| 37 | b | 514 | CLA | C1C-C2C-C3C | -3.61 | 103.19 | 106.98 |
| 48 | 16 | 313 | A86 | C8-C6-C5 | 3.61 | 124.68 | 119.01 |
| 37 | B | 504 | CLA | C3B-C2B-C1B | -3.60 | 102.92 | 107.17 |
| 37 | 21 | 206 | CLA | C1C-C2C-C3C | -3.60 | 103.19 | 106.98 |
| 37 | B | 510 | CLA | C1C-C2C-C3C | -3.60 | 103.19 | 106.98 |
| 44 | C | 517 | DGD | O6D-C1D-O3G | -3.60 | 101.53 | 110.04 |
| 48 | 14 | 315 | A86 | C12-C11-C13 | 3.60 | 121.84 | 116.00 |
| 47 | 13 | 302 | KC1 | CAA-CBA-CGA | -3.60 | 108.75 | 127.05 |
| 37 | 14 | 305 | CLA | C4A-NA-C1A | -3.60 | 105.04 | 106.68 |
| 37 | 21 | 205 | CLA | C4A-NA-C1A | -3.60 | 105.04 | 106.68 |
| 48 | 12 | 217 | A86 | C41-C32-C31 | -3.60 | 107.25 | 110.47 |
| 37 | 41 | 209 | CLA | C1C-C2C-C3C | -3.60 | 103.20 | 106.98 |
| 37 | 18 | 208 | CLA | C3C-C4C-NC | 3.60 | 115.04 | 110.43 |
| 47 | 11 | 306 | KC1 | C1A-NA-C4A | -3.59 | 105.04 | 106.68 |
| 47 | 33 | 302 | KC1 | CAA-CBA-CGA | -3.59 | 108.78 | 127.05 |
| 50 | 20 | 312 | DD6 | C21-C20-C15 | -3.59 | 116.39 | 122.30 |
| 47 | 12 | 206 | KC1 | C4C-C3C-C2C | -3.59 | 101.66 | 106.89 |
| 37 | 32 | 204 | CLA | CMC-C2C-C1C | 3.59 | 130.65 | 125.03 |
| 37 | B | 503 | CLA | CAA-C2A-C3A | -3.59 | 103.29 | 113.00 |
| 37 | B | 512 | CLA | C3B-C4B-NB | 3.59 | 113.74 | 110.53 |
| 48 | 12 | 202 | A86 | C25-C26-C27 | -3.59 | 122.24 | 127.28 |
| 37 | 32 | 213 | CLA | O2D-CGD-O1D | -3.59 | 116.86 | 123.85 |
| 47 | 32 | 207 | KC1 | C4C-C3C-C2C | -3.59 | 101.67 | 106.89 |
| 37 | b | 510 | CLA | C1C-C2C-C3C | -3.59 | 103.21 | 106.98 |
| 37 | b | 523 | CLA | C1C-C2C-C3C | -3.59 | 103.21 | 106.98 |
| 48 | 21 | 211 | A86 | C4-C5-C6 | -3.59 | 122.25 | 127.28 |
| 37 | 41 | 206 | CLA | CHD-C4C-NC | 3.59 | 129.79 | 124.23 |
| 37 | 31 | 301 | CLA | C3C-C4C-NC | 3.59 | 115.02 | 110.43 |
| 37 | c | 502 | CLA | CHD-C1D-ND | -3.59 | 119.76 | 124.80 |
| 44 | c | 517 | DGD | O6D-C1D-O3G | -3.58 | 101.57 | 110.04 |
| 37 | 12 | 203 | CLA | CMC-C2C-C1C | 3.58 | 130.63 | 125.03 |
| 37 | B | 511 | CLA | CAC-C3C-C4C | 3.58 | 129.45 | 124.79 |
| 37 | B | 516 | CLA | C3C-C4C-NC | 3.58 | 115.02 | 110.43 |
| 37 | d | 403 | CLA | C1C-C2C-C3C | -3.58 | 103.21 | 106.98 |
| 37 | 32 | 210 | CLA | C3C-C4C-NC | 3.58 | 115.02 | 110.43 |
| 47 | 17 | 305 | KC1 | C2C-C1C-NC | 3.58 | 114.88 | 110.45 |
| 47 | 17 | 308 | KC1 | C2C-C1C-NC | 3.58 | 114.88 | 110.45 |
| 48 | 12 | 213 | A86 | C12-C11-C13 | 3.58 | 121.81 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 503 | CLA | C1C-C2C-C3C | -3.58 | 103.22 | 106.98 |
| 37 | W | 102 | CLA | C3C-C4C-NC | 3.58 | 115.02 | 110.43 |
| 47 | 17 | 306 | KC1 | C1D-CHD-C4C | -3.58 | 117.83 | 126.25 |
| 37 | 31 | 306 | CLA | CAA-C2A-C3A | -3.58 | 103.33 | 113.00 |
| 37 | b | 514 | CLA | CHD-C1D-ND | -3.58 | 119.77 | 124.80 |
| 37 | b | 512 | CLA | C3B-C4B-NB | 3.58 | 113.72 | 110.53 |
| 48 | 35 | 315 | A86 | O2-C18-C17 | 3.58 | 117.06 | 109.75 |
| 37 | b | 511 | CLA | CAC-C3C-C4C | 3.58 | 129.44 | 124.79 |
| 37 | 11 | 305 | CLA | CAA-C2A-C3A | -3.58 | 103.33 | 113.00 |
| 47 | 20 | 302 | KC1 | C4B-C3B-C2B | -3.58 | 103.71 | 106.81 |
| 37 | 32 | 204 | CLA | C4A-NA-C1A | -3.58 | 105.05 | 106.68 |
| 48 | 32 | 203 | A86 | C25-C26-C27 | -3.58 | 122.26 | 127.28 |
| 47 | 37 | 304 | KC1 | C2C-C1C-NC | 3.58 | 114.88 | 110.45 |
| 48 | 41 | 215 | A86 | C34-O4-C38 | -3.58 | 111.53 | 117.85 |
| 48 | 32 | 214 | A86 | C3-C2-C1 | -3.58 | 122.26 | 127.28 |
| 48 | 41 | 215 | A86 | O1-C20-C15 | -3.58 | 57.79 | 59.23 |
| 47 | 40 | 204 | KC1 | C4B-C3B-C2B | -3.58 | 103.71 | 106.81 |
| 37 | 37 | 308 | CLA | C1C-C2C-C3C | -3.57 | 103.22 | 106.98 |
| 48 | 17 | 310 | A86 | C3-C2-C1 | -3.57 | 122.27 | 127.28 |
| 37 | B | 524 | CLA | O2A-CGA-CBA | 3.57 | 122.73 | 111.83 |
| 37 | 32 | 213 | CLA | C3C-C4C-NC | 3.57 | 115.01 | 110.43 |
| 37 | B | 503 | CLA | O2D-CGD-O1D | -3.57 | 116.89 | 123.85 |
| 37 | C | 502 | CLA | CHD-C1D-ND | -3.57 | 119.77 | 124.80 |
| 48 | 11 | 313 | A86 | C34-O4-C38 | -3.57 | 111.54 | 117.85 |
| 37 | 36 | 301 | CLA | CMC-C2C-C1C | 3.57 | 130.62 | 125.03 |
| 37 | 33 | 301 | CLA | C1C-C2C-C3C | -3.57 | 103.22 | 106.98 |
| 48 | 41 | 211 | A86 | C4-C5-C6 | -3.57 | 122.27 | 127.28 |
| 37 | B | 511 | CLA | C3C-C4C-NC | 3.57 | 115.00 | 110.43 |
| 37 | 15 | 301 | CLA | C4A-NA-C1A | -3.57 | 105.05 | 106.68 |
| 37 | 12 | 212 | CLA | C3C-C4C-NC | 3.57 | 115.00 | 110.43 |
| 37 | b | 503 | CLA | O2D-CGD-O1D | -3.57 | 116.91 | 123.85 |
| 37 | B | 506 | CLA | C1C-C2C-C3C | -3.57 | 103.23 | 106.98 |
| 37 | 39 | 303 | CLA | C3C-C4C-NC | 3.57 | 115.00 | 110.43 |
| 48 | 19 | 313 | A86 | C26-C25-C24 | -3.57 | 112.87 | 123.20 |
| 37 | 12 | 209 | CLA | C3C-C4C-NC | 3.57 | 115.00 | 110.43 |
| 37 | 12 | 212 | CLA | O2D-CGD-O1D | -3.56 | 116.91 | 123.85 |
| 37 | 18 | 201 | CLA | C3C-C4C-NC | 3.56 | 115.00 | 110.43 |
| 48 | 32 | 218 | A86 | C4-C3-C2 | -3.56 | 116.23 | 123.52 |
| 37 | b | 504 | CLA | C3B-C2B-C1B | -3.56 | 102.97 | 107.17 |
| 37 | 21 | 206 | CLA | CHD-C4C-NC | 3.56 | 129.76 | 124.23 |
| 37 | 35 | 303 | CLA | CBA-CAA-C2A | 3.56 | 124.39 | 113.79 |
| 47 | 17 | 303 | KC1 | CBA-CAA-C2A | -3.56 | 111.15 | 125.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 202 | CLA | C4A-NA-C1A | -3.56 | 105.05 | 106.68 |
| 37 | 41 | 206 | CLA | C1C-C2C-C3C | -3.56 | 103.23 | 106.98 |
| 47 | 37 | 302 | KC1 | CBA-CAA-C2A | -3.56 | 111.16 | 125.45 |
| 37 | b | 511 | CLA | C3C-C4C-NC | 3.56 | 114.99 | 110.43 |
| 47 | 37 | 305 | KC1 | C1D-CHD-C4C | -3.56 | 117.88 | 126.25 |
| 37 | 12 | 212 | CLA | C1C-C2C-C3C | -3.56 | 103.24 | 106.98 |
| 37 | B | 506 | CLA | C4C-C3C-C2C | -3.56 | 101.71 | 106.89 |
| 37 | 36 | 306 | CLA | CHD-C1D-ND | -3.56 | 119.80 | 124.80 |
| 37 | 16 | 303 | CLA | C1D-CHD-C4C | -3.56 | 118.46 | 126.02 |
| 47 | 15 | 302 | KC1 | C1D-CHD-C4C | -3.56 | 117.89 | 126.25 |
| 47 | 34 | 309 | KC1 | C4B-C3B-C2B | -3.56 | 103.73 | 106.81 |
| 37 | 38 | 204 | CLA | CMD-C2D-C3D | -3.56 | 119.54 | 127.69 |
| 48 | 21 | 215 | A86 | C34-O4-C38 | -3.55 | 111.57 | 117.85 |
| 37 | b | 506 | CLA | C4C-C3C-C2C | -3.55 | 101.72 | 106.89 |
| 48 | 32 | 214 | A86 | C12-C11-C13 | 3.55 | 121.76 | 116.00 |
| 48 | 33 | 311 | A86 | C3-C2-C1 | -3.55 | 122.29 | 127.28 |
| 47 | 35 | 306 | KC1 | C1A-NA-C4A | -3.55 | 105.06 | 106.68 |
| 37 | 17 | 307 | CLA | C1C-C2C-C3C | -3.55 | 103.24 | 106.98 |
| 37 | 18 | 204 | CLA | CMD-C2D-C3D | -3.55 | 119.54 | 127.69 |
| 37 | 16 | 301 | CLA | CMC-C2C-C1C | 3.55 | 130.58 | 125.03 |
| 48 | 21 | 215 | A86 | O1-C20-C15 | -3.55 | 57.80 | 59.23 |
| 37 | 16 | 303 | CLA | CBA-CAA-C2A | 3.55 | 124.36 | 113.79 |
| 37 | 20 | 307 | CLA | C1C-C2C-C3C | -3.55 | 103.25 | 106.98 |
| 37 | B | 512 | CLA | C4C-C3C-C2C | -3.55 | 101.73 | 106.89 |
| 47 | 11 | 304 | KC1 | CBA-CAA-C2A | -3.55 | 111.22 | 125.45 |
| 37 | 11 | 301 | CLA | C2C-C1C-NC | 3.54 | 113.70 | 109.98 |
| 37 | 36 | 303 | CLA | C1D-CHD-C4C | -3.54 | 118.49 | 126.02 |
| 37 | 15 | 303 | CLA | CBA-CAA-C2A | 3.54 | 124.34 | 113.79 |
| 37 | 21 | 208 | CLA | CAC-C3C-C4C | 3.54 | 129.40 | 124.79 |
| 37 | 36 | 303 | CLA | CBA-CAA-C2A | 3.54 | 124.33 | 113.79 |
| 47 | 35 | 309 | KC1 | C4B-C3B-C2B | -3.54 | 103.74 | 106.81 |
| 37 | 16 | 306 | CLA | CHD-C1D-ND | -3.54 | 119.82 | 124.80 |
| 37 | 13 | 301 | CLA | C1C-C2C-C3C | -3.54 | 103.26 | 106.98 |
| 37 | 17 | 309 | CLA | C1C-C2C-C3C | -3.54 | 103.26 | 106.98 |
| 44 | J | 101 | DGD | O6D-C1D-O3G | -3.54 | 101.68 | 110.04 |
| 40 | b | 521 | SQD | O8-S-C6 | 3.54 | 112.81 | 105.97 |
| 37 | c | 501 | CLA | C3B-C4B-NB | 3.54 | 113.69 | 110.53 |
| 44 | H | 102 | DGD | O3G-C3G-C2G | -3.54 | 102.21 | 110.82 |
| 37 | c | 503 | CLA | C3C-C4C-NC | 3.54 | 114.96 | 110.43 |
| 37 | 19 | 303 | CLA | C3C-C4C-NC | 3.54 | 114.96 | 110.43 |
| 47 | 35 | 309 | KC1 | CMA-C3A-C2A | -3.54 | 119.87 | 128.43 |
| 48 | 36 | 311 | A86 | C26-C25-C24 | -3.54 | 112.95 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 31 | 305 | KC1 | CBA-CAA-C2A | -3.54 | 111.26 | 125.45 |
| 37 | 37 | 306 | CLA | C1C-C2C-C3C | -3.53 | 103.26 | 106.98 |
| 37 | 40 | 209 | CLA | C1C-C2C-C3C | -3.53 | 103.26 | 106.98 |
| 47 | 14 | 309 | KC1 | C1C-C2C-C3C | -3.53 | 103.26 | 106.98 |
| 44 | j | 101 | DGD | O6D-C1D-O3G | -3.53 | 101.69 | 110.04 |
| 37 | 12 | 205 | CLA | C1C-C2C-C3C | -3.53 | 103.26 | 106.98 |
| 47 | 38 | 205 | KC1 | C1D-CHD-C4C | -3.53 | 117.94 | 126.25 |
| 48 | 16 | 311 | A86 | C26-C25-C24 | -3.53 | 112.96 | 123.20 |
| 37 | 14 | 301 | CLA | C4A-NA-C1A | -3.53 | 105.07 | 106.68 |
| 37 | C | 504 | CLA | C3B-C4B-NB | 3.53 | 113.68 | 110.53 |
| 37 | b | 506 | CLA | C1C-C2C-C3C | -3.53 | 103.26 | 106.98 |
| 37 | c | 510 | CLA | CAA-C2A-C3A | -3.53 | 103.45 | 113.00 |
| 40 | 16 | 315 | SQD | O47-C7-C8 | 3.53 | 119.12 | 111.48 |
| 37 | 32 | 213 | CLA | C1C-C2C-C3C | -3.53 | 103.27 | 106.98 |
| 37 | 41 | 208 | CLA | CAC-C3C-C4C | 3.53 | 129.38 | 124.79 |
| 40 | B | 522 | SQD | O8-S-C6 | 3.53 | 112.79 | 105.97 |
| 47 | 13 | 306 | KC1 | C1D-CHD-C4C | -3.53 | 117.95 | 126.25 |
| 47 | 20 | 304 | KC1 | CAA-CBA-CGA | -3.53 | 109.10 | 127.05 |
| 37 | 14 | 308 | CLA | C4A-NA-C1A | -3.53 | 105.07 | 106.68 |
| 47 | 33 | 306 | KC1 | C1D-CHD-C4C | -3.53 | 117.95 | 126.25 |
| 48 | 15 | 319 | A86 | C10-C9-C8 | -3.53 | 112.98 | 123.20 |
| 47 | 13 | 309 | KC1 | C1A-NA-C4A | -3.53 | 105.07 | 106.68 |
| 37 | C | 510 | CLA | CAA-C2A-C3A | -3.53 | 103.47 | 113.00 |
| 37 | 20 | 303 | CLA | C1C-C2C-C3C | -3.53 | 103.27 | 106.98 |
| 47 | 31 | 303 | KC1 | CBA-CAA-C2A | -3.53 | 111.30 | 125.45 |
| 48 | 14 | 316 | A86 | C33-C32-C31 | 3.53 | 112.64 | 109.21 |
| 47 | 11 | 302 | KC1 | CBA-CAA-C2A | -3.53 | 111.30 | 125.45 |
| 37 | 21 | 206 | CLA | CAA-C2A-C3A | -3.53 | 103.47 | 113.00 |
| 47 | 15 | 304 | KC1 | C1D-CHD-C4C | -3.53 | 117.96 | 126.25 |
| 47 | 38 | 207 | KC1 | C1A-NA-C4A | -3.52 | 105.07 | 106.68 |
| 37 | c | 504 | CLA | C3B-C4B-NB | 3.52 | 113.68 | 110.53 |
| 48 | 39 | 313 | A86 | C26-C25-C24 | -3.52 | 112.99 | 123.20 |
| 37 | c | 508 | CLA | C4C-C3C-C2C | -3.52 | 101.76 | 106.89 |
| 47 | 40 | 206 | KC1 | CAA-CBA-CGA | -3.52 | 109.14 | 127.05 |
| 37 | B | 501 | CLA | C4A-NA-C1A | -3.52 | 105.07 | 106.68 |
| 48 | 32 | 216 | A86 | C41-C32-C31 | -3.52 | 107.32 | 110.47 |
| 40 | 40 | 202 | SQD | O47-C7-C8 | 3.52 | 119.10 | 111.48 |
| 47 | 15 | 309 | KC1 | CMA-C3A-C2A | -3.52 | 119.91 | 128.43 |
| 37 | 31 | 302 | CLA | C2C-C1C-NC | 3.52 | 113.68 | 109.98 |
| 37 | 21 | 206 | CLA | C4A-NA-C1A | -3.52 | 105.07 | 106.68 |
| 37 | 41 | 206 | CLA | CAA-C2A-C3A | -3.52 | 103.49 | 113.00 |
| 50 | 16 | 312 | DD6 | C19-C18-C17 | 3.52 | 117.37 | 110.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 18 | 203 | CLA | C3C-C4C-NC | 3.52 | 114.94 | 110.43 |
| 48 | 37 | 309 | A86 | C3-C2-C1 | -3.52 | 122.34 | 127.28 |
| 37 | 31 | 302 | CLA | CAC-C3C-C4C | 3.52 | 129.37 | 124.79 |
| 48 | 37 | 312 | A86 | C12-C11-C13 | 3.52 | 121.70 | 116.00 |
| 47 | 18 | 205 | KC1 | C1D-CHD-C4C | -3.52 | 117.98 | 126.25 |
| 47 | 15 | 309 | KC1 | C4B-C3B-C2B | -3.52 | 103.77 | 106.81 |
| 37 | 14 | 307 | CLA | CHD-C1D-ND | -3.52 | 119.85 | 124.80 |
| 48 | 12 | 215 | A86 | C41-C32-C31 | -3.51 | 107.33 | 110.47 |
| 48 | 34 | 316 | A86 | C33-C32-C31 | 3.51 | 112.63 | 109.21 |
| 48 | 35 | 319 | A86 | C10-C9-C8 | -3.51 | 113.02 | 123.20 |
| 37 | 15 | 307 | CLA | C3C-C4C-NC | 3.51 | 114.93 | 110.43 |
| 47 | 20 | 302 | KC1 | CBA-CAA-C2A | -3.51 | 111.35 | 125.45 |
| 37 | 39 | 304 | CLA | C1C-C2C-C3C | -3.51 | 103.28 | 106.98 |
| 37 | 15 | 305 | CLA | C3B-C4B-NB | 3.51 | 113.67 | 110.53 |
| 44 | h | 102 | DGD | O3G-C3G-C2G | -3.51 | 102.27 | 110.82 |
| 37 | 38 | 203 | CLA | C3C-C4C-NC | 3.51 | 114.93 | 110.43 |
| 47 | 38 | 210 | KC1 | C1C-C2C-C3C | -3.51 | 103.29 | 106.98 |
| 37 | 38 | 201 | CLA | C1D-CHD-C4C | -3.51 | 118.56 | 126.02 |
| 37 | 35 | 307 | CLA | C3C-C4C-NC | 3.51 | 114.93 | 110.43 |
| 47 | 31 | 307 | KC1 | C2C-C1C-NC | 3.51 | 114.80 | 110.45 |
| 37 | 36 | 306 | CLA | C4B-C3B-C2B | -3.51 | 102.94 | 107.30 |
| 50 | 36 | 312 | DD6 | C19-C18-C17 | 3.51 | 117.36 | 110.79 |
| 47 | 40 | 204 | KC1 | CBA-CAA-C2A | -3.51 | 111.36 | 125.45 |
| 37 | c | 507 | CLA | CHD-C1D-ND | -3.51 | 119.86 | 124.80 |
| 37 | 34 | 307 | CLA | CHD-C1D-ND | -3.51 | 119.86 | 124.80 |
| 37 | 34 | 307 | CLA | C1C-C2C-C3C | -3.51 | 103.29 | 106.98 |
| 37 | 41 | 202 | CLA | C4B-C3B-C2B | -3.51 | 102.94 | 107.30 |
| 37 | C | 508 | CLA | C4C-C3C-C2C | -3.51 | 101.78 | 106.89 |
| 47 | 37 | 307 | KC1 | C2C-C1C-NC | 3.51 | 114.79 | 110.45 |
| 37 | 33 | 310 | CLA | C1C-C2C-C3C | -3.51 | 103.29 | 106.98 |
| 47 | 37 | 304 | KC1 | CBA-CAA-C2A | -3.51 | 111.38 | 125.45 |
| 37 | 34 | 307 | CLA | C3C-C4C-NC | 3.51 | 114.92 | 110.43 |
| 47 | 17 | 305 | KC1 | C1C-C2C-C3C | -3.51 | 103.29 | 106.98 |
| 48 | 31 | 312 | A86 | C4-C5-C6 | -3.51 | 122.36 | 127.28 |
| 48 | 17 | 312 | A86 | C40-C32-C31 | -3.51 | 107.33 | 110.47 |
| 37 | C | 503 | CLA | C3C-C4C-NC | 3.50 | 114.92 | 110.43 |
| 37 | 16 | 306 | CLA | C4B-C3B-C2B | -3.50 | 102.94 | 107.30 |
| 37 | 18 | 206 | CLA | C4B-C3B-C2B | -3.50 | 102.94 | 107.30 |
| 47 | 17 | 308 | KC1 | C1C-C2C-C3C | -3.50 | 103.30 | 106.98 |
| 37 | 21 | 210 | CLA | C3C-C4C-NC | 3.50 | 114.92 | 110.43 |
| 37 | 16 | 309 | CLA | C1C-C2C-C3C | -3.50 | 103.30 | 106.98 |
| 37 | 21 | 202 | CLA | C4B-C3B-C2B | -3.50 | 102.95 | 107.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 210 | CLA | C3B-C4B-NB | 3.50 | 113.66 | 110.53 |
| 37 | 35 | 310 | CLA | C3B-C4B-NB | 3.50 | 113.66 | 110.53 |
| 37 | 13 | 307 | CLA | C3D-C4D-ND | 3.50 | 115.68 | 109.99 |
| 48 | 18 | 212 | A86 | C34-O4-C38 | -3.50 | 111.66 | 117.85 |
| 37 | 16 | 301 | CLA | C4A-NA-C1A | -3.50 | 105.08 | 106.68 |
| 37 | 41 | 206 | CLA | C4A-NA-C1A | -3.50 | 105.08 | 106.68 |
| 48 | 14 | 312 | A86 | C36-C31-C32 | -3.50 | 116.22 | 119.70 |
| 48 | 37 | 312 | A86 | C25-C26-C27 | -3.50 | 122.37 | 127.28 |
| 37 | 14 | 307 | CLA | C3C-C4C-NC | 3.50 | 114.91 | 110.43 |
| 37 | 41 | 210 | CLA | C3C-C4C-NC | 3.50 | 114.91 | 110.43 |
| 37 | 14 | 307 | CLA | C1C-C2C-C3C | -3.50 | 103.30 | 106.98 |
| 37 | b | 510 | CLA | CHD-C1D-ND | -3.50 | 119.88 | 124.80 |
| 37 | 32 | 202 | CLA | C4B-C3B-C2B | -3.50 | 102.95 | 107.30 |
| 37 | C | 501 | CLA | C3B-C4B-NB | 3.50 | 113.65 | 110.53 |
| 40 | 16 | 315 | SQD | O5-C5-C4 | 3.50 | 116.00 | 109.70 |
| 37 | B | 510 | CLA | CHD-C1D-ND | -3.49 | 119.88 | 124.80 |
| 37 | 18 | 202 | CLA | C3C-C4C-NC | 3.49 | 114.91 | 110.43 |
| 47 | 37 | 307 | KC1 | CAC-C3C-C4C | 3.49 | 129.34 | 124.79 |
| 47 | 17 | 305 | KC1 | CBA-CAA-C2A | -3.49 | 111.44 | 125.45 |
| 37 | 33 | 307 | CLA | C3D-C4D-ND | 3.49 | 115.66 | 109.99 |
| 37 | b | 512 | CLA | C4C-C3C-C2C | -3.49 | 101.81 | 106.89 |
| 37 | 17 | 309 | CLA | C3C-C4C-NC | 3.49 | 114.90 | 110.43 |
| 48 | 14 | 316 | A86 | C41-C32-C31 | -3.49 | 107.35 | 110.47 |
| 41 | d | 409 | LMG | C1-C2-C3 | -3.49 | 102.67 | 110.01 |
| 37 | 32 | 205 | CLA | C4C-C3C-C2C | -3.49 | 101.81 | 106.89 |
| 37 | 41 | 210 | CLA | C3B-C4B-NB | 3.49 | 113.64 | 110.53 |
| 37 | A | 405 | CLA | C3C-C4C-NC | 3.49 | 114.90 | 110.43 |
| 47 | 33 | 309 | KC1 | C1A-NA-C4A | -3.49 | 105.09 | 106.68 |
| 40 | 40 | 202 | SQD | O5-C5-C4 | 3.49 | 115.98 | 109.70 |
| 47 | 31 | 307 | KC1 | CHD-C4C-NC | 3.49 | 129.56 | 124.31 |
| 37 | 32 | 213 | CLA | CAA-C2A-C3A | -3.49 | 103.58 | 113.00 |
| 37 | 19 | 303 | CLA | O2D-CGD-CBD | 3.49 | 117.32 | 111.23 |
| 37 | 15 | 308 | CLA | C1-C2-C3 | -3.49 | 120.49 | 126.20 |
| 37 | 11 | 301 | CLA | CMC-C2C-C1C | 3.49 | 130.48 | 125.03 |
| 37 | 32 | 206 | CLA | C3C-C4C-NC | 3.48 | 114.89 | 110.43 |
| 48 | 34 | 312 | A86 | C3-C4-C5 | -3.48 | 116.39 | 123.52 |
| 37 | 19 | 304 | CLA | C1C-C2C-C3C | -3.48 | 103.31 | 106.98 |
| 37 | b | 504 | CLA | C1-C2-C3 | -3.48 | 120.49 | 126.20 |
| 48 | 32 | 215 | A86 | C41-C32-C31 | -3.48 | 107.35 | 110.47 |
| 37 | 36 | 309 | CLA | C1C-C2C-C3C | -3.48 | 103.32 | 106.98 |
| 47 | 34 | 309 | KC1 | C1C-C2C-C3C | -3.48 | 103.32 | 106.98 |
| 37 | 11 | 301 | CLA | CAC-C3C-C4C | 3.48 | 129.32 | 124.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 506 | CLA | C4B-C3B-C2B | -3.48 | 102.97 | 107.30 |
| 47 | 37 | 302 | KC1 | C1D-CHD-C4C | -3.48 | 118.06 | 126.25 |
| 48 | 14 | 312 | A86 | C3-C4-C5 | -3.48 | 116.39 | 123.52 |
| 48 | 17 | 313 | A86 | C25-C26-C27 | -3.48 | 122.39 | 127.28 |
| 48 | 17 | 313 | A86 | C3-C4-C5 | -3.48 | 116.39 | 123.52 |
| 37 | b | 514 | CLA | CAC-C3C-C4C | 3.48 | 129.32 | 124.79 |
| 37 | 31 | 302 | CLA | CMC-C2C-C1C | 3.48 | 130.47 | 125.03 |
| 37 | 15 | 310 | CLA | C3B-C4B-NB | 3.48 | 113.64 | 110.53 |
| 37 | 12 | 209 | CLA | C1C-C2C-C3C | -3.48 | 103.32 | 106.98 |
| 37 | 32 | 211 | CLA | O2D-CGD-CBD | 3.48 | 117.31 | 111.23 |
| 37 | 12 | 203 | CLA | CAC-C3C-C4C | 3.48 | 129.32 | 124.79 |
| 37 | 32 | 204 | CLA | CAC-C3C-C4C | 3.48 | 129.32 | 124.79 |
| 48 | 34 | 315 | A86 | C33-C32-C31 | 3.48 | 112.59 | 109.21 |
| 37 | 12 | 210 | CLA | C3C-C4C-NC | 3.48 | 114.88 | 110.43 |
| 37 | B | 512 | CLA | C3D-C2D-C1D | -3.48 | 101.09 | 105.83 |
| 41 | D | 412 | LMG | C1-C2-C3 | -3.48 | 102.70 | 110.01 |
| 37 | 32 | 210 | CLA | C1C-C2C-C3C | -3.48 | 103.32 | 106.98 |
| 48 | 38 | 214 | A86 | C3-C4-C5 | -3.48 | 116.41 | 123.52 |
| 37 | 11 | 308 | CLA | C4B-C3B-C2B | -3.47 | 102.98 | 107.30 |
| 37 | B | 514 | CLA | CAC-C3C-C4C | 3.47 | 129.31 | 124.79 |
| 37 | 13 | 308 | CLA | O2A-CGA-CBA | 3.47 | 122.43 | 111.83 |
| 37 | 35 | 301 | CLA | C4A-NA-C1A | -3.47 | 105.09 | 106.68 |
| 37 | 12 | 212 | CLA | CAA-C2A-C3A | -3.47 | 103.61 | 113.00 |
| 37 | B | 516 | CLA | C4B-C3B-C2B | -3.47 | 102.98 | 107.30 |
| 37 | B | 506 | CLA | O2A-CGA-CBA | 3.47 | 122.42 | 111.83 |
| 37 | b | 506 | CLA | O2A-CGA-CBA | 3.47 | 122.42 | 111.83 |
| 37 | a | 407 | CLA | C3C-C4C-NC | 3.47 | 114.88 | 110.43 |
| 37 | 32 | 206 | CLA | C3B-C4B-NB | 3.47 | 113.63 | 110.53 |
| 37 | 38 | 204 | CLA | C3B-C4B-NB | 3.47 | 113.63 | 110.53 |
| 37 | 40 | 205 | CLA | C1C-C2C-C3C | -3.47 | 103.33 | 106.98 |
| 37 | 12 | 204 | CLA | C4C-C3C-C2C | -3.47 | 101.84 | 106.89 |
| 37 | b | 516 | CLA | C4B-C3B-C2B | -3.47 | 102.99 | 107.30 |
| 47 | 11 | 306 | KC1 | C2C-C1C-NC | 3.47 | 114.74 | 110.45 |
| 37 | b | 506 | CLA | C4B-C3B-C2B | -3.47 | 102.99 | 107.30 |
| 37 | b | 511 | CLA | C1C-C2C-C3C | -3.47 | 103.33 | 106.98 |
| 37 | 32 | 211 | CLA | C3B-C4B-NB | 3.47 | 113.62 | 110.53 |
| 37 | 17 | 302 | CLA | C3C-C4C-NC | 3.47 | 114.87 | 110.43 |
| 48 | 15 | 316 | A86 | C33-C32-C31 | 3.47 | 112.58 | 109.21 |
| 37 | 33 | 308 | CLA | O2A-CGA-CBA | 3.47 | 122.40 | 111.83 |
| 37 | 21 | 205 | CLA | C3B-C4B-NB | 3.47 | 113.62 | 110.53 |
| 47 | 32 | 212 | KC1 | C1A-NA-C4A | -3.47 | 105.10 | 106.68 |
| 37 | 38 | 209 | CLA | CMB-C2B-C1B | 3.46 | 130.69 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 507 | CLA | CHD-C1D-ND | -3.46 | 119.93 | 124.80 |
| 37 | 12 | 204 | CLA | C1C-C2C-C3C | -3.46 | 103.34 | 106.98 |
| 37 | 32 | 205 | CLA | C1C-C2C-C3C | -3.46 | 103.34 | 106.98 |
| 37 | B | 513 | CLA | C4B-C3B-C2B | -3.46 | 102.99 | 107.30 |
| 37 | b | 507 | CLA | C1C-C2C-C3C | -3.46 | 103.34 | 106.98 |
| 37 | a | 407 | CLA | C3B-C4B-NB | 3.46 | 113.62 | 110.53 |
| 37 | c | 503 | CLA | CAC-C3C-C4C | 3.46 | 129.29 | 124.79 |
| 37 | B | 511 | CLA | C1C-C2C-C3C | -3.46 | 103.34 | 106.98 |
| 48 | 34 | 312 | A86 | C36-C31-C32 | -3.46 | 116.26 | 119.70 |
| 37 | A | 405 | CLA | C3B-C4B-NB | 3.46 | 113.62 | 110.53 |
| 37 | 32 | 211 | CLA | C3C-C4C-NC | 3.46 | 114.86 | 110.43 |
| 47 | 17 | 303 | KC1 | C1D-CHD-C4C | -3.46 | 118.11 | 126.25 |
| 37 | 39 | 310 | CLA | C4A-NA-C1A | -3.46 | 105.10 | 106.68 |
| 48 | 36 | 311 | A86 | C4-C3-C2 | -3.46 | 116.44 | 123.52 |
| 37 | 18 | 209 | CLA | CMB-C2B-C1B | 3.46 | 130.69 | 125.42 |
| 37 | 38 | 208 | CLA | CAC-C3C-C4C | 3.46 | 129.29 | 124.79 |
| 37 | 11 | 308 | CLA | C3B-C4B-NB | 3.46 | 113.62 | 110.53 |
| 37 | 21 | 205 | CLA | C3C-C4C-NC | 3.46 | 114.86 | 110.43 |
| 37 | 41 | 205 | CLA | C3C-C4C-NC | 3.46 | 114.86 | 110.43 |
| 37 | W | 101 | CLA | O2D-CGD-O1D | -3.46 | 117.12 | 123.85 |
| 37 | 15 | 307 | CLA | C1C-C2C-C3C | -3.46 | 103.34 | 106.98 |
| 48 | 38 | 212 | A86 | C34-O4-C38 | -3.46 | 111.74 | 117.85 |
| 40 | A | 407 | SQD | O9-S-C6 | 3.46 | 111.92 | 106.76 |
| 48 | 11 | 312 | A86 | C4-C5-C6 | -3.46 | 122.43 | 127.28 |
| 47 | 12 | 211 | KC1 | C1A-NA-C4A | -3.46 | 105.10 | 106.68 |
| 48 | 34 | 311 | A86 | C3-C4-C5 | -3.46 | 116.45 | 123.52 |
| 47 | 20 | 305 | KC1 | C1D-CHD-C4C | -3.46 | 118.12 | 126.25 |
| 48 | 12 | 220 | A86 | C26-C25-C24 | -3.46 | 113.19 | 123.20 |
| 37 | 33 | 310 | CLA | C3B-C4B-NB | 3.45 | 113.61 | 110.53 |
| 47 | 35 | 304 | KC1 | CHD-C1D-ND | -3.45 | 118.87 | 124.05 |
| 37 | 33 | 303 | CLA | CBA-CAA-C2A | 3.45 | 124.07 | 113.79 |
| 47 | 14 | 309 | KC1 | C2C-C1C-NC | 3.45 | 114.72 | 110.45 |
| 37 | B | 507 | CLA | C1C-C2C-C3C | -3.45 | 103.35 | 106.98 |
| 47 | 11 | 306 | KC1 | CHD-C4C-NC | 3.45 | 129.51 | 124.31 |
| 37 | c | 505 | CLA | O2D-CGD-O1D | -3.45 | 117.13 | 123.85 |
| 37 | a | 403 | CLA | O2D-CGD-CBD | 3.45 | 117.26 | 111.23 |
| 48 | 18 | 214 | A86 | C4-C5-C6 | -3.45 | 122.44 | 127.28 |
| 37 | C | 506 | CLA | C3C-C4C-NC | 3.45 | 114.85 | 110.43 |
| 37 | A | 403 | CLA | O2D-CGD-CBD | 3.45 | 117.26 | 111.23 |
| 37 | 35 | 307 | CLA | C1C-C2C-C3C | -3.45 | 103.35 | 106.98 |
| 37 | C | 503 | CLA | O2A-CGA-CBA | 3.45 | 122.36 | 111.83 |
| 37 | 13 | 310 | CLA | C3B-C4B-NB | 3.45 | 113.61 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 509 | CLA | C4B-C3B-C2B | -3.45 | 103.01 | 107.30 |
| 37 | D | 401 | CLA | CHD-C4C-NC | 3.45 | 129.58 | 124.23 |
| 37 | 18 | 202 | CLA | CHD-C4C-NC | 3.45 | 129.58 | 124.23 |
| 37 | 35 | 303 | CLA | C4B-C3B-C2B | -3.45 | 103.01 | 107.30 |
| 48 | 16 | 310 | A86 | C3-C4-C5 | -3.45 | 116.46 | 123.52 |
| 47 | 15 | 304 | KC1 | CAA-CBA-CGA | -3.45 | 109.52 | 127.05 |
| 47 | 18 | 210 | KC1 | C1C-C2C-C3C | -3.45 | 103.35 | 106.98 |
| 37 | C | 505 | CLA | O2D-CGD-O1D | -3.45 | 117.14 | 123.85 |
| 37 | b | 512 | CLA | C3D-C2D-C1D | -3.45 | 101.13 | 105.83 |
| 48 | 14 | 315 | A86 | C33-C32-C31 | 3.45 | 112.56 | 109.21 |
| 47 | 37 | 302 | KC1 | C1A-NA-C4A | -3.45 | 105.11 | 106.68 |
| 48 | 17 | 313 | A86 | C12-C11-C13 | 3.44 | 121.58 | 116.00 |
| 48 | 16 | 311 | A86 | C4-C5-C6 | -3.44 | 122.45 | 127.28 |
| 37 | C | 503 | CLA | CAC-C3C-C4C | 3.44 | 129.27 | 124.79 |
| 37 | b | 513 | CLA | C4B-C3B-C2B | -3.44 | 103.02 | 107.30 |
| 48 | 11 | 312 | A86 | C36-C31-C32 | -3.44 | 116.28 | 119.70 |
| 37 | D | 405 | CLA | C3B-C4B-NB | 3.44 | 113.60 | 110.53 |
| 37 | 13 | 310 | CLA | C1C-C2C-C3C | -3.44 | 103.36 | 106.98 |
| 37 | B | 506 | CLA | CAC-C3C-C4C | 3.44 | 129.27 | 124.79 |
| 47 | 38 | 205 | KC1 | CHD-C1D-ND | -3.44 | 118.89 | 124.05 |
| 37 | c | 503 | CLA | O2A-CGA-CBA | 3.44 | 122.33 | 111.83 |
| 48 | 11 | 313 | A86 | C12-C11-C13 | 3.44 | 121.58 | 116.00 |
| 37 | B | 504 | CLA | C1-C2-C3 | -3.44 | 120.56 | 126.20 |
| 37 | b | 503 | CLA | C4-C3-C5 | 3.44 | 121.20 | 115.23 |
| 48 | 12 | 213 | A86 | C41-C32-C31 | -3.44 | 107.39 | 110.47 |
| 37 | B | 504 | CLA | CHC-C1C-C2C | -3.44 | 117.17 | 126.95 |
| 48 | 14 | 311 | A86 | C3-C4-C5 | -3.44 | 116.48 | 123.52 |
| 37 | b | 504 | CLA | CHC-C1C-C2C | -3.44 | 117.18 | 126.95 |
| 37 | c | 506 | CLA | C3C-C4C-NC | 3.44 | 114.83 | 110.43 |
| 37 | c | 504 | CLA | CAC-C3C-C4C | 3.44 | 129.26 | 124.79 |
| 37 | B | 505 | CLA | C1C-C2C-C3C | -3.44 | 103.36 | 106.98 |
| 37 | b | 515 | CLA | C1C-C2C-C3C | -3.44 | 103.36 | 106.98 |
| 37 | 18 | 203 | CLA | C4A-NA-C1A | -3.44 | 105.11 | 106.68 |
| 48 | 36 | 311 | A86 | C4-C5-C6 | -3.44 | 122.46 | 127.28 |
| 48 | 32 | 221 | A86 | C33-C32-C31 | 3.44 | 112.55 | 109.21 |
| 48 | 12 | 214 | A86 | C41-C32-C31 | -3.43 | 107.40 | 110.47 |
| 48 | 32 | 214 | A86 | C41-C32-C31 | -3.43 | 107.40 | 110.47 |
| 48 | 32 | 221 | A86 | C26-C25-C24 | -3.43 | 113.25 | 123.20 |
| 47 | 40 | 207 | KC1 | C1D-CHD-C4C | -3.43 | 118.17 | 126.25 |
| 37 | 20 | 303 | CLA | C3D-C4D-ND | 3.43 | 115.57 | 109.99 |
| 37 | 20 | 306 | CLA | C3C-C4C-NC | 3.43 | 114.83 | 110.43 |
| 37 | C | 502 | CLA | CHC-C1C-C2C | -3.43 | 117.19 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 11 | 310 | CLA | O2D-CGD-CBD | 3.43 | 117.23 | 111.23 |
| 37 | 32 | 202 | CLA | C3B-C4B-NB | 3.43 | 113.59 | 110.53 |
| 37 | 41 | 209 | CLA | C3B-C4B-NB | 3.43 | 113.59 | 110.53 |
| 37 | 18 | 206 | CLA | C3C-C4C-NC | 3.43 | 114.83 | 110.43 |
| 47 | 35 | 304 | KC1 | C1D-CHD-C4C | -3.43 | 118.17 | 126.25 |
| 47 | 35 | 304 | KC1 | CAA-CBA-CGA | -3.43 | 109.59 | 127.05 |
| 37 | 20 | 303 | CLA | C3B-C4B-NB | 3.43 | 113.59 | 110.53 |
| 37 | 33 | 308 | CLA | C3B-C4B-NB | 3.43 | 113.59 | 110.53 |
| 48 | 32 | 214 | A86 | C25-C24-C1 | -3.43 | 116.95 | 126.36 |
| 48 | 35 | 315 | A86 | C41-C32-C31 | -3.43 | 107.40 | 110.47 |
| 37 | B | 516 | CLA | C3B-C4B-NB | 3.43 | 113.59 | 110.53 |
| 37 | a | 404 | CLA | CHD-C4C-NC | 3.43 | 129.55 | 124.23 |
| 37 | 40 | 210 | CLA | CHD-C1D-ND | -3.43 | 119.98 | 124.80 |
| 37 | w | 101 | CLA | O2D-CGD-O1D | -3.43 | 117.17 | 123.85 |
| 37 | 17 | 302 | CLA | CHD-C1D-ND | -3.43 | 119.98 | 124.80 |
| 47 | 17 | 308 | KC1 | CAC-C3C-C4C | 3.43 | 129.25 | 124.79 |
| 37 | z | 101 | CLA | C3C-C4C-NC | 3.43 | 114.82 | 110.43 |
| 48 | 38 | 214 | A86 | C4-C5-C6 | -3.43 | 122.47 | 127.28 |
| 48 | 18 | 215 | A86 | C4-C3-C2 | -3.43 | 116.51 | 123.52 |
| 48 | 13 | 311 | A86 | C10-C9-C8 | -3.43 | 113.27 | 123.20 |
| 48 | 33 | 311 | A86 | C10-C9-C8 | -3.43 | 113.27 | 123.20 |
| 37 | 40 | 205 | CLA | C3D-C4D-ND | 3.43 | 115.56 | 109.99 |
| 47 | 18 | 205 | KC1 | CHD-C1D-ND | -3.43 | 118.91 | 124.05 |
| 47 | 16 | 304 | KC1 | CAA-CBA-CGA | -3.43 | 109.62 | 127.05 |
| 37 | d | 403 | CLA | C3B-C4B-NB | 3.43 | 113.59 | 110.53 |
| 37 | 11 | 303 | CLA | C3B-C4B-NB | 3.43 | 113.59 | 110.53 |
| 37 | 21 | 210 | CLA | C3B-C4B-NB | 3.43 | 113.59 | 110.53 |
| 37 | 31 | 304 | CLA | C3B-C4B-NB | 3.43 | 113.59 | 110.53 |
| 37 | B | 503 | CLA | C4-C3-C5 | 3.43 | 121.18 | 115.23 |
| 47 | 40 | 207 | KC1 | O2D-CGD-O1D | -3.43 | 117.18 | 123.85 |
| 47 | 36 | 304 | KC1 | CAA-CBA-CGA | -3.43 | 109.63 | 127.05 |
| 37 | 36 | 301 | CLA | C4A-NA-C1A | -3.43 | 105.12 | 106.68 |
| 47 | 17 | 303 | KC1 | C1A-NA-C4A | -3.43 | 105.12 | 106.68 |
| 37 | c | 502 | CLA | CHC-C1C-C2C | -3.43 | 117.21 | 126.95 |
| 48 | 31 | 315 | A86 | C25-C24-C1 | -3.43 | 116.97 | 126.36 |
| 48 | 15 | 315 | A86 | O2-C18-C17 | 3.43 | 116.75 | 109.75 |
| 48 | 11 | 315 | A86 | C25-C24-C1 | -3.42 | 116.97 | 126.36 |
| 37 | 18 | 201 | CLA | CAC-C3C-C4C | 3.42 | 129.25 | 124.79 |
| 48 | 16 | 311 | A86 | C4-C3-C2 | -3.42 | 116.51 | 123.52 |
| 48 | 14 | 315 | A86 | C10-C9-C8 | -3.42 | 113.28 | 123.20 |
| 48 | 34 | 315 | A86 | C10-C9-C8 | -3.42 | 113.28 | 123.20 |
| 47 | 36 | 302 | KC1 | C2A-C1A-NA | 3.42 | 114.83 | 109.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 205 | CLA | C1C-C2C-C3C | -3.42 | 103.38 | 106.98 |
| 37 | b | 503 | CLA | O2A-CGA-CBA | 3.42 | 122.27 | 111.83 |
| 37 | b | 516 | CLA | C3B-C4B-NB | 3.42 | 113.58 | 110.53 |
| 48 | 37 | 314 | A86 | C9-C8-C6 | -3.42 | 116.98 | 126.36 |
| 37 | 18 | 203 | CLA | CHC-C1C-C2C | -3.42 | 117.22 | 126.95 |
| 47 | 41 | 207 | KC1 | CMC-C2C-C1C | 3.42 | 130.38 | 125.03 |
| 48 | 34 | 316 | A86 | C41-C32-C31 | -3.42 | 107.41 | 110.47 |
| 37 | B | 507 | CLA | CHC-C1C-C2C | -3.42 | 117.22 | 126.95 |
| 47 | 37 | 307 | KC1 | C1C-C2C-C3C | -3.42 | 103.38 | 106.98 |
| 37 | 19 | 305 | CLA | CAA-C2A-C3A | -3.42 | 103.76 | 113.00 |
| 47 | 37 | 304 | KC1 | C1D-CHD-C4C | -3.42 | 118.21 | 126.25 |
| 37 | 15 | 303 | CLA | C4B-C3B-C2B | -3.42 | 103.05 | 107.30 |
| 48 | 32 | 203 | A86 | C12-C11-C13 | 3.42 | 121.54 | 116.00 |
| 37 | 20 | 308 | CLA | CHD-C1D-ND | -3.42 | 119.99 | 124.80 |
| 37 | 38 | 203 | CLA | C4A-NA-C1A | -3.42 | 105.12 | 106.68 |
| 37 | 13 | 303 | CLA | CBA-CAA-C2A | 3.42 | 123.96 | 113.79 |
| 37 | 16 | 303 | CLA | CAC-C3C-C4C | 3.42 | 129.24 | 124.79 |
| 48 | 38 | 215 | A86 | C4-C3-C2 | -3.41 | 116.53 | 123.52 |
| 48 | 36 | 310 | A86 | C3-C4-C5 | -3.41 | 116.53 | 123.52 |
| 48 | 31 | 312 | A86 | C36-C31-C32 | -3.41 | 116.31 | 119.70 |
| 48 | 15 | 313 | A86 | C12-C11-C13 | 3.41 | 121.53 | 116.00 |
| 37 | B | 503 | CLA | O2A-CGA-CBA | 3.41 | 122.24 | 111.83 |
| 40 | a | 409 | SQD | O9-S-C6 | 3.41 | 111.85 | 106.76 |
| 37 | b | 509 | CLA | C4B-C3B-C2B | -3.41 | 103.06 | 107.30 |
| 37 | 12 | 204 | CLA | O2D-CGD-O1D | -3.41 | 117.21 | 123.85 |
| 37 | c | 505 | CLA | C1C-C2C-C3C | -3.41 | 103.39 | 106.98 |
| 37 | 41 | 205 | CLA | C1C-C2C-C3C | -3.41 | 103.39 | 106.98 |
| 45 | d | 406 | PL9 | C7-C3-C4 | 3.41 | 119.72 | 116.91 |
| 37 | C | 513 | CLA | C1C-C2C-C3C | -3.41 | 103.39 | 106.98 |
| 37 | c | 509 | CLA | O2D-CGD-O1D | -3.41 | 117.21 | 123.85 |
| 48 | 37 | 312 | A86 | C10-C9-C8 | -3.41 | 113.32 | 123.20 |
| 37 | c | 509 | CLA | C4B-C3B-C2B | -3.41 | 103.06 | 107.30 |
| 37 | 37 | 308 | CLA | C3C-C4C-NC | 3.41 | 114.80 | 110.43 |
| 37 | B | 509 | CLA | CHD-C1D-ND | -3.41 | 120.00 | 124.80 |
| 37 | b | 509 | CLA | CHD-C1D-ND | -3.41 | 120.00 | 124.80 |
| 37 | 12 | 205 | CLA | C3B-C4B-NB | 3.41 | 113.57 | 110.53 |
| 47 | 34 | 309 | KC1 | C2C-C1C-NC | 3.41 | 114.67 | 110.45 |
| 47 | 32 | 207 | KC1 | C1A-NA-C4A | -3.41 | 105.12 | 106.68 |
| 37 | B | 508 | CLA | C3C-C4C-NC | 3.41 | 114.80 | 110.43 |
| 37 | 31 | 310 | CLA | O2D-CGD-CBD | 3.41 | 117.19 | 111.23 |
| 37 | 15 | 308 | CLA | CHC-C1C-C2C | -3.41 | 117.27 | 126.95 |
| 37 | B | 515 | CLA | C1C-C2C-C3C | -3.40 | 103.40 | 106.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 32 | 205 | CLA | O2D-CGD-O1D | -3.40 | 117.22 | 123.85 |
| 37 | 36 | 303 | CLA | CAC-C3C-C4C | 3.40 | 129.22 | 124.79 |
| 47 | 37 | 304 | KC1 | C4B-C3B-C2B | -3.40 | 103.86 | 106.81 |
| 48 | 13 | 314 | A86 | C12-C11-C13 | 3.40 | 121.52 | 116.00 |
| 48 | 17 | 315 | A86 | C9-C8-C6 | -3.40 | 117.04 | 126.36 |
| 37 | 39 | 306 | CLA | CHD-C1D-ND | -3.40 | 120.02 | 124.80 |
| 37 | 38 | 209 | CLA | C3B-C4B-NB | 3.40 | 113.56 | 110.53 |
| 37 | 19 | 303 | CLA | C1-C2-C3 | -3.40 | 120.63 | 126.20 |
| 37 | 11 | 305 | CLA | C3C-C4C-NC | 3.40 | 114.78 | 110.43 |
| 47 | 16 | 302 | KC1 | C2A-C1A-NA | 3.40 | 114.79 | 109.34 |
| 37 | 37 | 301 | CLA | C3C-C4C-NC | 3.40 | 114.78 | 110.43 |
| 37 | 13 | 308 | CLA | C3B-C4B-NB | 3.40 | 113.56 | 110.53 |
| 37 | 16 | 307 | CLA | C1-C2-C3 | -3.40 | 120.63 | 126.20 |
| 37 | 40 | 208 | CLA | C3C-C4C-NC | 3.40 | 114.78 | 110.43 |
| 48 | 35 | 312 | A86 | C36-C31-C32 | -3.40 | 116.33 | 119.70 |
| 47 | 13 | 306 | KC1 | CBC-CAC-C3C | -3.40 | 103.22 | 112.42 |
| 37 | b | 507 | CLA | CHC-C1C-C2C | -3.40 | 117.30 | 126.95 |
| 37 | C | 504 | CLA | CAC-C3C-C4C | 3.40 | 129.21 | 124.79 |
| 47 | 18 | 207 | KC1 | C1A-NA-C4A | -3.40 | 105.13 | 106.68 |
| 37 | 38 | 206 | CLA | C3B-C4B-NB | 3.39 | 113.56 | 110.53 |
| 37 | 36 | 307 | CLA | C1-C2-C3 | -3.39 | 120.64 | 126.20 |
| 37 | C | 509 | CLA | O2D-CGD-O1D | -3.39 | 117.24 | 123.85 |
| 47 | 12 | 206 | KC1 | C1A-NA-C4A | -3.39 | 105.13 | 106.68 |
| 37 | 21 | 206 | CLA | C3C-C4C-NC | 3.39 | 114.78 | 110.43 |
| 37 | 33 | 308 | CLA | C4B-C3B-C2B | -3.39 | 103.08 | 107.30 |
| 37 | b | 501 | CLA | C4A-NA-C1A | -3.39 | 105.13 | 106.68 |
| 48 | 12 | 202 | A86 | C12-C11-C13 | 3.39 | 121.50 | 116.00 |
| 47 | 17 | 305 | KC1 | C1D-CHD-C4C | -3.39 | 118.27 | 126.25 |
| 48 | 38 | 214 | A86 | C9-C8-C6 | -3.39 | 117.07 | 126.36 |
| 48 | 13 | 315 | A86 | C35-C34-C33 | 3.39 | 115.97 | 109.89 |
| 47 | 31 | 303 | KC1 | CAA-CBA-CGA | -3.39 | 109.82 | 127.05 |
| 37 | 19 | 306 | CLA | CHD-C1D-ND | -3.39 | 120.03 | 124.80 |
| 37 | 39 | 303 | CLA | C1-C2-C3 | -3.39 | 120.64 | 126.20 |
| 37 | 15 | 310 | CLA | C3C-C4C-NC | 3.39 | 114.77 | 110.43 |
| 41 | 16 | 316 | LMG | O6-C1-O1 | -3.39 | 102.04 | 110.04 |
| 37 | 40 | 205 | CLA | C3B-C4B-NB | 3.39 | 113.55 | 110.53 |
| 47 | 11 | 302 | KC1 | CAA-CBA-CGA | -3.39 | 109.83 | 127.05 |
| 37 | 41 | 202 | CLA | C3C-C4C-NC | 3.39 | 114.77 | 110.43 |
| 48 | 11 | 319 | A86 | C10-C9-C8 | -3.38 | 113.39 | 123.20 |
| 47 | 33 | 306 | KC1 | CBC-CAC-C3C | -3.38 | 103.25 | 112.42 |
| 48 | 18 | 214 | A86 | C36-C31-C32 | -3.38 | 116.34 | 119.70 |
| 47 | 20 | 305 | KC1 | O2D-CGD-O1D | -3.38 | 117.26 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 16 | 306 | CLA | CAC-C3C-C4C | 3.38 | 129.19 | 124.79 |
| 47 | 21 | 207 | KC1 | CMC-C2C-C1C | 3.38 | 130.32 | 125.03 |
| 48 | 37 | 311 | A86 | C4-C3-C2 | -3.38 | 116.60 | 123.52 |
| 48 | 38 | 214 | A86 | C36-C31-C32 | -3.38 | 116.34 | 119.70 |
| 48 | 31 | 319 | A86 | C10-C9-C8 | -3.38 | 113.40 | 123.20 |
| 37 | 12 | 207 | CLA | C3C-C4C-NC | 3.38 | 114.76 | 110.43 |
| 37 | b | 505 | CLA | C1C-C2C-C3C | -3.38 | 103.42 | 106.98 |
| 37 | b | 508 | CLA | C3C-C4C-NC | 3.38 | 114.76 | 110.43 |
| 37 | 36 | 306 | CLA | CAC-C3C-C4C | 3.38 | 129.19 | 124.79 |
| 37 | 20 | 307 | CLA | C3C-C4C-NC | 3.38 | 114.76 | 110.43 |
| 41 | 36 | 314 | LMG | O6-C1-O1 | -3.38 | 102.06 | 110.04 |
| 37 | C | 505 | CLA | C1C-C2C-C3C | -3.38 | 103.43 | 106.98 |
| 47 | 35 | 304 | KC1 | CAC-C3C-C4C | 3.38 | 129.19 | 124.79 |
| 47 | 40 | 204 | KC1 | CAA-CBA-CGA | -3.38 | 109.87 | 127.05 |
| 37 | 38 | 206 | CLA | C3C-C4C-NC | 3.38 | 114.76 | 110.43 |
| 37 | b | 506 | CLA | CAC-C3C-C4C | 3.38 | 129.19 | 124.79 |
| 37 | 16 | 307 | CLA | C3C-C4C-NC | 3.38 | 114.75 | 110.43 |
| 37 | 41 | 205 | CLA | C3B-C4B-NB | 3.38 | 113.54 | 110.53 |
| 37 | 17 | 309 | CLA | C1-C2-C3 | -3.37 | 120.67 | 126.20 |
| 37 | 39 | 305 | CLA | CAA-C2A-C3A | -3.37 | 103.88 | 113.00 |
| 37 | 15 | 303 | CLA | C3B-C4B-NB | 3.37 | 113.54 | 110.53 |
| 37 | 21 | 209 | CLA | C3B-C4B-NB | 3.37 | 113.54 | 110.53 |
| 47 | 20 | 302 | KC1 | CAA-CBA-CGA | -3.37 | 109.89 | 127.05 |
| 48 | 33 | 315 | A86 | C35-C34-C33 | 3.37 | 115.94 | 109.89 |
| 37 | C | 509 | CLA | C4B-C3B-C2B | -3.37 | 103.11 | 107.30 |
| 37 | 13 | 308 | CLA | C4B-C3B-C2B | -3.37 | 103.11 | 107.30 |
| 48 | 33 | 311 | A86 | C34-O4-C38 | -3.37 | 111.89 | 117.85 |
| 37 | Z | 101 | CLA | C3C-C4C-NC | 3.37 | 114.75 | 110.43 |
| 37 | 31 | 306 | CLA | C3C-C4C-NC | 3.37 | 114.75 | 110.43 |
| 48 | 12 | 213 | A86 | C10-C9-C8 | -3.37 | 113.43 | 123.20 |
| 37 | 41 | 208 | CLA | C3B-C4B-NB | 3.37 | 113.54 | 110.53 |
| 48 | 31 | 313 | A86 | C12-C11-C13 | 3.37 | 121.47 | 116.00 |
| 47 | 35 | 306 | KC1 | C4B-C3B-C2B | -3.37 | 103.89 | 106.81 |
| 37 | 18 | 209 | CLA | C3B-C4B-NB | 3.37 | 113.54 | 110.53 |
| 47 | 17 | 305 | KC1 | CHD-C1D-ND | -3.37 | 118.99 | 124.05 |
| 37 | 12 | 203 | CLA | C1C-C2C-C3C | -3.37 | 103.44 | 106.98 |
| 37 | 38 | 203 | CLA | CHC-C1C-C2C | -3.37 | 117.37 | 126.95 |
| 37 | 17 | 309 | CLA | C4C-C3C-C2C | -3.37 | 101.99 | 106.89 |
| 37 | w | 101 | CLA | CAA-C2A-C3A | -3.37 | 103.90 | 113.00 |
| 37 | 21 | 202 | CLA | C3C-C4C-NC | 3.37 | 114.75 | 110.43 |
| 37 | A | 403 | CLA | C4B-C3B-C2B | -3.37 | 103.11 | 107.30 |
| 37 | B | 514 | CLA | C3B-C4B-NB | 3.37 | 113.54 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 32 | 208 | CLA | C3C-C4C-NC | 3.37 | 114.74 | 110.43 |
| 37 | W | 101 | CLA | CAA-C2A-C3A | -3.37 | 103.90 | 113.00 |
| 37 | 41 | 206 | CLA | C3C-C4C-NC | 3.36 | 114.74 | 110.43 |
| 37 | 14 | 310 | CLA | C3B-C4B-NB | 3.36 | 113.53 | 110.53 |
| 48 | 17 | 315 | A86 | C33-C32-C31 | 3.36 | 112.48 | 109.21 |
| 47 | 40 | 206 | KC1 | C1A-NA-C4A | -3.36 | 105.14 | 106.68 |
| 37 | a | 403 | CLA | C4B-C3B-C2B | -3.36 | 103.12 | 107.30 |
| 48 | 13 | 315 | A86 | C41-C32-C31 | -3.36 | 107.46 | 110.47 |
| 47 | 15 | 302 | KC1 | CBA-CAA-C2A | -3.36 | 111.96 | 125.45 |
| 37 | 13 | 301 | CLA | C3C-C4C-NC | 3.36 | 114.74 | 110.43 |
| 37 | c | 513 | CLA | C1C-C2C-C3C | -3.36 | 103.44 | 106.98 |
| 37 | 35 | 308 | CLA | C1C-C2C-C3C | -3.36 | 103.44 | 106.98 |
| 48 | 12 | 220 | A86 | C33-C32-C31 | 3.36 | 112.48 | 109.21 |
| 48 | 12 | 216 | A86 | C3-C4-C5 | -3.36 | 116.65 | 123.52 |
| 37 | B | 504 | CLA | C3C-C4C-NC | 3.36 | 114.73 | 110.43 |
| 37 | 20 | 301 | CLA | C1-C2-C3 | -3.36 | 120.69 | 126.20 |
| 37 | 40 | 203 | CLA | C1-C2-C3 | -3.36 | 120.70 | 126.20 |
| 37 | 35 | 303 | CLA | C3B-C4B-NB | 3.36 | 113.53 | 110.53 |
| 48 | 16 | 313 | A86 | C36-C31-C32 | -3.36 | 116.37 | 119.70 |
| 48 | 37 | 314 | A86 | C33-C32-C31 | 3.36 | 112.47 | 109.21 |
| 37 | 19 | 302 | CLA | C3B-C4B-NB | 3.36 | 113.53 | 110.53 |
| 47 | 36 | 302 | KC1 | CMA-C3A-C2A | -3.35 | 120.31 | 128.43 |
| 37 | 40 | 210 | CLA | C3B-C4B-NB | 3.35 | 113.52 | 110.53 |
| 48 | 17 | 313 | A86 | C10-C9-C8 | -3.35 | 113.48 | 123.20 |
| 37 | C | 510 | CLA | C4B-C3B-C2B | -3.35 | 103.13 | 107.30 |
| 47 | 41 | 207 | KC1 | C1C-C2C-C3C | -3.35 | 103.45 | 106.98 |
| 47 | 15 | 306 | KC1 | C4B-C3B-C2B | -3.35 | 103.91 | 106.81 |
| 47 | 35 | 302 | KC1 | CBA-CAA-C2A | -3.35 | 112.01 | 125.45 |
| 37 | c | 510 | CLA | C4B-C3B-C2B | -3.35 | 103.14 | 107.30 |
| 37 | 34 | 308 | CLA | C4A-NA-C1A | -3.35 | 105.15 | 106.68 |
| 48 | 35 | 319 | A86 | C25-C24-C1 | -3.35 | 117.18 | 126.36 |
| 37 | 13 | 310 | CLA | CAC-C3C-C4C | 3.35 | 129.15 | 124.79 |
| 37 | 19 | 303 | CLA | C1C-C2C-C3C | -3.35 | 103.46 | 106.98 |
| 37 | 39 | 303 | CLA | C1C-C2C-C3C | -3.35 | 103.46 | 106.98 |
| 48 | 35 | 316 | A86 | C40-C32-C31 | 3.35 | 113.47 | 110.47 |
| 37 | 19 | 309 | CLA | C3C-C4C-NC | 3.35 | 114.72 | 110.43 |
| 37 | 38 | 201 | CLA | C3C-C4C-NC | 3.35 | 114.72 | 110.43 |
| 37 | 18 | 204 | CLA | C1C-C2C-C3C | -3.35 | 103.46 | 106.98 |
| 37 | b | 514 | CLA | C3B-C4B-NB | 3.35 | 113.52 | 110.53 |
| 37 | b | 504 | CLA | C3C-C4C-NC | 3.35 | 114.72 | 110.43 |
| 37 | 18 | 203 | CLA | C1-C2-C3 | -3.34 | 120.72 | 126.20 |
| 37 | 19 | 302 | CLA | C4B-C3B-C2B | -3.34 | 103.14 | 107.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 34 | 308 | CLA | CHC-C1C-C2C | -3.34 | 117.44 | 126.95 |
| 48 | 39 | 313 | A86 | C21-C20-C15 | -3.34 | 112.55 | 123.35 |
| 48 | 32 | 214 | A86 | C10-C9-C8 | -3.34 | 113.52 | 123.20 |
| 47 | 12 | 206 | KC1 | CHD-C4C-NC | 3.34 | 129.34 | 124.31 |
| 37 | 14 | 308 | CLA | CHC-C1C-C2C | -3.34 | 117.45 | 126.95 |
| 37 | 38 | 203 | CLA | C3B-C4B-NB | 3.34 | 113.51 | 110.53 |
| 48 | 15 | 319 | A86 | C25-C24-C1 | -3.34 | 117.20 | 126.36 |
| 48 | 40 | 201 | A86 | C36-C31-C32 | -3.34 | 116.38 | 119.70 |
| 37 | 34 | 310 | CLA | CHC-C1C-C2C | -3.34 | 117.46 | 126.95 |
| 48 | 13 | 311 | A86 | C34-O4-C38 | -3.34 | 111.95 | 117.85 |
| 48 | 32 | 217 | A86 | C3-C4-C5 | -3.34 | 116.69 | 123.52 |
| 37 | 39 | 303 | CLA | O2D-CGD-CBD | 3.34 | 117.06 | 111.23 |
| 37 | 33 | 310 | CLA | CAC-C3C-C4C | 3.34 | 129.13 | 124.79 |
| 37 | 12 | 205 | CLA | C3C-C4C-NC | 3.34 | 114.70 | 110.43 |
| 37 | 40 | 209 | CLA | C3C-C4C-NC | 3.34 | 114.70 | 110.43 |
| 37 | 32 | 204 | CLA | C1C-C2C-C3C | -3.34 | 103.47 | 106.98 |
| 48 | 21 | 213 | A86 | C35-C34-C33 | 3.34 | 115.88 | 109.89 |
| 37 | C | 511 | CLA | C4C-C3C-C2C | -3.34 | 102.04 | 106.89 |
| 37 | 36 | 307 | CLA | C3C-C4C-NC | 3.34 | 114.70 | 110.43 |
| 37 | 34 | 310 | CLA | C3B-C4B-NB | 3.33 | 113.51 | 110.53 |
| 48 | 35 | 313 | A86 | C12-C11-C13 | 3.33 | 121.41 | 116.00 |
| 48 | 36 | 311 | A86 | C36-C31-C32 | -3.33 | 116.39 | 119.70 |
| 47 | 16 | 302 | KC1 | CMA-C3A-C2A | -3.33 | 120.36 | 128.43 |
| 45 | D | 408 | PL9 | C7-C3-C4 | 3.33 | 119.66 | 116.91 |
| 37 | 35 | 310 | CLA | C3C-C4C-NC | 3.33 | 114.70 | 110.43 |
| 37 | 14 | 310 | CLA | CHC-C1C-C2C | -3.33 | 117.47 | 126.95 |
| 48 | 14 | 312 | A86 | C12-C11-C13 | 3.33 | 121.41 | 116.00 |
| 48 | 37 | 310 | A86 | C12-C11-C13 | 3.33 | 121.41 | 116.00 |
| 37 | 32 | 205 | CLA | CAA-C2A-C1A | 3.33 | 122.90 | 111.97 |
| 48 | 33 | 315 | A86 | C41-C32-C31 | -3.33 | 107.49 | 110.47 |
| 37 | 12 | 210 | CLA | O2D-CGD-CBD | 3.33 | 117.05 | 111.23 |
| 37 | 18 | 208 | CLA | C1C-C2C-C3C | -3.33 | 103.48 | 106.98 |
| 37 | 20 | 308 | CLA | C3B-C4B-NB | 3.33 | 113.50 | 110.53 |
| 48 | 41 | 213 | A86 | C35-C34-C33 | 3.33 | 115.87 | 109.89 |
| 37 | b | 505 | CLA | C3C-C4C-NC | 3.33 | 114.70 | 110.43 |
| 38 | A | 404 | PHO | O1D-CGD-CBD | 3.33 | 129.77 | 124.72 |
| 37 | 31 | 301 | CLA | CHD-C1D-ND | -3.33 | 120.12 | 124.80 |
| 37 | 11 | 301 | CLA | CHD-C4C-NC | 3.33 | 129.39 | 124.23 |
| 37 | 31 | 302 | CLA | CHD-C4C-NC | 3.33 | 129.39 | 124.23 |
| 48 | 39 | 311 | A86 | C12-C11-C13 | 3.33 | 121.40 | 116.00 |
| 37 | 39 | 302 | CLA | C4B-C3B-C2B | -3.33 | 103.16 | 107.30 |
| 37 | C | 507 | CLA | C3B-C4B-NB | 3.33 | 113.50 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 302 | KC1 | CAA-CBA-CGA | -3.33 | 110.13 | 127.05 |
| 47 | 32 | 207 | KC1 | CHD-C4C-NC | 3.33 | 129.32 | 124.31 |
| 48 | 16 | 311 | A86 | C36-C31-C32 | -3.33 | 116.39 | 119.70 |
| 37 | 37 | 308 | CLA | C1-C2-C3 | -3.33 | 120.75 | 126.20 |
| 48 | 19 | 311 | A86 | C12-C11-C13 | 3.33 | 121.39 | 116.00 |
| 48 | 34 | 312 | A86 | C41-C32-C31 | -3.33 | 107.50 | 110.47 |
| 37 | c | 505 | CLA | C4B-C3B-C2B | -3.33 | 103.17 | 107.30 |
| 47 | 15 | 302 | KC1 | CAA-CBA-CGA | -3.33 | 110.14 | 127.05 |
| 37 | 21 | 208 | CLA | C3B-C4B-NB | 3.33 | 113.50 | 110.53 |
| 37 | 33 | 301 | CLA | C3C-C4C-NC | 3.33 | 114.69 | 110.43 |
| 37 | 12 | 204 | CLA | C3D-C2D-C1D | -3.32 | 101.30 | 105.83 |
| 37 | 12 | 204 | CLA | CAA-C2A-C1A | 3.32 | 122.87 | 111.97 |
| 48 | 14 | 311 | A86 | C7-C6-C8 | 3.32 | 123.17 | 118.09 |
| 37 | 20 | 306 | CLA | CAA-C2A-C3A | -3.32 | 104.02 | 113.00 |
| 37 | c | 511 | CLA | C4C-C3C-C2C | -3.32 | 102.05 | 106.89 |
| 40 | 36 | 315 | SQD | O9-S-C6 | 3.32 | 111.72 | 106.76 |
| 47 | 15 | 304 | KC1 | CHD-C1D-ND | -3.32 | 119.06 | 124.05 |
| 37 | C | 505 | CLA | C4B-C3B-C2B | -3.32 | 103.17 | 107.30 |
| 48 | 18 | 213 | A86 | C7-C6-C5 | -3.32 | 117.43 | 122.82 |
| 40 | a | 409 | SQD | O7-S-C6 | 3.32 | 111.72 | 106.76 |
| 37 | 34 | 301 | CLA | CAC-C3C-C4C | 3.32 | 129.11 | 124.79 |
| 37 | W | 102 | CLA | CHD-C1D-ND | -3.32 | 120.13 | 124.80 |
| 37 | 40 | 210 | CLA | CAC-C3C-C4C | 3.32 | 129.11 | 124.79 |
| 37 | 14 | 301 | CLA | CAC-C3C-C4C | 3.32 | 129.11 | 124.79 |
| 47 | 37 | 302 | KC1 | CAA-CBA-CGA | -3.32 | 110.17 | 127.05 |
| 37 | z | 102 | CLA | C3C-C4C-NC | 3.32 | 114.68 | 110.43 |
| 37 | 18 | 208 | CLA | CAC-C3C-C4C | 3.32 | 129.11 | 124.79 |
| 37 | B | 505 | CLA | C3C-C4C-NC | 3.32 | 114.68 | 110.43 |
| 37 | 20 | 308 | CLA | CAC-C3C-C4C | 3.32 | 129.11 | 124.79 |
| 37 | 40 | 208 | CLA | CAA-C2A-C3A | -3.32 | 104.03 | 113.00 |
| 48 | 14 | 312 | A86 | C41-C32-C31 | -3.32 | 107.50 | 110.47 |
| 47 | 20 | 304 | KC1 | C1A-NA-C4A | -3.32 | 105.17 | 106.68 |
| 37 | 13 | 305 | CLA | C3C-C4C-NC | 3.32 | 114.68 | 110.43 |
| 37 | 33 | 305 | CLA | C3C-C4C-NC | 3.32 | 114.68 | 110.43 |
| 37 | c | 502 | CLA | C1-C2-C3 | -3.32 | 120.77 | 126.20 |
| 48 | 33 | 314 | A86 | C12-C11-C13 | 3.31 | 121.38 | 116.00 |
| 38 | a | 405 | PHO | C3B-C4B-NB | -3.31 | 105.30 | 107.46 |
| 40 | 17 | 301 | SQD | O9-S-C6 | 3.31 | 111.70 | 106.76 |
| 37 | b | 523 | CLA | C4C-C3C-C2C | -3.31 | 102.07 | 106.89 |
| 37 | b | 502 | CLA | C1-C2-C3 | -3.31 | 120.77 | 126.20 |
| 37 | D | 406 | CLA | C3C-C4C-NC | 3.31 | 114.67 | 110.43 |
| 37 | 39 | 307 | CLA | CAA-C2A-C3A | -3.31 | 104.05 | 113.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 35 | 305 | CLA | C3B-C4B-NB | 3.31 | 113.49 | 110.53 |
| 48 | 34 | 311 | A86 | C7-C6-C8 | 3.31 | 123.15 | 118.09 |
| 48 | 37 | 313 | A86 | C25-C24-C1 | -3.31 | 117.28 | 126.36 |
| 40 | A | 407 | SQD | O7-S-C6 | 3.31 | 111.70 | 106.76 |
| 37 | B | 516 | CLA | CAA-C2A-C3A | -3.31 | 104.05 | 113.00 |
| 37 | 39 | 302 | CLA | C3B-C4B-NB | 3.31 | 113.48 | 110.53 |
| 37 | 15 | 305 | CLA | C3C-C4C-NC | 3.31 | 114.67 | 110.43 |
| 37 | 16 | 309 | CLA | C3C-C4C-NC | 3.31 | 114.67 | 110.43 |
| 37 | C | 502 | CLA | CAC-C3C-C4C | 3.31 | 129.09 | 124.79 |
| 37 | 19 | 307 | CLA | CAA-C2A-C3A | -3.31 | 104.06 | 113.00 |
| 37 | c | 507 | CLA | C3B-C4B-NB | 3.31 | 113.48 | 110.53 |
| 48 | 13 | 314 | A86 | C4-C5-C6 | -3.31 | 122.64 | 127.28 |
| 37 | 39 | 309 | CLA | C3C-C4C-NC | 3.31 | 114.67 | 110.43 |
| 48 | 15 | 312 | A86 | C36-C31-C32 | -3.31 | 116.41 | 119.70 |
| 37 | 14 | 305 | CLA | CAA-C2A-C3A | -3.31 | 104.06 | 113.00 |
| 37 | 34 | 305 | CLA | CAA-C2A-C3A | -3.31 | 104.06 | 113.00 |
| 48 | 13 | 312 | A86 | C12-C11-C13 | 3.31 | 121.36 | 116.00 |
| 37 | 15 | 308 | CLA | C3C-C4C-NC | 3.31 | 114.67 | 110.43 |
| 37 | B | 502 | CLA | C1-C2-C3 | -3.31 | 120.78 | 126.20 |
| 47 | 21 | 203 | KC1 | CAA-CBA-CGA | -3.31 | 110.24 | 127.05 |
| 48 | 11 | 313 | A86 | C25-C26-C27 | -3.31 | 122.64 | 127.28 |
| 37 | 38 | 203 | CLA | C1-C2-C3 | -3.31 | 120.78 | 126.20 |
| 47 | 41 | 203 | KC1 | CAA-CBA-CGA | -3.30 | 110.25 | 127.05 |
| 48 | 37 | 319 | A86 | C4-C3-C2 | -3.30 | 116.76 | 123.52 |
| 48 | 39 | 313 | A86 | C9-C8-C6 | -3.30 | 117.31 | 126.36 |
| 37 | C | 508 | CLA | CAA-C2A-C3A | -3.30 | 104.07 | 113.00 |
| 37 | 35 | 308 | CLA | C3C-C4C-NC | 3.30 | 114.66 | 110.43 |
| 37 | D | 402 | CLA | CAA-C2A-C3A | -3.30 | 104.07 | 113.00 |
| 47 | 17 | 303 | KC1 | CAA-CBA-CGA | -3.30 | 110.26 | 127.05 |
| 37 | 33 | 303 | CLA | CAC-C3C-C4C | 3.30 | 129.09 | 124.79 |
| 47 | 32 | 212 | KC1 | CMA-C3A-C2A | -3.30 | 120.44 | 128.43 |
| 37 | d | 401 | CLA | CAA-C2A-C3A | -3.30 | 104.08 | 113.00 |
| 48 | 34 | 312 | A86 | C12-C11-C13 | 3.30 | 121.35 | 116.00 |
| 37 | 32 | 205 | CLA | C3D-C2D-C1D | -3.30 | 101.33 | 105.83 |
| 37 | w | 101 | CLA | O2A-CGA-CBA | 3.30 | 121.89 | 111.83 |
| 48 | 32 | 203 | A86 | C35-C34-C33 | 3.30 | 115.81 | 109.89 |
| 37 | b | 503 | CLA | C3B-C4B-NB | 3.30 | 113.47 | 110.53 |
| 47 | 33 | 309 | KC1 | CBC-CAC-C3C | -3.30 | 103.49 | 112.42 |
| 37 | a | 404 | CLA | CHC-C1C-C2C | -3.30 | 117.58 | 126.95 |
| 37 | Z | 102 | CLA | C3C-C4C-NC | 3.29 | 114.65 | 110.43 |
| 37 | b | 516 | CLA | CAA-C2A-C3A | -3.29 | 104.10 | 113.00 |
| 47 | 20 | 305 | KC1 | C1C-C2C-C3C | -3.29 | 103.52 | 106.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | W | 101 | CLA | O2A-CGA-CBA | 3.29 | 121.87 | 111.83 |
| 37 | 37 | 306 | CLA | C3C-C4C-NC | 3.29 | 114.65 | 110.43 |
| 37 | 38 | 211 | CLA | C3C-C4C-NC | 3.29 | 114.65 | 110.43 |
| 47 | 21 | 207 | KC1 | C1C-C2C-C3C | -3.29 | 103.52 | 106.98 |
| 37 | C | 502 | CLA | C1-C2-C3 | -3.29 | 120.81 | 126.20 |
| 37 | C | 505 | CLA | C4C-C3C-C2C | -3.29 | 102.10 | 106.89 |
| 48 | 33 | 312 | A86 | C12-C11-C13 | 3.29 | 121.33 | 116.00 |
| 48 | 14 | 311 | A86 | C4-C3-C2 | -3.29 | 116.79 | 123.52 |
| 37 | 34 | 308 | CLA | C3B-C4B-NB | 3.29 | 113.47 | 110.53 |
| 48 | 34 | 311 | A86 | C4-C3-C2 | -3.29 | 116.79 | 123.52 |
| 47 | 40 | 207 | KC1 | C1C-C2C-C3C | -3.29 | 103.52 | 106.98 |
| 47 | 15 | 304 | KC1 | CAC-C3C-C4C | 3.29 | 129.07 | 124.79 |
| 37 | c | 508 | CLA | CAA-C2A-C3A | -3.29 | 104.11 | 113.00 |
| 37 | b | 501 | CLA | O2D-CGD-O1D | -3.29 | 117.45 | 123.85 |
| 47 | 36 | 302 | KC1 | CAC-C3C-C4C | 3.29 | 129.07 | 124.79 |
| 37 | d | 404 | CLA | C3C-C4C-NC | 3.29 | 114.64 | 110.43 |
| 37 | B | 501 | CLA | O2D-CGD-O1D | -3.29 | 117.45 | 123.85 |
| 38 | a | 406 | PHO | O1D-CGD-CBD | 3.29 | 129.71 | 124.72 |
| 37 | b | 504 | CLA | C4B-C3B-C2B | -3.29 | 103.22 | 107.30 |
| 47 | 21 | 207 | KC1 | CAC-C3C-C4C | 3.28 | 129.06 | 124.79 |
| 47 | 13 | 309 | KC1 | CBC-CAC-C3C | -3.28 | 103.52 | 112.42 |
| 37 | 19 | 310 | CLA | CHC-C1C-C2C | -3.28 | 117.61 | 126.95 |
| 48 | 15 | 319 | A86 | C36-C31-C32 | -3.28 | 116.44 | 119.70 |
| 37 | C | 511 | CLA | C4A-NA-C1A | -3.28 | 105.18 | 106.68 |
| 37 | 18 | 204 | CLA | C3C-C4C-NC | 3.28 | 114.64 | 110.43 |
| 37 | c | 511 | CLA | C1C-C2C-C3C | -3.28 | 103.53 | 106.98 |
| 37 | z | 101 | CLA | CHC-C1C-C2C | -3.28 | 117.62 | 126.95 |
| 37 | B | 504 | CLA | C4B-C3B-C2B | -3.28 | 103.22 | 107.30 |
| 47 | 33 | 302 | KC1 | CAC-C3C-C4C | 3.28 | 129.06 | 124.79 |
| 37 | 14 | 308 | CLA | C3B-C4B-NB | 3.28 | 113.46 | 110.53 |
| 37 | 36 | 309 | CLA | C3C-C4C-NC | 3.28 | 114.63 | 110.43 |
| 48 | 17 | 311 | A86 | C34-O4-C38 | -3.28 | 112.05 | 117.85 |
| 48 | 12 | 202 | A86 | C35-C34-C33 | 3.28 | 115.78 | 109.89 |
| 37 | c | 505 | CLA | C4C-C3C-C2C | -3.28 | 102.12 | 106.89 |
| 37 | b | 509 | CLA | CHC-C1C-C2C | -3.28 | 117.63 | 126.95 |
| 37 | 37 | 308 | CLA | CED-O2D-CGD | 3.28 | 123.36 | 115.92 |
| 48 | 18 | 213 | A86 | C26-C25-C24 | -3.28 | 113.70 | 123.20 |
| 37 | 12 | 203 | CLA | C3C-C4C-NC | 3.28 | 114.63 | 110.43 |
| 37 | 14 | 305 | CLA | C3C-C4C-NC | 3.28 | 114.63 | 110.43 |
| 37 | D | 401 | CLA | CHC-C1C-C2C | -3.28 | 117.63 | 126.95 |
| 37 | 12 | 210 | CLA | CHC-C1C-C2C | -3.28 | 117.63 | 126.95 |
| 37 | B | 524 | CLA | C4C-C3C-C2C | -3.28 | 102.12 | 106.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 33 | 314 | A86 | C4-C5-C6 | -3.28 | 122.69 | 127.28 |
| 37 | b | 516 | CLA | CHC-C1C-C2C | -3.27 | 117.64 | 126.95 |
| 38 | D | 403 | PHO | C3B-C4B-NB | -3.27 | 105.33 | 107.46 |
| 44 | C | 516 | DGD | O6D-C1D-O3G | -3.27 | 102.31 | 110.04 |
| 37 | C | 511 | CLA | C1C-C2C-C3C | -3.27 | 103.54 | 106.98 |
| 37 | a | 403 | CLA | CAC-C3C-C4C | 3.27 | 129.05 | 124.79 |
| 37 | c | 502 | CLA | CAC-C3C-C4C | 3.27 | 129.05 | 124.79 |
| 37 | 17 | 307 | CLA | C3C-C4C-NC | 3.27 | 114.62 | 110.43 |
| 47 | 13 | 309 | KC1 | CAC-C3C-C4C | 3.27 | 129.05 | 124.79 |
| 37 | B | 516 | CLA | CHC-C1C-C2C | -3.27 | 117.65 | 126.95 |
| 37 | B | 508 | CLA | C4B-C3B-C2B | -3.27 | 103.23 | 107.30 |
| 37 | B | 509 | CLA | CHC-C1C-C2C | -3.27 | 117.65 | 126.95 |
| 37 | 39 | 310 | CLA | CHC-C1C-C2C | -3.27 | 117.65 | 126.95 |
| 37 | b | 506 | CLA | C1-C2-C3 | -3.27 | 120.84 | 126.20 |
| 48 | 35 | 314 | A86 | C41-C32-C31 | -3.27 | 107.55 | 110.47 |
| 37 | 32 | 204 | CLA | C3C-C4C-NC | 3.27 | 114.62 | 110.43 |
| 37 | C | 510 | CLA | CMD-C2D-C3D | -3.27 | 120.19 | 127.69 |
| 37 | 19 | 306 | CLA | CHD-C4C-NC | 3.27 | 129.30 | 124.23 |
| 47 | 12 | 211 | KC1 | CMA-C3A-C2A | -3.27 | 120.52 | 128.43 |
| 37 | 21 | 204 | CLA | C4-C3-C5 | 3.27 | 120.90 | 115.23 |
| 37 | Z | 101 | CLA | CHC-C1C-C2C | -3.27 | 117.66 | 126.95 |
| 37 | B | 506 | CLA | C1-C2-C3 | -3.27 | 120.84 | 126.20 |
| 37 | W | 101 | CLA | O1D-CGD-CBD | -3.27 | 118.08 | 124.52 |
| 37 | w | 101 | CLA | O1D-CGD-CBD | -3.27 | 118.08 | 124.52 |
| 37 | 32 | 204 | CLA | CHD-C4C-NC | 3.27 | 129.30 | 124.23 |
| 37 | C | 506 | CLA | CAC-C3C-C4C | 3.27 | 129.04 | 124.79 |
| 47 | 13 | 302 | KC1 | CAC-C3C-C4C | 3.27 | 129.04 | 124.79 |
| 48 | 31 | 314 | A86 | C34-O4-C38 | -3.26 | 112.08 | 117.85 |
| 37 | 32 | 205 | CLA | O2A-CGA-CBA | 3.26 | 121.79 | 111.83 |
| 47 | 15 | 306 | KC1 | CHD-C1D-ND | -3.26 | 119.15 | 124.05 |
| 48 | 15 | 314 | A86 | C41-C32-C31 | -3.26 | 107.55 | 110.47 |
| 37 | A | 403 | CLA | C3C-C4C-NC | 3.26 | 114.61 | 110.43 |
| 37 | 18 | 208 | CLA | CHD-C1D-ND | -3.26 | 120.21 | 124.80 |
| 37 | B | 503 | CLA | C3B-C4B-NB | 3.26 | 113.44 | 110.53 |
| 48 | 32 | 215 | A86 | C3-C4-C5 | -3.26 | 116.85 | 123.52 |
| 37 | A | 403 | CLA | CAC-C3C-C4C | 3.26 | 129.03 | 124.79 |
| 47 | 41 | 207 | KC1 | CAC-C3C-C4C | 3.26 | 129.03 | 124.79 |
| 37 | a | 403 | CLA | C3C-C4C-NC | 3.26 | 114.61 | 110.43 |
| 37 | B | 504 | CLA | C2B-C1B-NB | 3.26 | 113.70 | 110.33 |
| 37 | 34 | 301 | CLA | CHD-C4C-NC | 3.26 | 129.28 | 124.23 |
| 48 | 12 | 214 | A86 | C3-C4-C5 | -3.26 | 116.85 | 123.52 |
| 47 | 18 | 210 | KC1 | CAC-C3C-C4C | 3.26 | 129.03 | 124.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 14 | 301 | CLA | CHD-C4C-NC | 3.26 | 129.28 | 124.23 |
| 44 | c | 516 | DGD | O6D-C1D-O3G | -3.26 | 102.35 | 110.04 |
| 37 | 12 | 204 | CLA | O2A-CGA-CBA | 3.26 | 121.76 | 111.83 |
| 37 | b | 512 | CLA | O2D-CGD-O1D | -3.25 | 117.51 | 123.85 |
| 37 | b | 508 | CLA | C4B-C3B-C2B | -3.25 | 103.25 | 107.30 |
| 37 | 21 | 206 | CLA | C3B-C4B-NB | 3.25 | 113.44 | 110.53 |
| 37 | c | 510 | CLA | CMD-C2D-C3D | -3.25 | 120.23 | 127.69 |
| 37 | 41 | 209 | CLA | C4B-C3B-C2B | -3.25 | 103.26 | 107.30 |
| 37 | 20 | 308 | CLA | C4A-NA-C1A | -3.25 | 105.19 | 106.68 |
| 37 | 38 | 204 | CLA | C4B-C3B-C2B | -3.25 | 103.26 | 107.30 |
| 37 | 32 | 211 | CLA | CHC-C1C-C2C | -3.25 | 117.71 | 126.95 |
| 48 | 35 | 319 | A86 | C36-C31-C32 | -3.25 | 116.47 | 119.70 |
| 37 | C | 501 | CLA | CMB-C2B-C1B | 3.25 | 130.37 | 125.42 |
| 47 | 36 | 305 | KC1 | C4C-C3C-C2C | -3.25 | 102.16 | 106.89 |
| 37 | c | 510 | CLA | C3C-C4C-NC | 3.25 | 114.59 | 110.43 |
| 37 | 31 | 304 | CLA | C3C-C4C-NC | 3.25 | 114.59 | 110.43 |
| 48 | 17 | 312 | A86 | C4-C3-C2 | -3.25 | 116.87 | 123.52 |
| 37 | C | 501 | CLA | CHC-C1C-C2C | -3.25 | 117.71 | 126.95 |
| 47 | 14 | 304 | KC1 | C4B-C3B-C2B | -3.25 | 104.00 | 106.81 |
| 37 | 38 | 204 | CLA | C1C-C2C-C3C | -3.25 | 103.56 | 106.98 |
| 37 | d | 403 | CLA | C1D-CHD-C4C | -3.25 | 119.11 | 126.02 |
| 37 | 34 | 301 | CLA | CMC-C2C-C1C | 3.25 | 130.11 | 125.03 |
| 37 | c | 501 | CLA | CHC-C1C-C2C | -3.25 | 117.72 | 126.95 |
| 37 | D | 405 | CLA | C1D-CHD-C4C | -3.25 | 119.12 | 126.02 |
| 37 | 39 | 306 | CLA | CHD-C4C-NC | 3.25 | 129.27 | 124.23 |
| 37 | 18 | 204 | CLA | C3B-C4B-NB | 3.25 | 113.43 | 110.53 |
| 48 | 31 | 319 | A86 | C3-C4-C5 | -3.25 | 116.88 | 123.52 |
| 37 | 38 | 206 | CLA | C4B-C3B-C2B | -3.25 | 103.27 | 107.30 |
| 47 | 33 | 309 | KC1 | CAC-C3C-C4C | 3.25 | 129.01 | 124.79 |
| 47 | 35 | 306 | KC1 | CHD-C1D-ND | -3.25 | 119.18 | 124.05 |
| 37 | c | 506 | CLA | CAC-C3C-C4C | 3.25 | 129.01 | 124.79 |
| 37 | 13 | 303 | CLA | CAC-C3C-C4C | 3.25 | 129.01 | 124.79 |
| 37 | 32 | 206 | CLA | CAC-C3C-C4C | 3.25 | 129.01 | 124.79 |
| 37 | b | 502 | CLA | C3C-C4C-NC | 3.24 | 114.59 | 110.43 |
| 38 | D | 403 | PHO | CMB-C2B-C3B | 3.24 | 131.16 | 124.68 |
| 37 | 31 | 302 | CLA | C4C-C3C-C2C | -3.24 | 102.17 | 106.89 |
| 37 | 21 | 202 | CLA | C1-C2-C3 | -3.24 | 120.88 | 126.20 |
| 37 | 15 | 308 | CLA | C4B-C3B-C2B | -3.24 | 103.27 | 107.30 |
| 48 | 15 | 316 | A86 | C9-C10-C11 | -3.24 | 117.47 | 126.64 |
| 37 | 37 | 308 | CLA | C4C-C3C-C2C | -3.24 | 102.17 | 106.89 |
| 37 | c | 510 | CLA | CHC-C1C-C2C | -3.24 | 117.73 | 126.95 |
| 37 | 38 | 202 | CLA | CAC-C3C-C4C | 3.24 | 129.01 | 124.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 32 | 217 | A86 | C10-C9-C8 | -3.24 | 113.81 | 123.20 |
| 48 | 19 | 313 | A86 | C9-C8-C6 | -3.24 | 117.48 | 126.36 |
| 48 | 31 | 319 | A86 | C25-C24-C1 | -3.24 | 117.48 | 126.36 |
| 37 | 34 | 305 | CLA | C3C-C4C-NC | 3.24 | 114.58 | 110.43 |
| 37 | 35 | 305 | CLA | C3C-C4C-NC | 3.24 | 114.58 | 110.43 |
| 37 | C | 510 | CLA | CHC-C1C-C2C | -3.24 | 117.74 | 126.95 |
| 47 | 17 | 308 | KC1 | CBC-CAC-C3C | -3.24 | 103.64 | 112.42 |
| 37 | 38 | 208 | CLA | CHD-C1D-ND | -3.24 | 120.25 | 124.80 |
| 48 | 15 | 316 | A86 | C21-C20-C15 | -3.24 | 112.90 | 123.35 |
| 37 | 14 | 308 | CLA | CAC-C3C-C4C | 3.24 | 129.00 | 124.79 |
| 37 | 12 | 203 | CLA | CHD-C4C-NC | 3.24 | 129.25 | 124.23 |
| 37 | 18 | 201 | CLA | CMC-C2C-C1C | 3.24 | 130.09 | 125.03 |
| 37 | 41 | 204 | CLA | C4-C3-C5 | 3.24 | 120.85 | 115.23 |
| 37 | 31 | 301 | CLA | O2D-CGD-O1D | -3.24 | 117.55 | 123.85 |
| 48 | 12 | 216 | A86 | C10-C9-C8 | -3.24 | 113.82 | 123.20 |
| 37 | 11 | 310 | CLA | C4B-C3B-C2B | -3.24 | 103.28 | 107.30 |
| 47 | 16 | 305 | KC1 | C4C-C3C-C2C | -3.24 | 102.18 | 106.89 |
| 48 | 31 | 315 | A86 | C3-C4-C5 | -3.24 | 116.90 | 123.52 |
| 39 | A | 406 | BCR | C24-C23-C22 | -3.24 | 121.45 | 126.23 |
| 37 | 13 | 307 | CLA | C3B-C4B-NB | 3.24 | 113.42 | 110.53 |
| 37 | C | 501 | CLA | CAC-C3C-C4C | 3.23 | 129.00 | 124.79 |
| 37 | 11 | 303 | CLA | C3C-C4C-NC | 3.23 | 114.57 | 110.43 |
| 48 | 11 | 315 | A86 | C3-C4-C5 | -3.23 | 116.90 | 123.52 |
| 37 | 40 | 210 | CLA | C4A-NA-C1A | -3.23 | 105.20 | 106.68 |
| 37 | 16 | 309 | CLA | CAC-C3C-C4C | 3.23 | 129.00 | 124.79 |
| 37 | A | 403 | CLA | CHC-C1C-C2C | -3.23 | 117.76 | 126.95 |
| 37 | 33 | 308 | CLA | CHC-C1C-C2C | -3.23 | 117.76 | 126.95 |
| 47 | 15 | 306 | KC1 | CAA-CBA-CGA | -3.23 | 110.61 | 127.05 |
| 37 | 41 | 202 | CLA | C1-C2-C3 | -3.23 | 120.90 | 126.20 |
| 47 | 40 | 206 | KC1 | CHD-C1D-ND | -3.23 | 119.20 | 124.05 |
| 37 | W | 101 | CLA | C4C-C3C-C2C | -3.23 | 102.19 | 106.89 |
| 37 | 41 | 202 | CLA | CAC-C3C-C4C | 3.23 | 128.99 | 124.79 |
| 48 | 17 | 314 | A86 | C25-C24-C1 | -3.23 | 117.50 | 126.36 |
| 37 | c | 510 | CLA | C1-C2-C3 | -3.23 | 120.90 | 126.20 |
| 48 | 11 | 319 | A86 | C25-C24-C1 | -3.23 | 117.51 | 126.36 |
| 47 | 33 | 302 | KC1 | CMB-C2B-C1B | 3.23 | 130.42 | 124.73 |
| 48 | 21 | 213 | A86 | C36-C31-C32 | -3.23 | 116.49 | 119.70 |
| 47 | 36 | 308 | KC1 | CBA-CAA-C2A | -3.23 | 112.50 | 125.45 |
| 48 | 37 | 312 | A86 | C4-C5-C6 | -3.23 | 122.75 | 127.28 |
| 38 | a | 405 | PHO | CMB-C2B-C3B | 3.23 | 131.13 | 124.68 |
| 37 | w | 101 | CLA | C4C-C3C-C2C | -3.23 | 102.19 | 106.89 |
| 37 | b | 509 | CLA | CMB-C2B-C1B | 3.23 | 130.33 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 501 | CLA | CMB-C2B-C1B | 3.23 | 130.33 | 125.42 |
| 47 | 16 | 302 | KC1 | CBC-CAC-C3C | -3.23 | 103.68 | 112.42 |
| 48 | 19 | 311 | A86 | C4-C5-C6 | -3.23 | 122.75 | 127.28 |
| 37 | 37 | 306 | CLA | C3B-C4B-NB | 3.23 | 113.41 | 110.53 |
| 37 | 16 | 306 | CLA | C4C-C3C-C2C | -3.22 | 102.20 | 106.89 |
| 47 | 18 | 207 | KC1 | CAC-C3C-C4C | 3.22 | 128.99 | 124.79 |
| 48 | 37 | 310 | A86 | C34-O4-C38 | -3.22 | 112.15 | 117.85 |
| 48 | 38 | 213 | A86 | C3-C4-C5 | -3.22 | 116.92 | 123.52 |
| 39 | a | 408 | BCR | C24-C23-C22 | -3.22 | 121.47 | 126.23 |
| 37 | b | 501 | CLA | C3B-C4B-NB | 3.22 | 113.41 | 110.53 |
| 37 | W | 102 | CLA | O2D-CGD-O1D | -3.22 | 117.58 | 123.85 |
| 37 | B | 515 | CLA | CMB-C2B-C1B | 3.22 | 130.32 | 125.42 |
| 48 | 11 | 311 | A86 | C12-C11-C13 | 3.22 | 121.22 | 116.00 |
| 37 | D | 406 | CLA | C3B-C4B-NB | 3.22 | 113.41 | 110.53 |
| 37 | B | 502 | CLA | C3C-C4C-NC | 3.22 | 114.56 | 110.43 |
| 48 | 14 | 312 | A86 | C40-C32-C31 | -3.22 | 107.59 | 110.47 |
| 37 | b | 510 | CLA | O2A-CGA-CBA | 3.22 | 121.66 | 111.83 |
| 47 | 35 | 306 | KC1 | CAA-CBA-CGA | -3.22 | 110.67 | 127.05 |
| 37 | Z | 101 | CLA | C3B-C4B-NB | 3.22 | 113.41 | 110.53 |
| 37 | 14 | 301 | CLA | CMC-C2C-C1C | 3.22 | 130.07 | 125.03 |
| 47 | 16 | 308 | KC1 | CBA-CAA-C2A | -3.22 | 112.53 | 125.45 |
| 48 | 37 | 310 | A86 | C28-C27-C26 | 3.22 | 128.03 | 122.82 |
| 37 | 36 | 306 | CLA | C4C-C3C-C2C | -3.22 | 102.21 | 106.89 |
| 37 | B | 510 | CLA | O2A-CGA-CBA | 3.22 | 121.65 | 111.83 |
| 48 | 34 | 312 | A86 | C40-C32-C31 | -3.22 | 107.59 | 110.47 |
| 47 | 20 | 304 | KC1 | CHD-C1D-ND | -3.22 | 119.22 | 124.05 |
| 37 | 31 | 310 | CLA | C4B-C3B-C2B | -3.22 | 103.30 | 107.30 |
| 37 | 18 | 206 | CLA | CMA-C3A-C2A | -3.22 | 101.54 | 113.98 |
| 37 | 32 | 205 | CLA | CAC-C3C-C4C | 3.22 | 128.98 | 124.79 |
| 37 | 36 | 309 | CLA | CAC-C3C-C4C | 3.22 | 128.98 | 124.79 |
| 37 | b | 515 | CLA | CMB-C2B-C1B | 3.22 | 130.32 | 125.42 |
| 37 | 38 | 201 | CLA | C1C-C2C-C3C | -3.22 | 103.60 | 106.98 |
| 37 | 13 | 308 | CLA | CHC-C1C-C2C | -3.22 | 117.81 | 126.95 |
| 47 | 21 | 207 | KC1 | CHD-C4C-NC | 3.22 | 129.16 | 124.31 |
| 37 | B | 512 | CLA | O2D-CGD-O1D | -3.22 | 117.59 | 123.85 |
| 37 | a | 403 | CLA | CHC-C1C-C2C | -3.22 | 117.81 | 126.95 |
| 47 | 16 | 302 | KC1 | CAC-C3C-C4C | 3.21 | 128.97 | 124.79 |
| 47 | 36 | 302 | KC1 | CBC-CAC-C3C | -3.21 | 103.70 | 112.42 |
| 37 | D | 401 | CLA | C4B-C3B-C2B | -3.21 | 103.31 | 107.30 |
| 37 | Z | 102 | CLA | CHD-C4C-NC | 3.21 | 129.22 | 124.23 |
| 48 | 36 | 311 | A86 | C10-C9-C8 | -3.21 | 113.89 | 123.20 |
| 48 | 11 | 319 | A86 | C3-C4-C5 | -3.21 | 116.94 | 123.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 33 | 307 | CLA | C3B-C4B-NB | 3.21 | 113.40 | 110.53 |
| 37 | 21 | 209 | CLA | CAC-C3C-C4C | 3.21 | 128.97 | 124.79 |
| 37 | 11 | 301 | CLA | C4C-C3C-C2C | -3.21 | 102.22 | 106.89 |
| 37 | c | 502 | CLA | C4A-NA-C1A | -3.21 | 105.21 | 106.68 |
| 37 | 34 | 308 | CLA | C4B-C3B-C2B | -3.21 | 103.31 | 107.30 |
| 48 | 31 | 312 | A86 | C41-C32-C31 | -3.21 | 107.60 | 110.47 |
| 47 | 41 | 207 | KC1 | CHD-C4C-NC | 3.21 | 129.15 | 124.31 |
| 48 | 16 | 314 | A86 | C4-C3-C2 | -3.21 | 116.95 | 123.52 |
| 37 | 21 | 202 | CLA | CAC-C3C-C4C | 3.21 | 128.97 | 124.79 |
| 37 | 35 | 307 | CLA | CHD-C1D-ND | -3.21 | 120.29 | 124.80 |
| 37 | c | 501 | CLA | CAC-C3C-C4C | 3.21 | 128.96 | 124.79 |
| 37 | 38 | 208 | CLA | C1C-C2C-C3C | -3.21 | 103.61 | 106.98 |
| 37 | b | 510 | CLA | C4C-C3C-C2C | -3.21 | 102.22 | 106.89 |
| 37 | 17 | 309 | CLA | CHC-C1C-C2C | -3.21 | 117.83 | 126.95 |
| 37 | 34 | 305 | CLA | CHC-C1C-C2C | -3.21 | 117.83 | 126.95 |
| 37 | 13 | 303 | CLA | CHC-C1C-C2C | -3.21 | 117.83 | 126.95 |
| 37 | b | 514 | CLA | CAA-C2A-C3A | -3.21 | 104.33 | 113.00 |
| 37 | D | 405 | CLA | CMC-C2C-C1C | 3.21 | 130.04 | 125.03 |
| 37 | 19 | 309 | CLA | C3B-C4B-NB | 3.21 | 113.39 | 110.53 |
| 48 | 31 | 311 | A86 | C12-C11-C13 | 3.21 | 121.20 | 116.00 |
| 47 | 38 | 210 | KC1 | CAC-C3C-C4C | 3.21 | 128.96 | 124.79 |
| 37 | C | 510 | CLA | C1-C2-C3 | -3.21 | 120.94 | 126.20 |
| 47 | 12 | 208 | KC1 | C1A-NA-C4A | -3.20 | 105.22 | 106.68 |
| 37 | 11 | 308 | CLA | C3C-C4C-NC | 3.20 | 114.53 | 110.43 |
| 47 | 14 | 306 | KC1 | CMB-C2B-C1B | 3.20 | 130.37 | 124.73 |
| 48 | 17 | 320 | A86 | C4-C3-C2 | -3.20 | 116.96 | 123.52 |
| 37 | d | 404 | CLA | C3B-C4B-NB | 3.20 | 113.39 | 110.53 |
| 37 | 38 | 204 | CLA | C3C-C4C-NC | 3.20 | 114.53 | 110.43 |
| 37 | d | 403 | CLA | CMC-C2C-C1C | 3.20 | 130.04 | 125.03 |
| 37 | 12 | 204 | CLA | CHC-C1C-C2C | -3.20 | 117.84 | 126.95 |
| 37 | 32 | 205 | CLA | CHC-C1C-C2C | -3.20 | 117.84 | 126.95 |
| 37 | 19 | 301 | CLA | C1C-C2C-C3C | -3.20 | 103.61 | 106.98 |
| 37 | 33 | 308 | CLA | C4C-C3C-C2C | -3.20 | 102.23 | 106.89 |
| 47 | 17 | 306 | KC1 | O2D-CGD-O1D | -3.20 | 117.61 | 123.85 |
| 47 | 31 | 309 | KC1 | CAC-C3C-C4C | 3.20 | 128.96 | 124.79 |
| 37 | 39 | 306 | CLA | C4C-C3C-C2C | -3.20 | 102.23 | 106.89 |
| 37 | b | 523 | CLA | C3D-C2D-C1D | -3.20 | 101.46 | 105.83 |
| 37 | z | 102 | CLA | CHD-C4C-NC | 3.20 | 129.19 | 124.23 |
| 37 | 13 | 310 | CLA | C3C-C4C-NC | 3.20 | 114.53 | 110.43 |
| 37 | B | 510 | CLA | C4C-C3C-C2C | -3.20 | 102.23 | 106.89 |
| 48 | 37 | 313 | A86 | C33-C32-C31 | 3.20 | 112.32 | 109.21 |
| 37 | a | 404 | CLA | C1-C2-C3 | -3.20 | 120.95 | 126.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 210 | CLA | C4B-C3B-C2B | -3.20 | 103.32 | 107.30 |
| 37 | 39 | 301 | CLA | C1C-C2C-C3C | -3.20 | 103.61 | 106.98 |
| 37 | C | 510 | CLA | C3C-C4C-NC | 3.20 | 114.53 | 110.43 |
| 47 | 34 | 309 | KC1 | CHD-C1D-ND | -3.20 | 119.25 | 124.05 |
| 37 | 38 | 202 | CLA | CHD-C4C-NC | 3.20 | 129.19 | 124.23 |
| 37 | C | 505 | CLA | CHD-C1D-ND | -3.20 | 120.30 | 124.80 |
| 47 | 14 | 309 | KC1 | CAC-C3C-C4C | 3.20 | 128.95 | 124.79 |
| 37 | z | 101 | CLA | C3B-C4B-NB | 3.20 | 113.39 | 110.53 |
| 37 | 32 | 202 | CLA | C3C-C4C-NC | 3.20 | 114.53 | 110.43 |
| 37 | 33 | 303 | CLA | CHC-C1C-C2C | -3.20 | 117.86 | 126.95 |
| 37 | c | 511 | CLA | C4A-NA-C1A | -3.20 | 105.22 | 106.68 |
| 37 | 15 | 307 | CLA | CHD-C1D-ND | -3.20 | 120.30 | 124.80 |
| 37 | D | 401 | CLA | C1-C2-C3 | -3.20 | 120.96 | 126.20 |
| 37 | 19 | 306 | CLA | C4C-C3C-C2C | -3.20 | 102.24 | 106.89 |
| 37 | 32 | 208 | CLA | O2A-CGA-CBA | 3.20 | 121.58 | 111.83 |
| 37 | 37 | 308 | CLA | C3B-C4B-NB | 3.20 | 113.38 | 110.53 |
| 37 | 14 | 303 | CLA | C3C-C4C-NC | 3.20 | 114.52 | 110.43 |
| 48 | 32 | 203 | A86 | C41-C32-C31 | -3.20 | 107.61 | 110.47 |
| 37 | b | 504 | CLA | C2B-C1B-NB | 3.20 | 113.64 | 110.33 |
| 37 | D | 402 | CLA | C3C-C4C-NC | 3.20 | 114.52 | 110.43 |
| 47 | 36 | 305 | KC1 | CBA-CAA-C2A | -3.19 | 112.63 | 125.45 |
| 48 | 31 | 314 | A86 | C8-C6-C5 | -3.19 | 113.98 | 119.01 |
| 47 | 16 | 305 | KC1 | CBA-CAA-C2A | -3.19 | 112.63 | 125.45 |
| 37 | 38 | 211 | CLA | CHC-C1C-C2C | -3.19 | 117.87 | 126.95 |
| 47 | 11 | 309 | KC1 | CAC-C3C-C4C | 3.19 | 128.95 | 124.79 |
| 48 | 38 | 213 | A86 | C7-C6-C8 | 3.19 | 122.97 | 118.09 |
| 37 | 14 | 305 | CLA | CHC-C1C-C2C | -3.19 | 117.87 | 126.95 |
| 48 | 14 | 312 | A86 | C26-C25-C24 | -3.19 | 113.95 | 123.20 |
| 37 | b | 503 | CLA | C4B-C3B-C2B | -3.19 | 103.33 | 107.30 |
| 37 | 21 | 209 | CLA | C4B-C3B-C2B | -3.19 | 103.33 | 107.30 |
| 37 | 34 | 308 | CLA | CAC-C3C-C4C | 3.19 | 128.94 | 124.79 |
| 37 | B | 524 | CLA | C3D-C2D-C1D | -3.19 | 101.48 | 105.83 |
| 37 | 19 | 304 | CLA | C3C-C4C-NC | 3.19 | 114.52 | 110.43 |
| 48 | 16 | 311 | A86 | C10-C9-C8 | -3.19 | 113.95 | 123.20 |
| 37 | B | 514 | CLA | CAA-C2A-C3A | -3.19 | 104.38 | 113.00 |
| 37 | 40 | 203 | CLA | C4C-C3C-C2C | -3.19 | 102.25 | 106.89 |
| 48 | 11 | 312 | A86 | C41-C32-C31 | -3.19 | 107.62 | 110.47 |
| 47 | 41 | 207 | KC1 | C4B-C3B-C2B | -3.19 | 104.05 | 106.81 |
| 47 | 36 | 305 | KC1 | CAA-CBA-CGA | -3.19 | 110.83 | 127.05 |
| 37 | 35 | 307 | CLA | CHD-C4C-NC | 3.19 | 129.18 | 124.23 |
| 48 | 32 | 221 | A86 | C-C1-C24 | 3.19 | 122.96 | 118.09 |
| 48 | 35 | 316 | A86 | C9-C10-C11 | -3.19 | 117.63 | 126.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 13 | 308 | CLA | C4C-C3C-C2C | -3.19 | 102.25 | 106.89 |
| 47 | 16 | 305 | KC1 | CAA-CBA-CGA | -3.19 | 110.83 | 127.05 |
| 37 | 14 | 301 | CLA | CMB-C2B-C1B | 3.19 | 130.27 | 125.42 |
| 47 | 34 | 309 | KC1 | CAC-C3C-C4C | 3.19 | 128.94 | 124.79 |
| 37 | 18 | 202 | CLA | C4C-C3C-C2C | -3.19 | 102.25 | 106.89 |
| 37 | B | 511 | CLA | CHC-C1C-C2C | -3.19 | 117.89 | 126.95 |
| 47 | 12 | 208 | KC1 | CBA-CAA-C2A | -3.19 | 112.66 | 125.45 |
| 37 | b | 511 | CLA | CHC-C1C-C2C | -3.19 | 117.89 | 126.95 |
| 47 | 15 | 309 | KC1 | CAC-C3C-C4C | 3.19 | 128.94 | 124.79 |
| 48 | 34 | 312 | A86 | C26-C25-C24 | -3.19 | 113.97 | 123.20 |
| 47 | 15 | 302 | KC1 | CHD-C1D-ND | -3.19 | 119.27 | 124.05 |
| 37 | 11 | 303 | CLA | CHC-C1C-C2C | -3.19 | 117.89 | 126.95 |
| 37 | 41 | 202 | CLA | CMB-C2B-C1B | 3.19 | 130.27 | 125.42 |
| 37 | 11 | 307 | CLA | CHD-C4C-NC | 3.19 | 129.17 | 124.23 |
| 37 | 20 | 307 | CLA | CAC-C3C-C4C | 3.19 | 128.94 | 124.79 |
| 48 | 36 | 313 | A86 | C4-C3-C2 | -3.19 | 117.00 | 123.52 |
| 37 | Z | 102 | CLA | CHC-C1C-C2C | -3.19 | 117.90 | 126.95 |
| 47 | 14 | 309 | KC1 | CHD-C1D-ND | -3.19 | 119.27 | 124.05 |
| 37 | C | 513 | CLA | CMB-C2B-C1B | 3.18 | 130.27 | 125.42 |
| 37 | 15 | 310 | CLA | CHC-C1C-C2C | -3.18 | 117.90 | 126.95 |
| 37 | 31 | 308 | CLA | CHD-C4C-NC | 3.18 | 129.17 | 124.23 |
| 37 | 41 | 208 | CLA | CHC-C1C-C2C | -3.18 | 117.90 | 126.95 |
| 37 | 12 | 207 | CLA | O2A-CGA-CBA | 3.18 | 121.54 | 111.83 |
| 37 | 39 | 309 | CLA | C3B-C4B-NB | 3.18 | 113.37 | 110.53 |
| 37 | 38 | 209 | CLA | C1-C2-C3 | -3.18 | 120.98 | 126.20 |
| 48 | 35 | 316 | A86 | C21-C20-C15 | -3.18 | 113.08 | 123.35 |
| 37 | 14 | 308 | CLA | C4B-C3B-C2B | -3.18 | 103.35 | 107.30 |
| 48 | 36 | 313 | A86 | C26-C25-C24 | -3.18 | 113.98 | 123.20 |
| 37 | 41 | 209 | CLA | CAC-C3C-C4C | 3.18 | 128.93 | 124.79 |
| 48 | 41 | 213 | A86 | C36-C31-C32 | -3.18 | 116.54 | 119.70 |
| 48 | 16 | 311 | A86 | C41-C32-C31 | -3.18 | 107.63 | 110.47 |
| 37 | a | 404 | CLA | C4B-C3B-C2B | -3.18 | 103.35 | 107.30 |
| 37 | 12 | 204 | CLA | CAC-C3C-C4C | 3.18 | 128.93 | 124.79 |
| 37 | 21 | 208 | CLA | CHC-C1C-C2C | -3.18 | 117.91 | 126.95 |
| 48 | 38 | 213 | A86 | C26-C25-C24 | -3.18 | 113.99 | 123.20 |
| 47 | 34 | 309 | KC1 | CHD-C4C-NC | 3.18 | 129.10 | 124.31 |
| 37 | C | 506 | CLA | C3B-C2B-C1B | -3.18 | 103.42 | 107.17 |
| 37 | 40 | 209 | CLA | CAC-C3C-C4C | 3.18 | 128.93 | 124.79 |
| 37 | 21 | 202 | CLA | CMB-C2B-C1B | 3.18 | 130.26 | 125.42 |
| 37 | b | 515 | CLA | C4C-C3C-C2C | -3.18 | 102.27 | 106.89 |
| 47 | 34 | 306 | KC1 | CMB-C2B-C1B | 3.18 | 130.32 | 124.73 |
| 37 | 38 | 202 | CLA | C4C-C3C-C2C | -3.18 | 102.27 | 106.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 32 | 209 | KC1 | CBA-CAA-C2A | -3.18 | 112.70 | 125.45 |
| 48 | 39 | 311 | A86 | C4-C5-C6 | -3.18 | 122.82 | 127.28 |
| 37 | B | 506 | CLA | C3B-C4B-NB | 3.18 | 113.37 | 110.53 |
| 37 | 41 | 206 | CLA | C3B-C4B-NB | 3.18 | 113.36 | 110.53 |
| 37 | 37 | 308 | CLA | CHC-C1C-C2C | -3.18 | 117.92 | 126.95 |
| 37 | 32 | 206 | CLA | C4C-C3C-C2C | -3.18 | 102.27 | 106.89 |
| 37 | z | 102 | CLA | CHC-C1C-C2C | -3.17 | 117.92 | 126.95 |
| 47 | 41 | 207 | KC1 | C2C-C1C-NC | 3.17 | 114.38 | 110.45 |
| 37 | 16 | 301 | CLA | CHD-C4C-NC | 3.17 | 129.15 | 124.23 |
| 50 | 40 | 214 | DD6 | C14-C13-C11 | -3.17 | 120.61 | 125.53 |
| 37 | B | 503 | CLA | C4B-C3B-C2B | -3.17 | 103.36 | 107.30 |
| 48 | 18 | 214 | A86 | C12-C11-C13 | 3.17 | 121.14 | 116.00 |
| 37 | 14 | 303 | CLA | CBA-CAA-C2A | 3.17 | 123.23 | 113.79 |
| 37 | 34 | 303 | CLA | CBA-CAA-C2A | 3.17 | 123.23 | 113.79 |
| 37 | b | 502 | CLA | O2D-CGD-O1D | -3.17 | 117.67 | 123.85 |
| 37 | B | 512 | CLA | CAC-C3C-C4C | 3.17 | 128.92 | 124.79 |
| 48 | 36 | 311 | A86 | C41-C32-C31 | -3.17 | 107.63 | 110.47 |
| 37 | 36 | 301 | CLA | CHD-C4C-NC | 3.17 | 129.15 | 124.23 |
| 47 | 14 | 304 | KC1 | CHD-C4C-NC | 3.17 | 129.09 | 124.31 |
| 47 | 34 | 304 | KC1 | CHD-C4C-NC | 3.17 | 129.09 | 124.31 |
| 37 | 14 | 305 | CLA | C3B-C4B-NB | 3.17 | 113.36 | 110.53 |
| 37 | c | 505 | CLA | CHD-C1D-ND | -3.17 | 120.34 | 124.80 |
| 47 | 39 | 308 | KC1 | CHD-C4C-NC | 3.17 | 129.08 | 124.31 |
| 47 | 11 | 302 | KC1 | O2D-CGD-O1D | -3.17 | 117.68 | 123.85 |
| 48 | 14 | 314 | A86 | C10-C9-C8 | -3.17 | 114.02 | 123.20 |
| 37 | 11 | 307 | CLA | C4-C3-C5 | 3.17 | 120.73 | 115.23 |
| 48 | 16 | 314 | A86 | C26-C25-C24 | -3.17 | 114.02 | 123.20 |
| 37 | B | 509 | CLA | CMB-C2B-C1B | 3.17 | 130.24 | 125.42 |
| 37 | 39 | 302 | CLA | CHC-C1C-C2C | -3.17 | 117.95 | 126.95 |
| 37 | C | 513 | CLA | CHD-C4C-NC | 3.17 | 129.14 | 124.23 |
| 50 | 20 | 312 | DD6 | C14-C13-C11 | -3.17 | 120.62 | 125.53 |
| 37 | 34 | 303 | CLA | O2A-CGA-CBA | 3.17 | 121.49 | 111.83 |
| 37 | 17 | 304 | CLA | CHC-C1C-C2C | -3.17 | 117.95 | 126.95 |
| 37 | 35 | 310 | CLA | CHC-C1C-C2C | -3.17 | 117.95 | 126.95 |
| 47 | 37 | 305 | KC1 | O2D-CGD-O1D | -3.16 | 117.69 | 123.85 |
| 37 | 15 | 303 | CLA | C3C-C4C-NC | 3.16 | 114.48 | 110.43 |
| 37 | 14 | 303 | CLA | O2A-CGA-CBA | 3.16 | 121.48 | 111.83 |
| 37 | 17 | 309 | CLA | C3B-C4B-NB | 3.16 | 113.36 | 110.53 |
| 48 | 12 | 220 | A86 | C-C1-C24 | 3.16 | 122.92 | 118.09 |
| 37 | 18 | 204 | CLA | CHD-C4C-NC | 3.16 | 129.14 | 124.23 |
| 37 | 36 | 301 | CLA | C1-C2-C3 | -3.16 | 121.01 | 126.20 |
| 40 | 17 | 301 | SQD | O7-S-C6 | 3.16 | 111.48 | 106.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 40 | 36 | 315 | SQD | O7-S-C6 | 3.16 | 111.48 | 106.76 |
| 37 | 34 | 305 | CLA | C3B-C4B-NB | 3.16 | 113.35 | 110.53 |
| 37 | c | 508 | CLA | C1C-C2C-C3C | -3.16 | 103.65 | 106.98 |
| 37 | 21 | 205 | CLA | CHC-C1C-C2C | -3.16 | 117.96 | 126.95 |
| 37 | 41 | 209 | CLA | C3C-C4C-NC | 3.16 | 114.48 | 110.43 |
| 37 | 39 | 301 | CLA | C4C-C3C-C2C | -3.16 | 102.29 | 106.89 |
| 37 | 41 | 205 | CLA | CHC-C1C-C2C | -3.16 | 117.97 | 126.95 |
| 47 | 13 | 302 | KC1 | CMB-C2B-C1B | 3.16 | 130.29 | 124.73 |
| 47 | 11 | 306 | KC1 | O2D-CGD-O1D | -3.16 | 117.70 | 123.85 |
| 37 | 20 | 301 | CLA | C4C-C3C-C2C | -3.16 | 102.29 | 106.89 |
| 50 | 39 | 312 | DD6 | C37-C36-C35 | -3.16 | 108.61 | 114.42 |
| 37 | 21 | 204 | CLA | CHC-C1C-C2C | -3.16 | 117.97 | 126.95 |
| 47 | 31 | 307 | KC1 | CHD-C1D-ND | -3.16 | 119.31 | 124.05 |
| 37 | b | 507 | CLA | C3C-C4C-NC | 3.16 | 114.48 | 110.43 |
| 37 | 18 | 203 | CLA | C3B-C4B-NB | 3.16 | 113.35 | 110.53 |
| 37 | 19 | 309 | CLA | CAC-C3C-C4C | 3.16 | 128.90 | 124.79 |
| 37 | c | 508 | CLA | CHC-C1C-C2C | -3.16 | 117.97 | 126.95 |
| 37 | 31 | 304 | CLA | CHC-C1C-C2C | -3.16 | 117.97 | 126.95 |
| 37 | 32 | 211 | CLA | C4B-C3B-C2B | -3.16 | 103.38 | 107.30 |
| 40 | b | 521 | SQD | O9-S-O7 | -3.16 | 103.55 | 113.82 |
| 37 | B | 515 | CLA | C4C-C3C-C2C | -3.16 | 102.30 | 106.89 |
| 37 | 35 | 303 | CLA | C3C-C4C-NC | 3.16 | 114.47 | 110.43 |
| 37 | 13 | 303 | CLA | C3C-C4C-NC | 3.16 | 114.47 | 110.43 |
| 37 | 33 | 303 | CLA | C3C-C4C-NC | 3.16 | 114.47 | 110.43 |
| 40 | b | 521 | SQD | O47-C7-C8 | 3.16 | 118.31 | 111.48 |
| 37 | 37 | 303 | CLA | CHC-C1C-C2C | -3.16 | 117.98 | 126.95 |
| 37 | 16 | 307 | CLA | C4B-C3B-C2B | -3.16 | 103.38 | 107.30 |
| 37 | 34 | 301 | CLA | CMB-C2B-C1B | 3.16 | 130.22 | 125.42 |
| 48 | 32 | 217 | A86 | C4-C5-C6 | -3.16 | 122.85 | 127.28 |
| 40 | B | 522 | SQD | O9-S-O7 | -3.16 | 103.56 | 113.82 |
| 48 | 34 | 314 | A86 | C10-C9-C8 | -3.16 | 114.06 | 123.20 |
| 37 | c | 513 | CLA | CMB-C2B-C1B | 3.16 | 130.22 | 125.42 |
| 37 | B | 510 | CLA | O2D-CGD-O1D | -3.15 | 117.71 | 123.85 |
| 37 | 15 | 307 | CLA | CHD-C4C-NC | 3.15 | 129.12 | 124.23 |
| 48 | 11 | 314 | A86 | C8-C6-C5 | -3.15 | 114.05 | 119.01 |
| 37 | C | 508 | CLA | CHC-C1C-C2C | -3.15 | 117.98 | 126.95 |
| 47 | 37 | 302 | KC1 | CHD-C1D-ND | -3.15 | 119.32 | 124.05 |
| 37 | c | 503 | CLA | CHC-C1C-C2C | -3.15 | 117.98 | 126.95 |
| 37 | 33 | 310 | CLA | C4B-C3B-C2B | -3.15 | 103.38 | 107.30 |
| 37 | 38 | 203 | CLA | CAA-C2A-C1A | 3.15 | 122.31 | 111.97 |
| 47 | 40 | 204 | KC1 | CHD-C1D-ND | -3.15 | 119.32 | 124.05 |
| 47 | 17 | 303 | KC1 | CHD-C1D-ND | -3.15 | 119.32 | 124.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 19 | 308 | KC1 | CBA-CAA-C2A | -3.15 | 112.80 | 125.45 |
| 47 | 16 | 302 | KC1 | CMB-C2B-C1B | 3.15 | 130.28 | 124.73 |
| 48 | 12 | 202 | A86 | C41-C32-C31 | -3.15 | 107.65 | 110.47 |
| 48 | 17 | 311 | A86 | C12-C11-C13 | 3.15 | 121.11 | 116.00 |
| 37 | 36 | 307 | CLA | C4B-C3B-C2B | -3.15 | 103.38 | 107.30 |
| 37 | B | 507 | CLA | C3C-C4C-NC | 3.15 | 114.47 | 110.43 |
| 37 | b | 510 | CLA | O2D-CGD-O1D | -3.15 | 117.72 | 123.85 |
| 39 | B | 525 | BCR | C24-C23-C22 | -3.15 | 121.57 | 126.23 |
| 47 | 35 | 309 | KC1 | CAC-C3C-C4C | 3.15 | 128.89 | 124.79 |
| 37 | C | 509 | CLA | C1-O2A-CGA | 3.15 | 124.28 | 116.65 |
| 50 | 19 | 312 | DD6 | C37-C36-C35 | -3.15 | 108.63 | 114.42 |
| 37 | 15 | 303 | CLA | CAC-C3C-C4C | 3.15 | 128.89 | 124.79 |
| 37 | d | 401 | CLA | C3C-C4C-NC | 3.15 | 114.46 | 110.43 |
| 37 | 20 | 301 | CLA | C1C-C2C-C3C | -3.15 | 103.67 | 106.98 |
| 37 | 17 | 307 | CLA | C3B-C4B-NB | 3.15 | 113.34 | 110.53 |
| 37 | 39 | 306 | CLA | CAC-C3C-C4C | 3.15 | 128.89 | 124.79 |
| 37 | 41 | 205 | CLA | C4C-C3C-C2C | -3.15 | 102.31 | 106.89 |
| 37 | B | 501 | CLA | C3B-C4B-NB | 3.15 | 113.34 | 110.53 |
| 37 | b | 501 | CLA | CHC-C1C-C2C | -3.15 | 118.00 | 126.95 |
| 47 | 38 | 207 | KC1 | CAC-C3C-C4C | 3.15 | 128.88 | 124.79 |
| 37 | 19 | 301 | CLA | CHD-C4C-NC | 3.15 | 129.11 | 124.23 |
| 37 | 40 | 203 | CLA | C1C-C2C-C3C | -3.15 | 103.67 | 106.98 |
| 37 | 34 | 303 | CLA | C3C-C4C-NC | 3.15 | 114.46 | 110.43 |
| 37 | b | 505 | CLA | CMB-C2B-C1B | 3.15 | 130.21 | 125.42 |
| 37 | 36 | 301 | CLA | CMB-C2B-C1B | 3.15 | 130.21 | 125.42 |
| 37 | c | 513 | CLA | CHD-C4C-NC | 3.15 | 129.11 | 124.23 |
| 37 | c | 506 | CLA | C3B-C2B-C1B | -3.14 | 103.46 | 107.17 |
| 37 | 13 | 305 | CLA | C3B-C4B-NB | 3.14 | 113.34 | 110.53 |
| 37 | 21 | 209 | CLA | C3C-C4C-NC | 3.14 | 114.46 | 110.43 |
| 47 | 36 | 302 | KC1 | CMB-C2B-C1B | 3.14 | 130.26 | 124.73 |
| 47 | 39 | 308 | KC1 | CBA-CAA-C2A | -3.14 | 112.83 | 125.45 |
| 47 | 16 | 304 | KC1 | CHD-C1D-ND | -3.14 | 119.33 | 124.05 |
| 47 | 17 | 308 | KC1 | CHD-C1D-ND | -3.14 | 119.33 | 124.05 |
| 37 | 20 | 303 | CLA | CHD-C4C-NC | 3.14 | 129.10 | 124.23 |
| 37 | 20 | 303 | CLA | C1-O2A-CGA | 3.14 | 124.26 | 116.65 |
| 48 | 12 | 217 | A86 | C33-C32-C31 | 3.14 | 112.27 | 109.21 |
| 37 | 39 | 309 | CLA | CHC-C1C-C2C | -3.14 | 118.02 | 126.95 |
| 37 | b | 506 | CLA | C3B-C4B-NB | 3.14 | 113.33 | 110.53 |
| 47 | 21 | 207 | KC1 | C2C-C1C-NC | 3.14 | 114.34 | 110.45 |
| 47 | 34 | 304 | KC1 | C4B-C3B-C2B | -3.14 | 104.09 | 106.81 |
| 37 | 19 | 302 | CLA | C3C-C4C-NC | 3.14 | 114.45 | 110.43 |
| 47 | 14 | 309 | KC1 | CHD-C4C-NC | 3.14 | 129.04 | 124.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 502 | CLA | O2D-CGD-O1D | -3.14 | 117.73 | 123.85 |
| 47 | 32 | 209 | KC1 | C1A-NA-C4A | -3.14 | 105.25 | 106.68 |
| 37 | 36 | 307 | CLA | CHD-C4C-NC | 3.14 | 129.10 | 124.23 |
| 37 | 12 | 204 | CLA | C4B-C3B-C2B | -3.14 | 103.40 | 107.30 |
| 39 | b | 524 | BCR | C24-C23-C22 | -3.14 | 121.59 | 126.23 |
| 37 | 19 | 309 | CLA | CHC-C1C-C2C | -3.14 | 118.03 | 126.95 |
| 47 | 31 | 303 | KC1 | O2D-CGD-O1D | -3.14 | 117.74 | 123.85 |
| 37 | 41 | 204 | CLA | CHC-C1C-C2C | -3.14 | 118.03 | 126.95 |
| 47 | 11 | 306 | KC1 | CHD-C1D-ND | -3.14 | 119.34 | 124.05 |
| 37 | 19 | 302 | CLA | CHC-C1C-C2C | -3.14 | 118.03 | 126.95 |
| 48 | 13 | 311 | A86 | C7-C6-C8 | 3.14 | 122.88 | 118.09 |
| 37 | 14 | 302 | CLA | CMB-C2B-C1B | 3.14 | 130.20 | 125.42 |
| 40 | B | 522 | SQD | O47-C7-C8 | 3.14 | 118.27 | 111.48 |
| 37 | 35 | 308 | CLA | CHC-C1C-C2C | -3.14 | 118.03 | 126.95 |
| 37 | b | 523 | CLA | C1-C2-C3 | -3.14 | 121.06 | 126.20 |
| 37 | B | 507 | CLA | C4C-C3C-C2C | -3.14 | 102.33 | 106.89 |
| 37 | 21 | 205 | CLA | C4C-C3C-C2C | -3.14 | 102.33 | 106.89 |
| 37 | 40 | 205 | CLA | C1-O2A-CGA | 3.14 | 124.24 | 116.65 |
| 37 | 39 | 302 | CLA | C3C-C4C-NC | 3.14 | 114.45 | 110.43 |
| 47 | 36 | 304 | KC1 | CHD-C1D-ND | -3.14 | 119.34 | 124.05 |
| 48 | 12 | 213 | A86 | C3-C2-C1 | -3.14 | 122.88 | 127.28 |
| 37 | 39 | 309 | CLA | CAC-C3C-C4C | 3.14 | 128.87 | 124.79 |
| 37 | 16 | 301 | CLA | CMB-C2B-C1B | 3.13 | 130.19 | 125.42 |
| 48 | 12 | 216 | A86 | C4-C5-C6 | -3.13 | 122.88 | 127.28 |
| 47 | 21 | 207 | KC1 | C4B-C3B-C2B | -3.13 | 104.10 | 106.81 |
| 37 | C | 503 | CLA | CAA-C2A-C3A | -3.13 | 104.53 | 113.00 |
| 37 | B | 505 | CLA | CMB-C2B-C1B | 3.13 | 130.19 | 125.42 |
| 48 | 19 | 313 | A86 | C25-C26-C27 | -3.13 | 122.88 | 127.28 |
| 37 | 37 | 306 | CLA | C4B-C3B-C2B | -3.13 | 103.41 | 107.30 |
| 47 | 31 | 307 | KC1 | O2D-CGD-O1D | -3.13 | 117.75 | 123.85 |
| 37 | 31 | 306 | CLA | CHC-C1C-C2C | -3.13 | 118.05 | 126.95 |
| 37 | 37 | 303 | CLA | C3C-C4C-NC | 3.13 | 114.44 | 110.43 |
| 37 | B | 524 | CLA | C1-C2-C3 | -3.13 | 121.07 | 126.20 |
| 37 | B | 501 | CLA | CHC-C1C-C2C | -3.13 | 118.05 | 126.95 |
| 37 | C | 503 | CLA | CHC-C1C-C2C | -3.13 | 118.05 | 126.95 |
| 37 | 19 | 301 | CLA | C4C-C3C-C2C | -3.13 | 102.33 | 106.89 |
| 37 | c | 507 | CLA | O2D-CGD-O1D | -3.13 | 117.75 | 123.85 |
| 47 | 36 | 308 | KC1 | CMA-C3A-C2A | -3.13 | 120.85 | 128.43 |
| 47 | 35 | 302 | KC1 | CHD-C1D-ND | -3.13 | 119.35 | 124.05 |
| 48 | 33 | 312 | A86 | C3-C4-C5 | -3.13 | 117.11 | 123.52 |
| 37 | 39 | 301 | CLA | CHD-C4C-NC | 3.13 | 129.08 | 124.23 |
| 37 | 11 | 307 | CLA | O2A-CGA-CBA | 3.13 | 121.38 | 111.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 209 | CLA | C4-C3-C5 | 3.13 | 120.66 | 115.23 |
| 37 | 19 | 303 | CLA | CAC-C3C-C4C | 3.13 | 128.86 | 124.79 |
| 47 | 11 | 304 | KC1 | CHD-C1D-ND | -3.13 | 119.36 | 124.05 |
| 47 | 37 | 307 | KC1 | CHD-C1D-ND | -3.13 | 119.36 | 124.05 |
| 48 | 37 | 319 | A86 | C36-C31-C32 | -3.13 | 116.59 | 119.70 |
| 50 | 21 | 216 | DD6 | C23-C16-C15 | 3.13 | 118.49 | 110.05 |
| 37 | 11 | 305 | CLA | CHC-C1C-C2C | -3.13 | 118.06 | 126.95 |
| 48 | 32 | 218 | A86 | C33-C32-C31 | 3.13 | 112.25 | 109.21 |
| 37 | 32 | 210 | CLA | C4-C3-C5 | 3.13 | 120.65 | 115.23 |
| 47 | 35 | 302 | KC1 | C4B-C3B-C2B | -3.13 | 104.10 | 106.81 |
| 37 | 19 | 306 | CLA | CAC-C3C-C4C | 3.13 | 128.86 | 124.79 |
| 37 | 39 | 307 | CLA | CAC-C3C-C4C | 3.13 | 128.86 | 124.79 |
| 37 | 19 | 307 | CLA | CAC-C3C-C4C | 3.12 | 128.85 | 124.79 |
| 37 | 17 | 309 | CLA | CED-O2D-CGD | 3.12 | 123.00 | 115.92 |
| 37 | C | 504 | CLA | CHC-C1C-C2C | -3.12 | 118.07 | 126.95 |
| 47 | 17 | 306 | KC1 | C1A-NA-C4A | -3.12 | 105.25 | 106.68 |
| 37 | C | 508 | CLA | C1C-C2C-C3C | -3.12 | 103.69 | 106.98 |
| 37 | 17 | 304 | CLA | C3C-C4C-NC | 3.12 | 114.43 | 110.43 |
| 37 | 33 | 310 | CLA | CHC-C1C-C2C | -3.12 | 118.07 | 126.95 |
| 37 | 39 | 307 | CLA | CHC-C1C-C2C | -3.12 | 118.07 | 126.95 |
| 37 | 38 | 206 | CLA | CMA-C3A-C2A | -3.12 | 101.91 | 113.98 |
| 37 | 13 | 310 | CLA | C4B-C3B-C2B | -3.12 | 103.42 | 107.30 |
| 47 | 13 | 304 | KC1 | CHD-C4C-NC | 3.12 | 129.01 | 124.31 |
| 37 | c | 509 | CLA | C1-O2A-CGA | 3.12 | 124.21 | 116.65 |
| 47 | 20 | 302 | KC1 | CHD-C1D-ND | -3.12 | 119.37 | 124.05 |
| 37 | 16 | 301 | CLA | C1-C2-C3 | -3.12 | 121.08 | 126.20 |
| 50 | 41 | 216 | DD6 | C23-C16-C15 | 3.12 | 118.47 | 110.05 |
| 47 | 34 | 306 | KC1 | O2D-CGD-O1D | -3.12 | 117.78 | 123.85 |
| 48 | 37 | 311 | A86 | C36-C31-C32 | -3.12 | 116.60 | 119.70 |
| 41 | c | 518 | LMG | O6-C1-O1 | -3.12 | 102.67 | 110.04 |
| 37 | 40 | 210 | CLA | CHC-C1C-C2C | -3.12 | 118.08 | 126.95 |
| 37 | B | 513 | CLA | CHD-C4C-NC | 3.12 | 129.07 | 124.23 |
| 37 | b | 503 | CLA | CHC-C1C-C2C | -3.12 | 118.08 | 126.95 |
| 47 | 11 | 309 | KC1 | C2A-C1A-NA | 3.12 | 114.34 | 109.34 |
| 37 | 39 | 304 | CLA | C3C-C4C-NC | 3.12 | 114.42 | 110.43 |
| 48 | 32 | 203 | A86 | C3-C4-C5 | -3.12 | 117.14 | 123.52 |
| 37 | B | 505 | CLA | CHD-C4C-NC | 3.12 | 129.06 | 124.23 |
| 48 | 33 | 311 | A86 | C7-C6-C8 | 3.12 | 122.85 | 118.09 |
| 37 | b | 502 | CLA | CHC-C1C-C2C | -3.12 | 118.09 | 126.95 |
| 37 | c | 504 | CLA | CHC-C1C-C2C | -3.12 | 118.09 | 126.95 |
| 37 | 33 | 305 | CLA | C3B-C4B-NB | 3.12 | 113.31 | 110.53 |
| 37 | 31 | 308 | CLA | O2A-CGA-CBA | 3.12 | 121.34 | 111.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 503 | CLA | CAA-C2A-C3A | -3.12 | 104.58 | 113.00 |
| 48 | 12 | 202 | A86 | C26-C25-C24 | -3.12 | 114.17 | 123.20 |
| 37 | B | 502 | CLA | CHC-C1C-C2C | -3.12 | 118.09 | 126.95 |
| 37 | B | 503 | CLA | CHC-C1C-C2C | -3.12 | 118.09 | 126.95 |
| 37 | 12 | 204 | CLA | CMB-C2B-C1B | 3.12 | 130.16 | 125.42 |
| 48 | 37 | 309 | A86 | C23-C16-C22 | -3.12 | 102.84 | 107.37 |
| 37 | 19 | 307 | CLA | C4C-C3C-C2C | -3.11 | 102.36 | 106.89 |
| 37 | 40 | 205 | CLA | CHD-C4C-NC | 3.11 | 129.06 | 124.23 |
| 43 | 21 | 201 | LHG | O8-C23-C24 | 3.11 | 121.33 | 111.83 |
| 47 | 37 | 307 | KC1 | C2A-C1A-NA | 3.11 | 114.33 | 109.34 |
| 37 | b | 512 | CLA | CAC-C3C-C4C | 3.11 | 128.84 | 124.79 |
| 37 | 32 | 210 | CLA | CAC-C3C-C4C | 3.11 | 128.84 | 124.79 |
| 48 | 19 | 313 | A86 | C21-C20-C15 | -3.11 | 113.30 | 123.35 |
| 47 | 19 | 308 | KC1 | CHD-C4C-NC | 3.11 | 129.00 | 124.31 |
| 39 | c | 514 | BCR | C15-C16-C17 | -3.11 | 117.15 | 123.52 |
| 48 | 12 | 202 | A86 | C3-C4-C5 | -3.11 | 117.15 | 123.52 |
| 37 | 20 | 306 | CLA | C1-C2-C3 | -3.11 | 121.73 | 126.76 |
| 37 | 17 | 307 | CLA | C4B-C3B-C2B | -3.11 | 103.43 | 107.30 |
| 37 | 20 | 308 | CLA | CHC-C1C-C2C | -3.11 | 118.11 | 126.95 |
| 48 | 13 | 312 | A86 | C3-C4-C5 | -3.11 | 117.16 | 123.52 |
| 47 | 32 | 212 | KC1 | CAC-C3C-C4C | 3.11 | 128.84 | 124.79 |
| 47 | 16 | 308 | KC1 | CMA-C3A-C2A | -3.11 | 120.90 | 128.43 |
| 37 | Z | 101 | CLA | CHD-C4C-NC | 3.11 | 129.05 | 124.23 |
| 47 | 15 | 302 | KC1 | CMB-C2B-C1B | 3.11 | 130.20 | 124.73 |
| 37 | 18 | 201 | CLA | C4C-C3C-C2C | -3.11 | 102.37 | 106.89 |
| 37 | C | 502 | CLA | C4A-NA-C1A | -3.11 | 105.26 | 106.68 |
| 47 | 37 | 305 | KC1 | C1A-NA-C4A | -3.11 | 105.26 | 106.68 |
| 37 | z | 101 | CLA | CHD-C4C-NC | 3.11 | 129.05 | 124.23 |
| 37 | 17 | 304 | CLA | C4B-C3B-C2B | -3.11 | 103.44 | 107.30 |
| 37 | 17 | 302 | CLA | CHC-C1C-C2C | -3.11 | 118.12 | 126.95 |
| 37 | 13 | 310 | CLA | CHC-C1C-C2C | -3.11 | 118.12 | 126.95 |
| 37 | C | 511 | CLA | C4B-C3B-C2B | -3.11 | 103.44 | 107.30 |
| 37 | 20 | 306 | CLA | C4C-C3C-C2C | -3.11 | 102.37 | 106.89 |
| 37 | 40 | 205 | CLA | C4C-C3C-C2C | -3.11 | 102.37 | 106.89 |
| 37 | c | 507 | CLA | C4-C3-C5 | 3.11 | 120.62 | 115.23 |
| 37 | 14 | 303 | CLA | CHC-C1C-C2C | -3.11 | 118.12 | 126.95 |
| 37 | 31 | 301 | CLA | C3B-C4B-NB | 3.11 | 113.30 | 110.53 |
| 37 | 21 | 202 | CLA | C4C-C3C-C2C | -3.10 | 102.37 | 106.89 |
| 47 | 31 | 303 | KC1 | CHD-C4C-NC | 3.10 | 128.99 | 124.31 |
| 47 | 17 | 308 | KC1 | C2A-C1A-NA | 3.10 | 114.32 | 109.34 |
| 37 | 16 | 301 | CLA | C4C-C3C-C2C | -3.10 | 102.37 | 106.89 |
| 37 | 38 | 208 | CLA | C4C-C3C-C2C | -3.10 | 102.37 | 106.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 31 | 309 | KC1 | C2A-C1A-NA | 3.10 | 114.31 | 109.34 |
| 37 | d | 403 | CLA | CBC-CAC-C3C | -3.10 | 104.01 | 112.42 |
| 48 | 32 | 203 | A86 | C26-C25-C24 | -3.10 | 114.21 | 123.20 |
| 48 | 15 | 313 | A86 | C21-C20-C15 | -3.10 | 113.33 | 123.35 |
| 37 | c | 512 | CLA | C4C-C3C-C2C | -3.10 | 102.38 | 106.89 |
| 47 | 33 | 304 | KC1 | CHD-C4C-NC | 3.10 | 128.98 | 124.31 |
| 47 | 31 | 305 | KC1 | CHD-C1D-ND | -3.10 | 119.39 | 124.05 |
| 37 | 40 | 208 | CLA | C1-C2-C3 | -3.10 | 121.74 | 126.76 |
| 48 | 16 | 313 | A86 | C40-C32-C31 | -3.10 | 107.70 | 110.47 |
| 37 | b | 512 | CLA | CMC-C2C-C1C | 3.10 | 129.88 | 125.03 |
| 48 | 17 | 320 | A86 | C36-C31-C32 | -3.10 | 116.62 | 119.70 |
| 37 | 35 | 303 | CLA | CAC-C3C-C4C | 3.10 | 128.82 | 124.79 |
| 47 | 14 | 306 | KC1 | O2D-CGD-O1D | -3.10 | 117.81 | 123.85 |
| 47 | 34 | 304 | KC1 | CHD-C1D-ND | -3.10 | 119.40 | 124.05 |
| 47 | 16 | 302 | KC1 | CAA-CBA-CGA | -3.10 | 111.28 | 127.05 |
| 37 | C | 512 | CLA | C4C-C3C-C2C | -3.10 | 102.38 | 106.89 |
| 47 | 35 | 302 | KC1 | CAC-C3C-C4C | 3.10 | 128.82 | 124.79 |
| 37 | C | 507 | CLA | O2D-CGD-O1D | -3.10 | 117.81 | 123.85 |
| 47 | 36 | 308 | KC1 | C1A-NA-C4A | -3.10 | 105.27 | 106.68 |
| 37 | D | 405 | CLA | CBC-CAC-C3C | -3.10 | 104.02 | 112.42 |
| 39 | C | 514 | BCR | C2-C1-C6 | 3.10 | 114.94 | 110.44 |
| 48 | 35 | 313 | A86 | C21-C20-C15 | -3.10 | 113.35 | 123.35 |
| 37 | 39 | 303 | CLA | CAC-C3C-C4C | 3.10 | 128.82 | 124.79 |
| 37 | c | 501 | CLA | CAA-C2A-C3A | -3.10 | 104.63 | 113.00 |
| 37 | 33 | 310 | CLA | C3C-C4C-NC | 3.10 | 114.40 | 110.43 |
| 37 | 32 | 205 | CLA | CMB-C2B-C1B | 3.10 | 130.14 | 125.42 |
| 37 | 32 | 205 | CLA | C4B-C3B-C2B | -3.10 | 103.45 | 107.30 |
| 48 | 14 | 311 | A86 | C3-C2-C1 | -3.10 | 122.93 | 127.28 |
| 39 | C | 514 | BCR | C15-C16-C17 | -3.10 | 117.18 | 123.52 |
| 37 | b | 512 | CLA | C1C-C2C-C3C | -3.10 | 103.72 | 106.98 |
| 37 | 39 | 307 | CLA | C4C-C3C-C2C | -3.10 | 102.38 | 106.89 |
| 37 | 19 | 304 | CLA | C1D-CHD-C4C | -3.10 | 119.44 | 126.02 |
| 47 | 14 | 304 | KC1 | CHD-C1D-ND | -3.10 | 119.40 | 124.05 |
| 37 | 34 | 303 | CLA | CHC-C1C-C2C | -3.10 | 118.15 | 126.95 |
| 37 | 39 | 306 | CLA | CMC-C2C-C1C | 3.10 | 129.87 | 125.03 |
| 48 | 34 | 311 | A86 | C3-C2-C1 | -3.10 | 122.94 | 127.28 |
| 37 | 19 | 307 | CLA | CHC-C1C-C2C | -3.10 | 118.15 | 126.95 |
| 37 | 17 | 307 | CLA | CAA-C2A-C1A | 3.09 | 122.12 | 111.97 |
| 37 | 34 | 302 | CLA | CMB-C2B-C1B | 3.09 | 130.13 | 125.42 |
| 37 | 15 | 310 | CLA | C4B-C3B-C2B | -3.09 | 103.45 | 107.30 |
| 48 | 18 | 214 | A86 | C9-C8-C6 | -3.09 | 117.88 | 126.36 |
| 47 | 32 | 212 | KC1 | CHD-C1D-ND | -3.09 | 119.41 | 124.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 36 | 302 | KC1 | CAA-CBA-CGA | -3.09 | 111.31 | 127.05 |
| 39 | a | 413 | BCR | C11-C10-C9 | -3.09 | 122.94 | 127.28 |
| 37 | c | 511 | CLA | C4B-C3B-C2B | -3.09 | 103.45 | 107.30 |
| 37 | 37 | 303 | CLA | C4B-C3B-C2B | -3.09 | 103.45 | 107.30 |
| 37 | b | 505 | CLA | CHD-C4C-NC | 3.09 | 129.03 | 124.23 |
| 37 | 21 | 209 | CLA | CHC-C1C-C2C | -3.09 | 118.16 | 126.95 |
| 47 | 11 | 302 | KC1 | CHD-C4C-NC | 3.09 | 128.97 | 124.31 |
| 37 | 11 | 301 | CLA | C1-C2-C3 | -3.09 | 121.13 | 126.20 |
| 37 | 14 | 307 | CLA | CAC-C3C-C4C | 3.09 | 128.81 | 124.79 |
| 37 | B | 503 | CLA | C4C-C3C-C2C | -3.09 | 102.39 | 106.89 |
| 37 | Z | 101 | CLA | C4B-C3B-C2B | -3.09 | 103.46 | 107.30 |
| 37 | C | 501 | CLA | CAA-C2A-C3A | -3.09 | 104.65 | 113.00 |
| 37 | B | 512 | CLA | CMC-C2C-C1C | 3.09 | 129.86 | 125.03 |
| 37 | 31 | 310 | CLA | C3B-C4B-NB | 3.09 | 113.29 | 110.53 |
| 37 | z | 101 | CLA | C4B-C3B-C2B | -3.09 | 103.46 | 107.30 |
| 37 | 38 | 204 | CLA | CHD-C4C-NC | 3.09 | 129.02 | 124.23 |
| 37 | b | 515 | CLA | CHC-C1C-C2C | -3.09 | 118.17 | 126.95 |
| 47 | 37 | 307 | KC1 | CHD-C4C-NC | 3.09 | 128.97 | 124.31 |
| 37 | b | 507 | CLA | C4C-C3C-C2C | -3.09 | 102.39 | 106.89 |
| 47 | 12 | 211 | KC1 | CHD-C1D-ND | -3.09 | 119.41 | 124.05 |
| 37 | 35 | 310 | CLA | C4B-C3B-C2B | -3.09 | 103.46 | 107.30 |
| 48 | 34 | 313 | A86 | C21-C20-C15 | -3.09 | 113.38 | 123.35 |
| 37 | b | 511 | CLA | C4C-C3C-C2C | -3.09 | 102.40 | 106.89 |
| 37 | d | 404 | CLA | CHC-C1C-C2C | -3.09 | 118.17 | 126.95 |
| 37 | b | 504 | CLA | CAA-C2A-C3A | -3.09 | 104.65 | 113.00 |
| 37 | C | 512 | CLA | CMA-C3A-C4A | -3.09 | 103.47 | 111.77 |
| 37 | 16 | 303 | CLA | C3C-C4C-NC | 3.09 | 114.39 | 110.43 |
| 37 | 11 | 310 | CLA | C3B-C4B-NB | 3.09 | 113.29 | 110.53 |
| 37 | 18 | 204 | CLA | C4B-C3B-C2B | -3.09 | 103.46 | 107.30 |
| 37 | 15 | 307 | CLA | CMC-C2C-C1C | 3.09 | 129.86 | 125.03 |
| 39 | c | 514 | BCR | C2-C1-C6 | 3.09 | 114.92 | 110.44 |
| 37 | 39 | 304 | CLA | C1D-CHD-C4C | -3.09 | 119.46 | 126.02 |
| 37 | 13 | 307 | CLA | CAC-C3C-C4C | 3.09 | 128.81 | 124.79 |
| 37 | 36 | 303 | CLA | C3C-C4C-NC | 3.09 | 114.38 | 110.43 |
| 37 | 40 | 203 | CLA | C4-C3-C5 | 3.09 | 120.58 | 115.23 |
| 37 | 41 | 202 | CLA | C4C-C3C-C2C | -3.09 | 102.40 | 106.89 |
| 37 | 38 | 202 | CLA | C1C-C2C-C3C | -3.09 | 103.73 | 106.98 |
| 37 | 41 | 209 | CLA | CHC-C1C-C2C | -3.08 | 118.18 | 126.95 |
| 41 | C | 518 | LMG | O6-C1-O1 | -3.08 | 102.75 | 110.04 |
| 37 | b | 514 | CLA | C4C-C3C-C2C | -3.08 | 102.40 | 106.89 |
| 37 | c | 512 | CLA | CMA-C3A-C4A | -3.08 | 103.48 | 111.77 |
| 37 | B | 515 | CLA | CHC-C1C-C2C | -3.08 | 118.18 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | D | 406 | CLA | CHC-C1C-C2C | -3.08 | 118.18 | 126.95 |
| 37 | C | 503 | CLA | CMB-C2B-C1B | 3.08 | 130.11 | 125.42 |
| 48 | 14 | 313 | A86 | C21-C20-C15 | -3.08 | 113.40 | 123.35 |
| 37 | B | 511 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 37 | 36 | 301 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 37 | c | 503 | CLA | CMB-C2B-C1B | 3.08 | 130.11 | 125.42 |
| 37 | b | 513 | CLA | CHD-C4C-NC | 3.08 | 129.01 | 124.23 |
| 47 | 37 | 307 | KC1 | CBC-CAC-C3C | -3.08 | 104.06 | 112.42 |
| 47 | 13 | 306 | KC1 | CHD-C1D-ND | -3.08 | 119.43 | 124.05 |
| 37 | C | 509 | CLA | CHC-C1C-C2C | -3.08 | 118.19 | 126.95 |
| 37 | b | 503 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 37 | 21 | 202 | CLA | CHC-C1C-C2C | -3.08 | 118.19 | 126.95 |
| 37 | 40 | 203 | CLA | CAC-C3C-C4C | 3.08 | 128.80 | 124.79 |
| 48 | 39 | 313 | A86 | C25-C26-C27 | -3.08 | 122.96 | 127.28 |
| 37 | D | 406 | CLA | O2D-CGD-O1D | -3.08 | 117.85 | 123.85 |
| 37 | 19 | 306 | CLA | CMB-C2B-C1B | 3.08 | 130.11 | 125.42 |
| 37 | 20 | 301 | CLA | CHD-C4C-NC | 3.08 | 129.01 | 124.23 |
| 37 | 40 | 203 | CLA | CHD-C4C-NC | 3.08 | 129.01 | 124.23 |
| 48 | 34 | 311 | A86 | C25-C24-C1 | -3.08 | 117.92 | 126.36 |
| 37 | 12 | 209 | CLA | CAC-C3C-C4C | 3.08 | 128.80 | 124.79 |
| 37 | B | 504 | CLA | CAA-C2A-C3A | -3.08 | 104.68 | 113.00 |
| 48 | 17 | 312 | A86 | C36-C31-C32 | -3.08 | 116.64 | 119.70 |
| 37 | 41 | 202 | CLA | CHC-C1C-C2C | -3.08 | 118.20 | 126.95 |
| 37 | 16 | 307 | CLA | C3B-C4B-NB | 3.08 | 113.28 | 110.53 |
| 37 | 33 | 307 | CLA | CAC-C3C-C4C | 3.08 | 128.80 | 124.79 |
| 37 | 16 | 307 | CLA | CHD-C4C-NC | 3.08 | 129.00 | 124.23 |
| 48 | 38 | 214 | A86 | C7-C6-C8 | 3.08 | 122.79 | 118.09 |
| 48 | 34 | 312 | A86 | C10-C9-C8 | -3.08 | 114.28 | 123.20 |
| 37 | 19 | 303 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 37 | 39 | 303 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 37 | B | 506 | CLA | O2D-CGD-O1D | -3.08 | 117.86 | 123.85 |
| 37 | C | 507 | CLA | C4-C3-C5 | 3.08 | 120.57 | 115.23 |
| 37 | 20 | 301 | CLA | C4-C3-C5 | 3.08 | 120.57 | 115.23 |
| 37 | 18 | 202 | CLA | C4A-NA-C1A | -3.08 | 105.28 | 106.68 |
| 37 | 34 | 301 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 37 | 41 | 208 | CLA | C3C-C4C-NC | 3.08 | 114.37 | 110.43 |
| 48 | 38 | 213 | A86 | C21-C20-C15 | -3.08 | 113.42 | 123.35 |
| 37 | 36 | 307 | CLA | CHC-C1C-C2C | -3.08 | 118.20 | 126.95 |
| 48 | 18 | 214 | A86 | C7-C6-C8 | 3.08 | 122.79 | 118.09 |
| 37 | c | 509 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 37 | 17 | 302 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 48 | 40 | 201 | A86 | C12-C11-C10 | -3.08 | 116.19 | 123.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 310 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.89 |
| 37 | 34 | 307 | CLA | CAC-C3C-C4C | 3.08 | 128.79 | 124.79 |
| 50 | 41 | 212 | DD6 | C23-C16-C17 | -3.08 | 103.56 | 108.97 |
| 37 | 20 | 307 | CLA | C3B-C4B-NB | 3.07 | 113.28 | 110.53 |
| 47 | 12 | 211 | KC1 | CHD-C4C-NC | 3.07 | 128.94 | 124.31 |
| 37 | 38 | 209 | CLA | C4B-C3B-C2B | -3.07 | 103.48 | 107.30 |
| 48 | 14 | 312 | A86 | C10-C9-C8 | -3.07 | 114.29 | 123.20 |
| 37 | C | 509 | CLA | C4C-C3C-C2C | -3.07 | 102.42 | 106.89 |
| 37 | C | 512 | CLA | C3B-C4B-NB | 3.07 | 113.27 | 110.53 |
| 37 | B | 502 | CLA | C4B-C3B-C2B | -3.07 | 103.48 | 107.30 |
| 47 | 17 | 308 | KC1 | CHD-C4C-NC | 3.07 | 128.94 | 124.31 |
| 47 | 35 | 306 | KC1 | CHD-C4C-NC | 3.07 | 128.94 | 124.31 |
| 37 | 16 | 303 | CLA | CHC-C1C-C2C | -3.07 | 118.22 | 126.95 |
| 41 | c | 518 | LMG | O1-C7-C8 | -3.07 | 103.35 | 110.82 |
| 37 | 35 | 307 | CLA | CMC-C2C-C1C | 3.07 | 129.83 | 125.03 |
| 37 | 39 | 306 | CLA | CMB-C2B-C1B | 3.07 | 130.09 | 125.42 |
| 37 | B | 507 | CLA | CAC-C3C-C4C | 3.07 | 128.78 | 124.79 |
| 37 | 16 | 307 | CLA | CHC-C1C-C2C | -3.07 | 118.22 | 126.95 |
| 47 | 12 | 211 | KC1 | CAC-C3C-C4C | 3.07 | 128.78 | 124.79 |
| 37 | b | 506 | CLA | O2D-CGD-O1D | -3.07 | 117.87 | 123.85 |
| 37 | C | 502 | CLA | CAA-C2A-C3A | -3.07 | 104.70 | 113.00 |
| 48 | 39 | 313 | A86 | C4-C3-C2 | -3.07 | 117.24 | 123.52 |
| 37 | 37 | 306 | CLA | CAA-C2A-C1A | 3.07 | 122.03 | 111.97 |
| 48 | 36 | 310 | A86 | C10-C9-C8 | -3.07 | 114.31 | 123.20 |
| 47 | 11 | 309 | KC1 | CHD-C1D-ND | -3.07 | 119.45 | 124.05 |
| 37 | c | 509 | CLA | CHC-C1C-C2C | -3.07 | 118.23 | 126.95 |
| 37 | 40 | 208 | CLA | C4C-C3C-C2C | -3.07 | 102.43 | 106.89 |
| 48 | 16 | 313 | A86 | C12-C11-C10 | -3.07 | 116.22 | 123.67 |
| 37 | 11 | 305 | CLA | C3B-C4B-NB | 3.07 | 113.27 | 110.53 |
| 37 | 31 | 304 | CLA | O2D-CGD-O1D | -3.07 | 117.88 | 123.85 |
| 37 | 37 | 301 | CLA | CHC-C1C-C2C | -3.07 | 118.23 | 126.95 |
| 37 | 16 | 306 | CLA | C1C-C2C-C3C | -3.07 | 103.75 | 106.98 |
| 37 | 32 | 206 | CLA | C1C-C2C-C3C | -3.07 | 103.75 | 106.98 |
| 37 | 14 | 302 | CLA | CHC-C1C-C2C | -3.07 | 118.23 | 126.95 |
| 37 | 18 | 204 | CLA | CAC-C3C-C4C | 3.07 | 128.78 | 124.79 |
| 37 | 11 | 310 | CLA | C4C-C3C-C2C | -3.07 | 102.43 | 106.89 |
| 47 | 39 | 308 | KC1 | CAA-CBA-CGA | -3.07 | 111.46 | 127.05 |
| 39 | b | 517 | BCR | C11-C10-C9 | -3.06 | 122.98 | 127.28 |
| 37 | 11 | 303 | CLA | O2D-CGD-O1D | -3.06 | 117.88 | 123.85 |
| 37 | b | 506 | CLA | C1D-CHD-C4C | -3.06 | 119.51 | 126.02 |
| 37 | 12 | 209 | CLA | O2D-CGD-O1D | -3.06 | 117.88 | 123.85 |
| 48 | 37 | 319 | A86 | C41-C32-C31 | -3.06 | 107.73 | 110.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 18 | 208 | CLA | C3B-C4B-NB | 3.06 | 113.27 | 110.53 |
| 50 | 21 | 216 | DD6 | C21-C20-C15 | -3.06 | 117.26 | 122.30 |
| 41 | C | 518 | LMG | O1-C7-C8 | -3.06 | 103.37 | 110.82 |
| 37 | c | 508 | CLA | O2D-CGD-O1D | -3.06 | 117.89 | 123.85 |
| 37 | 14 | 301 | CLA | C4C-C3C-C2C | -3.06 | 102.43 | 106.89 |
| 37 | b | 507 | CLA | CAC-C3C-C4C | 3.06 | 128.78 | 124.79 |
| 47 | 33 | 306 | KC1 | CHD-C1D-ND | -3.06 | 119.45 | 124.05 |
| 47 | 19 | 308 | KC1 | CAA-CBA-CGA | -3.06 | 111.48 | 127.05 |
| 37 | 20 | 301 | CLA | CAC-C3C-C4C | 3.06 | 128.77 | 124.79 |
| 50 | 21 | 212 | DD6 | C23-C16-C17 | -3.06 | 103.59 | 108.97 |
| 37 | 40 | 209 | CLA | C3B-C4B-NB | 3.06 | 113.26 | 110.53 |
| 37 | 32 | 210 | CLA | O2D-CGD-O1D | -3.06 | 117.89 | 123.85 |
| 39 | A | 410 | BCR | C11-C10-C9 | -3.06 | 122.98 | 127.28 |
| 37 | 33 | 307 | CLA | CHC-C1C-C2C | -3.06 | 118.25 | 126.95 |
| 37 | B | 506 | CLA | C1D-CHD-C4C | -3.06 | 119.52 | 126.02 |
| 48 | 34 | 311 | A86 | C10-C9-C8 | -3.06 | 114.33 | 123.20 |
| 37 | 31 | 306 | CLA | C3B-C4B-NB | 3.06 | 113.26 | 110.53 |
| 37 | d | 404 | CLA | O2D-CGD-O1D | -3.06 | 117.89 | 123.85 |
| 37 | 20 | 303 | CLA | C4B-C3B-C2B | -3.06 | 103.50 | 107.30 |
| 48 | 14 | 311 | A86 | C25-C24-C1 | -3.06 | 117.98 | 126.36 |
| 37 | 38 | 208 | CLA | C3B-C4B-NB | 3.06 | 113.26 | 110.53 |
| 37 | 21 | 208 | CLA | C3C-C4C-NC | 3.06 | 114.35 | 110.43 |
| 39 | B | 517 | BCR | C11-C10-C9 | -3.06 | 122.99 | 127.28 |
| 48 | 16 | 310 | A86 | C10-C9-C8 | -3.06 | 114.34 | 123.20 |
| 37 | 36 | 303 | CLA | CHC-C1C-C2C | -3.06 | 118.26 | 126.95 |
| 37 | C | 511 | CLA | C1-C2-C3 | -3.06 | 121.19 | 126.20 |
| 37 | 31 | 302 | CLA | C1-C2-C3 | -3.06 | 121.19 | 126.20 |
| 37 | W | 101 | CLA | C3B-C4B-NB | 3.06 | 113.26 | 110.53 |
| 37 | 36 | 307 | CLA | C3B-C4B-NB | 3.06 | 113.26 | 110.53 |
| 37 | 13 | 307 | CLA | CHC-C1C-C2C | -3.06 | 118.26 | 126.95 |
| 37 | 39 | 305 | CLA | CHC-C1C-C2C | -3.06 | 118.26 | 126.95 |
| 39 | c | 514 | BCR | C11-C10-C9 | -3.06 | 122.99 | 127.28 |
| 37 | c | 502 | CLA | CAA-C2A-C3A | -3.06 | 104.74 | 113.00 |
| 37 | c | 512 | CLA | C3B-C4B-NB | 3.05 | 113.26 | 110.53 |
| 37 | 20 | 303 | CLA | C4C-C3C-C2C | -3.05 | 102.45 | 106.89 |
| 37 | 14 | 301 | CLA | C1C-C2C-C3C | -3.05 | 103.77 | 106.98 |
| 37 | 36 | 306 | CLA | C1C-C2C-C3C | -3.05 | 103.77 | 106.98 |
| 37 | 19 | 306 | CLA | CMC-C2C-C1C | 3.05 | 129.81 | 125.03 |
| 37 | 11 | 303 | CLA | CAC-C3C-C4C | 3.05 | 128.76 | 124.79 |
| 39 | C | 514 | BCR | C11-C10-C9 | -3.05 | 123.00 | 127.28 |
| 37 | 35 | 301 | CLA | CHD-C4C-NC | 3.05 | 128.97 | 124.23 |
| 37 | 16 | 306 | CLA | CMC-C2C-C1C | 3.05 | 129.80 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 501 | CLA | C4B-C3B-C2B | -3.05 | 103.51 | 107.30 |
| 47 | 13 | 302 | KC1 | CHD-C1D-ND | -3.05 | 119.47 | 124.05 |
| 37 | W | 102 | CLA | C3B-C4B-NB | 3.05 | 113.25 | 110.53 |
| 47 | 20 | 305 | KC1 | CBA-CAA-C2A | -3.05 | 113.22 | 125.45 |
| 37 | A | 405 | CLA | CAC-C3C-C4C | 3.05 | 128.76 | 124.79 |
| 37 | 15 | 303 | CLA | CHC-C1C-C2C | -3.05 | 118.28 | 126.95 |
| 37 | 14 | 307 | CLA | CHC-C1C-C2C | -3.05 | 118.28 | 126.95 |
| 37 | 34 | 302 | CLA | CHC-C1C-C2C | -3.05 | 118.29 | 126.95 |
| 47 | 33 | 302 | KC1 | CHD-C1D-ND | -3.05 | 119.48 | 124.05 |
| 48 | 15 | 316 | A86 | C3-C2-C1 | -3.05 | 123.00 | 127.28 |
| 37 | 20 | 307 | CLA | CHC-C1C-C2C | -3.05 | 118.29 | 126.95 |
| 47 | 31 | 309 | KC1 | CHD-C1D-ND | -3.05 | 119.48 | 124.05 |
| 50 | 36 | 312 | DD6 | C3-C4-C5 | -3.05 | 117.29 | 123.52 |
| 37 | 19 | 305 | CLA | CHC-C1C-C2C | -3.05 | 118.29 | 126.95 |
| 37 | b | 501 | CLA | C3C-C4C-NC | 3.05 | 114.33 | 110.43 |
| 48 | 31 | 314 | A86 | C7-C6-C8 | 3.05 | 122.74 | 118.09 |
| 37 | 12 | 205 | CLA | CAC-C3C-C4C | 3.05 | 128.75 | 124.79 |
| 37 | 12 | 207 | CLA | C3B-C4B-NB | 3.05 | 113.25 | 110.53 |
| 37 | 32 | 208 | CLA | C3B-C4B-NB | 3.05 | 113.25 | 110.53 |
| 37 | B | 514 | CLA | C4C-C3C-C2C | -3.05 | 102.46 | 106.89 |
| 48 | 14 | 311 | A86 | C10-C9-C8 | -3.05 | 114.38 | 123.20 |
| 37 | 37 | 308 | CLA | C4B-C3B-C2B | -3.05 | 103.52 | 107.30 |
| 37 | 12 | 212 | CLA | CHD-C4C-NC | 3.05 | 128.95 | 124.23 |
| 37 | 19 | 304 | CLA | C4C-C3C-C2C | -3.05 | 102.46 | 106.89 |
| 37 | 19 | 305 | CLA | C4C-C3C-C2C | -3.05 | 102.46 | 106.89 |
| 37 | b | 502 | CLA | C4B-C3B-C2B | -3.04 | 103.52 | 107.30 |
| 37 | 38 | 204 | CLA | CAC-C3C-C4C | 3.04 | 128.75 | 124.79 |
| 37 | 33 | 305 | CLA | CHD-C4C-NC | 3.04 | 128.95 | 124.23 |
| 37 | 31 | 304 | CLA | CAC-C3C-C4C | 3.04 | 128.75 | 124.79 |
| 50 | 16 | 312 | DD6 | C3-C4-C5 | -3.04 | 117.29 | 123.52 |
| 37 | 34 | 301 | CLA | C1C-C2C-C3C | -3.04 | 103.78 | 106.98 |
| 37 | c | 501 | CLA | C4B-C3B-C2B | -3.04 | 103.52 | 107.30 |
| 37 | 14 | 303 | CLA | CAC-C3C-C4C | 3.04 | 128.75 | 124.79 |
| 47 | 38 | 205 | KC1 | CAC-C3C-C4C | 3.04 | 128.75 | 124.79 |
| 37 | 18 | 206 | CLA | CHC-C1C-C2C | -3.04 | 118.30 | 126.95 |
| 37 | 39 | 301 | CLA | O2D-CGD-CBD | 3.04 | 116.55 | 111.23 |
| 37 | B | 513 | CLA | CHC-C1C-C2C | -3.04 | 118.31 | 126.95 |
| 40 | 36 | 315 | SQD | O47-C7-C8 | 3.04 | 118.06 | 111.48 |
| 37 | a | 407 | CLA | CAC-C3C-C4C | 3.04 | 128.75 | 124.79 |
| 37 | 34 | 307 | CLA | CHC-C1C-C2C | -3.04 | 118.31 | 126.95 |
| 50 | 20 | 310 | DD6 | C21-C20-C15 | -3.04 | 117.30 | 122.30 |
| 47 | 12 | 206 | KC1 | CHD-C1D-ND | -3.04 | 119.49 | 124.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 18 | 208 | CLA | C4C-C3C-C2C | -3.04 | 102.47 | 106.89 |
| 37 | D | 406 | CLA | CAA-C2A-C3A | -3.04 | 104.79 | 113.00 |
| 37 | d | 404 | CLA | CAA-C2A-C3A | -3.04 | 104.79 | 113.00 |
| 37 | 13 | 305 | CLA | CHD-C4C-NC | 3.04 | 128.94 | 124.23 |
| 47 | 32 | 209 | KC1 | CHD-C4C-NC | 3.04 | 128.89 | 124.31 |
| 44 | c | 516 | DGD | C3G-C2G-C1G | -3.04 | 104.70 | 111.78 |
| 47 | 20 | 302 | KC1 | CHD-C4C-NC | 3.04 | 128.88 | 124.31 |
| 47 | 40 | 204 | KC1 | CHD-C4C-NC | 3.04 | 128.88 | 124.31 |
| 47 | 35 | 309 | KC1 | C2A-C1A-NA | 3.04 | 114.21 | 109.34 |
| 47 | 35 | 302 | KC1 | CMB-C2B-C1B | 3.04 | 130.08 | 124.73 |
| 37 | C | 508 | CLA | O2D-CGD-O1D | -3.04 | 117.94 | 123.85 |
| 37 | 36 | 309 | CLA | C4C-C3C-C2C | -3.04 | 102.47 | 106.89 |
| 48 | 11 | 314 | A86 | C7-C6-C8 | 3.04 | 122.72 | 118.09 |
| 37 | 40 | 209 | CLA | CHC-C1C-C2C | -3.04 | 118.32 | 126.95 |
| 37 | 16 | 309 | CLA | C4C-C3C-C2C | -3.03 | 102.47 | 106.89 |
| 47 | 40 | 207 | KC1 | CBA-CAA-C2A | -3.03 | 113.27 | 125.45 |
| 40 | B | 519 | SQD | O5-C5-C4 | 3.03 | 115.17 | 109.70 |
| 47 | 18 | 205 | KC1 | CAA-CBA-CGA | -3.03 | 111.62 | 127.05 |
| 37 | 11 | 307 | CLA | CAC-C3C-C2C | 3.03 | 133.13 | 127.56 |
| 44 | C | 516 | DGD | C3G-C2G-C1G | -3.03 | 104.71 | 111.78 |
| 48 | 15 | 319 | A86 | C7-C6-C8 | 3.03 | 122.72 | 118.09 |
| 47 | 17 | 306 | KC1 | C4C-C3C-C2C | -3.03 | 102.48 | 106.89 |
| 37 | 19 | 309 | CLA | C4B-C3B-C2B | -3.03 | 103.53 | 107.30 |
| 37 | 36 | 306 | CLA | CMC-C2C-C1C | 3.03 | 129.77 | 125.03 |
| 37 | 35 | 303 | CLA | CHC-C1C-C2C | -3.03 | 118.33 | 126.95 |
| 37 | 19 | 303 | CLA | C3B-C4B-NB | 3.03 | 113.24 | 110.53 |
| 47 | 18 | 210 | KC1 | C2A-C1A-NA | 3.03 | 114.20 | 109.34 |
| 37 | 35 | 308 | CLA | C4C-C3C-C2C | -3.03 | 102.48 | 106.89 |
| 37 | B | 505 | CLA | CAC-C3C-C4C | 3.03 | 128.73 | 124.79 |
| 47 | 15 | 306 | KC1 | CHD-C4C-NC | 3.03 | 128.88 | 124.31 |
| 50 | 40 | 212 | DD6 | C21-C20-C15 | -3.03 | 117.31 | 122.30 |
| 37 | 40 | 205 | CLA | CAC-C3C-C4C | 3.03 | 128.73 | 124.79 |
| 40 | 17 | 301 | SQD | O47-C7-C8 | 3.03 | 118.03 | 111.48 |
| 37 | 18 | 203 | CLA | CAA-C2A-C1A | 3.03 | 121.90 | 111.97 |
| 37 | c | 511 | CLA | CAC-C3C-C4C | 3.03 | 128.73 | 124.79 |
| 47 | 12 | 208 | KC1 | CHD-C4C-NC | 3.03 | 128.87 | 124.31 |
| 37 | 19 | 301 | CLA | O2D-CGD-CBD | 3.03 | 116.52 | 111.23 |
| 37 | B | 512 | CLA | C1C-C2C-C3C | -3.03 | 103.80 | 106.98 |
| 48 | 34 | 312 | A86 | C4-C3-C2 | -3.03 | 117.32 | 123.52 |
| 37 | b | 501 | CLA | O2A-CGA-CBA | 3.03 | 121.07 | 111.83 |
| 48 | 40 | 201 | A86 | C40-C32-C31 | -3.03 | 107.76 | 110.47 |
| 47 | 38 | 205 | KC1 | CAA-CBA-CGA | -3.03 | 111.66 | 127.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 507 | CLA | C4A-NA-C1A | -3.03 | 105.30 | 106.68 |
| 48 | 14 | 312 | A86 | C4-C3-C2 | -3.03 | 117.33 | 123.52 |
| 48 | 34 | 315 | A86 | C36-C31-C32 | -3.03 | 116.69 | 119.70 |
| 48 | 33 | 312 | A86 | C4-C5-C6 | -3.03 | 123.03 | 127.28 |
| 37 | 17 | 309 | CLA | C4B-C3B-C2B | -3.03 | 103.54 | 107.30 |
| 37 | 38 | 203 | CLA | C4B-C3B-C2B | -3.03 | 103.54 | 107.30 |
| 37 | C | 511 | CLA | CAC-C3C-C4C | 3.03 | 128.73 | 124.79 |
| 40 | A | 407 | SQD | O5-C5-C4 | 3.02 | 115.15 | 109.70 |
| 37 | 18 | 211 | CLA | CHC-C1C-C2C | -3.02 | 118.35 | 126.95 |
| 48 | 14 | 316 | A86 | C12-C11-C13 | 3.02 | 120.90 | 116.00 |
| 37 | 37 | 308 | CLA | CAA-C2A-C1A | -3.02 | 102.06 | 111.97 |
| 47 | 38 | 210 | KC1 | C2A-C1A-NA | 3.02 | 114.19 | 109.34 |
| 38 | a | 405 | PHO | O2D-CGD-O1D | -3.02 | 117.96 | 123.85 |
| 37 | c | 501 | CLA | O2A-CGA-CBA | 3.02 | 121.06 | 111.83 |
| 37 | 39 | 309 | CLA | C4B-C3B-C2B | -3.02 | 103.54 | 107.30 |
| 40 | B | 519 | SQD | O6-C1-C2 | 3.02 | 112.86 | 108.27 |
| 37 | 34 | 303 | CLA | CAC-C3C-C4C | 3.02 | 128.72 | 124.79 |
| 47 | 16 | 308 | KC1 | O2D-CGD-O1D | -3.02 | 117.96 | 123.85 |
| 47 | 37 | 305 | KC1 | C4C-C3C-C2C | -3.02 | 102.49 | 106.89 |
| 40 | L | 101 | SQD | O6-C1-C2 | 3.02 | 112.86 | 108.27 |
| 47 | 16 | 308 | KC1 | C1A-NA-C4A | -3.02 | 105.30 | 106.68 |
| 47 | 19 | 308 | KC1 | CHD-C1D-ND | -3.02 | 119.52 | 124.05 |
| 37 | b | 513 | CLA | CHC-C1C-C2C | -3.02 | 118.36 | 126.95 |
| 47 | 18 | 210 | KC1 | C4C-C3C-C2C | -3.02 | 102.49 | 106.89 |
| 48 | 32 | 217 | A86 | C41-C32-C31 | -3.02 | 107.77 | 110.47 |
| 37 | C | 501 | CLA | O2A-CGA-CBA | 3.02 | 121.05 | 111.83 |
| 38 | D | 403 | PHO | O2D-CGD-O1D | -3.02 | 117.97 | 123.85 |
| 50 | 41 | 216 | DD6 | C21-C20-C15 | -3.02 | 117.33 | 122.30 |
| 48 | 19 | 313 | A86 | C4-C3-C2 | -3.02 | 117.34 | 123.52 |
| 48 | 36 | 311 | A86 | C7-C6-C8 | 3.02 | 122.70 | 118.09 |
| 37 | 39 | 305 | CLA | C4C-C3C-C2C | -3.02 | 102.50 | 106.89 |
| 37 | 40 | 205 | CLA | C4B-C3B-C2B | -3.02 | 103.55 | 107.30 |
| 48 | 41 | 214 | A86 | C4-C3-C2 | -3.02 | 117.34 | 123.52 |
| 37 | B | 504 | CLA | O2D-CGD-O1D | -3.02 | 117.97 | 123.85 |
| 37 | B | 524 | CLA | O2D-CGD-O1D | -3.02 | 117.97 | 123.85 |
| 47 | 18 | 205 | KC1 | CAC-C3C-C4C | 3.02 | 128.72 | 124.79 |
| 37 | 32 | 204 | CLA | C3B-C4B-NB | 3.02 | 113.22 | 110.53 |
| 37 | 39 | 303 | CLA | C3B-C4B-NB | 3.02 | 113.22 | 110.53 |
| 37 | 13 | 310 | CLA | CAA-C2A-C3A | -3.02 | 104.84 | 113.00 |
| 37 | 19 | 304 | CLA | CHC-C1C-C2C | -3.02 | 118.37 | 126.95 |
| 37 | 33 | 301 | CLA | C3B-C4B-NB | 3.02 | 113.22 | 110.53 |
| 37 | 31 | 308 | CLA | CAC-C3C-C2C | 3.02 | 133.10 | 127.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | d | 404 | CLA | CHD-C4C-NC | 3.02 | 128.91 | 124.23 |
| 37 | 39 | 304 | CLA | CHC-C1C-C2C | -3.02 | 118.38 | 126.95 |
| 48 | 35 | 319 | A86 | C7-C6-C8 | 3.02 | 122.69 | 118.09 |
| 37 | 40 | 208 | CLA | C1C-C2C-C3C | -3.01 | 103.81 | 106.98 |
| 37 | 37 | 301 | CLA | C4C-C3C-C2C | -3.01 | 102.50 | 106.89 |
| 48 | 17 | 320 | A86 | C41-C32-C31 | -3.01 | 107.77 | 110.47 |
| 37 | B | 514 | CLA | CMB-C2B-C1B | 3.01 | 130.01 | 125.42 |
| 47 | 33 | 304 | KC1 | CAA-CBA-CGA | -3.01 | 111.72 | 127.05 |
| 47 | 13 | 304 | KC1 | CAA-CBA-CGA | -3.01 | 111.72 | 127.05 |
| 45 | D | 408 | PL9 | C7-C8-C9 | -3.01 | 121.64 | 126.83 |
| 37 | c | 512 | CLA | CHC-C1C-C2C | -3.01 | 118.38 | 126.95 |
| 37 | b | 504 | CLA | O2D-CGD-O1D | -3.01 | 117.98 | 123.85 |
| 37 | 12 | 205 | CLA | C1-O2A-CGA | 3.01 | 123.94 | 116.65 |
| 47 | 16 | 308 | KC1 | CAC-C3C-C4C | 3.01 | 128.71 | 124.79 |
| 48 | 34 | 314 | A86 | C12-C11-C13 | 3.01 | 120.89 | 116.00 |
| 47 | 18 | 210 | KC1 | O2D-CGD-O1D | -3.01 | 117.98 | 123.85 |
| 37 | B | 501 | CLA | C3C-C4C-NC | 3.01 | 114.29 | 110.43 |
| 37 | B | 502 | CLA | CHD-C4C-NC | 3.01 | 128.90 | 124.23 |
| 37 | 36 | 301 | CLA | C1C-C2C-C3C | -3.01 | 103.81 | 106.98 |
| 37 | 13 | 310 | CLA | C4C-C3C-C2C | -3.01 | 102.51 | 106.89 |
| 48 | 15 | 315 | A86 | C21-C20-C15 | -3.01 | 113.63 | 123.35 |
| 37 | b | 514 | CLA | CMB-C2B-C1B | 3.01 | 130.00 | 125.42 |
| 47 | 32 | 207 | KC1 | CHD-C1D-ND | -3.01 | 119.53 | 124.05 |
| 48 | 21 | 214 | A86 | C4-C3-C2 | -3.01 | 117.36 | 123.52 |
| 37 | C | 502 | CLA | C4B-C3B-C2B | -3.01 | 103.56 | 107.30 |
| 37 | 15 | 305 | CLA | C4B-C3B-C2B | -3.01 | 103.56 | 107.30 |
| 37 | b | 505 | CLA | CAC-C3C-C4C | 3.01 | 128.71 | 124.79 |
| 48 | 34 | 316 | A86 | C12-C11-C13 | 3.01 | 120.88 | 116.00 |
| 47 | 32 | 212 | KC1 | CAA-CBA-CGA | -3.01 | 111.75 | 127.05 |
| 37 | 36 | 307 | CLA | CAA-C2A-C3A | -3.01 | 104.87 | 113.00 |
| 37 | 37 | 301 | CLA | C3B-C4B-NB | 3.01 | 113.22 | 110.53 |
| 37 | 35 | 305 | CLA | CHC-C1C-C2C | -3.01 | 118.40 | 126.95 |
| 37 | c | 501 | CLA | C3C-C4C-NC | 3.01 | 114.28 | 110.43 |
| 48 | 11 | 315 | A86 | C36-C31-C32 | -3.01 | 116.71 | 119.70 |
| 37 | w | 101 | CLA | C3B-C4B-NB | 3.01 | 113.22 | 110.53 |
| 37 | c | 502 | CLA | C4B-C3B-C2B | -3.01 | 103.56 | 107.30 |
| 37 | 18 | 202 | CLA | C1-C2-C3 | -3.01 | 121.27 | 126.20 |
| 37 | 15 | 305 | CLA | CHC-C1C-C2C | -3.01 | 118.41 | 126.95 |
| 37 | C | 507 | CLA | CHC-C1C-C2C | -3.01 | 118.41 | 126.95 |
| 37 | 20 | 303 | CLA | CAC-C3C-C4C | 3.01 | 128.70 | 124.79 |
| 37 | a | 407 | CLA | CMB-C2B-C1B | 3.00 | 129.99 | 125.42 |
| 37 | c | 505 | CLA | CHD-C4C-NC | 3.00 | 128.89 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 18 | 209 | CLA | C4B-C3B-C2B | -3.00 | 103.57 | 107.30 |
| 37 | b | 523 | CLA | O2D-CGD-O1D | -3.00 | 118.00 | 123.85 |
| 37 | 19 | 303 | CLA | CHD-C4C-NC | 3.00 | 128.89 | 124.23 |
| 37 | b | 504 | CLA | CHD-C1D-ND | -3.00 | 120.58 | 124.80 |
| 37 | C | 501 | CLA | C3C-C4C-NC | 3.00 | 114.28 | 110.43 |
| 37 | B | 501 | CLA | O2A-CGA-CBA | 3.00 | 120.99 | 111.83 |
| 48 | 17 | 315 | A86 | C41-C32-C31 | -3.00 | 107.78 | 110.47 |
| 48 | 35 | 316 | A86 | C3-C2-C1 | -3.00 | 123.07 | 127.28 |
| 48 | 14 | 314 | A86 | C12-C11-C13 | 3.00 | 120.87 | 116.00 |
| 47 | 12 | 211 | KC1 | CAA-CBA-CGA | -3.00 | 111.78 | 127.05 |
| 37 | B | 504 | CLA | CHD-C1D-ND | -3.00 | 120.58 | 124.80 |
| 37 | 35 | 303 | CLA | C1-C2-C3 | -3.00 | 121.28 | 126.20 |
| 40 | a | 409 | SQD | O5-C5-C4 | 3.00 | 115.11 | 109.70 |
| 47 | 15 | 309 | KC1 | C2A-C1A-NA | 3.00 | 114.15 | 109.34 |
| 37 | 16 | 307 | CLA | CAA-C2A-C3A | -3.00 | 104.89 | 113.00 |
| 37 | C | 512 | CLA | CHC-C1C-C2C | -3.00 | 118.42 | 126.95 |
| 39 | 0 | 101 | BCR | C11-C10-C9 | -3.00 | 123.07 | 127.28 |
| 48 | 18 | 212 | A86 | C7-C6-C8 | 3.00 | 122.67 | 118.09 |
| 48 | 18 | 212 | A86 | C25-C26-C27 | -3.00 | 123.07 | 127.28 |
| 37 | 31 | 308 | CLA | O2D-CGD-O1D | -3.00 | 118.01 | 123.85 |
| 47 | 33 | 304 | KC1 | CHD-C1D-ND | -3.00 | 119.55 | 124.05 |
| 37 | 32 | 206 | CLA | C1-O2A-CGA | 3.00 | 123.91 | 116.65 |
| 47 | 11 | 306 | KC1 | CMB-C2B-C1B | 3.00 | 130.01 | 124.73 |
| 47 | 32 | 209 | KC1 | CMB-C2B-C1B | 3.00 | 130.01 | 124.73 |
| 37 | 15 | 301 | CLA | CHD-C4C-NC | 3.00 | 128.88 | 124.23 |
| 37 | 15 | 307 | CLA | C4B-C3B-C2B | -3.00 | 103.57 | 107.30 |
| 37 | c | 507 | CLA | C4C-C3C-C2C | -3.00 | 102.53 | 106.89 |
| 40 | L | 101 | SQD | O5-C5-C4 | 3.00 | 115.10 | 109.70 |
| 48 | 34 | 316 | A86 | C21-C20-C15 | -3.00 | 113.67 | 123.35 |
| 37 | c | 511 | CLA | CHC-C1C-C2C | -3.00 | 118.43 | 126.95 |
| 48 | 35 | 315 | A86 | C21-C20-C15 | -3.00 | 113.67 | 123.35 |
| 47 | 18 | 210 | KC1 | CHD-C1D-ND | -3.00 | 119.55 | 124.05 |
| 37 | 34 | 310 | CLA | C3C-C4C-NC | 3.00 | 114.27 | 110.43 |
| 47 | 31 | 303 | KC1 | CHD-C1D-ND | -3.00 | 119.55 | 124.05 |
| 37 | 14 | 307 | CLA | C4-C3-C5 | 3.00 | 120.43 | 115.23 |
| 37 | 39 | 304 | CLA | C4C-C3C-C2C | -3.00 | 102.53 | 106.89 |
| 48 | 14 | 316 | A86 | C3-C2-C1 | -3.00 | 123.08 | 127.28 |
| 37 | C | 511 | CLA | CHC-C1C-C2C | -3.00 | 118.43 | 126.95 |
| 48 | 31 | 315 | A86 | C36-C31-C32 | -3.00 | 116.72 | 119.70 |
| 37 | W | 102 | CLA | C4C-C3C-C2C | -3.00 | 102.53 | 106.89 |
| 47 | 38 | 210 | KC1 | C4C-C3C-C2C | -3.00 | 102.53 | 106.89 |
| 37 | c | 507 | CLA | CHC-C1C-C2C | -3.00 | 118.44 | 126.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 14 | 316 | A86 | C21-C20-C15 | -3.00 | 113.68 | 123.35 |
| 48 | 12 | 214 | A86 | C36-C31-C32 | -2.99 | 116.72 | 119.70 |
| 37 | 21 | 205 | CLA | CAA-C2A-C3A | -2.99 | 104.91 | 113.00 |
| 48 | 17 | 312 | A86 | C21-C20-C15 | -2.99 | 113.68 | 123.35 |
| 48 | 37 | 311 | A86 | C21-C20-C15 | -2.99 | 113.68 | 123.35 |
| 37 | 15 | 301 | CLA | CMB-C2B-C1B | 2.99 | 129.98 | 125.42 |
| 37 | 32 | 202 | CLA | CHC-C1C-C2C | -2.99 | 118.44 | 126.95 |
| 37 | 18 | 208 | CLA | C4B-C3B-C2B | -2.99 | 103.58 | 107.30 |
| 37 | c | 513 | CLA | C4C-C3C-C2C | -2.99 | 102.53 | 106.89 |
| 37 | 20 | 308 | CLA | C4C-C3C-C2C | -2.99 | 102.53 | 106.89 |
| 37 | 39 | 307 | CLA | CMB-C2B-C1B | 2.99 | 129.98 | 125.42 |
| 47 | 12 | 208 | KC1 | CMB-C2B-C1B | 2.99 | 130.00 | 124.73 |
| 37 | 33 | 310 | CLA | CAA-C2A-C3A | -2.99 | 104.91 | 113.00 |
| 37 | 31 | 301 | CLA | C4C-C3C-C2C | -2.99 | 102.53 | 106.89 |
| 37 | 14 | 310 | CLA | C4B-C3B-C2B | -2.99 | 103.58 | 107.30 |
| 37 | 32 | 213 | CLA | CHD-C4C-NC | 2.99 | 128.87 | 124.23 |
| 47 | 16 | 308 | KC1 | CHD-C1D-ND | -2.99 | 119.56 | 124.05 |
| 37 | C | 505 | CLA | CHD-C4C-NC | 2.99 | 128.87 | 124.23 |
| 37 | c | 505 | CLA | CHC-C1C-C2C | -2.99 | 118.45 | 126.95 |
| 37 | 34 | 310 | CLA | C4B-C3B-C2B | -2.99 | 103.58 | 107.30 |
| 37 | 35 | 307 | CLA | C4B-C3B-C2B | -2.99 | 103.58 | 107.30 |
| 48 | 37 | 312 | A86 | C7-C6-C8 | 2.99 | 122.66 | 118.09 |
| 47 | 11 | 302 | KC1 | CHD-C1D-ND | -2.99 | 119.56 | 124.05 |
| 37 | B | 508 | CLA | CHC-C1C-C2C | -2.99 | 118.45 | 126.95 |
| 48 | 13 | 314 | A86 | C25-C24-C1 | -2.99 | 118.17 | 126.36 |
| 37 | 12 | 212 | CLA | C4C-C3C-C2C | -2.99 | 102.54 | 106.89 |
| 47 | 13 | 304 | KC1 | CHD-C1D-ND | -2.99 | 119.56 | 124.05 |
| 37 | 13 | 301 | CLA | CMB-C2B-C1B | 2.99 | 129.97 | 125.42 |
| 37 | C | 506 | CLA | C4C-C3C-C2C | -2.99 | 102.54 | 106.89 |
| 37 | 39 | 305 | CLA | C3B-C4B-NB | 2.99 | 113.20 | 110.53 |
| 37 | 18 | 201 | CLA | C1C-C2C-C3C | -2.99 | 103.84 | 106.98 |
| 48 | 35 | 315 | A86 | C36-C31-C32 | -2.99 | 116.73 | 119.70 |
| 48 | 12 | 216 | A86 | C41-C32-C31 | -2.99 | 107.80 | 110.47 |
| 37 | 11 | 308 | CLA | CHC-C1C-C2C | -2.99 | 118.46 | 126.95 |
| 37 | C | 507 | CLA | C4C-C3C-C2C | -2.99 | 102.54 | 106.89 |
| 37 | 19 | 305 | CLA | C4-C3-C5 | 2.99 | 119.64 | 116.13 |
| 48 | 15 | 316 | A86 | C40-C32-C31 | 2.99 | 113.14 | 110.47 |
| 37 | 11 | 307 | CLA | O2D-CGD-O1D | -2.99 | 118.03 | 123.85 |
| 48 | 16 | 311 | A86 | C7-C6-C8 | 2.99 | 122.65 | 118.09 |
| 37 | 18 | 211 | CLA | C4B-C3B-C2B | -2.99 | 103.59 | 107.30 |
| 37 | c | 511 | CLA | C1-C2-C3 | -2.99 | 121.31 | 126.20 |
| 48 | 17 | 311 | A86 | C28-C27-C26 | 2.99 | 127.65 | 122.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 504 | CLA | CMB-C2B-C1B | 2.99 | 129.97 | 125.42 |
| 37 | C | 505 | CLA | C3B-C4B-NB | 2.99 | 113.19 | 110.53 |
| 37 | 39 | 303 | CLA | CHD-C4C-NC | 2.99 | 128.86 | 124.23 |
| 37 | 38 | 208 | CLA | C4B-C3B-C2B | -2.98 | 103.59 | 107.30 |
| 37 | 32 | 206 | CLA | CHC-C1C-C2C | -2.98 | 118.47 | 126.95 |
| 47 | 36 | 308 | KC1 | O2D-CGD-O1D | -2.98 | 118.04 | 123.85 |
| 48 | 18 | 212 | A86 | C25-C24-C1 | -2.98 | 118.19 | 126.36 |
| 48 | 17 | 320 | A86 | C7-C6-C8 | 2.98 | 122.64 | 118.09 |
| 37 | 38 | 206 | CLA | CHC-C1C-C2C | -2.98 | 118.47 | 126.95 |
| 48 | 18 | 213 | A86 | C35-C34-C33 | 2.98 | 115.24 | 109.89 |
| 48 | 17 | 313 | A86 | C4-C5-C6 | -2.98 | 123.10 | 127.28 |
| 37 | b | 502 | CLA | CHD-C4C-NC | 2.98 | 128.85 | 124.23 |
| 37 | 20 | 306 | CLA | C1C-C2C-C3C | -2.98 | 103.84 | 106.98 |
| 48 | 36 | 310 | A86 | C35-C34-C33 | 2.98 | 115.24 | 109.89 |
| 48 | 33 | 314 | A86 | C25-C24-C1 | -2.98 | 118.19 | 126.36 |
| 37 | C | 507 | CLA | CHD-C4C-NC | 2.98 | 128.85 | 124.23 |
| 48 | 16 | 310 | A86 | C35-C34-C33 | 2.98 | 115.24 | 109.89 |
| 37 | b | 508 | CLA | CHC-C1C-C2C | -2.98 | 118.48 | 126.95 |
| 37 | z | 101 | CLA | C4C-C3C-C2C | -2.98 | 102.55 | 106.89 |
| 40 | 17 | 301 | SQD | C4-C3-C2 | 2.98 | 116.06 | 110.83 |
| 47 | 32 | 212 | KC1 | CHD-C4C-NC | 2.98 | 128.80 | 124.31 |
| 37 | Z | 102 | CLA | C3B-C4B-NB | 2.98 | 113.19 | 110.53 |
| 37 | C | 501 | CLA | O2D-CGD-O1D | -2.98 | 118.05 | 123.85 |
| 37 | c | 501 | CLA | O2D-CGD-O1D | -2.98 | 118.05 | 123.85 |
| 44 | h | 102 | DGD | C1D-C2D-C3D | -2.98 | 103.74 | 110.01 |
| 48 | 17 | 315 | A86 | C36-C31-C32 | -2.98 | 116.74 | 119.70 |
| 37 | b | 507 | CLA | C4A-NA-C1A | -2.98 | 105.32 | 106.68 |
| 37 | 11 | 303 | CLA | C1-O2A-CGA | 2.98 | 123.86 | 116.65 |
| 37 | 31 | 304 | CLA | C1-O2A-CGA | 2.98 | 123.86 | 116.65 |
| 37 | c | 505 | CLA | C3B-C4B-NB | 2.98 | 113.19 | 110.53 |
| 37 | 38 | 208 | CLA | CHC-C1C-C2C | -2.98 | 118.48 | 126.95 |
| 48 | 15 | 314 | A86 | C3-C4-C5 | -2.98 | 117.43 | 123.52 |
| 37 | 41 | 205 | CLA | CAA-C2A-C3A | -2.98 | 104.95 | 113.00 |
| 48 | 35 | 313 | A86 | C36-C31-C32 | -2.98 | 116.74 | 119.70 |
| 48 | 32 | 218 | A86 | C21-C20-C15 | -2.98 | 113.74 | 123.35 |
| 37 | 34 | 307 | CLA | C4-C3-C5 | 2.98 | 120.39 | 115.23 |
| 47 | 21 | 203 | KC1 | O2D-CGD-O1D | -2.98 | 118.06 | 123.85 |
| 37 | C | 504 | CLA | CMB-C2B-C1B | 2.98 | 129.95 | 125.42 |
| 37 | C | 513 | CLA | C4C-C3C-C2C | -2.98 | 102.56 | 106.89 |
| 48 | 18 | 213 | A86 | C21-C20-C15 | -2.98 | 113.75 | 123.35 |
| 48 | 41 | 214 | A86 | C12-C11-C13 | 2.98 | 120.82 | 116.00 |
| 37 | A | 405 | CLA | CMB-C2B-C1B | 2.98 | 129.95 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 39 | 308 | KC1 | CHD-C1D-ND | -2.98 | 119.59 | 124.05 |
| 37 | a | 407 | CLA | CHD-C4C-NC | 2.97 | 128.84 | 124.23 |
| 48 | 37 | 314 | A86 | C36-C31-C32 | -2.97 | 116.74 | 119.70 |
| 37 | 32 | 208 | CLA | CHD-C4C-NC | 2.97 | 128.84 | 124.23 |
| 48 | 35 | 314 | A86 | C7-C6-C8 | 2.97 | 122.63 | 118.09 |
| 37 | 12 | 205 | CLA | CHD-C4C-NC | 2.97 | 128.84 | 124.23 |
| 47 | 12 | 208 | KC1 | CAA-CBA-CGA | -2.97 | 111.93 | 127.05 |
| 48 | 34 | 316 | A86 | C3-C2-C1 | -2.97 | 123.11 | 127.28 |
| 37 | D | 406 | CLA | CHD-C4C-NC | 2.97 | 128.84 | 124.23 |
| 37 | 18 | 201 | CLA | CHD-C4C-NC | 2.97 | 128.84 | 124.23 |
| 50 | 39 | 312 | DD6 | C14-C13-C11 | -2.97 | 120.92 | 125.53 |
| 48 | 38 | 213 | A86 | C35-C34-C33 | 2.97 | 115.23 | 109.89 |
| 37 | 35 | 301 | CLA | CMB-C2B-C1B | 2.97 | 129.94 | 125.42 |
| 37 | A | 405 | CLA | CHD-C4C-NC | 2.97 | 128.84 | 124.23 |
| 37 | 32 | 213 | CLA | C4C-C3C-C2C | -2.97 | 102.56 | 106.89 |
| 47 | 38 | 207 | KC1 | C4C-C3C-C2C | -2.97 | 102.56 | 106.89 |
| 48 | 37 | 314 | A86 | C41-C32-C31 | -2.97 | 107.81 | 110.47 |
| 47 | 32 | 209 | KC1 | CAA-CBA-CGA | -2.97 | 111.94 | 127.05 |
| 37 | b | 507 | CLA | CAA-C2A-C3A | -2.97 | 104.97 | 113.00 |
| 48 | 31 | 311 | A86 | C10-C9-C8 | -2.97 | 114.59 | 123.20 |
| 47 | 31 | 307 | KC1 | CMB-C2B-C1B | 2.97 | 129.96 | 124.73 |
| 37 | 40 | 210 | CLA | C4C-C3C-C2C | -2.97 | 102.57 | 106.89 |
| 47 | 16 | 308 | KC1 | C4C-C3C-C2C | -2.97 | 102.57 | 106.89 |
| 37 | C | 505 | CLA | CHC-C1C-C2C | -2.97 | 118.50 | 126.95 |
| 47 | 31 | 305 | KC1 | CAC-C3C-C4C | 2.97 | 128.66 | 124.79 |
| 37 | 15 | 303 | CLA | C1-C2-C3 | -2.97 | 121.33 | 126.20 |
| 39 | 5 | 101 | BCR | C11-C10-C9 | -2.97 | 123.11 | 127.28 |
| 37 | 33 | 307 | CLA | C4-C3-C5 | 2.97 | 120.38 | 115.23 |
| 37 | C | 510 | CLA | CHD-C4C-NC | 2.97 | 128.84 | 124.23 |
| 37 | c | 507 | CLA | CHD-C4C-NC | 2.97 | 128.84 | 124.23 |
| 37 | 11 | 305 | CLA | CAC-C3C-C4C | 2.97 | 128.65 | 124.79 |
| 47 | 36 | 308 | KC1 | CAC-C3C-C4C | 2.97 | 128.65 | 124.79 |
| 41 | 17 | 317 | LMG | C1-C2-C3 | -2.97 | 103.76 | 110.01 |
| 44 | H | 102 | DGD | C1D-C2D-C3D | -2.97 | 103.76 | 110.01 |
| 37 | D | 402 | CLA | CHC-C1C-C2C | -2.97 | 118.51 | 126.95 |
| 37 | 16 | 301 | CLA | C1C-C2C-C3C | -2.97 | 103.86 | 106.98 |
| 37 | 38 | 211 | CLA | C4C-C3C-C2C | -2.97 | 102.57 | 106.89 |
| 37 | b | 509 | CLA | CBC-CAC-C3C | -2.97 | 104.37 | 112.42 |
| 37 | a | 404 | CLA | C3C-C4C-NC | 2.97 | 114.23 | 110.43 |
| 37 | 13 | 301 | CLA | CHD-C4C-NC | 2.97 | 128.83 | 124.23 |
| 48 | 35 | 319 | A86 | C4-C3-C2 | -2.97 | 117.45 | 123.52 |
| 37 | 19 | 310 | CLA | C1-C2-C3 | -2.97 | 121.34 | 126.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 503 | CLA | C4C-C3C-C2C | -2.97 | 102.57 | 106.89 |
| 37 | d | 403 | CLA | C4C-C3C-C2C | -2.97 | 102.57 | 106.89 |
| 47 | 14 | 304 | KC1 | CAA-CBA-CGA | -2.97 | 111.96 | 127.05 |
| 37 | 14 | 305 | CLA | C4B-C3B-C2B | -2.97 | 103.61 | 107.30 |
| 37 | 32 | 206 | CLA | CHD-C4C-NC | 2.97 | 128.83 | 124.23 |
| 48 | 13 | 312 | A86 | C4-C5-C6 | -2.97 | 123.12 | 127.28 |
| 40 | 36 | 315 | SQD | C4-C3-C2 | 2.97 | 116.04 | 110.83 |
| 37 | 18 | 202 | CLA | CBC-CAC-C3C | -2.97 | 104.38 | 112.42 |
| 48 | 32 | 215 | A86 | C36-C31-C32 | -2.97 | 116.75 | 119.70 |
| 37 | 14 | 310 | CLA | C3C-C4C-NC | 2.97 | 114.23 | 110.43 |
| 37 | 12 | 203 | CLA | C3B-C4B-NB | 2.97 | 113.18 | 110.53 |
| 37 | B | 509 | CLA | CBC-CAC-C3C | -2.97 | 104.38 | 112.42 |
| 47 | 15 | 302 | KC1 | C4B-C3B-C2B | -2.96 | 104.24 | 106.81 |
| 37 | 38 | 201 | CLA | CAC-C3C-C4C | 2.96 | 128.65 | 124.79 |
| 48 | 39 | 311 | A86 | C41-C32-C31 | -2.96 | 107.82 | 110.47 |
| 47 | 31 | 309 | KC1 | CBC-CAC-C3C | -2.96 | 104.38 | 112.42 |
| 47 | 34 | 304 | KC1 | CAA-CBA-CGA | -2.96 | 111.98 | 127.05 |
| 48 | 14 | 315 | A86 | C36-C31-C32 | -2.96 | 116.75 | 119.70 |
| 37 | 39 | 305 | CLA | C4-C3-C5 | 2.96 | 119.62 | 116.13 |
| 47 | 15 | 302 | KC1 | CAC-C3C-C4C | 2.96 | 128.65 | 124.79 |
| 37 | c | 506 | CLA | C4C-C3C-C2C | -2.96 | 102.58 | 106.89 |
| 48 | 12 | 217 | A86 | C21-C20-C15 | -2.96 | 113.79 | 123.35 |
| 47 | 41 | 203 | KC1 | CHD-C1D-ND | -2.96 | 119.61 | 124.05 |
| 37 | 37 | 306 | CLA | C1-C2-C3 | -2.96 | 121.34 | 126.20 |
| 37 | b | 509 | CLA | CHD-C4C-NC | 2.96 | 128.82 | 124.23 |
| 37 | C | 503 | CLA | C4C-C3C-C2C | -2.96 | 102.58 | 106.89 |
| 37 | 12 | 212 | CLA | CHC-C1C-C2C | -2.96 | 118.53 | 126.95 |
| 37 | 18 | 208 | CLA | CHC-C1C-C2C | -2.96 | 118.53 | 126.95 |
| 48 | 37 | 314 | A86 | C22-C16-C17 | -2.96 | 103.76 | 108.97 |
| 37 | 33 | 301 | CLA | CHD-C4C-NC | 2.96 | 128.82 | 124.23 |
| 37 | 19 | 302 | CLA | CAC-C3C-C4C | 2.96 | 128.64 | 124.79 |
| 47 | 31 | 307 | KC1 | C4B-C3B-C2B | -2.96 | 104.25 | 106.81 |
| 47 | 11 | 309 | KC1 | CBC-CAC-C3C | -2.96 | 104.39 | 112.42 |
| 48 | 15 | 319 | A86 | C4-C3-C2 | -2.96 | 117.46 | 123.52 |
| 37 | 32 | 210 | CLA | C4C-C3C-C2C | -2.96 | 102.58 | 106.89 |
| 37 | 31 | 306 | CLA | CAC-C3C-C4C | 2.96 | 128.64 | 124.79 |
| 47 | 38 | 210 | KC1 | O2D-CGD-O1D | -2.96 | 118.09 | 123.85 |
| 37 | 38 | 203 | CLA | C4-C3-C5 | 2.96 | 120.36 | 115.23 |
| 37 | c | 510 | CLA | CHD-C4C-NC | 2.96 | 128.82 | 124.23 |
| 48 | 11 | 311 | A86 | C10-C9-C8 | -2.96 | 114.63 | 123.20 |
| 37 | 17 | 309 | CLA | CAA-C2A-C1A | -2.96 | 102.28 | 111.97 |
| 47 | 35 | 306 | KC1 | CMB-C2B-C1B | 2.96 | 129.94 | 124.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | C | 517 | DGD | CDB-CCB-CBB | -2.96 | 99.42 | 114.37 |
| 37 | d | 401 | CLA | CHC-C1C-C2C | -2.96 | 118.54 | 126.95 |
| 44 | c | 517 | DGD | CDB-CCB-CBB | -2.96 | 99.42 | 114.37 |
| 37 | 38 | 211 | CLA | C4B-C3B-C2B | -2.96 | 103.62 | 107.30 |
| 48 | 32 | 218 | A86 | C8-C6-C5 | 2.96 | 123.66 | 119.01 |
| 37 | A | 405 | CLA | C4-C3-C5 | 2.96 | 120.36 | 115.23 |
| 37 | 21 | 210 | CLA | C4C-C3C-C2C | -2.96 | 102.59 | 106.89 |
| 37 | a | 407 | CLA | C4-C3-C5 | 2.96 | 120.36 | 115.23 |
| 47 | 11 | 304 | KC1 | CAC-C3C-C4C | 2.96 | 128.63 | 124.79 |
| 37 | 13 | 307 | CLA | C4C-C3C-C2C | -2.96 | 102.59 | 106.89 |
| 37 | 20 | 307 | CLA | C4C-C3C-C2C | -2.96 | 102.59 | 106.89 |
| 47 | 36 | 305 | KC1 | CHD-C1D-ND | -2.96 | 119.62 | 124.05 |
| 37 | 36 | 303 | CLA | C4B-C3B-C2B | -2.95 | 103.63 | 107.30 |
| 50 | 40 | 212 | DD6 | C12-C11-C13 | -2.95 | 113.58 | 118.09 |
| 37 | 41 | 210 | CLA | CAA-C2A-C3A | -2.95 | 105.02 | 113.00 |
| 47 | 38 | 210 | KC1 | CHD-C1D-ND | -2.95 | 119.62 | 124.05 |
| 37 | 20 | 303 | CLA | CAA-C2A-C1A | 2.95 | 121.65 | 111.97 |
| 48 | 15 | 315 | A86 | C41-C32-C31 | -2.95 | 107.83 | 110.47 |
| 47 | 18 | 207 | KC1 | C4C-C3C-C2C | -2.95 | 102.59 | 106.89 |
| 37 | 38 | 208 | CLA | CHD-C4C-NC | 2.95 | 128.81 | 124.23 |
| 37 | C | 512 | CLA | O2A-CGA-CBA | 2.95 | 120.84 | 111.83 |
| 47 | 16 | 305 | KC1 | CHD-C1D-ND | -2.95 | 119.62 | 124.05 |
| 37 | 11 | 305 | CLA | C4C-C3C-C2C | -2.95 | 102.59 | 106.89 |
| 37 | 12 | 207 | CLA | C4C-C3C-C2C | -2.95 | 102.59 | 106.89 |
| 37 | 11 | 301 | CLA | CMB-C2B-C1B | 2.95 | 129.91 | 125.42 |
| 37 | 31 | 302 | CLA | CMB-C2B-C1B | 2.95 | 129.91 | 125.42 |
| 37 | B | 512 | CLA | C4B-C3B-C2B | -2.95 | 103.63 | 107.30 |
| 37 | 16 | 303 | CLA | C4B-C3B-C2B | -2.95 | 103.63 | 107.30 |
| 45 | d | 406 | PL9 | C7-C8-C9 | -2.95 | 121.75 | 126.83 |
| 37 | B | 508 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 37 | 41 | 210 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 47 | 36 | 308 | KC1 | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 47 | 41 | 203 | KC1 | O2D-CGD-O1D | -2.95 | 118.10 | 123.85 |
| 37 | 18 | 203 | CLA | CAC-C3C-C4C | 2.95 | 128.63 | 124.79 |
| 37 | b | 510 | CLA | C4B-C3B-C2B | -2.95 | 103.63 | 107.30 |
| 50 | 20 | 310 | DD6 | C12-C11-C13 | -2.95 | 113.58 | 118.09 |
| 37 | 40 | 209 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 48 | 21 | 214 | A86 | C12-C11-C13 | 2.95 | 120.78 | 116.00 |
| 37 | 38 | 201 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 37 | 18 | 203 | CLA | CBA-CAA-C2A | -2.95 | 105.02 | 113.79 |
| 37 | 32 | 213 | CLA | CHC-C1C-C2C | -2.95 | 118.57 | 126.95 |
| 37 | 41 | 208 | CLA | C4B-C3B-C2B | -2.95 | 103.64 | 107.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 505 | CLA | CMC-C2C-C1C | 2.95 | 129.64 | 125.03 |
| 47 | 17 | 308 | KC1 | CMA-C3A-C2A | -2.95 | 121.29 | 128.43 |
| 47 | 37 | 307 | KC1 | CMA-C3A-C2A | -2.95 | 121.29 | 128.43 |
| 37 | 33 | 307 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 37 | 34 | 305 | CLA | C4B-C3B-C2B | -2.95 | 103.64 | 107.30 |
| 47 | 11 | 306 | KC1 | C4B-C3B-C2B | -2.95 | 104.26 | 106.81 |
| 37 | 31 | 308 | CLA | C4-C3-C5 | 2.95 | 120.34 | 115.23 |
| 37 | 40 | 205 | CLA | CAA-C2A-C1A | 2.95 | 121.63 | 111.97 |
| 37 | Z | 101 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 47 | 33 | 302 | KC1 | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 47 | 33 | 304 | KC1 | C4C-C3C-C2C | -2.95 | 102.60 | 106.89 |
| 37 | b | 512 | CLA | C4B-C3B-C2B | -2.95 | 103.64 | 107.30 |
| 37 | 39 | 305 | CLA | CHB-C4A-NA | 2.95 | 128.65 | 124.40 |
| 37 | B | 509 | CLA | CHD-C4C-NC | 2.95 | 128.80 | 124.23 |
| 47 | 13 | 302 | KC1 | C4C-C3C-C2C | -2.94 | 102.61 | 106.89 |
| 37 | 18 | 209 | CLA | CHC-C1C-C2C | -2.94 | 118.58 | 126.95 |
| 47 | 41 | 203 | KC1 | CAC-C3C-C4C | 2.94 | 128.62 | 124.79 |
| 48 | 14 | 315 | A86 | C7-C6-C8 | 2.94 | 122.59 | 118.09 |
| 37 | B | 507 | CLA | CAA-C2A-C3A | -2.94 | 105.04 | 113.00 |
| 41 | 37 | 316 | LMG | C1-C2-C3 | -2.94 | 103.82 | 110.01 |
| 37 | 36 | 309 | CLA | CHC-C1C-C2C | -2.94 | 118.58 | 126.95 |
| 37 | 39 | 302 | CLA | CAC-C3C-C4C | 2.94 | 128.62 | 124.79 |
| 37 | 33 | 301 | CLA | CMB-C2B-C1B | 2.94 | 129.90 | 125.42 |
| 47 | 19 | 308 | KC1 | C4C-C3C-C2C | -2.94 | 102.61 | 106.89 |
| 37 | 41 | 208 | CLA | CAA-C2A-C3A | -2.94 | 105.05 | 113.00 |
| 37 | 13 | 305 | CLA | CHC-C1C-C2C | -2.94 | 118.58 | 126.95 |
| 48 | 18 | 212 | A86 | C10-C9-C8 | -2.94 | 114.67 | 123.20 |
| 37 | 19 | 305 | CLA | C3B-C4B-NB | 2.94 | 113.16 | 110.53 |
| 37 | 12 | 207 | CLA | CAA-C2A-C1A | -2.94 | 102.33 | 111.97 |
| 37 | 21 | 210 | CLA | CAA-C2A-C3A | -2.94 | 105.05 | 113.00 |
| 37 | d | 404 | CLA | C4B-C3B-C2B | -2.94 | 103.64 | 107.30 |
| 47 | 13 | 306 | KC1 | CAA-CBA-CGA | -2.94 | 112.09 | 127.05 |
| 37 | 12 | 209 | CLA | C4C-C3C-C2C | -2.94 | 102.61 | 106.89 |
| 37 | 33 | 305 | CLA | CHC-C1C-C2C | -2.94 | 118.59 | 126.95 |
| 37 | 38 | 204 | CLA | C4C-C3C-C2C | -2.94 | 102.61 | 106.89 |
| 48 | 31 | 314 | A86 | C21-C20-C15 | -2.94 | 113.86 | 123.35 |
| 48 | 38 | 212 | A86 | C7-C6-C8 | 2.94 | 122.58 | 118.09 |
| 37 | d | 404 | CLA | CAC-C3C-C4C | 2.94 | 128.61 | 124.79 |
| 47 | 36 | 304 | KC1 | CHD-C4C-NC | 2.94 | 128.74 | 124.31 |
| 48 | 12 | 215 | A86 | C36-C31-C32 | -2.94 | 116.78 | 119.70 |
| 37 | 38 | 209 | CLA | CHC-C1C-C2C | -2.94 | 118.60 | 126.95 |
| 37 | 18 | 208 | CLA | CHD-C4C-NC | 2.94 | 128.79 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 210 | CLA | C4C-C3C-C2C | -2.94 | 102.61 | 106.89 |
| 37 | 21 | 208 | CLA | CAA-C2A-C3A | -2.94 | 105.06 | 113.00 |
| 50 | 19 | 312 | DD6 | C14-C13-C11 | -2.94 | 120.97 | 125.53 |
| 47 | 15 | 309 | KC1 | C4C-C3C-C2C | -2.94 | 102.62 | 106.89 |
| 48 | 32 | 216 | A86 | C36-C31-C32 | -2.94 | 116.78 | 119.70 |
| 47 | 16 | 304 | KC1 | CHD-C4C-NC | 2.94 | 128.73 | 124.31 |
| 48 | 34 | 315 | A86 | C7-C6-C8 | 2.94 | 122.57 | 118.09 |
| 37 | 32 | 211 | CLA | C4C-C3C-C2C | -2.94 | 102.62 | 106.89 |
| 37 | 37 | 306 | CLA | CHC-C1C-C2C | -2.94 | 118.61 | 126.95 |
| 37 | 16 | 309 | CLA | CHC-C1C-C2C | -2.94 | 118.61 | 126.95 |
| 50 | 40 | 212 | DD6 | C37-C36-C35 | -2.94 | 109.02 | 114.42 |
| 37 | D | 405 | CLA | C4C-C3C-C2C | -2.93 | 102.62 | 106.89 |
| 37 | b | 508 | CLA | C4C-C3C-C2C | -2.93 | 102.62 | 106.89 |
| 50 | 20 | 312 | DD6 | C19-C18-C17 | 2.93 | 116.28 | 110.79 |
| 37 | 18 | 203 | CLA | C4C-C3C-C2C | -2.93 | 102.62 | 106.89 |
| 48 | 13 | 315 | A86 | C21-C20-C15 | -2.93 | 113.88 | 123.35 |
| 48 | 15 | 315 | A86 | C4-C3-C2 | -2.93 | 117.52 | 123.52 |
| 37 | c | 512 | CLA | C4B-C3B-C2B | -2.93 | 103.66 | 107.30 |
| 37 | 11 | 310 | CLA | C4-C3-C5 | 2.93 | 119.58 | 116.13 |
| 48 | 33 | 311 | A86 | C25-C24-C1 | -2.93 | 118.32 | 126.36 |
| 37 | 36 | 303 | CLA | C1-C2-C3 | -2.93 | 121.39 | 126.20 |
| 50 | 40 | 214 | DD6 | C19-C18-C17 | 2.93 | 116.27 | 110.79 |
| 47 | 33 | 306 | KC1 | CAA-CBA-CGA | -2.93 | 112.14 | 127.05 |
| 37 | c | 512 | CLA | O2A-CGA-CBA | 2.93 | 120.78 | 111.83 |
| 37 | 32 | 208 | CLA | C4C-C3C-C2C | -2.93 | 102.62 | 106.89 |
| 37 | 12 | 207 | CLA | CHD-C4C-NC | 2.93 | 128.78 | 124.23 |
| 37 | 19 | 305 | CLA | CHB-C4A-NA | 2.93 | 128.63 | 124.40 |
| 37 | 32 | 208 | CLA | CAA-C2A-C1A | -2.93 | 102.37 | 111.97 |
| 47 | 36 | 304 | KC1 | CAC-C3C-C4C | 2.93 | 128.60 | 124.79 |
| 37 | Z | 101 | CLA | O2A-CGA-CBA | 2.93 | 120.77 | 111.83 |
| 48 | 35 | 314 | A86 | C3-C4-C5 | -2.93 | 117.52 | 123.52 |
| 48 | 12 | 217 | A86 | C8-C6-C5 | 2.93 | 123.62 | 119.01 |
| 37 | 17 | 304 | CLA | CAC-C3C-C4C | 2.93 | 128.60 | 124.79 |
| 37 | 37 | 303 | CLA | CAC-C3C-C4C | 2.93 | 128.60 | 124.79 |
| 37 | 31 | 301 | CLA | CHC-C1C-C2C | -2.93 | 118.62 | 126.95 |
| 48 | 11 | 314 | A86 | C21-C20-C15 | -2.93 | 113.89 | 123.35 |
| 37 | D | 406 | CLA | CAC-C3C-C4C | 2.93 | 128.60 | 124.79 |
| 47 | 21 | 207 | KC1 | C4C-C3C-C2C | -2.93 | 102.63 | 106.89 |
| 37 | b | 505 | CLA | CMC-C2C-C1C | 2.93 | 129.61 | 125.03 |
| 48 | 15 | 312 | A86 | C34-O4-C38 | -2.93 | 112.67 | 117.85 |
| 37 | B | 510 | CLA | C4B-C3B-C2B | -2.93 | 103.66 | 107.30 |
| 37 | 20 | 306 | CLA | CHD-C4C-NC | 2.93 | 128.77 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 306 | CLA | C4C-C3C-C2C | -2.93 | 102.63 | 106.89 |
| 48 | 17 | 310 | A86 | C23-C16-C22 | -2.93 | 103.12 | 107.37 |
| 37 | 21 | 208 | CLA | C4B-C3B-C2B | -2.93 | 103.66 | 107.30 |
| 48 | 33 | 315 | A86 | C21-C20-C15 | -2.93 | 113.90 | 123.35 |
| 37 | B | 509 | CLA | O2A-CGA-CBA | 2.93 | 120.76 | 111.83 |
| 43 | 41 | 201 | LHG | O8-C23-C24 | 2.93 | 120.76 | 111.83 |
| 37 | c | 513 | CLA | C3B-C4B-NB | 2.93 | 113.14 | 110.53 |
| 50 | 20 | 310 | DD6 | C37-C36-C35 | -2.93 | 109.04 | 114.42 |
| 37 | C | 513 | CLA | C3B-C4B-NB | 2.93 | 113.14 | 110.53 |
| 37 | z | 102 | CLA | C3B-C4B-NB | 2.93 | 113.14 | 110.53 |
| 37 | 40 | 208 | CLA | CHD-C4C-NC | 2.93 | 128.77 | 124.23 |
| 37 | 19 | 307 | CLA | CMB-C2B-C1B | 2.93 | 129.87 | 125.42 |
| 47 | 21 | 203 | KC1 | CAC-C3C-C4C | 2.93 | 128.60 | 124.79 |
| 48 | 11 | 314 | A86 | C34-O4-C38 | -2.92 | 112.68 | 117.85 |
| 47 | 13 | 304 | KC1 | C4C-C3C-C2C | -2.92 | 102.63 | 106.89 |
| 37 | d | 401 | CLA | C3B-C4B-NB | 2.92 | 113.14 | 110.53 |
| 37 | 17 | 302 | CLA | C3B-C4B-NB | 2.92 | 113.14 | 110.53 |
| 37 | 34 | 310 | CLA | CHD-C4C-NC | 2.92 | 128.77 | 124.23 |
| 37 | B | 511 | CLA | O2A-CGA-CBA | 2.92 | 120.75 | 111.83 |
| 47 | 38 | 207 | KC1 | CMB-C2B-C1B | 2.92 | 129.88 | 124.73 |
| 47 | 21 | 203 | KC1 | CHD-C1D-ND | -2.92 | 119.66 | 124.05 |
| 48 | 17 | 315 | A86 | C22-C16-C17 | -2.92 | 103.83 | 108.97 |
| 47 | 37 | 307 | KC1 | C4C-C3C-C2C | -2.92 | 102.64 | 106.89 |
| 48 | 17 | 313 | A86 | C25-C24-C1 | -2.92 | 118.35 | 126.36 |
| 37 | 13 | 301 | CLA | C3B-C4B-NB | 2.92 | 113.14 | 110.53 |
| 37 | 13 | 307 | CLA | C4-C3-C5 | 2.92 | 120.30 | 115.23 |
| 48 | 12 | 214 | A86 | C10-C9-C8 | -2.92 | 114.73 | 123.20 |
| 37 | D | 406 | CLA | C4B-C3B-C2B | -2.92 | 103.67 | 107.30 |
| 37 | D | 401 | CLA | C3C-C4C-NC | 2.92 | 114.17 | 110.43 |
| 48 | 32 | 215 | A86 | C10-C9-C8 | -2.92 | 114.73 | 123.20 |
| 37 | 15 | 310 | CLA | C4C-C3C-C2C | -2.92 | 102.64 | 106.89 |
| 37 | a | 403 | CLA | C4C-C3C-C2C | -2.92 | 102.64 | 106.89 |
| 47 | 36 | 308 | KC1 | CHD-C1D-ND | -2.92 | 119.67 | 124.05 |
| 37 | c | 512 | CLA | O2D-CGD-O1D | -2.92 | 118.17 | 123.85 |
| 37 | 37 | 308 | CLA | O2A-CGA-CBA | 2.92 | 120.74 | 111.83 |
| 37 | 34 | 305 | CLA | CHD-C4C-NC | 2.92 | 128.76 | 124.23 |
| 37 | 14 | 302 | CLA | C4C-C3C-C2C | -2.92 | 102.64 | 106.89 |
| 48 | 12 | 220 | A86 | C8-C6-C5 | -2.92 | 114.42 | 119.01 |
| 48 | 32 | 221 | A86 | C3-C4-C5 | -2.92 | 117.55 | 123.52 |
| 45 | D | 404 | PL9 | C40-C39-C41 | 2.92 | 120.29 | 115.23 |
| 48 | 40 | 201 | A86 | C25-C26-C27 | 2.92 | 131.37 | 127.28 |
| 48 | 32 | 217 | A86 | C36-C31-C32 | -2.92 | 116.80 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 17 | 307 | CLA | CHC-C1C-C2C | -2.92 | 118.66 | 126.95 |
| 37 | c | 508 | CLA | CAC-C3C-C4C | 2.92 | 128.59 | 124.79 |
| 37 | C | 512 | CLA | C4B-C3B-C2B | -2.92 | 103.67 | 107.30 |
| 37 | 21 | 205 | CLA | C4B-C3B-C2B | -2.92 | 103.67 | 107.30 |
| 48 | 15 | 319 | A86 | C41-C32-C31 | -2.92 | 107.86 | 110.47 |
| 48 | 19 | 311 | A86 | C41-C32-C31 | -2.92 | 107.86 | 110.47 |
| 37 | C | 509 | CLA | CAC-C3C-C4C | 2.92 | 128.59 | 124.79 |
| 37 | 38 | 203 | CLA | C4C-C3C-C2C | -2.92 | 102.65 | 106.89 |
| 37 | 31 | 306 | CLA | CHB-C4A-NA | 2.92 | 128.61 | 124.40 |
| 37 | 38 | 209 | CLA | C4C-C3C-C2C | -2.92 | 102.65 | 106.89 |
| 37 | 16 | 303 | CLA | C1-C2-C3 | -2.92 | 121.42 | 126.20 |
| 48 | 35 | 315 | A86 | C4-C3-C2 | -2.92 | 117.55 | 123.52 |
| 47 | 37 | 305 | KC1 | CBA-CAA-C2A | -2.92 | 113.75 | 125.45 |
| 37 | 19 | 304 | CLA | C3B-C4B-NB | 2.91 | 113.13 | 110.53 |
| 37 | 39 | 304 | CLA | C3B-C4B-NB | 2.91 | 113.13 | 110.53 |
| 47 | 39 | 308 | KC1 | C4C-C3C-C2C | -2.91 | 102.65 | 106.89 |
| 37 | z | 101 | CLA | O2A-CGA-CBA | 2.91 | 120.72 | 111.83 |
| 37 | 18 | 203 | CLA | C4-C3-C5 | 2.91 | 120.29 | 115.23 |
| 37 | A | 403 | CLA | C4C-C3C-C2C | -2.91 | 102.65 | 106.89 |
| 37 | d | 403 | CLA | CAC-C3C-C4C | 2.91 | 128.58 | 124.79 |
| 39 | A | 406 | BCR | C15-C16-C17 | -2.91 | 117.56 | 123.52 |
| 48 | 13 | 311 | A86 | C25-C24-C1 | -2.91 | 118.38 | 126.36 |
| 48 | 18 | 215 | A86 | C12-C11-C13 | 2.91 | 120.72 | 116.00 |
| 37 | 34 | 302 | CLA | C4C-C3C-C2C | -2.91 | 102.65 | 106.89 |
| 47 | 12 | 208 | KC1 | C4C-C3C-C2C | -2.91 | 102.65 | 106.89 |
| 47 | 32 | 209 | KC1 | C4C-C3C-C2C | -2.91 | 102.65 | 106.89 |
| 47 | 37 | 302 | KC1 | CAC-C3C-C4C | 2.91 | 128.58 | 124.79 |
| 37 | W | 102 | CLA | CHC-C1C-C2C | -2.91 | 118.67 | 126.95 |
| 37 | b | 505 | CLA | C4C-C3C-C2C | -2.91 | 102.65 | 106.89 |
| 37 | b | 510 | CLA | CHC-C1C-C2C | -2.91 | 118.67 | 126.95 |
| 48 | 37 | 312 | A86 | C25-C24-C1 | -2.91 | 118.38 | 126.36 |
| 37 | 21 | 206 | CLA | C4B-C3B-C2B | -2.91 | 103.68 | 107.30 |
| 37 | 31 | 308 | CLA | C4C-C3C-C2C | -2.91 | 102.65 | 106.89 |
| 37 | b | 511 | CLA | O2A-CGA-CBA | 2.91 | 120.71 | 111.83 |
| 37 | 14 | 307 | CLA | C4C-C3C-C2C | -2.91 | 102.66 | 106.89 |
| 48 | 38 | 212 | A86 | C25-C26-C27 | -2.91 | 123.20 | 127.28 |
| 37 | 19 | 302 | CLA | CGD-CBD-CAD | -2.91 | 101.43 | 110.85 |
| 39 | a | 408 | BCR | C15-C16-C17 | -2.91 | 117.57 | 123.52 |
| 37 | 41 | 204 | CLA | CHD-C4C-NC | 2.91 | 128.74 | 124.23 |
| 37 | 33 | 301 | CLA | CHC-C1C-C2C | -2.91 | 118.68 | 126.95 |
| 37 | 21 | 204 | CLA | CHD-C4C-NC | 2.91 | 128.74 | 124.23 |
| 37 | 11 | 305 | CLA | CHB-C4A-NA | 2.91 | 128.59 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 14 | 302 | CLA | CHD-C4C-NC | 2.91 | 128.74 | 124.23 |
| 37 | B | 501 | CLA | CMB-C2B-C1B | 2.91 | 129.84 | 125.42 |
| 37 | 15 | 301 | CLA | CMC-C2C-C1C | 2.91 | 129.57 | 125.03 |
| 37 | 31 | 310 | CLA | C4-C3-C5 | 2.91 | 119.55 | 116.13 |
| 37 | b | 510 | CLA | CHD-C4C-NC | 2.91 | 128.74 | 124.23 |
| 47 | 35 | 309 | KC1 | C4C-C3C-C2C | -2.90 | 102.66 | 106.89 |
| 37 | b | 514 | CLA | CHC-C1C-C2C | -2.90 | 118.69 | 126.95 |
| 37 | 38 | 202 | CLA | CMC-C2C-C1C | 2.90 | 129.57 | 125.03 |
| 47 | 17 | 306 | KC1 | CBA-CAA-C2A | -2.90 | 113.80 | 125.45 |
| 37 | 12 | 205 | CLA | CHC-C1C-C2C | -2.90 | 118.69 | 126.95 |
| 48 | 41 | 214 | A86 | C41-C32-C31 | -2.90 | 107.87 | 110.47 |
| 37 | 35 | 301 | CLA | C1-C2-C3 | -2.90 | 121.44 | 126.20 |
| 37 | 34 | 307 | CLA | C4C-C3C-C2C | -2.90 | 102.67 | 106.89 |
| 37 | b | 509 | CLA | O2A-CGA-CBA | 2.90 | 120.69 | 111.83 |
| 48 | 32 | 214 | A86 | C34-O4-C38 | -2.90 | 112.72 | 117.85 |
| 37 | C | 506 | CLA | O2A-CGA-CBA | 2.90 | 120.68 | 111.83 |
| 37 | B | 524 | CLA | C4B-C3B-C2B | -2.90 | 103.69 | 107.30 |
| 47 | 16 | 304 | KC1 | CAC-C3C-C4C | 2.90 | 128.56 | 124.79 |
| 37 | D | 402 | CLA | C3B-C4B-NB | 2.90 | 113.12 | 110.53 |
| 37 | 18 | 209 | CLA | C4C-C3C-C2C | -2.90 | 102.67 | 106.89 |
| 37 | 20 | 303 | CLA | C4-C3-C5 | 2.90 | 120.26 | 115.23 |
| 48 | 12 | 216 | A86 | C36-C31-C32 | -2.90 | 116.82 | 119.70 |
| 37 | B | 514 | CLA | CHC-C1C-C2C | -2.90 | 118.71 | 126.95 |
| 37 | C | 510 | CLA | CBC-CAC-C3C | -2.90 | 104.56 | 112.42 |
| 48 | 12 | 213 | A86 | C34-O4-C38 | -2.90 | 112.72 | 117.85 |
| 47 | 41 | 203 | KC1 | C4C-C3C-C2C | -2.90 | 102.67 | 106.89 |
| 37 | B | 510 | CLA | CHC-C1C-C2C | -2.90 | 118.71 | 126.95 |
| 37 | B | 510 | CLA | CHD-C4C-NC | 2.90 | 128.73 | 124.23 |
| 37 | 19 | 310 | CLA | C3B-C4B-NB | 2.90 | 113.12 | 110.53 |
| 37 | 11 | 303 | CLA | C4-C3-C5 | 2.90 | 120.26 | 115.23 |
| 45 | d | 402 | PL9 | C40-C39-C41 | 2.90 | 120.26 | 115.23 |
| 37 | 37 | 306 | CLA | CAC-C3C-C4C | 2.90 | 128.56 | 124.79 |
| 37 | 13 | 301 | CLA | CHC-C1C-C2C | -2.90 | 118.71 | 126.95 |
| 37 | C | 504 | CLA | CHB-C4A-NA | 2.90 | 128.58 | 124.40 |
| 37 | 15 | 301 | CLA | C1-C2-C3 | -2.90 | 121.45 | 126.20 |
| 37 | 18 | 204 | CLA | C4C-C3C-C2C | -2.90 | 102.68 | 106.89 |
| 37 | 39 | 310 | CLA | C3B-C4B-NB | 2.90 | 113.11 | 110.53 |
| 47 | 21 | 203 | KC1 | CHD-C4C-NC | 2.89 | 128.67 | 124.31 |
| 37 | 33 | 310 | CLA | C4C-C3C-C2C | -2.89 | 102.68 | 106.89 |
| 47 | 41 | 207 | KC1 | C4C-C3C-C2C | -2.89 | 102.68 | 106.89 |
| 37 | 14 | 305 | CLA | CHD-C4C-NC | 2.89 | 128.72 | 124.23 |
| 37 | D | 402 | CLA | C4C-C3C-C2C | -2.89 | 102.68 | 106.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 35 | 316 | A86 | C12-C11-C13 | 2.89 | 120.69 | 116.00 |
| 37 | b | 523 | CLA | C4B-C3B-C2B | -2.89 | 103.70 | 107.30 |
| 37 | 40 | 205 | CLA | C4-C3-C5 | 2.89 | 120.25 | 115.23 |
| 37 | b | 508 | CLA | C1-C2-C3 | -2.89 | 121.46 | 126.20 |
| 48 | 12 | 214 | A86 | C21-C20-C15 | -2.89 | 114.01 | 123.35 |
| 48 | 32 | 215 | A86 | C21-C20-C15 | -2.89 | 114.01 | 123.35 |
| 37 | 32 | 206 | CLA | CAA-C2A-C1A | 2.89 | 121.45 | 111.97 |
| 37 | B | 505 | CLA | C4C-C3C-C2C | -2.89 | 102.68 | 106.89 |
| 47 | 21 | 203 | KC1 | C4C-C3C-C2C | -2.89 | 102.68 | 106.89 |
| 37 | 40 | 209 | CLA | C4B-C3B-C2B | -2.89 | 103.71 | 107.30 |
| 37 | 31 | 304 | CLA | C4-C3-C5 | 2.89 | 120.25 | 115.23 |
| 37 | 17 | 307 | CLA | CAC-C3C-C4C | 2.89 | 128.55 | 124.79 |
| 47 | 14 | 309 | KC1 | C4C-C3C-C2C | -2.89 | 102.69 | 106.89 |
| 37 | 32 | 202 | CLA | C1-C2-C3 | -2.89 | 121.46 | 126.20 |
| 37 | 13 | 303 | CLA | C4-C3-C5 | 2.89 | 120.24 | 115.23 |
| 37 | c | 509 | CLA | CAC-C3C-C4C | 2.89 | 128.55 | 124.79 |
| 37 | C | 512 | CLA | O2D-CGD-O1D | -2.89 | 118.22 | 123.85 |
| 37 | C | 501 | CLA | CHD-C4C-NC | 2.89 | 128.71 | 124.23 |
| 37 | 12 | 209 | CLA | CHD-C4C-NC | 2.89 | 128.71 | 124.23 |
| 48 | 15 | 314 | A86 | C7-C6-C8 | 2.89 | 122.50 | 118.09 |
| 47 | 36 | 308 | KC1 | CAA-CBA-CGA | -2.89 | 112.36 | 127.05 |
| 37 | 39 | 301 | CLA | CMB-C2B-C1B | 2.89 | 129.82 | 125.42 |
| 37 | 21 | 202 | CLA | O2A-CGA-CBA | 2.89 | 120.64 | 111.83 |
| 44 | H | 102 | DGD | O6D-C1D-O3G | -2.89 | 103.22 | 110.04 |
| 37 | 17 | 309 | CLA | O2A-CGA-CBA | 2.89 | 120.64 | 111.83 |
| 48 | 16 | 313 | A86 | C25-C26-C27 | 2.89 | 131.33 | 127.28 |
| 47 | 34 | 309 | KC1 | C4C-C3C-C2C | -2.89 | 102.69 | 106.89 |
| 37 | c | 504 | CLA | C4A-NA-C1A | -2.89 | 105.36 | 106.68 |
| 48 | 17 | 314 | A86 | C3-C2-C1 | -2.89 | 123.23 | 127.28 |
| 44 | h | 102 | DGD | O6D-C1D-O3G | -2.89 | 103.22 | 110.04 |
| 37 | 38 | 201 | CLA | CMB-C2B-C1B | 2.89 | 129.81 | 125.42 |
| 37 | A | 405 | CLA | CHC-C1C-C2C | -2.89 | 118.75 | 126.95 |
| 48 | 35 | 311 | A86 | C12-C11-C13 | 2.89 | 120.68 | 116.00 |
| 47 | 38 | 210 | KC1 | CHD-C4C-NC | 2.88 | 128.66 | 124.31 |
| 37 | 14 | 307 | CLA | CHD-C4C-NC | 2.88 | 128.70 | 124.23 |
| 37 | c | 510 | CLA | CBC-CAC-C3C | -2.88 | 104.60 | 112.42 |
| 37 | 41 | 202 | CLA | O2A-CGA-CBA | 2.88 | 120.63 | 111.83 |
| 37 | 41 | 206 | CLA | CHC-C1C-C2C | -2.88 | 118.75 | 126.95 |
| 37 | d | 404 | CLA | C4-C3-C5 | 2.88 | 120.23 | 115.23 |
| 47 | 37 | 302 | KC1 | CHD-C4C-NC | 2.88 | 128.65 | 124.31 |
| 44 | j | 101 | DGD | C3G-C2G-C1G | -2.88 | 105.06 | 111.78 |
| 37 | 32 | 210 | CLA | CHD-C4C-NC | 2.88 | 128.70 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 17 | 304 | CLA | O1D-CGD-CBD | -2.88 | 118.83 | 124.52 |
| 37 | 18 | 206 | CLA | C4C-C3C-C2C | -2.88 | 102.70 | 106.89 |
| 48 | 34 | 313 | A86 | C35-C34-C33 | 2.88 | 115.06 | 109.89 |
| 38 | a | 406 | PHO | CBC-CAC-C3C | 2.88 | 117.00 | 112.87 |
| 37 | D | 406 | CLA | C4C-C3C-C2C | -2.88 | 102.70 | 106.89 |
| 47 | 17 | 308 | KC1 | C4C-C3C-C2C | -2.88 | 102.70 | 106.89 |
| 37 | 17 | 304 | CLA | CHD-C4C-NC | 2.88 | 128.70 | 124.23 |
| 37 | 40 | 203 | CLA | CAA-C2A-C3A | -2.88 | 105.22 | 113.00 |
| 37 | 21 | 202 | CLA | CHB-C4A-NA | 2.88 | 128.56 | 124.40 |
| 37 | a | 407 | CLA | CHC-C1C-C2C | -2.88 | 118.76 | 126.95 |
| 37 | 21 | 206 | CLA | CHC-C1C-C2C | -2.88 | 118.76 | 126.95 |
| 37 | D | 405 | CLA | CAC-C3C-C4C | 2.88 | 128.54 | 124.79 |
| 37 | 12 | 205 | CLA | CAA-C2A-C1A | 2.88 | 121.41 | 111.97 |
| 37 | 14 | 307 | CLA | CAA-C2A-C1A | 2.88 | 121.41 | 111.97 |
| 48 | 15 | 316 | A86 | C12-C11-C13 | 2.88 | 120.67 | 116.00 |
| 47 | 16 | 308 | KC1 | CAA-CBA-CGA | -2.88 | 112.41 | 127.05 |
| 48 | 38 | 212 | A86 | C25-C24-C1 | -2.88 | 118.47 | 126.36 |
| 37 | 15 | 308 | CLA | C4C-C3C-C2C | -2.88 | 102.70 | 106.89 |
| 37 | D | 406 | CLA | C4-C3-C5 | 2.88 | 120.22 | 115.23 |
| 37 | 20 | 301 | CLA | CAA-C2A-C3A | -2.88 | 105.22 | 113.00 |
| 37 | C | 508 | CLA | CAC-C3C-C4C | 2.88 | 128.53 | 124.79 |
| 37 | 40 | 205 | CLA | CHC-C1C-C2C | -2.88 | 118.77 | 126.95 |
| 37 | c | 506 | CLA | O2A-CGA-CBA | 2.88 | 120.61 | 111.83 |
| 37 | 20 | 303 | CLA | CHC-C1C-C2C | -2.88 | 118.77 | 126.95 |
| 47 | 41 | 203 | KC1 | CHD-C4C-NC | 2.88 | 128.65 | 124.31 |
| 37 | 11 | 308 | CLA | C1-C2-C3 | -2.88 | 121.48 | 126.20 |
| 37 | b | 512 | CLA | CHD-C4C-NC | 2.88 | 128.69 | 124.23 |
| 37 | A | 405 | CLA | C4C-C3C-C2C | -2.88 | 102.70 | 106.89 |
| 37 | 37 | 301 | CLA | C4-C3-C5 | 2.88 | 120.22 | 115.23 |
| 47 | 15 | 309 | KC1 | CHD-C1D-ND | -2.88 | 119.73 | 124.05 |
| 39 | K | 101 | BCR | C24-C23-C22 | -2.88 | 121.98 | 126.23 |
| 37 | b | 516 | CLA | CHD-C4C-NC | 2.88 | 128.69 | 124.23 |
| 37 | 38 | 203 | CLA | CHD-C4C-NC | 2.87 | 128.69 | 124.23 |
| 38 | A | 404 | PHO | CBC-CAC-C3C | 2.87 | 116.99 | 112.87 |
| 47 | 13 | 306 | KC1 | CAC-C3C-C4C | 2.87 | 128.53 | 124.79 |
| 37 | 39 | 302 | CLA | CGD-CBD-CAD | -2.87 | 101.54 | 110.85 |
| 37 | b | 510 | CLA | CAC-C3C-C4C | 2.87 | 128.53 | 124.79 |
| 48 | 32 | 221 | A86 | C8-C6-C5 | -2.87 | 114.49 | 119.01 |
| 37 | 41 | 202 | CLA | CHB-C4A-NA | 2.87 | 128.55 | 124.40 |
| 47 | 11 | 306 | KC1 | CAA-CBA-CGA | -2.87 | 112.44 | 127.05 |
| 37 | 41 | 206 | CLA | C4B-C3B-C2B | -2.87 | 103.73 | 107.30 |
| 48 | 37 | 319 | A86 | C7-C6-C8 | 2.87 | 122.47 | 118.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 32 | 206 | CLA | C4B-C3B-C2B | -2.87 | 103.73 | 107.30 |
| 37 | 35 | 305 | CLA | C4B-C3B-C2B | -2.87 | 103.73 | 107.30 |
| 37 | B | 516 | CLA | CHD-C4C-NC | 2.87 | 128.68 | 124.23 |
| 47 | 17 | 303 | KC1 | CHD-C4C-NC | 2.87 | 128.64 | 124.31 |
| 47 | 11 | 309 | KC1 | C4C-C3C-C2C | -2.87 | 102.71 | 106.89 |
| 37 | 34 | 307 | CLA | CAA-C2A-C1A | 2.87 | 121.38 | 111.97 |
| 37 | D | 405 | CLA | C4B-C3B-C2B | -2.87 | 103.73 | 107.30 |
| 37 | 36 | 309 | CLA | C4B-C3B-C2B | -2.87 | 103.73 | 107.30 |
| 47 | 17 | 303 | KC1 | CAC-C3C-C4C | 2.87 | 128.53 | 124.79 |
| 37 | 35 | 301 | CLA | CMC-C2C-C1C | 2.87 | 129.52 | 125.03 |
| 37 | d | 404 | CLA | C4C-C3C-C2C | -2.87 | 102.71 | 106.89 |
| 37 | 11 | 307 | CLA | C4C-C3C-C2C | -2.87 | 102.71 | 106.89 |
| 48 | 14 | 313 | A86 | C35-C34-C33 | 2.87 | 115.04 | 109.89 |
| 39 | A | 406 | BCR | C11-C10-C9 | -2.87 | 123.25 | 127.28 |
| 37 | 38 | 206 | CLA | CHD-C4C-NC | 2.87 | 128.68 | 124.23 |
| 37 | B | 510 | CLA | CAC-C3C-C4C | 2.87 | 128.52 | 124.79 |
| 37 | B | 512 | CLA | CHD-C4C-NC | 2.87 | 128.68 | 124.23 |
| 37 | c | 501 | CLA | CHD-C4C-NC | 2.87 | 128.68 | 124.23 |
| 39 | a | 408 | BCR | C11-C10-C9 | -2.87 | 123.25 | 127.28 |
| 47 | 12 | 208 | KC1 | CAC-C3C-C4C | 2.87 | 128.52 | 124.79 |
| 47 | 32 | 209 | KC1 | CAC-C3C-C4C | 2.87 | 128.52 | 124.79 |
| 48 | 35 | 319 | A86 | C41-C32-C31 | -2.87 | 107.91 | 110.47 |
| 37 | b | 508 | CLA | CHD-C4C-NC | 2.87 | 128.68 | 124.23 |
| 47 | 33 | 306 | KC1 | CAC-C3C-C4C | 2.87 | 128.52 | 124.79 |
| 48 | 12 | 220 | A86 | C3-C4-C5 | -2.87 | 117.65 | 123.52 |
| 37 | 37 | 303 | CLA | O1D-CGD-CBD | -2.87 | 118.86 | 124.52 |
| 48 | 39 | 311 | A86 | C35-C34-C33 | 2.87 | 115.03 | 109.89 |
| 37 | 31 | 306 | CLA | C4B-C3B-C2B | -2.87 | 103.74 | 107.30 |
| 37 | 14 | 310 | CLA | CHD-C4C-NC | 2.87 | 128.67 | 124.23 |
| 47 | 14 | 306 | KC1 | C4C-C3C-C2C | -2.87 | 102.72 | 106.89 |
| 47 | 34 | 306 | KC1 | C4C-C3C-C2C | -2.87 | 102.72 | 106.89 |
| 37 | b | 513 | CLA | C1-C2-C3 | -2.86 | 121.50 | 126.20 |
| 37 | 18 | 204 | CLA | CMC-C2C-C1C | 2.86 | 129.51 | 125.03 |
| 48 | 21 | 214 | A86 | C41-C32-C31 | -2.86 | 107.91 | 110.47 |
| 47 | 19 | 308 | KC1 | CAA-C2A-C1A | -2.86 | 112.09 | 124.64 |
| 48 | 19 | 311 | A86 | C35-C34-C33 | 2.86 | 115.03 | 109.89 |
| 47 | 39 | 308 | KC1 | CAA-C2A-C1A | -2.86 | 112.09 | 124.64 |
| 37 | 20 | 306 | CLA | O2A-CGA-CBA | 2.86 | 120.57 | 111.83 |
| 37 | 20 | 307 | CLA | C4B-C3B-C2B | -2.86 | 103.74 | 107.30 |
| 37 | 12 | 207 | CLA | CHC-C1C-C2C | -2.86 | 118.81 | 126.95 |
| 37 | 39 | 306 | CLA | C1C-C2C-C3C | -2.86 | 103.97 | 106.98 |
| 37 | B | 508 | CLA | C1-C2-C3 | -2.86 | 121.51 | 126.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 14 | 309 | KC1 | CBC-CAC-C3C | -2.86 | 104.66 | 112.42 |
| 44 | J | 101 | DGD | C3G-C2G-C1G | -2.86 | 105.11 | 111.78 |
| 37 | 14 | 305 | CLA | CAC-C3C-C4C | 2.86 | 128.51 | 124.79 |
| 37 | 41 | 204 | CLA | C4B-C3B-C2B | -2.86 | 103.74 | 107.30 |
| 37 | 20 | 306 | CLA | CHC-C1C-C2C | -2.86 | 118.82 | 126.95 |
| 37 | 40 | 208 | CLA | CHC-C1C-C2C | -2.86 | 118.82 | 126.95 |
| 37 | c | 504 | CLA | CHB-C4A-NA | 2.86 | 128.53 | 124.40 |
| 47 | 40 | 207 | KC1 | CHD-C1D-ND | -2.86 | 119.76 | 124.05 |
| 37 | 18 | 203 | CLA | CHD-C4C-NC | 2.86 | 128.67 | 124.23 |
| 47 | 35 | 309 | KC1 | CHD-C1D-ND | -2.86 | 119.76 | 124.05 |
| 37 | 38 | 204 | CLA | C4-C3-C5 | 2.86 | 120.19 | 115.23 |
| 37 | 35 | 310 | CLA | C4C-C3C-C2C | -2.86 | 102.73 | 106.89 |
| 37 | 18 | 201 | CLA | C4B-C3B-C2B | -2.86 | 103.75 | 107.30 |
| 37 | d | 403 | CLA | C4B-C3B-C2B | -2.86 | 103.75 | 107.30 |
| 37 | 11 | 305 | CLA | C4B-C3B-C2B | -2.86 | 103.75 | 107.30 |
| 37 | 12 | 212 | CLA | C4B-C3B-C2B | -2.86 | 103.75 | 107.30 |
| 47 | 18 | 210 | KC1 | CHD-C4C-NC | 2.86 | 128.61 | 124.31 |
| 37 | 18 | 202 | CLA | C1C-C2C-C3C | -2.86 | 103.98 | 106.98 |
| 37 | 34 | 305 | CLA | CAC-C3C-C4C | 2.86 | 128.51 | 124.79 |
| 47 | 17 | 305 | KC1 | CAA-CBA-CGA | -2.86 | 112.53 | 127.05 |
| 48 | 39 | 311 | A86 | C21-C20-C15 | -2.86 | 114.13 | 123.35 |
| 37 | B | 515 | CLA | O2D-CGD-O1D | -2.86 | 118.29 | 123.85 |
| 37 | 12 | 204 | CLA | CMD-C2D-C1D | 2.86 | 129.76 | 124.73 |
| 37 | 32 | 205 | CLA | CMD-C2D-C1D | 2.86 | 129.76 | 124.73 |
| 47 | 37 | 304 | KC1 | CAA-CBA-CGA | -2.85 | 112.53 | 127.05 |
| 48 | 12 | 202 | A86 | C9-C8-C6 | -2.85 | 118.54 | 126.36 |
| 37 | 18 | 202 | CLA | CHC-C1C-C2C | -2.85 | 118.84 | 126.95 |
| 37 | 38 | 203 | CLA | CAC-C3C-C4C | 2.85 | 128.50 | 124.79 |
| 37 | b | 501 | CLA | CMB-C2B-C1B | 2.85 | 129.76 | 125.42 |
| 37 | 35 | 307 | CLA | C4C-C3C-C2C | -2.85 | 102.74 | 106.89 |
| 37 | 38 | 209 | CLA | CAC-C3C-C4C | 2.85 | 128.50 | 124.79 |
| 37 | 40 | 208 | CLA | O2A-CGA-CBA | 2.85 | 120.53 | 111.83 |
| 47 | 31 | 305 | KC1 | CHD-C4C-NC | 2.85 | 128.61 | 124.31 |
| 37 | 41 | 205 | CLA | C4B-C3B-C2B | -2.85 | 103.76 | 107.30 |
| 37 | 15 | 301 | CLA | C4C-C3C-C2C | -2.85 | 102.74 | 106.89 |
| 47 | 31 | 309 | KC1 | C4C-C3C-C2C | -2.85 | 102.74 | 106.89 |
| 47 | 34 | 309 | KC1 | CBC-CAC-C3C | -2.85 | 104.69 | 112.42 |
| 37 | 34 | 302 | CLA | CHD-C4C-NC | 2.85 | 128.65 | 124.23 |
| 47 | 41 | 207 | KC1 | CHD-C1D-ND | -2.85 | 119.77 | 124.05 |
| 37 | B | 513 | CLA | C1-C2-C3 | -2.85 | 121.53 | 126.20 |
| 37 | 32 | 208 | CLA | CHC-C1C-C2C | -2.85 | 118.85 | 126.95 |
| 37 | B | 513 | CLA | C4C-C3C-C2C | -2.85 | 102.74 | 106.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 20 | 305 | KC1 | CHD-C1D-ND | -2.85 | 119.77 | 124.05 |
| 47 | 31 | 307 | KC1 | CAA-CBA-CGA | -2.85 | 112.56 | 127.05 |
| 37 | 19 | 303 | CLA | CHC-C1C-C2C | -2.85 | 118.85 | 126.95 |
| 37 | 39 | 303 | CLA | CHC-C1C-C2C | -2.85 | 118.85 | 126.95 |
| 37 | 34 | 307 | CLA | CHD-C4C-NC | 2.85 | 128.65 | 124.23 |
| 37 | 37 | 303 | CLA | CHD-C4C-NC | 2.85 | 128.65 | 124.23 |
| 37 | w | 101 | CLA | CHC-C1C-C2C | -2.85 | 118.85 | 126.95 |
| 37 | 12 | 205 | CLA | C4C-C3C-C2C | -2.85 | 102.75 | 106.89 |
| 37 | 17 | 302 | CLA | C4-C3-C5 | 2.85 | 120.17 | 115.23 |
| 39 | b | 518 | BCR | C27-C26-C25 | 2.85 | 126.55 | 122.70 |
| 37 | b | 502 | CLA | C4C-C3C-C2C | -2.85 | 102.75 | 106.89 |
| 37 | 35 | 307 | CLA | CAC-C3C-C4C | 2.85 | 128.49 | 124.79 |
| 37 | 40 | 209 | CLA | CHD-C4C-NC | 2.85 | 128.64 | 124.23 |
| 37 | d | 401 | CLA | C4C-C3C-C2C | -2.85 | 102.75 | 106.89 |
| 37 | 34 | 303 | CLA | C4C-C3C-C2C | -2.85 | 102.75 | 106.89 |
| 37 | 41 | 209 | CLA | C4C-C3C-C2C | -2.85 | 102.75 | 106.89 |
| 48 | 38 | 212 | A86 | C10-C9-C8 | -2.85 | 114.95 | 123.20 |
| 48 | 15 | 312 | A86 | C7-C6-C8 | 2.85 | 122.44 | 118.09 |
| 37 | 31 | 301 | CLA | C4B-C3B-C2B | -2.85 | 103.76 | 107.30 |
| 37 | 19 | 301 | CLA | CMB-C2B-C1B | 2.85 | 129.75 | 125.42 |
| 47 | 35 | 302 | KC1 | CHD-C4C-NC | 2.85 | 128.60 | 124.31 |
| 37 | 39 | 310 | CLA | C1-C2-C3 | -2.84 | 121.54 | 126.20 |
| 37 | a | 407 | CLA | C4C-C3C-C2C | -2.84 | 102.75 | 106.89 |
| 37 | 38 | 206 | CLA | C4C-C3C-C2C | -2.84 | 102.75 | 106.89 |
| 37 | 21 | 204 | CLA | C4B-C3B-C2B | -2.84 | 103.77 | 107.30 |
| 37 | 18 | 204 | CLA | C4-C3-C5 | 2.84 | 120.17 | 115.23 |
| 37 | b | 515 | CLA | O2D-CGD-O1D | -2.84 | 118.31 | 123.85 |
| 47 | 34 | 306 | KC1 | CHD-C4C-NC | 2.84 | 128.59 | 124.31 |
| 48 | 32 | 217 | A86 | C25-C24-C1 | -2.84 | 118.57 | 126.36 |
| 39 | c | 515 | BCR | C15-C16-C17 | -2.84 | 117.70 | 123.52 |
| 37 | 12 | 209 | CLA | CHC-C1C-C2C | -2.84 | 118.87 | 126.95 |
| 37 | D | 405 | CLA | CHD-C4C-NC | 2.84 | 128.64 | 124.23 |
| 48 | 32 | 203 | A86 | C9-C8-C6 | -2.84 | 118.57 | 126.36 |
| 37 | 13 | 301 | CLA | C4C-C3C-C2C | -2.84 | 102.75 | 106.89 |
| 37 | d | 403 | CLA | CHD-C4C-NC | 2.84 | 128.64 | 124.23 |
| 48 | 11 | 312 | A86 | C12-C11-C13 | 2.84 | 120.61 | 116.00 |
| 37 | c | 504 | CLA | C4B-C3B-C2B | -2.84 | 103.77 | 107.30 |
| 37 | 12 | 205 | CLA | C4B-C3B-C2B | -2.84 | 103.77 | 107.30 |
| 37 | 38 | 203 | CLA | CBA-CAA-C2A | -2.84 | 105.34 | 113.79 |
| 47 | 14 | 306 | KC1 | CHD-C4C-NC | 2.84 | 128.59 | 124.31 |
| 48 | 36 | 313 | A86 | C21-C20-C15 | -2.84 | 114.18 | 123.35 |
| 48 | 35 | 312 | A86 | C34-O4-C38 | -2.84 | 112.83 | 117.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 14 | 303 | CLA | C4C-C3C-C2C | -2.84 | 102.76 | 106.89 |
| 37 | 19 | 309 | CLA | C4C-C3C-C2C | -2.84 | 102.76 | 106.89 |
| 48 | 15 | 314 | A86 | C34-O4-C38 | -2.84 | 112.83 | 117.85 |
| 48 | 15 | 311 | A86 | C12-C11-C13 | 2.84 | 120.60 | 116.00 |
| 37 | c | 504 | CLA | C3C-C4C-NC | 2.84 | 114.07 | 110.43 |
| 37 | B | 508 | CLA | CHD-C4C-NC | 2.84 | 128.63 | 124.23 |
| 37 | A | 405 | CLA | C4B-C3B-C2B | -2.84 | 103.77 | 107.30 |
| 48 | 19 | 311 | A86 | C21-C20-C15 | -2.84 | 114.19 | 123.35 |
| 48 | 15 | 314 | A86 | C4-C5-C6 | -2.84 | 123.30 | 127.28 |
| 37 | 21 | 205 | CLA | CMB-C2B-C1B | 2.84 | 129.74 | 125.42 |
| 48 | 15 | 313 | A86 | C36-C31-C32 | -2.84 | 116.88 | 119.70 |
| 39 | b | 524 | BCR | C15-C14-C13 | -2.84 | 123.30 | 127.28 |
| 37 | 16 | 309 | CLA | C4B-C3B-C2B | -2.84 | 103.77 | 107.30 |
| 37 | 32 | 213 | CLA | C4B-C3B-C2B | -2.84 | 103.77 | 107.30 |
| 48 | 17 | 310 | A86 | C4-C3-C2 | -2.84 | 117.71 | 123.52 |
| 37 | C | 504 | CLA | C4B-C3B-C2B | -2.84 | 103.78 | 107.30 |
| 37 | 21 | 209 | CLA | C4C-C3C-C2C | -2.84 | 102.76 | 106.89 |
| 37 | 38 | 211 | CLA | O2D-CGD-O1D | -2.84 | 118.33 | 123.85 |
| 48 | 14 | 316 | A86 | C36-C31-C32 | -2.84 | 116.88 | 119.70 |
| 37 | 21 | 210 | CLA | CMB-C2B-C1B | 2.84 | 129.74 | 125.42 |
| 37 | a | 407 | CLA | C4B-C3B-C2B | -2.83 | 103.78 | 107.30 |
| 39 | B | 518 | BCR | C15-C16-C17 | -2.83 | 117.72 | 123.52 |
| 37 | 12 | 207 | CLA | C1-C2-C3 | -2.83 | 122.18 | 126.76 |
| 37 | b | 513 | CLA | C4C-C3C-C2C | -2.83 | 102.77 | 106.89 |
| 48 | 16 | 314 | A86 | C21-C20-C15 | -2.83 | 114.20 | 123.35 |
| 37 | D | 402 | CLA | C4B-C3B-C2B | -2.83 | 103.78 | 107.30 |
| 37 | W | 102 | CLA | C4B-C3B-C2B | -2.83 | 103.78 | 107.30 |
| 47 | 11 | 309 | KC1 | CHD-C4C-NC | 2.83 | 128.58 | 124.31 |
| 37 | 21 | 209 | CLA | CHD-C4C-NC | 2.83 | 128.62 | 124.23 |
| 47 | 37 | 305 | KC1 | CHD-C1D-ND | -2.83 | 119.80 | 124.05 |
| 48 | 17 | 311 | A86 | C21-C20-C15 | -2.83 | 114.21 | 123.35 |
| 37 | W | 101 | CLA | CHC-C1C-C2C | -2.83 | 118.90 | 126.95 |
| 37 | 35 | 301 | CLA | C4C-C3C-C2C | -2.83 | 102.77 | 106.89 |
| 48 | 34 | 312 | A86 | C7-C6-C8 | 2.83 | 122.41 | 118.09 |
| 37 | 11 | 310 | CLA | CAA-C2A-C3A | -2.83 | 105.35 | 113.00 |
| 37 | 31 | 310 | CLA | CAA-C2A-C3A | -2.83 | 105.35 | 113.00 |
| 37 | Z | 102 | CLA | CED-O2D-CGD | 2.83 | 122.34 | 115.92 |
| 48 | 12 | 216 | A86 | C25-C24-C1 | -2.83 | 118.60 | 126.36 |
| 48 | 37 | 309 | A86 | C9-C10-C11 | -2.83 | 118.64 | 126.64 |
| 37 | 32 | 210 | CLA | CHC-C1C-C2C | -2.83 | 118.91 | 126.95 |
| 37 | B | 505 | CLA | C3B-C4B-NB | 2.83 | 113.06 | 110.53 |
| 37 | 32 | 208 | CLA | C1-C2-C3 | -2.83 | 122.18 | 126.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 502 | CLA | CHD-C4C-NC | 2.83 | 128.62 | 124.23 |
| 39 | y | 101 | BCR | C24-C23-C22 | -2.83 | 122.05 | 126.23 |
| 37 | z | 102 | CLA | CED-O2D-CGD | 2.83 | 122.33 | 115.92 |
| 47 | 16 | 308 | KC1 | CHD-C4C-NC | 2.83 | 128.57 | 124.31 |
| 48 | 37 | 309 | A86 | C4-C3-C2 | -2.83 | 117.73 | 123.52 |
| 37 | 15 | 307 | CLA | C4C-C3C-C2C | -2.83 | 102.78 | 106.89 |
| 37 | 41 | 210 | CLA | CMB-C2B-C1B | 2.83 | 129.72 | 125.42 |
| 37 | 41 | 209 | CLA | CHD-C4C-NC | 2.83 | 128.62 | 124.23 |
| 48 | 31 | 312 | A86 | C12-C11-C13 | 2.83 | 120.58 | 116.00 |
| 39 | C | 515 | BCR | C15-C16-C17 | -2.83 | 117.73 | 123.52 |
| 47 | 17 | 305 | KC1 | C4C-C3C-C2C | -2.83 | 102.78 | 106.89 |
| 47 | 33 | 306 | KC1 | CHD-C4C-NC | 2.83 | 128.57 | 124.31 |
| 37 | 18 | 203 | CLA | C4B-C3B-C2B | -2.83 | 103.79 | 107.30 |
| 37 | 13 | 303 | CLA | C4C-C3C-C2C | -2.83 | 102.78 | 106.89 |
| 47 | 11 | 304 | KC1 | CHD-C4C-NC | 2.83 | 128.57 | 124.31 |
| 47 | 16 | 305 | KC1 | CMB-C2B-C1B | 2.83 | 129.71 | 124.73 |
| 37 | 14 | 307 | CLA | C1-C2-C3 | -2.83 | 121.57 | 126.20 |
| 37 | 31 | 310 | CLA | CHC-C1C-C2C | -2.83 | 118.92 | 126.95 |
| 37 | 20 | 303 | CLA | OBD-CAD-C3D | -2.83 | 121.81 | 128.42 |
| 39 | b | 518 | BCR | C15-C16-C17 | -2.83 | 117.74 | 123.52 |
| 37 | 36 | 309 | CLA | C3B-C4B-NB | 2.83 | 113.05 | 110.53 |
| 37 | 15 | 305 | CLA | CAC-C3C-C4C | 2.82 | 128.47 | 124.79 |
| 48 | 16 | 313 | A86 | C21-C20-C15 | -2.82 | 114.23 | 123.35 |
| 47 | 17 | 306 | KC1 | CAC-C3C-C4C | 2.82 | 128.46 | 124.79 |
| 48 | 15 | 312 | A86 | C12-C11-C13 | 2.82 | 120.58 | 116.00 |
| 37 | d | 401 | CLA | CHD-C4C-NC | 2.82 | 128.61 | 124.23 |
| 37 | b | 505 | CLA | C3B-C4B-NB | 2.82 | 113.05 | 110.53 |
| 37 | 33 | 303 | CLA | C4-C3-C5 | 2.82 | 120.13 | 115.23 |
| 37 | 32 | 210 | CLA | C4B-C3B-C2B | -2.82 | 103.79 | 107.30 |
| 48 | 18 | 213 | A86 | C12-C11-C13 | 2.82 | 120.57 | 116.00 |
| 37 | 39 | 310 | CLA | CAA-C2A-C3A | -2.82 | 105.38 | 113.00 |
| 47 | 11 | 309 | KC1 | CMB-C2B-C1B | 2.82 | 129.69 | 124.73 |
| 37 | 11 | 310 | CLA | CHC-C1C-C2C | -2.82 | 118.93 | 126.95 |
| 47 | 21 | 207 | KC1 | CHD-C1D-ND | -2.82 | 119.82 | 124.05 |
| 37 | B | 514 | CLA | C4B-C3B-C2B | -2.82 | 103.80 | 107.30 |
| 37 | d | 401 | CLA | C4B-C3B-C2B | -2.82 | 103.80 | 107.30 |
| 37 | 32 | 211 | CLA | C1-C2-C3 | -2.82 | 121.58 | 126.20 |
| 37 | 38 | 211 | CLA | CAC-C3C-C4C | 2.82 | 128.46 | 124.79 |
| 37 | B | 502 | CLA | C4C-C3C-C2C | -2.82 | 102.79 | 106.89 |
| 37 | 11 | 308 | CLA | C4C-C3C-C2C | -2.82 | 102.79 | 106.89 |
| 37 | C | 502 | CLA | CHD-C4C-NC | 2.82 | 128.60 | 124.23 |
| 48 | 37 | 310 | A86 | C21-C20-C15 | -2.82 | 114.25 | 123.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 210 | CLA | C1-C2-C3 | -2.82 | 121.58 | 126.20 |
| 38 | a | 405 | PHO | O1D-CGD-CBD | 2.82 | 129.00 | 124.72 |
| 37 | 12 | 212 | CLA | C3B-C4B-NB | 2.82 | 113.05 | 110.53 |
| 37 | 40 | 205 | CLA | OBD-CAD-C3D | -2.82 | 121.83 | 128.42 |
| 37 | B | 501 | CLA | C4-C3-C5 | 2.82 | 120.12 | 115.23 |
| 47 | 38 | 205 | KC1 | CHD-C4C-NC | 2.82 | 128.55 | 124.31 |
| 37 | 13 | 307 | CLA | C4B-C3B-C2B | -2.82 | 103.80 | 107.30 |
| 47 | 11 | 306 | KC1 | C4C-C3C-C2C | -2.82 | 102.79 | 106.89 |
| 48 | 33 | 311 | A86 | C3-C4-C5 | -2.82 | 117.75 | 123.52 |
| 48 | 21 | 215 | A86 | C12-C11-C13 | 2.82 | 120.57 | 116.00 |
| 39 | D | 407 | BCR | C24-C23-C22 | -2.82 | 122.07 | 126.23 |
| 48 | 40 | 201 | A86 | C21-C20-C15 | -2.82 | 114.26 | 123.35 |
| 47 | 31 | 309 | KC1 | CMB-C2B-C1B | 2.82 | 129.69 | 124.73 |
| 37 | c | 510 | CLA | O2A-CGA-CBA | 2.82 | 120.42 | 111.83 |
| 37 | 33 | 301 | CLA | C4C-C3C-C2C | -2.82 | 102.79 | 106.89 |
| 48 | 35 | 312 | A86 | C7-C6-C8 | 2.82 | 122.39 | 118.09 |
| 48 | 14 | 312 | A86 | C7-C6-C8 | 2.81 | 122.39 | 118.09 |
| 37 | b | 514 | CLA | C4B-C3B-C2B | -2.81 | 103.80 | 107.30 |
| 37 | D | 401 | CLA | C4A-NA-C1A | -2.81 | 105.39 | 106.68 |
| 37 | 32 | 202 | CLA | C4C-C3C-C2C | -2.81 | 102.80 | 106.89 |
| 37 | 19 | 310 | CLA | CAA-C2A-C3A | -2.81 | 105.40 | 113.00 |
| 37 | 13 | 301 | CLA | CHB-C4A-NA | 2.81 | 128.46 | 124.40 |
| 47 | 37 | 305 | KC1 | CAC-C3C-C4C | 2.81 | 128.45 | 124.79 |
| 37 | 39 | 301 | CLA | C3B-C4B-NB | 2.81 | 113.04 | 110.53 |
| 38 | a | 406 | PHO | C2D-C1D-ND | -2.81 | 107.40 | 109.43 |
| 47 | 13 | 309 | KC1 | CHD-C1D-ND | -2.81 | 119.83 | 124.05 |
| 47 | 17 | 306 | KC1 | CHD-C1D-ND | -2.81 | 119.83 | 124.05 |
| 39 | B | 518 | BCR | C27-C26-C25 | 2.81 | 126.50 | 122.70 |
| 37 | 35 | 305 | CLA | CHD-C4C-NC | 2.81 | 128.59 | 124.23 |
| 39 | A | 410 | BCR | C15-C16-C17 | -2.81 | 117.77 | 123.52 |
| 37 | b | 516 | CLA | O1D-CGD-CBD | -2.81 | 118.97 | 124.52 |
| 45 | d | 406 | PL9 | C7-C3-C2 | -2.81 | 120.07 | 123.39 |
| 37 | 35 | 303 | CLA | O2D-CGD-O1D | -2.81 | 118.38 | 123.85 |
| 37 | c | 511 | CLA | CHD-C4C-NC | 2.81 | 128.59 | 124.23 |
| 37 | B | 509 | CLA | C4C-C3C-C2C | -2.81 | 102.80 | 106.89 |
| 48 | 13 | 311 | A86 | C3-C4-C5 | -2.81 | 117.77 | 123.52 |
| 37 | B | 505 | CLA | C1-C2-C3 | -2.81 | 121.59 | 126.20 |
| 37 | A | 403 | CLA | CHD-C4C-NC | 2.81 | 128.59 | 124.23 |
| 48 | 14 | 314 | A86 | C21-C20-C15 | -2.81 | 114.28 | 123.35 |
| 37 | 41 | 210 | CLA | C4B-C3B-C2B | -2.81 | 103.81 | 107.30 |
| 45 | D | 408 | PL9 | C7-C3-C2 | -2.81 | 120.08 | 123.39 |
| 37 | 33 | 305 | CLA | CAC-C3C-C4C | 2.81 | 128.44 | 124.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 38 | 213 | A86 | C41-C32-C31 | -2.81 | 107.96 | 110.47 |
| 37 | 41 | 205 | CLA | CMB-C2B-C1B | 2.81 | 129.70 | 125.42 |
| 37 | 13 | 305 | CLA | C4C-C3C-C2C | -2.81 | 102.80 | 106.89 |
| 37 | 19 | 310 | CLA | C4C-C3C-C2C | -2.81 | 102.80 | 106.89 |
| 37 | 18 | 208 | CLA | CAA-C2A-C3A | -2.81 | 105.41 | 113.00 |
| 39 | C | 519 | BCR | C27-C26-C25 | 2.81 | 126.50 | 122.70 |
| 48 | 35 | 314 | A86 | C34-O4-C38 | -2.81 | 112.89 | 117.85 |
| 37 | 13 | 305 | CLA | CMB-C2B-C1B | 2.81 | 129.69 | 125.42 |
| 47 | 32 | 212 | KC1 | O2D-CGD-O1D | -2.81 | 118.38 | 123.85 |
| 48 | 11 | 319 | A86 | O4-C38-O5 | -2.81 | 117.57 | 122.99 |
| 47 | 36 | 308 | KC1 | CHD-C4C-NC | 2.81 | 128.54 | 124.31 |
| 47 | 20 | 305 | KC1 | O1D-CGD-CBD | -2.81 | 118.98 | 124.52 |
| 37 | C | 513 | CLA | C1-C2-C3 | -2.81 | 121.60 | 126.20 |
| 37 | 21 | 210 | CLA | CHC-C1C-C2C | -2.81 | 118.97 | 126.95 |
| 39 | d | 405 | BCR | C24-C23-C22 | -2.81 | 122.08 | 126.23 |
| 37 | C | 508 | CLA | CHD-C4C-NC | 2.81 | 128.58 | 124.23 |
| 37 | 37 | 306 | CLA | CHD-C4C-NC | 2.81 | 128.58 | 124.23 |
| 37 | C | 510 | CLA | O2A-CGA-CBA | 2.81 | 120.39 | 111.83 |
| 37 | B | 510 | CLA | C1-C2-C3 | -2.81 | 121.60 | 126.20 |
| 37 | 19 | 301 | CLA | C3B-C4B-NB | 2.81 | 113.03 | 110.53 |
| 37 | B | 524 | CLA | CMC-C2C-C1C | 2.81 | 129.42 | 125.03 |
| 37 | b | 501 | CLA | C4B-C3B-C2B | -2.81 | 103.81 | 107.30 |
| 37 | b | 510 | CLA | C1-C2-C3 | -2.81 | 121.60 | 126.20 |
| 37 | C | 504 | CLA | C3C-C4C-NC | 2.81 | 114.02 | 110.43 |
| 48 | 16 | 310 | A86 | C21-C20-C15 | -2.81 | 114.29 | 123.35 |
| 48 | 31 | 313 | A86 | C4-C3-C2 | -2.80 | 117.78 | 123.52 |
| 37 | b | 509 | CLA | C4C-C3C-C2C | -2.80 | 102.81 | 106.89 |
| 37 | D | 402 | CLA | CHD-C4C-NC | 2.80 | 128.58 | 124.23 |
| 37 | 15 | 307 | CLA | CAC-C3C-C4C | 2.80 | 128.44 | 124.79 |
| 37 | c | 505 | CLA | CAA-C2A-C3A | -2.80 | 105.42 | 113.00 |
| 39 | B | 525 | BCR | C15-C14-C13 | -2.80 | 123.35 | 127.28 |
| 37 | b | 513 | CLA | CAA-C2A-C3A | -2.80 | 105.42 | 113.00 |
| 48 | 37 | 313 | A86 | C41-C32-C31 | -2.80 | 107.96 | 110.47 |
| 47 | 14 | 309 | KC1 | C2A-C1A-NA | 2.80 | 113.83 | 109.34 |
| 47 | 34 | 309 | KC1 | C2A-C1A-NA | 2.80 | 113.83 | 109.34 |
| 37 | 18 | 206 | CLA | CHD-C4C-NC | 2.80 | 128.58 | 124.23 |
| 47 | 13 | 306 | KC1 | CHD-C4C-NC | 2.80 | 128.53 | 124.31 |
| 37 | a | 403 | CLA | CHD-C4C-NC | 2.80 | 128.58 | 124.23 |
| 37 | 39 | 310 | CLA | C4C-C3C-C2C | -2.80 | 102.81 | 106.89 |
| 37 | 21 | 210 | CLA | C4B-C3B-C2B | -2.80 | 103.82 | 107.30 |
| 47 | 41 | 207 | KC1 | O2D-CGD-O1D | -2.80 | 118.40 | 123.85 |
| 37 | 36 | 306 | CLA | CHD-C4C-NC | 2.80 | 128.57 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 40 | 208 | CLA | C3B-C4B-NB | 2.80 | 113.03 | 110.53 |
| 48 | 14 | 311 | A86 | C34-O4-C38 | -2.80 | 112.90 | 117.85 |
| 37 | 41 | 210 | CLA | CHC-C1C-C2C | -2.80 | 118.99 | 126.95 |
| 47 | 35 | 309 | KC1 | CHD-C4C-NC | 2.80 | 128.53 | 124.31 |
| 47 | 33 | 309 | KC1 | CHD-C1D-ND | -2.80 | 119.85 | 124.05 |
| 48 | 17 | 320 | A86 | C26-C25-C24 | -2.80 | 115.09 | 123.20 |
| 48 | 36 | 310 | A86 | C21-C20-C15 | -2.80 | 114.31 | 123.35 |
| 37 | 21 | 208 | CLA | O2A-CGA-CBA | 2.80 | 120.37 | 111.83 |
| 38 | D | 403 | PHO | O1D-CGD-CBD | 2.80 | 128.97 | 124.72 |
| 47 | 31 | 307 | KC1 | C4C-C3C-C2C | -2.80 | 102.82 | 106.89 |
| 37 | c | 507 | CLA | C4A-NA-C1A | -2.80 | 105.40 | 106.68 |
| 48 | 32 | 218 | A86 | C40-C32-C31 | 2.80 | 112.98 | 110.47 |
| 47 | 36 | 305 | KC1 | CMB-C2B-C1B | 2.80 | 129.66 | 124.73 |
| 37 | b | 511 | CLA | CHD-C4C-NC | 2.80 | 128.57 | 124.23 |
| 37 | B | 513 | CLA | CAA-C2A-C3A | -2.80 | 105.44 | 113.00 |
| 37 | 12 | 209 | CLA | C4B-C3B-C2B | -2.80 | 103.82 | 107.30 |
| 37 | 39 | 301 | CLA | CAC-C3C-C4C | 2.80 | 128.43 | 124.79 |
| 37 | B | 503 | CLA | CHD-C4C-NC | 2.80 | 128.57 | 124.23 |
| 48 | 17 | 313 | A86 | C7-C6-C8 | 2.80 | 122.36 | 118.09 |
| 48 | 34 | 311 | A86 | C34-O4-C38 | -2.80 | 112.91 | 117.85 |
| 37 | 17 | 307 | CLA | CHD-C4C-NC | 2.80 | 128.57 | 124.23 |
| 48 | 35 | 312 | A86 | C12-C11-C13 | 2.80 | 120.53 | 116.00 |
| 47 | 31 | 309 | KC1 | CHD-C4C-NC | 2.80 | 128.52 | 124.31 |
| 48 | 14 | 313 | A86 | C25-C24-C1 | -2.80 | 118.70 | 126.36 |
| 37 | 34 | 307 | CLA | C1-C2-C3 | -2.79 | 121.62 | 126.20 |
| 37 | 19 | 303 | CLA | C4B-C3B-C2B | -2.79 | 103.83 | 107.30 |
| 37 | 33 | 307 | CLA | C4B-C3B-C2B | -2.79 | 103.83 | 107.30 |
| 47 | 13 | 306 | KC1 | C4C-C3C-C2C | -2.79 | 102.82 | 106.89 |
| 37 | 16 | 309 | CLA | C3B-C4B-NB | 2.79 | 113.02 | 110.53 |
| 37 | 33 | 303 | CLA | C4C-C3C-C2C | -2.79 | 102.83 | 106.89 |
| 37 | B | 511 | CLA | CHD-C4C-NC | 2.79 | 128.56 | 124.23 |
| 37 | 39 | 302 | CLA | CHD-C4C-NC | 2.79 | 128.56 | 124.23 |
| 37 | b | 509 | CLA | CAC-C3C-C4C | 2.79 | 128.42 | 124.79 |
| 47 | 14 | 306 | KC1 | CAC-C3C-C4C | 2.79 | 128.42 | 124.79 |
| 48 | 35 | 315 | A86 | C10-C9-C8 | -2.79 | 115.11 | 123.20 |
| 37 | 31 | 310 | CLA | CHD-C4C-NC | 2.79 | 128.56 | 124.23 |
| 37 | 39 | 306 | CLA | O2A-CGA-CBA | 2.79 | 120.35 | 111.83 |
| 37 | C | 504 | CLA | C4A-NA-C1A | -2.79 | 105.41 | 106.68 |
| 47 | 34 | 306 | KC1 | CHD-C1D-ND | -2.79 | 119.86 | 124.05 |
| 37 | c | 511 | CLA | O2A-CGA-CBA | 2.79 | 120.35 | 111.83 |
| 37 | B | 509 | CLA | CAC-C3C-C4C | 2.79 | 128.42 | 124.79 |
| 47 | 15 | 306 | KC1 | CMB-C2B-C1B | 2.79 | 129.65 | 124.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 523 | CLA | CMC-C2C-C1C | 2.79 | 129.40 | 125.03 |
| 37 | 39 | 303 | CLA | CMB-C2B-C1B | 2.79 | 129.67 | 125.42 |
| 47 | 21 | 207 | KC1 | O2D-CGD-O1D | -2.79 | 118.41 | 123.85 |
| 37 | b | 505 | CLA | C1-C2-C3 | -2.79 | 121.62 | 126.20 |
| 37 | c | 513 | CLA | C1-C2-C3 | -2.79 | 121.62 | 126.20 |
| 37 | 37 | 306 | CLA | C4C-C3C-C2C | -2.79 | 102.83 | 106.89 |
| 48 | 31 | 319 | A86 | O4-C38-O5 | -2.79 | 117.60 | 122.99 |
| 48 | 17 | 310 | A86 | C9-C10-C11 | -2.79 | 118.75 | 126.64 |
| 37 | 19 | 303 | CLA | CMB-C2B-C1B | 2.79 | 129.67 | 125.42 |
| 37 | 33 | 305 | CLA | C4C-C3C-C2C | -2.79 | 102.83 | 106.89 |
| 37 | b | 501 | CLA | C4-C3-C5 | 2.79 | 120.07 | 115.23 |
| 37 | 20 | 307 | CLA | CHD-C4C-NC | 2.79 | 128.56 | 124.23 |
| 37 | 13 | 305 | CLA | C4B-C3B-C2B | -2.79 | 103.83 | 107.30 |
| 37 | 33 | 301 | CLA | CHB-C4A-NA | 2.79 | 128.43 | 124.40 |
| 48 | 34 | 314 | A86 | C21-C20-C15 | -2.79 | 114.34 | 123.35 |
| 50 | 20 | 312 | DD6 | C24-C1-C2 | -2.79 | 114.62 | 119.01 |
| 37 | 14 | 305 | CLA | C4C-C3C-C2C | -2.79 | 102.83 | 106.89 |
| 46 | V | 201 | HEM | CAC-C3C-C4C | 2.79 | 131.48 | 124.82 |
| 37 | 18 | 211 | CLA | O2D-CGD-O1D | -2.79 | 118.42 | 123.85 |
| 37 | b | 507 | CLA | O2D-CGD-O1D | -2.79 | 118.42 | 123.85 |
| 37 | C | 511 | CLA | CHD-C4C-NC | 2.79 | 128.55 | 124.23 |
| 37 | z | 102 | CLA | C4B-C3B-C2B | -2.79 | 103.84 | 107.30 |
| 37 | 13 | 305 | CLA | CAC-C3C-C4C | 2.79 | 128.42 | 124.79 |
| 46 | v | 201 | HEM | CAC-C3C-C4C | 2.79 | 131.47 | 124.82 |
| 48 | 17 | 311 | A86 | C25-C24-C1 | -2.79 | 118.72 | 126.36 |
| 37 | 40 | 205 | CLA | CMC-C2C-C1C | 2.79 | 129.39 | 125.03 |
| 39 | a | 413 | BCR | C15-C16-C17 | -2.79 | 117.82 | 123.52 |
| 48 | 41 | 215 | A86 | C12-C11-C13 | 2.79 | 120.52 | 116.00 |
| 37 | b | 507 | CLA | C1-C2-C3 | -2.79 | 121.63 | 126.20 |
| 47 | 12 | 211 | KC1 | O2D-CGD-O1D | -2.79 | 118.43 | 123.85 |
| 39 | c | 519 | BCR | C27-C26-C25 | 2.79 | 126.47 | 122.70 |
| 47 | 36 | 302 | KC1 | C4C-C3C-C2C | -2.79 | 102.84 | 106.89 |
| 37 | 19 | 301 | CLA | CAC-C3C-C4C | 2.79 | 128.41 | 124.79 |
| 37 | c | 508 | CLA | CHD-C4C-NC | 2.79 | 128.55 | 124.23 |
| 48 | 19 | 311 | A86 | C28-C27-C26 | 2.78 | 127.33 | 122.82 |
| 37 | Z | 102 | CLA | C4B-C3B-C2B | -2.78 | 103.84 | 107.30 |
| 37 | B | 516 | CLA | O1D-CGD-CBD | -2.78 | 119.03 | 124.52 |
| 37 | b | 503 | CLA | CAC-C3C-C4C | 2.78 | 128.41 | 124.79 |
| 37 | 39 | 309 | CLA | C4C-C3C-C2C | -2.78 | 102.84 | 106.89 |
| 37 | 41 | 206 | CLA | C4C-C3C-C2C | -2.78 | 102.84 | 106.89 |
| 37 | W | 101 | CLA | CAC-C3C-C4C | 2.78 | 128.41 | 124.79 |
| 47 | 16 | 302 | KC1 | CHD-C1D-ND | -2.78 | 119.87 | 124.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 503 | CLA | CHD-C4C-NC | 2.78 | 128.55 | 124.23 |
| 47 | 15 | 309 | KC1 | CHD-C4C-NC | 2.78 | 128.50 | 124.31 |
| 37 | C | 511 | CLA | O2A-CGA-CBA | 2.78 | 120.32 | 111.83 |
| 37 | B | 503 | CLA | CAC-C3C-C4C | 2.78 | 128.41 | 124.79 |
| 47 | 15 | 302 | KC1 | CHD-C4C-NC | 2.78 | 128.50 | 124.31 |
| 40 | 40 | 202 | SQD | O48-C23-C24 | 2.78 | 120.32 | 111.83 |
| 37 | w | 101 | CLA | CAC-C3C-C4C | 2.78 | 128.41 | 124.79 |
| 37 | 13 | 301 | CLA | CAC-C3C-C4C | 2.78 | 128.41 | 124.79 |
| 40 | a | 409 | SQD | O48-C23-C24 | 2.78 | 120.32 | 111.83 |
| 37 | 15 | 305 | CLA | C4C-C3C-C2C | -2.78 | 102.84 | 106.89 |
| 37 | b | 515 | CLA | O2A-CGA-O1A | -2.78 | 116.67 | 123.63 |
| 50 | 40 | 214 | DD6 | C24-C1-C2 | -2.78 | 114.64 | 119.01 |
| 37 | 33 | 307 | CLA | CHB-C4A-NA | 2.78 | 128.41 | 124.40 |
| 37 | C | 505 | CLA | CAA-C2A-C3A | -2.78 | 105.48 | 113.00 |
| 37 | 20 | 303 | CLA | CMC-C2C-C1C | 2.78 | 129.38 | 125.03 |
| 37 | c | 513 | CLA | CAC-C3C-C4C | 2.78 | 128.41 | 124.79 |
| 47 | 11 | 309 | KC1 | O2D-CGD-O1D | -2.78 | 118.44 | 123.85 |
| 37 | 37 | 303 | CLA | C4-C3-C5 | 2.78 | 120.05 | 115.23 |
| 47 | 18 | 205 | KC1 | C4C-C3C-C2C | -2.78 | 102.85 | 106.89 |
| 37 | 19 | 301 | CLA | CHC-C1C-C2C | -2.78 | 119.05 | 126.95 |
| 37 | 19 | 302 | CLA | CHD-C4C-NC | 2.78 | 128.54 | 124.23 |
| 40 | 40 | 202 | SQD | O9-S-C6 | 2.78 | 110.91 | 106.76 |
| 37 | 41 | 208 | CLA | O2A-CGA-CBA | 2.78 | 120.31 | 111.83 |
| 37 | C | 513 | CLA | CMC-C2C-C1C | 2.78 | 129.38 | 125.03 |
| 37 | 38 | 209 | CLA | O2A-CGA-CBA | 2.78 | 120.31 | 111.83 |
| 37 | 19 | 306 | CLA | O2A-CGA-CBA | 2.78 | 120.31 | 111.83 |
| 37 | 17 | 307 | CLA | C4C-C3C-C2C | -2.78 | 102.85 | 106.89 |
| 37 | C | 504 | CLA | CHD-C4C-NC | 2.78 | 128.54 | 124.23 |
| 37 | 39 | 305 | CLA | CHD-C4C-NC | 2.78 | 128.54 | 124.23 |
| 48 | 38 | 214 | A86 | C21-C20-C15 | -2.78 | 114.39 | 123.35 |
| 41 | b | 519 | LMG | C1-C2-C3 | -2.78 | 104.17 | 110.01 |
| 41 | d | 409 | LMG | O6-C1-O1 | -2.78 | 103.48 | 110.04 |
| 37 | W | 101 | CLA | C4B-C3B-C2B | -2.78 | 103.85 | 107.30 |
| 48 | 15 | 315 | A86 | C10-C9-C8 | -2.78 | 115.16 | 123.20 |
| 37 | B | 506 | CLA | O2A-CGA-O1A | -2.77 | 116.69 | 123.63 |
| 37 | 18 | 201 | CLA | C3B-C4B-NB | 2.77 | 113.01 | 110.53 |
| 37 | B | 515 | CLA | O2A-CGA-O1A | -2.77 | 116.69 | 123.63 |
| 37 | 19 | 306 | CLA | C1C-C2C-C3C | -2.77 | 104.06 | 106.98 |
| 37 | 21 | 204 | CLA | C3C-C4C-NC | 2.77 | 113.98 | 110.43 |
| 37 | 14 | 308 | CLA | C4C-C3C-C2C | -2.77 | 102.85 | 106.89 |
| 37 | B | 507 | CLA | C1-C2-C3 | -2.77 | 121.65 | 126.20 |
| 37 | 33 | 305 | CLA | CMB-C2B-C1B | 2.77 | 129.64 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 36 | 313 | A86 | C41-C32-C31 | -2.77 | 107.99 | 110.47 |
| 48 | 12 | 213 | A86 | C23-C16-C22 | -2.77 | 103.34 | 107.37 |
| 48 | 34 | 316 | A86 | C36-C31-C32 | -2.77 | 116.94 | 119.70 |
| 37 | b | 507 | CLA | CHB-C4A-NA | 2.77 | 128.40 | 124.40 |
| 37 | 41 | 204 | CLA | C3C-C4C-NC | 2.77 | 113.98 | 110.43 |
| 48 | 12 | 202 | A86 | C21-C20-C15 | -2.77 | 114.40 | 123.35 |
| 47 | 40 | 204 | KC1 | CAC-C3C-C4C | 2.77 | 128.40 | 124.79 |
| 48 | 39 | 311 | A86 | C28-C27-C26 | 2.77 | 127.31 | 122.82 |
| 37 | 39 | 303 | CLA | C4B-C3B-C2B | -2.77 | 103.86 | 107.30 |
| 37 | W | 102 | CLA | CHD-C4C-NC | 2.77 | 128.53 | 124.23 |
| 37 | B | 507 | CLA | CHB-C4A-NA | 2.77 | 128.40 | 124.40 |
| 47 | 38 | 207 | KC1 | CHD-C4C-NC | 2.77 | 128.49 | 124.31 |
| 37 | B | 501 | CLA | C4B-C3B-C2B | -2.77 | 103.86 | 107.30 |
| 37 | 11 | 305 | CLA | CHD-C4C-NC | 2.77 | 128.53 | 124.23 |
| 37 | 37 | 308 | CLA | CAA-CBA-CGA | -2.77 | 105.34 | 113.21 |
| 37 | 13 | 307 | CLA | CHB-C4A-NA | 2.77 | 128.40 | 124.40 |
| 37 | D | 406 | CLA | O2A-CGA-CBA | 2.77 | 120.28 | 111.83 |
| 37 | B | 516 | CLA | O2D-CGD-O1D | -2.77 | 118.45 | 123.85 |
| 41 | 11 | 317 | LMG | O6-C1-O1 | -2.77 | 103.50 | 110.04 |
| 37 | 33 | 305 | CLA | C4B-C3B-C2B | -2.77 | 103.86 | 107.30 |
| 47 | 32 | 212 | KC1 | CBC-CAC-C3C | -2.77 | 104.91 | 112.42 |
| 47 | 35 | 302 | KC1 | CBC-CAC-C3C | -2.77 | 104.91 | 112.42 |
| 37 | Z | 101 | CLA | C1-C2-C3 | -2.77 | 121.66 | 126.20 |
| 37 | C | 505 | CLA | CAC-C3C-C4C | 2.77 | 128.39 | 124.79 |
| 37 | 34 | 308 | CLA | C4C-C3C-C2C | -2.77 | 102.86 | 106.89 |
| 37 | 17 | 304 | CLA | CBC-CAC-C3C | -2.77 | 104.91 | 112.42 |
| 37 | z | 101 | CLA | C1-C2-C3 | -2.77 | 121.66 | 126.20 |
| 47 | 36 | 304 | KC1 | C4C-C3C-C2C | -2.77 | 102.86 | 106.89 |
| 47 | 40 | 207 | KC1 | O1D-CGD-CBD | -2.77 | 119.06 | 124.52 |
| 37 | b | 516 | CLA | O2D-CGD-O1D | -2.77 | 118.46 | 123.85 |
| 37 | 32 | 213 | CLA | C3B-C4B-NB | 2.77 | 113.00 | 110.53 |
| 37 | Z | 102 | CLA | C4C-C3C-C2C | -2.77 | 102.86 | 106.89 |
| 47 | 33 | 306 | KC1 | C4C-C3C-C2C | -2.77 | 102.86 | 106.89 |
| 37 | 11 | 308 | CLA | CMB-C2B-C1B | 2.77 | 129.63 | 125.42 |
| 50 | 36 | 312 | DD6 | C35-C36-C31 | -2.77 | 114.74 | 120.50 |
| 41 | 31 | 316 | LMG | C1-O6-C5 | -2.77 | 108.32 | 113.72 |
| 48 | 39 | 311 | A86 | C7-C6-C8 | 2.77 | 122.31 | 118.09 |
| 48 | 37 | 309 | A86 | C25-C24-C1 | -2.77 | 118.78 | 126.36 |
| 47 | 34 | 306 | KC1 | CAC-C3C-C4C | 2.77 | 128.39 | 124.79 |
| 37 | 37 | 303 | CLA | CBC-CAC-C3C | -2.77 | 104.92 | 112.42 |
| 48 | 32 | 203 | A86 | C21-C20-C15 | -2.77 | 114.42 | 123.35 |
| 37 | b | 509 | CLA | CMC-C2C-C1C | 2.77 | 129.36 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 20 | 301 | CLA | CMB-C2B-C1B | 2.77 | 129.63 | 125.42 |
| 37 | 34 | 305 | CLA | C4C-C3C-C2C | -2.77 | 102.87 | 106.89 |
| 47 | 12 | 211 | KC1 | CBC-CAC-C3C | -2.77 | 104.92 | 112.42 |
| 40 | A | 407 | SQD | O48-C23-C24 | 2.77 | 120.27 | 111.83 |
| 47 | 20 | 305 | KC1 | CAC-C3C-C4C | 2.77 | 128.39 | 124.79 |
| 37 | B | 505 | CLA | CHC-C1C-C2C | -2.77 | 119.09 | 126.95 |
| 37 | 39 | 301 | CLA | CHC-C1C-C2C | -2.77 | 119.09 | 126.95 |
| 48 | 35 | 319 | A86 | C-C1-C24 | 2.77 | 122.31 | 118.09 |
| 37 | 32 | 210 | CLA | C3B-C4B-NB | 2.76 | 113.00 | 110.53 |
| 37 | 11 | 307 | CLA | CHC-C1C-C2C | -2.76 | 119.09 | 126.95 |
| 48 | 34 | 313 | A86 | C25-C24-C1 | -2.76 | 118.78 | 126.36 |
| 37 | z | 102 | CLA | C4C-C3C-C2C | -2.76 | 102.87 | 106.89 |
| 47 | 18 | 205 | KC1 | CHD-C4C-NC | 2.76 | 128.47 | 124.31 |
| 48 | 15 | 319 | A86 | C-C1-C24 | 2.76 | 122.31 | 118.09 |
| 37 | 32 | 210 | CLA | C1-C2-C3 | -2.76 | 121.67 | 126.20 |
| 37 | 32 | 202 | CLA | CMB-C2B-C1B | 2.76 | 129.63 | 125.42 |
| 37 | B | 510 | CLA | C3B-C4B-NB | 2.76 | 113.00 | 110.53 |
| 37 | A | 405 | CLA | CMC-C2C-C1C | 2.76 | 129.35 | 125.03 |
| 37 | 18 | 209 | CLA | CAC-C3C-C4C | 2.76 | 128.38 | 124.79 |
| 48 | 12 | 215 | A86 | C21-C20-C15 | -2.76 | 114.43 | 123.35 |
| 37 | d | 404 | CLA | O2A-CGA-CBA | 2.76 | 120.26 | 111.83 |
| 37 | 19 | 310 | CLA | CHD-C4C-NC | 2.76 | 128.51 | 124.23 |
| 44 | J | 101 | DGD | CDB-CCB-CBB | -2.76 | 100.40 | 114.37 |
| 40 | 16 | 315 | SQD | O48-C23-C24 | 2.76 | 120.26 | 111.83 |
| 44 | j | 101 | DGD | CDB-CCB-CBB | -2.76 | 100.41 | 114.37 |
| 47 | 16 | 304 | KC1 | C4C-C3C-C2C | -2.76 | 102.87 | 106.89 |
| 48 | 15 | 315 | A86 | C36-C31-C32 | -2.76 | 116.96 | 119.70 |
| 48 | 34 | 314 | A86 | C40-C32-C31 | -2.76 | 108.00 | 110.47 |
| 37 | 35 | 305 | CLA | CAC-C3C-C4C | 2.76 | 128.38 | 124.79 |
| 37 | 15 | 305 | CLA | CHD-C4C-NC | 2.76 | 128.51 | 124.23 |
| 50 | 41 | 212 | DD6 | C19-C18-C17 | 2.76 | 115.95 | 110.79 |
| 47 | 11 | 304 | KC1 | CAA-CBA-CGA | -2.76 | 113.01 | 127.05 |
| 48 | 18 | 214 | A86 | C21-C20-C15 | -2.76 | 114.44 | 123.35 |
| 37 | 20 | 306 | CLA | C3B-C4B-NB | 2.76 | 112.99 | 110.53 |
| 47 | 16 | 302 | KC1 | C4C-C3C-C2C | -2.76 | 102.87 | 106.89 |
| 37 | b | 506 | CLA | CAA-C2A-C3A | -2.76 | 105.54 | 113.00 |
| 41 | B | 520 | LMG | C1-C2-C3 | -2.76 | 104.20 | 110.01 |
| 47 | 11 | 309 | KC1 | CAA-CBA-CGA | -2.76 | 113.02 | 127.05 |
| 50 | 16 | 312 | DD6 | C35-C36-C31 | -2.76 | 114.76 | 120.50 |
| 50 | 21 | 216 | DD6 | C37-C36-C35 | -2.76 | 109.35 | 114.42 |
| 37 | b | 506 | CLA | O2A-CGA-O1A | -2.76 | 116.73 | 123.63 |
| 37 | C | 505 | CLA | O1D-CGD-CBD | -2.76 | 119.08 | 124.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 19 | 305 | CLA | CHD-C4C-NC | 2.76 | 128.51 | 124.23 |
| 48 | 19 | 311 | A86 | C7-C6-C8 | 2.76 | 122.30 | 118.09 |
| 47 | 31 | 309 | KC1 | CAA-CBA-CGA | -2.76 | 113.03 | 127.05 |
| 37 | 16 | 306 | CLA | CHD-C4C-NC | 2.76 | 128.51 | 124.23 |
| 37 | b | 505 | CLA | CHC-C1C-C2C | -2.76 | 119.11 | 126.95 |
| 37 | 11 | 307 | CLA | C3B-C4B-NB | 2.76 | 112.99 | 110.53 |
| 47 | 15 | 306 | KC1 | CAC-C3C-C4C | 2.76 | 128.38 | 124.79 |
| 37 | B | 506 | CLA | CAA-C2A-C3A | -2.76 | 105.55 | 113.00 |
| 41 | a | 410 | LMG | C1-C2-C3 | -2.76 | 104.21 | 110.01 |
| 37 | 32 | 204 | CLA | C4-C3-C5 | 2.75 | 120.01 | 115.23 |
| 41 | D | 412 | LMG | O6-C1-O1 | -2.75 | 103.53 | 110.04 |
| 37 | 39 | 310 | CLA | CHD-C4C-NC | 2.75 | 128.50 | 124.23 |
| 37 | A | 405 | CLA | O2D-CGD-O1D | -2.75 | 118.49 | 123.85 |
| 37 | B | 507 | CLA | O2D-CGD-O1D | -2.75 | 118.49 | 123.85 |
| 37 | 14 | 308 | CLA | CAA-C2A-C3A | -2.75 | 105.56 | 113.00 |
| 37 | 34 | 308 | CLA | CAA-C2A-C3A | -2.75 | 105.56 | 113.00 |
| 37 | 13 | 307 | CLA | CGD-CBD-CAD | -2.75 | 101.93 | 110.85 |
| 37 | C | 513 | CLA | CAC-C3C-C4C | 2.75 | 128.37 | 124.79 |
| 37 | 11 | 303 | CLA | C4C-C3C-C2C | -2.75 | 102.88 | 106.89 |
| 37 | 16 | 307 | CLA | C4C-C3C-C2C | -2.75 | 102.89 | 106.89 |
| 37 | 21 | 208 | CLA | C4C-C3C-C2C | -2.75 | 102.89 | 106.89 |
| 37 | c | 504 | CLA | CHD-C4C-NC | 2.75 | 128.50 | 124.23 |
| 37 | 11 | 310 | CLA | CHD-C4C-NC | 2.75 | 128.50 | 124.23 |
| 37 | 33 | 301 | CLA | CAC-C3C-C4C | 2.75 | 128.37 | 124.79 |
| 37 | b | 514 | CLA | CMC-C2C-C1C | 2.75 | 129.34 | 125.03 |
| 37 | 37 | 301 | CLA | CHB-C4A-NA | 2.75 | 128.37 | 124.40 |
| 48 | 33 | 314 | A86 | C40-C32-C31 | -2.75 | 108.01 | 110.47 |
| 50 | 41 | 216 | DD6 | C37-C36-C35 | -2.75 | 109.36 | 114.42 |
| 37 | 31 | 306 | CLA | CHD-C4C-NC | 2.75 | 128.50 | 124.23 |
| 48 | 40 | 201 | A86 | O4-C34-C35 | 2.75 | 114.68 | 107.64 |
| 47 | 36 | 308 | KC1 | CMB-C2B-C1B | 2.75 | 129.57 | 124.73 |
| 37 | 31 | 308 | CLA | C3B-C4B-NB | 2.75 | 112.99 | 110.53 |
| 37 | b | 504 | CLA | CMC-C2C-C1C | 2.75 | 129.33 | 125.03 |
| 48 | 31 | 312 | A86 | C10-C9-C8 | -2.75 | 115.23 | 123.20 |
| 48 | 31 | 314 | A86 | C35-C34-C33 | 2.75 | 114.83 | 109.89 |
| 48 | 11 | 314 | A86 | C36-C31-C32 | -2.75 | 116.97 | 119.70 |
| 41 | 11 | 316 | LMG | C1-O6-C5 | -2.75 | 108.35 | 113.72 |
| 37 | B | 509 | CLA | CMC-C2C-C1C | 2.75 | 129.33 | 125.03 |
| 37 | 40 | 208 | CLA | CMC-C2C-C1C | 2.75 | 129.33 | 125.03 |
| 47 | 20 | 302 | KC1 | CMB-C2B-C1B | 2.75 | 129.57 | 124.73 |
| 37 | 31 | 301 | CLA | CAC-C3C-C4C | 2.75 | 128.37 | 124.79 |
| 47 | 20 | 302 | KC1 | CAC-C3C-C4C | 2.75 | 128.37 | 124.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 206 | CLA | C4C-C3C-C2C | -2.75 | 102.89 | 106.89 |
| 48 | 32 | 214 | A86 | C3-C4-C5 | -2.75 | 117.89 | 123.52 |
| 47 | 15 | 302 | KC1 | CBC-CAC-C3C | -2.75 | 104.97 | 112.42 |
| 37 | 38 | 201 | CLA | CHC-C1C-C2C | -2.75 | 119.14 | 126.95 |
| 37 | B | 507 | CLA | CHD-C4C-NC | 2.75 | 128.49 | 124.23 |
| 37 | 21 | 208 | CLA | CHD-C4C-NC | 2.75 | 128.49 | 124.23 |
| 37 | 12 | 209 | CLA | C3B-C4B-NB | 2.75 | 112.98 | 110.53 |
| 37 | w | 101 | CLA | CMB-C2B-C1B | 2.75 | 129.60 | 125.42 |
| 37 | 36 | 307 | CLA | C4C-C3C-C2C | -2.75 | 102.89 | 106.89 |
| 48 | 20 | 311 | A86 | C41-C32-C31 | -2.75 | 108.01 | 110.47 |
| 37 | 11 | 308 | CLA | CBC-CAC-C3C | -2.75 | 104.97 | 112.42 |
| 37 | 38 | 201 | CLA | CHD-C4C-NC | 2.75 | 128.49 | 124.23 |
| 47 | 32 | 207 | KC1 | CAA-CBA-CGA | -2.75 | 113.08 | 127.05 |
| 37 | c | 505 | CLA | O1D-CGD-CBD | -2.75 | 119.10 | 124.52 |
| 37 | W | 102 | CLA | CAC-C3C-C4C | 2.75 | 128.36 | 124.79 |
| 37 | c | 505 | CLA | CAC-C3C-C4C | 2.75 | 128.36 | 124.79 |
| 47 | 31 | 305 | KC1 | CAA-CBA-CGA | -2.75 | 113.09 | 127.05 |
| 47 | 16 | 308 | KC1 | CMB-C2B-C1B | 2.75 | 129.56 | 124.73 |
| 48 | 12 | 217 | A86 | C40-C32-C31 | 2.75 | 112.93 | 110.47 |
| 37 | 38 | 202 | CLA | C1-C2-C3 | -2.74 | 121.70 | 126.20 |
| 48 | 32 | 216 | A86 | C21-C20-C15 | -2.74 | 114.49 | 123.35 |
| 37 | 19 | 305 | CLA | CAC-C3C-C4C | 2.74 | 128.36 | 124.79 |
| 37 | 31 | 308 | CLA | CHC-C1C-C2C | -2.74 | 119.15 | 126.95 |
| 37 | 31 | 304 | CLA | C4C-C3C-C2C | -2.74 | 102.90 | 106.89 |
| 37 | 20 | 306 | CLA | CMC-C2C-C1C | 2.74 | 129.32 | 125.03 |
| 37 | 32 | 202 | CLA | CMC-C2C-C1C | 2.74 | 129.32 | 125.03 |
| 37 | 35 | 301 | CLA | C3B-C4B-NB | 2.74 | 112.98 | 110.53 |
| 37 | b | 505 | CLA | CAA-C2A-C3A | -2.74 | 105.59 | 113.00 |
| 37 | B | 504 | CLA | CMC-C2C-C1C | 2.74 | 129.32 | 125.03 |
| 37 | 31 | 301 | CLA | CHD-C4C-NC | 2.74 | 128.48 | 124.23 |
| 37 | 34 | 302 | CLA | CAC-C3C-C4C | 2.74 | 128.36 | 124.79 |
| 48 | 13 | 314 | A86 | C40-C32-C31 | -2.74 | 108.02 | 110.47 |
| 37 | 19 | 304 | CLA | C4B-C3B-C2B | -2.74 | 103.89 | 107.30 |
| 48 | 11 | 312 | A86 | C10-C9-C8 | -2.74 | 115.26 | 123.20 |
| 37 | 39 | 305 | CLA | CBC-CAC-C3C | -2.74 | 104.99 | 112.42 |
| 37 | 33 | 307 | CLA | CGD-CBD-CAD | -2.74 | 101.97 | 110.85 |
| 37 | 19 | 309 | CLA | CHD-C4C-NC | 2.74 | 128.48 | 124.23 |
| 37 | 38 | 209 | CLA | CHD-C4C-NC | 2.74 | 128.48 | 124.23 |
| 39 | B | 517 | BCR | C7-C8-C9 | -2.74 | 122.18 | 126.23 |
| 47 | 12 | 206 | KC1 | CAA-CBA-CGA | -2.74 | 113.11 | 127.05 |
| 48 | 17 | 311 | A86 | C10-C9-C8 | -2.74 | 115.26 | 123.20 |
| 37 | 16 | 303 | CLA | CHD-C4C-NC | 2.74 | 128.48 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 508 | CLA | C3B-C4B-NB | 2.74 | 112.98 | 110.53 |
| 48 | 34 | 314 | A86 | C25-C24-C1 | -2.74 | 118.85 | 126.36 |
| 48 | 11 | 319 | A86 | C8-C6-C5 | -2.74 | 114.70 | 119.01 |
| 48 | 14 | 314 | A86 | C40-C32-C31 | -2.74 | 108.02 | 110.47 |
| 47 | 31 | 309 | KC1 | O2D-CGD-O1D | -2.74 | 118.52 | 123.85 |
| 37 | a | 407 | CLA | CMC-C2C-C1C | 2.74 | 129.31 | 125.03 |
| 37 | 15 | 303 | CLA | C4C-C3C-C2C | -2.74 | 102.91 | 106.89 |
| 37 | W | 101 | CLA | CMB-C2B-C1B | 2.74 | 129.59 | 125.42 |
| 40 | 16 | 315 | SQD | O9-S-C6 | 2.74 | 110.84 | 106.76 |
| 37 | B | 506 | CLA | CHC-C1C-C2C | -2.74 | 119.17 | 126.95 |
| 50 | 21 | 212 | DD6 | C19-C18-C17 | 2.74 | 115.91 | 110.79 |
| 48 | 16 | 314 | A86 | C41-C32-C31 | -2.74 | 108.02 | 110.47 |
| 45 | D | 404 | PL9 | C7-C8-C9 | -2.74 | 122.12 | 126.83 |
| 37 | c | 513 | CLA | CMC-C2C-C1C | 2.74 | 129.31 | 125.03 |
| 48 | 32 | 218 | A86 | C36-C31-C32 | -2.73 | 116.98 | 119.70 |
| 39 | b | 517 | BCR | C7-C8-C9 | -2.73 | 122.19 | 126.23 |
| 37 | 39 | 305 | CLA | CAC-C3C-C4C | 2.73 | 128.35 | 124.79 |
| 37 | 35 | 305 | CLA | CMB-C2B-C1B | 2.73 | 129.58 | 125.42 |
| 48 | 37 | 310 | A86 | C25-C24-C1 | -2.73 | 118.86 | 126.36 |
| 37 | b | 510 | CLA | C3B-C4B-NB | 2.73 | 112.97 | 110.53 |
| 37 | a | 404 | CLA | O2D-CGD-O1D | -2.73 | 118.53 | 123.85 |
| 48 | 40 | 213 | A86 | C41-C32-C31 | -2.73 | 108.03 | 110.47 |
| 41 | A | 408 | LMG | C1-C2-C3 | -2.73 | 104.26 | 110.01 |
| 37 | B | 504 | CLA | C4C-C3C-C2C | -2.73 | 102.91 | 106.89 |
| 48 | 16 | 313 | A86 | O4-C34-C35 | 2.73 | 114.63 | 107.64 |
| 37 | 18 | 202 | CLA | C4B-C3B-C2B | -2.73 | 103.91 | 107.30 |
| 37 | B | 505 | CLA | CAA-C2A-C3A | -2.73 | 105.62 | 113.00 |
| 37 | b | 523 | CLA | CHD-C4C-NC | 2.73 | 128.47 | 124.23 |
| 37 | 38 | 208 | CLA | CAA-C2A-C3A | -2.73 | 105.62 | 113.00 |
| 37 | C | 507 | CLA | C4A-NA-C1A | -2.73 | 105.43 | 106.68 |
| 37 | w | 101 | CLA | C4B-C3B-C2B | -2.73 | 103.91 | 107.30 |
| 37 | w | 101 | CLA | CHD-C4C-NC | 2.73 | 128.47 | 124.23 |
| 37 | B | 524 | CLA | CHC-C1C-C2C | -2.73 | 119.19 | 126.95 |
| 48 | 32 | 217 | A86 | C34-O4-C38 | -2.73 | 113.03 | 117.85 |
| 37 | 11 | 308 | CLA | CMC-C2C-C1C | 2.73 | 129.30 | 125.03 |
| 48 | 38 | 214 | A86 | C12-C11-C13 | 2.73 | 120.42 | 116.00 |
| 37 | b | 507 | CLA | CHD-C4C-NC | 2.73 | 128.46 | 124.23 |
| 48 | 37 | 319 | A86 | C26-C25-C24 | -2.73 | 115.30 | 123.20 |
| 37 | b | 523 | CLA | CHC-C1C-C2C | -2.73 | 119.19 | 126.95 |
| 47 | 37 | 307 | KC1 | O2D-CGD-O1D | -2.73 | 118.54 | 123.85 |
| 37 | 39 | 309 | CLA | CHD-C4C-NC | 2.73 | 128.46 | 124.23 |
| 41 | 31 | 317 | LMG | O6-C1-O1 | -2.73 | 103.60 | 110.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 14 | 306 | KC1 | CHD-C1D-ND | -2.73 | 119.96 | 124.05 |
| 43 | D | 409 | LHG | O8-C23-C24 | 2.73 | 120.15 | 111.83 |
| 37 | 14 | 302 | CLA | CHB-C4A-NA | 2.73 | 128.34 | 124.40 |
| 47 | 11 | 309 | KC1 | CHB-C4A-NA | 2.73 | 128.46 | 124.23 |
| 37 | 39 | 304 | CLA | C4B-C3B-C2B | -2.73 | 103.91 | 107.30 |
| 37 | C | 513 | CLA | CHB-C4A-NA | 2.73 | 128.34 | 124.40 |
| 37 | b | 501 | CLA | C4C-C3C-C2C | -2.73 | 102.92 | 106.89 |
| 48 | 12 | 216 | A86 | C34-O4-C38 | -2.73 | 113.03 | 117.85 |
| 37 | 40 | 203 | CLA | CMB-C2B-C1B | 2.73 | 129.57 | 125.42 |
| 37 | B | 524 | CLA | CHD-C4C-NC | 2.73 | 128.46 | 124.23 |
| 37 | B | 505 | CLA | O2D-CGD-O1D | -2.72 | 118.54 | 123.85 |
| 43 | d | 407 | LHG | O8-C23-C24 | 2.72 | 120.14 | 111.83 |
| 40 | A | 407 | SQD | C1-C2-C3 | -2.72 | 104.28 | 110.01 |
| 37 | b | 501 | CLA | CHD-C4C-NC | 2.72 | 128.46 | 124.23 |
| 37 | C | 502 | CLA | C1C-C2C-C3C | -2.72 | 104.11 | 106.98 |
| 48 | 12 | 217 | A86 | C36-C31-C32 | -2.72 | 116.99 | 119.70 |
| 37 | 32 | 202 | CLA | CBC-CAC-C3C | -2.72 | 105.04 | 112.42 |
| 39 | B | 517 | BCR | C15-C16-C17 | -2.72 | 117.95 | 123.52 |
| 37 | 35 | 308 | CLA | CBC-CAC-C3C | -2.72 | 105.04 | 112.42 |
| 48 | 14 | 314 | A86 | C25-C24-C1 | -2.72 | 118.90 | 126.36 |
| 37 | 34 | 303 | CLA | CHD-C4C-NC | 2.72 | 128.45 | 124.23 |
| 37 | 19 | 310 | CLA | CAC-C3C-C4C | 2.72 | 128.33 | 124.79 |
| 47 | 15 | 304 | KC1 | CHD-C4C-NC | 2.72 | 128.41 | 124.31 |
| 37 | b | 505 | CLA | CHB-C4A-NA | 2.72 | 128.33 | 124.40 |
| 47 | 36 | 302 | KC1 | CHD-C1D-ND | -2.72 | 119.97 | 124.05 |
| 47 | 31 | 303 | KC1 | CAC-C3C-C4C | 2.72 | 128.33 | 124.79 |
| 37 | b | 506 | CLA | CHC-C1C-C2C | -2.72 | 119.21 | 126.95 |
| 39 | b | 524 | BCR | C15-C16-C17 | -2.72 | 117.95 | 123.52 |
| 48 | 31 | 319 | A86 | C8-C6-C5 | -2.72 | 114.73 | 119.01 |
| 37 | 12 | 209 | CLA | C1-C2-C3 | -2.72 | 121.74 | 126.20 |
| 48 | 18 | 213 | A86 | C41-C32-C31 | -2.72 | 108.04 | 110.47 |
| 39 | b | 517 | BCR | C15-C16-C17 | -2.72 | 117.95 | 123.52 |
| 47 | 16 | 302 | KC1 | C1A-NA-C4A | -2.72 | 105.44 | 106.68 |
| 37 | 14 | 303 | CLA | C1-O2A-CGA | 2.72 | 123.23 | 116.65 |
| 47 | 38 | 205 | KC1 | C4C-C3C-C2C | -2.72 | 102.93 | 106.89 |
| 48 | 13 | 315 | A86 | C12-C11-C13 | 2.72 | 120.41 | 116.00 |
| 37 | 12 | 203 | CLA | C4-C3-C5 | 2.72 | 119.95 | 115.23 |
| 37 | C | 513 | CLA | CHC-C1C-C2C | -2.72 | 119.22 | 126.95 |
| 37 | 17 | 307 | CLA | O2A-CGA-CBA | 2.72 | 120.12 | 111.83 |
| 37 | C | 509 | CLA | CHD-C4C-NC | 2.72 | 128.45 | 124.23 |
| 39 | B | 525 | BCR | C15-C16-C17 | -2.72 | 117.96 | 123.52 |
| 37 | 36 | 303 | CLA | CHD-C4C-NC | 2.72 | 128.45 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 33 | 315 | A86 | C12-C11-C13 | 2.72 | 120.41 | 116.00 |
| 37 | a | 404 | CLA | C4A-NA-C1A | -2.72 | 105.44 | 106.68 |
| 47 | 17 | 308 | KC1 | O2D-CGD-O1D | -2.72 | 118.56 | 123.85 |
| 37 | 32 | 204 | CLA | C4C-C3C-C2C | -2.72 | 102.94 | 106.89 |
| 37 | 41 | 206 | CLA | O2A-CGA-CBA | 2.72 | 120.12 | 111.83 |
| 47 | 11 | 302 | KC1 | CAC-C3C-C4C | 2.72 | 128.32 | 124.79 |
| 37 | B | 514 | CLA | CMC-C2C-C1C | 2.72 | 129.28 | 125.03 |
| 37 | 12 | 207 | CLA | C4B-C3B-C2B | -2.72 | 103.92 | 107.30 |
| 37 | 32 | 208 | CLA | C4B-C3B-C2B | -2.72 | 103.92 | 107.30 |
| 48 | 15 | 311 | A86 | C10-C9-C8 | -2.72 | 115.33 | 123.20 |
| 37 | 21 | 206 | CLA | O2A-CGA-CBA | 2.72 | 120.11 | 111.83 |
| 37 | 41 | 206 | CLA | CMC-C2C-C1C | 2.72 | 129.28 | 125.03 |
| 48 | 17 | 310 | A86 | C25-C24-C1 | -2.72 | 118.92 | 126.36 |
| 37 | B | 501 | CLA | CHD-C4C-NC | 2.71 | 128.44 | 124.23 |
| 37 | 13 | 303 | CLA | CHD-C4C-NC | 2.71 | 128.44 | 124.23 |
| 37 | 37 | 306 | CLA | CHB-C4A-NA | 2.71 | 128.32 | 124.40 |
| 37 | 41 | 208 | CLA | C4C-C3C-C2C | -2.71 | 102.94 | 106.89 |
| 48 | 32 | 214 | A86 | C23-C16-C22 | -2.71 | 103.43 | 107.37 |
| 37 | 35 | 305 | CLA | C4C-C3C-C2C | -2.71 | 102.94 | 106.89 |
| 47 | 35 | 306 | KC1 | CAC-C3C-C4C | 2.71 | 128.32 | 124.79 |
| 37 | b | 504 | CLA | C4C-C3C-C2C | -2.71 | 102.94 | 106.89 |
| 47 | 40 | 207 | KC1 | CAC-C3C-C4C | 2.71 | 128.32 | 124.79 |
| 37 | 40 | 205 | CLA | CMB-C2B-C1B | 2.71 | 129.55 | 125.42 |
| 48 | 17 | 313 | A86 | C34-O4-C38 | -2.71 | 113.06 | 117.85 |
| 37 | 14 | 302 | CLA | CAC-C3C-C4C | 2.71 | 128.32 | 124.79 |
| 48 | 35 | 311 | A86 | C10-C9-C8 | -2.71 | 115.34 | 123.20 |
| 47 | 40 | 204 | KC1 | CMB-C2B-C1B | 2.71 | 129.50 | 124.73 |
| 37 | 35 | 303 | CLA | C4C-C3C-C2C | -2.71 | 102.95 | 106.89 |
| 40 | a | 409 | SQD | C1-C2-C3 | -2.71 | 104.31 | 110.01 |
| 37 | c | 513 | CLA | CHB-C4A-NA | 2.71 | 128.31 | 124.40 |
| 37 | 31 | 310 | CLA | O2A-CGA-CBA | 2.71 | 120.10 | 111.83 |
| 47 | 31 | 309 | KC1 | CHB-C4A-NA | 2.71 | 128.43 | 124.23 |
| 37 | 12 | 203 | CLA | C4C-C3C-C2C | -2.71 | 102.95 | 106.89 |
| 37 | 16 | 306 | CLA | CHC-C1C-C2C | -2.71 | 119.25 | 126.95 |
| 37 | 18 | 209 | CLA | CHD-C4C-NC | 2.71 | 128.43 | 124.23 |
| 37 | 33 | 307 | CLA | CBC-CAC-C3C | -2.71 | 105.08 | 112.42 |
| 48 | 37 | 312 | A86 | C21-C20-C15 | -2.71 | 114.61 | 123.35 |
| 37 | A | 403 | CLA | C1-C2-C3 | -2.71 | 121.76 | 126.20 |
| 47 | 12 | 208 | KC1 | CHD-C1D-ND | -2.71 | 119.99 | 124.05 |
| 37 | C | 512 | CLA | CHD-C4C-NC | 2.71 | 128.43 | 124.23 |
| 48 | 12 | 215 | A86 | C12-C11-C13 | 2.71 | 120.39 | 116.00 |
| 47 | 38 | 210 | KC1 | CBC-CAC-C3C | -2.71 | 105.08 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 14 | 316 | A86 | C7-C6-C5 | -2.71 | 118.43 | 122.82 |
| 37 | 14 | 307 | CLA | C4B-C3B-C2B | -2.71 | 103.94 | 107.30 |
| 47 | 36 | 302 | KC1 | C1A-NA-C4A | -2.70 | 105.44 | 106.68 |
| 37 | a | 407 | CLA | O2D-CGD-O1D | -2.70 | 118.58 | 123.85 |
| 37 | z | 102 | CLA | O1D-CGD-CBD | -2.70 | 119.18 | 124.52 |
| 37 | c | 509 | CLA | CHD-C4C-NC | 2.70 | 128.42 | 124.23 |
| 37 | 34 | 303 | CLA | C1-O2A-CGA | 2.70 | 123.20 | 116.65 |
| 37 | C | 501 | CLA | CBC-CAC-C3C | -2.70 | 105.09 | 112.42 |
| 37 | 13 | 307 | CLA | CBC-CAC-C3C | -2.70 | 105.09 | 112.42 |
| 48 | 35 | 314 | A86 | C21-C20-C15 | -2.70 | 114.62 | 123.35 |
| 37 | 17 | 309 | CLA | CAA-CBA-CGA | -2.70 | 105.53 | 113.21 |
| 37 | 19 | 305 | CLA | CBC-CAC-C3C | -2.70 | 105.09 | 112.42 |
| 37 | 11 | 308 | CLA | O2A-CGA-CBA | 2.70 | 120.08 | 111.83 |
| 48 | 34 | 311 | A86 | C23-C16-C22 | -2.70 | 103.44 | 107.37 |
| 37 | c | 501 | CLA | CBC-CAC-C3C | -2.70 | 105.09 | 112.42 |
| 37 | 11 | 301 | CLA | C1C-C2C-C3C | -2.70 | 104.14 | 106.98 |
| 37 | 41 | 208 | CLA | CHD-C4C-NC | 2.70 | 128.42 | 124.23 |
| 37 | 31 | 308 | CLA | C1-C2-C3 | -2.70 | 121.77 | 126.20 |
| 48 | 32 | 217 | A86 | C21-C20-C15 | -2.70 | 114.63 | 123.35 |
| 37 | B | 524 | CLA | CAC-C3C-C4C | 2.70 | 128.31 | 124.79 |
| 48 | 12 | 216 | A86 | C21-C20-C15 | -2.70 | 114.63 | 123.35 |
| 37 | 39 | 301 | CLA | CHB-C4A-NA | 2.70 | 128.30 | 124.40 |
| 47 | 18 | 210 | KC1 | CBC-CAC-C3C | -2.70 | 105.10 | 112.42 |
| 37 | 34 | 303 | CLA | C4B-C3B-C2B | -2.70 | 103.94 | 107.30 |
| 37 | 39 | 305 | CLA | C1-O2A-CGA | 2.70 | 123.19 | 116.65 |
| 45 | d | 402 | PL9 | C7-C8-C9 | -2.70 | 122.18 | 126.83 |
| 37 | 32 | 202 | CLA | O2A-CGA-CBA | 2.70 | 120.06 | 111.83 |
| 37 | D | 405 | CLA | CMB-C2B-C1B | 2.70 | 129.53 | 125.42 |
| 37 | b | 508 | CLA | C3B-C4B-NB | 2.70 | 112.94 | 110.53 |
| 47 | 33 | 309 | KC1 | CMB-C2B-C1B | 2.70 | 129.48 | 124.73 |
| 37 | b | 506 | CLA | CMC-C2C-C1C | 2.70 | 129.25 | 125.03 |
| 37 | 36 | 306 | CLA | CHC-C1C-C2C | -2.70 | 119.28 | 126.95 |
| 37 | a | 403 | CLA | C1-C2-C3 | -2.70 | 121.78 | 126.20 |
| 47 | 13 | 309 | KC1 | O2D-CGD-O1D | -2.70 | 118.60 | 123.85 |
| 47 | 16 | 302 | KC1 | CAB-C3B-C4B | 2.70 | 131.26 | 124.82 |
| 48 | 19 | 313 | A86 | C-C1-C24 | 2.70 | 122.21 | 118.09 |
| 48 | 13 | 314 | A86 | C22-C16-C17 | -2.70 | 104.23 | 108.97 |
| 37 | D | 401 | CLA | O2D-CGD-O1D | -2.70 | 118.60 | 123.85 |
| 48 | 15 | 314 | A86 | C25-C24-C1 | -2.70 | 118.97 | 126.36 |
| 48 | 32 | 214 | A86 | C21-C20-C15 | -2.70 | 114.65 | 123.35 |
| 39 | a | 408 | BCR | C15-C14-C13 | -2.70 | 123.50 | 127.28 |
| 48 | 18 | 212 | A86 | C12-C11-C13 | 2.70 | 120.37 | 116.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 505 | CLA | O2D-CGD-O1D | -2.70 | 118.60 | 123.85 |
| 37 | 33 | 301 | CLA | C4-C3-C5 | 2.70 | 119.91 | 115.23 |
| 37 | W | 101 | CLA | CHD-C4C-NC | 2.69 | 128.41 | 124.23 |
| 47 | 15 | 302 | KC1 | C4C-C3C-C2C | -2.69 | 102.97 | 106.89 |
| 37 | c | 512 | CLA | CHD-C4C-NC | 2.69 | 128.41 | 124.23 |
| 47 | 15 | 306 | KC1 | C4C-C3C-C2C | -2.69 | 102.97 | 106.89 |
| 48 | 35 | 312 | A86 | C10-C9-C8 | -2.69 | 115.39 | 123.20 |
| 48 | 12 | 213 | A86 | C21-C20-C15 | -2.69 | 114.65 | 123.35 |
| 37 | c | 513 | CLA | CHC-C1C-C2C | -2.69 | 119.29 | 126.95 |
| 47 | 35 | 302 | KC1 | C4C-C3C-C2C | -2.69 | 102.97 | 106.89 |
| 47 | 17 | 306 | KC1 | CHC-C4B-C3B | -2.69 | 120.67 | 125.21 |
| 47 | 21 | 207 | KC1 | CAA-C2A-C1A | -2.69 | 112.84 | 124.64 |
| 37 | w | 101 | CLA | CGD-CBD-CAD | 2.69 | 119.56 | 110.85 |
| 47 | 41 | 207 | KC1 | CAA-C2A-C1A | -2.69 | 112.85 | 124.64 |
| 48 | 34 | 316 | A86 | C7-C6-C5 | -2.69 | 118.45 | 122.82 |
| 37 | 14 | 303 | CLA | CHD-C4C-NC | 2.69 | 128.41 | 124.23 |
| 37 | C | 505 | CLA | CMB-C2B-C1B | 2.69 | 129.52 | 125.42 |
| 47 | 36 | 308 | KC1 | O1D-CGD-CBD | -2.69 | 119.21 | 124.52 |
| 48 | 31 | 313 | A86 | C34-O4-C38 | -2.69 | 113.09 | 117.85 |
| 48 | 13 | 311 | A86 | C21-C20-C15 | -2.69 | 114.66 | 123.35 |
| 37 | 14 | 307 | CLA | C3B-C4B-NB | 2.69 | 112.93 | 110.53 |
| 48 | 33 | 312 | A86 | C34-O4-C38 | -2.69 | 113.09 | 117.85 |
| 38 | A | 404 | PHO | C2D-C1D-ND | -2.69 | 107.49 | 109.43 |
| 37 | 34 | 307 | CLA | C3B-C4B-NB | 2.69 | 112.93 | 110.53 |
| 47 | 35 | 309 | KC1 | C1A-NA-C4A | -2.69 | 105.45 | 106.68 |
| 37 | C | 504 | CLA | O2D-CGD-O1D | -2.69 | 118.61 | 123.85 |
| 37 | b | 523 | CLA | CAC-C3C-C4C | 2.69 | 128.29 | 124.79 |
| 37 | 19 | 301 | CLA | CHB-C4A-NA | 2.69 | 128.28 | 124.40 |
| 48 | 34 | 313 | A86 | C9-C8-C6 | -2.69 | 118.99 | 126.36 |
| 48 | 33 | 311 | A86 | C21-C20-C15 | -2.69 | 114.67 | 123.35 |
| 37 | W | 101 | CLA | CGD-CBD-CAD | 2.69 | 119.55 | 110.85 |
| 47 | 13 | 302 | KC1 | CHD-C4C-NC | 2.69 | 128.36 | 124.31 |
| 37 | 13 | 301 | CLA | C4-C3-C5 | 2.69 | 119.89 | 115.23 |
| 37 | c | 502 | CLA | O2D-CGD-O1D | -2.69 | 118.62 | 123.85 |
| 37 | 21 | 210 | CLA | O2D-CGD-O1D | -2.69 | 118.62 | 123.85 |
| 48 | 32 | 216 | A86 | C12-C11-C13 | 2.69 | 120.36 | 116.00 |
| 37 | 13 | 307 | CLA | CHD-C1D-ND | -2.69 | 121.02 | 124.80 |
| 47 | 13 | 309 | KC1 | CHD-C4C-NC | 2.69 | 128.36 | 124.31 |
| 37 | c | 502 | CLA | C1C-C2C-C3C | -2.69 | 104.15 | 106.98 |
| 37 | 14 | 303 | CLA | C4B-C3B-C2B | -2.69 | 103.96 | 107.30 |
| 37 | B | 501 | CLA | C4C-C3C-C2C | -2.69 | 102.98 | 106.89 |
| 37 | B | 501 | CLA | CHB-C4A-NA | 2.69 | 128.28 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 21 | 206 | CLA | CMC-C2C-C1C | 2.69 | 129.23 | 125.03 |
| 37 | 11 | 310 | CLA | O2A-CGA-CBA | 2.69 | 120.03 | 111.83 |
| 37 | 38 | 208 | CLA | O2A-CGA-CBA | 2.69 | 120.03 | 111.83 |
| 37 | b | 504 | CLA | C4-C3-C5 | 2.69 | 119.89 | 115.23 |
| 37 | 17 | 307 | CLA | C4-C3-C5 | 2.69 | 119.89 | 115.23 |
| 37 | B | 506 | CLA | CMC-C2C-C1C | 2.69 | 129.23 | 125.03 |
| 37 | 20 | 308 | CLA | C4B-C3B-C2B | -2.69 | 103.96 | 107.30 |
| 37 | 12 | 203 | CLA | CHC-C1C-C2C | -2.69 | 119.32 | 126.95 |
| 47 | 14 | 309 | KC1 | O2D-CGD-O1D | -2.68 | 118.62 | 123.85 |
| 37 | 12 | 209 | CLA | O1D-CGD-CBD | -2.68 | 119.22 | 124.52 |
| 37 | 39 | 310 | CLA | CAC-C3C-C4C | 2.68 | 128.28 | 124.79 |
| 37 | 18 | 209 | CLA | O2A-CGA-CBA | 2.68 | 120.02 | 111.83 |
| 37 | B | 505 | CLA | C4B-C3B-C2B | -2.68 | 103.97 | 107.30 |
| 37 | c | 504 | CLA | O2D-CGD-O1D | -2.68 | 118.63 | 123.85 |
| 37 | 11 | 303 | CLA | CHD-C4C-NC | 2.68 | 128.39 | 124.23 |
| 47 | 31 | 305 | KC1 | C4C-C3C-C2C | -2.68 | 102.99 | 106.89 |
| 37 | d | 403 | CLA | CMB-C2B-C1B | 2.68 | 129.50 | 125.42 |
| 37 | 19 | 305 | CLA | C1-O2A-CGA | 2.68 | 123.14 | 116.65 |
| 37 | Z | 102 | CLA | O1D-CGD-CBD | -2.68 | 119.23 | 124.52 |
| 48 | 17 | 313 | A86 | C21-C20-C15 | -2.68 | 114.69 | 123.35 |
| 47 | 11 | 304 | KC1 | C4C-C3C-C2C | -2.68 | 102.99 | 106.89 |
| 47 | 35 | 306 | KC1 | C4C-C3C-C2C | -2.68 | 102.99 | 106.89 |
| 47 | 13 | 309 | KC1 | CMB-C2B-C1B | 2.68 | 129.45 | 124.73 |
| 37 | 31 | 304 | CLA | CHD-C4C-NC | 2.68 | 128.39 | 124.23 |
| 37 | 36 | 303 | CLA | CMB-C2B-C1B | 2.68 | 129.50 | 125.42 |
| 37 | 21 | 210 | CLA | CHD-C4C-NC | 2.68 | 128.39 | 124.23 |
| 37 | 34 | 308 | CLA | CHD-C4C-NC | 2.68 | 128.39 | 124.23 |
| 37 | 35 | 307 | CLA | CHC-C1C-C2C | -2.68 | 119.33 | 126.95 |
| 37 | 41 | 210 | CLA | O2D-CGD-O1D | -2.68 | 118.63 | 123.85 |
| 37 | d | 401 | CLA | O2A-CGA-CBA | 2.68 | 120.00 | 111.83 |
| 37 | 15 | 308 | CLA | CBC-CAC-C3C | -2.68 | 105.16 | 112.42 |
| 37 | 15 | 303 | CLA | O2D-CGD-O1D | -2.68 | 118.63 | 123.85 |
| 37 | B | 515 | CLA | C4B-C3B-C2B | -2.68 | 103.97 | 107.30 |
| 37 | b | 523 | CLA | CHA-C1A-NA | -2.68 | 120.33 | 126.39 |
| 37 | 33 | 307 | CLA | CHD-C1D-ND | -2.68 | 121.03 | 124.80 |
| 37 | 37 | 303 | CLA | C4C-C3C-C2C | -2.68 | 102.99 | 106.89 |
| 48 | 13 | 312 | A86 | C34-O4-C38 | -2.68 | 113.12 | 117.85 |
| 48 | 14 | 313 | A86 | C9-C8-C6 | -2.68 | 119.02 | 126.36 |
| 37 | B | 504 | CLA | C4-C3-C5 | 2.68 | 119.88 | 115.23 |
| 37 | C | 502 | CLA | O2D-CGD-O1D | -2.68 | 118.64 | 123.85 |
| 48 | 35 | 314 | A86 | C25-C24-C1 | -2.68 | 119.02 | 126.36 |
| 37 | 11 | 303 | CLA | CBC-CAC-C3C | -2.68 | 105.16 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 19 | 302 | CLA | CBC-CAC-C3C | -2.68 | 105.16 | 112.42 |
| 48 | 13 | 312 | A86 | C25-C24-C1 | -2.68 | 119.02 | 126.36 |
| 48 | 32 | 218 | A86 | C7-C6-C5 | -2.68 | 118.48 | 122.82 |
| 37 | 39 | 310 | CLA | C4B-C3B-C2B | -2.68 | 103.97 | 107.30 |
| 47 | 38 | 210 | KC1 | CHB-C4A-NA | 2.68 | 128.38 | 124.23 |
| 37 | 20 | 303 | CLA | CMB-C2B-C1B | 2.68 | 129.49 | 125.42 |
| 48 | 37 | 319 | A86 | C21-C20-C15 | -2.68 | 114.71 | 123.35 |
| 47 | 35 | 304 | KC1 | CHD-C4C-NC | 2.68 | 128.34 | 124.31 |
| 47 | 12 | 206 | KC1 | O2D-CGD-O1D | -2.68 | 118.64 | 123.85 |
| 47 | 37 | 305 | KC1 | CHC-C4B-C3B | -2.67 | 120.70 | 125.21 |
| 47 | 34 | 309 | KC1 | O2D-CGD-O1D | -2.67 | 118.64 | 123.85 |
| 48 | 35 | 312 | A86 | C21-C20-C15 | -2.67 | 114.72 | 123.35 |
| 37 | 21 | 209 | CLA | CAA-C2A-C3A | -2.67 | 105.77 | 113.00 |
| 47 | 33 | 309 | KC1 | CHD-C4C-NC | 2.67 | 128.34 | 124.31 |
| 47 | 14 | 309 | KC1 | CAA-CBA-CGA | -2.67 | 113.45 | 127.05 |
| 48 | 32 | 214 | A86 | C4-C3-C2 | -2.67 | 118.05 | 123.52 |
| 37 | 14 | 308 | CLA | O2A-CGA-CBA | 2.67 | 119.99 | 111.83 |
| 37 | C | 503 | CLA | CHB-C4A-NA | 2.67 | 128.26 | 124.40 |
| 43 | D | 409 | LHG | C11-C10-C9 | -2.67 | 100.86 | 114.37 |
| 48 | 17 | 315 | A86 | C21-C20-C15 | -2.67 | 114.72 | 123.35 |
| 37 | 38 | 204 | CLA | CHC-C1C-C2C | -2.67 | 119.35 | 126.95 |
| 37 | D | 405 | CLA | C4-C3-C5 | 2.67 | 119.87 | 115.23 |
| 39 | b | 518 | BCR | C15-C14-C13 | -2.67 | 123.53 | 127.28 |
| 48 | 13 | 312 | A86 | C21-C20-C15 | -2.67 | 114.73 | 123.35 |
| 37 | 19 | 310 | CLA | C4B-C3B-C2B | -2.67 | 103.98 | 107.30 |
| 37 | 34 | 307 | CLA | C4B-C3B-C2B | -2.67 | 103.98 | 107.30 |
| 37 | B | 524 | CLA | CHA-C1A-NA | -2.67 | 120.34 | 126.39 |
| 39 | 0 | 101 | BCR | C29-C30-C25 | 2.67 | 114.32 | 110.44 |
| 39 | A | 406 | BCR | C15-C14-C13 | -2.67 | 123.53 | 127.28 |
| 37 | 36 | 306 | CLA | C2A-C3A-C4A | -2.67 | 97.55 | 101.87 |
| 37 | D | 402 | CLA | O2A-CGA-CBA | 2.67 | 119.98 | 111.83 |
| 37 | 32 | 210 | CLA | CHB-C4A-NA | 2.67 | 128.25 | 124.40 |
| 37 | B | 512 | CLA | CMB-C2B-C3B | 2.67 | 132.83 | 126.55 |
| 48 | 33 | 312 | A86 | C21-C20-C15 | -2.67 | 114.73 | 123.35 |
| 37 | C | 505 | CLA | C1-C2-C3 | -2.67 | 121.82 | 126.20 |
| 37 | b | 512 | CLA | CMB-C2B-C3B | 2.67 | 132.83 | 126.55 |
| 37 | 17 | 307 | CLA | CHB-C4A-NA | 2.67 | 128.25 | 124.40 |
| 37 | 41 | 209 | CLA | CAA-C2A-C3A | -2.67 | 105.78 | 113.00 |
| 37 | 16 | 306 | CLA | C2A-C3A-C4A | -2.67 | 97.56 | 101.87 |
| 37 | b | 501 | CLA | CHB-C4A-NA | 2.67 | 128.25 | 124.40 |
| 47 | 18 | 210 | KC1 | O1D-CGD-CBD | -2.67 | 119.25 | 124.52 |
| 47 | 36 | 302 | KC1 | CHD-C4C-NC | 2.67 | 128.33 | 124.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 13 | 312 | A86 | C7-C6-C8 | 2.67 | 122.16 | 118.09 |
| 37 | 31 | 304 | CLA | CBC-CAC-C3C | -2.67 | 105.19 | 112.42 |
| 37 | 39 | 302 | CLA | CBC-CAC-C3C | -2.67 | 105.19 | 112.42 |
| 37 | a | 407 | CLA | CHB-C4A-NA | 2.67 | 128.25 | 124.40 |
| 48 | 39 | 313 | A86 | C-C1-C24 | 2.67 | 122.16 | 118.09 |
| 37 | b | 515 | CLA | C4B-C3B-C2B | -2.67 | 103.98 | 107.30 |
| 37 | 14 | 308 | CLA | CBC-CAC-C3C | -2.67 | 105.19 | 112.42 |
| 47 | 16 | 308 | KC1 | O1D-CGD-CBD | -2.67 | 119.26 | 124.52 |
| 37 | 33 | 301 | CLA | CMC-C2C-C1C | 2.67 | 129.20 | 125.03 |
| 47 | 32 | 209 | KC1 | CHD-C1D-ND | -2.67 | 120.05 | 124.05 |
| 37 | 15 | 307 | CLA | CHC-C1C-C2C | -2.67 | 119.37 | 126.95 |
| 48 | 12 | 217 | A86 | C7-C6-C5 | -2.67 | 118.50 | 122.82 |
| 43 | d | 407 | LHG | C11-C10-C9 | -2.67 | 100.89 | 114.37 |
| 48 | 37 | 314 | A86 | C21-C20-C15 | -2.67 | 114.74 | 123.35 |
| 47 | 34 | 309 | KC1 | CAA-CBA-CGA | -2.67 | 113.49 | 127.05 |
| 37 | 37 | 301 | CLA | CMB-C2B-C1B | 2.67 | 129.48 | 125.42 |
| 50 | 16 | 312 | DD6 | C25-C24-C1 | -2.67 | 119.06 | 126.36 |
| 37 | 40 | 210 | CLA | C4B-C3B-C2B | -2.67 | 103.99 | 107.30 |
| 37 | d | 404 | CLA | CBC-CAC-C3C | -2.66 | 105.20 | 112.42 |
| 37 | b | 505 | CLA | C4B-C3B-C2B | -2.66 | 103.99 | 107.30 |
| 37 | 40 | 203 | CLA | CMC-C2C-C1C | 2.66 | 129.20 | 125.03 |
| 47 | 18 | 210 | KC1 | CHB-C4A-NA | 2.66 | 128.36 | 124.23 |
| 37 | 32 | 204 | CLA | CHC-C1C-C2C | -2.66 | 119.38 | 126.95 |
| 37 | 18 | 201 | CLA | C1-O2A-CGA | 2.66 | 123.10 | 116.65 |
| 47 | 32 | 212 | KC1 | C4C-C3C-C2C | -2.66 | 103.02 | 106.89 |
| 47 | 38 | 210 | KC1 | CAA-CBA-CGA | -2.66 | 113.51 | 127.05 |
| 48 | 13 | 311 | A86 | C4-C3-C2 | -2.66 | 118.07 | 123.52 |
| 37 | 41 | 210 | CLA | CHD-C4C-NC | 2.66 | 128.36 | 124.23 |
| 37 | 18 | 201 | CLA | CHC-C1C-C2C | -2.66 | 119.38 | 126.95 |
| 47 | 36 | 302 | KC1 | CAB-C3B-C4B | 2.66 | 131.18 | 124.82 |
| 37 | C | 502 | CLA | CHB-C4A-NA | 2.66 | 128.24 | 124.40 |
| 37 | 16 | 303 | CLA | CMB-C2B-C1B | 2.66 | 129.47 | 125.42 |
| 37 | 39 | 302 | CLA | C4-C3-C5 | 2.66 | 119.85 | 115.23 |
| 39 | B | 517 | BCR | C27-C26-C25 | 2.66 | 126.30 | 122.70 |
| 37 | 15 | 303 | CLA | CHD-C4C-NC | 2.66 | 128.36 | 124.23 |
| 47 | 18 | 210 | KC1 | CAA-CBA-CGA | -2.66 | 113.52 | 127.05 |
| 37 | D | 406 | CLA | CBC-CAC-C3C | -2.66 | 105.21 | 112.42 |
| 47 | 14 | 309 | KC1 | CHB-C4A-NA | 2.66 | 128.35 | 124.23 |
| 37 | C | 509 | CLA | C4-C3-C5 | 2.66 | 119.84 | 115.23 |
| 37 | 19 | 301 | CLA | CMA-C3A-C2A | -2.66 | 103.70 | 113.98 |
| 37 | d | 403 | CLA | C1-C2-C3 | -2.66 | 121.84 | 126.20 |
| 48 | 15 | 312 | A86 | C21-C20-C15 | -2.66 | 114.77 | 123.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | 5 | 101 | BCR | C29-C30-C25 | 2.66 | 114.30 | 110.44 |
| 37 | 38 | 202 | CLA | CHC-C1C-C2C | -2.66 | 119.40 | 126.95 |
| 47 | 14 | 306 | KC1 | CAA-CBA-CGA | -2.66 | 113.54 | 127.05 |
| 47 | 13 | 309 | KC1 | CAA-CBA-CGA | -2.66 | 113.54 | 127.05 |
| 47 | 34 | 306 | KC1 | CAA-CBA-CGA | -2.66 | 113.54 | 127.05 |
| 47 | 14 | 309 | KC1 | C1A-NA-C4A | -2.66 | 105.47 | 106.68 |
| 47 | 34 | 309 | KC1 | C1A-NA-C4A | -2.66 | 105.47 | 106.68 |
| 37 | 34 | 308 | CLA | O2A-CGA-CBA | 2.66 | 119.94 | 111.83 |
| 37 | 31 | 302 | CLA | C1C-C2C-C3C | -2.66 | 104.19 | 106.98 |
| 44 | H | 102 | DGD | CDB-CCB-CBB | -2.66 | 100.94 | 114.37 |
| 37 | 17 | 304 | CLA | C4C-C3C-C2C | -2.66 | 103.03 | 106.89 |
| 44 | h | 102 | DGD | CDB-CCB-CBB | -2.66 | 100.94 | 114.37 |
| 48 | 11 | 315 | A86 | C21-C20-C15 | -2.66 | 114.78 | 123.35 |
| 48 | 31 | 315 | A86 | C21-C20-C15 | -2.66 | 114.78 | 123.35 |
| 37 | B | 505 | CLA | CHB-C4A-NA | 2.66 | 128.23 | 124.40 |
| 37 | 39 | 301 | CLA | C4B-C3B-C2B | -2.65 | 104.00 | 107.30 |
| 37 | 11 | 307 | CLA | C1-C2-C3 | -2.65 | 121.85 | 126.20 |
| 47 | 12 | 211 | KC1 | C4C-C3C-C2C | -2.65 | 103.03 | 106.89 |
| 48 | 38 | 215 | A86 | C21-C20-C15 | -2.65 | 114.78 | 123.35 |
| 37 | 12 | 210 | CLA | CED-O2D-CGD | 2.65 | 121.94 | 115.92 |
| 37 | 12 | 209 | CLA | CMC-C2C-C1C | 2.65 | 129.18 | 125.03 |
| 47 | 33 | 302 | KC1 | CHD-C4C-NC | 2.65 | 128.31 | 124.31 |
| 37 | 11 | 303 | CLA | C4B-C3B-C2B | -2.65 | 104.00 | 107.30 |
| 37 | 31 | 304 | CLA | C4B-C3B-C2B | -2.65 | 104.00 | 107.30 |
| 37 | c | 505 | CLA | C1-C2-C3 | -2.65 | 121.85 | 126.20 |
| 40 | 17 | 301 | SQD | C44-O6-C1 | 2.65 | 119.48 | 113.80 |
| 47 | 37 | 304 | KC1 | CMB-C2B-C1B | 2.65 | 129.40 | 124.73 |
| 37 | 35 | 303 | CLA | CHD-C4C-NC | 2.65 | 128.34 | 124.23 |
| 37 | 17 | 304 | CLA | C4-C3-C5 | 2.65 | 119.83 | 115.23 |
| 37 | d | 403 | CLA | CHC-C1C-C2C | -2.65 | 119.41 | 126.95 |
| 37 | 21 | 204 | CLA | O1D-CGD-CBD | -2.65 | 119.29 | 124.52 |
| 48 | 12 | 202 | A86 | C34-O4-C38 | -2.65 | 113.16 | 117.85 |
| 48 | 32 | 203 | A86 | C34-O4-C38 | -2.65 | 113.16 | 117.85 |
| 37 | D | 405 | CLA | C1-C2-C3 | -2.65 | 121.85 | 126.20 |
| 37 | B | 507 | CLA | CBC-CAC-C3C | -2.65 | 105.23 | 112.42 |
| 47 | 14 | 309 | KC1 | CMC-C2C-C1C | 2.65 | 129.18 | 125.03 |
| 47 | 15 | 309 | KC1 | CAA-CBA-CGA | -2.65 | 113.56 | 127.05 |
| 37 | 14 | 308 | CLA | CHD-C4C-NC | 2.65 | 128.34 | 124.23 |
| 47 | 33 | 309 | KC1 | O2D-CGD-O1D | -2.65 | 118.69 | 123.85 |
| 37 | 19 | 301 | CLA | C4B-C3B-C2B | -2.65 | 104.00 | 107.30 |
| 48 | 33 | 311 | A86 | C4-C3-C2 | -2.65 | 118.09 | 123.52 |
| 37 | D | 401 | CLA | O2A-CGA-CBA | 2.65 | 119.92 | 111.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 505 | CLA | CMB-C2B-C1B | 2.65 | 129.46 | 125.42 |
| 37 | c | 503 | CLA | CHB-C4A-NA | 2.65 | 128.22 | 124.40 |
| 37 | 12 | 212 | CLA | CHB-C4A-NA | 2.65 | 128.22 | 124.40 |
| 47 | 33 | 309 | KC1 | CAA-CBA-CGA | -2.65 | 113.57 | 127.05 |
| 37 | 13 | 301 | CLA | CMC-C2C-C1C | 2.65 | 129.18 | 125.03 |
| 48 | 14 | 316 | A86 | C8-C6-C5 | 2.65 | 123.18 | 119.01 |
| 37 | b | 507 | CLA | CBC-CAC-C3C | -2.65 | 105.24 | 112.42 |
| 47 | 34 | 309 | KC1 | CMC-C2C-C1C | 2.65 | 129.17 | 125.03 |
| 48 | 34 | 314 | A86 | C7-C6-C8 | 2.65 | 122.14 | 118.09 |
| 47 | 21 | 207 | KC1 | CBC-CAC-C3C | -2.65 | 105.24 | 112.42 |
| 37 | 20 | 308 | CLA | CHD-C4C-NC | 2.65 | 128.34 | 124.23 |
| 37 | 17 | 302 | CLA | CHB-C4A-NA | 2.65 | 128.22 | 124.40 |
| 37 | 11 | 303 | CLA | CAA-C2A-C1A | 2.65 | 120.65 | 111.97 |
| 37 | 31 | 304 | CLA | CAA-C2A-C1A | 2.65 | 120.65 | 111.97 |
| 37 | 21 | 208 | CLA | C4-C3-C5 | 2.65 | 119.82 | 115.23 |
| 37 | 34 | 308 | CLA | CBC-CAC-C3C | -2.65 | 105.24 | 112.42 |
| 37 | 20 | 301 | CLA | CMC-C2C-C1C | 2.65 | 129.17 | 125.03 |
| 47 | 32 | 207 | KC1 | O2D-CGD-O1D | -2.65 | 118.69 | 123.85 |
| 50 | 36 | 312 | DD6 | C25-C24-C1 | -2.65 | 119.11 | 126.36 |
| 37 | d | 403 | CLA | C4-C3-C5 | 2.65 | 119.82 | 115.23 |
| 47 | 17 | 308 | KC1 | CHB-C4A-NA | 2.65 | 128.34 | 124.23 |
| 48 | 40 | 211 | A86 | C4-C3-C2 | -2.65 | 118.10 | 123.52 |
| 37 | 34 | 302 | CLA | CHB-C4A-NA | 2.65 | 128.22 | 124.40 |
| 37 | 18 | 204 | CLA | C1-O2A-CGA | 2.65 | 123.06 | 116.65 |
| 37 | a | 404 | CLA | O2A-CGA-CBA | 2.65 | 119.90 | 111.83 |
| 48 | 33 | 312 | A86 | C25-C24-C1 | -2.65 | 119.11 | 126.36 |
| 48 | 21 | 211 | A86 | C21-C20-C15 | -2.65 | 114.81 | 123.35 |
| 37 | c | 509 | CLA | C4-C3-C5 | 2.65 | 119.82 | 115.23 |
| 37 | 39 | 310 | CLA | CMB-C2B-C1B | 2.65 | 129.45 | 125.42 |
| 48 | 18 | 213 | A86 | C9-C8-C6 | -2.65 | 119.11 | 126.36 |
| 48 | 33 | 314 | A86 | C21-C20-C15 | -2.64 | 114.81 | 123.35 |
| 47 | 35 | 309 | KC1 | CAA-CBA-CGA | -2.64 | 113.60 | 127.05 |
| 37 | b | 516 | CLA | CMB-C2B-C1B | 2.64 | 129.45 | 125.42 |
| 47 | 20 | 304 | KC1 | CMB-C2B-C1B | 2.64 | 129.38 | 124.73 |
| 37 | 12 | 209 | CLA | CHB-C4A-NA | 2.64 | 128.22 | 124.40 |
| 37 | 40 | 208 | CLA | C4B-C3B-C2B | -2.64 | 104.01 | 107.30 |
| 48 | 41 | 211 | A86 | C21-C20-C15 | -2.64 | 114.81 | 123.35 |
| 47 | 16 | 305 | KC1 | CAC-C3C-C4C | 2.64 | 128.23 | 124.79 |
| 37 | 38 | 206 | CLA | CAA-C2A-C3A | -2.64 | 105.86 | 113.00 |
| 37 | 19 | 310 | CLA | CMB-C2B-C1B | 2.64 | 129.44 | 125.42 |
| 37 | 38 | 201 | CLA | C4B-C3B-C2B | -2.64 | 104.02 | 107.30 |
| 37 | 39 | 302 | CLA | C4C-C3C-C2C | -2.64 | 103.04 | 106.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 18 | 211 | CLA | C1C-C2C-C3C | -2.64 | 104.20 | 106.98 |
| 40 | 36 | 315 | SQD | C44-O6-C1 | 2.64 | 119.46 | 113.80 |
| 50 | 39 | 312 | DD6 | C4-C3-C2 | -2.64 | 118.11 | 123.52 |
| 48 | 16 | 310 | A86 | C36-C31-C32 | -2.64 | 117.07 | 119.70 |
| 37 | c | 511 | CLA | CAA-C2A-C3A | -2.64 | 105.86 | 113.00 |
| 37 | 33 | 307 | CLA | CHD-C4C-NC | 2.64 | 128.33 | 124.23 |
| 39 | b | 517 | BCR | C27-C26-C25 | 2.64 | 126.27 | 122.70 |
| 37 | 41 | 204 | CLA | O1D-CGD-CBD | -2.64 | 119.31 | 124.52 |
| 37 | c | 502 | CLA | CHB-C4A-NA | 2.64 | 128.21 | 124.40 |
| 41 | c | 518 | LMG | O1-C1-C2 | -2.64 | 104.26 | 108.27 |
| 37 | 33 | 303 | CLA | CHD-C4C-NC | 2.64 | 128.33 | 124.23 |
| 47 | 34 | 309 | KC1 | CHB-C4A-NA | 2.64 | 128.33 | 124.23 |
| 47 | 16 | 302 | KC1 | CHD-C4C-NC | 2.64 | 128.29 | 124.31 |
| 37 | 38 | 209 | CLA | C4-C3-C5 | 2.64 | 119.81 | 115.23 |
| 37 | D | 405 | CLA | CHC-C1C-C2C | -2.64 | 119.45 | 126.95 |
| 37 | C | 503 | CLA | C4-C3-C5 | 2.64 | 119.81 | 115.23 |
| 37 | 41 | 208 | CLA | C4-C3-C5 | 2.64 | 119.81 | 115.23 |
| 48 | 13 | 314 | A86 | C34-O4-C38 | -2.64 | 113.19 | 117.85 |
| 39 | C | 514 | BCR | C15-C14-C13 | -2.64 | 123.58 | 127.28 |
| 39 | B | 525 | BCR | C27-C26-C25 | 2.64 | 126.27 | 122.70 |
| 48 | 15 | 312 | A86 | C10-C9-C8 | -2.64 | 115.55 | 123.20 |
| 48 | 33 | 314 | A86 | C34-O4-C38 | -2.64 | 113.19 | 117.85 |
| 39 | c | 514 | BCR | C7-C8-C9 | -2.64 | 122.33 | 126.23 |
| 47 | 40 | 206 | KC1 | CMB-C2B-C1B | 2.64 | 129.37 | 124.73 |
| 37 | C | 511 | CLA | CAA-C2A-C3A | -2.64 | 105.87 | 113.00 |
| 47 | 33 | 306 | KC1 | CMB-C2B-C1B | 2.64 | 129.37 | 124.73 |
| 47 | 35 | 309 | KC1 | CHB-C4A-NA | 2.64 | 128.32 | 124.23 |
| 37 | 12 | 210 | CLA | CMB-C2B-C1B | 2.64 | 129.44 | 125.42 |
| 48 | 37 | 310 | A86 | C10-C9-C8 | -2.64 | 115.56 | 123.20 |
| 37 | C | 503 | CLA | CHD-C4C-NC | 2.64 | 128.32 | 124.23 |
| 37 | 33 | 310 | CLA | CHD-C4C-NC | 2.64 | 128.32 | 124.23 |
| 47 | 21 | 207 | KC1 | CBA-CAA-C2A | -2.64 | 114.87 | 125.45 |
| 37 | 38 | 203 | CLA | CHB-C4A-NA | 2.64 | 128.20 | 124.40 |
| 47 | 15 | 309 | KC1 | CHB-C4A-NA | 2.64 | 128.32 | 124.23 |
| 37 | b | 512 | CLA | CHC-C1C-C2C | -2.64 | 119.46 | 126.95 |
| 37 | 19 | 302 | CLA | C4C-C3C-C2C | -2.63 | 103.06 | 106.89 |
| 37 | 17 | 307 | CLA | CBC-CAC-C3C | -2.63 | 105.28 | 112.42 |
| 48 | 13 | 314 | A86 | C21-C20-C15 | -2.63 | 114.85 | 123.35 |
| 37 | B | 516 | CLA | CMB-C2B-C1B | 2.63 | 129.43 | 125.42 |
| 37 | 38 | 204 | CLA | C1-O2A-CGA | 2.63 | 123.03 | 116.65 |
| 47 | 18 | 207 | KC1 | CHD-C4C-NC | 2.63 | 128.28 | 124.31 |
| 47 | 41 | 207 | KC1 | CBC-CAC-C3C | -2.63 | 105.28 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 21 | 215 | A86 | C19-C18-C17 | -2.63 | 105.86 | 110.79 |
| 37 | 18 | 208 | CLA | O2A-CGA-CBA | 2.63 | 119.86 | 111.83 |
| 37 | 14 | 302 | CLA | C3B-C4B-NB | 2.63 | 112.88 | 110.53 |
| 39 | c | 514 | BCR | C15-C14-C13 | -2.63 | 123.58 | 127.28 |
| 48 | 40 | 201 | A86 | C7-C6-C5 | -2.63 | 118.55 | 122.82 |
| 37 | 12 | 203 | CLA | CHB-C4A-NA | 2.63 | 128.20 | 124.40 |
| 39 | B | 518 | BCR | C15-C14-C13 | -2.63 | 123.59 | 127.28 |
| 48 | 20 | 309 | A86 | C4-C3-C2 | -2.63 | 118.13 | 123.52 |
| 37 | C | 509 | CLA | O2A-CGA-CBA | 2.63 | 119.86 | 111.83 |
| 37 | 16 | 303 | CLA | CBC-CAC-C3C | -2.63 | 105.29 | 112.42 |
| 37 | 13 | 307 | CLA | CHD-C4C-NC | 2.63 | 128.31 | 124.23 |
| 48 | 14 | 314 | A86 | C7-C6-C8 | 2.63 | 122.11 | 118.09 |
| 37 | b | 512 | CLA | C4-C3-C5 | 2.63 | 119.79 | 115.23 |
| 50 | 19 | 312 | DD6 | C4-C3-C2 | -2.63 | 118.14 | 123.52 |
| 37 | 39 | 309 | CLA | O2D-CGD-O1D | -2.63 | 118.73 | 123.85 |
| 37 | 40 | 203 | CLA | CHC-C1C-C2C | -2.63 | 119.48 | 126.95 |
| 37 | 32 | 213 | CLA | CHB-C4A-NA | 2.63 | 128.19 | 124.40 |
| 48 | 17 | 315 | A86 | C12-C11-C13 | 2.63 | 120.26 | 116.00 |
| 37 | 20 | 307 | CLA | CAA-C2A-C3A | -2.63 | 105.90 | 113.00 |
| 47 | 41 | 207 | KC1 | CBA-CAA-C2A | -2.63 | 114.91 | 125.45 |
| 48 | 35 | 312 | A86 | C25-C24-C1 | -2.63 | 119.16 | 126.36 |
| 37 | 16 | 306 | CLA | O2D-CGD-O1D | -2.63 | 118.73 | 123.85 |
| 41 | C | 518 | LMG | O1-C1-C2 | -2.63 | 104.28 | 108.27 |
| 37 | 17 | 302 | CLA | CMB-C2B-C1B | 2.63 | 129.42 | 125.42 |
| 37 | 36 | 303 | CLA | CBC-CAC-C3C | -2.63 | 105.30 | 112.42 |
| 48 | 15 | 314 | A86 | C21-C20-C15 | -2.63 | 114.88 | 123.35 |
| 37 | 34 | 305 | CLA | O2D-CGD-O1D | -2.63 | 118.74 | 123.85 |
| 37 | 38 | 206 | CLA | CAC-C3C-C4C | 2.62 | 128.21 | 124.79 |
| 37 | 39 | 301 | CLA | CMA-C3A-C2A | -2.62 | 103.83 | 113.98 |
| 47 | 13 | 309 | KC1 | C4C-C3C-C2C | -2.62 | 103.07 | 106.89 |
| 48 | 37 | 314 | A86 | C12-C11-C13 | 2.62 | 120.25 | 116.00 |
| 48 | 31 | 314 | A86 | C25-C24-C1 | -2.62 | 119.17 | 126.36 |
| 37 | 16 | 306 | CLA | CHB-C1B-C2B | -2.62 | 119.81 | 127.43 |
| 37 | a | 403 | CLA | CMD-C2D-C3D | -2.62 | 121.67 | 127.69 |
| 47 | 18 | 210 | KC1 | C1A-NA-C4A | -2.62 | 105.48 | 106.68 |
| 47 | 17 | 308 | KC1 | CMB-C2B-C1B | 2.62 | 129.35 | 124.73 |
| 47 | 37 | 307 | KC1 | CHB-C4A-NA | 2.62 | 128.30 | 124.23 |
| 48 | 37 | 312 | A86 | C34-O4-C38 | -2.62 | 113.21 | 117.85 |
| 47 | 15 | 306 | KC1 | O2D-CGD-O1D | -2.62 | 118.74 | 123.85 |
| 48 | 11 | 314 | A86 | C25-C24-C1 | -2.62 | 119.17 | 126.36 |
| 39 | 0 | 101 | BCR | C3-C4-C5 | -2.62 | 109.38 | 114.06 |
| 41 | D | 412 | LMG | C6-C5-C4 | -2.62 | 106.58 | 113.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 11 | 312 | A86 | C23-C16-C22 | -2.62 | 103.56 | 107.37 |
| 44 | h | 102 | DGD | CBB-CAB-C9B | -2.62 | 101.11 | 114.37 |
| 37 | 14 | 301 | CLA | CHC-C1C-C2C | -2.62 | 119.50 | 126.95 |
| 37 | 18 | 203 | CLA | CHB-C4A-NA | 2.62 | 128.18 | 124.40 |
| 37 | 41 | 208 | CLA | CHB-C4A-NA | 2.62 | 128.18 | 124.40 |
| 39 | b | 524 | BCR | C27-C26-C25 | 2.62 | 126.25 | 122.70 |
| 47 | 38 | 210 | KC1 | O1D-CGD-CBD | -2.62 | 119.35 | 124.52 |
| 47 | 39 | 308 | KC1 | O2D-CGD-O1D | -2.62 | 118.75 | 123.85 |
| 37 | 34 | 301 | CLA | CHC-C1C-C2C | -2.62 | 119.50 | 126.95 |
| 37 | 37 | 306 | CLA | CBC-CAC-C3C | -2.62 | 105.31 | 112.42 |
| 37 | A | 405 | CLA | CHB-C4A-NA | 2.62 | 128.18 | 124.40 |
| 44 | H | 102 | DGD | CBB-CAB-C9B | -2.62 | 101.12 | 114.37 |
| 37 | b | 501 | CLA | CMC-C2C-C1C | 2.62 | 129.13 | 125.03 |
| 48 | 35 | 314 | A86 | C4-C5-C6 | -2.62 | 123.60 | 127.28 |
| 37 | 18 | 206 | CLA | CBC-CAC-C3C | -2.62 | 105.32 | 112.42 |
| 37 | 21 | 208 | CLA | CHB-C4A-NA | 2.62 | 128.18 | 124.40 |
| 37 | 32 | 210 | CLA | CMC-C2C-C1C | 2.62 | 129.13 | 125.03 |
| 48 | 33 | 312 | A86 | C7-C6-C8 | 2.62 | 122.09 | 118.09 |
| 48 | 36 | 310 | A86 | C36-C31-C32 | -2.62 | 117.10 | 119.70 |
| 37 | b | 511 | CLA | C1-C2-C3 | -2.62 | 121.91 | 126.20 |
| 37 | B | 512 | CLA | C4-C3-C5 | 2.62 | 119.77 | 115.23 |
| 47 | 36 | 305 | KC1 | CAC-C3C-C4C | 2.62 | 128.20 | 124.79 |
| 48 | 19 | 313 | A86 | C22-C16-C17 | -2.62 | 104.37 | 108.97 |
| 37 | 39 | 307 | CLA | C1-C2-C3 | -2.62 | 121.91 | 126.20 |
| 47 | 13 | 306 | KC1 | CMB-C2B-C1B | 2.62 | 129.34 | 124.73 |
| 47 | 17 | 306 | KC1 | O1D-CGD-CBD | -2.62 | 119.36 | 124.52 |
| 37 | 20 | 306 | CLA | C4B-C3B-C2B | -2.62 | 104.05 | 107.30 |
| 37 | 15 | 301 | CLA | C3B-C4B-NB | 2.62 | 112.87 | 110.53 |
| 37 | 15 | 307 | CLA | CHB-C1B-C2B | -2.62 | 119.83 | 127.43 |
| 47 | 37 | 304 | KC1 | CHD-C4C-NC | 2.62 | 128.25 | 124.31 |
| 37 | 18 | 206 | CLA | CAA-C2A-C3A | -2.62 | 105.93 | 113.00 |
| 37 | 32 | 202 | CLA | CAA-C2A-C3A | -2.62 | 105.93 | 113.00 |
| 37 | 32 | 211 | CLA | O2A-CGA-CBA | 2.62 | 119.81 | 111.83 |
| 48 | 14 | 313 | A86 | C12-C11-C13 | 2.62 | 120.24 | 116.00 |
| 48 | 14 | 311 | A86 | C23-C16-C22 | -2.62 | 103.57 | 107.37 |
| 47 | 35 | 306 | KC1 | O2D-CGD-O1D | -2.62 | 118.76 | 123.85 |
| 37 | 38 | 202 | CLA | C4B-C3B-C2B | -2.62 | 104.05 | 107.30 |
| 37 | 36 | 306 | CLA | CHB-C1B-C2B | -2.61 | 119.84 | 127.43 |
| 37 | 36 | 301 | CLA | C3B-C4B-NB | 2.61 | 112.86 | 110.53 |
| 37 | B | 512 | CLA | CHC-C1C-C2C | -2.61 | 119.52 | 126.95 |
| 37 | B | 514 | CLA | CHD-C4C-NC | 2.61 | 128.28 | 124.23 |
| 37 | 36 | 306 | CLA | O2D-CGD-O1D | -2.61 | 118.76 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 34 | 310 | CLA | CMB-C2B-C1B | 2.61 | 129.40 | 125.42 |
| 37 | 15 | 305 | CLA | CHB-C4A-NA | 2.61 | 128.17 | 124.40 |
| 37 | A | 403 | CLA | CMD-C2D-C3D | -2.61 | 121.69 | 127.69 |
| 37 | 14 | 305 | CLA | O2D-CGD-O1D | -2.61 | 118.76 | 123.85 |
| 48 | 38 | 215 | A86 | C36-C31-C32 | -2.61 | 117.10 | 119.70 |
| 37 | B | 511 | CLA | CAA-C2A-C3A | -2.61 | 105.94 | 113.00 |
| 37 | 38 | 204 | CLA | O2D-CGD-O1D | -2.61 | 118.76 | 123.85 |
| 37 | 40 | 210 | CLA | CHD-C4C-NC | 2.61 | 128.28 | 124.23 |
| 37 | c | 503 | CLA | C4-C3-C5 | 2.61 | 119.76 | 115.23 |
| 37 | b | 512 | CLA | CHB-C4A-NA | 2.61 | 128.17 | 124.40 |
| 47 | 34 | 304 | KC1 | C4C-C3C-C2C | -2.61 | 103.09 | 106.89 |
| 37 | 41 | 204 | CLA | O2A-CGA-CBA | 2.61 | 119.80 | 111.83 |
| 37 | 11 | 308 | CLA | CAA-C2A-C3A | -2.61 | 105.94 | 113.00 |
| 47 | 15 | 309 | KC1 | O2D-CGD-O1D | -2.61 | 118.77 | 123.85 |
| 37 | d | 403 | CLA | O2A-CGA-CBA | 2.61 | 119.80 | 111.83 |
| 37 | 18 | 206 | CLA | CMB-C2B-C1B | 2.61 | 129.40 | 125.42 |
| 37 | c | 503 | CLA | C4B-C3B-C2B | -2.61 | 104.06 | 107.30 |
| 47 | 18 | 207 | KC1 | CAA-CBA-CGA | -2.61 | 113.77 | 127.05 |
| 37 | D | 405 | CLA | O2A-CGA-CBA | 2.61 | 119.80 | 111.83 |
| 40 | B | 519 | SQD | C44-O6-C1 | 2.61 | 119.39 | 113.80 |
| 50 | 19 | 312 | DD6 | C25-C24-C1 | -2.61 | 119.20 | 126.36 |
| 37 | 40 | 205 | CLA | C1-C2-C3 | -2.61 | 121.92 | 126.20 |
| 37 | 12 | 203 | CLA | C4B-C3B-C2B | -2.61 | 104.06 | 107.30 |
| 37 | c | 509 | CLA | O2A-CGA-CBA | 2.61 | 119.79 | 111.83 |
| 47 | 37 | 305 | KC1 | O1D-CGD-CBD | -2.61 | 119.37 | 124.52 |
| 39 | C | 515 | BCR | C7-C8-C9 | -2.61 | 122.37 | 126.23 |
| 48 | 19 | 313 | A86 | C7-C6-C5 | -2.61 | 118.59 | 122.82 |
| 37 | B | 512 | CLA | CHB-C4A-NA | 2.61 | 128.17 | 124.40 |
| 37 | 17 | 304 | CLA | CHB-C4A-NA | 2.61 | 128.16 | 124.40 |
| 48 | 34 | 316 | A86 | C8-C6-C5 | 2.61 | 123.11 | 119.01 |
| 37 | 34 | 302 | CLA | C3B-C4B-NB | 2.61 | 112.86 | 110.53 |
| 37 | 21 | 205 | CLA | CHB-C4A-NA | 2.61 | 128.16 | 124.40 |
| 39 | c | 515 | BCR | C7-C8-C9 | -2.61 | 122.38 | 126.23 |
| 37 | 40 | 209 | CLA | CAA-C2A-C3A | -2.61 | 105.95 | 113.00 |
| 37 | 32 | 204 | CLA | CHB-C4A-NA | 2.61 | 128.16 | 124.40 |
| 37 | c | 504 | CLA | CBC-CAC-C3C | -2.61 | 105.35 | 112.42 |
| 37 | 35 | 305 | CLA | CHB-C4A-NA | 2.61 | 128.16 | 124.40 |
| 48 | 16 | 313 | A86 | C7-C6-C5 | -2.61 | 118.59 | 122.82 |
| 37 | 12 | 207 | CLA | CMB-C2B-C1B | 2.61 | 129.39 | 125.42 |
| 47 | 36 | 302 | KC1 | CHB-C4A-NA | 2.61 | 128.27 | 124.23 |
| 37 | 12 | 210 | CLA | O2A-CGA-CBA | 2.61 | 119.78 | 111.83 |
| 37 | 36 | 303 | CLA | C4C-C3C-C2C | -2.61 | 103.10 | 106.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 309 | KC1 | O2D-CGD-O1D | -2.60 | 118.78 | 123.85 |
| 48 | 34 | 313 | A86 | C12-C11-C13 | 2.60 | 120.22 | 116.00 |
| 37 | 20 | 301 | CLA | CHC-C1C-C2C | -2.60 | 119.55 | 126.95 |
| 47 | 36 | 304 | KC1 | O2D-CGD-O1D | -2.60 | 118.78 | 123.85 |
| 37 | 20 | 303 | CLA | C1-C2-C3 | -2.60 | 121.93 | 126.20 |
| 50 | 39 | 312 | DD6 | C25-C24-C1 | -2.60 | 119.22 | 126.36 |
| 47 | 35 | 309 | KC1 | CMB-C2B-C1B | 2.60 | 129.31 | 124.73 |
| 41 | d | 409 | LMG | C6-C5-C4 | -2.60 | 106.63 | 113.02 |
| 37 | 19 | 309 | CLA | O2D-CGD-O1D | -2.60 | 118.78 | 123.85 |
| 47 | 21 | 203 | KC1 | CHB-C1B-C2B | -2.60 | 120.08 | 125.49 |
| 46 | V | 201 | HEM | CMB-C2B-C1B | -2.60 | 120.97 | 125.03 |
| 37 | 21 | 204 | CLA | O2A-CGA-CBA | 2.60 | 119.77 | 111.83 |
| 37 | 39 | 307 | CLA | O2A-CGA-CBA | 2.60 | 119.77 | 111.83 |
| 47 | 38 | 210 | KC1 | CMB-C2B-C1B | 2.60 | 129.31 | 124.73 |
| 48 | 37 | 309 | A86 | C21-C20-C15 | -2.60 | 114.95 | 123.35 |
| 37 | b | 511 | CLA | CAA-C2A-C3A | -2.60 | 105.97 | 113.00 |
| 37 | 33 | 303 | CLA | CMB-C2B-C1B | 2.60 | 129.38 | 125.42 |
| 46 | v | 201 | HEM | CMB-C2B-C1B | -2.60 | 120.97 | 125.03 |
| 37 | 21 | 210 | CLA | CAC-C3C-C4C | 2.60 | 128.17 | 124.79 |
| 37 | c | 503 | CLA | CHD-C4C-NC | 2.60 | 128.26 | 124.23 |
| 37 | 16 | 303 | CLA | C4C-C3C-C2C | -2.60 | 103.11 | 106.89 |
| 37 | C | 504 | CLA | CBC-CAC-C3C | -2.60 | 105.37 | 112.42 |
| 37 | c | 504 | CLA | C4-C3-C5 | 2.60 | 119.74 | 115.23 |
| 37 | 13 | 303 | CLA | CMB-C2B-C1B | 2.60 | 129.38 | 125.42 |
| 37 | 21 | 206 | CLA | CMB-C2B-C1B | 2.60 | 129.38 | 125.42 |
| 37 | 18 | 202 | CLA | C3B-C4B-NB | 2.60 | 112.85 | 110.53 |
| 37 | 13 | 310 | CLA | CHD-C4C-NC | 2.60 | 128.26 | 124.23 |
| 47 | 16 | 302 | KC1 | CHB-C4A-NA | 2.60 | 128.26 | 124.23 |
| 37 | 35 | 307 | CLA | CHB-C1B-C2B | -2.60 | 119.89 | 127.43 |
| 48 | 41 | 215 | A86 | C19-C18-C17 | -2.60 | 105.93 | 110.79 |
| 48 | 38 | 212 | A86 | C12-C11-C13 | 2.60 | 120.21 | 116.00 |
| 37 | 21 | 204 | CLA | CHB-C4A-NA | 2.60 | 128.15 | 124.40 |
| 37 | 19 | 307 | CLA | CHB-C4A-NA | 2.60 | 128.15 | 124.40 |
| 37 | 32 | 211 | CLA | CMB-C2B-C1B | 2.60 | 129.37 | 125.42 |
| 37 | C | 504 | CLA | C4-C3-C5 | 2.60 | 119.73 | 115.23 |
| 37 | 39 | 304 | CLA | CHB-C4A-NA | 2.60 | 128.15 | 124.40 |
| 39 | c | 515 | BCR | C11-C10-C9 | -2.60 | 123.64 | 127.28 |
| 47 | 19 | 308 | KC1 | O2D-CGD-O1D | -2.60 | 118.80 | 123.85 |
| 47 | 15 | 309 | KC1 | C1A-NA-C4A | -2.60 | 105.50 | 106.68 |
| 48 | 15 | 312 | A86 | C25-C24-C1 | -2.60 | 119.25 | 126.36 |
| 48 | 18 | 215 | A86 | C36-C31-C32 | -2.59 | 117.12 | 119.70 |
| 37 | 19 | 304 | CLA | CMB-C2B-C1B | 2.59 | 129.37 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 31 | 319 | A86 | C4-C5-C6 | -2.59 | 123.64 | 127.28 |
| 37 | 12 | 209 | CLA | CAA-C2A-C1A | 2.59 | 120.48 | 111.97 |
| 37 | 14 | 303 | CLA | O2D-CGD-O1D | -2.59 | 118.80 | 123.85 |
| 37 | 35 | 310 | CLA | CHD-C4C-NC | 2.59 | 128.25 | 124.23 |
| 50 | 41 | 212 | DD6 | C33-C32-C31 | 2.59 | 114.60 | 109.49 |
| 48 | 40 | 213 | A86 | C9-C8-C6 | -2.59 | 119.25 | 126.36 |
| 47 | 41 | 203 | KC1 | CHB-C1B-C2B | -2.59 | 120.09 | 125.49 |
| 48 | 11 | 319 | A86 | C4-C5-C6 | -2.59 | 123.64 | 127.28 |
| 37 | 38 | 201 | CLA | C1-O2A-CGA | 2.59 | 122.93 | 116.65 |
| 37 | C | 501 | CLA | C4-C3-C5 | 2.59 | 119.73 | 115.23 |
| 37 | 33 | 303 | CLA | O2D-CGD-O1D | -2.59 | 118.80 | 123.85 |
| 40 | L | 101 | SQD | C44-O6-C1 | 2.59 | 119.36 | 113.80 |
| 47 | 40 | 206 | KC1 | CHD-C4C-NC | 2.59 | 128.22 | 124.31 |
| 37 | 12 | 205 | CLA | O2D-CGD-O1D | -2.59 | 118.80 | 123.85 |
| 48 | 18 | 212 | A86 | C21-C20-C15 | -2.59 | 114.98 | 123.35 |
| 39 | C | 514 | BCR | C7-C8-C9 | -2.59 | 122.40 | 126.23 |
| 48 | 31 | 312 | A86 | C23-C16-C22 | -2.59 | 103.60 | 107.37 |
| 48 | 11 | 315 | A86 | C19-C18-C17 | -2.59 | 105.94 | 110.79 |
| 37 | b | 508 | CLA | O2A-CGA-CBA | 2.59 | 119.74 | 111.83 |
| 37 | d | 404 | CLA | CHB-C4A-NA | 2.59 | 128.14 | 124.40 |
| 37 | 32 | 210 | CLA | CAA-C2A-C1A | 2.59 | 120.47 | 111.97 |
| 47 | 33 | 309 | KC1 | C4C-C3C-C2C | -2.59 | 103.12 | 106.89 |
| 48 | 12 | 220 | A86 | C21-C20-C15 | -2.59 | 114.99 | 123.35 |
| 48 | 32 | 221 | A86 | C21-C20-C15 | -2.59 | 114.99 | 123.35 |
| 37 | 13 | 305 | CLA | CAA-C2A-C3A | -2.59 | 106.00 | 113.00 |
| 37 | 39 | 306 | CLA | C4-C3-C5 | 2.59 | 119.72 | 115.23 |
| 37 | B | 511 | CLA | C1-C2-C3 | -2.59 | 121.95 | 126.20 |
| 37 | 19 | 307 | CLA | C1-C2-C3 | -2.59 | 121.95 | 126.20 |
| 37 | 15 | 310 | CLA | CAC-C3C-C4C | 2.59 | 128.16 | 124.79 |
| 48 | 31 | 314 | A86 | C41-C32-C31 | -2.59 | 108.15 | 110.47 |
| 37 | 19 | 307 | CLA | CHD-C4C-NC | 2.59 | 128.25 | 124.23 |
| 37 | 41 | 210 | CLA | CAC-C3C-C4C | 2.59 | 128.16 | 124.79 |
| 37 | 34 | 302 | CLA | O2A-CGA-CBA | 2.59 | 119.73 | 111.83 |
| 37 | 39 | 307 | CLA | CHB-C4A-NA | 2.59 | 128.14 | 124.40 |
| 37 | 17 | 307 | CLA | C1-C2-C3 | -2.59 | 121.96 | 126.20 |
| 37 | D | 406 | CLA | CHB-C4A-NA | 2.59 | 128.13 | 124.40 |
| 37 | 16 | 301 | CLA | C3B-C4B-NB | 2.59 | 112.84 | 110.53 |
| 37 | 16 | 306 | CLA | C3B-C4B-NB | 2.59 | 112.84 | 110.53 |
| 47 | 14 | 304 | KC1 | C4C-C3C-C2C | -2.59 | 103.12 | 106.89 |
| 39 | 5 | 101 | BCR | C3-C4-C5 | -2.59 | 109.44 | 114.06 |
| 37 | B | 508 | CLA | O2A-CGA-CBA | 2.59 | 119.72 | 111.83 |
| 37 | 34 | 307 | CLA | CHA-C1A-NA | -2.59 | 120.53 | 126.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 14 | 310 | CLA | CMB-C2B-C1B | 2.59 | 129.36 | 125.42 |
| 37 | 32 | 206 | CLA | O2D-CGD-O1D | -2.59 | 118.81 | 123.85 |
| 37 | 34 | 303 | CLA | O2D-CGD-O1D | -2.59 | 118.81 | 123.85 |
| 37 | 19 | 306 | CLA | C4-C3-C5 | 2.59 | 119.72 | 115.23 |
| 37 | 14 | 307 | CLA | CHA-C1A-NA | -2.59 | 120.53 | 126.39 |
| 47 | 37 | 307 | KC1 | CMB-C2B-C1B | 2.59 | 129.28 | 124.73 |
| 37 | 19 | 307 | CLA | O2A-CGA-CBA | 2.59 | 119.72 | 111.83 |
| 47 | 31 | 309 | KC1 | O1D-CGD-CBD | -2.59 | 119.42 | 124.52 |
| 47 | 16 | 304 | KC1 | O2D-CGD-O1D | -2.59 | 118.82 | 123.85 |
| 48 | 17 | 310 | A86 | C21-C20-C15 | -2.58 | 115.01 | 123.35 |
| 47 | 11 | 309 | KC1 | C1A-NA-C4A | -2.58 | 105.50 | 106.68 |
| 43 | 37 | 315 | LHG | O8-C23-C24 | 2.58 | 119.71 | 111.83 |
| 47 | 20 | 304 | KC1 | CHD-C4C-NC | 2.58 | 128.20 | 124.31 |
| 48 | 31 | 311 | A86 | C21-C20-C15 | -2.58 | 115.01 | 123.35 |
| 48 | 41 | 214 | A86 | C21-C20-C15 | -2.58 | 115.01 | 123.35 |
| 48 | 17 | 311 | A86 | C7-C6-C8 | 2.58 | 122.03 | 118.09 |
| 37 | 32 | 204 | CLA | C4B-C3B-C2B | -2.58 | 104.09 | 107.30 |
| 48 | 11 | 311 | A86 | C21-C20-C15 | -2.58 | 115.01 | 123.35 |
| 39 | C | 519 | BCR | C15-C16-C17 | -2.58 | 118.23 | 123.52 |
| 37 | 32 | 210 | CLA | O1D-CGD-CBD | -2.58 | 119.42 | 124.52 |
| 47 | 11 | 309 | KC1 | O1D-CGD-CBD | -2.58 | 119.42 | 124.52 |
| 41 | L | 102 | LMG | O2-C2-C1 | -2.58 | 103.92 | 110.08 |
| 37 | c | 508 | CLA | C1-C2-C3 | -2.58 | 121.97 | 126.20 |
| 37 | 36 | 306 | CLA | C3B-C4B-NB | 2.58 | 112.83 | 110.53 |
| 37 | b | 514 | CLA | CHD-C4C-NC | 2.58 | 128.23 | 124.23 |
| 37 | b | 503 | CLA | O1D-CGD-CBD | -2.58 | 119.43 | 124.52 |
| 37 | 34 | 307 | CLA | CHB-C4A-NA | 2.58 | 128.12 | 124.40 |
| 48 | 31 | 315 | A86 | C19-C18-C17 | -2.58 | 105.96 | 110.79 |
| 37 | 33 | 305 | CLA | CAA-C2A-C3A | -2.58 | 106.03 | 113.00 |
| 37 | 37 | 303 | CLA | CHB-C4A-NA | 2.58 | 128.12 | 124.40 |
| 48 | 20 | 311 | A86 | C9-C8-C6 | -2.58 | 119.29 | 126.36 |
| 37 | 33 | 305 | CLA | CHB-C4A-NA | 2.58 | 128.12 | 124.40 |
| 48 | 35 | 311 | A86 | C21-C20-C15 | -2.58 | 115.03 | 123.35 |
| 37 | B | 501 | CLA | CMC-C2C-C1C | 2.58 | 129.06 | 125.03 |
| 37 | a | 404 | CLA | CBC-CAC-C3C | -2.58 | 105.43 | 112.42 |
| 48 | 11 | 313 | A86 | C3-C4-C5 | -2.58 | 118.24 | 123.52 |
| 45 | D | 408 | PL9 | C22-C23-C24 | -2.58 | 121.72 | 127.62 |
| 37 | 40 | 210 | CLA | O2A-CGA-CBA | 2.58 | 119.69 | 111.83 |
| 48 | 38 | 212 | A86 | C21-C20-C15 | -2.58 | 115.03 | 123.35 |
| 37 | 40 | 210 | CLA | CMB-C2B-C1B | 2.58 | 129.34 | 125.42 |
| 41 | l | 101 | LMG | O2-C2-C1 | -2.58 | 103.93 | 110.08 |
| 37 | 11 | 307 | CLA | C4B-C3B-C2B | -2.58 | 104.10 | 107.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 40 | a | 409 | SQD | O48-C23-O10 | -2.58 | 117.18 | 123.63 |
| 37 | 14 | 302 | CLA | O2A-CGA-CBA | 2.58 | 119.69 | 111.83 |
| 37 | 41 | 206 | CLA | CMB-C2B-C1B | 2.58 | 129.34 | 125.42 |
| 48 | 38 | 215 | A86 | C35-C34-C33 | 2.58 | 114.52 | 109.89 |
| 37 | 15 | 308 | CLA | CAA-C2A-C3A | -2.58 | 106.04 | 113.00 |
| 47 | 35 | 309 | KC1 | CBC-CAC-C3C | -2.58 | 105.44 | 112.42 |
| 37 | 39 | 304 | CLA | CMB-C2B-C1B | 2.58 | 129.34 | 125.42 |
| 48 | 21 | 214 | A86 | C21-C20-C15 | -2.58 | 115.04 | 123.35 |
| 37 | 19 | 304 | CLA | CHB-C4A-NA | 2.57 | 128.12 | 124.40 |
| 43 | B | 523 | LHG | O8-C23-C24 | 2.57 | 119.68 | 111.83 |
| 37 | 16 | 307 | CLA | O2A-CGA-CBA | 2.57 | 119.68 | 111.83 |
| 37 | 13 | 307 | CLA | CMC-C2C-C1C | 2.57 | 129.06 | 125.03 |
| 39 | c | 515 | BCR | C15-C14-C13 | -2.57 | 123.67 | 127.28 |
| 37 | 39 | 304 | CLA | CAA-C2A-C3A | -2.57 | 106.05 | 113.00 |
| 37 | 13 | 310 | CLA | O2D-CGD-O1D | -2.57 | 118.84 | 123.85 |
| 38 | A | 404 | PHO | O2D-CGD-O1D | -2.57 | 118.84 | 123.85 |
| 37 | c | 513 | CLA | CBC-CAC-C3C | -2.57 | 105.45 | 112.42 |
| 37 | 36 | 307 | CLA | CAC-C3C-C4C | 2.57 | 128.14 | 124.79 |
| 47 | 15 | 304 | KC1 | C4C-C3C-C2C | -2.57 | 103.15 | 106.89 |
| 37 | 34 | 302 | CLA | CAA-C2A-C1A | 2.57 | 120.41 | 111.97 |
| 47 | 15 | 309 | KC1 | CMB-C2B-C1B | 2.57 | 129.26 | 124.73 |
| 37 | 39 | 310 | CLA | CHB-C4A-NA | 2.57 | 128.11 | 124.40 |
| 40 | B | 522 | SQD | C1-O5-C5 | 2.57 | 118.74 | 113.72 |
| 37 | 20 | 308 | CLA | O2A-CGA-CBA | 2.57 | 119.68 | 111.83 |
| 43 | b | 522 | LHG | O8-C23-C24 | 2.57 | 119.68 | 111.83 |
| 37 | c | 511 | CLA | CMB-C2B-C1B | 2.57 | 129.34 | 125.42 |
| 37 | B | 524 | CLA | C4-C3-C5 | 2.57 | 119.69 | 115.23 |
| 37 | 36 | 307 | CLA | O2A-CGA-CBA | 2.57 | 119.67 | 111.83 |
| 48 | 18 | 215 | A86 | C35-C34-C33 | 2.57 | 114.50 | 109.89 |
| 37 | 41 | 205 | CLA | CHB-C4A-NA | 2.57 | 128.11 | 124.40 |
| 45 | d | 406 | PL9 | C22-C23-C24 | -2.57 | 121.74 | 127.62 |
| 37 | 14 | 301 | CLA | C1-C2-C3 | -2.57 | 121.99 | 126.20 |
| 37 | 35 | 307 | CLA | C3B-C4B-NB | 2.57 | 112.82 | 110.53 |
| 50 | 21 | 212 | DD6 | C33-C32-C31 | 2.57 | 114.55 | 109.49 |
| 37 | 19 | 302 | CLA | C4-C3-C5 | 2.57 | 119.69 | 115.23 |
| 37 | 39 | 306 | CLA | CAA-C2A-C3A | -2.57 | 106.06 | 113.00 |
| 43 | 17 | 316 | LHG | O8-C23-C24 | 2.57 | 119.66 | 111.83 |
| 37 | 38 | 211 | CLA | CMB-C2B-C1B | 2.57 | 129.33 | 125.42 |
| 47 | 11 | 302 | KC1 | C4C-C3C-C2C | -2.57 | 103.16 | 106.89 |
| 47 | 35 | 309 | KC1 | CMC-C2C-C1C | 2.57 | 129.04 | 125.03 |
| 37 | 13 | 305 | CLA | CHB-C4A-NA | 2.57 | 128.10 | 124.40 |
| 37 | 32 | 208 | CLA | CMB-C2B-C1B | 2.57 | 129.33 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 11 | 305 | CLA | O2D-CGD-O1D | -2.57 | 118.85 | 123.85 |
| 37 | C | 513 | CLA | CBC-CAC-C3C | -2.57 | 105.47 | 112.42 |
| 39 | C | 515 | BCR | C15-C14-C13 | -2.57 | 123.68 | 127.28 |
| 39 | c | 519 | BCR | C15-C16-C17 | -2.57 | 118.27 | 123.52 |
| 47 | 38 | 207 | KC1 | CAA-CBA-CGA | -2.57 | 114.00 | 127.05 |
| 37 | C | 508 | CLA | C1-C2-C3 | -2.56 | 122.00 | 126.20 |
| 37 | 36 | 309 | CLA | O2D-CGD-O1D | -2.56 | 118.86 | 123.85 |
| 37 | B | 503 | CLA | O1D-CGD-CBD | -2.56 | 119.46 | 124.52 |
| 37 | 14 | 302 | CLA | CAA-C2A-C1A | 2.56 | 120.38 | 111.97 |
| 37 | 36 | 301 | CLA | CHC-C1C-C2C | -2.56 | 119.66 | 126.95 |
| 37 | 14 | 310 | CLA | CHB-C4A-NA | 2.56 | 128.10 | 124.40 |
| 37 | C | 503 | CLA | C4B-C3B-C2B | -2.56 | 104.11 | 107.30 |
| 37 | c | 501 | CLA | C4-C3-C5 | 2.56 | 119.68 | 115.23 |
| 37 | 12 | 207 | CLA | CHB-C4A-NA | 2.56 | 128.10 | 124.40 |
| 37 | 39 | 302 | CLA | O2A-CGA-CBA | 2.56 | 119.65 | 111.83 |
| 37 | 33 | 307 | CLA | CMC-C2C-C1C | 2.56 | 129.04 | 125.03 |
| 48 | 12 | 213 | A86 | C3-C4-C5 | -2.56 | 118.28 | 123.52 |
| 40 | 36 | 315 | SQD | C1-O5-C5 | 2.56 | 118.72 | 113.72 |
| 37 | 16 | 309 | CLA | O2D-CGD-O1D | -2.56 | 118.86 | 123.85 |
| 37 | B | 507 | CLA | O2A-CGA-CBA | 2.56 | 119.65 | 111.83 |
| 43 | 21 | 201 | LHG | C11-C10-C9 | -2.56 | 101.42 | 114.37 |
| 37 | 15 | 307 | CLA | C3B-C4B-NB | 2.56 | 112.82 | 110.53 |
| 40 | b | 521 | SQD | C1-O5-C5 | 2.56 | 118.72 | 113.72 |
| 37 | 21 | 206 | CLA | CHB-C4A-NA | 2.56 | 128.10 | 124.40 |
| 37 | b | 507 | CLA | O2A-CGA-CBA | 2.56 | 119.65 | 111.83 |
| 37 | 18 | 204 | CLA | CHC-C1C-C2C | -2.56 | 119.67 | 126.95 |
| 37 | D | 401 | CLA | CBC-CAC-C3C | -2.56 | 105.48 | 112.42 |
| 37 | 38 | 209 | CLA | C1-O2A-CGA | 2.56 | 122.85 | 116.65 |
| 47 | 17 | 305 | KC1 | CMB-C2B-C1B | 2.56 | 129.24 | 124.73 |
| 37 | B | 504 | CLA | CAA-CBA-CGA | -2.56 | 105.94 | 113.21 |
| 40 | A | 407 | SQD | O48-C23-O10 | -2.56 | 117.23 | 123.63 |
| 37 | 21 | 202 | CLA | CHD-C4C-NC | 2.56 | 128.20 | 124.23 |
| 37 | 19 | 310 | CLA | CHB-C4A-NA | 2.56 | 128.09 | 124.40 |
| 37 | 32 | 208 | CLA | CHB-C4A-NA | 2.56 | 128.09 | 124.40 |
| 37 | 20 | 308 | CLA | CMB-C2B-C1B | 2.56 | 129.31 | 125.42 |
| 37 | 19 | 304 | CLA | CAA-C2A-C3A | -2.56 | 106.09 | 113.00 |
| 37 | 16 | 306 | CLA | C1-C2-C3 | -2.56 | 122.01 | 126.20 |
| 37 | 18 | 204 | CLA | O2D-CGD-O1D | -2.56 | 118.87 | 123.85 |
| 37 | 34 | 301 | CLA | C1-C2-C3 | -2.55 | 122.01 | 126.20 |
| 37 | b | 502 | CLA | CAA-CBA-CGA | -2.55 | 105.95 | 113.21 |
| 37 | b | 504 | CLA | CAA-CBA-CGA | -2.55 | 105.95 | 113.21 |
| 37 | 39 | 303 | CLA | CMC-C2C-C1C | 2.55 | 129.03 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 13 | 313 | A86 | C9-C10-C11 | -2.55 | 119.42 | 126.64 |
| 48 | 33 | 313 | A86 | C9-C10-C11 | -2.55 | 119.42 | 126.64 |
| 37 | 40 | 203 | CLA | CBC-CAC-C3C | -2.55 | 105.50 | 112.42 |
| 43 | b | 522 | LHG | C11-C10-C9 | -2.55 | 101.46 | 114.37 |
| 48 | 37 | 311 | A86 | C41-C32-C31 | -2.55 | 108.19 | 110.47 |
| 48 | 18 | 215 | A86 | C21-C20-C15 | -2.55 | 115.11 | 123.35 |
| 37 | 31 | 306 | CLA | CMB-C2B-C1B | 2.55 | 129.31 | 125.42 |
| 37 | 39 | 301 | CLA | CMC-C2C-C1C | 2.55 | 129.02 | 125.03 |
| 43 | 41 | 201 | LHG | C11-C10-C9 | -2.55 | 101.47 | 114.37 |
| 48 | 31 | 319 | A86 | C21-C20-C15 | -2.55 | 115.11 | 123.35 |
| 37 | 41 | 204 | CLA | CHB-C4A-NA | 2.55 | 128.08 | 124.40 |
| 37 | B | 502 | CLA | CAA-CBA-CGA | -2.55 | 105.96 | 113.21 |
| 47 | 31 | 303 | KC1 | C4C-C3C-C2C | -2.55 | 103.18 | 106.89 |
| 37 | 13 | 303 | CLA | O2D-CGD-O1D | -2.55 | 118.88 | 123.85 |
| 37 | b | 515 | CLA | C4-C3-C5 | 2.55 | 119.66 | 115.23 |
| 37 | 37 | 301 | CLA | C1-O2A-CGA | 2.55 | 122.83 | 116.65 |
| 37 | c | 512 | CLA | CMB-C2B-C1B | 2.55 | 129.30 | 125.42 |
| 37 | 41 | 206 | CLA | CHB-C4A-NA | 2.55 | 128.08 | 124.40 |
| 40 | 17 | 301 | SQD | C1-O5-C5 | 2.55 | 118.70 | 113.72 |
| 47 | 18 | 207 | KC1 | CHB-C1B-NB | -2.55 | 121.21 | 124.80 |
| 37 | 39 | 307 | CLA | CHD-C4C-NC | 2.55 | 128.19 | 124.23 |
| 37 | Z | 101 | CLA | CBC-CAC-C3C | -2.55 | 105.51 | 112.42 |
| 37 | 20 | 301 | CLA | CBC-CAC-C3C | -2.55 | 105.51 | 112.42 |
| 37 | B | 515 | CLA | C4-C3-C5 | 2.55 | 119.66 | 115.23 |
| 37 | 15 | 305 | CLA | CMB-C2B-C1B | 2.55 | 129.30 | 125.42 |
| 37 | 18 | 204 | CLA | CBC-CAC-C3C | -2.55 | 105.51 | 112.42 |
| 43 | B | 523 | LHG | C11-C10-C9 | -2.55 | 101.48 | 114.37 |
| 47 | 31 | 309 | KC1 | C1A-NA-C4A | -2.55 | 105.52 | 106.68 |
| 47 | 32 | 209 | KC1 | O2D-CGD-O1D | -2.55 | 118.89 | 123.85 |
| 37 | 38 | 206 | CLA | CBC-CAC-C3C | -2.55 | 105.51 | 112.42 |
| 37 | 12 | 209 | CLA | CHA-C1A-NA | -2.55 | 120.62 | 126.39 |
| 37 | 18 | 208 | CLA | CBC-CAC-C3C | -2.55 | 105.51 | 112.42 |
| 37 | 16 | 307 | CLA | CAC-C3C-C4C | 2.55 | 128.10 | 124.79 |
| 37 | 16 | 301 | CLA | CHC-C1C-C2C | -2.55 | 119.71 | 126.95 |
| 37 | C | 512 | CLA | CMB-C2B-C1B | 2.55 | 129.30 | 125.42 |
| 48 | 12 | 213 | A86 | C7-C6-C8 | 2.55 | 121.98 | 118.09 |
| 50 | 19 | 312 | DD6 | C10-C9-C8 | -2.55 | 115.82 | 123.20 |
| 48 | 12 | 213 | A86 | C4-C3-C2 | -2.55 | 118.31 | 123.52 |
| 37 | 14 | 307 | CLA | CHB-C4A-NA | 2.55 | 128.07 | 124.40 |
| 47 | 15 | 309 | KC1 | CBC-CAC-C3C | -2.55 | 105.52 | 112.42 |
| 37 | 35 | 301 | CLA | O2A-CGA-CBA | 2.55 | 119.60 | 111.83 |
| 37 | 19 | 306 | CLA | CAA-C2A-C3A | -2.55 | 106.12 | 113.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 308 | CLA | CHA-C1A-NA | -2.55 | 120.63 | 126.39 |
| 37 | c | 503 | CLA | O2D-CGD-O1D | -2.55 | 118.89 | 123.85 |
| 37 | 20 | 306 | CLA | O2D-CGD-O1D | -2.55 | 118.89 | 123.85 |
| 39 | C | 515 | BCR | C11-C10-C9 | -2.55 | 123.71 | 127.28 |
| 37 | 31 | 302 | CLA | CHB-C4A-NA | 2.55 | 128.07 | 124.40 |
| 37 | 15 | 310 | CLA | CHD-C4C-NC | 2.54 | 128.18 | 124.23 |
| 48 | 11 | 319 | A86 | C21-C20-C15 | -2.54 | 115.14 | 123.35 |
| 37 | B | 509 | CLA | C1-C2-C3 | -2.54 | 122.03 | 126.20 |
| 48 | 17 | 313 | A86 | C36-C31-C32 | -2.54 | 117.17 | 119.70 |
| 50 | 39 | 312 | DD6 | C10-C9-C8 | -2.54 | 115.83 | 123.20 |
| 47 | 12 | 208 | KC1 | O2D-CGD-O1D | -2.54 | 118.90 | 123.85 |
| 37 | 31 | 308 | CLA | C4B-C3B-C2B | -2.54 | 104.14 | 107.30 |
| 37 | 11 | 305 | CLA | CMB-C2B-C1B | 2.54 | 129.29 | 125.42 |
| 37 | 15 | 307 | CLA | CHB-C4A-NA | 2.54 | 128.07 | 124.40 |
| 48 | 34 | 314 | A86 | C34-O4-C38 | -2.54 | 113.36 | 117.85 |
| 37 | b | 509 | CLA | C1-C2-C3 | -2.54 | 122.03 | 126.20 |
| 37 | B | 502 | CLA | CHB-C4A-NA | 2.54 | 128.07 | 124.40 |
| 37 | c | 513 | CLA | O2A-CGA-CBA | 2.54 | 119.58 | 111.83 |
| 37 | 12 | 203 | CLA | O2A-CGA-CBA | 2.54 | 119.58 | 111.83 |
| 37 | 34 | 310 | CLA | CHB-C4A-NA | 2.54 | 128.07 | 124.40 |
| 37 | 35 | 310 | CLA | O1D-CGD-CBD | -2.54 | 119.50 | 124.52 |
| 45 | d | 402 | PL9 | O2-C1-C6 | 2.54 | 124.52 | 120.48 |
| 48 | 11 | 315 | A86 | C41-C32-C31 | -2.54 | 108.20 | 110.47 |
| 37 | 32 | 204 | CLA | O2A-CGA-CBA | 2.54 | 119.58 | 111.83 |
| 47 | 34 | 306 | KC1 | C1A-NA-C4A | -2.54 | 105.52 | 106.68 |
| 37 | 34 | 305 | CLA | CHB-C4A-NA | 2.54 | 128.07 | 124.40 |
| 48 | 19 | 313 | A86 | C24-C1-C2 | -2.54 | 115.02 | 119.01 |
| 37 | 41 | 202 | CLA | CHD-C4C-NC | 2.54 | 128.17 | 124.23 |
| 37 | C | 501 | CLA | C4C-C3C-C2C | -2.54 | 103.20 | 106.89 |
| 37 | C | 513 | CLA | O2A-CGA-CBA | 2.54 | 119.58 | 111.83 |
| 37 | 18 | 202 | CLA | O2A-CGA-CBA | 2.54 | 119.58 | 111.83 |
| 48 | 34 | 316 | A86 | C40-C32-C31 | 2.54 | 112.74 | 110.47 |
| 37 | 33 | 305 | CLA | CMC-C2C-C1C | 2.54 | 129.00 | 125.03 |
| 37 | 36 | 306 | CLA | C1-C2-C3 | -2.54 | 122.04 | 126.20 |
| 47 | 36 | 305 | KC1 | CHD-C4C-NC | 2.54 | 128.13 | 124.31 |
| 45 | D | 404 | PL9 | C22-C23-C24 | -2.54 | 121.81 | 127.62 |
| 37 | C | 511 | CLA | CMB-C2B-C1B | 2.54 | 129.28 | 125.42 |
| 47 | 16 | 305 | KC1 | CHD-C4C-NC | 2.54 | 128.13 | 124.31 |
| 48 | 14 | 316 | A86 | C40-C32-C31 | 2.54 | 112.74 | 110.47 |
| 37 | 11 | 307 | CLA | CHA-C1A-NA | -2.54 | 120.64 | 126.39 |
| 37 | C | 505 | CLA | O2A-CGA-CBA | 2.54 | 119.57 | 111.83 |
| 37 | c | 505 | CLA | O2A-CGA-CBA | 2.54 | 119.57 | 111.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 39 | 312 | DD6 | C23-C16-C15 | 2.54 | 116.89 | 110.05 |
| 37 | D | 402 | CLA | C4-C3-C5 | 2.54 | 119.63 | 115.23 |
| 48 | 36 | 311 | A86 | C21-C20-C15 | -2.54 | 115.16 | 123.35 |
| 48 | 33 | 315 | A86 | C36-C31-C32 | -2.54 | 117.18 | 119.70 |
| 37 | 15 | 310 | CLA | CMB-C2B-C1B | 2.54 | 129.28 | 125.42 |
| 47 | 11 | 309 | KC1 | CMA-C3A-C2A | -2.54 | 122.29 | 128.43 |
| 47 | 21 | 203 | KC1 | CBC-CAC-C3C | -2.54 | 105.55 | 112.42 |
| 48 | 14 | 314 | A86 | C34-O4-C38 | -2.53 | 113.37 | 117.85 |
| 37 | a | 404 | CLA | CHB-C4A-NA | 2.53 | 128.06 | 124.40 |
| 37 | b | 515 | CLA | CHB-C4A-NA | 2.53 | 128.06 | 124.40 |
| 48 | 15 | 311 | A86 | C21-C20-C15 | -2.53 | 115.17 | 123.35 |
| 48 | 16 | 311 | A86 | C21-C20-C15 | -2.53 | 115.17 | 123.35 |
| 37 | 18 | 211 | CLA | CMB-C2B-C1B | 2.53 | 129.28 | 125.42 |
| 37 | 17 | 307 | CLA | CMB-C2B-C3B | 2.53 | 132.51 | 126.55 |
| 50 | 41 | 216 | DD6 | C19-C18-C17 | 2.53 | 115.53 | 110.79 |
| 37 | z | 101 | CLA | CBC-CAC-C3C | -2.53 | 105.55 | 112.42 |
| 37 | 11 | 301 | CLA | CHB-C4A-NA | 2.53 | 128.06 | 124.40 |
| 39 | b | 518 | BCR | C30-C25-C26 | -2.53 | 119.17 | 122.64 |
| 37 | 32 | 210 | CLA | CHA-C1A-NA | -2.53 | 120.66 | 126.39 |
| 47 | 41 | 203 | KC1 | CBC-CAC-C3C | -2.53 | 105.56 | 112.42 |
| 37 | 15 | 301 | CLA | O2A-CGA-CBA | 2.53 | 119.56 | 111.83 |
| 47 | 38 | 207 | KC1 | CHD-C1D-ND | -2.53 | 120.25 | 124.05 |
| 50 | 21 | 216 | DD6 | C19-C18-C17 | 2.53 | 115.53 | 110.79 |
| 37 | 14 | 305 | CLA | CHB-C4A-NA | 2.53 | 128.05 | 124.40 |
| 43 | d | 408 | LHG | O8-C23-C24 | 2.53 | 119.55 | 111.83 |
| 48 | 31 | 319 | A86 | C7-C6-C8 | 2.53 | 121.95 | 118.09 |
| 48 | 32 | 214 | A86 | C7-C6-C8 | 2.53 | 121.95 | 118.09 |
| 37 | c | 512 | CLA | CHB-C4A-NA | 2.53 | 128.05 | 124.40 |
| 37 | 12 | 203 | CLA | C1-C2-C3 | -2.53 | 122.05 | 126.20 |
| 47 | 17 | 308 | KC1 | CAA-CBA-CGA | -2.53 | 114.19 | 127.05 |
| 37 | 13 | 307 | CLA | O2A-CGA-CBA | 2.53 | 119.55 | 111.83 |
| 37 | 15 | 308 | CLA | CMC-C2C-C1C | 2.53 | 128.99 | 125.03 |
| 37 | 21 | 204 | CLA | O2D-CGD-O1D | -2.53 | 118.92 | 123.85 |
| 48 | 33 | 313 | A86 | C35-C34-C33 | 2.53 | 114.43 | 109.89 |
| 47 | 35 | 306 | KC1 | CMC-C2C-C1C | 2.53 | 128.99 | 125.03 |
| 37 | 13 | 305 | CLA | CMC-C2C-C1C | 2.53 | 128.99 | 125.03 |
| 37 | 32 | 204 | CLA | C1-C2-C3 | -2.53 | 122.06 | 126.20 |
| 37 | 37 | 308 | CLA | O2A-CGA-O1A | -2.53 | 117.31 | 123.63 |
| 37 | b | 509 | CLA | CHA-C1A-NA | -2.53 | 120.67 | 126.39 |
| 37 | 19 | 303 | CLA | CMC-C2C-C1C | 2.53 | 128.98 | 125.03 |
| 37 | 11 | 308 | CLA | CHD-C4C-NC | 2.53 | 128.15 | 124.23 |
| 37 | 32 | 202 | CLA | CHD-C4C-NC | 2.53 | 128.15 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 18 | 210 | KC1 | CMB-C2B-C1B | 2.53 | 129.18 | 124.73 |
| 37 | C | 512 | CLA | CHB-C4A-NA | 2.53 | 128.04 | 124.40 |
| 37 | b | 506 | CLA | C4-C3-C5 | 2.53 | 119.61 | 115.23 |
| 38 | a | 406 | PHO | O2D-CGD-O1D | -2.53 | 118.93 | 123.85 |
| 47 | 35 | 304 | KC1 | C4C-C3C-C2C | -2.53 | 103.22 | 106.89 |
| 37 | 40 | 208 | CLA | O2D-CGD-O1D | -2.53 | 118.93 | 123.85 |
| 50 | 19 | 312 | DD6 | C23-C16-C15 | 2.52 | 116.86 | 110.05 |
| 48 | 21 | 215 | A86 | C25-C24-C1 | -2.52 | 119.44 | 126.36 |
| 48 | 11 | 319 | A86 | C7-C6-C8 | 2.52 | 121.94 | 118.09 |
| 37 | 32 | 211 | CLA | CED-O2D-CGD | 2.52 | 121.64 | 115.92 |
| 47 | 34 | 309 | KC1 | CHB-C1B-C2B | -2.52 | 120.24 | 125.49 |
| 44 | J | 101 | DGD | C1D-C2D-C3D | -2.52 | 104.70 | 110.01 |
| 47 | 31 | 303 | KC1 | C1A-NA-C4A | -2.52 | 105.53 | 106.68 |
| 44 | j | 101 | DGD | C1D-C2D-C3D | -2.52 | 104.70 | 110.01 |
| 37 | 18 | 209 | CLA | C1-C2-C3 | -2.52 | 122.06 | 126.20 |
| 37 | B | 515 | CLA | CHB-C4A-NA | 2.52 | 128.04 | 124.40 |
| 37 | 34 | 307 | CLA | CBC-CAC-C3C | -2.52 | 105.58 | 112.42 |
| 37 | C | 503 | CLA | O2D-CGD-O1D | -2.52 | 118.94 | 123.85 |
| 47 | 14 | 309 | KC1 | CHB-C1B-C2B | -2.52 | 120.24 | 125.49 |
| 37 | B | 509 | CLA | CHA-C1A-NA | -2.52 | 120.68 | 126.39 |
| 37 | 39 | 306 | CLA | CHC-C1C-C2C | -2.52 | 119.78 | 126.95 |
| 37 | B | 506 | CLA | C4-C3-C5 | 2.52 | 119.60 | 115.23 |
| 37 | b | 502 | CLA | CHB-C4A-NA | 2.52 | 128.04 | 124.40 |
| 48 | 34 | 313 | A86 | C19-C18-C17 | -2.52 | 106.08 | 110.79 |
| 37 | A | 405 | CLA | O2A-CGA-CBA | 2.52 | 119.52 | 111.83 |
| 37 | a | 407 | CLA | O2A-CGA-CBA | 2.52 | 119.52 | 111.83 |
| 45 | d | 402 | PL9 | C22-C23-C24 | -2.52 | 121.86 | 127.62 |
| 37 | 31 | 306 | CLA | O2D-CGD-O1D | -2.52 | 118.94 | 123.85 |
| 48 | 11 | 314 | A86 | C41-C32-C31 | -2.52 | 108.22 | 110.47 |
| 47 | 14 | 306 | KC1 | CHB-C1B-NB | -2.52 | 121.26 | 124.80 |
| 41 | b | 519 | LMG | C38-C37-C36 | -2.52 | 101.64 | 114.37 |
| 37 | b | 511 | CLA | CBC-CAC-C3C | -2.52 | 105.60 | 112.42 |
| 43 | D | 410 | LHG | O8-C23-C24 | 2.52 | 119.51 | 111.83 |
| 48 | 37 | 312 | A86 | C36-C31-C32 | -2.52 | 117.20 | 119.70 |
| 37 | 14 | 307 | CLA | CBC-CAC-C3C | -2.52 | 105.60 | 112.42 |
| 37 | 41 | 204 | CLA | O2D-CGD-O1D | -2.52 | 118.95 | 123.85 |
| 37 | c | 510 | CLA | C4C-C3C-C2C | -2.52 | 103.23 | 106.89 |
| 37 | 15 | 310 | CLA | O1D-CGD-CBD | -2.52 | 119.56 | 124.52 |
| 41 | B | 520 | LMG | C38-C37-C36 | -2.52 | 101.65 | 114.37 |
| 47 | 37 | 307 | KC1 | CAA-CBA-CGA | -2.52 | 114.26 | 127.05 |
| 37 | 14 | 301 | CLA | C3B-C4B-NB | 2.51 | 112.78 | 110.53 |
| 37 | 37 | 306 | CLA | CMB-C2B-C3B | 2.51 | 132.47 | 126.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 34 | 310 | CLA | C4C-C3C-C2C | -2.51 | 103.23 | 106.89 |
| 37 | 12 | 212 | CLA | CMB-C2B-C1B | 2.51 | 129.25 | 125.42 |
| 47 | 31 | 309 | KC1 | CMA-C3A-C2A | -2.51 | 122.34 | 128.43 |
| 43 | d | 407 | LHG | C20-C19-C18 | -2.51 | 101.66 | 114.37 |
| 47 | 38 | 210 | KC1 | C1A-NA-C4A | -2.51 | 105.53 | 106.68 |
| 43 | D | 409 | LHG | C20-C19-C18 | -2.51 | 101.66 | 114.37 |
| 48 | 14 | 312 | A86 | C34-O4-C38 | -2.51 | 113.41 | 117.85 |
| 37 | 20 | 307 | CLA | CMB-C2B-C1B | 2.51 | 129.25 | 125.42 |
| 47 | 12 | 211 | KC1 | CHB-C4A-NA | 2.51 | 128.13 | 124.23 |
| 37 | 13 | 307 | CLA | C4D-CHA-C1A | -2.51 | 118.25 | 121.24 |
| 37 | B | 504 | CLA | CHD-C4C-NC | 2.51 | 128.13 | 124.23 |
| 37 | 33 | 307 | CLA | O2A-CGA-CBA | 2.51 | 119.49 | 111.83 |
| 48 | 34 | 314 | A86 | C8-C6-C5 | -2.51 | 115.06 | 119.01 |
| 47 | 32 | 212 | KC1 | CHB-C4A-NA | 2.51 | 128.13 | 124.23 |
| 48 | 14 | 315 | A86 | C21-C20-C15 | -2.51 | 115.24 | 123.35 |
| 37 | 19 | 306 | CLA | C4B-C3B-C2B | -2.51 | 104.18 | 107.30 |
| 37 | B | 511 | CLA | CBC-CAC-C3C | -2.51 | 105.61 | 112.42 |
| 48 | 36 | 310 | A86 | C7-C6-C8 | 2.51 | 121.92 | 118.09 |
| 37 | 19 | 301 | CLA | CMC-C2C-C1C | 2.51 | 128.96 | 125.03 |
| 37 | 41 | 206 | CLA | CBC-CAC-C3C | -2.51 | 105.61 | 112.42 |
| 37 | 36 | 309 | CLA | CAA-CBA-CGA | -2.51 | 105.79 | 112.49 |
| 48 | 21 | 215 | A86 | C40-C32-C31 | 2.51 | 112.72 | 110.47 |
| 37 | 33 | 310 | CLA | O2D-CGD-O1D | -2.51 | 118.96 | 123.85 |
| 47 | 32 | 212 | KC1 | CMC-C2C-C1C | 2.51 | 128.96 | 125.03 |
| 48 | 20 | 311 | A86 | C34-O4-C38 | -2.51 | 113.41 | 117.85 |
| 37 | 13 | 303 | CLA | CBC-CAC-C3C | -2.51 | 105.62 | 112.42 |
| 47 | 15 | 306 | KC1 | CMC-C2C-C1C | 2.51 | 128.96 | 125.03 |
| 37 | 13 | 303 | CLA | CAA-C2A-C1A | 2.51 | 120.20 | 111.97 |
| 39 | c | 514 | BCR | C27-C26-C25 | 2.51 | 126.09 | 122.70 |
| 37 | 16 | 309 | CLA | CAA-CBA-CGA | -2.51 | 105.80 | 112.49 |
| 37 | c | 501 | CLA | C4C-C3C-C2C | -2.51 | 103.24 | 106.89 |
| 48 | 41 | 215 | A86 | C25-C24-C1 | -2.51 | 119.48 | 126.36 |
| 37 | 13 | 303 | CLA | CHB-C4A-NA | 2.51 | 128.02 | 124.40 |
| 48 | 41 | 214 | A86 | C10-C9-C8 | -2.51 | 115.93 | 123.20 |
| 47 | 38 | 207 | KC1 | O1D-CGD-CBD | -2.51 | 119.57 | 124.52 |
| 37 | 35 | 301 | CLA | CHC-C1C-C2C | -2.51 | 119.82 | 126.95 |
| 37 | 18 | 209 | CLA | C4-C3-C5 | 2.51 | 119.58 | 115.23 |
| 48 | 13 | 315 | A86 | C36-C31-C32 | -2.51 | 117.21 | 119.70 |
| 46 | F | 101 | HEM | CAA-C2A-C1A | 2.51 | 129.84 | 124.94 |
| 37 | c | 511 | CLA | CAA-CBA-CGA | -2.51 | 106.09 | 113.21 |
| 37 | d | 401 | CLA | C4-C3-C5 | 2.51 | 119.58 | 115.23 |
| 37 | 31 | 306 | CLA | CBC-CAC-C3C | -2.51 | 105.62 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 21 | 213 | A86 | C21-C20-C15 | -2.51 | 115.26 | 123.35 |
| 48 | 17 | 313 | A86 | C8-C6-C5 | -2.51 | 115.07 | 119.01 |
| 47 | 33 | 304 | KC1 | CMB-C2B-C1B | 2.51 | 129.14 | 124.73 |
| 37 | 12 | 205 | CLA | C4-C3-C5 | 2.50 | 119.58 | 115.23 |
| 37 | 39 | 301 | CLA | CMA-C3A-C4A | -2.50 | 105.04 | 111.77 |
| 37 | 20 | 303 | CLA | CHB-C4A-NA | 2.50 | 128.01 | 124.40 |
| 37 | 35 | 307 | CLA | CHB-C4A-NA | 2.50 | 128.01 | 124.40 |
| 37 | 15 | 301 | CLA | CHC-C1C-C2C | -2.50 | 119.83 | 126.95 |
| 37 | 39 | 305 | CLA | C4B-C3B-C2B | -2.50 | 104.19 | 107.30 |
| 37 | b | 523 | CLA | C4-C3-C5 | 2.50 | 119.57 | 115.23 |
| 37 | B | 515 | CLA | C1-C2-C3 | -2.50 | 122.10 | 126.20 |
| 37 | 14 | 308 | CLA | C1-C2-C3 | -2.50 | 122.10 | 126.20 |
| 48 | 21 | 211 | A86 | C9-C8-C6 | -2.50 | 119.50 | 126.36 |
| 44 | c | 516 | DGD | CDB-CCB-CBB | -2.50 | 101.72 | 114.37 |
| 48 | 34 | 315 | A86 | C21-C20-C15 | -2.50 | 115.27 | 123.35 |
| 37 | 21 | 208 | CLA | C1-C2-C3 | -2.50 | 122.10 | 126.20 |
| 43 | b | 522 | LHG | C20-C19-C18 | -2.50 | 101.72 | 114.37 |
| 48 | 41 | 213 | A86 | C21-C20-C15 | -2.50 | 115.28 | 123.35 |
| 37 | 34 | 307 | CLA | CMC-C2C-C1C | 2.50 | 128.94 | 125.03 |
| 37 | b | 504 | CLA | CHD-C4C-NC | 2.50 | 128.11 | 124.23 |
| 47 | 35 | 304 | KC1 | CAA-C2A-C1A | -2.50 | 113.68 | 124.64 |
| 37 | 19 | 305 | CLA | C4B-C3B-C2B | -2.50 | 104.19 | 107.30 |
| 37 | c | 510 | CLA | O2D-CGD-O1D | -2.50 | 118.98 | 123.85 |
| 37 | 37 | 301 | CLA | CHD-C4C-NC | 2.50 | 128.11 | 124.23 |
| 43 | B | 523 | LHG | C20-C19-C18 | -2.50 | 101.73 | 114.37 |
| 47 | 20 | 304 | KC1 | C4C-C3C-C2C | -2.50 | 103.25 | 106.89 |
| 37 | 40 | 209 | CLA | CMB-C2B-C1B | 2.50 | 129.23 | 125.42 |
| 39 | C | 514 | BCR | C27-C26-C25 | 2.50 | 126.08 | 122.70 |
| 48 | 40 | 213 | A86 | C34-O4-C38 | -2.50 | 113.43 | 117.85 |
| 48 | 14 | 313 | A86 | C19-C18-C17 | -2.50 | 106.11 | 110.79 |
| 48 | 34 | 315 | A86 | C35-C34-C33 | 2.50 | 114.38 | 109.89 |
| 37 | 36 | 301 | CLA | CBC-CAC-C3C | -2.50 | 105.64 | 112.42 |
| 47 | 34 | 306 | KC1 | CHB-C1B-NB | -2.50 | 121.28 | 124.80 |
| 47 | 34 | 304 | KC1 | CMB-C2B-C1B | 2.50 | 129.13 | 124.73 |
| 45 | D | 404 | PL9 | O2-C1-C6 | 2.50 | 124.45 | 120.48 |
| 37 | 41 | 208 | CLA | C1-C2-C3 | -2.50 | 122.11 | 126.20 |
| 46 | f | 101 | HEM | CAA-C2A-C1A | 2.50 | 129.82 | 124.94 |
| 37 | C | 504 | CLA | CMC-C2C-C1C | 2.50 | 128.94 | 125.03 |
| 37 | 16 | 303 | CLA | CMC-C2C-C1C | 2.50 | 128.94 | 125.03 |
| 37 | 16 | 309 | CLA | CHD-C4C-NC | 2.50 | 128.10 | 124.23 |
| 37 | 18 | 206 | CLA | O2D-CGD-O1D | -2.50 | 118.99 | 123.85 |
| 37 | C | 504 | CLA | C1-C2-C3 | -2.50 | 122.11 | 126.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 36 | 309 | CLA | CHD-C4C-NC | 2.50 | 128.10 | 124.23 |
| 47 | 37 | 304 | KC1 | C4C-C3C-C2C | -2.50 | 103.26 | 106.89 |
| 37 | 18 | 209 | CLA | CBC-CAC-C3C | -2.50 | 105.65 | 112.42 |
| 48 | 31 | 315 | A86 | C41-C32-C31 | -2.50 | 108.24 | 110.47 |
| 37 | c | 513 | CLA | C4B-C3B-C2B | -2.50 | 104.20 | 107.30 |
| 48 | 16 | 310 | A86 | C7-C6-C8 | 2.50 | 121.90 | 118.09 |
| 37 | 21 | 206 | CLA | CBC-CAC-C3C | -2.50 | 105.65 | 112.42 |
| 44 | C | 516 | DGD | CDB-CCB-CBB | -2.50 | 101.75 | 114.37 |
| 37 | 35 | 310 | CLA | CMB-C2B-C1B | 2.50 | 129.22 | 125.42 |
| 37 | 35 | 301 | CLA | C4B-C3B-C2B | -2.50 | 104.20 | 107.30 |
| 37 | b | 515 | CLA | C1-C2-C3 | -2.50 | 122.11 | 126.20 |
| 48 | 41 | 215 | A86 | C40-C32-C31 | 2.50 | 112.70 | 110.47 |
| 47 | 15 | 309 | KC1 | CMC-C2C-C1C | 2.50 | 128.93 | 125.03 |
| 39 | b | 518 | BCR | C40-C30-C25 | 2.49 | 114.16 | 110.24 |
| 39 | B | 518 | BCR | C30-C25-C26 | -2.49 | 119.23 | 122.64 |
| 47 | 14 | 306 | KC1 | O1D-CGD-CBD | -2.49 | 119.60 | 124.52 |
| 47 | 34 | 306 | KC1 | O1D-CGD-CBD | -2.49 | 119.60 | 124.52 |
| 37 | c | 504 | CLA | C1-C2-C3 | -2.49 | 122.11 | 126.20 |
| 48 | 14 | 314 | A86 | C8-C6-C5 | -2.49 | 115.09 | 119.01 |
| 37 | 32 | 213 | CLA | CMB-C2B-C1B | 2.49 | 129.21 | 125.42 |
| 47 | 14 | 304 | KC1 | CMB-C2B-C1B | 2.49 | 129.12 | 124.73 |
| 37 | C | 511 | CLA | CAA-CBA-CGA | -2.49 | 106.13 | 113.21 |
| 48 | 41 | 211 | A86 | C9-C8-C6 | -2.49 | 119.53 | 126.36 |
| 37 | 11 | 301 | CLA | CHC-C1C-C2C | -2.49 | 119.87 | 126.95 |
| 37 | 35 | 307 | CLA | CMB-C2B-C3B | 2.49 | 132.41 | 126.55 |
| 37 | 33 | 301 | CLA | C4B-C3B-C2B | -2.49 | 104.20 | 107.30 |
| 47 | 12 | 211 | KC1 | CMC-C2C-C1C | 2.49 | 128.93 | 125.03 |
| 37 | 33 | 307 | CLA | C4D-CHA-C1A | -2.49 | 118.27 | 121.24 |
| 37 | 38 | 206 | CLA | O2D-CGD-O1D | -2.49 | 119.00 | 123.85 |
| 37 | b | 502 | CLA | C4-C3-C5 | 2.49 | 119.55 | 115.23 |
| 37 | 31 | 308 | CLA | CHB-C4A-NA | 2.49 | 127.99 | 124.40 |
| 37 | B | 514 | CLA | CMA-C3A-C2A | -2.49 | 104.36 | 113.98 |
| 37 | 38 | 202 | CLA | CBC-CAC-C3C | -2.49 | 105.67 | 112.42 |
| 48 | 37 | 319 | A86 | C40-C32-C31 | -2.49 | 108.24 | 110.47 |
| 37 | 21 | 204 | CLA | CMC-C2C-C1C | 2.49 | 128.92 | 125.03 |
| 39 | b | 524 | BCR | C11-C10-C9 | -2.49 | 123.79 | 127.28 |
| 48 | 18 | 212 | A86 | C4-C3-C2 | -2.49 | 118.43 | 123.52 |
| 37 | c | 504 | CLA | CMC-C2C-C1C | 2.49 | 128.92 | 125.03 |
| 47 | 11 | 302 | KC1 | C1A-NA-C4A | -2.49 | 105.54 | 106.68 |
| 37 | d | 404 | CLA | CMB-C2B-C1B | 2.49 | 129.21 | 125.42 |
| 37 | C | 510 | CLA | C4C-C3C-C2C | -2.49 | 103.27 | 106.89 |
| 37 | 41 | 205 | CLA | CHD-C4C-NC | 2.49 | 128.09 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | A | 403 | CLA | O2A-CGA-CBA | 2.49 | 119.42 | 111.83 |
| 37 | 19 | 302 | CLA | O2A-CGA-CBA | 2.49 | 119.42 | 111.83 |
| 41 | B | 521 | LMG | O6-C1-O1 | -2.49 | 104.17 | 110.04 |
| 48 | 34 | 313 | A86 | C36-C31-C32 | -2.49 | 117.23 | 119.70 |
| 37 | 32 | 206 | CLA | C4-C3-C5 | 2.49 | 119.54 | 115.23 |
| 37 | D | 406 | CLA | CMB-C2B-C1B | 2.49 | 129.20 | 125.42 |
| 37 | 19 | 301 | CLA | CMA-C3A-C4A | -2.49 | 105.09 | 111.77 |
| 48 | 21 | 215 | A86 | C10-C9-C8 | -2.49 | 116.00 | 123.20 |
| 37 | 17 | 302 | CLA | C1-O2A-CGA | 2.49 | 122.67 | 116.65 |
| 37 | C | 510 | CLA | O2D-CGD-O1D | -2.48 | 119.01 | 123.85 |
| 37 | 34 | 308 | CLA | CMB-C2B-C1B | 2.48 | 129.20 | 125.42 |
| 37 | 38 | 208 | CLA | CBC-CAC-C3C | -2.48 | 105.69 | 112.42 |
| 37 | b | 514 | CLA | CMA-C3A-C2A | -2.48 | 104.38 | 113.98 |
| 37 | 12 | 210 | CLA | CAA-C2A-C3A | -2.48 | 106.29 | 113.00 |
| 47 | 13 | 302 | KC1 | CHB-C4A-NA | 2.48 | 128.08 | 124.23 |
| 47 | 41 | 207 | KC1 | CHB-C4A-NA | 2.48 | 128.08 | 124.23 |
| 37 | 39 | 306 | CLA | C4B-C3B-C2B | -2.48 | 104.21 | 107.30 |
| 39 | B | 518 | BCR | C40-C30-C25 | 2.48 | 114.14 | 110.24 |
| 37 | 14 | 307 | CLA | CMC-C2C-C1C | 2.48 | 128.91 | 125.03 |
| 37 | 36 | 303 | CLA | CMC-C2C-C1C | 2.48 | 128.91 | 125.03 |
| 37 | 41 | 206 | CLA | C1-C2-C3 | -2.48 | 122.13 | 126.20 |
| 41 | b | 520 | LMG | O6-C1-O1 | -2.48 | 104.18 | 110.04 |
| 48 | 39 | 313 | A86 | C24-C1-C2 | -2.48 | 115.10 | 119.01 |
| 37 | 34 | 308 | CLA | C1-C2-C3 | -2.48 | 122.13 | 126.20 |
| 39 | D | 407 | BCR | C15-C16-C17 | -2.48 | 118.44 | 123.52 |
| 37 | b | 502 | CLA | CAC-C3C-C4C | 2.48 | 128.02 | 124.79 |
| 37 | a | 403 | CLA | O2A-CGA-CBA | 2.48 | 119.40 | 111.83 |
| 37 | B | 502 | CLA | C4-C3-C5 | 2.48 | 119.53 | 115.23 |
| 37 | 40 | 205 | CLA | CHB-C4A-NA | 2.48 | 127.98 | 124.40 |
| 48 | 13 | 313 | A86 | C35-C34-C33 | 2.48 | 114.34 | 109.89 |
| 37 | 20 | 301 | CLA | O2A-CGA-CBA | 2.48 | 119.40 | 111.83 |
| 48 | 21 | 214 | A86 | C10-C9-C8 | -2.48 | 116.01 | 123.20 |
| 37 | 16 | 306 | CLA | CMB-C2B-C3B | 2.48 | 132.38 | 126.55 |
| 39 | d | 405 | BCR | C15-C16-C17 | -2.48 | 118.44 | 123.52 |
| 37 | 38 | 202 | CLA | C3B-C4B-NB | 2.48 | 112.74 | 110.53 |
| 48 | 37 | 310 | A86 | C8-C6-C5 | -2.48 | 115.11 | 119.01 |
| 37 | B | 508 | CLA | O2D-CGD-O1D | -2.48 | 119.02 | 123.85 |
| 47 | 19 | 308 | KC1 | CMB-C2B-C1B | 2.48 | 129.09 | 124.73 |
| 47 | 39 | 308 | KC1 | CMB-C2B-C1B | 2.48 | 129.09 | 124.73 |
| 37 | 21 | 204 | CLA | C4C-C3C-C2C | -2.48 | 103.28 | 106.89 |
| 37 | 41 | 204 | CLA | C4C-C3C-C2C | -2.48 | 103.28 | 106.89 |
| 37 | 38 | 201 | CLA | CAA-C2A-C3A | -2.48 | 106.30 | 113.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | D | 402 | CLA | CMB-C2B-C1B | 2.48 | 129.19 | 125.42 |
| 48 | 17 | 314 | A86 | O-C13-C14 | -2.48 | 116.68 | 121.76 |
| 47 | 17 | 306 | KC1 | CAA-CBA-CGA | -2.48 | 114.45 | 127.05 |
| 37 | 15 | 307 | CLA | CMB-C2B-C3B | 2.48 | 132.38 | 126.55 |
| 48 | 15 | 311 | A86 | C7-C6-C8 | 2.48 | 121.87 | 118.09 |
| 47 | 37 | 305 | KC1 | CAA-CBA-CGA | -2.48 | 114.46 | 127.05 |
| 37 | 19 | 310 | CLA | O2D-CGD-O1D | -2.48 | 119.03 | 123.85 |
| 37 | b | 511 | CLA | CMB-C2B-C3B | 2.48 | 132.37 | 126.55 |
| 47 | 21 | 207 | KC1 | CHB-C4A-NA | 2.48 | 128.07 | 124.23 |
| 37 | 34 | 301 | CLA | C3B-C4B-NB | 2.48 | 112.74 | 110.53 |
| 48 | 19 | 311 | A86 | C8-C6-C5 | -2.47 | 115.12 | 119.01 |
| 37 | 17 | 307 | CLA | O1D-CGD-CBD | -2.47 | 119.64 | 124.52 |
| 37 | 11 | 305 | CLA | CBC-CAC-C3C | -2.47 | 105.71 | 112.42 |
| 37 | 34 | 310 | CLA | CBC-CAC-C3C | -2.47 | 105.71 | 112.42 |
| 39 | D | 407 | BCR | C29-C30-C25 | 2.47 | 114.03 | 110.44 |
| 39 | D | 407 | BCR | C28-C27-C26 | -2.47 | 109.64 | 114.06 |
| 37 | 17 | 307 | CLA | CMC-C2C-C1C | 2.47 | 128.90 | 125.03 |
| 37 | 37 | 306 | CLA | CMC-C2C-C1C | 2.47 | 128.90 | 125.03 |
| 47 | 13 | 304 | KC1 | CMB-C2B-C1B | 2.47 | 129.08 | 124.73 |
| 37 | 41 | 204 | CLA | CMC-C2C-C1C | 2.47 | 128.90 | 125.03 |
| 48 | 32 | 217 | A86 | C7-C6-C8 | 2.47 | 121.86 | 118.09 |
| 37 | D | 401 | CLA | CHB-C4A-NA | 2.47 | 127.97 | 124.40 |
| 37 | 19 | 306 | CLA | CHC-C1C-C2C | -2.47 | 119.92 | 126.95 |
| 48 | 34 | 312 | A86 | C34-O4-C38 | -2.47 | 113.48 | 117.85 |
| 37 | B | 511 | CLA | CMB-C2B-C3B | 2.47 | 132.36 | 126.55 |
| 37 | 32 | 211 | CLA | CAA-C2A-C3A | -2.47 | 106.32 | 113.00 |
| 47 | 14 | 306 | KC1 | CHB-C4A-NA | 2.47 | 128.06 | 124.23 |
| 48 | 14 | 313 | A86 | C36-C31-C32 | -2.47 | 117.24 | 119.70 |
| 37 | 35 | 310 | CLA | O2D-CGD-O1D | -2.47 | 119.04 | 123.85 |
| 37 | 11 | 307 | CLA | CHB-C4A-NA | 2.47 | 127.97 | 124.40 |
| 37 | 12 | 204 | CLA | C3B-C4B-NB | 2.47 | 112.73 | 110.53 |
| 48 | 16 | 310 | A86 | C25-C26-C27 | -2.47 | 123.81 | 127.28 |
| 37 | 39 | 310 | CLA | CBC-CAC-C3C | -2.47 | 105.72 | 112.42 |
| 37 | 13 | 303 | CLA | C4B-C3B-C2B | -2.47 | 104.23 | 107.30 |
| 37 | C | 512 | CLA | O1D-CGD-CBD | -2.47 | 119.65 | 124.52 |
| 37 | 21 | 205 | CLA | CHD-C4C-NC | 2.47 | 128.06 | 124.23 |
| 37 | d | 401 | CLA | CMB-C2B-C1B | 2.47 | 129.18 | 125.42 |
| 37 | 40 | 203 | CLA | O2A-CGA-CBA | 2.47 | 119.36 | 111.83 |
| 48 | 31 | 313 | A86 | C9-C10-C11 | -2.47 | 119.66 | 126.64 |
| 37 | b | 501 | CLA | CBC-CAC-C3C | -2.47 | 105.73 | 112.42 |
| 37 | 12 | 205 | CLA | CBC-CAC-C3C | -2.47 | 105.73 | 112.42 |
| 37 | 35 | 308 | CLA | CHB-C4A-NA | 2.47 | 127.96 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 33 | 303 | CLA | CBC-CAC-C3C | -2.47 | 105.73 | 112.42 |
| 37 | 33 | 303 | CLA | C4B-C3B-C2B | -2.47 | 104.23 | 107.30 |
| 37 | 18 | 201 | CLA | CAA-C2A-C3A | -2.47 | 106.33 | 113.00 |
| 37 | 15 | 310 | CLA | O2D-CGD-O1D | -2.47 | 119.05 | 123.85 |
| 48 | 14 | 311 | A86 | C21-C20-C15 | -2.47 | 115.39 | 123.35 |
| 47 | 33 | 304 | KC1 | CAC-C3C-C4C | 2.46 | 128.00 | 124.79 |
| 37 | 16 | 301 | CLA | CBC-CAC-C3C | -2.46 | 105.74 | 112.42 |
| 37 | 14 | 308 | CLA | CMB-C2B-C1B | 2.46 | 129.17 | 125.42 |
| 47 | 34 | 306 | KC1 | CHB-C4A-NA | 2.46 | 128.05 | 124.23 |
| 37 | C | 507 | CLA | O1D-CGD-CBD | -2.46 | 119.66 | 124.52 |
| 37 | 35 | 310 | CLA | CAC-C3C-C4C | 2.46 | 128.00 | 124.79 |
| 48 | 15 | 319 | A86 | C21-C20-C15 | -2.46 | 115.40 | 123.35 |
| 48 | 34 | 311 | A86 | C21-C20-C15 | -2.46 | 115.40 | 123.35 |
| 39 | d | 405 | BCR | C29-C30-C25 | 2.46 | 114.02 | 110.44 |
| 43 | 41 | 201 | LHG | O3-C3-C2 | -2.46 | 99.48 | 109.63 |
| 37 | 14 | 310 | CLA | C4C-C3C-C2C | -2.46 | 103.31 | 106.89 |
| 37 | 38 | 209 | CLA | CBC-CAC-C3C | -2.46 | 105.75 | 112.42 |
| 47 | 14 | 306 | KC1 | C1A-NA-C4A | -2.46 | 105.56 | 106.68 |
| 37 | 31 | 302 | CLA | CHC-C1C-C2C | -2.46 | 119.95 | 126.95 |
| 37 | D | 402 | CLA | CAC-C3C-C4C | 2.46 | 127.99 | 124.79 |
| 37 | 18 | 208 | CLA | CMC-C2C-C1C | 2.46 | 128.88 | 125.03 |
| 47 | 18 | 207 | KC1 | CHD-C1D-ND | -2.46 | 120.36 | 124.05 |
| 37 | 32 | 202 | CLA | CAA-CBA-CGA | -2.46 | 106.22 | 113.21 |
| 48 | 35 | 319 | A86 | C21-C20-C15 | -2.46 | 115.41 | 123.35 |
| 47 | 31 | 303 | KC1 | CHB-C4A-NA | 2.46 | 128.05 | 124.23 |
| 37 | B | 502 | CLA | CAC-C3C-C4C | 2.46 | 127.99 | 124.79 |
| 48 | 36 | 310 | A86 | C25-C26-C27 | -2.46 | 123.83 | 127.28 |
| 37 | 11 | 305 | CLA | CMA-C3A-C4A | -2.46 | 105.16 | 111.77 |
| 37 | 19 | 307 | CLA | CHB-C1B-C2B | -2.46 | 120.29 | 127.43 |
| 39 | d | 405 | BCR | C28-C27-C26 | -2.46 | 109.67 | 114.06 |
| 48 | 32 | 218 | A86 | C22-C16-C17 | -2.46 | 104.65 | 108.97 |
| 39 | B | 525 | BCR | C11-C10-C9 | -2.46 | 123.83 | 127.28 |
| 48 | 14 | 315 | A86 | C35-C34-C33 | 2.46 | 114.30 | 109.89 |
| 37 | 17 | 302 | CLA | C4B-C3B-C2B | -2.46 | 104.25 | 107.30 |
| 37 | B | 501 | CLA | CBC-CAC-C3C | -2.46 | 105.76 | 112.42 |
| 37 | 13 | 301 | CLA | C4B-C3B-C2B | -2.46 | 104.25 | 107.30 |
| 37 | 35 | 303 | CLA | O1D-CGD-CBD | -2.46 | 119.67 | 124.52 |
| 37 | b | 508 | CLA | O2D-CGD-O1D | -2.46 | 119.07 | 123.85 |
| 37 | C | 513 | CLA | C4B-C3B-C2B | -2.46 | 104.25 | 107.30 |
| 48 | 17 | 320 | A86 | C40-C32-C31 | -2.45 | 108.28 | 110.47 |
| 37 | c | 512 | CLA | O1D-CGD-CBD | -2.45 | 119.68 | 124.52 |
| 37 | 14 | 310 | CLA | CBC-CAC-C3C | -2.45 | 105.77 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 16 | 304 | KC1 | O2A-CGA-O1A | -2.45 | 117.70 | 122.70 |
| 37 | 36 | 306 | CLA | CMB-C2B-C3B | 2.45 | 132.32 | 126.55 |
| 37 | b | 508 | CLA | CHB-C1B-C2B | -2.45 | 120.31 | 127.43 |
| 37 | 18 | 206 | CLA | CAC-C3C-C4C | 2.45 | 127.98 | 124.79 |
| 47 | 13 | 302 | KC1 | CBC-CAC-C3C | -2.45 | 105.77 | 112.42 |
| 37 | 33 | 308 | CLA | CMB-C2B-C1B | 2.45 | 129.15 | 125.42 |
| 48 | 15 | 311 | A86 | C8-C6-C5 | -2.45 | 115.15 | 119.01 |
| 37 | 19 | 303 | CLA | O2A-CGA-CBA | 2.45 | 119.31 | 111.83 |
| 47 | 11 | 302 | KC1 | CHB-C4A-NA | 2.45 | 128.03 | 124.23 |
| 37 | 15 | 308 | CLA | CMB-C2B-C1B | 2.45 | 129.15 | 125.42 |
| 37 | 21 | 209 | CLA | CMB-C2B-C1B | 2.45 | 129.15 | 125.42 |
| 47 | 37 | 304 | KC1 | CMC-C2C-C1C | 2.45 | 128.86 | 125.03 |
| 45 | d | 406 | PL9 | O1-C4-C3 | -2.45 | 118.15 | 120.73 |
| 37 | c | 507 | CLA | O1D-CGD-CBD | -2.45 | 119.68 | 124.52 |
| 47 | 32 | 209 | KC1 | CAB-C3B-C4B | 2.45 | 130.67 | 124.82 |
| 47 | 15 | 304 | KC1 | CAA-C2A-C1A | -2.45 | 113.91 | 124.64 |
| 47 | 40 | 206 | KC1 | C4C-C3C-C2C | -2.45 | 103.33 | 106.89 |
| 37 | B | 508 | CLA | CAC-C3C-C4C | 2.45 | 127.98 | 124.79 |
| 48 | 39 | 311 | A86 | C8-C6-C5 | -2.45 | 115.16 | 119.01 |
| 37 | 41 | 209 | CLA | CMB-C2B-C1B | 2.45 | 129.15 | 125.42 |
| 47 | 36 | 304 | KC1 | O2A-CGA-O1A | -2.45 | 117.71 | 122.70 |
| 37 | 31 | 304 | CLA | O1D-CGD-CBD | -2.45 | 119.69 | 124.52 |
| 37 | 14 | 308 | CLA | C1-O2A-CGA | 2.45 | 122.58 | 116.65 |
| 37 | D | 405 | CLA | CMA-C3A-C2A | -2.45 | 104.52 | 113.98 |
| 48 | 41 | 215 | A86 | C10-C9-C8 | -2.45 | 116.11 | 123.20 |
| 37 | 31 | 306 | CLA | CMA-C3A-C4A | -2.45 | 105.20 | 111.77 |
| 37 | 11 | 308 | CLA | CAA-CBA-CGA | -2.45 | 106.26 | 113.21 |
| 37 | C | 508 | CLA | CHB-C4A-NA | 2.45 | 127.93 | 124.40 |
| 37 | 15 | 305 | CLA | CAA-C2A-C3A | -2.45 | 106.39 | 113.00 |
| 37 | C | 502 | CLA | CHC-C1C-NC | 2.45 | 128.00 | 124.31 |
| 37 | 37 | 306 | CLA | O1D-CGD-CBD | -2.45 | 119.69 | 124.52 |
| 37 | 19 | 310 | CLA | CBC-CAC-C3C | -2.45 | 105.79 | 112.42 |
| 48 | 17 | 311 | A86 | C8-C6-C5 | -2.45 | 115.16 | 119.01 |
| 39 | a | 413 | BCR | C15-C14-C13 | -2.45 | 123.85 | 127.28 |
| 37 | 11 | 303 | CLA | O1D-CGD-CBD | -2.44 | 119.70 | 124.52 |
| 37 | 14 | 303 | CLA | CHB-C4A-NA | 2.44 | 127.93 | 124.40 |
| 37 | B | 512 | CLA | O2A-CGA-CBA | 2.44 | 119.29 | 111.83 |
| 37 | 20 | 301 | CLA | C3B-C4B-NB | 2.44 | 112.71 | 110.53 |
| 48 | 12 | 216 | A86 | C7-C6-C8 | 2.44 | 121.82 | 118.09 |
| 48 | 35 | 311 | A86 | C7-C6-C8 | 2.44 | 121.82 | 118.09 |
| 37 | 39 | 310 | CLA | O2D-CGD-O1D | -2.44 | 119.09 | 123.85 |
| 47 | 33 | 304 | KC1 | O2D-CGD-O1D | -2.44 | 119.09 | 123.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 32 | 210 | CLA | O2A-CGA-CBA | 2.44 | 119.28 | 111.83 |
| 47 | 33 | 302 | KC1 | CBC-CAC-C3C | -2.44 | 105.80 | 112.42 |
| 37 | C | 504 | CLA | C4C-C3C-C2C | -2.44 | 103.34 | 106.89 |
| 37 | c | 504 | CLA | C4C-C3C-C2C | -2.44 | 103.34 | 106.89 |
| 37 | b | 513 | CLA | O2A-CGA-CBA | 2.44 | 119.28 | 111.83 |
| 37 | B | 510 | CLA | CAA-CBA-CGA | -2.44 | 106.28 | 113.21 |
| 37 | W | 102 | CLA | C4-C3-C5 | 2.44 | 119.47 | 115.23 |
| 37 | 15 | 301 | CLA | C4B-C3B-C2B | -2.44 | 104.27 | 107.30 |
| 37 | 38 | 202 | CLA | O2A-CGA-CBA | 2.44 | 119.28 | 111.83 |
| 37 | b | 508 | CLA | CAC-C3C-C4C | 2.44 | 127.97 | 124.79 |
| 37 | 37 | 306 | CLA | C4-C3-C5 | 2.44 | 119.47 | 115.23 |
| 37 | 34 | 308 | CLA | C1-O2A-CGA | 2.44 | 122.56 | 116.65 |
| 37 | 18 | 204 | CLA | O1D-CGD-CBD | -2.44 | 119.70 | 124.52 |
| 37 | 38 | 204 | CLA | O1D-CGD-CBD | -2.44 | 119.70 | 124.52 |
| 37 | b | 512 | CLA | O2A-CGA-CBA | 2.44 | 119.28 | 111.83 |
| 37 | a | 403 | CLA | CHB-C4A-NA | 2.44 | 127.92 | 124.40 |
| 48 | 31 | 313 | A86 | C9-C8-C6 | -2.44 | 119.68 | 126.36 |
| 37 | 12 | 209 | CLA | O2A-CGA-CBA | 2.44 | 119.27 | 111.83 |
| 48 | 11 | 312 | A86 | C7-C6-C8 | 2.44 | 121.81 | 118.09 |
| 47 | 33 | 302 | KC1 | CHB-C4A-NA | 2.44 | 128.01 | 124.23 |
| 48 | 12 | 217 | A86 | C22-C16-C17 | -2.44 | 104.69 | 108.97 |
| 37 | c | 502 | CLA | CHC-C1C-NC | 2.44 | 127.98 | 124.31 |
| 37 | 39 | 303 | CLA | O2A-CGA-CBA | 2.44 | 119.27 | 111.83 |
| 37 | d | 403 | CLA | CMA-C3A-C2A | -2.44 | 104.56 | 113.98 |
| 48 | 15 | 312 | A86 | C8-C6-C5 | -2.44 | 115.18 | 119.01 |
| 39 | B | 517 | BCR | C15-C14-C13 | -2.44 | 123.86 | 127.28 |
| 37 | B | 508 | CLA | CBC-CAC-C3C | -2.44 | 105.82 | 112.42 |
| 41 | L | 102 | LMG | O6-C1-O1 | -2.44 | 104.29 | 110.04 |
| 47 | 15 | 302 | KC1 | CHB-C4A-NA | 2.44 | 128.01 | 124.23 |
| 37 | 36 | 303 | CLA | CHB-C4A-NA | 2.44 | 127.91 | 124.40 |
| 37 | 21 | 206 | CLA | C1-C2-C3 | -2.43 | 122.21 | 126.20 |
| 37 | 31 | 301 | CLA | C4-C3-C5 | 2.43 | 119.45 | 115.23 |
| 37 | 35 | 308 | CLA | CHD-C4C-NC | 2.43 | 128.01 | 124.23 |
| 37 | 35 | 305 | CLA | CAA-C2A-C3A | -2.43 | 106.42 | 113.00 |
| 48 | 31 | 312 | A86 | C7-C6-C8 | 2.43 | 121.81 | 118.09 |
| 47 | 14 | 304 | KC1 | CAA-C2A-C1A | -2.43 | 113.98 | 124.64 |
| 47 | 37 | 305 | KC1 | CHB-C4A-NA | 2.43 | 128.00 | 124.23 |
| 37 | b | 510 | CLA | CAA-CBA-CGA | -2.43 | 106.30 | 113.21 |
| 37 | b | 512 | CLA | C1-C2-C3 | -2.43 | 122.21 | 126.20 |
| 37 | A | 403 | CLA | CHB-C4A-NA | 2.43 | 127.91 | 124.40 |
| 37 | 13 | 301 | CLA | CBC-CAC-C3C | -2.43 | 105.83 | 112.42 |
| 48 | 15 | 316 | A86 | C36-C31-C32 | -2.43 | 117.28 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 12 | 203 | CLA | CMB-C2B-C1B | 2.43 | 129.12 | 125.42 |
| 37 | 16 | 307 | CLA | CBC-CAC-C3C | -2.43 | 105.83 | 112.42 |
| 48 | 19 | 311 | A86 | C10-C9-C8 | -2.43 | 116.15 | 123.20 |
| 48 | 32 | 216 | A86 | C3-C4-C5 | -2.43 | 118.54 | 123.52 |
| 37 | 13 | 307 | CLA | C1-C2-C3 | -2.43 | 122.21 | 126.20 |
| 48 | 17 | 312 | A86 | C41-C32-C31 | -2.43 | 108.30 | 110.47 |
| 37 | 39 | 306 | CLA | CBC-CAC-C3C | -2.43 | 105.83 | 112.42 |
| 47 | 13 | 309 | KC1 | CHB-C4A-NA | 2.43 | 128.00 | 124.23 |
| 48 | 39 | 311 | A86 | C10-C9-C8 | -2.43 | 116.16 | 123.20 |
| 37 | 13 | 308 | CLA | CMB-C2B-C1B | 2.43 | 129.12 | 125.42 |
| 47 | 37 | 305 | KC1 | CMB-C2B-C1B | 2.43 | 129.01 | 124.73 |
| 37 | W | 102 | CLA | CGD-CBD-CAD | -2.43 | 102.98 | 110.85 |
| 37 | 32 | 205 | CLA | C3B-C4B-NB | 2.43 | 112.70 | 110.53 |
| 50 | 21 | 212 | DD6 | C4-C3-C2 | -2.43 | 118.55 | 123.52 |
| 47 | 34 | 304 | KC1 | CAA-C2A-C1A | -2.43 | 114.00 | 124.64 |
| 37 | B | 508 | CLA | CHB-C1B-C2B | -2.43 | 120.38 | 127.43 |
| 37 | 31 | 301 | CLA | CGD-CBD-CAD | -2.43 | 102.98 | 110.85 |
| 37 | c | 507 | CLA | CHB-C4A-NA | 2.43 | 127.91 | 124.40 |
| 37 | A | 403 | CLA | C6-C7-C8 | -2.43 | 107.89 | 115.97 |
| 47 | 12 | 208 | KC1 | CAB-C3B-C4B | 2.43 | 130.62 | 124.82 |
| 37 | d | 401 | CLA | CAC-C3C-C4C | 2.43 | 127.95 | 124.79 |
| 47 | 13 | 304 | KC1 | CAC-C3C-C4C | 2.43 | 127.95 | 124.79 |
| 37 | b | 507 | CLA | CHB-C1B-C2B | -2.43 | 120.38 | 127.43 |
| 37 | 37 | 301 | CLA | C4B-C3B-C2B | -2.43 | 104.28 | 107.30 |
| 37 | 13 | 305 | CLA | CBC-CAC-C3C | -2.43 | 105.84 | 112.42 |
| 37 | 12 | 212 | CLA | CAC-C3C-C4C | 2.43 | 127.95 | 124.79 |
| 37 | 33 | 301 | CLA | CBC-CAC-C3C | -2.43 | 105.84 | 112.42 |
| 37 | b | 508 | CLA | CBC-CAC-C3C | -2.43 | 105.84 | 112.42 |
| 37 | 32 | 204 | CLA | CMB-C2B-C1B | 2.43 | 129.11 | 125.42 |
| 47 | 33 | 309 | KC1 | CHB-C4A-NA | 2.43 | 127.99 | 124.23 |
| 41 | l | 101 | LMG | O6-C1-O1 | -2.43 | 104.31 | 110.04 |
| 37 | a | 403 | CLA | C6-C7-C8 | -2.43 | 107.90 | 115.97 |
| 37 | C | 504 | CLA | CAA-C2A-C3A | -2.42 | 106.45 | 113.00 |
| 37 | 11 | 303 | CLA | C7-C6-C5 | -2.42 | 106.80 | 113.26 |
| 37 | B | 512 | CLA | C1-C2-C3 | -2.42 | 122.22 | 126.20 |
| 37 | c | 506 | CLA | CBC-CAC-C3C | -2.42 | 105.85 | 112.42 |
| 37 | 32 | 208 | CLA | CBC-CAC-C3C | -2.42 | 105.85 | 112.42 |
| 47 | 15 | 304 | KC1 | CMB-C2B-C1B | 2.42 | 129.00 | 124.73 |
| 37 | B | 506 | CLA | CHB-C4A-NA | 2.42 | 127.90 | 124.40 |
| 37 | 19 | 306 | CLA | CBC-CAC-C3C | -2.42 | 105.85 | 112.42 |
| 37 | 34 | 303 | CLA | CHB-C4A-NA | 2.42 | 127.90 | 124.40 |
| 37 | 14 | 308 | CLA | CED-O2D-CGD | 2.42 | 121.41 | 115.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 37 | 303 | CLA | C1-O2A-CGA | 2.42 | 122.52 | 116.65 |
| 37 | 17 | 302 | CLA | CHD-C4C-NC | 2.42 | 127.99 | 124.23 |
| 37 | 33 | 303 | CLA | CHB-C4A-NA | 2.42 | 127.90 | 124.40 |
| 37 | 12 | 209 | CLA | CHB-C1B-C2B | -2.42 | 120.39 | 127.43 |
| 47 | 17 | 306 | KC1 | CHB-C4A-NA | 2.42 | 127.99 | 124.23 |
| 43 | D | 411 | LHG | C20-C19-C18 | -2.42 | 102.12 | 114.37 |
| 37 | c | 511 | CLA | O2D-CGD-O1D | -2.42 | 119.13 | 123.85 |
| 37 | 36 | 307 | CLA | CBC-CAC-C3C | -2.42 | 105.86 | 112.42 |
| 37 | 18 | 209 | CLA | CAA-C2A-C3A | -2.42 | 106.45 | 113.00 |
| 47 | 17 | 305 | KC1 | CHB-C4A-NA | 2.42 | 127.99 | 124.23 |
| 37 | B | 511 | CLA | C7-C6-C5 | -2.42 | 106.81 | 113.26 |
| 43 | a | 412 | LHG | C20-C19-C18 | -2.42 | 102.13 | 114.37 |
| 48 | 17 | 312 | A86 | C19-C18-C17 | -2.42 | 106.26 | 110.79 |
| 48 | 32 | 216 | A86 | C23-C16-C22 | -2.42 | 103.85 | 107.37 |
| 37 | 12 | 207 | CLA | C5-C3-C4 | 2.42 | 120.16 | 114.59 |
| 47 | 16 | 308 | KC1 | CHB-C4A-NA | 2.42 | 127.98 | 124.23 |
| 37 | C | 512 | CLA | CAA-C2A-C3A | -2.42 | 106.46 | 113.00 |
| 37 | 11 | 310 | CLA | C1-C2-C3 | -2.42 | 122.23 | 126.20 |
| 47 | 14 | 309 | KC1 | CMB-C2B-C1B | 2.42 | 128.99 | 124.73 |
| 48 | 12 | 215 | A86 | C23-C16-C22 | -2.42 | 103.86 | 107.37 |
| 41 | 12 | 201 | LMG | O3-C3-C2 | -2.42 | 104.67 | 110.38 |
| 37 | b | 511 | CLA | C7-C6-C5 | -2.42 | 106.82 | 113.26 |
| 37 | 12 | 207 | CLA | CBC-CAC-C3C | -2.42 | 105.86 | 112.42 |
| 39 | b | 517 | BCR | C15-C14-C13 | -2.42 | 123.89 | 127.28 |
| 37 | 32 | 208 | CLA | C5-C3-C4 | 2.42 | 120.15 | 114.59 |
| 44 | J | 101 | DGD | O6E-C1E-O5D | -2.42 | 104.33 | 110.04 |
| 37 | c | 512 | CLA | CAA-C2A-C3A | -2.42 | 106.47 | 113.00 |
| 37 | B | 513 | CLA | O2A-CGA-CBA | 2.42 | 119.20 | 111.83 |
| 37 | B | 507 | CLA | CHB-C1B-C2B | -2.42 | 120.41 | 127.43 |
| 48 | 12 | 215 | A86 | C3-C4-C5 | -2.42 | 118.57 | 123.52 |
| 47 | 13 | 304 | KC1 | O2D-CGD-O1D | -2.42 | 119.14 | 123.85 |
| 48 | 35 | 312 | A86 | C8-C6-C5 | -2.42 | 115.21 | 119.01 |
| 37 | 33 | 307 | CLA | C1-C2-C3 | -2.42 | 122.24 | 126.20 |
| 48 | 16 | 313 | A86 | C-C1-C24 | -2.42 | 114.40 | 118.09 |
| 37 | 11 | 307 | CLA | O1D-CGD-CBD | -2.42 | 119.75 | 124.52 |
| 39 | 5 | 101 | BCR | C24-C23-C22 | -2.42 | 122.66 | 126.23 |
| 48 | 37 | 313 | A86 | O-C13-C14 | -2.41 | 116.81 | 121.76 |
| 47 | 17 | 305 | KC1 | O2D-CGD-O1D | -2.41 | 119.15 | 123.85 |
| 37 | 15 | 308 | CLA | O2A-CGA-CBA | 2.41 | 119.19 | 111.83 |
| 37 | 31 | 304 | CLA | C7-C6-C5 | -2.41 | 106.83 | 113.26 |
| 37 | 33 | 307 | CLA | CAA-C2A-C3A | -2.41 | 106.48 | 113.00 |
| 47 | 17 | 306 | KC1 | CMB-C2B-C1B | 2.41 | 128.98 | 124.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | 32 | 201 | LMG | O3-C3-C2 | -2.41 | 104.69 | 110.38 |
| 50 | 41 | 212 | DD6 | C4-C3-C2 | -2.41 | 118.58 | 123.52 |
| 48 | 11 | 314 | A86 | C35-C34-C33 | 2.41 | 114.22 | 109.89 |
| 37 | 41 | 204 | CLA | C1-C2-C3 | -2.41 | 122.25 | 126.20 |
| 48 | 35 | 315 | A86 | C7-C6-C8 | 2.41 | 121.77 | 118.09 |
| 48 | 14 | 311 | A86 | C8-C6-C5 | -2.41 | 115.22 | 119.01 |
| 37 | 12 | 205 | CLA | CMC-C2C-C1C | 2.41 | 128.80 | 125.03 |
| 37 | 12 | 204 | CLA | CHA-C1A-NA | -2.41 | 120.93 | 126.39 |
| 37 | C | 511 | CLA | O2D-CGD-O1D | -2.41 | 119.16 | 123.85 |
| 37 | 11 | 308 | CLA | C4-C3-C5 | 2.41 | 119.41 | 115.23 |
| 37 | 13 | 307 | CLA | CAA-C2A-C3A | -2.41 | 106.48 | 113.00 |
| 37 | C | 506 | CLA | CBC-CAC-C3C | -2.41 | 105.89 | 112.42 |
| 37 | 31 | 310 | CLA | C1-C2-C3 | -2.41 | 122.25 | 126.20 |
| 39 | A | 410 | BCR | C15-C14-C13 | -2.41 | 123.90 | 127.28 |
| 37 | b | 516 | CLA | CHC-C1C-NC | 2.41 | 127.94 | 124.31 |
| 37 | C | 507 | CLA | CHB-C4A-NA | 2.41 | 127.88 | 124.40 |
| 48 | 40 | 201 | A86 | C-C1-C24 | -2.41 | 114.41 | 118.09 |
| 37 | 21 | 204 | CLA | C1-C2-C3 | -2.41 | 122.25 | 126.20 |
| 37 | 33 | 305 | CLA | CBC-CAC-C3C | -2.41 | 105.89 | 112.42 |
| 41 | C | 518 | LMG | O2-C2-C1 | -2.41 | 104.34 | 110.08 |
| 48 | 38 | 212 | A86 | C4-C3-C2 | -2.41 | 118.59 | 123.52 |
| 48 | 35 | 311 | A86 | C8-C6-C5 | -2.41 | 115.22 | 119.01 |
| 37 | C | 508 | CLA | CMB-C2B-C3B | 2.41 | 132.21 | 126.55 |
| 48 | 35 | 312 | A86 | C41-C32-C31 | -2.41 | 108.32 | 110.47 |
| 37 | 38 | 202 | CLA | CMB-C2B-C1B | 2.41 | 129.08 | 125.42 |
| 37 | 32 | 205 | CLA | O2A-CGA-O1A | -2.41 | 117.61 | 123.63 |
| 37 | 16 | 303 | CLA | CHB-C4A-NA | 2.41 | 127.87 | 124.40 |
| 37 | 38 | 208 | CLA | CMC-C2C-C1C | 2.40 | 128.79 | 125.03 |
| 37 | B | 508 | CLA | C4-C3-C5 | 2.40 | 119.40 | 115.23 |
| 48 | 31 | 319 | A86 | C19-C18-C17 | -2.40 | 106.29 | 110.79 |
| 37 | 34 | 302 | CLA | CBC-CAC-C3C | -2.40 | 105.90 | 112.42 |
| 37 | 39 | 307 | CLA | CHB-C1B-C2B | -2.40 | 120.45 | 127.43 |
| 48 | 12 | 202 | A86 | C7-C6-C5 | -2.40 | 118.92 | 122.82 |
| 37 | 14 | 303 | CLA | CBC-CAC-C3C | -2.40 | 105.90 | 112.42 |
| 37 | 40 | 210 | CLA | CMC-C2C-C1C | 2.40 | 128.79 | 125.03 |
| 37 | B | 515 | CLA | CHD-C4C-NC | 2.40 | 127.96 | 124.23 |
| 37 | c | 504 | CLA | CAA-C2A-C3A | -2.40 | 106.50 | 113.00 |
| 37 | c | 508 | CLA | CHB-C4A-NA | 2.40 | 127.87 | 124.40 |
| 48 | 38 | 212 | A86 | C3-C4-C5 | -2.40 | 118.60 | 123.52 |
| 50 | 39 | 312 | DD6 | C33-C32-C31 | 2.40 | 114.22 | 109.49 |
| 41 | c | 518 | LMG | O2-C2-C1 | -2.40 | 104.35 | 110.08 |
| 37 | C | 507 | CLA | O2A-CGA-CBA | 2.40 | 119.16 | 111.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 39 | 0 | 101 | BCR | C24-C23-C22 | -2.40 | 122.68 | 126.23 |
| 37 | b | 504 | CLA | O2A-CGA-O1A | -2.40 | 117.62 | 123.63 |
| 37 | b | 508 | CLA | C4-C3-C5 | 2.40 | 119.40 | 115.23 |
| 37 | c | 507 | CLA | O2A-CGA-CBA | 2.40 | 119.16 | 111.83 |
| 37 | 20 | 308 | CLA | CMC-C2C-C1C | 2.40 | 128.79 | 125.03 |
| 47 | 21 | 203 | KC1 | CMC-C2C-C1C | 2.40 | 128.79 | 125.03 |
| 37 | 21 | 202 | CLA | O2A-CGA-O1A | -2.40 | 117.62 | 123.63 |
| 50 | 19 | 312 | DD6 | C33-C32-C31 | 2.40 | 114.22 | 109.49 |
| 44 | j | 101 | DGD | O6E-C1E-O5D | -2.40 | 104.37 | 110.04 |
| 48 | 13 | 313 | A86 | C7-C6-C5 | -2.40 | 118.93 | 122.82 |
| 37 | 39 | 307 | CLA | C4B-C3B-C2B | -2.40 | 104.32 | 107.30 |
| 37 | B | 513 | CLA | CMC-C2C-C1C | 2.40 | 128.78 | 125.03 |
| 48 | 40 | 213 | A86 | C9-C10-C11 | -2.40 | 119.86 | 126.64 |
| 45 | D | 408 | PL9 | O1-C4-C3 | -2.40 | 118.20 | 120.73 |
| 37 | c | 508 | CLA | CMB-C2B-C3B | 2.40 | 132.19 | 126.55 |
| 37 | 32 | 211 | CLA | C4-C3-C5 | 2.40 | 119.39 | 115.23 |
| 37 | B | 504 | CLA | O1D-CGD-CBD | -2.40 | 119.79 | 124.52 |
| 37 | 15 | 308 | CLA | CHD-C4C-NC | 2.40 | 127.95 | 124.23 |
| 48 | 11 | 319 | A86 | C19-C18-C17 | -2.40 | 106.31 | 110.79 |
| 37 | 41 | 202 | CLA | O2A-CGA-O1A | -2.40 | 117.63 | 123.63 |
| 37 | 20 | 301 | CLA | CHB-C4A-NA | 2.40 | 127.86 | 124.40 |
| 47 | 34 | 309 | KC1 | CMB-C2B-C1B | 2.40 | 128.95 | 124.73 |
| 41 | L | 102 | LMG | C1-C2-C3 | -2.40 | 104.97 | 110.01 |
| 37 | 39 | 310 | CLA | O2A-CGA-CBA | 2.40 | 119.14 | 111.83 |
| 47 | 21 | 207 | KC1 | CMB-C2B-C1B | 2.40 | 128.95 | 124.73 |
| 45 | D | 404 | PL9 | C37-C38-C39 | -2.40 | 122.14 | 127.62 |
| 37 | 38 | 201 | CLA | C3B-C4B-NB | 2.40 | 112.67 | 110.53 |
| 37 | 41 | 202 | CLA | O2D-CGD-O1D | -2.40 | 119.18 | 123.85 |
| 37 | 38 | 204 | CLA | CMC-C2C-C1C | 2.40 | 128.78 | 125.03 |
| 37 | 19 | 305 | CLA | C4A-NA-C1A | -2.40 | 105.59 | 106.68 |
| 47 | 15 | 306 | KC1 | CAA-C2A-C1A | -2.40 | 114.14 | 124.64 |
| 43 | 21 | 217 | LHG | C11-C10-C9 | -2.40 | 102.26 | 114.37 |
| 43 | 37 | 321 | LHG | C11-C10-C9 | -2.39 | 102.26 | 114.37 |
| 44 | c | 517 | DGD | CBB-CAB-C9B | -2.39 | 102.27 | 114.37 |
| 37 | B | 509 | CLA | CHB-C4A-NA | 2.39 | 127.86 | 124.40 |
| 47 | 13 | 306 | KC1 | C3D-C2D-C1D | -2.39 | 98.75 | 106.40 |
| 47 | 35 | 306 | KC1 | O1D-CGD-CBD | -2.39 | 119.80 | 124.52 |
| 37 | 14 | 302 | CLA | CBC-CAC-C3C | -2.39 | 105.93 | 112.42 |
| 37 | B | 502 | CLA | O2A-CGA-CBA | 2.39 | 119.13 | 111.83 |
| 37 | 14 | 301 | CLA | C4B-C3B-C2B | -2.39 | 104.33 | 107.30 |
| 37 | 31 | 308 | CLA | O1D-CGD-CBD | -2.39 | 119.80 | 124.52 |
| 37 | 40 | 203 | CLA | C3B-C4B-NB | 2.39 | 112.67 | 110.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 34 | 308 | CLA | CED-O2D-CGD | 2.39 | 121.34 | 115.92 |
| 47 | 38 | 207 | KC1 | CHB-C4A-NA | 2.39 | 127.94 | 124.23 |
| 37 | 39 | 305 | CLA | C4A-NA-C1A | -2.39 | 105.59 | 106.68 |
| 37 | W | 101 | CLA | CHB-C4A-NA | 2.39 | 127.85 | 124.40 |
| 37 | 32 | 205 | CLA | CHA-C1A-NA | -2.39 | 120.98 | 126.39 |
| 37 | 18 | 208 | CLA | CHB-C4A-NA | 2.39 | 127.85 | 124.40 |
| 44 | C | 517 | DGD | CBB-CAB-C9B | -2.39 | 102.28 | 114.37 |
| 41 | 17 | 317 | LMG | O6-C1-O1 | -2.39 | 104.39 | 110.04 |
| 37 | 32 | 210 | CLA | CHB-C1B-C2B | -2.39 | 120.49 | 127.43 |
| 47 | 41 | 207 | KC1 | CMB-C2B-C1B | 2.39 | 128.94 | 124.73 |
| 48 | 35 | 311 | A86 | C23-C16-C22 | -2.39 | 103.90 | 107.37 |
| 48 | 20 | 311 | A86 | C9-C10-C11 | -2.39 | 119.88 | 126.64 |
| 37 | 34 | 303 | CLA | CBC-CAC-C3C | -2.39 | 105.94 | 112.42 |
| 37 | 32 | 206 | CLA | O1D-CGD-CBD | -2.39 | 119.81 | 124.52 |
| 37 | 35 | 310 | CLA | CHB-C4A-NA | 2.39 | 127.85 | 124.40 |
| 37 | 14 | 302 | CLA | C4-C3-C5 | 2.39 | 119.38 | 115.23 |
| 48 | 32 | 203 | A86 | C7-C6-C5 | -2.39 | 118.95 | 122.82 |
| 37 | 31 | 301 | CLA | O2A-CGA-CBA | 2.39 | 119.12 | 111.83 |
| 46 | f | 101 | HEM | CMC-C2C-C1C | -2.39 | 120.52 | 124.73 |
| 47 | 35 | 306 | KC1 | CAA-C2A-C1A | -2.39 | 114.18 | 124.64 |
| 50 | 41 | 212 | DD6 | C22-C16-C17 | 2.39 | 113.17 | 108.97 |
| 41 | l | 101 | LMG | C1-C2-C3 | -2.39 | 104.99 | 110.01 |
| 47 | 36 | 308 | KC1 | CHB-C4A-NA | 2.39 | 127.93 | 124.23 |
| 44 | h | 102 | DGD | C3G-C2G-C1G | -2.39 | 106.22 | 111.78 |
| 47 | 41 | 203 | KC1 | CMC-C2C-C1C | 2.39 | 128.76 | 125.03 |
| 37 | W | 102 | CLA | O2A-CGA-CBA | 2.39 | 119.11 | 111.83 |
| 37 | b | 515 | CLA | CHD-C4C-NC | 2.39 | 127.93 | 124.23 |
| 37 | 19 | 309 | CLA | CMB-C2B-C1B | 2.39 | 129.05 | 125.42 |
| 37 | 32 | 213 | CLA | CAC-C3C-C4C | 2.39 | 127.89 | 124.79 |
| 37 | 39 | 309 | CLA | CMB-C2B-C1B | 2.38 | 129.05 | 125.42 |
| 37 | 16 | 301 | CLA | CBA-CAA-C2A | 2.38 | 120.89 | 113.79 |
| 48 | 17 | 312 | A86 | C25-C24-C1 | -2.38 | 119.83 | 126.36 |
| 38 | a | 405 | PHO | C2D-C1D-ND | -2.38 | 107.71 | 109.43 |
| 37 | b | 506 | CLA | CHB-C4A-NA | 2.38 | 127.84 | 124.40 |
| 48 | 35 | 315 | A86 | C26-C25-C24 | -2.38 | 116.29 | 123.20 |
| 48 | 37 | 311 | A86 | C40-C32-C31 | -2.38 | 108.34 | 110.47 |
| 37 | 35 | 303 | CLA | CBC-CAC-C3C | -2.38 | 105.96 | 112.42 |
| 37 | b | 504 | CLA | O1D-CGD-CBD | -2.38 | 119.82 | 124.52 |
| 43 | D | 410 | LHG | C20-C19-C18 | -2.38 | 102.33 | 114.37 |
| 47 | 32 | 212 | KC1 | CGD-CBD-CAD | -2.38 | 103.14 | 110.85 |
| 37 | B | 516 | CLA | CHC-C1C-NC | 2.38 | 127.90 | 124.31 |
| 37 | 38 | 204 | CLA | CBC-CAC-C3C | -2.38 | 105.96 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 502 | CLA | O2A-CGA-CBA | 2.38 | 119.10 | 111.83 |
| 47 | 20 | 302 | KC1 | O2D-CGD-O1D | -2.38 | 119.21 | 123.85 |
| 37 | B | 508 | CLA | CHB-C4A-NA | 2.38 | 127.84 | 124.40 |
| 47 | 41 | 207 | KC1 | O1D-CGD-CBD | -2.38 | 119.82 | 124.52 |
| 47 | 33 | 306 | KC1 | C3D-C2D-C1D | -2.38 | 98.80 | 106.40 |
| 39 | B | 525 | BCR | C7-C8-C9 | -2.38 | 122.71 | 126.23 |
| 37 | 33 | 303 | CLA | CAA-C2A-C1A | 2.38 | 119.78 | 111.97 |
| 37 | w | 101 | CLA | CHB-C4A-NA | 2.38 | 127.83 | 124.40 |
| 37 | 15 | 303 | CLA | CBC-CAC-C3C | -2.38 | 105.97 | 112.42 |
| 37 | 12 | 207 | CLA | CAC-C3C-C4C | 2.38 | 127.89 | 124.79 |
| 47 | 35 | 302 | KC1 | CHB-C4A-NA | 2.38 | 127.92 | 124.23 |
| 47 | 32 | 212 | KC1 | CMB-C2B-C1B | 2.38 | 128.92 | 124.73 |
| 39 | C | 515 | BCR | C27-C26-C25 | 2.38 | 125.92 | 122.70 |
| 48 | 33 | 313 | A86 | C7-C6-C5 | -2.38 | 118.96 | 122.82 |
| 48 | 38 | 213 | A86 | C19-C18-C17 | -2.38 | 106.34 | 110.79 |
| 47 | 15 | 306 | KC1 | CBC-CAC-C3C | -2.38 | 105.97 | 112.42 |
| 44 | H | 102 | DGD | C3G-C2G-C1G | -2.38 | 106.24 | 111.78 |
| 37 | 21 | 202 | CLA | O2D-CGD-O1D | -2.38 | 119.22 | 123.85 |
| 41 | C | 518 | LMG | C40-C39-C38 | -2.38 | 102.35 | 114.37 |
| 43 | d | 408 | LHG | C20-C19-C18 | -2.38 | 102.35 | 114.37 |
| 47 | 40 | 207 | KC1 | CHB-C4A-NA | 2.38 | 127.92 | 124.23 |
| 37 | 12 | 210 | CLA | C4-C3-C5 | 2.38 | 119.36 | 115.23 |
| 41 | c | 518 | LMG | C40-C39-C38 | -2.38 | 102.35 | 114.37 |
| 37 | b | 508 | CLA | CHB-C4A-NA | 2.38 | 127.83 | 124.40 |
| 37 | 37 | 306 | CLA | CHA-C1A-NA | -2.38 | 121.01 | 126.39 |
| 37 | B | 504 | CLA | O2A-CGA-O1A | -2.38 | 117.68 | 123.63 |
| 37 | b | 513 | CLA | CMC-C2C-C1C | 2.38 | 128.75 | 125.03 |
| 50 | 21 | 212 | DD6 | C22-C16-C17 | 2.38 | 113.15 | 108.97 |
| 37 | 35 | 307 | CLA | O2D-CGD-O1D | -2.38 | 119.22 | 123.85 |
| 37 | 12 | 204 | CLA | O2A-CGA-O1A | -2.38 | 117.68 | 123.63 |
| 37 | b | 509 | CLA | O2D-CGD-O1D | -2.38 | 119.22 | 123.85 |
| 37 | a | 404 | CLA | C4C-C3C-C2C | -2.38 | 103.43 | 106.89 |
| 37 | Z | 102 | CLA | CAC-C3C-C4C | 2.38 | 127.88 | 124.79 |
| 47 | 18 | 207 | KC1 | O1D-CGD-CBD | -2.38 | 119.83 | 124.52 |
| 47 | 12 | 211 | KC1 | CGD-CBD-CAD | -2.38 | 103.16 | 110.85 |
| 38 | D | 403 | PHO | C2D-C1D-ND | -2.38 | 107.71 | 109.43 |
| 37 | 32 | 202 | CLA | C4-C3-C5 | 2.38 | 119.35 | 115.23 |
| 48 | 34 | 311 | A86 | C8-C6-C5 | -2.38 | 115.27 | 119.01 |
| 37 | d | 401 | CLA | O2D-CGD-O1D | -2.38 | 119.22 | 123.85 |
| 37 | z | 101 | CLA | O2D-CGD-O1D | -2.38 | 119.22 | 123.85 |
| 37 | W | 101 | CLA | C1-C2-C3 | -2.37 | 122.31 | 126.20 |
| 37 | 40 | 205 | CLA | O1D-CGD-CBD | -2.37 | 119.84 | 124.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 18 | 207 | KC1 | O2A-CGA-O1A | -2.37 | 117.87 | 122.70 |
| 37 | 35 | 308 | CLA | O2A-CGA-CBA | 2.37 | 119.07 | 111.83 |
| 37 | 36 | 301 | CLA | CBA-CAA-C2A | 2.37 | 120.85 | 113.79 |
| 48 | 33 | 315 | A86 | C4-C3-C2 | -2.37 | 118.67 | 123.52 |
| 37 | b | 523 | CLA | C3B-C4B-NB | 2.37 | 112.65 | 110.53 |
| 47 | 40 | 204 | KC1 | O2D-CGD-O1D | -2.37 | 119.23 | 123.85 |
| 47 | 21 | 207 | KC1 | O1D-CGD-CBD | -2.37 | 119.84 | 124.52 |
| 37 | c | 507 | CLA | CBC-CAC-C3C | -2.37 | 105.99 | 112.42 |
| 47 | 17 | 305 | KC1 | CHD-C4C-NC | 2.37 | 127.88 | 124.31 |
| 47 | 12 | 211 | KC1 | CMB-C2B-C1B | 2.37 | 128.90 | 124.73 |
| 37 | 18 | 211 | CLA | CHD-C4C-NC | 2.37 | 127.91 | 124.23 |
| 47 | 16 | 304 | KC1 | CHB-C4A-NA | 2.37 | 127.91 | 124.23 |
| 41 | 37 | 316 | LMG | O6-C1-O1 | -2.37 | 104.44 | 110.04 |
| 47 | 35 | 306 | KC1 | CBC-CAC-C3C | -2.37 | 106.00 | 112.42 |
| 45 | d | 402 | PL9 | C37-C38-C39 | -2.37 | 122.20 | 127.62 |
| 48 | 39 | 313 | A86 | C7-C6-C5 | -2.37 | 118.98 | 122.82 |
| 37 | 36 | 301 | CLA | CHB-C4A-NA | 2.37 | 127.82 | 124.40 |
| 37 | C | 512 | CLA | C4-C3-C5 | 2.37 | 119.34 | 115.23 |
| 39 | c | 515 | BCR | C27-C26-C25 | 2.37 | 125.91 | 122.70 |
| 47 | 20 | 305 | KC1 | CHB-C4A-NA | 2.37 | 127.90 | 124.23 |
| 37 | 17 | 307 | CLA | CHA-C1A-NA | -2.37 | 121.03 | 126.39 |
| 47 | 40 | 204 | KC1 | C4C-C3C-C2C | -2.37 | 103.44 | 106.89 |
| 37 | C | 507 | CLA | CBC-CAC-C3C | -2.37 | 106.00 | 112.42 |
| 37 | 38 | 209 | CLA | CAA-C2A-C3A | -2.37 | 106.60 | 113.00 |
| 48 | 31 | 314 | A86 | C23-C16-C22 | -2.37 | 103.93 | 107.37 |
| 37 | 12 | 205 | CLA | O1D-CGD-CBD | -2.37 | 119.85 | 124.52 |
| 37 | 34 | 302 | CLA | C4-C3-C5 | 2.37 | 119.33 | 115.23 |
| 37 | 38 | 211 | CLA | CHB-C4A-NA | 2.37 | 127.81 | 124.40 |
| 37 | z | 102 | CLA | CMB-C2B-C1B | 2.37 | 129.02 | 125.42 |
| 37 | Z | 102 | CLA | CMB-C2B-C1B | 2.36 | 129.02 | 125.42 |
| 42 | a | 411 | BCT | O3-C-O1 | -2.36 | 113.63 | 119.68 |
| 37 | d | 403 | CLA | O2D-CGD-O1D | -2.36 | 119.25 | 123.85 |
| 37 | 34 | 301 | CLA | C4B-C3B-C2B | -2.36 | 104.36 | 107.30 |
| 37 | 32 | 208 | CLA | CAC-C3C-C4C | 2.36 | 127.86 | 124.79 |
| 48 | 15 | 314 | A86 | C8-C6-C5 | -2.36 | 115.29 | 119.01 |
| 37 | C | 506 | CLA | CHA-C1A-NA | -2.36 | 121.04 | 126.39 |
| 37 | D | 402 | CLA | CHB-C4A-NA | 2.36 | 127.81 | 124.40 |
| 37 | 33 | 308 | CLA | CAA-C2A-C3A | -2.36 | 106.61 | 113.00 |
| 48 | 15 | 315 | A86 | C26-C25-C24 | -2.36 | 116.35 | 123.20 |
| 48 | 37 | 311 | A86 | C19-C18-C17 | -2.36 | 106.37 | 110.79 |
| 37 | C | 501 | CLA | CMC-C2C-C1C | 2.36 | 128.73 | 125.03 |
| 48 | 15 | 316 | A86 | C10-C9-C8 | -2.36 | 116.36 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 509 | CLA | CHB-C4A-NA | 2.36 | 127.81 | 124.40 |
| 37 | 40 | 203 | CLA | CHB-C4A-NA | 2.36 | 127.81 | 124.40 |
| 48 | 37 | 313 | A86 | C34-O4-C38 | -2.36 | 113.67 | 117.85 |
| 50 | 41 | 216 | DD6 | C14-C13-C11 | -2.36 | 121.86 | 125.53 |
| 48 | 35 | 314 | A86 | C8-C6-C5 | -2.36 | 115.29 | 119.01 |
| 37 | 38 | 208 | CLA | CHB-C4A-NA | 2.36 | 127.81 | 124.40 |
| 37 | C | 502 | CLA | CBC-CAC-C3C | -2.36 | 106.02 | 112.42 |
| 37 | D | 401 | CLA | C4C-C3C-C2C | -2.36 | 103.45 | 106.89 |
| 47 | 36 | 304 | KC1 | CHB-C4A-NA | 2.36 | 127.89 | 124.23 |
| 48 | 11 | 314 | A86 | C23-C16-C22 | -2.36 | 103.94 | 107.37 |
| 37 | 34 | 301 | CLA | CHB-C4A-NA | 2.36 | 127.81 | 124.40 |
| 47 | 11 | 304 | KC1 | O2D-CGD-O1D | -2.36 | 119.25 | 123.85 |
| 48 | 31 | 314 | A86 | C36-C31-C32 | -2.36 | 117.35 | 119.70 |
| 48 | 37 | 313 | A86 | C36-C31-C32 | -2.36 | 117.35 | 119.70 |
| 48 | 15 | 315 | A86 | C40-C32-C31 | -2.36 | 108.36 | 110.47 |
| 37 | z | 102 | CLA | CAC-C3C-C4C | 2.36 | 127.86 | 124.79 |
| 37 | D | 402 | CLA | O2D-CGD-O1D | -2.36 | 119.25 | 123.85 |
| 37 | Z | 101 | CLA | O2D-CGD-O1D | -2.36 | 119.26 | 123.85 |
| 37 | 13 | 308 | CLA | CAA-C2A-C3A | -2.36 | 106.62 | 113.00 |
| 37 | 34 | 303 | CLA | CMB-C2B-C1B | 2.36 | 129.01 | 125.42 |
| 37 | d | 401 | CLA | CHB-C4A-NA | 2.36 | 127.80 | 124.40 |
| 37 | 36 | 307 | CLA | CHB-C4A-NA | 2.36 | 127.80 | 124.40 |
| 37 | C | 513 | CLA | O2D-CGD-O1D | -2.36 | 119.26 | 123.85 |
| 50 | 40 | 214 | DD6 | C37-C36-C35 | -2.36 | 110.08 | 114.42 |
| 44 | c | 517 | DGD | O6E-C1E-O5D | -2.36 | 104.47 | 110.04 |
| 37 | c | 503 | CLA | CAA-CBA-CGA | -2.36 | 106.51 | 113.21 |
| 42 | A | 409 | BCT | O3-C-O1 | -2.36 | 113.64 | 119.68 |
| 47 | 15 | 306 | KC1 | O1D-CGD-CBD | -2.36 | 119.87 | 124.52 |
| 50 | 21 | 216 | DD6 | C14-C13-C11 | -2.36 | 121.87 | 125.53 |
| 37 | w | 101 | CLA | C1-C2-C3 | -2.36 | 122.33 | 126.20 |
| 37 | 21 | 208 | CLA | CMC-C2C-C1C | 2.36 | 128.72 | 125.03 |
| 37 | C | 506 | CLA | CGD-CBD-CAD | -2.36 | 103.22 | 110.85 |
| 37 | 40 | 209 | CLA | CBC-CAC-C3C | -2.36 | 106.03 | 112.42 |
| 48 | 37 | 310 | A86 | C7-C6-C8 | 2.36 | 121.69 | 118.09 |
| 41 | L | 102 | LMG | O3-C3-C2 | -2.36 | 104.82 | 110.38 |
| 48 | 39 | 313 | A86 | C41-C32-C31 | -2.36 | 108.36 | 110.47 |
| 37 | 35 | 307 | CLA | CAA-C2A-C3A | -2.36 | 106.63 | 113.00 |
| 51 | 39 | 315 | LMU | C1B-O1B-C4' | -2.36 | 112.39 | 117.98 |
| 37 | 11 | 303 | CLA | CHB-C4A-NA | 2.36 | 127.80 | 124.40 |
| 48 | 34 | 312 | A86 | C21-C20-C15 | -2.36 | 115.75 | 123.35 |
| 37 | b | 508 | CLA | CAA-C2A-C3A | -2.36 | 106.63 | 113.00 |
| 41 | B | 520 | LMG | C40-C39-C38 | -2.36 | 102.46 | 114.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | B | 509 | CLA | O2D-CGD-O1D | -2.36 | 119.26 | 123.85 |
| 37 | 21 | 208 | CLA | O2D-CGD-O1D | -2.36 | 119.26 | 123.85 |
| 47 | 31 | 305 | KC1 | O2D-CGD-O1D | -2.36 | 119.26 | 123.85 |
| 51 | 19 | 315 | LMU | C1B-O1B-C4' | -2.35 | 112.40 | 117.98 |
| 48 | 32 | 203 | A86 | C22-C16-C17 | -2.35 | 104.83 | 108.97 |
| 37 | 17 | 309 | CLA | O2A-CGA-O1A | -2.35 | 117.74 | 123.63 |
| 41 | l | 101 | LMG | O3-C3-C2 | -2.35 | 104.83 | 110.38 |
| 39 | d | 405 | BCR | C33-C5-C6 | -2.35 | 121.92 | 124.48 |
| 37 | 17 | 304 | CLA | C1-O2A-CGA | 2.35 | 122.35 | 116.65 |
| 37 | B | 508 | CLA | CAA-C2A-C3A | -2.35 | 106.64 | 113.00 |
| 47 | 35 | 304 | KC1 | CMB-C2B-C1B | 2.35 | 128.87 | 124.73 |
| 47 | 19 | 308 | KC1 | CBC-CAC-C3C | -2.35 | 106.04 | 112.42 |
| 47 | 17 | 308 | KC1 | CMC-C2C-C1C | 2.35 | 128.71 | 125.03 |
| 37 | Z | 101 | CLA | C1-O2A-CGA | 2.35 | 122.35 | 116.65 |
| 37 | c | 512 | CLA | C4-C3-C5 | 2.35 | 119.31 | 115.23 |
| 37 | 32 | 210 | CLA | CAA-C2A-C3A | -2.35 | 106.64 | 113.00 |
| 37 | B | 524 | CLA | C3B-C4B-NB | 2.35 | 112.63 | 110.53 |
| 47 | 20 | 302 | KC1 | C4C-C3C-C2C | -2.35 | 103.47 | 106.89 |
| 37 | 20 | 307 | CLA | CBC-CAC-C3C | -2.35 | 106.04 | 112.42 |
| 41 | b | 519 | LMG | C40-C39-C38 | -2.35 | 102.48 | 114.37 |
| 37 | 12 | 204 | CLA | CHD-C4C-NC | 2.35 | 127.88 | 124.23 |
| 37 | 32 | 205 | CLA | CHD-C4C-NC | 2.35 | 127.88 | 124.23 |
| 37 | 35 | 308 | CLA | CMC-C2C-C1C | 2.35 | 128.71 | 125.03 |
| 37 | D | 406 | CLA | C1-C2-C3 | -2.35 | 122.34 | 126.20 |
| 37 | c | 502 | CLA | CBC-CAC-C3C | -2.35 | 106.05 | 112.42 |
| 41 | A | 408 | LMG | C6-C5-C4 | -2.35 | 107.25 | 113.02 |
| 48 | 31 | 312 | A86 | C9-C10-C11 | -2.35 | 119.99 | 126.64 |
| 47 | 39 | 308 | KC1 | CBC-CAC-C3C | -2.35 | 106.05 | 112.42 |
| 37 | d | 404 | CLA | C1-C2-C3 | -2.35 | 122.35 | 126.20 |
| 37 | c | 506 | CLA | CHA-C1A-NA | -2.35 | 121.07 | 126.39 |
| 48 | 13 | 315 | A86 | C4-C3-C2 | -2.35 | 118.71 | 123.52 |
| 37 | 14 | 303 | CLA | C1-C2-C3 | -2.35 | 122.35 | 126.20 |
| 47 | 32 | 209 | KC1 | CMC-C2C-C1C | 2.35 | 128.71 | 125.03 |
| 37 | 38 | 209 | CLA | CED-O2D-CGD | 2.35 | 121.24 | 115.92 |
| 48 | 15 | 315 | A86 | C19-C18-C17 | -2.35 | 106.40 | 110.79 |
| 37 | C | 507 | CLA | C4B-C3B-C2B | -2.35 | 104.38 | 107.30 |
| 37 | 41 | 208 | CLA | CMB-C2B-C1B | 2.35 | 128.99 | 125.42 |
| 48 | 14 | 312 | A86 | C21-C20-C15 | -2.35 | 115.77 | 123.35 |
| 37 | c | 513 | CLA | O2D-CGD-O1D | -2.35 | 119.28 | 123.85 |
| 37 | 20 | 301 | CLA | O2D-CGD-O1D | -2.35 | 119.28 | 123.85 |
| 50 | 20 | 312 | DD6 | C37-C36-C35 | -2.35 | 110.11 | 114.42 |
| 48 | 17 | 320 | A86 | C21-C20-C15 | -2.35 | 115.77 | 123.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 506 | CLA | CGD-CBD-CAD | -2.35 | 103.25 | 110.85 |
| 47 | 34 | 304 | KC1 | O2D-CGD-O1D | -2.35 | 119.28 | 123.85 |
| 48 | 12 | 202 | A86 | C22-C16-C17 | -2.35 | 104.85 | 108.97 |
| 39 | b | 517 | BCR | C33-C5-C6 | -2.35 | 121.92 | 124.48 |
| 37 | 34 | 307 | CLA | O2A-CGA-CBA | 2.34 | 118.98 | 111.83 |
| 37 | 16 | 307 | CLA | CHB-C4A-NA | 2.34 | 127.78 | 124.40 |
| 37 | 31 | 304 | CLA | CHB-C4A-NA | 2.34 | 127.78 | 124.40 |
| 37 | 38 | 201 | CLA | CMC-C2C-C1C | 2.34 | 128.70 | 125.03 |
| 37 | 38 | 209 | CLA | CMC-C2C-C1C | 2.34 | 128.70 | 125.03 |
| 37 | 15 | 310 | CLA | CHB-C4A-NA | 2.34 | 127.78 | 124.40 |
| 48 | 32 | 221 | A86 | C41-C32-C31 | -2.34 | 108.37 | 110.47 |
| 39 | b | 524 | BCR | C7-C8-C9 | -2.34 | 122.77 | 126.23 |
| 47 | 12 | 208 | KC1 | CMC-C2C-C1C | 2.34 | 128.70 | 125.03 |
| 48 | 11 | 312 | A86 | C19-C18-C17 | 2.34 | 115.17 | 110.79 |
| 39 | B | 517 | BCR | C33-C5-C6 | -2.34 | 121.93 | 124.48 |
| 37 | 11 | 310 | CLA | CMC-C2C-C1C | 2.34 | 128.69 | 125.03 |
| 37 | D | 405 | CLA | O2D-CGD-O1D | -2.34 | 119.29 | 123.85 |
| 37 | 14 | 307 | CLA | O2A-CGA-CBA | 2.34 | 118.98 | 111.83 |
| 47 | 37 | 307 | KC1 | CMC-C2C-C1C | 2.34 | 128.69 | 125.03 |
| 37 | 21 | 208 | CLA | CMB-C2B-C1B | 2.34 | 128.99 | 125.42 |
| 44 | j | 101 | DGD | CAB-C9B-C8B | -2.34 | 102.53 | 114.37 |
| 48 | 37 | 312 | A86 | C-C1-C24 | 2.34 | 121.67 | 118.09 |
| 37 | 14 | 301 | CLA | CHB-C4A-NA | 2.34 | 127.78 | 124.40 |
| 37 | 20 | 308 | CLA | CHB-C4A-NA | 2.34 | 127.78 | 124.40 |
| 37 | 15 | 307 | CLA | CAA-C2A-C3A | -2.34 | 106.67 | 113.00 |
| 37 | 40 | 210 | CLA | O2D-CGD-O1D | -2.34 | 119.29 | 123.85 |
| 47 | 37 | 307 | KC1 | C1A-NA-C4A | -2.34 | 105.61 | 106.68 |
| 44 | J | 101 | DGD | CAB-C9B-C8B | -2.34 | 102.53 | 114.37 |
| 40 | b | 521 | SQD | O48-C23-O10 | -2.34 | 117.77 | 123.63 |
| 37 | 37 | 308 | CLA | CHD-C4C-NC | 2.34 | 127.86 | 124.23 |
| 39 | h | 101 | BCR | C15-C14-C13 | -2.34 | 124.00 | 127.28 |
| 48 | 21 | 213 | A86 | C10-C9-C8 | -2.34 | 116.42 | 123.20 |
| 37 | 40 | 210 | CLA | CBC-CAC-C3C | -2.34 | 106.08 | 112.42 |
| 37 | 20 | 308 | CLA | O2D-CGD-O1D | -2.34 | 119.30 | 123.85 |
| 37 | 36 | 306 | CLA | C1-O2A-CGA | 2.34 | 122.31 | 116.65 |
| 43 | D | 410 | LHG | C5-O7-C7 | -2.34 | 112.20 | 117.80 |
| 47 | 38 | 207 | KC1 | O2A-CGA-O1A | -2.34 | 117.94 | 122.70 |
| 37 | 34 | 307 | CLA | CHB-C1B-C2B | -2.34 | 120.64 | 127.43 |
| 37 | 12 | 205 | CLA | O2A-CGA-CBA | 2.34 | 118.96 | 111.83 |
| 37 | 16 | 301 | CLA | CHB-C4A-NA | 2.34 | 127.77 | 124.40 |
| 37 | 37 | 306 | CLA | CHB-C1B-C2B | -2.34 | 120.64 | 127.43 |
| 37 | c | 507 | CLA | C4B-C3B-C2B | -2.34 | 104.39 | 107.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 17 | 303 | KC1 | CHB-C4A-NA | 2.34 | 127.86 | 124.23 |
| 37 | z | 101 | CLA | C1-O2A-CGA | 2.34 | 122.31 | 116.65 |
| 37 | C | 503 | CLA | CAA-CBA-CGA | -2.34 | 106.57 | 113.21 |
| 37 | 38 | 201 | CLA | O2A-CGA-CBA | 2.34 | 118.96 | 111.83 |
| 37 | 21 | 209 | CLA | CHB-C4A-NA | 2.34 | 127.77 | 124.40 |
| 41 | a | 410 | LMG | C38-C37-C36 | -2.34 | 102.56 | 114.37 |
| 43 | B | 523 | LHG | C18-C17-C16 | -2.34 | 102.56 | 114.37 |
| 48 | 35 | 319 | A86 | C34-O4-C38 | -2.34 | 113.72 | 117.85 |
| 47 | 17 | 303 | KC1 | O2D-CGD-O1D | -2.34 | 119.30 | 123.85 |
| 37 | 20 | 303 | CLA | CHA-C1A-NA | -2.34 | 121.10 | 126.39 |
| 37 | 17 | 302 | CLA | CAA-CBA-CGA | -2.34 | 106.58 | 113.21 |
| 41 | a | 410 | LMG | C6-C5-C4 | -2.34 | 107.28 | 113.02 |
| 44 | c | 516 | DGD | O5D-C6D-C5D | -2.34 | 104.16 | 109.42 |
| 39 | D | 407 | BCR | C11-C10-C9 | -2.34 | 124.00 | 127.28 |
| 48 | 41 | 213 | A86 | C10-C9-C8 | -2.34 | 116.43 | 123.20 |
| 37 | 39 | 302 | CLA | CMC-C2C-C1C | 2.34 | 128.68 | 125.03 |
| 48 | 17 | 314 | A86 | C23-C16-C17 | -2.34 | 104.86 | 108.97 |
| 37 | 31 | 310 | CLA | CMC-C2C-C1C | 2.33 | 128.68 | 125.03 |
| 46 | F | 101 | HEM | CMC-C2C-C1C | -2.33 | 120.62 | 124.73 |
| 37 | c | 503 | CLA | O2A-C1-C2 | 2.33 | 117.09 | 108.11 |
| 48 | 17 | 311 | A86 | C41-C32-C31 | -2.33 | 108.38 | 110.47 |
| 47 | 14 | 304 | KC1 | O2D-CGD-O1D | -2.33 | 119.31 | 123.85 |
| 48 | 37 | 313 | A86 | C23-C16-C17 | -2.33 | 104.87 | 108.97 |
| 44 | C | 517 | DGD | O6E-C1E-O5D | -2.33 | 104.53 | 110.04 |
| 41 | A | 408 | LMG | C38-C37-C36 | -2.33 | 102.57 | 114.37 |
| 37 | 33 | 310 | CLA | O1D-CGD-CBD | -2.33 | 119.92 | 124.52 |
| 47 | 37 | 304 | KC1 | O2D-CGD-O1D | -2.33 | 119.31 | 123.85 |
| 37 | 18 | 203 | CLA | O2A-CGA-CBA | 2.33 | 118.95 | 111.83 |
| 37 | 40 | 205 | CLA | CHA-C1A-NA | -2.33 | 121.11 | 126.39 |
| 37 | 19 | 310 | CLA | O2A-CGA-CBA | 2.33 | 118.95 | 111.83 |
| 37 | 38 | 208 | CLA | C4-C3-C5 | 2.33 | 119.28 | 115.23 |
| 48 | 12 | 220 | A86 | C41-C32-C31 | -2.33 | 108.39 | 110.47 |
| 37 | 15 | 303 | CLA | CMC-C2C-C1C | 2.33 | 128.68 | 125.03 |
| 37 | 32 | 206 | CLA | O2A-CGA-CBA | 2.33 | 118.94 | 111.83 |
| 47 | 15 | 306 | KC1 | CHB-C4A-NA | 2.33 | 127.85 | 124.23 |
| 37 | 38 | 204 | CLA | C1-C2-C3 | -2.33 | 122.38 | 126.20 |
| 37 | 14 | 308 | CLA | CMC-C2C-C1C | 2.33 | 128.68 | 125.03 |
| 44 | C | 516 | DGD | O5D-C6D-C5D | -2.33 | 104.17 | 109.42 |
| 37 | 34 | 303 | CLA | C1-C2-C3 | -2.33 | 122.38 | 126.20 |
| 43 | 21 | 217 | LHG | C27-C26-C25 | -2.33 | 102.59 | 114.37 |
| 48 | 14 | 311 | A86 | C4-C5-C6 | -2.33 | 124.01 | 127.28 |
| 37 | C | 503 | CLA | O2A-C1-C2 | 2.33 | 117.07 | 108.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 32 | 206 | CLA | CHB-C4A-NA | 2.33 | 127.76 | 124.40 |
| 37 | 41 | 208 | CLA | O2D-CGD-O1D | -2.33 | 119.31 | 123.85 |
| 47 | 37 | 302 | KC1 | O2D-CGD-O1D | -2.33 | 119.31 | 123.85 |
| 39 | D | 407 | BCR | C33-C5-C6 | -2.33 | 121.94 | 124.48 |
| 43 | d | 408 | LHG | C5-O7-C7 | -2.33 | 112.22 | 117.80 |
| 37 | 12 | 209 | CLA | CAA-C2A-C3A | -2.33 | 106.71 | 113.00 |
| 37 | 14 | 302 | CLA | CMC-C2C-C1C | 2.33 | 128.67 | 125.03 |
| 39 | a | 413 | BCR | C7-C8-C9 | -2.33 | 122.79 | 126.23 |
| 37 | c | 506 | CLA | CHD-C4C-NC | 2.33 | 127.84 | 124.23 |
| 37 | 37 | 308 | CLA | CHB-C4A-NA | 2.33 | 127.76 | 124.40 |
| 40 | B | 522 | SQD | O48-C23-O10 | -2.33 | 117.81 | 123.63 |
| 48 | 31 | 312 | A86 | C40-C32-C31 | -2.33 | 108.39 | 110.47 |
| 43 | 37 | 321 | LHG | C27-C26-C25 | -2.33 | 102.60 | 114.37 |
| 50 | 41 | 212 | DD6 | C23-C16-C22 | -2.33 | 103.99 | 107.37 |
| 47 | 17 | 305 | KC1 | CMC-C2C-C1C | 2.33 | 128.67 | 125.03 |
| 37 | 18 | 211 | CLA | CAA-C2A-C3A | -2.33 | 106.71 | 113.00 |
| 37 | 17 | 309 | CLA | CHB-C4A-NA | 2.33 | 127.76 | 124.40 |
| 41 | a | 410 | LMG | O2-C2-C1 | -2.33 | 104.53 | 110.08 |
| 46 | V | 201 | HEM | CAC-C3C-C2C | -2.33 | 120.87 | 128.43 |
| 37 | 14 | 307 | CLA | CHB-C1B-C2B | -2.33 | 120.67 | 127.43 |
| 37 | 18 | 209 | CLA | CED-O2D-CGD | 2.33 | 121.19 | 115.92 |
| 37 | B | 512 | CLA | O1D-CGD-CBD | -2.33 | 119.93 | 124.52 |
| 43 | b | 522 | LHG | C18-C17-C16 | -2.33 | 102.61 | 114.37 |
| 37 | C | 509 | CLA | CBC-CAC-C3C | -2.33 | 106.12 | 112.42 |
| 46 | v | 201 | HEM | CAC-C3C-C2C | -2.33 | 120.87 | 128.43 |
| 47 | 37 | 302 | KC1 | CHB-C4A-NA | 2.33 | 127.84 | 124.23 |
| 37 | c | 505 | CLA | CBC-CAC-C3C | -2.33 | 106.12 | 112.42 |
| 44 | C | 517 | DGD | O3E-C3E-C2E | -2.32 | 104.90 | 110.38 |
| 37 | c | 509 | CLA | CBC-CAC-C3C | -2.32 | 106.12 | 112.42 |
| 37 | 20 | 306 | CLA | CHB-C4A-NA | 2.32 | 127.75 | 124.40 |
| 48 | 37 | 314 | A86 | C7-C6-C5 | -2.32 | 119.05 | 122.82 |
| 37 | 17 | 307 | CLA | CHB-C1B-C2B | -2.32 | 120.68 | 127.43 |
| 37 | C | 505 | CLA | CBC-CAC-C3C | -2.32 | 106.12 | 112.42 |
| 37 | 40 | 203 | CLA | O2D-CGD-O1D | -2.32 | 119.33 | 123.85 |
| 48 | 38 | 215 | A86 | C8-C6-C5 | 2.32 | 122.66 | 119.01 |
| 47 | 33 | 304 | KC1 | CMC-C2C-C1C | 2.32 | 128.66 | 125.03 |
| 37 | 14 | 303 | CLA | CMB-C2B-C1B | 2.32 | 128.96 | 125.42 |
| 48 | 37 | 311 | A86 | C-C1-C24 | 2.32 | 121.64 | 118.09 |
| 47 | 38 | 207 | KC1 | CMC-C2C-C1C | 2.32 | 128.66 | 125.03 |
| 37 | B | 503 | CLA | CMB-C2B-C1B | 2.32 | 128.96 | 125.42 |
| 37 | 20 | 303 | CLA | O1D-CGD-CBD | -2.32 | 119.94 | 124.52 |
| 48 | 17 | 315 | A86 | C7-C6-C5 | -2.32 | 119.05 | 122.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 503 | CLA | CMB-C2B-C1B | 2.32 | 128.95 | 125.42 |
| 37 | 32 | 210 | CLA | CMB-C2B-C3B | 2.32 | 132.01 | 126.55 |
| 37 | 11 | 301 | CLA | C4-C3-C5 | 2.32 | 119.26 | 115.23 |
| 48 | 31 | 312 | A86 | C19-C18-C17 | 2.32 | 115.13 | 110.79 |
| 37 | 31 | 308 | CLA | CAA-C2A-C1A | 2.32 | 119.58 | 111.97 |
| 48 | 11 | 312 | A86 | C9-C10-C11 | -2.32 | 120.08 | 126.64 |
| 37 | C | 513 | CLA | CAA-C2A-C3A | -2.32 | 106.73 | 113.00 |
| 37 | c | 501 | CLA | CMC-C2C-C1C | 2.32 | 128.66 | 125.03 |
| 47 | 37 | 304 | KC1 | CHB-C4A-NA | 2.32 | 127.83 | 124.23 |
| 41 | C | 518 | LMG | C38-C37-C36 | -2.32 | 102.64 | 114.37 |
| 39 | H | 101 | BCR | C27-C26-C25 | 2.32 | 125.84 | 122.70 |
| 44 | c | 517 | DGD | C3D-C4D-C5D | -2.32 | 106.03 | 110.23 |
| 47 | 33 | 302 | KC1 | CHB-C1B-C2B | -2.32 | 120.66 | 125.49 |
| 39 | H | 101 | BCR | C15-C14-C13 | -2.32 | 124.03 | 127.28 |
| 41 | c | 518 | LMG | C38-C37-C36 | -2.32 | 102.65 | 114.37 |
| 37 | 20 | 308 | CLA | CBC-CAC-C3C | -2.32 | 106.14 | 112.42 |
| 41 | c | 518 | LMG | O3-C3-C2 | -2.32 | 104.91 | 110.38 |
| 37 | 12 | 205 | CLA | CHB-C4A-NA | 2.32 | 127.74 | 124.40 |
| 37 | 40 | 210 | CLA | CHB-C4A-NA | 2.32 | 127.74 | 124.40 |
| 41 | C | 518 | LMG | O3-C3-C2 | -2.32 | 104.91 | 110.38 |
| 37 | 34 | 302 | CLA | CHA-C1A-NA | -2.32 | 121.14 | 126.39 |
| 48 | 34 | 311 | A86 | C4-C5-C6 | -2.32 | 124.03 | 127.28 |
| 44 | c | 517 | DGD | O3E-C3E-C2E | -2.32 | 104.92 | 110.38 |
| 47 | 12 | 206 | KC1 | C3D-C2D-C1D | -2.32 | 99.00 | 106.40 |
| 37 | 18 | 209 | CLA | CMC-C2C-C1C | 2.32 | 128.65 | 125.03 |
| 37 | 41 | 208 | CLA | CMC-C2C-C1C | 2.32 | 128.65 | 125.03 |
| 48 | 38 | 215 | A86 | C12-C11-C13 | 2.32 | 119.75 | 116.00 |
| 37 | 40 | 208 | CLA | CHB-C4A-NA | 2.32 | 127.74 | 124.40 |
| 37 | C | 508 | CLA | O2A-CGA-CBA | 2.32 | 118.89 | 111.83 |
| 37 | 35 | 307 | CLA | CAA-C2A-C1A | 2.31 | 119.56 | 111.97 |
| 47 | 12 | 211 | KC1 | O1D-CGD-CBD | -2.31 | 119.95 | 124.52 |
| 46 | F | 101 | HEM | CMB-C2B-C1B | -2.31 | 121.42 | 125.03 |
| 37 | 34 | 305 | CLA | CMB-C2B-C1B | 2.31 | 128.94 | 125.42 |
| 48 | 33 | 315 | A86 | C26-C25-C24 | -2.31 | 116.50 | 123.20 |
| 48 | 18 | 212 | A86 | C3-C4-C5 | -2.31 | 118.78 | 123.52 |
| 47 | 16 | 308 | KC1 | CBC-CAC-C3C | -2.31 | 106.15 | 112.42 |
| 37 | 16 | 307 | CLA | CMC-C2C-C1C | 2.31 | 128.65 | 125.03 |
| 41 | A | 408 | LMG | O2-C2-C1 | -2.31 | 104.56 | 110.08 |
| 37 | c | 503 | CLA | CMC-C2C-C1C | 2.31 | 128.65 | 125.03 |
| 37 | b | 512 | CLA | O1D-CGD-CBD | -2.31 | 119.96 | 124.52 |
| 37 | 13 | 305 | CLA | O2D-CGD-O1D | -2.31 | 119.35 | 123.85 |
| 47 | 32 | 207 | KC1 | C3D-C2D-C1D | -2.31 | 99.02 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 44 | c | 516 | DGD | C1D-C2D-C3D | -2.31 | 105.15 | 110.01 |
| 37 | 19 | 302 | CLA | CMC-C2C-C1C | 2.31 | 128.65 | 125.03 |
| 48 | 31 | 314 | A86 | C-C1-C24 | 2.31 | 121.62 | 118.09 |
| 37 | 35 | 303 | CLA | CMC-C2C-C1C | 2.31 | 128.65 | 125.03 |
| 37 | 37 | 301 | CLA | CAA-CBA-CGA | -2.31 | 106.64 | 113.21 |
| 37 | 37 | 306 | CLA | O2A-CGA-CBA | 2.31 | 118.88 | 111.83 |
| 37 | 36 | 301 | CLA | C4B-C3B-C2B | -2.31 | 104.43 | 107.30 |
| 37 | C | 503 | CLA | O2A-CGA-O1A | -2.31 | 117.85 | 123.63 |
| 37 | 19 | 309 | CLA | CBC-CAC-C3C | -2.31 | 106.16 | 112.42 |
| 39 | h | 101 | BCR | C27-C26-C25 | 2.31 | 125.83 | 122.70 |
| 37 | B | 516 | CLA | O2A-CGA-CBA | 2.31 | 118.88 | 111.83 |
| 37 | 34 | 308 | CLA | CMC-C2C-C1C | 2.31 | 128.64 | 125.03 |
| 47 | 13 | 302 | KC1 | CHB-C1B-C2B | -2.31 | 120.68 | 125.49 |
| 48 | 19 | 311 | A86 | O4-C38-O5 | -2.31 | 118.53 | 122.99 |
| 37 | B | 512 | CLA | CAA-C2A-C3A | -2.31 | 106.76 | 113.00 |
| 37 | 16 | 306 | CLA | C1-O2A-CGA | 2.31 | 122.24 | 116.65 |
| 48 | 15 | 312 | A86 | C41-C32-C31 | -2.31 | 108.41 | 110.47 |
| 48 | 19 | 313 | A86 | C41-C32-C31 | -2.31 | 108.41 | 110.47 |
| 48 | 14 | 313 | A86 | C4-C3-C2 | -2.31 | 118.80 | 123.52 |
| 48 | 34 | 313 | A86 | C4-C3-C2 | -2.31 | 118.80 | 123.52 |
| 37 | 36 | 307 | CLA | CMC-C2C-C1C | 2.31 | 128.64 | 125.03 |
| 48 | 15 | 319 | A86 | C34-O4-C38 | -2.31 | 113.77 | 117.85 |
| 48 | 32 | 221 | A86 | C34-O4-C38 | -2.31 | 113.77 | 117.85 |
| 43 | 21 | 201 | LHG | O3-C3-C2 | -2.31 | 100.12 | 109.63 |
| 47 | 15 | 302 | KC1 | O1D-CGD-CBD | -2.31 | 119.97 | 124.52 |
| 37 | c | 508 | CLA | O2A-CGA-CBA | 2.31 | 118.87 | 111.83 |
| 48 | 12 | 220 | A86 | C34-O4-C38 | -2.31 | 113.77 | 117.85 |
| 37 | w | 101 | CLA | C4-C3-C5 | 2.31 | 119.23 | 115.23 |
| 48 | 35 | 316 | A86 | C36-C31-C32 | -2.31 | 117.41 | 119.70 |
| 37 | 15 | 303 | CLA | O1D-CGD-CBD | -2.31 | 119.97 | 124.52 |
| 48 | 13 | 315 | A86 | C26-C25-C24 | -2.31 | 116.52 | 123.20 |
| 50 | 21 | 212 | DD6 | C23-C16-C22 | -2.31 | 104.02 | 107.37 |
| 37 | 13 | 303 | CLA | C1-O2A-CGA | 2.31 | 122.23 | 116.65 |
| 37 | 19 | 307 | CLA | C4B-C3B-C2B | -2.31 | 104.44 | 107.30 |
| 37 | c | 503 | CLA | O2A-CGA-O1A | -2.31 | 117.86 | 123.63 |
| 37 | 41 | 209 | CLA | CHB-C4A-NA | 2.31 | 127.73 | 124.40 |
| 37 | 18 | 202 | CLA | CMB-C2B-C1B | 2.31 | 128.93 | 125.42 |
| 47 | 16 | 304 | KC1 | CAA-C2A-C1A | -2.31 | 114.54 | 124.64 |
| 37 | 39 | 309 | CLA | CBC-CAC-C3C | -2.30 | 106.17 | 112.42 |
| 47 | 13 | 304 | KC1 | CBC-CAC-C3C | -2.30 | 106.17 | 112.42 |
| 47 | 36 | 308 | KC1 | CBC-CAC-C3C | -2.30 | 106.17 | 112.42 |
| 37 | 18 | 202 | CLA | CED-O2D-CGD | 2.30 | 121.14 | 115.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 513 | CLA | CAA-C2A-C3A | -2.30 | 106.77 | 113.00 |
| 37 | C | 512 | CLA | CAC-C3C-C4C | 2.30 | 127.79 | 124.79 |
| 37 | 14 | 302 | CLA | CHA-C1A-NA | -2.30 | 121.17 | 126.39 |
| 37 | W | 102 | CLA | CAA-C2A-C3A | -2.30 | 106.78 | 113.00 |
| 41 | B | 521 | LMG | C1-C2-C3 | -2.30 | 105.17 | 110.01 |
| 48 | 11 | 312 | A86 | C40-C32-C31 | -2.30 | 108.41 | 110.47 |
| 47 | 32 | 212 | KC1 | O1D-CGD-CBD | -2.30 | 119.98 | 124.52 |
| 37 | C | 506 | CLA | CHD-C4C-NC | 2.30 | 127.80 | 124.23 |
| 48 | 17 | 313 | A86 | C-C1-C24 | 2.30 | 121.61 | 118.09 |
| 47 | 35 | 306 | KC1 | CHB-C4A-NA | 2.30 | 127.80 | 124.23 |
| 37 | 31 | 302 | CLA | C4-C3-C5 | 2.30 | 119.22 | 115.23 |
| 45 | d | 402 | PL9 | C20-C19-C21 | 2.30 | 119.22 | 115.23 |
| 47 | 15 | 304 | KC1 | CBC-CAC-C3C | -2.30 | 106.18 | 112.42 |
| 37 | 12 | 210 | CLA | CMC-C2C-C1C | 2.30 | 128.63 | 125.03 |
| 48 | 36 | 310 | A86 | C23-C16-C22 | -2.30 | 104.03 | 107.37 |
| 37 | 15 | 307 | CLA | O2D-CGD-O1D | -2.30 | 119.37 | 123.85 |
| 48 | 13 | 311 | A86 | C8-C6-C5 | -2.30 | 115.39 | 119.01 |
| 37 | 14 | 305 | CLA | O1D-CGD-CBD | -2.30 | 119.98 | 124.52 |
| 37 | 14 | 305 | CLA | CMB-C2B-C1B | 2.30 | 128.92 | 125.42 |
| 47 | 38 | 207 | KC1 | CAB-C3B-C4B | 2.30 | 130.31 | 124.82 |
| 41 | d | 409 | LMG | C40-C39-C38 | -2.30 | 102.74 | 114.37 |
| 37 | 21 | 209 | CLA | CBC-CAC-C3C | -2.30 | 106.18 | 112.42 |
| 37 | z | 102 | CLA | CBC-CAC-C3C | -2.30 | 106.19 | 112.42 |
| 48 | 11 | 314 | A86 | C-C1-C24 | 2.30 | 121.60 | 118.09 |
| 44 | C | 517 | DGD | C3D-C4D-C5D | -2.30 | 106.06 | 110.23 |
| 37 | 16 | 301 | CLA | C4B-C3B-C2B | -2.30 | 104.44 | 107.30 |
| 44 | C | 516 | DGD | C1D-C2D-C3D | -2.30 | 105.17 | 110.01 |
| 37 | 36 | 309 | CLA | CHB-C4A-NA | 2.30 | 127.72 | 124.40 |
| 40 | 17 | 301 | SQD | O6-C1-C2 | 2.30 | 111.76 | 108.27 |
| 48 | 37 | 311 | A86 | O4-C34-C33 | 2.30 | 113.52 | 107.64 |
| 37 | b | 515 | CLA | CMC-C2C-C1C | 2.30 | 128.62 | 125.03 |
| 37 | b | 511 | CLA | CHB-C4A-NA | 2.30 | 127.72 | 124.40 |
| 37 | 15 | 307 | CLA | CAA-C2A-C1A | 2.30 | 119.50 | 111.97 |
| 37 | 12 | 209 | CLA | CMB-C2B-C3B | 2.30 | 131.95 | 126.55 |
| 41 | D | 412 | LMG | C40-C39-C38 | -2.30 | 102.76 | 114.37 |
| 39 | C | 514 | BCR | C31-C1-C6 | 2.30 | 113.84 | 110.24 |
| 39 | d | 405 | BCR | C11-C10-C9 | -2.30 | 124.06 | 127.28 |
| 37 | 37 | 308 | CLA | CAC-C3C-C4C | 2.30 | 127.78 | 124.79 |
| 37 | 33 | 305 | CLA | O2D-CGD-O1D | -2.30 | 119.38 | 123.85 |
| 48 | 16 | 310 | A86 | C23-C16-C22 | -2.30 | 104.03 | 107.37 |
| 37 | 41 | 209 | CLA | CBC-CAC-C3C | -2.30 | 106.20 | 112.42 |
| 37 | B | 512 | CLA | CMA-C3A-C2A | -2.30 | 105.11 | 113.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 17 | 312 | A86 | O4-C34-C33 | 2.30 | 113.51 | 107.64 |
| 47 | 11 | 306 | KC1 | C3D-C2D-C1D | -2.30 | 99.07 | 106.40 |
| 47 | 36 | 304 | KC1 | CAA-C2A-C1A | -2.29 | 114.59 | 124.64 |
| 37 | 11 | 307 | CLA | CAA-C2A-C1A | 2.29 | 119.50 | 111.97 |
| 37 | 13 | 307 | CLA | CMB-C2B-C1B | 2.29 | 128.91 | 125.42 |
| 48 | 20 | 309 | A86 | C25-C24-C1 | -2.29 | 120.07 | 126.36 |
| 48 | 17 | 311 | A86 | C4-C5-C6 | -2.29 | 124.06 | 127.28 |
| 37 | b | 512 | CLA | CAA-C2A-C3A | -2.29 | 106.80 | 113.00 |
| 37 | b | 511 | CLA | O2D-CGD-O1D | -2.29 | 119.38 | 123.85 |
| 48 | 40 | 211 | A86 | C25-C24-C1 | -2.29 | 120.08 | 126.36 |
| 41 | b | 520 | LMG | C1-C2-C3 | -2.29 | 105.19 | 110.01 |
| 37 | B | 513 | CLA | C4-C3-C5 | 2.29 | 119.21 | 115.23 |
| 37 | b | 516 | CLA | O2A-CGA-CBA | 2.29 | 118.82 | 111.83 |
| 37 | B | 514 | CLA | CBC-CAC-C3C | -2.29 | 106.21 | 112.42 |
| 37 | 38 | 211 | CLA | CAA-C2A-C3A | -2.29 | 106.81 | 113.00 |
| 37 | 41 | 206 | CLA | CAC-C3C-C4C | 2.29 | 127.77 | 124.79 |
| 37 | b | 514 | CLA | CBC-CAC-C3C | -2.29 | 106.21 | 112.42 |
| 37 | 18 | 211 | CLA | CHB-C4A-NA | 2.29 | 127.70 | 124.40 |
| 50 | 40 | 212 | DD6 | C3-C4-C5 | -2.29 | 118.83 | 123.52 |
| 48 | 15 | 316 | A86 | C22-C16-C17 | -2.29 | 104.94 | 108.97 |
| 47 | 15 | 302 | KC1 | CGD-CBD-CAD | -2.29 | 103.43 | 110.85 |
| 37 | b | 510 | CLA | C4-C3-C5 | 2.29 | 119.20 | 115.23 |
| 37 | 19 | 310 | CLA | C4-C3-C5 | 2.29 | 119.20 | 115.23 |
| 37 | b | 512 | CLA | CMA-C3A-C2A | -2.29 | 105.13 | 113.98 |
| 37 | 21 | 206 | CLA | CAC-C3C-C4C | 2.29 | 127.77 | 124.79 |
| 47 | 35 | 302 | KC1 | CGD-CBD-CAD | -2.29 | 103.43 | 110.85 |
| 47 | 38 | 205 | KC1 | O2D-CGD-O1D | -2.29 | 119.39 | 123.85 |
| 40 | 36 | 315 | SQD | O48-C23-C24 | 2.29 | 118.82 | 111.83 |
| 45 | D | 404 | PL9 | C20-C19-C21 | 2.29 | 119.20 | 115.23 |
| 38 | a | 406 | PHO | C3B-C4B-NB | -2.29 | 105.97 | 107.46 |
| 37 | Z | 102 | CLA | CBC-CAC-C3C | -2.29 | 106.22 | 112.42 |
| 50 | 20 | 310 | DD6 | C3-C4-C5 | -2.29 | 118.84 | 123.52 |
| 37 | 31 | 301 | CLA | CAA-C2A-C3A | -2.29 | 106.82 | 113.00 |
| 47 | 31 | 303 | KC1 | CMC-C2C-C1C | 2.29 | 128.61 | 125.03 |
| 39 | B | 525 | BCR | C33-C5-C6 | -2.29 | 121.99 | 124.48 |
| 47 | 37 | 302 | KC1 | C4C-C3C-C2C | -2.29 | 103.56 | 106.89 |
| 37 | 18 | 204 | CLA | CHB-C1B-C2B | -2.29 | 120.79 | 127.43 |
| 37 | B | 510 | CLA | C4-C3-C5 | 2.29 | 119.20 | 115.23 |
| 37 | 32 | 211 | CLA | CMC-C2C-C1C | 2.29 | 128.61 | 125.03 |
| 37 | 15 | 307 | CLA | CHA-C1A-NA | -2.29 | 121.21 | 126.39 |
| 37 | Z | 102 | CLA | CGD-CBD-CAD | -2.29 | 103.44 | 110.85 |
| 39 | A | 410 | BCR | C7-C8-C9 | -2.29 | 122.85 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 18 | 202 | CLA | CAA-CBA-CGA | -2.29 | 106.72 | 113.21 |
| 37 | 11 | 310 | CLA | CHB-C4A-NA | 2.29 | 127.70 | 124.40 |
| 37 | 41 | 208 | CLA | CBC-CAC-C3C | -2.29 | 106.22 | 112.42 |
| 47 | 31 | 307 | KC1 | C3D-C2D-C1D | -2.29 | 99.10 | 106.40 |
| 37 | b | 511 | CLA | CMC-C2C-C1C | 2.29 | 128.61 | 125.03 |
| 47 | 38 | 205 | KC1 | CHB-C4A-NA | 2.29 | 127.78 | 124.23 |
| 48 | 31 | 314 | A86 | C4-C5-C6 | -2.29 | 124.07 | 127.28 |
| 37 | 37 | 308 | CLA | C2A-C3A-C4A | -2.28 | 98.18 | 101.87 |
| 37 | B | 524 | CLA | CMB-C2B-C1B | 2.28 | 128.90 | 125.42 |
| 37 | 39 | 306 | CLA | CHB-C4A-NA | 2.28 | 127.70 | 124.40 |
| 37 | 16 | 303 | CLA | O1D-CGD-CBD | -2.28 | 120.01 | 124.52 |
| 40 | 17 | 301 | SQD | O48-C23-C24 | 2.28 | 118.80 | 111.83 |
| 37 | 39 | 310 | CLA | C4-C3-C5 | 2.28 | 119.19 | 115.23 |
| 48 | 39 | 313 | A86 | C3-C2-C1 | -2.28 | 124.08 | 127.28 |
| 38 | D | 403 | PHO | C1-C2-C3 | -2.28 | 122.46 | 126.20 |
| 46 | f | 101 | HEM | CMB-C2B-C1B | -2.28 | 121.47 | 125.03 |
| 47 | 35 | 302 | KC1 | O1D-CGD-CBD | -2.28 | 120.02 | 124.52 |
| 48 | 17 | 314 | A86 | C36-C31-C32 | -2.28 | 117.43 | 119.70 |
| 39 | b | 524 | BCR | C33-C5-C6 | -2.28 | 121.99 | 124.48 |
| 37 | c | 511 | CLA | CHB-C4A-NA | 2.28 | 127.69 | 124.40 |
| 48 | 35 | 315 | A86 | C40-C32-C31 | -2.28 | 108.43 | 110.47 |
| 37 | 16 | 306 | CLA | C4-C3-C5 | 2.28 | 119.19 | 115.23 |
| 37 | 36 | 306 | CLA | C4-C3-C5 | 2.28 | 119.19 | 115.23 |
| 39 | c | 514 | BCR | C31-C1-C6 | 2.28 | 113.82 | 110.24 |
| 37 | 21 | 208 | CLA | CBC-CAC-C3C | -2.28 | 106.24 | 112.42 |
| 37 | B | 511 | CLA | CMC-C2C-C1C | 2.28 | 128.60 | 125.03 |
| 48 | 13 | 315 | A86 | C23-C16-C17 | -2.28 | 104.96 | 108.97 |
| 37 | w | 101 | CLA | CMC-C2C-C1C | 2.28 | 128.60 | 125.03 |
| 37 | b | 502 | CLA | CMB-C2B-C1B | 2.28 | 128.89 | 125.42 |
| 37 | 35 | 307 | CLA | CHA-C1A-NA | -2.28 | 121.23 | 126.39 |
| 48 | 15 | 319 | A86 | C8-C6-C5 | -2.28 | 115.42 | 119.01 |
| 37 | 38 | 204 | CLA | CHB-C1B-C2B | -2.28 | 120.81 | 127.43 |
| 48 | 41 | 211 | A86 | C25-C24-C1 | -2.28 | 120.12 | 126.36 |
| 48 | 39 | 311 | A86 | O4-C38-O5 | -2.28 | 118.59 | 122.99 |
| 47 | 31 | 309 | KC1 | CGD-CBD-CAD | -2.28 | 103.47 | 110.85 |
| 37 | 34 | 305 | CLA | O1D-CGD-CBD | -2.28 | 120.03 | 124.52 |
| 47 | 40 | 204 | KC1 | CAB-C3B-C4B | 2.28 | 130.26 | 124.82 |
| 48 | 15 | 311 | A86 | C23-C16-C22 | -2.28 | 104.06 | 107.37 |
| 46 | F | 101 | HEM | CBA-CAA-C2A | 2.28 | 118.83 | 112.53 |
| 47 | 34 | 306 | KC1 | C3D-C2D-C1D | -2.28 | 99.13 | 106.40 |
| 37 | 35 | 305 | CLA | CMC-C2C-C1C | 2.28 | 128.59 | 125.03 |
| 47 | 33 | 304 | KC1 | CBC-CAC-C3C | -2.28 | 106.25 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 46 | f | 101 | HEM | CBA-CAA-C2A | 2.28 | 118.83 | 112.53 |
| 37 | 15 | 305 | CLA | CMC-C2C-C1C | 2.28 | 128.59 | 125.03 |
| 48 | 35 | 313 | A86 | C9-C8-C6 | -2.28 | 120.12 | 126.36 |
| 48 | 11 | 311 | A86 | C9-C10-C11 | -2.28 | 120.21 | 126.64 |
| 38 | A | 404 | PHO | C3B-C4B-NB | -2.28 | 105.98 | 107.46 |
| 37 | B | 506 | CLA | CHB-C1B-C2B | -2.27 | 120.82 | 127.43 |
| 41 | B | 521 | LMG | O3-C3-C2 | -2.27 | 105.01 | 110.38 |
| 37 | 19 | 307 | CLA | CHA-C1A-NA | -2.27 | 121.24 | 126.39 |
| 45 | d | 406 | PL9 | C8-C7-C3 | 2.27 | 117.91 | 112.03 |
| 37 | 34 | 310 | CLA | CAC-C3C-C4C | 2.27 | 127.75 | 124.79 |
| 37 | 15 | 307 | CLA | O1D-CGD-CBD | -2.27 | 120.03 | 124.52 |
| 37 | 12 | 203 | CLA | CBC-CAC-C3C | -2.27 | 106.26 | 112.42 |
| 37 | 33 | 310 | CLA | CMB-C2B-C1B | 2.27 | 128.88 | 125.42 |
| 37 | 35 | 305 | CLA | O2D-CGD-O1D | -2.27 | 119.42 | 123.85 |
| 37 | z | 102 | CLA | CGD-CBD-CAD | -2.27 | 103.49 | 110.85 |
| 37 | B | 516 | CLA | CBC-CAC-C3C | -2.27 | 106.26 | 112.42 |
| 45 | D | 404 | PL9 | C41-C39-C38 | -2.27 | 116.07 | 121.17 |
| 37 | b | 513 | CLA | C4-C3-C5 | 2.27 | 119.17 | 115.23 |
| 48 | 31 | 311 | A86 | C8-C6-C5 | -2.27 | 115.44 | 119.01 |
| 37 | d | 401 | CLA | CBC-CAC-C3C | -2.27 | 106.26 | 112.42 |
| 40 | 36 | 315 | SQD | O6-C1-C2 | 2.27 | 111.72 | 108.27 |
| 37 | B | 514 | CLA | O2A-CGA-CBA | 2.27 | 118.76 | 111.83 |
| 37 | 36 | 303 | CLA | O1D-CGD-CBD | -2.27 | 120.04 | 124.52 |
| 37 | B | 511 | CLA | CHB-C4A-NA | 2.27 | 127.68 | 124.40 |
| 37 | D | 402 | CLA | CBC-CAC-C3C | -2.27 | 106.27 | 112.42 |
| 37 | B | 502 | CLA | CMB-C2B-C1B | 2.27 | 128.88 | 125.42 |
| 47 | 20 | 302 | KC1 | CAB-C3B-C4B | 2.27 | 130.24 | 124.82 |
| 37 | 41 | 209 | CLA | O2D-CGD-O1D | -2.27 | 119.43 | 123.85 |
| 37 | 19 | 305 | CLA | O2A-CGA-CBA | 2.27 | 118.76 | 111.83 |
| 48 | 21 | 211 | A86 | C25-C24-C1 | -2.27 | 120.14 | 126.36 |
| 37 | B | 515 | CLA | CMC-C2C-C1C | 2.27 | 128.58 | 125.03 |
| 37 | B | 511 | CLA | O2D-CGD-O1D | -2.27 | 119.43 | 123.85 |
| 48 | 16 | 311 | A86 | C8-C6-C5 | -2.27 | 115.44 | 119.01 |
| 48 | 33 | 311 | A86 | C8-C6-C5 | -2.27 | 115.44 | 119.01 |
| 37 | B | 515 | CLA | O2A-CGA-CBA | 2.27 | 118.75 | 111.83 |
| 37 | b | 514 | CLA | O2A-CGA-CBA | 2.27 | 118.75 | 111.83 |
| 37 | 20 | 303 | CLA | O2A-CGA-CBA | 2.27 | 118.75 | 111.83 |
| 45 | d | 402 | PL9 | C41-C39-C38 | -2.27 | 116.07 | 121.17 |
| 47 | 18 | 205 | KC1 | CHB-C4A-NA | 2.27 | 127.75 | 124.23 |
| 37 | 34 | 302 | CLA | CMC-C2C-C1C | 2.27 | 128.58 | 125.03 |
| 48 | 33 | 315 | A86 | C23-C16-C17 | -2.27 | 104.98 | 108.97 |
| 48 | 11 | 312 | A86 | C21-C20-C15 | -2.27 | 116.03 | 123.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 38 | 212 | A86 | C23-C16-C17 | -2.27 | 104.98 | 108.97 |
| 48 | 11 | 313 | A86 | C9-C10-C11 | -2.27 | 120.23 | 126.64 |
| 37 | 18 | 202 | CLA | O2A-CGA-O1A | -2.27 | 117.96 | 123.63 |
| 37 | c | 512 | CLA | CAC-C3C-C4C | 2.27 | 127.74 | 124.79 |
| 37 | b | 505 | CLA | CHB-C1B-C2B | -2.27 | 120.85 | 127.43 |
| 48 | 36 | 311 | A86 | C8-C6-C5 | -2.27 | 115.44 | 119.01 |
| 37 | 32 | 204 | CLA | CBC-CAC-C3C | -2.27 | 106.28 | 112.42 |
| 37 | 15 | 305 | CLA | O1D-CGD-CBD | -2.27 | 120.05 | 124.52 |
| 48 | 37 | 311 | A86 | C25-C24-C1 | -2.27 | 120.15 | 126.36 |
| 37 | 19 | 307 | CLA | C4-C3-C5 | 2.27 | 119.16 | 115.23 |
| 37 | 19 | 306 | CLA | CHB-C4A-NA | 2.27 | 127.67 | 124.40 |
| 48 | 35 | 319 | A86 | C8-C6-C5 | -2.27 | 115.45 | 119.01 |
| 50 | 16 | 312 | DD6 | C10-C9-C8 | -2.27 | 116.64 | 123.20 |
| 37 | 16 | 309 | CLA | CHB-C4A-NA | 2.26 | 127.67 | 124.40 |
| 37 | 33 | 307 | CLA | CMB-C2B-C1B | 2.26 | 128.87 | 125.42 |
| 48 | 14 | 316 | A86 | C26-C25-C24 | -2.26 | 116.64 | 123.20 |
| 41 | A | 408 | LMG | C40-C39-C38 | -2.26 | 102.92 | 114.37 |
| 48 | 19 | 313 | A86 | C3-C2-C1 | -2.26 | 124.10 | 127.28 |
| 43 | 37 | 315 | LHG | C20-C19-C18 | -2.26 | 102.92 | 114.37 |
| 37 | D | 406 | CLA | CMC-C2C-C1C | 2.26 | 128.57 | 125.03 |
| 37 | 31 | 310 | CLA | CHB-C4A-NA | 2.26 | 127.67 | 124.40 |
| 47 | 18 | 205 | KC1 | O2D-CGD-O1D | -2.26 | 119.44 | 123.85 |
| 37 | W | 101 | CLA | C4-C3-C5 | 2.26 | 119.16 | 115.23 |
| 37 | 16 | 303 | CLA | C4-C3-C5 | 2.26 | 119.16 | 115.23 |
| 47 | 20 | 302 | KC1 | CMC-C2C-C1C | 2.26 | 128.57 | 125.03 |
| 37 | B | 512 | CLA | CBC-CAC-C3C | -2.26 | 106.29 | 112.42 |
| 37 | 35 | 301 | CLA | CHB-C4A-NA | 2.26 | 127.67 | 124.40 |
| 48 | 38 | 212 | A86 | C3-C2-C1 | -2.26 | 124.11 | 127.28 |
| 37 | b | 516 | CLA | CBC-CAC-C3C | -2.26 | 106.29 | 112.42 |
| 37 | 38 | 204 | CLA | O2A-CGA-CBA | 2.26 | 118.73 | 111.83 |
| 47 | 39 | 308 | KC1 | CMC-C2C-C1C | 2.26 | 128.57 | 125.03 |
| 47 | 40 | 206 | KC1 | CMC-C2C-C1C | 2.26 | 128.57 | 125.03 |
| 37 | 40 | 205 | CLA | O2A-CGA-CBA | 2.26 | 118.73 | 111.83 |
| 37 | 40 | 208 | CLA | CMB-C2B-C1B | 2.26 | 128.86 | 125.42 |
| 37 | 12 | 210 | CLA | CHB-C4A-NA | 2.26 | 127.66 | 124.40 |
| 37 | 38 | 202 | CLA | CAA-CBA-CGA | -2.26 | 106.79 | 113.21 |
| 37 | b | 515 | CLA | O2A-CGA-CBA | 2.26 | 118.73 | 111.83 |
| 47 | 35 | 304 | KC1 | O2D-CGD-O1D | -2.26 | 119.45 | 123.85 |
| 48 | 34 | 316 | A86 | C9-C10-C11 | -2.26 | 120.25 | 126.64 |
| 37 | 38 | 202 | CLA | CHA-C1A-NA | -2.26 | 121.27 | 126.39 |
| 37 | c | 509 | CLA | CHB-C4A-NA | 2.26 | 127.66 | 124.40 |
| 47 | 16 | 305 | KC1 | CHB-C4A-NA | 2.26 | 127.74 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 31 | 311 | A86 | C9-C10-C11 | -2.26 | 120.25 | 126.64 |
| 39 | K | 101 | BCR | C29-C30-C25 | 2.26 | 113.72 | 110.44 |
| 48 | 11 | 311 | A86 | C8-C6-C5 | -2.26 | 115.45 | 119.01 |
| 37 | 34 | 310 | CLA | O2D-CGD-O1D | -2.26 | 119.45 | 123.85 |
| 47 | 17 | 308 | KC1 | C1A-NA-C4A | -2.26 | 105.65 | 106.68 |
| 48 | 31 | 311 | A86 | C23-C16-C22 | -2.26 | 104.09 | 107.37 |
| 45 | D | 408 | PL9 | C8-C7-C3 | 2.26 | 117.87 | 112.03 |
| 39 | d | 405 | BCR | C7-C8-C9 | -2.26 | 122.89 | 126.23 |
| 48 | 31 | 312 | A86 | C21-C20-C15 | -2.26 | 116.06 | 123.35 |
| 37 | b | 506 | CLA | CHB-C1B-C2B | -2.26 | 120.87 | 127.43 |
| 47 | 37 | 302 | KC1 | CMC-C2C-C1C | 2.26 | 128.56 | 125.03 |
| 47 | 11 | 309 | KC1 | CGD-CBD-CAD | -2.26 | 103.53 | 110.85 |
| 37 | 39 | 307 | CLA | CHA-C1A-NA | -2.26 | 121.28 | 126.39 |
| 47 | 14 | 306 | KC1 | C3D-C2D-C1D | -2.26 | 99.19 | 106.40 |
| 47 | 13 | 309 | KC1 | CAB-C3B-C4B | 2.26 | 130.21 | 124.82 |
| 47 | 35 | 304 | KC1 | CED-O2D-CGD | 2.26 | 121.04 | 115.92 |
| 48 | 15 | 313 | A86 | C9-C8-C6 | -2.26 | 120.17 | 126.36 |
| 37 | 39 | 305 | CLA | O2A-CGA-CBA | 2.26 | 118.72 | 111.83 |
| 37 | B | 514 | CLA | CHB-C4A-NA | 2.26 | 127.66 | 124.40 |
| 41 | a | 410 | LMG | C40-C39-C38 | -2.26 | 102.96 | 114.37 |
| 37 | W | 101 | CLA | CMC-C2C-C1C | 2.26 | 128.56 | 125.03 |
| 37 | 15 | 303 | CLA | CAA-C2A-C1A | 2.26 | 119.37 | 111.97 |
| 37 | 39 | 307 | CLA | C4-C3-C5 | 2.26 | 119.14 | 115.23 |
| 47 | 17 | 303 | KC1 | C4C-C3C-C2C | -2.26 | 103.61 | 106.89 |
| 47 | 15 | 304 | KC1 | CHB-C4A-NA | 2.26 | 127.73 | 124.23 |
| 37 | 38 | 201 | CLA | CBC-CAC-C3C | -2.26 | 106.31 | 112.42 |
| 37 | 35 | 307 | CLA | O1D-CGD-CBD | -2.26 | 120.07 | 124.52 |
| 47 | 13 | 304 | KC1 | CMC-C2C-C1C | 2.26 | 128.56 | 125.03 |
| 47 | 40 | 204 | KC1 | CMC-C2C-C1C | 2.26 | 128.56 | 125.03 |
| 39 | h | 101 | BCR | C7-C8-C9 | -2.25 | 122.90 | 126.23 |
| 48 | 21 | 213 | A86 | C25-C24-C1 | -2.25 | 120.18 | 126.36 |
| 37 | B | 507 | CLA | CHC-C1C-NC | 2.25 | 127.71 | 124.31 |
| 39 | B | 518 | BCR | C11-C10-C9 | -2.25 | 124.12 | 127.28 |
| 37 | C | 504 | CLA | O1D-CGD-CBD | -2.25 | 120.07 | 124.52 |
| 37 | B | 516 | CLA | C1C-C2C-C3C | -2.25 | 104.61 | 106.98 |
| 41 | b | 519 | LMG | O6-C1-O1 | -2.25 | 104.72 | 110.04 |
| 39 | a | 408 | BCR | C16-C15-C14 | -2.25 | 118.91 | 123.52 |
| 37 | C | 507 | CLA | CMC-C2C-C1C | 2.25 | 128.56 | 125.03 |
| 37 | 36 | 303 | CLA | C4-C3-C5 | 2.25 | 119.14 | 115.23 |
| 38 | a | 405 | PHO | C4B-NB-C1B | 2.25 | 112.10 | 108.82 |
| 37 | B | 509 | CLA | C7-C6-C5 | -2.25 | 107.26 | 113.26 |
| 37 | B | 505 | CLA | CHB-C1B-C2B | -2.25 | 120.89 | 127.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | 17 | 316 | LHG | C20-C19-C18 | -2.25 | 102.98 | 114.37 |
| 37 | 11 | 303 | CLA | O2A-CGA-CBA | 2.25 | 118.70 | 111.83 |
| 37 | 31 | 304 | CLA | O2A-CGA-CBA | 2.25 | 118.70 | 111.83 |
| 39 | A | 410 | BCR | C27-C26-C25 | 2.25 | 125.75 | 122.70 |
| 50 | 36 | 312 | DD6 | C10-C9-C8 | -2.25 | 116.67 | 123.20 |
| 37 | 34 | 302 | CLA | C4B-C3B-C2B | -2.25 | 104.50 | 107.30 |
| 37 | b | 509 | CLA | C7-C6-C5 | -2.25 | 107.26 | 113.26 |
| 43 | B | 523 | LHG | C27-C26-C25 | -2.25 | 102.98 | 114.37 |
| 48 | 14 | 316 | A86 | C9-C10-C11 | -2.25 | 120.27 | 126.64 |
| 38 | a | 405 | PHO | C1-C2-C3 | -2.25 | 122.51 | 126.20 |
| 48 | 34 | 316 | A86 | C26-C25-C24 | -2.25 | 116.68 | 123.20 |
| 47 | 18 | 205 | KC1 | CMB-C2B-C1B | 2.25 | 128.69 | 124.73 |
| 37 | d | 404 | CLA | CMC-C2C-C1C | 2.25 | 128.55 | 125.03 |
| 37 | C | 503 | CLA | CMC-C2C-C1C | 2.25 | 128.55 | 125.03 |
| 37 | 35 | 303 | CLA | CAA-C2A-C1A | 2.25 | 119.35 | 111.97 |
| 47 | 13 | 302 | KC1 | C4B-C3B-C2B | -2.25 | 104.86 | 106.81 |
| 37 | 32 | 206 | CLA | CBC-CAC-C3C | -2.25 | 106.32 | 112.42 |
| 47 | 33 | 304 | KC1 | CHB-C4A-NA | 2.25 | 127.72 | 124.23 |
| 41 | b | 520 | LMG | O3-C3-C2 | -2.25 | 105.07 | 110.38 |
| 37 | 15 | 305 | CLA | O2D-CGD-O1D | -2.25 | 119.47 | 123.85 |
| 41 | B | 520 | LMG | O6-C1-O1 | -2.25 | 104.73 | 110.04 |
| 37 | 39 | 305 | CLA | CMC-C2C-C1C | 2.25 | 128.55 | 125.03 |
| 37 | b | 512 | CLA | CBC-CAC-C3C | -2.25 | 106.33 | 112.42 |
| 47 | 11 | 302 | KC1 | CMC-C2C-C1C | 2.25 | 128.55 | 125.03 |
| 47 | 13 | 304 | KC1 | CHB-C4A-NA | 2.25 | 127.72 | 124.23 |
| 40 | B | 519 | SQD | O48-C23-C24 | 2.25 | 118.69 | 111.83 |
| 37 | 12 | 203 | CLA | O2D-CGD-O1D | -2.25 | 119.47 | 123.85 |
| 37 | 35 | 308 | CLA | C1-O2A-CGA | 2.25 | 122.09 | 116.65 |
| 47 | 11 | 309 | KC1 | C3D-C2D-C1D | -2.25 | 99.22 | 106.40 |
| 37 | 19 | 309 | CLA | CHB-C4A-NA | 2.25 | 127.64 | 124.40 |
| 37 | 31 | 301 | CLA | C1-C2-C3 | -2.25 | 122.52 | 126.20 |
| 47 | 14 | 304 | KC1 | CHB-C4A-NA | 2.25 | 127.71 | 124.23 |
| 47 | 31 | 309 | KC1 | C3D-C2D-C1D | -2.25 | 99.23 | 106.40 |
| 37 | 38 | 201 | CLA | C4-C3-C5 | 2.25 | 119.13 | 115.23 |
| 47 | 36 | 305 | KC1 | CAA-C2A-C1A | -2.25 | 114.80 | 124.64 |
| 37 | 20 | 303 | CLA | CBC-CAC-C3C | -2.25 | 106.33 | 112.42 |
| 37 | c | 504 | CLA | O1D-CGD-CBD | -2.25 | 120.09 | 124.52 |
| 37 | 13 | 303 | CLA | O2A-CGA-CBA | 2.24 | 118.68 | 111.83 |
| 48 | 11 | 313 | A86 | C-C1-C24 | 2.24 | 121.52 | 118.09 |
| 38 | D | 403 | PHO | C4B-NB-C1B | 2.24 | 112.09 | 108.82 |
| 48 | 13 | 315 | A86 | C22-C16-C17 | -2.24 | 105.02 | 108.97 |
| 37 | 41 | 210 | CLA | CHB-C4A-NA | 2.24 | 127.64 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 31 | 310 | CLA | CAC-C3C-C4C | 2.24 | 127.71 | 124.79 |
| 37 | b | 516 | CLA | C1C-C2C-C3C | -2.24 | 104.62 | 106.98 |
| 48 | 21 | 214 | A86 | C25-C24-C1 | -2.24 | 120.21 | 126.36 |
| 48 | 40 | 211 | A86 | C21-C20-C15 | -2.24 | 116.11 | 123.35 |
| 48 | 38 | 213 | A86 | C23-C16-C17 | -2.24 | 105.03 | 108.97 |
| 37 | 17 | 309 | CLA | CHD-C4C-NC | 2.24 | 127.71 | 124.23 |
| 37 | 13 | 310 | CLA | CMB-C2B-C1B | 2.24 | 128.84 | 125.42 |
| 39 | K | 101 | BCR | C1-C6-C5 | -2.24 | 119.57 | 122.64 |
| 39 | A | 406 | BCR | C16-C15-C14 | -2.24 | 118.93 | 123.52 |
| 47 | 16 | 305 | KC1 | O2D-CGD-O1D | -2.24 | 119.48 | 123.85 |
| 47 | 19 | 308 | KC1 | CAC-C3C-C4C | 2.24 | 127.71 | 124.79 |
| 39 | H | 101 | BCR | C7-C8-C9 | -2.24 | 122.92 | 126.23 |
| 45 | D | 408 | PL9 | C20-C19-C21 | 2.24 | 119.12 | 115.23 |
| 37 | b | 509 | CLA | C4-C3-C5 | 2.24 | 119.12 | 115.23 |
| 37 | b | 501 | CLA | CAA-C2A-C3A | -2.24 | 106.94 | 113.00 |
| 37 | b | 523 | CLA | CMB-C2B-C1B | 2.24 | 128.83 | 125.42 |
| 37 | c | 507 | CLA | CMC-C2C-C1C | 2.24 | 128.54 | 125.03 |
| 37 | 15 | 303 | CLA | C4-C3-C5 | 2.24 | 119.12 | 115.23 |
| 37 | 14 | 310 | CLA | O2D-CGD-O1D | -2.24 | 119.48 | 123.85 |
| 37 | 14 | 302 | CLA | C4B-C3B-C2B | -2.24 | 104.52 | 107.30 |
| 47 | 16 | 305 | KC1 | CAA-C2A-C1A | -2.24 | 114.82 | 124.64 |
| 43 | b | 522 | LHG | C27-C26-C25 | -2.24 | 103.04 | 114.37 |
| 37 | 38 | 203 | CLA | CHA-C1A-NA | -2.24 | 121.32 | 126.39 |
| 47 | 20 | 304 | KC1 | CMC-C2C-C1C | 2.24 | 128.54 | 125.03 |
| 43 | d | 407 | LHG | C18-C17-C16 | -2.24 | 103.04 | 114.37 |
| 48 | 11 | 311 | A86 | C23-C16-C22 | -2.24 | 104.11 | 107.37 |
| 47 | 21 | 207 | KC1 | CHB-C1B-C2B | -2.24 | 120.83 | 125.49 |
| 48 | 11 | 312 | A86 | C34-O4-C38 | -2.24 | 113.89 | 117.85 |
| 37 | 34 | 305 | CLA | CBC-CAC-C3C | -2.24 | 106.35 | 112.42 |
| 37 | 17 | 309 | CLA | C2A-C3A-C4A | -2.24 | 98.25 | 101.87 |
| 37 | 35 | 303 | CLA | C4-C3-C5 | 2.24 | 119.11 | 115.23 |
| 37 | 38 | 201 | CLA | CHB-C1B-C2B | -2.24 | 120.93 | 127.43 |
| 37 | C | 512 | CLA | CHB-C1B-C2B | -2.24 | 120.93 | 127.43 |
| 47 | 33 | 309 | KC1 | CAB-C3B-C4B | 2.24 | 130.17 | 124.82 |
| 37 | 14 | 305 | CLA | CBC-CAC-C3C | -2.24 | 106.35 | 112.42 |
| 37 | C | 509 | CLA | CHB-C4A-NA | 2.24 | 127.63 | 124.40 |
| 40 | L | 101 | SQD | O48-C23-C24 | 2.24 | 118.66 | 111.83 |
| 39 | a | 413 | BCR | C27-C26-C25 | 2.24 | 125.73 | 122.70 |
| 43 | D | 409 | LHG | C18-C17-C16 | -2.24 | 103.06 | 114.37 |
| 47 | 19 | 308 | KC1 | CMC-C2C-C1C | 2.24 | 128.53 | 125.03 |
| 43 | 17 | 316 | LHG | C27-C26-C25 | -2.24 | 103.06 | 114.37 |
| 47 | 31 | 307 | KC1 | CHB-C4A-NA | 2.24 | 127.70 | 124.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 39 | 309 | CLA | CHB-C4A-NA | 2.24 | 127.63 | 124.40 |
| 48 | 16 | 314 | A86 | C3-C4-C5 | -2.24 | 118.94 | 123.52 |
| 37 | 40 | 205 | CLA | CBC-CAC-C3C | -2.24 | 106.36 | 112.42 |
| 48 | 18 | 214 | A86 | C8-C6-C5 | -2.24 | 115.49 | 119.01 |
| 37 | 18 | 201 | CLA | O2A-CGA-CBA | 2.24 | 118.66 | 111.83 |
| 37 | 18 | 204 | CLA | C1-C2-C3 | -2.24 | 122.53 | 126.20 |
| 37 | 32 | 204 | CLA | O2D-CGD-O1D | -2.24 | 119.49 | 123.85 |
| 39 | b | 518 | BCR | C11-C10-C9 | -2.24 | 124.14 | 127.28 |
| 37 | 18 | 201 | CLA | C1-C2-C3 | -2.24 | 122.53 | 126.20 |
| 37 | b | 514 | CLA | CHB-C4A-NA | 2.24 | 127.63 | 124.40 |
| 47 | 41 | 207 | KC1 | CHB-C1B-C2B | -2.24 | 120.84 | 125.49 |
| 39 | y | 101 | BCR | C1-C6-C5 | -2.24 | 119.58 | 122.64 |
| 43 | 37 | 315 | LHG | C27-C26-C25 | -2.24 | 103.06 | 114.37 |
| 39 | y | 101 | BCR | C29-C30-C25 | 2.24 | 113.69 | 110.44 |
| 48 | 41 | 214 | A86 | C25-C24-C1 | -2.24 | 120.23 | 126.36 |
| 37 | b | 516 | CLA | C4-C3-C5 | 2.24 | 119.11 | 115.23 |
| 48 | 20 | 309 | A86 | C21-C20-C15 | -2.24 | 116.13 | 123.35 |
| 47 | 12 | 208 | KC1 | CBC-CAC-C3C | -2.24 | 106.36 | 112.42 |
| 37 | 11 | 301 | CLA | C4B-C3B-C2B | -2.24 | 104.52 | 107.30 |
| 37 | 37 | 308 | CLA | CMB-C2B-C1B | 2.24 | 128.82 | 125.42 |
| 37 | 38 | 203 | CLA | CMB-C2B-C1B | 2.24 | 128.82 | 125.42 |
| 37 | 35 | 305 | CLA | O1D-CGD-CBD | -2.24 | 120.11 | 124.52 |
| 48 | 35 | 316 | A86 | C22-C16-C17 | -2.23 | 105.04 | 108.97 |
| 37 | 31 | 302 | CLA | C4B-C3B-C2B | -2.23 | 104.52 | 107.30 |
| 39 | C | 514 | BCR | C24-C23-C22 | -2.23 | 122.93 | 126.23 |
| 39 | c | 514 | BCR | C24-C23-C22 | -2.23 | 122.93 | 126.23 |
| 41 | 31 | 316 | LMG | O1-C7-C8 | -2.23 | 105.38 | 110.82 |
| 37 | 14 | 310 | CLA | CAC-C3C-C4C | 2.23 | 127.70 | 124.79 |
| 37 | 18 | 203 | CLA | CHA-C1A-NA | -2.23 | 121.33 | 126.39 |
| 37 | 21 | 209 | CLA | O2D-CGD-O1D | -2.23 | 119.50 | 123.85 |
| 47 | 16 | 308 | KC1 | CMC-C2C-C1C | 2.23 | 128.52 | 125.03 |
| 48 | 38 | 213 | A86 | C4-C3-C2 | -2.23 | 118.95 | 123.52 |
| 37 | C | 511 | CLA | CHB-C4A-NA | 2.23 | 127.62 | 124.40 |
| 37 | b | 503 | CLA | CMC-C2C-C1C | 2.23 | 128.52 | 125.03 |
| 48 | 11 | 314 | A86 | C4-C5-C6 | -2.23 | 124.15 | 127.28 |
| 37 | b | 506 | CLA | CHD-C4C-NC | 2.23 | 127.69 | 124.23 |
| 37 | C | 503 | CLA | CHB-C1B-C2B | -2.23 | 120.95 | 127.43 |
| 48 | 13 | 311 | A86 | C35-C34-C33 | 2.23 | 113.90 | 109.89 |
| 48 | 33 | 315 | A86 | C22-C16-C17 | -2.23 | 105.05 | 108.97 |
| 37 | c | 512 | CLA | CHB-C1B-C2B | -2.23 | 120.95 | 127.43 |
| 37 | 38 | 211 | CLA | CHD-C4C-NC | 2.23 | 127.69 | 124.23 |
| 48 | 41 | 213 | A86 | C25-C24-C1 | -2.23 | 120.25 | 126.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 37 | 302 | KC1 | CMB-C2B-C1B | 2.23 | 128.66 | 124.73 |
| 37 | a | 407 | CLA | CBC-CAC-C3C | -2.23 | 106.37 | 112.42 |
| 47 | 13 | 306 | KC1 | CMC-C2C-C1C | 2.23 | 128.52 | 125.03 |
| 37 | 11 | 301 | CLA | O2D-CGD-O1D | -2.23 | 119.51 | 123.85 |
| 37 | 17 | 309 | CLA | OBD-CAD-C3D | -2.23 | 123.21 | 128.42 |
| 48 | 38 | 215 | A86 | C7-C6-C5 | -2.23 | 119.20 | 122.82 |
| 47 | 35 | 306 | KC1 | C3D-C2D-C1D | -2.23 | 99.28 | 106.40 |
| 47 | 31 | 303 | KC1 | C3D-C2D-C1D | -2.23 | 99.28 | 106.40 |
| 37 | W | 102 | CLA | C1-C2-C3 | -2.23 | 122.55 | 126.20 |
| 37 | B | 509 | CLA | C4-C3-C5 | 2.23 | 119.10 | 115.23 |
| 37 | 20 | 306 | CLA | CMB-C2B-C1B | 2.23 | 128.81 | 125.42 |
| 37 | 12 | 204 | CLA | CHB-C4A-NA | 2.23 | 127.61 | 124.40 |
| 37 | 38 | 209 | CLA | CHB-C4A-NA | 2.23 | 127.61 | 124.40 |
| 37 | 19 | 305 | CLA | C1-C2-C3 | -2.23 | 122.55 | 126.20 |
| 37 | c | 503 | CLA | CHB-C1B-C2B | -2.23 | 120.96 | 127.43 |
| 37 | 11 | 310 | CLA | CAC-C3C-C4C | 2.23 | 127.69 | 124.79 |
| 37 | 11 | 308 | CLA | CHB-C4A-NA | 2.23 | 127.61 | 124.40 |
| 47 | 11 | 302 | KC1 | C3D-C2D-C1D | -2.23 | 99.29 | 106.40 |
| 47 | 40 | 204 | KC1 | CHB-C4A-NA | 2.23 | 127.68 | 124.23 |
| 37 | 32 | 205 | CLA | C4-C3-C5 | 2.23 | 119.09 | 115.23 |
| 37 | 38 | 206 | CLA | CMC-C2C-C1C | 2.23 | 128.51 | 125.03 |
| 37 | 36 | 301 | CLA | O1D-CGD-CBD | -2.23 | 120.13 | 124.52 |
| 37 | B | 514 | CLA | C4-C3-C5 | 2.23 | 119.09 | 115.23 |
| 37 | 21 | 204 | CLA | CBC-CAC-C3C | -2.23 | 106.39 | 112.42 |
| 48 | 37 | 309 | A86 | C12-C11-C13 | 2.23 | 119.61 | 116.00 |
| 47 | 34 | 309 | KC1 | C3D-C2D-C1D | -2.23 | 99.29 | 106.40 |
| 48 | 35 | 316 | A86 | C8-C6-C5 | 2.23 | 122.51 | 119.01 |
| 37 | 41 | 204 | CLA | CBC-CAC-C3C | -2.23 | 106.39 | 112.42 |
| 47 | 39 | 308 | KC1 | CAB-C3B-C4B | 2.23 | 130.13 | 124.82 |
| 37 | 11 | 308 | CLA | O2D-CGD-O1D | -2.23 | 119.52 | 123.85 |
| 47 | 18 | 207 | KC1 | CMC-C2C-C1C | 2.23 | 128.51 | 125.03 |
| 47 | 14 | 309 | KC1 | C3D-C2D-C1D | -2.22 | 99.29 | 106.40 |
| 37 | B | 503 | CLA | CMC-C2C-C1C | 2.22 | 128.51 | 125.03 |
| 48 | 33 | 311 | A86 | C35-C34-C33 | 2.22 | 113.88 | 109.89 |
| 48 | 37 | 314 | A86 | C25-C24-C1 | -2.22 | 120.27 | 126.36 |
| 37 | 37 | 308 | CLA | OBD-CAD-C3D | -2.22 | 123.22 | 128.42 |
| 45 | d | 406 | PL9 | C20-C19-C21 | 2.22 | 119.09 | 115.23 |
| 47 | 33 | 306 | KC1 | CMC-C2C-C1C | 2.22 | 128.51 | 125.03 |
| 37 | 32 | 211 | CLA | CHB-C4A-NA | 2.22 | 127.61 | 124.40 |
| 37 | A | 403 | CLA | C11-C10-C8 | -2.22 | 108.58 | 115.97 |
| 47 | 32 | 209 | KC1 | CBC-CAC-C3C | -2.22 | 106.39 | 112.42 |
| 47 | 32 | 209 | KC1 | C3D-C2D-C1D | -2.22 | 99.30 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 32 | 208 | CLA | O2A-CGA-O1A | -2.22 | 118.07 | 123.63 |
| 47 | 11 | 304 | KC1 | C3D-C2D-C1D | -2.22 | 99.30 | 106.40 |
| 48 | 38 | 215 | A86 | C29-C30-C31 | -2.22 | 175.04 | 177.66 |
| 47 | 13 | 304 | KC1 | C3D-C2D-C1D | -2.22 | 99.30 | 106.40 |
| 37 | 38 | 202 | CLA | CHB-C4A-NA | 2.22 | 127.61 | 124.40 |
| 37 | 38 | 211 | CLA | O1D-CGD-CBD | -2.22 | 120.14 | 124.52 |
| 37 | 18 | 201 | CLA | C4-C3-C5 | 2.22 | 119.08 | 115.23 |
| 48 | 32 | 217 | A86 | C8-C6-C5 | -2.22 | 115.51 | 119.01 |
| 37 | 18 | 206 | CLA | O1D-CGD-CBD | -2.22 | 120.14 | 124.52 |
| 37 | B | 501 | CLA | CAA-C2A-C3A | -2.22 | 107.00 | 113.00 |
| 41 | 11 | 316 | LMG | O1-C7-C8 | -2.22 | 105.42 | 110.82 |
| 37 | 38 | 206 | CLA | O1D-CGD-CBD | -2.22 | 120.14 | 124.52 |
| 37 | 17 | 309 | CLA | CMB-C2B-C1B | 2.22 | 128.80 | 125.42 |
| 37 | 39 | 305 | CLA | C1-C2-C3 | -2.22 | 122.56 | 126.20 |
| 47 | 15 | 306 | KC1 | C3D-C2D-C1D | -2.22 | 99.31 | 106.40 |
| 37 | 15 | 308 | CLA | C4-C3-C5 | 2.22 | 119.08 | 115.23 |
| 48 | 15 | 315 | A86 | C7-C6-C8 | 2.22 | 121.48 | 118.09 |
| 48 | 37 | 313 | A86 | C3-C2-C1 | -2.22 | 124.16 | 127.28 |
| 37 | 32 | 202 | CLA | O2D-CGD-O1D | -2.22 | 119.53 | 123.85 |
| 48 | 33 | 313 | A86 | C10-C9-C8 | -2.22 | 116.77 | 123.20 |
| 48 | 21 | 213 | A86 | C12-C11-C13 | 2.22 | 119.60 | 116.00 |
| 50 | 41 | 216 | DD6 | C9-C8-C6 | -2.22 | 120.28 | 126.36 |
| 37 | 12 | 207 | CLA | O2A-CGA-O1A | -2.22 | 118.08 | 123.63 |
| 48 | 38 | 213 | A86 | C10-C9-C8 | -2.22 | 116.77 | 123.20 |
| 37 | b | 507 | CLA | CHC-C1C-NC | 2.22 | 127.65 | 124.31 |
| 48 | 17 | 315 | A86 | C25-C24-C1 | -2.22 | 120.28 | 126.36 |
| 48 | 32 | 215 | A86 | C34-O4-C38 | -2.22 | 113.93 | 117.85 |
| 43 | D | 410 | LHG | C18-C17-C16 | -2.22 | 103.16 | 114.37 |
| 37 | 33 | 303 | CLA | O2A-CGA-CBA | 2.22 | 118.60 | 111.83 |
| 48 | 38 | 214 | A86 | C40-C32-C31 | -2.22 | 108.49 | 110.47 |
| 47 | 11 | 306 | KC1 | O2A-CGA-O1A | -2.22 | 118.18 | 122.70 |
| 47 | 17 | 303 | KC1 | CHC-C4B-C3B | -2.22 | 121.47 | 125.21 |
| 47 | 13 | 302 | KC1 | CAB-C3B-C4B | 2.22 | 130.12 | 124.82 |
| 37 | 15 | 301 | CLA | CHB-C4A-NA | 2.22 | 127.60 | 124.40 |
| 47 | 38 | 205 | KC1 | CMB-C2B-C1B | 2.22 | 128.63 | 124.73 |
| 47 | 31 | 307 | KC1 | O2A-CGA-O1A | -2.22 | 118.19 | 122.70 |
| 37 | a | 403 | CLA | C11-C10-C8 | -2.22 | 108.60 | 115.97 |
| 47 | 15 | 304 | KC1 | O2D-CGD-O1D | -2.22 | 119.53 | 123.85 |
| 37 | 39 | 309 | CLA | CMC-C2C-C1C | 2.22 | 128.50 | 125.03 |
| 47 | 12 | 208 | KC1 | C3D-C2D-C1D | -2.22 | 99.32 | 106.40 |
| 47 | 20 | 302 | KC1 | CHB-C4A-NA | 2.22 | 127.67 | 124.23 |
| 44 | c | 517 | DGD | O5D-C6D-C5D | -2.22 | 104.43 | 109.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 40 | 204 | KC1 | C3D-C2D-C1D | -2.22 | 99.32 | 106.40 |
| 47 | 11 | 306 | KC1 | CHB-C4A-NA | 2.22 | 127.67 | 124.23 |
| 47 | 32 | 209 | KC1 | CHB-C4A-NA | 2.22 | 127.67 | 124.23 |
| 37 | B | 516 | CLA | C4-C3-C5 | 2.21 | 119.07 | 115.23 |
| 47 | 20 | 302 | KC1 | C3D-C2D-C1D | -2.21 | 99.33 | 106.40 |
| 48 | 31 | 312 | A86 | C34-O4-C38 | -2.21 | 113.94 | 117.85 |
| 37 | 12 | 204 | CLA | C1-C2-C3 | -2.21 | 122.57 | 126.20 |
| 47 | 37 | 305 | KC1 | CHD-C4C-NC | 2.21 | 127.65 | 124.31 |
| 47 | 18 | 207 | KC1 | CBC-CAC-C3C | -2.21 | 106.42 | 112.42 |
| 48 | 13 | 313 | A86 | C10-C9-C8 | -2.21 | 116.79 | 123.20 |
| 37 | 18 | 202 | CLA | CHB-C4A-NA | 2.21 | 127.59 | 124.40 |
| 37 | 38 | 204 | CLA | CHB-C4A-NA | 2.21 | 127.59 | 124.40 |
| 45 | d | 402 | PL9 | O2-C1-C2 | -2.21 | 116.80 | 121.83 |
| 44 | C | 516 | DGD | CBB-CAB-C9B | -2.21 | 103.18 | 114.37 |
| 48 | 12 | 214 | A86 | C34-O4-C38 | -2.21 | 113.94 | 117.85 |
| 37 | A | 405 | CLA | CBC-CAC-C3C | -2.21 | 106.42 | 112.42 |
| 37 | 12 | 210 | CLA | CHD-C4C-NC | 2.21 | 127.66 | 124.23 |
| 47 | 31 | 305 | KC1 | C3D-C2D-C1D | -2.21 | 99.33 | 106.40 |
| 48 | 13 | 312 | A86 | C41-C32-C31 | -2.21 | 108.49 | 110.47 |
| 37 | 31 | 302 | CLA | O2D-CGD-O1D | -2.21 | 119.54 | 123.85 |
| 39 | D | 407 | BCR | C7-C8-C9 | -2.21 | 122.96 | 126.23 |
| 47 | 18 | 205 | KC1 | C3D-C2D-C1D | -2.21 | 99.34 | 106.40 |
| 44 | c | 516 | DGD | CBB-CAB-C9B | -2.21 | 103.20 | 114.37 |
| 37 | 32 | 205 | CLA | C1-C2-C3 | -2.21 | 122.58 | 126.20 |
| 50 | 21 | 216 | DD6 | C9-C8-C6 | -2.21 | 120.30 | 126.36 |
| 47 | 36 | 305 | KC1 | O1D-CGD-CBD | -2.21 | 120.16 | 124.52 |
| 37 | 32 | 202 | CLA | CHB-C4A-NA | 2.21 | 127.59 | 124.40 |
| 48 | 37 | 319 | A86 | C19-C18-C17 | -2.21 | 106.66 | 110.79 |
| 37 | C | 511 | CLA | OBD-CAD-C3D | -2.21 | 123.25 | 128.42 |
| 37 | 41 | 204 | CLA | CGD-CBD-CAD | -2.21 | 103.69 | 110.85 |
| 47 | 36 | 305 | KC1 | CHB-C4A-NA | 2.21 | 127.66 | 124.23 |
| 48 | 36 | 313 | A86 | C3-C4-C5 | -2.21 | 119.00 | 123.52 |
| 37 | 16 | 303 | CLA | O2A-CGA-CBA | 2.21 | 118.57 | 111.83 |
| 37 | 11 | 301 | CLA | CBC-CAC-C3C | -2.21 | 106.43 | 112.42 |
| 44 | C | 517 | DGD | O5D-C6D-C5D | -2.21 | 104.44 | 109.42 |
| 41 | 17 | 317 | LMG | O7-C10-O9 | -2.21 | 118.54 | 123.70 |
| 37 | 16 | 301 | CLA | O1D-CGD-CBD | -2.21 | 120.16 | 124.52 |
| 47 | 33 | 304 | KC1 | C3D-C2D-C1D | -2.21 | 99.35 | 106.40 |
| 37 | 19 | 309 | CLA | CMC-C2C-C1C | 2.21 | 128.48 | 125.03 |
| 47 | 36 | 308 | KC1 | CMC-C2C-C1C | 2.21 | 128.48 | 125.03 |
| 37 | 12 | 207 | CLA | O2D-CGD-O1D | -2.21 | 119.55 | 123.85 |
| 37 | 39 | 307 | CLA | CBC-CAC-C3C | -2.21 | 106.44 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 304 | KC1 | CBC-CAC-C3C | -2.21 | 106.44 | 112.42 |
| 47 | 33 | 306 | KC1 | CHB-C4A-NA | 2.21 | 127.65 | 124.23 |
| 37 | b | 514 | CLA | C4-C3-C5 | 2.21 | 119.06 | 115.23 |
| 43 | d | 408 | LHG | C18-C17-C16 | -2.21 | 103.22 | 114.37 |
| 48 | 15 | 319 | A86 | C3-C4-C5 | -2.21 | 119.00 | 123.52 |
| 48 | 17 | 314 | A86 | C34-O4-C38 | -2.21 | 113.95 | 117.85 |
| 47 | 19 | 308 | KC1 | CAB-C3B-C4B | 2.21 | 130.09 | 124.82 |
| 48 | 19 | 313 | A86 | C10-C9-C8 | 2.21 | 129.59 | 123.20 |
| 48 | 33 | 313 | A86 | C21-C20-C15 | -2.21 | 116.23 | 123.35 |
| 47 | 20 | 304 | KC1 | CHB-C4A-NA | 2.21 | 127.65 | 124.23 |
| 48 | 35 | 314 | A86 | C12-C11-C13 | 2.21 | 119.58 | 116.00 |
| 48 | 41 | 213 | A86 | C12-C11-C13 | 2.20 | 119.57 | 116.00 |
| 37 | 19 | 305 | CLA | CMC-C2C-C1C | 2.20 | 128.48 | 125.03 |
| 37 | 34 | 301 | CLA | CBC-CAC-C3C | -2.20 | 106.44 | 112.42 |
| 37 | 21 | 205 | CLA | CED-O2D-CGD | 2.20 | 120.92 | 115.92 |
| 37 | 17 | 304 | CLA | O2A-CGA-CBA | 2.20 | 118.55 | 111.83 |
| 47 | 16 | 305 | KC1 | O1D-CGD-CBD | -2.20 | 120.17 | 124.52 |
| 47 | 32 | 207 | KC1 | CAB-C3B-C4B | 2.20 | 130.08 | 124.82 |
| 37 | 12 | 204 | CLA | C4-C3-C5 | 2.20 | 119.05 | 115.23 |
| 37 | 34 | 307 | CLA | O2D-CGD-O1D | -2.20 | 119.56 | 123.85 |
| 46 | V | 201 | HEM | CHD-C4C-C3C | 2.20 | 128.92 | 125.21 |
| 37 | d | 401 | CLA | C1-C2-C3 | -2.20 | 122.59 | 126.20 |
| 47 | 20 | 302 | KC1 | CHB-C1B-C2B | -2.20 | 120.91 | 125.49 |
| 37 | 14 | 307 | CLA | O2D-CGD-O1D | -2.20 | 119.56 | 123.85 |
| 47 | 36 | 305 | KC1 | O2D-CGD-O1D | -2.20 | 119.56 | 123.85 |
| 41 | 32 | 201 | LMG | O2-C2-C1 | -2.20 | 104.83 | 110.08 |
| 37 | 18 | 208 | CLA | C4-C3-C5 | 2.20 | 119.05 | 115.23 |
| 41 | 31 | 316 | LMG | O2-C2-C1 | -2.20 | 104.83 | 110.08 |
| 37 | 31 | 302 | CLA | CBC-CAC-C3C | -2.20 | 106.45 | 112.42 |
| 37 | 36 | 303 | CLA | O2A-CGA-CBA | 2.20 | 118.54 | 111.83 |
| 37 | B | 506 | CLA | CHD-C4C-NC | 2.20 | 127.64 | 124.23 |
| 48 | 37 | 310 | A86 | C41-C32-C31 | -2.20 | 108.50 | 110.47 |
| 47 | 35 | 304 | KC1 | O1D-CGD-CBD | -2.20 | 120.18 | 124.52 |
| 47 | 13 | 306 | KC1 | CHB-C4A-NA | 2.20 | 127.64 | 124.23 |
| 37 | c | 506 | CLA | C4-C3-C5 | 2.20 | 119.05 | 115.23 |
| 37 | 32 | 205 | CLA | CHB-C4A-NA | 2.20 | 127.57 | 124.40 |
| 37 | 18 | 206 | CLA | CMC-C2C-C1C | 2.20 | 128.47 | 125.03 |
| 37 | 14 | 301 | CLA | CBC-CAC-C3C | -2.20 | 106.46 | 112.42 |
| 48 | 18 | 214 | A86 | C40-C32-C31 | -2.20 | 108.50 | 110.47 |
| 48 | 35 | 319 | A86 | C3-C4-C5 | -2.20 | 119.02 | 123.52 |
| 37 | 18 | 204 | CLA | CHB-C4A-NA | 2.20 | 127.57 | 124.40 |
| 48 | 18 | 215 | A86 | C29-C30-C31 | -2.20 | 175.07 | 177.66 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | c | 506 | CLA | CHC-C1C-NC | 2.20 | 127.62 | 124.31 |
| 37 | C | 510 | CLA | CMC-C2C-C1C | 2.20 | 128.47 | 125.03 |
| 37 | 41 | 205 | CLA | CED-O2D-CGD | 2.20 | 120.90 | 115.92 |
| 47 | 33 | 309 | KC1 | CHB-C1B-C2B | -2.20 | 120.92 | 125.49 |
| 37 | 32 | 211 | CLA | CHD-C4C-NC | 2.20 | 127.64 | 124.23 |
| 37 | c | 510 | CLA | CAC-C3C-C4C | 2.20 | 127.65 | 124.79 |
| 48 | 37 | 311 | A86 | C10-C9-C8 | -2.20 | 116.83 | 123.20 |
| 37 | c | 511 | CLA | OBD-CAD-C3D | -2.20 | 123.28 | 128.42 |
| 37 | 41 | 202 | CLA | CAA-C2A-C3A | -2.20 | 107.06 | 113.00 |
| 47 | 38 | 205 | KC1 | CMC-C2C-C1C | 2.20 | 128.47 | 125.03 |
| 48 | 13 | 315 | A86 | C7-C6-C5 | -2.20 | 119.26 | 122.82 |
| 37 | 21 | 205 | CLA | CHA-C1A-NA | -2.20 | 121.42 | 126.39 |
| 47 | 18 | 207 | KC1 | CHB-C4A-NA | 2.20 | 127.64 | 124.23 |
| 37 | 19 | 307 | CLA | CBC-CAC-C3C | -2.20 | 106.47 | 112.42 |
| 44 | j | 101 | DGD | O5D-C6D-C5D | -2.20 | 104.47 | 109.42 |
| 48 | 17 | 314 | A86 | C23-C16-C22 | -2.20 | 104.18 | 107.37 |
| 48 | 18 | 214 | A86 | C34-O4-C38 | -2.20 | 113.97 | 117.85 |
| 37 | 31 | 302 | CLA | CHA-C1A-NA | -2.20 | 121.42 | 126.39 |
| 37 | 33 | 303 | CLA | C1-O2A-CGA | 2.20 | 121.97 | 116.65 |
| 47 | 33 | 309 | KC1 | O1D-CGD-CBD | -2.20 | 120.19 | 124.52 |
| 41 | b | 520 | LMG | C38-C37-C36 | -2.20 | 103.27 | 114.37 |
| 48 | 13 | 313 | A86 | C21-C20-C15 | -2.19 | 116.27 | 123.35 |
| 50 | 20 | 312 | DD6 | C3-C4-C5 | -2.19 | 119.03 | 123.52 |
| 43 | 17 | 316 | LHG | C18-C17-C16 | -2.19 | 103.28 | 114.37 |
| 47 | 38 | 205 | KC1 | C3D-C2D-C1D | -2.19 | 99.39 | 106.40 |
| 41 | D | 412 | LMG | C38-C37-C36 | -2.19 | 103.28 | 114.37 |
| 37 | 21 | 202 | CLA | CAA-C2A-C3A | -2.19 | 107.07 | 113.00 |
| 37 | 21 | 210 | CLA | CMC-C2C-C1C | 2.19 | 128.46 | 125.03 |
| 44 | J | 101 | DGD | O5D-C6D-C5D | -2.19 | 104.48 | 109.42 |
| 41 | 37 | 316 | LMG | O7-C10-O9 | -2.19 | 118.58 | 123.70 |
| 47 | 34 | 304 | KC1 | CHB-C4A-NA | 2.19 | 127.63 | 124.23 |
| 47 | 40 | 206 | KC1 | CHB-C4A-NA | 2.19 | 127.63 | 124.23 |
| 48 | 36 | 311 | A86 | C3-C4-C5 | -2.19 | 119.03 | 123.52 |
| 37 | 12 | 210 | CLA | CBC-CAC-C3C | -2.19 | 106.48 | 112.42 |
| 41 | 16 | 316 | LMG | O3-C3-C2 | -2.19 | 105.21 | 110.38 |
| 47 | 17 | 306 | KC1 | CHD-C4C-NC | 2.19 | 127.61 | 124.31 |
| 43 | 37 | 315 | LHG | C18-C17-C16 | -2.19 | 103.29 | 114.37 |
| 37 | 37 | 303 | CLA | O2A-CGA-CBA | 2.19 | 118.52 | 111.83 |
| 37 | 21 | 206 | CLA | C4-C3-C5 | 2.19 | 119.03 | 115.23 |
| 48 | 12 | 213 | A86 | C8-C6-C5 | -2.19 | 115.56 | 119.01 |
| 37 | 21 | 204 | CLA | CGD-CBD-CAD | -2.19 | 103.76 | 110.85 |
| 37 | 33 | 303 | CLA | C1-C2-C3 | -2.19 | 122.61 | 126.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 45 | D | 404 | PL9 | O2-C1-C2 | -2.19 | 116.85 | 121.83 |
| 41 | 36 | 314 | LMG | O3-C3-C2 | -2.19 | 105.21 | 110.38 |
| 47 | 17 | 303 | KC1 | CMB-C2B-C1B | 2.19 | 128.58 | 124.73 |
| 50 | 40 | 214 | DD6 | C3-C4-C5 | -2.19 | 119.04 | 123.52 |
| 48 | 33 | 312 | A86 | C-C1-C2 | -2.19 | 119.27 | 122.82 |
| 37 | C | 506 | CLA | C4-C3-C5 | 2.19 | 119.03 | 115.23 |
| 37 | 41 | 205 | CLA | CHA-C1A-NA | -2.19 | 121.44 | 126.39 |
| 37 | 18 | 204 | CLA | O2A-CGA-CBA | 2.19 | 118.51 | 111.83 |
| 48 | 17 | 310 | A86 | C12-C11-C13 | 2.19 | 119.55 | 116.00 |
| 48 | 31 | 315 | A86 | C8-C6-C5 | -2.19 | 115.57 | 119.01 |
| 37 | 11 | 301 | CLA | CHA-C1A-NA | -2.19 | 121.44 | 126.39 |
| 47 | 20 | 304 | KC1 | O1D-CGD-CBD | -2.19 | 120.20 | 124.52 |
| 47 | 38 | 207 | KC1 | CBC-CAC-C3C | -2.19 | 106.49 | 112.42 |
| 41 | 11 | 316 | LMG | O2-C2-C1 | -2.19 | 104.86 | 110.08 |
| 48 | 38 | 214 | A86 | C25-C24-C1 | -2.19 | 120.37 | 126.36 |
| 47 | 11 | 304 | KC1 | CMB-C2B-C1B | 2.19 | 128.58 | 124.73 |
| 46 | v | 201 | HEM | CHD-C4C-C3C | 2.19 | 128.90 | 125.21 |
| 37 | 12 | 212 | CLA | CHB-C1B-C2B | -2.19 | 121.08 | 127.43 |
| 47 | 40 | 206 | KC1 | O2D-CGD-O1D | -2.19 | 119.59 | 123.85 |
| 48 | 17 | 310 | A86 | C3-C4-C5 | -2.19 | 119.05 | 123.52 |
| 48 | 35 | 315 | A86 | C19-C18-C17 | -2.19 | 106.70 | 110.79 |
| 47 | 40 | 207 | KC1 | O2A-CGA-O1A | -2.19 | 118.25 | 122.70 |
| 37 | z | 101 | CLA | CAC-C3C-C4C | 2.19 | 127.63 | 124.79 |
| 47 | 39 | 308 | KC1 | CAC-C3C-C4C | 2.19 | 127.63 | 124.79 |
| 37 | A | 403 | CLA | CMC-C2C-C1C | 2.18 | 128.45 | 125.03 |
| 48 | 17 | 310 | A86 | C7-C6-C8 | 2.18 | 121.42 | 118.09 |
| 48 | 11 | 315 | A86 | C8-C6-C5 | -2.18 | 115.57 | 119.01 |
| 48 | 38 | 214 | A86 | C34-O4-C38 | -2.18 | 113.99 | 117.85 |
| 48 | 13 | 312 | A86 | C10-C9-C8 | -2.18 | 116.87 | 123.20 |
| 48 | 33 | 312 | A86 | C10-C9-C8 | -2.18 | 116.87 | 123.20 |
| 37 | 32 | 206 | CLA | CHA-C1A-NA | -2.18 | 121.44 | 126.39 |
| 37 | 19 | 301 | CLA | CBC-CAC-C3C | -2.18 | 106.50 | 112.42 |
| 37 | 32 | 211 | CLA | CBC-CAC-C3C | -2.18 | 106.50 | 112.42 |
| 48 | 32 | 218 | A86 | C9-C8-C6 | -2.18 | 120.38 | 126.36 |
| 47 | 40 | 204 | KC1 | CHB-C1B-C2B | -2.18 | 120.94 | 125.49 |
| 37 | b | 510 | CLA | CHB-C4A-NA | 2.18 | 127.55 | 124.40 |
| 37 | C | 511 | CLA | CBC-CAC-C3C | -2.18 | 106.50 | 112.42 |
| 47 | 12 | 206 | KC1 | CAB-C3B-C4B | 2.18 | 130.03 | 124.82 |
| 40 | a | 409 | SQD | O8-S-C6 | 2.18 | 110.19 | 105.97 |
| 48 | 17 | 315 | A86 | C4-C3-C2 | -2.18 | 119.05 | 123.52 |
| 41 | d | 409 | LMG | C38-C37-C36 | -2.18 | 103.34 | 114.37 |
| 37 | 17 | 307 | CLA | CBA-CAA-C2A | -2.18 | 107.30 | 113.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 20 | 301 | CLA | C4B-C3B-C2B | -2.18 | 104.59 | 107.30 |
| 37 | b | 513 | CLA | O2D-CGD-O1D | -2.18 | 119.60 | 123.85 |
| 48 | 12 | 213 | A86 | C36-C31-C32 | -2.18 | 117.53 | 119.70 |
| 47 | 33 | 302 | KC1 | CAB-C3B-C4B | 2.18 | 130.03 | 124.82 |
| 48 | 32 | 214 | A86 | C8-C6-C5 | -2.18 | 115.58 | 119.01 |
| 48 | 37 | 309 | A86 | C3-C4-C5 | -2.18 | 119.06 | 123.52 |
| 41 | 12 | 201 | LMG | O2-C2-C1 | -2.18 | 104.88 | 110.08 |
| 47 | 12 | 208 | KC1 | CHB-C4A-NA | 2.18 | 127.61 | 124.23 |
| 37 | 40 | 210 | CLA | CHA-C1A-NA | -2.18 | 121.46 | 126.39 |
| 37 | B | 513 | CLA | O2D-CGD-O1D | -2.18 | 119.61 | 123.85 |
| 37 | c | 510 | CLA | CMC-C2C-C1C | 2.18 | 128.44 | 125.03 |
| 41 | B | 521 | LMG | C38-C37-C36 | -2.18 | 103.36 | 114.37 |
| 37 | 15 | 303 | CLA | CHB-C4A-NA | 2.18 | 127.54 | 124.40 |
| 37 | 21 | 210 | CLA | CHB-C4A-NA | 2.18 | 127.54 | 124.40 |
| 39 | A | 406 | BCR | C27-C26-C25 | 2.18 | 125.65 | 122.70 |
| 37 | b | 505 | CLA | CBC-CAC-C3C | -2.18 | 106.51 | 112.42 |
| 47 | 17 | 303 | KC1 | CMC-C2C-C1C | 2.18 | 128.44 | 125.03 |
| 37 | B | 505 | CLA | CBC-CAC-C3C | -2.18 | 106.52 | 112.42 |
| 39 | B | 517 | BCR | C16-C15-C14 | -2.18 | 119.06 | 123.52 |
| 37 | C | 505 | CLA | C1-O2A-CGA | 2.18 | 121.92 | 116.65 |
| 37 | a | 403 | CLA | CMA-C3A-C2A | -2.18 | 105.57 | 113.98 |
| 40 | A | 407 | SQD | O8-S-C6 | 2.18 | 110.17 | 105.97 |
| 47 | 13 | 309 | KC1 | CHB-C1B-C2B | -2.18 | 120.96 | 125.49 |
| 48 | 18 | 215 | A86 | C8-C6-C5 | 2.18 | 122.43 | 119.01 |
| 37 | 12 | 205 | CLA | CHA-C1A-NA | -2.18 | 121.47 | 126.39 |
| 37 | C | 510 | CLA | CAC-C3C-C4C | 2.18 | 127.62 | 124.79 |
| 37 | C | 509 | CLA | C12-C11-C10 | -2.18 | 103.53 | 113.28 |
| 39 | K | 101 | BCR | C27-C26-C25 | 2.17 | 125.64 | 122.70 |
| 39 | C | 515 | BCR | C2-C1-C6 | 2.17 | 113.60 | 110.44 |
| 37 | 33 | 308 | CLA | O2A-CGA-O1A | -2.17 | 118.19 | 123.63 |
| 37 | 35 | 308 | CLA | C4-C3-C5 | 2.17 | 119.00 | 115.23 |
| 37 | 13 | 308 | CLA | O2A-CGA-O1A | -2.17 | 118.19 | 123.63 |
| 48 | 12 | 217 | A86 | C9-C8-C6 | -2.17 | 120.40 | 126.36 |
| 44 | j | 101 | DGD | CBB-CAB-C9B | -2.17 | 103.38 | 114.37 |
| 44 | J | 101 | DGD | CBB-CAB-C9B | -2.17 | 103.38 | 114.37 |
| 37 | 32 | 213 | CLA | CHB-C1B-C2B | -2.17 | 121.12 | 127.43 |
| 37 | 41 | 210 | CLA | CMC-C2C-C1C | 2.17 | 128.43 | 125.03 |
| 47 | 31 | 305 | KC1 | CMB-C2B-C1B | 2.17 | 128.55 | 124.73 |
| 37 | 18 | 202 | CLA | C4-C3-C5 | 2.17 | 119.00 | 115.23 |
| 37 | C | 506 | CLA | CHC-C1C-NC | 2.17 | 127.58 | 124.31 |
| 39 | b | 517 | BCR | C16-C15-C14 | -2.17 | 119.07 | 123.52 |
| 37 | 39 | 301 | CLA | CBC-CAC-C3C | -2.17 | 106.53 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 13 | 307 | CLA | OBD-CAD-C3D | -2.17 | 123.34 | 128.42 |
| 37 | 32 | 208 | CLA | O2D-CGD-O1D | -2.17 | 119.62 | 123.85 |
| 47 | 15 | 309 | KC1 | O1D-CGD-CBD | -2.17 | 120.23 | 124.52 |
| 47 | 40 | 206 | KC1 | O1D-CGD-CBD | -2.17 | 120.23 | 124.52 |
| 37 | c | 511 | CLA | CBC-CAC-C3C | -2.17 | 106.53 | 112.42 |
| 37 | 15 | 308 | CLA | CHB-C4A-NA | 2.17 | 127.53 | 124.40 |
| 37 | 13 | 310 | CLA | O1D-CGD-CBD | -2.17 | 120.23 | 124.52 |
| 48 | 37 | 309 | A86 | C7-C6-C8 | 2.17 | 121.41 | 118.09 |
| 37 | 41 | 206 | CLA | C4-C3-C5 | 2.17 | 119.00 | 115.23 |
| 47 | 20 | 304 | KC1 | O2D-CGD-O1D | -2.17 | 119.62 | 123.85 |
| 37 | c | 509 | CLA | C12-C11-C10 | -2.17 | 103.55 | 113.28 |
| 37 | A | 403 | CLA | CMA-C3A-C2A | -2.17 | 105.59 | 113.98 |
| 37 | 41 | 209 | CLA | CMC-C2C-C1C | 2.17 | 128.43 | 125.03 |
| 40 | B | 522 | SQD | O47-C7-O49 | -2.17 | 118.63 | 123.70 |
| 37 | 32 | 213 | CLA | O1D-CGD-CBD | -2.17 | 120.24 | 124.52 |
| 37 | 20 | 303 | CLA | CED-O2D-CGD | 2.17 | 120.84 | 115.92 |
| 47 | 20 | 305 | KC1 | O2A-CGA-O1A | -2.17 | 118.28 | 122.70 |
| 48 | 12 | 216 | A86 | C8-C6-C5 | -2.17 | 115.60 | 119.01 |
| 37 | 20 | 308 | CLA | CHA-C1A-NA | -2.17 | 121.48 | 126.39 |
| 47 | 16 | 304 | KC1 | O1D-CGD-CBD | -2.17 | 120.24 | 124.52 |
| 48 | 32 | 214 | A86 | C36-C31-C32 | -2.17 | 117.55 | 119.70 |
| 37 | Z | 102 | CLA | CHB-C4A-NA | 2.17 | 127.53 | 124.40 |
| 48 | 16 | 311 | A86 | C3-C4-C5 | -2.17 | 119.08 | 123.52 |
| 37 | C | 512 | CLA | CHA-C1A-NA | -2.17 | 121.48 | 126.39 |
| 40 | 16 | 315 | SQD | C1-O5-C5 | 2.17 | 117.95 | 113.72 |
| 37 | B | 510 | CLA | CHB-C4A-NA | 2.17 | 127.53 | 124.40 |
| 37 | 18 | 201 | CLA | CHB-C4A-NA | 2.17 | 127.53 | 124.40 |
| 41 | 17 | 317 | LMG | O3-C3-C2 | -2.17 | 105.27 | 110.38 |
| 47 | 32 | 209 | KC1 | O1D-CGD-CBD | -2.17 | 120.25 | 124.52 |
| 37 | 33 | 308 | CLA | O2D-CGD-O1D | -2.17 | 119.63 | 123.85 |
| 47 | 39 | 308 | KC1 | CHB-C4A-NA | 2.17 | 127.59 | 124.23 |
| 37 | c | 512 | CLA | CHA-C1A-NA | -2.17 | 121.49 | 126.39 |
| 37 | 33 | 301 | CLA | CHA-C1A-NA | -2.17 | 121.49 | 126.39 |
| 47 | 33 | 309 | KC1 | CMC-C2C-C1C | 2.16 | 128.42 | 125.03 |
| 48 | 33 | 313 | A86 | C25-C24-C1 | -2.16 | 120.43 | 126.36 |
| 37 | 20 | 307 | CLA | CHB-C4A-NA | 2.16 | 127.52 | 124.40 |
| 37 | 18 | 209 | CLA | CHB-C4A-NA | 2.16 | 127.52 | 124.40 |
| 37 | 21 | 209 | CLA | CMC-C2C-C1C | 2.16 | 128.41 | 125.03 |
| 37 | 15 | 307 | CLA | O2A-CGA-CBA | 2.16 | 118.43 | 111.83 |
| 48 | 12 | 220 | A86 | C40-C32-C31 | -2.16 | 108.54 | 110.47 |
| 37 | 38 | 203 | CLA | CBC-CAC-C3C | -2.16 | 106.56 | 112.42 |
| 37 | D | 402 | CLA | C1-C2-C3 | -2.16 | 122.65 | 126.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 13 | 314 | A86 | C3-C4-C5 | -2.16 | 119.09 | 123.52 |
| 48 | 32 | 221 | A86 | C40-C32-C31 | -2.16 | 108.54 | 110.47 |
| 37 | b | 511 | CLA | CHA-C1A-NA | -2.16 | 121.50 | 126.39 |
| 37 | 35 | 303 | CLA | CHB-C4A-NA | 2.16 | 127.52 | 124.40 |
| 47 | 31 | 305 | KC1 | CMC-C2C-C1C | 2.16 | 128.41 | 125.03 |
| 47 | 12 | 208 | KC1 | O1D-CGD-CBD | -2.16 | 120.25 | 124.52 |
| 43 | D | 411 | LHG | C27-C26-C25 | -2.16 | 103.44 | 114.37 |
| 40 | 40 | 202 | SQD | C1-O5-C5 | 2.16 | 117.94 | 113.72 |
| 37 | a | 404 | CLA | C1-O2A-CGA | 2.16 | 121.88 | 116.65 |
| 37 | 40 | 205 | CLA | CED-O2D-CGD | 2.16 | 120.82 | 115.92 |
| 37 | 37 | 303 | CLA | CHB-C1B-C2B | -2.16 | 121.16 | 127.43 |
| 47 | 15 | 302 | KC1 | CMC-C2C-C1C | 2.16 | 128.41 | 125.03 |
| 51 | 39 | 315 | LMU | C2'-C3'-C4' | 2.16 | 114.58 | 109.68 |
| 37 | 33 | 307 | CLA | OBD-CAD-C3D | -2.16 | 123.37 | 128.42 |
| 48 | 40 | 211 | A86 | C9-C8-C6 | -2.16 | 120.44 | 126.36 |
| 47 | 33 | 302 | KC1 | C3D-C2D-C1D | -2.16 | 99.50 | 106.40 |
| 47 | 31 | 305 | KC1 | CAA-C2A-C1A | -2.16 | 115.18 | 124.64 |
| 48 | 13 | 313 | A86 | C25-C24-C1 | -2.16 | 120.44 | 126.36 |
| 48 | 14 | 315 | A86 | C8-C6-C5 | -2.16 | 115.61 | 119.01 |
| 47 | 35 | 304 | KC1 | CHB-C4A-NA | 2.16 | 127.58 | 124.23 |
| 39 | a | 408 | BCR | C27-C26-C25 | 2.16 | 125.62 | 122.70 |
| 37 | a | 403 | CLA | CMC-C2C-C1C | 2.16 | 128.41 | 125.03 |
| 48 | 31 | 313 | A86 | C-C1-C24 | 2.16 | 121.39 | 118.09 |
| 37 | B | 503 | CLA | O2A-CGA-O1A | -2.16 | 118.23 | 123.63 |
| 47 | 36 | 305 | KC1 | C3D-C2D-C1D | -2.16 | 99.51 | 106.40 |
| 37 | D | 405 | CLA | C2A-C1A-CHA | -2.16 | 120.12 | 123.87 |
| 37 | 34 | 301 | CLA | C4-C3-C5 | 2.16 | 118.97 | 115.23 |
| 47 | 14 | 309 | KC1 | CGD-CBD-CAD | -2.16 | 103.87 | 110.85 |
| 47 | 16 | 308 | KC1 | C3D-C2D-C1D | -2.16 | 99.51 | 106.40 |
| 37 | 17 | 304 | CLA | CHB-C1B-C2B | -2.16 | 121.17 | 127.43 |
| 37 | 19 | 307 | CLA | CMC-C2C-C1C | 2.16 | 128.40 | 125.03 |
| 43 | a | 412 | LHG | C27-C26-C25 | -2.16 | 103.47 | 114.37 |
| 47 | 17 | 306 | KC1 | C3D-C2D-C1D | -2.16 | 99.52 | 106.40 |
| 47 | 41 | 203 | KC1 | C3D-C2D-C1D | -2.16 | 99.52 | 106.40 |
| 48 | 40 | 213 | A86 | C3-C4-C5 | -2.16 | 119.11 | 123.52 |
| 41 | 31 | 317 | LMG | O1-C7-C8 | -2.16 | 105.58 | 110.82 |
| 37 | 34 | 308 | CLA | CMA-C3A-C2A | -2.16 | 105.65 | 113.98 |
| 37 | D | 401 | CLA | CAC-C3C-C2C | 2.15 | 131.52 | 127.56 |
| 37 | 14 | 303 | CLA | C4-C3-C5 | 2.15 | 118.97 | 115.23 |
| 37 | 39 | 301 | CLA | O2A-CGA-CBA | 2.15 | 118.40 | 111.83 |
| 40 | 17 | 301 | SQD | O8-S-C6 | 2.15 | 110.13 | 105.97 |
| 47 | 36 | 304 | KC1 | O1D-CGD-CBD | -2.15 | 120.27 | 124.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 37 | 305 | KC1 | C3D-C2D-C1D | -2.15 | 99.52 | 106.40 |
| 48 | 33 | 314 | A86 | C3-C4-C5 | -2.15 | 119.11 | 123.52 |
| 48 | 20 | 309 | A86 | C9-C8-C6 | -2.15 | 120.46 | 126.36 |
| 47 | 13 | 309 | KC1 | O1D-CGD-CBD | -2.15 | 120.27 | 124.52 |
| 47 | 18 | 205 | KC1 | O1D-CGD-CBD | -2.15 | 120.27 | 124.52 |
| 47 | 40 | 207 | KC1 | CAA-CBA-CGA | -2.15 | 116.10 | 127.05 |
| 37 | 14 | 301 | CLA | C4-C3-C5 | 2.15 | 118.97 | 115.23 |
| 47 | 20 | 305 | KC1 | CAA-CBA-CGA | -2.15 | 116.10 | 127.05 |
| 37 | a | 403 | CLA | C6-C5-C3 | -2.15 | 108.22 | 113.47 |
| 47 | 11 | 304 | KC1 | CMC-C2C-C1C | 2.15 | 128.40 | 125.03 |
| 47 | 37 | 307 | KC1 | C3D-C2D-C1D | -2.15 | 99.53 | 106.40 |
| 47 | 16 | 305 | KC1 | C3D-C2D-C1D | -2.15 | 99.53 | 106.40 |
| 37 | 17 | 304 | CLA | CHA-C1A-NA | -2.15 | 121.52 | 126.39 |
| 40 | b | 521 | SQD | O47-C7-O49 | -2.15 | 118.67 | 123.70 |
| 37 | b | 503 | CLA | O2A-CGA-O1A | -2.15 | 118.25 | 123.63 |
| 37 | 36 | 309 | CLA | CAA-C2A-C1A | -2.15 | 104.92 | 111.97 |
| 37 | c | 502 | CLA | CHA-C1A-NA | -2.15 | 121.52 | 126.39 |
| 37 | A | 403 | CLA | C6-C5-C3 | -2.15 | 108.23 | 113.47 |
| 37 | 12 | 212 | CLA | O1D-CGD-CBD | -2.15 | 120.27 | 124.52 |
| 37 | 14 | 303 | CLA | O2A-CGA-O1A | -2.15 | 118.25 | 123.63 |
| 37 | 20 | 303 | CLA | O2D-CGD-O1D | -2.15 | 119.66 | 123.85 |
| 47 | 36 | 304 | KC1 | C3D-C2D-C1D | -2.15 | 99.53 | 106.40 |
| 47 | 13 | 309 | KC1 | CMC-C2C-C1C | 2.15 | 128.40 | 125.03 |
| 43 | D | 411 | LHG | C11-C10-C9 | -2.15 | 103.49 | 114.37 |
| 37 | 13 | 303 | CLA | C1-C2-C3 | -2.15 | 122.67 | 126.20 |
| 37 | 19 | 301 | CLA | O2A-CGA-CBA | 2.15 | 118.39 | 111.83 |
| 47 | 36 | 302 | KC1 | C3D-C2D-C1D | -2.15 | 99.53 | 106.40 |
| 47 | 13 | 302 | KC1 | C3D-C2D-C1D | -2.15 | 99.53 | 106.40 |
| 39 | c | 515 | BCR | C2-C1-C6 | 2.15 | 113.56 | 110.44 |
| 47 | 34 | 309 | KC1 | CGD-CBD-CAD | -2.15 | 103.88 | 110.85 |
| 48 | 33 | 315 | A86 | C7-C6-C5 | -2.15 | 119.33 | 122.82 |
| 48 | 32 | 218 | A86 | C26-C25-C24 | -2.15 | 116.97 | 123.20 |
| 48 | 36 | 311 | A86 | C23-C16-C22 | -2.15 | 104.25 | 107.37 |
| 37 | 12 | 203 | CLA | CHA-C1A-NA | -2.15 | 121.52 | 126.39 |
| 48 | 37 | 313 | A86 | C23-C16-C22 | -2.15 | 104.25 | 107.37 |
| 44 | C | 516 | DGD | O2D-C2D-C1D | -2.15 | 104.95 | 110.08 |
| 43 | a | 412 | LHG | C11-C10-C9 | -2.15 | 103.50 | 114.37 |
| 44 | C | 517 | DGD | CAB-C9B-C8B | -2.15 | 103.50 | 114.37 |
| 37 | B | 516 | CLA | C4-C3-C2 | -2.15 | 118.11 | 123.63 |
| 37 | 13 | 301 | CLA | CHA-C1A-NA | -2.15 | 121.53 | 126.39 |
| 47 | 12 | 211 | KC1 | CHB-C1B-C2B | -2.15 | 121.02 | 125.49 |
| 47 | 35 | 309 | KC1 | CHB-C1B-C2B | -2.15 | 121.02 | 125.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 21 | 203 | KC1 | C3D-C2D-C1D | -2.15 | 99.54 | 106.40 |
| 48 | 39 | 311 | A86 | C23-C16-C22 | -2.15 | 104.25 | 107.37 |
| 48 | 38 | 213 | A86 | C12-C11-C13 | 2.15 | 119.48 | 116.00 |
| 37 | 41 | 204 | CLA | C1-O2A-CGA | 2.15 | 121.85 | 116.65 |
| 48 | 12 | 217 | A86 | C26-C25-C24 | -2.15 | 116.98 | 123.20 |
| 37 | Z | 102 | CLA | C2A-C3A-C4A | -2.15 | 98.40 | 101.87 |
| 47 | 16 | 304 | KC1 | C3D-C2D-C1D | -2.15 | 99.54 | 106.40 |
| 41 | 37 | 316 | LMG | O3-C3-C2 | -2.15 | 105.32 | 110.38 |
| 47 | 16 | 302 | KC1 | C3D-C2D-C1D | -2.15 | 99.54 | 106.40 |
| 37 | c | 505 | CLA | C1-O2A-CGA | 2.15 | 121.85 | 116.65 |
| 48 | 20 | 311 | A86 | C3-C4-C5 | -2.15 | 119.13 | 123.52 |
| 37 | D | 401 | CLA | C1-O2A-CGA | 2.15 | 121.84 | 116.65 |
| 48 | 14 | 316 | A86 | C23-C16-C17 | -2.15 | 105.20 | 108.97 |
| 37 | B | 510 | CLA | CMB-C2B-C1B | 2.15 | 128.69 | 125.42 |
| 47 | 17 | 306 | KC1 | CHC-C1C-NC | 2.15 | 127.56 | 124.23 |
| 47 | 37 | 305 | KC1 | CHC-C1C-NC | 2.15 | 127.56 | 124.23 |
| 37 | 34 | 303 | CLA | O2A-CGA-O1A | -2.15 | 118.26 | 123.63 |
| 37 | a | 404 | CLA | CAC-C3C-C2C | 2.15 | 131.50 | 127.56 |
| 37 | z | 102 | CLA | CHB-C4A-NA | 2.14 | 127.50 | 124.40 |
| 37 | 13 | 310 | CLA | CHB-C4A-NA | 2.14 | 127.50 | 124.40 |
| 37 | 39 | 302 | CLA | CHB-C4A-NA | 2.14 | 127.50 | 124.40 |
| 47 | 14 | 304 | KC1 | C3D-C2D-C1D | -2.14 | 99.55 | 106.40 |
| 37 | 19 | 302 | CLA | CHB-C4A-NA | 2.14 | 127.49 | 124.40 |
| 44 | c | 517 | DGD | CAB-C9B-C8B | -2.14 | 103.54 | 114.37 |
| 48 | 35 | 316 | A86 | C10-C9-C8 | -2.14 | 116.99 | 123.20 |
| 48 | 18 | 215 | A86 | C7-C6-C5 | -2.14 | 119.34 | 122.82 |
| 41 | 11 | 317 | LMG | O1-C7-C8 | -2.14 | 105.61 | 110.82 |
| 37 | 16 | 306 | CLA | CBC-CAC-C3C | -2.14 | 106.61 | 112.42 |
| 37 | 38 | 201 | CLA | C1-C2-C3 | -2.14 | 122.69 | 126.20 |
| 37 | 16 | 309 | CLA | CAA-C2A-C1A | -2.14 | 104.96 | 111.97 |
| 37 | 14 | 308 | CLA | CMA-C3A-C2A | -2.14 | 105.70 | 113.98 |
| 37 | 40 | 203 | CLA | C4B-C3B-C2B | -2.14 | 104.64 | 107.30 |
| 37 | B | 504 | CLA | CHB-C4A-NA | 2.14 | 127.49 | 124.40 |
| 37 | B | 507 | CLA | O1D-CGD-CBD | -2.14 | 120.30 | 124.52 |
| 47 | 17 | 308 | KC1 | C3D-C2D-C1D | -2.14 | 99.56 | 106.40 |
| 48 | 37 | 310 | A86 | C40-C32-C31 | -2.14 | 108.56 | 110.47 |
| 37 | 12 | 207 | CLA | CMA-C3A-C4A | -2.14 | 106.02 | 111.77 |
| 37 | 34 | 303 | CLA | O1D-CGD-CBD | -2.14 | 120.30 | 124.52 |
| 37 | 31 | 301 | CLA | CMC-C2C-C1C | 2.14 | 128.38 | 125.03 |
| 40 | 36 | 315 | SQD | O8-S-C6 | 2.14 | 110.11 | 105.97 |
| 48 | 36 | 310 | A86 | C19-C18-C17 | -2.14 | 106.79 | 110.79 |
| 44 | c | 516 | DGD | O2D-C2D-C1D | -2.14 | 104.97 | 110.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 18 | 203 | CLA | CMB-C2B-C1B | 2.14 | 128.68 | 125.42 |
| 37 | 34 | 303 | CLA | C4-C3-C5 | 2.14 | 118.94 | 115.23 |
| 37 | B | 511 | CLA | CHA-C1A-NA | -2.14 | 121.55 | 126.39 |
| 37 | 36 | 301 | CLA | CED-O2D-CGD | 2.14 | 120.77 | 115.92 |
| 47 | 37 | 302 | KC1 | CHC-C4B-C3B | -2.14 | 121.60 | 125.21 |
| 37 | 35 | 307 | CLA | C4-C3-C5 | 2.14 | 118.94 | 115.23 |
| 37 | z | 102 | CLA | C2A-C3A-C4A | -2.14 | 98.41 | 101.87 |
| 48 | 34 | 315 | A86 | C8-C6-C5 | -2.14 | 115.65 | 119.01 |
| 39 | 0 | 101 | BCR | C27-C26-C25 | 2.14 | 125.59 | 122.70 |
| 48 | 13 | 312 | A86 | C-C1-C24 | 2.14 | 121.35 | 118.09 |
| 39 | C | 514 | BCR | C16-C15-C14 | -2.14 | 119.15 | 123.52 |
| 37 | d | 403 | CLA | C2A-C1A-CHA | -2.14 | 120.16 | 123.87 |
| 48 | 17 | 320 | A86 | C22-C16-C17 | -2.14 | 105.21 | 108.97 |
| 47 | 37 | 302 | KC1 | C3D-C2D-C1D | -2.14 | 99.58 | 106.40 |
| 43 | 37 | 315 | LHG | C11-C10-C9 | -2.14 | 103.57 | 114.37 |
| 37 | 38 | 202 | CLA | CHB-C1B-C2B | -2.14 | 121.23 | 127.43 |
| 37 | 13 | 308 | CLA | O2D-CGD-O1D | -2.14 | 119.69 | 123.85 |
| 37 | 19 | 310 | CLA | CMC-C2C-C1C | 2.14 | 128.37 | 125.03 |
| 45 | D | 404 | PL9 | C27-C28-C29 | -2.14 | 122.74 | 127.62 |
| 47 | 17 | 303 | KC1 | C3D-C2D-C1D | -2.14 | 99.58 | 106.40 |
| 47 | 17 | 305 | KC1 | O2A-CGA-O1A | -2.14 | 118.35 | 122.70 |
| 43 | 41 | 201 | LHG | C27-C26-C25 | -2.13 | 103.58 | 114.37 |
| 48 | 37 | 314 | A86 | C4-C3-C2 | -2.13 | 119.15 | 123.52 |
| 48 | 13 | 312 | A86 | C-C1-C2 | -2.13 | 119.36 | 122.82 |
| 37 | 16 | 301 | CLA | CED-O2D-CGD | 2.13 | 120.76 | 115.92 |
| 47 | 33 | 306 | KC1 | CHB-C1B-NB | -2.13 | 121.80 | 124.80 |
| 43 | 21 | 201 | LHG | C27-C26-C25 | -2.13 | 103.58 | 114.37 |
| 37 | 35 | 308 | CLA | CAA-C2A-C3A | -2.13 | 107.23 | 113.00 |
| 46 | V | 201 | HEM | C4D-ND-C1D | 2.13 | 107.73 | 105.21 |
| 37 | W | 101 | CLA | O2A-CGA-O1A | -2.13 | 118.29 | 123.63 |
| 37 | C | 502 | CLA | CHA-C1A-NA | -2.13 | 121.56 | 126.39 |
| 37 | B | 510 | CLA | CMC-C2C-C1C | 2.13 | 128.37 | 125.03 |
| 37 | b | 509 | CLA | CAA-C2A-C3A | -2.13 | 107.24 | 113.00 |
| 47 | 35 | 304 | KC1 | C3D-C2D-C1D | -2.13 | 99.59 | 106.40 |
| 37 | 40 | 205 | CLA | O2D-CGD-O1D | -2.13 | 119.70 | 123.85 |
| 37 | 16 | 309 | CLA | CMB-C2B-C1B | 2.13 | 128.67 | 125.42 |
| 37 | 41 | 210 | CLA | O1D-CGD-CBD | -2.13 | 120.31 | 124.52 |
| 47 | 36 | 308 | KC1 | C3D-C2D-C1D | -2.13 | 99.59 | 106.40 |
| 37 | 21 | 210 | CLA | O1D-CGD-CBD | -2.13 | 120.31 | 124.52 |
| 48 | 32 | 217 | A86 | C23-C16-C22 | -2.13 | 104.27 | 107.37 |
| 47 | 35 | 302 | KC1 | C3D-C2D-C1D | -2.13 | 99.59 | 106.40 |
| 47 | 16 | 308 | KC1 | O2A-CGA-O1A | -2.13 | 118.36 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 19 | 308 | KC1 | CHB-C4A-NA | 2.13 | 127.53 | 124.23 |
| 37 | 20 | 307 | CLA | O2D-CGD-O1D | -2.13 | 119.70 | 123.85 |
| 37 | 38 | 204 | CLA | CMB-C2B-C3B | 2.13 | 131.56 | 126.55 |
| 37 | 39 | 310 | CLA | CMC-C2C-C1C | 2.13 | 128.36 | 125.03 |
| 37 | 40 | 209 | CLA | CHB-C4A-NA | 2.13 | 127.47 | 124.40 |
| 47 | 12 | 206 | KC1 | CHB-C4A-NA | 2.13 | 127.53 | 124.23 |
| 43 | D | 411 | LHG | C18-C17-C16 | -2.13 | 103.61 | 114.37 |
| 43 | a | 412 | LHG | C18-C17-C16 | -2.13 | 103.61 | 114.37 |
| 37 | 38 | 201 | CLA | CHB-C4A-NA | 2.13 | 127.47 | 124.40 |
| 47 | 38 | 207 | KC1 | CHB-C1B-NB | -2.13 | 121.81 | 124.80 |
| 43 | D | 410 | LHG | O8-C6-C5 | -2.13 | 102.26 | 108.40 |
| 37 | b | 510 | CLA | CMB-C2B-C1B | 2.13 | 128.66 | 125.42 |
| 37 | b | 516 | CLA | C4-C3-C2 | -2.13 | 118.16 | 123.63 |
| 41 | B | 521 | LMG | C40-C39-C38 | -2.13 | 103.61 | 114.37 |
| 41 | b | 520 | LMG | C40-C39-C38 | -2.13 | 103.61 | 114.37 |
| 37 | Z | 101 | CLA | CAC-C3C-C4C | 2.13 | 127.56 | 124.79 |
| 37 | 20 | 306 | CLA | CHA-C1A-NA | -2.13 | 121.57 | 126.39 |
| 48 | 34 | 316 | A86 | C23-C16-C17 | -2.13 | 105.23 | 108.97 |
| 47 | 38 | 205 | KC1 | O1D-CGD-CBD | -2.13 | 120.32 | 124.52 |
| 47 | 20 | 304 | KC1 | C3D-C2D-C1D | -2.13 | 99.61 | 106.40 |
| 51 | 19 | 315 | LMU | C2'-C3'-C4' | 2.13 | 114.51 | 109.68 |
| 37 | b | 523 | CLA | CHB-C4A-NA | 2.13 | 127.47 | 124.40 |
| 48 | 32 | 215 | A86 | C9-C10-C11 | -2.13 | 120.63 | 126.64 |
| 50 | 20 | 310 | DD6 | C9-C8-C6 | -2.13 | 120.53 | 126.36 |
| 37 | 36 | 309 | CLA | CMB-C2B-C1B | 2.13 | 128.66 | 125.42 |
| 37 | 41 | 202 | CLA | C4-C3-C5 | 2.13 | 118.92 | 115.23 |
| 37 | 11 | 303 | CLA | CHA-C1A-NA | -2.13 | 121.58 | 126.39 |
| 39 | C | 519 | BCR | C15-C14-C13 | -2.13 | 124.30 | 127.28 |
| 48 | 16 | 311 | A86 | C23-C16-C22 | -2.13 | 104.28 | 107.37 |
| 39 | A | 410 | BCR | C33-C5-C6 | -2.13 | 122.16 | 124.48 |
| 37 | 37 | 303 | CLA | CAA-C2A-C1A | 2.13 | 118.94 | 111.97 |
| 37 | 38 | 208 | CLA | O2D-CGD-O1D | -2.13 | 119.71 | 123.85 |
| 37 | 36 | 306 | CLA | CBC-CAC-C3C | -2.13 | 106.66 | 112.42 |
| 37 | 40 | 208 | CLA | CHB-C1B-C2B | -2.13 | 121.26 | 127.43 |
| 44 | c | 516 | DGD | C1E-O6E-C5E | 2.13 | 117.87 | 113.72 |
| 48 | 21 | 214 | A86 | C7-C6-C8 | 2.13 | 121.33 | 118.09 |
| 37 | 33 | 308 | CLA | CBC-CAC-C3C | -2.13 | 106.66 | 112.42 |
| 47 | 32 | 207 | KC1 | CHB-C4A-NA | 2.13 | 127.53 | 124.23 |
| 37 | 36 | 309 | CLA | CHB-C1B-C2B | -2.13 | 121.26 | 127.43 |
| 48 | 17 | 312 | A86 | C10-C9-C8 | -2.12 | 117.04 | 123.20 |
| 37 | w | 101 | CLA | O2A-CGA-O1A | -2.12 | 118.31 | 123.63 |
| 48 | 35 | 316 | A86 | C19-C18-C17 | -2.12 | 106.82 | 110.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 37 | 303 | CLA | CHA-C1A-NA | -2.12 | 121.58 | 126.39 |
| 37 | 12 | 207 | CLA | CMC-C2C-C1C | 2.12 | 128.35 | 125.03 |
| 37 | B | 509 | CLA | CAA-C2A-C3A | -2.12 | 107.26 | 113.00 |
| 48 | 33 | 312 | A86 | C-C1-C24 | 2.12 | 121.33 | 118.09 |
| 37 | 31 | 304 | CLA | CHA-C1A-NA | -2.12 | 121.58 | 126.39 |
| 48 | 38 | 214 | A86 | C8-C6-C5 | -2.12 | 115.67 | 119.01 |
| 48 | 40 | 201 | A86 | C4-C3-C2 | 2.12 | 127.86 | 123.52 |
| 37 | 32 | 208 | CLA | CMA-C3A-C4A | -2.12 | 106.06 | 111.77 |
| 48 | 35 | 312 | A86 | C4-C5-C6 | -2.12 | 124.30 | 127.28 |
| 48 | 36 | 310 | A86 | C8-C6-C5 | -2.12 | 115.67 | 119.01 |
| 37 | 13 | 307 | CLA | CMA-C3A-C4A | -2.12 | 106.07 | 111.77 |
| 37 | 33 | 307 | CLA | CMA-C3A-C4A | -2.12 | 106.07 | 111.77 |
| 43 | 17 | 316 | LHG | C11-C10-C9 | -2.12 | 103.64 | 114.37 |
| 37 | 12 | 212 | CLA | CMC-C2C-C1C | 2.12 | 128.35 | 125.03 |
| 37 | 32 | 204 | CLA | CHA-C1A-NA | -2.12 | 121.58 | 126.39 |
| 37 | 20 | 307 | CLA | O2A-CGA-CBA | 2.12 | 120.71 | 114.00 |
| 37 | 21 | 204 | CLA | C1-O2A-CGA | 2.12 | 121.79 | 116.65 |
| 47 | 18 | 205 | KC1 | CMC-C2C-C1C | 2.12 | 128.35 | 125.03 |
| 39 | c | 514 | BCR | C16-C15-C14 | -2.12 | 119.18 | 123.52 |
| 43 | D | 409 | LHG | O8-C23-O10 | -2.12 | 118.32 | 123.63 |
| 37 | 40 | 210 | CLA | CAA-C2A-C1A | 2.12 | 118.93 | 111.97 |
| 37 | 11 | 307 | CLA | CMB-C2B-C1B | 2.12 | 128.65 | 125.42 |
| 37 | 20 | 306 | CLA | CHB-C1B-C2B | -2.12 | 121.27 | 127.43 |
| 37 | 37 | 308 | CLA | C4-C3-C5 | 2.12 | 118.91 | 115.23 |
| 37 | 20 | 308 | CLA | CAA-C2A-C1A | 2.12 | 118.93 | 111.97 |
| 47 | 17 | 308 | KC1 | CHB-C1B-C2B | -2.12 | 121.07 | 125.49 |
| 37 | b | 504 | CLA | CHB-C4A-NA | 2.12 | 127.46 | 124.40 |
| 37 | 32 | 208 | CLA | CMC-C2C-C1C | 2.12 | 128.35 | 125.03 |
| 47 | 11 | 304 | KC1 | CAA-C2A-C1A | -2.12 | 115.35 | 124.64 |
| 47 | 34 | 304 | KC1 | C3D-C2D-C1D | -2.12 | 99.63 | 106.40 |
| 47 | 15 | 304 | KC1 | C3D-C2D-C1D | -2.12 | 99.63 | 106.40 |
| 48 | 17 | 312 | A86 | C-C1-C24 | 2.12 | 121.33 | 118.09 |
| 41 | 36 | 314 | LMG | O7-C10-O9 | -2.12 | 118.75 | 123.70 |
| 44 | C | 516 | DGD | C1E-O6E-C5E | 2.12 | 117.86 | 113.72 |
| 45 | d | 402 | PL9 | C27-C28-C29 | -2.12 | 122.78 | 127.62 |
| 47 | 15 | 309 | KC1 | CHB-C1B-C2B | -2.12 | 121.08 | 125.49 |
| 37 | 16 | 309 | CLA | CHB-C1B-C2B | -2.12 | 121.28 | 127.43 |
| 48 | 12 | 214 | A86 | C9-C10-C11 | -2.12 | 120.65 | 126.64 |
| 47 | 37 | 304 | KC1 | O2A-CGA-O1A | -2.12 | 118.39 | 122.70 |
| 48 | 15 | 316 | A86 | C19-C18-C17 | -2.12 | 106.83 | 110.79 |
| 45 | d | 402 | PL9 | C36-C34-C33 | -2.12 | 116.41 | 121.17 |
| 37 | C | 501 | CLA | CHB-C4A-NA | 2.12 | 127.46 | 124.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 35 | 309 | KC1 | O1D-CGD-CBD | -2.12 | 120.34 | 124.52 |
| 47 | 13 | 306 | KC1 | O2D-CGD-O1D | -2.12 | 119.73 | 123.85 |
| 47 | 12 | 211 | KC1 | C3D-C2D-C1D | -2.12 | 99.64 | 106.40 |
| 41 | 31 | 317 | LMG | O2-C2-C1 | -2.12 | 105.03 | 110.08 |
| 37 | 31 | 308 | CLA | CMB-C2B-C1B | 2.12 | 128.64 | 125.42 |
| 37 | 13 | 308 | CLA | CBC-CAC-C3C | -2.12 | 106.68 | 112.42 |
| 47 | 32 | 212 | KC1 | C3D-C2D-C1D | -2.12 | 99.64 | 106.40 |
| 37 | 34 | 307 | CLA | CMB-C2B-C3B | 2.12 | 131.53 | 126.55 |
| 39 | A | 406 | BCR | C7-C8-C9 | -2.12 | 123.11 | 126.23 |
| 37 | 38 | 201 | CLA | O2D-CGD-O1D | -2.12 | 119.73 | 123.85 |
| 47 | 33 | 306 | KC1 | O2D-CGD-O1D | -2.12 | 119.73 | 123.85 |
| 39 | h | 101 | BCR | C11-C10-C9 | -2.12 | 124.31 | 127.28 |
| 37 | 38 | 206 | CLA | CMB-C2B-C1B | 2.12 | 128.64 | 125.42 |
| 48 | 13 | 315 | A86 | O4-C38-O5 | -2.12 | 118.91 | 122.99 |
| 48 | 14 | 312 | A86 | C19-C18-C17 | 2.11 | 114.75 | 110.79 |
| 37 | 18 | 204 | CLA | CAA-C2A-C1A | 2.11 | 118.90 | 111.97 |
| 50 | 40 | 212 | DD6 | C9-C8-C6 | -2.11 | 120.57 | 126.36 |
| 48 | 16 | 310 | A86 | C19-C18-C17 | -2.11 | 106.84 | 110.79 |
| 43 | d | 407 | LHG | O8-C23-O10 | -2.11 | 118.34 | 123.63 |
| 37 | B | 524 | CLA | CHD-C1D-ND | -2.11 | 121.83 | 124.80 |
| 47 | 40 | 206 | KC1 | C3D-C2D-C1D | -2.11 | 99.65 | 106.40 |
| 37 | 40 | 209 | CLA | O2A-CGA-CBA | 2.11 | 120.68 | 114.00 |
| 47 | 15 | 302 | KC1 | C3D-C2D-C1D | -2.11 | 99.65 | 106.40 |
| 47 | 36 | 308 | KC1 | O2A-CGA-O1A | -2.11 | 118.40 | 122.70 |
| 48 | 17 | 320 | A86 | C-C1-C24 | 2.11 | 121.31 | 118.09 |
| 37 | b | 510 | CLA | CMC-C2C-C1C | 2.11 | 128.34 | 125.03 |
| 41 | d | 409 | LMG | O3-C3-C2 | -2.11 | 105.40 | 110.38 |
| 39 | c | 519 | BCR | C15-C14-C13 | -2.11 | 124.32 | 127.28 |
| 37 | 17 | 304 | CLA | CMC-C2C-C1C | 2.11 | 128.33 | 125.03 |
| 37 | a | 403 | CLA | CMB-C2B-C3B | 2.11 | 131.52 | 126.55 |
| 48 | 19 | 313 | A86 | O4-C38-O5 | -2.11 | 118.92 | 122.99 |
| 48 | 35 | 314 | A86 | C9-C8-C6 | -2.11 | 120.57 | 126.36 |
| 43 | D | 410 | LHG | C27-C26-C25 | -2.11 | 103.70 | 114.37 |
| 37 | 37 | 303 | CLA | CMC-C2C-C1C | 2.11 | 128.33 | 125.03 |
| 39 | a | 413 | BCR | C33-C5-C6 | -2.11 | 122.18 | 124.48 |
| 39 | y | 101 | BCR | C27-C26-C25 | 2.11 | 125.56 | 122.70 |
| 37 | 40 | 209 | CLA | O2D-CGD-O1D | -2.11 | 119.74 | 123.85 |
| 37 | B | 516 | CLA | CHB-C1B-C2B | -2.11 | 121.30 | 127.43 |
| 43 | d | 408 | LHG | O8-C6-C5 | -2.11 | 102.32 | 108.40 |
| 37 | b | 507 | CLA | O1D-CGD-CBD | -2.11 | 120.36 | 124.52 |
| 48 | 15 | 314 | A86 | C9-C8-C6 | -2.11 | 120.58 | 126.36 |
| 47 | 15 | 309 | KC1 | C3D-C2D-C1D | -2.11 | 99.67 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 39 | 306 | CLA | C3B-C4B-NB | 2.11 | 112.41 | 110.53 |
| 37 | 14 | 303 | CLA | O1D-CGD-CBD | -2.11 | 120.36 | 124.52 |
| 47 | 13 | 306 | KC1 | CHB-C1B-NB | -2.11 | 121.84 | 124.80 |
| 48 | 41 | 214 | A86 | C9-C10-C11 | -2.11 | 120.68 | 126.64 |
| 46 | v | 201 | HEM | C4D-ND-C1D | 2.11 | 107.70 | 105.21 |
| 41 | B | 521 | LMG | O2-C2-C1 | -2.11 | 105.05 | 110.08 |
| 37 | 14 | 308 | CLA | C4-C3-C5 | 2.11 | 118.89 | 115.23 |
| 48 | 16 | 313 | A86 | C4-C3-C2 | 2.11 | 127.83 | 123.52 |
| 37 | b | 523 | CLA | CHD-C1D-ND | -2.11 | 121.84 | 124.80 |
| 48 | 15 | 314 | A86 | C12-C11-C13 | 2.11 | 119.42 | 116.00 |
| 48 | 12 | 216 | A86 | C23-C16-C22 | -2.11 | 104.31 | 107.37 |
| 37 | B | 524 | CLA | CHB-C4A-NA | 2.11 | 127.44 | 124.40 |
| 48 | 18 | 214 | A86 | C25-C24-C1 | -2.11 | 120.59 | 126.36 |
| 37 | c | 512 | CLA | CBC-CAC-C3C | -2.11 | 106.71 | 112.42 |
| 43 | d | 408 | LHG | C27-C26-C25 | -2.11 | 103.72 | 114.37 |
| 41 | B | 520 | LMG | O2-C2-C1 | -2.11 | 105.06 | 110.08 |
| 37 | 32 | 213 | CLA | CMC-C2C-C1C | 2.11 | 128.32 | 125.03 |
| 43 | a | 412 | LHG | O8-C23-C24 | 2.11 | 118.25 | 111.83 |
| 37 | B | 510 | CLA | CHB-C1B-C2B | -2.10 | 121.32 | 127.43 |
| 37 | 39 | 306 | CLA | CHA-C1A-NA | -2.10 | 121.63 | 126.39 |
| 48 | 31 | 313 | A86 | C19-C18-C17 | -2.10 | 106.86 | 110.79 |
| 48 | 19 | 311 | A86 | C23-C16-C22 | -2.10 | 104.31 | 107.37 |
| 44 | j | 101 | DGD | O5E-C6E-C5E | -2.10 | 104.17 | 111.33 |
| 37 | 18 | 201 | CLA | CBC-CAC-C3C | -2.10 | 106.72 | 112.42 |
| 48 | 41 | 214 | A86 | C7-C6-C8 | 2.10 | 121.30 | 118.09 |
| 45 | D | 404 | PL9 | C36-C34-C33 | -2.10 | 116.45 | 121.17 |
| 47 | 35 | 309 | KC1 | C3D-C2D-C1D | -2.10 | 99.69 | 106.40 |
| 39 | c | 514 | BCR | C20-C21-C22 | -2.10 | 124.33 | 127.28 |
| 44 | C | 517 | DGD | C5B-C4B-C3B | -2.10 | 103.74 | 114.37 |
| 48 | 33 | 312 | A86 | C41-C32-C31 | -2.10 | 108.59 | 110.47 |
| 37 | 39 | 301 | CLA | CBA-CAA-C2A | 2.10 | 120.05 | 113.79 |
| 47 | 33 | 302 | KC1 | CMC-C2C-C1C | 2.10 | 128.32 | 125.03 |
| 48 | 14 | 312 | A86 | C8-C6-C5 | -2.10 | 115.70 | 119.01 |
| 37 | 18 | 211 | CLA | O1D-CGD-CBD | -2.10 | 120.37 | 124.52 |
| 39 | 5 | 101 | BCR | C27-C26-C25 | 2.10 | 125.54 | 122.70 |
| 47 | 19 | 308 | KC1 | C3D-C2D-C1D | -2.10 | 99.69 | 106.40 |
| 48 | 34 | 312 | A86 | C8-C6-C5 | -2.10 | 115.70 | 119.01 |
| 37 | c | 503 | CLA | CBC-CAC-C3C | -2.10 | 106.73 | 112.42 |
| 37 | B | 516 | CLA | CHA-C1A-NA | -2.10 | 121.64 | 126.39 |
| 37 | 19 | 306 | CLA | CHA-C1A-NA | -2.10 | 121.64 | 126.39 |
| 37 | 15 | 310 | CLA | O2A-CGA-CBA | 2.10 | 120.63 | 114.00 |
| 37 | 38 | 202 | CLA | C4-C3-C5 | 2.10 | 118.87 | 115.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 34 | 312 | A86 | C19-C18-C17 | 2.10 | 114.72 | 110.79 |
| 37 | B | 503 | CLA | CHB-C4A-NA | 2.10 | 127.43 | 124.40 |
| 37 | 33 | 308 | CLA | CHD-C4C-NC | 2.10 | 127.48 | 124.23 |
| 48 | 18 | 215 | A86 | C9-C8-C6 | -2.10 | 120.61 | 126.36 |
| 48 | 11 | 313 | A86 | C19-C18-C17 | -2.10 | 106.87 | 110.79 |
| 41 | 16 | 316 | LMG | O1-C1-C2 | -2.10 | 105.09 | 108.27 |
| 50 | 21 | 212 | DD6 | C22-C16-C15 | 2.10 | 115.71 | 110.05 |
| 37 | 21 | 202 | CLA | C4-C3-C5 | 2.10 | 118.87 | 115.23 |
| 48 | 35 | 312 | A86 | C-C1-C2 | -2.10 | 119.42 | 122.82 |
| 37 | 14 | 307 | CLA | CMB-C2B-C3B | 2.10 | 131.48 | 126.55 |
| 44 | J | 101 | DGD | C8B-C7B-C6B | -2.10 | 103.77 | 114.37 |
| 45 | D | 408 | PL9 | C40-C39-C41 | 2.10 | 118.87 | 115.23 |
| 41 | b | 520 | LMG | O2-C2-C1 | -2.10 | 105.08 | 110.08 |
| 39 | y | 101 | BCR | C33-C5-C6 | -2.10 | 122.20 | 124.48 |
| 40 | b | 521 | SQD | O48-C23-C24 | 2.10 | 118.23 | 111.83 |
| 37 | 11 | 301 | CLA | C3B-C4B-NB | 2.10 | 112.40 | 110.53 |
| 37 | 31 | 302 | CLA | C3B-C4B-NB | 2.10 | 112.40 | 110.53 |
| 37 | 40 | 208 | CLA | CHA-C1A-NA | -2.10 | 121.64 | 126.39 |
| 47 | 32 | 212 | KC1 | CHB-C1B-C2B | -2.10 | 121.13 | 125.49 |
| 44 | c | 517 | DGD | C5B-C4B-C3B | -2.10 | 103.78 | 114.37 |
| 37 | 34 | 301 | CLA | O2D-CGD-O1D | -2.10 | 119.77 | 123.85 |
| 44 | j | 101 | DGD | C8B-C7B-C6B | -2.10 | 103.78 | 114.37 |
| 37 | b | 516 | CLA | CHB-C1B-C2B | -2.10 | 121.34 | 127.43 |
| 37 | 32 | 202 | CLA | CED-O2D-CGD | 2.10 | 120.67 | 115.92 |
| 37 | 39 | 307 | CLA | CMC-C2C-C1C | 2.10 | 128.31 | 125.03 |
| 37 | b | 510 | CLA | CHB-C1B-C2B | -2.09 | 121.34 | 127.43 |
| 41 | 36 | 314 | LMG | O1-C1-C2 | -2.09 | 105.09 | 108.27 |
| 37 | 31 | 301 | CLA | CHA-C1A-NA | -2.09 | 121.65 | 126.39 |
| 48 | 15 | 316 | A86 | C8-C6-C5 | 2.09 | 122.30 | 119.01 |
| 37 | W | 102 | CLA | CHA-C1A-NA | -2.09 | 121.65 | 126.39 |
| 48 | 34 | 311 | A86 | C36-C31-C32 | -2.09 | 117.62 | 119.70 |
| 37 | 15 | 308 | CLA | C1-O2A-CGA | 2.09 | 121.72 | 116.65 |
| 37 | 39 | 307 | CLA | C3B-C4B-NB | 2.09 | 112.40 | 110.53 |
| 37 | 17 | 304 | CLA | CAA-C2A-C1A | 2.09 | 118.83 | 111.97 |
| 43 | a | 412 | LHG | C29-C28-C27 | -2.09 | 103.79 | 114.37 |
| 48 | 17 | 314 | A86 | C41-C32-C31 | -2.09 | 108.60 | 110.47 |
| 47 | 39 | 308 | KC1 | C3D-C2D-C1D | -2.09 | 99.72 | 106.40 |
| 37 | 40 | 209 | CLA | CMC-C2C-C1C | 2.09 | 128.30 | 125.03 |
| 37 | 38 | 202 | CLA | O2D-CGD-O1D | -2.09 | 119.78 | 123.85 |
| 37 | 39 | 303 | CLA | C4-C3-C5 | 2.09 | 118.86 | 115.23 |
| 48 | 14 | 312 | A86 | C9-C10-C11 | -2.09 | 120.72 | 126.64 |
| 37 | 35 | 301 | CLA | CAC-C3C-C4C | 2.09 | 127.51 | 124.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 509 | CLA | O2A-CGA-O1A | -2.09 | 118.39 | 123.63 |
| 37 | Z | 102 | CLA | CMC-C2C-C1C | 2.09 | 128.30 | 125.03 |
| 41 | D | 412 | LMG | O3-C3-C2 | -2.09 | 105.44 | 110.38 |
| 48 | 40 | 201 | A86 | C-C1-C2 | -2.09 | 119.43 | 122.82 |
| 41 | 16 | 316 | LMG | O7-C10-O9 | -2.09 | 118.81 | 123.70 |
| 37 | 35 | 310 | CLA | O2A-CGA-CBA | 2.09 | 120.61 | 114.00 |
| 37 | 19 | 306 | CLA | C3B-C4B-NB | 2.09 | 112.40 | 110.53 |
| 37 | 34 | 308 | CLA | C4-C3-C5 | 2.09 | 118.86 | 115.23 |
| 43 | D | 411 | LHG | C29-C28-C27 | -2.09 | 103.80 | 114.37 |
| 48 | 16 | 310 | A86 | C8-C6-C5 | -2.09 | 115.72 | 119.01 |
| 37 | D | 402 | CLA | CMD-C2D-C3D | -2.09 | 122.89 | 127.69 |
| 40 | 16 | 315 | SQD | O8-S-C6 | 2.09 | 110.01 | 105.97 |
| 47 | 35 | 302 | KC1 | CMC-C2C-C1C | 2.09 | 128.30 | 125.03 |
| 39 | K | 101 | BCR | C33-C5-C6 | -2.09 | 122.20 | 124.48 |
| 48 | 15 | 315 | A86 | C34-O4-C38 | -2.09 | 114.15 | 117.85 |
| 48 | 15 | 316 | A86 | C-C1-C24 | 2.09 | 121.28 | 118.09 |
| 47 | 13 | 304 | KC1 | O1D-CGD-CBD | -2.09 | 120.40 | 124.52 |
| 45 | D | 408 | PL9 | C50-C49-C48 | -2.09 | 116.38 | 122.66 |
| 41 | b | 519 | LMG | O2-C2-C1 | -2.09 | 105.10 | 110.08 |
| 48 | 33 | 314 | A86 | C22-C16-C17 | -2.09 | 105.30 | 108.97 |
| 44 | J | 101 | DGD | O2D-C2D-C1D | -2.09 | 105.10 | 110.08 |
| 37 | 11 | 308 | CLA | CED-O2D-CGD | 2.09 | 120.65 | 115.92 |
| 37 | C | 512 | CLA | CBC-CAC-C3C | -2.09 | 106.76 | 112.42 |
| 37 | 32 | 206 | CLA | C7-C6-C5 | -2.09 | 107.69 | 113.26 |
| 37 | 15 | 303 | CLA | O2A-CGA-CBA | 2.09 | 118.20 | 111.83 |
| 37 | A | 403 | CLA | CMB-C2B-C3B | 2.09 | 131.46 | 126.55 |
| 37 | C | 503 | CLA | CBC-CAC-C3C | -2.09 | 106.76 | 112.42 |
| 37 | 19 | 303 | CLA | CHB-C4A-NA | 2.09 | 127.41 | 124.40 |
| 44 | j | 101 | DGD | O2D-C2D-C1D | -2.09 | 105.10 | 110.08 |
| 37 | W | 102 | CLA | CMC-C2C-C1C | 2.09 | 128.29 | 125.03 |
| 41 | a | 410 | LMG | O1-C1-C2 | -2.09 | 105.10 | 108.27 |
| 44 | J | 101 | DGD | O5E-C6E-C5E | -2.09 | 104.23 | 111.33 |
| 37 | 19 | 301 | CLA | CBA-CAA-C2A | 2.09 | 120.00 | 113.79 |
| 43 | D | 411 | LHG | O8-C23-C24 | 2.09 | 118.19 | 111.83 |
| 39 | C | 514 | BCR | C20-C21-C22 | -2.09 | 124.35 | 127.28 |
| 37 | b | 516 | CLA | CHA-C1A-NA | -2.09 | 121.67 | 126.39 |
| 37 | c | 503 | CLA | CHA-C1A-NA | -2.09 | 121.67 | 126.39 |
| 47 | 11 | 302 | KC1 | CHB-C1B-NB | -2.09 | 121.87 | 124.80 |
| 37 | d | 401 | CLA | CMD-C2D-C3D | -2.09 | 122.91 | 127.69 |
| 47 | 18 | 207 | KC1 | C3D-C2D-C1D | -2.08 | 99.74 | 106.40 |
| 38 | a | 406 | PHO | O2A-CGA-O1A | -2.08 | 118.41 | 123.63 |
| 41 | 11 | 317 | LMG | O2-C2-C1 | -2.08 | 105.11 | 110.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 51 | 19 | 315 | LMU | O1'-C1'-C2' | 2.08 | 111.44 | 108.27 |
| 39 | a | 408 | BCR | C7-C8-C9 | -2.08 | 123.15 | 126.23 |
| 40 | 40 | 202 | SQD | O8-S-C6 | 2.08 | 110.00 | 105.97 |
| 50 | 41 | 212 | DD6 | C22-C16-C15 | 2.08 | 115.67 | 110.05 |
| 37 | 31 | 310 | CLA | CBC-CAC-C3C | -2.08 | 106.77 | 112.42 |
| 37 | b | 503 | CLA | CHB-C4A-NA | 2.08 | 127.41 | 124.40 |
| 37 | b | 504 | CLA | C6-C7-C8 | -2.08 | 109.04 | 115.97 |
| 37 | 20 | 307 | CLA | CMC-C2C-C1C | 2.08 | 128.29 | 125.03 |
| 37 | C | 503 | CLA | CHA-C1A-NA | -2.08 | 121.67 | 126.39 |
| 48 | 39 | 313 | A86 | O4-C38-O5 | -2.08 | 118.97 | 122.99 |
| 37 | 33 | 308 | CLA | CED-O2D-CGD | 2.08 | 120.64 | 115.92 |
| 47 | 37 | 307 | KC1 | CHB-C1B-C2B | -2.08 | 121.15 | 125.49 |
| 37 | 14 | 301 | CLA | O2A-CGA-CBA | 2.08 | 118.19 | 111.83 |
| 48 | 17 | 314 | A86 | C21-C20-C15 | -2.08 | 116.63 | 123.35 |
| 48 | 31 | 311 | A86 | C19-C18-C17 | -2.08 | 106.89 | 110.79 |
| 40 | B | 522 | SQD | O6-C1-C2 | 2.08 | 111.44 | 108.27 |
| 45 | d | 406 | PL9 | C50-C49-C48 | -2.08 | 116.41 | 122.66 |
| 48 | 11 | 313 | A86 | C10-C9-C8 | -2.08 | 117.17 | 123.20 |
| 37 | B | 512 | CLA | CHD-C1D-ND | -2.08 | 121.87 | 124.80 |
| 47 | 17 | 305 | KC1 | C3D-C2D-C1D | -2.08 | 99.75 | 106.40 |
| 37 | 19 | 303 | CLA | C4-C3-C5 | 2.08 | 118.84 | 115.23 |
| 38 | A | 404 | PHO | O2A-CGA-O1A | -2.08 | 118.42 | 123.63 |
| 41 | A | 408 | LMG | O3-C3-C2 | -2.08 | 105.47 | 110.38 |
| 48 | 15 | 312 | A86 | C-C1-C2 | -2.08 | 119.44 | 122.82 |
| 37 | C | 507 | CLA | C1-C2-C3 | -2.08 | 122.79 | 126.20 |
| 37 | 41 | 204 | CLA | CMB-C2B-C1B | 2.08 | 128.59 | 125.42 |
| 47 | 38 | 207 | KC1 | C3D-C2D-C1D | -2.08 | 99.76 | 106.40 |
| 37 | C | 506 | CLA | O2D-CGD-O1D | -2.08 | 119.80 | 123.85 |
| 37 | c | 511 | CLA | CHA-C1A-NA | -2.08 | 121.68 | 126.39 |
| 37 | 41 | 205 | CLA | O2A-CGA-CBA | 2.08 | 120.57 | 114.00 |
| 47 | 33 | 302 | KC1 | C4B-C3B-C2B | -2.08 | 105.01 | 106.81 |
| 37 | B | 504 | CLA | C6-C7-C8 | -2.08 | 109.06 | 115.97 |
| 41 | 11 | 317 | LMG | O3-C3-C2 | -2.08 | 105.48 | 110.38 |
| 47 | 18 | 207 | KC1 | CAB-C3B-C4B | 2.08 | 129.78 | 124.82 |
| 37 | c | 505 | CLA | C4-C3-C5 | 2.08 | 118.83 | 115.23 |
| 37 | c | 509 | CLA | CMC-C2C-C1C | 2.08 | 128.28 | 125.03 |
| 37 | 15 | 305 | CLA | CBC-CAC-C3C | -2.08 | 106.79 | 112.42 |
| 47 | 15 | 302 | KC1 | CBB-CAB-C3B | -2.08 | 117.14 | 127.53 |
| 37 | 21 | 205 | CLA | O2A-CGA-CBA | 2.08 | 120.56 | 114.00 |
| 48 | 34 | 312 | A86 | C9-C10-C11 | -2.08 | 120.77 | 126.64 |
| 37 | c | 508 | CLA | C4-C3-C5 | 2.08 | 118.83 | 115.23 |
| 48 | 35 | 316 | A86 | O4-C38-O5 | -2.08 | 118.98 | 122.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | 14 | 301 | CLA | O2D-CGD-O1D | -2.08 | 119.81 | 123.85 |
| 37 | 17 | 309 | CLA | CAC-C3C-C4C | 2.08 | 127.49 | 124.79 |
| 45 | d | 402 | PL9 | C50-C49-C48 | -2.08 | 116.42 | 122.66 |
| 37 | 39 | 303 | CLA | CHB-C4A-NA | 2.08 | 127.40 | 124.40 |
| 41 | 31 | 317 | LMG | O3-C3-C2 | -2.08 | 105.48 | 110.38 |
| 37 | 17 | 309 | CLA | CHB-C1B-C2B | -2.08 | 121.40 | 127.43 |
| 37 | b | 515 | CLA | CHA-C1A-NA | -2.08 | 121.69 | 126.39 |
| 37 | c | 502 | CLA | O2A-CGA-CBA | 2.08 | 118.16 | 111.83 |
| 37 | 35 | 307 | CLA | O2A-CGA-CBA | 2.08 | 118.16 | 111.83 |
| 48 | 35 | 315 | A86 | C34-O4-C38 | -2.08 | 114.18 | 117.85 |
| 37 | D | 405 | CLA | CHB-C4A-NA | 2.08 | 127.39 | 124.40 |
| 48 | 35 | 316 | A86 | C-C1-C24 | 2.08 | 121.26 | 118.09 |
| 41 | A | 408 | LMG | O1-C1-C2 | -2.07 | 105.12 | 108.27 |
| 47 | 15 | 304 | KC1 | O1D-CGD-CBD | -2.07 | 120.43 | 124.52 |
| 48 | 21 | 214 | A86 | C9-C10-C11 | -2.07 | 120.78 | 126.64 |
| 37 | 38 | 203 | CLA | CGD-CBD-CAD | -2.07 | 104.13 | 110.85 |
| 37 | A | 403 | CLA | C11-C12-C13 | -2.07 | 109.07 | 115.97 |
| 40 | B | 522 | SQD | O48-C23-C24 | 2.07 | 118.16 | 111.83 |
| 37 | c | 501 | CLA | CHB-C4A-NA | 2.07 | 127.39 | 124.40 |
| 48 | 16 | 313 | A86 | C-C1-C2 | -2.07 | 119.46 | 122.82 |
| 47 | 11 | 304 | KC1 | CHB-C4A-NA | 2.07 | 127.45 | 124.23 |
| 47 | 14 | 309 | KC1 | O1D-CGD-CBD | -2.07 | 120.43 | 124.52 |
| 37 | C | 508 | CLA | C4-C3-C5 | 2.07 | 118.83 | 115.23 |
| 48 | 37 | 313 | A86 | C21-C20-C15 | -2.07 | 116.66 | 123.35 |
| 37 | B | 513 | CLA | CHB-C4A-NA | 2.07 | 127.39 | 124.40 |
| 44 | c | 517 | DGD | O6D-C5D-C6D | -2.07 | 102.59 | 106.69 |
| 37 | C | 511 | CLA | CHA-C1A-NA | -2.07 | 121.70 | 126.39 |
| 43 | D | 409 | LHG | C27-C26-C25 | -2.07 | 103.90 | 114.37 |
| 47 | 38 | 210 | KC1 | C3D-C2D-C1D | -2.07 | 99.78 | 106.40 |
| 44 | C | 517 | DGD | C1D-C2D-C3D | -2.07 | 105.65 | 110.01 |
| 37 | 34 | 301 | CLA | O2A-CGA-CBA | 2.07 | 118.15 | 111.83 |
| 37 | Z | 101 | CLA | CAA-C2A-C3A | -2.07 | 107.41 | 113.00 |
| 48 | 33 | 315 | A86 | O4-C38-O5 | -2.07 | 119.00 | 122.99 |
| 48 | 18 | 212 | A86 | C3-C2-C1 | -2.07 | 124.38 | 127.28 |
| 41 | a | 410 | LMG | O3-C3-C2 | -2.07 | 105.50 | 110.38 |
| 37 | 21 | 204 | CLA | CMB-C2B-C1B | 2.07 | 128.57 | 125.42 |
| 37 | 12 | 205 | CLA | C7-C6-C5 | -2.07 | 107.75 | 113.26 |
| 43 | d | 407 | LHG | C27-C26-C25 | -2.07 | 103.91 | 114.37 |
| 37 | B | 514 | CLA | C1-C2-C3 | -2.07 | 122.81 | 126.20 |
| 37 | 19 | 304 | CLA | O2D-CGD-O1D | -2.07 | 119.82 | 123.85 |
| 37 | B | 509 | CLA | O2A-CGA-O1A | -2.07 | 118.45 | 123.63 |
| 48 | 12 | 214 | A86 | C7-C6-C8 | 2.07 | 121.25 | 118.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | C | 502 | CLA | O2A-CGA-CBA | 2.07 | 118.14 | 111.83 |
| 48 | 32 | 203 | A86 | C19-C18-C17 | -2.07 | 106.92 | 110.79 |
| 37 | 37 | 306 | CLA | CBA-CAA-C2A | -2.07 | 107.64 | 113.79 |
| 37 | 33 | 310 | CLA | CHB-C1B-C2B | -2.07 | 121.42 | 127.43 |
| 40 | b | 521 | SQD | O5-C5-C4 | 2.07 | 113.42 | 109.70 |
| 37 | 11 | 310 | CLA | CBC-CAC-C3C | -2.07 | 106.81 | 112.42 |
| 47 | 37 | 307 | KC1 | CHC-C1C-NC | 2.07 | 127.44 | 124.23 |
| 37 | 41 | 209 | CLA | O1D-CGD-CBD | -2.07 | 120.44 | 124.52 |
| 37 | 13 | 308 | CLA | CED-O2D-CGD | 2.07 | 120.60 | 115.92 |
| 37 | 19 | 304 | CLA | CMC-C2C-C1C | 2.07 | 128.26 | 125.03 |
| 48 | 34 | 316 | A86 | O4-C38-O5 | -2.07 | 119.00 | 122.99 |
| 44 | c | 516 | DGD | O6E-C1E-O5D | -2.07 | 105.16 | 110.04 |
| 37 | b | 514 | CLA | C1-C2-C3 | -2.07 | 122.81 | 126.20 |
| 37 | 18 | 204 | CLA | CMB-C2B-C3B | 2.07 | 131.41 | 126.55 |
| 45 | d | 406 | PL9 | C40-C39-C41 | 2.07 | 118.81 | 115.23 |
| 44 | C | 517 | DGD | O6D-C5D-C6D | -2.07 | 102.60 | 106.69 |
| 37 | 38 | 201 | CLA | CHA-C1A-NA | -2.07 | 121.71 | 126.39 |
| 48 | 35 | 313 | A86 | C23-C16-C22 | -2.07 | 104.37 | 107.37 |
| 47 | 17 | 308 | KC1 | CHC-C1C-NC | 2.07 | 127.43 | 124.23 |
| 37 | 39 | 304 | CLA | CMC-C2C-C1C | 2.07 | 128.26 | 125.03 |
| 37 | 15 | 307 | CLA | C1-C2-C3 | -2.06 | 122.81 | 126.20 |
| 37 | Z | 102 | CLA | CHB-C1B-C2B | -2.06 | 121.43 | 127.43 |
| 40 | 40 | 202 | SQD | O48-C23-O10 | -2.06 | 118.46 | 123.63 |
| 44 | C | 516 | DGD | CAB-C9B-C8B | -2.06 | 103.93 | 114.37 |
| 37 | c | 507 | CLA | C1-C2-C3 | -2.06 | 122.81 | 126.20 |
| 37 | c | 508 | CLA | CHB-C1B-C2B | -2.06 | 121.44 | 127.43 |
| 45 | D | 408 | PL9 | C27-C28-C29 | -2.06 | 122.90 | 127.62 |
| 44 | c | 517 | DGD | C1D-C2D-C3D | -2.06 | 105.67 | 110.01 |
| 45 | d | 406 | PL9 | C27-C28-C29 | -2.06 | 122.90 | 127.62 |
| 47 | 18 | 210 | KC1 | C3D-C2D-C1D | -2.06 | 99.81 | 106.40 |
| 37 | 14 | 303 | CLA | CHB-C1B-C2B | -2.06 | 121.44 | 127.43 |
| 37 | z | 102 | CLA | CMC-C2C-C1C | 2.06 | 128.26 | 125.03 |
| 37 | c | 509 | CLA | C1-C2-C3 | -2.06 | 122.82 | 126.20 |
| 37 | 18 | 202 | CLA | CHA-C1A-NA | -2.06 | 121.72 | 126.39 |
| 48 | 37 | 319 | A86 | C-C1-C24 | 2.06 | 121.24 | 118.09 |
| 48 | 14 | 316 | A86 | O4-C38-O5 | -2.06 | 119.01 | 122.99 |
| 37 | C | 506 | CLA | CHB-C4A-NA | 2.06 | 127.37 | 124.40 |
| 37 | c | 505 | CLA | CHB-C4A-NA | 2.06 | 127.37 | 124.40 |
| 48 | 11 | 311 | A86 | C19-C18-C17 | -2.06 | 106.94 | 110.79 |
| 48 | 14 | 313 | A86 | C23-C16-C22 | -2.06 | 104.38 | 107.37 |
| 44 | C | 516 | DGD | O6E-C1E-O5D | -2.06 | 105.18 | 110.04 |
| 47 | 14 | 306 | KC1 | CMC-C2C-C1C | 2.06 | 128.25 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 15 | 304 | KC1 | CED-O2D-CGD | 2.06 | 120.59 | 115.92 |
| 37 | z | 102 | CLA | CHB-C1B-C2B | -2.06 | 121.45 | 127.43 |
| 37 | 35 | 303 | CLA | O2A-CGA-CBA | 2.06 | 118.11 | 111.83 |
| 37 | 34 | 303 | CLA | CHB-C1B-C2B | -2.06 | 121.45 | 127.43 |
| 47 | 34 | 309 | KC1 | O1D-CGD-CBD | -2.06 | 120.46 | 124.52 |
| 37 | B | 515 | CLA | CHA-C1A-NA | -2.06 | 121.73 | 126.39 |
| 37 | 37 | 301 | CLA | CHA-C1A-NA | -2.06 | 121.73 | 126.39 |
| 37 | b | 515 | CLA | C11-C10-C8 | -2.06 | 109.12 | 115.97 |
| 37 | 33 | 310 | CLA | CHB-C4A-NA | 2.06 | 127.37 | 124.40 |
| 47 | 17 | 308 | KC1 | O1D-CGD-CBD | -2.06 | 120.46 | 124.52 |
| 40 | b | 521 | SQD | O6-C1-C2 | 2.06 | 111.40 | 108.27 |
| 48 | 15 | 312 | A86 | C4-C5-C6 | -2.06 | 124.39 | 127.28 |
| 37 | 39 | 304 | CLA | O2D-CGD-O1D | -2.06 | 119.84 | 123.85 |
| 37 | 21 | 209 | CLA | O1D-CGD-CBD | -2.06 | 120.46 | 124.52 |
| 48 | 32 | 215 | A86 | C7-C6-C8 | 2.06 | 121.23 | 118.09 |
| 44 | H | 102 | DGD | C5B-C4B-C3B | -2.06 | 103.97 | 114.37 |
| 37 | 17 | 309 | CLA | C4-C3-C5 | 2.06 | 118.80 | 115.23 |
| 37 | b | 513 | CLA | CHB-C4A-NA | 2.06 | 127.37 | 124.40 |
| 37 | 12 | 209 | CLA | CBC-CAC-C3C | -2.06 | 106.85 | 112.42 |
| 37 | 13 | 308 | CLA | CHD-C4C-NC | 2.06 | 127.42 | 124.23 |
| 37 | C | 509 | CLA | CMC-C2C-C1C | 2.06 | 128.25 | 125.03 |
| 37 | z | 101 | CLA | CAA-C2A-C3A | -2.06 | 107.44 | 113.00 |
| 48 | 12 | 202 | A86 | C19-C18-C17 | -2.06 | 106.95 | 110.79 |
| 37 | 14 | 303 | CLA | CHA-C1A-NA | -2.06 | 121.74 | 126.39 |
| 50 | 20 | 312 | DD6 | C23-C16-C17 | -2.06 | 105.36 | 108.97 |
| 48 | 12 | 202 | A86 | C25-C24-C1 | -2.06 | 120.73 | 126.36 |
| 44 | c | 516 | DGD | CAB-C9B-C8B | -2.06 | 103.98 | 114.37 |
| 37 | 37 | 308 | CLA | CHB-C1B-C2B | -2.05 | 121.46 | 127.43 |
| 37 | c | 510 | CLA | O1D-CGD-CBD | -2.05 | 120.47 | 124.52 |
| 37 | C | 505 | CLA | CHB-C4A-NA | 2.05 | 127.36 | 124.40 |
| 48 | 34 | 313 | A86 | C23-C16-C22 | -2.05 | 104.39 | 107.37 |
| 37 | b | 513 | CLA | C1-O2A-CGA | 2.05 | 121.62 | 116.65 |
| 47 | 31 | 303 | KC1 | CHB-C1B-NB | -2.05 | 121.91 | 124.80 |
| 37 | a | 403 | CLA | C11-C12-C13 | -2.05 | 109.14 | 115.97 |
| 37 | 33 | 303 | CLA | CHA-C1A-NA | -2.05 | 121.74 | 126.39 |
| 37 | c | 506 | CLA | CHB-C4A-NA | 2.05 | 127.36 | 124.40 |
| 45 | D | 404 | PL9 | C50-C49-C48 | -2.05 | 116.49 | 122.66 |
| 46 | v | 201 | HEM | C2D-C1D-ND | -2.05 | 107.53 | 109.90 |
| 47 | 14 | 306 | KC1 | CBC-CAC-C3C | -2.05 | 106.86 | 112.42 |
| 40 | B | 522 | SQD | O5-C5-C4 | 2.05 | 113.40 | 109.70 |
| 37 | 15 | 301 | CLA | CHA-C1A-NA | -2.05 | 121.74 | 126.39 |
| 37 | 41 | 202 | CLA | CBC-CAC-C3C | -2.05 | 106.86 | 112.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 37 | 312 | A86 | C8-C6-C5 | -2.05 | 115.78 | 119.01 |
| 37 | 35 | 301 | CLA | CHA-C1A-NA | -2.05 | 121.74 | 126.39 |
| 48 | 35 | 315 | A86 | C9-C8-C6 | -2.05 | 120.74 | 126.36 |
| 47 | 11 | 309 | KC1 | CHB-C1B-C2B | -2.05 | 121.22 | 125.49 |
| 44 | h | 102 | DGD | C5B-C4B-C3B | -2.05 | 104.00 | 114.37 |
| 47 | 33 | 304 | KC1 | O1D-CGD-CBD | -2.05 | 120.47 | 124.52 |
| 47 | 37 | 307 | KC1 | O1D-CGD-CBD | -2.05 | 120.47 | 124.52 |
| 37 | 18 | 203 | CLA | CHC-C1C-NC | 2.05 | 127.40 | 124.31 |
| 47 | 19 | 308 | KC1 | O2A-CGA-O1A | -2.05 | 118.53 | 122.70 |
| 37 | 40 | 203 | CLA | CHA-C1A-NA | -2.05 | 121.75 | 126.39 |
| 37 | b | 513 | CLA | CHA-C1A-NA | -2.05 | 121.75 | 126.39 |
| 46 | V | 201 | HEM | C2D-C1D-ND | -2.05 | 107.53 | 109.90 |
| 39 | H | 101 | BCR | C11-C10-C9 | -2.05 | 124.40 | 127.28 |
| 37 | B | 515 | CLA | C11-C10-C8 | -2.05 | 109.15 | 115.97 |
| 37 | C | 508 | CLA | CHB-C1B-C2B | -2.05 | 121.48 | 127.43 |
| 37 | d | 404 | CLA | CHB-C1B-C2B | -2.05 | 121.48 | 127.43 |
| 37 | 41 | 206 | CLA | CHA-C1A-NA | -2.05 | 121.75 | 126.39 |
| 47 | 36 | 304 | KC1 | CMC-C2C-C1C | 2.05 | 128.24 | 125.03 |
| 37 | 21 | 202 | CLA | CBC-CAC-C3C | -2.05 | 106.87 | 112.42 |
| 47 | 31 | 305 | KC1 | CHB-C4A-NA | 2.05 | 127.41 | 124.23 |
| 37 | 38 | 203 | CLA | CED-O2D-CGD | 2.05 | 120.56 | 115.92 |
| 37 | 19 | 302 | CLA | CMB-C2B-C1B | 2.05 | 128.54 | 125.42 |
| 37 | 19 | 304 | CLA | O1D-CGD-CBD | -2.05 | 120.48 | 124.52 |
| 37 | D | 406 | CLA | CHB-C1B-C2B | -2.05 | 121.48 | 127.43 |
| 38 | a | 405 | PHO | CBA-CAA-C2A | -2.05 | 107.75 | 113.78 |
| 44 | C | 516 | DGD | O6E-C5E-C6E | -2.05 | 101.37 | 106.44 |
| 37 | 35 | 305 | CLA | CBC-CAC-C3C | -2.05 | 106.87 | 112.42 |
| 37 | 18 | 202 | CLA | CHC-C1C-NC | 2.05 | 127.39 | 124.31 |
| 44 | c | 516 | DGD | O6E-C5E-C6E | -2.05 | 101.37 | 106.44 |
| 37 | B | 513 | CLA | CHA-C1A-NA | -2.05 | 121.76 | 126.39 |
| 47 | 33 | 302 | KC1 | O1D-CGD-CBD | -2.05 | 120.48 | 124.52 |
| 47 | 34 | 306 | KC1 | CBC-CAC-C3C | -2.05 | 106.87 | 112.42 |
| 37 | b | 512 | CLA | CHD-C1D-ND | -2.05 | 121.92 | 124.80 |
| 37 | c | 501 | CLA | O2A-CGA-O1A | -2.05 | 118.51 | 123.63 |
| 38 | D | 403 | PHO | CBA-CAA-C2A | -2.05 | 107.75 | 113.78 |
| 48 | 32 | 218 | A86 | O4-C38-O5 | -2.05 | 119.04 | 122.99 |
| 37 | z | 101 | CLA | CHA-C1A-NA | -2.05 | 121.76 | 126.39 |
| 37 | 20 | 301 | CLA | CHA-C1A-NA | -2.05 | 121.76 | 126.39 |
| 37 | B | 512 | CLA | CMA-C3A-C4A | -2.05 | 106.28 | 111.77 |
| 37 | b | 512 | CLA | CMA-C3A-C4A | -2.05 | 106.28 | 111.77 |
| 37 | 31 | 306 | CLA | CMC-C2C-C1C | 2.05 | 128.23 | 125.03 |
| 37 | c | 507 | CLA | CMB-C2B-C1B | 2.05 | 128.53 | 125.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 15 | 315 | A86 | C9-C8-C6 | -2.04 | 120.76 | 126.36 |
| 37 | c | 506 | CLA | O2D-CGD-O1D | -2.04 | 119.87 | 123.85 |
| 40 | 16 | 315 | SQD | O48-C23-O10 | -2.04 | 118.52 | 123.63 |
| 37 | 34 | 307 | CLA | O1D-CGD-CBD | -2.04 | 120.49 | 124.52 |
| 37 | 31 | 301 | CLA | CHB-C4A-NA | 2.04 | 127.35 | 124.40 |
| 48 | 13 | 313 | A86 | C4-C3-C2 | -2.04 | 119.34 | 123.52 |
| 48 | 33 | 313 | A86 | C4-C3-C2 | -2.04 | 119.34 | 123.52 |
| 45 | D | 408 | PL9 | C12-C13-C14 | -2.04 | 122.95 | 127.62 |
| 37 | 34 | 308 | CLA | CHB-C4A-NA | 2.04 | 127.35 | 124.40 |
| 47 | 13 | 302 | KC1 | CMC-C2C-C1C | 2.04 | 128.22 | 125.03 |
| 48 | 36 | 313 | A86 | C25-C24-C1 | -2.04 | 120.77 | 126.36 |
| 37 | b | 513 | CLA | CAC-C3C-C4C | 2.04 | 127.44 | 124.79 |
| 37 | 14 | 310 | CLA | CMD-C2D-C3D | -2.04 | 123.01 | 127.69 |
| 48 | 18 | 213 | A86 | C34-O4-C38 | -2.04 | 114.24 | 117.85 |
| 37 | B | 513 | CLA | C1-O2A-CGA | 2.04 | 121.59 | 116.65 |
| 37 | 19 | 306 | CLA | CHB-C1B-C2B | -2.04 | 121.50 | 127.43 |
| 37 | 18 | 203 | CLA | O2D-CGD-O1D | -2.04 | 119.88 | 123.85 |
| 37 | C | 505 | CLA | C4-C3-C5 | 2.04 | 118.77 | 115.23 |
| 37 | 36 | 303 | CLA | O2D-CGD-O1D | -2.04 | 119.88 | 123.85 |
| 37 | 16 | 309 | CLA | CMC-C2C-C1C | 2.04 | 128.22 | 125.03 |
| 37 | 21 | 206 | CLA | CHA-C1A-NA | -2.04 | 121.77 | 126.39 |
| 37 | B | 513 | CLA | CAC-C3C-C4C | 2.04 | 127.44 | 124.79 |
| 37 | a | 407 | CLA | C1-O2A-CGA | 2.04 | 121.59 | 116.65 |
| 37 | 34 | 302 | CLA | CAA-C2A-C3A | -2.04 | 107.49 | 113.00 |
| 37 | 34 | 310 | CLA | CMD-C2D-C3D | -2.04 | 123.01 | 127.69 |
| 37 | Z | 101 | CLA | CHA-C1A-NA | -2.04 | 121.78 | 126.39 |
| 37 | B | 503 | CLA | CHB-C1B-C2B | -2.04 | 121.51 | 127.43 |
| 48 | 13 | 313 | A86 | O4-C34-C33 | 2.04 | 112.85 | 107.64 |
| 48 | 32 | 203 | A86 | C25-C24-C1 | -2.04 | 120.77 | 126.36 |
| 37 | 11 | 303 | CLA | CMC-C2C-C1C | 2.04 | 128.22 | 125.03 |
| 37 | 31 | 304 | CLA | CMC-C2C-C1C | 2.04 | 128.22 | 125.03 |
| 37 | 11 | 310 | CLA | CED-O2D-CGD | 2.04 | 120.54 | 115.92 |
| 37 | C | 513 | CLA | CHB-C1B-C2B | -2.04 | 121.51 | 127.43 |
| 37 | C | 510 | CLA | O1D-CGD-CBD | -2.04 | 120.50 | 124.52 |
| 47 | 20 | 305 | KC1 | C3D-C2D-C1D | -2.04 | 99.89 | 106.40 |
| 37 | d | 403 | CLA | CHB-C4A-NA | 2.04 | 127.34 | 124.40 |
| 41 | 12 | 201 | LMG | O7-C10-O9 | -2.04 | 118.94 | 123.70 |
| 47 | 13 | 309 | KC1 | CHC-C1C-NC | 2.04 | 127.39 | 124.23 |
| 47 | 33 | 309 | KC1 | CHC-C1C-NC | 2.04 | 127.39 | 124.23 |
| 39 | h | 101 | BCR | C15-C16-C17 | -2.04 | 119.35 | 123.52 |
| 48 | 32 | 203 | A86 | C4-C3-C2 | -2.04 | 119.35 | 123.52 |
| 48 | 12 | 217 | A86 | O4-C38-O5 | -2.04 | 119.06 | 122.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | b | 503 | CLA | CHA-C1A-NA | -2.04 | 121.78 | 126.39 |
| 37 | D | 402 | CLA | CHB-C1B-C2B | -2.04 | 121.52 | 127.43 |
| 48 | 16 | 314 | A86 | C25-C24-C1 | -2.04 | 120.78 | 126.36 |
| 37 | 41 | 208 | CLA | O1D-CGD-CBD | -2.04 | 120.50 | 124.52 |
| 37 | 18 | 203 | CLA | CHB-C1B-C2B | -2.04 | 121.52 | 127.43 |
| 40 | 17 | 301 | SQD | O47-C7-O49 | -2.04 | 118.94 | 123.70 |
| 44 | H | 102 | DGD | O3E-C3E-C2E | -2.04 | 105.58 | 110.38 |
| 47 | 37 | 304 | KC1 | CBC-CAC-C3C | -2.04 | 106.90 | 112.42 |
| 37 | B | 503 | CLA | CHA-C1A-NA | -2.04 | 121.78 | 126.39 |
| 37 | C | 511 | CLA | CMC-C2C-C1C | 2.04 | 128.22 | 125.03 |
| 37 | C | 509 | CLA | C1-C2-C3 | -2.04 | 122.86 | 126.20 |
| 48 | 37 | 319 | A86 | C25-C24-C1 | -2.04 | 120.78 | 126.36 |
| 37 | 36 | 306 | CLA | CBA-CAA-C2A | 2.04 | 119.85 | 113.79 |
| 37 | 31 | 306 | CLA | CHB-C1B-C2B | -2.04 | 121.52 | 127.43 |
| 44 | C | 517 | DGD | C8B-C7B-C6B | -2.04 | 104.08 | 114.37 |
| 47 | 33 | 309 | KC1 | C3D-C2D-C1D | -2.04 | 99.90 | 106.40 |
| 47 | 40 | 207 | KC1 | C3D-C2D-C1D | -2.03 | 99.90 | 106.40 |
| 37 | 18 | 203 | CLA | CBC-CAC-C3C | -2.03 | 106.90 | 112.42 |
| 39 | H | 101 | BCR | C15-C16-C17 | -2.03 | 119.36 | 123.52 |
| 37 | 14 | 302 | CLA | CAA-C2A-C3A | -2.03 | 107.50 | 113.00 |
| 37 | 13 | 310 | CLA | CHB-C1B-C2B | -2.03 | 121.52 | 127.43 |
| 37 | 18 | 202 | CLA | CHB-C1B-C2B | -2.03 | 121.52 | 127.43 |
| 37 | c | 507 | CLA | CHA-C1A-NA | -2.03 | 121.78 | 126.39 |
| 37 | 38 | 203 | CLA | O2D-CGD-O1D | -2.03 | 119.89 | 123.85 |
| 47 | 41 | 207 | KC1 | CAB-C3B-C4B | 2.03 | 129.68 | 124.82 |
| 37 | 13 | 308 | CLA | CHA-C1A-NA | -2.03 | 121.79 | 126.39 |
| 37 | Z | 101 | CLA | O1D-CGD-CBD | -2.03 | 120.51 | 124.52 |
| 37 | 11 | 305 | CLA | CMC-C2C-C1C | 2.03 | 128.21 | 125.03 |
| 37 | 34 | 303 | CLA | CHA-C1A-NA | -2.03 | 121.79 | 126.39 |
| 44 | c | 517 | DGD | C8B-C7B-C6B | -2.03 | 104.10 | 114.37 |
| 50 | 40 | 214 | DD6 | C23-C16-C17 | -2.03 | 105.40 | 108.97 |
| 37 | 14 | 301 | CLA | C6-C7-C8 | -2.03 | 109.21 | 115.97 |
| 48 | 39 | 313 | A86 | C10-C9-C8 | 2.03 | 129.09 | 123.20 |
| 37 | 16 | 306 | CLA | CBA-CAA-C2A | 2.03 | 119.84 | 113.79 |
| 48 | 13 | 311 | A86 | C23-C16-C22 | -2.03 | 104.42 | 107.37 |
| 37 | B | 511 | CLA | O2A-CGA-O1A | -2.03 | 118.55 | 123.63 |
| 37 | c | 511 | CLA | CMC-C2C-C1C | 2.03 | 128.21 | 125.03 |
| 37 | c | 505 | CLA | CHB-C1B-C2B | -2.03 | 121.53 | 127.43 |
| 37 | b | 502 | CLA | CBC-CAC-C3C | -2.03 | 106.92 | 112.42 |
| 37 | 15 | 303 | CLA | CMB-C2B-C1B | 2.03 | 128.51 | 125.42 |
| 37 | 14 | 308 | CLA | C6-C7-C8 | -2.03 | 109.22 | 115.97 |
| 37 | C | 505 | CLA | CHB-C1B-C2B | -2.03 | 121.53 | 127.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 31 | 309 | KC1 | CHB-C1B-C2B | -2.03 | 121.27 | 125.49 |
| 37 | d | 401 | CLA | CHB-C1B-C2B | -2.03 | 121.53 | 127.43 |
| 37 | b | 516 | CLA | CHB-C4A-NA | 2.03 | 127.33 | 124.40 |
| 47 | 39 | 308 | KC1 | O2A-CGA-O1A | -2.03 | 118.57 | 122.70 |
| 37 | 11 | 305 | CLA | CHB-C1B-C2B | -2.03 | 121.53 | 127.43 |
| 48 | 38 | 213 | A86 | C-C1-C24 | 2.03 | 121.19 | 118.09 |
| 37 | 14 | 307 | CLA | O1D-CGD-CBD | -2.03 | 120.52 | 124.52 |
| 44 | C | 516 | DGD | C5B-C4B-C3B | -2.03 | 104.11 | 114.37 |
| 47 | 34 | 306 | KC1 | O2A-CGA-O1A | -2.03 | 118.57 | 122.70 |
| 37 | 13 | 301 | CLA | C1-C2-C3 | -2.03 | 122.87 | 126.20 |
| 45 | d | 406 | PL9 | C12-C13-C14 | -2.03 | 122.98 | 127.62 |
| 37 | 36 | 307 | CLA | CHB-C1B-C2B | -2.03 | 121.54 | 127.43 |
| 37 | 17 | 302 | CLA | CED-O2D-CGD | 2.03 | 120.52 | 115.92 |
| 37 | C | 501 | CLA | O2A-CGA-O1A | -2.03 | 118.56 | 123.63 |
| 37 | B | 502 | CLA | CHB-C1B-C2B | -2.03 | 121.54 | 127.43 |
| 47 | 16 | 304 | KC1 | CBC-CAC-C3C | -2.03 | 106.92 | 112.42 |
| 37 | 18 | 201 | CLA | CHA-C1A-NA | -2.03 | 121.80 | 126.39 |
| 47 | 13 | 309 | KC1 | C3D-C2D-C1D | -2.03 | 99.93 | 106.40 |
| 37 | 11 | 310 | CLA | CHB-C1B-C2B | -2.03 | 121.55 | 127.43 |
| 48 | 17 | 311 | A86 | C40-C32-C31 | -2.03 | 108.66 | 110.47 |
| 37 | B | 510 | CLA | CBC-CAC-C3C | -2.03 | 106.93 | 112.42 |
| 37 | 33 | 303 | CLA | CMC-C2C-C1C | 2.03 | 128.20 | 125.03 |
| 37 | c | 513 | CLA | CHB-C1B-C2B | -2.03 | 121.55 | 127.43 |
| 44 | h | 102 | DGD | O3E-C3E-C2E | -2.03 | 105.60 | 110.38 |
| 48 | 33 | 313 | A86 | O4-C34-C33 | 2.03 | 112.82 | 107.64 |
| 37 | b | 503 | CLA | CHB-C1B-C2B | -2.03 | 121.55 | 127.43 |
| 47 | 38 | 210 | KC1 | CHC-C1C-NC | 2.02 | 127.37 | 124.23 |
| 47 | 31 | 309 | KC1 | CMC-C2C-C1C | 2.02 | 128.20 | 125.03 |
| 48 | 12 | 202 | A86 | C7-C6-C8 | 2.02 | 121.18 | 118.09 |
| 37 | 15 | 301 | CLA | CAC-C3C-C4C | 2.02 | 127.42 | 124.79 |
| 37 | 31 | 306 | CLA | O2A-CGA-CBA | 2.02 | 120.40 | 114.00 |
| 41 | 37 | 316 | LMG | C6-C5-C4 | -2.02 | 108.05 | 113.02 |
| 37 | W | 102 | CLA | CHB-C4A-NA | 2.02 | 127.32 | 124.40 |
| 37 | 39 | 306 | CLA | CHB-C1B-C2B | -2.02 | 121.55 | 127.43 |
| 37 | 33 | 303 | CLA | O1D-CGD-CBD | -2.02 | 120.53 | 124.52 |
| 37 | b | 516 | CLA | C6-C7-C8 | -2.02 | 109.24 | 115.97 |
| 37 | 34 | 301 | CLA | C6-C7-C8 | -2.02 | 109.24 | 115.97 |
| 44 | c | 516 | DGD | C5B-C4B-C3B | -2.02 | 104.14 | 114.37 |
| 48 | 33 | 311 | A86 | C23-C16-C22 | -2.02 | 104.43 | 107.37 |
| 37 | Z | 101 | CLA | C6-C7-C8 | -2.02 | 109.24 | 115.97 |
| 37 | 37 | 301 | CLA | CED-O2D-CGD | 2.02 | 120.50 | 115.92 |
| 37 | 31 | 310 | CLA | CHB-C1B-C2B | -2.02 | 121.56 | 127.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 48 | 31 | 312 | A86 | C8-C6-C5 | -2.02 | 115.83 | 119.01 |
| 37 | B | 516 | CLA | CHB-C4A-NA | 2.02 | 127.32 | 124.40 |
| 47 | 38 | 205 | KC1 | CAA-C2A-C1A | -2.02 | 115.78 | 124.64 |
| 37 | 36 | 309 | CLA | CMC-C2C-C1C | 2.02 | 128.19 | 125.03 |
| 37 | 32 | 208 | CLA | O1D-CGD-CBD | -2.02 | 120.53 | 124.52 |
| 37 | d | 404 | CLA | CHA-C1A-NA | -2.02 | 121.81 | 126.39 |
| 48 | 32 | 221 | A86 | C25-C24-C1 | -2.02 | 120.82 | 126.36 |
| 37 | 18 | 203 | CLA | CGD-CBD-CAD | -2.02 | 104.31 | 110.85 |
| 39 | 5 | 101 | BCR | C15-C16-C17 | -2.02 | 119.39 | 123.52 |
| 37 | B | 502 | CLA | CBC-CAC-C3C | -2.02 | 106.94 | 112.42 |
| 47 | 37 | 304 | KC1 | C3D-C2D-C1D | -2.02 | 99.95 | 106.40 |
| 37 | 14 | 302 | CLA | CHB-C1B-C2B | -2.02 | 121.56 | 127.43 |
| 37 | B | 516 | CLA | C6-C7-C8 | -2.02 | 109.25 | 115.97 |
| 37 | 20 | 301 | CLA | O1D-CGD-CBD | -2.02 | 120.53 | 124.52 |
| 37 | b | 515 | CLA | C2A-C3A-C4A | -2.02 | 98.61 | 101.87 |
| 44 | c | 516 | DGD | C7A-C6A-C5A | -2.02 | 104.16 | 114.37 |
| 37 | 34 | 305 | CLA | CMC-C2C-C1C | 2.02 | 128.19 | 125.03 |
| 39 | K | 101 | BCR | C4-C5-C6 | 2.02 | 125.43 | 122.70 |
| 37 | 34 | 308 | CLA | C6-C7-C8 | -2.02 | 109.25 | 115.97 |
| 37 | C | 507 | CLA | CHA-C1A-NA | -2.02 | 121.82 | 126.39 |
| 37 | 39 | 302 | CLA | CMB-C2B-C1B | 2.02 | 128.49 | 125.42 |
| 37 | 12 | 205 | CLA | CHB-C1B-C2B | -2.02 | 121.57 | 127.43 |
| 37 | 38 | 203 | CLA | O2A-CGA-CBA | 2.02 | 117.99 | 111.83 |
| 40 | 36 | 315 | SQD | O47-C7-O49 | -2.02 | 118.99 | 123.70 |
| 37 | z | 102 | CLA | CHA-C1A-NA | -2.02 | 121.82 | 126.39 |
| 37 | 13 | 310 | CLA | CHA-C1A-NA | -2.02 | 121.82 | 126.39 |
| 37 | 38 | 208 | CLA | CHA-C1A-NA | -2.02 | 121.82 | 126.39 |
| 37 | 35 | 308 | CLA | CMB-C2B-C1B | 2.02 | 128.49 | 125.42 |
| 37 | 31 | 308 | CLA | CHB-C1B-C2B | -2.02 | 121.57 | 127.43 |
| 37 | 40 | 203 | CLA | CBB-CAB-C3B | -2.02 | 117.45 | 127.53 |
| 47 | 14 | 306 | KC1 | O2A-CGA-O1A | -2.02 | 118.59 | 122.70 |
| 44 | C | 516 | DGD | C7A-C6A-C5A | -2.02 | 104.17 | 114.37 |
| 44 | c | 517 | DGD | O2D-C2D-C1D | -2.02 | 105.27 | 110.08 |
| 37 | 11 | 307 | CLA | CHB-C1B-C2B | -2.02 | 121.57 | 127.43 |
| 47 | 13 | 302 | KC1 | O1D-CGD-CBD | -2.02 | 120.54 | 124.52 |
| 47 | 12 | 208 | KC1 | CHB-C1B-NB | -2.02 | 121.97 | 124.80 |
| 47 | 32 | 209 | KC1 | CHB-C1B-NB | -2.02 | 121.97 | 124.80 |
| 37 | 32 | 210 | CLA | CBC-CAC-C3C | -2.02 | 106.95 | 112.42 |
| 37 | b | 502 | CLA | CHB-C1B-C2B | -2.02 | 121.57 | 127.43 |
| 37 | b | 510 | CLA | CBC-CAC-C3C | -2.02 | 106.95 | 112.42 |
| 37 | B | 510 | CLA | O1D-CGD-CBD | -2.02 | 120.54 | 124.52 |
| 47 | 34 | 306 | KC1 | CMC-C2C-C1C | 2.02 | 128.18 | 125.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 18 | 210 | KC1 | CHC-C1C-NC | 2.02 | 127.36 | 124.23 |
| 37 | 20 | 301 | CLA | CBB-CAB-C3B | -2.02 | 117.45 | 127.53 |
| 37 | 13 | 303 | CLA | CMC-C2C-C1C | 2.02 | 128.18 | 125.03 |
| 37 | 33 | 308 | CLA | CHA-C1A-NA | -2.02 | 121.83 | 126.39 |
| 37 | b | 511 | CLA | O2A-CGA-O1A | -2.01 | 118.59 | 123.63 |
| 37 | z | 101 | CLA | C6-C7-C8 | -2.01 | 109.27 | 115.97 |
| 48 | 32 | 215 | A86 | C4-C3-C2 | -2.01 | 119.40 | 123.52 |
| 47 | 16 | 304 | KC1 | CMC-C2C-C1C | 2.01 | 128.18 | 125.03 |
| 48 | 14 | 311 | A86 | C36-C31-C32 | -2.01 | 117.70 | 119.70 |
| 44 | C | 517 | DGD | O2D-C2D-C1D | -2.01 | 105.28 | 110.08 |
| 37 | c | 507 | CLA | CAC-C3C-C4C | 2.01 | 127.41 | 124.79 |
| 37 | 18 | 208 | CLA | CHA-C1A-NA | -2.01 | 121.83 | 126.39 |
| 48 | 15 | 313 | A86 | C4-C3-C2 | -2.01 | 119.40 | 123.52 |
| 37 | 21 | 204 | CLA | CHA-C1A-NA | -2.01 | 121.83 | 126.39 |
| 48 | 12 | 214 | A86 | C4-C3-C2 | -2.01 | 119.40 | 123.52 |
| 41 | 32 | 201 | LMG | O7-C10-O9 | -2.01 | 119.00 | 123.70 |
| 37 | 16 | 303 | CLA | O2D-CGD-O1D | -2.01 | 119.93 | 123.85 |
| 37 | 39 | 304 | CLA | CHD-C4C-NC | 2.01 | 127.35 | 124.23 |
| 37 | A | 405 | CLA | C1-O2A-CGA | 2.01 | 121.52 | 116.65 |
| 37 | 14 | 308 | CLA | CHB-C4A-NA | 2.01 | 127.30 | 124.40 |
| 39 | h | 101 | BCR | C29-C30-C25 | 2.01 | 113.36 | 110.44 |
| 37 | 34 | 302 | CLA | CHB-C1B-C2B | -2.01 | 121.59 | 127.43 |
| 37 | 11 | 305 | CLA | O2A-CGA-CBA | 2.01 | 120.35 | 114.00 |
| 37 | 39 | 304 | CLA | O1D-CGD-CBD | -2.01 | 120.55 | 124.52 |
| 37 | C | 501 | CLA | CMD-C2D-C3D | -2.01 | 123.08 | 127.69 |
| 39 | 0 | 101 | BCR | C15-C16-C17 | -2.01 | 119.41 | 123.52 |
| 37 | b | 510 | CLA | O1D-CGD-CBD | -2.01 | 120.55 | 124.52 |
| 37 | 31 | 310 | CLA | CED-O2D-CGD | 2.01 | 120.47 | 115.92 |
| 48 | 12 | 202 | A86 | C4-C3-C2 | -2.01 | 119.41 | 123.52 |
| 48 | 15 | 316 | A86 | O4-C38-O5 | -2.01 | 119.11 | 122.99 |
| 48 | 11 | 312 | A86 | C8-C6-C5 | -2.01 | 115.85 | 119.01 |
| 47 | 15 | 304 | KC1 | CMC-C2C-C1C | 2.01 | 128.17 | 125.03 |
| 47 | 18 | 205 | KC1 | CAA-C2A-C1A | -2.01 | 115.84 | 124.64 |
| 37 | b | 506 | CLA | CBC-CAC-C3C | -2.01 | 106.98 | 112.42 |
| 39 | K | 101 | BCR | C30-C25-C26 | -2.01 | 119.89 | 122.64 |
| 37 | W | 102 | CLA | CMB-C2B-C1B | 2.01 | 128.48 | 125.42 |
| 47 | 19 | 308 | KC1 | O1D-CGD-CBD | -2.01 | 120.56 | 124.52 |
| 48 | 15 | 313 | A86 | C23-C16-C22 | -2.01 | 104.45 | 107.37 |
| 44 | C | 517 | DGD | C7B-C6B-C5B | -2.01 | 104.22 | 114.37 |
| 37 | 41 | 204 | CLA | CHA-C1A-NA | -2.01 | 121.85 | 126.39 |
| 37 | B | 515 | CLA | C2A-C3A-C4A | -2.01 | 98.63 | 101.87 |
| 47 | 12 | 211 | KC1 | CAB-C3B-C4B | 2.01 | 129.61 | 124.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 47 | 14 | 309 | KC1 | CAB-C3B-C4B | 2.01 | 129.61 | 124.82 |
| 37 | c | 508 | CLA | CHA-C1A-NA | -2.01 | 121.85 | 126.39 |
| 48 | 21 | 213 | A86 | C28-C27-C26 | -2.01 | 119.57 | 122.82 |
| 37 | 20 | 306 | CLA | O2A-CGA-O1A | -2.01 | 118.61 | 123.63 |
| 47 | 36 | 304 | KC1 | CBC-CAC-C3C | -2.01 | 106.98 | 112.42 |
| 37 | z | 101 | CLA | O1D-CGD-CBD | -2.01 | 120.56 | 124.52 |
| 37 | 18 | 201 | CLA | O2D-CGD-O1D | -2.01 | 119.94 | 123.85 |
| 48 | 21 | 215 | A86 | C22-C16-C17 | -2.01 | 105.44 | 108.97 |
| 37 | 16 | 307 | CLA | CHB-C1B-C2B | -2.01 | 121.61 | 127.43 |
| 47 | 37 | 305 | KC1 | CHB-C1B-NB | -2.00 | 121.98 | 124.80 |
| 37 | 38 | 209 | CLA | O2A-CGA-O1A | -2.00 | 118.61 | 123.63 |
| 48 | 41 | 215 | A86 | C22-C16-C17 | -2.00 | 105.45 | 108.97 |
| 37 | 19 | 307 | CLA | O2D-CGD-O1D | -2.00 | 119.95 | 123.85 |
| 48 | 17 | 315 | A86 | C34-O4-C38 | -2.00 | 114.31 | 117.85 |
| 48 | 32 | 203 | A86 | C7-C6-C8 | 2.00 | 121.15 | 118.09 |
| 48 | 31 | 315 | A86 | O4-C38-O5 | -2.00 | 119.12 | 122.99 |
| 47 | 40 | 206 | KC1 | CBC-CAC-C3C | -2.00 | 106.99 | 112.42 |
| 40 | 16 | 315 | SQD | O47-C7-O49 | -2.00 | 119.02 | 123.70 |
| 37 | 39 | 305 | CLA | CMA-C3A-C4A | -2.00 | 106.39 | 111.77 |
| 37 | 33 | 310 | CLA | CHA-C1A-NA | -2.00 | 121.86 | 126.39 |
| 37 | C | 507 | CLA | CAC-C3C-C4C | 2.00 | 127.39 | 124.79 |
| 37 | 38 | 204 | CLA | CAA-C2A-C1A | 2.00 | 118.53 | 111.97 |
| 37 | Z | 102 | CLA | CHA-C1A-NA | -2.00 | 121.86 | 126.39 |
| 37 | 31 | 301 | CLA | CBC-CAC-C3C | -2.00 | 107.00 | 112.42 |
| 37 | 14 | 308 | CLA | O2D-CGD-O1D | -2.00 | 119.95 | 123.85 |
| 37 | 16 | 301 | CLA | O2A-CGA-CBA | 2.00 | 117.94 | 111.83 |
| 37 | 35 | 308 | CLA | CHA-C1A-NA | -2.00 | 121.86 | 126.39 |
| 37 | 18 | 208 | CLA | O1D-CGD-CBD | -2.00 | 120.57 | 124.52 |
| 37 | 40 | 203 | CLA | O1D-CGD-CBD | -2.00 | 120.57 | 124.52 |
| 37 | 36 | 301 | CLA | O2A-CGA-CBA | 2.00 | 117.93 | 111.83 |
| 37 | 12 | 212 | CLA | O2A-CGA-CBA | 2.00 | 120.32 | 114.00 |
| 48 | 11 | 315 | A86 | O4-C38-O5 | -2.00 | 119.13 | 122.99 |

All (177) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 37 | A | 403 | CLA | ND |
| 37 | B | 501 | CLA | ND |
| 37 | B | 502 | CLA | ND |
| 37 | B | 503 | CLA | ND |
| 37 | B | 504 | CLA | ND |
| 37 | B | 505 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 37 | B | 506 | CLA | ND |
| 37 | B | 507 | CLA | ND |
| 37 | B | 509 | CLA | ND |
| 37 | B | 510 | CLA | ND |
| 37 | B | 511 | CLA | ND |
| 37 | B | 512 | CLA | ND |
| 37 | B | 513 | CLA | ND |
| 37 | B | 514 | CLA | ND |
| 37 | B | 515 | CLA | ND |
| 37 | B | 516 | CLA | ND |
| 37 | B | 524 | CLA | ND |
| 37 | C | 501 | CLA | ND |
| 37 | C | 502 | CLA | ND |
| 37 | C | 503 | CLA | ND |
| 37 | C | 504 | CLA | ND |
| 37 | C | 505 | CLA | ND |
| 37 | C | 506 | CLA | ND |
| 37 | C | 507 | CLA | ND |
| 37 | C | 508 | CLA | ND |
| 37 | C | 509 | CLA | ND |
| 37 | C | 510 | CLA | ND |
| 37 | C | 511 | CLA | ND |
| 37 | C | 512 | CLA | ND |
| 37 | C | 513 | CLA | ND |
| 37 | D | 401 | CLA | ND |
| 37 | D | 405 | CLA | ND |
| 37 | D | 406 | CLA | ND |
| 37 | Z | 101 | CLA | ND |
| 37 | Z | 102 | CLA | ND |
| 37 | W | 101 | CLA | ND |
| 37 | W | 102 | CLA | ND |
| 37 | a | 403 | CLA | ND |
| 37 | a | 404 | CLA | ND |
| 37 | b | 501 | CLA | ND |
| 37 | b | 502 | CLA | ND |
| 37 | b | 503 | CLA | ND |
| 37 | b | 504 | CLA | ND |
| 37 | b | 505 | CLA | ND |
| 37 | b | 506 | CLA | ND |
| 37 | b | 507 | CLA | ND |
| 37 | b | 509 | CLA | ND |
| 37 | b | 510 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 37 | b | 511 | CLA | ND |
| 37 | b | 512 | CLA | ND |
| 37 | b | 513 | CLA | ND |
| 37 | b | 514 | CLA | ND |
| 37 | b | 515 | CLA | ND |
| 37 | b | 516 | CLA | ND |
| 37 | b | 523 | CLA | ND |
| 37 | c | 501 | CLA | ND |
| 37 | c | 502 | CLA | ND |
| 37 | c | 503 | CLA | ND |
| 37 | c | 504 | CLA | ND |
| 37 | c | 505 | CLA | ND |
| 37 | c | 506 | CLA | ND |
| 37 | c | 507 | CLA | ND |
| 37 | c | 508 | CLA | ND |
| 37 | c | 509 | CLA | ND |
| 37 | c | 510 | CLA | ND |
| 37 | c | 511 | CLA | ND |
| 37 | c | 512 | CLA | ND |
| 37 | c | 513 | CLA | ND |
| 37 | d | 403 | CLA | ND |
| 37 | d | 404 | CLA | ND |
| 37 | z | 101 | CLA | ND |
| 37 | z | 102 | CLA | ND |
| 37 | w | 101 | CLA | ND |
| 37 | 11 | 303 | CLA | ND |
| 37 | 11 | 305 | CLA | ND |
| 37 | 11 | 308 | CLA | ND |
| 37 | 11 | 310 | CLA | ND |
| 37 | 12 | 203 | CLA | ND |
| 37 | 12 | 204 | CLA | ND |
| 37 | 12 | 205 | CLA | ND |
| 37 | 12 | 207 | CLA | ND |
| 37 | 12 | 209 | CLA | ND |
| 37 | 12 | 212 | CLA | ND |
| 37 | 13 | 303 | CLA | ND |
| 37 | 13 | 305 | CLA | ND |
| 37 | 13 | 307 | CLA | ND |
| 37 | 14 | 302 | CLA | ND |
| 37 | 14 | 305 | CLA | ND |
| 37 | 14 | 307 | CLA | ND |
| 37 | 14 | 308 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 37 | 14 | 310 | CLA | ND |
| 37 | 15 | 305 | CLA | ND |
| 37 | 15 | 307 | CLA | ND |
| 37 | 15 | 308 | CLA | ND |
| 37 | 15 | 310 | CLA | ND |
| 37 | 16 | 303 | CLA | ND |
| 37 | 16 | 306 | CLA | ND |
| 37 | 16 | 307 | CLA | ND |
| 37 | 16 | 309 | CLA | ND |
| 37 | 17 | 304 | CLA | ND |
| 37 | 17 | 307 | CLA | ND |
| 37 | 17 | 309 | CLA | ND |
| 37 | 18 | 201 | CLA | ND |
| 37 | 18 | 203 | CLA | ND |
| 37 | 18 | 204 | CLA | ND |
| 37 | 18 | 206 | CLA | ND |
| 37 | 18 | 208 | CLA | ND |
| 37 | 18 | 209 | CLA | ND |
| 37 | 19 | 301 | CLA | ND |
| 37 | 19 | 302 | CLA | ND |
| 37 | 19 | 303 | CLA | ND |
| 37 | 19 | 304 | CLA | ND |
| 37 | 19 | 305 | CLA | ND |
| 37 | 19 | 306 | CLA | ND |
| 37 | 19 | 307 | CLA | ND |
| 37 | 19 | 309 | CLA | ND |
| 37 | 19 | 310 | CLA | ND |
| 37 | 20 | 303 | CLA | ND |
| 37 | 20 | 306 | CLA | ND |
| 37 | 20 | 307 | CLA | ND |
| 37 | 20 | 308 | CLA | ND |
| 37 | 21 | 202 | CLA | ND |
| 37 | 21 | 205 | CLA | ND |
| 37 | 21 | 206 | CLA | ND |
| 37 | 21 | 208 | CLA | ND |
| 37 | 21 | 209 | CLA | ND |
| 37 | 31 | 301 | CLA | ND |
| 37 | 31 | 304 | CLA | ND |
| 37 | 31 | 306 | CLA | ND |
| 37 | 31 | 310 | CLA | ND |
| 37 | 32 | 202 | CLA | ND |
| 37 | 32 | 204 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 37 | 32 | 205 | CLA | ND |
| 37 | 32 | 206 | CLA | ND |
| 37 | 32 | 208 | CLA | ND |
| 37 | 32 | 210 | CLA | ND |
| 37 | 32 | 213 | CLA | ND |
| 37 | 33 | 303 | CLA | ND |
| 37 | 33 | 305 | CLA | ND |
| 37 | 33 | 307 | CLA | ND |
| 37 | 34 | 302 | CLA | ND |
| 37 | 34 | 305 | CLA | ND |
| 37 | 34 | 307 | CLA | ND |
| 37 | 34 | 308 | CLA | ND |
| 37 | 34 | 310 | CLA | ND |
| 37 | 35 | 305 | CLA | ND |
| 37 | 35 | 307 | CLA | ND |
| 37 | 35 | 310 | CLA | ND |
| 37 | 36 | 303 | CLA | ND |
| 37 | 36 | 306 | CLA | ND |
| 37 | 36 | 307 | CLA | ND |
| 37 | 36 | 309 | CLA | ND |
| 37 | 37 | 303 | CLA | ND |
| 37 | 37 | 306 | CLA | ND |
| 37 | 37 | 308 | CLA | ND |
| 37 | 38 | 201 | CLA | ND |
| 37 | 38 | 203 | CLA | ND |
| 37 | 38 | 204 | CLA | ND |
| 37 | 38 | 208 | CLA | ND |
| 37 | 38 | 209 | CLA | ND |
| 37 | 39 | 301 | CLA | ND |
| 37 | 39 | 302 | CLA | ND |
| 37 | 39 | 303 | CLA | ND |
| 37 | 39 | 304 | CLA | ND |
| 37 | 39 | 305 | CLA | ND |
| 37 | 39 | 307 | CLA | ND |
| 37 | 39 | 309 | CLA | ND |
| 37 | 39 | 310 | CLA | ND |
| 37 | 40 | 205 | CLA | ND |
| 37 | 40 | 208 | CLA | ND |
| 37 | 40 | 209 | CLA | ND |
| 37 | 40 | 210 | CLA | ND |
| 37 | 41 | 202 | CLA | ND |
| 37 | 41 | 205 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 37 | 41 | 206 | CLA | ND |
| 37 | 41 | 208 | CLA | ND |
| 37 | 41 | 209 | CLA | ND |

All (5098) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | B | 503 | CLA | C2B-C3B-CAB-CBB |
| 37 | B | 503 | CLA | C4B-C3B-CAB-CBB |
| 37 | B | 504 | CLA | C2B-C3B-CAB-CBB |
| 37 | B | 504 | CLA | C4B-C3B-CAB-CBB |
| 37 | B | 514 | CLA | CAD-CBD-CGD-O1D |
| 37 | B | 514 | CLA | CAD-CBD-CGD-O2D |
| 37 | B | 516 | CLA | CHA-CBD-CGD-O1D |
| 37 | B | 516 | CLA | CHA-CBD-CGD-O2D |
| 37 | C | 501 | CLA | C1A-C2A-CAA-CBA |
| 37 | C | 501 | CLA | C2-C3-C5-C6 |
| 37 | C | 501 | CLA | C4-C3-C5-C6 |
| 37 | C | 502 | CLA | C2B-C3B-CAB-CBB |
| 37 | C | 502 | CLA | C4B-C3B-CAB-CBB |
| 37 | C | 503 | CLA | C4B-C3B-CAB-CBB |
| 37 | C | 503 | CLA | C14-C13-C15-C16 |
| 37 | C | 504 | CLA | C2-C3-C5-C6 |
| 37 | C | 504 | CLA | C4-C3-C5-C6 |
| 37 | C | 506 | CLA | C1A-C2A-CAA-CBA |
| 37 | D | 405 | CLA | C1A-C2A-CAA-CBA |
| 37 | D | 405 | CLA | C3A-C2A-CAA-CBA |
| 37 | a | 404 | CLA | C1A-C2A-CAA-CBA |
| 37 | b | 503 | CLA | C2B-C3B-CAB-CBB |
| 37 | b | 503 | CLA | C4B-C3B-CAB-CBB |
| 37 | b | 504 | CLA | C2B-C3B-CAB-CBB |
| 37 | b | 504 | CLA | C4B-C3B-CAB-CBB |
| 37 | b | 514 | CLA | CAD-CBD-CGD-O1D |
| 37 | b | 514 | CLA | CAD-CBD-CGD-O2D |
| 37 | b | 516 | CLA | CHA-CBD-CGD-O1D |
| 37 | b | 516 | CLA | CHA-CBD-CGD-O2D |
| 37 | c | 501 | CLA | C1A-C2A-CAA-CBA |
| 37 | c | 501 | CLA | C2-C3-C5-C6 |
| 37 | c | 501 | CLA | C4-C3-C5-C6 |
| 37 | c | 502 | CLA | C2B-C3B-CAB-CBB |
| 37 | c | 502 | CLA | C4B-C3B-CAB-CBB |
| 37 | c | 503 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | c | 503 | CLA | C14-C13-C15-C16 |
| 37 | c | 504 | CLA | C2-C3-C5-C6 |
| 37 | c | 504 | CLA | C4-C3-C5-C6 |
| 37 | c | 506 | CLA | C1A-C2A-CAA-CBA |
| 37 | d | 403 | CLA | C1A-C2A-CAA-CBA |
| 37 | d | 403 | CLA | C3A-C2A-CAA-CBA |
| 37 | 11 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 11 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 11 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 11 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 11 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 11 | 310 | CLA | CBD-CGD-O2D-CED |
| 37 | 12 | 203 | CLA | C3A-C2A-CAA-CBA |
| 37 | 12 | 204 | CLA | C1A-C2A-CAA-CBA |
| 37 | 12 | 205 | CLA | C1A-C2A-CAA-CBA |
| 37 | 12 | 212 | CLA | CHA-CBD-CGD-O1D |
| 37 | 12 | 212 | CLA | CHA-CBD-CGD-O2D |
| 37 | 13 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 13 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 13 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 13 | 307 | CLA | CHA-CBD-CGD-O1D |
| 37 | 13 | 307 | CLA | CHA-CBD-CGD-O2D |
| 37 | 14 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 14 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 14 | 302 | CLA | C6-C7-C8-C9 |
| 37 | 14 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 14 | 303 | CLA | C4B-C3B-CAB-CBB |
| 37 | 14 | 307 | CLA | C2B-C3B-CAB-CBB |
| 37 | 14 | 307 | CLA | C4B-C3B-CAB-CBB |
| 37 | 15 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 15 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 15 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 15 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 15 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 15 | 310 | CLA | CHA-CBD-CGD-O1D |
| 37 | 15 | 310 | CLA | CHA-CBD-CGD-O2D |
| 37 | 16 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 16 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 16 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 16 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 16 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 16 | 306 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 16 | 306 | CLA | C2B-C3B-CAB-CBB |
| 37 | 16 | 306 | CLA | C4B-C3B-CAB-CBB |
| 37 | 16 | 309 | CLA | C1A-C2A-CAA-CBA |
| 37 | 17 | 302 | CLA | C4B-C3B-CAB-CBB |
| 37 | 17 | 304 | CLA | C1A-C2A-CAA-CBA |
| 37 | 17 | 309 | CLA | CHA-CBD-CGD-O1D |
| 37 | 17 | 309 | CLA | CHA-CBD-CGD-O2D |
| 37 | 18 | 202 | CLA | C1A-C2A-CAA-CBA |
| 37 | 18 | 202 | CLA | C3A-C2A-CAA-CBA |
| 37 | 18 | 204 | CLA | C1A-C2A-CAA-CBA |
| 37 | 18 | 208 | CLA | C4B-C3B-CAB-CBB |
| 37 | 18 | 208 | CLA | CHA-CBD-CGD-O2D |
| 37 | 19 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 19 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 19 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 19 | 303 | CLA | C4B-C3B-CAB-CBB |
| 37 | 19 | 305 | CLA | C2-C3-C5-C6 |
| 37 | 20 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 20 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 20 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 20 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 20 | 307 | CLA | CHA-CBD-CGD-O1D |
| 37 | 20 | 307 | CLA | CHA-CBD-CGD-O2D |
| 37 | 21 | 204 | CLA | C1A-C2A-CAA-CBA |
| 37 | 21 | 208 | CLA | C2-C3-C5-C6 |
| 37 | 21 | 208 | CLA | C4-C3-C5-C6 |
| 37 | 21 | 209 | CLA | CHA-CBD-CGD-O1D |
| 37 | 21 | 209 | CLA | CHA-CBD-CGD-O2D |
| 37 | 21 | 210 | CLA | CHA-CBD-CGD-O1D |
| 37 | 21 | 210 | CLA | CHA-CBD-CGD-O2D |
| 37 | 31 | 302 | CLA | C1A-C2A-CAA-CBA |
| 37 | 31 | 302 | CLA | C3A-C2A-CAA-CBA |
| 37 | 31 | 302 | CLA | C2B-C3B-CAB-CBB |
| 37 | 31 | 302 | CLA | C4B-C3B-CAB-CBB |
| 37 | 31 | 304 | CLA | C1A-C2A-CAA-CBA |
| 37 | 31 | 310 | CLA | CBD-CGD-O2D-CED |
| 37 | 32 | 204 | CLA | C3A-C2A-CAA-CBA |
| 37 | 32 | 205 | CLA | C1A-C2A-CAA-CBA |
| 37 | 32 | 206 | CLA | C1A-C2A-CAA-CBA |
| 37 | 32 | 213 | CLA | CHA-CBD-CGD-O1D |
| 37 | 32 | 213 | CLA | CHA-CBD-CGD-O2D |
| 37 | 33 | 301 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 33 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 33 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 33 | 307 | CLA | CHA-CBD-CGD-O1D |
| 37 | 33 | 307 | CLA | CHA-CBD-CGD-O2D |
| 37 | 34 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 34 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 34 | 302 | CLA | C6-C7-C8-C9 |
| 37 | 34 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 34 | 303 | CLA | C4B-C3B-CAB-CBB |
| 37 | 34 | 307 | CLA | C2B-C3B-CAB-CBB |
| 37 | 34 | 307 | CLA | C4B-C3B-CAB-CBB |
| 37 | 35 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 35 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 35 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 35 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 35 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 35 | 310 | CLA | CHA-CBD-CGD-O1D |
| 37 | 35 | 310 | CLA | CHA-CBD-CGD-O2D |
| 37 | 36 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 36 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 36 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 36 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 36 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 36 | 306 | CLA | C1A-C2A-CAA-CBA |
| 37 | 36 | 306 | CLA | C2B-C3B-CAB-CBB |
| 37 | 36 | 306 | CLA | C4B-C3B-CAB-CBB |
| 37 | 36 | 309 | CLA | C1A-C2A-CAA-CBA |
| 37 | 37 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 37 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 37 | 308 | CLA | CHA-CBD-CGD-O1D |
| 37 | 37 | 308 | CLA | CHA-CBD-CGD-O2D |
| 37 | 37 | 308 | CLA | CBD-CGD-O2D-CED |
| 37 | 38 | 202 | CLA | C1A-C2A-CAA-CBA |
| 37 | 38 | 202 | CLA | C3A-C2A-CAA-CBA |
| 37 | 38 | 202 | CLA | CBD-CGD-O2D-CED |
| 37 | 38 | 204 | CLA | C1A-C2A-CAA-CBA |
| 37 | 38 | 208 | CLA | C4B-C3B-CAB-CBB |
| 37 | 38 | 208 | CLA | CHA-CBD-CGD-O2D |
| 37 | 39 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 39 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 39 | 302 | CLA | C4-C3-C5-C6 |
| 37 | 39 | 303 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 39 | 305 | CLA | C2-C3-C5-C6 |
| 37 | 40 | 203 | CLA | C1A-C2A-CAA-CBA |
| 37 | 40 | 203 | CLA | C2B-C3B-CAB-CBB |
| 37 | 40 | 203 | CLA | C4B-C3B-CAB-CBB |
| 37 | 40 | 205 | CLA | C1A-C2A-CAA-CBA |
| 37 | 40 | 209 | CLA | CHA-CBD-CGD-O1D |
| 37 | 40 | 209 | CLA | CHA-CBD-CGD-O2D |
| 37 | 41 | 204 | CLA | C1A-C2A-CAA-CBA |
| 37 | 41 | 208 | CLA | C2-C3-C5-C6 |
| 37 | 41 | 208 | CLA | C4-C3-C5-C6 |
| 37 | 41 | 209 | CLA | CHA-CBD-CGD-O1D |
| 37 | 41 | 209 | CLA | CHA-CBD-CGD-O2D |
| 37 | 41 | 210 | CLA | CHA-CBD-CGD-O1D |
| 37 | 41 | 210 | CLA | CHA-CBD-CGD-O2D |
| 39 | A | 406 | BCR | C7-C8-C9-C10 |
| 39 | A | 406 | BCR | C7-C8-C9-C34 |
| 39 | A | 410 | BCR | C6-C7-C8-C9 |
| 39 | A | 410 | BCR | C7-C8-C9-C10 |
| 39 | B | 517 | BCR | C20-C21-C22-C37 |
| 39 | B | 517 | BCR | C21-C22-C23-C24 |
| 39 | B | 518 | BCR | C7-C8-C9-C10 |
| 39 | B | 525 | BCR | C11-C10-C9-C8 |
| 39 | B | 525 | BCR | C10-C11-C12-C13 |
| 39 | B | 525 | BCR | C37-C22-C23-C24 |
| 39 | C | 514 | BCR | C21-C22-C23-C24 |
| 39 | C | 514 | BCR | C37-C22-C23-C24 |
| 39 | C | 515 | BCR | C7-C8-C9-C10 |
| 39 | C | 515 | BCR | C7-C8-C9-C34 |
| 39 | D | 407 | BCR | C7-C8-C9-C10 |
| 39 | D | 407 | BCR | C7-C8-C9-C34 |
| 39 | D | 407 | BCR | C11-C10-C9-C34 |
| 39 | D | 407 | BCR | C21-C22-C23-C24 |
| 39 | D | 407 | BCR | C22-C23-C24-C25 |
| 39 | H | 101 | BCR | C21-C22-C23-C24 |
| 39 | H | 101 | BCR | C37-C22-C23-C24 |
| 39 | K | 101 | BCR | C6-C7-C8-C9 |
| 39 | K | 101 | BCR | C10-C11-C12-C13 |
| 39 | K | 101 | BCR | C11-C12-C13-C14 |
| 39 | K | 101 | BCR | C11-C12-C13-C35 |
| 39 | K | 101 | BCR | C18-C19-C20-C21 |
| 39 | K | 101 | BCR | C21-C22-C23-C24 |
| 39 | 0 | 101 | BCR | C7-C8-C9-C10 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | a | 408 | BCR | C7-C8-C9-C10 |
| 39 | a | 408 | BCR | C7-C8-C9-C34 |
| 39 | a | 413 | BCR | C6-C7-C8-C9 |
| 39 | a | 413 | BCR | C7-C8-C9-C10 |
| 39 | b | 517 | BCR | C20-C21-C22-C37 |
| 39 | b | 517 | BCR | C21-C22-C23-C24 |
| 39 | b | 518 | BCR | C7-C8-C9-C10 |
| 39 | b | 524 | BCR | C11-C10-C9-C8 |
| 39 | b | 524 | BCR | C10-C11-C12-C13 |
| 39 | b | 524 | BCR | C37-C22-C23-C24 |
| 39 | c | 514 | BCR | C21-C22-C23-C24 |
| 39 | c | 514 | BCR | C37-C22-C23-C24 |
| 39 | c | 515 | BCR | C7-C8-C9-C10 |
| 39 | c | 515 | BCR | C7-C8-C9-C34 |
| 39 | d | 405 | BCR | C7-C8-C9-C10 |
| 39 | d | 405 | BCR | C7-C8-C9-C34 |
| 39 | d | 405 | BCR | C11-C10-C9-C34 |
| 39 | d | 405 | BCR | C21-C22-C23-C24 |
| 39 | d | 405 | BCR | C22-C23-C24-C25 |
| 39 | h | 101 | BCR | C21-C22-C23-C24 |
| 39 | h | 101 | BCR | C37-C22-C23-C24 |
| 39 | y | 101 | BCR | C6-C7-C8-C9 |
| 39 | y | 101 | BCR | C10-C11-C12-C13 |
| 39 | y | 101 | BCR | C11-C12-C13-C14 |
| 39 | y | 101 | BCR | C11-C12-C13-C35 |
| 39 | y | 101 | BCR | C18-C19-C20-C21 |
| 39 | y | 101 | BCR | C21-C22-C23-C24 |
| 39 | 5 | 101 | BCR | C7-C8-C9-C10 |
| 40 | A | 407 | SQD | C5-C6-S-O7 |
| 40 | B | 519 | SQD | O5-C1-O6-C44 |
| 40 | B | 519 | SQD | C8-C7-O47-C45 |
| 40 | B | 519 | SQD | O5-C5-C6-S |
| 40 | L | 101 | SQD | O5-C1-O6-C44 |
| 40 | L | 101 | SQD | C8-C7-O47-C45 |
| 40 | L | 101 | SQD | O5-C5-C6-S |
| 40 | a | 409 | SQD | C5-C6-S-O7 |
| 40 | 16 | 315 | SQD | O5-C5-C6-S |
| 40 | 17 | 301 | SQD | C2-C1-O6-C44 |
| 40 | 17 | 301 | SQD | O5-C1-O6-C44 |
| 40 | 17 | 301 | SQD | C8-C7-O47-C45 |
| 40 | 17 | 301 | SQD | C5-C6-S-O7 |
| 40 | 17 | 301 | SQD | C5-C6-S-O8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 40 | 17 | 301 | SQD | C5-C6-S-O9 |
| 40 | 36 | 315 | SQD | C2-C1-O6-C44 |
| 40 | 36 | 315 | SQD | O5-C1-O6-C44 |
| 40 | 36 | 315 | SQD | C8-C7-O47-C45 |
| 40 | 36 | 315 | SQD | C5-C6-S-O7 |
| 40 | 36 | 315 | SQD | C5-C6-S-O8 |
| 40 | 36 | 315 | SQD | C5-C6-S-O9 |
| 40 | 40 | 202 | SQD | O5-C5-C6-S |
| 41 | A | 408 | LMG | O1-C7-C8-O7 |
| 41 | L | 102 | LMG | O9-C10-O7-C8 |
| 41 | a | 410 | LMG | O1-C7-C8-O7 |
| 41 | l | 101 | LMG | O9-C10-O7-C8 |
| 41 | 11 | 316 | LMG | O9-C10-O7-C8 |
| 41 | 11 | 316 | LMG | C11-C10-O7-C8 |
| 41 | 12 | 201 | LMG | O6-C1-O1-C7 |
| 41 | 17 | 317 | LMG | O9-C10-O7-C8 |
| 41 | 17 | 317 | LMG | C11-C10-O7-C8 |
| 41 | 31 | 316 | LMG | O9-C10-O7-C8 |
| 41 | 31 | 316 | LMG | C11-C10-O7-C8 |
| 41 | 32 | 201 | LMG | O6-C1-O1-C7 |
| 41 | 37 | 316 | LMG | O9-C10-O7-C8 |
| 41 | 37 | 316 | LMG | C11-C10-O7-C8 |
| 43 | B | 523 | LHG | C4-O6-P-O5 |
| 43 | D | 409 | LHG | O1-C1-C2-C3 |
| 43 | D | 409 | LHG | C1-C2-C3-O3 |
| 43 | D | 410 | LHG | C3-O3-P-O4 |
| 43 | D | 410 | LHG | C4-O6-P-O3 |
| 43 | D | 410 | LHG | C4-O6-P-O4 |
| 43 | D | 410 | LHG | C4-O6-P-O5 |
| 43 | D | 410 | LHG | C8-C7-O7-C5 |
| 43 | D | 411 | LHG | C4-O6-P-O3 |
| 43 | D | 411 | LHG | C4-O6-P-O4 |
| 43 | D | 411 | LHG | C4-O6-P-O5 |
| 43 | D | 411 | LHG | C8-C7-O7-C5 |
| 43 | a | 412 | LHG | C4-O6-P-O3 |
| 43 | a | 412 | LHG | C4-O6-P-O4 |
| 43 | a | 412 | LHG | C4-O6-P-O5 |
| 43 | a | 412 | LHG | C8-C7-O7-C5 |
| 43 | b | 522 | LHG | C4-O6-P-O5 |
| 43 | d | 407 | LHG | O1-C1-C2-C3 |
| 43 | d | 407 | LHG | C1-C2-C3-O3 |
| 43 | d | 408 | LHG | C3-O3-P-O4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | d | 408 | LHG | C4-O6-P-O3 |
| 43 | d | 408 | LHG | C4-O6-P-O4 |
| 43 | d | 408 | LHG | C4-O6-P-O5 |
| 43 | d | 408 | LHG | C8-C7-O7-C5 |
| 43 | 17 | 316 | LHG | C4-O6-P-O5 |
| 43 | 19 | 314 | LHG | C3-O3-P-O4 |
| 43 | 21 | 201 | LHG | C3-O3-P-O4 |
| 43 | 21 | 201 | LHG | C3-O3-P-O6 |
| 43 | 21 | 201 | LHG | C4-O6-P-O3 |
| 43 | 21 | 201 | LHG | C4-O6-P-O4 |
| 43 | 21 | 217 | LHG | O1-C1-C2-C3 |
| 43 | 21 | 217 | LHG | C3-O3-P-O5 |
| 43 | 21 | 217 | LHG | C4-O6-P-O3 |
| 43 | 21 | 217 | LHG | C4-O6-P-O4 |
| 43 | 21 | 217 | LHG | O7-C5-C6-O8 |
| 43 | 37 | 315 | LHG | C4-O6-P-O5 |
| 43 | 37 | 321 | LHG | O1-C1-C2-C3 |
| 43 | 37 | 321 | LHG | C3-O3-P-O5 |
| 43 | 37 | 321 | LHG | C4-O6-P-O3 |
| 43 | 37 | 321 | LHG | C4-O6-P-O4 |
| 43 | 37 | 321 | LHG | O7-C5-C6-O8 |
| 43 | 39 | 314 | LHG | C3-O3-P-O4 |
| 43 | 41 | 201 | LHG | C3-O3-P-O4 |
| 43 | 41 | 201 | LHG | C3-O3-P-O6 |
| 43 | 41 | 201 | LHG | C4-O6-P-O3 |
| 43 | 41 | 201 | LHG | C4-O6-P-O4 |
| 45 | D | 404 | PL9 | C9-C11-C12-C13 |
| 45 | D | 404 | PL9 | C32-C33-C34-C36 |
| 45 | D | 404 | PL9 | C37-C38-C39-C40 |
| 45 | D | 404 | PL9 | C44-C46-C47-C48 |
| 45 | D | 408 | PL9 | C39-C41-C42-C43 |
| 45 | d | 402 | PL9 | C9-C11-C12-C13 |
| 45 | d | 402 | PL9 | C32-C33-C34-C36 |
| 45 | d | 402 | PL9 | C37-C38-C39-C40 |
| 45 | d | 402 | PL9 | C44-C46-C47-C48 |
| 45 | d | 406 | PL9 | C39-C41-C42-C43 |
| 46 | F | 101 | HEM | C1A-C2A-CAA-CBA |
| 46 | V | 201 | HEM | C2B-C3B-CAB-CBB |
| 46 | V | 201 | HEM | C4B-C3B-CAB-CBB |
| 46 | f | 101 | HEM | C1A-C2A-CAA-CBA |
| 46 | v | 201 | HEM | C2B-C3B-CAB-CBB |
| 46 | v | 201 | HEM | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 46 | v | 201 | HEM | C2C-C3C-CAC-CBC |
| 46 | v | 201 | HEM | C4C-C3C-CAC-CBC |
| 47 | 11 | 302 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 11 | 302 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 11 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 11 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 11 | 306 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 11 | 306 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 11 | 306 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 11 | 309 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 11 | 309 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 11 | 309 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 11 | 309 | KC1 | CHA-CBD-CGD-O2D |
| 47 | 12 | 206 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 12 | 206 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 12 | 206 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 12 | 208 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 12 | 211 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 12 | 211 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 13 | 302 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 13 | 302 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 13 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 13 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 13 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 13 | 306 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 13 | 306 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 13 | 309 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 13 | 309 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 14 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 14 | 306 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 14 | 306 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 14 | 309 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 15 | 302 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 15 | 302 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 15 | 302 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 15 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 15 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 15 | 306 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 15 | 306 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 15 | 309 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 15 | 309 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 16 | 302 | KC1 | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 47 | 16 | 302 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 16 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 16 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 16 | 305 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 16 | 308 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 16 | 308 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 17 | 303 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 17 | 303 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 17 | 305 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 17 | 306 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 17 | 306 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 17 | 308 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 17 | 308 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 18 | 205 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 18 | 205 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 18 | 207 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 18 | 207 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 18 | 207 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 18 | 207 | KC1 | CHA-CBD-CGD-O2D |
| 47 | 18 | 210 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 19 | 308 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 20 | 302 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 20 | 302 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 20 | 302 | KC1 | CBD-CGD-O2D-CED |
| 47 | 20 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 20 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 20 | 305 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 20 | 305 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 21 | 203 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 21 | 203 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 21 | 207 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 31 | 303 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 31 | 303 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 31 | 305 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 31 | 305 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 31 | 307 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 31 | 307 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 31 | 307 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 31 | 309 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 31 | 309 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 31 | 309 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 31 | 309 | KC1 | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 47 | 32 | 207 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 32 | 207 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 32 | 207 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 32 | 209 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 32 | 212 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 32 | 212 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 33 | 302 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 33 | 302 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 33 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 33 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 33 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 33 | 306 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 33 | 306 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 33 | 309 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 33 | 309 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 34 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 34 | 306 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 34 | 306 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 34 | 309 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 35 | 302 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 35 | 302 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 35 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 35 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 35 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 35 | 306 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 35 | 306 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 35 | 309 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 35 | 309 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 36 | 302 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 36 | 302 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 36 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 36 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 36 | 305 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 36 | 308 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 36 | 308 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 37 | 302 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 37 | 302 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 37 | 304 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 37 | 305 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 37 | 305 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 37 | 307 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 37 | 307 | KC1 | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 47 | 38 | 205 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 38 | 205 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 38 | 207 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 38 | 207 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 38 | 207 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 38 | 207 | KC1 | CHA-CBD-CGD-O2D |
| 47 | 38 | 210 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 39 | 308 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 40 | 204 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 40 | 204 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 40 | 204 | KC1 | CBD-CGD-O2D-CED |
| 47 | 40 | 206 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 40 | 206 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 40 | 207 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 40 | 207 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 41 | 203 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 41 | 203 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 41 | 207 | KC1 | C2B-C3B-CAB-CBB |
| 48 | 11 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 11 | 311 | A86 | O5-C38-O4-C34 |
| 48 | 11 | 312 | A86 | C24-C25-C26-C27 |
| 48 | 11 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 11 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 11 | 314 | A86 | C-C1-C24-C25 |
| 48 | 11 | 314 | A86 | C2-C1-C24-C25 |
| 48 | 11 | 314 | A86 | C12-C11-C13-O |
| 48 | 11 | 315 | A86 | C39-C38-O4-C34 |
| 48 | 11 | 315 | A86 | O5-C38-O4-C34 |
| 48 | 12 | 202 | A86 | C11-C10-C9-C8 |
| 48 | 12 | 202 | A86 | C10-C11-C13-O |
| 48 | 12 | 202 | A86 | C12-C11-C13-O |
| 48 | 12 | 202 | A86 | C13-C14-C15-C16 |
| 48 | 12 | 202 | A86 | C39-C38-O4-C34 |
| 48 | 12 | 202 | A86 | C5-C6-C8-C9 |
| 48 | 12 | 213 | A86 | C2-C1-C24-C25 |
| 48 | 12 | 215 | A86 | C26-C27-C29-C30 |
| 48 | 12 | 215 | A86 | C35-C34-O4-C38 |
| 48 | 12 | 216 | A86 | C-C1-C24-C25 |
| 48 | 12 | 216 | A86 | C2-C1-C24-C25 |
| 48 | 12 | 216 | A86 | C39-C38-O4-C34 |
| 48 | 12 | 216 | A86 | C5-C6-C8-C9 |
| 48 | 12 | 217 | A86 | O-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 12 | 217 | A86 | C11-C13-C14-C15 |
| 48 | 12 | 217 | A86 | C13-C14-C15-C16 |
| 48 | 12 | 217 | A86 | O5-C38-O4-C34 |
| 48 | 12 | 220 | A86 | C-C1-C24-C25 |
| 48 | 12 | 220 | A86 | C2-C1-C24-C25 |
| 48 | 12 | 220 | A86 | C11-C10-C9-C8 |
| 48 | 12 | 220 | A86 | O5-C38-O4-C34 |
| 48 | 12 | 220 | A86 | C3-C4-C5-C6 |
| 48 | 13 | 311 | A86 | C-C1-C24-C25 |
| 48 | 13 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 13 | 312 | A86 | C39-C38-O4-C34 |
| 48 | 13 | 312 | A86 | C5-C6-C8-C9 |
| 48 | 13 | 312 | A86 | C7-C6-C8-C9 |
| 48 | 13 | 313 | A86 | C12-C11-C13-C14 |
| 48 | 13 | 313 | A86 | O-C13-C14-C15 |
| 48 | 13 | 313 | A86 | C11-C13-C14-C15 |
| 48 | 13 | 313 | A86 | C33-C34-O4-C38 |
| 48 | 13 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 13 | 314 | A86 | C11-C10-C9-C8 |
| 48 | 13 | 314 | A86 | C13-C14-C15-C16 |
| 48 | 13 | 314 | A86 | C24-C25-C26-C27 |
| 48 | 13 | 314 | A86 | C39-C38-O4-C34 |
| 48 | 13 | 315 | A86 | C11-C10-C9-C8 |
| 48 | 13 | 315 | A86 | C13-C14-C15-C16 |
| 48 | 13 | 315 | A86 | O5-C38-O4-C34 |
| 48 | 13 | 315 | A86 | C5-C6-C8-C9 |
| 48 | 13 | 315 | A86 | C7-C6-C8-C9 |
| 48 | 14 | 311 | A86 | O-C13-C14-C15 |
| 48 | 14 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 14 | 313 | A86 | C-C1-C24-C25 |
| 48 | 14 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 14 | 313 | A86 | O-C13-C14-C15 |
| 48 | 14 | 313 | A86 | C24-C25-C26-C27 |
| 48 | 14 | 313 | A86 | C26-C27-C29-C30 |
| 48 | 14 | 313 | A86 | C33-C34-O4-C38 |
| 48 | 14 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 14 | 313 | A86 | C5-C6-C8-C9 |
| 48 | 14 | 313 | A86 | C7-C6-C8-C9 |
| 48 | 14 | 314 | A86 | C-C1-C24-C25 |
| 48 | 14 | 314 | A86 | C2-C1-C24-C25 |
| 48 | 14 | 314 | A86 | C39-C38-O4-C34 |
| 48 | 14 | 314 | A86 | C5-C6-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 14 | 314 | A86 | C7-C6-C8-C9 |
| 48 | 14 | 316 | A86 | O-C13-C14-C15 |
| 48 | 14 | 316 | A86 | C11-C13-C14-C15 |
| 48 | 14 | 316 | A86 | C13-C14-C15-C16 |
| 48 | 15 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 15 | 311 | A86 | O5-C38-O4-C34 |
| 48 | 15 | 312 | A86 | C39-C38-O4-C34 |
| 48 | 15 | 312 | A86 | C5-C6-C8-C9 |
| 48 | 15 | 312 | A86 | C7-C6-C8-C9 |
| 48 | 15 | 313 | A86 | O-C13-C14-C15 |
| 48 | 15 | 313 | A86 | C26-C27-C29-C30 |
| 48 | 15 | 314 | A86 | C2-C1-C24-C25 |
| 48 | 15 | 314 | A86 | C11-C10-C9-C8 |
| 48 | 15 | 314 | A86 | C39-C38-O4-C34 |
| 48 | 15 | 315 | A86 | C2-C1-C24-C25 |
| 48 | 15 | 315 | A86 | C39-C38-O4-C34 |
| 48 | 15 | 315 | A86 | O5-C38-O4-C34 |
| 48 | 15 | 315 | A86 | C5-C6-C8-C9 |
| 48 | 15 | 315 | A86 | C7-C6-C8-C9 |
| 48 | 15 | 316 | A86 | O-C13-C14-C15 |
| 48 | 15 | 316 | A86 | C11-C13-C14-C15 |
| 48 | 15 | 316 | A86 | C13-C14-C15-C16 |
| 48 | 15 | 316 | A86 | O5-C38-O4-C34 |
| 48 | 15 | 319 | A86 | C39-C38-O4-C34 |
| 48 | 15 | 319 | A86 | C5-C6-C8-C9 |
| 48 | 15 | 319 | A86 | C7-C6-C8-C9 |
| 48 | 16 | 310 | A86 | C39-C38-O4-C34 |
| 48 | 16 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 16 | 313 | A86 | C12-C11-C13-C14 |
| 48 | 16 | 314 | A86 | C10-C11-C13-O |
| 48 | 16 | 314 | A86 | C12-C11-C13-O |
| 48 | 16 | 314 | A86 | O5-C38-O4-C34 |
| 48 | 17 | 310 | A86 | C12-C11-C13-C14 |
| 48 | 17 | 311 | A86 | C5-C6-C8-C9 |
| 48 | 17 | 311 | A86 | C7-C6-C8-C9 |
| 48 | 17 | 312 | A86 | C24-C25-C26-C27 |
| 48 | 17 | 312 | A86 | C33-C34-O4-C38 |
| 48 | 17 | 312 | A86 | C39-C38-O4-C34 |
| 48 | 17 | 313 | A86 | C-C1-C24-C25 |
| 48 | 17 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 17 | 314 | A86 | C-C1-C24-C25 |
| 48 | 17 | 314 | A86 | C2-C1-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 17 | 314 | A86 | O-C13-C14-C15 |
| 48 | 17 | 314 | A86 | C11-C13-C14-C15 |
| 48 | 17 | 314 | A86 | C5-C6-C8-C9 |
| 48 | 17 | 314 | A86 | C7-C6-C8-C9 |
| 48 | 17 | 315 | A86 | C11-C10-C9-C8 |
| 48 | 17 | 315 | A86 | C10-C11-C13-O |
| 48 | 17 | 315 | A86 | C12-C11-C13-O |
| 48 | 17 | 315 | A86 | C11-C13-C14-C15 |
| 48 | 17 | 315 | A86 | C13-C14-C15-C16 |
| 48 | 17 | 320 | A86 | C-C1-C24-C25 |
| 48 | 17 | 320 | A86 | C2-C1-C24-C25 |
| 48 | 17 | 320 | A86 | C39-C38-O4-C34 |
| 48 | 17 | 320 | A86 | C5-C6-C8-C9 |
| 48 | 18 | 212 | A86 | O-C13-C14-C15 |
| 48 | 18 | 212 | A86 | C24-C25-C26-C27 |
| 48 | 18 | 212 | A86 | C39-C38-O4-C34 |
| 48 | 18 | 213 | A86 | C5-C6-C8-C9 |
| 48 | 18 | 213 | A86 | C7-C6-C8-C9 |
| 48 | 18 | 214 | A86 | C-C1-C24-C25 |
| 48 | 18 | 214 | A86 | C2-C1-C24-C25 |
| 48 | 18 | 214 | A86 | C11-C10-C9-C8 |
| 48 | 18 | 215 | A86 | O-C13-C14-C15 |
| 48 | 18 | 215 | A86 | C11-C13-C14-C15 |
| 48 | 18 | 215 | A86 | C13-C14-C15-C16 |
| 48 | 18 | 215 | A86 | C39-C38-O4-C34 |
| 48 | 18 | 215 | A86 | O5-C38-O4-C34 |
| 48 | 19 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 20 | 309 | A86 | C11-C10-C9-C8 |
| 48 | 20 | 309 | A86 | O-C13-C14-C15 |
| 48 | 20 | 311 | A86 | C10-C11-C13-O |
| 48 | 20 | 311 | A86 | O-C13-C14-C15 |
| 48 | 20 | 311 | A86 | C11-C13-C14-C15 |
| 48 | 20 | 311 | A86 | C26-C27-C29-C30 |
| 48 | 21 | 211 | A86 | C-C1-C24-C25 |
| 48 | 21 | 211 | A86 | C2-C1-C24-C25 |
| 48 | 21 | 211 | A86 | O-C13-C14-C15 |
| 48 | 21 | 211 | A86 | O5-C38-O4-C34 |
| 48 | 21 | 213 | A86 | O-C13-C14-C15 |
| 48 | 21 | 214 | A86 | C-C1-C24-C25 |
| 48 | 21 | 214 | A86 | C2-C1-C24-C25 |
| 48 | 21 | 214 | A86 | O-C13-C14-C15 |
| 48 | 21 | 215 | A86 | C-C1-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 21 | 215 | A86 | C2-C1-C24-C25 |
| 48 | 31 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 31 | 311 | A86 | O5-C38-O4-C34 |
| 48 | 31 | 312 | A86 | C24-C25-C26-C27 |
| 48 | 31 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 31 | 314 | A86 | C-C1-C24-C25 |
| 48 | 31 | 314 | A86 | C2-C1-C24-C25 |
| 48 | 31 | 314 | A86 | C12-C11-C13-O |
| 48 | 31 | 315 | A86 | C39-C38-O4-C34 |
| 48 | 31 | 315 | A86 | O5-C38-O4-C34 |
| 48 | 32 | 203 | A86 | C11-C10-C9-C8 |
| 48 | 32 | 203 | A86 | C10-C11-C13-O |
| 48 | 32 | 203 | A86 | C12-C11-C13-O |
| 48 | 32 | 203 | A86 | C13-C14-C15-C16 |
| 48 | 32 | 203 | A86 | C39-C38-O4-C34 |
| 48 | 32 | 203 | A86 | C5-C6-C8-C9 |
| 48 | 32 | 214 | A86 | C2-C1-C24-C25 |
| 48 | 32 | 216 | A86 | C26-C27-C29-C30 |
| 48 | 32 | 216 | A86 | C35-C34-O4-C38 |
| 48 | 32 | 217 | A86 | C-C1-C24-C25 |
| 48 | 32 | 217 | A86 | C2-C1-C24-C25 |
| 48 | 32 | 217 | A86 | C39-C38-O4-C34 |
| 48 | 32 | 217 | A86 | C5-C6-C8-C9 |
| 48 | 32 | 218 | A86 | O-C13-C14-C15 |
| 48 | 32 | 218 | A86 | C11-C13-C14-C15 |
| 48 | 32 | 218 | A86 | C13-C14-C15-C16 |
| 48 | 32 | 218 | A86 | O5-C38-O4-C34 |
| 48 | 32 | 221 | A86 | C-C1-C24-C25 |
| 48 | 32 | 221 | A86 | C2-C1-C24-C25 |
| 48 | 32 | 221 | A86 | C11-C10-C9-C8 |
| 48 | 32 | 221 | A86 | O5-C38-O4-C34 |
| 48 | 32 | 221 | A86 | C3-C4-C5-C6 |
| 48 | 33 | 311 | A86 | C-C1-C24-C25 |
| 48 | 33 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 33 | 312 | A86 | C39-C38-O4-C34 |
| 48 | 33 | 312 | A86 | C5-C6-C8-C9 |
| 48 | 33 | 312 | A86 | C7-C6-C8-C9 |
| 48 | 33 | 313 | A86 | C12-C11-C13-C14 |
| 48 | 33 | 313 | A86 | O-C13-C14-C15 |
| 48 | 33 | 313 | A86 | C11-C13-C14-C15 |
| 48 | 33 | 313 | A86 | C33-C34-O4-C38 |
| 48 | 33 | 313 | A86 | C39-C38-O4-C34 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 33 | 314 | A86 | C11-C10-C9-C8 |
| 48 | 33 | 314 | A86 | C13-C14-C15-C16 |
| 48 | 33 | 314 | A86 | C13-C14-C15-O1 |
| 48 | 33 | 314 | A86 | C24-C25-C26-C27 |
| 48 | 33 | 314 | A86 | C39-C38-O4-C34 |
| 48 | 33 | 315 | A86 | C11-C10-C9-C8 |
| 48 | 33 | 315 | A86 | C13-C14-C15-C16 |
| 48 | 33 | 315 | A86 | O5-C38-O4-C34 |
| 48 | 33 | 315 | A86 | C5-C6-C8-C9 |
| 48 | 33 | 315 | A86 | C7-C6-C8-C9 |
| 48 | 34 | 311 | A86 | O-C13-C14-C15 |
| 48 | 34 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 34 | 313 | A86 | C-C1-C24-C25 |
| 48 | 34 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 34 | 313 | A86 | O-C13-C14-C15 |
| 48 | 34 | 313 | A86 | C24-C25-C26-C27 |
| 48 | 34 | 313 | A86 | C26-C27-C29-C30 |
| 48 | 34 | 313 | A86 | C33-C34-O4-C38 |
| 48 | 34 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 34 | 313 | A86 | C5-C6-C8-C9 |
| 48 | 34 | 313 | A86 | C7-C6-C8-C9 |
| 48 | 34 | 314 | A86 | C-C1-C24-C25 |
| 48 | 34 | 314 | A86 | C2-C1-C24-C25 |
| 48 | 34 | 314 | A86 | C39-C38-O4-C34 |
| 48 | 34 | 314 | A86 | C5-C6-C8-C9 |
| 48 | 34 | 314 | A86 | C7-C6-C8-C9 |
| 48 | 34 | 316 | A86 | O-C13-C14-C15 |
| 48 | 34 | 316 | A86 | C11-C13-C14-C15 |
| 48 | 34 | 316 | A86 | C13-C14-C15-C16 |
| 48 | 35 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 35 | 312 | A86 | C39-C38-O4-C34 |
| 48 | 35 | 312 | A86 | C5-C6-C8-C9 |
| 48 | 35 | 312 | A86 | C7-C6-C8-C9 |
| 48 | 35 | 313 | A86 | O-C13-C14-C15 |
| 48 | 35 | 313 | A86 | C26-C27-C29-C30 |
| 48 | 35 | 314 | A86 | C2-C1-C24-C25 |
| 48 | 35 | 314 | A86 | C11-C10-C9-C8 |
| 48 | 35 | 314 | A86 | C39-C38-O4-C34 |
| 48 | 35 | 315 | A86 | C2-C1-C24-C25 |
| 48 | 35 | 315 | A86 | C39-C38-O4-C34 |
| 48 | 35 | 315 | A86 | O5-C38-O4-C34 |
| 48 | 35 | 315 | A86 | C5-C6-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 35 | 315 | A86 | C7-C6-C8-C9 |
| 48 | 35 | 316 | A86 | O-C13-C14-C15 |
| 48 | 35 | 316 | A86 | C11-C13-C14-C15 |
| 48 | 35 | 316 | A86 | C13-C14-C15-C16 |
| 48 | 35 | 316 | A86 | O5-C38-O4-C34 |
| 48 | 35 | 319 | A86 | C39-C38-O4-C34 |
| 48 | 35 | 319 | A86 | C5-C6-C8-C9 |
| 48 | 35 | 319 | A86 | C7-C6-C8-C9 |
| 48 | 36 | 310 | A86 | C39-C38-O4-C34 |
| 48 | 36 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 36 | 313 | A86 | C10-C11-C13-O |
| 48 | 36 | 313 | A86 | C12-C11-C13-O |
| 48 | 36 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 37 | 309 | A86 | C12-C11-C13-C14 |
| 48 | 37 | 310 | A86 | C5-C6-C8-C9 |
| 48 | 37 | 310 | A86 | C7-C6-C8-C9 |
| 48 | 37 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 37 | 311 | A86 | C33-C34-O4-C38 |
| 48 | 37 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 37 | 312 | A86 | C-C1-C24-C25 |
| 48 | 37 | 312 | A86 | C2-C1-C24-C25 |
| 48 | 37 | 313 | A86 | C-C1-C24-C25 |
| 48 | 37 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 37 | 313 | A86 | O-C13-C14-C15 |
| 48 | 37 | 313 | A86 | C11-C13-C14-C15 |
| 48 | 37 | 313 | A86 | C5-C6-C8-C9 |
| 48 | 37 | 313 | A86 | C7-C6-C8-C9 |
| 48 | 37 | 314 | A86 | C11-C10-C9-C8 |
| 48 | 37 | 314 | A86 | C10-C11-C13-O |
| 48 | 37 | 314 | A86 | C12-C11-C13-O |
| 48 | 37 | 314 | A86 | C11-C13-C14-C15 |
| 48 | 37 | 314 | A86 | C13-C14-C15-C16 |
| 48 | 37 | 319 | A86 | C-C1-C24-C25 |
| 48 | 37 | 319 | A86 | C2-C1-C24-C25 |
| 48 | 37 | 319 | A86 | C39-C38-O4-C34 |
| 48 | 37 | 319 | A86 | C5-C6-C8-C9 |
| 48 | 38 | 212 | A86 | O-C13-C14-C15 |
| 48 | 38 | 212 | A86 | C24-C25-C26-C27 |
| 48 | 38 | 212 | A86 | C39-C38-O4-C34 |
| 48 | 38 | 213 | A86 | C5-C6-C8-C9 |
| 48 | 38 | 213 | A86 | C7-C6-C8-C9 |
| 48 | 38 | 214 | A86 | C-C1-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 38 | 214 | A86 | C2-C1-C24-C25 |
| 48 | 38 | 214 | A86 | C11-C10-C9-C8 |
| 48 | 38 | 215 | A86 | O-C13-C14-C15 |
| 48 | 38 | 215 | A86 | C11-C13-C14-C15 |
| 48 | 38 | 215 | A86 | C13-C14-C15-C16 |
| 48 | 38 | 215 | A86 | C39-C38-O4-C34 |
| 48 | 38 | 215 | A86 | O5-C38-O4-C34 |
| 48 | 39 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 40 | 201 | A86 | C12-C11-C13-C14 |
| 48 | 40 | 211 | A86 | C11-C10-C9-C8 |
| 48 | 40 | 211 | A86 | O-C13-C14-C15 |
| 48 | 40 | 213 | A86 | C10-C11-C13-O |
| 48 | 40 | 213 | A86 | O-C13-C14-C15 |
| 48 | 40 | 213 | A86 | C11-C13-C14-C15 |
| 48 | 40 | 213 | A86 | C26-C27-C29-C30 |
| 48 | 41 | 211 | A86 | C-C1-C24-C25 |
| 48 | 41 | 211 | A86 | C2-C1-C24-C25 |
| 48 | 41 | 211 | A86 | O-C13-C14-C15 |
| 48 | 41 | 211 | A86 | O5-C38-O4-C34 |
| 48 | 41 | 213 | A86 | O-C13-C14-C15 |
| 48 | 41 | 214 | A86 | C-C1-C24-C25 |
| 48 | 41 | 214 | A86 | C2-C1-C24-C25 |
| 48 | 41 | 214 | A86 | O-C13-C14-C15 |
| 48 | 41 | 215 | A86 | C-C1-C24-C25 |
| 48 | 41 | 215 | A86 | C2-C1-C24-C25 |
| 50 | 16 | 312 | DD6 | C-C1-C2-C3 |
| 50 | 16 | 312 | DD6 | C-C1-C24-C25 |
| 50 | 16 | 312 | DD6 | C2-C1-C24-C25 |
| 50 | 16 | 312 | DD6 | C9-C10-C11-C13 |
| 50 | 16 | 312 | DD6 | C10-C11-C13-C14 |
| 50 | 16 | 312 | DD6 | C4-C5-C6-C7 |
| 50 | 16 | 312 | DD6 | C7-C6-C8-C9 |
| 50 | 19 | 312 | DD6 | C-C1-C2-C3 |
| 50 | 19 | 312 | DD6 | C-C1-C24-C25 |
| 50 | 19 | 312 | DD6 | C9-C10-C11-C12 |
| 50 | 19 | 312 | DD6 | C4-C5-C6-C7 |
| 50 | 19 | 312 | DD6 | C5-C6-C8-C9 |
| 50 | 20 | 310 | DD6 | C-C1-C2-C3 |
| 50 | 20 | 310 | DD6 | C-C1-C24-C25 |
| 50 | 20 | 310 | DD6 | C2-C1-C24-C25 |
| 50 | 20 | 310 | DD6 | C9-C10-C11-C12 |
| 50 | 20 | 310 | DD6 | C9-C10-C11-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 50 | 20 | 310 | DD6 | C10-C11-C13-C14 |
| 50 | 20 | 310 | DD6 | C1-C2-C3-C4 |
| 50 | 20 | 310 | DD6 | C3-C4-C5-C6 |
| 50 | 20 | 310 | DD6 | C4-C5-C6-C7 |
| 50 | 20 | 310 | DD6 | C4-C5-C6-C8 |
| 50 | 20 | 312 | DD6 | C-C1-C2-C3 |
| 50 | 20 | 312 | DD6 | C2-C1-C24-C25 |
| 50 | 20 | 312 | DD6 | C9-C10-C11-C12 |
| 50 | 20 | 312 | DD6 | C13-C14-C15-C16 |
| 50 | 20 | 312 | DD6 | C4-C5-C6-C7 |
| 50 | 20 | 312 | DD6 | C7-C6-C8-C9 |
| 50 | 21 | 212 | DD6 | C-C1-C2-C3 |
| 50 | 21 | 212 | DD6 | C24-C1-C2-C3 |
| 50 | 21 | 212 | DD6 | C9-C10-C11-C12 |
| 50 | 21 | 212 | DD6 | C12-C11-C13-C14 |
| 50 | 21 | 212 | DD6 | C4-C5-C6-C8 |
| 50 | 21 | 212 | DD6 | C7-C6-C8-C9 |
| 50 | 21 | 216 | DD6 | C-C1-C2-C3 |
| 50 | 21 | 216 | DD6 | C2-C1-C24-C25 |
| 50 | 21 | 216 | DD6 | C9-C10-C11-C12 |
| 50 | 21 | 216 | DD6 | C10-C11-C13-C14 |
| 50 | 21 | 216 | DD6 | C4-C5-C6-C7 |
| 50 | 21 | 216 | DD6 | C4-C5-C6-C8 |
| 50 | 21 | 216 | DD6 | C5-C6-C8-C9 |
| 50 | 36 | 312 | DD6 | C-C1-C2-C3 |
| 50 | 36 | 312 | DD6 | C-C1-C24-C25 |
| 50 | 36 | 312 | DD6 | C2-C1-C24-C25 |
| 50 | 36 | 312 | DD6 | C9-C10-C11-C13 |
| 50 | 36 | 312 | DD6 | C10-C11-C13-C14 |
| 50 | 36 | 312 | DD6 | C4-C5-C6-C7 |
| 50 | 36 | 312 | DD6 | C7-C6-C8-C9 |
| 50 | 39 | 312 | DD6 | C-C1-C2-C3 |
| 50 | 39 | 312 | DD6 | C-C1-C24-C25 |
| 50 | 39 | 312 | DD6 | C9-C10-C11-C12 |
| 50 | 39 | 312 | DD6 | C4-C5-C6-C7 |
| 50 | 39 | 312 | DD6 | C5-C6-C8-C9 |
| 50 | 40 | 212 | DD6 | C-C1-C2-C3 |
| 50 | 40 | 212 | DD6 | C-C1-C24-C25 |
| 50 | 40 | 212 | DD6 | C2-C1-C24-C25 |
| 50 | 40 | 212 | DD6 | C9-C10-C11-C12 |
| 50 | 40 | 212 | DD6 | C9-C10-C11-C13 |
| 50 | 40 | 212 | DD6 | C10-C11-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 50 | 40 | 212 | DD6 | C1-C2-C3-C4 |
| 50 | 40 | 212 | DD6 | C3-C4-C5-C6 |
| 50 | 40 | 212 | DD6 | C4-C5-C6-C7 |
| 50 | 40 | 212 | DD6 | C4-C5-C6-C8 |
| 50 | 40 | 214 | DD6 | C-C1-C2-C3 |
| 50 | 40 | 214 | DD6 | C2-C1-C24-C25 |
| 50 | 40 | 214 | DD6 | C9-C10-C11-C12 |
| 50 | 40 | 214 | DD6 | C13-C14-C15-C16 |
| 50 | 40 | 214 | DD6 | C4-C5-C6-C7 |
| 50 | 40 | 214 | DD6 | C7-C6-C8-C9 |
| 50 | 41 | 212 | DD6 | C-C1-C2-C3 |
| 50 | 41 | 212 | DD6 | C24-C1-C2-C3 |
| 50 | 41 | 212 | DD6 | C9-C10-C11-C12 |
| 50 | 41 | 212 | DD6 | C12-C11-C13-C14 |
| 50 | 41 | 212 | DD6 | C4-C5-C6-C8 |
| 50 | 41 | 212 | DD6 | C7-C6-C8-C9 |
| 50 | 41 | 216 | DD6 | C-C1-C2-C3 |
| 50 | 41 | 216 | DD6 | C2-C1-C24-C25 |
| 50 | 41 | 216 | DD6 | C9-C10-C11-C12 |
| 50 | 41 | 216 | DD6 | C10-C11-C13-C14 |
| 50 | 41 | 216 | DD6 | C4-C5-C6-C7 |
| 50 | 41 | 216 | DD6 | C4-C5-C6-C8 |
| 50 | 41 | 216 | DD6 | C5-C6-C8-C9 |
| 37 | 17 | 309 | CLA | O1D-CGD-O2D-CED |
| 37 | 37 | 308 | CLA | O1D-CGD-O2D-CED |
| 48 | 11 | 314 | A86 | C39-C38-O4-C34 |
| 48 | 12 | 202 | A86 | O5-C38-O4-C34 |
| 48 | 12 | 215 | A86 | C39-C38-O4-C34 |
| 48 | 12 | 220 | A86 | C39-C38-O4-C34 |
| 48 | 13 | 312 | A86 | O5-C38-O4-C34 |
| 48 | 13 | 314 | A86 | O5-C38-O4-C34 |
| 48 | 14 | 314 | A86 | O5-C38-O4-C34 |
| 48 | 15 | 312 | A86 | O5-C38-O4-C34 |
| 48 | 15 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 15 | 316 | A86 | C39-C38-O4-C34 |
| 48 | 16 | 314 | A86 | C39-C38-O4-C34 |
| 48 | 17 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 17 | 315 | A86 | C39-C38-O4-C34 |
| 48 | 18 | 212 | A86 | O5-C38-O4-C34 |
| 48 | 18 | 214 | A86 | C39-C38-O4-C34 |
| 48 | 21 | 211 | A86 | C39-C38-O4-C34 |
| 48 | 21 | 213 | A86 | C39-C38-O4-C34 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 21 | 215 | A86 | C39-C38-O4-C34 |
| 48 | 31 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 31 | 314 | A86 | C39-C38-O4-C34 |
| 48 | 32 | 203 | A86 | O5-C38-O4-C34 |
| 48 | 32 | 216 | A86 | C39-C38-O4-C34 |
| 48 | 32 | 221 | A86 | C39-C38-O4-C34 |
| 48 | 33 | 312 | A86 | O5-C38-O4-C34 |
| 48 | 33 | 314 | A86 | O5-C38-O4-C34 |
| 48 | 34 | 314 | A86 | O5-C38-O4-C34 |
| 48 | 35 | 312 | A86 | O5-C38-O4-C34 |
| 48 | 35 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 36 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 37 | 310 | A86 | C39-C38-O4-C34 |
| 48 | 37 | 314 | A86 | C39-C38-O4-C34 |
| 48 | 38 | 212 | A86 | O5-C38-O4-C34 |
| 48 | 38 | 214 | A86 | C39-C38-O4-C34 |
| 48 | 41 | 211 | A86 | C39-C38-O4-C34 |
| 48 | 41 | 213 | A86 | C39-C38-O4-C34 |
| 48 | 41 | 215 | A86 | C39-C38-O4-C34 |
| 48 | 12 | 216 | A86 | O5-C38-O4-C34 |
| 48 | 13 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 14 | 311 | A86 | O5-C38-O4-C34 |
| 48 | 14 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 15 | 314 | A86 | O5-C38-O4-C34 |
| 48 | 17 | 312 | A86 | O5-C38-O4-C34 |
| 48 | 17 | 320 | A86 | O5-C38-O4-C34 |
| 48 | 32 | 217 | A86 | O5-C38-O4-C34 |
| 48 | 33 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 34 | 311 | A86 | O5-C38-O4-C34 |
| 48 | 34 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 35 | 314 | A86 | O5-C38-O4-C34 |
| 48 | 35 | 316 | A86 | C39-C38-O4-C34 |
| 48 | 37 | 311 | A86 | O5-C38-O4-C34 |
| 48 | 37 | 319 | A86 | O5-C38-O4-C34 |
| 37 | 14 | 301 | CLA | CBD-CGD-O2D-CED |
| 37 | 17 | 309 | CLA | CBD-CGD-O2D-CED |
| 37 | 18 | 201 | CLA | CBD-CGD-O2D-CED |
| 37 | 18 | 202 | CLA | CBD-CGD-O2D-CED |
| 37 | 21 | 206 | CLA | CBD-CGD-O2D-CED |
| 37 | 34 | 301 | CLA | CBD-CGD-O2D-CED |
| 37 | 38 | 201 | CLA | CBD-CGD-O2D-CED |
| 37 | 41 | 206 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | C | 513 | CLA | O1A-CGA-O2A-C1 |
| 37 | c | 513 | CLA | O1A-CGA-O2A-C1 |
| 47 | 12 | 206 | KC1 | C4C-C3C-CAC-CBC |
| 47 | 32 | 207 | KC1 | C4C-C3C-CAC-CBC |
| 48 | 11 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 12 | 217 | A86 | C39-C38-O4-C34 |
| 48 | 13 | 315 | A86 | C39-C38-O4-C34 |
| 48 | 14 | 312 | A86 | C39-C38-O4-C34 |
| 48 | 15 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 16 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 31 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 32 | 218 | A86 | C39-C38-O4-C34 |
| 48 | 33 | 315 | A86 | C39-C38-O4-C34 |
| 48 | 34 | 312 | A86 | C39-C38-O4-C34 |
| 48 | 35 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 36 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 15 | 313 | A86 | C35-C34-O4-C38 |
| 48 | 21 | 213 | A86 | C35-C34-O4-C38 |
| 48 | 35 | 313 | A86 | C35-C34-O4-C38 |
| 48 | 41 | 213 | A86 | C35-C34-O4-C38 |
| 45 | D | 404 | PL9 | C47-C48-C49-C50 |
| 45 | D | 404 | PL9 | C47-C48-C49-C51 |
| 45 | d | 402 | PL9 | C47-C48-C49-C50 |
| 45 | d | 402 | PL9 | C47-C48-C49-C51 |
| 37 | 21 | 206 | CLA | O1D-CGD-O2D-CED |
| 37 | 41 | 206 | CLA | O1D-CGD-O2D-CED |
| 47 | 20 | 302 | KC1 | O1D-CGD-O2D-CED |
| 47 | 40 | 204 | KC1 | O1D-CGD-O2D-CED |
| 48 | 12 | 215 | A86 | O5-C38-O4-C34 |
| 48 | 15 | 319 | A86 | O5-C38-O4-C34 |
| 48 | 16 | 310 | A86 | O5-C38-O4-C34 |
| 48 | 17 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 19 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 19 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 32 | 216 | A86 | O5-C38-O4-C34 |
| 48 | 35 | 311 | A86 | O5-C38-O4-C34 |
| 48 | 35 | 319 | A86 | O5-C38-O4-C34 |
| 48 | 36 | 310 | A86 | O5-C38-O4-C34 |
| 48 | 39 | 313 | A86 | C39-C38-O4-C34 |
| 48 | 39 | 313 | A86 | O5-C38-O4-C34 |
| 37 | C | 512 | CLA | O1A-CGA-O2A-C1 |
| 37 | c | 512 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 13 | 308 | CLA | O1A-CGA-O2A-C1 |
| 37 | 18 | 203 | CLA | O1A-CGA-O2A-C1 |
| 37 | 33 | 308 | CLA | O1A-CGA-O2A-C1 |
| 37 | 38 | 203 | CLA | O1A-CGA-O2A-C1 |
| 41 | 17 | 317 | LMG | O10-C28-O8-C9 |
| 41 | 37 | 316 | LMG | O10-C28-O8-C9 |
| 37 | 18 | 202 | CLA | O1D-CGD-O2D-CED |
| 48 | 37 | 312 | A86 | C39-C38-O4-C34 |
| 37 | 38 | 202 | CLA | O1D-CGD-O2D-CED |
| 48 | 11 | 312 | A86 | C39-C38-O4-C34 |
| 48 | 14 | 316 | A86 | C39-C38-O4-C34 |
| 48 | 15 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 17 | 315 | A86 | O5-C38-O4-C34 |
| 48 | 18 | 214 | A86 | O5-C38-O4-C34 |
| 48 | 21 | 213 | A86 | O5-C38-O4-C34 |
| 48 | 31 | 312 | A86 | C39-C38-O4-C34 |
| 48 | 34 | 316 | A86 | C39-C38-O4-C34 |
| 48 | 35 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 37 | 314 | A86 | O5-C38-O4-C34 |
| 48 | 38 | 214 | A86 | O5-C38-O4-C34 |
| 48 | 41 | 213 | A86 | O5-C38-O4-C34 |
| 37 | 16 | 307 | CLA | CBD-CGD-O2D-CED |
| 37 | 32 | 213 | CLA | CBD-CGD-O2D-CED |
| 37 | 36 | 307 | CLA | CBD-CGD-O2D-CED |
| 47 | 12 | 206 | KC1 | C2C-C3C-CAC-CBC |
| 47 | 32 | 207 | KC1 | C2C-C3C-CAC-CBC |
| 40 | B | 519 | SQD | O49-C7-O47-C45 |
| 40 | L | 101 | SQD | O49-C7-O47-C45 |
| 43 | D | 411 | LHG | O9-C7-O7-C5 |
| 43 | a | 412 | LHG | O9-C7-O7-C5 |
| 43 | 21 | 201 | LHG | O9-C7-O7-C5 |
| 43 | 41 | 201 | LHG | O9-C7-O7-C5 |
| 48 | 14 | 316 | A86 | O5-C38-O4-C34 |
| 48 | 34 | 316 | A86 | O5-C38-O4-C34 |
| 37 | B | 507 | CLA | C3-C5-C6-C7 |
| 37 | B | 514 | CLA | C3-C5-C6-C7 |
| 37 | C | 511 | CLA | C3-C5-C6-C7 |
| 37 | C | 512 | CLA | C3-C5-C6-C7 |
| 37 | b | 507 | CLA | C3-C5-C6-C7 |
| 37 | b | 514 | CLA | C3-C5-C6-C7 |
| 37 | c | 511 | CLA | C3-C5-C6-C7 |
| 37 | c | 512 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 13 | 301 | CLA | C3-C5-C6-C7 |
| 37 | 15 | 308 | CLA | C3-C5-C6-C7 |
| 37 | 17 | 302 | CLA | C3-C5-C6-C7 |
| 37 | 21 | 202 | CLA | C3-C5-C6-C7 |
| 37 | 21 | 206 | CLA | C3-C5-C6-C7 |
| 37 | 33 | 301 | CLA | C3-C5-C6-C7 |
| 37 | 35 | 308 | CLA | C3-C5-C6-C7 |
| 37 | 37 | 301 | CLA | C3-C5-C6-C7 |
| 37 | 38 | 208 | CLA | C3-C5-C6-C7 |
| 37 | 41 | 202 | CLA | C3-C5-C6-C7 |
| 37 | 41 | 206 | CLA | C3-C5-C6-C7 |
| 38 | A | 404 | PHO | C3-C5-C6-C7 |
| 38 | a | 406 | PHO | C3-C5-C6-C7 |
| 37 | C | 513 | CLA | CBA-CGA-O2A-C1 |
| 37 | c | 513 | CLA | CBA-CGA-O2A-C1 |
| 37 | 18 | 203 | CLA | CBA-CGA-O2A-C1 |
| 41 | 17 | 317 | LMG | C29-C28-O8-C9 |
| 41 | 37 | 316 | LMG | C29-C28-O8-C9 |
| 48 | 31 | 314 | A86 | O5-C38-O4-C34 |
| 37 | C | 501 | CLA | CBD-CGD-O2D-CED |
| 37 | C | 502 | CLA | CBD-CGD-O2D-CED |
| 37 | c | 501 | CLA | CBD-CGD-O2D-CED |
| 37 | c | 502 | CLA | CBD-CGD-O2D-CED |
| 37 | 11 | 301 | CLA | CBD-CGD-O2D-CED |
| 37 | 12 | 212 | CLA | CBD-CGD-O2D-CED |
| 37 | 16 | 306 | CLA | CBD-CGD-O2D-CED |
| 37 | 17 | 302 | CLA | CBD-CGD-O2D-CED |
| 37 | 19 | 301 | CLA | CBD-CGD-O2D-CED |
| 37 | 31 | 302 | CLA | CBD-CGD-O2D-CED |
| 37 | 36 | 306 | CLA | CBD-CGD-O2D-CED |
| 37 | 37 | 301 | CLA | CBD-CGD-O2D-CED |
| 37 | 39 | 301 | CLA | CBD-CGD-O2D-CED |
| 41 | B | 521 | LMG | C11-C10-O7-C8 |
| 41 | L | 102 | LMG | C11-C10-O7-C8 |
| 41 | b | 520 | LMG | C11-C10-O7-C8 |
| 41 | l | 101 | LMG | C11-C10-O7-C8 |
| 37 | 11 | 310 | CLA | O1D-CGD-O2D-CED |
| 37 | 31 | 310 | CLA | O1D-CGD-O2D-CED |
| 48 | 11 | 314 | A86 | O5-C38-O4-C34 |
| 48 | 14 | 315 | A86 | C39-C38-O4-C34 |
| 48 | 34 | 315 | A86 | C39-C38-O4-C34 |
| 48 | 11 | 319 | A86 | C39-C38-O4-C34 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 31 | 319 | A86 | C39-C38-O4-C34 |
| 48 | 37 | 309 | A86 | C39-C38-O4-C34 |
| 47 | 11 | 306 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 11 | 306 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 31 | 307 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 31 | 307 | KC1 | CAA-CBA-CGA-O2A |
| 37 | B | 514 | CLA | C4-C3-C5-C6 |
| 37 | C | 507 | CLA | C4-C3-C5-C6 |
| 37 | D | 406 | CLA | C4-C3-C5-C6 |
| 37 | b | 514 | CLA | C4-C3-C5-C6 |
| 37 | c | 507 | CLA | C4-C3-C5-C6 |
| 37 | d | 404 | CLA | C4-C3-C5-C6 |
| 37 | 15 | 308 | CLA | C4-C3-C5-C6 |
| 37 | 19 | 302 | CLA | C4-C3-C5-C6 |
| 37 | 19 | 310 | CLA | C4-C3-C5-C6 |
| 37 | 20 | 303 | CLA | C4-C3-C5-C6 |
| 37 | 21 | 204 | CLA | C4-C3-C5-C6 |
| 37 | 35 | 308 | CLA | C4-C3-C5-C6 |
| 37 | 39 | 310 | CLA | C4-C3-C5-C6 |
| 37 | 40 | 205 | CLA | C4-C3-C5-C6 |
| 37 | 41 | 204 | CLA | C4-C3-C5-C6 |
| 37 | B | 514 | CLA | C2-C3-C5-C6 |
| 37 | D | 406 | CLA | C2-C3-C5-C6 |
| 37 | b | 514 | CLA | C2-C3-C5-C6 |
| 37 | d | 404 | CLA | C2-C3-C5-C6 |
| 37 | 15 | 308 | CLA | C2-C3-C5-C6 |
| 37 | 19 | 302 | CLA | C2-C3-C5-C6 |
| 37 | 20 | 303 | CLA | C2-C3-C5-C6 |
| 37 | 35 | 308 | CLA | C2-C3-C5-C6 |
| 37 | 39 | 302 | CLA | C2-C3-C5-C6 |
| 37 | 39 | 310 | CLA | C2-C3-C5-C6 |
| 37 | 40 | 205 | CLA | C2-C3-C5-C6 |
| 48 | 11 | 319 | A86 | O5-C38-O4-C34 |
| 48 | 17 | 311 | A86 | O5-C38-O4-C34 |
| 48 | 21 | 215 | A86 | O5-C38-O4-C34 |
| 48 | 31 | 319 | A86 | O5-C38-O4-C34 |
| 48 | 37 | 309 | A86 | O5-C38-O4-C34 |
| 48 | 37 | 310 | A86 | O5-C38-O4-C34 |
| 48 | 41 | 215 | A86 | O5-C38-O4-C34 |
| 41 | 11 | 316 | LMG | O6-C5-C6-O5 |
| 41 | 17 | 317 | LMG | O6-C5-C6-O5 |
| 41 | 31 | 316 | LMG | O6-C5-C6-O5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 37 | 316 | LMG | O6-C5-C6-O5 |
| 37 | 11 | 307 | CLA | C3-C5-C6-C7 |
| 37 | 12 | 209 | CLA | C3-C5-C6-C7 |
| 37 | 13 | 307 | CLA | C3-C5-C6-C7 |
| 37 | 14 | 307 | CLA | C3-C5-C6-C7 |
| 37 | 15 | 307 | CLA | C3-C5-C6-C7 |
| 37 | 17 | 307 | CLA | C3-C5-C6-C7 |
| 37 | 31 | 308 | CLA | C3-C5-C6-C7 |
| 37 | 32 | 210 | CLA | C3-C5-C6-C7 |
| 37 | 33 | 307 | CLA | C3-C5-C6-C7 |
| 37 | 34 | 307 | CLA | C3-C5-C6-C7 |
| 37 | 35 | 307 | CLA | C3-C5-C6-C7 |
| 37 | 37 | 306 | CLA | C3-C5-C6-C7 |
| 37 | 11 | 301 | CLA | C3-C5-C6-C7 |
| 37 | 12 | 204 | CLA | C3-C5-C6-C7 |
| 37 | 18 | 208 | CLA | C3-C5-C6-C7 |
| 37 | 31 | 302 | CLA | C3-C5-C6-C7 |
| 37 | 32 | 205 | CLA | C3-C5-C6-C7 |
| 37 | C | 512 | CLA | CBA-CGA-O2A-C1 |
| 37 | c | 512 | CLA | CBA-CGA-O2A-C1 |
| 37 | 13 | 308 | CLA | CBA-CGA-O2A-C1 |
| 37 | 33 | 308 | CLA | CBA-CGA-O2A-C1 |
| 37 | 38 | 203 | CLA | CBA-CGA-O2A-C1 |
| 45 | D | 404 | PL9 | C37-C38-C39-C41 |
| 45 | d | 402 | PL9 | C37-C38-C39-C41 |
| 48 | 17 | 310 | A86 | C39-C38-O4-C34 |
| 39 | B | 525 | BCR | C13-C14-C15-C16 |
| 39 | b | 524 | BCR | C13-C14-C15-C16 |
| 48 | 11 | 313 | A86 | C24-C25-C26-C27 |
| 48 | 11 | 315 | A86 | C24-C25-C26-C27 |
| 48 | 11 | 319 | A86 | C24-C25-C26-C27 |
| 48 | 12 | 214 | A86 | C24-C25-C26-C27 |
| 48 | 12 | 215 | A86 | C24-C25-C26-C27 |
| 48 | 12 | 217 | A86 | C11-C10-C9-C8 |
| 48 | 12 | 220 | A86 | C24-C25-C26-C27 |
| 48 | 13 | 312 | A86 | C24-C25-C26-C27 |
| 48 | 13 | 313 | A86 | C24-C25-C26-C27 |
| 48 | 14 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 14 | 315 | A86 | C24-C25-C26-C27 |
| 48 | 15 | 313 | A86 | C24-C25-C26-C27 |
| 48 | 16 | 310 | A86 | C24-C25-C26-C27 |
| 48 | 17 | 310 | A86 | C11-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 17 | 310 | A86 | C24-C25-C26-C27 |
| 48 | 18 | 212 | A86 | C11-C10-C9-C8 |
| 48 | 18 | 213 | A86 | C11-C10-C9-C8 |
| 48 | 18 | 215 | A86 | C11-C10-C9-C8 |
| 48 | 20 | 311 | A86 | C11-C10-C9-C8 |
| 48 | 21 | 211 | A86 | C11-C10-C9-C8 |
| 48 | 21 | 214 | A86 | C24-C25-C26-C27 |
| 48 | 31 | 315 | A86 | C24-C25-C26-C27 |
| 48 | 31 | 319 | A86 | C24-C25-C26-C27 |
| 48 | 32 | 215 | A86 | C24-C25-C26-C27 |
| 48 | 32 | 216 | A86 | C24-C25-C26-C27 |
| 48 | 32 | 218 | A86 | C11-C10-C9-C8 |
| 48 | 32 | 221 | A86 | C24-C25-C26-C27 |
| 48 | 33 | 312 | A86 | C24-C25-C26-C27 |
| 48 | 33 | 313 | A86 | C24-C25-C26-C27 |
| 48 | 34 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 34 | 315 | A86 | C24-C25-C26-C27 |
| 48 | 35 | 313 | A86 | C24-C25-C26-C27 |
| 48 | 36 | 310 | A86 | C24-C25-C26-C27 |
| 48 | 37 | 309 | A86 | C11-C10-C9-C8 |
| 48 | 37 | 309 | A86 | C24-C25-C26-C27 |
| 48 | 37 | 312 | A86 | C24-C25-C26-C27 |
| 48 | 38 | 212 | A86 | C11-C10-C9-C8 |
| 48 | 38 | 213 | A86 | C11-C10-C9-C8 |
| 48 | 38 | 215 | A86 | C11-C10-C9-C8 |
| 48 | 40 | 213 | A86 | C11-C10-C9-C8 |
| 48 | 41 | 211 | A86 | C11-C10-C9-C8 |
| 48 | 41 | 214 | A86 | C24-C25-C26-C27 |
| 50 | 16 | 312 | DD6 | C24-C25-C26-C27 |
| 50 | 20 | 312 | DD6 | C24-C25-C26-C27 |
| 50 | 21 | 212 | DD6 | C24-C25-C26-C27 |
| 50 | 21 | 212 | DD6 | C3-C4-C5-C6 |
| 50 | 21 | 216 | DD6 | C1-C2-C3-C4 |
| 50 | 36 | 312 | DD6 | C24-C25-C26-C27 |
| 50 | 40 | 214 | DD6 | C24-C25-C26-C27 |
| 50 | 41 | 212 | DD6 | C24-C25-C26-C27 |
| 50 | 41 | 212 | DD6 | C3-C4-C5-C6 |
| 50 | 41 | 216 | DD6 | C1-C2-C3-C4 |
| 41 | 16 | 316 | LMG | O9-C10-O7-C8 |
| 41 | 36 | 314 | LMG | O9-C10-O7-C8 |
| 48 | 14 | 312 | A86 | O5-C38-O4-C34 |
| 48 | 34 | 312 | A86 | O5-C38-O4-C34 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 17 | 310 | A86 | O5-C38-O4-C34 |
| 48 | 19 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 39 | 311 | A86 | C39-C38-O4-C34 |
| 37 | B | 502 | CLA | C3-C5-C6-C7 |
| 37 | b | 502 | CLA | C3-C5-C6-C7 |
| 37 | 19 | 307 | CLA | C3-C5-C6-C7 |
| 37 | 19 | 310 | CLA | C3-C5-C6-C7 |
| 37 | 39 | 307 | CLA | C3-C5-C6-C7 |
| 37 | 39 | 310 | CLA | C3-C5-C6-C7 |
| 37 | 13 | 307 | CLA | CBD-CGD-O2D-CED |
| 37 | 33 | 307 | CLA | CBD-CGD-O2D-CED |
| 43 | D | 409 | LHG | O2-C2-C3-O3 |
| 43 | d | 407 | LHG | O2-C2-C3-O3 |
| 43 | 17 | 316 | LHG | O2-C2-C3-O3 |
| 43 | 37 | 315 | LHG | O2-C2-C3-O3 |
| 37 | C | 511 | CLA | CBA-CGA-O2A-C1 |
| 37 | c | 511 | CLA | CBA-CGA-O2A-C1 |
| 41 | 16 | 316 | LMG | C29-C28-O8-C9 |
| 41 | 36 | 314 | LMG | C29-C28-O8-C9 |
| 48 | 16 | 311 | A86 | O5-C38-O4-C34 |
| 48 | 36 | 311 | A86 | O5-C38-O4-C34 |
| 40 | 17 | 301 | SQD | O10-C23-O48-C46 |
| 40 | 36 | 315 | SQD | O10-C23-O48-C46 |
| 48 | 19 | 311 | A86 | O5-C38-O4-C34 |
| 48 | 39 | 311 | A86 | O5-C38-O4-C34 |
| 44 | C | 516 | DGD | O6E-C5E-C6E-O5E |
| 44 | c | 516 | DGD | O6E-C5E-C6E-O5E |
| 37 | W | 102 | CLA | CBD-CGD-O2D-CED |
| 37 | 31 | 301 | CLA | CBD-CGD-O2D-CED |
| 43 | 21 | 201 | LHG | C8-C7-O7-C5 |
| 43 | 41 | 201 | LHG | C8-C7-O7-C5 |
| 48 | 20 | 311 | A86 | C39-C38-O4-C34 |
| 48 | 40 | 213 | A86 | C39-C38-O4-C34 |
| 37 | 14 | 301 | CLA | O1D-CGD-O2D-CED |
| 37 | 34 | 301 | CLA | O1D-CGD-O2D-CED |
| 37 | D | 406 | CLA | C3-C5-C6-C7 |
| 37 | W | 101 | CLA | C3-C5-C6-C7 |
| 37 | d | 404 | CLA | C3-C5-C6-C7 |
| 37 | w | 101 | CLA | C3-C5-C6-C7 |
| 37 | 14 | 302 | CLA | C3-C5-C6-C7 |
| 37 | 34 | 302 | CLA | C3-C5-C6-C7 |
| 37 | 21 | 205 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 38 | 203 | CLA | CBD-CGD-O2D-CED |
| 37 | 41 | 205 | CLA | CBD-CGD-O2D-CED |
| 41 | 11 | 317 | LMG | O6-C5-C6-O5 |
| 41 | 31 | 317 | LMG | O6-C5-C6-O5 |
| 37 | Z | 101 | CLA | CBA-CGA-O2A-C1 |
| 37 | z | 101 | CLA | CBA-CGA-O2A-C1 |
| 47 | 11 | 309 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 14 | 309 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 15 | 306 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 21 | 207 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 31 | 309 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 34 | 309 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 35 | 304 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 35 | 306 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 41 | 207 | KC1 | CAA-CBA-CGA-O2A |
| 37 | B | 503 | CLA | C4-C3-C5-C6 |
| 37 | B | 505 | CLA | C4-C3-C5-C6 |
| 37 | b | 503 | CLA | C4-C3-C5-C6 |
| 37 | b | 505 | CLA | C4-C3-C5-C6 |
| 37 | 20 | 301 | CLA | C4-C3-C5-C6 |
| 37 | 40 | 203 | CLA | C4-C3-C5-C6 |
| 37 | B | 503 | CLA | C2-C3-C5-C6 |
| 37 | B | 505 | CLA | C2-C3-C5-C6 |
| 37 | C | 503 | CLA | C2-C3-C5-C6 |
| 37 | C | 507 | CLA | C2-C3-C5-C6 |
| 37 | b | 503 | CLA | C2-C3-C5-C6 |
| 37 | b | 505 | CLA | C2-C3-C5-C6 |
| 37 | c | 503 | CLA | C2-C3-C5-C6 |
| 37 | c | 507 | CLA | C2-C3-C5-C6 |
| 37 | 20 | 301 | CLA | C2-C3-C5-C6 |
| 37 | 21 | 204 | CLA | C2-C3-C5-C6 |
| 37 | 40 | 203 | CLA | C2-C3-C5-C6 |
| 37 | 41 | 204 | CLA | C2-C3-C5-C6 |
| 43 | 17 | 316 | LHG | O9-C7-O7-C5 |
| 43 | 37 | 315 | LHG | O9-C7-O7-C5 |
| 45 | D | 404 | PL9 | C24-C26-C27-C28 |
| 45 | D | 404 | PL9 | C29-C31-C32-C33 |
| 45 | D | 404 | PL9 | C34-C36-C37-C38 |
| 45 | d | 402 | PL9 | C24-C26-C27-C28 |
| 45 | d | 402 | PL9 | C29-C31-C32-C33 |
| 45 | d | 402 | PL9 | C34-C36-C37-C38 |
| 41 | 11 | 316 | LMG | C4-C5-C6-O5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 31 | 316 | LMG | C4-C5-C6-O5 |
| 37 | 18 | 203 | CLA | CBD-CGD-O2D-CED |
| 41 | 17 | 317 | LMG | C4-C5-C6-O5 |
| 41 | 37 | 316 | LMG | C4-C5-C6-O5 |
| 37 | 12 | 204 | CLA | C2A-CAA-CBA-CGA |
| 37 | 19 | 309 | CLA | C2A-CAA-CBA-CGA |
| 37 | 32 | 205 | CLA | C2A-CAA-CBA-CGA |
| 37 | 39 | 309 | CLA | C2A-CAA-CBA-CGA |
| 37 | C | 511 | CLA | O1A-CGA-O2A-C1 |
| 37 | c | 511 | CLA | O1A-CGA-O2A-C1 |
| 37 | 39 | 307 | CLA | O1A-CGA-O2A-C1 |
| 37 | b | 523 | CLA | C3-C5-C6-C7 |
| 40 | 16 | 315 | SQD | O5-C1-O6-C44 |
| 40 | 40 | 202 | SQD | O5-C1-O6-C44 |
| 41 | A | 408 | LMG | O6-C1-O1-C7 |
| 41 | a | 410 | LMG | O6-C1-O1-C7 |
| 37 | C | 505 | CLA | CBA-CGA-O2A-C1 |
| 37 | W | 102 | CLA | CBA-CGA-O2A-C1 |
| 37 | 19 | 307 | CLA | CBA-CGA-O2A-C1 |
| 37 | 31 | 301 | CLA | CBA-CGA-O2A-C1 |
| 37 | 39 | 307 | CLA | CBA-CGA-O2A-C1 |
| 37 | B | 516 | CLA | CBD-CGD-O2D-CED |
| 37 | D | 406 | CLA | CBD-CGD-O2D-CED |
| 37 | b | 516 | CLA | CBD-CGD-O2D-CED |
| 37 | d | 404 | CLA | CBD-CGD-O2D-CED |
| 37 | 12 | 209 | CLA | CBD-CGD-O2D-CED |
| 37 | 32 | 210 | CLA | CBD-CGD-O2D-CED |
| 47 | 11 | 309 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 15 | 304 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 31 | 309 | KC1 | CAA-CBA-CGA-O1A |
| 37 | C | 505 | CLA | O1A-CGA-O2A-C1 |
| 37 | c | 505 | CLA | O1A-CGA-O2A-C1 |
| 37 | 19 | 307 | CLA | O1A-CGA-O2A-C1 |
| 41 | C | 518 | LMG | O6-C5-C6-O5 |
| 41 | c | 518 | LMG | O6-C5-C6-O5 |
| 41 | 16 | 316 | LMG | C11-C10-O7-C8 |
| 41 | 36 | 314 | LMG | C11-C10-O7-C8 |
| 37 | B | 524 | CLA | C3-C5-C6-C7 |
| 48 | 11 | 314 | A86 | C24-C25-C26-C27 |
| 48 | 14 | 316 | A86 | C11-C10-C9-C8 |
| 48 | 15 | 314 | A86 | C24-C25-C26-C27 |
| 48 | 16 | 313 | A86 | C1-C2-C3-C4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 17 | 313 | A86 | C24-C25-C26-C27 |
| 48 | 21 | 211 | A86 | C24-C25-C26-C27 |
| 48 | 31 | 314 | A86 | C24-C25-C26-C27 |
| 48 | 34 | 316 | A86 | C11-C10-C9-C8 |
| 48 | 35 | 314 | A86 | C24-C25-C26-C27 |
| 48 | 40 | 201 | A86 | C1-C2-C3-C4 |
| 48 | 41 | 211 | A86 | C24-C25-C26-C27 |
| 50 | 21 | 216 | DD6 | C24-C25-C26-C27 |
| 50 | 41 | 216 | DD6 | C24-C25-C26-C27 |
| 37 | Z | 101 | CLA | O1A-CGA-O2A-C1 |
| 37 | z | 101 | CLA | O1A-CGA-O2A-C1 |
| 37 | C | 506 | CLA | CBA-CGA-O2A-C1 |
| 37 | C | 510 | CLA | CBA-CGA-O2A-C1 |
| 37 | c | 505 | CLA | CBA-CGA-O2A-C1 |
| 37 | c | 506 | CLA | CBA-CGA-O2A-C1 |
| 37 | c | 510 | CLA | CBA-CGA-O2A-C1 |
| 37 | 19 | 305 | CLA | CBA-CGA-O2A-C1 |
| 37 | 39 | 305 | CLA | CBA-CGA-O2A-C1 |
| 40 | 17 | 301 | SQD | C24-C23-O48-C46 |
| 40 | 36 | 315 | SQD | C24-C23-O48-C46 |
| 41 | 11 | 317 | LMG | C29-C28-O8-C9 |
| 41 | 31 | 317 | LMG | C29-C28-O8-C9 |
| 37 | 21 | 209 | CLA | CBD-CGD-O2D-CED |
| 37 | 41 | 209 | CLA | CBD-CGD-O2D-CED |
| 43 | 19 | 314 | LHG | C27-C28-C29-C30 |
| 43 | 39 | 314 | LHG | C27-C28-C29-C30 |
| 37 | 18 | 201 | CLA | O1D-CGD-O2D-CED |
| 37 | 38 | 201 | CLA | O1D-CGD-O2D-CED |
| 41 | 11 | 317 | LMG | C4-C5-C6-O5 |
| 41 | 31 | 317 | LMG | C4-C5-C6-O5 |
| 47 | 13 | 304 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 13 | 304 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 14 | 309 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 15 | 302 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 15 | 302 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 15 | 306 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 16 | 304 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 16 | 304 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 18 | 205 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 21 | 207 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 33 | 304 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 33 | 304 | KC1 | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 47 | 34 | 309 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 35 | 302 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 35 | 302 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 35 | 306 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 36 | 304 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 36 | 304 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 38 | 205 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 41 | 207 | KC1 | CAA-CBA-CGA-O1A |
| 37 | B | 502 | CLA | C4-C3-C5-C6 |
| 37 | C | 503 | CLA | C4-C3-C5-C6 |
| 37 | b | 502 | CLA | C4-C3-C5-C6 |
| 37 | c | 503 | CLA | C4-C3-C5-C6 |
| 37 | B | 502 | CLA | C2-C3-C5-C6 |
| 37 | b | 502 | CLA | C2-C3-C5-C6 |
| 37 | 19 | 310 | CLA | C2-C3-C5-C6 |
| 37 | C | 508 | CLA | C3-C5-C6-C7 |
| 37 | c | 508 | CLA | C3-C5-C6-C7 |
| 37 | A | 405 | CLA | C11-C10-C8-C9 |
| 37 | B | 501 | CLA | C11-C10-C8-C9 |
| 37 | Z | 101 | CLA | C11-C12-C13-C14 |
| 37 | a | 407 | CLA | C11-C10-C8-C9 |
| 37 | b | 501 | CLA | C11-C10-C8-C9 |
| 37 | z | 101 | CLA | C11-C12-C13-C14 |
| 37 | 21 | 206 | CLA | C11-C12-C13-C14 |
| 37 | 41 | 206 | CLA | C11-C12-C13-C14 |
| 37 | 12 | 212 | CLA | O1D-CGD-O2D-CED |
| 37 | 32 | 213 | CLA | O1D-CGD-O2D-CED |
| 40 | 16 | 315 | SQD | C2-C1-O6-C44 |
| 40 | 40 | 202 | SQD | C2-C1-O6-C44 |
| 43 | D | 411 | LHG | C7-C8-C9-C10 |
| 43 | a | 412 | LHG | C7-C8-C9-C10 |
| 37 | W | 101 | CLA | CBD-CGD-O2D-CED |
| 37 | w | 101 | CLA | CBD-CGD-O2D-CED |
| 37 | 16 | 307 | CLA | O1D-CGD-O2D-CED |
| 37 | 36 | 307 | CLA | O1D-CGD-O2D-CED |
| 39 | A | 410 | BCR | C7-C8-C9-C34 |
| 39 | B | 518 | BCR | C7-C8-C9-C34 |
| 39 | K | 101 | BCR | C7-C8-C9-C34 |
| 39 | a | 413 | BCR | C7-C8-C9-C34 |
| 39 | b | 518 | BCR | C7-C8-C9-C34 |
| 39 | y | 101 | BCR | C7-C8-C9-C34 |
| 48 | 11 | 312 | A86 | C-C1-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 12 | 202 | A86 | C7-C6-C8-C9 |
| 48 | 12 | 213 | A86 | C-C1-C24-C25 |
| 48 | 12 | 215 | A86 | C-C1-C24-C25 |
| 48 | 12 | 216 | A86 | C7-C6-C8-C9 |
| 48 | 12 | 217 | A86 | C-C1-C24-C25 |
| 48 | 12 | 220 | A86 | C7-C6-C8-C9 |
| 48 | 13 | 313 | A86 | C-C1-C24-C25 |
| 48 | 13 | 313 | A86 | C7-C6-C8-C9 |
| 48 | 13 | 314 | A86 | C-C1-C24-C25 |
| 48 | 15 | 312 | A86 | C-C1-C24-C25 |
| 48 | 15 | 313 | A86 | C-C1-C24-C25 |
| 48 | 15 | 314 | A86 | C-C1-C24-C25 |
| 48 | 15 | 314 | A86 | C7-C6-C8-C9 |
| 48 | 15 | 315 | A86 | C-C1-C24-C25 |
| 48 | 16 | 313 | A86 | C-C1-C24-C25 |
| 48 | 16 | 313 | A86 | C7-C6-C8-C9 |
| 48 | 17 | 310 | A86 | C7-C6-C8-C9 |
| 48 | 17 | 311 | A86 | C-C1-C24-C25 |
| 48 | 17 | 320 | A86 | C7-C6-C8-C9 |
| 48 | 19 | 313 | A86 | C-C1-C24-C25 |
| 48 | 20 | 311 | A86 | C-C1-C24-C25 |
| 48 | 21 | 211 | A86 | C7-C6-C8-C9 |
| 48 | 21 | 213 | A86 | C-C1-C24-C25 |
| 48 | 31 | 312 | A86 | C-C1-C24-C25 |
| 48 | 32 | 203 | A86 | C7-C6-C8-C9 |
| 48 | 32 | 214 | A86 | C-C1-C24-C25 |
| 48 | 32 | 216 | A86 | C-C1-C24-C25 |
| 48 | 32 | 217 | A86 | C7-C6-C8-C9 |
| 48 | 32 | 218 | A86 | C-C1-C24-C25 |
| 48 | 32 | 221 | A86 | C7-C6-C8-C9 |
| 48 | 33 | 313 | A86 | C-C1-C24-C25 |
| 48 | 33 | 313 | A86 | C7-C6-C8-C9 |
| 48 | 33 | 314 | A86 | C-C1-C24-C25 |
| 48 | 35 | 312 | A86 | C-C1-C24-C25 |
| 48 | 35 | 313 | A86 | C-C1-C24-C25 |
| 48 | 35 | 314 | A86 | C-C1-C24-C25 |
| 48 | 35 | 314 | A86 | C7-C6-C8-C9 |
| 48 | 35 | 315 | A86 | C-C1-C24-C25 |
| 48 | 37 | 309 | A86 | C7-C6-C8-C9 |
| 48 | 37 | 319 | A86 | C7-C6-C8-C9 |
| 48 | 39 | 313 | A86 | C-C1-C24-C25 |
| 48 | 40 | 201 | A86 | C-C1-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 40 | 201 | A86 | C7-C6-C8-C9 |
| 48 | 40 | 213 | A86 | C-C1-C24-C25 |
| 48 | 41 | 211 | A86 | C7-C6-C8-C9 |
| 48 | 41 | 213 | A86 | C-C1-C24-C25 |
| 50 | 16 | 312 | DD6 | C12-C11-C13-C14 |
| 50 | 19 | 312 | DD6 | C7-C6-C8-C9 |
| 50 | 20 | 310 | DD6 | C7-C6-C8-C9 |
| 50 | 20 | 312 | DD6 | C-C1-C24-C25 |
| 50 | 21 | 212 | DD6 | C-C1-C24-C25 |
| 50 | 21 | 216 | DD6 | C-C1-C24-C25 |
| 50 | 21 | 216 | DD6 | C12-C11-C13-C14 |
| 50 | 21 | 216 | DD6 | C7-C6-C8-C9 |
| 50 | 36 | 312 | DD6 | C12-C11-C13-C14 |
| 50 | 39 | 312 | DD6 | C7-C6-C8-C9 |
| 50 | 40 | 212 | DD6 | C7-C6-C8-C9 |
| 50 | 40 | 214 | DD6 | C-C1-C24-C25 |
| 50 | 41 | 212 | DD6 | C-C1-C24-C25 |
| 50 | 41 | 216 | DD6 | C-C1-C24-C25 |
| 50 | 41 | 216 | DD6 | C12-C11-C13-C14 |
| 50 | 41 | 216 | DD6 | C7-C6-C8-C9 |
| 39 | K | 101 | BCR | C7-C8-C9-C10 |
| 39 | y | 101 | BCR | C7-C8-C9-C10 |
| 48 | 11 | 312 | A86 | C2-C1-C24-C25 |
| 48 | 12 | 215 | A86 | C2-C1-C24-C25 |
| 48 | 12 | 220 | A86 | C5-C6-C8-C9 |
| 48 | 13 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 13 | 313 | A86 | C5-C6-C8-C9 |
| 48 | 13 | 314 | A86 | C2-C1-C24-C25 |
| 48 | 15 | 312 | A86 | C2-C1-C24-C25 |
| 48 | 16 | 313 | A86 | C5-C6-C8-C9 |
| 48 | 17 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 21 | 213 | A86 | C2-C1-C24-C25 |
| 48 | 31 | 312 | A86 | C2-C1-C24-C25 |
| 48 | 32 | 216 | A86 | C2-C1-C24-C25 |
| 48 | 32 | 221 | A86 | C5-C6-C8-C9 |
| 48 | 33 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 33 | 313 | A86 | C5-C6-C8-C9 |
| 48 | 33 | 314 | A86 | C2-C1-C24-C25 |
| 48 | 35 | 312 | A86 | C2-C1-C24-C25 |
| 48 | 37 | 310 | A86 | C2-C1-C24-C25 |
| 48 | 40 | 201 | A86 | C5-C6-C8-C9 |
| 48 | 41 | 213 | A86 | C2-C1-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 19 | 305 | CLA | O1A-CGA-O2A-C1 |
| 37 | 39 | 305 | CLA | O1A-CGA-O2A-C1 |
| 37 | B | 510 | CLA | CBD-CGD-O2D-CED |
| 37 | b | 510 | CLA | CBD-CGD-O2D-CED |
| 47 | 13 | 302 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 15 | 304 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 19 | 308 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 20 | 302 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 33 | 302 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 35 | 304 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 39 | 308 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 40 | 204 | KC1 | CAA-CBA-CGA-O1A |
| 37 | D | 406 | CLA | CBA-CGA-O2A-C1 |
| 37 | d | 404 | CLA | CBA-CGA-O2A-C1 |
| 37 | 19 | 306 | CLA | CBA-CGA-O2A-C1 |
| 37 | 39 | 306 | CLA | CBA-CGA-O2A-C1 |
| 37 | 16 | 306 | CLA | O1D-CGD-O2D-CED |
| 37 | 17 | 302 | CLA | O1D-CGD-O2D-CED |
| 37 | 33 | 307 | CLA | O1D-CGD-O2D-CED |
| 37 | 36 | 306 | CLA | O1D-CGD-O2D-CED |
| 37 | 37 | 301 | CLA | O1D-CGD-O2D-CED |
| 37 | 13 | 301 | CLA | CBD-CGD-O2D-CED |
| 37 | 16 | 309 | CLA | CBD-CGD-O2D-CED |
| 37 | 33 | 301 | CLA | CBD-CGD-O2D-CED |
| 37 | 36 | 309 | CLA | CBD-CGD-O2D-CED |
| 45 | D | 408 | PL9 | C42-C43-C44-C45 |
| 45 | d | 406 | PL9 | C42-C43-C44-C45 |
| 37 | B | 513 | CLA | C8-C10-C11-C12 |
| 37 | C | 508 | CLA | C8-C10-C11-C12 |
| 37 | W | 101 | CLA | C8-C10-C11-C12 |
| 37 | b | 501 | CLA | C8-C10-C11-C12 |
| 37 | b | 513 | CLA | C8-C10-C11-C12 |
| 37 | c | 503 | CLA | C8-C10-C11-C12 |
| 37 | c | 508 | CLA | C8-C10-C11-C12 |
| 37 | w | 101 | CLA | C8-C10-C11-C12 |
| 37 | 13 | 308 | CLA | C10-C11-C12-C13 |
| 37 | 33 | 308 | CLA | C10-C11-C12-C13 |
| 37 | 12 | 203 | CLA | C3-C5-C6-C7 |
| 37 | 32 | 204 | CLA | C3-C5-C6-C7 |
| 41 | B | 521 | LMG | C10-C11-C12-C13 |
| 41 | b | 520 | LMG | C10-C11-C12-C13 |
| 43 | 21 | 217 | LHG | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 13 | 307 | CLA | O1D-CGD-O2D-CED |
| 41 | L | 102 | LMG | O10-C28-O8-C9 |
| 41 | l | 101 | LMG | O10-C28-O8-C9 |
| 37 | C | 503 | CLA | C8-C10-C11-C12 |
| 37 | C | 508 | CLA | C5-C6-C7-C8 |
| 37 | 11 | 308 | CLA | CBA-CGA-O2A-C1 |
| 37 | 32 | 202 | CLA | CBA-CGA-O2A-C1 |
| 40 | B | 522 | SQD | C24-C23-O48-C46 |
| 40 | b | 521 | SQD | C24-C23-O48-C46 |
| 48 | 17 | 313 | A86 | O5-C38-O4-C34 |
| 48 | 37 | 312 | A86 | O5-C38-O4-C34 |
| 47 | 18 | 205 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 19 | 308 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 20 | 302 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 38 | 205 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 39 | 308 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 40 | 204 | KC1 | CAA-CBA-CGA-O2A |
| 44 | C | 517 | DGD | O6E-C5E-C6E-O5E |
| 44 | c | 517 | DGD | O6E-C5E-C6E-O5E |
| 37 | B | 501 | CLA | C8-C10-C11-C12 |
| 43 | B | 523 | LHG | C23-C24-C25-C26 |
| 43 | b | 522 | LHG | C23-C24-C25-C26 |
| 43 | 37 | 321 | LHG | C23-C24-C25-C26 |
| 39 | K | 101 | BCR | C9-C10-C11-C12 |
| 39 | y | 101 | BCR | C9-C10-C11-C12 |
| 48 | 12 | 216 | A86 | C24-C25-C26-C27 |
| 48 | 13 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 13 | 313 | A86 | C11-C10-C9-C8 |
| 48 | 14 | 312 | A86 | C24-C25-C26-C27 |
| 48 | 14 | 314 | A86 | C24-C25-C26-C27 |
| 48 | 15 | 319 | A86 | C24-C25-C26-C27 |
| 48 | 15 | 319 | A86 | C3-C4-C5-C6 |
| 48 | 16 | 314 | A86 | C11-C10-C9-C8 |
| 48 | 17 | 314 | A86 | C11-C10-C9-C8 |
| 48 | 18 | 214 | A86 | C24-C25-C26-C27 |
| 48 | 21 | 213 | A86 | C3-C4-C5-C6 |
| 48 | 21 | 215 | A86 | C24-C25-C26-C27 |
| 48 | 32 | 217 | A86 | C24-C25-C26-C27 |
| 48 | 33 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 33 | 313 | A86 | C11-C10-C9-C8 |
| 48 | 34 | 312 | A86 | C24-C25-C26-C27 |
| 48 | 34 | 314 | A86 | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 35 | 319 | A86 | C24-C25-C26-C27 |
| 48 | 35 | 319 | A86 | C3-C4-C5-C6 |
| 48 | 36 | 313 | A86 | C11-C10-C9-C8 |
| 48 | 37 | 313 | A86 | C11-C10-C9-C8 |
| 48 | 38 | 214 | A86 | C24-C25-C26-C27 |
| 48 | 41 | 213 | A86 | C3-C4-C5-C6 |
| 48 | 41 | 215 | A86 | C24-C25-C26-C27 |
| 50 | 20 | 310 | DD6 | C11-C10-C9-C8 |
| 50 | 40 | 212 | DD6 | C11-C10-C9-C8 |
| 48 | 31 | 312 | A86 | O5-C38-O4-C34 |
| 45 | D | 408 | PL9 | C44-C46-C47-C48 |
| 45 | d | 406 | PL9 | C44-C46-C47-C48 |
| 41 | C | 518 | LMG | C4-C5-C6-O5 |
| 48 | 11 | 312 | A86 | O5-C38-O4-C34 |
| 37 | Z | 101 | CLA | C8-C10-C11-C12 |
| 37 | z | 101 | CLA | C8-C10-C11-C12 |
| 41 | c | 518 | LMG | C4-C5-C6-O5 |
| 41 | 11 | 317 | LMG | C10-C11-C12-C13 |
| 41 | 31 | 317 | LMG | C10-C11-C12-C13 |
| 44 | J | 101 | DGD | C1A-C2A-C3A-C4A |
| 44 | j | 101 | DGD | C1A-C2A-C3A-C4A |
| 37 | C | 506 | CLA | O1A-CGA-O2A-C1 |
| 37 | 11 | 308 | CLA | O1A-CGA-O2A-C1 |
| 37 | 32 | 202 | CLA | O1A-CGA-O2A-C1 |
| 37 | c | 502 | CLA | O1D-CGD-O2D-CED |
| 37 | B | 516 | CLA | CBA-CGA-O2A-C1 |
| 37 | b | 516 | CLA | CBA-CGA-O2A-C1 |
| 37 | B | 501 | CLA | C13-C15-C16-C17 |
| 37 | B | 507 | CLA | C13-C15-C16-C17 |
| 37 | C | 512 | CLA | C15-C16-C17-C18 |
| 37 | b | 501 | CLA | C13-C15-C16-C17 |
| 37 | b | 507 | CLA | C13-C15-C16-C17 |
| 37 | c | 508 | CLA | C5-C6-C7-C8 |
| 37 | c | 512 | CLA | C15-C16-C17-C18 |
| 37 | 19 | 307 | CLA | C10-C11-C12-C13 |
| 37 | 39 | 303 | CLA | C13-C15-C16-C17 |
| 37 | 39 | 307 | CLA | C10-C11-C12-C13 |
| 37 | B | 501 | CLA | C2A-CAA-CBA-CGA |
| 37 | B | 506 | CLA | C2A-CAA-CBA-CGA |
| 37 | C | 513 | CLA | C2A-CAA-CBA-CGA |
| 37 | b | 501 | CLA | C2A-CAA-CBA-CGA |
| 37 | b | 506 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | c | 513 | CLA | C2A-CAA-CBA-CGA |
| 37 | 11 | 301 | CLA | C2A-CAA-CBA-CGA |
| 37 | 11 | 307 | CLA | C2A-CAA-CBA-CGA |
| 37 | 14 | 302 | CLA | C2A-CAA-CBA-CGA |
| 37 | 17 | 302 | CLA | C2A-CAA-CBA-CGA |
| 37 | 18 | 208 | CLA | C2A-CAA-CBA-CGA |
| 37 | 31 | 302 | CLA | C2A-CAA-CBA-CGA |
| 37 | 31 | 308 | CLA | C2A-CAA-CBA-CGA |
| 37 | 34 | 302 | CLA | C2A-CAA-CBA-CGA |
| 37 | 35 | 307 | CLA | C2A-CAA-CBA-CGA |
| 37 | 37 | 301 | CLA | C2A-CAA-CBA-CGA |
| 37 | 38 | 208 | CLA | C2A-CAA-CBA-CGA |
| 37 | C | 502 | CLA | O1D-CGD-O2D-CED |
| 47 | 13 | 302 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 33 | 302 | KC1 | CAA-CBA-CGA-O1A |
| 39 | B | 525 | BCR | C18-C19-C20-C21 |
| 39 | b | 524 | BCR | C18-C19-C20-C21 |
| 37 | B | 502 | CLA | C5-C6-C7-C8 |
| 37 | b | 502 | CLA | C5-C6-C7-C8 |
| 37 | 19 | 303 | CLA | C13-C15-C16-C17 |
| 37 | 32 | 211 | CLA | C10-C11-C12-C13 |
| 37 | 39 | 303 | CLA | C8-C10-C11-C12 |
| 41 | 16 | 316 | LMG | C10-C11-C12-C13 |
| 41 | 32 | 201 | LMG | C10-C11-C12-C13 |
| 41 | 36 | 314 | LMG | C10-C11-C12-C13 |
| 43 | D | 409 | LHG | C23-C24-C25-C26 |
| 43 | a | 412 | LHG | C23-C24-C25-C26 |
| 43 | d | 407 | LHG | C23-C24-C25-C26 |
| 37 | W | 102 | CLA | O1A-CGA-O2A-C1 |
| 37 | c | 506 | CLA | O1A-CGA-O2A-C1 |
| 37 | 31 | 301 | CLA | O1A-CGA-O2A-C1 |
| 41 | C | 518 | LMG | O10-C28-O8-C9 |
| 41 | c | 518 | LMG | O10-C28-O8-C9 |
| 37 | D | 402 | CLA | C3-C5-C6-C7 |
| 37 | d | 401 | CLA | C3-C5-C6-C7 |
| 37 | 19 | 301 | CLA | C3-C5-C6-C7 |
| 37 | 39 | 301 | CLA | C3-C5-C6-C7 |
| 37 | 15 | 307 | CLA | CBD-CGD-O2D-CED |
| 44 | C | 517 | DGD | O6E-C1E-O5D-C6D |
| 44 | c | 517 | DGD | O6E-C1E-O5D-C6D |
| 37 | B | 506 | CLA | C10-C11-C12-C13 |
| 37 | B | 507 | CLA | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | B | 511 | CLA | C15-C16-C17-C18 |
| 37 | B | 513 | CLA | C10-C11-C12-C13 |
| 37 | B | 524 | CLA | C15-C16-C17-C18 |
| 37 | C | 505 | CLA | C13-C15-C16-C17 |
| 37 | C | 506 | CLA | C10-C11-C12-C13 |
| 37 | C | 507 | CLA | C10-C11-C12-C13 |
| 37 | C | 513 | CLA | C10-C11-C12-C13 |
| 37 | W | 101 | CLA | C13-C15-C16-C17 |
| 37 | b | 506 | CLA | C10-C11-C12-C13 |
| 37 | b | 507 | CLA | C15-C16-C17-C18 |
| 37 | b | 511 | CLA | C15-C16-C17-C18 |
| 37 | b | 513 | CLA | C10-C11-C12-C13 |
| 37 | b | 523 | CLA | C15-C16-C17-C18 |
| 37 | c | 505 | CLA | C13-C15-C16-C17 |
| 37 | c | 506 | CLA | C10-C11-C12-C13 |
| 37 | c | 507 | CLA | C10-C11-C12-C13 |
| 37 | c | 513 | CLA | C10-C11-C12-C13 |
| 37 | w | 101 | CLA | C13-C15-C16-C17 |
| 37 | 12 | 203 | CLA | C8-C10-C11-C12 |
| 37 | 12 | 203 | CLA | C15-C16-C17-C18 |
| 37 | 12 | 210 | CLA | C10-C11-C12-C13 |
| 37 | 13 | 301 | CLA | C15-C16-C17-C18 |
| 37 | 19 | 303 | CLA | C8-C10-C11-C12 |
| 37 | 32 | 204 | CLA | C8-C10-C11-C12 |
| 37 | 33 | 301 | CLA | C15-C16-C17-C18 |
| 37 | 21 | 208 | CLA | CBA-CGA-O2A-C1 |
| 37 | 40 | 208 | CLA | CBA-CGA-O2A-C1 |
| 37 | 41 | 208 | CLA | CBA-CGA-O2A-C1 |
| 41 | A | 408 | LMG | C29-C28-O8-C9 |
| 41 | a | 410 | LMG | C29-C28-O8-C9 |
| 37 | C | 510 | CLA | O1A-CGA-O2A-C1 |
| 37 | c | 510 | CLA | O1A-CGA-O2A-C1 |
| 41 | 16 | 316 | LMG | O10-C28-O8-C9 |
| 41 | 36 | 314 | LMG | O10-C28-O8-C9 |
| 41 | 11 | 316 | LMG | C28-C29-C30-C31 |
| 41 | 12 | 201 | LMG | C10-C11-C12-C13 |
| 41 | 31 | 316 | LMG | C28-C29-C30-C31 |
| 43 | D | 411 | LHG | C23-C24-C25-C26 |
| 43 | 19 | 314 | LHG | C23-C24-C25-C26 |
| 43 | 21 | 217 | LHG | C7-C8-C9-C10 |
| 43 | 37 | 321 | LHG | C7-C8-C9-C10 |
| 43 | 39 | 314 | LHG | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | B | 501 | CLA | C5-C6-C7-C8 |
| 37 | B | 506 | CLA | C15-C16-C17-C18 |
| 37 | W | 101 | CLA | C10-C11-C12-C13 |
| 37 | b | 501 | CLA | C5-C6-C7-C8 |
| 37 | b | 506 | CLA | C15-C16-C17-C18 |
| 37 | w | 101 | CLA | C10-C11-C12-C13 |
| 37 | 18 | 209 | CLA | C10-C11-C12-C13 |
| 37 | 19 | 306 | CLA | C10-C11-C12-C13 |
| 37 | 32 | 204 | CLA | C15-C16-C17-C18 |
| 37 | 38 | 209 | CLA | C10-C11-C12-C13 |
| 37 | 39 | 306 | CLA | C10-C11-C12-C13 |
| 40 | 36 | 315 | SQD | O49-C7-O47-C45 |
| 37 | C | 512 | CLA | C10-C11-C12-C13 |
| 37 | D | 401 | CLA | C13-C15-C16-C17 |
| 37 | a | 404 | CLA | C13-C15-C16-C17 |
| 37 | c | 512 | CLA | C10-C11-C12-C13 |
| 37 | 35 | 307 | CLA | CBD-CGD-O2D-CED |
| 44 | C | 517 | DGD | C4E-C5E-C6E-O5E |
| 44 | c | 517 | DGD | C4E-C5E-C6E-O5E |
| 37 | C | 501 | CLA | O1D-CGD-O2D-CED |
| 37 | c | 501 | CLA | O1D-CGD-O2D-CED |
| 37 | 31 | 302 | CLA | O1D-CGD-O2D-CED |
| 41 | D | 412 | LMG | O6-C5-C6-O5 |
| 41 | d | 409 | LMG | O6-C5-C6-O5 |
| 37 | A | 405 | CLA | C5-C6-C7-C8 |
| 37 | B | 507 | CLA | C8-C10-C11-C12 |
| 37 | a | 407 | CLA | C5-C6-C7-C8 |
| 37 | b | 507 | CLA | C8-C10-C11-C12 |
| 37 | 14 | 308 | CLA | CBA-CGA-O2A-C1 |
| 37 | 20 | 306 | CLA | CBA-CGA-O2A-C1 |
| 37 | 34 | 308 | CLA | CBA-CGA-O2A-C1 |
| 37 | 39 | 310 | CLA | CBA-CGA-O2A-C1 |
| 37 | B | 509 | CLA | CBD-CGD-O2D-CED |
| 37 | b | 509 | CLA | CBD-CGD-O2D-CED |
| 37 | 20 | 301 | CLA | CBD-CGD-O2D-CED |
| 37 | 40 | 203 | CLA | CBD-CGD-O2D-CED |
| 47 | 14 | 309 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 18 | 210 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 34 | 309 | KC1 | C2A-CAA-CBA-CGA |
| 47 | 38 | 210 | KC1 | C2A-CAA-CBA-CGA |
| 37 | 11 | 301 | CLA | O1D-CGD-O2D-CED |
| 37 | B | 515 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | b | 515 | CLA | C10-C11-C12-C13 |
| 39 | B | 525 | BCR | C15-C16-C17-C18 |
| 39 | b | 524 | BCR | C15-C16-C17-C18 |
| 48 | 12 | 213 | A86 | C24-C25-C26-C27 |
| 48 | 15 | 315 | A86 | C24-C25-C26-C27 |
| 48 | 15 | 316 | A86 | C11-C10-C9-C8 |
| 48 | 16 | 313 | A86 | C3-C4-C5-C6 |
| 48 | 17 | 320 | A86 | C3-C4-C5-C6 |
| 48 | 20 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 32 | 214 | A86 | C24-C25-C26-C27 |
| 48 | 35 | 315 | A86 | C11-C10-C9-C8 |
| 48 | 35 | 315 | A86 | C24-C25-C26-C27 |
| 48 | 35 | 316 | A86 | C11-C10-C9-C8 |
| 48 | 40 | 201 | A86 | C3-C4-C5-C6 |
| 48 | 40 | 213 | A86 | C24-C25-C26-C27 |
| 50 | 20 | 310 | DD6 | C24-C25-C26-C27 |
| 50 | 40 | 212 | DD6 | C24-C25-C26-C27 |
| 37 | D | 406 | CLA | O1A-CGA-O2A-C1 |
| 47 | 18 | 210 | KC1 | CAA-CBA-CGA-O2A |
| 40 | 17 | 301 | SQD | O49-C7-O47-C45 |
| 43 | 17 | 316 | LHG | C1-C2-C3-O3 |
| 43 | 37 | 315 | LHG | C1-C2-C3-O3 |
| 37 | W | 102 | CLA | C2A-CAA-CBA-CGA |
| 37 | 13 | 301 | CLA | C2A-CAA-CBA-CGA |
| 37 | 31 | 301 | CLA | C2A-CAA-CBA-CGA |
| 37 | 33 | 301 | CLA | C2A-CAA-CBA-CGA |
| 37 | 19 | 310 | CLA | CBA-CGA-O2A-C1 |
| 40 | B | 519 | SQD | C24-C23-O48-C46 |
| 40 | L | 101 | SQD | C24-C23-O48-C46 |
| 37 | B | 524 | CLA | C8-C10-C11-C12 |
| 37 | C | 506 | CLA | C13-C15-C16-C17 |
| 37 | C | 510 | CLA | C8-C10-C11-C12 |
| 37 | W | 102 | CLA | C13-C15-C16-C17 |
| 37 | b | 523 | CLA | C8-C10-C11-C12 |
| 37 | c | 506 | CLA | C13-C15-C16-C17 |
| 37 | c | 510 | CLA | C8-C10-C11-C12 |
| 37 | 11 | 308 | CLA | C10-C11-C12-C13 |
| 37 | 14 | 302 | CLA | C8-C10-C11-C12 |
| 37 | 18 | 201 | CLA | C13-C15-C16-C17 |
| 37 | 31 | 301 | CLA | C13-C15-C16-C17 |
| 37 | 34 | 302 | CLA | C8-C10-C11-C12 |
| 37 | 38 | 201 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | d | 404 | CLA | O1A-CGA-O2A-C1 |
| 37 | C | 503 | CLA | C5-C6-C7-C8 |
| 37 | C | 503 | CLA | C10-C11-C12-C13 |
| 37 | c | 503 | CLA | C5-C6-C7-C8 |
| 37 | c | 503 | CLA | C10-C11-C12-C13 |
| 37 | 32 | 202 | CLA | C10-C11-C12-C13 |
| 48 | 14 | 315 | A86 | O5-C38-O4-C34 |
| 48 | 34 | 315 | A86 | O5-C38-O4-C34 |
| 37 | A | 405 | CLA | C8-C10-C11-C12 |
| 37 | B | 516 | CLA | C8-C10-C11-C12 |
| 37 | a | 407 | CLA | C8-C10-C11-C12 |
| 37 | b | 516 | CLA | C8-C10-C11-C12 |
| 37 | 19 | 307 | CLA | C13-C15-C16-C17 |
| 37 | 39 | 307 | CLA | C13-C15-C16-C17 |
| 47 | 12 | 208 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 32 | 209 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 38 | 210 | KC1 | CAA-CBA-CGA-O2A |
| 37 | 12 | 203 | CLA | C13-C15-C16-C17 |
| 37 | 14 | 302 | CLA | C10-C11-C12-C13 |
| 37 | 18 | 209 | CLA | C13-C15-C16-C17 |
| 37 | 32 | 204 | CLA | C13-C15-C16-C17 |
| 37 | 34 | 302 | CLA | C10-C11-C12-C13 |
| 37 | 38 | 209 | CLA | C13-C15-C16-C17 |
| 37 | C | 503 | CLA | C3-C5-C6-C7 |
| 37 | c | 503 | CLA | C3-C5-C6-C7 |
| 37 | 18 | 204 | CLA | C3-C5-C6-C7 |
| 37 | 20 | 301 | CLA | C3-C5-C6-C7 |
| 37 | 38 | 204 | CLA | C3-C5-C6-C7 |
| 37 | 40 | 203 | CLA | C3-C5-C6-C7 |
| 43 | 21 | 217 | LHG | C8-C7-O7-C5 |
| 43 | 37 | 321 | LHG | C8-C7-O7-C5 |
| 40 | B | 519 | SQD | C2-C1-O6-C44 |
| 40 | L | 101 | SQD | C2-C1-O6-C44 |
| 41 | 12 | 201 | LMG | C2-C1-O1-C7 |
| 41 | 32 | 201 | LMG | C2-C1-O1-C7 |
| 44 | C | 517 | DGD | C2E-C1E-O5D-C6D |
| 44 | c | 517 | DGD | C2E-C1E-O5D-C6D |
| 37 | C | 509 | CLA | C13-C15-C16-C17 |
| 37 | c | 509 | CLA | C13-C15-C16-C17 |
| 37 | B | 502 | CLA | CBA-CGA-O2A-C1 |
| 37 | b | 502 | CLA | CBA-CGA-O2A-C1 |
| 37 | 18 | 201 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 38 | 201 | CLA | C10-C11-C12-C13 |
| 37 | B | 516 | CLA | O1A-CGA-O2A-C1 |
| 39 | B | 525 | BCR | C11-C10-C9-C34 |
| 39 | C | 515 | BCR | C20-C21-C22-C37 |
| 39 | 0 | 101 | BCR | C20-C21-C22-C37 |
| 39 | b | 524 | BCR | C11-C10-C9-C34 |
| 39 | c | 515 | BCR | C20-C21-C22-C37 |
| 39 | 5 | 101 | BCR | C20-C21-C22-C37 |
| 47 | 15 | 309 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 35 | 309 | KC1 | CAA-CBA-CGA-O2A |
| 37 | C | 503 | CLA | C13-C15-C16-C17 |
| 37 | c | 503 | CLA | C13-C15-C16-C17 |
| 39 | K | 101 | BCR | C37-C22-C23-C24 |
| 39 | y | 101 | BCR | C37-C22-C23-C24 |
| 48 | 11 | 313 | A86 | C-C1-C24-C25 |
| 48 | 11 | 319 | A86 | C-C1-C24-C25 |
| 48 | 13 | 312 | A86 | C-C1-C24-C25 |
| 48 | 13 | 315 | A86 | C-C1-C24-C25 |
| 48 | 14 | 316 | A86 | C-C1-C24-C25 |
| 48 | 15 | 316 | A86 | C7-C6-C8-C9 |
| 48 | 16 | 311 | A86 | C-C1-C24-C25 |
| 48 | 19 | 311 | A86 | C-C1-C24-C25 |
| 48 | 31 | 319 | A86 | C-C1-C24-C25 |
| 48 | 33 | 312 | A86 | C-C1-C24-C25 |
| 48 | 33 | 315 | A86 | C-C1-C24-C25 |
| 48 | 34 | 316 | A86 | C-C1-C24-C25 |
| 48 | 35 | 316 | A86 | C7-C6-C8-C9 |
| 48 | 36 | 311 | A86 | C-C1-C24-C25 |
| 48 | 39 | 311 | A86 | C-C1-C24-C25 |
| 50 | 19 | 312 | DD6 | C12-C11-C13-C14 |
| 50 | 20 | 312 | DD6 | C12-C11-C13-C14 |
| 50 | 39 | 312 | DD6 | C12-C11-C13-C14 |
| 50 | 40 | 214 | DD6 | C12-C11-C13-C14 |
| 44 | H | 102 | DGD | O6E-C5E-C6E-O5E |
| 39 | B | 525 | BCR | C21-C22-C23-C24 |
| 39 | b | 524 | BCR | C21-C22-C23-C24 |
| 48 | 11 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 11 | 319 | A86 | C2-C1-C24-C25 |
| 48 | 12 | 217 | A86 | C2-C1-C24-C25 |
| 48 | 13 | 312 | A86 | C2-C1-C24-C25 |
| 48 | 15 | 314 | A86 | C5-C6-C8-C9 |
| 48 | 15 | 316 | A86 | C5-C6-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 16 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 19 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 20 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 21 | 211 | A86 | C5-C6-C8-C9 |
| 48 | 31 | 319 | A86 | C2-C1-C24-C25 |
| 48 | 32 | 218 | A86 | C2-C1-C24-C25 |
| 48 | 33 | 312 | A86 | C2-C1-C24-C25 |
| 48 | 35 | 314 | A86 | C5-C6-C8-C9 |
| 48 | 35 | 316 | A86 | C5-C6-C8-C9 |
| 48 | 39 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 40 | 201 | A86 | C2-C1-C24-C25 |
| 48 | 40 | 213 | A86 | C2-C1-C24-C25 |
| 48 | 41 | 211 | A86 | C5-C6-C8-C9 |
| 37 | 19 | 306 | CLA | O1A-CGA-O2A-C1 |
| 37 | 39 | 306 | CLA | O1A-CGA-O2A-C1 |
| 37 | C | 507 | CLA | C2A-CAA-CBA-CGA |
| 37 | c | 507 | CLA | C2A-CAA-CBA-CGA |
| 37 | 12 | 212 | CLA | C2A-CAA-CBA-CGA |
| 37 | 15 | 307 | CLA | C2A-CAA-CBA-CGA |
| 37 | 18 | 202 | CLA | C2A-CAA-CBA-CGA |
| 37 | 19 | 306 | CLA | C2A-CAA-CBA-CGA |
| 37 | 32 | 213 | CLA | C2A-CAA-CBA-CGA |
| 37 | 38 | 202 | CLA | C2A-CAA-CBA-CGA |
| 37 | 39 | 306 | CLA | C2A-CAA-CBA-CGA |
| 48 | 18 | 213 | A86 | C39-C38-O4-C34 |
| 37 | B | 510 | CLA | C15-C16-C17-C18 |
| 37 | C | 506 | CLA | C8-C10-C11-C12 |
| 37 | b | 510 | CLA | C15-C16-C17-C18 |
| 37 | c | 506 | CLA | C8-C10-C11-C12 |
| 43 | D | 410 | LHG | O1-C1-C2-C3 |
| 43 | D | 411 | LHG | O1-C1-C2-C3 |
| 43 | a | 412 | LHG | O1-C1-C2-C3 |
| 43 | d | 408 | LHG | O1-C1-C2-C3 |
| 44 | h | 102 | DGD | O6E-C5E-C6E-O5E |
| 40 | B | 519 | SQD | C46-C45-O47-C7 |
| 40 | L | 101 | SQD | C46-C45-O47-C7 |
| 37 | 11 | 307 | CLA | C2C-C3C-CAC-CBC |
| 48 | 38 | 213 | A86 | C39-C38-O4-C34 |
| 48 | 14 | 316 | A86 | C3-C4-C5-C6 |
| 48 | 34 | 316 | A86 | C3-C4-C5-C6 |
| 48 | 37 | 310 | A86 | C11-C10-C9-C8 |
| 37 | D | 402 | CLA | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | d | 401 | CLA | C16-C17-C18-C19 |
| 37 | 11 | 308 | CLA | C16-C17-C18-C20 |
| 37 | 16 | 306 | CLA | C16-C17-C18-C20 |
| 37 | 32 | 202 | CLA | C16-C17-C18-C20 |
| 37 | 36 | 306 | CLA | C16-C17-C18-C20 |
| 37 | b | 516 | CLA | O1A-CGA-O2A-C1 |
| 37 | 14 | 308 | CLA | O1A-CGA-O2A-C1 |
| 37 | B | 501 | CLA | C3-C5-C6-C7 |
| 37 | C | 509 | CLA | C3-C5-C6-C7 |
| 37 | c | 509 | CLA | C3-C5-C6-C7 |
| 37 | 17 | 309 | CLA | C3-C5-C6-C7 |
| 37 | 31 | 308 | CLA | C2C-C3C-CAC-CBC |
| 44 | C | 516 | DGD | C4E-C5E-C6E-O5E |
| 44 | c | 516 | DGD | C4E-C5E-C6E-O5E |
| 39 | A | 406 | BCR | C20-C21-C22-C23 |
| 39 | B | 525 | BCR | C16-C17-C18-C19 |
| 39 | B | 525 | BCR | C20-C21-C22-C23 |
| 39 | a | 408 | BCR | C20-C21-C22-C23 |
| 39 | b | 524 | BCR | C16-C17-C18-C19 |
| 39 | b | 524 | BCR | C20-C21-C22-C23 |
| 50 | 16 | 312 | DD6 | C24-C1-C2-C3 |
| 50 | 19 | 312 | DD6 | C4-C5-C6-C8 |
| 50 | 21 | 216 | DD6 | C24-C1-C2-C3 |
| 50 | 36 | 312 | DD6 | C24-C1-C2-C3 |
| 50 | 39 | 312 | DD6 | C4-C5-C6-C8 |
| 50 | 41 | 216 | DD6 | C24-C1-C2-C3 |
| 46 | F | 101 | HEM | C3A-C2A-CAA-CBA |
| 46 | f | 101 | HEM | C3A-C2A-CAA-CBA |
| 41 | C | 518 | LMG | O6-C1-O1-C7 |
| 41 | c | 518 | LMG | O6-C1-O1-C7 |
| 41 | 16 | 316 | LMG | O6-C1-O1-C7 |
| 41 | 36 | 314 | LMG | O6-C1-O1-C7 |
| 44 | C | 517 | DGD | O6D-C1D-O3G-C3G |
| 44 | c | 517 | DGD | O6D-C1D-O3G-C3G |
| 47 | 12 | 208 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 15 | 309 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 16 | 305 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 17 | 303 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 18 | 210 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 32 | 209 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 35 | 309 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 36 | 305 | KC1 | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 47 | 37 | 302 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 38 | 210 | KC1 | CAA-CBA-CGA-O1A |
| 37 | 19 | 301 | CLA | O1D-CGD-O2D-CED |
| 37 | 39 | 301 | CLA | O1D-CGD-O2D-CED |
| 37 | 34 | 308 | CLA | O1A-CGA-O2A-C1 |
| 37 | 12 | 210 | CLA | CBA-CGA-O2A-C1 |
| 37 | 32 | 211 | CLA | CBA-CGA-O2A-C1 |
| 37 | 15 | 308 | CLA | C5-C6-C7-C8 |
| 37 | 16 | 301 | CLA | C8-C10-C11-C12 |
| 37 | 16 | 306 | CLA | C8-C10-C11-C12 |
| 37 | 36 | 301 | CLA | C8-C10-C11-C12 |
| 37 | 36 | 306 | CLA | C8-C10-C11-C12 |
| 44 | H | 102 | DGD | C1A-C2A-C3A-C4A |
| 44 | h | 102 | DGD | C1A-C2A-C3A-C4A |
| 37 | b | 501 | CLA | C3-C5-C6-C7 |
| 37 | 41 | 205 | CLA | O1D-CGD-O2D-CED |
| 37 | C | 509 | CLA | C2-C1-O2A-CGA |
| 37 | c | 509 | CLA | C2-C1-O2A-CGA |
| 37 | Z | 101 | CLA | C16-C17-C18-C20 |
| 37 | z | 101 | CLA | C16-C17-C18-C20 |
| 37 | 11 | 308 | CLA | C16-C17-C18-C19 |
| 37 | 32 | 202 | CLA | C16-C17-C18-C19 |
| 37 | 20 | 306 | CLA | O1A-CGA-O2A-C1 |
| 37 | 40 | 208 | CLA | O1A-CGA-O2A-C1 |
| 37 | C | 507 | CLA | C13-C15-C16-C17 |
| 37 | c | 507 | CLA | C13-C15-C16-C17 |
| 40 | B | 519 | SQD | C32-C33-C34-C35 |
| 40 | 40 | 202 | SQD | C14-C15-C16-C17 |
| 41 | B | 521 | LMG | C18-C19-C20-C21 |
| 41 | b | 520 | LMG | C18-C19-C20-C21 |
| 41 | c | 518 | LMG | C19-C20-C21-C22 |
| 43 | 17 | 316 | LHG | C11-C10-C9-C8 |
| 43 | 19 | 314 | LHG | C18-C19-C20-C21 |
| 43 | 39 | 314 | LHG | C18-C19-C20-C21 |
| 44 | H | 102 | DGD | C3A-C4A-C5A-C6A |
| 44 | h | 102 | DGD | C3A-C4A-C5A-C6A |
| 39 | A | 406 | BCR | C14-C15-C16-C17 |
| 39 | a | 408 | BCR | C14-C15-C16-C17 |
| 40 | A | 407 | SQD | C16-C17-C18-C19 |
| 40 | L | 101 | SQD | C32-C33-C34-C35 |
| 40 | 16 | 315 | SQD | C14-C15-C16-C17 |
| 41 | C | 518 | LMG | C19-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | D | 410 | LHG | C32-C33-C34-C35 |
| 43 | D | 410 | LHG | C33-C34-C35-C36 |
| 43 | D | 411 | LHG | C16-C17-C18-C19 |
| 43 | a | 412 | LHG | C16-C17-C18-C19 |
| 43 | d | 408 | LHG | C32-C33-C34-C35 |
| 43 | d | 408 | LHG | C33-C34-C35-C36 |
| 43 | 37 | 315 | LHG | C11-C10-C9-C8 |
| 37 | 21 | 205 | CLA | O1D-CGD-O2D-CED |
| 41 | 36 | 314 | LMG | O6-C5-C6-O5 |
| 37 | 35 | 308 | CLA | C5-C6-C7-C8 |
| 47 | 17 | 303 | KC1 | CAA-CBA-CGA-O2A |
| 40 | A | 407 | SQD | C14-C15-C16-C17 |
| 40 | a | 409 | SQD | C14-C15-C16-C17 |
| 40 | a | 409 | SQD | C16-C17-C18-C19 |
| 43 | 21 | 201 | LHG | C11-C10-C9-C8 |
| 44 | H | 102 | DGD | CBA-CCA-CDA-CEA |
| 44 | h | 102 | DGD | CBA-CCA-CDA-CEA |
| 37 | 21 | 208 | CLA | O1A-CGA-O2A-C1 |
| 37 | 39 | 310 | CLA | O1A-CGA-O2A-C1 |
| 37 | 41 | 208 | CLA | O1A-CGA-O2A-C1 |
| 40 | A | 407 | SQD | C18-C19-C20-C21 |
| 40 | a | 409 | SQD | C18-C19-C20-C21 |
| 43 | 39 | 314 | LHG | C31-C32-C33-C34 |
| 41 | 16 | 316 | LMG | O6-C5-C6-O5 |
| 43 | D | 409 | LHG | O1-C1-C2-O2 |
| 43 | d | 407 | LHG | O1-C1-C2-O2 |
| 40 | 17 | 301 | SQD | C9-C10-C11-C12 |
| 40 | 36 | 315 | SQD | C9-C10-C11-C12 |
| 41 | A | 408 | LMG | C32-C33-C34-C35 |
| 41 | a | 410 | LMG | C32-C33-C34-C35 |
| 43 | 19 | 314 | LHG | C31-C32-C33-C34 |
| 43 | 41 | 201 | LHG | C11-C10-C9-C8 |
| 37 | b | 501 | CLA | C10-C11-C12-C13 |
| 37 | A | 405 | CLA | C4B-C3B-CAB-CBB |
| 37 | B | 515 | CLA | C4B-C3B-CAB-CBB |
| 37 | C | 513 | CLA | C4B-C3B-CAB-CBB |
| 37 | D | 405 | CLA | C4B-C3B-CAB-CBB |
| 37 | a | 407 | CLA | C4B-C3B-CAB-CBB |
| 37 | b | 515 | CLA | C4B-C3B-CAB-CBB |
| 37 | c | 513 | CLA | C4B-C3B-CAB-CBB |
| 37 | d | 403 | CLA | C4B-C3B-CAB-CBB |
| 37 | 11 | 307 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 13 | 303 | CLA | C4B-C3B-CAB-CBB |
| 37 | 14 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 14 | 302 | CLA | C4B-C3B-CAB-CBB |
| 37 | 31 | 308 | CLA | C4B-C3B-CAB-CBB |
| 37 | 33 | 303 | CLA | C4B-C3B-CAB-CBB |
| 37 | 34 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 34 | 302 | CLA | C4B-C3B-CAB-CBB |
| 37 | 16 | 306 | CLA | C16-C17-C18-C19 |
| 37 | 36 | 306 | CLA | C16-C17-C18-C19 |
| 37 | 18 | 203 | CLA | O1D-CGD-O2D-CED |
| 37 | 19 | 310 | CLA | O1A-CGA-O2A-C1 |
| 41 | B | 521 | LMG | C19-C20-C21-C22 |
| 41 | b | 520 | LMG | C19-C20-C21-C22 |
| 37 | B | 501 | CLA | C10-C11-C12-C13 |
| 37 | W | 101 | CLA | C5-C6-C7-C8 |
| 37 | w | 101 | CLA | C5-C6-C7-C8 |
| 37 | 21 | 208 | CLA | C13-C15-C16-C17 |
| 37 | 41 | 208 | CLA | C13-C15-C16-C17 |
| 40 | B | 522 | SQD | C8-C7-O47-C45 |
| 40 | b | 521 | SQD | C8-C7-O47-C45 |
| 41 | A | 408 | LMG | C11-C10-O7-C8 |
| 41 | a | 410 | LMG | C11-C10-O7-C8 |
| 43 | 41 | 201 | LHG | C10-C11-C12-C13 |
| 37 | W | 102 | CLA | O1D-CGD-O2D-CED |
| 41 | A | 408 | LMG | C4-C5-C6-O5 |
| 41 | a | 410 | LMG | C4-C5-C6-O5 |
| 37 | 19 | 306 | CLA | C11-C12-C13-C15 |
| 37 | 39 | 306 | CLA | C11-C12-C13-C15 |
| 40 | B | 519 | SQD | C10-C11-C12-C13 |
| 40 | L | 101 | SQD | C10-C11-C12-C13 |
| 43 | B | 523 | LHG | C16-C17-C18-C19 |
| 43 | b | 522 | LHG | C16-C17-C18-C19 |
| 44 | H | 102 | DGD | C3B-C4B-C5B-C6B |
| 44 | h | 102 | DGD | C3B-C4B-C5B-C6B |
| 40 | A | 407 | SQD | C7-C8-C9-C10 |
| 40 | B | 522 | SQD | C7-C8-C9-C10 |
| 40 | a | 409 | SQD | C7-C8-C9-C10 |
| 40 | b | 521 | SQD | C7-C8-C9-C10 |
| 37 | C | 507 | CLA | C8-C10-C11-C12 |
| 37 | c | 507 | CLA | C8-C10-C11-C12 |
| 40 | A | 407 | SQD | C17-C18-C19-C20 |
| 40 | a | 409 | SQD | C17-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | L | 102 | LMG | C14-C15-C16-C17 |
| 41 | l | 101 | LMG | C14-C15-C16-C17 |
| 43 | D | 411 | LHG | C11-C10-C9-C8 |
| 43 | a | 412 | LHG | C11-C10-C9-C8 |
| 43 | 21 | 201 | LHG | C10-C11-C12-C13 |
| 37 | 31 | 304 | CLA | C3-C5-C6-C7 |
| 37 | 37 | 308 | CLA | C3-C5-C6-C7 |
| 47 | 16 | 305 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 17 | 306 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 36 | 305 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 37 | 305 | KC1 | CAA-CBA-CGA-O1A |
| 37 | B | 524 | CLA | C3A-C2A-CAA-CBA |
| 37 | C | 506 | CLA | C3A-C2A-CAA-CBA |
| 37 | Z | 101 | CLA | C3A-C2A-CAA-CBA |
| 37 | W | 102 | CLA | C3A-C2A-CAA-CBA |
| 37 | b | 523 | CLA | C3A-C2A-CAA-CBA |
| 37 | c | 506 | CLA | C3A-C2A-CAA-CBA |
| 37 | z | 101 | CLA | C3A-C2A-CAA-CBA |
| 37 | 11 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 12 | 205 | CLA | C3A-C2A-CAA-CBA |
| 37 | 13 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 15 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 16 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 16 | 306 | CLA | C3A-C2A-CAA-CBA |
| 37 | 17 | 304 | CLA | C3A-C2A-CAA-CBA |
| 37 | 17 | 309 | CLA | C3A-C2A-CAA-CBA |
| 37 | 18 | 203 | CLA | C3A-C2A-CAA-CBA |
| 37 | 18 | 204 | CLA | C3A-C2A-CAA-CBA |
| 37 | 19 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 20 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 20 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 20 | 308 | CLA | C3A-C2A-CAA-CBA |
| 37 | 21 | 204 | CLA | C3A-C2A-CAA-CBA |
| 37 | 21 | 205 | CLA | C3A-C2A-CAA-CBA |
| 37 | 31 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 31 | 304 | CLA | C3A-C2A-CAA-CBA |
| 37 | 32 | 206 | CLA | C3A-C2A-CAA-CBA |
| 37 | 33 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 35 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 36 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 36 | 306 | CLA | C3A-C2A-CAA-CBA |
| 37 | 37 | 303 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 37 | 308 | CLA | C3A-C2A-CAA-CBA |
| 37 | 38 | 203 | CLA | C3A-C2A-CAA-CBA |
| 37 | 38 | 204 | CLA | C3A-C2A-CAA-CBA |
| 37 | 39 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 40 | 203 | CLA | C3A-C2A-CAA-CBA |
| 37 | 40 | 205 | CLA | C3A-C2A-CAA-CBA |
| 37 | 40 | 210 | CLA | C3A-C2A-CAA-CBA |
| 37 | 41 | 204 | CLA | C3A-C2A-CAA-CBA |
| 37 | 41 | 205 | CLA | C3A-C2A-CAA-CBA |
| 38 | D | 403 | PHO | C3A-C2A-CAA-CBA |
| 38 | a | 405 | PHO | C3A-C2A-CAA-CBA |
| 37 | 31 | 301 | CLA | O1D-CGD-O2D-CED |
| 37 | 38 | 203 | CLA | O1D-CGD-O2D-CED |
| 40 | a | 409 | SQD | C10-C11-C12-C13 |
| 40 | 17 | 301 | SQD | C27-C28-C29-C30 |
| 40 | 36 | 315 | SQD | C27-C28-C29-C30 |
| 43 | 39 | 314 | LHG | C34-C35-C36-C37 |
| 40 | A | 407 | SQD | C10-C11-C12-C13 |
| 37 | C | 503 | CLA | C15-C16-C17-C18 |
| 37 | b | 508 | CLA | C8-C10-C11-C12 |
| 37 | c | 503 | CLA | C15-C16-C17-C18 |
| 44 | H | 102 | DGD | C4E-C5E-C6E-O5E |
| 44 | h | 102 | DGD | C4E-C5E-C6E-O5E |
| 48 | 15 | 315 | A86 | C11-C10-C9-C8 |
| 48 | 17 | 311 | A86 | C11-C10-C9-C8 |
| 48 | 18 | 213 | A86 | C24-C25-C26-C27 |
| 48 | 20 | 311 | A86 | C3-C4-C5-C6 |
| 48 | 38 | 213 | A86 | C24-C25-C26-C27 |
| 48 | 40 | 213 | A86 | C3-C4-C5-C6 |
| 50 | 21 | 216 | DD6 | C3-C4-C5-C6 |
| 50 | 41 | 216 | DD6 | C3-C4-C5-C6 |
| 37 | B | 502 | CLA | O1A-CGA-O2A-C1 |
| 37 | b | 502 | CLA | O1A-CGA-O2A-C1 |
| 40 | B | 519 | SQD | C33-C34-C35-C36 |
| 40 | L | 101 | SQD | C33-C34-C35-C36 |
| 40 | 17 | 301 | SQD | C29-C30-C31-C32 |
| 40 | 36 | 315 | SQD | C29-C30-C31-C32 |
| 41 | B | 520 | LMG | C12-C13-C14-C15 |
| 41 | a | 410 | LMG | C18-C19-C20-C21 |
| 41 | b | 519 | LMG | C12-C13-C14-C15 |
| 43 | B | 523 | LHG | C27-C28-C29-C30 |
| 43 | D | 409 | LHG | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | a | 412 | LHG | C14-C15-C16-C17 |
| 43 | b | 522 | LHG | C27-C28-C29-C30 |
| 37 | B | 508 | CLA | C8-C10-C11-C12 |
| 37 | Z | 102 | CLA | CBD-CGD-O2D-CED |
| 41 | A | 408 | LMG | C18-C19-C20-C21 |
| 41 | 11 | 316 | LMG | C13-C14-C15-C16 |
| 41 | 31 | 316 | LMG | C13-C14-C15-C16 |
| 43 | B | 523 | LHG | C28-C29-C30-C31 |
| 43 | D | 411 | LHG | C14-C15-C16-C17 |
| 43 | a | 412 | LHG | C15-C16-C17-C18 |
| 43 | b | 522 | LHG | C28-C29-C30-C31 |
| 43 | d | 407 | LHG | C32-C33-C34-C35 |
| 37 | W | 101 | CLA | CBA-CGA-O2A-C1 |
| 37 | w | 101 | CLA | CBA-CGA-O2A-C1 |
| 40 | 16 | 315 | SQD | C24-C23-O48-C46 |
| 40 | 40 | 202 | SQD | C24-C23-O48-C46 |
| 41 | B | 521 | LMG | C29-C28-O8-C9 |
| 41 | C | 518 | LMG | C29-C28-O8-C9 |
| 41 | b | 520 | LMG | C29-C28-O8-C9 |
| 41 | c | 518 | LMG | C29-C28-O8-C9 |
| 51 | 39 | 315 | LMU | C1-C2-C3-C4 |
| 41 | A | 408 | LMG | C7-C8-C9-O8 |
| 41 | a | 410 | LMG | C7-C8-C9-O8 |
| 41 | C | 518 | LMG | C18-C19-C20-C21 |
| 41 | c | 518 | LMG | C18-C19-C20-C21 |
| 43 | D | 411 | LHG | C15-C16-C17-C18 |
| 43 | b | 522 | LHG | C13-C14-C15-C16 |
| 43 | 19 | 314 | LHG | C34-C35-C36-C37 |
| 43 | 37 | 315 | LHG | C16-C17-C18-C19 |
| 44 | H | 102 | DGD | C7A-C8A-C9A-CAA |
| 44 | h | 102 | DGD | C7A-C8A-C9A-CAA |
| 37 | 11 | 303 | CLA | C3-C5-C6-C7 |
| 40 | 16 | 315 | SQD | C18-C19-C20-C21 |
| 40 | 40 | 202 | SQD | C18-C19-C20-C21 |
| 43 | B | 523 | LHG | C13-C14-C15-C16 |
| 43 | 17 | 316 | LHG | C16-C17-C18-C19 |
| 51 | 19 | 315 | LMU | C1-C2-C3-C4 |
| 47 | 37 | 302 | KC1 | CAA-CBA-CGA-O2A |
| 43 | B | 523 | LHG | C32-C33-C34-C35 |
| 43 | b | 522 | LHG | C32-C33-C34-C35 |
| 43 | 21 | 217 | LHG | C30-C31-C32-C33 |
| 43 | 37 | 321 | LHG | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 44 | J | 101 | DGD | C3A-C4A-C5A-C6A |
| 44 | j | 101 | DGD | C3A-C4A-C5A-C6A |
| 43 | D | 410 | LHG | C13-C14-C15-C16 |
| 43 | 21 | 201 | LHG | C24-C25-C26-C27 |
| 48 | 20 | 311 | A86 | O5-C38-O4-C34 |
| 37 | D | 406 | CLA | O1D-CGD-O2D-CED |
| 37 | d | 404 | CLA | O1D-CGD-O2D-CED |
| 41 | D | 412 | LMG | C35-C36-C37-C38 |
| 41 | d | 409 | LMG | C35-C36-C37-C38 |
| 43 | D | 410 | LHG | C34-C35-C36-C37 |
| 43 | D | 411 | LHG | C27-C28-C29-C30 |
| 43 | a | 412 | LHG | C27-C28-C29-C30 |
| 43 | d | 408 | LHG | C13-C14-C15-C16 |
| 44 | C | 516 | DGD | C7B-C8B-C9B-CAB |
| 44 | c | 516 | DGD | C7B-C8B-C9B-CAB |
| 37 | 12 | 210 | CLA | O1A-CGA-O2A-C1 |
| 37 | 32 | 211 | CLA | O1A-CGA-O2A-C1 |
| 37 | C | 503 | CLA | C2B-C3B-CAB-CBB |
| 37 | C | 513 | CLA | C2B-C3B-CAB-CBB |
| 37 | c | 503 | CLA | C2B-C3B-CAB-CBB |
| 37 | c | 513 | CLA | C2B-C3B-CAB-CBB |
| 37 | 14 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 14 | 302 | CLA | C2B-C3B-CAB-CBB |
| 37 | 17 | 302 | CLA | C2B-C3B-CAB-CBB |
| 37 | 18 | 203 | CLA | C2B-C3B-CAB-CBB |
| 37 | 19 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 20 | 308 | CLA | C2B-C3B-CAB-CBB |
| 37 | 34 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 34 | 302 | CLA | C2B-C3B-CAB-CBB |
| 37 | 37 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 38 | 208 | CLA | C2B-C3B-CAB-CBB |
| 37 | 39 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 39 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 40 | 210 | CLA | C2B-C3B-CAB-CBB |
| 39 | A | 410 | BCR | C1-C6-C7-C8 |
| 39 | A | 410 | BCR | C5-C6-C7-C8 |
| 39 | B | 517 | BCR | C1-C6-C7-C8 |
| 39 | B | 517 | BCR | C5-C6-C7-C8 |
| 39 | B | 525 | BCR | C1-C6-C7-C8 |
| 39 | B | 525 | BCR | C5-C6-C7-C8 |
| 39 | K | 101 | BCR | C5-C6-C7-C8 |
| 39 | a | 413 | BCR | C1-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | a | 413 | BCR | C5-C6-C7-C8 |
| 39 | b | 517 | BCR | C1-C6-C7-C8 |
| 39 | b | 517 | BCR | C5-C6-C7-C8 |
| 39 | b | 524 | BCR | C1-C6-C7-C8 |
| 39 | b | 524 | BCR | C5-C6-C7-C8 |
| 39 | y | 101 | BCR | C5-C6-C7-C8 |
| 37 | z | 102 | CLA | CBD-CGD-O2D-CED |
| 37 | 32 | 211 | CLA | CBD-CGD-O2D-CED |
| 41 | L | 102 | LMG | C29-C28-O8-C9 |
| 41 | l | 101 | LMG | C29-C28-O8-C9 |
| 41 | D | 412 | LMG | C37-C38-C39-C40 |
| 43 | d | 408 | LHG | C34-C35-C36-C37 |
| 43 | 41 | 201 | LHG | C24-C25-C26-C27 |
| 48 | 40 | 213 | A86 | O5-C38-O4-C34 |
| 41 | L | 102 | LMG | C15-C16-C17-C18 |
| 41 | d | 409 | LMG | C37-C38-C39-C40 |
| 43 | D | 409 | LHG | C28-C29-C30-C31 |
| 43 | d | 407 | LHG | C28-C29-C30-C31 |
| 37 | B | 510 | CLA | C2A-CAA-CBA-CGA |
| 37 | C | 506 | CLA | C2A-CAA-CBA-CGA |
| 37 | b | 510 | CLA | C2A-CAA-CBA-CGA |
| 37 | c | 506 | CLA | C2A-CAA-CBA-CGA |
| 41 | C | 518 | LMG | C10-C11-C12-C13 |
| 41 | c | 518 | LMG | C10-C11-C12-C13 |
| 41 | l | 101 | LMG | C15-C16-C17-C18 |
| 37 | C | 513 | CLA | CBD-CGD-O2D-CED |
| 37 | 14 | 307 | CLA | CBD-CGD-O2D-CED |
| 37 | B | 514 | CLA | C13-C15-C16-C17 |
| 37 | b | 514 | CLA | C13-C15-C16-C17 |
| 47 | 17 | 306 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 37 | 305 | KC1 | CAA-CBA-CGA-O2A |
| 37 | 13 | 303 | CLA | C4-C3-C5-C6 |
| 37 | 33 | 303 | CLA | C4-C3-C5-C6 |
| 37 | 37 | 306 | CLA | C4-C3-C5-C6 |
| 39 | D | 407 | BCR | C10-C11-C12-C13 |
| 39 | d | 405 | BCR | C10-C11-C12-C13 |
| 37 | B | 506 | CLA | C13-C15-C16-C17 |
| 37 | b | 506 | CLA | C13-C15-C16-C17 |
| 37 | 39 | 303 | CLA | C10-C11-C12-C13 |
| 41 | A | 408 | LMG | C19-C20-C21-C22 |
| 41 | a | 410 | LMG | C19-C20-C21-C22 |
| 43 | B | 523 | LHG | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | b | 522 | LHG | C30-C31-C32-C33 |
| 43 | d | 408 | LHG | C24-C25-C26-C27 |
| 37 | 11 | 310 | CLA | CBA-CGA-O2A-C1 |
| 37 | 31 | 310 | CLA | CBA-CGA-O2A-C1 |
| 44 | J | 101 | DGD | C2A-C1A-O1G-C1G |
| 44 | j | 101 | DGD | C2A-C1A-O1G-C1G |
| 37 | 33 | 303 | CLA | C3-C5-C6-C7 |
| 37 | c | 513 | CLA | CBD-CGD-O2D-CED |
| 41 | a | 410 | LMG | C17-C18-C19-C20 |
| 43 | D | 410 | LHG | C24-C25-C26-C27 |
| 43 | D | 411 | LHG | C31-C32-C33-C34 |
| 43 | a | 412 | LHG | C31-C32-C33-C34 |
| 37 | 19 | 303 | CLA | C10-C11-C12-C13 |
| 40 | 36 | 315 | SQD | C11-C12-C13-C14 |
| 41 | A | 408 | LMG | C17-C18-C19-C20 |
| 39 | H | 101 | BCR | C22-C23-C24-C25 |
| 39 | h | 101 | BCR | C22-C23-C24-C25 |
| 40 | A | 407 | SQD | C11-C12-C13-C14 |
| 40 | 17 | 301 | SQD | C11-C12-C13-C14 |
| 41 | B | 520 | LMG | C31-C32-C33-C34 |
| 41 | L | 102 | LMG | C33-C34-C35-C36 |
| 41 | b | 519 | LMG | C31-C32-C33-C34 |
| 41 | l | 101 | LMG | C33-C34-C35-C36 |
| 43 | 19 | 314 | LHG | C25-C26-C27-C28 |
| 43 | 39 | 314 | LHG | C25-C26-C27-C28 |
| 41 | 16 | 316 | LMG | C2-C1-O1-C7 |
| 41 | 36 | 314 | LMG | C2-C1-O1-C7 |
| 37 | 34 | 307 | CLA | CBD-CGD-O2D-CED |
| 40 | a | 409 | SQD | C11-C12-C13-C14 |
| 41 | c | 518 | LMG | C17-C18-C19-C20 |
| 41 | d | 409 | LMG | C30-C31-C32-C33 |
| 41 | B | 520 | LMG | C13-C14-C15-C16 |
| 41 | C | 518 | LMG | C17-C18-C19-C20 |
| 41 | D | 412 | LMG | C30-C31-C32-C33 |
| 41 | b | 519 | LMG | C13-C14-C15-C16 |
| 41 | 11 | 316 | LMG | C30-C31-C32-C33 |
| 41 | 31 | 316 | LMG | C30-C31-C32-C33 |
| 37 | 13 | 303 | CLA | C3-C5-C6-C7 |
| 37 | 39 | 303 | CLA | C3-C5-C6-C7 |
| 48 | 11 | 319 | A86 | C3-C4-C5-C6 |
| 48 | 14 | 314 | A86 | C3-C4-C5-C6 |
| 48 | 31 | 319 | A86 | C3-C4-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 34 | 314 | A86 | C3-C4-C5-C6 |
| 48 | 35 | 314 | A86 | C3-C4-C5-C6 |
| 50 | 19 | 312 | DD6 | C3-C4-C5-C6 |
| 50 | 39 | 312 | DD6 | C3-C4-C5-C6 |
| 37 | D | 402 | CLA | C16-C17-C18-C20 |
| 37 | d | 401 | CLA | C16-C17-C18-C20 |
| 37 | b | 523 | CLA | C10-C11-C12-C13 |
| 41 | B | 521 | LMG | O9-C10-O7-C8 |
| 41 | b | 520 | LMG | O9-C10-O7-C8 |
| 43 | 21 | 217 | LHG | O9-C7-O7-C5 |
| 47 | 20 | 305 | KC1 | C2C-C3C-CAC-CBC |
| 47 | 40 | 207 | KC1 | C2C-C3C-CAC-CBC |
| 37 | B | 524 | CLA | C10-C11-C12-C13 |
| 39 | D | 407 | BCR | C37-C22-C23-C24 |
| 39 | 0 | 101 | BCR | C7-C8-C9-C34 |
| 39 | 0 | 101 | BCR | C37-C22-C23-C24 |
| 39 | d | 405 | BCR | C37-C22-C23-C24 |
| 39 | 5 | 101 | BCR | C7-C8-C9-C34 |
| 39 | 5 | 101 | BCR | C37-C22-C23-C24 |
| 48 | 37 | 310 | A86 | C-C1-C24-C25 |
| 40 | 17 | 301 | SQD | C7-C8-C9-C10 |
| 40 | 36 | 315 | SQD | C7-C8-C9-C10 |
| 43 | D | 410 | LHG | C23-C24-C25-C26 |
| 43 | d | 408 | LHG | C23-C24-C25-C26 |
| 40 | B | 522 | SQD | C11-C10-C9-C8 |
| 40 | b | 521 | SQD | C11-C10-C9-C8 |
| 41 | A | 408 | LMG | C15-C16-C17-C18 |
| 41 | A | 408 | LMG | C20-C21-C22-C23 |
| 41 | B | 520 | LMG | C17-C18-C19-C20 |
| 41 | a | 410 | LMG | C15-C16-C17-C18 |
| 41 | a | 410 | LMG | C20-C21-C22-C23 |
| 43 | D | 409 | LHG | C25-C26-C27-C28 |
| 43 | D | 411 | LHG | C12-C13-C14-C15 |
| 43 | d | 407 | LHG | C25-C26-C27-C28 |
| 37 | 19 | 303 | CLA | C3-C5-C6-C7 |
| 39 | K | 101 | BCR | C17-C18-C19-C20 |
| 39 | y | 101 | BCR | C17-C18-C19-C20 |
| 48 | 16 | 310 | A86 | C2-C1-C24-C25 |
| 48 | 17 | 310 | A86 | C5-C6-C8-C9 |
| 48 | 36 | 310 | A86 | C2-C1-C24-C25 |
| 48 | 37 | 309 | A86 | C5-C6-C8-C9 |
| 50 | 20 | 310 | DD6 | C5-C6-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 50 | 40 | 212 | DD6 | C5-C6-C8-C9 |
| 41 | b | 519 | LMG | C17-C18-C19-C20 |
| 43 | a | 412 | LHG | C12-C13-C14-C15 |
| 37 | D | 401 | CLA | C2A-CAA-CBA-CGA |
| 37 | a | 404 | CLA | C2A-CAA-CBA-CGA |
| 47 | 20 | 305 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 40 | 207 | KC1 | CAA-CBA-CGA-O1A |
| 41 | B | 520 | LMG | C30-C31-C32-C33 |
| 41 | b | 519 | LMG | C30-C31-C32-C33 |
| 44 | C | 516 | DGD | C4B-C5B-C6B-C7B |
| 44 | c | 516 | DGD | C4B-C5B-C6B-C7B |
| 37 | 15 | 307 | CLA | C4-C3-C5-C6 |
| 37 | 17 | 307 | CLA | C4-C3-C5-C6 |
| 37 | 17 | 307 | CLA | C2-C3-C5-C6 |
| 47 | 11 | 309 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 14 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 14 | 306 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 15 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 15 | 306 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 15 | 309 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 16 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 16 | 305 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 17 | 305 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 17 | 308 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 18 | 205 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 20 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 31 | 309 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 34 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 34 | 306 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 35 | 302 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 35 | 306 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 35 | 309 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 36 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 36 | 305 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 37 | 304 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 37 | 307 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 38 | 205 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 40 | 206 | KC1 | C2B-C3B-CAB-CBB |
| 41 | A | 408 | LMG | C35-C36-C37-C38 |
| 41 | a | 410 | LMG | C35-C36-C37-C38 |
| 43 | 39 | 314 | LHG | C13-C14-C15-C16 |
| 44 | H | 102 | DGD | CBB-CCB-CDB-CEB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 44 | h | 102 | DGD | CBB-CCB-CDB-CEB |
| 37 | W | 102 | CLA | C15-C16-C17-C18 |
| 37 | 31 | 301 | CLA | C15-C16-C17-C18 |
| 41 | L | 102 | LMG | C29-C30-C31-C32 |
| 41 | l | 101 | LMG | C29-C30-C31-C32 |
| 43 | 19 | 314 | LHG | C13-C14-C15-C16 |
| 43 | 39 | 314 | LHG | C11-C12-C13-C14 |
| 40 | B | 519 | SQD | C17-C18-C19-C20 |
| 43 | 19 | 314 | LHG | C11-C12-C13-C14 |
| 37 | W | 101 | CLA | O1A-CGA-O2A-C1 |
| 37 | w | 101 | CLA | O1A-CGA-O2A-C1 |
| 41 | B | 521 | LMG | O10-C28-O8-C9 |
| 41 | b | 520 | LMG | O10-C28-O8-C9 |
| 37 | 13 | 308 | CLA | C3-C5-C6-C7 |
| 37 | 33 | 308 | CLA | C3-C5-C6-C7 |
| 37 | B | 512 | CLA | C10-C11-C12-C13 |
| 37 | C | 502 | CLA | C13-C15-C16-C17 |
| 37 | b | 512 | CLA | C10-C11-C12-C13 |
| 37 | c | 502 | CLA | C13-C15-C16-C17 |
| 37 | 12 | 203 | CLA | C10-C11-C12-C13 |
| 37 | 32 | 204 | CLA | C10-C11-C12-C13 |
| 38 | D | 403 | PHO | C13-C15-C16-C17 |
| 40 | L | 101 | SQD | C17-C18-C19-C20 |
| 43 | 37 | 321 | LHG | O9-C7-O7-C5 |
| 37 | B | 508 | CLA | C13-C15-C16-C17 |
| 37 | b | 508 | CLA | C13-C15-C16-C17 |
| 37 | 13 | 308 | CLA | C5-C6-C7-C8 |
| 37 | 33 | 308 | CLA | C5-C6-C7-C8 |
| 38 | a | 405 | PHO | C13-C15-C16-C17 |
| 44 | C | 517 | DGD | C5A-C6A-C7A-C8A |
| 44 | c | 517 | DGD | C5A-C6A-C7A-C8A |
| 41 | 11 | 317 | LMG | O10-C28-O8-C9 |
| 41 | 31 | 317 | LMG | O10-C28-O8-C9 |
| 41 | B | 521 | LMG | C16-C17-C18-C19 |
| 43 | d | 407 | LHG | C14-C15-C16-C17 |
| 41 | 11 | 316 | LMG | C10-C11-C12-C13 |
| 41 | 17 | 317 | LMG | C28-C29-C30-C31 |
| 41 | 31 | 316 | LMG | C10-C11-C12-C13 |
| 41 | b | 520 | LMG | C16-C17-C18-C19 |
| 43 | D | 409 | LHG | C14-C15-C16-C17 |
| 41 | C | 518 | LMG | O7-C8-C9-O8 |
| 41 | c | 518 | LMG | O7-C8-C9-O8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | c | 518 | LMG | C16-C17-C18-C19 |
| 43 | 17 | 316 | LHG | C13-C14-C15-C16 |
| 43 | 21 | 217 | LHG | C29-C30-C31-C32 |
| 43 | 37 | 315 | LHG | C13-C14-C15-C16 |
| 43 | 37 | 321 | LHG | C29-C30-C31-C32 |
| 37 | 16 | 307 | CLA | CBA-CGA-O2A-C1 |
| 37 | 36 | 307 | CLA | CBA-CGA-O2A-C1 |
| 43 | 17 | 316 | LHG | C24-C23-O8-C6 |
| 43 | 37 | 315 | LHG | C24-C23-O8-C6 |
| 41 | C | 518 | LMG | C16-C17-C18-C19 |
| 43 | D | 409 | LHG | C11-C10-C9-C8 |
| 43 | D | 411 | LHG | C28-C29-C30-C31 |
| 43 | a | 412 | LHG | C28-C29-C30-C31 |
| 43 | d | 407 | LHG | C11-C10-C9-C8 |
| 43 | 37 | 315 | LHG | C27-C28-C29-C30 |
| 37 | C | 510 | CLA | C13-C15-C16-C17 |
| 37 | c | 510 | CLA | C13-C15-C16-C17 |
| 41 | 32 | 201 | LMG | C33-C34-C35-C36 |
| 43 | 17 | 316 | LHG | C27-C28-C29-C30 |
| 37 | 19 | 302 | CLA | CBD-CGD-O2D-CED |
| 41 | 12 | 201 | LMG | C33-C34-C35-C36 |
| 44 | J | 101 | DGD | C5B-C6B-C7B-C8B |
| 44 | j | 101 | DGD | C5B-C6B-C7B-C8B |
| 37 | B | 511 | CLA | C4-C3-C5-C6 |
| 37 | b | 511 | CLA | C4-C3-C5-C6 |
| 37 | 13 | 308 | CLA | C4-C3-C5-C6 |
| 37 | 33 | 308 | CLA | C4-C3-C5-C6 |
| 37 | 16 | 306 | CLA | C3-C5-C6-C7 |
| 37 | 36 | 306 | CLA | C3-C5-C6-C7 |
| 37 | 37 | 306 | CLA | C2-C3-C5-C6 |
| 45 | D | 404 | PL9 | C12-C11-C9-C8 |
| 45 | D | 408 | PL9 | C13-C14-C16-C17 |
| 45 | d | 402 | PL9 | C12-C11-C9-C8 |
| 45 | d | 406 | PL9 | C13-C14-C16-C17 |
| 40 | L | 101 | SQD | C31-C32-C33-C34 |
| 41 | B | 521 | LMG | C31-C32-C33-C34 |
| 41 | b | 520 | LMG | C31-C32-C33-C34 |
| 37 | B | 503 | CLA | C2A-CAA-CBA-CGA |
| 37 | b | 503 | CLA | C2A-CAA-CBA-CGA |
| 37 | 16 | 303 | CLA | CBD-CGD-O2D-CED |
| 37 | 36 | 303 | CLA | CBD-CGD-O2D-CED |
| 37 | 21 | 206 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 41 | 206 | CLA | CBA-CGA-O2A-C1 |
| 41 | l | 101 | LMG | O6-C5-C6-O5 |
| 40 | B | 519 | SQD | C31-C32-C33-C34 |
| 44 | C | 517 | DGD | CBA-CCA-CDA-CEA |
| 41 | 37 | 316 | LMG | C28-C29-C30-C31 |
| 44 | H | 102 | DGD | CCB-CDB-CEB-CFB |
| 44 | c | 517 | DGD | CBA-CCA-CDA-CEA |
| 44 | h | 102 | DGD | CCB-CDB-CEB-CFB |
| 37 | B | 515 | CLA | C16-C17-C18-C19 |
| 37 | b | 515 | CLA | C16-C17-C18-C19 |
| 41 | L | 102 | LMG | O6-C5-C6-O5 |
| 43 | D | 411 | LHG | O1-C1-C2-O2 |
| 43 | a | 412 | LHG | O1-C1-C2-O2 |
| 43 | 21 | 217 | LHG | O1-C1-C2-O2 |
| 43 | 37 | 321 | LHG | O1-C1-C2-O2 |
| 44 | C | 516 | DGD | C8A-C9A-CAA-CBA |
| 44 | c | 516 | DGD | C8A-C9A-CAA-CBA |
| 37 | A | 405 | CLA | C1A-C2A-CAA-CBA |
| 37 | B | 503 | CLA | C1A-C2A-CAA-CBA |
| 37 | B | 524 | CLA | C1A-C2A-CAA-CBA |
| 37 | C | 502 | CLA | C1A-C2A-CAA-CBA |
| 37 | C | 503 | CLA | C1A-C2A-CAA-CBA |
| 37 | C | 508 | CLA | C1A-C2A-CAA-CBA |
| 37 | C | 511 | CLA | C1A-C2A-CAA-CBA |
| 37 | D | 401 | CLA | C1A-C2A-CAA-CBA |
| 37 | D | 402 | CLA | C1A-C2A-CAA-CBA |
| 37 | D | 406 | CLA | C1A-C2A-CAA-CBA |
| 37 | W | 102 | CLA | C1A-C2A-CAA-CBA |
| 37 | a | 407 | CLA | C1A-C2A-CAA-CBA |
| 37 | b | 503 | CLA | C1A-C2A-CAA-CBA |
| 37 | b | 523 | CLA | C1A-C2A-CAA-CBA |
| 37 | c | 502 | CLA | C1A-C2A-CAA-CBA |
| 37 | c | 503 | CLA | C1A-C2A-CAA-CBA |
| 37 | c | 508 | CLA | C1A-C2A-CAA-CBA |
| 37 | c | 511 | CLA | C1A-C2A-CAA-CBA |
| 37 | d | 401 | CLA | C1A-C2A-CAA-CBA |
| 37 | d | 404 | CLA | C1A-C2A-CAA-CBA |
| 37 | 11 | 305 | CLA | C1A-C2A-CAA-CBA |
| 37 | 11 | 308 | CLA | C1A-C2A-CAA-CBA |
| 37 | 11 | 310 | CLA | C1A-C2A-CAA-CBA |
| 37 | 12 | 203 | CLA | C1A-C2A-CAA-CBA |
| 37 | 12 | 210 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 13 | 308 | CLA | C1A-C2A-CAA-CBA |
| 37 | 14 | 305 | CLA | C1A-C2A-CAA-CBA |
| 37 | 16 | 307 | CLA | C1A-C2A-CAA-CBA |
| 37 | 17 | 309 | CLA | C1A-C2A-CAA-CBA |
| 37 | 18 | 201 | CLA | C1A-C2A-CAA-CBA |
| 37 | 18 | 203 | CLA | C1A-C2A-CAA-CBA |
| 37 | 19 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 19 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 19 | 305 | CLA | C1A-C2A-CAA-CBA |
| 37 | 19 | 306 | CLA | C1A-C2A-CAA-CBA |
| 37 | 19 | 307 | CLA | C1A-C2A-CAA-CBA |
| 37 | 20 | 308 | CLA | C1A-C2A-CAA-CBA |
| 37 | 21 | 205 | CLA | C1A-C2A-CAA-CBA |
| 37 | 21 | 206 | CLA | C1A-C2A-CAA-CBA |
| 37 | 21 | 208 | CLA | C1A-C2A-CAA-CBA |
| 37 | 31 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 31 | 306 | CLA | C1A-C2A-CAA-CBA |
| 37 | 31 | 310 | CLA | C1A-C2A-CAA-CBA |
| 37 | 32 | 202 | CLA | C1A-C2A-CAA-CBA |
| 37 | 32 | 204 | CLA | C1A-C2A-CAA-CBA |
| 37 | 32 | 211 | CLA | C1A-C2A-CAA-CBA |
| 37 | 33 | 308 | CLA | C1A-C2A-CAA-CBA |
| 37 | 34 | 305 | CLA | C1A-C2A-CAA-CBA |
| 37 | 36 | 307 | CLA | C1A-C2A-CAA-CBA |
| 37 | 37 | 308 | CLA | C1A-C2A-CAA-CBA |
| 37 | 38 | 201 | CLA | C1A-C2A-CAA-CBA |
| 37 | 38 | 203 | CLA | C1A-C2A-CAA-CBA |
| 37 | 39 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 39 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 39 | 305 | CLA | C1A-C2A-CAA-CBA |
| 37 | 39 | 306 | CLA | C1A-C2A-CAA-CBA |
| 37 | 39 | 307 | CLA | C1A-C2A-CAA-CBA |
| 37 | 40 | 210 | CLA | C1A-C2A-CAA-CBA |
| 37 | 41 | 205 | CLA | C1A-C2A-CAA-CBA |
| 37 | 41 | 206 | CLA | C1A-C2A-CAA-CBA |
| 37 | 41 | 208 | CLA | C1A-C2A-CAA-CBA |
| 37 | 11 | 310 | CLA | O1A-CGA-O2A-C1 |
| 43 | D | 410 | LHG | O9-C7-O7-C5 |
| 43 | d | 408 | LHG | O9-C7-O7-C5 |
| 40 | 16 | 315 | SQD | C23-C24-C25-C26 |
| 40 | 40 | 202 | SQD | C23-C24-C25-C26 |
| 37 | b | 516 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | A | 405 | CLA | C11-C10-C8-C7 |
| 37 | B | 506 | CLA | C11-C10-C8-C7 |
| 37 | B | 507 | CLA | C12-C13-C15-C16 |
| 37 | B | 508 | CLA | C12-C13-C15-C16 |
| 37 | B | 511 | CLA | C12-C13-C15-C16 |
| 37 | B | 524 | CLA | C6-C7-C8-C10 |
| 37 | B | 524 | CLA | C11-C10-C8-C7 |
| 37 | C | 510 | CLA | C12-C13-C15-C16 |
| 37 | Z | 101 | CLA | C6-C7-C8-C10 |
| 37 | Z | 101 | CLA | C11-C12-C13-C15 |
| 37 | a | 407 | CLA | C11-C10-C8-C7 |
| 37 | b | 506 | CLA | C11-C10-C8-C7 |
| 37 | b | 507 | CLA | C12-C13-C15-C16 |
| 37 | b | 508 | CLA | C12-C13-C15-C16 |
| 37 | b | 511 | CLA | C12-C13-C15-C16 |
| 37 | b | 523 | CLA | C6-C7-C8-C10 |
| 37 | b | 523 | CLA | C11-C10-C8-C7 |
| 37 | c | 510 | CLA | C12-C13-C15-C16 |
| 37 | z | 101 | CLA | C6-C7-C8-C10 |
| 37 | z | 101 | CLA | C11-C12-C13-C15 |
| 37 | 14 | 301 | CLA | C6-C7-C8-C10 |
| 37 | 14 | 301 | CLA | C12-C13-C15-C16 |
| 37 | 18 | 202 | CLA | C11-C10-C8-C7 |
| 37 | 18 | 202 | CLA | C12-C13-C15-C16 |
| 37 | 21 | 204 | CLA | C6-C7-C8-C10 |
| 37 | 34 | 301 | CLA | C6-C7-C8-C10 |
| 37 | 34 | 301 | CLA | C12-C13-C15-C16 |
| 37 | 38 | 202 | CLA | C11-C10-C8-C7 |
| 37 | 38 | 202 | CLA | C12-C13-C15-C16 |
| 37 | 41 | 204 | CLA | C6-C7-C8-C10 |
| 37 | 12 | 205 | CLA | C10-C11-C12-C13 |
| 37 | 32 | 206 | CLA | C10-C11-C12-C13 |
| 37 | 31 | 310 | CLA | O1A-CGA-O2A-C1 |
| 37 | 39 | 302 | CLA | CBD-CGD-O2D-CED |
| 47 | 40 | 207 | KC1 | CBD-CGD-O2D-CED |
| 47 | 20 | 304 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 20 | 305 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 32 | 212 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 40 | 206 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 40 | 207 | KC1 | CAA-CBA-CGA-O2A |
| 37 | C | 509 | CLA | C15-C16-C17-C18 |
| 37 | c | 509 | CLA | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 21 | 206 | CLA | C10-C11-C12-C13 |
| 37 | 41 | 206 | CLA | C10-C11-C12-C13 |
| 37 | B | 509 | CLA | C4-C3-C5-C6 |
| 37 | b | 509 | CLA | C4-C3-C5-C6 |
| 37 | 18 | 209 | CLA | C4-C3-C5-C6 |
| 45 | D | 404 | PL9 | C30-C29-C31-C32 |
| 45 | d | 402 | PL9 | C30-C29-C31-C32 |
| 37 | B | 509 | CLA | C2-C3-C5-C6 |
| 37 | b | 509 | CLA | C2-C3-C5-C6 |
| 37 | b | 511 | CLA | C2-C3-C5-C6 |
| 37 | 41 | 209 | CLA | O1D-CGD-O2D-CED |
| 41 | a | 410 | LMG | C13-C14-C15-C16 |
| 37 | 13 | 301 | CLA | C5-C6-C7-C8 |
| 47 | 20 | 305 | KC1 | CBD-CGD-O2D-CED |
| 37 | B | 508 | CLA | C14-C13-C15-C16 |
| 37 | C | 509 | CLA | C14-C13-C15-C16 |
| 37 | b | 508 | CLA | C14-C13-C15-C16 |
| 37 | c | 509 | CLA | C14-C13-C15-C16 |
| 37 | 11 | 308 | CLA | C14-C13-C15-C16 |
| 37 | 14 | 301 | CLA | C6-C7-C8-C9 |
| 37 | 14 | 301 | CLA | C14-C13-C15-C16 |
| 37 | 19 | 307 | CLA | C14-C13-C15-C16 |
| 37 | 32 | 202 | CLA | C14-C13-C15-C16 |
| 37 | 34 | 301 | CLA | C6-C7-C8-C9 |
| 37 | 34 | 301 | CLA | C14-C13-C15-C16 |
| 37 | 39 | 307 | CLA | C14-C13-C15-C16 |
| 40 | 16 | 315 | SQD | C13-C14-C15-C16 |
| 40 | 40 | 202 | SQD | C13-C14-C15-C16 |
| 43 | B | 523 | LHG | C11-C12-C13-C14 |
| 43 | b | 522 | LHG | C11-C12-C13-C14 |
| 37 | 11 | 307 | CLA | C4C-C3C-CAC-CBC |
| 41 | A | 408 | LMG | C13-C14-C15-C16 |
| 41 | 32 | 201 | LMG | C32-C33-C34-C35 |
| 43 | D | 409 | LHG | C9-C10-C11-C12 |
| 43 | d | 407 | LHG | C9-C10-C11-C12 |
| 37 | B | 516 | CLA | O1D-CGD-O2D-CED |
| 37 | B | 512 | CLA | CBA-CGA-O2A-C1 |
| 37 | b | 512 | CLA | CBA-CGA-O2A-C1 |
| 38 | D | 403 | PHO | CBA-CGA-O2A-C1 |
| 38 | a | 405 | PHO | CBA-CGA-O2A-C1 |
| 37 | 33 | 301 | CLA | C5-C6-C7-C8 |
| 37 | B | 504 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | b | 504 | CLA | CBD-CGD-O2D-CED |
| 37 | 21 | 209 | CLA | O1D-CGD-O2D-CED |
| 41 | 12 | 201 | LMG | C32-C33-C34-C35 |
| 44 | c | 516 | DGD | CCA-CDA-CEA-CFA |
| 37 | A | 403 | CLA | C5-C6-C7-C8 |
| 37 | a | 403 | CLA | C5-C6-C7-C8 |
| 44 | C | 516 | DGD | CCA-CDA-CEA-CFA |
| 51 | 19 | 315 | LMU | C11-C10-C9-C8 |
| 47 | 12 | 211 | KC1 | CAA-CBA-CGA-O1A |
| 40 | A | 407 | SQD | O6-C44-C45-C46 |
| 40 | a | 409 | SQD | O6-C44-C45-C46 |
| 41 | A | 408 | LMG | O1-C7-C8-C9 |
| 41 | C | 518 | LMG | C7-C8-C9-O8 |
| 41 | a | 410 | LMG | O1-C7-C8-C9 |
| 41 | c | 518 | LMG | C7-C8-C9-O8 |
| 41 | 11 | 317 | LMG | C7-C8-C9-O8 |
| 41 | 31 | 317 | LMG | C7-C8-C9-O8 |
| 43 | 21 | 201 | LHG | C4-C5-C6-O8 |
| 43 | 41 | 201 | LHG | C4-C5-C6-O8 |
| 37 | 31 | 308 | CLA | C4C-C3C-CAC-CBC |
| 43 | 19 | 314 | LHG | C10-C11-C12-C13 |
| 51 | 39 | 315 | LMU | C11-C10-C9-C8 |
| 37 | 16 | 301 | CLA | C3-C5-C6-C7 |
| 37 | 36 | 301 | CLA | C3-C5-C6-C7 |
| 41 | D | 412 | LMG | C20-C21-C22-C23 |
| 41 | d | 409 | LMG | C20-C21-C22-C23 |
| 37 | b | 514 | CLA | C8-C10-C11-C12 |
| 37 | 16 | 307 | CLA | C10-C11-C12-C13 |
| 37 | 36 | 307 | CLA | C10-C11-C12-C13 |
| 37 | B | 505 | CLA | CBA-CGA-O2A-C1 |
| 37 | B | 509 | CLA | CBA-CGA-O2A-C1 |
| 37 | b | 505 | CLA | CBA-CGA-O2A-C1 |
| 37 | b | 509 | CLA | CBA-CGA-O2A-C1 |
| 37 | 15 | 307 | CLA | CBA-CGA-O2A-C1 |
| 37 | 35 | 307 | CLA | CBA-CGA-O2A-C1 |
| 41 | A | 408 | LMG | C36-C37-C38-C39 |
| 41 | B | 520 | LMG | C29-C30-C31-C32 |
| 41 | a | 410 | LMG | C36-C37-C38-C39 |
| 41 | b | 519 | LMG | C29-C30-C31-C32 |
| 43 | 39 | 314 | LHG | C10-C11-C12-C13 |
| 37 | 17 | 309 | CLA | C2C-C3C-CAC-CBC |
| 37 | B | 514 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | B | 520 | LMG | C4-C5-C6-O5 |
| 41 | b | 519 | LMG | C4-C5-C6-O5 |
| 39 | A | 410 | BCR | C11-C10-C9-C34 |
| 39 | a | 413 | BCR | C11-C10-C9-C34 |
| 37 | 39 | 310 | CLA | C5-C6-C7-C8 |
| 43 | B | 523 | LHG | C29-C30-C31-C32 |
| 43 | b | 522 | LHG | C29-C30-C31-C32 |
| 43 | 17 | 316 | LHG | C7-C8-C9-C10 |
| 43 | 37 | 315 | LHG | C7-C8-C9-C10 |
| 39 | B | 525 | BCR | C14-C15-C16-C17 |
| 37 | 16 | 307 | CLA | O1A-CGA-O2A-C1 |
| 37 | 36 | 307 | CLA | O1A-CGA-O2A-C1 |
| 41 | 11 | 316 | LMG | O10-C28-O8-C9 |
| 41 | 31 | 316 | LMG | O10-C28-O8-C9 |
| 44 | C | 516 | DGD | O1A-C1A-O1G-C1G |
| 44 | c | 516 | DGD | O1A-C1A-O1G-C1G |
| 41 | A | 408 | LMG | C38-C39-C40-C41 |
| 41 | a | 410 | LMG | C38-C39-C40-C41 |
| 44 | H | 102 | DGD | C2B-C3B-C4B-C5B |
| 37 | B | 511 | CLA | C2-C3-C5-C6 |
| 37 | 13 | 303 | CLA | C2-C3-C5-C6 |
| 37 | 13 | 308 | CLA | C2-C3-C5-C6 |
| 37 | 15 | 307 | CLA | C2-C3-C5-C6 |
| 37 | 33 | 308 | CLA | C2-C3-C5-C6 |
| 44 | h | 102 | DGD | C2B-C3B-C4B-C5B |
| 41 | A | 408 | LMG | O6-C5-C6-O5 |
| 41 | a | 410 | LMG | O6-C5-C6-O5 |
| 48 | 12 | 217 | A86 | C7-C6-C8-C9 |
| 48 | 16 | 310 | A86 | C-C1-C24-C25 |
| 48 | 18 | 215 | A86 | C7-C6-C8-C9 |
| 48 | 32 | 218 | A86 | C7-C6-C8-C9 |
| 48 | 36 | 310 | A86 | C-C1-C24-C25 |
| 48 | 38 | 215 | A86 | C7-C6-C8-C9 |
| 41 | D | 412 | LMG | C36-C37-C38-C39 |
| 37 | B | 515 | CLA | C16-C17-C18-C20 |
| 37 | b | 515 | CLA | C16-C17-C18-C20 |
| 41 | d | 409 | LMG | C36-C37-C38-C39 |
| 48 | 11 | 315 | A86 | C2-C1-C24-C25 |
| 48 | 12 | 217 | A86 | C5-C6-C8-C9 |
| 48 | 14 | 315 | A86 | C2-C1-C24-C25 |
| 48 | 14 | 316 | A86 | C2-C1-C24-C25 |
| 48 | 14 | 316 | A86 | C5-C6-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 15 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 18 | 215 | A86 | C5-C6-C8-C9 |
| 48 | 31 | 315 | A86 | C2-C1-C24-C25 |
| 48 | 32 | 218 | A86 | C5-C6-C8-C9 |
| 48 | 34 | 315 | A86 | C2-C1-C24-C25 |
| 48 | 34 | 316 | A86 | C2-C1-C24-C25 |
| 48 | 34 | 316 | A86 | C5-C6-C8-C9 |
| 48 | 35 | 313 | A86 | C2-C1-C24-C25 |
| 48 | 38 | 215 | A86 | C5-C6-C8-C9 |
| 50 | 20 | 312 | DD6 | C10-C11-C13-C14 |
| 50 | 40 | 214 | DD6 | C10-C11-C13-C14 |
| 37 | B | 509 | CLA | O1A-CGA-O2A-C1 |
| 37 | b | 509 | CLA | O1A-CGA-O2A-C1 |
| 37 | W | 101 | CLA | C15-C16-C17-C18 |
| 37 | w | 101 | CLA | C15-C16-C17-C18 |
| 43 | B | 523 | LHG | C14-C15-C16-C17 |
| 43 | b | 522 | LHG | C14-C15-C16-C17 |
| 43 | 21 | 217 | LHG | C11-C10-C9-C8 |
| 43 | 37 | 321 | LHG | C11-C10-C9-C8 |
| 37 | 13 | 307 | CLA | C2A-CAA-CBA-CGA |
| 37 | 33 | 307 | CLA | C2A-CAA-CBA-CGA |
| 43 | D | 410 | LHG | C7-C8-C9-C10 |
| 43 | d | 408 | LHG | C7-C8-C9-C10 |
| 41 | 17 | 317 | LMG | C16-C17-C18-C19 |
| 41 | 37 | 316 | LMG | C16-C17-C18-C19 |
| 43 | b | 522 | LHG | C33-C34-C35-C36 |
| 37 | 32 | 210 | CLA | O1D-CGD-O2D-CED |
| 37 | B | 503 | CLA | CBA-CGA-O2A-C1 |
| 37 | b | 503 | CLA | CBA-CGA-O2A-C1 |
| 37 | C | 503 | CLA | O2A-C1-C2-C3 |
| 37 | c | 503 | CLA | O2A-C1-C2-C3 |
| 43 | 17 | 316 | LHG | C4-C5-O7-C7 |
| 43 | 37 | 315 | LHG | C4-C5-O7-C7 |
| 40 | B | 519 | SQD | C27-C28-C29-C30 |
| 40 | L | 101 | SQD | C27-C28-C29-C30 |
| 43 | B | 523 | LHG | C33-C34-C35-C36 |
| 43 | D | 411 | LHG | C9-C10-C11-C12 |
| 43 | a | 412 | LHG | C9-C10-C11-C12 |
| 37 | Z | 101 | CLA | C13-C15-C16-C17 |
| 37 | W | 102 | CLA | C8-C10-C11-C12 |
| 37 | z | 101 | CLA | C13-C15-C16-C17 |
| 37 | 31 | 301 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | A | 408 | LMG | C37-C38-C39-C40 |
| 41 | a | 410 | LMG | C37-C38-C39-C40 |
| 48 | 15 | 314 | A86 | C3-C4-C5-C6 |
| 48 | 15 | 316 | A86 | C3-C4-C5-C6 |
| 48 | 35 | 316 | A86 | C3-C4-C5-C6 |
| 44 | J | 101 | DGD | C5A-C6A-C7A-C8A |
| 44 | j | 101 | DGD | C5A-C6A-C7A-C8A |
| 43 | 17 | 316 | LHG | C23-C24-C25-C26 |
| 43 | 37 | 315 | LHG | C23-C24-C25-C26 |
| 37 | B | 512 | CLA | O1A-CGA-O2A-C1 |
| 37 | b | 505 | CLA | O1A-CGA-O2A-C1 |
| 37 | b | 512 | CLA | O1A-CGA-O2A-C1 |
| 37 | C | 504 | CLA | C3-C5-C6-C7 |
| 37 | c | 504 | CLA | C3-C5-C6-C7 |
| 37 | 12 | 210 | CLA | CBD-CGD-O2D-CED |
| 50 | 16 | 312 | DD6 | C4-C5-C6-C8 |
| 50 | 20 | 312 | DD6 | C9-C10-C11-C13 |
| 50 | 36 | 312 | DD6 | C4-C5-C6-C8 |
| 50 | 40 | 214 | DD6 | C9-C10-C11-C13 |
| 40 | 17 | 301 | SQD | C12-C13-C14-C15 |
| 40 | 36 | 315 | SQD | C12-C13-C14-C15 |
| 41 | A | 408 | LMG | C30-C31-C32-C33 |
| 43 | D | 411 | LHG | O6-C4-C5-O7 |
| 43 | a | 412 | LHG | O6-C4-C5-O7 |
| 41 | a | 410 | LMG | C30-C31-C32-C33 |
| 43 | 37 | 321 | LHG | C26-C27-C28-C29 |
| 37 | 38 | 208 | CLA | CBA-CGA-O2A-C1 |
| 37 | B | 505 | CLA | O1A-CGA-O2A-C1 |
| 43 | 21 | 217 | LHG | C26-C27-C28-C29 |
| 44 | H | 102 | DGD | CCA-CDA-CEA-CFA |
| 43 | 39 | 314 | LHG | C32-C33-C34-C35 |
| 44 | h | 102 | DGD | CCA-CDA-CEA-CFA |
| 51 | 19 | 315 | LMU | C7-C8-C9-C10 |
| 51 | 39 | 315 | LMU | C7-C8-C9-C10 |
| 37 | 38 | 209 | CLA | C4-C3-C5-C6 |
| 37 | 21 | 206 | CLA | C2-C3-C5-C6 |
| 37 | 35 | 307 | CLA | C2-C3-C5-C6 |
| 37 | 41 | 206 | CLA | C2-C3-C5-C6 |
| 41 | B | 520 | LMG | C37-C38-C39-C40 |
| 41 | b | 519 | LMG | C37-C38-C39-C40 |
| 37 | 16 | 307 | CLA | C3-C5-C6-C7 |
| 40 | B | 522 | SQD | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 40 | b | 521 | SQD | C12-C13-C14-C15 |
| 40 | 40 | 202 | SQD | C12-C13-C14-C15 |
| 41 | B | 521 | LMG | C34-C35-C36-C37 |
| 43 | 19 | 314 | LHG | C32-C33-C34-C35 |
| 41 | 12 | 201 | LMG | C16-C17-C18-C19 |
| 41 | 32 | 201 | LMG | C16-C17-C18-C19 |
| 40 | 16 | 315 | SQD | C12-C13-C14-C15 |
| 41 | b | 520 | LMG | C34-C35-C36-C37 |
| 40 | A | 407 | SQD | O6-C44-C45-O47 |
| 40 | B | 519 | SQD | O47-C45-C46-O48 |
| 40 | B | 522 | SQD | O47-C45-C46-O48 |
| 40 | L | 101 | SQD | O47-C45-C46-O48 |
| 40 | a | 409 | SQD | O6-C44-C45-O47 |
| 40 | b | 521 | SQD | O47-C45-C46-O48 |
| 41 | 11 | 317 | LMG | C32-C33-C34-C35 |
| 43 | 17 | 316 | LHG | C9-C10-C11-C12 |
| 37 | 38 | 201 | CLA | CBA-CGA-O2A-C1 |
| 41 | 31 | 317 | LMG | C32-C33-C34-C35 |
| 43 | 19 | 314 | LHG | C19-C20-C21-C22 |
| 40 | B | 519 | SQD | C18-C19-C20-C21 |
| 40 | L | 101 | SQD | C18-C19-C20-C21 |
| 41 | D | 412 | LMG | C32-C33-C34-C35 |
| 43 | 37 | 315 | LHG | C9-C10-C11-C12 |
| 37 | 12 | 209 | CLA | O1D-CGD-O2D-CED |
| 41 | d | 409 | LMG | C32-C33-C34-C35 |
| 44 | C | 516 | DGD | CBA-CCA-CDA-CEA |
| 44 | c | 516 | DGD | CBA-CCA-CDA-CEA |
| 37 | 36 | 307 | CLA | C3-C5-C6-C7 |
| 43 | 39 | 314 | LHG | C19-C20-C21-C22 |
| 41 | L | 102 | LMG | C16-C17-C18-C19 |
| 41 | l | 101 | LMG | C16-C17-C18-C19 |
| 37 | 18 | 201 | CLA | CBA-CGA-O2A-C1 |
| 37 | 18 | 208 | CLA | CBA-CGA-O2A-C1 |
| 41 | 37 | 316 | LMG | C15-C16-C17-C18 |
| 40 | 17 | 301 | SQD | C35-C36-C37-C38 |
| 40 | 36 | 315 | SQD | C35-C36-C37-C38 |
| 41 | 17 | 317 | LMG | C15-C16-C17-C18 |
| 37 | 19 | 310 | CLA | C5-C6-C7-C8 |
| 37 | B | 516 | CLA | C3-C5-C6-C7 |
| 39 | b | 524 | BCR | C14-C15-C16-C17 |
| 44 | j | 101 | DGD | CCA-CDA-CEA-CFA |
| 37 | B | 511 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | B | 524 | CLA | C13-C15-C16-C17 |
| 37 | C | 504 | CLA | C15-C16-C17-C18 |
| 37 | b | 511 | CLA | C10-C11-C12-C13 |
| 37 | c | 504 | CLA | C15-C16-C17-C18 |
| 37 | 16 | 309 | CLA | O1D-CGD-O2D-CED |
| 37 | 36 | 309 | CLA | O1D-CGD-O2D-CED |
| 48 | 17 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 19 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 19 | 313 | A86 | C11-C10-C9-C8 |
| 48 | 31 | 313 | A86 | C24-C25-C26-C27 |
| 48 | 37 | 310 | A86 | C24-C25-C26-C27 |
| 48 | 39 | 311 | A86 | C24-C25-C26-C27 |
| 48 | 39 | 313 | A86 | C11-C10-C9-C8 |
| 44 | J | 101 | DGD | CCA-CDA-CEA-CFA |
| 37 | 12 | 209 | CLA | C4-C3-C5-C6 |
| 37 | 14 | 307 | CLA | C4-C3-C5-C6 |
| 37 | 21 | 206 | CLA | C4-C3-C5-C6 |
| 37 | 32 | 210 | CLA | C4-C3-C5-C6 |
| 37 | 41 | 206 | CLA | C4-C3-C5-C6 |
| 37 | 21 | 202 | CLA | CBA-CGA-O2A-C1 |
| 37 | 41 | 202 | CLA | CBA-CGA-O2A-C1 |
| 37 | D | 405 | CLA | C15-C16-C17-C18 |
| 37 | d | 403 | CLA | C15-C16-C17-C18 |
| 37 | 11 | 301 | CLA | C8-C10-C11-C12 |
| 37 | 31 | 302 | CLA | C8-C10-C11-C12 |
| 43 | a | 412 | LHG | C13-C14-C15-C16 |
| 37 | b | 516 | CLA | C3-C5-C6-C7 |
| 37 | B | 506 | CLA | C11-C10-C8-C9 |
| 37 | B | 507 | CLA | C14-C13-C15-C16 |
| 37 | B | 510 | CLA | C11-C12-C13-C14 |
| 37 | B | 524 | CLA | C11-C10-C8-C9 |
| 37 | Z | 101 | CLA | C6-C7-C8-C9 |
| 37 | b | 506 | CLA | C11-C10-C8-C9 |
| 37 | b | 507 | CLA | C14-C13-C15-C16 |
| 37 | b | 510 | CLA | C11-C12-C13-C14 |
| 37 | b | 523 | CLA | C11-C10-C8-C9 |
| 37 | z | 101 | CLA | C6-C7-C8-C9 |
| 37 | 16 | 306 | CLA | C14-C13-C15-C16 |
| 37 | 18 | 202 | CLA | C11-C10-C8-C9 |
| 37 | 18 | 202 | CLA | C14-C13-C15-C16 |
| 37 | 21 | 204 | CLA | C6-C7-C8-C9 |
| 37 | 36 | 306 | CLA | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 38 | 202 | CLA | C11-C10-C8-C9 |
| 37 | 38 | 202 | CLA | C14-C13-C15-C16 |
| 37 | 41 | 204 | CLA | C6-C7-C8-C9 |
| 41 | b | 520 | LMG | C17-C18-C19-C20 |
| 43 | D | 411 | LHG | C13-C14-C15-C16 |
| 37 | C | 510 | CLA | C10-C11-C12-C13 |
| 37 | c | 510 | CLA | C10-C11-C12-C13 |
| 37 | 21 | 208 | CLA | C10-C11-C12-C13 |
| 37 | 41 | 208 | CLA | C10-C11-C12-C13 |
| 37 | B | 514 | CLA | C4B-C3B-CAB-CBB |
| 37 | C | 511 | CLA | C4B-C3B-CAB-CBB |
| 37 | b | 514 | CLA | C4B-C3B-CAB-CBB |
| 37 | c | 511 | CLA | C4B-C3B-CAB-CBB |
| 37 | 11 | 303 | CLA | C4B-C3B-CAB-CBB |
| 37 | 12 | 203 | CLA | C4B-C3B-CAB-CBB |
| 37 | 12 | 207 | CLA | C4B-C3B-CAB-CBB |
| 37 | 13 | 307 | CLA | C4B-C3B-CAB-CBB |
| 37 | 16 | 303 | CLA | C4B-C3B-CAB-CBB |
| 37 | 17 | 307 | CLA | C4B-C3B-CAB-CBB |
| 37 | 18 | 203 | CLA | C4B-C3B-CAB-CBB |
| 37 | 19 | 304 | CLA | C4B-C3B-CAB-CBB |
| 37 | 20 | 303 | CLA | C4B-C3B-CAB-CBB |
| 37 | 20 | 306 | CLA | C4B-C3B-CAB-CBB |
| 37 | 20 | 308 | CLA | C4B-C3B-CAB-CBB |
| 37 | 31 | 304 | CLA | C4B-C3B-CAB-CBB |
| 37 | 32 | 204 | CLA | C4B-C3B-CAB-CBB |
| 37 | 32 | 208 | CLA | C4B-C3B-CAB-CBB |
| 37 | 33 | 307 | CLA | C4B-C3B-CAB-CBB |
| 37 | 36 | 303 | CLA | C4B-C3B-CAB-CBB |
| 37 | 37 | 306 | CLA | C4B-C3B-CAB-CBB |
| 37 | 39 | 304 | CLA | C4B-C3B-CAB-CBB |
| 37 | 40 | 205 | CLA | C4B-C3B-CAB-CBB |
| 37 | 40 | 208 | CLA | C4B-C3B-CAB-CBB |
| 37 | 40 | 210 | CLA | C4B-C3B-CAB-CBB |
| 41 | B | 521 | LMG | C17-C18-C19-C20 |
| 41 | C | 518 | LMG | C37-C38-C39-C40 |
| 41 | c | 518 | LMG | C37-C38-C39-C40 |
| 43 | 17 | 316 | LHG | C29-C30-C31-C32 |
| 43 | 21 | 217 | LHG | C32-C33-C34-C35 |
| 43 | 37 | 315 | LHG | C29-C30-C31-C32 |
| 43 | 37 | 321 | LHG | C32-C33-C34-C35 |
| 41 | B | 521 | LMG | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 40 | 16 | 315 | SQD | C9-C10-C11-C12 |
| 40 | 40 | 202 | SQD | C9-C10-C11-C12 |
| 41 | b | 520 | LMG | C22-C23-C24-C25 |
| 41 | 37 | 316 | LMG | C31-C32-C33-C34 |
| 48 | 12 | 214 | A86 | C39-C38-O4-C34 |
| 47 | 12 | 211 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 32 | 212 | KC1 | CAA-CBA-CGA-O2A |
| 37 | 12 | 209 | CLA | C2A-CAA-CBA-CGA |
| 37 | 32 | 210 | CLA | C2A-CAA-CBA-CGA |
| 41 | C | 518 | LMG | C2-C1-O1-C7 |
| 41 | c | 518 | LMG | C2-C1-O1-C7 |
| 41 | 11 | 316 | LMG | C2-C1-O1-C7 |
| 41 | 31 | 316 | LMG | C2-C1-O1-C7 |
| 37 | b | 523 | CLA | C13-C15-C16-C17 |
| 41 | C | 518 | LMG | C33-C34-C35-C36 |
| 41 | c | 518 | LMG | C33-C34-C35-C36 |
| 43 | 19 | 314 | LHG | C15-C16-C17-C18 |
| 43 | 39 | 314 | LHG | C15-C16-C17-C18 |
| 37 | B | 502 | CLA | C12-C13-C15-C16 |
| 37 | C | 503 | CLA | C12-C13-C15-C16 |
| 37 | C | 509 | CLA | C12-C13-C15-C16 |
| 37 | b | 501 | CLA | C11-C10-C8-C7 |
| 37 | b | 502 | CLA | C12-C13-C15-C16 |
| 37 | c | 503 | CLA | C12-C13-C15-C16 |
| 37 | c | 509 | CLA | C12-C13-C15-C16 |
| 37 | 11 | 308 | CLA | C12-C13-C15-C16 |
| 37 | 16 | 306 | CLA | C12-C13-C15-C16 |
| 37 | 19 | 302 | CLA | C6-C7-C8-C10 |
| 37 | 19 | 307 | CLA | C12-C13-C15-C16 |
| 37 | 32 | 202 | CLA | C12-C13-C15-C16 |
| 37 | 35 | 308 | CLA | C12-C13-C15-C16 |
| 37 | 36 | 306 | CLA | C12-C13-C15-C16 |
| 37 | 39 | 302 | CLA | C6-C7-C8-C10 |
| 37 | 39 | 307 | CLA | C12-C13-C15-C16 |
| 41 | 17 | 317 | LMG | C31-C32-C33-C34 |
| 48 | 32 | 215 | A86 | C39-C38-O4-C34 |
| 37 | 14 | 302 | CLA | C5-C6-C7-C8 |
| 37 | 34 | 302 | CLA | C5-C6-C7-C8 |
| 40 | 17 | 301 | SQD | C14-C15-C16-C17 |
| 40 | 36 | 315 | SQD | C14-C15-C16-C17 |
| 37 | 21 | 206 | CLA | O1A-CGA-O2A-C1 |
| 37 | 35 | 307 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 41 | 206 | CLA | O1A-CGA-O2A-C1 |
| 37 | B | 501 | CLA | C3A-C2A-CAA-CBA |
| 37 | b | 501 | CLA | C3A-C2A-CAA-CBA |
| 37 | 11 | 307 | CLA | C4-C3-C5-C6 |
| 37 | 16 | 309 | CLA | C3A-C2A-CAA-CBA |
| 37 | 21 | 202 | CLA | C3A-C2A-CAA-CBA |
| 37 | 31 | 308 | CLA | C4-C3-C5-C6 |
| 37 | 34 | 307 | CLA | C4-C3-C5-C6 |
| 37 | 35 | 307 | CLA | C4-C3-C5-C6 |
| 37 | 36 | 309 | CLA | C3A-C2A-CAA-CBA |
| 37 | 41 | 202 | CLA | C3A-C2A-CAA-CBA |
| 37 | 14 | 301 | CLA | C8-C10-C11-C12 |
| 37 | 34 | 301 | CLA | C8-C10-C11-C12 |
| 37 | 38 | 208 | CLA | C2-C3-C5-C6 |
| 37 | 15 | 307 | CLA | O1A-CGA-O2A-C1 |
| 38 | D | 403 | PHO | O1A-CGA-O2A-C1 |
| 38 | a | 405 | PHO | O1A-CGA-O2A-C1 |
| 37 | 12 | 203 | CLA | C5-C6-C7-C8 |
| 37 | 32 | 204 | CLA | C5-C6-C7-C8 |
| 37 | B | 510 | CLA | O1D-CGD-O2D-CED |
| 37 | 19 | 301 | CLA | CBA-CGA-O2A-C1 |
| 37 | 39 | 301 | CLA | CBA-CGA-O2A-C1 |
| 48 | 11 | 315 | A86 | C3-C4-C5-C6 |
| 48 | 13 | 311 | A86 | C11-C10-C9-C8 |
| 48 | 15 | 312 | A86 | C24-C25-C26-C27 |
| 48 | 16 | 311 | A86 | C1-C2-C3-C4 |
| 48 | 21 | 214 | A86 | C3-C4-C5-C6 |
| 48 | 31 | 315 | A86 | C3-C4-C5-C6 |
| 48 | 33 | 311 | A86 | C11-C10-C9-C8 |
| 48 | 35 | 312 | A86 | C24-C25-C26-C27 |
| 48 | 36 | 311 | A86 | C1-C2-C3-C4 |
| 48 | 38 | 213 | A86 | C3-C4-C5-C6 |
| 48 | 41 | 214 | A86 | C3-C4-C5-C6 |
| 48 | 11 | 315 | A86 | C-C1-C24-C25 |
| 48 | 14 | 316 | A86 | C7-C6-C8-C9 |
| 48 | 31 | 315 | A86 | C-C1-C24-C25 |
| 48 | 34 | 316 | A86 | C7-C6-C8-C9 |
| 37 | 11 | 310 | CLA | C4-C3-C5-C6 |
| 37 | 19 | 305 | CLA | C4-C3-C5-C6 |
| 37 | 31 | 310 | CLA | C4-C3-C5-C6 |
| 37 | 39 | 305 | CLA | C4-C3-C5-C6 |
| 43 | 21 | 201 | LHG | C2-C3-O3-P |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | 41 | 201 | LHG | C2-C3-O3-P |
| 37 | b | 510 | CLA | O1D-CGD-O2D-CED |
| 41 | 16 | 316 | LMG | C15-C16-C17-C18 |
| 41 | 36 | 314 | LMG | C15-C16-C17-C18 |
| 48 | 18 | 213 | A86 | O5-C38-O4-C34 |
| 41 | 11 | 317 | LMG | O9-C10-O7-C8 |
| 41 | 31 | 317 | LMG | O9-C10-O7-C8 |
| 40 | 16 | 315 | SQD | O6-C44-C45-C46 |
| 40 | 40 | 202 | SQD | O6-C44-C45-C46 |
| 41 | C | 518 | LMG | O1-C7-C8-C9 |
| 41 | c | 518 | LMG | O1-C7-C8-C9 |
| 41 | 11 | 316 | LMG | C7-C8-C9-O8 |
| 41 | 11 | 317 | LMG | O1-C7-C8-C9 |
| 41 | 12 | 201 | LMG | O1-C7-C8-C9 |
| 41 | 31 | 316 | LMG | C7-C8-C9-O8 |
| 41 | 31 | 317 | LMG | O1-C7-C8-C9 |
| 41 | 32 | 201 | LMG | O1-C7-C8-C9 |
| 48 | 14 | 314 | A86 | C12-C11-C13-O |
| 48 | 15 | 314 | A86 | C12-C11-C13-O |
| 48 | 16 | 313 | A86 | C12-C11-C13-O |
| 48 | 18 | 214 | A86 | C12-C11-C13-O |
| 48 | 18 | 215 | A86 | C12-C11-C13-O |
| 48 | 20 | 311 | A86 | C12-C11-C13-O |
| 48 | 34 | 314 | A86 | C12-C11-C13-O |
| 48 | 35 | 314 | A86 | C12-C11-C13-O |
| 48 | 38 | 214 | A86 | C12-C11-C13-O |
| 48 | 40 | 201 | A86 | C12-C11-C13-O |
| 48 | 40 | 213 | A86 | C12-C11-C13-O |
| 38 | D | 403 | PHO | C1A-C2A-CAA-CBA |
| 38 | a | 405 | PHO | C1A-C2A-CAA-CBA |
| 41 | A | 408 | LMG | C39-C40-C41-C42 |
| 41 | a | 410 | LMG | C39-C40-C41-C42 |
| 43 | D | 409 | LHG | C34-C35-C36-C37 |
| 44 | C | 517 | DGD | C5B-C6B-C7B-C8B |
| 44 | c | 517 | DGD | C5B-C6B-C7B-C8B |
| 37 | 38 | 208 | CLA | C4-C3-C5-C6 |
| 47 | 20 | 305 | KC1 | C4C-C3C-CAC-CBC |
| 47 | 40 | 207 | KC1 | C4C-C3C-CAC-CBC |
| 43 | d | 407 | LHG | C34-C35-C36-C37 |
| 37 | 11 | 307 | CLA | C2-C3-C5-C6 |
| 37 | 12 | 209 | CLA | C2-C3-C5-C6 |
| 37 | 31 | 308 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 32 | 210 | CLA | C2-C3-C5-C6 |
| 37 | 12 | 205 | CLA | C3-C5-C6-C7 |
| 37 | z | 102 | CLA | O1D-CGD-O2D-CED |
| 48 | 38 | 213 | A86 | O5-C38-O4-C34 |
| 48 | 11 | 314 | A86 | C10-C11-C13-O |
| 48 | 12 | 215 | A86 | C10-C11-C13-O |
| 48 | 14 | 314 | A86 | C10-C11-C13-O |
| 48 | 15 | 314 | A86 | C10-C11-C13-O |
| 48 | 16 | 313 | A86 | C10-C11-C13-O |
| 48 | 18 | 214 | A86 | C10-C11-C13-O |
| 48 | 31 | 314 | A86 | C10-C11-C13-O |
| 48 | 32 | 216 | A86 | C10-C11-C13-O |
| 48 | 34 | 314 | A86 | C10-C11-C13-O |
| 48 | 35 | 314 | A86 | C10-C11-C13-O |
| 48 | 38 | 214 | A86 | C10-C11-C13-O |
| 48 | 40 | 201 | A86 | C10-C11-C13-O |
| 37 | Z | 102 | CLA | O1D-CGD-O2D-CED |
| 37 | 13 | 301 | CLA | O1D-CGD-O2D-CED |
| 37 | 33 | 301 | CLA | O1D-CGD-O2D-CED |
| 43 | D | 411 | LHG | C18-C19-C20-C21 |
| 43 | a | 412 | LHG | C18-C19-C20-C21 |
| 37 | C | 503 | CLA | C16-C17-C18-C20 |
| 37 | c | 503 | CLA | C16-C17-C18-C20 |
| 40 | B | 522 | SQD | C9-C10-C11-C12 |
| 43 | D | 409 | LHG | C33-C34-C35-C36 |
| 43 | d | 407 | LHG | C33-C34-C35-C36 |
| 37 | C | 504 | CLA | C2B-C3B-CAB-CBB |
| 37 | c | 504 | CLA | C2B-C3B-CAB-CBB |
| 37 | 12 | 207 | CLA | C2B-C3B-CAB-CBB |
| 37 | 18 | 208 | CLA | C2B-C3B-CAB-CBB |
| 37 | 18 | 211 | CLA | C2B-C3B-CAB-CBB |
| 37 | 19 | 304 | CLA | C2B-C3B-CAB-CBB |
| 37 | 32 | 208 | CLA | C2B-C3B-CAB-CBB |
| 37 | 39 | 304 | CLA | C2B-C3B-CAB-CBB |
| 39 | A | 406 | BCR | C1-C6-C7-C8 |
| 39 | C | 519 | BCR | C1-C6-C7-C8 |
| 39 | C | 519 | BCR | C23-C24-C25-C30 |
| 39 | D | 407 | BCR | C1-C6-C7-C8 |
| 39 | D | 407 | BCR | C5-C6-C7-C8 |
| 39 | H | 101 | BCR | C1-C6-C7-C8 |
| 39 | K | 101 | BCR | C1-C6-C7-C8 |
| 39 | 0 | 101 | BCR | C1-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | a | 408 | BCR | C1-C6-C7-C8 |
| 39 | c | 519 | BCR | C1-C6-C7-C8 |
| 39 | c | 519 | BCR | C23-C24-C25-C30 |
| 39 | d | 405 | BCR | C1-C6-C7-C8 |
| 39 | d | 405 | BCR | C5-C6-C7-C8 |
| 39 | h | 101 | BCR | C1-C6-C7-C8 |
| 39 | y | 101 | BCR | C1-C6-C7-C8 |
| 39 | 5 | 101 | BCR | C1-C6-C7-C8 |
| 43 | 19 | 314 | LHG | O2-C2-C3-O3 |
| 43 | 39 | 314 | LHG | O2-C2-C3-O3 |
| 37 | 32 | 206 | CLA | C3-C5-C6-C7 |
| 40 | b | 521 | SQD | C9-C10-C11-C12 |
| 43 | 37 | 315 | LHG | C30-C31-C32-C33 |
| 41 | D | 412 | LMG | C17-C18-C19-C20 |
| 37 | 11 | 303 | CLA | C10-C11-C12-C13 |
| 37 | 31 | 304 | CLA | C10-C11-C12-C13 |
| 43 | 17 | 316 | LHG | C30-C31-C32-C33 |
| 41 | d | 409 | LMG | C17-C18-C19-C20 |
| 44 | H | 102 | DGD | C9B-CAB-CBB-CCB |
| 44 | h | 102 | DGD | C9B-CAB-CBB-CCB |
| 37 | W | 102 | CLA | C10-C11-C12-C13 |
| 37 | 31 | 301 | CLA | C10-C11-C12-C13 |
| 40 | 16 | 315 | SQD | O47-C45-C46-O48 |
| 40 | 40 | 202 | SQD | O47-C45-C46-O48 |
| 41 | 11 | 316 | LMG | O7-C8-C9-O8 |
| 41 | 11 | 317 | LMG | O1-C7-C8-O7 |
| 41 | 17 | 317 | LMG | O1-C7-C8-O7 |
| 41 | 31 | 316 | LMG | O7-C8-C9-O8 |
| 41 | 31 | 317 | LMG | O1-C7-C8-O7 |
| 41 | 37 | 316 | LMG | O1-C7-C8-O7 |
| 43 | D | 411 | LHG | O7-C5-C6-O8 |
| 43 | a | 412 | LHG | O7-C5-C6-O8 |
| 43 | 21 | 201 | LHG | O7-C5-C6-O8 |
| 43 | 41 | 201 | LHG | O7-C5-C6-O8 |
| 45 | D | 408 | PL9 | C4-C3-C7-C8 |
| 45 | d | 406 | PL9 | C4-C3-C7-C8 |
| 37 | 18 | 208 | CLA | C4-C3-C5-C6 |
| 37 | 35 | 308 | CLA | C13-C15-C16-C17 |
| 37 | 18 | 208 | CLA | C2-C3-C5-C6 |
| 43 | 17 | 316 | LHG | C12-C13-C14-C15 |
| 43 | 39 | 314 | LHG | C16-C17-C18-C19 |
| 43 | 17 | 316 | LHG | C8-C7-O7-C5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | B | 511 | CLA | C14-C13-C15-C16 |
| 37 | b | 511 | CLA | C14-C13-C15-C16 |
| 37 | b | 523 | CLA | C11-C12-C13-C14 |
| 40 | A | 407 | SQD | C28-C29-C30-C31 |
| 40 | a | 409 | SQD | C28-C29-C30-C31 |
| 43 | 19 | 314 | LHG | C30-C31-C32-C33 |
| 51 | 19 | 315 | LMU | C3-C4-C5-C6 |
| 51 | 39 | 315 | LMU | C3-C4-C5-C6 |
| 47 | 20 | 304 | KC1 | CAA-CBA-CGA-O2A |
| 47 | 40 | 206 | KC1 | CAA-CBA-CGA-O2A |
| 41 | 31 | 316 | LMG | C29-C30-C31-C32 |
| 43 | D | 410 | LHG | C12-C13-C14-C15 |
| 43 | d | 408 | LHG | C12-C13-C14-C15 |
| 43 | 37 | 315 | LHG | C12-C13-C14-C15 |
| 40 | 17 | 301 | SQD | C26-C27-C28-C29 |
| 40 | 36 | 315 | SQD | C26-C27-C28-C29 |
| 41 | 11 | 316 | LMG | C29-C30-C31-C32 |
| 43 | d | 408 | LHG | C26-C27-C28-C29 |
| 43 | 39 | 314 | LHG | C30-C31-C32-C33 |
| 37 | Z | 101 | CLA | C16-C17-C18-C19 |
| 37 | z | 101 | CLA | C16-C17-C18-C19 |
| 43 | D | 410 | LHG | C26-C27-C28-C29 |
| 43 | 19 | 314 | LHG | C16-C17-C18-C19 |
| 44 | c | 516 | DGD | C4A-C5A-C6A-C7A |
| 44 | C | 516 | DGD | C4A-C5A-C6A-C7A |
| 40 | L | 101 | SQD | C29-C30-C31-C32 |
| 44 | C | 516 | DGD | C3A-C4A-C5A-C6A |
| 44 | c | 516 | DGD | C3A-C4A-C5A-C6A |
| 43 | 19 | 314 | LHG | C35-C36-C37-C38 |
| 43 | 39 | 314 | LHG | C35-C36-C37-C38 |
| 37 | a | 407 | CLA | C13-C15-C16-C17 |
| 43 | D | 410 | LHG | O1-C1-C2-O2 |
| 43 | d | 408 | LHG | O1-C1-C2-O2 |
| 37 | 16 | 303 | CLA | CBA-CGA-O2A-C1 |
| 37 | 36 | 303 | CLA | CBA-CGA-O2A-C1 |
| 37 | 37 | 303 | CLA | C4-C3-C5-C6 |
| 48 | 13 | 315 | A86 | C3-C4-C5-C6 |
| 48 | 18 | 213 | A86 | C3-C4-C5-C6 |
| 48 | 18 | 214 | A86 | C3-C4-C5-C6 |
| 48 | 33 | 315 | A86 | C3-C4-C5-C6 |
| 37 | B | 501 | CLA | CAA-CBA-CGA-O2A |
| 37 | b | 501 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 14 | 307 | CLA | C2-C3-C5-C6 |
| 37 | 33 | 303 | CLA | C2-C3-C5-C6 |
| 37 | 34 | 307 | CLA | C2-C3-C5-C6 |
| 40 | B | 519 | SQD | C29-C30-C31-C32 |
| 43 | 37 | 315 | LHG | C8-C7-O7-C5 |
| 37 | B | 513 | CLA | C13-C15-C16-C17 |
| 37 | b | 513 | CLA | C13-C15-C16-C17 |
| 37 | b | 509 | CLA | O1D-CGD-O2D-CED |
| 44 | C | 516 | DGD | C9A-CAA-CBA-CCA |
| 44 | c | 516 | DGD | C9A-CAA-CBA-CCA |
| 37 | A | 405 | CLA | C13-C15-C16-C17 |
| 41 | c | 518 | LMG | C32-C33-C34-C35 |
| 39 | B | 525 | BCR | C16-C17-C18-C36 |
| 41 | C | 518 | LMG | C32-C33-C34-C35 |
| 43 | 19 | 314 | LHG | C24-C25-C26-C27 |
| 43 | D | 409 | LHG | O6-C4-C5-C6 |
| 43 | d | 407 | LHG | O6-C4-C5-C6 |
| 37 | B | 509 | CLA | O1D-CGD-O2D-CED |
| 40 | B | 522 | SQD | C10-C11-C12-C13 |
| 40 | b | 521 | SQD | C10-C11-C12-C13 |
| 43 | 39 | 314 | LHG | C24-C25-C26-C27 |
| 39 | H | 101 | BCR | C7-C8-C9-C34 |
| 39 | h | 101 | BCR | C7-C8-C9-C34 |
| 48 | 11 | 311 | A86 | C-C1-C24-C25 |
| 48 | 14 | 315 | A86 | C-C1-C24-C25 |
| 48 | 15 | 311 | A86 | C-C1-C24-C25 |
| 48 | 15 | 319 | A86 | C-C1-C24-C25 |
| 48 | 17 | 312 | A86 | C-C1-C24-C25 |
| 48 | 17 | 315 | A86 | C-C1-C24-C25 |
| 48 | 18 | 214 | A86 | C7-C6-C8-C9 |
| 48 | 20 | 309 | A86 | C7-C6-C8-C9 |
| 48 | 31 | 311 | A86 | C-C1-C24-C25 |
| 48 | 34 | 315 | A86 | C-C1-C24-C25 |
| 48 | 35 | 311 | A86 | C-C1-C24-C25 |
| 48 | 35 | 319 | A86 | C-C1-C24-C25 |
| 48 | 37 | 311 | A86 | C-C1-C24-C25 |
| 48 | 38 | 214 | A86 | C7-C6-C8-C9 |
| 48 | 40 | 211 | A86 | C7-C6-C8-C9 |
| 37 | B | 501 | CLA | C11-C10-C8-C7 |
| 37 | B | 514 | CLA | C12-C13-C15-C16 |
| 37 | C | 502 | CLA | C11-C12-C13-C15 |
| 37 | C | 511 | CLA | C6-C7-C8-C10 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | D | 406 | CLA | C11-C12-C13-C15 |
| 37 | D | 406 | CLA | C12-C13-C15-C16 |
| 37 | W | 101 | CLA | C6-C7-C8-C10 |
| 37 | W | 102 | CLA | C11-C12-C13-C15 |
| 37 | b | 514 | CLA | C12-C13-C15-C16 |
| 37 | c | 502 | CLA | C11-C12-C13-C15 |
| 37 | c | 511 | CLA | C6-C7-C8-C10 |
| 37 | d | 404 | CLA | C11-C12-C13-C15 |
| 37 | d | 404 | CLA | C12-C13-C15-C16 |
| 37 | w | 101 | CLA | C6-C7-C8-C10 |
| 37 | 14 | 308 | CLA | C12-C13-C15-C16 |
| 37 | 15 | 308 | CLA | C12-C13-C15-C16 |
| 37 | 31 | 301 | CLA | C11-C12-C13-C15 |
| 37 | 34 | 308 | CLA | C6-C7-C8-C10 |
| 37 | 34 | 308 | CLA | C12-C13-C15-C16 |
| 44 | c | 517 | DGD | C8B-C9B-CAB-CBB |
| 44 | C | 517 | DGD | C8B-C9B-CAB-CBB |
| 44 | J | 101 | DGD | CDA-CEA-CFA-CGA |
| 44 | j | 101 | DGD | CDA-CEA-CFA-CGA |
| 48 | 11 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 13 | 315 | A86 | C2-C1-C24-C25 |
| 48 | 15 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 15 | 319 | A86 | C2-C1-C24-C25 |
| 48 | 17 | 312 | A86 | C2-C1-C24-C25 |
| 48 | 18 | 212 | A86 | C2-C1-C24-C25 |
| 48 | 18 | 214 | A86 | C5-C6-C8-C9 |
| 48 | 20 | 309 | A86 | C5-C6-C8-C9 |
| 48 | 31 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 33 | 315 | A86 | C2-C1-C24-C25 |
| 48 | 35 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 35 | 319 | A86 | C2-C1-C24-C25 |
| 48 | 37 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 38 | 212 | A86 | C2-C1-C24-C25 |
| 48 | 38 | 214 | A86 | C5-C6-C8-C9 |
| 48 | 40 | 211 | A86 | C5-C6-C8-C9 |
| 37 | 18 | 209 | CLA | CBA-CGA-O2A-C1 |
| 37 | 19 | 303 | CLA | CBA-CGA-O2A-C1 |
| 37 | 39 | 303 | CLA | CBA-CGA-O2A-C1 |
| 41 | A | 408 | LMG | C16-C17-C18-C19 |
| 41 | a | 410 | LMG | C16-C17-C18-C19 |
| 37 | 38 | 208 | CLA | O1A-CGA-O2A-C1 |
| 41 | A | 408 | LMG | O10-C28-O8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | a | 410 | LMG | O10-C28-O8-C9 |
| 40 | A | 407 | SQD | C5-C6-S-O8 |
| 40 | a | 409 | SQD | C5-C6-S-O8 |
| 37 | 14 | 303 | CLA | C2A-CAA-CBA-CGA |
| 37 | 34 | 303 | CLA | C2A-CAA-CBA-CGA |
| 41 | A | 408 | LMG | O9-C10-O7-C8 |
| 41 | a | 410 | LMG | O9-C10-O7-C8 |
| 40 | B | 519 | SQD | C12-C13-C14-C15 |
| 40 | 16 | 315 | SQD | C11-C10-C9-C8 |
| 40 | 40 | 202 | SQD | C11-C10-C9-C8 |
| 37 | C | 506 | CLA | C4-C3-C5-C6 |
| 37 | c | 506 | CLA | C4-C3-C5-C6 |
| 37 | B | 503 | CLA | O1A-CGA-O2A-C1 |
| 37 | b | 503 | CLA | O1A-CGA-O2A-C1 |
| 37 | 38 | 201 | CLA | O1A-CGA-O2A-C1 |
| 37 | 18 | 209 | CLA | C2-C3-C5-C6 |
| 47 | 13 | 306 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 14 | 309 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 17 | 303 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 17 | 306 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 18 | 210 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 20 | 305 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 33 | 306 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 34 | 309 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 36 | 308 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 37 | 302 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 37 | 305 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 38 | 210 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 40 | 207 | KC1 | C2B-C3B-CAB-CBB |
| 40 | L | 101 | SQD | C12-C13-C14-C15 |
| 41 | 16 | 316 | LMG | C9-C8-O7-C10 |
| 41 | 36 | 314 | LMG | C9-C8-O7-C10 |
| 37 | 16 | 303 | CLA | O1A-CGA-O2A-C1 |
| 37 | 18 | 201 | CLA | O1A-CGA-O2A-C1 |
| 37 | 18 | 208 | CLA | O1A-CGA-O2A-C1 |
| 37 | 21 | 202 | CLA | O1A-CGA-O2A-C1 |
| 37 | 36 | 303 | CLA | O1A-CGA-O2A-C1 |
| 43 | 41 | 201 | LHG | C25-C26-C27-C28 |
| 37 | D | 402 | CLA | C13-C15-C16-C17 |
| 37 | d | 401 | CLA | C13-C15-C16-C17 |
| 48 | 13 | 312 | A86 | C11-C10-C9-C8 |
| 48 | 33 | 312 | A86 | C11-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 37 | 319 | A86 | C3-C4-C5-C6 |
| 48 | 38 | 214 | A86 | C3-C4-C5-C6 |
| 43 | B | 523 | LHG | C31-C32-C33-C34 |
| 37 | B | 513 | CLA | C16-C17-C18-C20 |
| 37 | b | 513 | CLA | C16-C17-C18-C20 |
| 41 | b | 520 | LMG | C11-C12-C13-C14 |
| 37 | 41 | 202 | CLA | O1A-CGA-O2A-C1 |
| 41 | b | 520 | LMG | C13-C14-C15-C16 |
| 43 | b | 522 | LHG | C31-C32-C33-C34 |
| 41 | B | 521 | LMG | C11-C12-C13-C14 |
| 41 | B | 521 | LMG | C13-C14-C15-C16 |
| 50 | 19 | 312 | DD6 | C24-C1-C2-C3 |
| 50 | 39 | 312 | DD6 | C24-C1-C2-C3 |
| 40 | 16 | 315 | SQD | C19-C20-C21-C22 |
| 40 | 17 | 301 | SQD | C30-C31-C32-C33 |
| 40 | 36 | 315 | SQD | C30-C31-C32-C33 |
| 43 | B | 523 | LHG | O6-C4-C5-O7 |
| 43 | D | 409 | LHG | O6-C4-C5-O7 |
| 43 | b | 522 | LHG | O6-C4-C5-O7 |
| 43 | d | 407 | LHG | O6-C4-C5-O7 |
| 43 | 21 | 201 | LHG | C25-C26-C27-C28 |
| 40 | B | 522 | SQD | C44-C45-C46-O48 |
| 40 | b | 521 | SQD | C44-C45-C46-O48 |
| 41 | B | 521 | LMG | O1-C7-C8-C9 |
| 41 | b | 520 | LMG | O1-C7-C8-C9 |
| 43 | 21 | 217 | LHG | C4-C5-C6-O8 |
| 43 | 37 | 321 | LHG | C4-C5-C6-O8 |
| 40 | 40 | 202 | SQD | C19-C20-C21-C22 |
| 47 | 11 | 304 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 11 | 306 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 13 | 304 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 13 | 306 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 14 | 309 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 15 | 302 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 16 | 304 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 21 | 207 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 31 | 305 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 31 | 307 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 33 | 304 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 33 | 306 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 34 | 309 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 36 | 304 | KC1 | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 47 | 41 | 207 | KC1 | C4B-C3B-CAB-CBB |
| 40 | 16 | 315 | SQD | C26-C27-C28-C29 |
| 40 | 40 | 202 | SQD | C26-C27-C28-C29 |
| 41 | B | 521 | LMG | C35-C36-C37-C38 |
| 43 | D | 409 | LHG | C30-C31-C32-C33 |
| 43 | d | 407 | LHG | C30-C31-C32-C33 |
| 37 | 13 | 307 | CLA | C4-C3-C5-C6 |
| 37 | 33 | 307 | CLA | C4-C3-C5-C6 |
| 45 | D | 404 | PL9 | C12-C11-C9-C10 |
| 45 | d | 402 | PL9 | C12-C11-C9-C10 |
| 37 | 38 | 209 | CLA | C2-C3-C5-C6 |
| 41 | b | 520 | LMG | C35-C36-C37-C38 |
| 43 | 21 | 201 | LHG | O2-C2-C3-O3 |
| 43 | 41 | 201 | LHG | O2-C2-C3-O3 |
| 48 | 12 | 215 | A86 | C28-C27-C29-C30 |
| 48 | 15 | 313 | A86 | C28-C27-C29-C30 |
| 48 | 16 | 311 | A86 | C28-C27-C29-C30 |
| 48 | 20 | 311 | A86 | C28-C27-C29-C30 |
| 48 | 32 | 216 | A86 | C28-C27-C29-C30 |
| 48 | 35 | 313 | A86 | C28-C27-C29-C30 |
| 48 | 36 | 311 | A86 | C28-C27-C29-C30 |
| 48 | 40 | 213 | A86 | C28-C27-C29-C30 |
| 37 | 17 | 309 | CLA | C4C-C3C-CAC-CBC |
| 37 | 13 | 301 | CLA | C10-C11-C12-C13 |
| 37 | 33 | 301 | CLA | C10-C11-C12-C13 |
| 44 | C | 516 | DGD | C9B-CAB-CBB-CCB |
| 44 | c | 516 | DGD | C9B-CAB-CBB-CCB |
| 41 | B | 521 | LMG | O1-C7-C8-O7 |
| 41 | C | 518 | LMG | O1-C7-C8-O7 |
| 41 | b | 520 | LMG | O1-C7-C8-O7 |
| 41 | c | 518 | LMG | O1-C7-C8-O7 |
| 41 | 11 | 317 | LMG | O7-C8-C9-O8 |
| 41 | 12 | 201 | LMG | O1-C7-C8-O7 |
| 41 | 31 | 317 | LMG | O7-C8-C9-O8 |
| 41 | 32 | 201 | LMG | O1-C7-C8-O7 |
| 37 | B | 524 | CLA | C11-C12-C13-C14 |
| 37 | D | 406 | CLA | C14-C13-C15-C16 |
| 37 | W | 101 | CLA | C6-C7-C8-C9 |
| 37 | d | 404 | CLA | C14-C13-C15-C16 |
| 37 | w | 101 | CLA | C6-C7-C8-C9 |
| 37 | 14 | 308 | CLA | C14-C13-C15-C16 |
| 37 | 34 | 308 | CLA | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | d | 407 | LHG | C13-C14-C15-C16 |
| 44 | C | 516 | DGD | CAB-CBB-CCB-CDB |
| 43 | D | 409 | LHG | C13-C14-C15-C16 |
| 43 | D | 409 | LHG | C17-C18-C19-C20 |
| 43 | d | 407 | LHG | C17-C18-C19-C20 |
| 43 | 37 | 321 | LHG | C31-C32-C33-C34 |
| 44 | c | 516 | DGD | CAB-CBB-CCB-CDB |
| 37 | 18 | 209 | CLA | O1A-CGA-O2A-C1 |
| 37 | 19 | 303 | CLA | O1A-CGA-O2A-C1 |
| 37 | 39 | 303 | CLA | O1A-CGA-O2A-C1 |
| 43 | 21 | 217 | LHG | C31-C32-C33-C34 |
| 48 | 12 | 202 | A86 | C13-C14-C15-O1 |
| 48 | 12 | 217 | A86 | C13-C14-C15-O1 |
| 48 | 13 | 313 | A86 | C13-C14-C15-O1 |
| 48 | 13 | 314 | A86 | C13-C14-C15-O1 |
| 48 | 13 | 315 | A86 | C13-C14-C15-O1 |
| 48 | 14 | 316 | A86 | C13-C14-C15-O1 |
| 48 | 15 | 316 | A86 | C13-C14-C15-O1 |
| 48 | 16 | 314 | A86 | C13-C14-C15-O1 |
| 48 | 17 | 315 | A86 | C13-C14-C15-O1 |
| 48 | 18 | 215 | A86 | C13-C14-C15-O1 |
| 48 | 32 | 203 | A86 | C13-C14-C15-O1 |
| 48 | 32 | 218 | A86 | C13-C14-C15-O1 |
| 48 | 33 | 313 | A86 | C13-C14-C15-O1 |
| 48 | 33 | 315 | A86 | C13-C14-C15-O1 |
| 48 | 34 | 316 | A86 | C13-C14-C15-O1 |
| 48 | 35 | 316 | A86 | C13-C14-C15-O1 |
| 48 | 36 | 313 | A86 | C13-C14-C15-O1 |
| 48 | 37 | 314 | A86 | C13-C14-C15-O1 |
| 48 | 38 | 215 | A86 | C13-C14-C15-O1 |
| 43 | D | 409 | LHG | C11-C12-C13-C14 |
| 43 | d | 407 | LHG | C11-C12-C13-C14 |
| 37 | 37 | 301 | CLA | C8-C10-C11-C12 |
| 37 | 20 | 301 | CLA | O1D-CGD-O2D-CED |
| 44 | J | 101 | DGD | C6A-C7A-C8A-C9A |
| 44 | j | 101 | DGD | C6A-C7A-C8A-C9A |
| 43 | 21 | 201 | LHG | C5-C4-O6-P |
| 37 | 40 | 203 | CLA | O1D-CGD-O2D-CED |
| 40 | 40 | 202 | SQD | C11-C12-C13-C14 |
| 46 | F | 101 | HEM | C2A-CAA-CBA-CGA |
| 46 | f | 101 | HEM | C2A-CAA-CBA-CGA |
| 44 | c | 517 | DGD | C1B-C2B-C3B-C4B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | c | 506 | CLA | C2-C3-C5-C6 |
| 40 | 16 | 315 | SQD | C11-C12-C13-C14 |
| 44 | J | 101 | DGD | O1B-C1B-O2G-C2G |
| 40 | B | 519 | SQD | C26-C27-C28-C29 |
| 40 | L | 101 | SQD | C26-C27-C28-C29 |
| 37 | B | 514 | CLA | C2A-CAA-CBA-CGA |
| 37 | b | 514 | CLA | C2A-CAA-CBA-CGA |
| 37 | 21 | 204 | CLA | C5-C6-C7-C8 |
| 37 | 41 | 204 | CLA | C5-C6-C7-C8 |
| 41 | A | 408 | LMG | C34-C35-C36-C37 |
| 41 | a | 410 | LMG | C34-C35-C36-C37 |
| 43 | 17 | 316 | LHG | C11-C12-C13-C14 |
| 43 | 37 | 315 | LHG | C11-C12-C13-C14 |
| 44 | C | 517 | DGD | C1B-C2B-C3B-C4B |
| 37 | C | 504 | CLA | O1A-CGA-O2A-C1 |
| 37 | c | 504 | CLA | O1A-CGA-O2A-C1 |
| 41 | B | 520 | LMG | C15-C16-C17-C18 |
| 41 | b | 519 | LMG | C15-C16-C17-C18 |
| 37 | 13 | 307 | CLA | CBA-CGA-O2A-C1 |
| 37 | 20 | 301 | CLA | CBA-CGA-O2A-C1 |
| 37 | 33 | 307 | CLA | CBA-CGA-O2A-C1 |
| 37 | 40 | 203 | CLA | CBA-CGA-O2A-C1 |
| 44 | j | 101 | DGD | O1B-C1B-O2G-C2G |
| 37 | C | 513 | CLA | O1D-CGD-O2D-CED |
| 37 | c | 513 | CLA | O1D-CGD-O2D-CED |
| 37 | 35 | 303 | CLA | O1A-CGA-O2A-C1 |
| 41 | B | 520 | LMG | O6-C5-C6-O5 |
| 37 | 14 | 308 | CLA | C13-C15-C16-C17 |
| 37 | 34 | 308 | CLA | C13-C15-C16-C17 |
| 39 | C | 519 | BCR | C37-C22-C23-C24 |
| 39 | c | 519 | BCR | C37-C22-C23-C24 |
| 48 | 18 | 212 | A86 | C-C1-C24-C25 |
| 48 | 37 | 314 | A86 | C-C1-C24-C25 |
| 44 | J | 101 | DGD | C7B-C8B-C9B-CAB |
| 37 | B | 501 | CLA | C4B-C3B-CAB-CBB |
| 37 | B | 524 | CLA | C4B-C3B-CAB-CBB |
| 37 | C | 501 | CLA | C4B-C3B-CAB-CBB |
| 37 | C | 504 | CLA | C4B-C3B-CAB-CBB |
| 37 | D | 402 | CLA | C4B-C3B-CAB-CBB |
| 37 | D | 406 | CLA | C4B-C3B-CAB-CBB |
| 37 | Z | 101 | CLA | C1A-C2A-CAA-CBA |
| 37 | Z | 101 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | Z | 102 | CLA | C4B-C3B-CAB-CBB |
| 37 | W | 101 | CLA | C4B-C3B-CAB-CBB |
| 37 | W | 102 | CLA | C4B-C3B-CAB-CBB |
| 37 | b | 501 | CLA | C4B-C3B-CAB-CBB |
| 37 | b | 523 | CLA | C4B-C3B-CAB-CBB |
| 37 | c | 501 | CLA | C4B-C3B-CAB-CBB |
| 37 | c | 504 | CLA | C4B-C3B-CAB-CBB |
| 37 | d | 401 | CLA | C4B-C3B-CAB-CBB |
| 37 | d | 404 | CLA | C4B-C3B-CAB-CBB |
| 37 | z | 101 | CLA | C1A-C2A-CAA-CBA |
| 37 | z | 101 | CLA | C4B-C3B-CAB-CBB |
| 37 | z | 102 | CLA | C4B-C3B-CAB-CBB |
| 37 | w | 101 | CLA | C4B-C3B-CAB-CBB |
| 37 | 11 | 305 | CLA | C4B-C3B-CAB-CBB |
| 37 | 13 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 13 | 305 | CLA | C4B-C3B-CAB-CBB |
| 37 | 14 | 305 | CLA | C4B-C3B-CAB-CBB |
| 37 | 15 | 305 | CLA | C4B-C3B-CAB-CBB |
| 37 | 15 | 307 | CLA | C4B-C3B-CAB-CBB |
| 37 | 15 | 308 | CLA | C4B-C3B-CAB-CBB |
| 37 | 18 | 206 | CLA | C4B-C3B-CAB-CBB |
| 37 | 18 | 211 | CLA | C4B-C3B-CAB-CBB |
| 37 | 19 | 305 | CLA | C4B-C3B-CAB-CBB |
| 37 | 19 | 309 | CLA | C4B-C3B-CAB-CBB |
| 37 | 19 | 310 | CLA | C1A-C2A-CAA-CBA |
| 37 | 19 | 310 | CLA | C4B-C3B-CAB-CBB |
| 37 | 20 | 307 | CLA | C4B-C3B-CAB-CBB |
| 37 | 21 | 202 | CLA | C4B-C3B-CAB-CBB |
| 37 | 21 | 205 | CLA | C4B-C3B-CAB-CBB |
| 37 | 21 | 206 | CLA | C4B-C3B-CAB-CBB |
| 37 | 21 | 208 | CLA | C4B-C3B-CAB-CBB |
| 37 | 21 | 210 | CLA | C4B-C3B-CAB-CBB |
| 37 | 31 | 301 | CLA | C4B-C3B-CAB-CBB |
| 37 | 31 | 306 | CLA | C4B-C3B-CAB-CBB |
| 37 | 33 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 33 | 305 | CLA | C4B-C3B-CAB-CBB |
| 37 | 34 | 305 | CLA | C4B-C3B-CAB-CBB |
| 37 | 34 | 310 | CLA | C4B-C3B-CAB-CBB |
| 37 | 35 | 305 | CLA | C4B-C3B-CAB-CBB |
| 37 | 35 | 307 | CLA | C4B-C3B-CAB-CBB |
| 37 | 35 | 308 | CLA | C4B-C3B-CAB-CBB |
| 37 | 38 | 201 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 38 | 203 | CLA | C4B-C3B-CAB-CBB |
| 37 | 38 | 206 | CLA | C4B-C3B-CAB-CBB |
| 37 | 38 | 211 | CLA | C4B-C3B-CAB-CBB |
| 37 | 39 | 305 | CLA | C4B-C3B-CAB-CBB |
| 37 | 39 | 309 | CLA | C4B-C3B-CAB-CBB |
| 37 | 39 | 310 | CLA | C1A-C2A-CAA-CBA |
| 37 | 39 | 310 | CLA | C4B-C3B-CAB-CBB |
| 37 | 40 | 209 | CLA | C4B-C3B-CAB-CBB |
| 37 | 41 | 202 | CLA | C4B-C3B-CAB-CBB |
| 37 | 41 | 205 | CLA | C4B-C3B-CAB-CBB |
| 37 | 41 | 206 | CLA | C4B-C3B-CAB-CBB |
| 37 | 41 | 208 | CLA | C4B-C3B-CAB-CBB |
| 37 | 41 | 210 | CLA | C4B-C3B-CAB-CBB |
| 48 | 11 | 313 | A86 | O-C13-C14-C15 |
| 48 | 12 | 213 | A86 | O-C13-C14-C15 |
| 48 | 12 | 215 | A86 | O-C13-C14-C15 |
| 48 | 13 | 311 | A86 | O-C13-C14-C15 |
| 48 | 14 | 314 | A86 | O-C13-C14-C15 |
| 48 | 15 | 311 | A86 | O-C13-C14-C15 |
| 48 | 16 | 313 | A86 | O-C13-C14-C15 |
| 48 | 17 | 310 | A86 | O-C13-C14-C15 |
| 48 | 17 | 313 | A86 | O-C13-C14-C15 |
| 48 | 17 | 315 | A86 | O-C13-C14-C15 |
| 48 | 18 | 213 | A86 | O-C13-C14-C15 |
| 48 | 19 | 311 | A86 | O-C13-C14-C15 |
| 48 | 31 | 313 | A86 | O-C13-C14-C15 |
| 48 | 32 | 214 | A86 | O-C13-C14-C15 |
| 48 | 32 | 216 | A86 | O-C13-C14-C15 |
| 48 | 33 | 311 | A86 | O-C13-C14-C15 |
| 48 | 34 | 314 | A86 | O-C13-C14-C15 |
| 48 | 35 | 311 | A86 | O-C13-C14-C15 |
| 48 | 37 | 309 | A86 | O-C13-C14-C15 |
| 48 | 37 | 312 | A86 | O-C13-C14-C15 |
| 48 | 37 | 314 | A86 | O-C13-C14-C15 |
| 48 | 38 | 213 | A86 | O-C13-C14-C15 |
| 48 | 39 | 311 | A86 | O-C13-C14-C15 |
| 48 | 40 | 201 | A86 | O-C13-C14-C15 |
| 37 | 32 | 211 | CLA | O1D-CGD-O2D-CED |
| 44 | j | 101 | DGD | C7B-C8B-C9B-CAB |
| 41 | 11 | 317 | LMG | C28-C29-C30-C31 |
| 41 | 31 | 317 | LMG | C28-C29-C30-C31 |
| 37 | 14 | 301 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 18 | 202 | CLA | C4-C3-C5-C6 |
| 37 | 32 | 206 | CLA | C4-C3-C5-C6 |
| 37 | 34 | 301 | CLA | C4-C3-C5-C6 |
| 37 | 38 | 202 | CLA | C4-C3-C5-C6 |
| 37 | 38 | 204 | CLA | C4-C3-C5-C6 |
| 37 | 17 | 302 | CLA | C8-C10-C11-C12 |
| 39 | B | 525 | BCR | C22-C23-C24-C25 |
| 39 | D | 407 | BCR | C6-C7-C8-C9 |
| 39 | b | 524 | BCR | C22-C23-C24-C25 |
| 39 | d | 405 | BCR | C6-C7-C8-C9 |
| 37 | C | 506 | CLA | C2-C3-C5-C6 |
| 41 | 11 | 316 | LMG | C20-C21-C22-C23 |
| 44 | C | 516 | DGD | C4D-C5D-C6D-O5D |
| 44 | c | 516 | DGD | C4D-C5D-C6D-O5D |
| 37 | 19 | 301 | CLA | O1A-CGA-O2A-C1 |
| 37 | 39 | 301 | CLA | O1A-CGA-O2A-C1 |
| 41 | A | 408 | LMG | C14-C15-C16-C17 |
| 41 | 31 | 316 | LMG | C20-C21-C22-C23 |
| 41 | a | 410 | LMG | C14-C15-C16-C17 |
| 37 | 15 | 308 | CLA | C13-C15-C16-C17 |
| 37 | B | 516 | CLA | C6-C7-C8-C10 |
| 37 | B | 516 | CLA | C11-C10-C8-C7 |
| 37 | C | 503 | CLA | C11-C12-C13-C15 |
| 37 | C | 508 | CLA | C6-C7-C8-C10 |
| 37 | D | 402 | CLA | C12-C13-C15-C16 |
| 37 | Z | 101 | CLA | C12-C13-C15-C16 |
| 37 | W | 101 | CLA | C11-C10-C8-C7 |
| 37 | b | 516 | CLA | C6-C7-C8-C10 |
| 37 | b | 516 | CLA | C11-C10-C8-C7 |
| 37 | c | 503 | CLA | C11-C12-C13-C15 |
| 37 | c | 508 | CLA | C6-C7-C8-C10 |
| 37 | d | 401 | CLA | C12-C13-C15-C16 |
| 37 | z | 101 | CLA | C12-C13-C15-C16 |
| 37 | w | 101 | CLA | C11-C10-C8-C7 |
| 37 | 14 | 308 | CLA | C6-C7-C8-C10 |
| 37 | 21 | 206 | CLA | C11-C12-C13-C15 |
| 37 | 41 | 206 | CLA | C11-C12-C13-C15 |
| 38 | A | 404 | PHO | C6-C7-C8-C10 |
| 38 | a | 406 | PHO | C6-C7-C8-C10 |
| 40 | B | 519 | SQD | C19-C20-C21-C22 |
| 37 | C | 503 | CLA | C16-C17-C18-C19 |
| 37 | D | 406 | CLA | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | c | 503 | CLA | C16-C17-C18-C19 |
| 38 | A | 404 | PHO | C16-C17-C18-C20 |
| 40 | L | 101 | SQD | C19-C20-C21-C22 |
| 44 | c | 517 | DGD | C8A-C9A-CAA-CBA |
| 37 | 15 | 307 | CLA | O1D-CGD-O2D-CED |
| 37 | 15 | 303 | CLA | O1A-CGA-O2A-C1 |
| 43 | D | 409 | LHG | C18-C19-C20-C21 |
| 43 | d | 407 | LHG | C18-C19-C20-C21 |
| 44 | C | 517 | DGD | C8A-C9A-CAA-CBA |
| 37 | C | 504 | CLA | CBA-CGA-O2A-C1 |
| 37 | c | 504 | CLA | CBA-CGA-O2A-C1 |
| 43 | 41 | 201 | LHG | C15-C16-C17-C18 |
| 41 | b | 519 | LMG | O6-C5-C6-O5 |
| 41 | 37 | 316 | LMG | C11-C12-C13-C14 |
| 41 | 17 | 317 | LMG | C11-C12-C13-C14 |
| 37 | 20 | 301 | CLA | O1A-CGA-O2A-C1 |
| 37 | 40 | 203 | CLA | O1A-CGA-O2A-C1 |
| 37 | W | 101 | CLA | O1D-CGD-O2D-CED |
| 37 | w | 101 | CLA | O1D-CGD-O2D-CED |
| 43 | 41 | 201 | LHG | C5-C4-O6-P |
| 37 | 18 | 204 | CLA | C4-C3-C5-C6 |
| 45 | D | 404 | PL9 | C20-C19-C21-C22 |
| 45 | d | 402 | PL9 | C20-C19-C21-C22 |
| 37 | C | 506 | CLA | C16-C17-C18-C19 |
| 37 | c | 506 | CLA | C16-C17-C18-C19 |
| 37 | d | 404 | CLA | C16-C17-C18-C19 |
| 38 | a | 406 | PHO | C16-C17-C18-C20 |
| 37 | 13 | 307 | CLA | C2-C3-C5-C6 |
| 37 | 33 | 307 | CLA | C2-C3-C5-C6 |
| 37 | 37 | 308 | CLA | C2C-C3C-CAC-CBC |
| 43 | 21 | 217 | LHG | O6-C4-C5-O7 |
| 43 | 37 | 321 | LHG | O6-C4-C5-O7 |
| 37 | 35 | 307 | CLA | O1D-CGD-O2D-CED |
| 37 | 15 | 305 | CLA | C2A-CAA-CBA-CGA |
| 37 | 35 | 305 | CLA | C2A-CAA-CBA-CGA |
| 37 | B | 514 | CLA | C14-C13-C15-C16 |
| 37 | B | 516 | CLA | C6-C7-C8-C9 |
| 37 | C | 510 | CLA | C14-C13-C15-C16 |
| 37 | D | 406 | CLA | C11-C12-C13-C14 |
| 37 | W | 102 | CLA | C11-C12-C13-C14 |
| 37 | b | 514 | CLA | C14-C13-C15-C16 |
| 37 | b | 516 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | c | 510 | CLA | C14-C13-C15-C16 |
| 37 | d | 404 | CLA | C11-C12-C13-C14 |
| 37 | 15 | 308 | CLA | C14-C13-C15-C16 |
| 37 | 31 | 301 | CLA | C11-C12-C13-C14 |
| 41 | C | 518 | LMG | C14-C15-C16-C17 |
| 41 | c | 518 | LMG | C14-C15-C16-C17 |
| 44 | C | 517 | DGD | CBB-CCB-CDB-CEB |
| 44 | c | 517 | DGD | CBB-CCB-CDB-CEB |
| 48 | 11 | 319 | A86 | C1-C2-C3-C4 |
| 48 | 20 | 309 | A86 | C24-C25-C26-C27 |
| 48 | 21 | 213 | A86 | C11-C10-C9-C8 |
| 48 | 31 | 311 | A86 | C1-C2-C3-C4 |
| 48 | 31 | 319 | A86 | C1-C2-C3-C4 |
| 48 | 40 | 211 | A86 | C24-C25-C26-C27 |
| 48 | 41 | 213 | A86 | C11-C10-C9-C8 |
| 41 | 11 | 316 | LMG | C14-C15-C16-C17 |
| 41 | 31 | 316 | LMG | C14-C15-C16-C17 |
| 47 | 11 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 12 | 208 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 14 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 14 | 306 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 16 | 305 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 17 | 305 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 20 | 305 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 21 | 207 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 31 | 305 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 32 | 209 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 34 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 34 | 306 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 36 | 305 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 37 | 304 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 40 | 207 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 41 | 207 | KC1 | C3A-C2A-CAA-CBA |
| 48 | 16 | 311 | A86 | C26-C27-C29-C30 |
| 48 | 36 | 311 | A86 | C26-C27-C29-C30 |
| 44 | J | 101 | DGD | C8A-C9A-CAA-CBA |
| 44 | j | 101 | DGD | C8A-C9A-CAA-CBA |
| 40 | 36 | 315 | SQD | O6-C44-C45-O47 |
| 41 | A | 408 | LMG | O7-C8-C9-O8 |
| 41 | a | 410 | LMG | O7-C8-C9-O8 |
| 37 | 39 | 303 | CLA | C5-C6-C7-C8 |
| 37 | 40 | 205 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 40 | 17 | 301 | SQD | C44-C45-C46-O48 |
| 40 | 36 | 315 | SQD | C44-C45-C46-O48 |
| 43 | D | 411 | LHG | C4-C5-C6-O8 |
| 43 | a | 412 | LHG | C4-C5-C6-O8 |
| 43 | d | 407 | LHG | C4-C5-C6-O8 |
| 41 | 32 | 201 | LMG | O6-C5-C6-O5 |
| 37 | 19 | 303 | CLA | C5-C6-C7-C8 |
| 37 | 20 | 303 | CLA | CBD-CGD-O2D-CED |
| 37 | B | 501 | CLA | CAD-CBD-CGD-O2D |
| 37 | B | 503 | CLA | CAD-CBD-CGD-O2D |
| 37 | B | 507 | CLA | CAD-CBD-CGD-O2D |
| 37 | b | 501 | CLA | CAD-CBD-CGD-O2D |
| 37 | b | 503 | CLA | CAD-CBD-CGD-O2D |
| 37 | b | 507 | CLA | CAD-CBD-CGD-O2D |
| 37 | 12 | 204 | CLA | CAD-CBD-CGD-O2D |
| 37 | 13 | 303 | CLA | CAD-CBD-CGD-O2D |
| 37 | 14 | 302 | CLA | CAD-CBD-CGD-O2D |
| 37 | 15 | 303 | CLA | CAD-CBD-CGD-O2D |
| 37 | 18 | 211 | CLA | CAD-CBD-CGD-O2D |
| 37 | 19 | 303 | CLA | CAD-CBD-CGD-O2D |
| 37 | 32 | 205 | CLA | CAD-CBD-CGD-O2D |
| 37 | 33 | 303 | CLA | CAD-CBD-CGD-O2D |
| 37 | 34 | 302 | CLA | CAD-CBD-CGD-O2D |
| 37 | 38 | 211 | CLA | CAD-CBD-CGD-O2D |
| 37 | 39 | 303 | CLA | CAD-CBD-CGD-O2D |
| 37 | 33 | 307 | CLA | O1A-CGA-O2A-C1 |
| 37 | Z | 101 | CLA | C5-C6-C7-C8 |
| 37 | z | 101 | CLA | C5-C6-C7-C8 |
| 44 | j | 101 | DGD | CBB-CCB-CDB-CEB |
| 41 | 16 | 316 | LMG | C13-C14-C15-C16 |
| 41 | 36 | 314 | LMG | C13-C14-C15-C16 |
| 44 | J | 101 | DGD | CBB-CCB-CDB-CEB |
| 37 | A | 403 | CLA | C2A-CAA-CBA-CGA |
| 43 | 17 | 316 | LHG | C10-C11-C12-C13 |
| 37 | 13 | 307 | CLA | O1A-CGA-O2A-C1 |
| 37 | 38 | 209 | CLA | O1A-CGA-O2A-C1 |
| 37 | 16 | 303 | CLA | O1D-CGD-O2D-CED |
| 43 | d | 407 | LHG | C26-C27-C28-C29 |
| 41 | 11 | 316 | LMG | C31-C32-C33-C34 |
| 43 | D | 409 | LHG | C26-C27-C28-C29 |
| 43 | D | 410 | LHG | C31-C32-C33-C34 |
| 43 | d | 408 | LHG | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | 37 | 315 | LHG | C10-C11-C12-C13 |
| 44 | C | 517 | DGD | C6B-C7B-C8B-C9B |
| 44 | c | 517 | DGD | C6B-C7B-C8B-C9B |
| 37 | B | 501 | CLA | CAD-CBD-CGD-O1D |
| 37 | B | 503 | CLA | CAD-CBD-CGD-O1D |
| 37 | B | 507 | CLA | CAD-CBD-CGD-O1D |
| 37 | C | 507 | CLA | CHA-CBD-CGD-O1D |
| 37 | C | 507 | CLA | CHA-CBD-CGD-O2D |
| 37 | W | 102 | CLA | CHA-CBD-CGD-O1D |
| 37 | b | 501 | CLA | CAD-CBD-CGD-O1D |
| 37 | b | 503 | CLA | CAD-CBD-CGD-O1D |
| 37 | b | 507 | CLA | CAD-CBD-CGD-O1D |
| 37 | c | 507 | CLA | CHA-CBD-CGD-O1D |
| 37 | c | 507 | CLA | CHA-CBD-CGD-O2D |
| 37 | 12 | 204 | CLA | CAD-CBD-CGD-O1D |
| 37 | 13 | 303 | CLA | CAD-CBD-CGD-O1D |
| 37 | 14 | 302 | CLA | CAD-CBD-CGD-O1D |
| 37 | 14 | 307 | CLA | CHA-CBD-CGD-O1D |
| 37 | 14 | 307 | CLA | CHA-CBD-CGD-O2D |
| 37 | 15 | 303 | CLA | CAD-CBD-CGD-O1D |
| 37 | 17 | 307 | CLA | CHA-CBD-CGD-O1D |
| 37 | 17 | 307 | CLA | CHA-CBD-CGD-O2D |
| 37 | 18 | 208 | CLA | CHA-CBD-CGD-O1D |
| 37 | 18 | 211 | CLA | CAD-CBD-CGD-O1D |
| 37 | 19 | 303 | CLA | CAD-CBD-CGD-O1D |
| 37 | 31 | 301 | CLA | CHA-CBD-CGD-O1D |
| 37 | 32 | 205 | CLA | CAD-CBD-CGD-O1D |
| 37 | 33 | 303 | CLA | CAD-CBD-CGD-O1D |
| 37 | 34 | 302 | CLA | CAD-CBD-CGD-O1D |
| 37 | 34 | 307 | CLA | CHA-CBD-CGD-O1D |
| 37 | 34 | 307 | CLA | CHA-CBD-CGD-O2D |
| 37 | 35 | 303 | CLA | CAD-CBD-CGD-O1D |
| 37 | 37 | 306 | CLA | CHA-CBD-CGD-O1D |
| 37 | 37 | 306 | CLA | CHA-CBD-CGD-O2D |
| 37 | 38 | 206 | CLA | CAD-CBD-CGD-O1D |
| 37 | 38 | 208 | CLA | CHA-CBD-CGD-O1D |
| 37 | 38 | 211 | CLA | CAD-CBD-CGD-O1D |
| 37 | 39 | 303 | CLA | CAD-CBD-CGD-O1D |
| 43 | D | 409 | LHG | C4-O6-P-O5 |
| 43 | d | 407 | LHG | C4-O6-P-O5 |
| 43 | 19 | 314 | LHG | C3-O3-P-O5 |
| 43 | 19 | 314 | LHG | C3-O3-P-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | 21 | 217 | LHG | C4-O6-P-O5 |
| 43 | 37 | 321 | LHG | C4-O6-P-O5 |
| 43 | 39 | 314 | LHG | C3-O3-P-O5 |
| 43 | 39 | 314 | LHG | C3-O3-P-O6 |
| 47 | 12 | 211 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 15 | 309 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 15 | 309 | KC1 | CHA-CBD-CGD-O2D |
| 47 | 18 | 210 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 18 | 210 | KC1 | CHA-CBD-CGD-O2D |
| 47 | 20 | 305 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 21 | 207 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 21 | 207 | KC1 | CHA-CBD-CGD-O2D |
| 47 | 32 | 212 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 35 | 309 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 35 | 309 | KC1 | CHA-CBD-CGD-O2D |
| 47 | 38 | 210 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 38 | 210 | KC1 | CHA-CBD-CGD-O2D |
| 47 | 40 | 207 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 41 | 207 | KC1 | CHA-CBD-CGD-O1D |
| 47 | 41 | 207 | KC1 | CHA-CBD-CGD-O2D |
| 48 | 11 | 311 | A86 | C1-C2-C3-C4 |
| 48 | 11 | 314 | A86 | C10-C11-C13-C14 |
| 48 | 12 | 202 | A86 | C3-C4-C5-C6 |
| 48 | 12 | 215 | A86 | C10-C11-C13-C14 |
| 48 | 12 | 216 | A86 | C3-C4-C5-C6 |
| 48 | 13 | 313 | A86 | C10-C11-C13-C14 |
| 48 | 14 | 313 | A86 | C11-C10-C9-C8 |
| 48 | 14 | 314 | A86 | C10-C11-C13-C14 |
| 48 | 15 | 314 | A86 | C10-C11-C13-C14 |
| 48 | 20 | 311 | A86 | C10-C11-C13-C14 |
| 48 | 31 | 314 | A86 | C10-C11-C13-C14 |
| 48 | 32 | 203 | A86 | C3-C4-C5-C6 |
| 48 | 32 | 216 | A86 | C10-C11-C13-C14 |
| 48 | 32 | 217 | A86 | C3-C4-C5-C6 |
| 48 | 33 | 313 | A86 | C10-C11-C13-C14 |
| 48 | 34 | 313 | A86 | C11-C10-C9-C8 |
| 48 | 34 | 314 | A86 | C10-C11-C13-C14 |
| 48 | 35 | 314 | A86 | C10-C11-C13-C14 |
| 48 | 37 | 319 | A86 | C24-C25-C26-C27 |
| 48 | 40 | 213 | A86 | C10-C11-C13-C14 |
| 50 | 21 | 216 | DD6 | C11-C10-C9-C8 |
| 50 | 41 | 216 | DD6 | C11-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 36 | 301 | CLA | C15-C16-C17-C18 |
| 41 | b | 520 | LMG | C8-C9-O8-C28 |
| 40 | B | 519 | SQD | C16-C17-C18-C19 |
| 41 | 31 | 316 | LMG | C31-C32-C33-C34 |
| 40 | L | 101 | SQD | C16-C17-C18-C19 |
| 44 | J | 101 | DGD | C4B-C5B-C6B-C7B |
| 37 | 16 | 301 | CLA | C15-C16-C17-C18 |
| 37 | 12 | 205 | CLA | C4-C3-C5-C6 |
| 37 | 17 | 304 | CLA | C4-C3-C5-C6 |
| 37 | A | 405 | CLA | C2B-C3B-CAB-CBB |
| 37 | B | 509 | CLA | C2B-C3B-CAB-CBB |
| 37 | B | 515 | CLA | C2B-C3B-CAB-CBB |
| 37 | D | 402 | CLA | C2B-C3B-CAB-CBB |
| 37 | D | 405 | CLA | C2B-C3B-CAB-CBB |
| 37 | D | 406 | CLA | C2B-C3B-CAB-CBB |
| 37 | Z | 101 | CLA | C2B-C3B-CAB-CBB |
| 37 | W | 102 | CLA | C2B-C3B-CAB-CBB |
| 37 | a | 407 | CLA | C2B-C3B-CAB-CBB |
| 37 | b | 509 | CLA | C2B-C3B-CAB-CBB |
| 37 | b | 515 | CLA | C2B-C3B-CAB-CBB |
| 37 | d | 401 | CLA | C2B-C3B-CAB-CBB |
| 37 | d | 403 | CLA | C2B-C3B-CAB-CBB |
| 37 | d | 404 | CLA | C2B-C3B-CAB-CBB |
| 37 | z | 101 | CLA | C2B-C3B-CAB-CBB |
| 37 | 11 | 307 | CLA | C2B-C3B-CAB-CBB |
| 37 | 13 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 18 | 204 | CLA | C2B-C3B-CAB-CBB |
| 37 | 18 | 206 | CLA | C2B-C3B-CAB-CBB |
| 37 | 18 | 209 | CLA | C2B-C3B-CAB-CBB |
| 37 | 19 | 305 | CLA | C2B-C3B-CAB-CBB |
| 37 | 19 | 310 | CLA | C2B-C3B-CAB-CBB |
| 37 | 21 | 205 | CLA | C2B-C3B-CAB-CBB |
| 37 | 21 | 206 | CLA | C2B-C3B-CAB-CBB |
| 37 | 21 | 208 | CLA | C2B-C3B-CAB-CBB |
| 37 | 21 | 210 | CLA | C2B-C3B-CAB-CBB |
| 37 | 31 | 301 | CLA | C2B-C3B-CAB-CBB |
| 37 | 31 | 308 | CLA | C2B-C3B-CAB-CBB |
| 37 | 33 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 38 | 204 | CLA | C2B-C3B-CAB-CBB |
| 37 | 38 | 211 | CLA | C2B-C3B-CAB-CBB |
| 37 | 39 | 305 | CLA | C2B-C3B-CAB-CBB |
| 37 | 39 | 310 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 41 | 205 | CLA | C2B-C3B-CAB-CBB |
| 37 | 41 | 206 | CLA | C2B-C3B-CAB-CBB |
| 37 | 41 | 208 | CLA | C2B-C3B-CAB-CBB |
| 37 | 41 | 210 | CLA | C2B-C3B-CAB-CBB |
| 39 | B | 518 | BCR | C1-C6-C7-C8 |
| 39 | b | 518 | BCR | C1-C6-C7-C8 |
| 43 | 39 | 314 | LHG | C14-C15-C16-C17 |
| 44 | C | 516 | DGD | O6D-C5D-C6D-O5D |
| 44 | c | 516 | DGD | O6D-C5D-C6D-O5D |
| 44 | j | 101 | DGD | C4B-C5B-C6B-C7B |
| 43 | 17 | 316 | LHG | C2-C3-O3-P |
| 43 | 37 | 315 | LHG | C2-C3-O3-P |
| 48 | 38 | 212 | A86 | C-C1-C24-C25 |
| 41 | B | 521 | LMG | C8-C9-O8-C28 |
| 44 | c | 517 | DGD | C1A-C2A-C3A-C4A |
| 40 | B | 519 | SQD | O10-C23-O48-C46 |
| 48 | 11 | 314 | A86 | C12-C11-C13-C14 |
| 48 | 12 | 202 | A86 | C12-C11-C13-C14 |
| 48 | 12 | 215 | A86 | C12-C11-C13-C14 |
| 48 | 14 | 314 | A86 | C12-C11-C13-C14 |
| 48 | 15 | 314 | A86 | C12-C11-C13-C14 |
| 48 | 17 | 315 | A86 | C12-C11-C13-C14 |
| 48 | 20 | 311 | A86 | C12-C11-C13-C14 |
| 48 | 31 | 314 | A86 | C12-C11-C13-C14 |
| 48 | 32 | 203 | A86 | C12-C11-C13-C14 |
| 48 | 32 | 216 | A86 | C12-C11-C13-C14 |
| 48 | 34 | 314 | A86 | C12-C11-C13-C14 |
| 48 | 35 | 314 | A86 | C12-C11-C13-C14 |
| 48 | 37 | 314 | A86 | C12-C11-C13-C14 |
| 48 | 40 | 213 | A86 | C12-C11-C13-C14 |
| 44 | C | 517 | DGD | C1A-C2A-C3A-C4A |
| 37 | 36 | 303 | CLA | O1D-CGD-O2D-CED |
| 40 | L | 101 | SQD | O10-C23-O48-C46 |
| 45 | D | 404 | PL9 | C4-C3-C7-C8 |
| 45 | d | 402 | PL9 | C4-C3-C7-C8 |
| 37 | 19 | 302 | CLA | O1D-CGD-O2D-CED |
| 43 | 39 | 314 | LHG | O1-C1-C2-C3 |
| 41 | C | 518 | LMG | C28-C29-C30-C31 |
| 41 | c | 518 | LMG | C28-C29-C30-C31 |
| 40 | A | 407 | SQD | C25-C26-C27-C28 |
| 40 | a | 409 | SQD | C25-C26-C27-C28 |
| 47 | 33 | 309 | KC1 | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 16 | 307 | CLA | C12-C13-C15-C16 |
| 37 | 36 | 307 | CLA | C12-C13-C15-C16 |
| 40 | 16 | 315 | SQD | C32-C33-C34-C35 |
| 41 | C | 518 | LMG | C36-C37-C38-C39 |
| 40 | 40 | 202 | SQD | C32-C33-C34-C35 |
| 41 | c | 518 | LMG | C36-C37-C38-C39 |
| 41 | L | 102 | LMG | C35-C36-C37-C38 |
| 41 | l | 101 | LMG | C35-C36-C37-C38 |
| 50 | 21 | 212 | DD6 | C1-C24-C25-C26 |
| 50 | 41 | 212 | DD6 | C1-C24-C25-C26 |
| 41 | 12 | 201 | LMG | C14-C15-C16-C17 |
| 48 | 14 | 315 | A86 | C3-C4-C5-C6 |
| 48 | 17 | 320 | A86 | C24-C25-C26-C27 |
| 48 | 34 | 315 | A86 | C3-C4-C5-C6 |
| 43 | B | 523 | LHG | O6-C4-C5-C6 |
| 43 | D | 410 | LHG | O6-C4-C5-C6 |
| 43 | D | 411 | LHG | O6-C4-C5-C6 |
| 43 | a | 412 | LHG | O6-C4-C5-C6 |
| 43 | b | 522 | LHG | O6-C4-C5-C6 |
| 43 | d | 408 | LHG | O6-C4-C5-C6 |
| 51 | 19 | 315 | LMU | C4-C5-C6-C7 |
| 37 | B | 511 | CLA | O1A-CGA-O2A-C1 |
| 37 | b | 511 | CLA | O1A-CGA-O2A-C1 |
| 51 | 39 | 315 | LMU | C4-C5-C6-C7 |
| 37 | 37 | 301 | CLA | CAA-CBA-CGA-O2A |
| 37 | B | 502 | CLA | C14-C13-C15-C16 |
| 37 | B | 516 | CLA | C11-C10-C8-C9 |
| 37 | C | 502 | CLA | C11-C12-C13-C14 |
| 37 | C | 508 | CLA | C6-C7-C8-C9 |
| 37 | C | 509 | CLA | C6-C7-C8-C9 |
| 37 | C | 511 | CLA | C6-C7-C8-C9 |
| 37 | b | 502 | CLA | C14-C13-C15-C16 |
| 37 | b | 516 | CLA | C11-C10-C8-C9 |
| 37 | c | 502 | CLA | C11-C12-C13-C14 |
| 37 | c | 508 | CLA | C6-C7-C8-C9 |
| 37 | c | 509 | CLA | C6-C7-C8-C9 |
| 37 | c | 511 | CLA | C6-C7-C8-C9 |
| 37 | 19 | 302 | CLA | C6-C7-C8-C9 |
| 37 | 35 | 308 | CLA | C14-C13-C15-C16 |
| 37 | 39 | 302 | CLA | C6-C7-C8-C9 |
| 47 | 13 | 309 | KC1 | CAA-CBA-CGA-O1A |
| 43 | 21 | 201 | LHG | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | B | 512 | CLA | C11-C10-C8-C7 |
| 37 | b | 512 | CLA | C11-C10-C8-C7 |
| 37 | 12 | 204 | CLA | C6-C7-C8-C10 |
| 37 | 32 | 205 | CLA | C6-C7-C8-C10 |
| 50 | 20 | 312 | DD6 | C24-C1-C2-C3 |
| 50 | 40 | 214 | DD6 | C24-C1-C2-C3 |
| 41 | D | 412 | LMG | C13-C14-C15-C16 |
| 43 | 19 | 314 | LHG | O6-C4-C5-O7 |
| 43 | 39 | 314 | LHG | O6-C4-C5-O7 |
| 41 | d | 409 | LMG | C13-C14-C15-C16 |
| 37 | 12 | 210 | CLA | O1D-CGD-O2D-CED |
| 37 | 17 | 302 | CLA | CAA-CBA-CGA-O2A |
| 47 | 20 | 305 | KC1 | O1D-CGD-O2D-CED |
| 44 | C | 517 | DGD | C2D-C1D-O3G-C3G |
| 44 | c | 517 | DGD | C2D-C1D-O3G-C3G |
| 48 | 12 | 214 | A86 | O5-C38-O4-C34 |
| 48 | 32 | 215 | A86 | O5-C38-O4-C34 |
| 38 | a | 406 | PHO | C8-C10-C11-C12 |
| 41 | c | 518 | LMG | C35-C36-C37-C38 |
| 41 | C | 518 | LMG | C35-C36-C37-C38 |
| 41 | C | 518 | LMG | C39-C40-C41-C42 |
| 41 | c | 518 | LMG | C39-C40-C41-C42 |
| 37 | a | 404 | CLA | C3-C5-C6-C7 |
| 37 | 15 | 303 | CLA | CBA-CGA-O2A-C1 |
| 37 | 35 | 303 | CLA | CBA-CGA-O2A-C1 |
| 37 | B | 513 | CLA | C16-C17-C18-C19 |
| 37 | b | 513 | CLA | C16-C17-C18-C19 |
| 38 | A | 404 | PHO | C8-C10-C11-C12 |
| 47 | 40 | 207 | KC1 | O1D-CGD-O2D-CED |
| 41 | 32 | 201 | LMG | C14-C15-C16-C17 |
| 40 | 40 | 202 | SQD | C17-C18-C19-C20 |
| 40 | 16 | 315 | SQD | C17-C18-C19-C20 |
| 40 | 17 | 301 | SQD | O6-C44-C45-O47 |
| 41 | 36 | 314 | LMG | C16-C17-C18-C19 |
| 37 | 17 | 302 | CLA | C2C-C3C-CAC-CBC |
| 41 | 16 | 316 | LMG | C16-C17-C18-C19 |
| 40 | 40 | 202 | SQD | C10-C11-C12-C13 |
| 43 | B | 523 | LHG | C18-C19-C20-C21 |
| 40 | 16 | 315 | SQD | C10-C11-C12-C13 |
| 37 | a | 403 | CLA | C2A-CAA-CBA-CGA |
| 37 | D | 401 | CLA | C3-C5-C6-C7 |
| 37 | 38 | 208 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 40 | L | 101 | SQD | C9-C10-C11-C12 |
| 43 | b | 522 | LHG | C18-C19-C20-C21 |
| 37 | 14 | 302 | CLA | C4-C3-C5-C6 |
| 37 | 34 | 302 | CLA | C4-C3-C5-C6 |
| 40 | B | 519 | SQD | C9-C10-C11-C12 |
| 44 | H | 102 | DGD | C4A-C5A-C6A-C7A |
| 44 | h | 102 | DGD | C4A-C5A-C6A-C7A |
| 43 | D | 409 | LHG | C4-C5-C6-O8 |
| 43 | 19 | 314 | LHG | C14-C15-C16-C17 |
| 41 | 32 | 201 | LMG | C11-C12-C13-C14 |
| 37 | 33 | 301 | CLA | CAA-CBA-CGA-O2A |
| 48 | 14 | 311 | A86 | C-C1-C24-C25 |
| 48 | 34 | 311 | A86 | C-C1-C24-C25 |
| 47 | 33 | 309 | KC1 | CAA-CBA-CGA-O2A |
| 41 | 12 | 201 | LMG | C11-C12-C13-C14 |
| 40 | 40 | 202 | SQD | O10-C23-O48-C46 |
| 40 | 16 | 315 | SQD | O10-C23-O48-C46 |
| 37 | 11 | 308 | CLA | C13-C15-C16-C17 |
| 37 | 32 | 202 | CLA | C8-C10-C11-C12 |
| 37 | 32 | 202 | CLA | C13-C15-C16-C17 |
| 37 | D | 402 | CLA | C2A-CAA-CBA-CGA |
| 37 | d | 401 | CLA | C2A-CAA-CBA-CGA |
| 39 | C | 519 | BCR | C19-C20-C21-C22 |
| 39 | c | 519 | BCR | C19-C20-C21-C22 |
| 48 | 12 | 217 | A86 | C3-C4-C5-C6 |
| 48 | 15 | 316 | A86 | C24-C25-C26-C27 |
| 48 | 17 | 313 | A86 | C3-C4-C5-C6 |
| 48 | 35 | 316 | A86 | C24-C25-C26-C27 |
| 43 | D | 410 | LHG | C25-C26-C27-C28 |
| 43 | d | 408 | LHG | C25-C26-C27-C28 |
| 48 | 38 | 215 | A86 | C33-C34-O4-C38 |
| 37 | C | 510 | CLA | C4-C3-C5-C6 |
| 37 | c | 510 | CLA | C4-C3-C5-C6 |
| 37 | 13 | 301 | CLA | C4-C3-C5-C6 |
| 37 | 33 | 301 | CLA | C4-C3-C5-C6 |
| 45 | d | 406 | PL9 | C15-C14-C16-C17 |
| 37 | d | 404 | CLA | C10-C11-C12-C13 |
| 37 | 11 | 308 | CLA | C8-C10-C11-C12 |
| 37 | 13 | 301 | CLA | CAA-CBA-CGA-O2A |
| 47 | 16 | 308 | KC1 | C2B-C3B-CAB-CBB |
| 37 | 34 | 307 | CLA | O1D-CGD-O2D-CED |
| 37 | 39 | 302 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 38 | 209 | CLA | CBA-CGA-O2A-C1 |
| 37 | D | 406 | CLA | C10-C11-C12-C13 |
| 37 | 14 | 307 | CLA | O1D-CGD-O2D-CED |
| 43 | 19 | 314 | LHG | C1-C2-C3-O3 |
| 43 | 39 | 314 | LHG | C1-C2-C3-O3 |
| 48 | 12 | 213 | A86 | C13-C14-C15-C16 |
| 48 | 13 | 313 | A86 | C13-C14-C15-C16 |
| 48 | 14 | 311 | A86 | C13-C14-C15-C16 |
| 48 | 16 | 314 | A86 | C13-C14-C15-C16 |
| 48 | 17 | 313 | A86 | C13-C14-C15-C16 |
| 48 | 18 | 212 | A86 | C13-C14-C15-C16 |
| 48 | 18 | 213 | A86 | C13-C14-C15-C16 |
| 48 | 31 | 313 | A86 | C13-C14-C15-C16 |
| 48 | 32 | 214 | A86 | C13-C14-C15-C16 |
| 48 | 33 | 313 | A86 | C13-C14-C15-C16 |
| 48 | 34 | 311 | A86 | C13-C14-C15-C16 |
| 48 | 36 | 313 | A86 | C13-C14-C15-C16 |
| 48 | 37 | 312 | A86 | C13-C14-C15-C16 |
| 48 | 38 | 212 | A86 | C13-C14-C15-C16 |
| 48 | 38 | 213 | A86 | C13-C14-C15-C16 |
| 37 | 16 | 301 | CLA | C16-C17-C18-C19 |
| 37 | 36 | 301 | CLA | C16-C17-C18-C19 |
| 47 | 13 | 309 | KC1 | CAA-CBA-CGA-O2A |
| 37 | B | 512 | CLA | C11-C10-C8-C9 |
| 37 | b | 512 | CLA | C11-C10-C8-C9 |
| 37 | 14 | 308 | CLA | C6-C7-C8-C9 |
| 37 | 34 | 308 | CLA | C6-C7-C8-C9 |
| 37 | B | 511 | CLA | CBA-CGA-O2A-C1 |
| 37 | b | 511 | CLA | CBA-CGA-O2A-C1 |
| 37 | B | 509 | CLA | C4B-C3B-CAB-CBB |
| 37 | b | 509 | CLA | C4B-C3B-CAB-CBB |
| 37 | 12 | 205 | CLA | C4B-C3B-CAB-CBB |
| 37 | 12 | 209 | CLA | C4B-C3B-CAB-CBB |
| 37 | 14 | 310 | CLA | C4B-C3B-CAB-CBB |
| 37 | 15 | 310 | CLA | C4B-C3B-CAB-CBB |
| 37 | 18 | 204 | CLA | C4B-C3B-CAB-CBB |
| 37 | 18 | 209 | CLA | C4B-C3B-CAB-CBB |
| 37 | 32 | 206 | CLA | C4B-C3B-CAB-CBB |
| 37 | 32 | 210 | CLA | C4B-C3B-CAB-CBB |
| 37 | 35 | 310 | CLA | C4B-C3B-CAB-CBB |
| 37 | 38 | 204 | CLA | C4B-C3B-CAB-CBB |
| 37 | 38 | 209 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 39 | 302 | CLA | O1A-CGA-O2A-C1 |
| 37 | 39 | 302 | CLA | CBA-CGA-O2A-C1 |
| 43 | D | 409 | LHG | C24-C23-O8-C6 |
| 43 | d | 407 | LHG | C24-C23-O8-C6 |
| 37 | 21 | 205 | CLA | C2A-CAA-CBA-CGA |
| 37 | 41 | 205 | CLA | C2A-CAA-CBA-CGA |
| 41 | 11 | 316 | LMG | C12-C13-C14-C15 |
| 41 | 16 | 316 | LMG | C29-C30-C31-C32 |
| 41 | 36 | 314 | LMG | C29-C30-C31-C32 |
| 37 | 12 | 203 | CLA | C4-C3-C5-C6 |
| 37 | 32 | 204 | CLA | C4-C3-C5-C6 |
| 45 | D | 408 | PL9 | C15-C14-C16-C17 |
| 37 | 14 | 302 | CLA | C2-C3-C5-C6 |
| 37 | 34 | 302 | CLA | C2-C3-C5-C6 |
| 37 | 37 | 303 | CLA | C2-C3-C5-C6 |
| 43 | 21 | 201 | LHG | O6-C4-C5-O7 |
| 41 | 31 | 316 | LMG | C12-C13-C14-C15 |
| 44 | J | 101 | DGD | C2B-C3B-C4B-C5B |
| 37 | 37 | 308 | CLA | C4C-C3C-CAC-CBC |
| 40 | B | 519 | SQD | C15-C16-C17-C18 |
| 44 | j | 101 | DGD | C2B-C3B-C4B-C5B |
| 48 | 16 | 311 | A86 | C3-C4-C5-C6 |
| 48 | 32 | 218 | A86 | C3-C4-C5-C6 |
| 48 | 36 | 311 | A86 | C3-C4-C5-C6 |
| 46 | V | 201 | HEM | C4C-C3C-CAC-CBC |
| 47 | 11 | 309 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 14 | 304 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 14 | 306 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 15 | 304 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 15 | 306 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 15 | 309 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 16 | 305 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 17 | 305 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 17 | 308 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 18 | 205 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 20 | 304 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 31 | 309 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 34 | 304 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 34 | 306 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 35 | 302 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 35 | 304 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 35 | 306 | KC1 | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 47 | 35 | 309 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 36 | 305 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 37 | 304 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 37 | 307 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 38 | 205 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 38 | 210 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 40 | 206 | KC1 | C4B-C3B-CAB-CBB |
| 40 | L | 101 | SQD | C15-C16-C17-C18 |
| 41 | B | 521 | LMG | C21-C22-C23-C24 |
| 41 | b | 519 | LMG | C28-C29-C30-C31 |
| 41 | b | 520 | LMG | C21-C22-C23-C24 |
| 37 | 11 | 308 | CLA | C11-C10-C8-C7 |
| 37 | 12 | 205 | CLA | C6-C7-C8-C10 |
| 37 | 14 | 302 | CLA | C6-C7-C8-C10 |
| 37 | 32 | 202 | CLA | C11-C10-C8-C7 |
| 37 | 32 | 206 | CLA | C6-C7-C8-C10 |
| 37 | 34 | 302 | CLA | C6-C7-C8-C10 |
| 37 | C | 503 | CLA | O1A-CGA-O2A-C1 |
| 43 | 37 | 321 | LHG | C25-C26-C27-C28 |
| 41 | 12 | 201 | LMG | O6-C5-C6-O5 |
| 37 | c | 503 | CLA | O1A-CGA-O2A-C1 |
| 37 | 13 | 303 | CLA | O1A-CGA-O2A-C1 |
| 37 | 19 | 302 | CLA | O1A-CGA-O2A-C1 |
| 43 | 21 | 217 | LHG | C25-C26-C27-C28 |
| 48 | 18 | 215 | A86 | C33-C34-O4-C38 |
| 41 | b | 519 | LMG | C21-C22-C23-C24 |
| 37 | D | 406 | CLA | C16-C17-C18-C20 |
| 37 | d | 404 | CLA | C16-C17-C18-C20 |
| 37 | 17 | 302 | CLA | C4C-C3C-CAC-CBC |
| 41 | B | 520 | LMG | C28-C29-C30-C31 |
| 47 | 21 | 203 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 41 | 203 | KC1 | CAA-CBA-CGA-O1A |
| 41 | 17 | 317 | LMG | O7-C8-C9-O8 |
| 41 | 37 | 316 | LMG | O7-C8-C9-O8 |
| 43 | D | 409 | LHG | O7-C5-C6-O8 |
| 43 | d | 407 | LHG | O7-C5-C6-O8 |
| 41 | B | 520 | LMG | C21-C22-C23-C24 |
| 37 | B | 509 | CLA | C3A-C2A-CAA-CBA |
| 37 | C | 501 | CLA | C3A-C2A-CAA-CBA |
| 37 | b | 509 | CLA | C3A-C2A-CAA-CBA |
| 37 | c | 501 | CLA | C3A-C2A-CAA-CBA |
| 37 | 12 | 204 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 13 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 32 | 205 | CLA | C3A-C2A-CAA-CBA |
| 37 | 33 | 301 | CLA | C3A-C2A-CAA-CBA |
| 37 | 34 | 301 | CLA | C2-C3-C5-C6 |
| 37 | 37 | 301 | CLA | C2C-C3C-CAC-CBC |
| 46 | F | 101 | HEM | CAA-CBA-CGA-O1A |
| 46 | f | 101 | HEM | CAA-CBA-CGA-O1A |
| 39 | b | 524 | BCR | C16-C17-C18-C36 |
| 41 | B | 520 | LMG | O6-C1-O1-C7 |
| 41 | b | 519 | LMG | O6-C1-O1-C7 |
| 48 | 16 | 313 | A86 | C25-C26-C27-C28 |
| 48 | 40 | 201 | A86 | C25-C26-C27-C28 |
| 50 | 21 | 212 | DD6 | C4-C5-C6-C7 |
| 50 | 41 | 212 | DD6 | C4-C5-C6-C7 |
| 37 | 16 | 307 | CLA | C14-C13-C15-C16 |
| 37 | 36 | 307 | CLA | C14-C13-C15-C16 |
| 37 | Z | 101 | CLA | C2-C1-O2A-CGA |
| 37 | z | 101 | CLA | C2-C1-O2A-CGA |
| 48 | 14 | 312 | A86 | C11-C10-C9-C8 |
| 48 | 17 | 312 | A86 | C3-C4-C5-C6 |
| 48 | 18 | 215 | A86 | C3-C4-C5-C6 |
| 48 | 34 | 312 | A86 | C11-C10-C9-C8 |
| 48 | 38 | 215 | A86 | C3-C4-C5-C6 |
| 50 | 16 | 312 | DD6 | C3-C4-C5-C6 |
| 50 | 36 | 312 | DD6 | C3-C4-C5-C6 |
| 43 | D | 411 | LHG | C2-C3-O3-P |
| 43 | a | 412 | LHG | C2-C3-O3-P |
| 48 | 12 | 202 | A86 | C-C1-C24-C25 |
| 48 | 32 | 203 | A86 | C-C1-C24-C25 |
| 48 | 35 | 316 | A86 | C-C1-C24-C25 |
| 46 | F | 101 | HEM | CAD-CBD-CGD-O2D |
| 46 | f | 101 | HEM | CAD-CBD-CGD-O2D |
| 38 | D | 403 | PHO | C15-C16-C17-C18 |
| 38 | a | 405 | PHO | C15-C16-C17-C18 |
| 43 | b | 522 | LHG | C10-C11-C12-C13 |
| 47 | 41 | 203 | KC1 | CAA-CBA-CGA-O2A |
| 40 | A | 407 | SQD | C9-C10-C11-C12 |
| 40 | a | 409 | SQD | C9-C10-C11-C12 |
| 43 | B | 523 | LHG | C10-C11-C12-C13 |
| 48 | 17 | 315 | A86 | C2-C1-C24-C25 |
| 44 | c | 517 | DGD | C7B-C8B-C9B-CAB |
| 37 | C | 505 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | c | 505 | CLA | C4-C3-C5-C6 |
| 46 | F | 101 | HEM | C3D-CAD-CBD-CGD |
| 46 | f | 101 | HEM | C3D-CAD-CBD-CGD |
| 37 | 14 | 301 | CLA | C2-C3-C5-C6 |
| 37 | 18 | 202 | CLA | C2-C3-C5-C6 |
| 37 | 38 | 202 | CLA | C2-C3-C5-C6 |
| 37 | B | 501 | CLA | C16-C17-C18-C20 |
| 37 | b | 501 | CLA | C16-C17-C18-C20 |
| 43 | 21 | 217 | LHG | C12-C13-C14-C15 |
| 44 | C | 517 | DGD | C7B-C8B-C9B-CAB |
| 37 | 32 | 204 | CLA | C2A-CAA-CBA-CGA |
| 37 | 20 | 307 | CLA | CAA-CBA-CGA-O2A |
| 37 | 40 | 209 | CLA | CAA-CBA-CGA-O2A |
| 46 | f | 101 | HEM | CAD-CBD-CGD-O1D |
| 40 | a | 409 | SQD | C19-C20-C21-C22 |
| 37 | 19 | 302 | CLA | CBA-CGA-O2A-C1 |
| 48 | 12 | 215 | A86 | C12-C11-C13-O |
| 48 | 13 | 313 | A86 | C12-C11-C13-O |
| 48 | 14 | 316 | A86 | C12-C11-C13-O |
| 48 | 15 | 316 | A86 | C12-C11-C13-O |
| 48 | 32 | 216 | A86 | C12-C11-C13-O |
| 48 | 33 | 313 | A86 | C12-C11-C13-O |
| 48 | 34 | 316 | A86 | C12-C11-C13-O |
| 48 | 35 | 316 | A86 | C12-C11-C13-O |
| 48 | 38 | 215 | A86 | C12-C11-C13-O |
| 43 | 37 | 321 | LHG | C12-C13-C14-C15 |
| 40 | A | 407 | SQD | C19-C20-C21-C22 |
| 47 | 21 | 203 | KC1 | CAA-CBA-CGA-O2A |
| 37 | C | 510 | CLA | CBD-CGD-O2D-CED |
| 44 | J | 101 | DGD | O6E-C5E-C6E-O5E |
| 46 | F | 101 | HEM | CAD-CBD-CGD-O1D |
| 37 | B | 510 | CLA | C14-C13-C15-C16 |
| 37 | C | 504 | CLA | C11-C10-C8-C9 |
| 37 | Z | 101 | CLA | C14-C13-C15-C16 |
| 37 | b | 510 | CLA | C14-C13-C15-C16 |
| 37 | c | 504 | CLA | C11-C10-C8-C9 |
| 37 | z | 101 | CLA | C14-C13-C15-C16 |
| 37 | 11 | 308 | CLA | C11-C12-C13-C14 |
| 37 | 12 | 205 | CLA | C6-C7-C8-C9 |
| 37 | 32 | 202 | CLA | C11-C12-C13-C14 |
| 37 | 32 | 206 | CLA | C6-C7-C8-C9 |
| 43 | 19 | 314 | LHG | O1-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | b | 512 | CLA | C13-C15-C16-C17 |
| 37 | c | 510 | CLA | CBD-CGD-O2D-CED |
| 44 | j | 101 | DGD | O6E-C5E-C6E-O5E |
| 37 | 14 | 303 | CLA | CAA-CBA-CGA-O2A |
| 37 | 34 | 303 | CLA | CAA-CBA-CGA-O2A |
| 37 | B | 512 | CLA | C13-C15-C16-C17 |
| 40 | L | 101 | SQD | C11-C10-C9-C8 |
| 41 | A | 408 | LMG | C40-C41-C42-C43 |
| 41 | a | 410 | LMG | C40-C41-C42-C43 |
| 40 | B | 519 | SQD | C11-C10-C9-C8 |
| 37 | 20 | 303 | CLA | C3-C5-C6-C7 |
| 37 | 40 | 205 | CLA | C3-C5-C6-C7 |
| 37 | 20 | 307 | CLA | CAA-CBA-CGA-O1A |
| 37 | 40 | 209 | CLA | CAA-CBA-CGA-O1A |
| 46 | F | 101 | HEM | CAA-CBA-CGA-O2A |
| 46 | f | 101 | HEM | CAA-CBA-CGA-O2A |
| 37 | 12 | 203 | CLA | C2A-CAA-CBA-CGA |
| 37 | 18 | 206 | CLA | C2A-CAA-CBA-CGA |
| 37 | 19 | 301 | CLA | C2A-CAA-CBA-CGA |
| 37 | 34 | 307 | CLA | C2A-CAA-CBA-CGA |
| 37 | 38 | 206 | CLA | C2A-CAA-CBA-CGA |
| 37 | 39 | 301 | CLA | C2A-CAA-CBA-CGA |
| 37 | B | 501 | CLA | C1A-C2A-CAA-CBA |
| 37 | B | 506 | CLA | C1A-C2A-CAA-CBA |
| 37 | B | 511 | CLA | C1A-C2A-CAA-CBA |
| 37 | b | 501 | CLA | C1A-C2A-CAA-CBA |
| 37 | b | 506 | CLA | C1A-C2A-CAA-CBA |
| 37 | b | 511 | CLA | C1A-C2A-CAA-CBA |
| 37 | 14 | 308 | CLA | C1A-C2A-CAA-CBA |
| 37 | 17 | 302 | CLA | C1A-C2A-CAA-CBA |
| 37 | 17 | 307 | CLA | C1A-C2A-CAA-CBA |
| 37 | 18 | 209 | CLA | C1A-C2A-CAA-CBA |
| 37 | 19 | 304 | CLA | C1A-C2A-CAA-CBA |
| 37 | 21 | 202 | CLA | C1A-C2A-CAA-CBA |
| 37 | 34 | 308 | CLA | C1A-C2A-CAA-CBA |
| 37 | 37 | 301 | CLA | C1A-C2A-CAA-CBA |
| 37 | 39 | 304 | CLA | C1A-C2A-CAA-CBA |
| 37 | 41 | 202 | CLA | C1A-C2A-CAA-CBA |
| 48 | 13 | 313 | A86 | C10-C11-C13-O |
| 48 | 16 | 313 | A86 | C25-C26-C27-C29 |
| 48 | 18 | 215 | A86 | C10-C11-C13-O |
| 48 | 33 | 313 | A86 | C10-C11-C13-O |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 38 | 215 | A86 | C10-C11-C13-O |
| 48 | 40 | 201 | A86 | C25-C26-C27-C29 |
| 41 | 11 | 316 | LMG | C29-C28-O8-C9 |
| 41 | 31 | 316 | LMG | C29-C28-O8-C9 |
| 37 | 37 | 301 | CLA | C4C-C3C-CAC-CBC |
| 43 | 41 | 201 | LHG | O6-C4-C5-O7 |
| 43 | 37 | 321 | LHG | C10-C11-C12-C13 |
| 37 | 33 | 303 | CLA | O1A-CGA-O2A-C1 |
| 37 | B | 501 | CLA | C2B-C3B-CAB-CBB |
| 37 | B | 524 | CLA | C2B-C3B-CAB-CBB |
| 37 | C | 501 | CLA | C2B-C3B-CAB-CBB |
| 37 | Z | 102 | CLA | C2B-C3B-CAB-CBB |
| 37 | W | 101 | CLA | C2B-C3B-CAB-CBB |
| 37 | b | 501 | CLA | C2B-C3B-CAB-CBB |
| 37 | b | 523 | CLA | C2B-C3B-CAB-CBB |
| 37 | c | 501 | CLA | C2B-C3B-CAB-CBB |
| 37 | z | 102 | CLA | C2B-C3B-CAB-CBB |
| 37 | w | 101 | CLA | C2B-C3B-CAB-CBB |
| 37 | 11 | 305 | CLA | C2B-C3B-CAB-CBB |
| 37 | 12 | 203 | CLA | C2B-C3B-CAB-CBB |
| 37 | 12 | 205 | CLA | C2B-C3B-CAB-CBB |
| 37 | 12 | 209 | CLA | C2B-C3B-CAB-CBB |
| 37 | 13 | 305 | CLA | C2B-C3B-CAB-CBB |
| 37 | 13 | 307 | CLA | C2B-C3B-CAB-CBB |
| 37 | 13 | 310 | CLA | C2B-C3B-CAB-CBB |
| 37 | 14 | 305 | CLA | C2B-C3B-CAB-CBB |
| 37 | 14 | 310 | CLA | C2B-C3B-CAB-CBB |
| 37 | 15 | 305 | CLA | C2B-C3B-CAB-CBB |
| 37 | 15 | 307 | CLA | C2B-C3B-CAB-CBB |
| 37 | 15 | 308 | CLA | C2B-C3B-CAB-CBB |
| 37 | 15 | 310 | CLA | C2B-C3B-CAB-CBB |
| 37 | 16 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 17 | 307 | CLA | C2B-C3B-CAB-CBB |
| 37 | 19 | 309 | CLA | C2B-C3B-CAB-CBB |
| 37 | 20 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 20 | 306 | CLA | C2B-C3B-CAB-CBB |
| 37 | 20 | 307 | CLA | C2B-C3B-CAB-CBB |
| 37 | 21 | 202 | CLA | C2B-C3B-CAB-CBB |
| 37 | 21 | 204 | CLA | C2B-C3B-CAB-CBB |
| 37 | 31 | 306 | CLA | C2B-C3B-CAB-CBB |
| 37 | 32 | 204 | CLA | C2B-C3B-CAB-CBB |
| 37 | 32 | 206 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 32 | 210 | CLA | C2B-C3B-CAB-CBB |
| 37 | 33 | 305 | CLA | C2B-C3B-CAB-CBB |
| 37 | 33 | 307 | CLA | C2B-C3B-CAB-CBB |
| 37 | 33 | 310 | CLA | C2B-C3B-CAB-CBB |
| 37 | 34 | 305 | CLA | C2B-C3B-CAB-CBB |
| 37 | 34 | 310 | CLA | C2B-C3B-CAB-CBB |
| 37 | 35 | 305 | CLA | C2B-C3B-CAB-CBB |
| 37 | 35 | 307 | CLA | C2B-C3B-CAB-CBB |
| 37 | 35 | 308 | CLA | C2B-C3B-CAB-CBB |
| 37 | 35 | 310 | CLA | C2B-C3B-CAB-CBB |
| 37 | 36 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 37 | 306 | CLA | C2B-C3B-CAB-CBB |
| 37 | 38 | 203 | CLA | C2B-C3B-CAB-CBB |
| 37 | 38 | 206 | CLA | C2B-C3B-CAB-CBB |
| 37 | 38 | 209 | CLA | C2B-C3B-CAB-CBB |
| 37 | 39 | 309 | CLA | C2B-C3B-CAB-CBB |
| 37 | 40 | 205 | CLA | C2B-C3B-CAB-CBB |
| 37 | 40 | 208 | CLA | C2B-C3B-CAB-CBB |
| 37 | 40 | 209 | CLA | C2B-C3B-CAB-CBB |
| 37 | 41 | 202 | CLA | C2B-C3B-CAB-CBB |
| 37 | 41 | 204 | CLA | C2B-C3B-CAB-CBB |
| 39 | A | 406 | BCR | C5-C6-C7-C8 |
| 39 | A | 406 | BCR | C23-C24-C25-C30 |
| 39 | B | 517 | BCR | C23-C24-C25-C30 |
| 39 | B | 518 | BCR | C5-C6-C7-C8 |
| 39 | B | 525 | BCR | C23-C24-C25-C30 |
| 39 | C | 514 | BCR | C5-C6-C7-C8 |
| 39 | C | 514 | BCR | C23-C24-C25-C30 |
| 39 | C | 515 | BCR | C23-C24-C25-C30 |
| 39 | C | 519 | BCR | C5-C6-C7-C8 |
| 39 | C | 519 | BCR | C23-C24-C25-C26 |
| 39 | D | 407 | BCR | C23-C24-C25-C30 |
| 39 | H | 101 | BCR | C5-C6-C7-C8 |
| 39 | 0 | 101 | BCR | C5-C6-C7-C8 |
| 39 | 0 | 101 | BCR | C23-C24-C25-C26 |
| 39 | 0 | 101 | BCR | C23-C24-C25-C30 |
| 39 | a | 408 | BCR | C5-C6-C7-C8 |
| 39 | a | 408 | BCR | C23-C24-C25-C30 |
| 39 | b | 517 | BCR | C23-C24-C25-C30 |
| 39 | b | 518 | BCR | C5-C6-C7-C8 |
| 39 | b | 524 | BCR | C23-C24-C25-C30 |
| 39 | c | 514 | BCR | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | c | 515 | BCR | C23-C24-C25-C30 |
| 39 | c | 519 | BCR | C5-C6-C7-C8 |
| 39 | c | 519 | BCR | C23-C24-C25-C26 |
| 39 | d | 405 | BCR | C23-C24-C25-C30 |
| 39 | h | 101 | BCR | C5-C6-C7-C8 |
| 39 | 5 | 101 | BCR | C5-C6-C7-C8 |
| 39 | 5 | 101 | BCR | C23-C24-C25-C30 |
| 43 | 21 | 217 | LHG | C10-C11-C12-C13 |
| 37 | C | 503 | CLA | CBA-CGA-O2A-C1 |
| 37 | c | 503 | CLA | CBA-CGA-O2A-C1 |
| 43 | 19 | 314 | LHG | O6-C4-C5-C6 |
| 43 | 21 | 217 | LHG | O6-C4-C5-C6 |
| 43 | 37 | 321 | LHG | O6-C4-C5-C6 |
| 43 | 39 | 314 | LHG | O6-C4-C5-C6 |
| 43 | 41 | 201 | LHG | O6-C4-C5-C6 |
| 37 | 13 | 301 | CLA | C2-C3-C5-C6 |
| 37 | 33 | 301 | CLA | C2-C3-C5-C6 |
| 45 | D | 404 | PL9 | C18-C19-C21-C22 |
| 45 | d | 402 | PL9 | C18-C19-C21-C22 |
| 37 | 21 | 208 | CLA | C12-C13-C15-C16 |
| 37 | 41 | 208 | CLA | C12-C13-C15-C16 |
| 37 | c | 506 | CLA | C16-C17-C18-C20 |
| 41 | D | 412 | LMG | C4-C5-C6-O5 |
| 40 | 16 | 315 | SQD | O6-C44-C45-O47 |
| 40 | 40 | 202 | SQD | O6-C44-C45-O47 |
| 43 | 17 | 316 | LHG | O7-C5-C6-O8 |
| 43 | 37 | 315 | LHG | O7-C5-C6-O8 |
| 37 | 21 | 205 | CLA | CAA-CBA-CGA-O1A |
| 37 | 41 | 205 | CLA | CAA-CBA-CGA-O1A |
| 41 | d | 409 | LMG | C4-C5-C6-O5 |
| 43 | 17 | 316 | LHG | C26-C27-C28-C29 |
| 43 | 37 | 315 | LHG | C26-C27-C28-C29 |
| 37 | 17 | 309 | CLA | CAA-CBA-CGA-O2A |
| 37 | C | 506 | CLA | C16-C17-C18-C20 |
| 48 | 15 | 316 | A86 | C-C1-C24-C25 |
| 43 | 19 | 314 | LHG | C12-C13-C14-C15 |
| 37 | a | 403 | CLA | O1A-CGA-O2A-C1 |
| 37 | 11 | 303 | CLA | C4-C3-C5-C6 |
| 37 | 31 | 304 | CLA | C4-C3-C5-C6 |
| 37 | 18 | 208 | CLA | CBD-CGD-O2D-CED |
| 37 | A | 403 | CLA | CBA-CGA-O2A-C1 |
| 37 | a | 403 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | C | 510 | CLA | C2-C3-C5-C6 |
| 37 | c | 510 | CLA | C2-C3-C5-C6 |
| 37 | 12 | 203 | CLA | C2-C3-C5-C6 |
| 37 | 32 | 204 | CLA | C2-C3-C5-C6 |
| 41 | 11 | 316 | LMG | C19-C20-C21-C22 |
| 37 | b | 511 | CLA | O1D-CGD-O2D-CED |
| 37 | 16 | 301 | CLA | C2-C1-O2A-CGA |
| 37 | 18 | 209 | CLA | C2-C1-O2A-CGA |
| 41 | 31 | 316 | LMG | C19-C20-C21-C22 |
| 37 | 35 | 305 | CLA | CAA-CBA-CGA-O2A |
| 48 | 37 | 314 | A86 | C2-C1-C24-C25 |
| 37 | 37 | 308 | CLA | CAA-CBA-CGA-O2A |
| 37 | C | 510 | CLA | O1D-CGD-O2D-CED |
| 37 | 14 | 307 | CLA | C2A-CAA-CBA-CGA |
| 37 | 37 | 306 | CLA | C2A-CAA-CBA-CGA |
| 37 | z | 102 | CLA | CAA-CBA-CGA-O2A |
| 37 | 15 | 305 | CLA | CAA-CBA-CGA-O2A |
| 43 | 41 | 201 | LHG | C27-C28-C29-C30 |
| 37 | Z | 102 | CLA | CAA-CBA-CGA-O2A |
| 37 | D | 401 | CLA | C2C-C3C-CAC-CBC |
| 37 | c | 510 | CLA | O1D-CGD-O2D-CED |
| 43 | 21 | 201 | LHG | C27-C28-C29-C30 |
| 37 | A | 403 | CLA | O1A-CGA-O2A-C1 |
| 37 | C | 505 | CLA | C2-C3-C5-C6 |
| 37 | c | 505 | CLA | C2-C3-C5-C6 |
| 37 | 12 | 205 | CLA | C2-C3-C5-C6 |
| 37 | 17 | 304 | CLA | C2-C3-C5-C6 |
| 37 | 32 | 206 | CLA | C2-C3-C5-C6 |
| 47 | 11 | 306 | KC1 | CBD-CGD-O2D-CED |
| 44 | H | 102 | DGD | C5A-C6A-C7A-C8A |
| 44 | h | 102 | DGD | C5A-C6A-C7A-C8A |
| 37 | a | 404 | CLA | C2C-C3C-CAC-CBC |
| 37 | B | 511 | CLA | O1D-CGD-O2D-CED |
| 44 | j | 101 | DGD | C4A-C5A-C6A-C7A |
| 40 | 16 | 315 | SQD | C44-C45-C46-O48 |
| 40 | 40 | 202 | SQD | C44-C45-C46-O48 |
| 41 | 17 | 317 | LMG | C7-C8-C9-O8 |
| 41 | 37 | 316 | LMG | C7-C8-C9-O8 |
| 44 | J | 101 | DGD | C4A-C5A-C6A-C7A |
| 37 | 20 | 303 | CLA | O1D-CGD-O2D-CED |
| 38 | D | 403 | PHO | C2A-CAA-CBA-CGA |
| 38 | a | 405 | PHO | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 40 | 205 | CLA | O1D-CGD-O2D-CED |
| 38 | A | 404 | PHO | CAA-CBA-CGA-O2A |
| 38 | a | 406 | PHO | CAA-CBA-CGA-O2A |
| 41 | L | 102 | LMG | C30-C31-C32-C33 |
| 41 | l | 101 | LMG | C30-C31-C32-C33 |
| 37 | 21 | 205 | CLA | CAA-CBA-CGA-O2A |
| 37 | 41 | 205 | CLA | CAA-CBA-CGA-O2A |
| 37 | D | 405 | CLA | C13-C15-C16-C17 |
| 37 | d | 403 | CLA | C13-C15-C16-C17 |
| 43 | 39 | 314 | LHG | C12-C13-C14-C15 |
| 37 | B | 504 | CLA | C4-C3-C5-C6 |
| 37 | b | 504 | CLA | C4-C3-C5-C6 |
| 37 | 18 | 206 | CLA | CAA-CBA-CGA-O2A |
| 37 | 38 | 206 | CLA | CAA-CBA-CGA-O2A |
| 37 | C | 506 | CLA | C15-C16-C17-C18 |
| 41 | B | 521 | LMG | C20-C21-C22-C23 |
| 41 | b | 520 | LMG | C20-C21-C22-C23 |
| 37 | B | 502 | CLA | C4B-C3B-CAB-CBB |
| 37 | b | 502 | CLA | C4B-C3B-CAB-CBB |
| 37 | 21 | 204 | CLA | C4B-C3B-CAB-CBB |
| 37 | 37 | 303 | CLA | C4B-C3B-CAB-CBB |
| 37 | 41 | 204 | CLA | C4B-C3B-CAB-CBB |
| 37 | c | 506 | CLA | C15-C16-C17-C18 |
| 37 | 32 | 213 | CLA | CAA-CBA-CGA-O2A |
| 44 | H | 102 | DGD | O2G-C1B-C2B-C3B |
| 44 | h | 102 | DGD | O2G-C1B-C2B-C3B |
| 37 | 12 | 212 | CLA | CAA-CBA-CGA-O2A |
| 37 | 16 | 301 | CLA | C16-C17-C18-C20 |
| 37 | 36 | 301 | CLA | C16-C17-C18-C20 |
| 43 | d | 407 | LHG | C19-C20-C21-C22 |
| 47 | 31 | 307 | KC1 | CBD-CGD-O2D-CED |
| 39 | K | 101 | BCR | C11-C10-C9-C34 |
| 39 | y | 101 | BCR | C11-C10-C9-C34 |
| 44 | C | 517 | DGD | O1A-C1A-O1G-C1G |
| 44 | c | 517 | DGD | O1A-C1A-O1G-C1G |
| 43 | D | 409 | LHG | C19-C20-C21-C22 |
| 37 | B | 511 | CLA | CBD-CGD-O2D-CED |
| 47 | 37 | 304 | KC1 | CAA-CBA-CGA-O1A |
| 47 | 37 | 304 | KC1 | CAA-CBA-CGA-O2A |
| 41 | D | 412 | LMG | C34-C35-C36-C37 |
| 43 | 21 | 201 | LHG | O6-C4-C5-C6 |
| 37 | C | 505 | CLA | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 46 | V | 201 | HEM | CAD-CBD-CGD-O2D |
| 46 | v | 201 | HEM | CAD-CBD-CGD-O2D |
| 37 | b | 511 | CLA | CBD-CGD-O2D-CED |
| 41 | 12 | 201 | LMG | C11-C10-O7-C8 |
| 41 | d | 409 | LMG | C34-C35-C36-C37 |
| 37 | c | 505 | CLA | C15-C16-C17-C18 |
| 41 | b | 520 | LMG | C28-C29-C30-C31 |
| 37 | z | 102 | CLA | CAA-CBA-CGA-O1A |
| 37 | 13 | 305 | CLA | CAA-CBA-CGA-O2A |
| 37 | 16 | 309 | CLA | CAA-CBA-CGA-O2A |
| 37 | 33 | 305 | CLA | CAA-CBA-CGA-O2A |
| 37 | 35 | 305 | CLA | CAA-CBA-CGA-O1A |
| 37 | 36 | 309 | CLA | CAA-CBA-CGA-O2A |
| 37 | 39 | 304 | CLA | CAA-CBA-CGA-O2A |
| 37 | D | 402 | CLA | C6-C7-C8-C9 |
| 37 | D | 402 | CLA | C14-C13-C15-C16 |
| 37 | W | 102 | CLA | C6-C7-C8-C9 |
| 37 | d | 401 | CLA | C6-C7-C8-C9 |
| 37 | d | 401 | CLA | C14-C13-C15-C16 |
| 37 | 11 | 301 | CLA | C6-C7-C8-C9 |
| 37 | 14 | 302 | CLA | C11-C12-C13-C14 |
| 37 | 31 | 301 | CLA | C6-C7-C8-C9 |
| 37 | 34 | 302 | CLA | C11-C12-C13-C14 |
| 40 | B | 519 | SQD | C45-C44-O6-C1 |
| 40 | L | 101 | SQD | C45-C44-O6-C1 |
| 41 | B | 521 | LMG | C28-C29-C30-C31 |
| 37 | Z | 102 | CLA | CAA-CBA-CGA-O1A |
| 37 | 15 | 305 | CLA | CAA-CBA-CGA-O1A |
| 37 | 19 | 304 | CLA | CAA-CBA-CGA-O2A |
| 37 | 21 | 209 | CLA | CAA-CBA-CGA-O2A |
| 37 | 41 | 209 | CLA | CAA-CBA-CGA-O2A |
| 37 | B | 509 | CLA | C2-C1-O2A-CGA |
| 37 | b | 509 | CLA | C2-C1-O2A-CGA |
| 37 | 11 | 308 | CLA | C2-C1-O2A-CGA |
| 37 | 14 | 308 | CLA | C2-C1-O2A-CGA |
| 37 | 15 | 308 | CLA | C2-C1-O2A-CGA |
| 37 | 32 | 202 | CLA | C2-C1-O2A-CGA |
| 37 | 34 | 308 | CLA | C2-C1-O2A-CGA |
| 37 | 36 | 301 | CLA | C2-C1-O2A-CGA |
| 37 | 19 | 303 | CLA | C16-C17-C18-C20 |
| 37 | 39 | 303 | CLA | C16-C17-C18-C20 |
| 37 | 14 | 307 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 34 | 307 | CLA | CBA-CGA-O2A-C1 |
| 37 | 20 | 307 | CLA | C3A-C2A-CAA-CBA |
| 37 | 40 | 209 | CLA | C3A-C2A-CAA-CBA |
| 40 | 16 | 315 | SQD | C30-C31-C32-C33 |
| 40 | 40 | 202 | SQD | C30-C31-C32-C33 |
| 37 | 38 | 204 | CLA | C2-C3-C5-C6 |
| 46 | V | 201 | HEM | C2C-C3C-CAC-CBC |
| 47 | 12 | 206 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 13 | 302 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 18 | 207 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 20 | 302 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 33 | 302 | KC1 | C2B-C3B-CAB-CBB |
| 47 | 40 | 204 | KC1 | C2B-C3B-CAB-CBB |
| 37 | 35 | 301 | CLA | C13-C15-C16-C17 |
| 41 | 11 | 317 | LMG | C31-C32-C33-C34 |
| 41 | 31 | 317 | LMG | C31-C32-C33-C34 |
| 47 | 17 | 305 | KC1 | CAA-CBA-CGA-O1A |
| 40 | b | 521 | SQD | O10-C23-O48-C46 |
| 37 | 14 | 310 | CLA | CAA-CBA-CGA-O2A |
| 37 | B | 513 | CLA | C3-C5-C6-C7 |
| 40 | 17 | 301 | SQD | C11-C10-C9-C8 |
| 40 | 36 | 315 | SQD | C11-C10-C9-C8 |
| 37 | 12 | 212 | CLA | CAA-CBA-CGA-O1A |
| 37 | 32 | 213 | CLA | CAA-CBA-CGA-O1A |
| 47 | 17 | 305 | KC1 | CAA-CBA-CGA-O2A |
| 37 | C | 505 | CLA | C2A-CAA-CBA-CGA |
| 37 | c | 505 | CLA | C2A-CAA-CBA-CGA |
| 47 | 34 | 304 | KC1 | C2C-C3C-CAC-CBC |
| 37 | b | 513 | CLA | C3-C5-C6-C7 |
| 37 | B | 501 | CLA | CAA-CBA-CGA-O1A |
| 37 | 21 | 209 | CLA | CAA-CBA-CGA-O1A |
| 37 | 21 | 210 | CLA | CAA-CBA-CGA-O2A |
| 37 | 34 | 310 | CLA | CAA-CBA-CGA-O2A |
| 37 | 39 | 304 | CLA | CAA-CBA-CGA-O1A |
| 37 | 41 | 209 | CLA | CAA-CBA-CGA-O1A |
| 37 | 18 | 204 | CLA | C2-C3-C5-C6 |
| 51 | 39 | 315 | LMU | O1'-C1-C2-C3 |
| 37 | C | 501 | CLA | C5-C6-C7-C8 |
| 37 | c | 501 | CLA | C5-C6-C7-C8 |
| 41 | d | 409 | LMG | C14-C15-C16-C17 |
| 47 | 14 | 304 | KC1 | C2C-C3C-CAC-CBC |
| 50 | 19 | 312 | DD6 | C13-C14-C15-O1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 50 | 39 | 312 | DD6 | C13-C14-C15-O1 |
| 37 | 18 | 206 | CLA | CAA-CBA-CGA-O1A |
| 37 | 38 | 206 | CLA | CAA-CBA-CGA-O1A |
| 43 | 17 | 316 | LHG | O6-C4-C5-O7 |
| 43 | 37 | 315 | LHG | O6-C4-C5-O7 |
| 40 | B | 522 | SQD | O10-C23-O48-C46 |
| 37 | b | 501 | CLA | CAA-CBA-CGA-O1A |
| 37 | 12 | 209 | CLA | CBA-CGA-O2A-C1 |
| 37 | 13 | 303 | CLA | CBA-CGA-O2A-C1 |
| 37 | 32 | 210 | CLA | CBA-CGA-O2A-C1 |
| 37 | 19 | 304 | CLA | CAA-CBA-CGA-O1A |
| 40 | B | 519 | SQD | C44-C45-C46-O48 |
| 40 | L | 101 | SQD | C44-C45-C46-O48 |
| 43 | d | 408 | LHG | C4-C5-C6-O8 |
| 44 | C | 516 | DGD | C1G-C2G-C3G-O3G |
| 44 | H | 102 | DGD | C1G-C2G-C3G-O3G |
| 44 | c | 516 | DGD | C1G-C2G-C3G-O3G |
| 44 | h | 102 | DGD | C1G-C2G-C3G-O3G |
| 37 | 36 | 307 | CLA | C8-C10-C11-C12 |
| 47 | 16 | 308 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 17 | 303 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 17 | 306 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 18 | 210 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 20 | 305 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 36 | 308 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 37 | 302 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 37 | 305 | KC1 | C4B-C3B-CAB-CBB |
| 47 | 40 | 207 | KC1 | C4B-C3B-CAB-CBB |
| 41 | D | 412 | LMG | C14-C15-C16-C17 |
| 51 | 19 | 315 | LMU | O1'-C1-C2-C3 |
| 37 | 41 | 210 | CLA | CAA-CBA-CGA-O2A |
| 37 | b | 504 | CLA | O1D-CGD-O2D-CED |
| 41 | A | 408 | LMG | C33-C34-C35-C36 |
| 41 | a | 410 | LMG | C33-C34-C35-C36 |
| 37 | 16 | 301 | CLA | C4-C3-C5-C6 |
| 37 | 36 | 301 | CLA | C4-C3-C5-C6 |
| 37 | 17 | 307 | CLA | C2A-CAA-CBA-CGA |
| 45 | D | 408 | PL9 | C12-C11-C9-C8 |
| 45 | d | 406 | PL9 | C12-C11-C9-C8 |
| 48 | 13 | 313 | A86 | C3-C4-C5-C6 |
| 48 | 33 | 313 | A86 | C3-C4-C5-C6 |
| 48 | 37 | 311 | A86 | C3-C4-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 37 | 313 | A86 | C24-C25-C26-C27 |
| 50 | 21 | 212 | DD6 | C11-C10-C9-C8 |
| 48 | 11 | 312 | A86 | C28-C27-C29-C30 |
| 48 | 14 | 313 | A86 | C28-C27-C29-C30 |
| 48 | 31 | 312 | A86 | C28-C27-C29-C30 |
| 48 | 34 | 313 | A86 | C28-C27-C29-C30 |
| 43 | d | 408 | LHG | C29-C30-C31-C32 |
| 37 | 16 | 307 | CLA | C8-C10-C11-C12 |
| 43 | D | 410 | LHG | C29-C30-C31-C32 |
| 43 | D | 410 | LHG | O7-C7-C8-C9 |
| 44 | c | 516 | DGD | O2G-C1B-C2B-C3B |
| 37 | 13 | 305 | CLA | CAA-CBA-CGA-O1A |
| 37 | W | 101 | CLA | C11-C10-C8-C9 |
| 37 | w | 101 | CLA | C11-C10-C8-C9 |
| 37 | 21 | 208 | CLA | C14-C13-C15-C16 |
| 37 | 31 | 302 | CLA | C6-C7-C8-C9 |
| 37 | 37 | 301 | CLA | C11-C12-C13-C14 |
| 37 | 41 | 208 | CLA | C14-C13-C15-C16 |
| 38 | A | 404 | PHO | C6-C7-C8-C9 |
| 38 | a | 406 | PHO | C6-C7-C8-C9 |
| 47 | 37 | 305 | KC1 | C2C-C3C-CAC-CBC |
| 37 | 14 | 307 | CLA | CAA-CBA-CGA-O2A |
| 37 | 34 | 307 | CLA | CAA-CBA-CGA-O2A |
| 43 | d | 408 | LHG | O7-C7-C8-C9 |
| 44 | C | 516 | DGD | O2G-C1B-C2B-C3B |
| 43 | D | 410 | LHG | C35-C36-C37-C38 |
| 43 | d | 408 | LHG | C35-C36-C37-C38 |
| 43 | 17 | 316 | LHG | O6-C4-C5-C6 |
| 43 | 37 | 315 | LHG | O6-C4-C5-C6 |
| 37 | 33 | 305 | CLA | CAA-CBA-CGA-O1A |
| 48 | 14 | 311 | A86 | C2-C1-C24-C25 |
| 48 | 34 | 311 | A86 | C2-C1-C24-C25 |
| 41 | 32 | 201 | LMG | C31-C32-C33-C34 |
| 48 | 16 | 313 | A86 | C13-C14-C15-O1 |
| 48 | 20 | 311 | A86 | C13-C14-C15-O1 |
| 48 | 40 | 201 | A86 | C13-C14-C15-O1 |
| 48 | 40 | 213 | A86 | C13-C14-C15-O1 |
| 37 | B | 504 | CLA | O1D-CGD-O2D-CED |
| 47 | 17 | 306 | KC1 | C2C-C3C-CAC-CBC |
| 41 | a | 410 | LMG | C21-C22-C23-C24 |
| 37 | 18 | 208 | CLA | CAA-CBA-CGA-O2A |
| 37 | 16 | 309 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 36 | 309 | CLA | CAA-CBA-CGA-O1A |
| 46 | V | 201 | HEM | CAD-CBD-CGD-O1D |
| 46 | v | 201 | HEM | CAD-CBD-CGD-O1D |
| 41 | A | 408 | LMG | C21-C22-C23-C24 |
| 37 | B | 510 | CLA | C12-C13-C15-C16 |
| 37 | D | 402 | CLA | C6-C7-C8-C10 |
| 37 | D | 402 | CLA | C11-C10-C8-C7 |
| 37 | W | 102 | CLA | C6-C7-C8-C10 |
| 37 | b | 510 | CLA | C12-C13-C15-C16 |
| 37 | d | 401 | CLA | C6-C7-C8-C10 |
| 37 | d | 401 | CLA | C11-C10-C8-C7 |
| 37 | 14 | 302 | CLA | C11-C12-C13-C15 |
| 37 | 31 | 301 | CLA | C6-C7-C8-C10 |
| 37 | 34 | 302 | CLA | C11-C12-C13-C15 |
| 37 | B | 514 | CLA | C2B-C3B-CAB-CBB |
| 37 | C | 511 | CLA | C2B-C3B-CAB-CBB |
| 37 | b | 514 | CLA | C2B-C3B-CAB-CBB |
| 37 | c | 511 | CLA | C2B-C3B-CAB-CBB |
| 37 | 11 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 17 | 304 | CLA | C2B-C3B-CAB-CBB |
| 37 | 19 | 302 | CLA | C2B-C3B-CAB-CBB |
| 37 | 31 | 304 | CLA | C2B-C3B-CAB-CBB |
| 37 | 37 | 303 | CLA | C2B-C3B-CAB-CBB |
| 37 | 39 | 302 | CLA | C2B-C3B-CAB-CBB |
| 37 | 39 | 306 | CLA | C2B-C3B-CAB-CBB |
| 39 | A | 406 | BCR | C23-C24-C25-C26 |
| 39 | A | 410 | BCR | C23-C24-C25-C26 |
| 39 | B | 517 | BCR | C23-C24-C25-C26 |
| 39 | B | 518 | BCR | C23-C24-C25-C26 |
| 39 | B | 518 | BCR | C23-C24-C25-C30 |
| 39 | B | 525 | BCR | C23-C24-C25-C26 |
| 39 | C | 514 | BCR | C1-C6-C7-C8 |
| 39 | C | 514 | BCR | C23-C24-C25-C26 |
| 39 | C | 515 | BCR | C1-C6-C7-C8 |
| 39 | C | 515 | BCR | C5-C6-C7-C8 |
| 39 | C | 515 | BCR | C23-C24-C25-C26 |
| 39 | D | 407 | BCR | C23-C24-C25-C26 |
| 39 | K | 101 | BCR | C23-C24-C25-C26 |
| 39 | a | 408 | BCR | C23-C24-C25-C26 |
| 39 | a | 413 | BCR | C23-C24-C25-C26 |
| 39 | b | 517 | BCR | C23-C24-C25-C26 |
| 39 | b | 518 | BCR | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 39 | b | 518 | BCR | C23-C24-C25-C30 |
| 39 | b | 524 | BCR | C23-C24-C25-C26 |
| 39 | c | 514 | BCR | C1-C6-C7-C8 |
| 39 | c | 514 | BCR | C5-C6-C7-C8 |
| 39 | c | 514 | BCR | C23-C24-C25-C26 |
| 39 | c | 515 | BCR | C1-C6-C7-C8 |
| 39 | c | 515 | BCR | C5-C6-C7-C8 |
| 39 | c | 515 | BCR | C23-C24-C25-C26 |
| 39 | d | 405 | BCR | C23-C24-C25-C26 |
| 39 | y | 101 | BCR | C23-C24-C25-C26 |
| 39 | 5 | 101 | BCR | C23-C24-C25-C26 |
| 41 | 32 | 201 | LMG | C11-C10-O7-C8 |
| 41 | 12 | 201 | LMG | C31-C32-C33-C34 |
| 37 | C | 505 | CLA | C2-C1-O2A-CGA |
| 37 | c | 505 | CLA | C2-C1-O2A-CGA |
| 37 | 12 | 210 | CLA | C2-C1-O2A-CGA |
| 37 | 16 | 307 | CLA | C2-C1-O2A-CGA |
| 37 | 32 | 211 | CLA | C2-C1-O2A-CGA |
| 37 | 36 | 307 | CLA | C2-C1-O2A-CGA |
| 37 | 37 | 308 | CLA | C2-C1-O2A-CGA |
| 37 | 38 | 209 | CLA | C2-C1-O2A-CGA |
| 48 | 21 | 215 | A86 | C33-C34-O4-C38 |
| 37 | 38 | 208 | CLA | CAA-CBA-CGA-O2A |
| 43 | 21 | 217 | LHG | C28-C29-C30-C31 |
| 43 | 37 | 321 | LHG | C28-C29-C30-C31 |
| 37 | 33 | 303 | CLA | CBA-CGA-O2A-C1 |
| 41 | l | 101 | LMG | C8-C9-O8-C28 |
| 41 | B | 520 | LMG | O8-C28-C29-C30 |
| 41 | b | 519 | LMG | O8-C28-C29-C30 |
| 45 | D | 404 | PL9 | C28-C29-C31-C32 |
| 45 | d | 402 | PL9 | C28-C29-C31-C32 |
| 37 | 14 | 310 | CLA | CAA-CBA-CGA-O1A |
| 48 | 41 | 215 | A86 | C33-C34-O4-C38 |
| 41 | L | 102 | LMG | C8-C9-O8-C28 |
| 37 | 34 | 310 | CLA | CAA-CBA-CGA-O1A |
| 37 | 15 | 301 | CLA | O1A-CGA-O2A-C1 |
| 37 | 35 | 301 | CLA | O1A-CGA-O2A-C1 |
| 37 | W | 102 | CLA | CAA-CBA-CGA-O2A |
| 37 | 31 | 301 | CLA | CAA-CBA-CGA-O2A |
| 37 | 35 | 307 | CLA | CAA-CBA-CGA-O2A |
| 37 | 15 | 301 | CLA | C13-C15-C16-C17 |
| 47 | 34 | 304 | KC1 | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 15 | 307 | CLA | CAA-CBA-CGA-O2A |
| 37 | 37 | 306 | CLA | CAA-CBA-CGA-O2A |
| 50 | 41 | 212 | DD6 | C11-C10-C9-C8 |
| 47 | 14 | 304 | KC1 | C4C-C3C-CAC-CBC |
| 37 | B | 512 | CLA | CAA-CBA-CGA-O2A |
| 37 | C | 501 | CLA | CAA-CBA-CGA-O2A |
| 37 | b | 513 | CLA | CAA-CBA-CGA-O2A |
| 37 | c | 501 | CLA | CAA-CBA-CGA-O2A |
| 37 | c | 505 | CLA | CAA-CBA-CGA-O2A |
| 37 | 17 | 307 | CLA | CAA-CBA-CGA-O2A |
| 37 | 21 | 206 | CLA | CAA-CBA-CGA-O2A |
| 37 | 41 | 206 | CLA | CAA-CBA-CGA-O2A |
| 45 | D | 408 | PL9 | C18-C19-C21-C22 |
| 45 | d | 406 | PL9 | C18-C19-C21-C22 |
| 37 | B | 513 | CLA | CAA-CBA-CGA-O2A |
| 37 | C | 505 | CLA | CAA-CBA-CGA-O2A |
| 37 | b | 512 | CLA | CAA-CBA-CGA-O2A |
| 37 | 17 | 304 | CLA | O1A-CGA-O2A-C1 |
| 37 | 14 | 301 | CLA | C13-C15-C16-C17 |
| 37 | 34 | 301 | CLA | C13-C15-C16-C17 |
| 40 | 36 | 315 | SQD | C34-C35-C36-C37 |
| 37 | 21 | 210 | CLA | CAA-CBA-CGA-O1A |
| 37 | 41 | 210 | CLA | CAA-CBA-CGA-O1A |
| 37 | 12 | 204 | CLA | C11-C12-C13-C14 |
| 37 | 17 | 302 | CLA | C11-C12-C13-C14 |
| 40 | 17 | 301 | SQD | C34-C35-C36-C37 |
| 43 | d | 408 | LHG | C16-C17-C18-C19 |
| 37 | 11 | 301 | CLA | O1A-CGA-O2A-C1 |
| 37 | 12 | 209 | CLA | O1A-CGA-O2A-C1 |
| 37 | 34 | 307 | CLA | O1A-CGA-O2A-C1 |
| 41 | 17 | 317 | LMG | O1-C7-C8-C9 |
| 41 | 37 | 316 | LMG | O1-C7-C8-C9 |
| 43 | D | 410 | LHG | C4-C5-C6-O8 |
| 43 | D | 410 | LHG | C16-C17-C18-C19 |
| 37 | 12 | 209 | CLA | C1A-C2A-CAA-CBA |
| 37 | 12 | 210 | CLA | C4B-C3B-CAB-CBB |
| 37 | 13 | 310 | CLA | C4B-C3B-CAB-CBB |
| 37 | 14 | 302 | CLA | C1A-C2A-CAA-CBA |
| 37 | 14 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 14 | 307 | CLA | C1A-C2A-CAA-CBA |
| 37 | 14 | 308 | CLA | C4B-C3B-CAB-CBB |
| 37 | 16 | 307 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 17 | 304 | CLA | C4B-C3B-CAB-CBB |
| 37 | 18 | 202 | CLA | C4B-C3B-CAB-CBB |
| 37 | 19 | 302 | CLA | C4B-C3B-CAB-CBB |
| 37 | 19 | 306 | CLA | C4B-C3B-CAB-CBB |
| 37 | 20 | 307 | CLA | C1A-C2A-CAA-CBA |
| 37 | 32 | 210 | CLA | C1A-C2A-CAA-CBA |
| 37 | 32 | 211 | CLA | C4B-C3B-CAB-CBB |
| 37 | 33 | 310 | CLA | C4B-C3B-CAB-CBB |
| 37 | 34 | 302 | CLA | C1A-C2A-CAA-CBA |
| 37 | 34 | 303 | CLA | C1A-C2A-CAA-CBA |
| 37 | 34 | 307 | CLA | C1A-C2A-CAA-CBA |
| 37 | 34 | 308 | CLA | C4B-C3B-CAB-CBB |
| 37 | 36 | 307 | CLA | C4B-C3B-CAB-CBB |
| 37 | 37 | 306 | CLA | C1A-C2A-CAA-CBA |
| 37 | 38 | 202 | CLA | C4B-C3B-CAB-CBB |
| 37 | 39 | 302 | CLA | C4B-C3B-CAB-CBB |
| 37 | 39 | 306 | CLA | C4B-C3B-CAB-CBB |
| 37 | 40 | 209 | CLA | C1A-C2A-CAA-CBA |
| 48 | 12 | 202 | A86 | O-C13-C14-C15 |
| 48 | 12 | 216 | A86 | O-C13-C14-C15 |
| 48 | 13 | 314 | A86 | O-C13-C14-C15 |
| 48 | 13 | 315 | A86 | O-C13-C14-C15 |
| 48 | 15 | 314 | A86 | O-C13-C14-C15 |
| 48 | 16 | 314 | A86 | O-C13-C14-C15 |
| 48 | 17 | 312 | A86 | O-C13-C14-C15 |
| 48 | 18 | 214 | A86 | O-C13-C14-C15 |
| 48 | 19 | 313 | A86 | O-C13-C14-C15 |
| 48 | 32 | 203 | A86 | O-C13-C14-C15 |
| 48 | 32 | 217 | A86 | O-C13-C14-C15 |
| 48 | 33 | 314 | A86 | O-C13-C14-C15 |
| 48 | 33 | 315 | A86 | O-C13-C14-C15 |
| 48 | 35 | 314 | A86 | O-C13-C14-C15 |
| 48 | 36 | 313 | A86 | O-C13-C14-C15 |
| 48 | 38 | 214 | A86 | O-C13-C14-C15 |
| 48 | 39 | 313 | A86 | O-C13-C14-C15 |
| 37 | 21 | 204 | CLA | C10-C11-C12-C13 |
| 37 | B | 507 | CLA | C4-C3-C5-C6 |
| 37 | W | 101 | CLA | C4-C3-C5-C6 |
| 37 | b | 507 | CLA | C4-C3-C5-C6 |
| 37 | w | 101 | CLA | C4-C3-C5-C6 |
| 37 | 11 | 301 | CLA | C4-C3-C5-C6 |
| 37 | 31 | 302 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 41 | 204 | CLA | C10-C11-C12-C13 |
| 37 | 12 | 209 | CLA | CAA-CBA-CGA-O2A |
| 37 | 32 | 210 | CLA | CAA-CBA-CGA-O2A |
| 37 | 38 | 202 | CLA | CAA-CBA-CGA-O2A |
| 43 | 21 | 217 | LHG | O7-C7-C8-C9 |
| 48 | 12 | 202 | A86 | C2-C1-C24-C25 |
| 48 | 15 | 316 | A86 | C2-C1-C24-C25 |
| 48 | 32 | 203 | A86 | C2-C1-C24-C25 |
| 48 | 35 | 316 | A86 | C2-C1-C24-C25 |
| 48 | 17 | 314 | A86 | C24-C25-C26-C27 |
| 48 | 19 | 313 | A86 | C3-C4-C5-C6 |
| 50 | 19 | 312 | DD6 | C24-C25-C26-C27 |
| 50 | 39 | 312 | DD6 | C24-C25-C26-C27 |
| 47 | 33 | 306 | KC1 | CBD-CGD-O2D-CED |
| 37 | 31 | 301 | CLA | C16-C17-C18-C20 |
| 41 | A | 408 | LMG | C22-C23-C24-C25 |
| 41 | a | 410 | LMG | C22-C23-C24-C25 |
| 37 | 16 | 303 | CLA | CAA-CBA-CGA-O2A |
| 37 | 18 | 204 | CLA | CAA-CBA-CGA-O2A |
| 37 | 21 | 208 | CLA | CAA-CBA-CGA-O2A |
| 37 | 36 | 303 | CLA | CAA-CBA-CGA-O2A |
| 37 | 40 | 203 | CLA | CAA-CBA-CGA-O2A |
| 37 | 41 | 208 | CLA | CAA-CBA-CGA-O2A |
| 41 | B | 521 | LMG | O8-C28-C29-C30 |
| 41 | C | 518 | LMG | O7-C10-C11-C12 |
| 41 | b | 520 | LMG | O8-C28-C29-C30 |
| 41 | c | 518 | LMG | O7-C10-C11-C12 |
| 43 | 37 | 321 | LHG | O7-C7-C8-C9 |
| 37 | C | 501 | CLA | C2A-CAA-CBA-CGA |
| 37 | c | 501 | CLA | C2A-CAA-CBA-CGA |
| 37 | B | 502 | CLA | C8-C10-C11-C12 |
| 37 | 14 | 307 | CLA | O1A-CGA-O2A-C1 |
| 37 | 31 | 302 | CLA | O1A-CGA-O2A-C1 |
| 37 | 32 | 210 | CLA | O1A-CGA-O2A-C1 |
| 43 | 39 | 314 | LHG | C29-C30-C31-C32 |
| 37 | W | 102 | CLA | C16-C17-C18-C20 |
| 37 | d | 403 | CLA | CAA-CBA-CGA-O2A |
| 37 | 18 | 202 | CLA | CAA-CBA-CGA-O2A |
| 37 | 20 | 301 | CLA | CAA-CBA-CGA-O2A |
| 37 | 21 | 202 | CLA | CAA-CBA-CGA-O2A |
| 37 | b | 502 | CLA | C8-C10-C11-C12 |
| 41 | L | 102 | LMG | C4-C5-C6-O5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 40 | A | 407 | SQD | C5-C6-S-O9 |
| 40 | a | 409 | SQD | C5-C6-S-O9 |
| 37 | 15 | 301 | CLA | C8-C10-C11-C12 |
| 37 | B | 516 | CLA | C2-C1-O2A-CGA |
| 37 | C | 502 | CLA | C2-C1-O2A-CGA |
| 37 | C | 503 | CLA | C2-C1-O2A-CGA |
| 37 | D | 406 | CLA | C2-C1-O2A-CGA |
| 37 | b | 516 | CLA | C2-C1-O2A-CGA |
| 37 | c | 502 | CLA | C2-C1-O2A-CGA |
| 37 | c | 503 | CLA | C2-C1-O2A-CGA |
| 37 | d | 404 | CLA | C2-C1-O2A-CGA |
| 37 | 17 | 309 | CLA | C2-C1-O2A-CGA |
| 37 | 35 | 308 | CLA | C2-C1-O2A-CGA |
| 37 | B | 514 | CLA | CAA-CBA-CGA-O2A |
| 37 | D | 405 | CLA | CAA-CBA-CGA-O2A |
| 37 | b | 514 | CLA | CAA-CBA-CGA-O2A |
| 37 | 15 | 301 | CLA | CAA-CBA-CGA-O2A |
| 37 | 35 | 301 | CLA | CAA-CBA-CGA-O2A |
| 37 | 41 | 202 | CLA | CAA-CBA-CGA-O2A |
| 43 | B | 523 | LHG | C11-C10-C9-C8 |
| 41 | l | 101 | LMG | C4-C5-C6-O5 |
| 37 | 16 | 307 | CLA | C11-C10-C8-C7 |
| 37 | 19 | 302 | CLA | C12-C13-C15-C16 |
| 37 | 36 | 307 | CLA | C11-C10-C8-C7 |
| 37 | 39 | 302 | CLA | C12-C13-C15-C16 |
| 37 | 15 | 301 | CLA | CBA-CGA-O2A-C1 |
| 37 | 35 | 301 | CLA | CBA-CGA-O2A-C1 |
| 37 | 16 | 306 | CLA | C10-C11-C12-C13 |
| 37 | 31 | 304 | CLA | O1A-CGA-O2A-C1 |
| 37 | 37 | 303 | CLA | O1A-CGA-O2A-C1 |
| 37 | C | 512 | CLA | C16-C17-C18-C20 |
| 37 | c | 512 | CLA | C16-C17-C18-C20 |
| 43 | D | 410 | LHG | C17-C18-C19-C20 |
| 37 | 36 | 306 | CLA | C10-C11-C12-C13 |
| 43 | b | 522 | LHG | C11-C10-C9-C8 |
| 47 | 13 | 306 | KC1 | CBD-CGD-O2D-CED |
| 40 | 17 | 301 | SQD | O47-C7-C8-C9 |
| 40 | 36 | 315 | SQD | O47-C7-C8-C9 |
| 37 | 15 | 303 | CLA | C5-C6-C7-C8 |
| 37 | 35 | 303 | CLA | C5-C6-C7-C8 |
| 37 | 41 | 204 | CLA | C3-C5-C6-C7 |
| 41 | A | 408 | LMG | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 41 | 36 | 314 | LMG | C14-C15-C16-C17 |
| 43 | d | 408 | LHG | C17-C18-C19-C20 |
| 41 | C | 518 | LMG | O9-C10-C11-C12 |
| 41 | c | 518 | LMG | O9-C10-C11-C12 |
| 48 | 15 | 312 | A86 | C11-C10-C9-C8 |
| 41 | 16 | 316 | LMG | C14-C15-C16-C17 |
| 37 | B | 505 | CLA | C2A-CAA-CBA-CGA |
| 37 | b | 505 | CLA | C2A-CAA-CBA-CGA |
| 37 | 11 | 303 | CLA | O1A-CGA-O2A-C1 |
| 37 | 14 | 305 | CLA | CAA-CBA-CGA-O2A |
| 37 | 34 | 305 | CLA | CAA-CBA-CGA-O2A |
| 41 | a | 410 | LMG | C31-C32-C33-C34 |
| 37 | 20 | 306 | CLA | CAA-CBA-CGA-O2A |
| 37 | 38 | 204 | CLA | CAA-CBA-CGA-O2A |
| 37 | C | 508 | CLA | O1A-CGA-O2A-C1 |
| 37 | c | 508 | CLA | O1A-CGA-O2A-C1 |
| 37 | Z | 102 | CLA | C3A-C2A-CAA-CBA |
| 37 | z | 102 | CLA | C3A-C2A-CAA-CBA |
| 37 | 14 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 34 | 303 | CLA | C3A-C2A-CAA-CBA |
| 37 | 35 | 301 | CLA | C8-C10-C11-C12 |
| 37 | 40 | 208 | CLA | CAA-CBA-CGA-O2A |
| 37 | 11 | 303 | CLA | C2-C3-C5-C6 |
| 37 | 31 | 304 | CLA | C2-C3-C5-C6 |
| 39 | B | 525 | BCR | C12-C13-C14-C15 |
| 37 | D | 405 | CLA | CAA-CBA-CGA-O1A |
| 37 | W | 102 | CLA | CAA-CBA-CGA-O1A |
| 37 | 12 | 209 | CLA | CAA-CBA-CGA-O1A |
| 37 | 34 | 302 | CLA | O1A-CGA-O2A-C1 |
| 43 | d | 407 | LHG | C15-C16-C17-C18 |
| 45 | D | 408 | PL9 | C2-C3-C7-C8 |
| 45 | d | 406 | PL9 | C2-C3-C7-C8 |
| 43 | D | 409 | LHG | C15-C16-C17-C18 |
| 37 | 14 | 302 | CLA | O1A-CGA-O2A-C1 |
| 37 | 31 | 301 | CLA | CAA-CBA-CGA-O1A |
| 38 | a | 405 | PHO | C16-C17-C18-C19 |
| 37 | 21 | 204 | CLA | C3-C5-C6-C7 |
| 43 | 17 | 316 | LHG | C19-C20-C21-C22 |
| 37 | C | 508 | CLA | CBA-CGA-O2A-C1 |
| 37 | C | 503 | CLA | C11-C12-C13-C14 |
| 37 | c | 503 | CLA | C11-C12-C13-C14 |
| 37 | 12 | 204 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 32 | 205 | CLA | C6-C7-C8-C9 |
| 37 | 32 | 205 | CLA | C11-C12-C13-C14 |
| 37 | 32 | 210 | CLA | CAA-CBA-CGA-O1A |
| 44 | C | 517 | DGD | CCB-CDB-CEB-CFB |
| 44 | c | 517 | DGD | CCB-CDB-CEB-CFB |
| 48 | 35 | 312 | A86 | C11-C10-C9-C8 |
| 37 | d | 404 | CLA | C5-C6-C7-C8 |
| 37 | 14 | 308 | CLA | C5-C6-C7-C8 |
| 37 | 34 | 308 | CLA | C5-C6-C7-C8 |
| 37 | B | 508 | CLA | C4-C3-C5-C6 |
| 37 | D | 402 | CLA | C4-C3-C5-C6 |
| 37 | b | 508 | CLA | C4-C3-C5-C6 |
| 37 | d | 401 | CLA | C4-C3-C5-C6 |
| 37 | d | 403 | CLA | CAA-CBA-CGA-O1A |
| 37 | 17 | 307 | CLA | CAA-CBA-CGA-O1A |
| 37 | 38 | 208 | CLA | CAA-CBA-CGA-O1A |
| 37 | 41 | 206 | CLA | CAA-CBA-CGA-O1A |
| 43 | 19 | 314 | LHG | C29-C30-C31-C32 |
| 37 | c | 508 | CLA | CBA-CGA-O2A-C1 |
| 43 | 37 | 315 | LHG | C19-C20-C21-C22 |
| 47 | 11 | 306 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 13 | 304 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 13 | 306 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 17 | 306 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 18 | 207 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 19 | 308 | KC1 | C3A-C2A-CAA-CBA |
| 47 | 31 | 307 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 33 | 304 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 33 | 306 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 37 | 305 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 38 | 207 | KC1 | C1A-C2A-CAA-CBA |
| 47 | 39 | 308 | KC1 | C3A-C2A-CAA-CBA |
| 48 | 31 | 313 | A86 | C26-C27-C29-C30 |
| 37 | 14 | 307 | CLA | CAA-CBA-CGA-O1A |
| 37 | 15 | 307 | CLA | CAA-CBA-CGA-O1A |
| 37 | 21 | 206 | CLA | CAA-CBA-CGA-O1A |
| 37 | 34 | 307 | CLA | CAA-CBA-CGA-O1A |
| 37 | 37 | 306 | CLA | CAA-CBA-CGA-O1A |
| 40 | a | 409 | SQD | O49-C7-C8-C9 |
| 37 | B | 503 | CLA | C13-C15-C16-C17 |
| 37 | b | 503 | CLA | C13-C15-C16-C17 |
| 37 | Z | 101 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | z | 101 | CLA | CAA-CBA-CGA-O2A |
| 37 | D | 406 | CLA | C5-C6-C7-C8 |
| 37 | 14 | 302 | CLA | CBD-CGD-O2D-CED |
| 37 | 34 | 302 | CLA | CBD-CGD-O2D-CED |
| 37 | b | 513 | CLA | CAA-CBA-CGA-O1A |
| 43 | 21 | 217 | LHG | O9-C7-C8-C9 |
| 41 | L | 102 | LMG | C8-C7-O1-C1 |
| 41 | l | 101 | LMG | C8-C7-O1-C1 |
| 41 | 12 | 201 | LMG | C8-C7-O1-C1 |
| 41 | 32 | 201 | LMG | C8-C7-O1-C1 |
| 43 | 19 | 314 | LHG | O9-C7-O7-C5 |
| 43 | 39 | 314 | LHG | O9-C7-O7-C5 |
| 37 | B | 512 | CLA | CAA-CBA-CGA-O1A |
| 37 | B | 513 | CLA | CAA-CBA-CGA-O1A |
| 37 | b | 512 | CLA | CAA-CBA-CGA-O1A |
| 37 | c | 505 | CLA | CAA-CBA-CGA-O1A |
| 37 | 38 | 202 | CLA | CAA-CBA-CGA-O1A |
| 40 | A | 407 | SQD | O49-C7-C8-C9 |
| 43 | 17 | 316 | LHG | O9-C7-C8-C9 |
| 43 | 37 | 315 | LHG | O9-C7-C8-C9 |
| 43 | 37 | 321 | LHG | O9-C7-C8-C9 |
| 37 | Z | 101 | CLA | C2A-CAA-CBA-CGA |
| 37 | z | 101 | CLA | C2A-CAA-CBA-CGA |
| 44 | c | 517 | DGD | C9A-CAA-CBA-CCA |
| 48 | 12 | 217 | A86 | C12-C11-C13-O |
| 48 | 19 | 313 | A86 | C12-C11-C13-O |
| 48 | 32 | 218 | A86 | C12-C11-C13-O |
| 48 | 39 | 313 | A86 | C12-C11-C13-O |
| 37 | C | 505 | CLA | CAA-CBA-CGA-O1A |
| 37 | 18 | 208 | CLA | CAA-CBA-CGA-O1A |
| 37 | 20 | 301 | CLA | CAA-CBA-CGA-O1A |
| 37 | 21 | 202 | CLA | CAA-CBA-CGA-O1A |
| 37 | 40 | 203 | CLA | CAA-CBA-CGA-O1A |
| 37 | 41 | 202 | CLA | CAA-CBA-CGA-O1A |
| 40 | B | 522 | SQD | O10-C23-C24-C25 |
| 40 | b | 521 | SQD | O10-C23-C24-C25 |
| 37 | a | 404 | CLA | C4C-C3C-CAC-CBC |
| 37 | B | 505 | CLA | C8-C10-C11-C12 |
| 37 | b | 505 | CLA | C8-C10-C11-C12 |
| 37 | 32 | 206 | CLA | CAA-CBA-CGA-O2A |
| 47 | 32 | 207 | KC1 | C2B-C3B-CAB-CBB |
| 37 | c | 501 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 35 | 307 | CLA | CAA-CBA-CGA-O1A |
| 37 | D | 401 | CLA | C4C-C3C-CAC-CBC |
| 44 | C | 517 | DGD | C9A-CAA-CBA-CCA |
| 37 | B | 509 | CLA | CAD-CBD-CGD-O2D |
| 37 | C | 513 | CLA | CAD-CBD-CGD-O2D |
| 37 | b | 509 | CLA | CAD-CBD-CGD-O2D |
| 37 | c | 513 | CLA | CAD-CBD-CGD-O2D |
| 37 | 19 | 304 | CLA | CAD-CBD-CGD-O2D |
| 37 | 35 | 303 | CLA | CAD-CBD-CGD-O2D |
| 37 | 39 | 304 | CLA | CAD-CBD-CGD-O2D |
| 47 | 12 | 211 | KC1 | CAD-CBD-CGD-O2D |
| 47 | 14 | 306 | KC1 | CAD-CBD-CGD-O2D |
| 47 | 32 | 212 | KC1 | CAD-CBD-CGD-O2D |
| 47 | 34 | 306 | KC1 | CAD-CBD-CGD-O2D |
| 37 | 12 | 205 | CLA | CAA-CBA-CGA-O2A |
| 40 | 16 | 315 | SQD | O47-C7-C8-C9 |
| 40 | 40 | 202 | SQD | O47-C7-C8-C9 |
| 37 | 39 | 309 | CLA | CAA-CBA-CGA-O2A |
| 37 | C | 501 | CLA | CAA-CBA-CGA-O1A |
| 37 | 18 | 202 | CLA | CAA-CBA-CGA-O1A |
| 37 | 21 | 208 | CLA | CAA-CBA-CGA-O1A |
| 41 | B | 521 | LMG | O10-C28-C29-C30 |
| 41 | D | 412 | LMG | O9-C10-C11-C12 |
| 41 | b | 520 | LMG | O10-C28-C29-C30 |
| 37 | 18 | 204 | CLA | O1A-CGA-O2A-C1 |
| 37 | 12 | 203 | CLA | C2-C1-O2A-CGA |
| 37 | 32 | 204 | CLA | C2-C1-O2A-CGA |
| 37 | 39 | 309 | CLA | CAA-CBA-CGA-O1A |
| 37 | 41 | 208 | CLA | CAA-CBA-CGA-O1A |
| 41 | d | 409 | LMG | O9-C10-C11-C12 |
| 37 | 21 | 204 | CLA | CAA-CBA-CGA-O2A |
| 37 | 41 | 204 | CLA | CAA-CBA-CGA-O2A |
| 38 | D | 403 | PHO | C16-C17-C18-C19 |
| 41 | B | 521 | LMG | C32-C33-C34-C35 |
| 41 | b | 520 | LMG | C32-C33-C34-C35 |
| 47 | 37 | 305 | KC1 | C4C-C3C-CAC-CBC |
| 38 | D | 403 | PHO | C3-C5-C6-C7 |
| 38 | a | 405 | PHO | C3-C5-C6-C7 |
| 43 | D | 411 | LHG | C32-C33-C34-C35 |
| 37 | 16 | 303 | CLA | CAA-CBA-CGA-O1A |
| 37 | c | 510 | CLA | CAA-CBA-CGA-O2A |
| 37 | 11 | 303 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 37 | 20 | 303 | CLA | CAA-CBA-CGA-O2A |
| 37 | 31 | 304 | CLA | CAA-CBA-CGA-O2A |
| 37 | 33 | 303 | CLA | CAA-CBA-CGA-O2A |
| 37 | 40 | 205 | CLA | CAA-CBA-CGA-O2A |
| 43 | a | 412 | LHG | C32-C33-C34-C35 |
| 43 | 21 | 217 | LHG | C35-C36-C37-C38 |
| 37 | 12 | 210 | CLA | C5-C6-C7-C8 |
| 37 | 19 | 309 | CLA | CAA-CBA-CGA-O1A |
| 37 | 19 | 309 | CLA | CAA-CBA-CGA-O2A |
| 37 | B | 501 | CLA | C16-C17-C18-C19 |
| 37 | 36 | 303 | CLA | CAA-CBA-CGA-O1A |
| 48 | 37 | 313 | A86 | C39-C38-O4-C34 |
| 37 | 32 | 211 | CLA | C5-C6-C7-C8 |
| 43 | 37 | 321 | LHG | C35-C36-C37-C38 |
| 37 | C | 510 | CLA | CAA-CBA-CGA-O2A |
| 37 | 17 | 304 | CLA | CAA-CBA-CGA-O2A |
| 37 | 35 | 303 | CLA | CAA-CBA-CGA-O2A |
| 37 | 37 | 303 | CLA | CAA-CBA-CGA-O2A |
| 37 | 15 | 301 | CLA | CAA-CBA-CGA-O1A |
| 37 | 18 | 204 | CLA | CAA-CBA-CGA-O1A |
| 37 | 35 | 301 | CLA | CAA-CBA-CGA-O1A |
| 41 | B | 520 | LMG | O10-C28-C29-C30 |
| 41 | b | 519 | LMG | O10-C28-C29-C30 |

All (2) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 48 | 31 | 313 | A86 | C31-C32-C33-C34-C35-C36 |
| 48 | 11 | 313 | A86 | C31-C32-C33-C34-C35-C36 |

281 monomers are involved in 580 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 37 | 19 | 306 | CLA | 1 | 0 |
| 37 | c | 508 | CLA | 1 | 0 |
| 47 | 20 | 302 | KC1 | 1 | 0 |
| 37 | C | 512 | CLA | 4 | 0 |
| 37 | b | 511 | CLA | 1 | 0 |
| 47 | 38 | 205 | KC1 | 2 | 0 |
| 37 | b | 514 | CLA | 3 | 0 |
| 37 | 17 | 302 | CLA | 3 | 0 |
| 37 | b | 504 | CLA | 5 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 37 | 32 | 210 | CLA | 1 | 0 |
| 37 | 15 | 307 | CLA | 1 | 0 |
| 39 | C | 514 | BCR | 2 | 0 |
| 37 | B | 513 | CLA | 2 | 0 |
| 37 | 12 | 205 | CLA | 3 | 0 |
| 37 | 35 | 307 | CLA | 1 | 0 |
| 37 | 41 | 202 | CLA | 2 | 0 |
| 37 | 11 | 301 | CLA | 1 | 0 |
| 37 | 11 | 308 | CLA | 5 | 0 |
| 37 | 37 | 306 | CLA | 1 | 0 |
| 47 | 17 | 303 | KC1 | 2 | 0 |
| 37 | 14 | 301 | CLA | 2 | 0 |
| 37 | C | 503 | CLA | 3 | 0 |
| 41 | d | 409 | LMG | 2 | 0 |
| 37 | c | 513 | CLA | 2 | 0 |
| 37 | c | 511 | CLA | 5 | 0 |
| 37 | b | 503 | CLA | 3 | 0 |
| 39 | b | 518 | BCR | 2 | 0 |
| 44 | J | 101 | DGD | 1 | 0 |
| 48 | 18 | 212 | A86 | 1 | 0 |
| 37 | c | 512 | CLA | 3 | 0 |
| 37 | 19 | 307 | CLA | 2 | 0 |
| 39 | c | 515 | BCR | 2 | 0 |
| 39 | D | 407 | BCR | 4 | 0 |
| 37 | 17 | 309 | CLA | 4 | 0 |
| 40 | 16 | 315 | SQD | 1 | 0 |
| 37 | w | 101 | CLA | 1 | 0 |
| 48 | 34 | 315 | A86 | 1 | 0 |
| 37 | 36 | 301 | CLA | 4 | 0 |
| 37 | 14 | 302 | CLA | 3 | 0 |
| 37 | 34 | 308 | CLA | 1 | 0 |
| 44 | c | 516 | DGD | 4 | 0 |
| 41 | C | 518 | LMG | 1 | 0 |
| 37 | Z | 102 | CLA | 2 | 0 |
| 37 | z | 101 | CLA | 2 | 0 |
| 39 | H | 101 | BCR | 2 | 0 |
| 37 | z | 102 | CLA | 1 | 0 |
| 37 | 32 | 206 | CLA | 3 | 0 |
| 37 | C | 511 | CLA | 4 | 0 |
| 37 | 33 | 310 | CLA | 1 | 0 |
| 41 | b | 519 | LMG | 4 | 0 |
| 37 | 18 | 208 | CLA | 4 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 37 | 21 | 206 | CLA | 5 | 0 |
| 39 | C | 515 | BCR | 2 | 0 |
| 40 | 40 | 202 | SQD | 2 | 0 |
| 37 | c | 510 | CLA | 4 | 0 |
| 37 | 31 | 302 | CLA | 1 | 0 |
| 40 | b | 521 | SQD | 1 | 0 |
| 46 | F | 101 | HEM | 2 | 0 |
| 39 | h | 101 | BCR | 1 | 0 |
| 45 | D | 408 | PL9 | 1 | 0 |
| 37 | 12 | 212 | CLA | 1 | 0 |
| 37 | 15 | 308 | CLA | 2 | 0 |
| 37 | 33 | 307 | CLA | 1 | 0 |
| 42 | A | 409 | BCT | 1 | 0 |
| 37 | 35 | 301 | CLA | 4 | 0 |
| 48 | 34 | 314 | A86 | 1 | 0 |
| 37 | 21 | 208 | CLA | 1 | 0 |
| 43 | 39 | 314 | LHG | 8 | 0 |
| 37 | 32 | 211 | CLA | 2 | 0 |
| 39 | y | 101 | BCR | 4 | 0 |
| 37 | c | 504 | CLA | 3 | 0 |
| 37 | 38 | 201 | CLA | 4 | 0 |
| 37 | B | 509 | CLA | 2 | 0 |
| 37 | C | 508 | CLA | 2 | 0 |
| 37 | 38 | 208 | CLA | 3 | 0 |
| 37 | B | 503 | CLA | 2 | 0 |
| 37 | C | 510 | CLA | 4 | 0 |
| 44 | C | 516 | DGD | 4 | 0 |
| 37 | 13 | 310 | CLA | 2 | 0 |
| 37 | c | 503 | CLA | 4 | 0 |
| 43 | 19 | 314 | LHG | 10 | 0 |
| 37 | B | 524 | CLA | 3 | 0 |
| 39 | B | 517 | BCR | 3 | 0 |
| 37 | b | 509 | CLA | 2 | 0 |
| 37 | 34 | 301 | CLA | 2 | 0 |
| 38 | A | 404 | PHO | 2 | 0 |
| 37 | Z | 101 | CLA | 3 | 0 |
| 37 | 41 | 209 | CLA | 1 | 0 |
| 43 | 37 | 315 | LHG | 1 | 0 |
| 39 | b | 524 | BCR | 2 | 0 |
| 43 | D | 410 | LHG | 2 | 0 |
| 41 | L | 102 | LMG | 2 | 0 |
| 40 | B | 519 | SQD | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 37 | C | 504 | CLA | 2 | 0 |
| 37 | 14 | 303 | CLA | 1 | 0 |
| 43 | D | 411 | LHG | 3 | 0 |
| 37 | 34 | 303 | CLA | 1 | 0 |
| 37 | 12 | 203 | CLA | 2 | 0 |
| 37 | c | 506 | CLA | 2 | 0 |
| 37 | 12 | 204 | CLA | 2 | 0 |
| 37 | 16 | 307 | CLA | 3 | 0 |
| 37 | B | 511 | CLA | 1 | 0 |
| 38 | D | 403 | PHO | 1 | 0 |
| 50 | 20 | 312 | DD6 | 1 | 0 |
| 37 | d | 403 | CLA | 4 | 0 |
| 48 | 15 | 311 | A86 | 1 | 0 |
| 37 | 19 | 305 | CLA | 2 | 0 |
| 37 | C | 501 | CLA | 3 | 0 |
| 47 | 11 | 306 | KC1 | 4 | 0 |
| 37 | D | 405 | CLA | 4 | 0 |
| 37 | 18 | 202 | CLA | 2 | 0 |
| 37 | 14 | 307 | CLA | 1 | 0 |
| 37 | 33 | 308 | CLA | 4 | 0 |
| 39 | B | 525 | BCR | 2 | 0 |
| 48 | 11 | 313 | A86 | 9 | 0 |
| 37 | b | 515 | CLA | 1 | 0 |
| 37 | b | 505 | CLA | 3 | 0 |
| 37 | 15 | 303 | CLA | 1 | 0 |
| 37 | 19 | 301 | CLA | 1 | 0 |
| 37 | C | 506 | CLA | 2 | 0 |
| 37 | C | 509 | CLA | 1 | 0 |
| 37 | 39 | 310 | CLA | 5 | 0 |
| 37 | 36 | 309 | CLA | 1 | 0 |
| 48 | 13 | 311 | A86 | 1 | 0 |
| 46 | v | 201 | HEM | 2 | 0 |
| 37 | 21 | 202 | CLA | 2 | 0 |
| 47 | 33 | 302 | KC1 | 1 | 0 |
| 37 | B | 501 | CLA | 1 | 0 |
| 37 | 32 | 204 | CLA | 3 | 0 |
| 37 | 37 | 308 | CLA | 1 | 0 |
| 37 | 19 | 303 | CLA | 1 | 0 |
| 37 | 31 | 308 | CLA | 3 | 0 |
| 37 | 17 | 307 | CLA | 1 | 0 |
| 37 | B | 512 | CLA | 3 | 0 |
| 37 | c | 502 | CLA | 5 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 47 | 40 | 204 | KC1 | 1 | 0 |
| 37 | 20 | 306 | CLA | 1 | 0 |
| 50 | 40 | 214 | DD6 | 1 | 0 |
| 43 | 21 | 217 | LHG | 3 | 0 |
| 37 | 19 | 302 | CLA | 3 | 0 |
| 37 | c | 509 | CLA | 1 | 0 |
| 37 | b | 506 | CLA | 3 | 0 |
| 46 | f | 101 | HEM | 2 | 0 |
| 48 | 35 | 311 | A86 | 1 | 0 |
| 37 | B | 514 | CLA | 3 | 0 |
| 37 | 11 | 307 | CLA | 4 | 0 |
| 37 | 40 | 205 | CLA | 1 | 0 |
| 37 | b | 508 | CLA | 1 | 0 |
| 37 | 34 | 302 | CLA | 3 | 0 |
| 37 | 32 | 205 | CLA | 2 | 0 |
| 39 | 5 | 101 | BCR | 3 | 0 |
| 37 | 13 | 307 | CLA | 1 | 0 |
| 41 | 16 | 316 | LMG | 1 | 0 |
| 37 | 19 | 304 | CLA | 2 | 0 |
| 37 | 14 | 308 | CLA | 1 | 0 |
| 48 | 31 | 311 | A86 | 2 | 0 |
| 37 | 39 | 303 | CLA | 1 | 0 |
| 37 | 13 | 308 | CLA | 4 | 0 |
| 37 | 32 | 202 | CLA | 4 | 0 |
| 45 | D | 404 | PL9 | 4 | 0 |
| 37 | C | 513 | CLA | 2 | 0 |
| 37 | 40 | 203 | CLA | 1 | 0 |
| 41 | l | 101 | LMG | 1 | 0 |
| 48 | 11 | 319 | A86 | 1 | 0 |
| 37 | W | 101 | CLA | 3 | 0 |
| 40 | 17 | 301 | SQD | 3 | 0 |
| 37 | 18 | 211 | CLA | 1 | 0 |
| 37 | 31 | 301 | CLA | 2 | 0 |
| 37 | b | 502 | CLA | 7 | 0 |
| 37 | W | 102 | CLA | 2 | 0 |
| 43 | 37 | 321 | LHG | 3 | 0 |
| 37 | B | 505 | CLA | 2 | 0 |
| 47 | 31 | 309 | KC1 | 1 | 0 |
| 47 | 40 | 206 | KC1 | 1 | 0 |
| 44 | h | 102 | DGD | 3 | 0 |
| 37 | 12 | 210 | CLA | 2 | 0 |
| 37 | 41 | 206 | CLA | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 37 | 31 | 304 | CLA | 1 | 0 |
| 37 | 21 | 209 | CLA | 1 | 0 |
| 48 | 14 | 315 | A86 | 1 | 0 |
| 48 | 31 | 319 | A86 | 1 | 0 |
| 37 | 39 | 306 | CLA | 1 | 0 |
| 43 | a | 412 | LHG | 3 | 0 |
| 37 | B | 508 | CLA | 2 | 0 |
| 37 | c | 505 | CLA | 2 | 0 |
| 43 | d | 407 | LHG | 1 | 0 |
| 37 | B | 504 | CLA | 5 | 0 |
| 48 | 14 | 311 | A86 | 1 | 0 |
| 37 | A | 405 | CLA | 6 | 0 |
| 40 | L | 101 | SQD | 3 | 0 |
| 41 | a | 410 | LMG | 4 | 0 |
| 37 | 16 | 301 | CLA | 4 | 0 |
| 37 | 36 | 307 | CLA | 4 | 0 |
| 41 | c | 518 | LMG | 3 | 0 |
| 45 | d | 406 | PL9 | 3 | 0 |
| 48 | 31 | 313 | A86 | 11 | 0 |
| 37 | B | 506 | CLA | 3 | 0 |
| 37 | 18 | 209 | CLA | 1 | 0 |
| 38 | a | 405 | PHO | 2 | 0 |
| 47 | 37 | 302 | KC1 | 2 | 0 |
| 43 | D | 409 | LHG | 1 | 0 |
| 37 | 20 | 301 | CLA | 1 | 0 |
| 39 | b | 517 | BCR | 4 | 0 |
| 38 | a | 406 | PHO | 1 | 0 |
| 48 | 38 | 212 | A86 | 1 | 0 |
| 43 | 17 | 316 | LHG | 1 | 0 |
| 37 | 19 | 310 | CLA | 5 | 0 |
| 40 | A | 407 | SQD | 1 | 0 |
| 39 | A | 410 | BCR | 2 | 0 |
| 50 | 39 | 312 | DD6 | 2 | 0 |
| 37 | 12 | 207 | CLA | 1 | 0 |
| 45 | d | 402 | PL9 | 2 | 0 |
| 44 | j | 101 | DGD | 2 | 0 |
| 37 | c | 501 | CLA | 4 | 0 |
| 37 | 15 | 301 | CLA | 5 | 0 |
| 37 | b | 507 | CLA | 2 | 0 |
| 37 | a | 407 | CLA | 6 | 0 |
| 37 | A | 403 | CLA | 4 | 0 |
| 37 | D | 401 | CLA | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 37 | 41 | 208 | CLA | 1 | 0 |
| 46 | V | 201 | HEM | 2 | 0 |
| 39 | A | 406 | BCR | 4 | 0 |
| 48 | 14 | 314 | A86 | 1 | 0 |
| 37 | B | 502 | CLA | 4 | 0 |
| 37 | b | 512 | CLA | 3 | 0 |
| 41 | b | 520 | LMG | 4 | 0 |
| 37 | a | 404 | CLA | 2 | 0 |
| 37 | 11 | 303 | CLA | 1 | 0 |
| 41 | B | 521 | LMG | 4 | 0 |
| 40 | 36 | 315 | SQD | 3 | 0 |
| 48 | 33 | 311 | A86 | 1 | 0 |
| 48 | 34 | 311 | A86 | 1 | 0 |
| 47 | 16 | 304 | KC1 | 1 | 0 |
| 47 | 18 | 205 | KC1 | 1 | 0 |
| 37 | 39 | 305 | CLA | 2 | 0 |
| 37 | 39 | 307 | CLA | 3 | 0 |
| 37 | 38 | 211 | CLA | 1 | 0 |
| 37 | B | 515 | CLA | 1 | 0 |
| 37 | 39 | 301 | CLA | 2 | 0 |
| 37 | b | 513 | CLA | 2 | 0 |
| 37 | 38 | 203 | CLA | 2 | 0 |
| 37 | C | 505 | CLA | 1 | 0 |
| 37 | B | 516 | CLA | 2 | 0 |
| 44 | H | 102 | DGD | 2 | 0 |
| 37 | D | 406 | CLA | 2 | 0 |
| 50 | 19 | 312 | DD6 | 2 | 0 |
| 39 | B | 518 | BCR | 2 | 0 |
| 37 | 18 | 203 | CLA | 3 | 0 |
| 39 | d | 405 | BCR | 3 | 0 |
| 48 | 11 | 311 | A86 | 1 | 0 |
| 47 | 20 | 304 | KC1 | 1 | 0 |
| 40 | B | 522 | SQD | 2 | 0 |
| 37 | 35 | 308 | CLA | 6 | 0 |
| 37 | 40 | 208 | CLA | 1 | 0 |
| 37 | 18 | 201 | CLA | 6 | 0 |
| 37 | b | 516 | CLA | 1 | 0 |
| 41 | B | 520 | LMG | 3 | 0 |
| 43 | d | 408 | LHG | 2 | 0 |
| 41 | D | 412 | LMG | 2 | 0 |
| 39 | C | 519 | BCR | 1 | 0 |
| 41 | A | 408 | LMG | 4 | 0 |

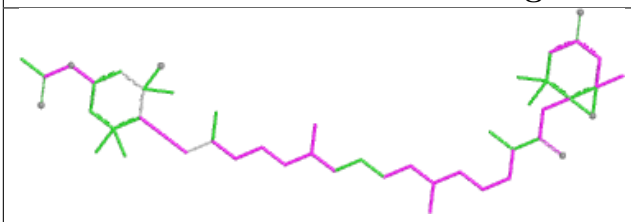
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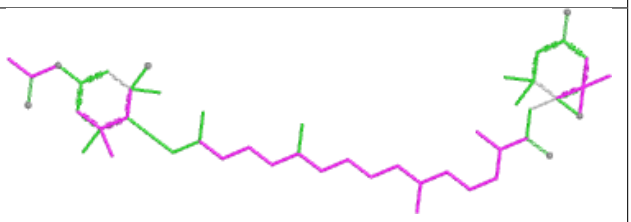
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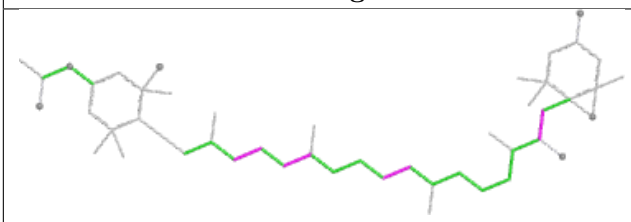
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 48 | 39 | 313 | A86 | 1 | 0 |
| 37 | b | 523 | CLA | 4 | 0 |
| 39 | c | 514 | BCR | 2 | 0 |
| 37 | 37 | 301 | CLA | 2 | 0 |
| 37 | 34 | 307 | CLA | 1 | 0 |
| 47 | 36 | 304 | KC1 | 1 | 0 |
| 37 | b | 501 | CLA | 3 | 0 |
| 37 | B | 507 | CLA | 2 | 0 |
| 37 | a | 403 | CLA | 6 | 0 |
| 42 | a | 411 | BCT | 1 | 0 |
| 37 | d | 404 | CLA | 1 | 0 |
| 37 | 16 | 309 | CLA | 1 | 0 |
| 37 | 32 | 213 | CLA | 1 | 0 |
| 39 | K | 101 | BCR | 4 | 0 |
| 37 | 39 | 302 | CLA | 3 | 0 |
| 37 | C | 502 | CLA | 4 | 0 |
| 39 | a | 408 | BCR | 5 | 0 |
| 37 | 36 | 306 | CLA | 2 | 0 |
| 37 | 35 | 310 | CLA | 1 | 0 |
| 39 | 0 | 101 | BCR | 5 | 0 |

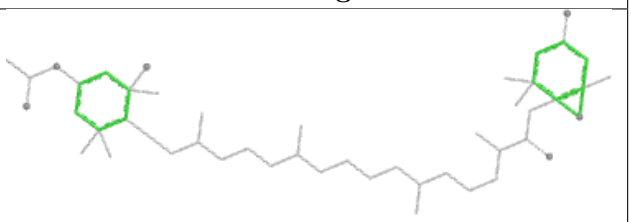
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight $> 250$ and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand A86 41 214

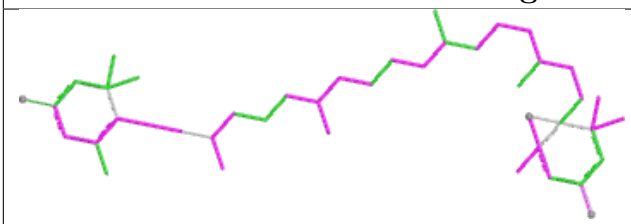

Bond lengths

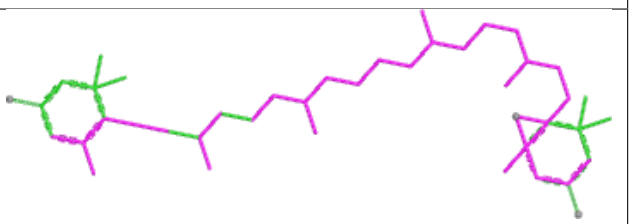

Bond angles

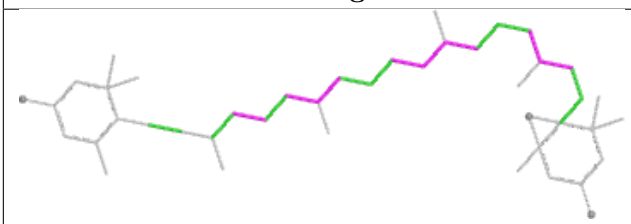

Torsions

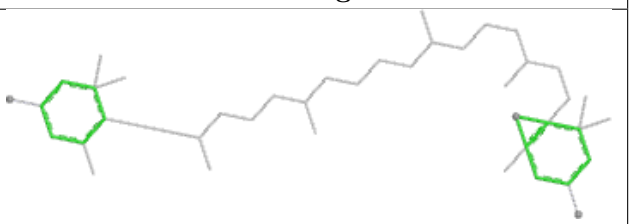

Rings

## Ligand DD6 16 312

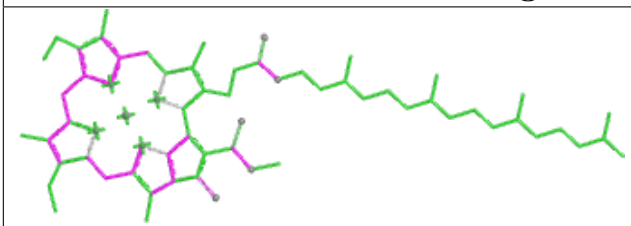

Bond lengths

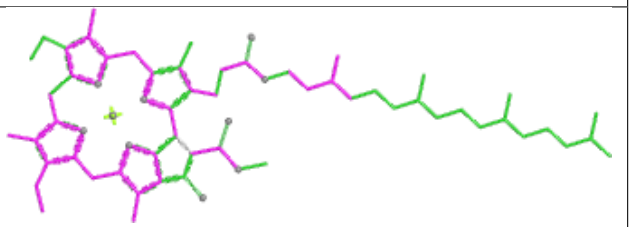

Bond angles

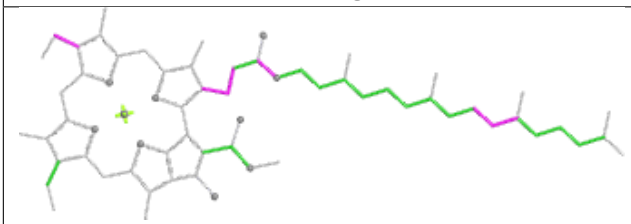

Torsions

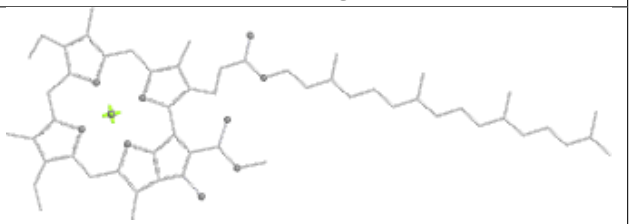

Rings

## Ligand CLA 19 306

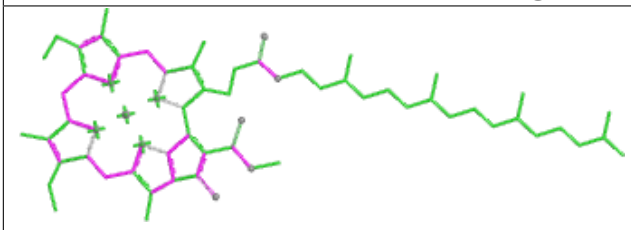

Bond lengths


Bond angles

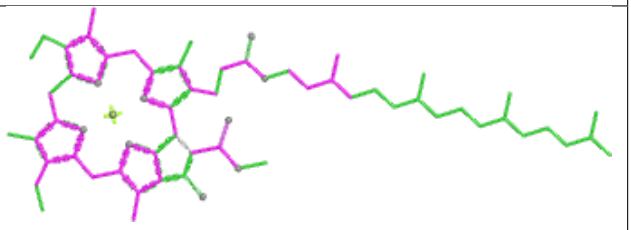

Torsions


Rings

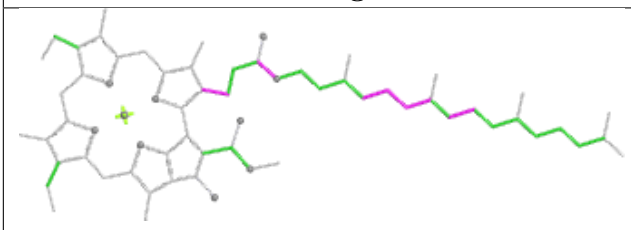
## Ligand CLA c 508



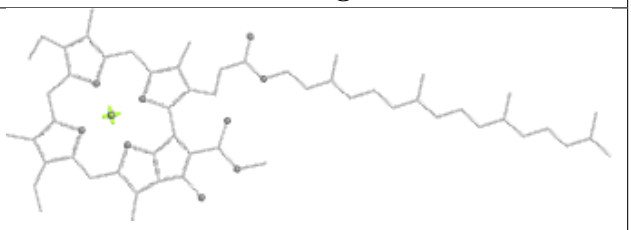
Bond lengths



Bond angles

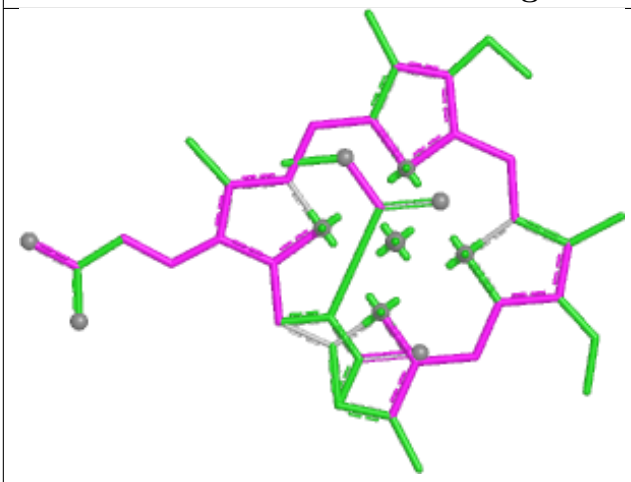


Torsions

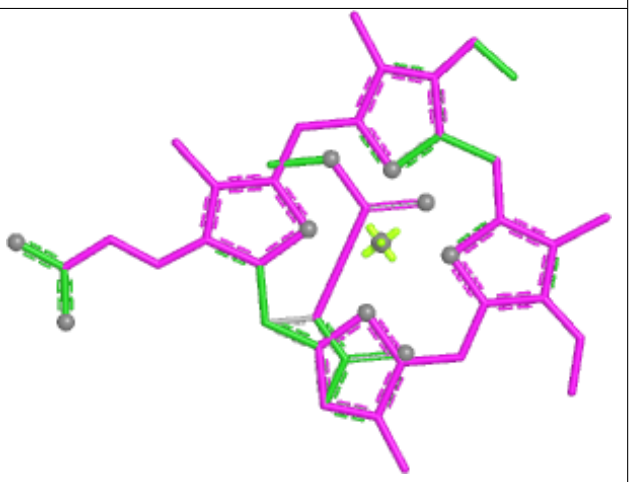


Rings

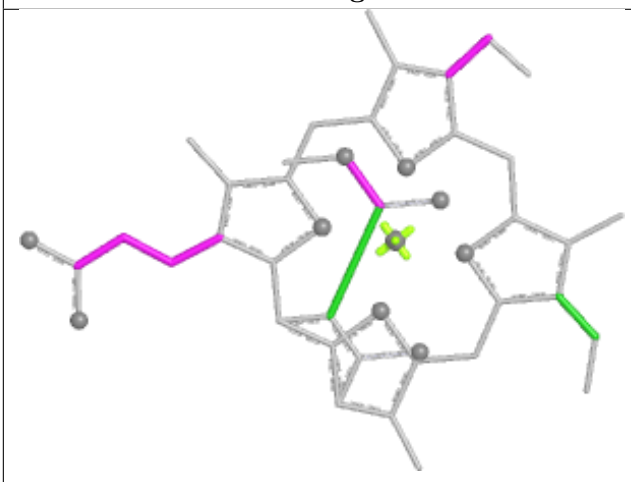
## Ligand KC1 20 302



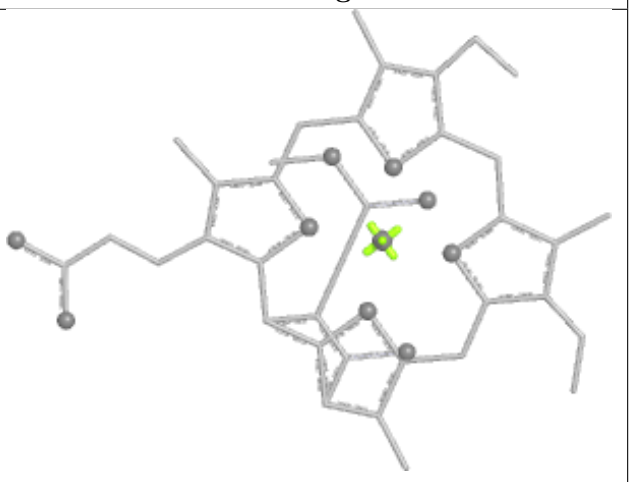
Bond lengths



Bond angles

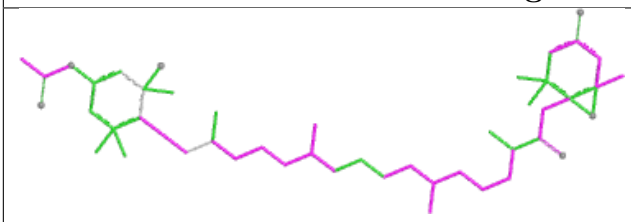


Torsions

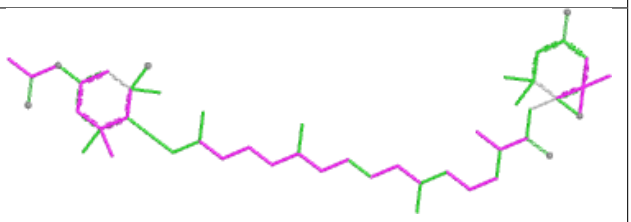


Rings

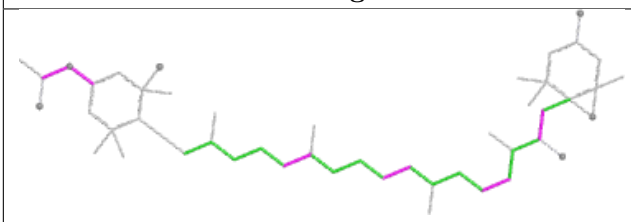
**Ligand A86 41 213**



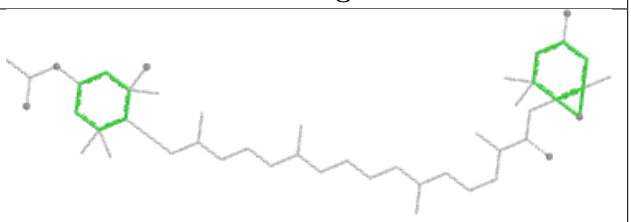
Bond lengths



Bond angles

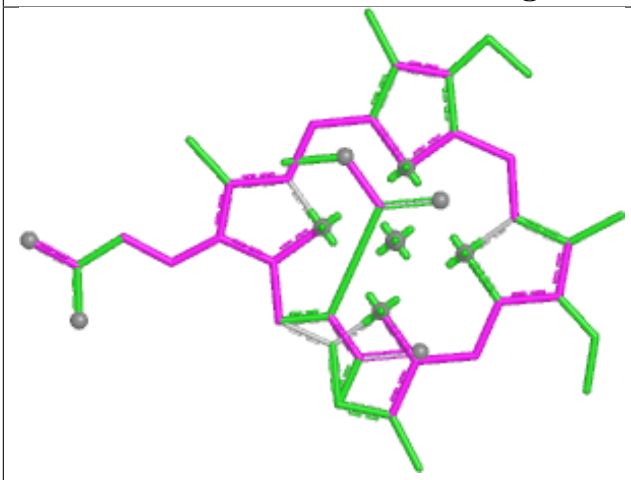


Torsions

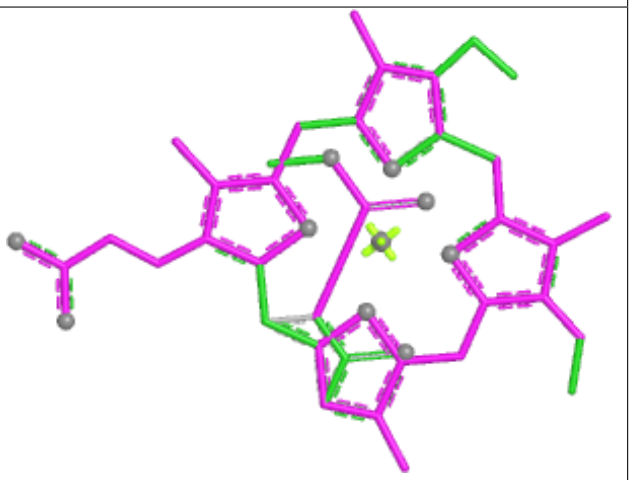


Rings

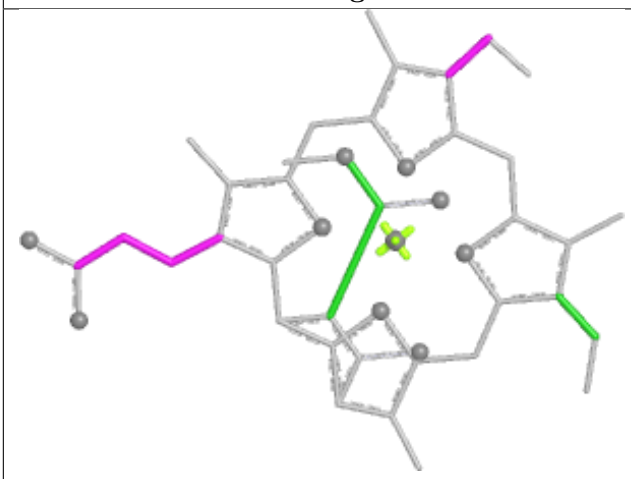
**Ligand KC1 17 305**



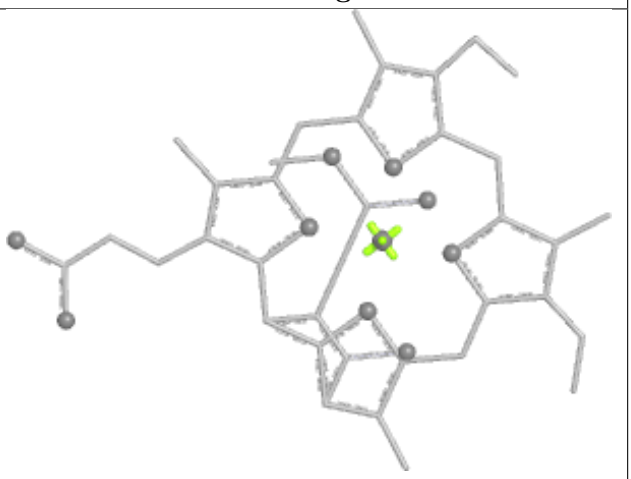
Bond lengths



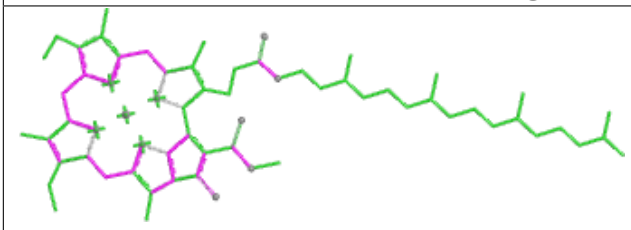
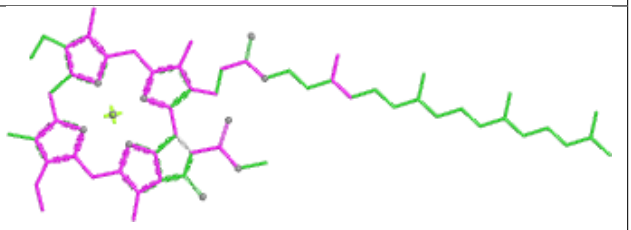
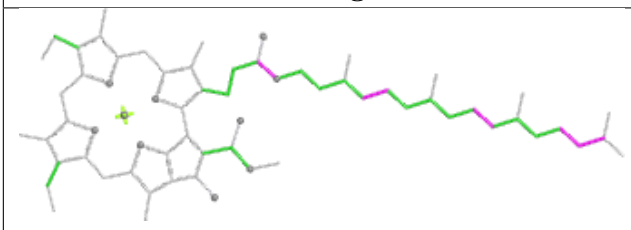
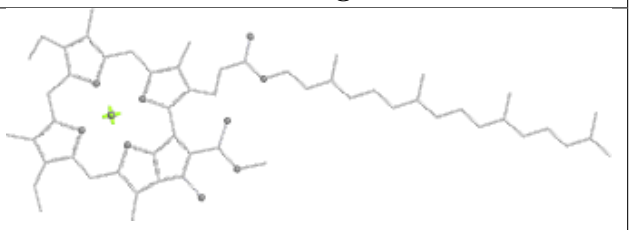
Bond angles

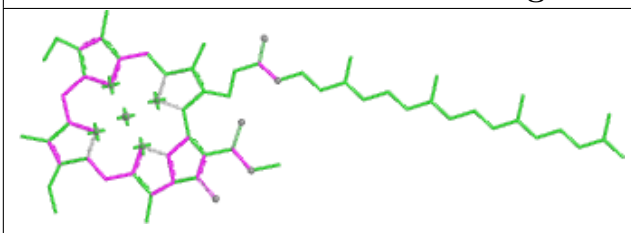
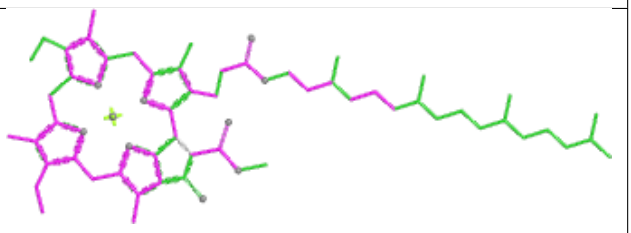
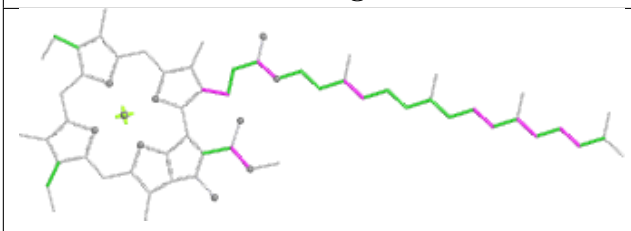
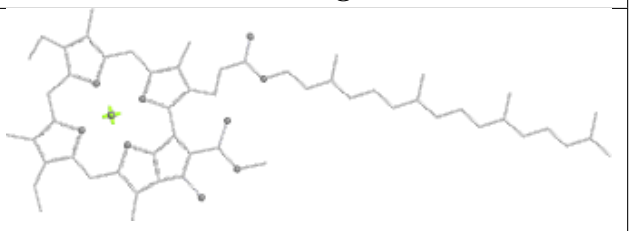


Torsions

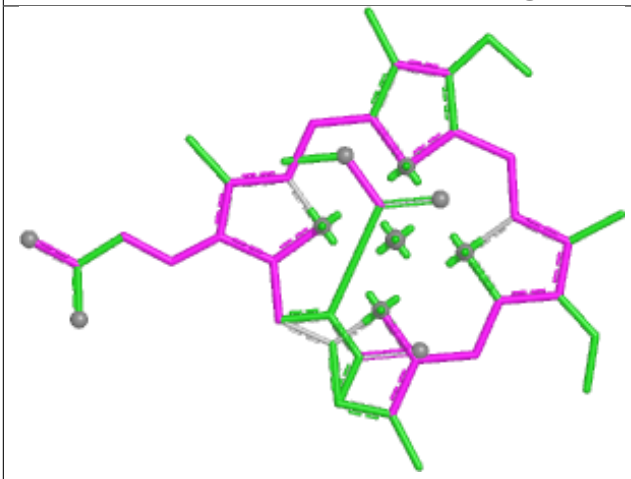


Rings

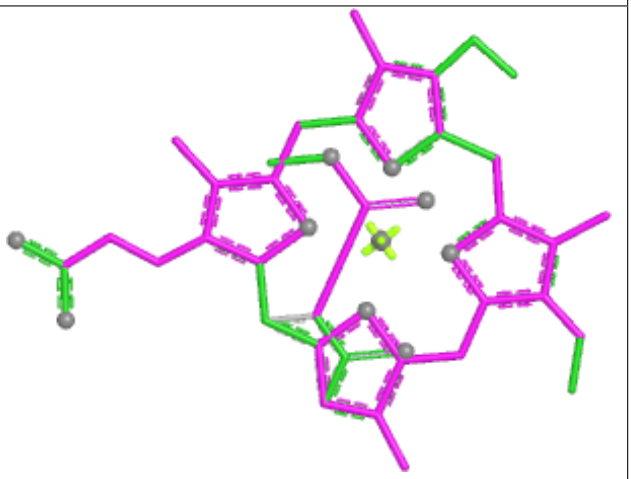
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|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA b 511 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

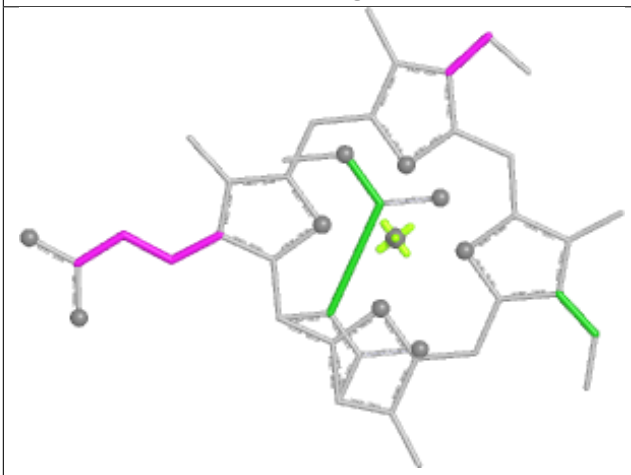
**Ligand KC1 38 205**



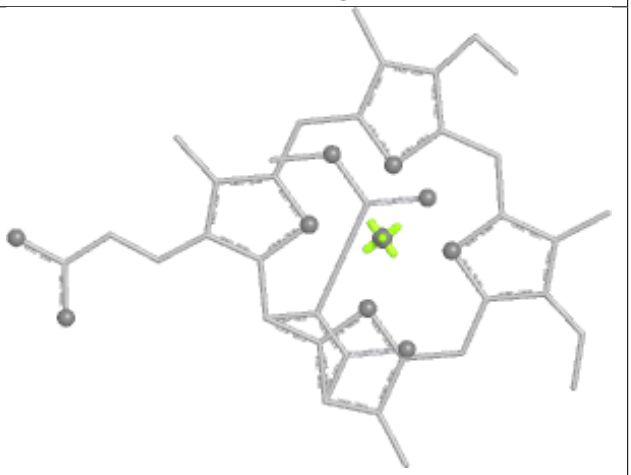
Bond lengths



Bond angles

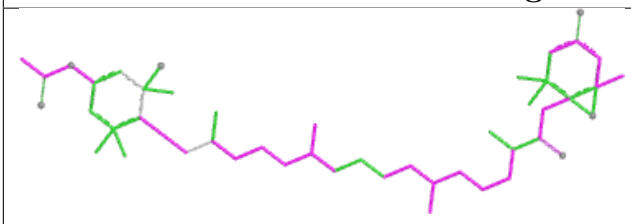


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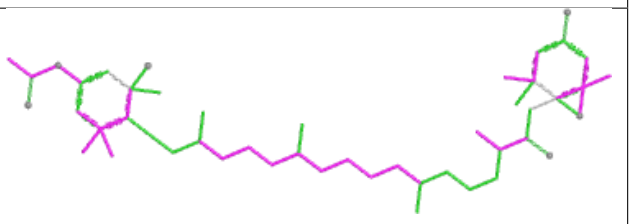


Rings

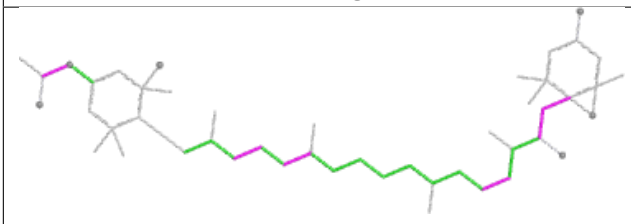
**Ligand A86 33 314**



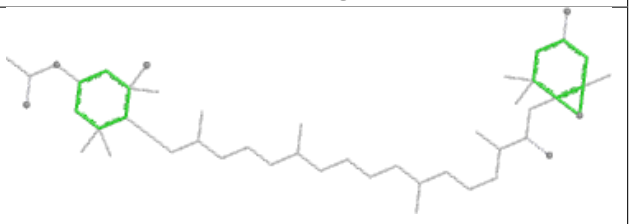
Bond lengths



Bond angles

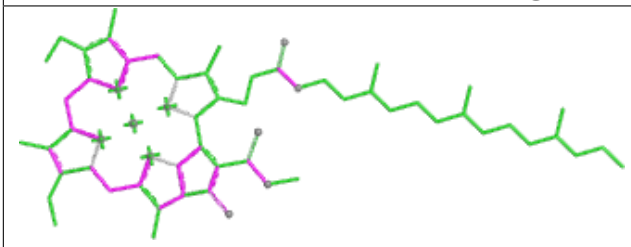


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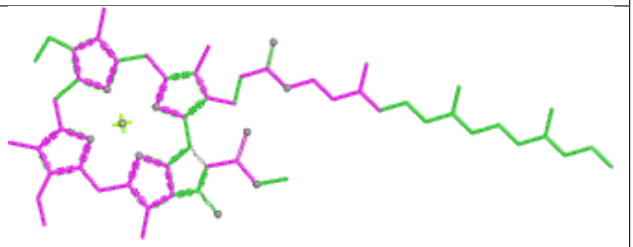


Rings

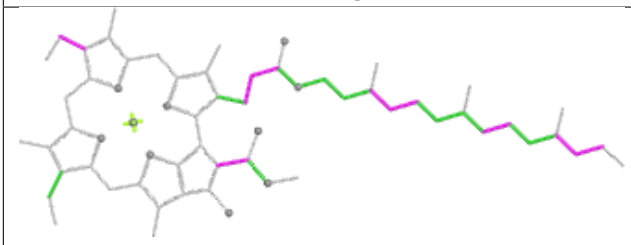
## Ligand CLA b 514



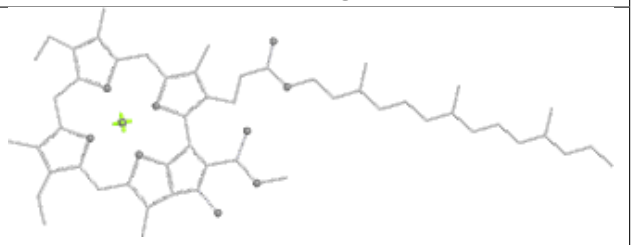
Bond lengths



Bond angles

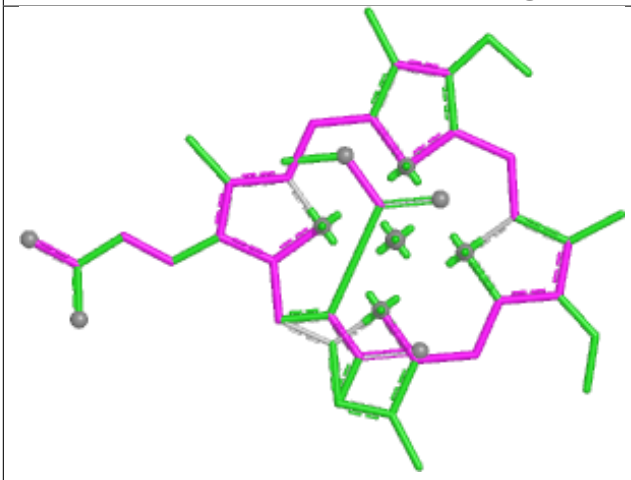


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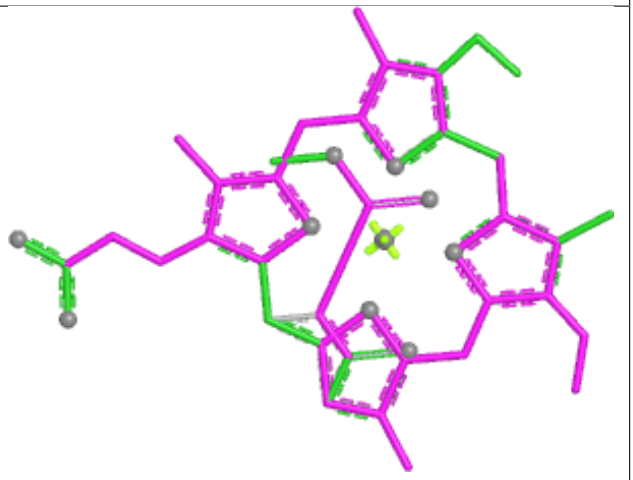


Rings

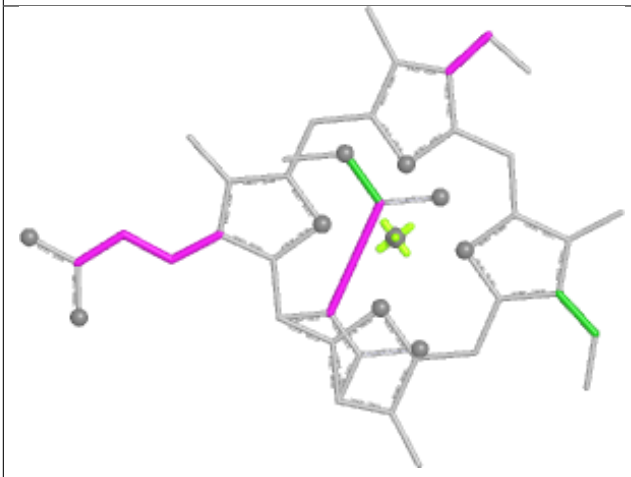
## Ligand KC1 11 309



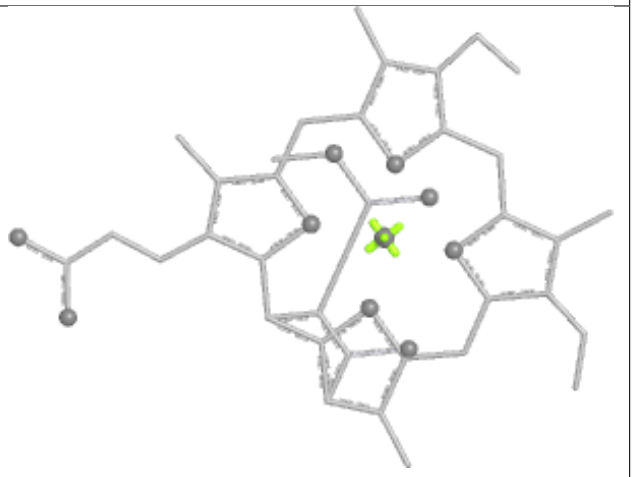
Bond lengths



Bond angles

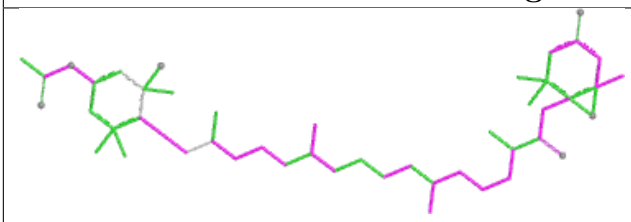


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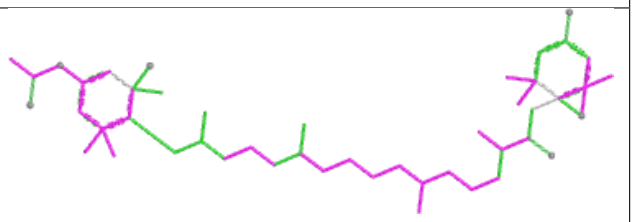


Rings

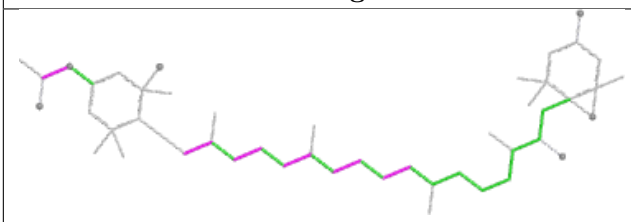
## Ligand A86 16 311



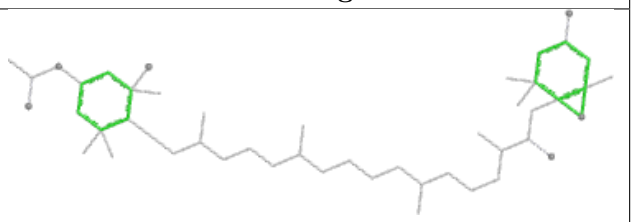
Bond lengths



Bond angles

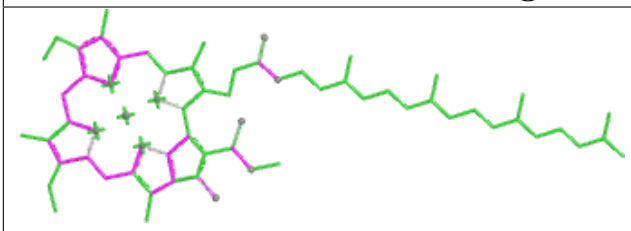


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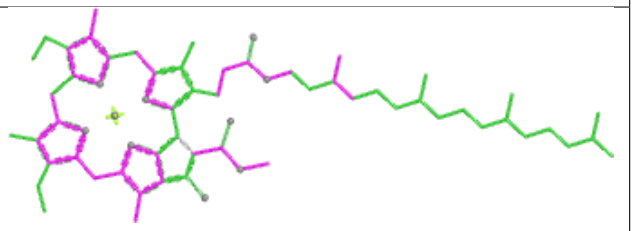


Rings

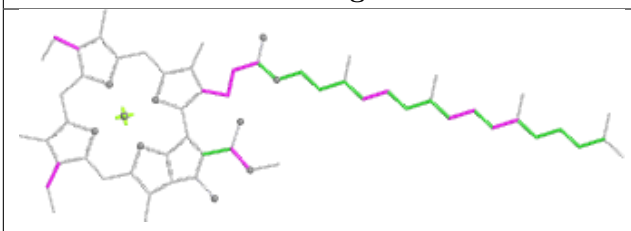
## Ligand CLA 17 302



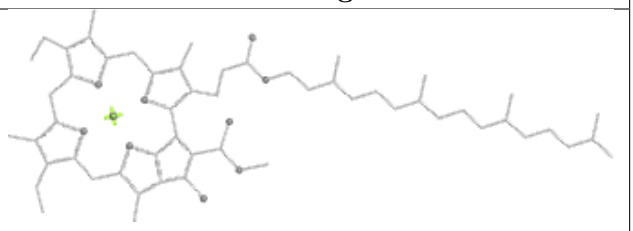
Bond lengths



Bond angles

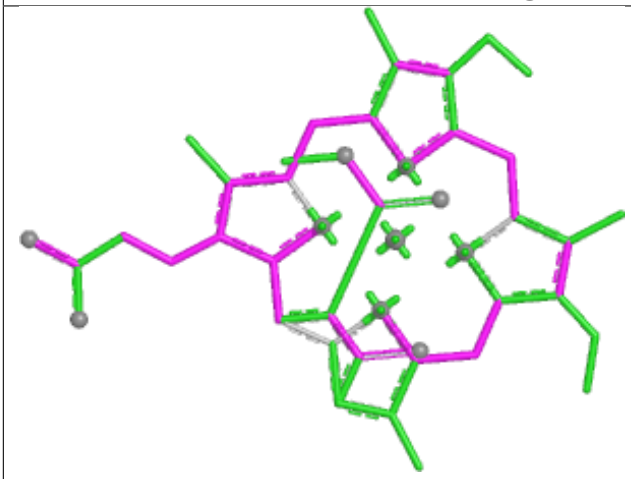


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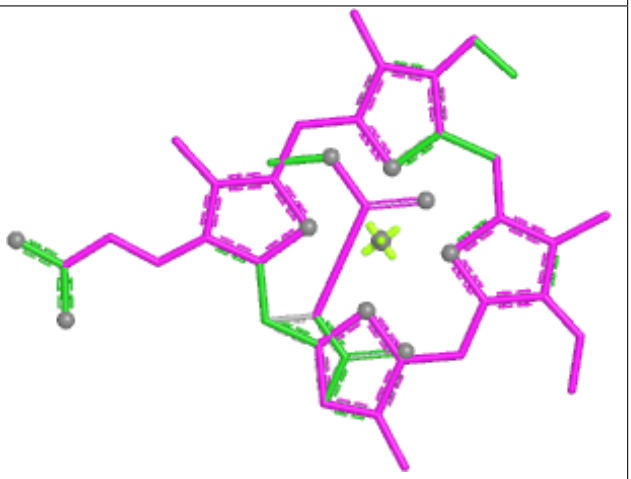


Rings

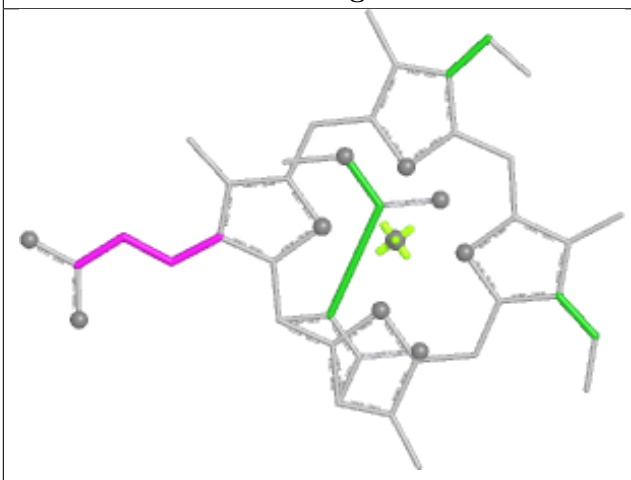
**Ligand KC1 12 208**



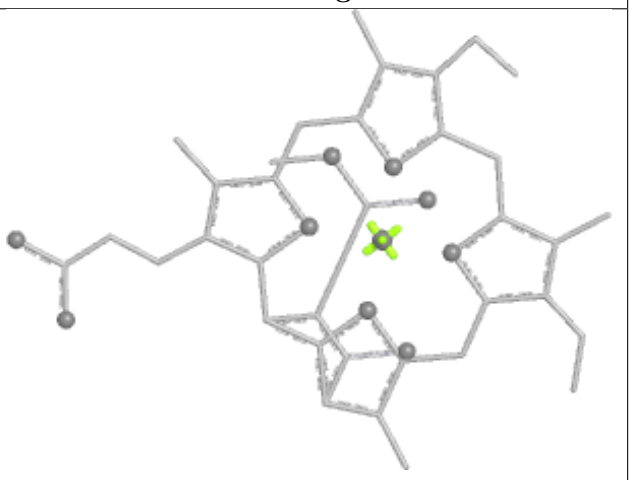
**Bond lengths**



**Bond angles**

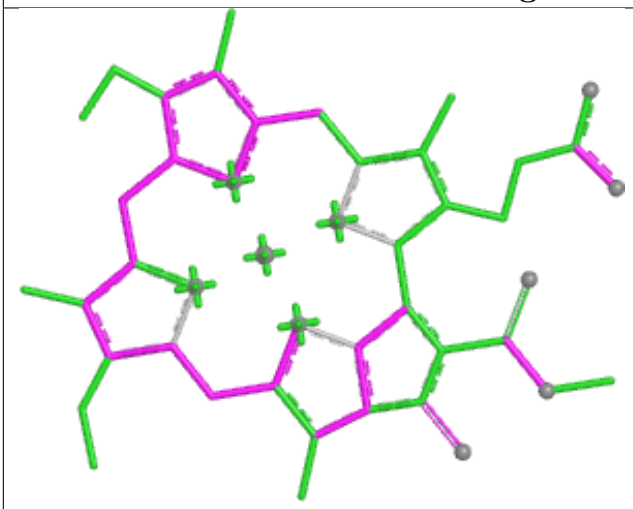


**Torsions**

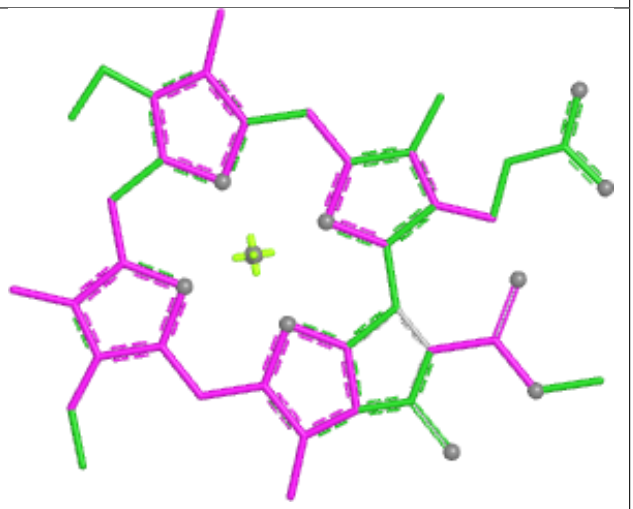


**Rings**

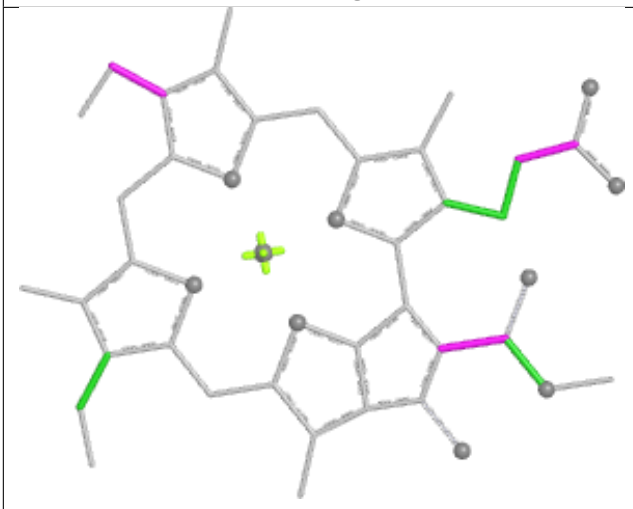
**Ligand CLA 41 210**



**Bond lengths**



**Bond angles**

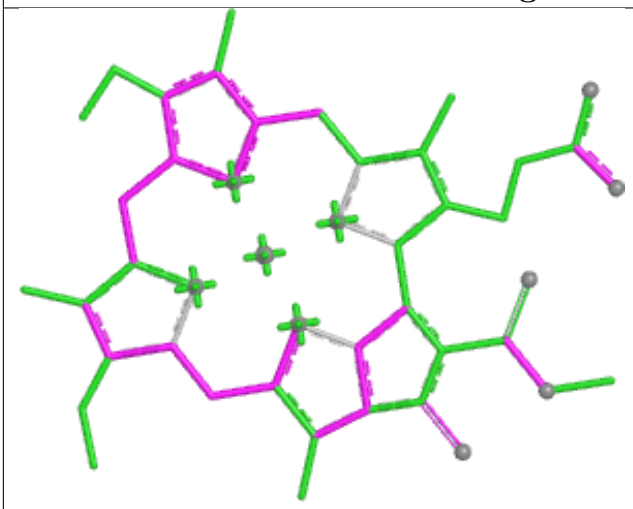


**Torsions**

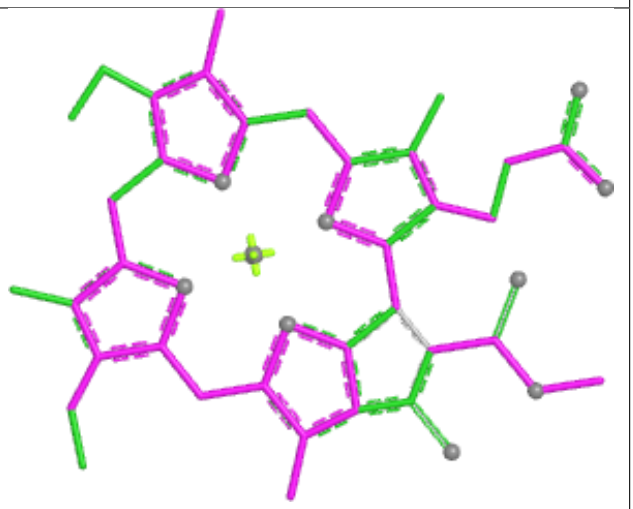


**Rings**

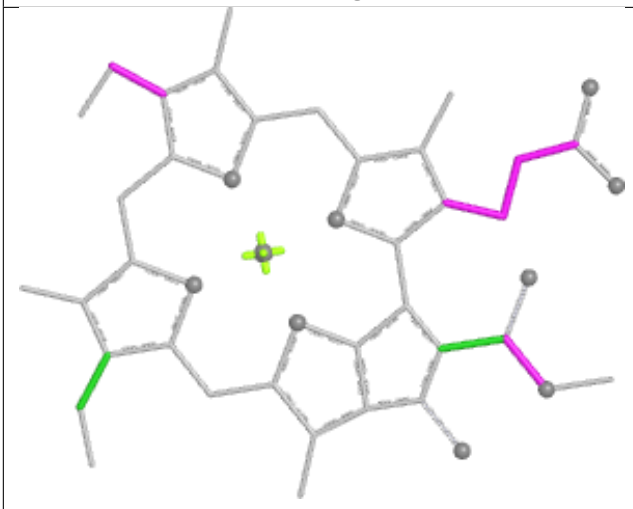
## Ligand CLA 41 205



Bond lengths



Bond angles

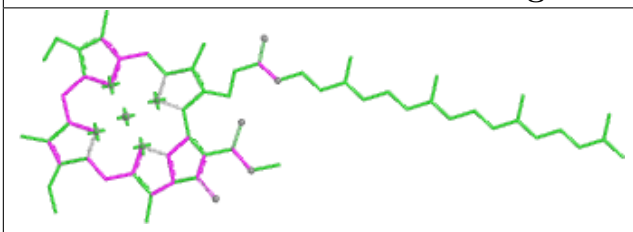


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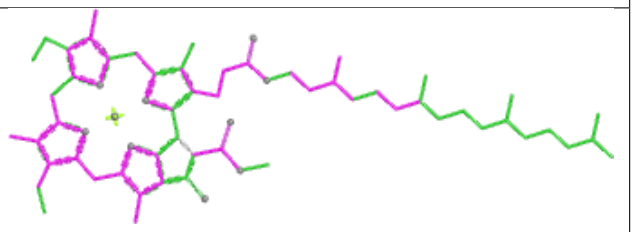


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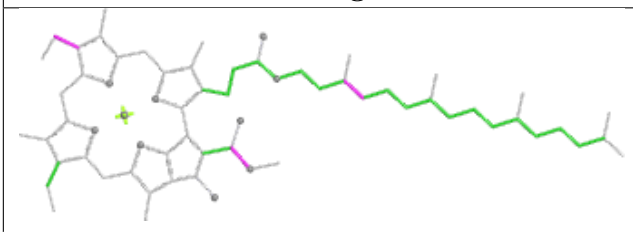
## Ligand CLA b 504



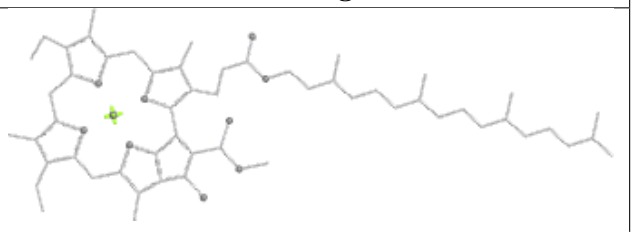
Bond lengths



Bond angles

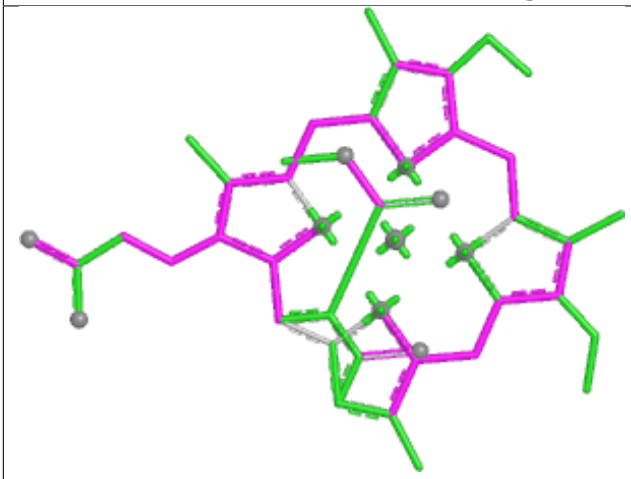


Torsions

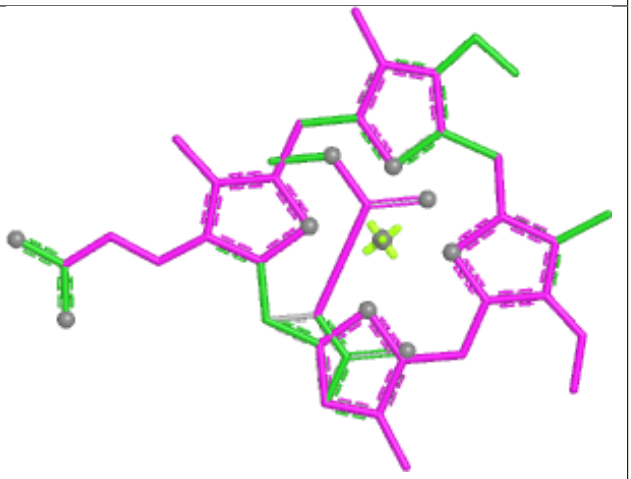


Rings

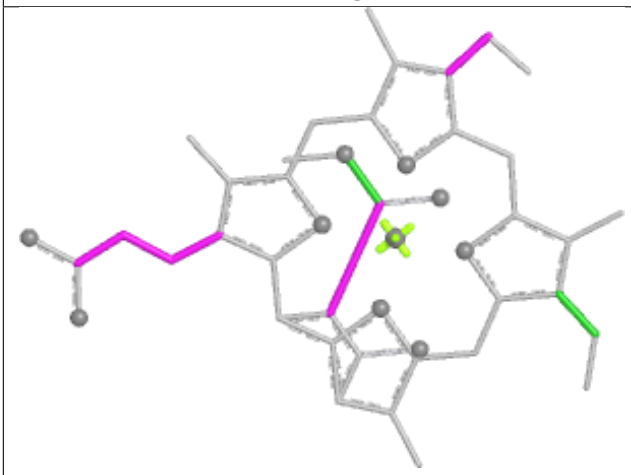
## Ligand KC1 38 210



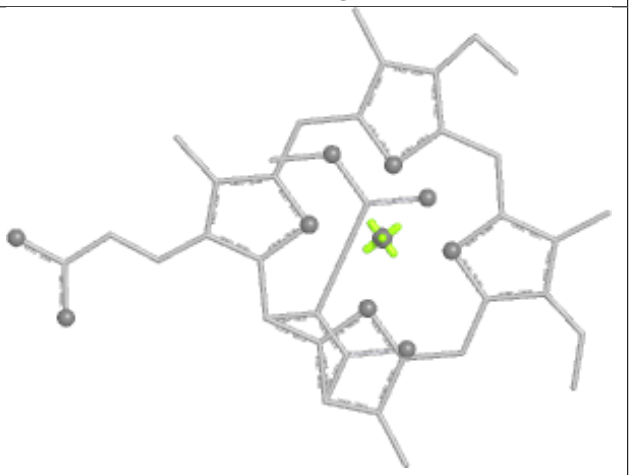
Bond lengths



Bond angles

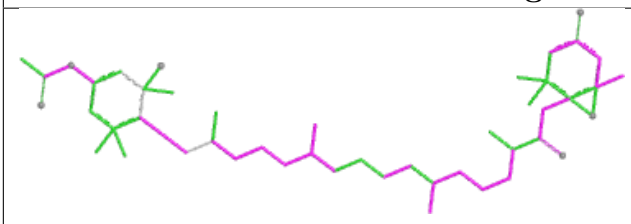


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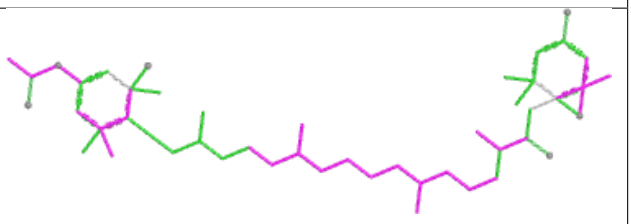


Rings

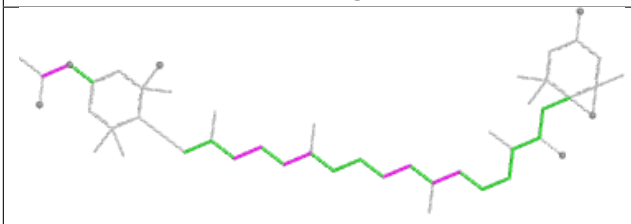
## Ligand A86 15 319



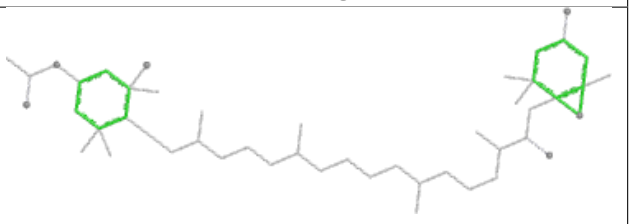
Bond lengths



Bond angles

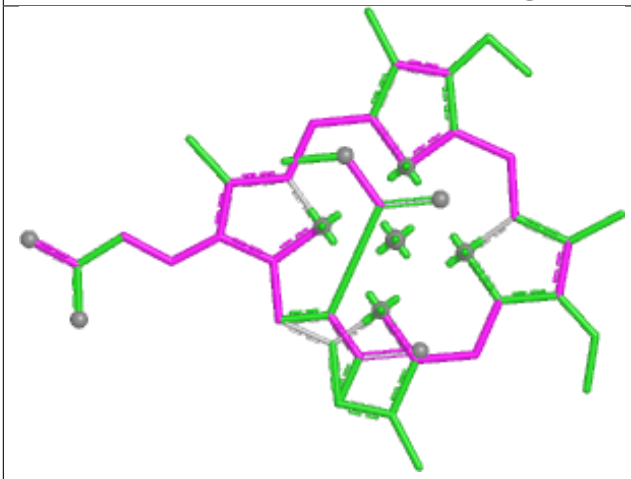


Torsions

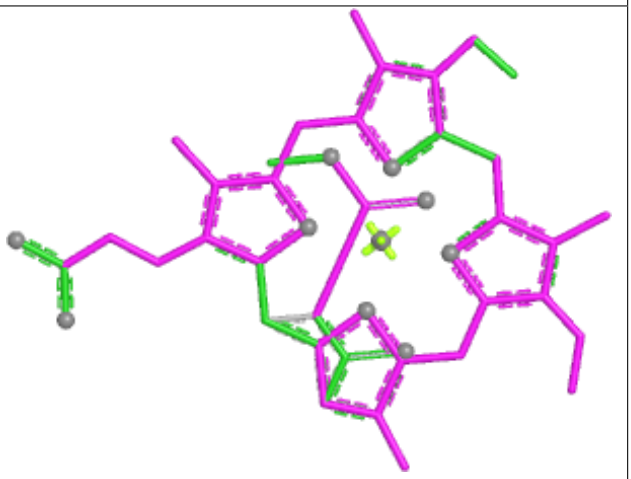


Rings

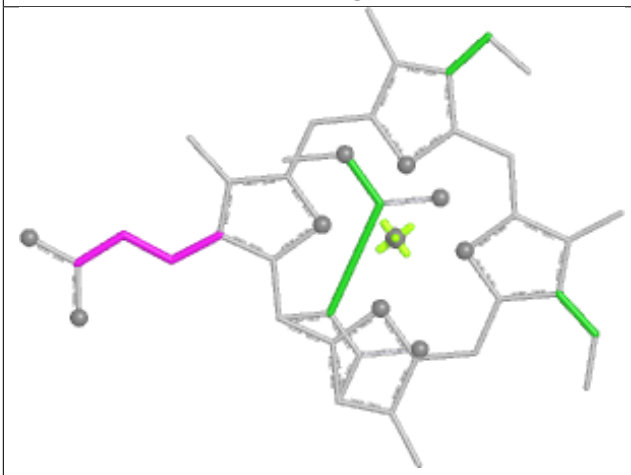
**Ligand KC1 32 209**



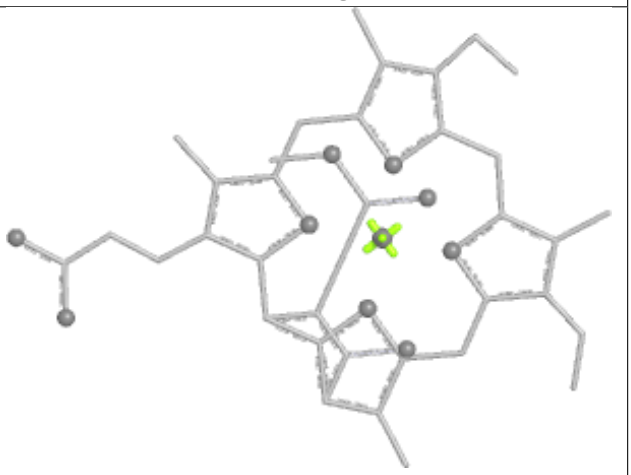
**Bond lengths**



**Bond angles**

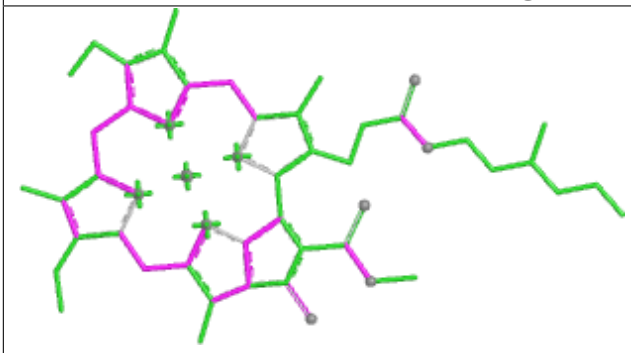


**Torsions**

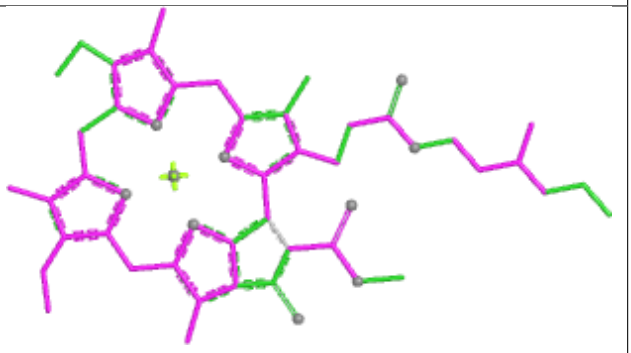


**Rings**

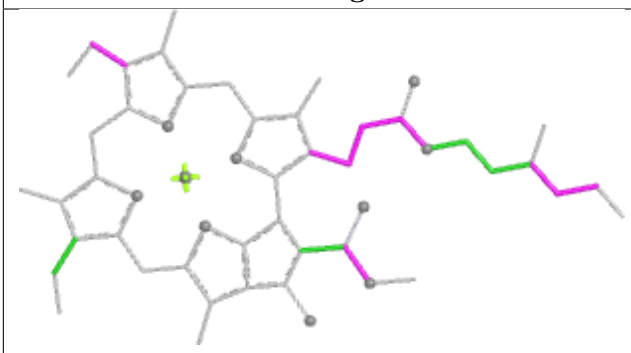
**Ligand CLA 32 210**



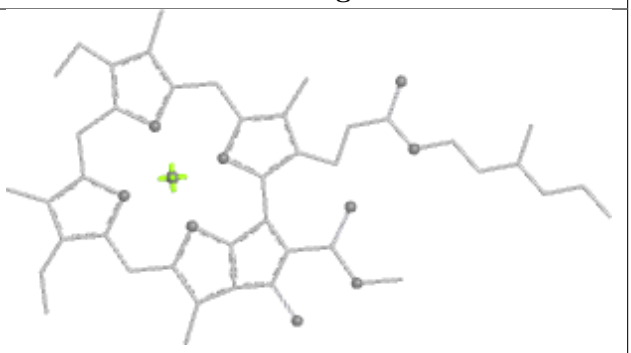
Bond lengths



Bond angles

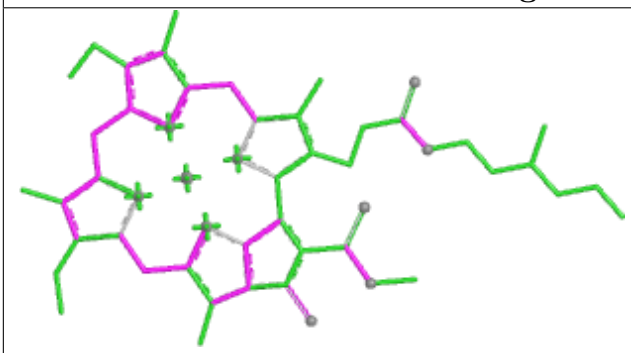


Torsions

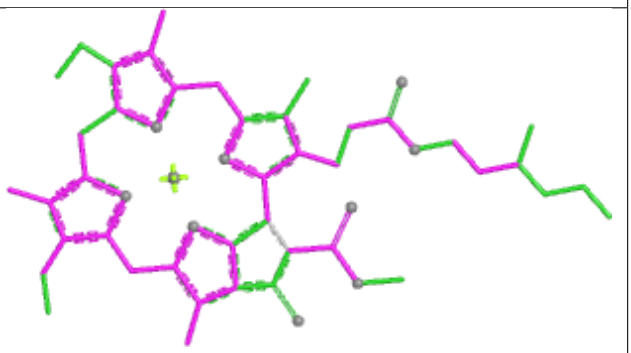


Rings

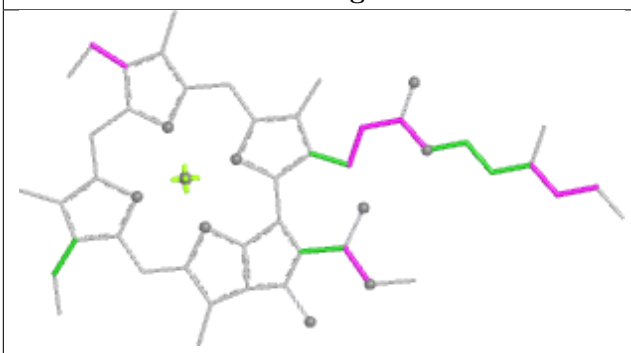
**Ligand CLA 15 307**



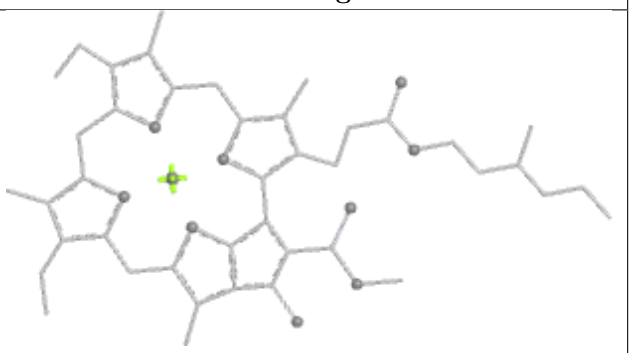
Bond lengths



Bond angles

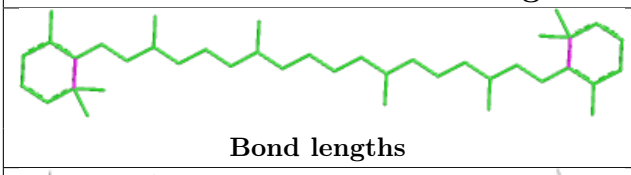


Torsions

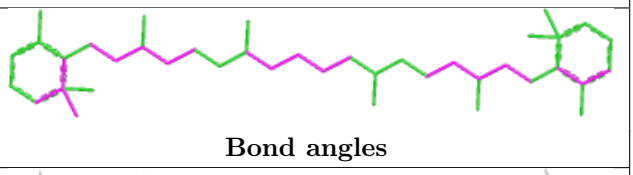


Rings

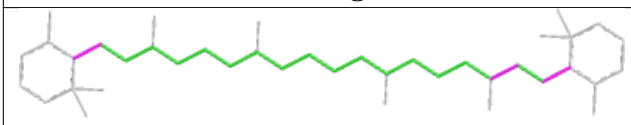
## Ligand BCR C 514



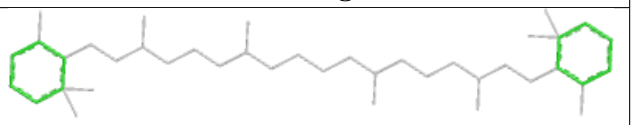
Bond lengths



Bond angles

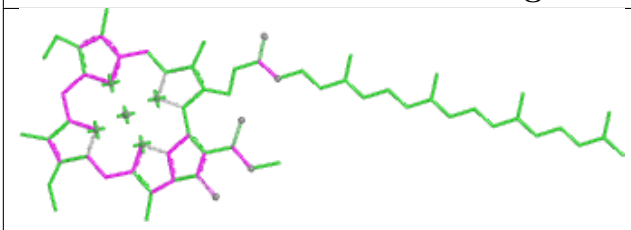


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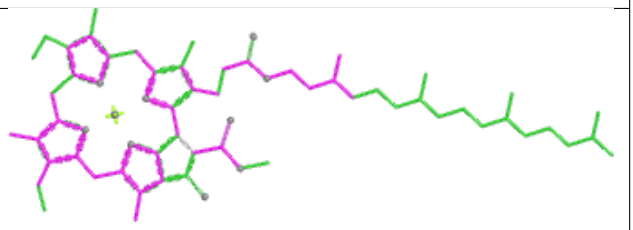


Rings

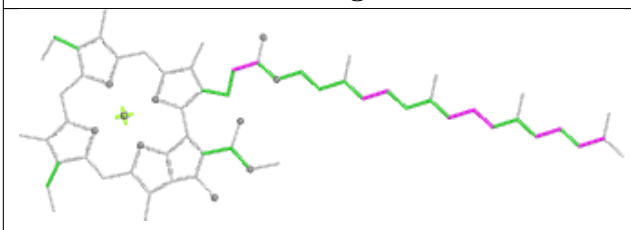
## Ligand CLA B 513



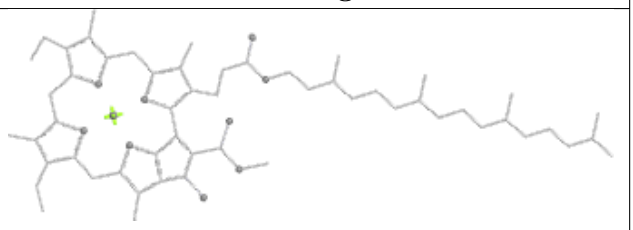
Bond lengths



Bond angles

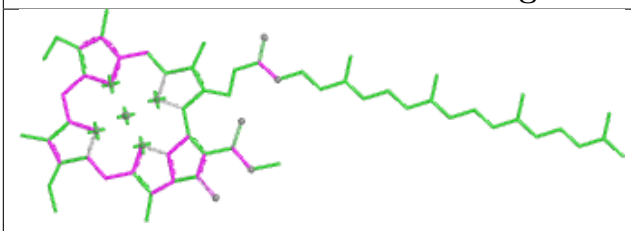


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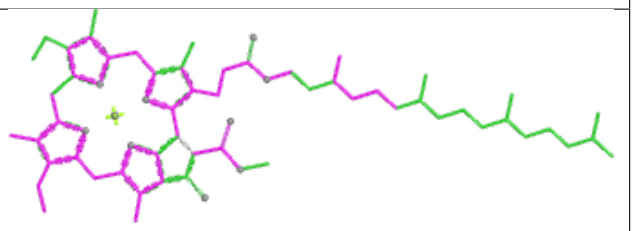


Rings

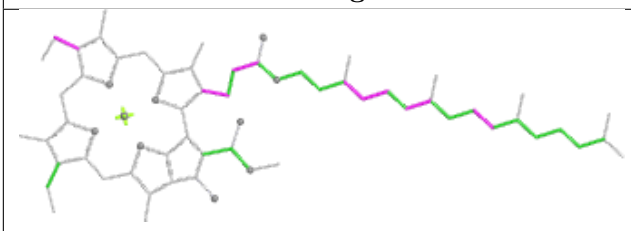
## Ligand CLA 12 205



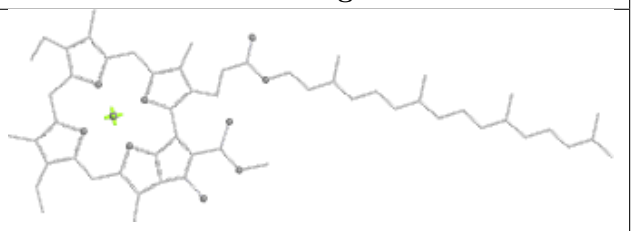
Bond lengths



Bond angles

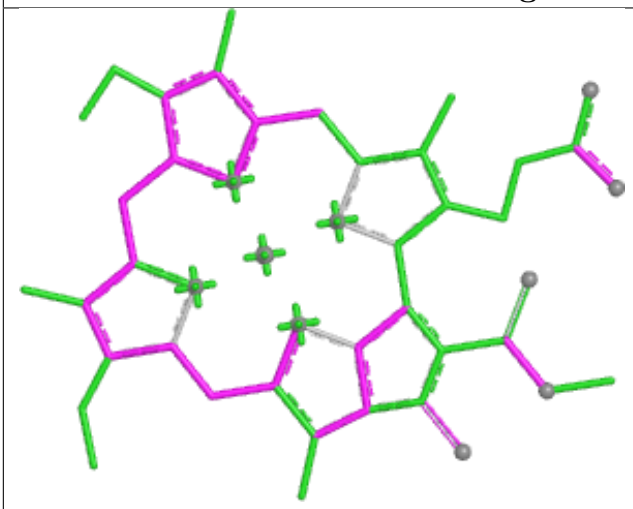


Torsions

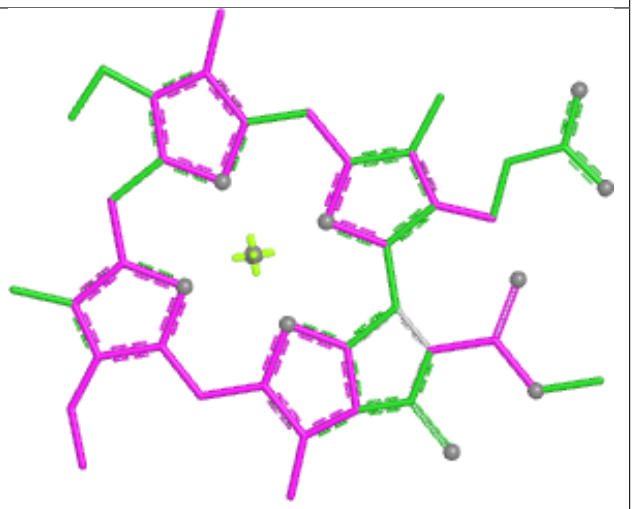


Rings

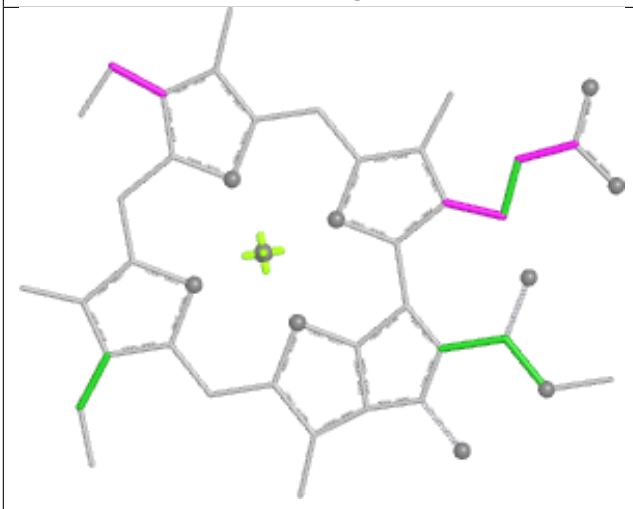
**Ligand CLA 14 305**



**Bond lengths**



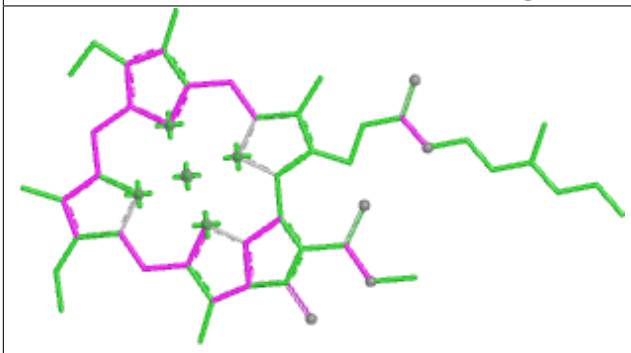
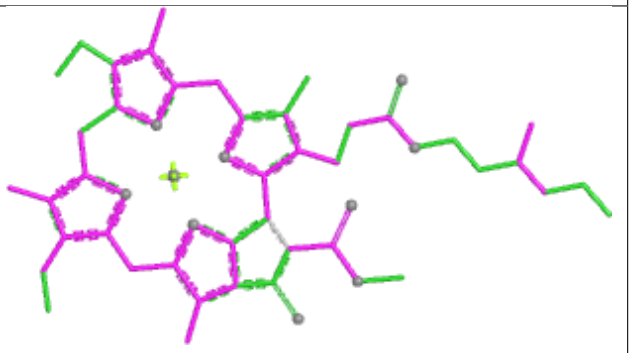
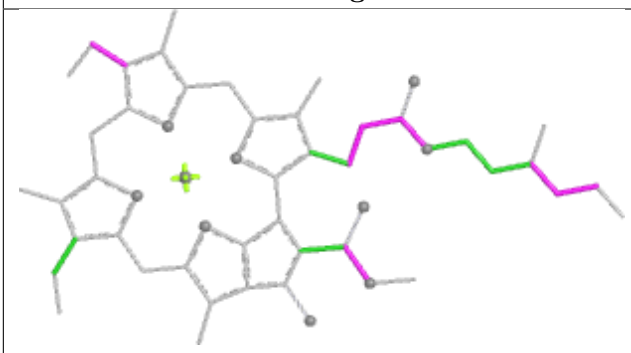
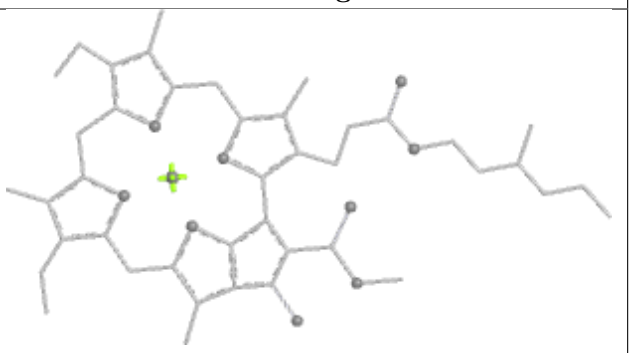
**Bond angles**

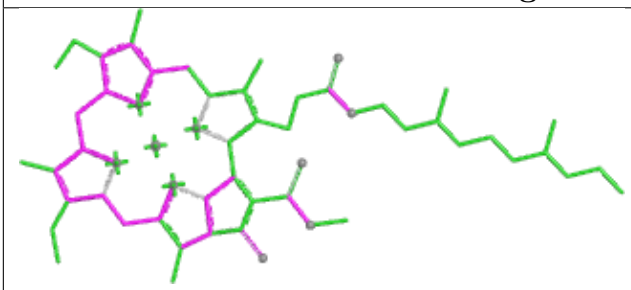
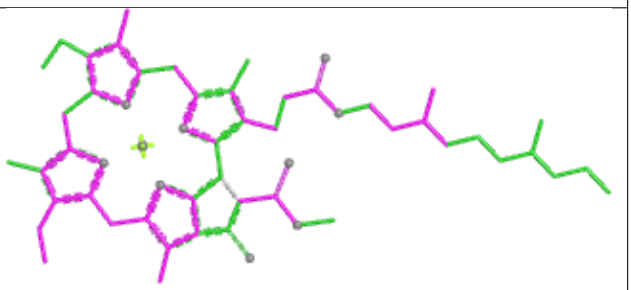
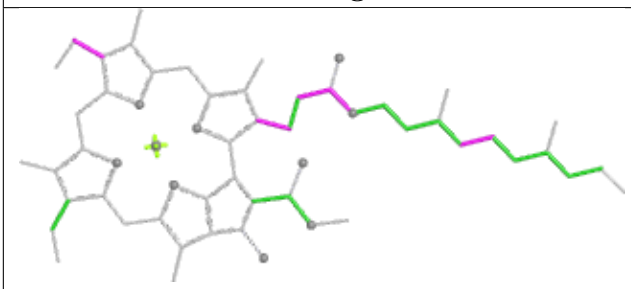
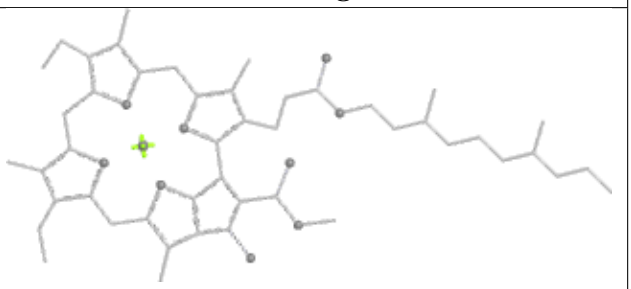


**Torsions**

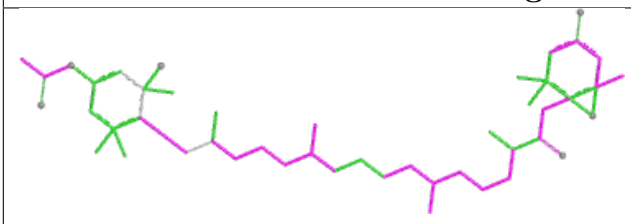


**Rings**

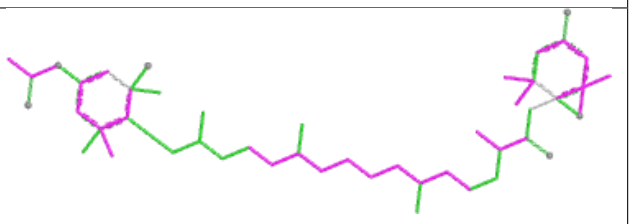
| Ligand CLA 35 307 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 41 202 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

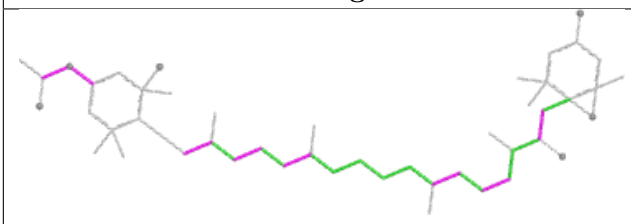
## Ligand A86 34 313



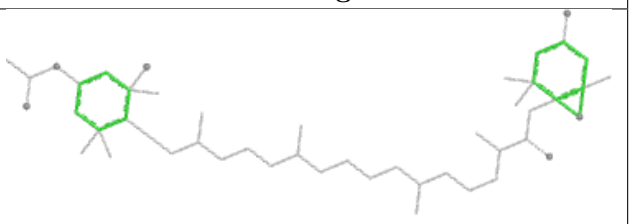
Bond lengths



Bond angles

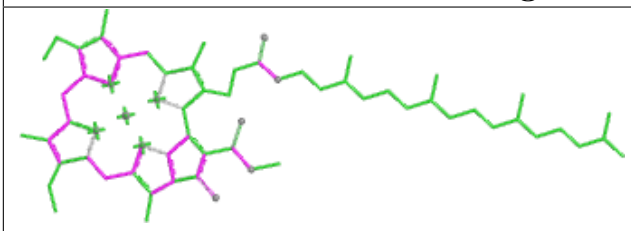


Torsions

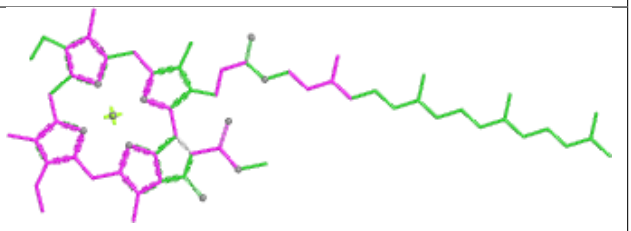


Rings

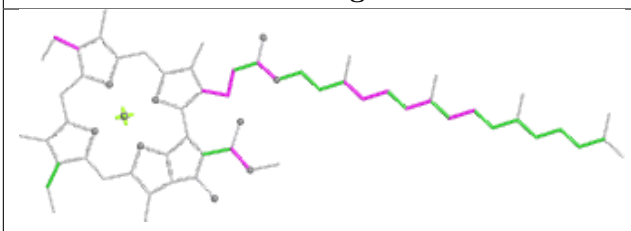
## Ligand CLA 11 301



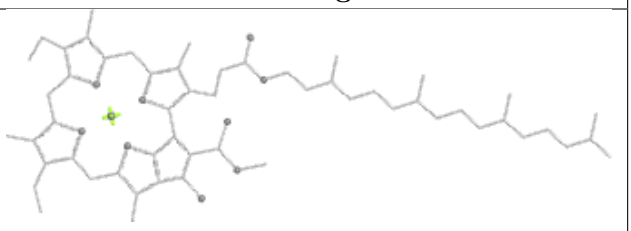
Bond lengths



Bond angles

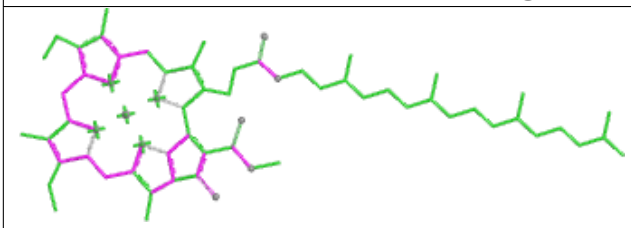


Torsions

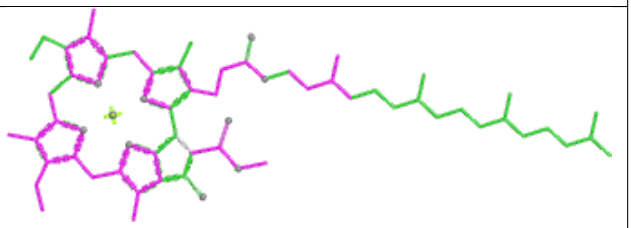


Rings

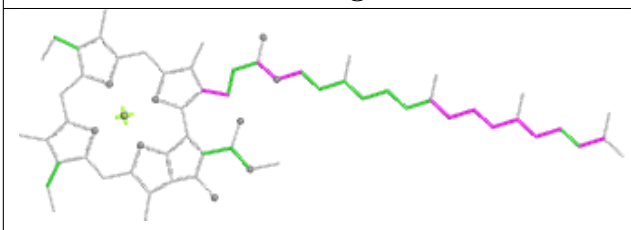
## Ligand CLA 11 308



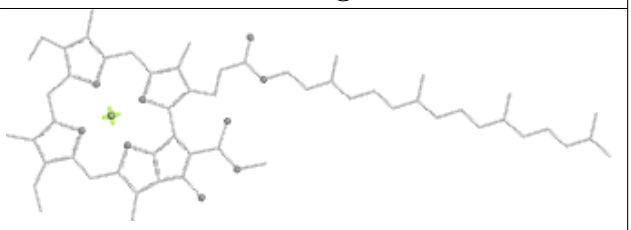
Bond lengths



Bond angles

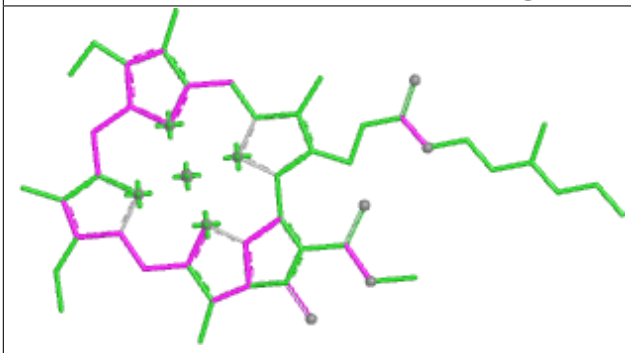


Torsions

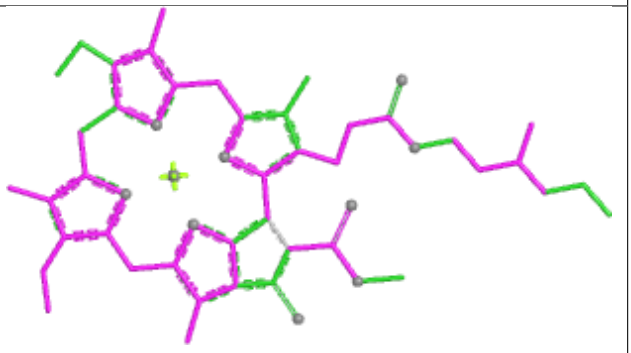


Rings

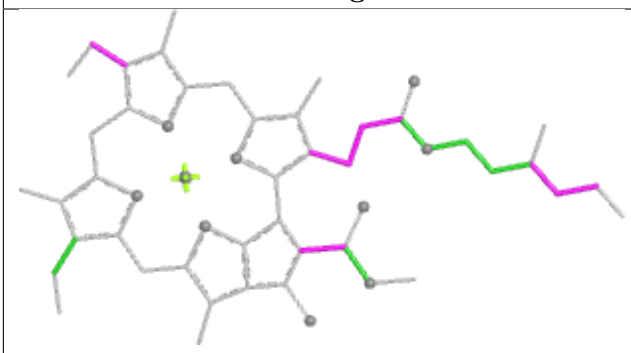
## Ligand CLA 37 306



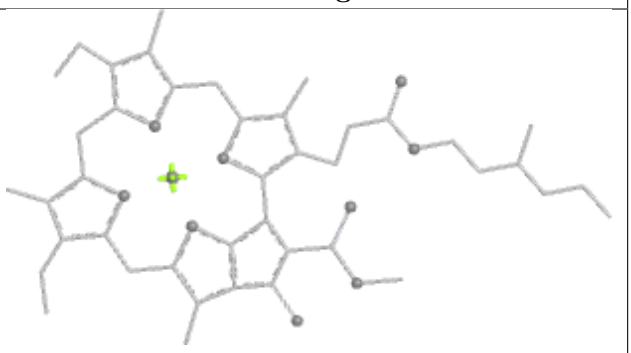
Bond lengths



Bond angles

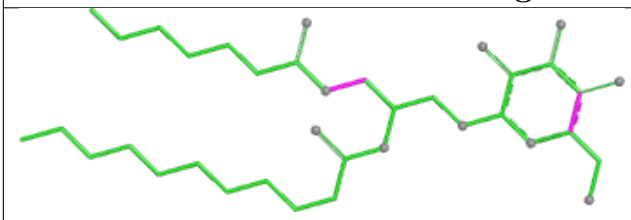


Torsions

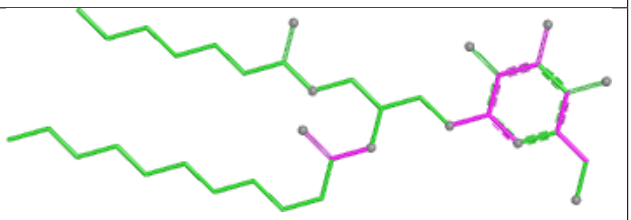


Rings

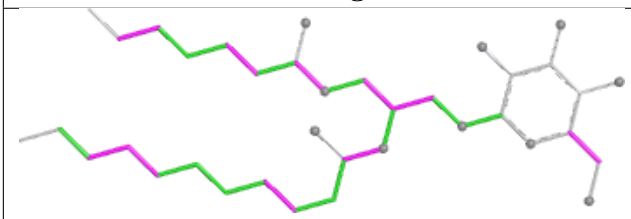
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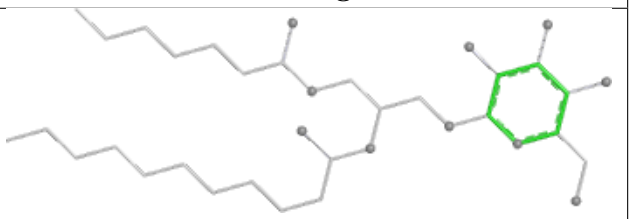
Bond lengths



Bond angles

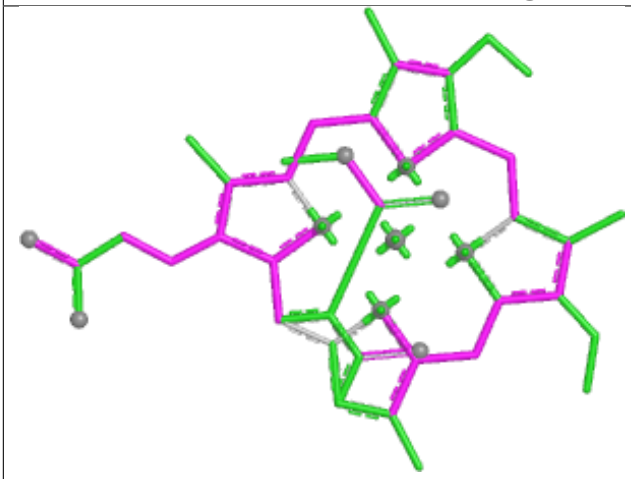


Torsions

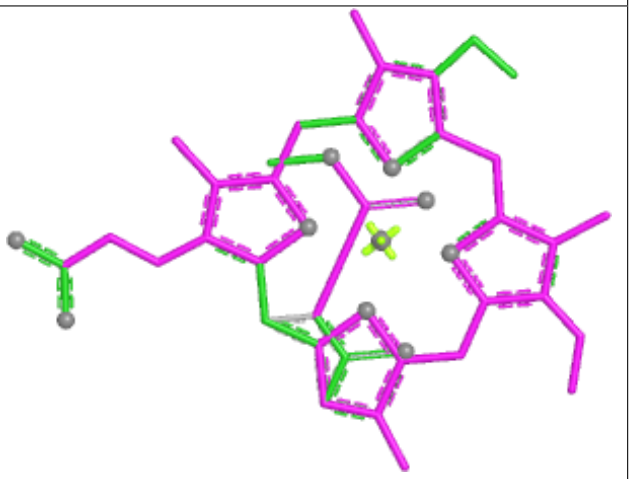


Rings

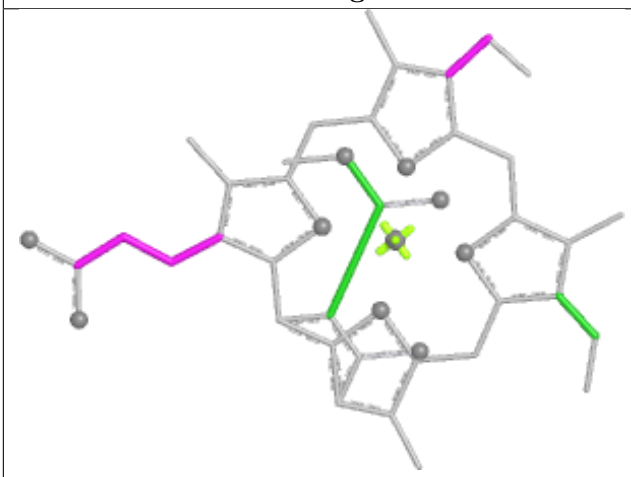
**Ligand KC1 17 303**



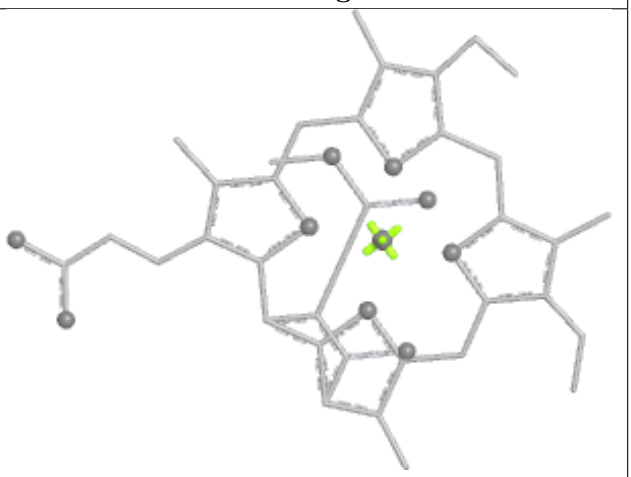
Bond lengths



Bond angles

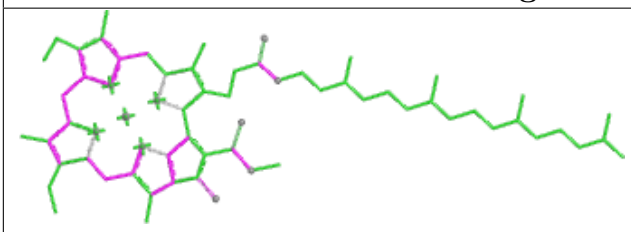


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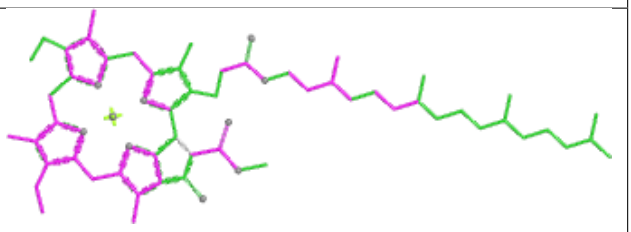


Rings

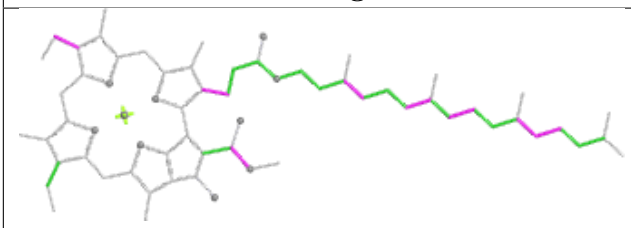
**Ligand CLA 14 301**



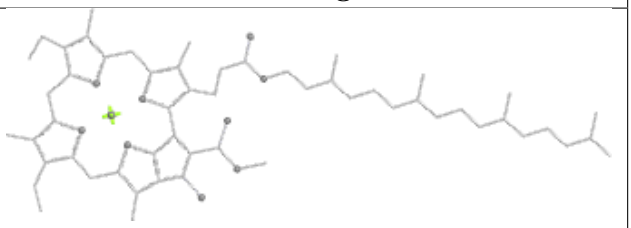
Bond lengths



Bond angles

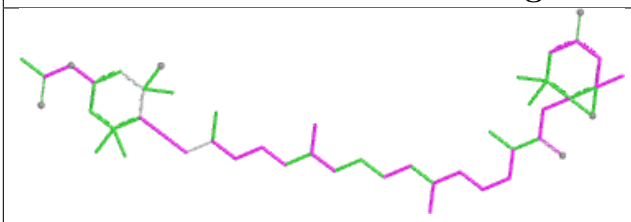


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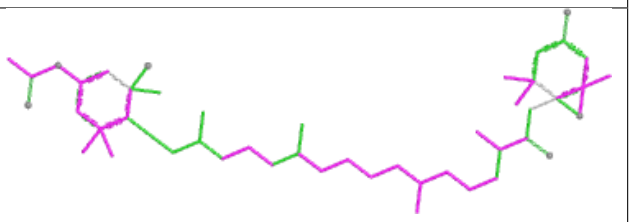


Rings

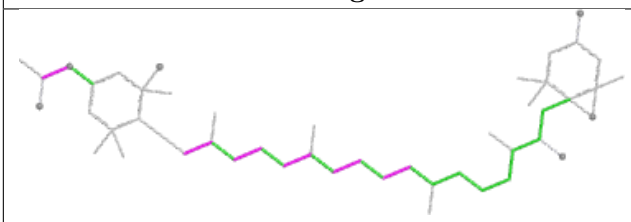
## Ligand A86 36 311



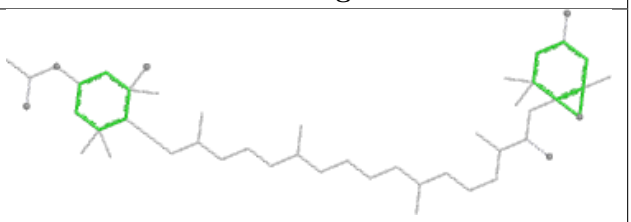
Bond lengths



Bond angles

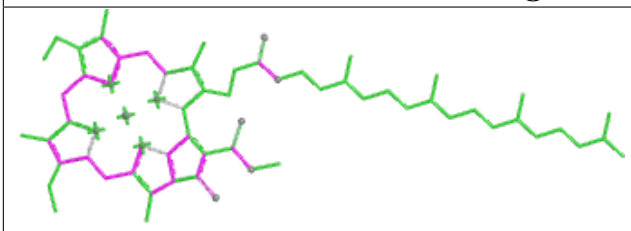


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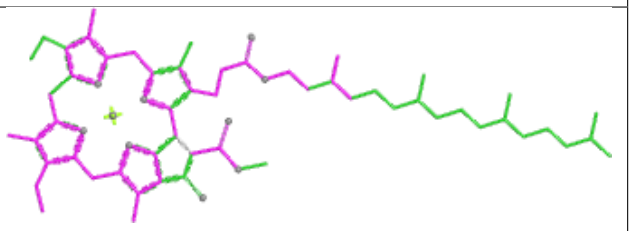


Rings

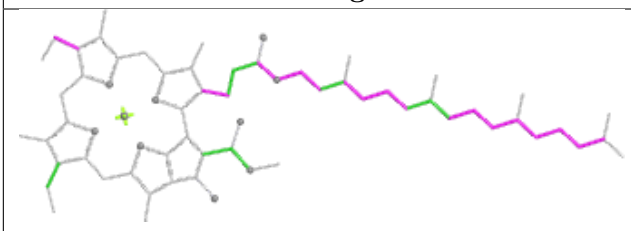
## Ligand CLA C 503



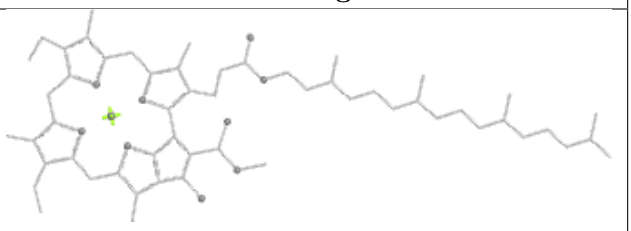
Bond lengths



Bond angles

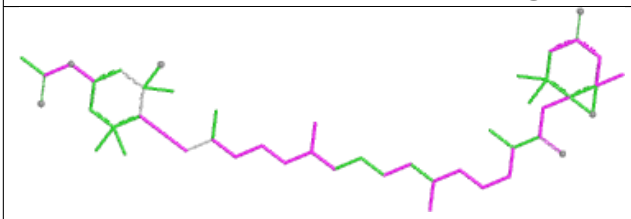


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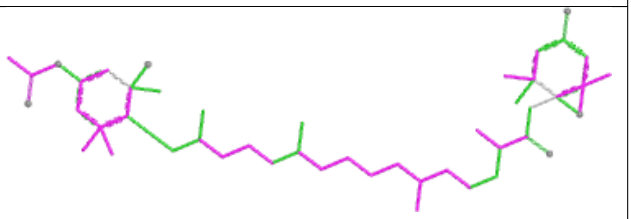


Rings

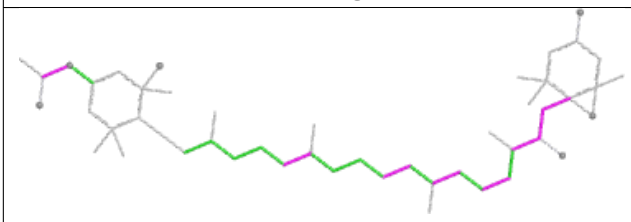
## Ligand A86 32 218



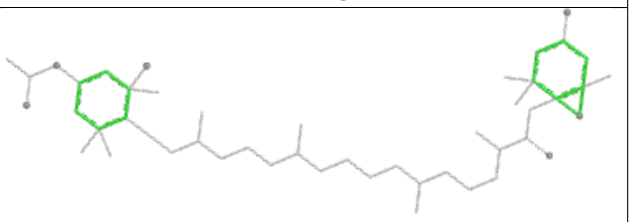
Bond lengths



Bond angles

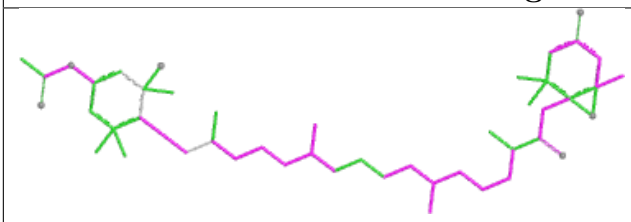


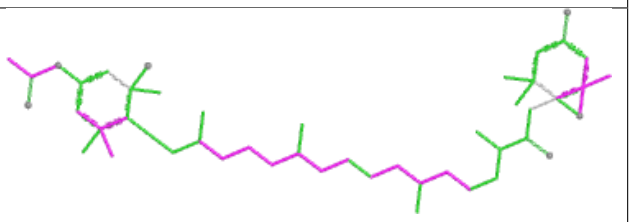
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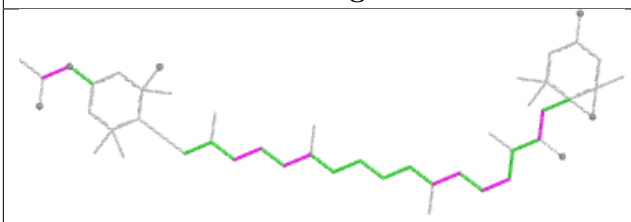


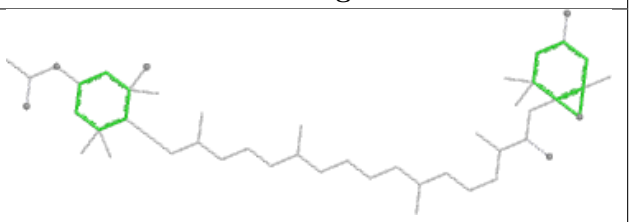
Rings

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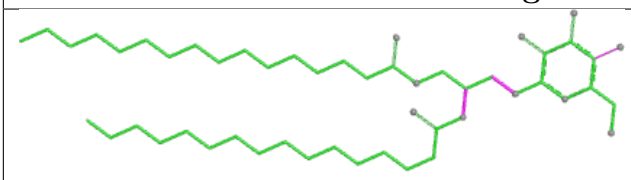

Bond lengths

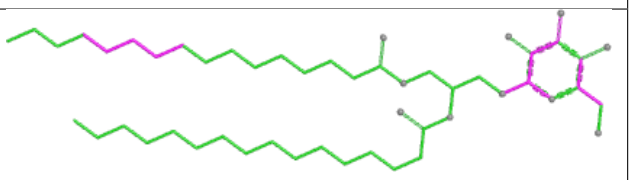

Bond angles

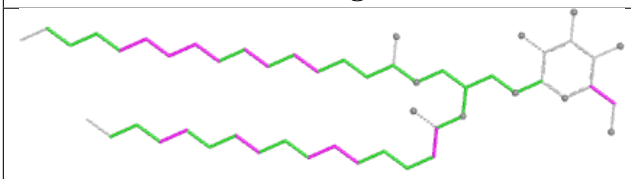

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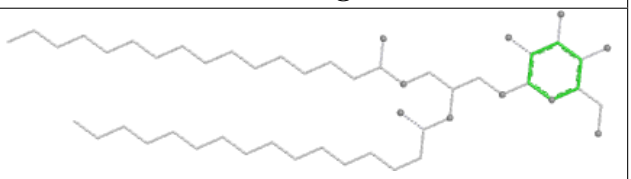

Rings

## Ligand LMG d 409

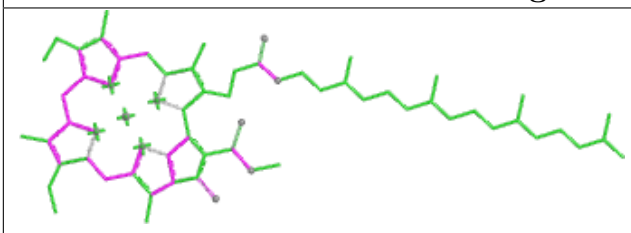

Bond lengths

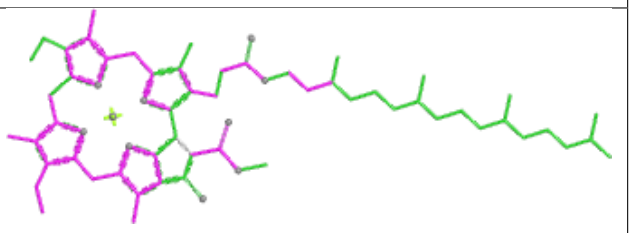

Bond angles

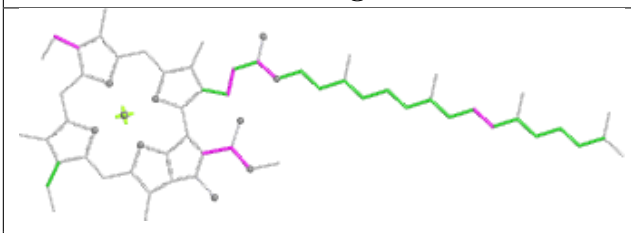

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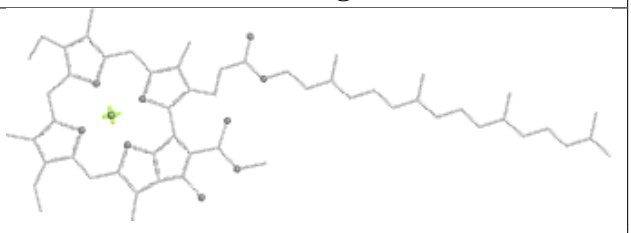

Rings

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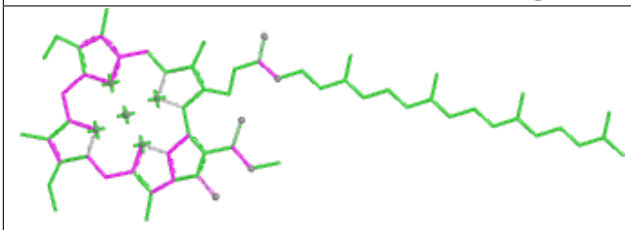

Bond lengths


Bond angles

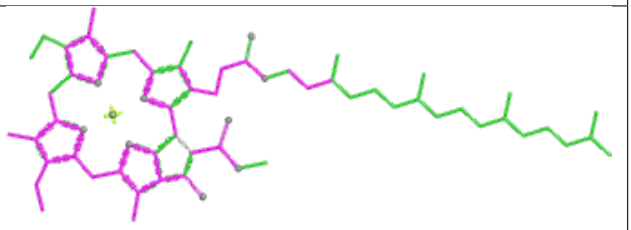

Torsions


Rings

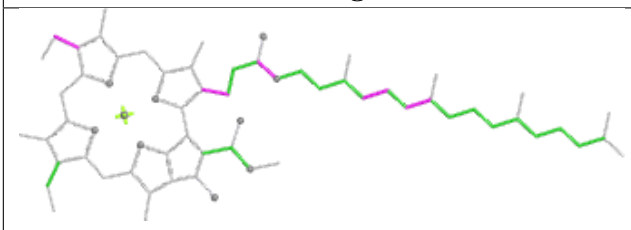
## Ligand CLA c 511



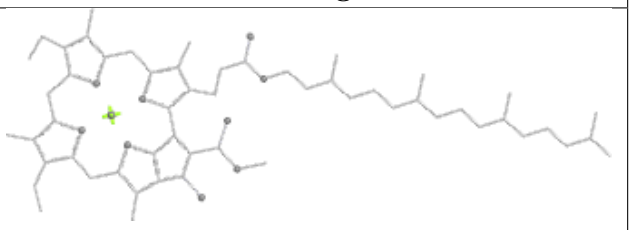
Bond lengths



Bond angles

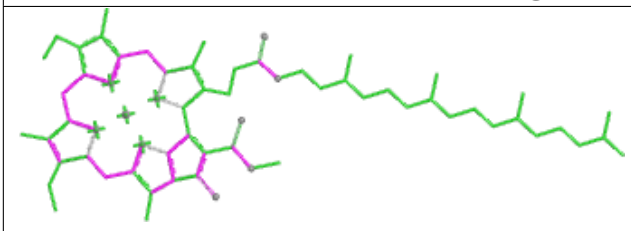


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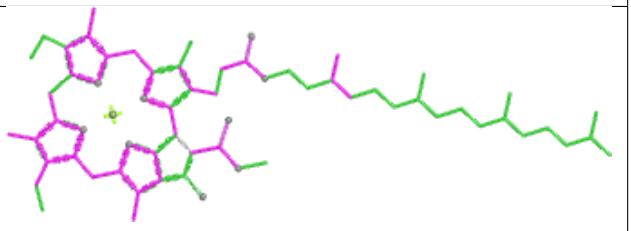


Rings

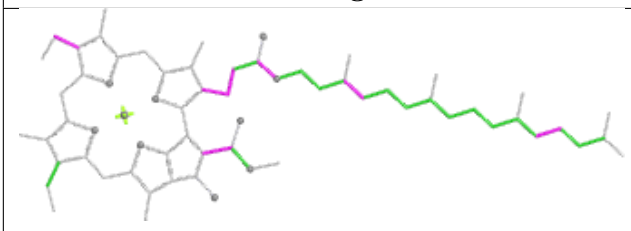
## Ligand CLA b 503



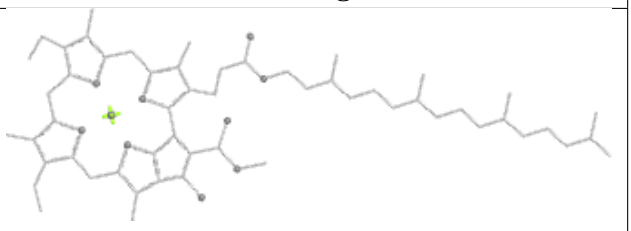
Bond lengths



Bond angles

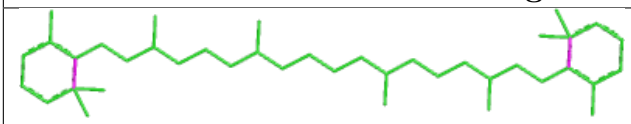


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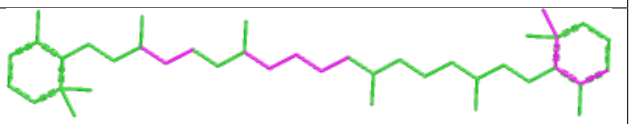


Rings

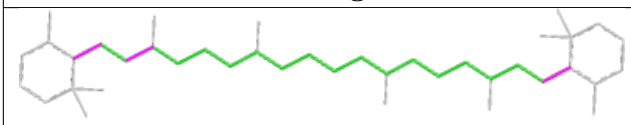
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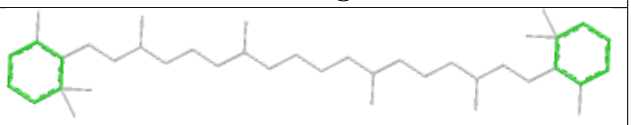
Bond lengths



Bond angles

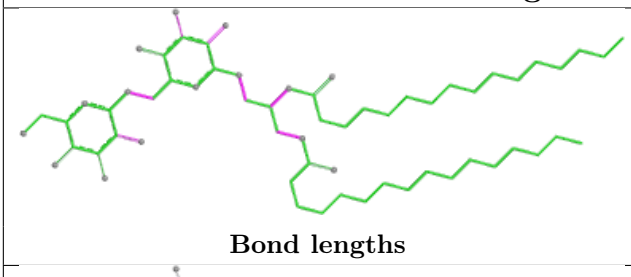


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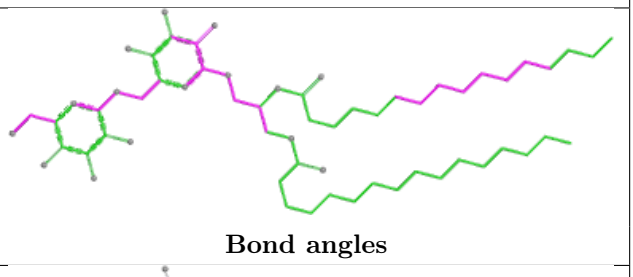


Rings

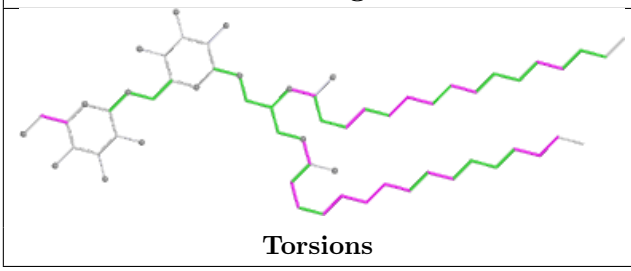
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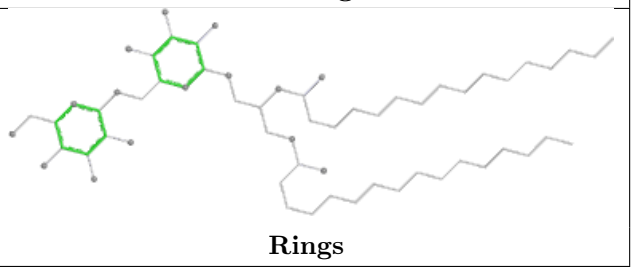
Bond lengths



Bond angles

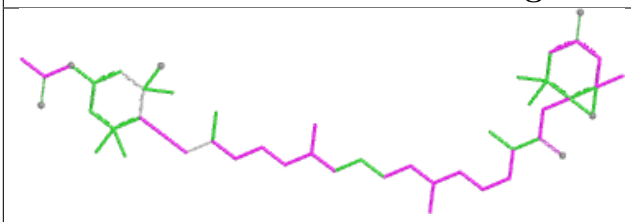


Torsions

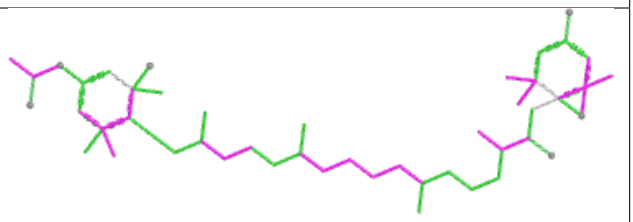


Rings

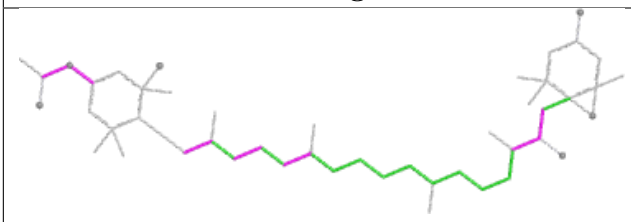
## Ligand A86 32 216



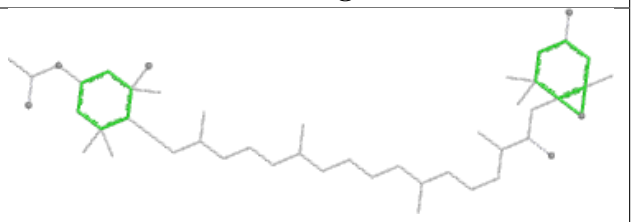
Bond lengths



Bond angles

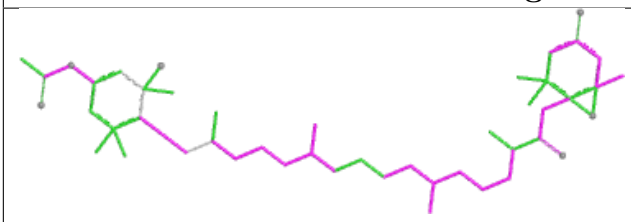


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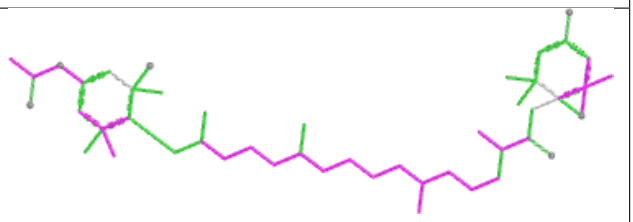


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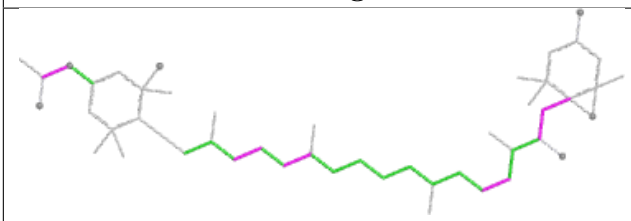
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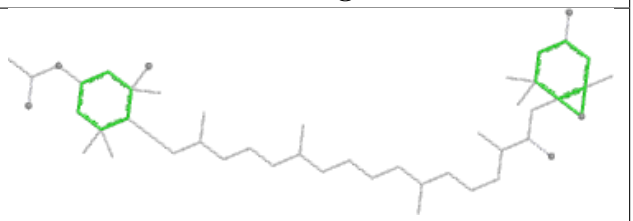
Bond lengths



Bond angles

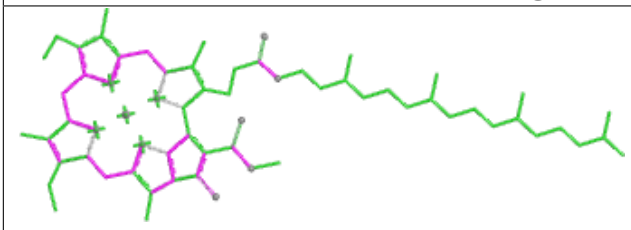


Torsions

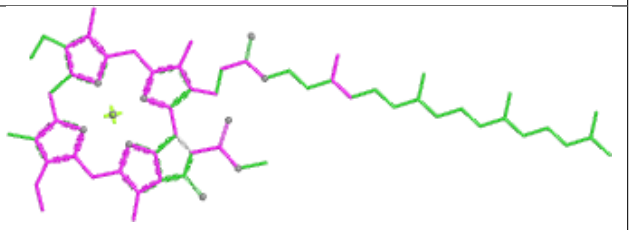


Rings

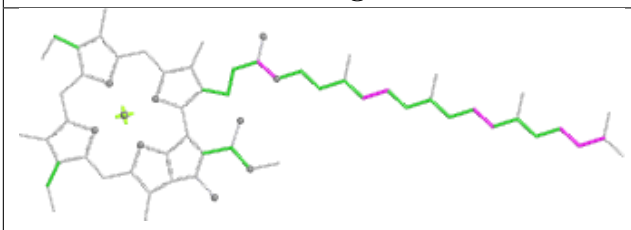
**Ligand CLA c 512**



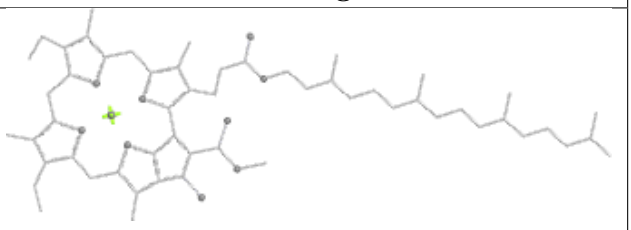
Bond lengths



Bond angles

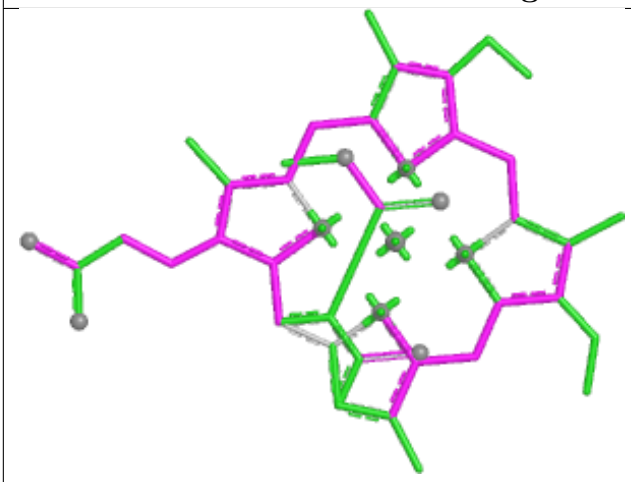


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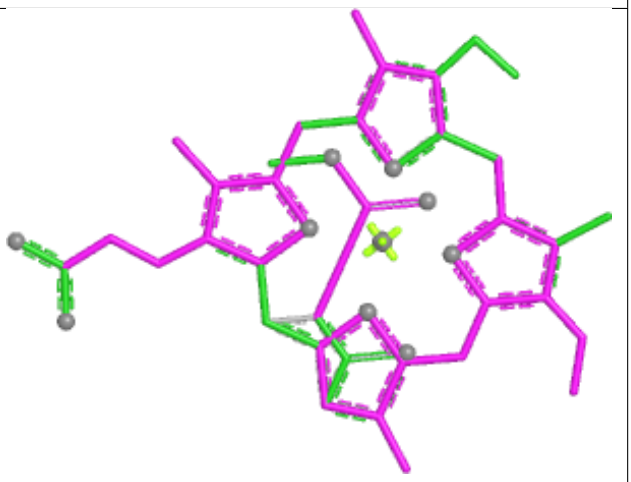


Rings

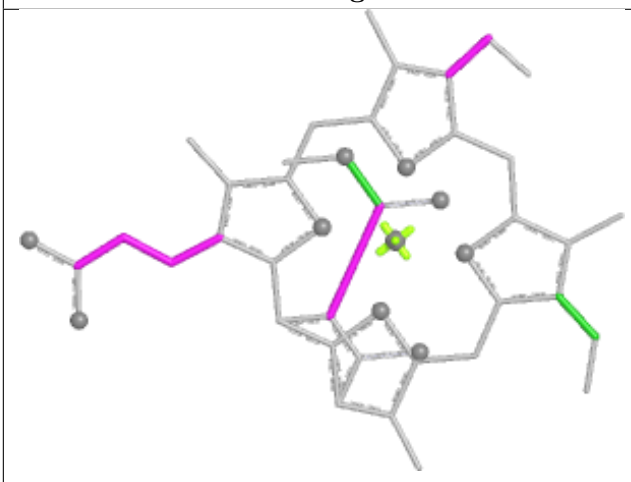
**Ligand KC1 18 210**



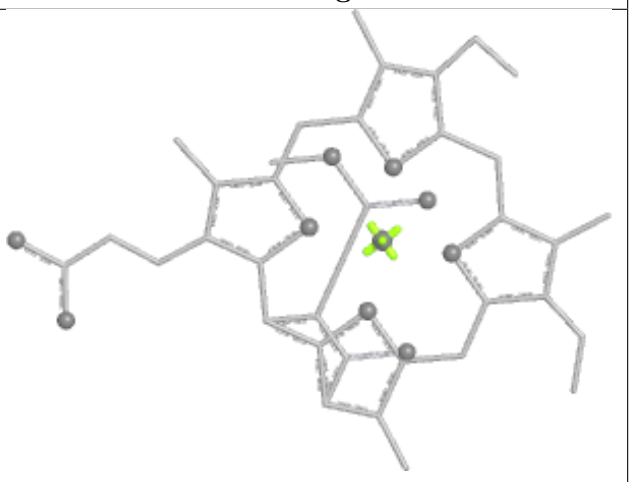
Bond lengths



Bond angles

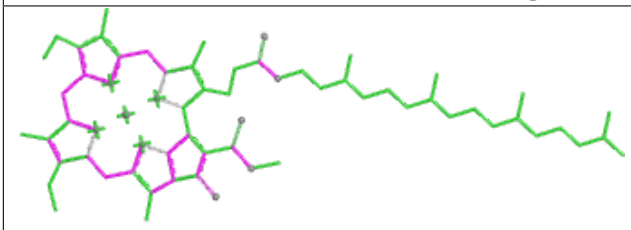


Torsions

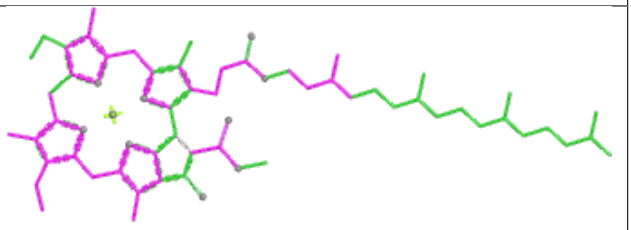


Rings

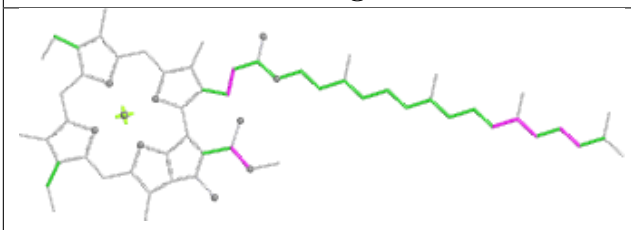
**Ligand CLA B 510**



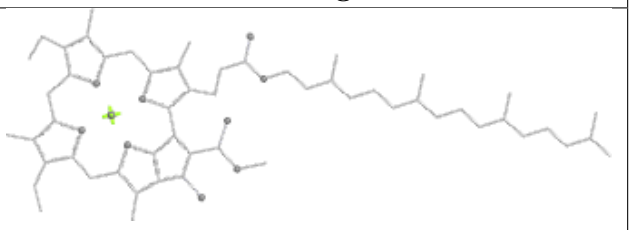
Bond lengths



Bond angles

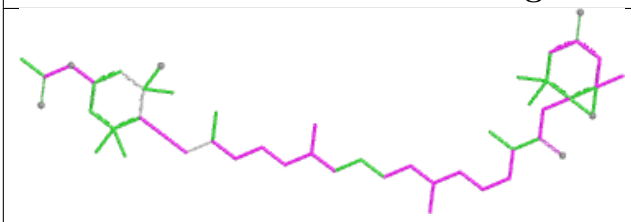


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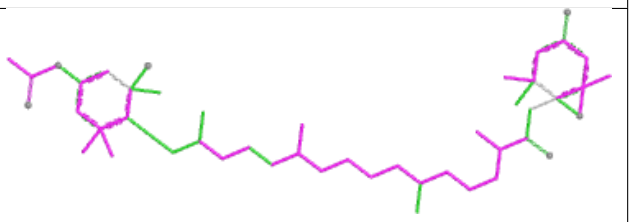


Rings

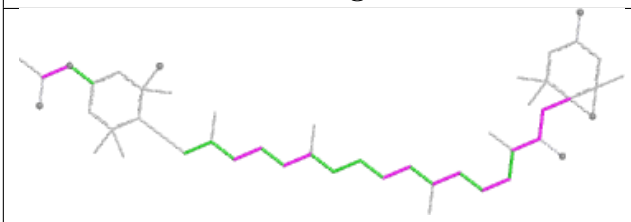
**Ligand A86 35 316**



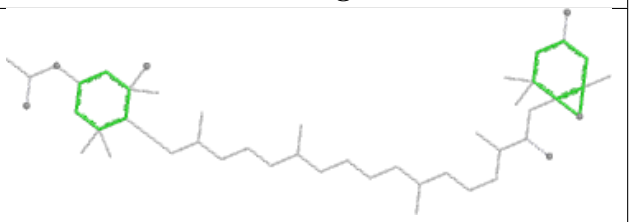
Bond lengths



Bond angles

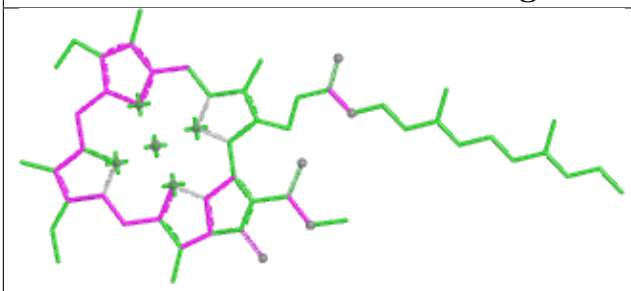


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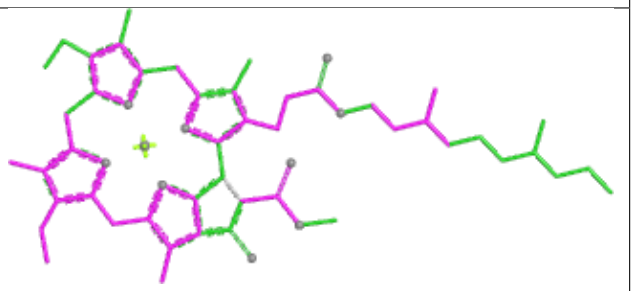


Rings

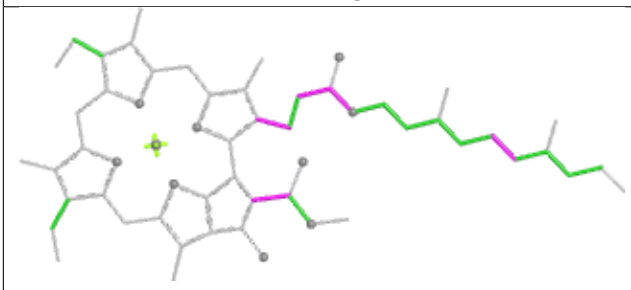
## Ligand CLA 35 303



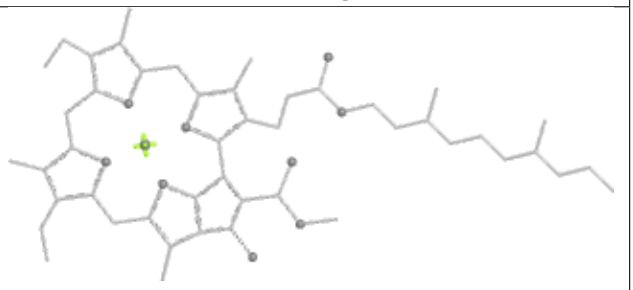
Bond lengths



Bond angles

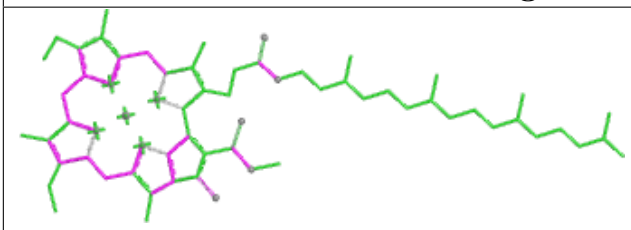


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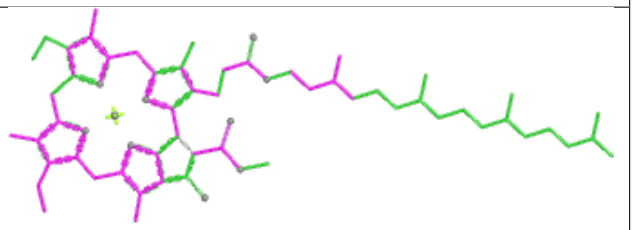


Rings

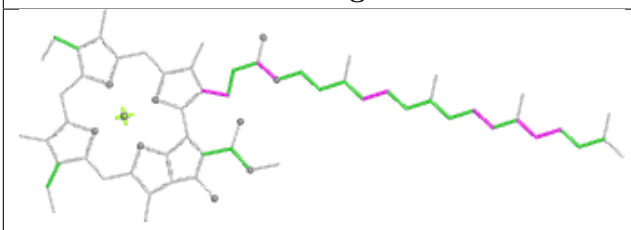
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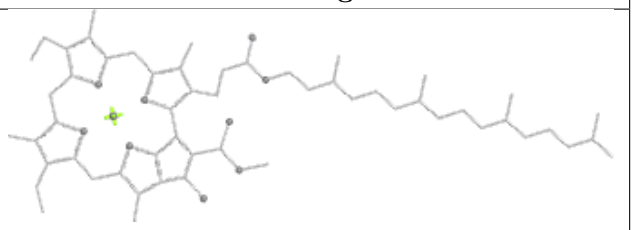
Bond lengths



Bond angles

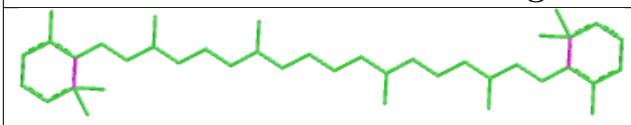


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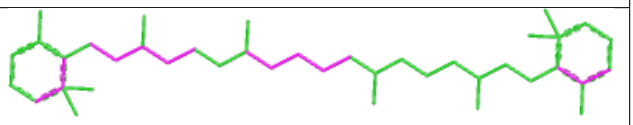


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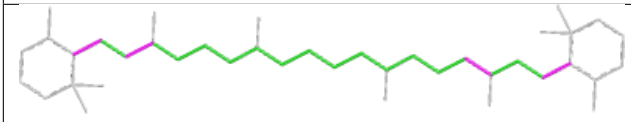
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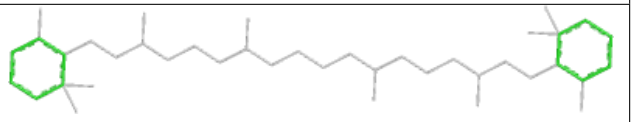
Bond lengths



Bond angles

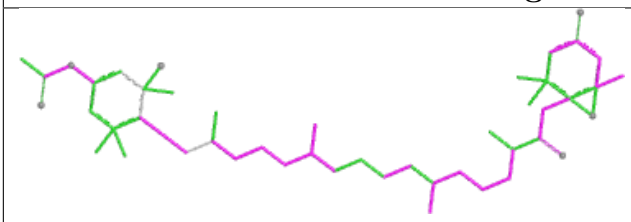


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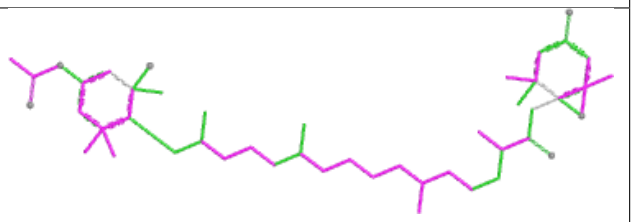


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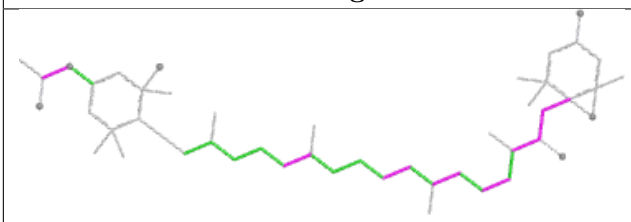
## Ligand A86 12 217



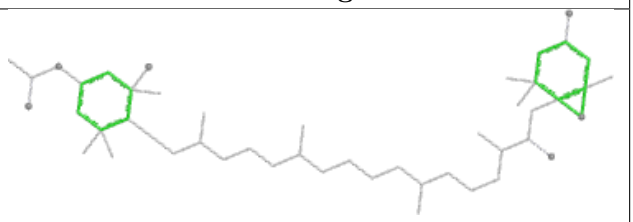
Bond lengths



Bond angles

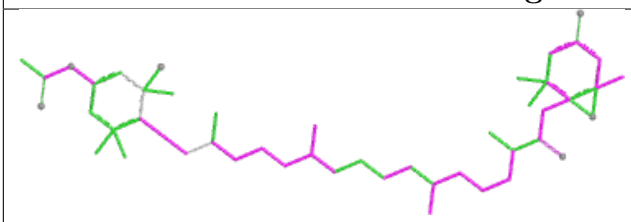


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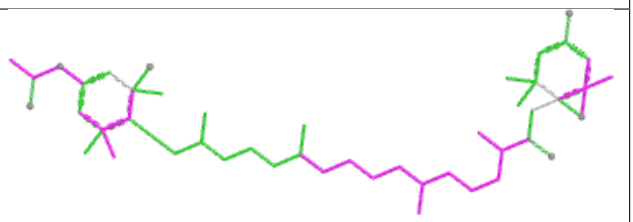


Rings

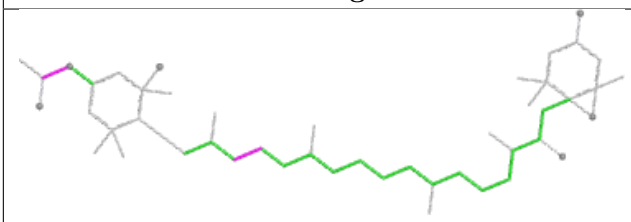
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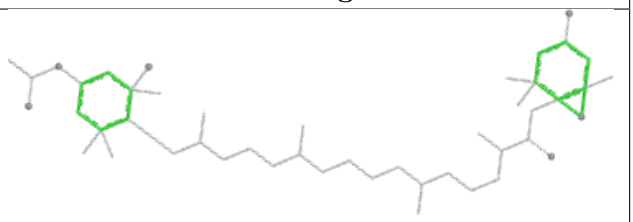
Bond lengths



Bond angles

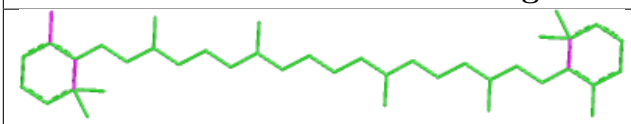


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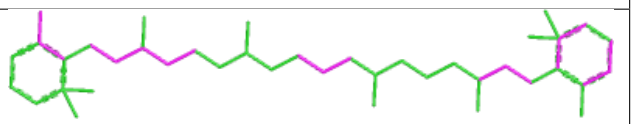


Rings

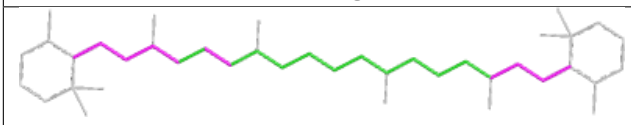
## Ligand BCR D 407



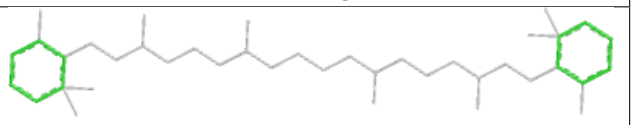
Bond lengths



Bond angles

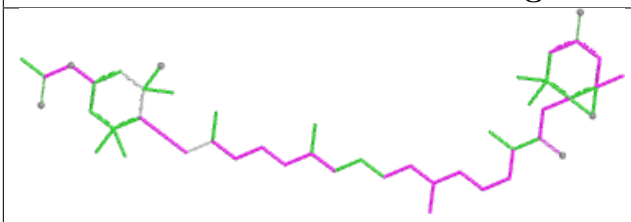


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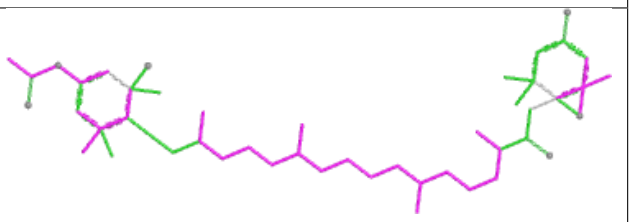


Rings

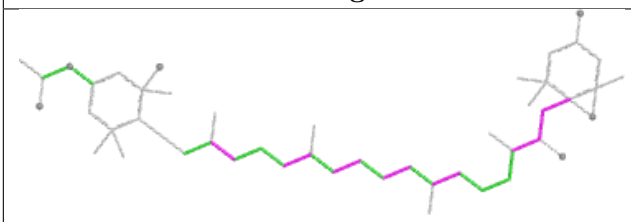
## Ligand A86 16 313



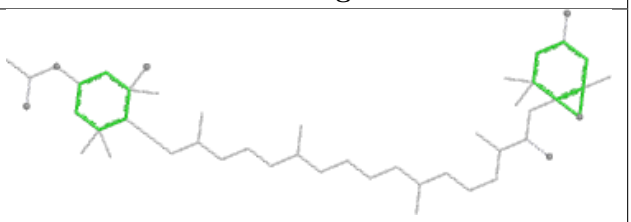
Bond lengths



Bond angles

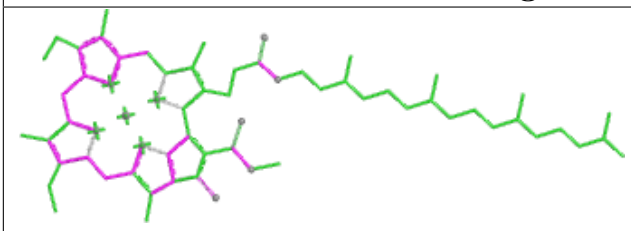


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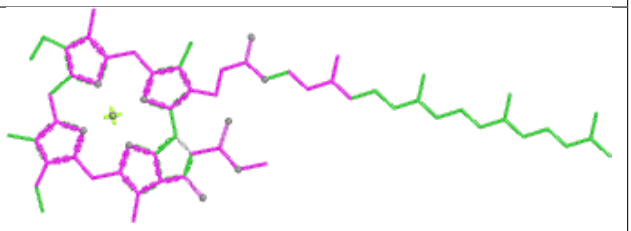


Rings

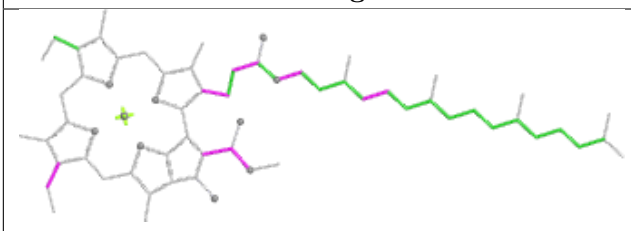
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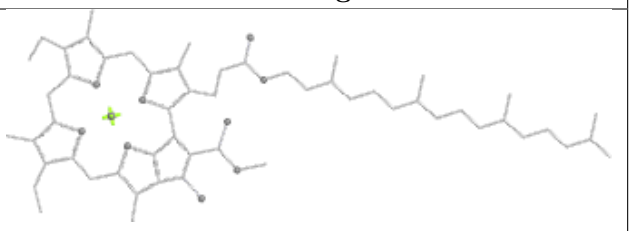
Bond lengths



Bond angles

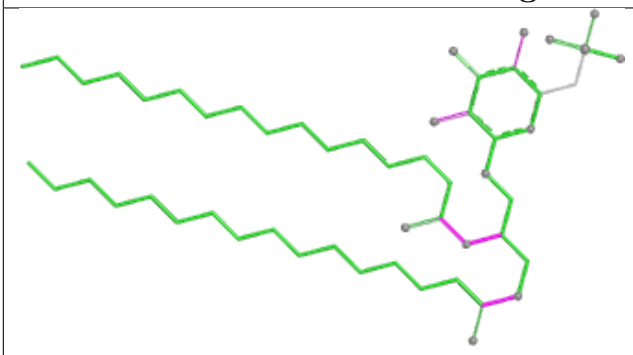


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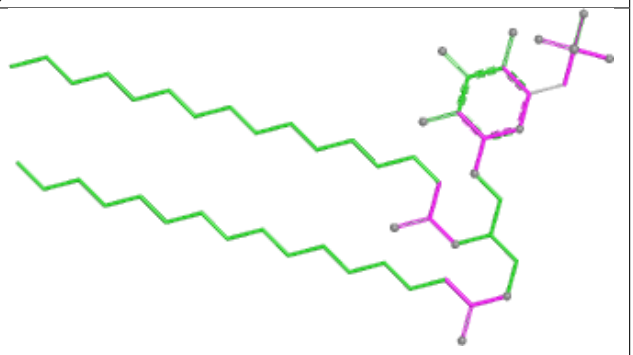


Rings

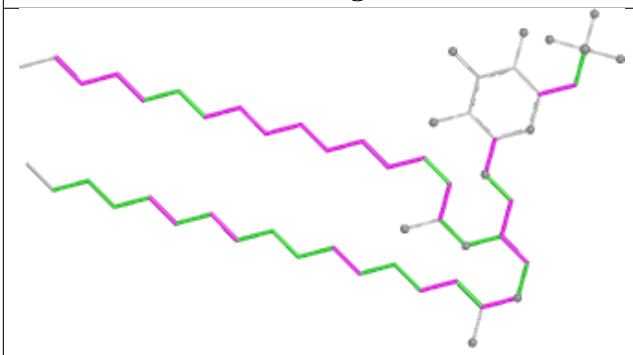
## Ligand SQD 16 315



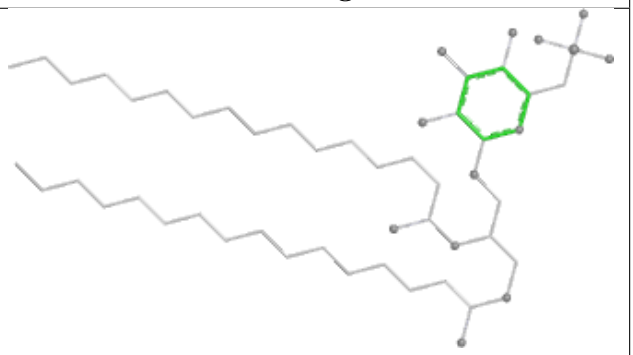
Bond lengths



Bond angles

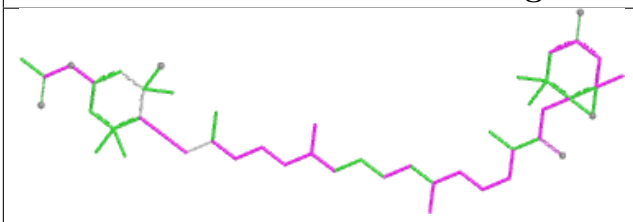


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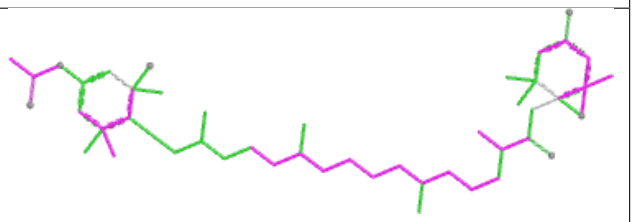


Rings

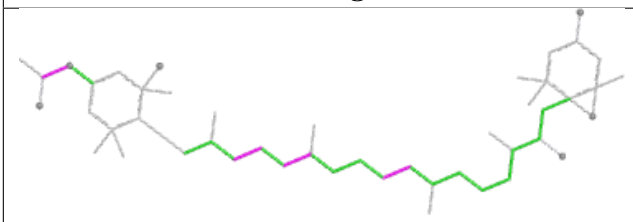
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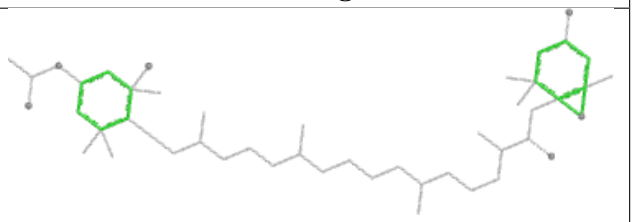
Bond lengths



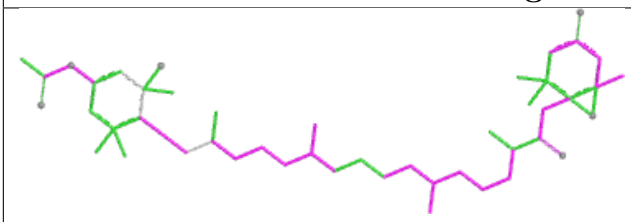
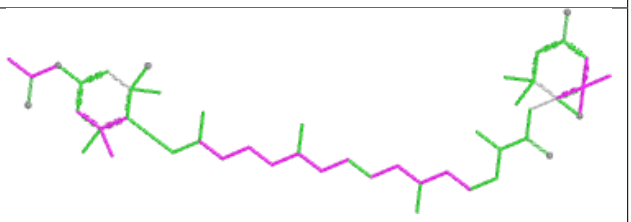
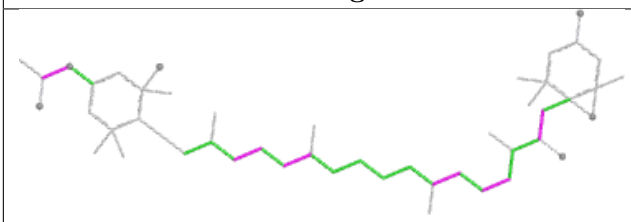
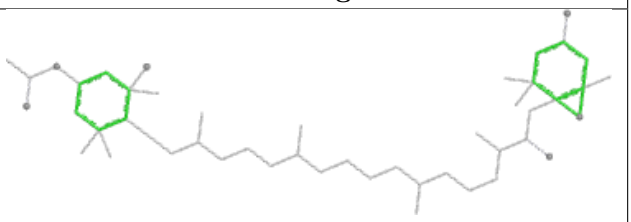
Bond angles

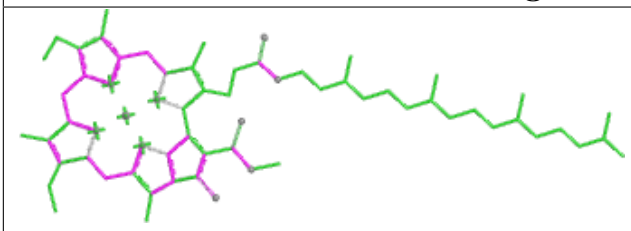
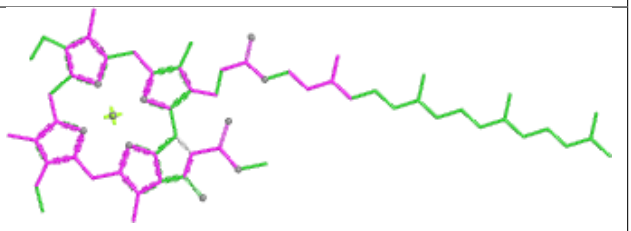
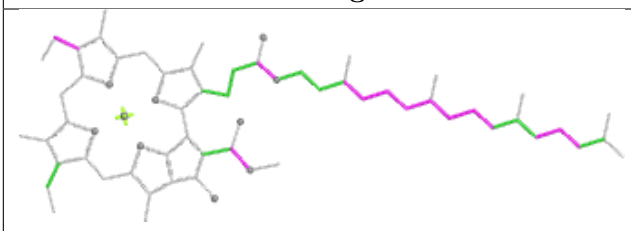
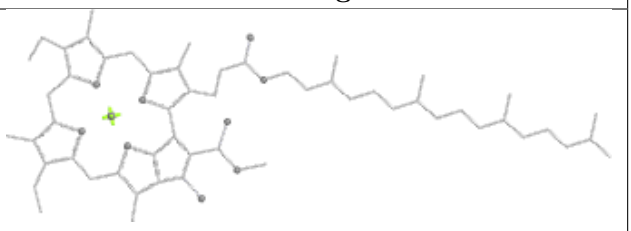


Torsions

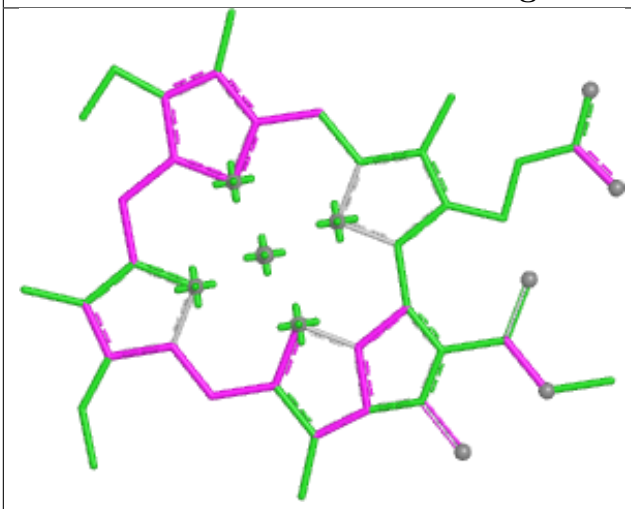


Rings

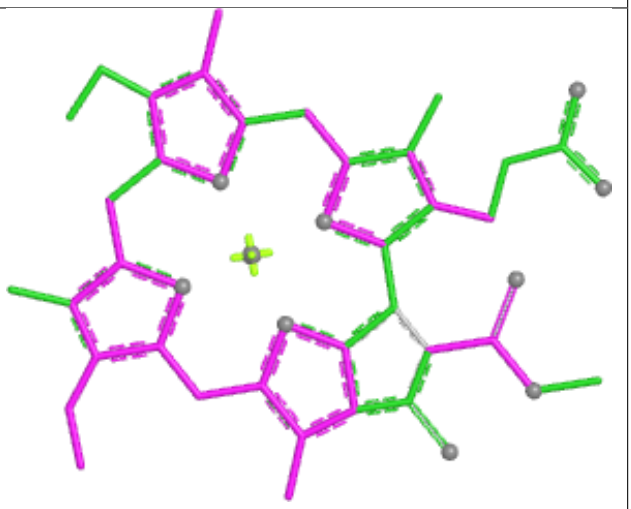
| Ligand A86 41 211 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA w 101 | |
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|  Bond lengths |  Bond angles |
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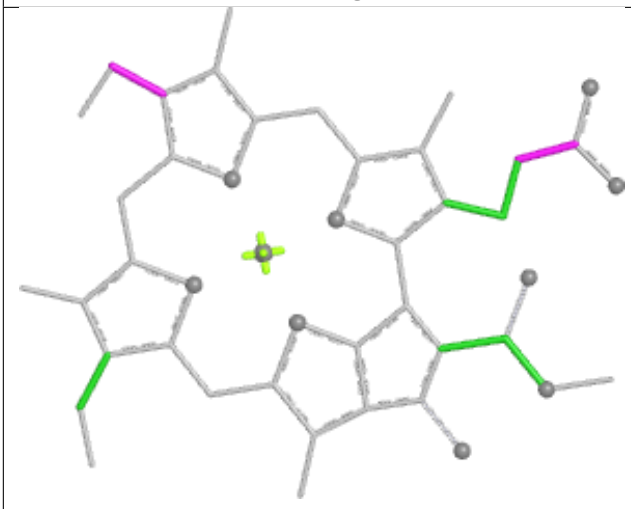
## Ligand CLA 14 310



Bond lengths



Bond angles

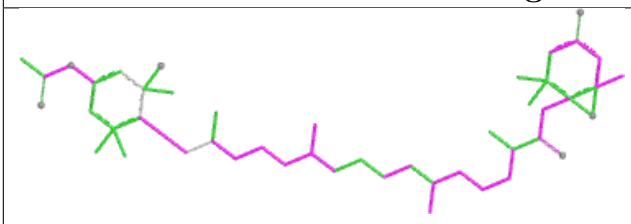


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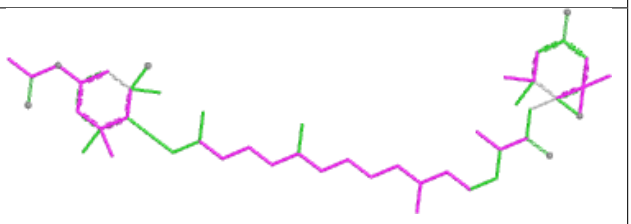


Rings

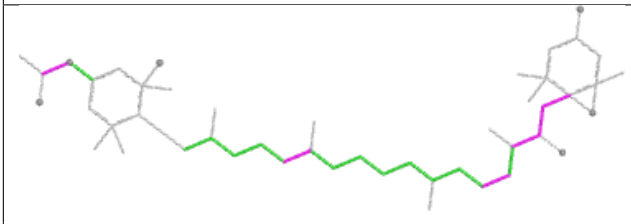
## Ligand A86 17 315



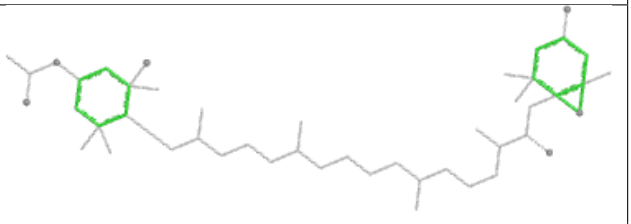
Bond lengths



Bond angles

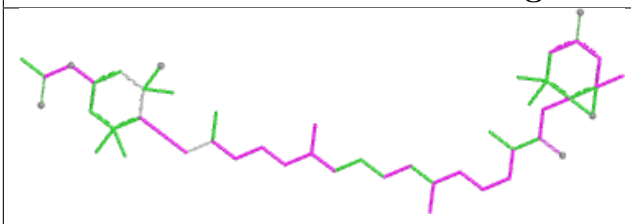


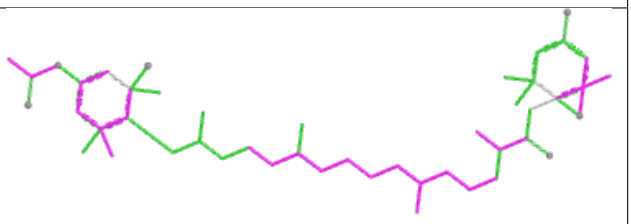
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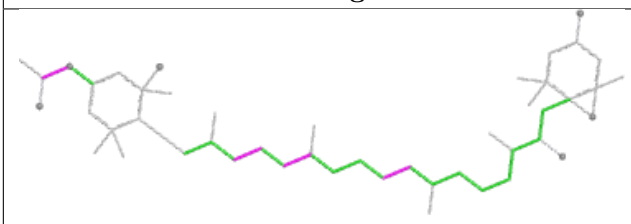


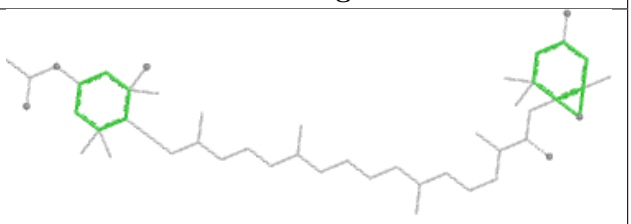
Rings

## Ligand A86 34 315

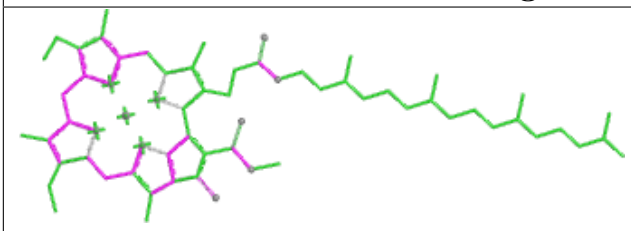

Bond lengths

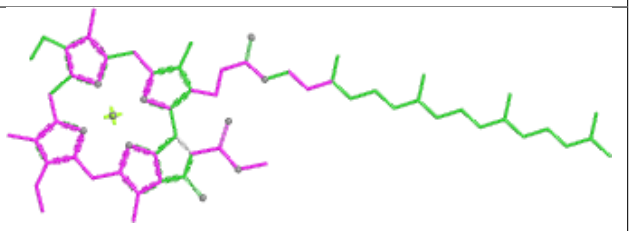

Bond angles

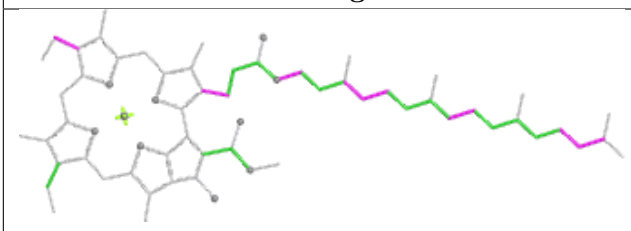

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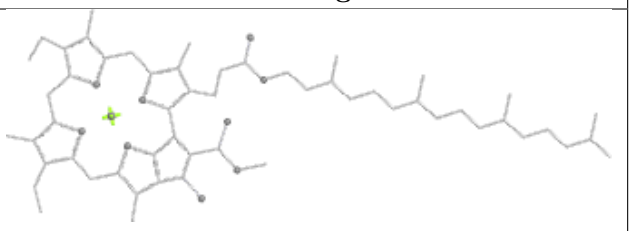

Rings

## Ligand CLA 36 301

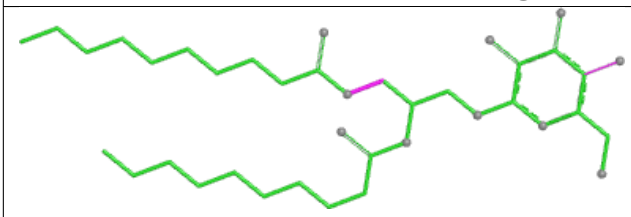

Bond lengths

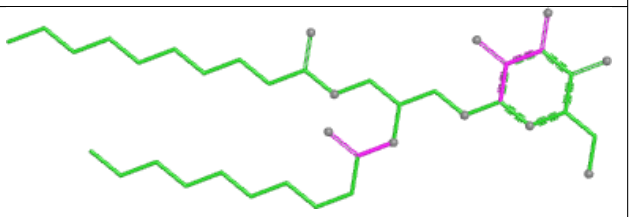

Bond angles

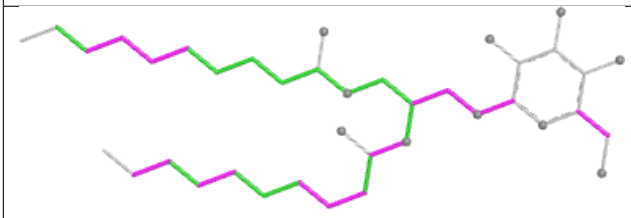

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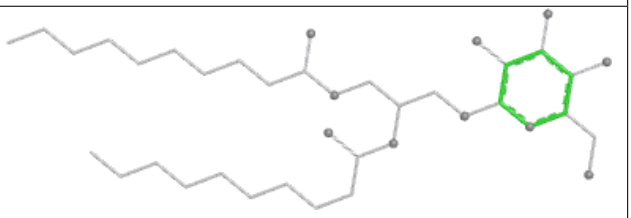

Rings

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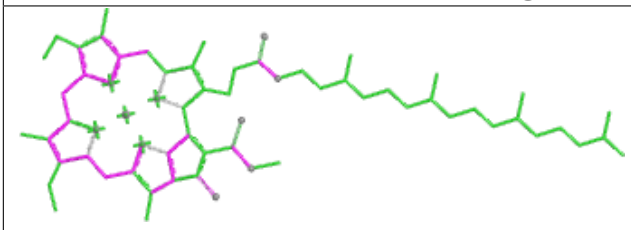

Bond lengths


Bond angles

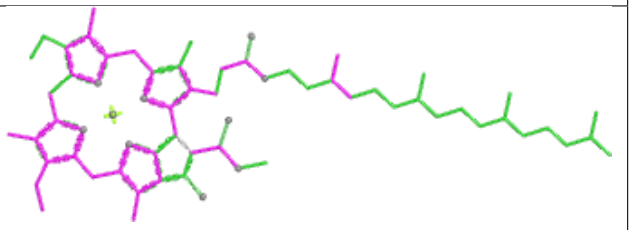

Torsions


Rings

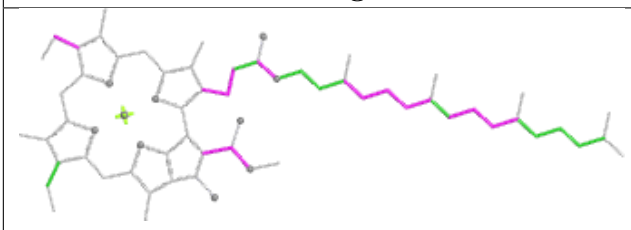
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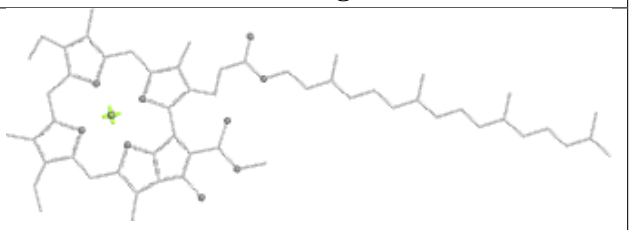
Bond lengths



Bond angles

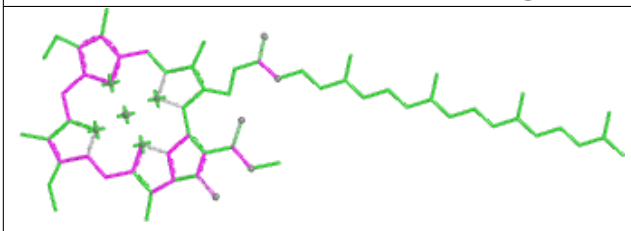


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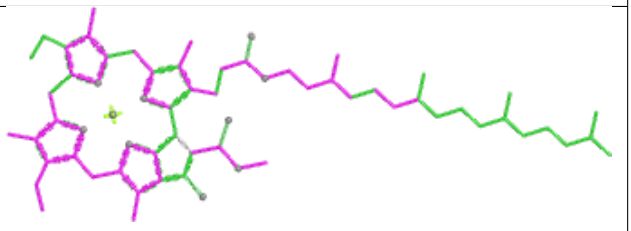


Rings

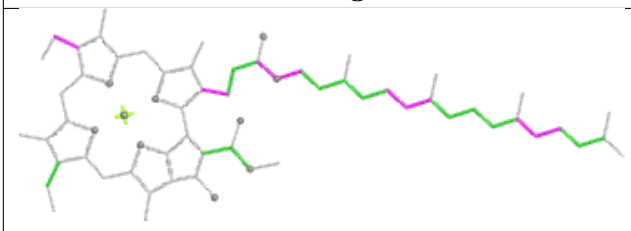
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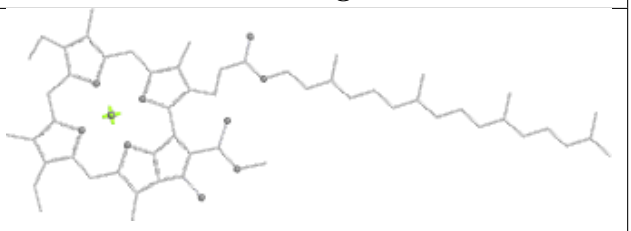
Bond lengths



Bond angles

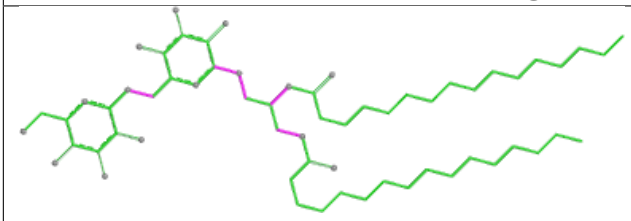


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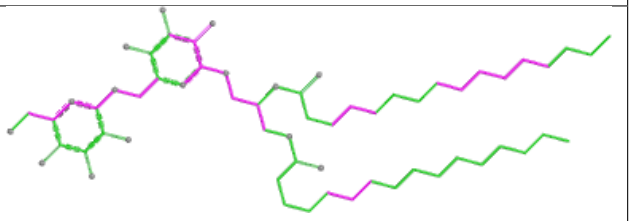


Rings

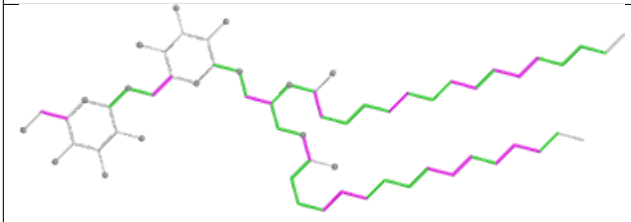
## Ligand DGD c 516



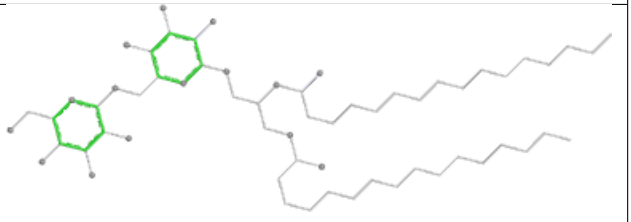
Bond lengths



Bond angles

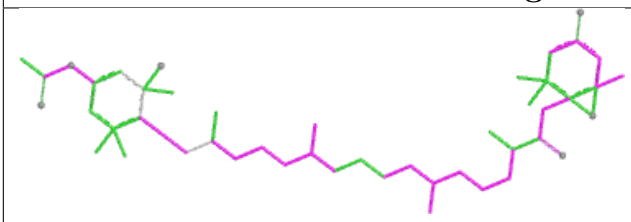


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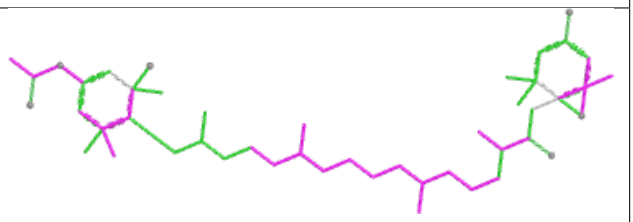


Rings

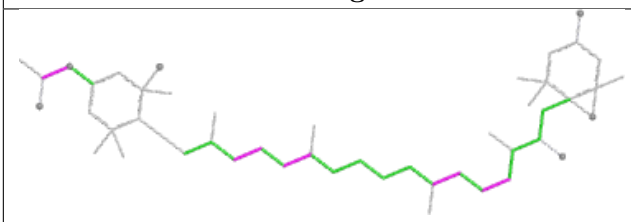
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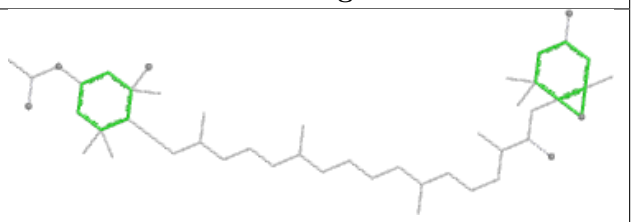
Bond lengths



Bond angles

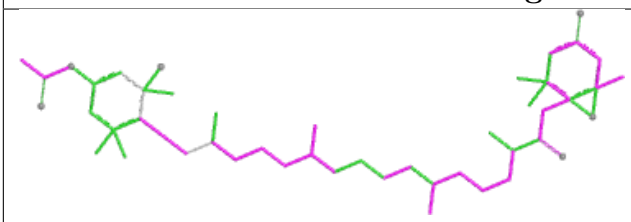


Torsions

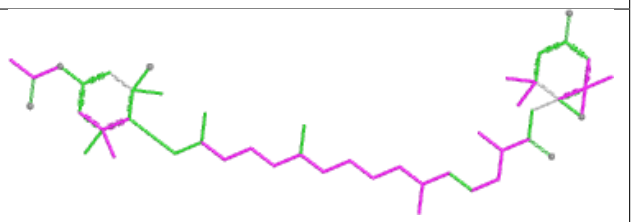


Rings

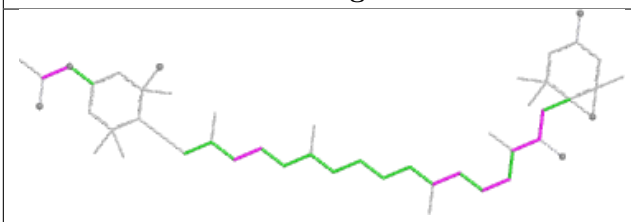
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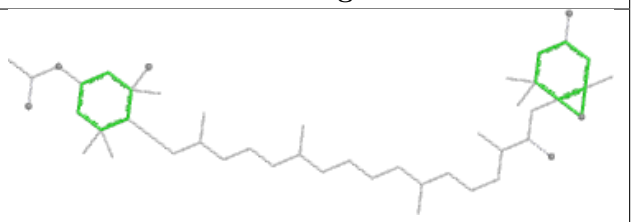
Bond lengths



Bond angles

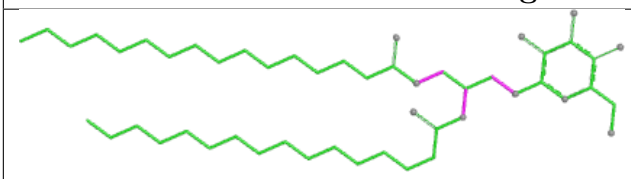


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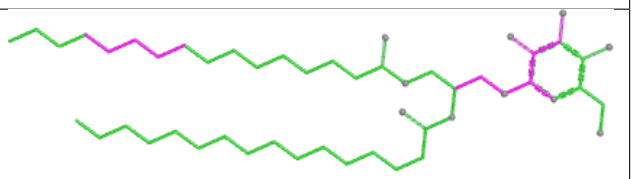


Rings

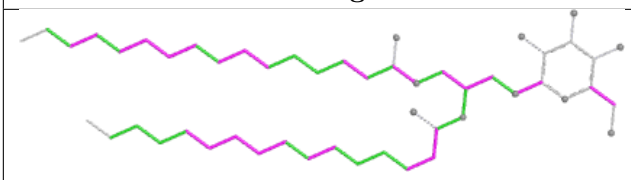
## Ligand LMG C 518



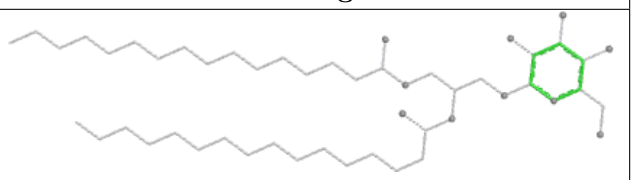
Bond lengths



Bond angles

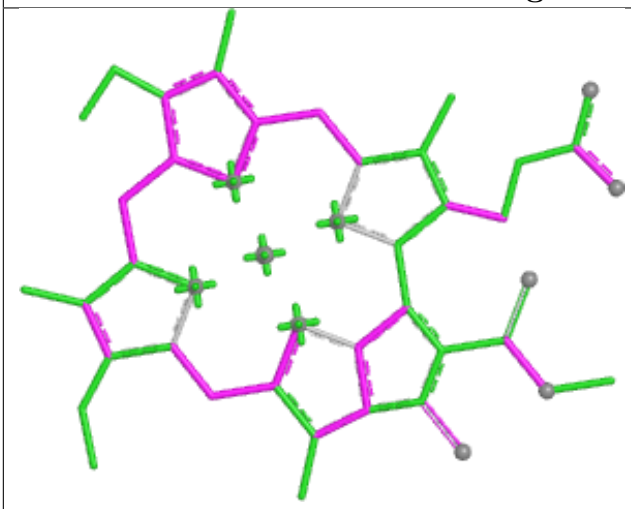


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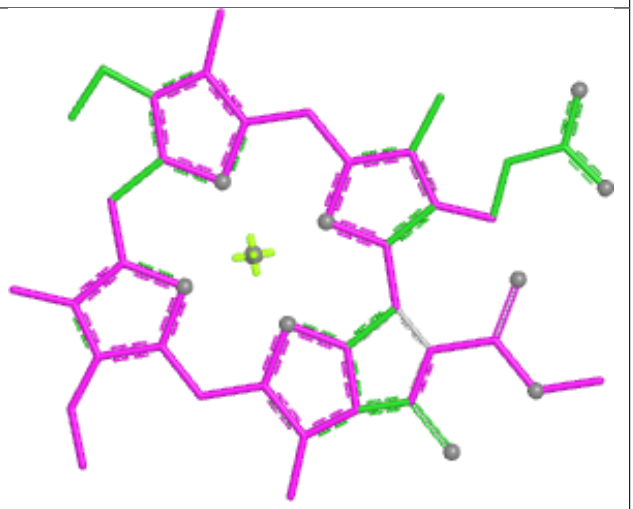


Rings

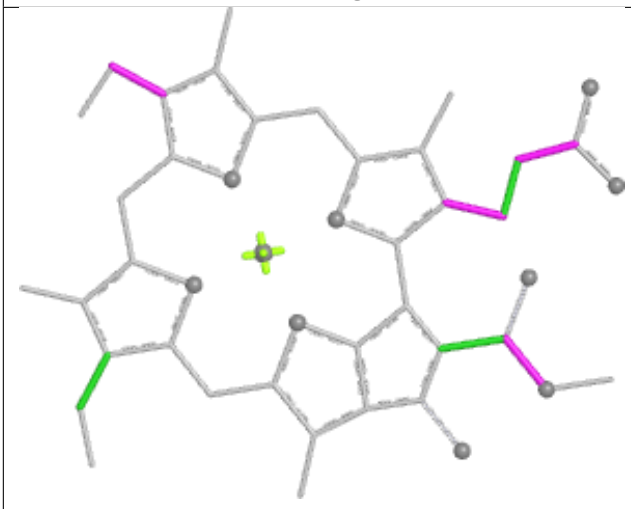
## Ligand CLA Z 102



Bond lengths



Bond angles

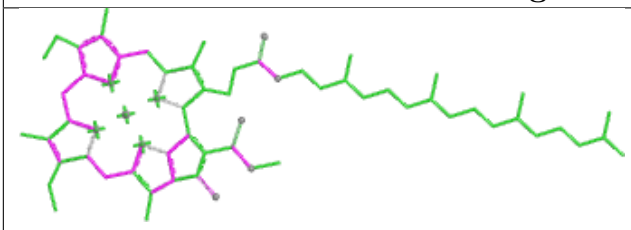


Torsions

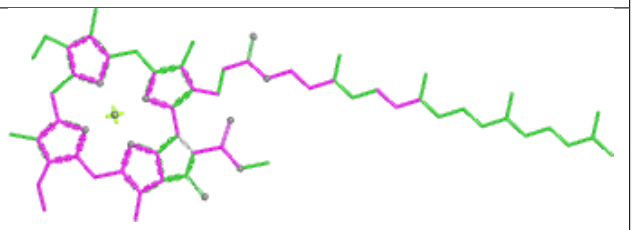


Rings

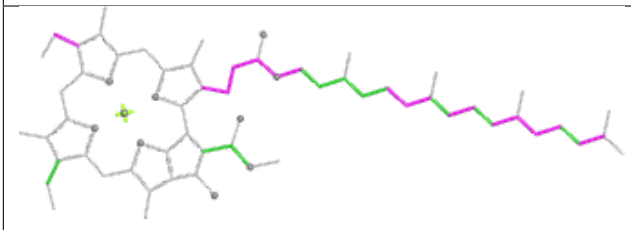
## Ligand CLA z 101



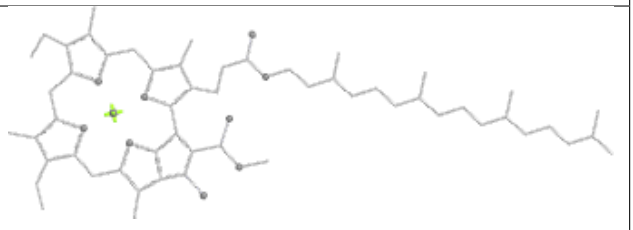
Bond lengths



Bond angles

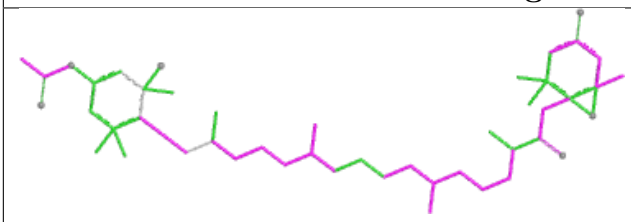


Torsions

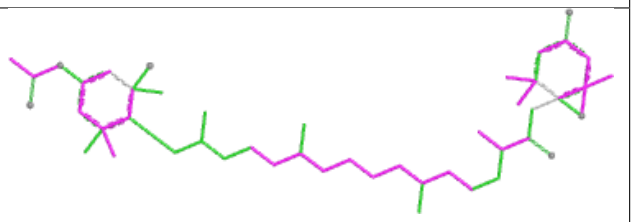


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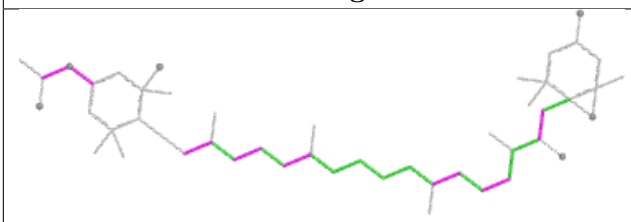
## Ligand A86 14 313



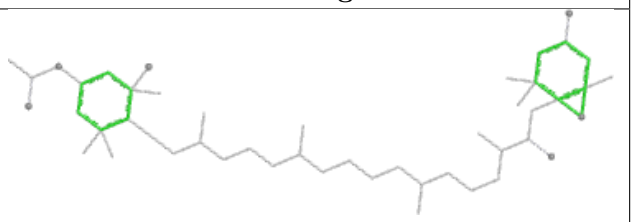
Bond lengths



Bond angles



Torsions

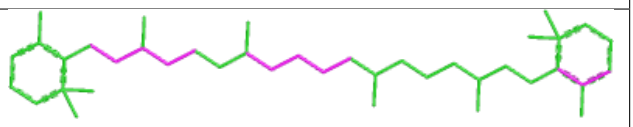


Rings

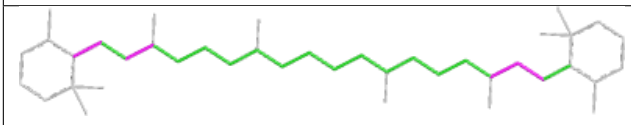
## Ligand BCR H 101



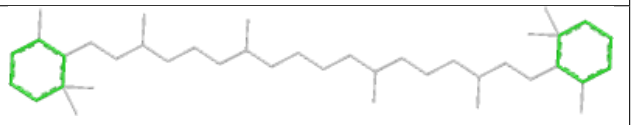
Bond lengths



Bond angles

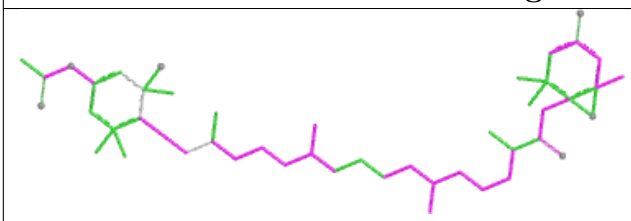


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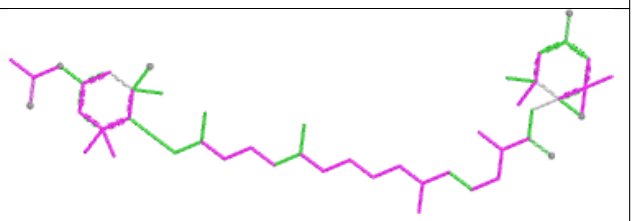


Rings

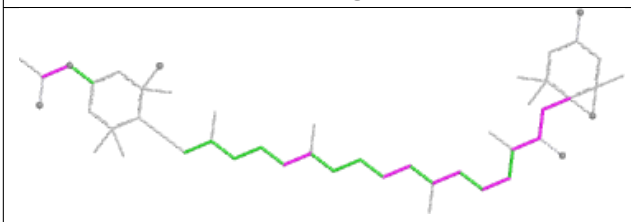
## Ligand A86 14 316



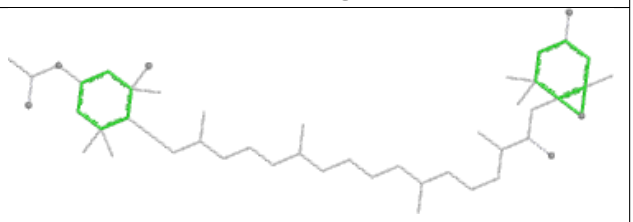
Bond lengths



Bond angles

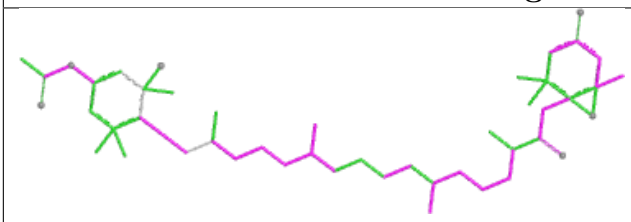


Torsions

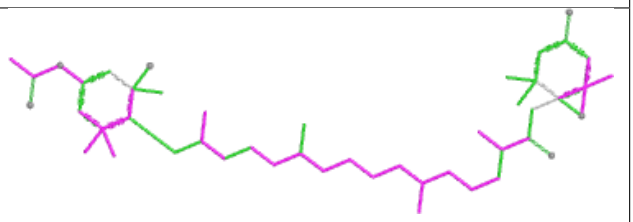


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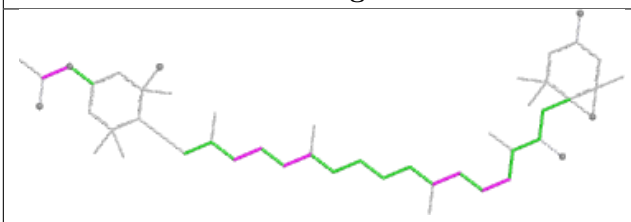
## Ligand A86 17 311



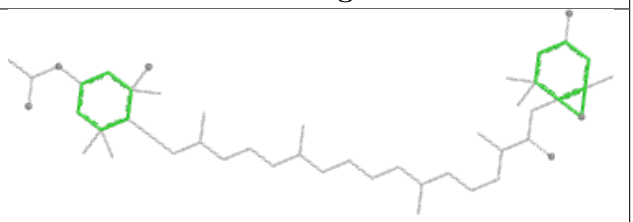
Bond lengths



Bond angles

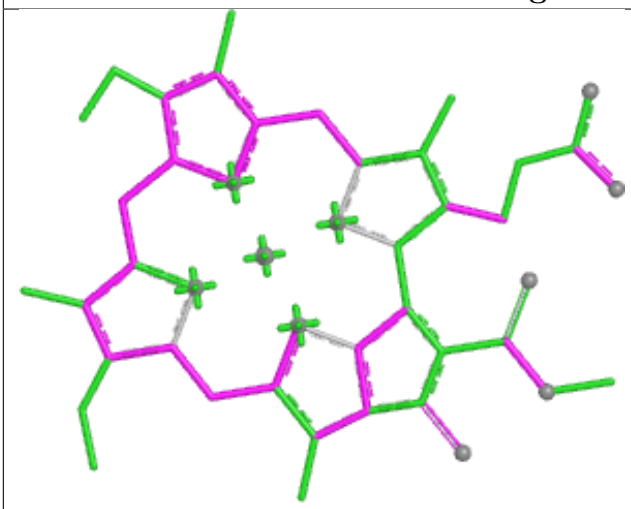


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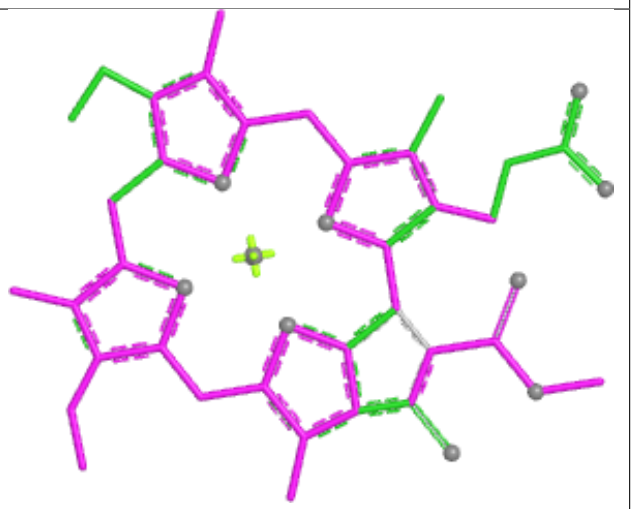


Rings

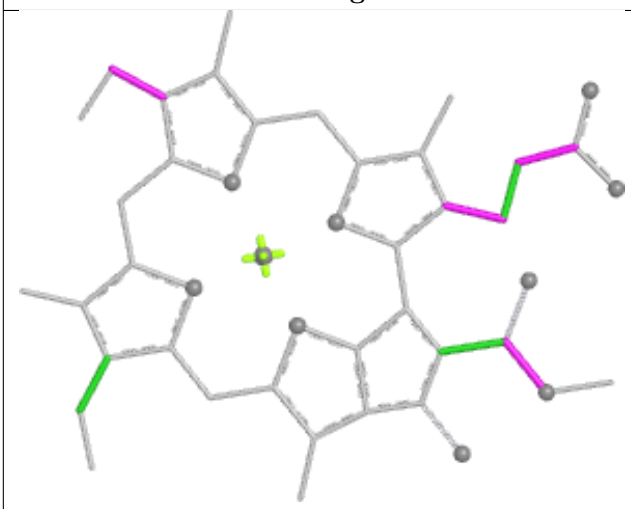
## Ligand CLA z 102



Bond lengths



Bond angles

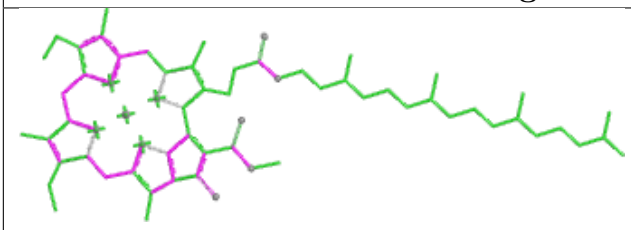


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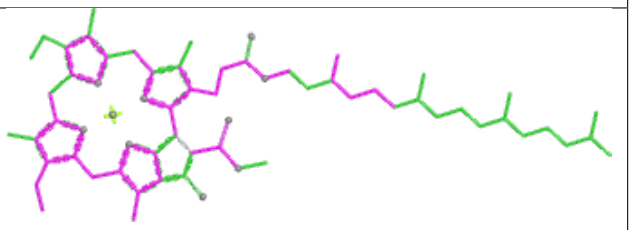


Rings

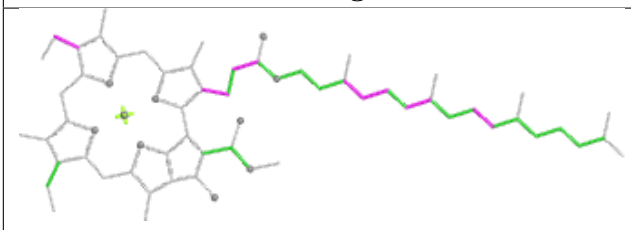
**Ligand CLA 32 206**



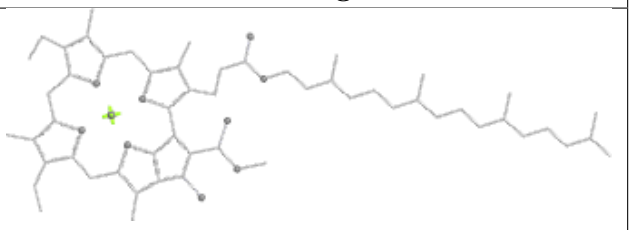
Bond lengths



Bond angles

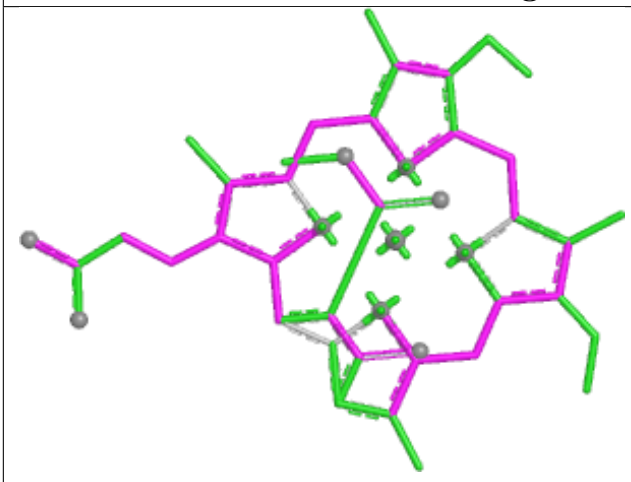


Torsions

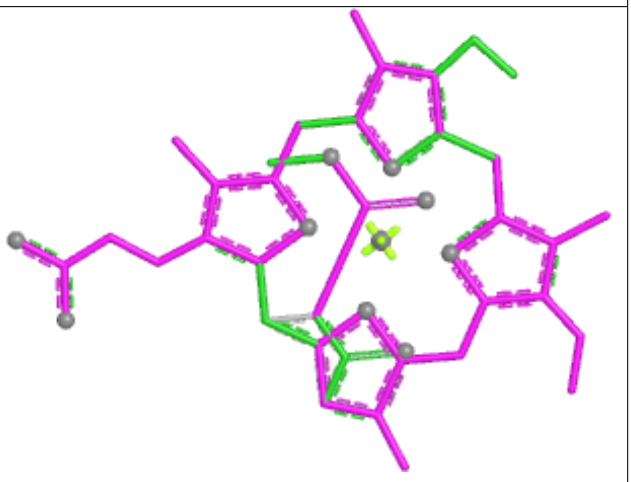


Rings

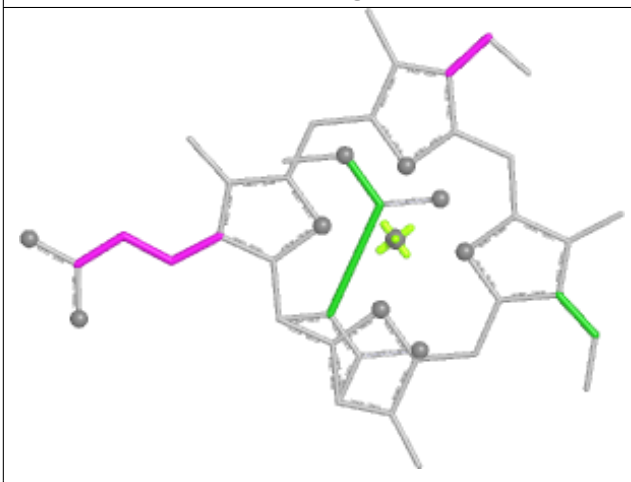
**Ligand KC1 37 304**



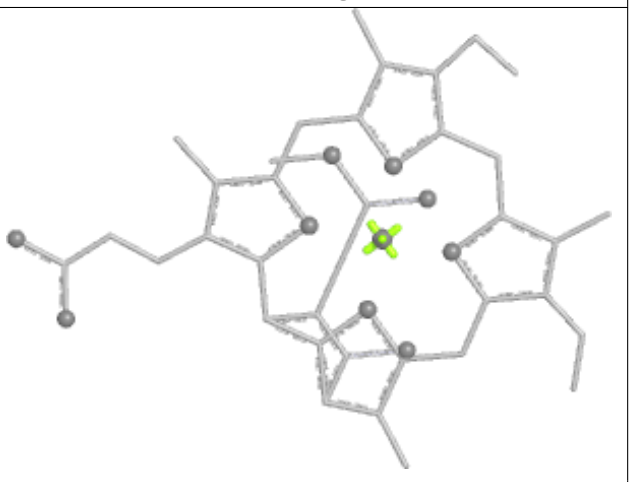
Bond lengths



Bond angles

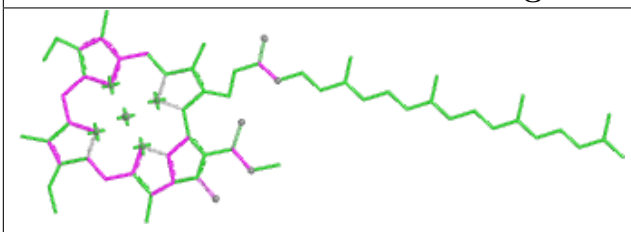


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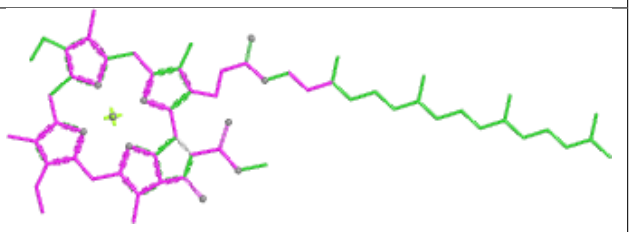


Rings

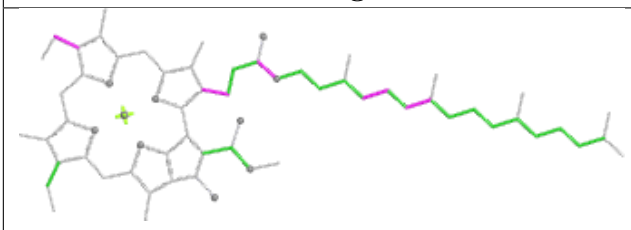
## Ligand CLA C 511



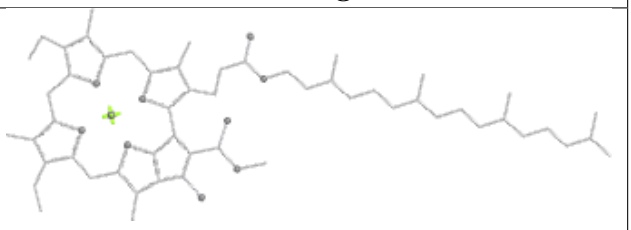
Bond lengths



Bond angles

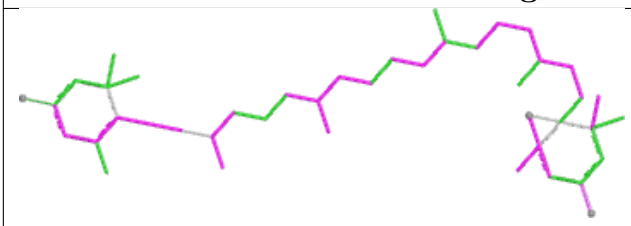


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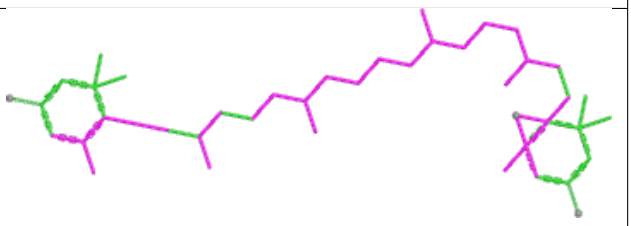


Rings

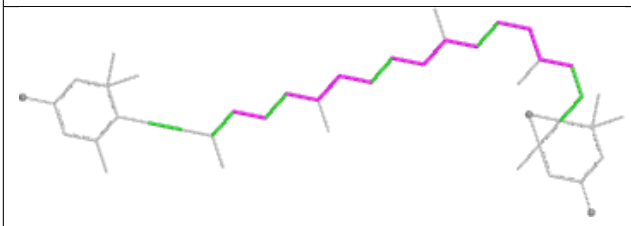
## Ligand DD6 20 310



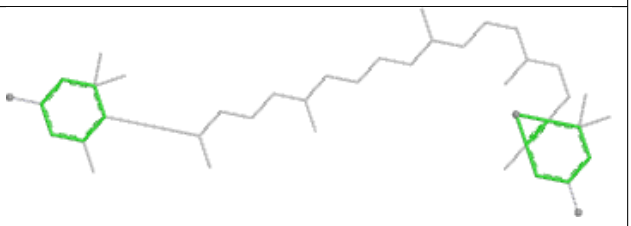
Bond lengths



Bond angles

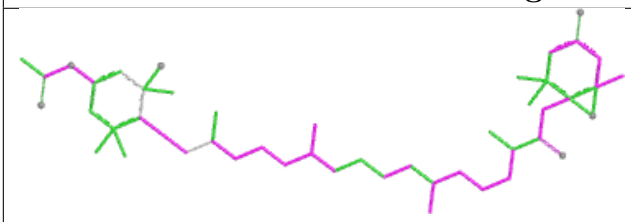


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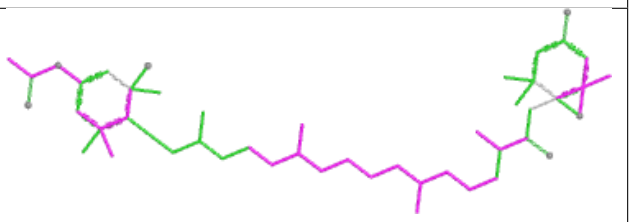


Rings

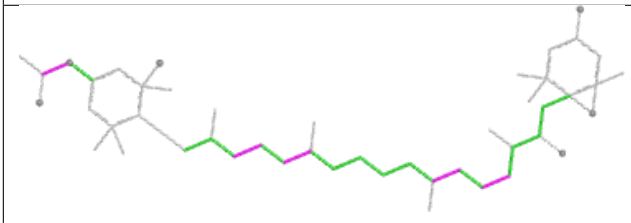
## Ligand A86 33 312



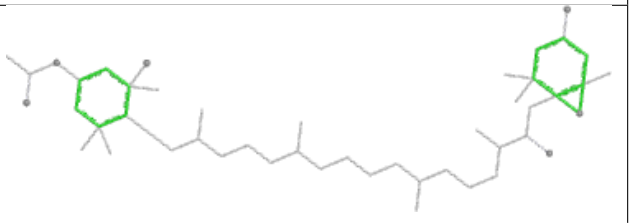
Bond lengths



Bond angles

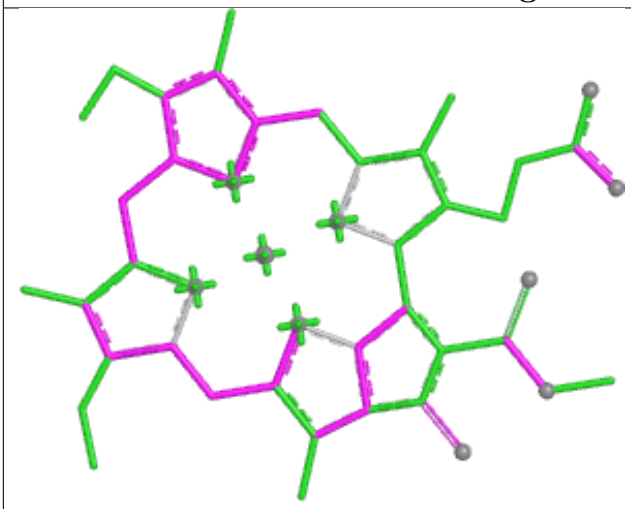


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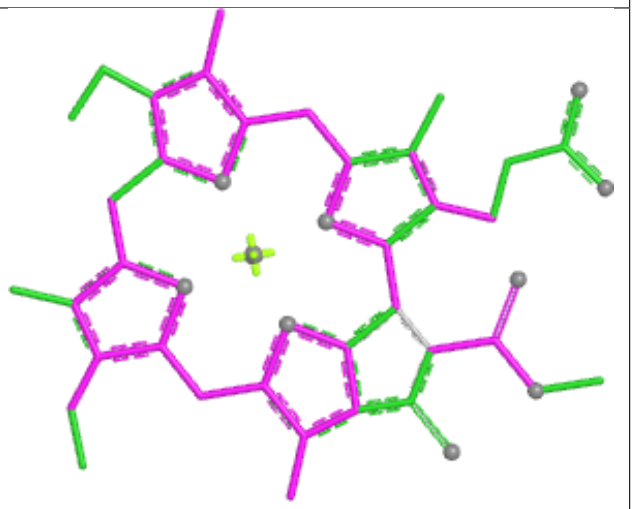


Rings

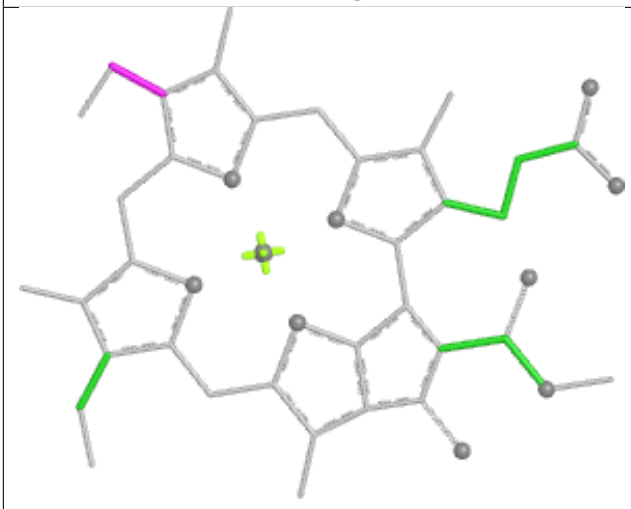
## Ligand CLA 33 310



Bond lengths



Bond angles

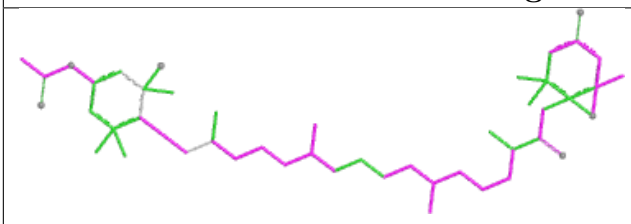


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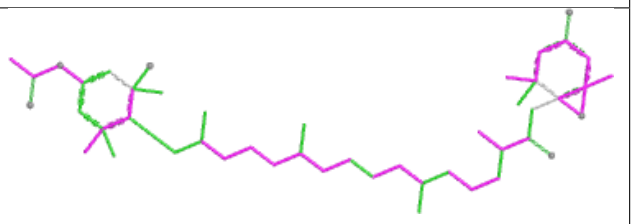


Rings

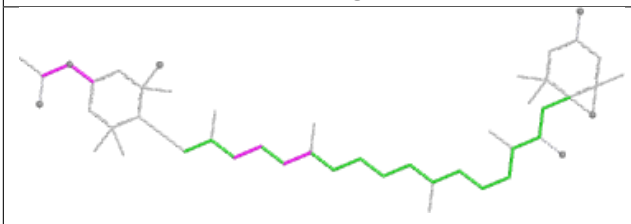
## Ligand A86 21 215



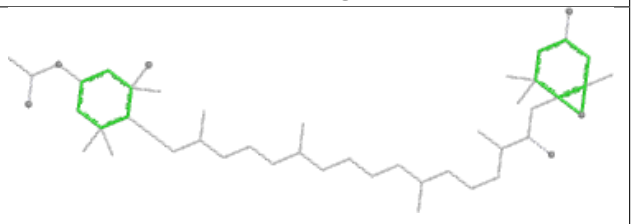
Bond lengths



Bond angles

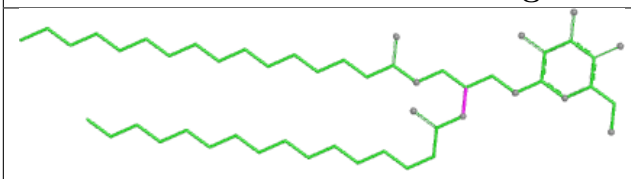


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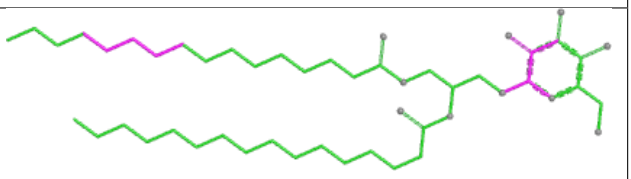


Rings

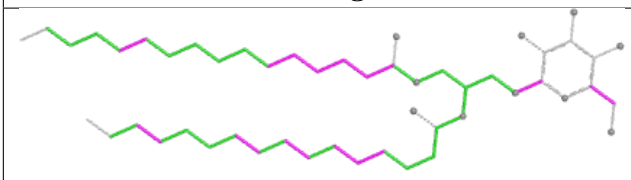
**Ligand LMG b 519**



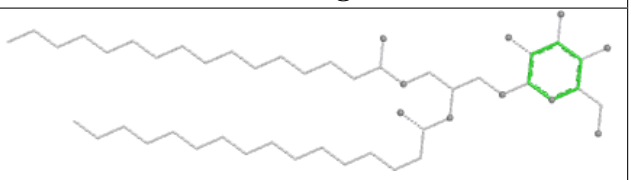
Bond lengths



Bond angles

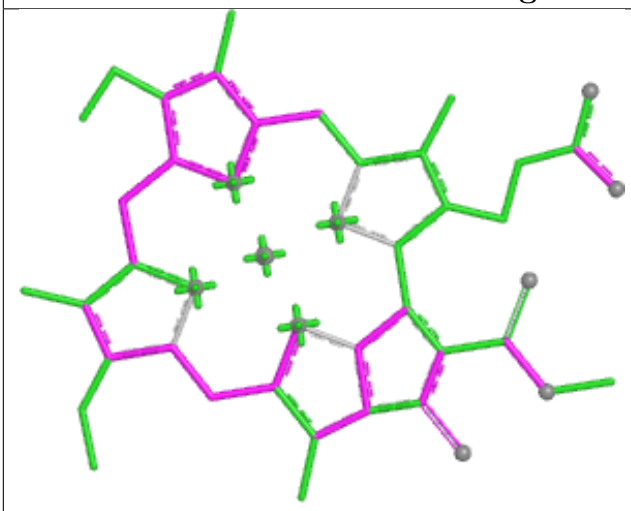


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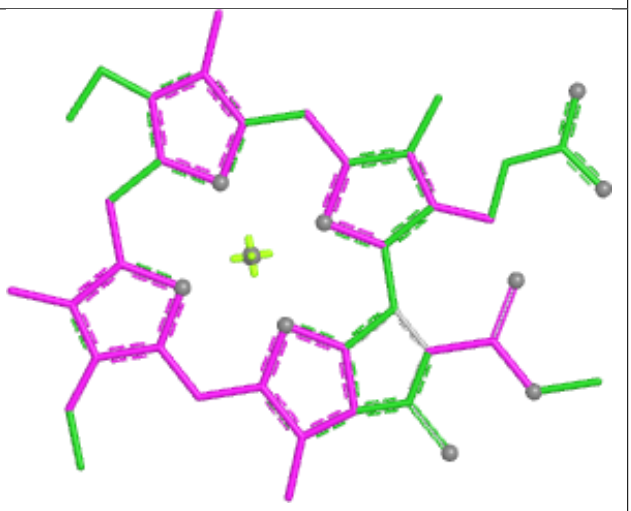


Rings

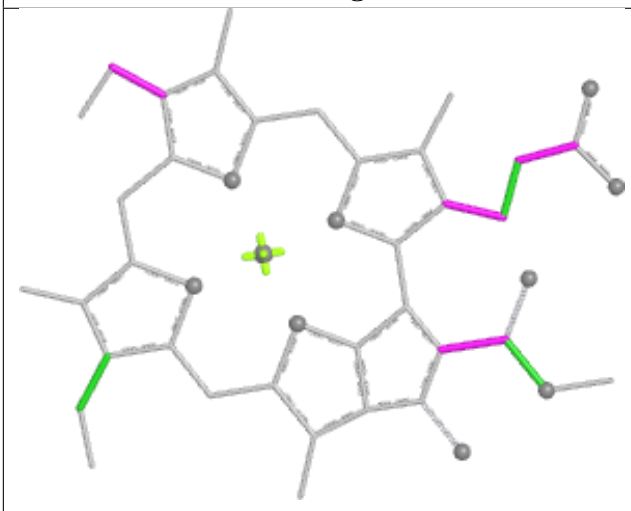
**Ligand CLA 39 304**



Bond lengths



Bond angles

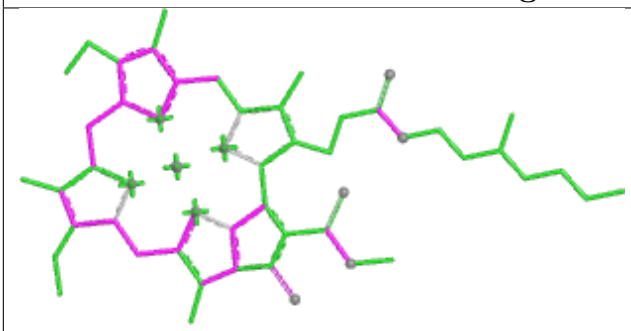


Torsions

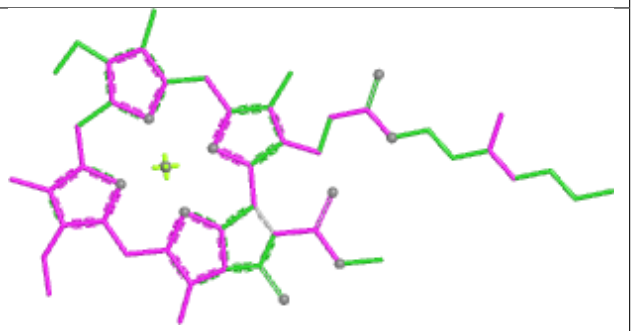


Rings

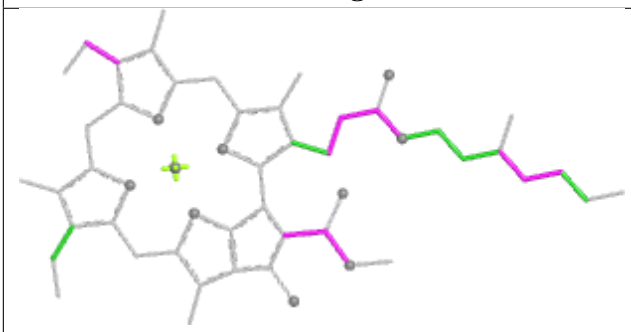
## Ligand CLA 18 208



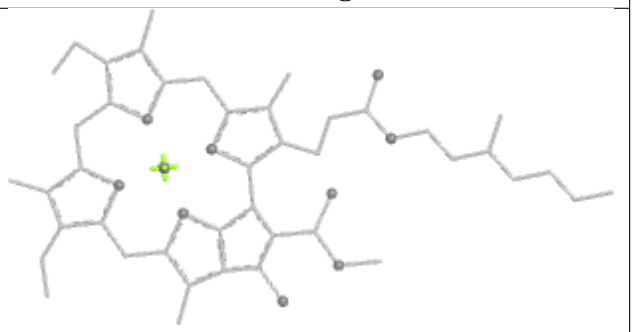
Bond lengths



Bond angles

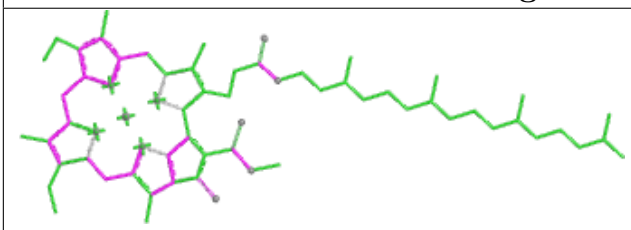


Torsions

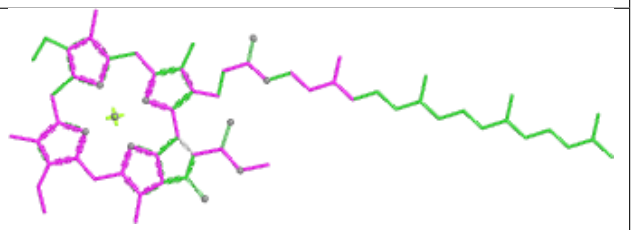


Rings

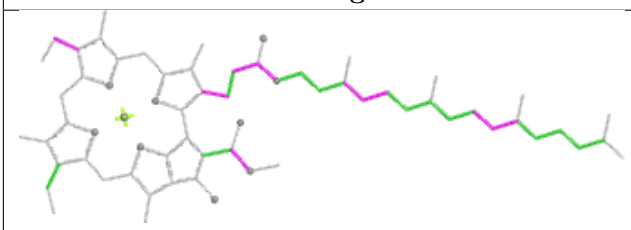
## Ligand CLA 21 206



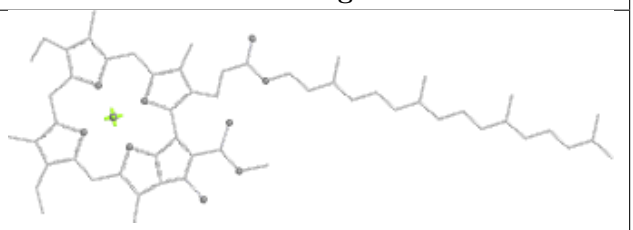
Bond lengths



Bond angles

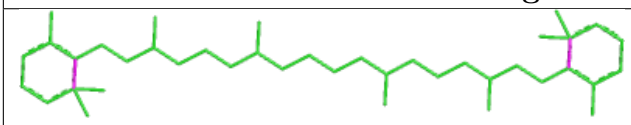


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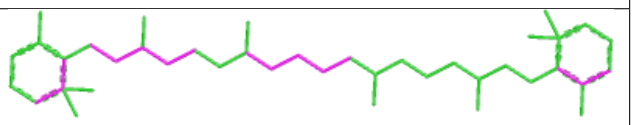


Rings

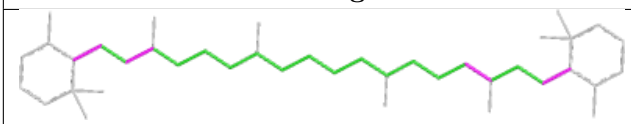
## Ligand BCR C 515



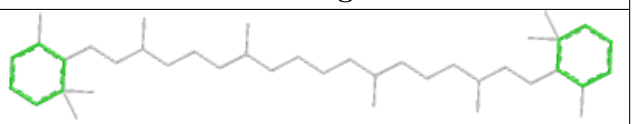
Bond lengths



Bond angles

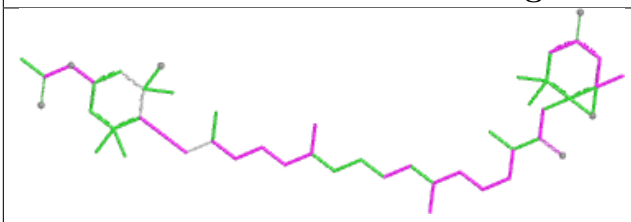


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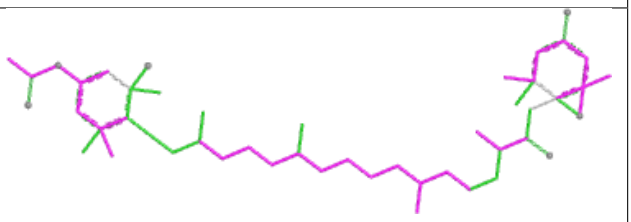


Rings

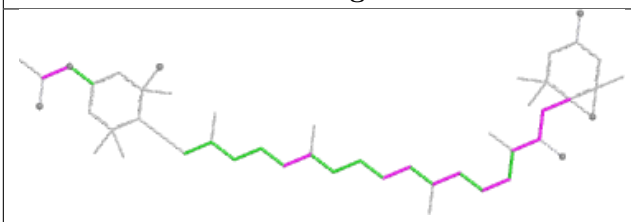
## Ligand A86 12 202



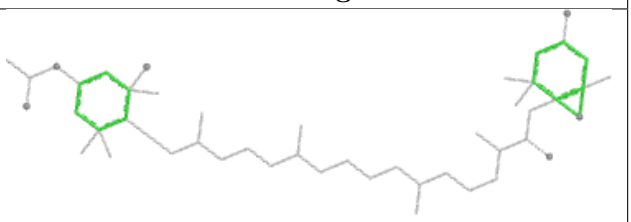
Bond lengths



Bond angles

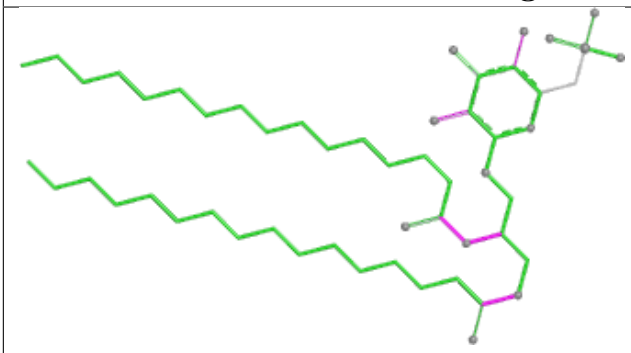


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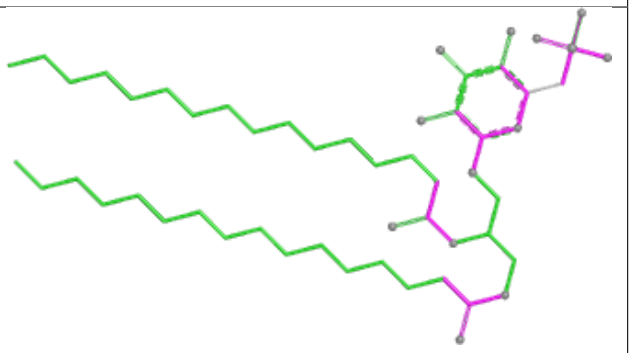


Rings

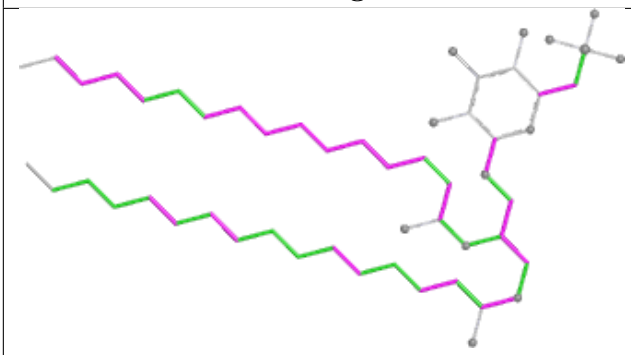
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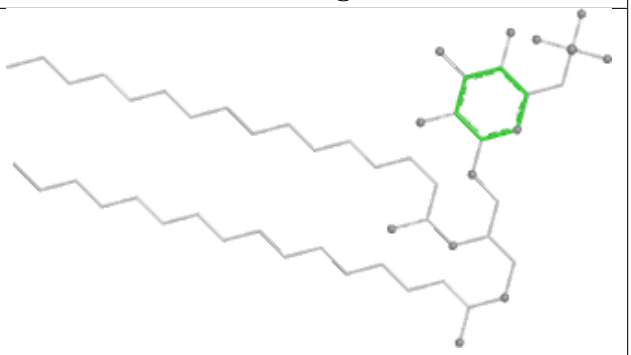
Bond lengths



Bond angles

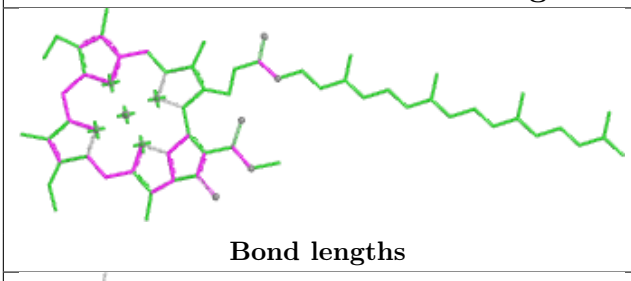


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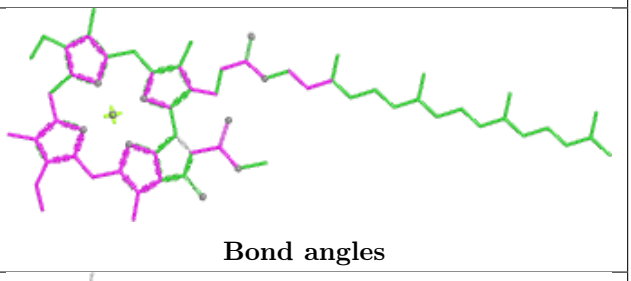


Rings

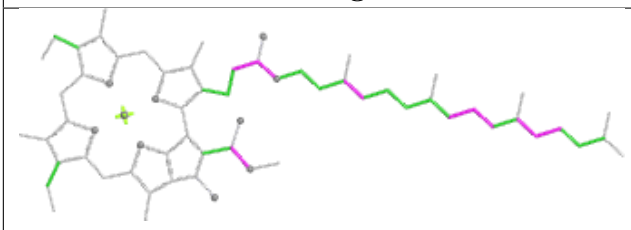
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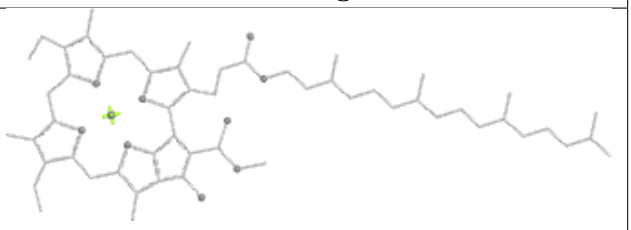
Bond lengths



Bond angles

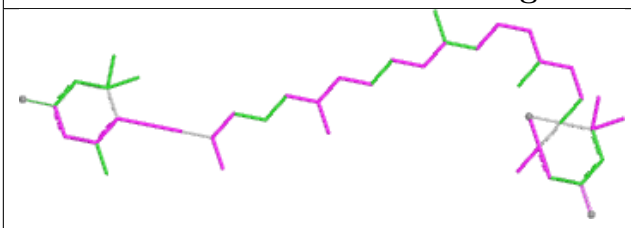


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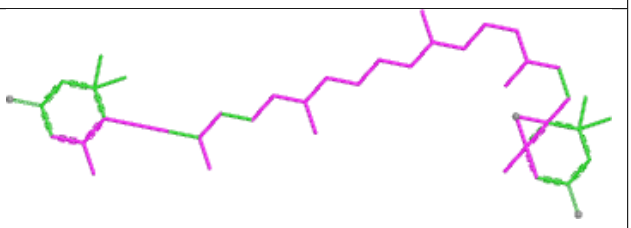


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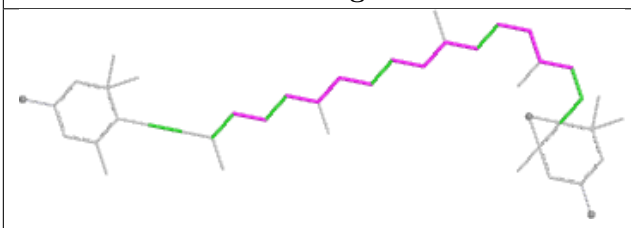
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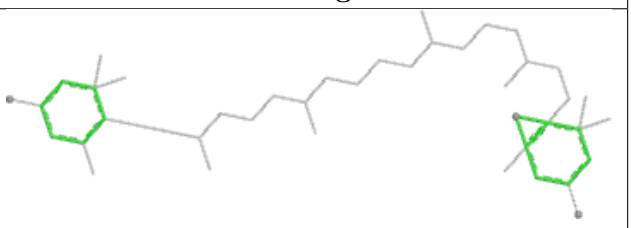
Bond lengths



Bond angles

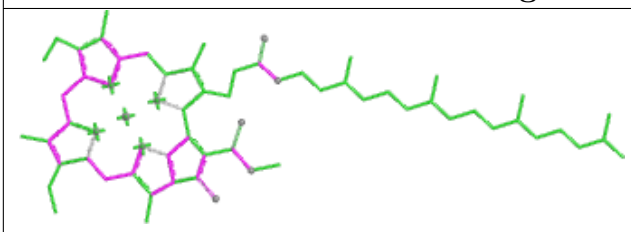


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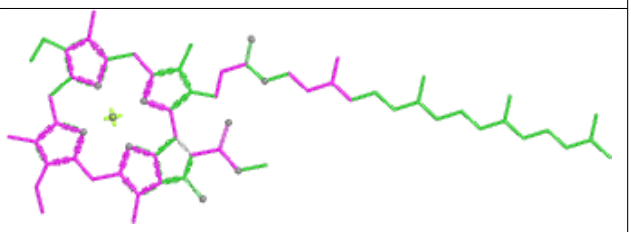


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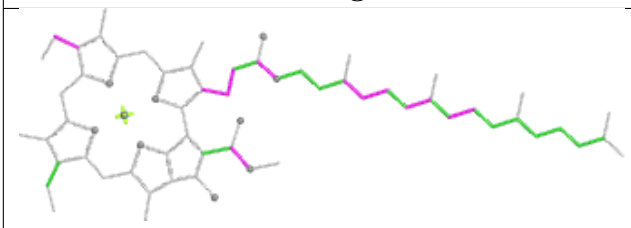
## Ligand CLA 31 302



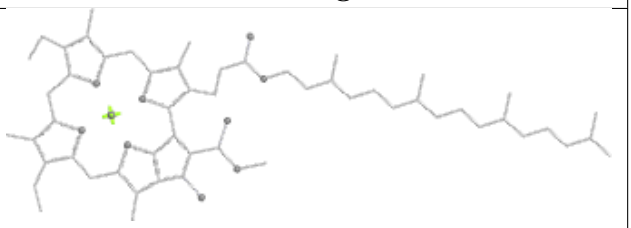
Bond lengths



Bond angles

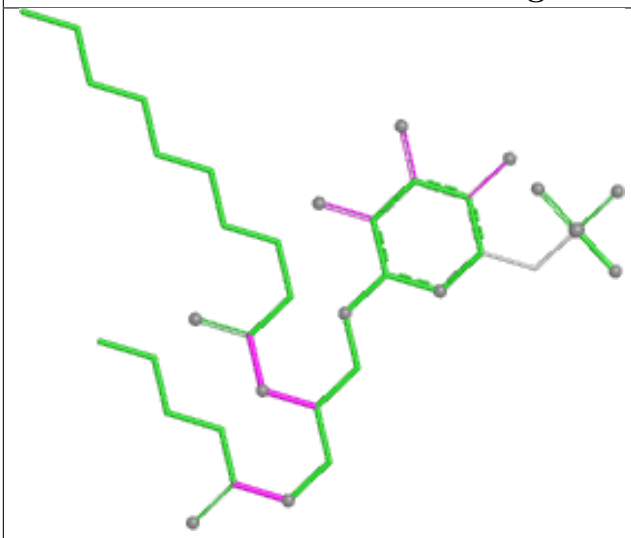


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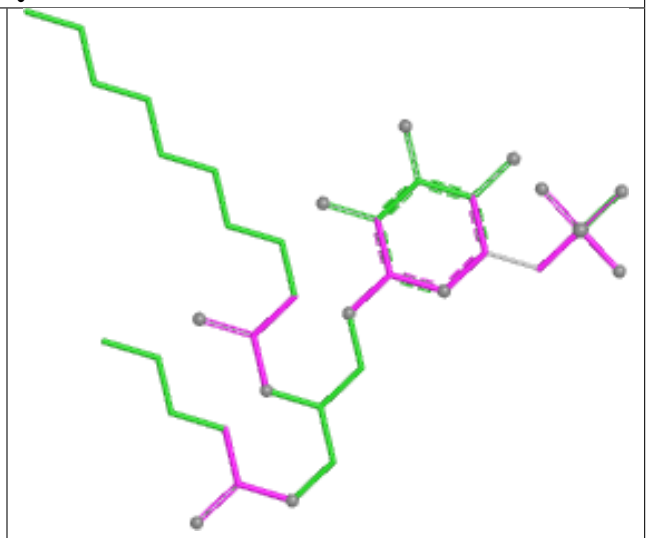


Rings

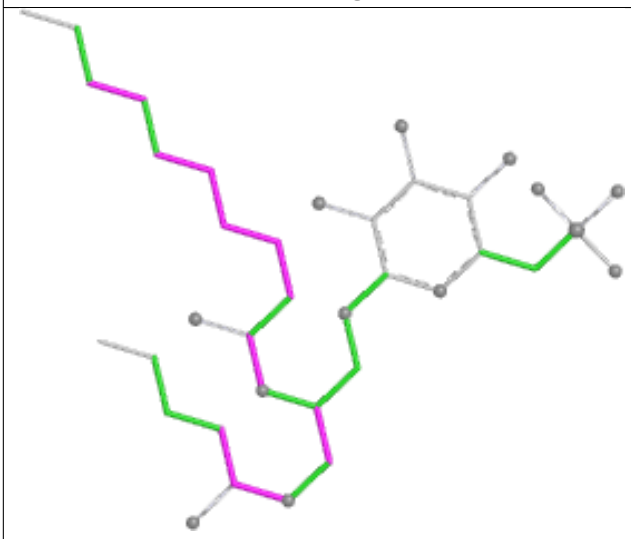
**Ligand SQD b 521**



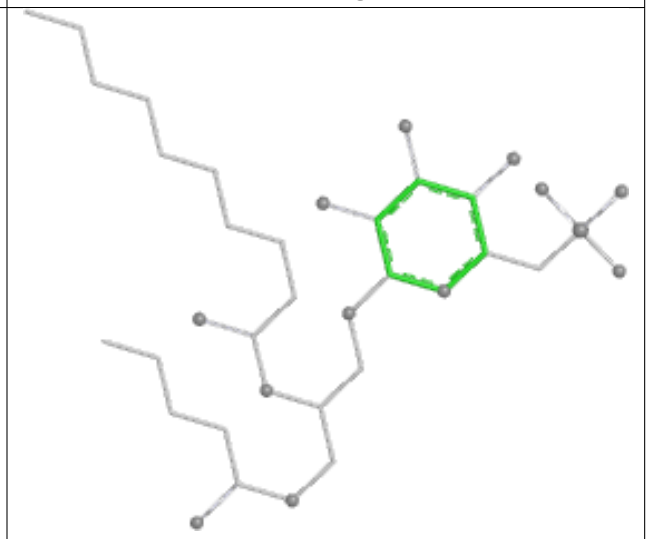
**Bond lengths**



**Bond angles**

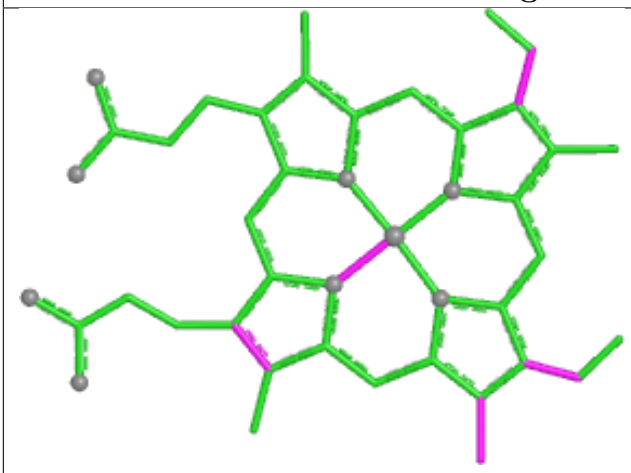


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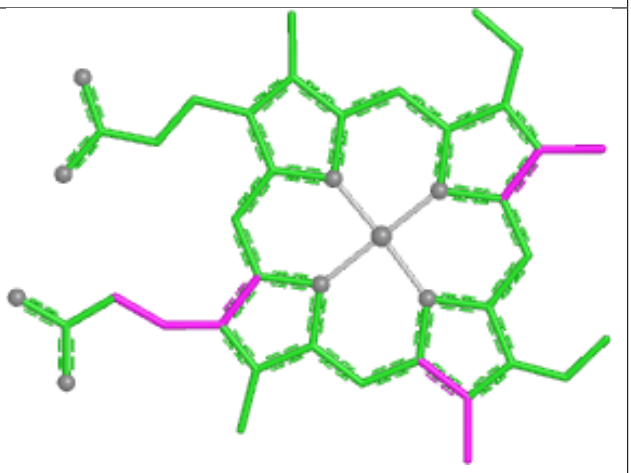


**Rings**

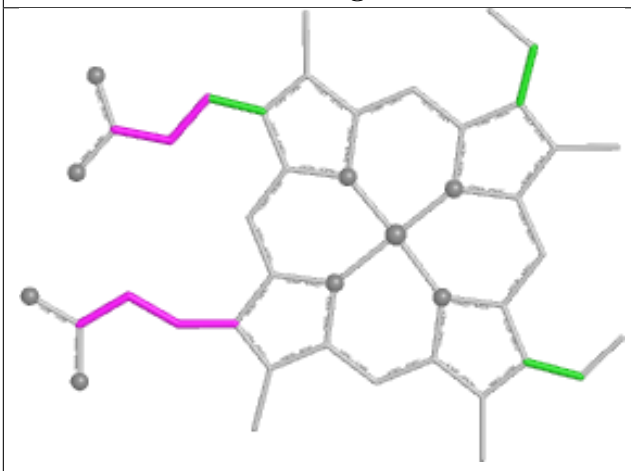
**Ligand HEM F 101**



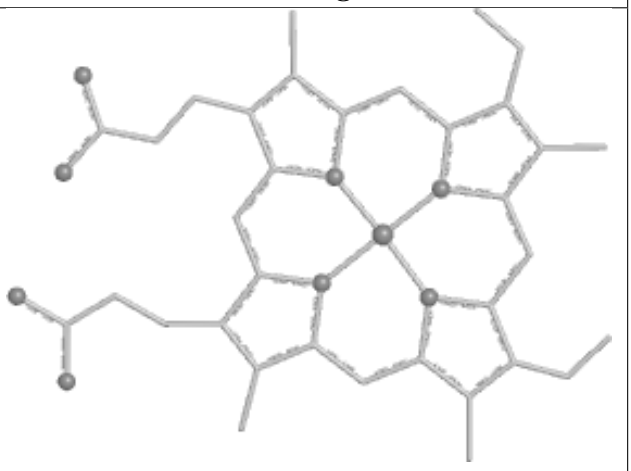
**Bond lengths**



**Bond angles**

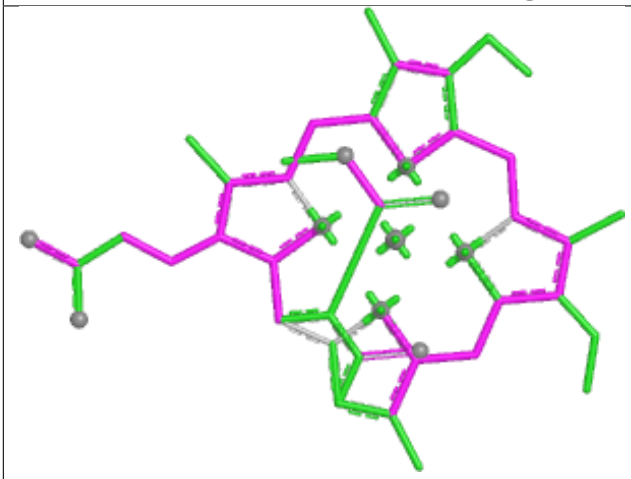


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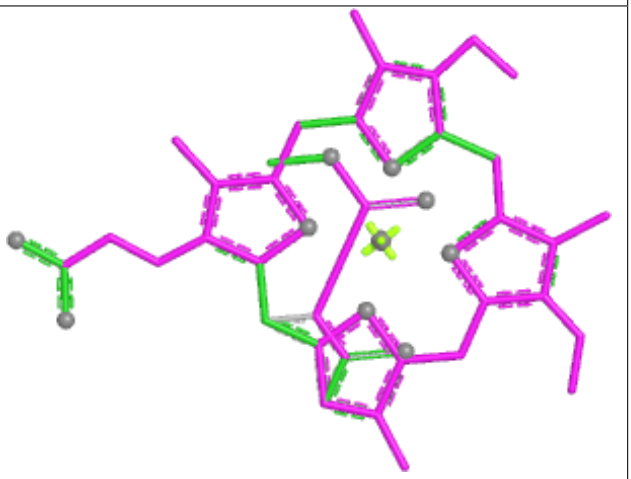


**Rings**

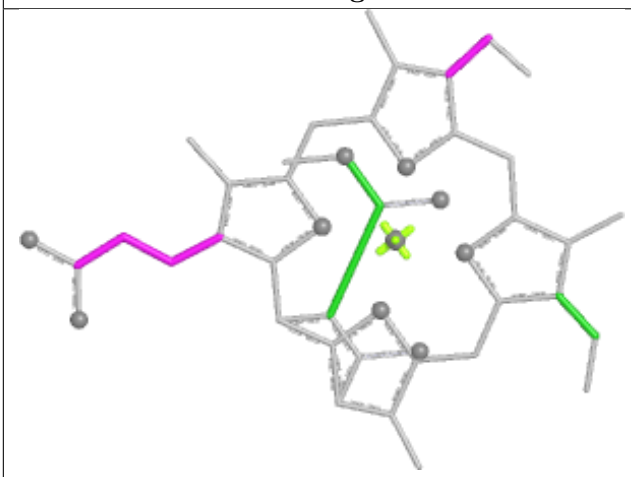
**Ligand KC1 15 302**



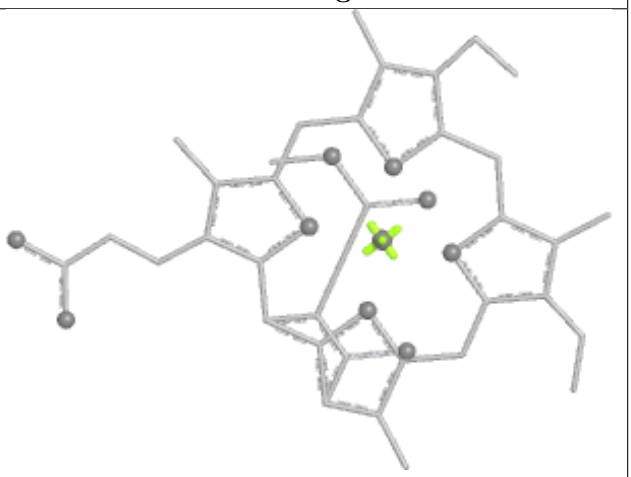
Bond lengths



Bond angles

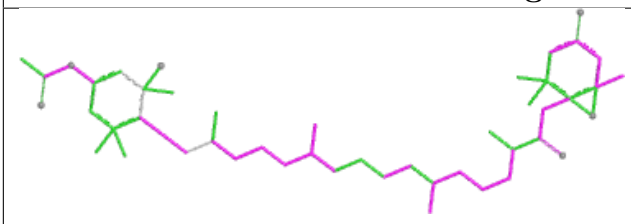


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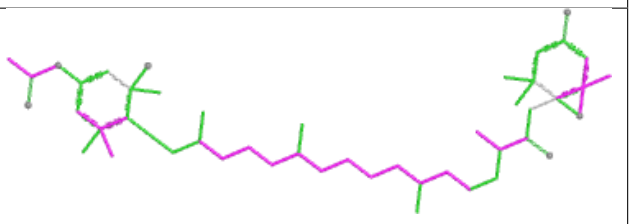


Rings

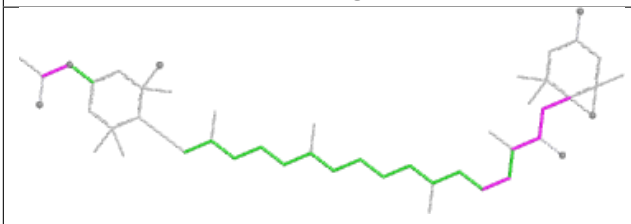
**Ligand A86 36 313**



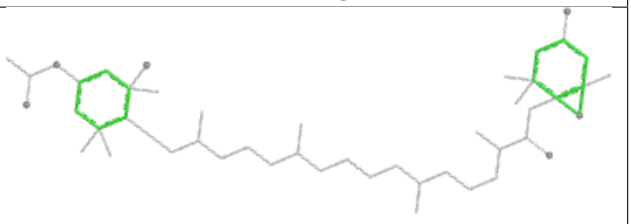
Bond lengths



Bond angles

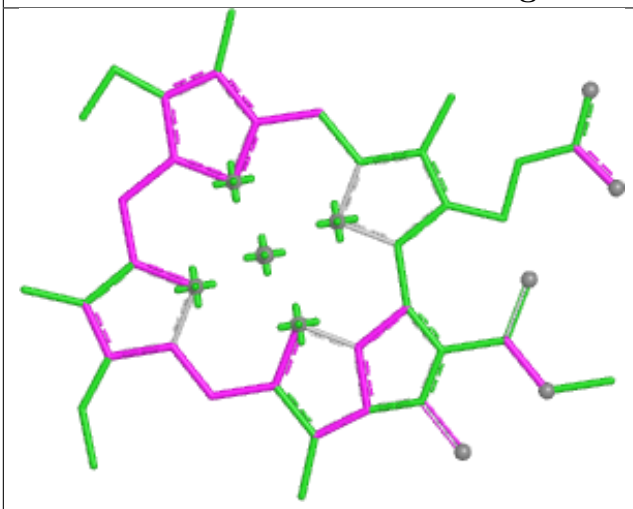


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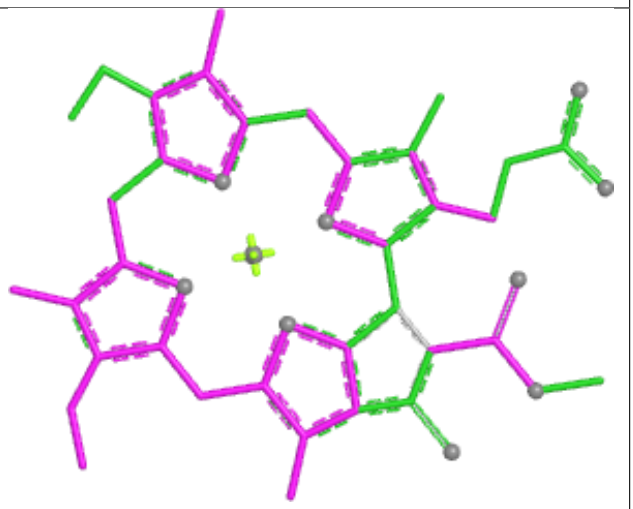


Rings

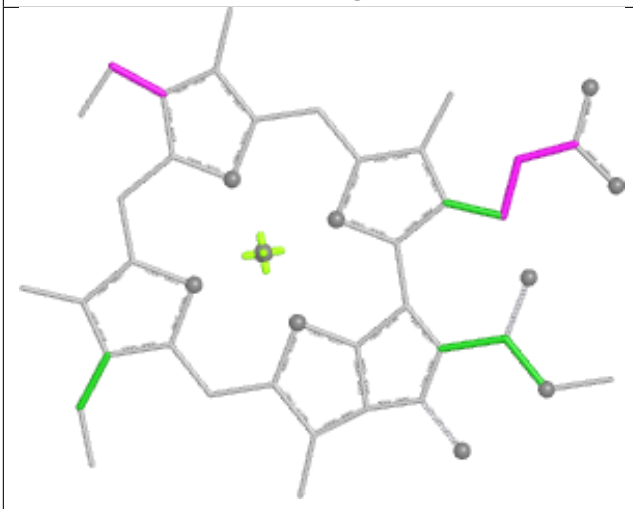
## Ligand CLA 19 309



Bond lengths



Bond angles

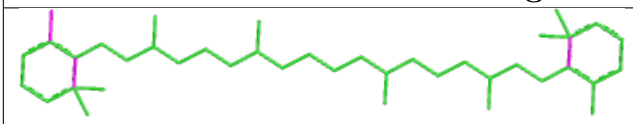


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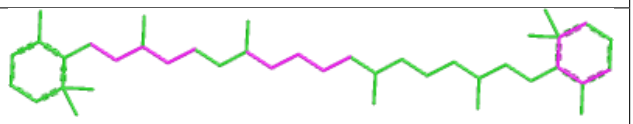


Rings

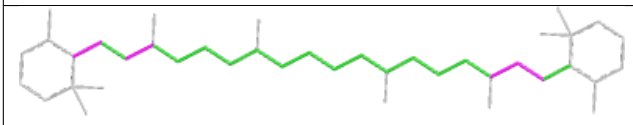
## Ligand BCR h 101



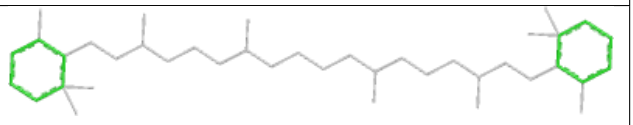
Bond lengths



Bond angles

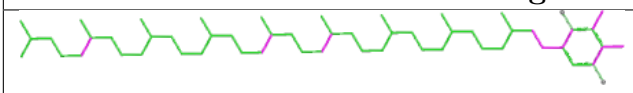


Torsions

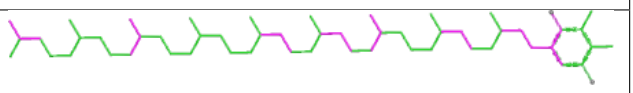


Rings

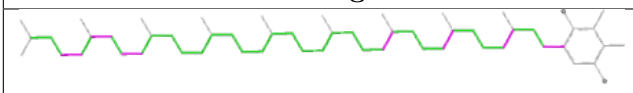
## Ligand PL9 D 408



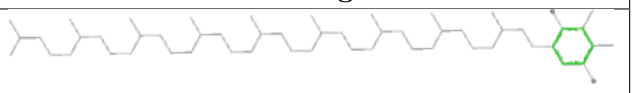
Bond lengths



Bond angles

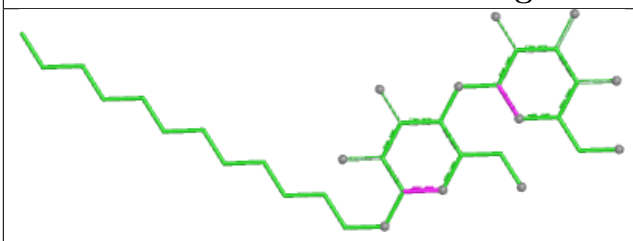


Torsions

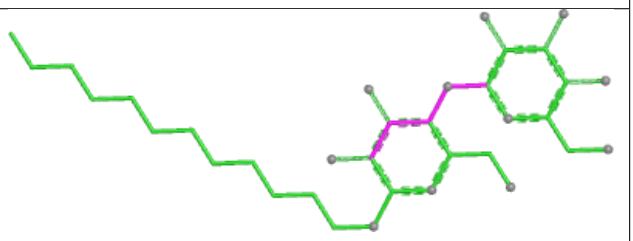


Rings

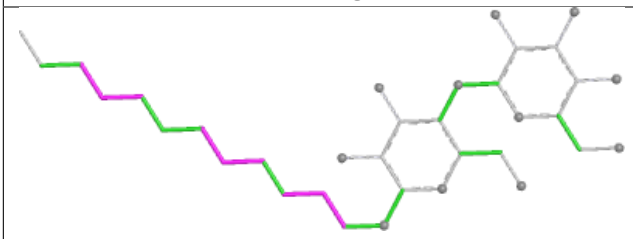
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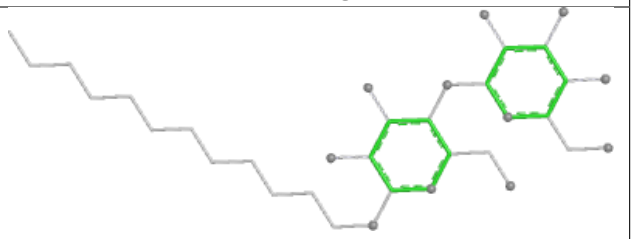
Bond lengths



Bond angles



Torsions

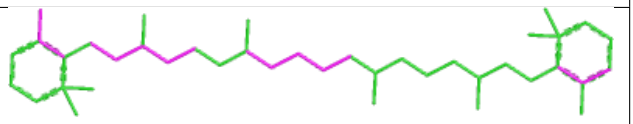


Rings

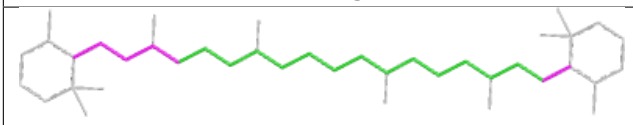
## Ligand BCR a 413



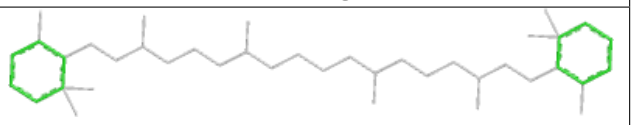
Bond lengths



Bond angles

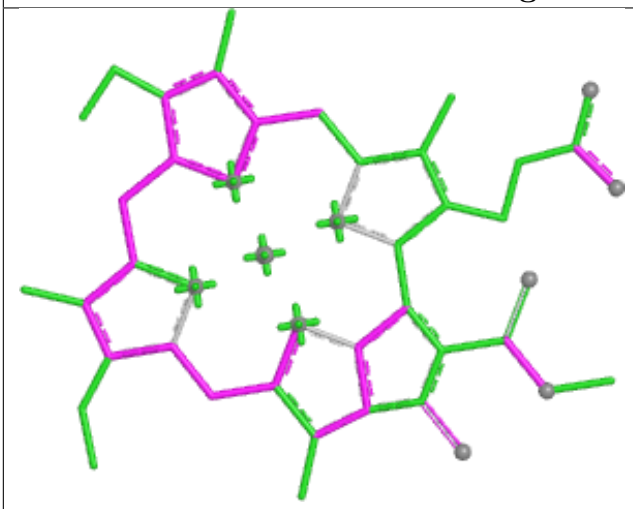


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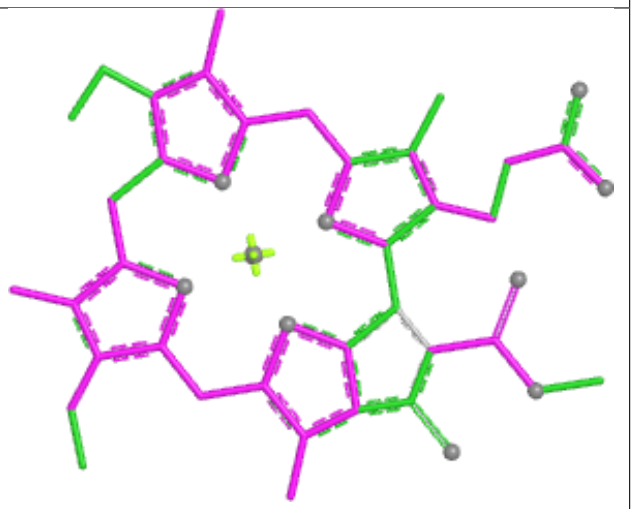


Rings

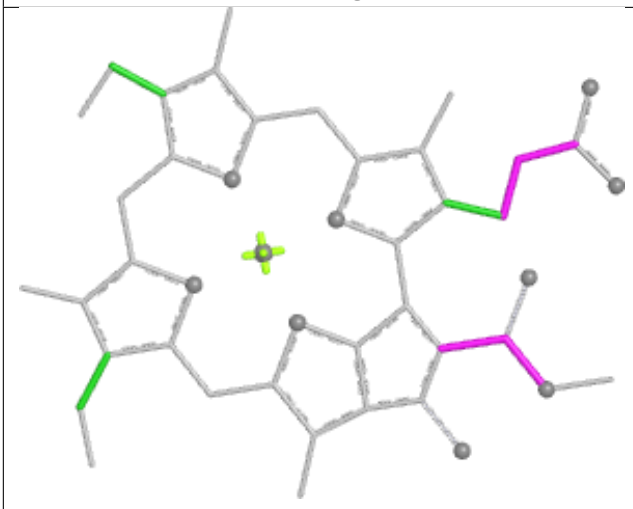
## Ligand CLA 12 212



Bond lengths



Bond angles

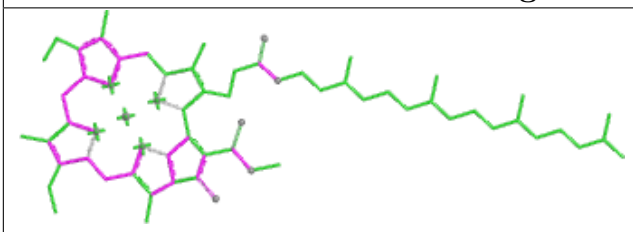


Torsions

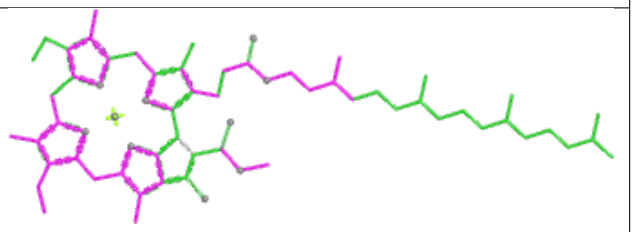


Rings

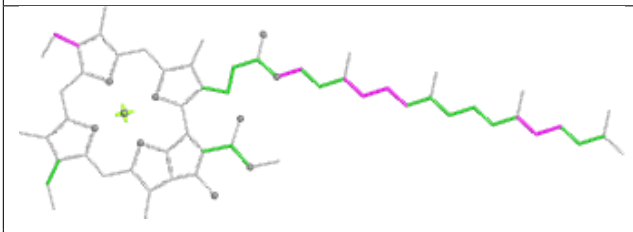
## Ligand CLA 15 308



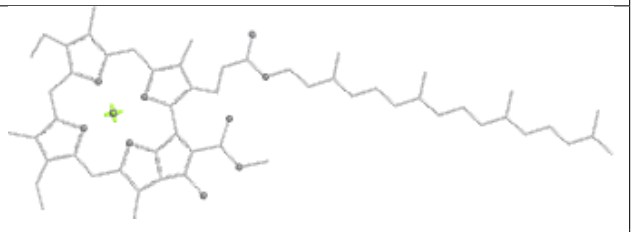
Bond lengths



Bond angles

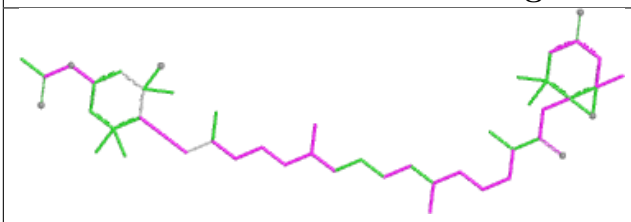


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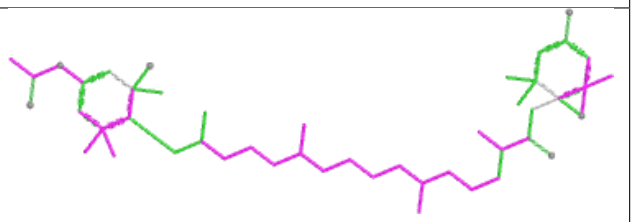


Rings

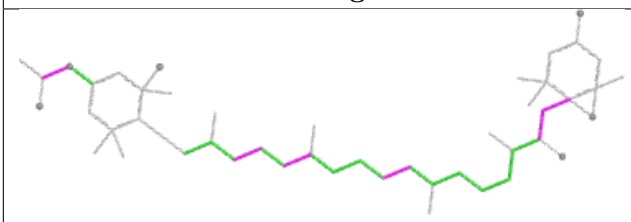
## Ligand A86 17 313



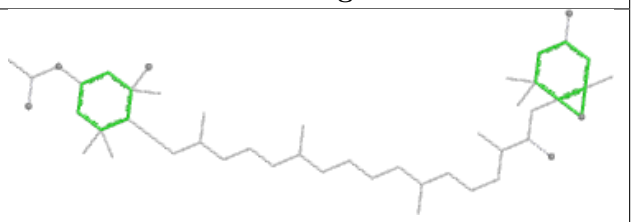
Bond lengths



Bond angles

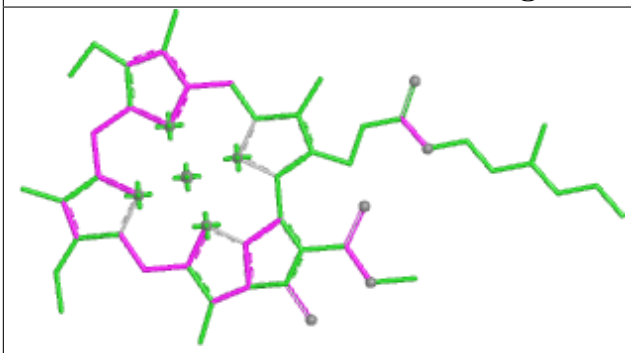


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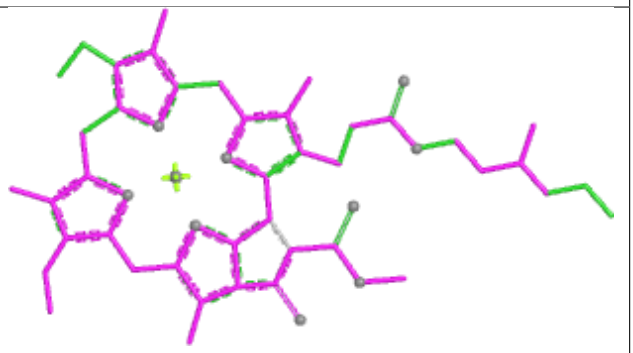


Rings

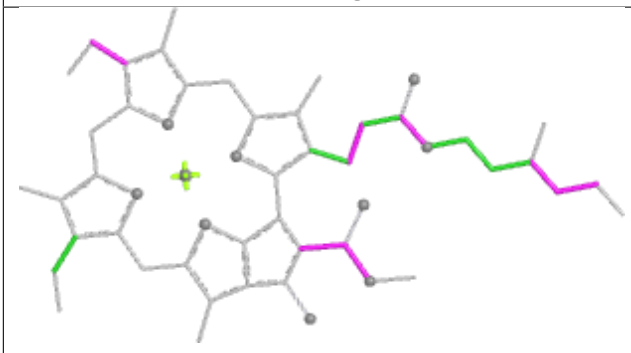
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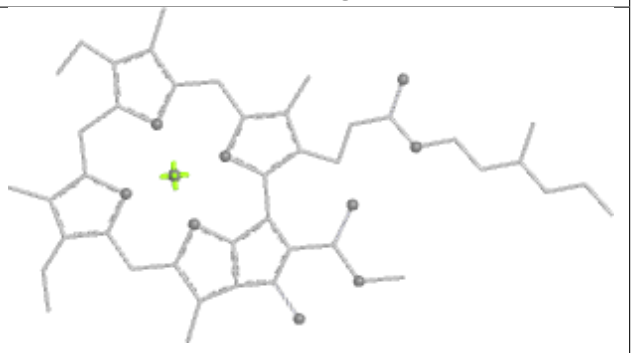
Bond lengths



Bond angles

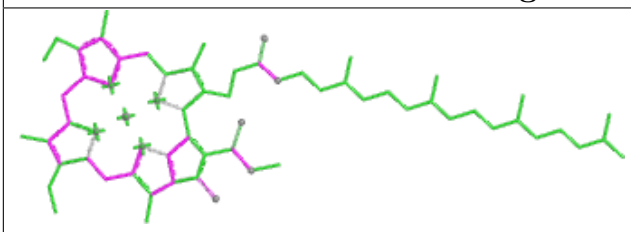


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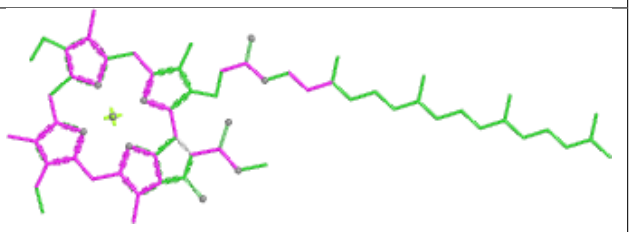


Rings

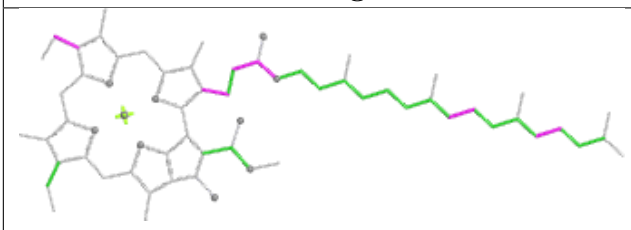
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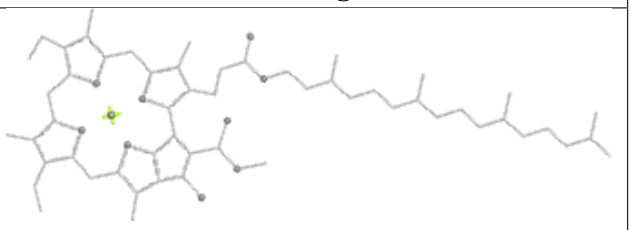
Bond lengths



Bond angles

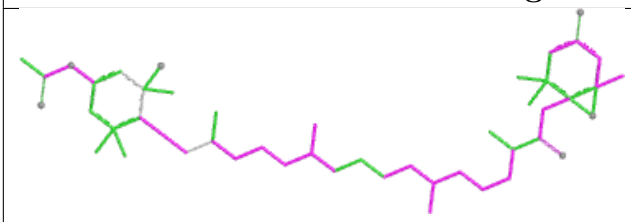


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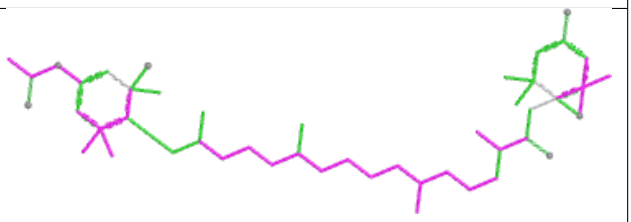


Rings

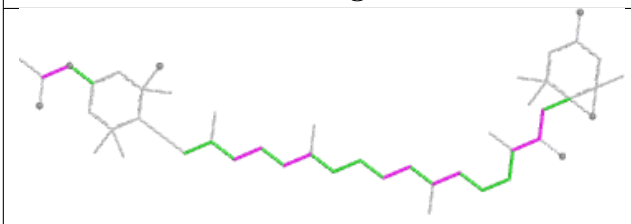
## Ligand A86 34 314



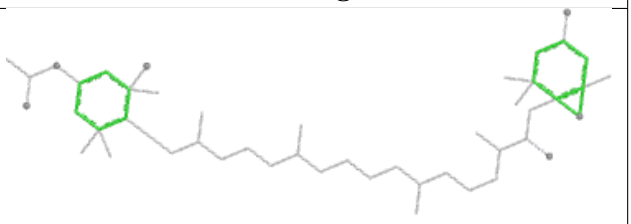
Bond lengths



Bond angles

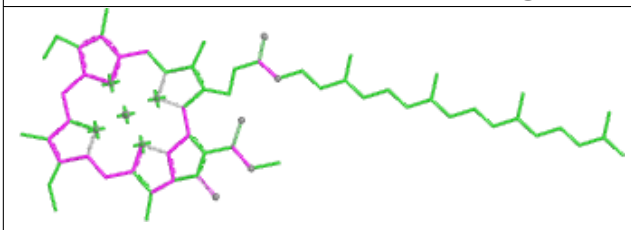


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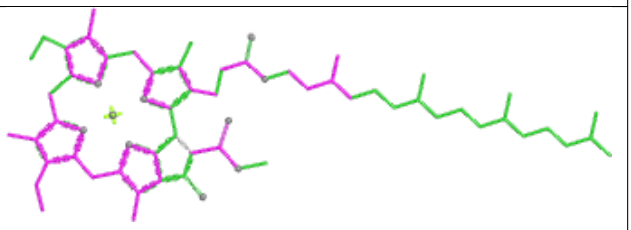


Rings

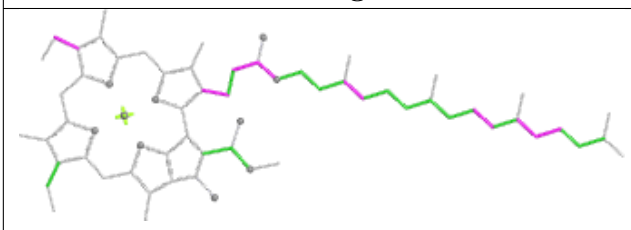
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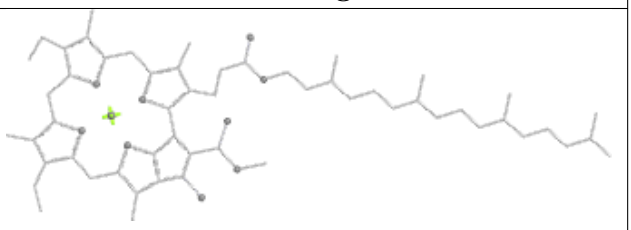
Bond lengths



Bond angles

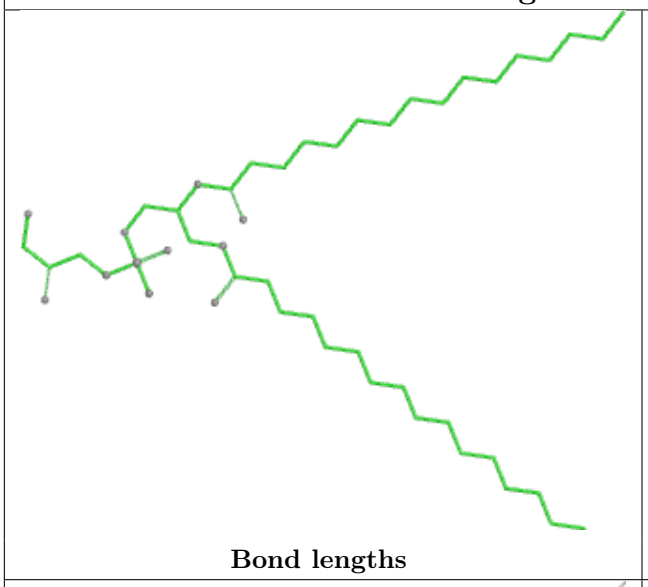


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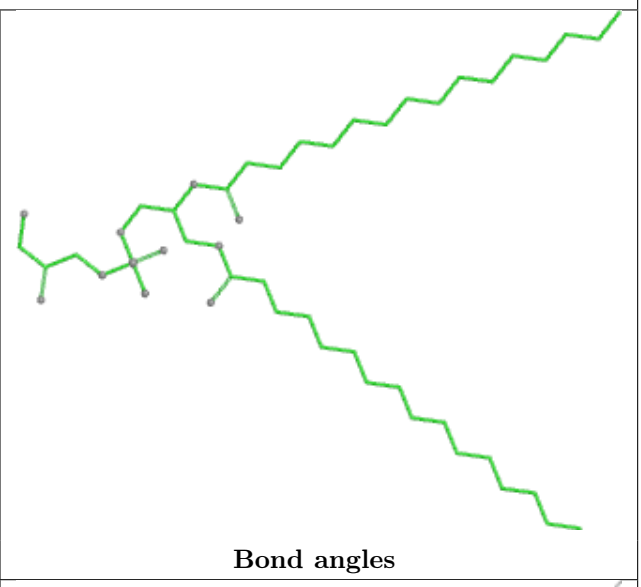


Rings

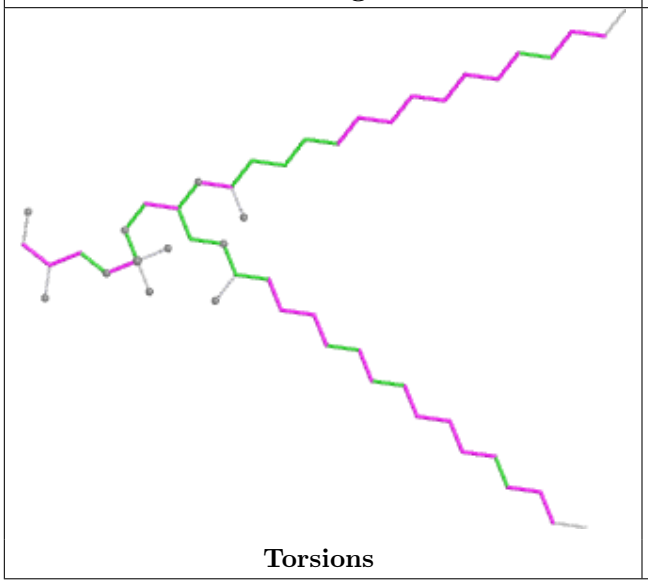
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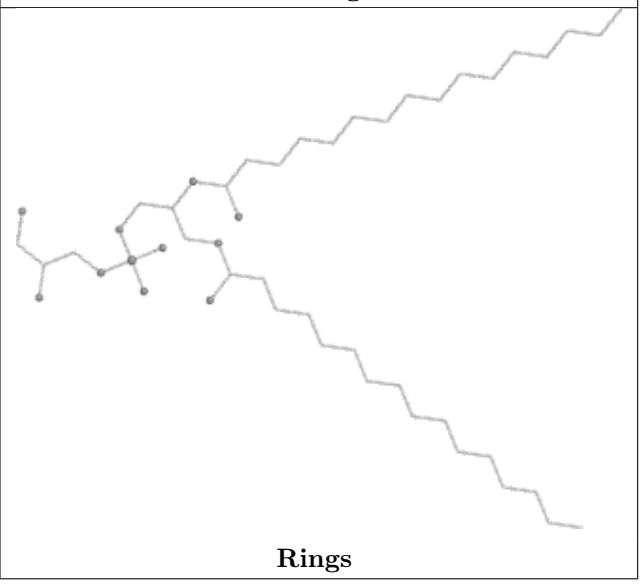
Bond lengths



Bond angles

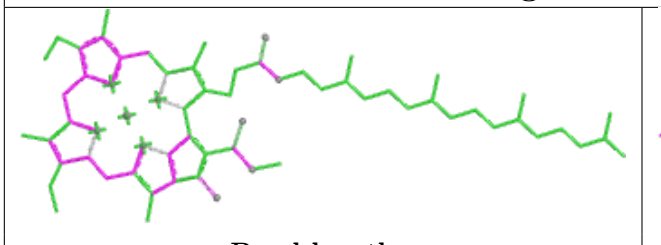


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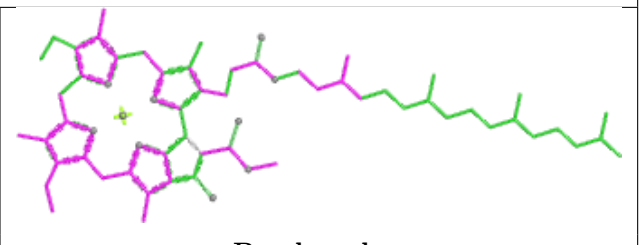


Rings

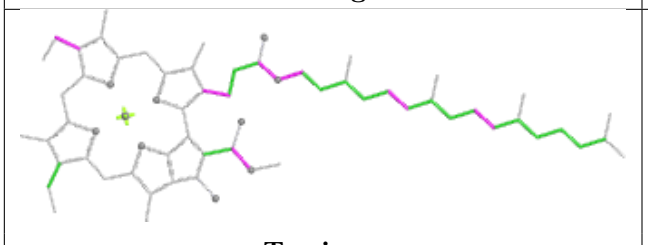
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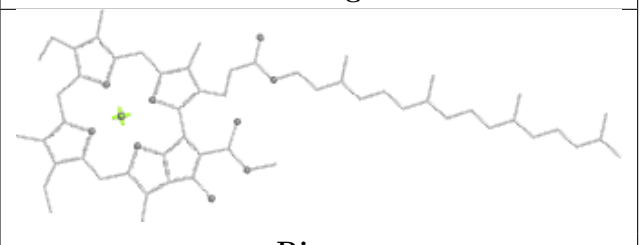
Bond lengths



Bond angles

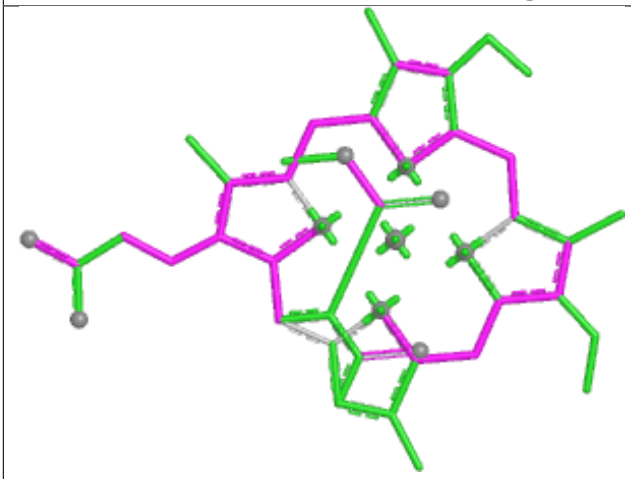


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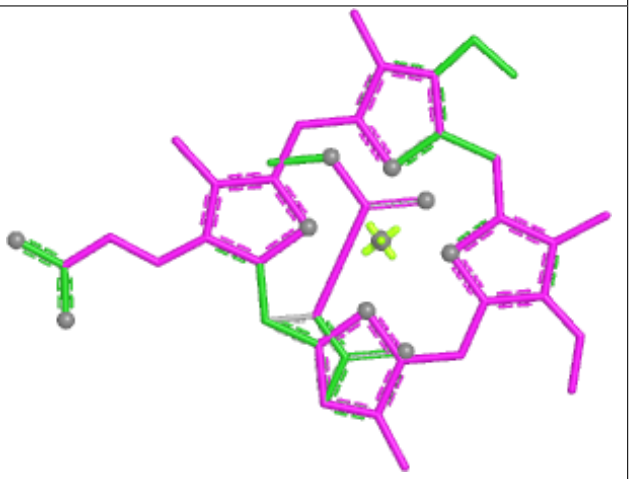


Rings

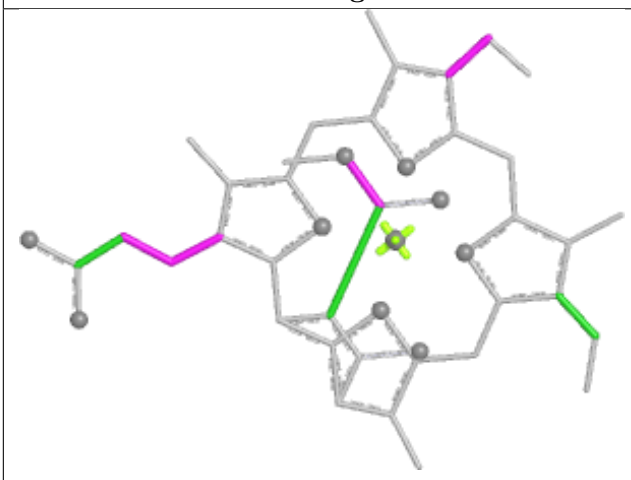
**Ligand KC1 13 306**



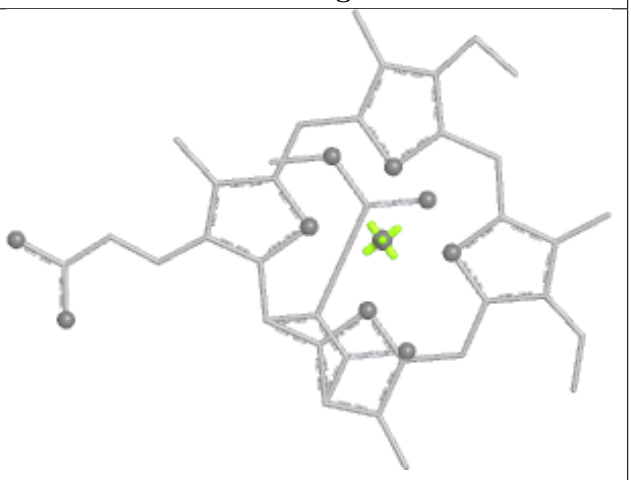
**Bond lengths**



**Bond angles**

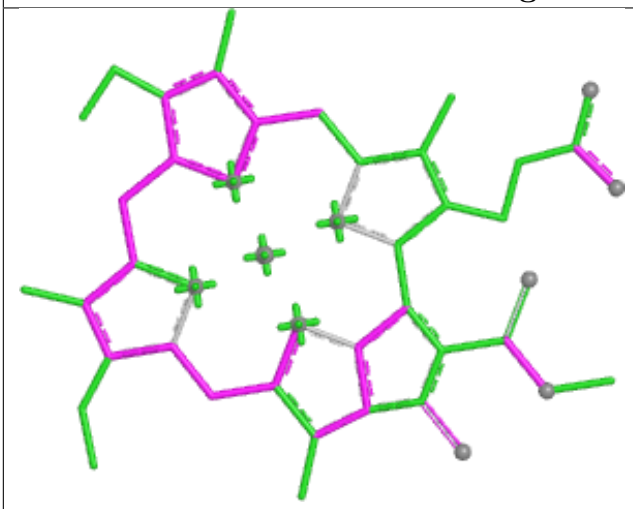


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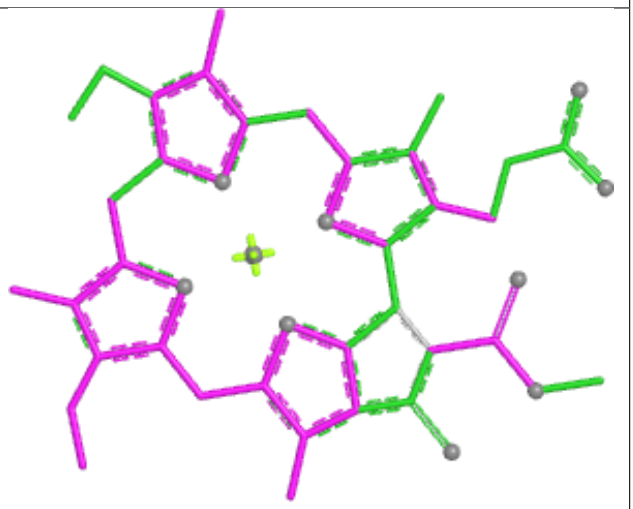


**Rings**

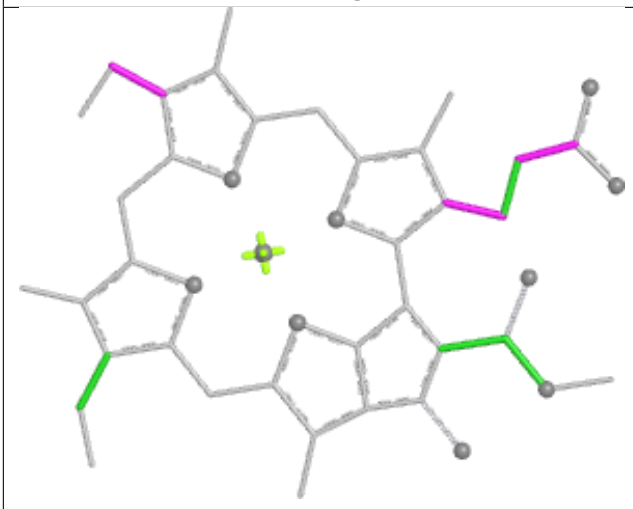
## Ligand CLA 34 305



Bond lengths



Bond angles

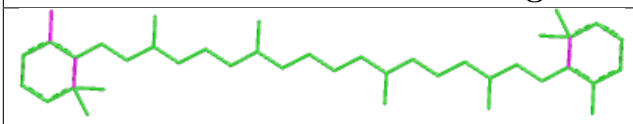


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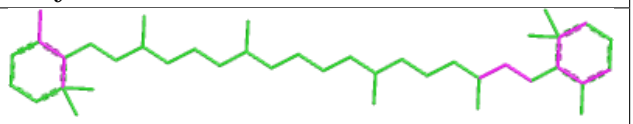


Rings

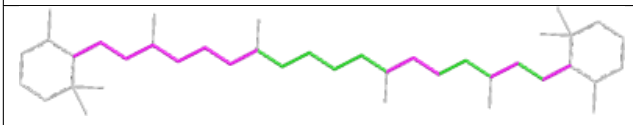
## Ligand BCR y 101



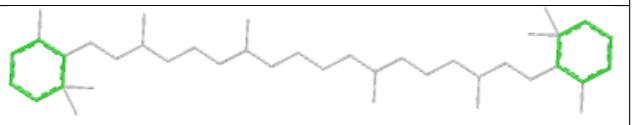
Bond lengths



Bond angles

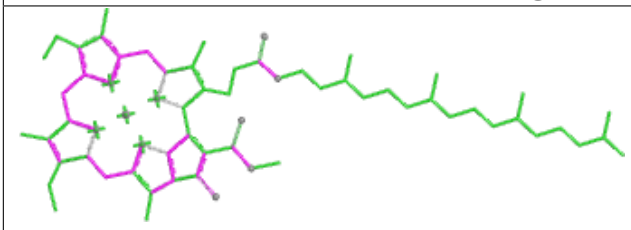


Torsions

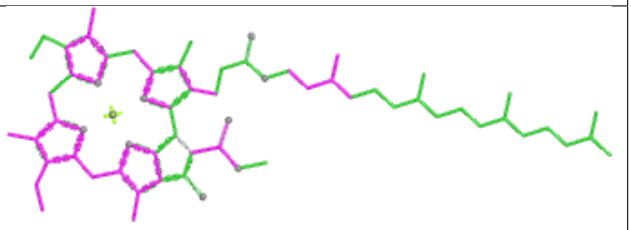


Rings

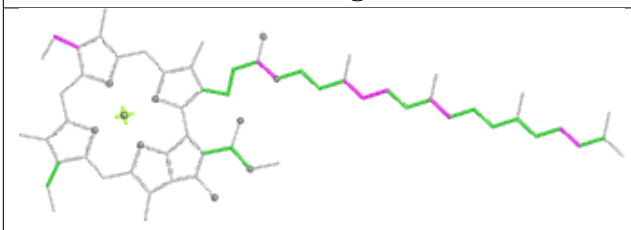
## Ligand CLA c 504



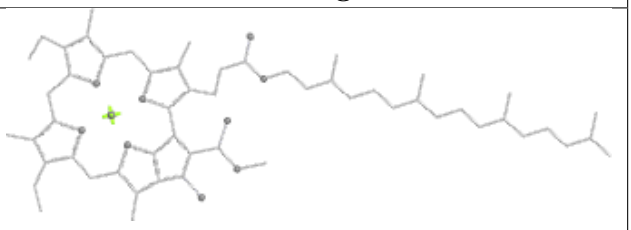
Bond lengths



Bond angles

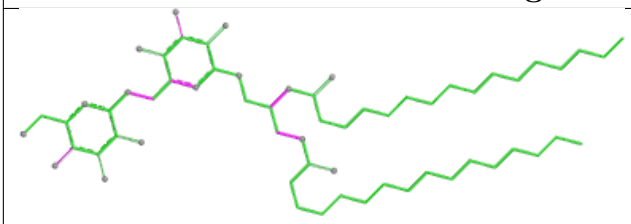


Torsions

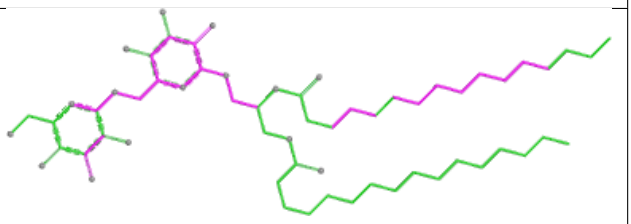


Rings

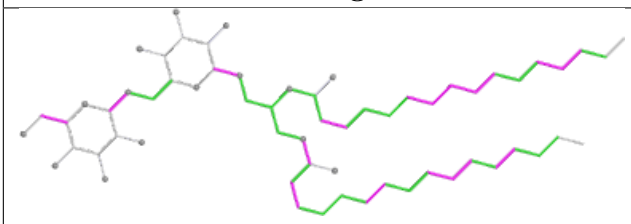
## Ligand DGD c 517



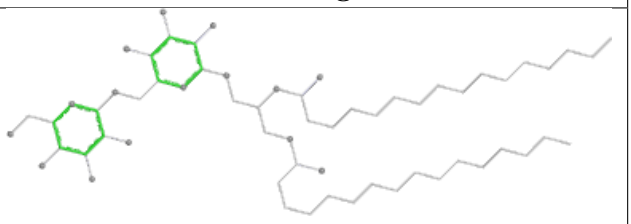
Bond lengths



Bond angles

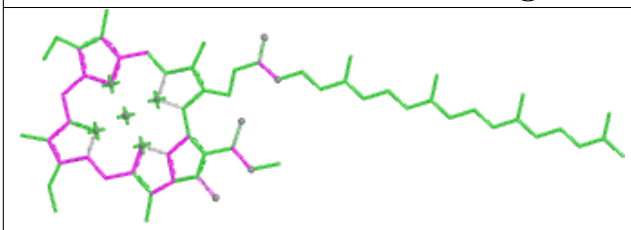


Torsions

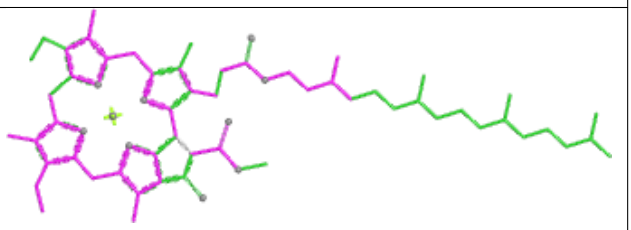


Rings

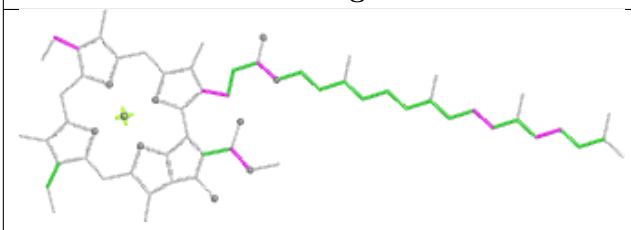
## Ligand CLA 38 201



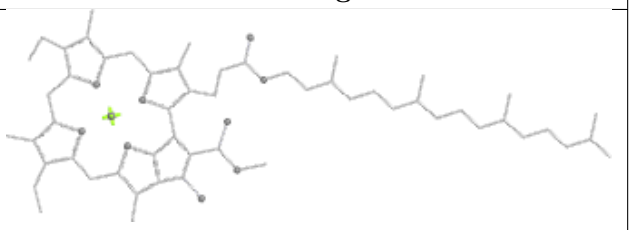
Bond lengths



Bond angles

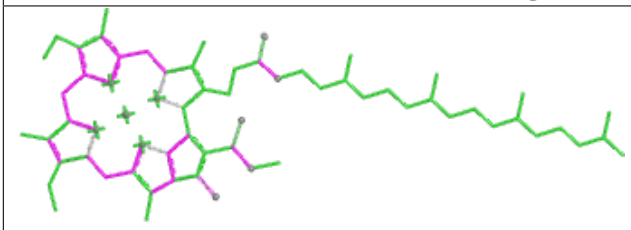


Torsions

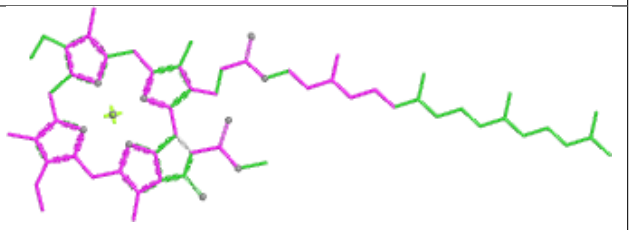


Rings

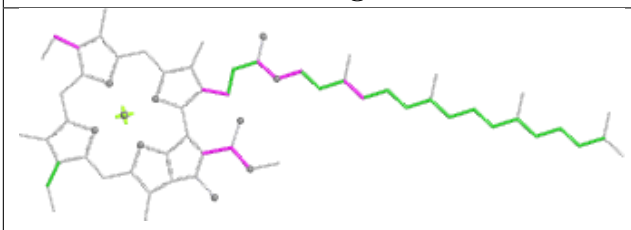
## Ligand CLA B 509



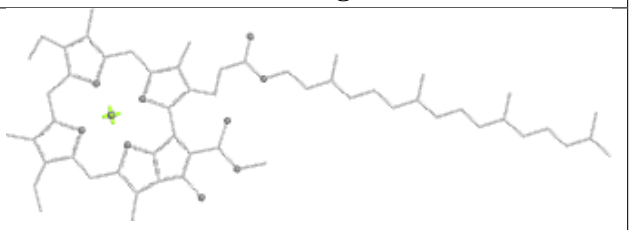
Bond lengths



Bond angles

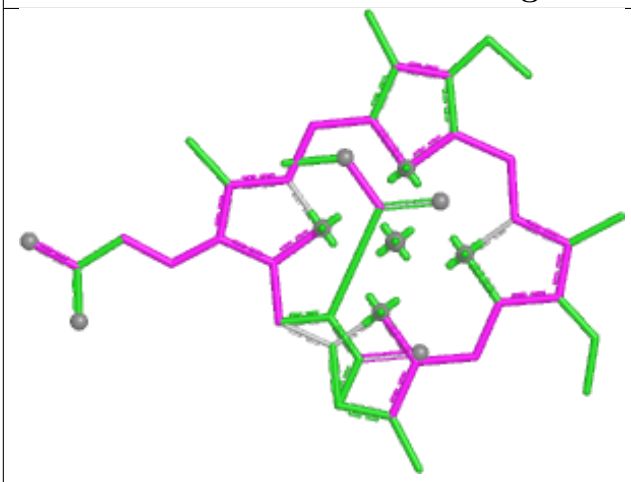


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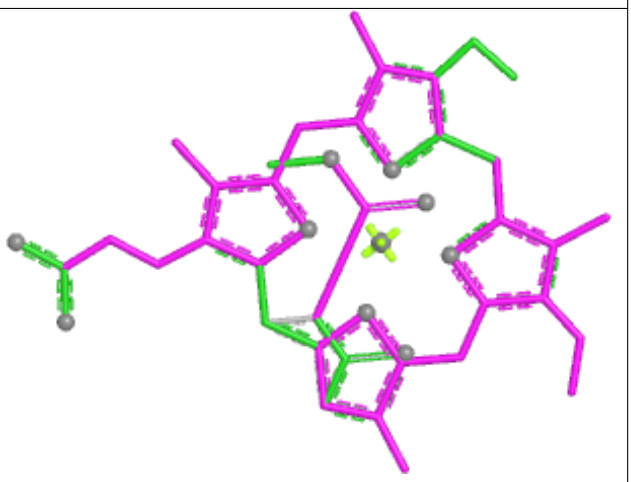


Rings

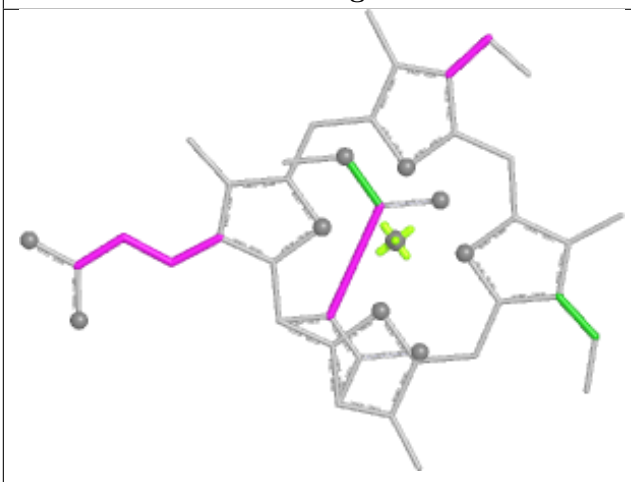
## Ligand KC1 35 309



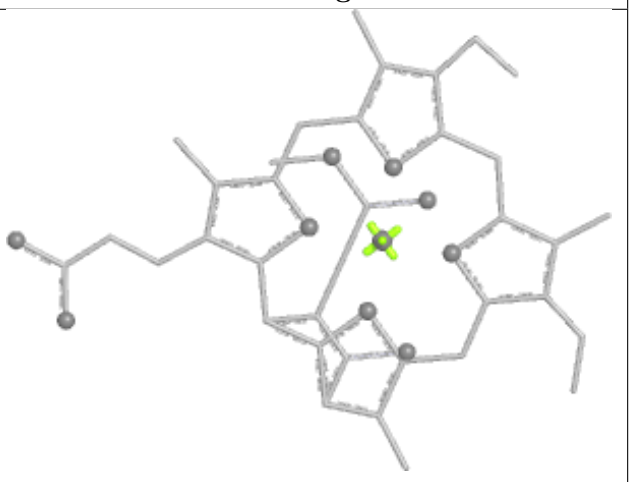
Bond lengths



Bond angles

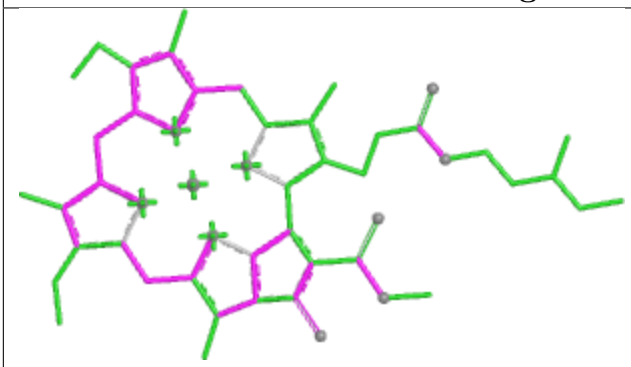


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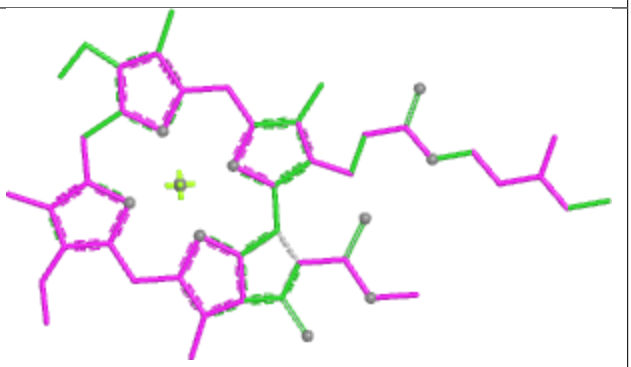


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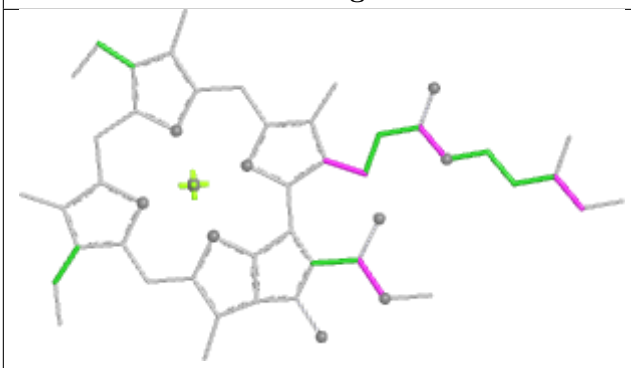
**Ligand CLA 31 310**



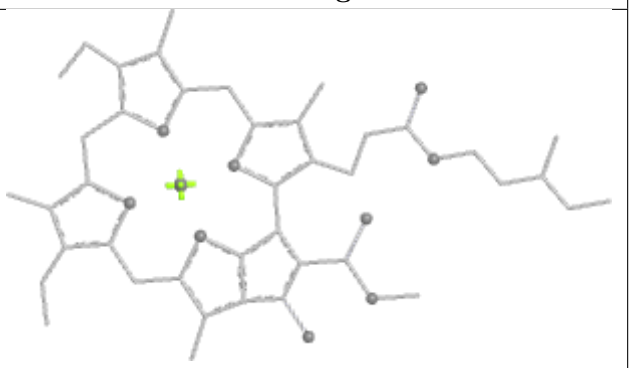
**Bond lengths**



**Bond angles**

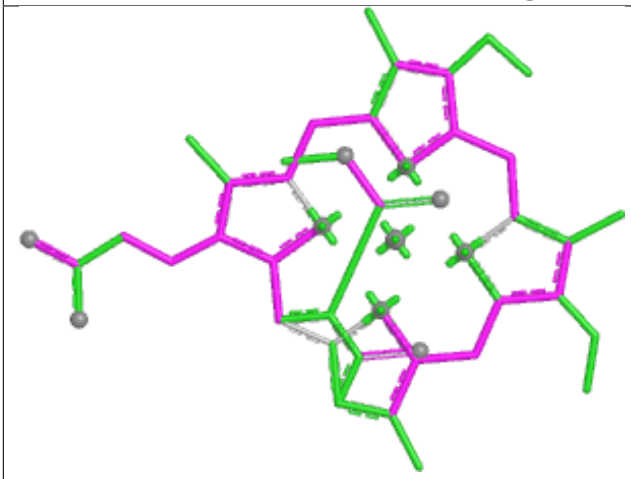


**Torsions**

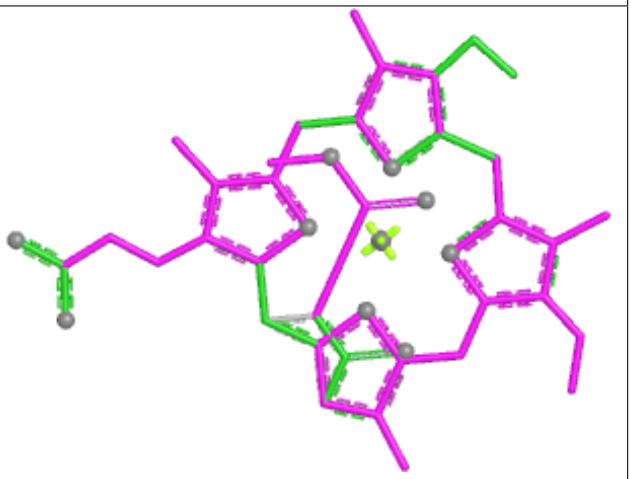


**Rings**

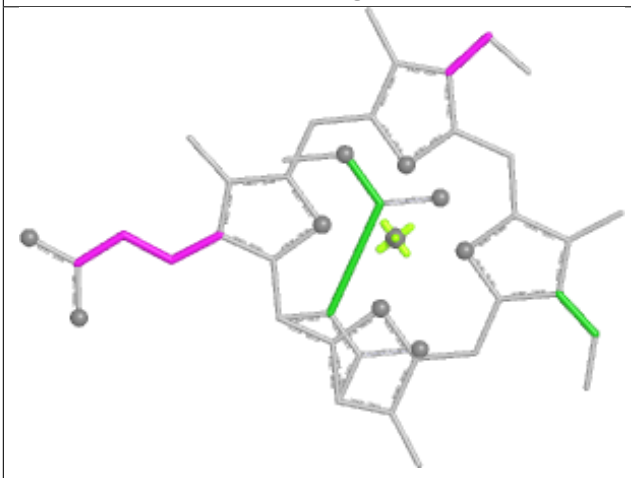
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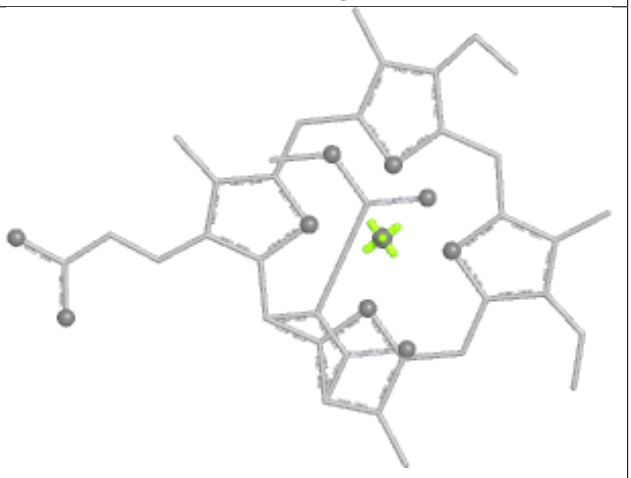
**Bond lengths**



**Bond angles**

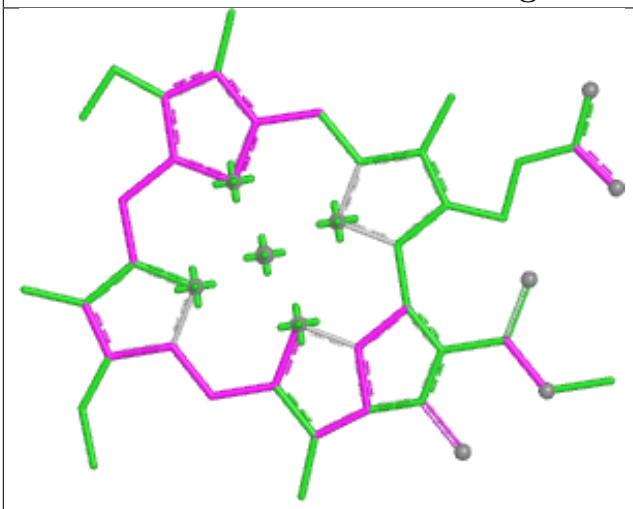


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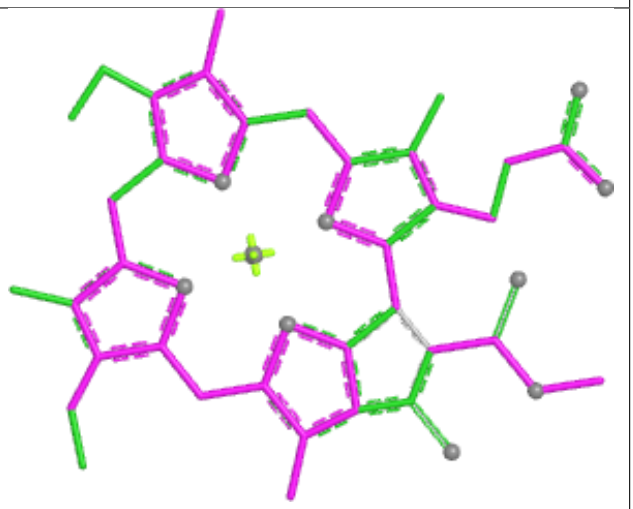


**Rings**

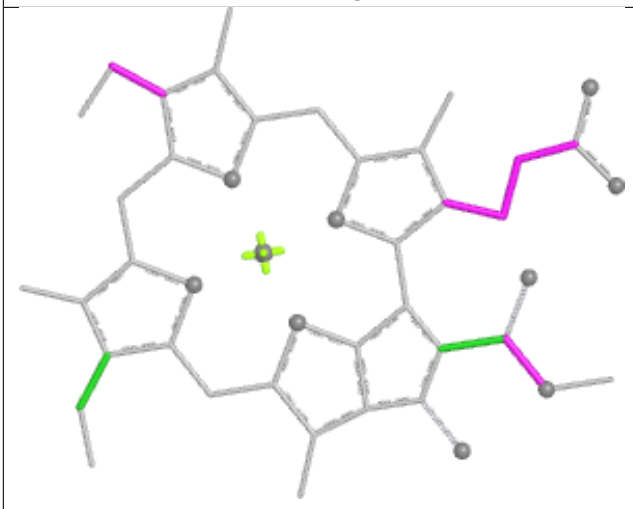
## Ligand CLA 21 205



Bond lengths



Bond angles

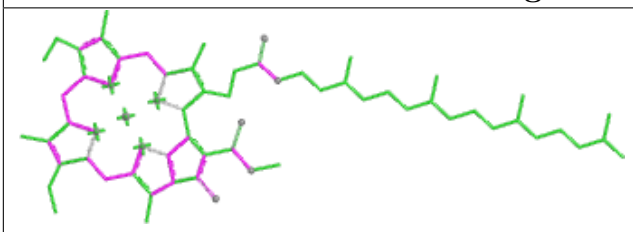


Torsions

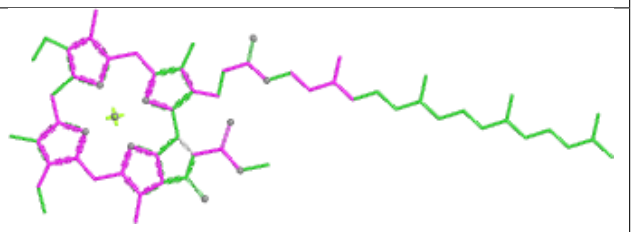


Rings

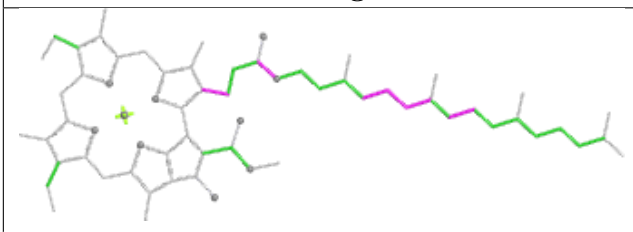
## Ligand CLA C 508



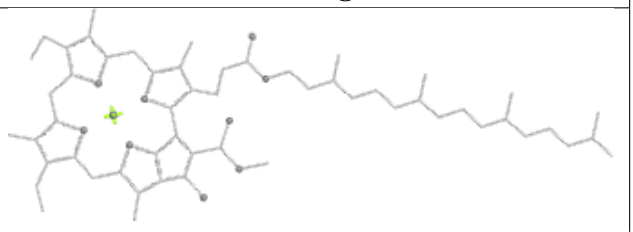
Bond lengths



Bond angles

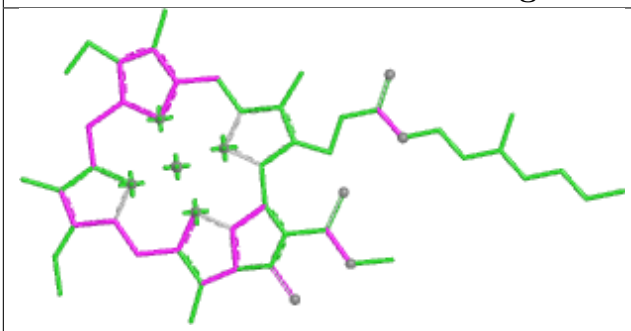


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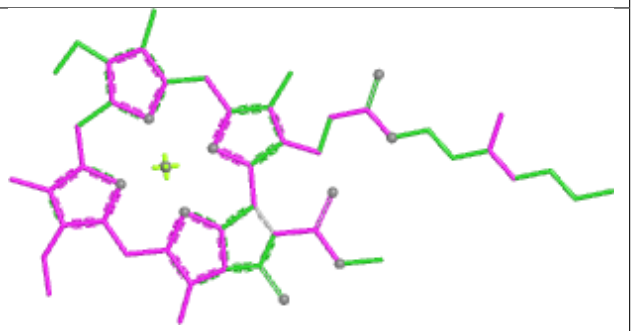


Rings

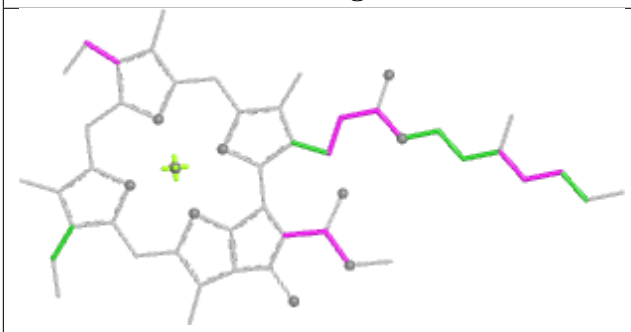
## Ligand CLA 38 208



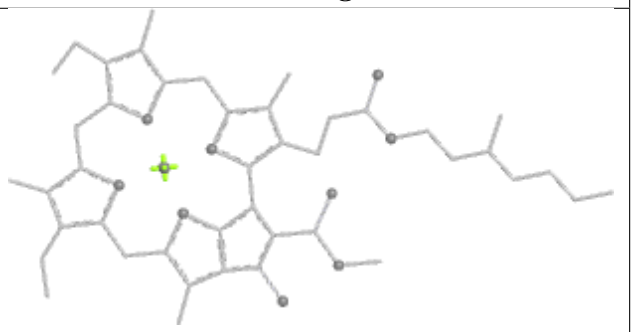
Bond lengths



Bond angles

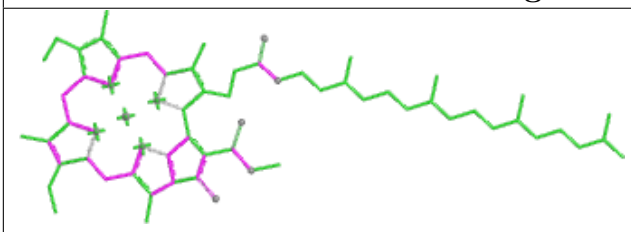


Torsions

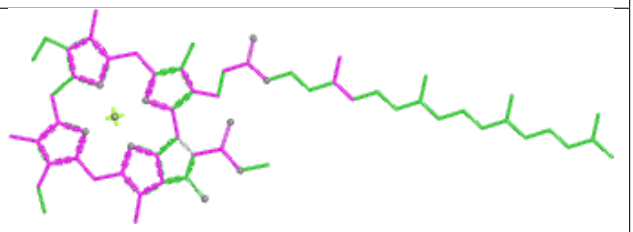


Rings

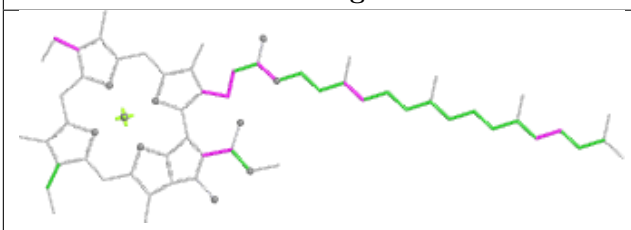
## Ligand CLA B 503



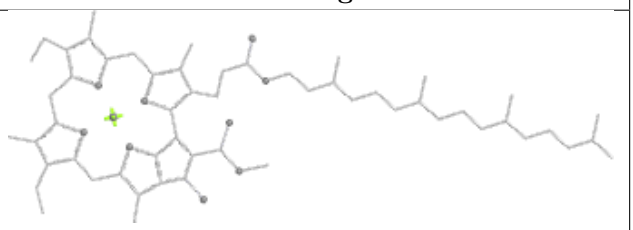
Bond lengths



Bond angles

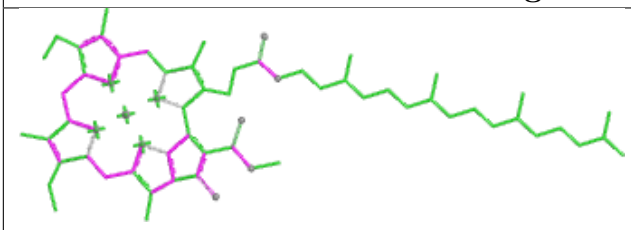


Torsions

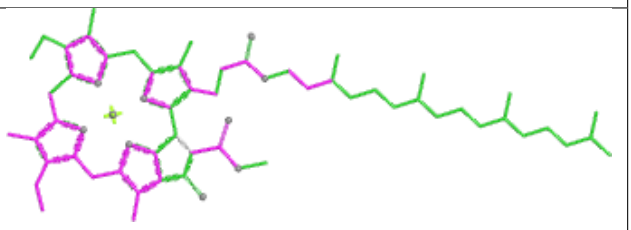


Rings

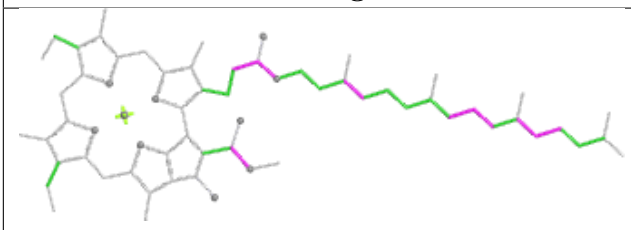
**Ligand CLA C 510**



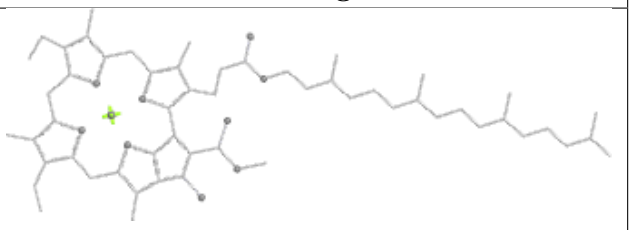
Bond lengths



Bond angles

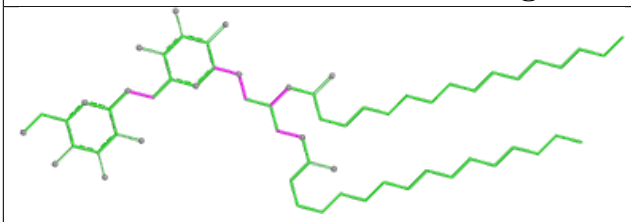


Torsions

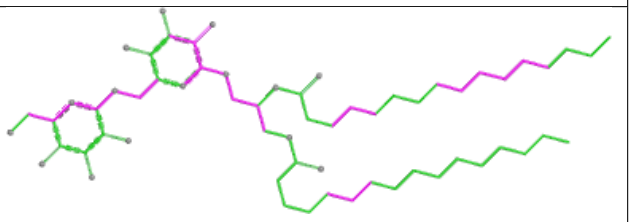


Rings

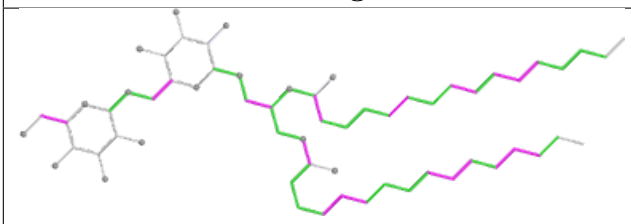
**Ligand DGD C 516**



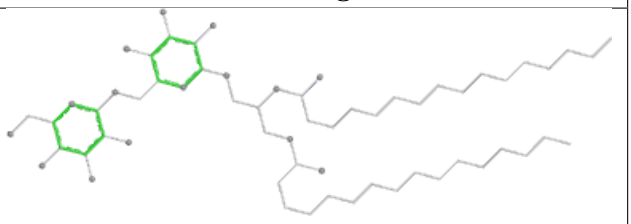
Bond lengths



Bond angles

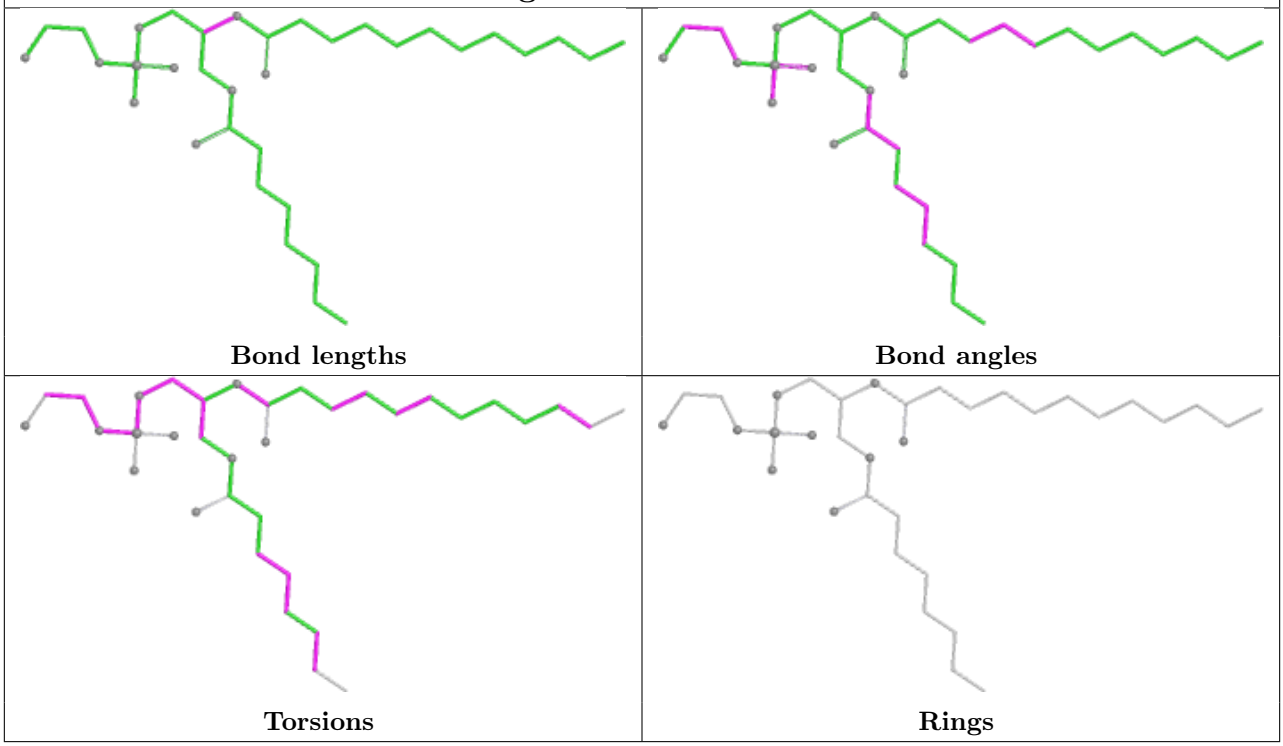


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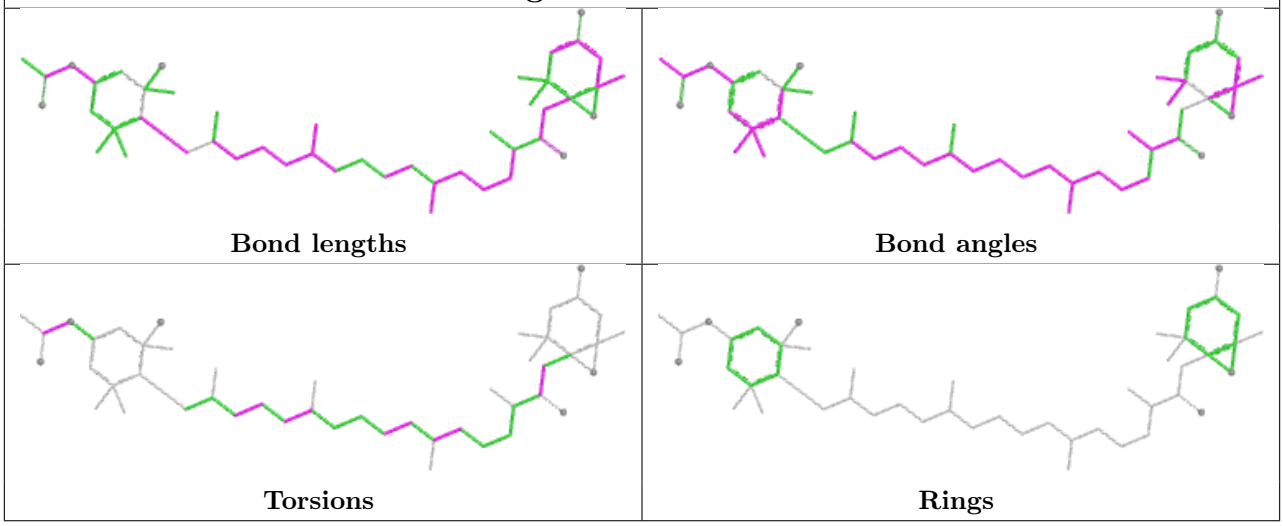


Rings

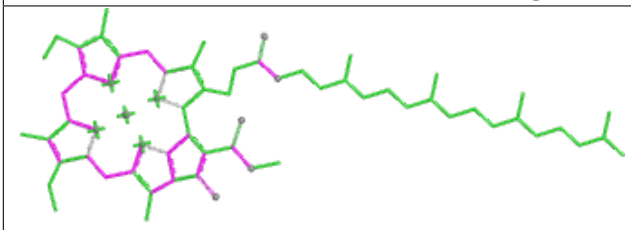
## Ligand LHG 41 201



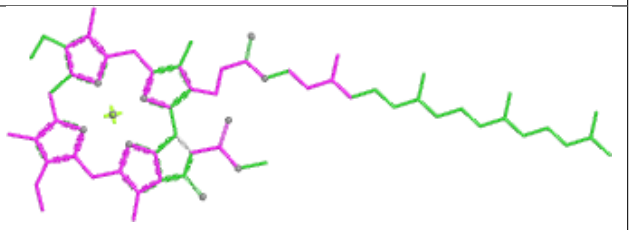

## Ligand A86 12 216



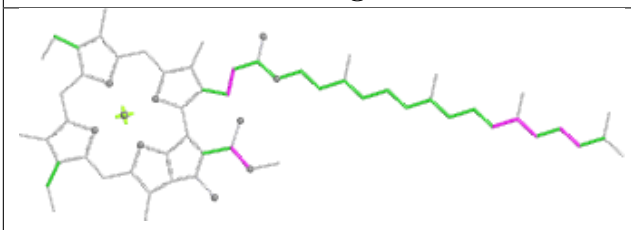
## Ligand CLA b 510



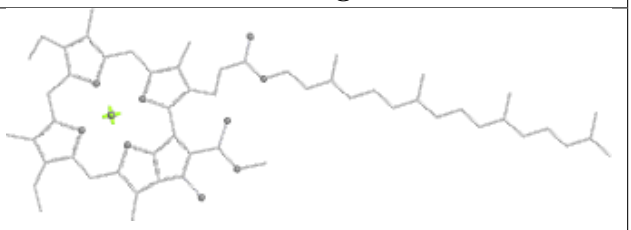
Bond lengths



Bond angles

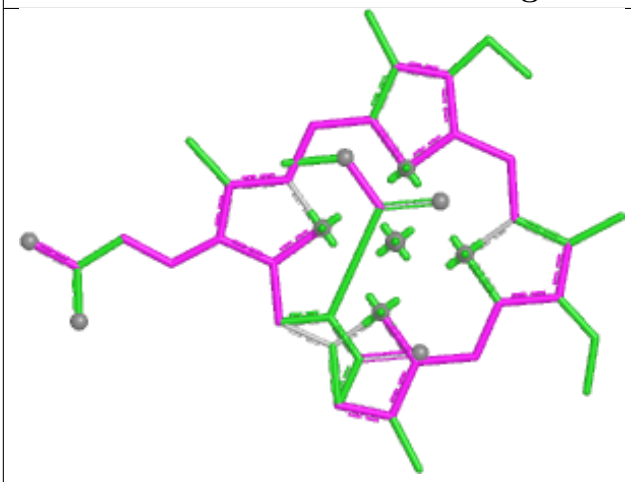


Torsions

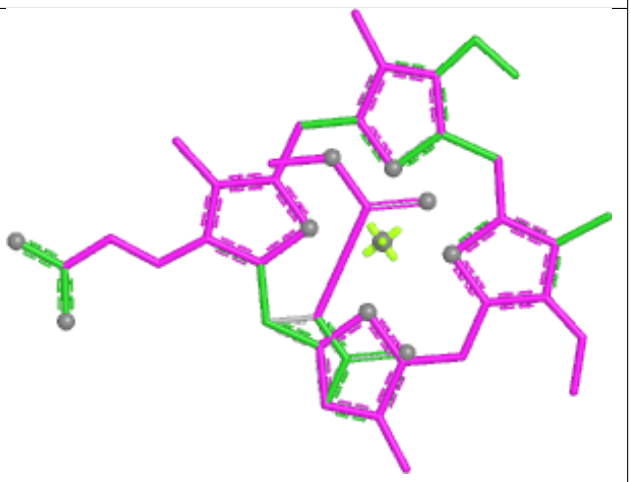


Rings

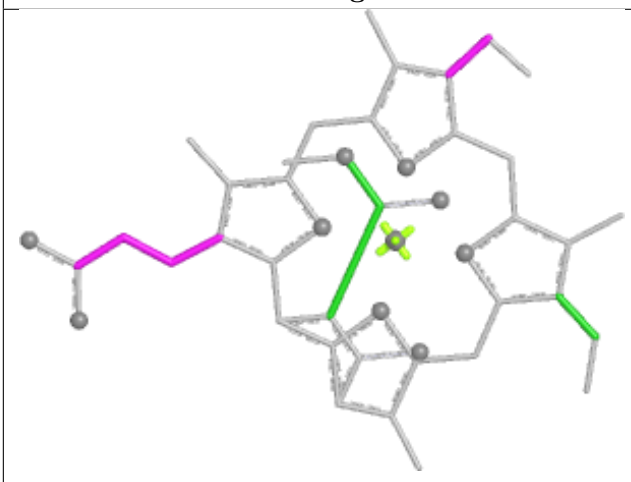
## Ligand KC1 35 304



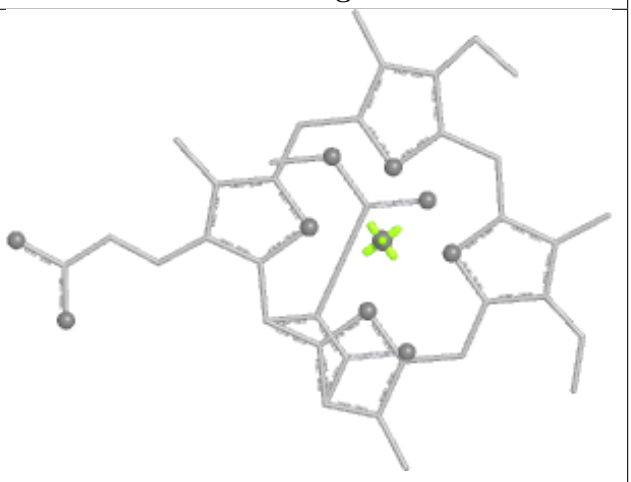
Bond lengths



Bond angles

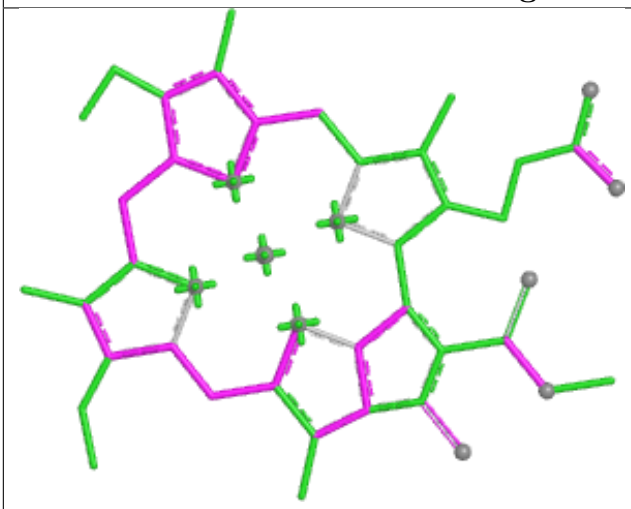


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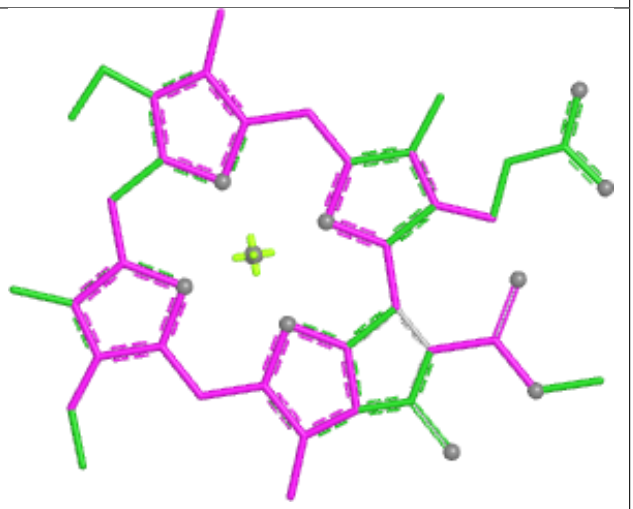


Rings

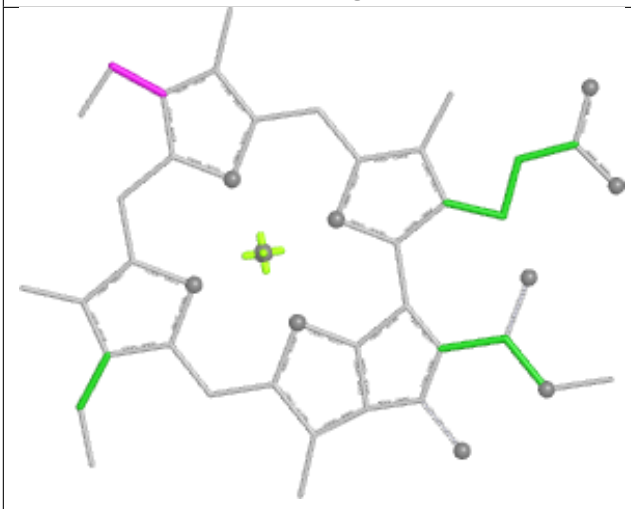
## Ligand CLA 13 310



Bond lengths



Bond angles

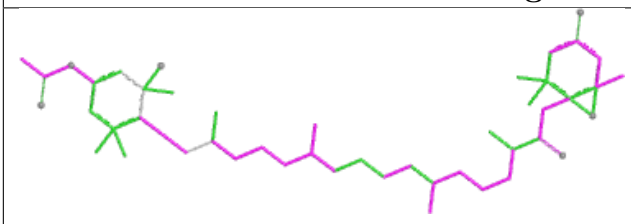


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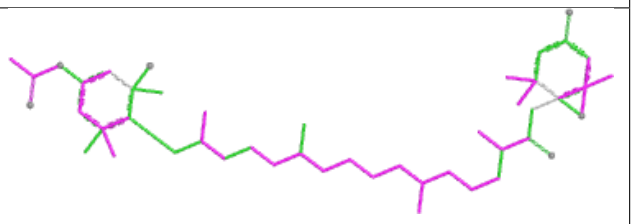


Rings

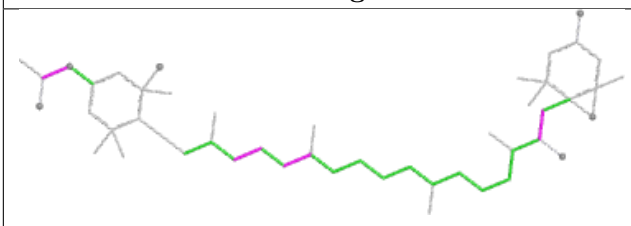
## Ligand A86 19 311



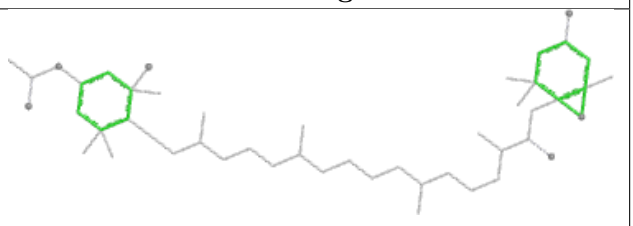
Bond lengths



Bond angles

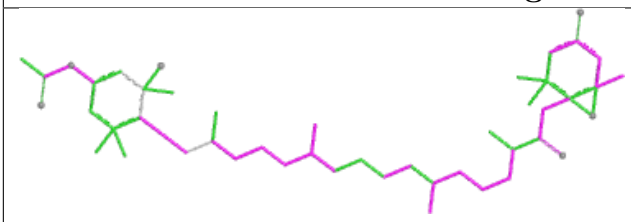


Torsions

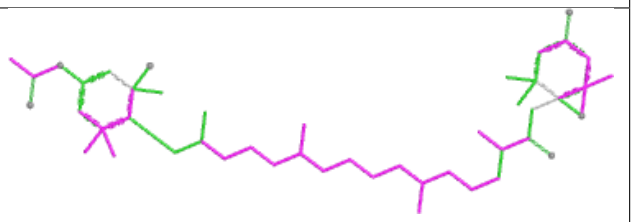


Rings

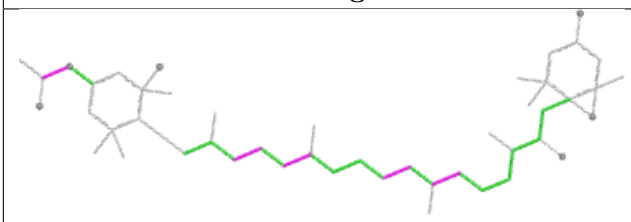
## Ligand A86 37 319



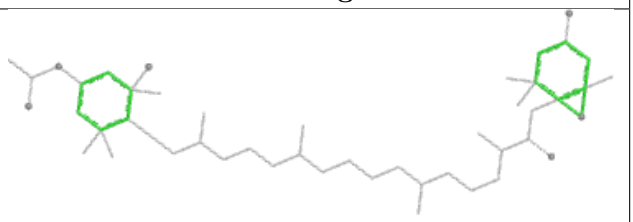
Bond lengths



Bond angles

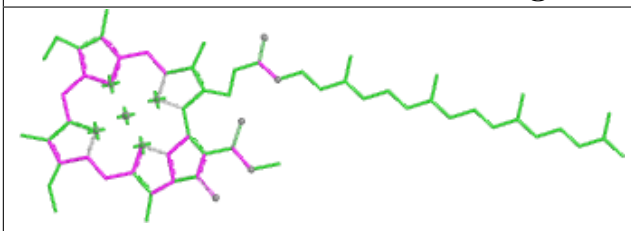


Torsions

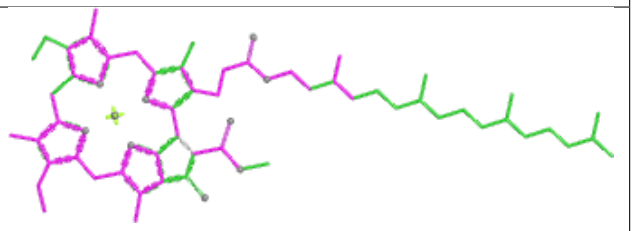


Rings

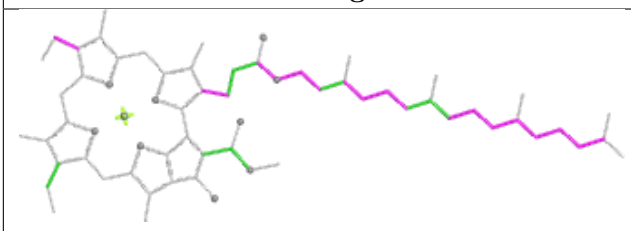
## Ligand CLA c 503



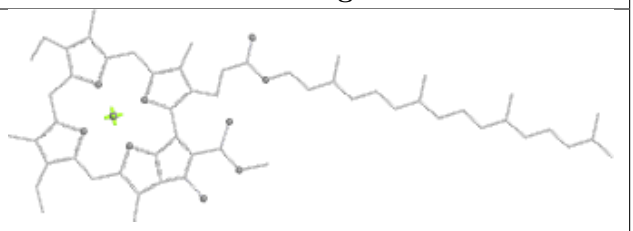
Bond lengths



Bond angles

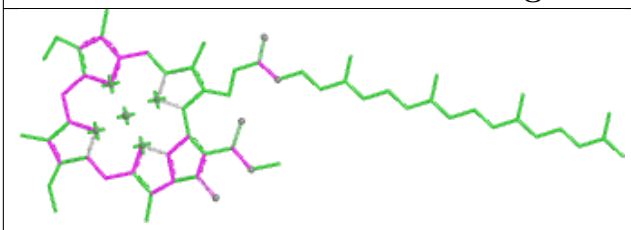


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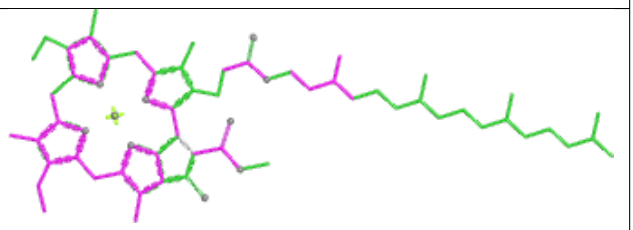


Rings

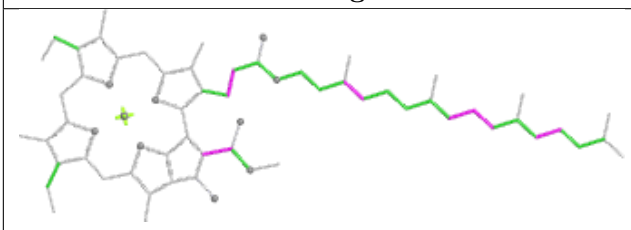
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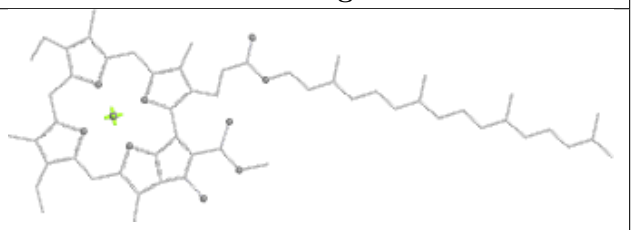
Bond lengths



Bond angles

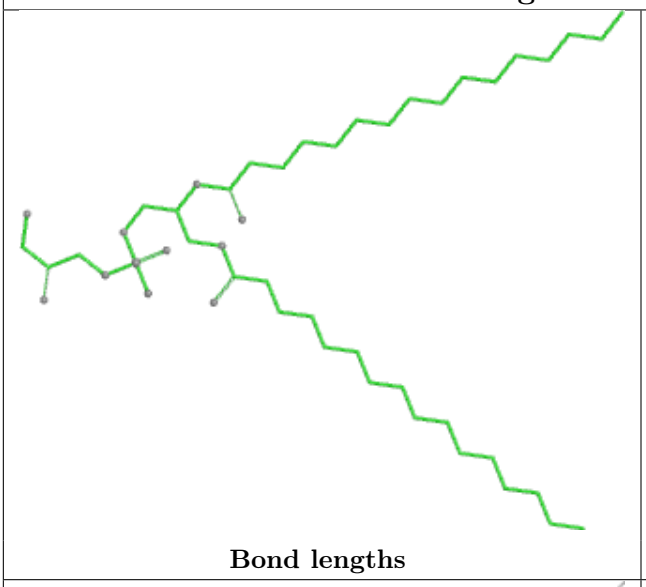


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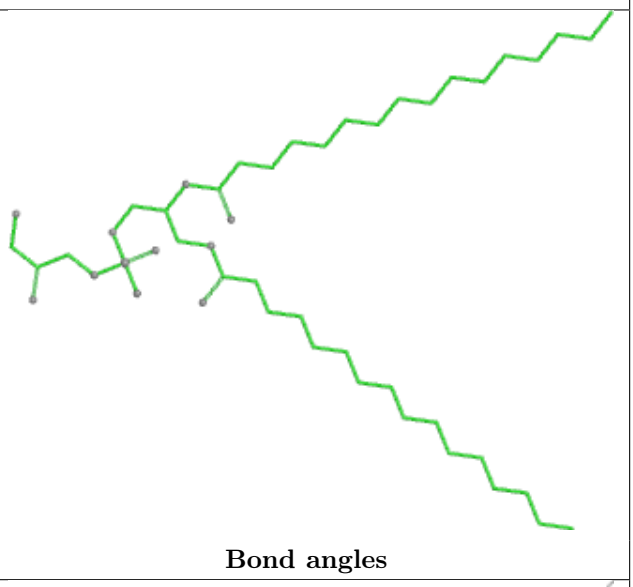


Rings

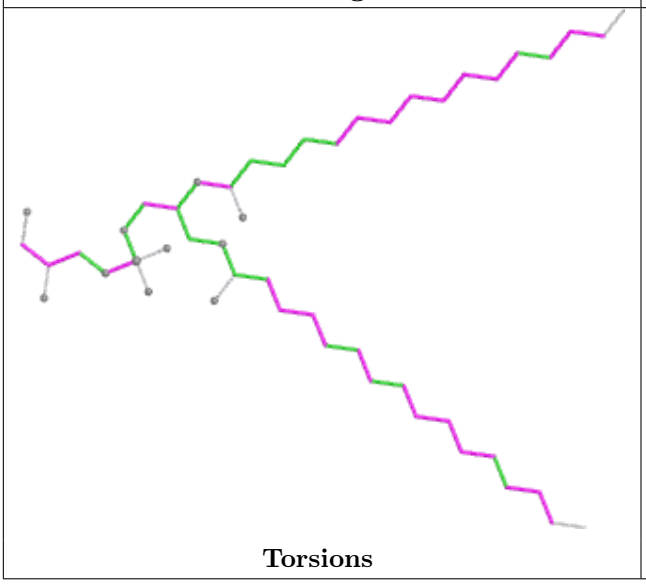
## Ligand LHG 19 314



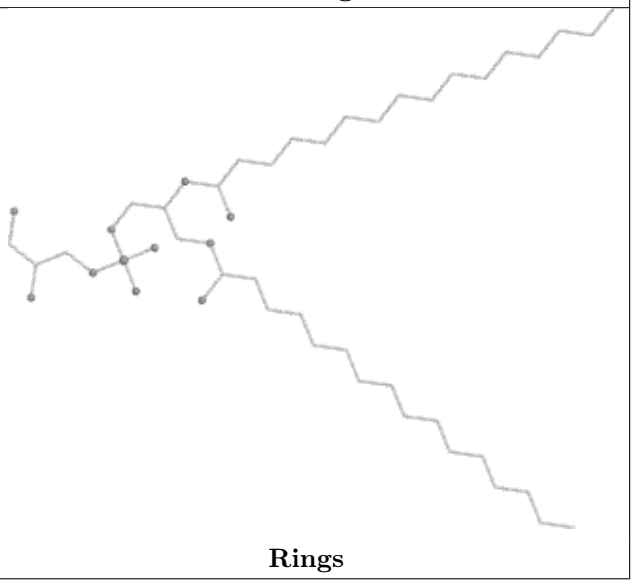
Bond lengths



Bond angles

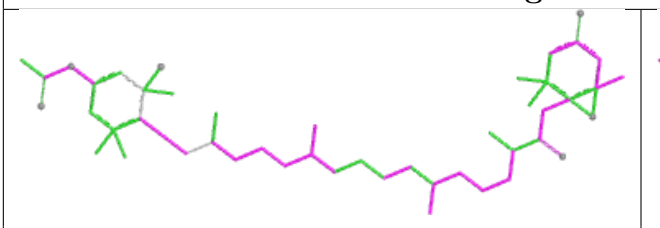


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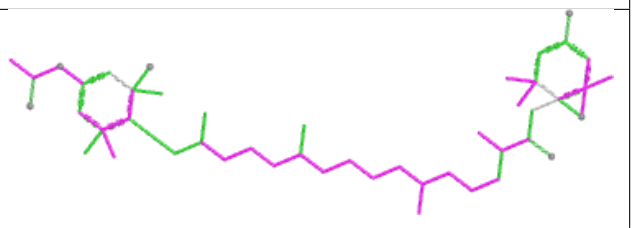


Rings

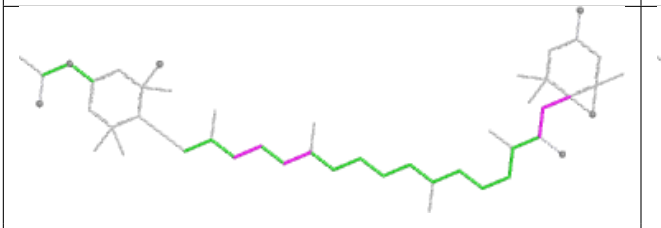
## Ligand A86 32 214



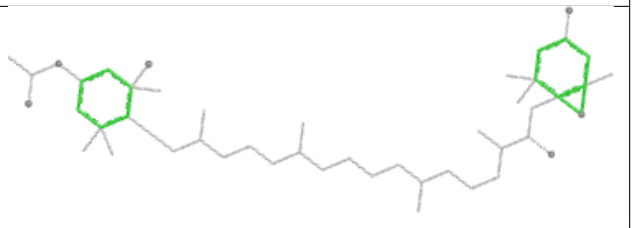
Bond lengths



Bond angles

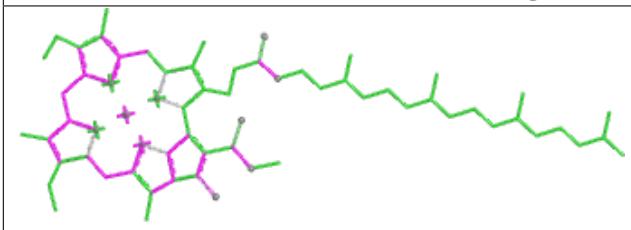


Torsions

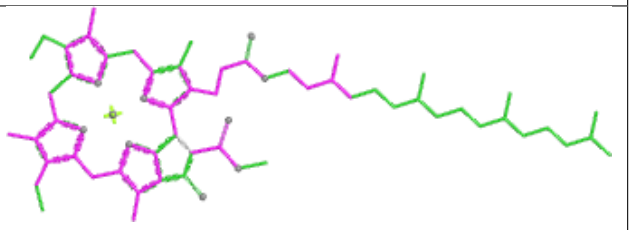


Rings

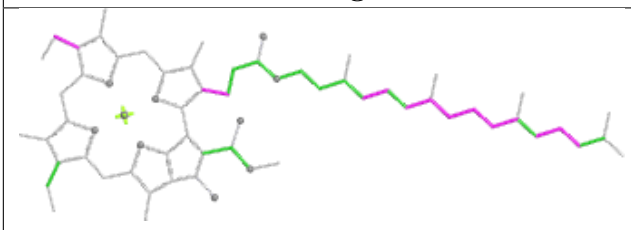
## Ligand CLA B 524



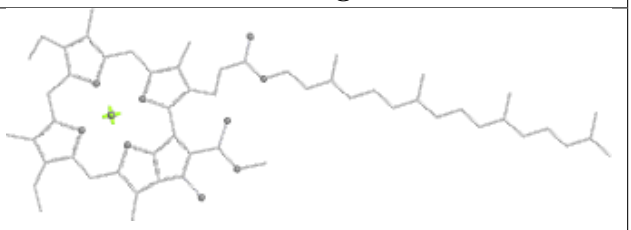
Bond lengths



Bond angles



Torsions

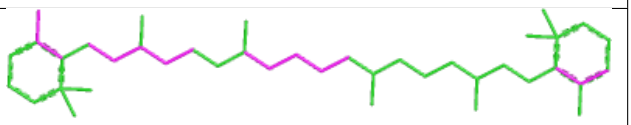


Rings

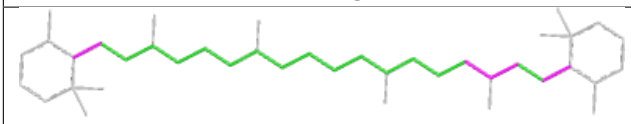
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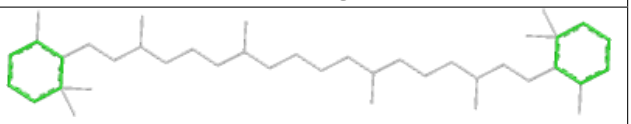
Bond lengths



Bond angles

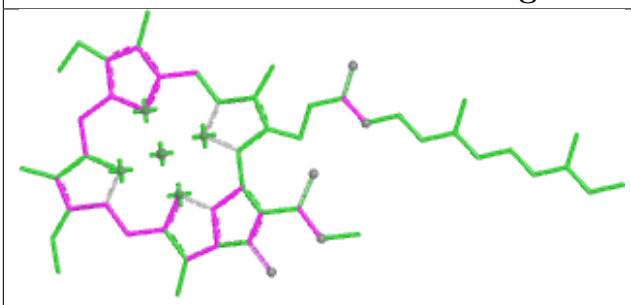


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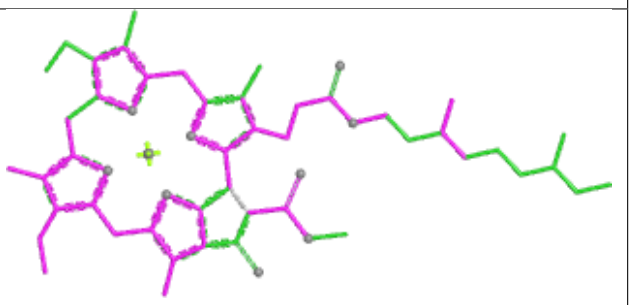


Rings

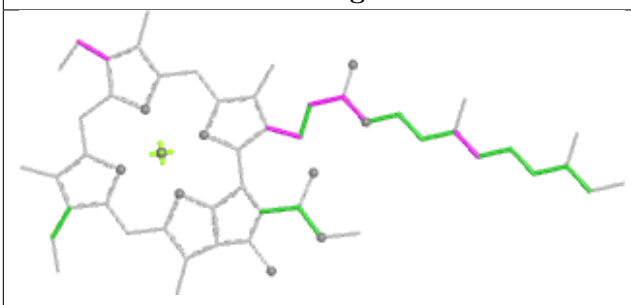
## Ligand CLA 37 303



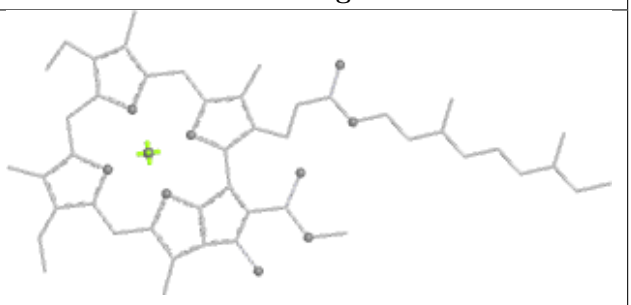
Bond lengths



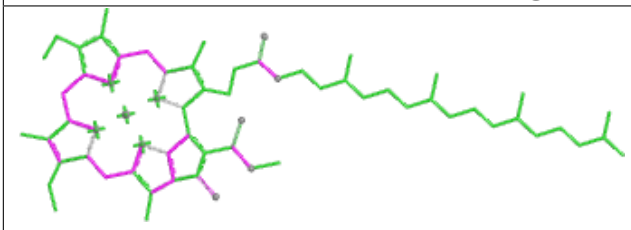
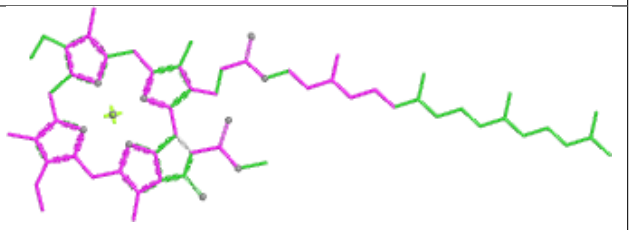
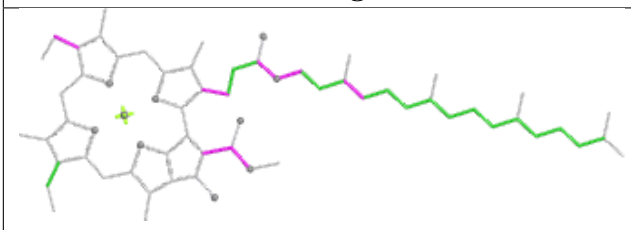
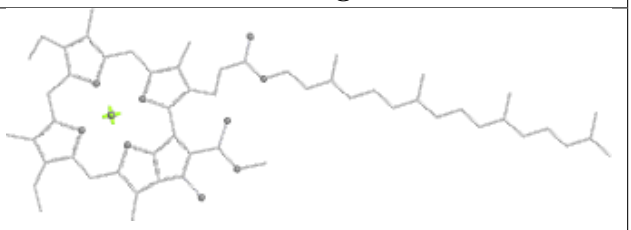
Bond angles

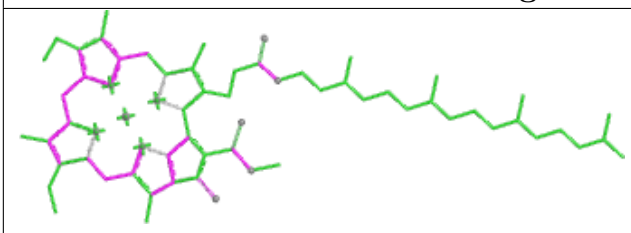
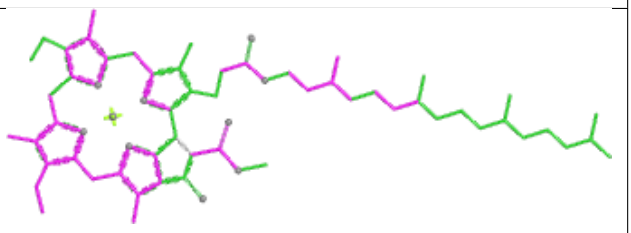
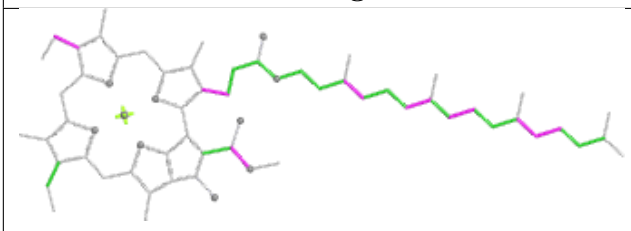
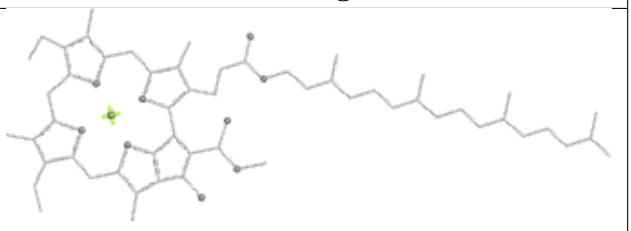


Torsions

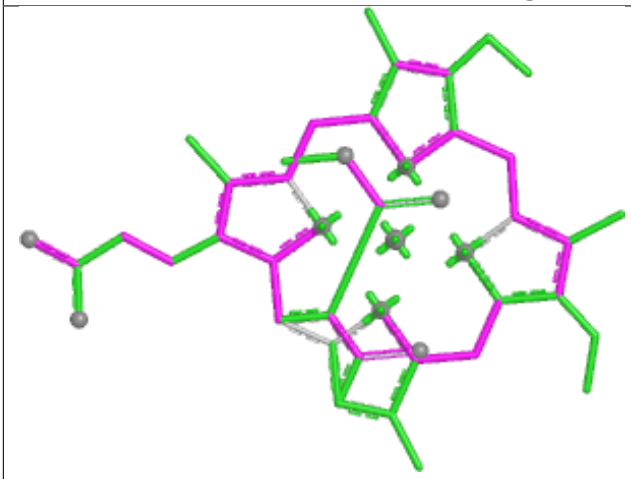


Rings

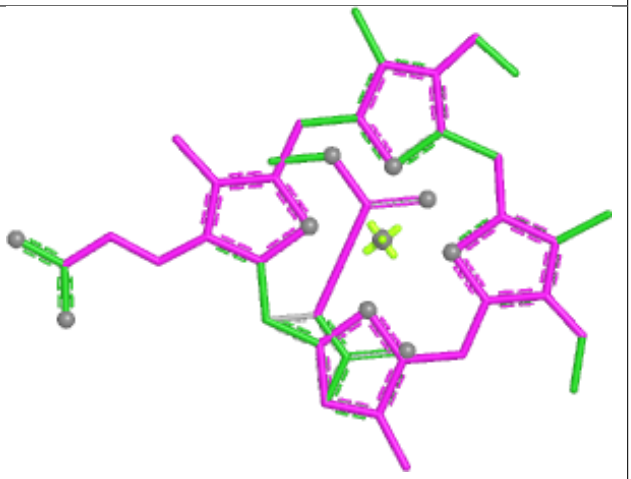
| Ligand CLA b 509 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 34 301 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

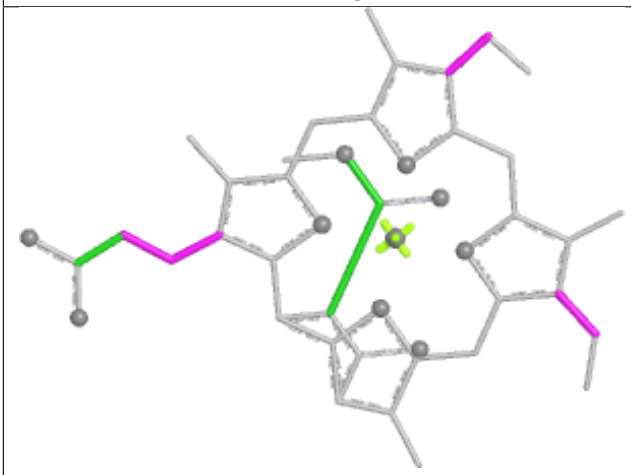
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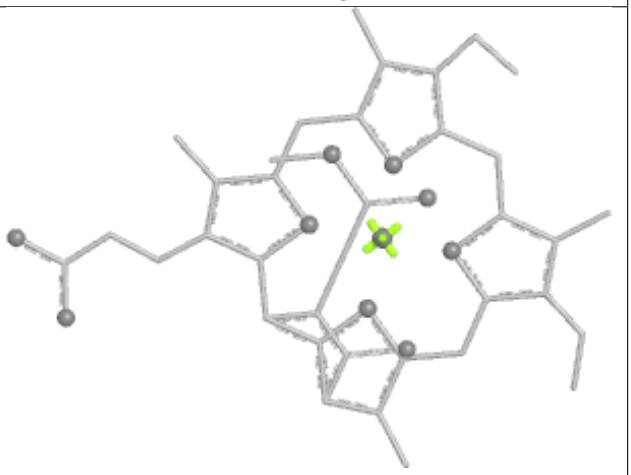
Bond lengths



Bond angles

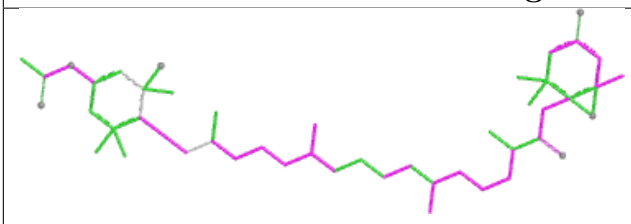


Torsions

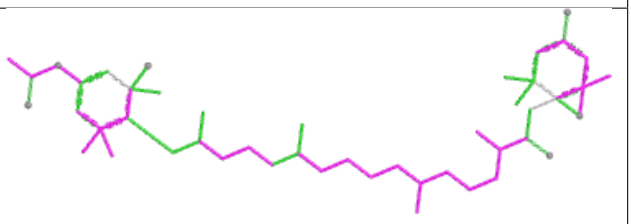


Rings

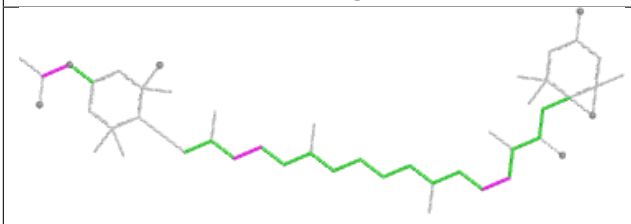
**Ligand A86 34 312**



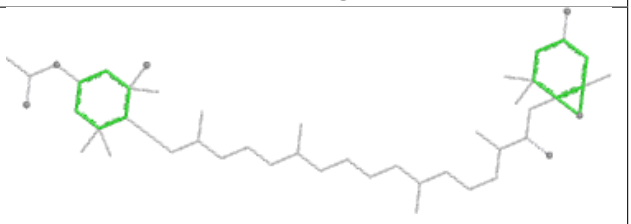
Bond lengths



Bond angles

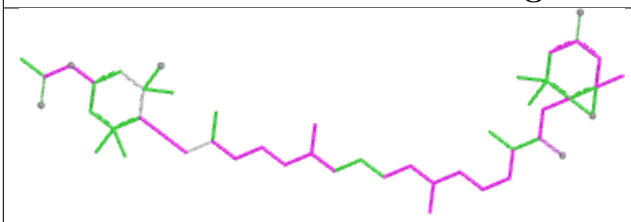


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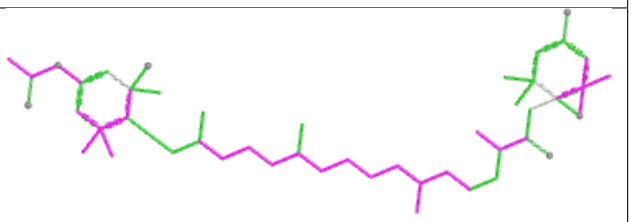


Rings

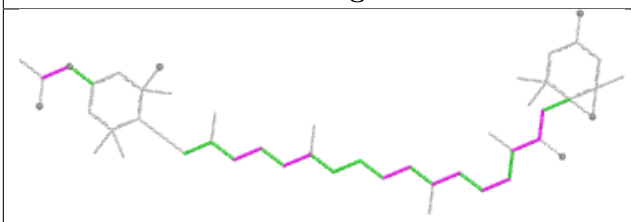
## Ligand A86 18 214



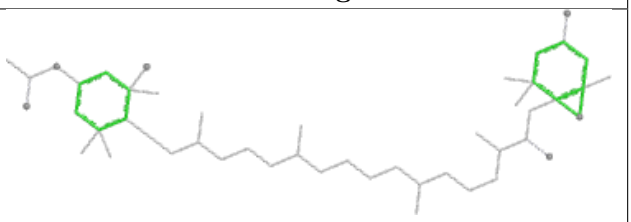
Bond lengths



Bond angles

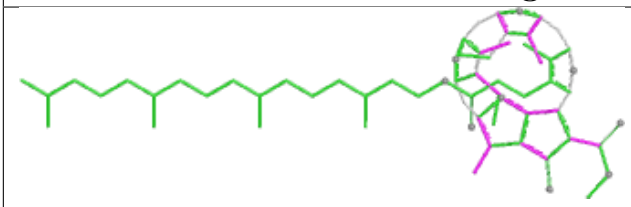


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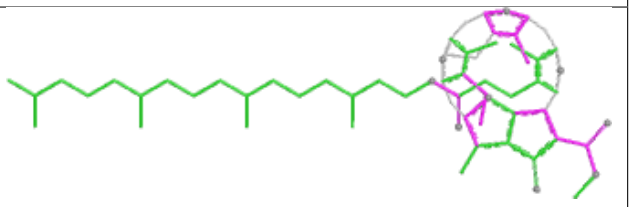


Rings

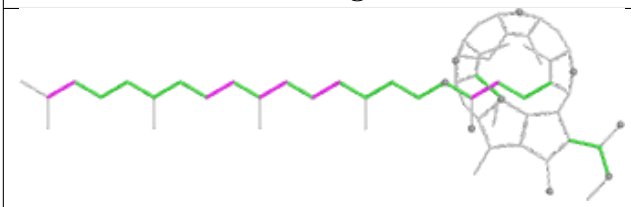
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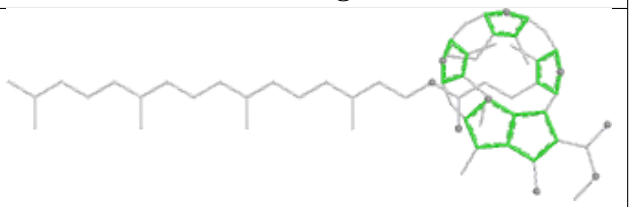
Bond lengths



Bond angles

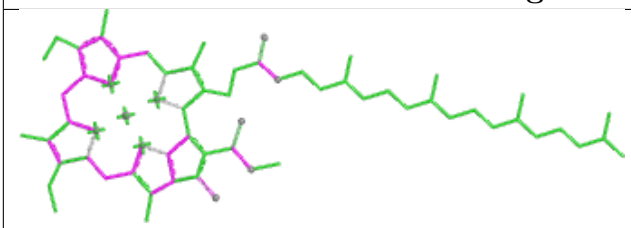


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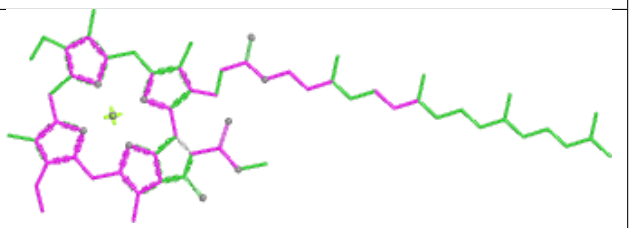


Rings

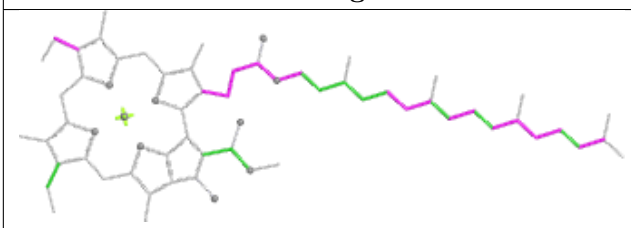
## Ligand CLA Z 101



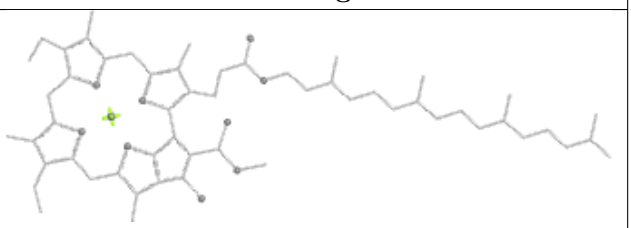
Bond lengths



Bond angles

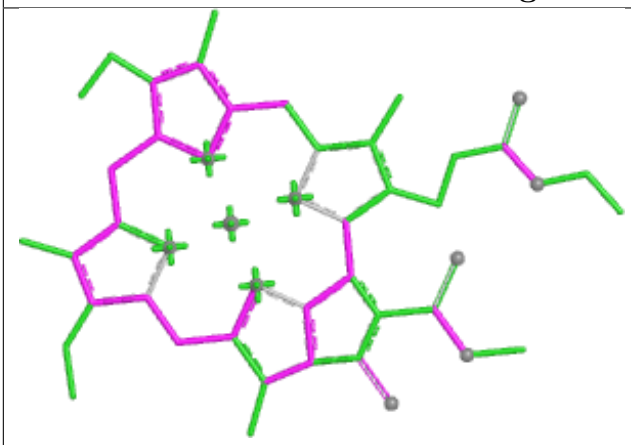


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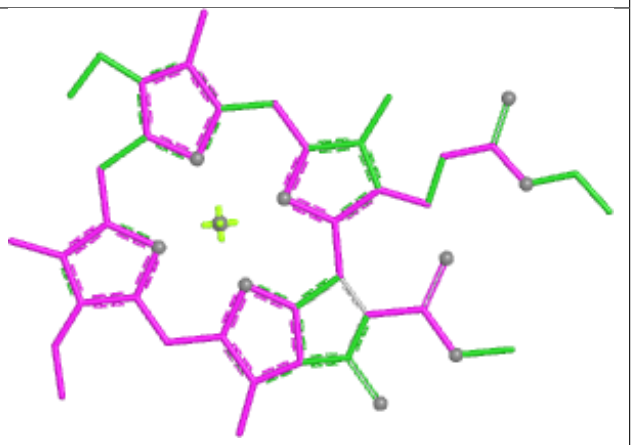


Rings

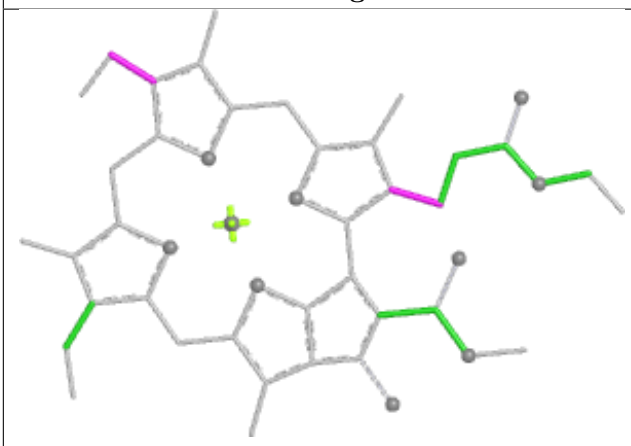
**Ligand CLA 40 210**



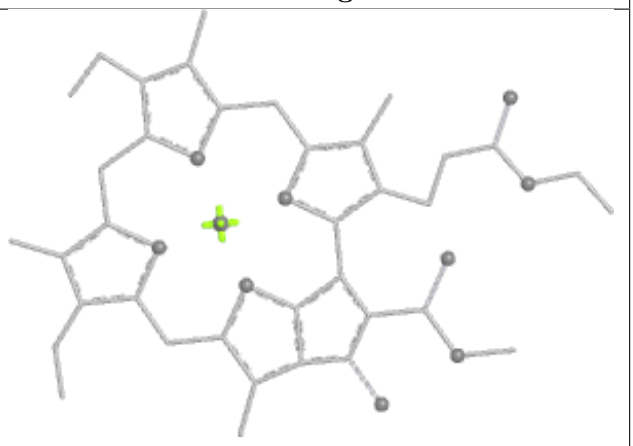
**Bond lengths**



**Bond angles**

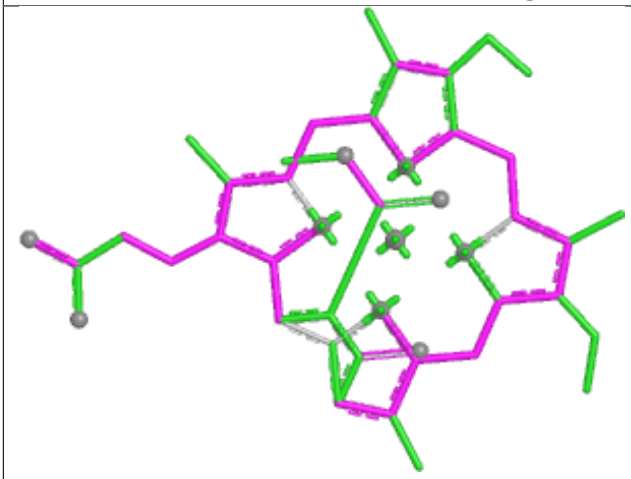


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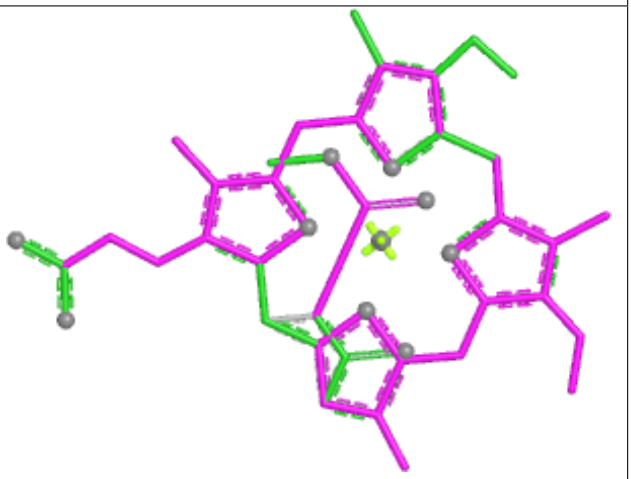


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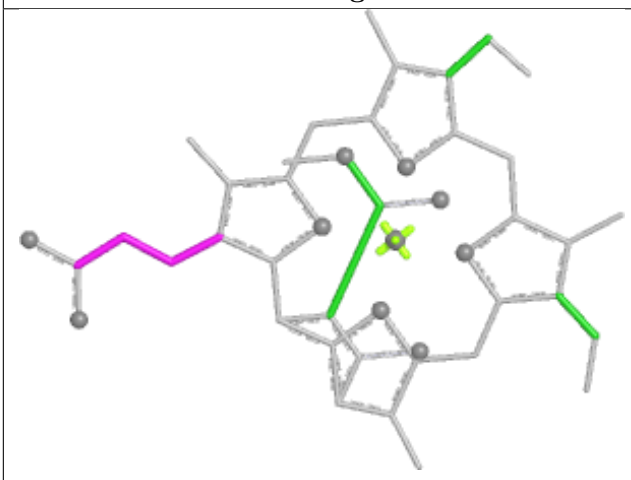
**Ligand KC1 41 203**



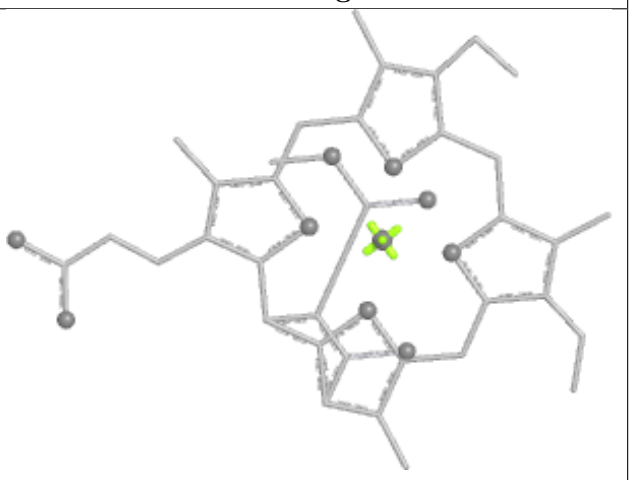
**Bond lengths**



**Bond angles**

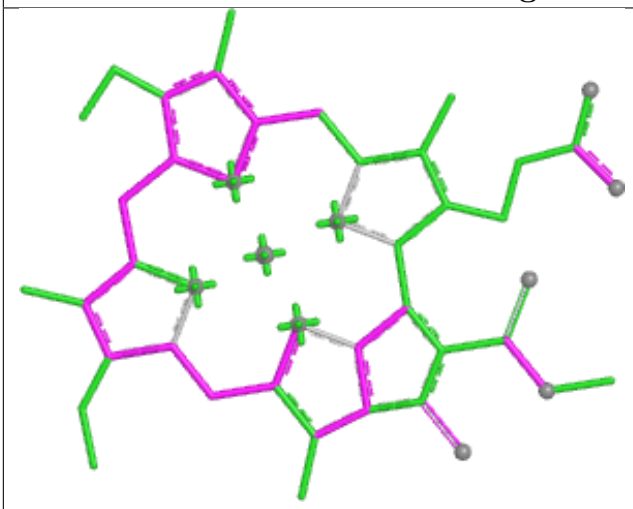


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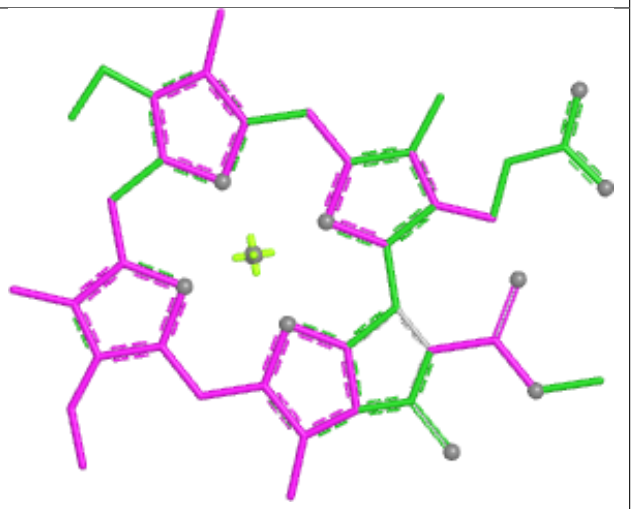


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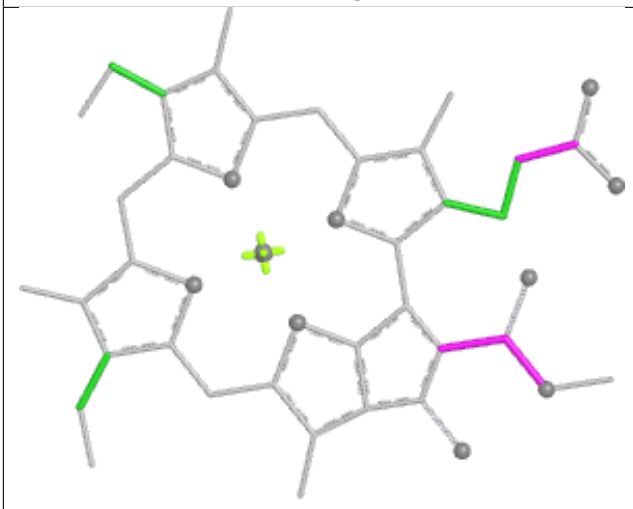
**Ligand CLA 41 209**



**Bond lengths**



**Bond angles**

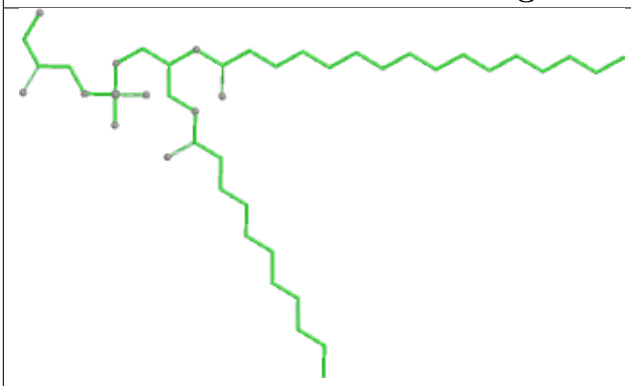


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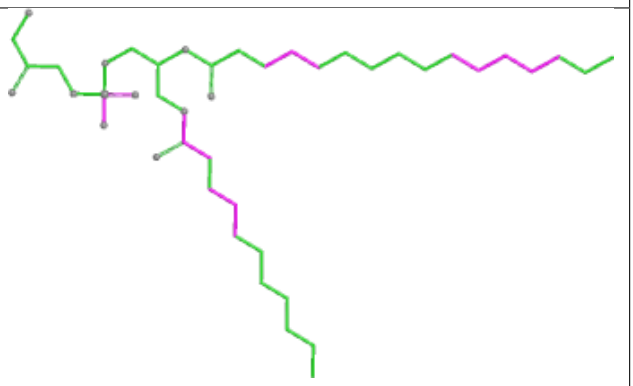


**Rings**

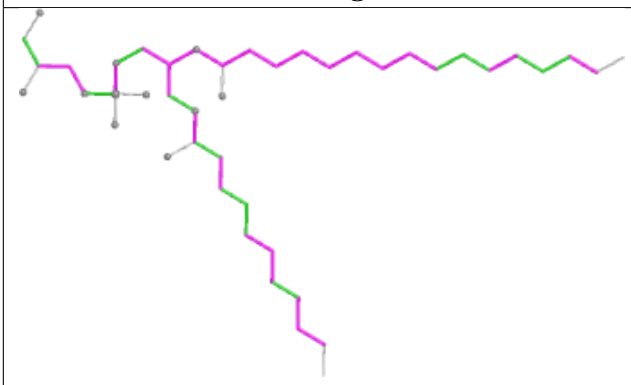
## Ligand LHG 37 315



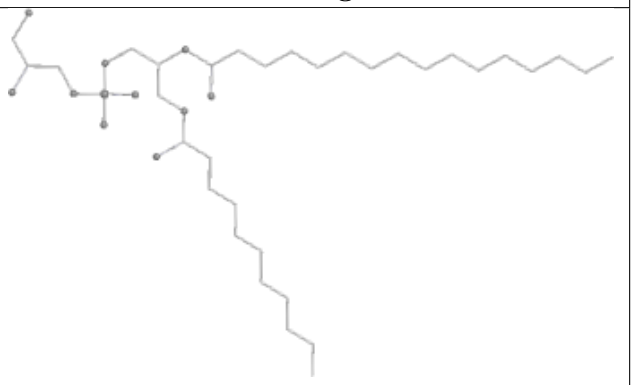
Bond lengths



Bond angles

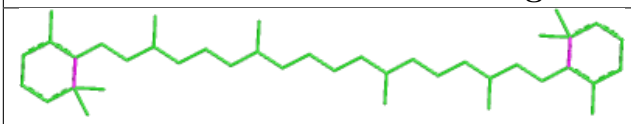


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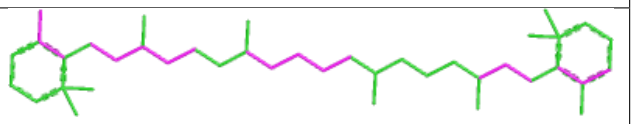


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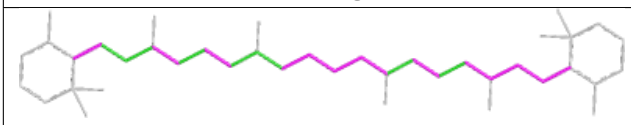
## Ligand BCR b 524



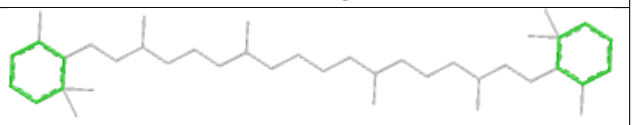
Bond lengths



Bond angles

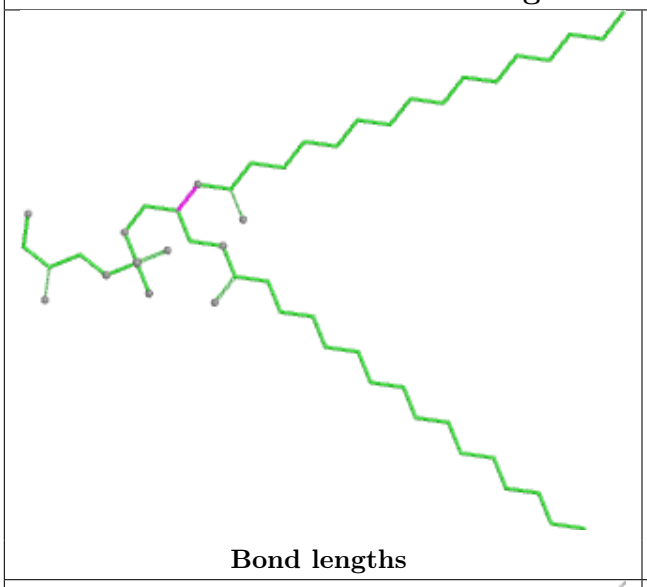


Torsions

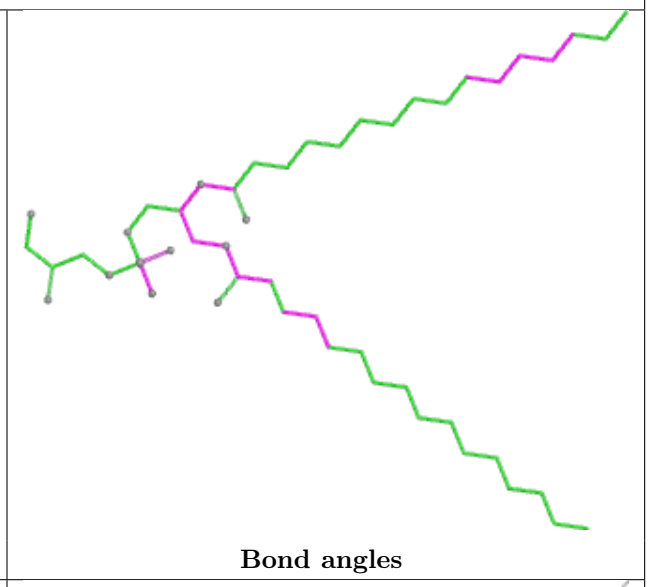


Rings

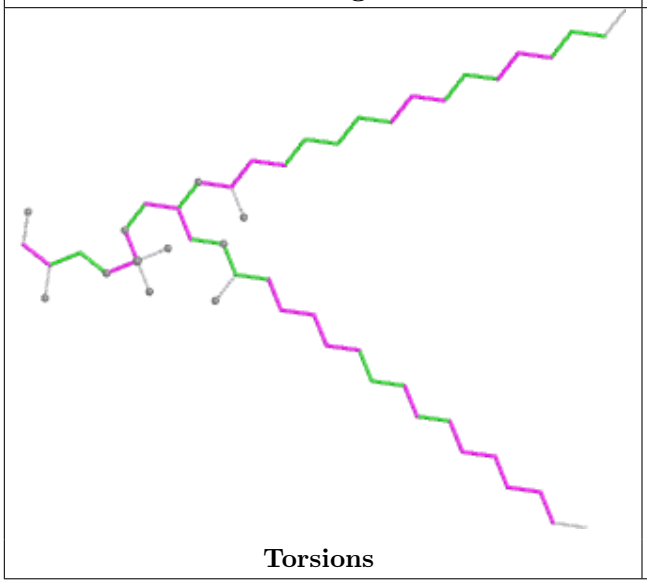
## Ligand LHG D 410



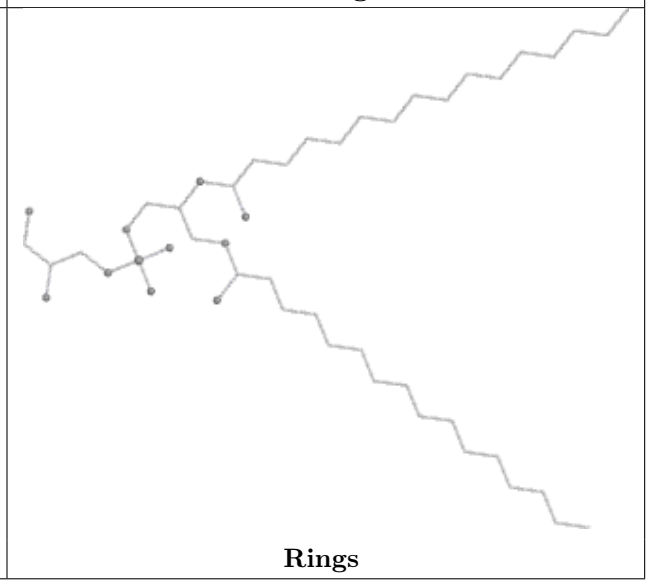
Bond lengths



Bond angles

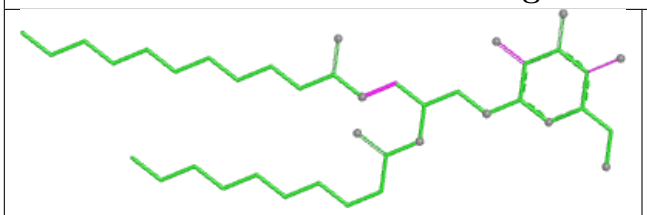


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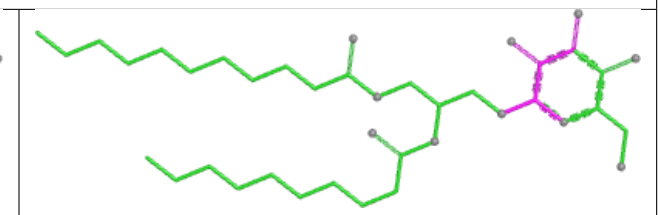


Rings

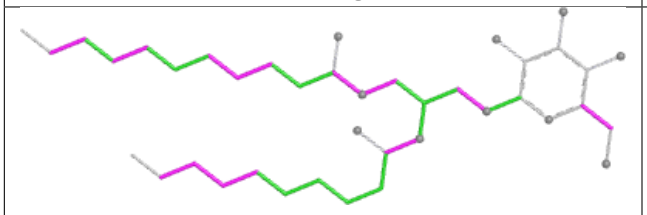
## Ligand LMG L 102



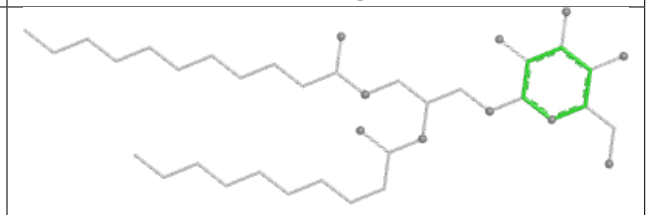
Bond lengths



Bond angles

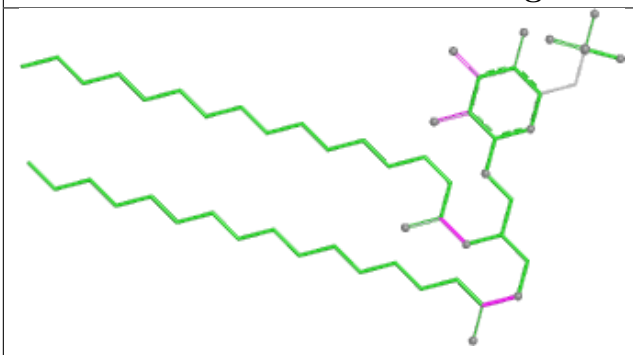


Torsions

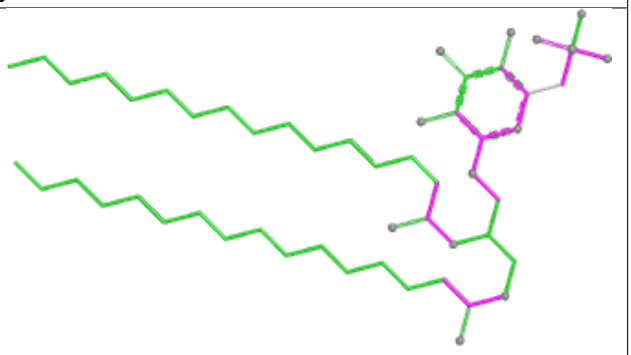


Rings

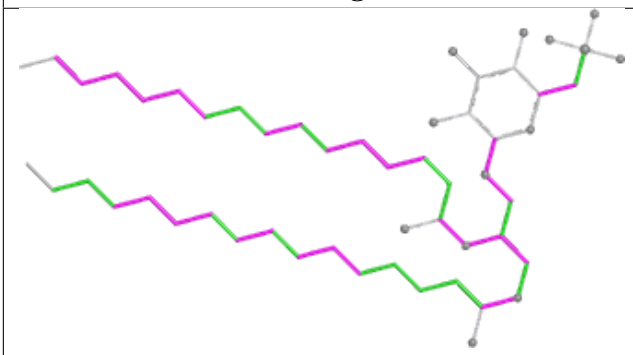
## Ligand SQD B 519



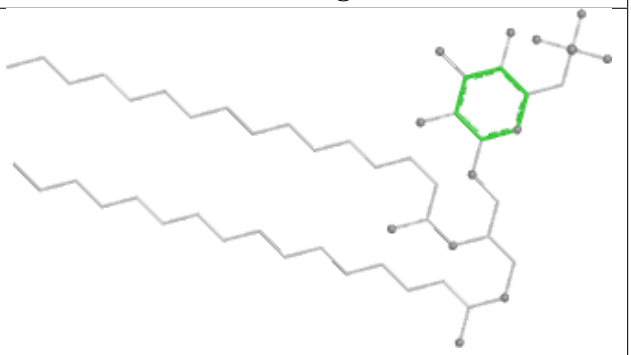
Bond lengths



Bond angles

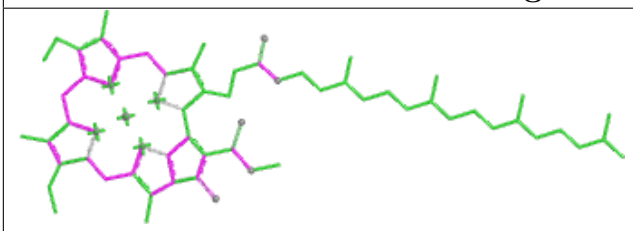


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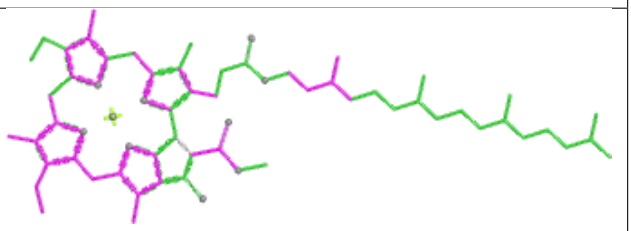


Rings

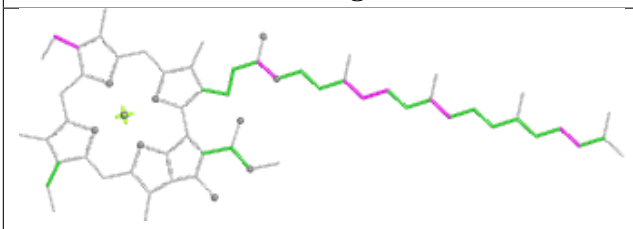
## Ligand CLA C 504



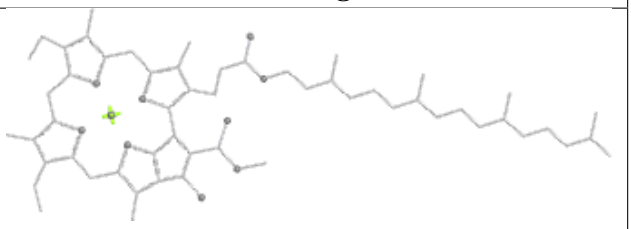
Bond lengths



Bond angles

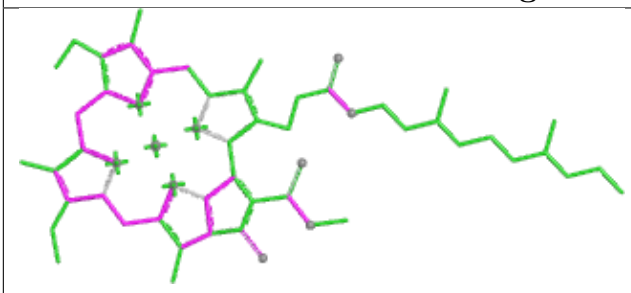


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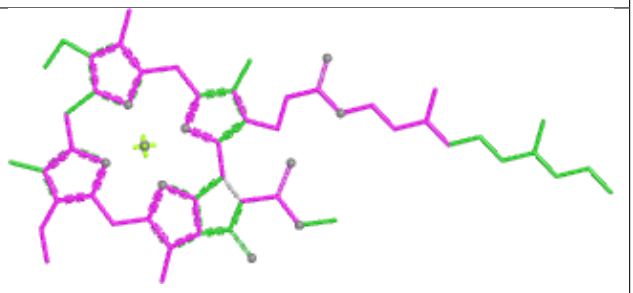


Rings

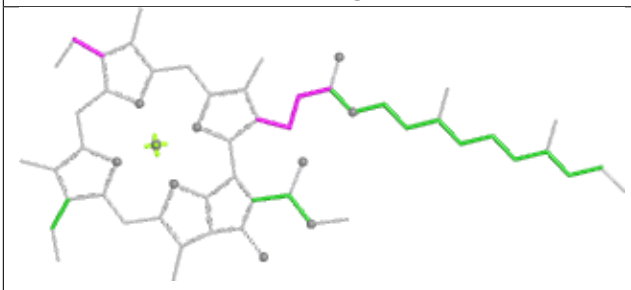
## Ligand CLA 14 303



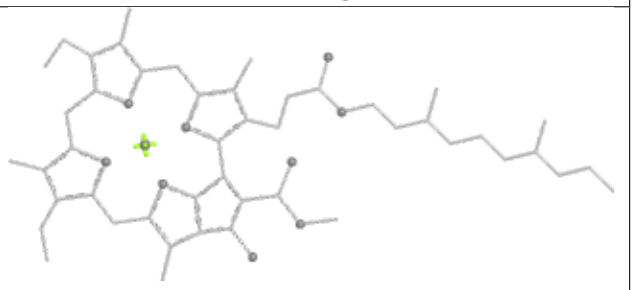
Bond lengths



Bond angles

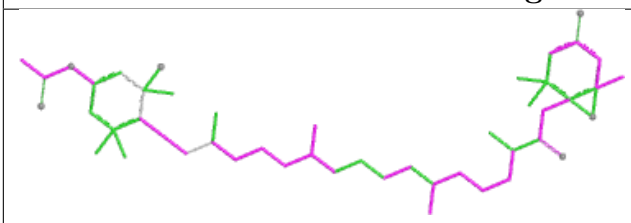


Torsions

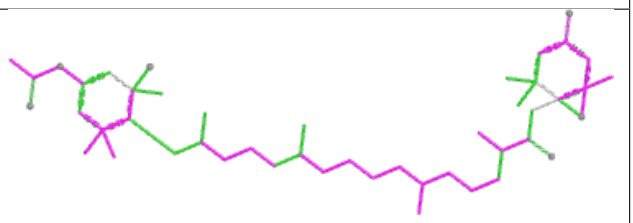


Rings

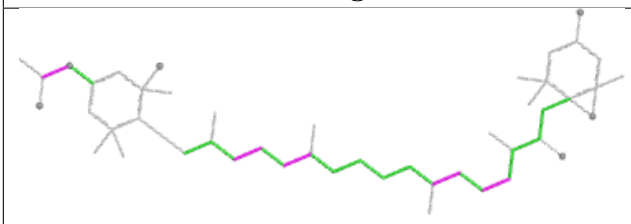
## Ligand A86 15 315



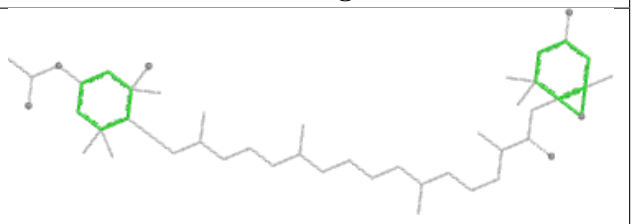
Bond lengths



Bond angles

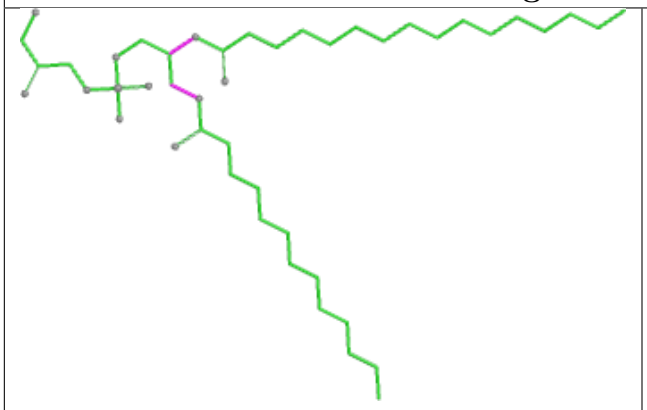


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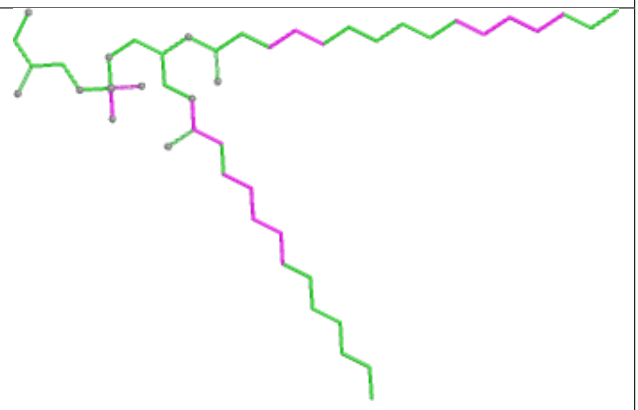


Rings

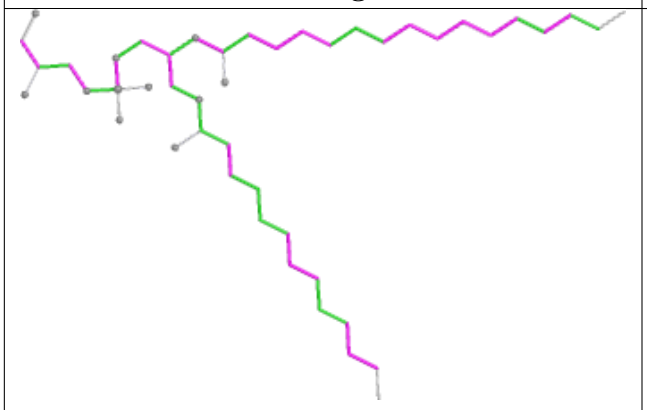
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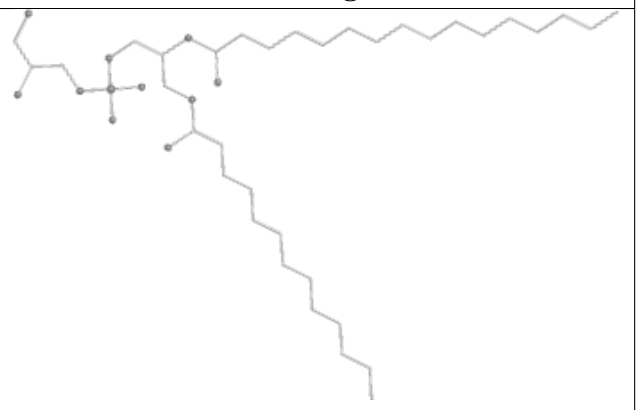
Bond lengths



Bond angles

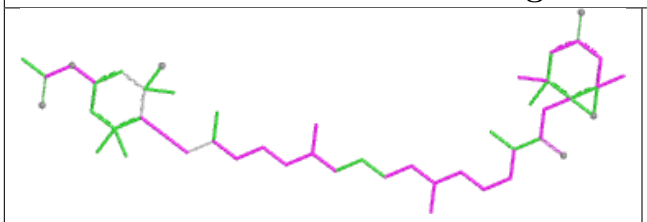


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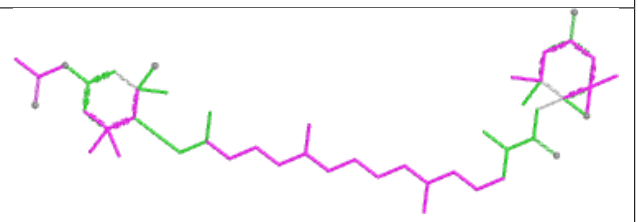


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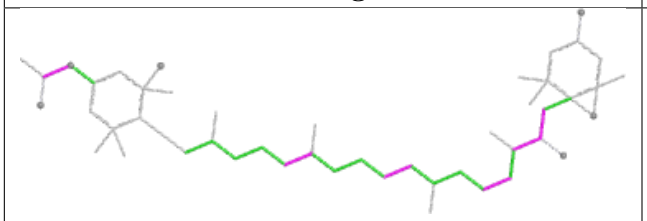
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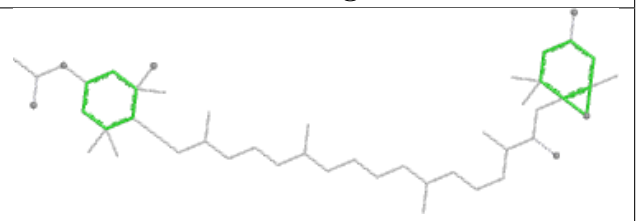
Bond lengths



Bond angles

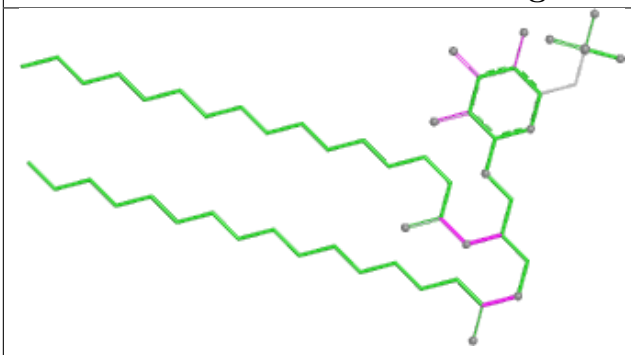


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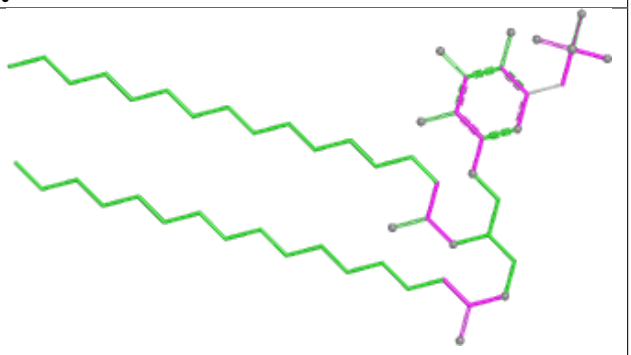


Rings

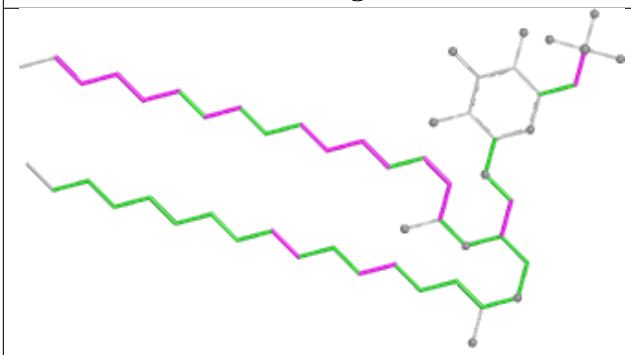
**Ligand SQD a 409**



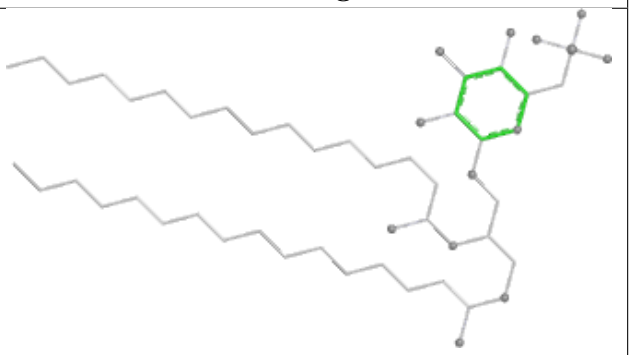
Bond lengths



Bond angles

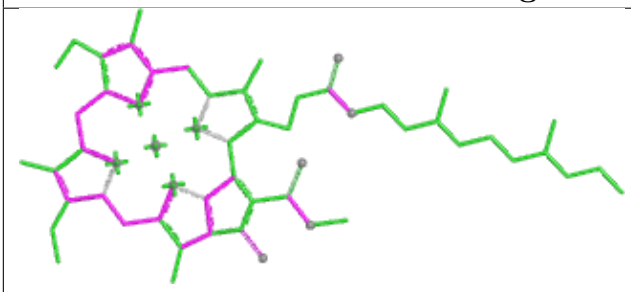


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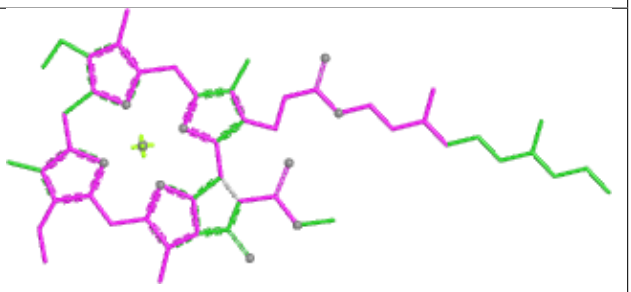


Rings

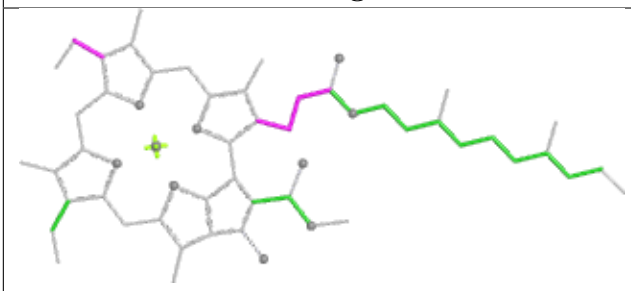
**Ligand CLA 34 303**



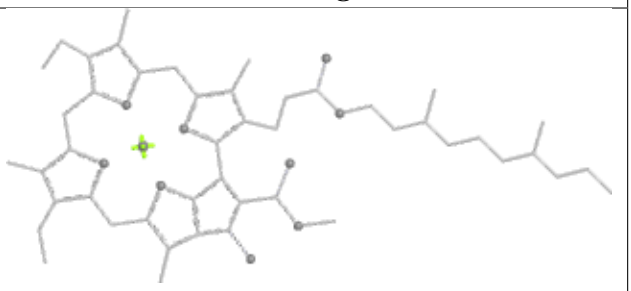
Bond lengths



Bond angles

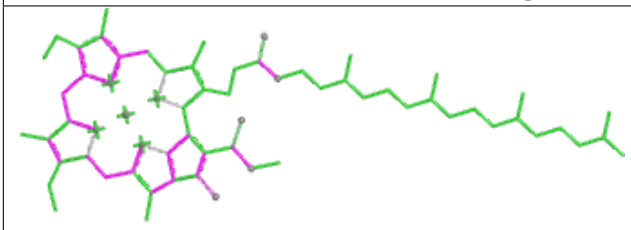


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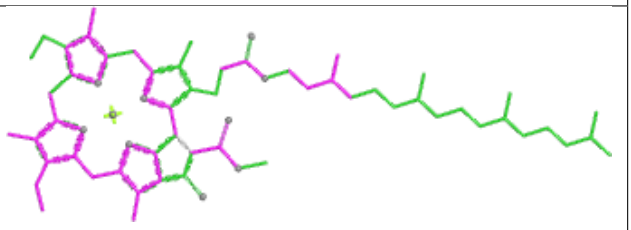


Rings

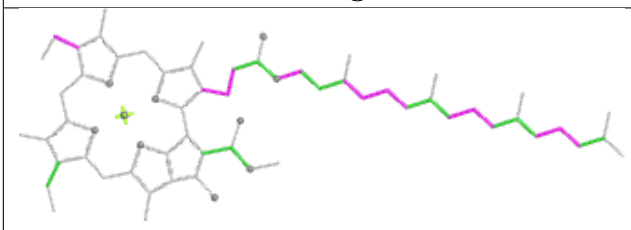
## Ligand CLA 12 203



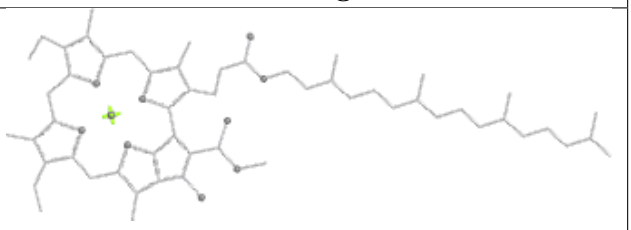
Bond lengths



Bond angles

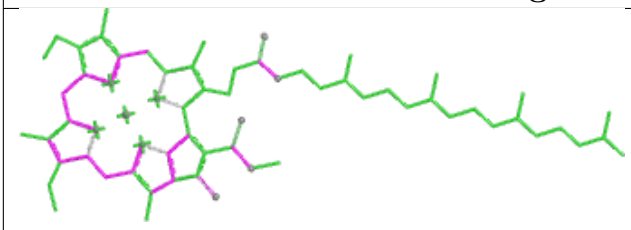


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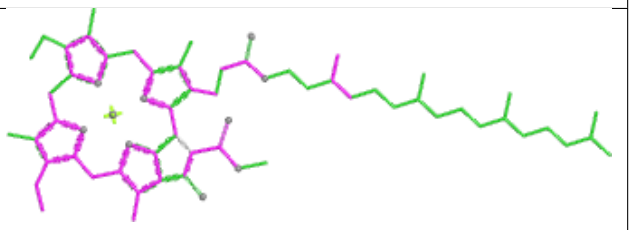


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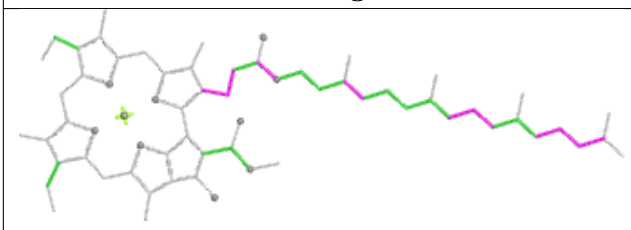
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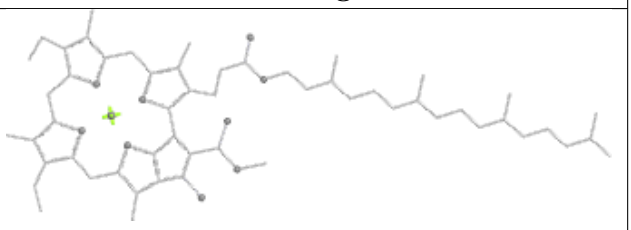
Bond lengths



Bond angles

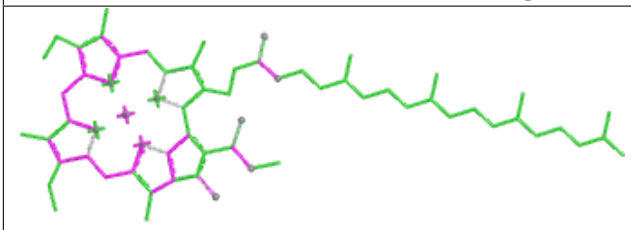


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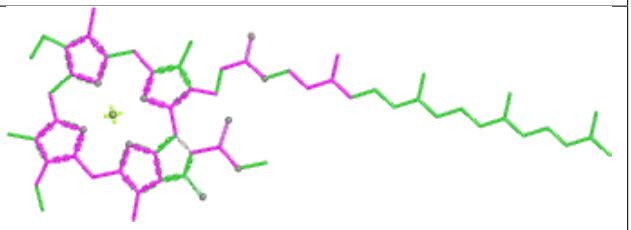


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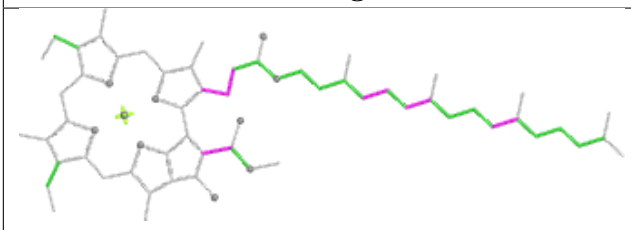
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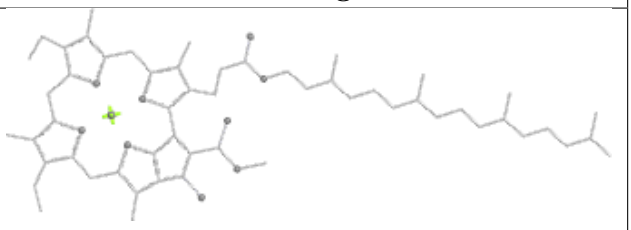
Bond lengths



Bond angles

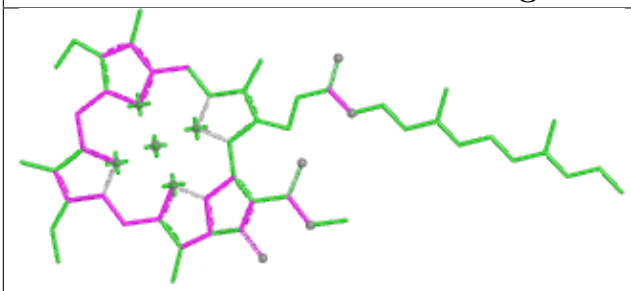


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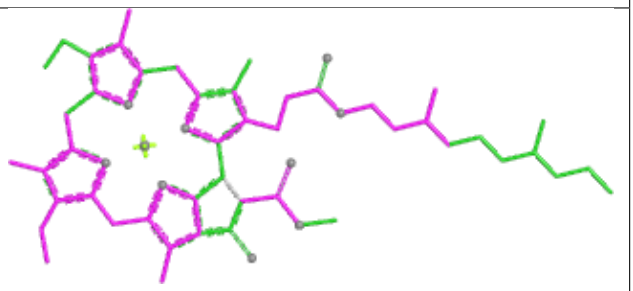


Rings

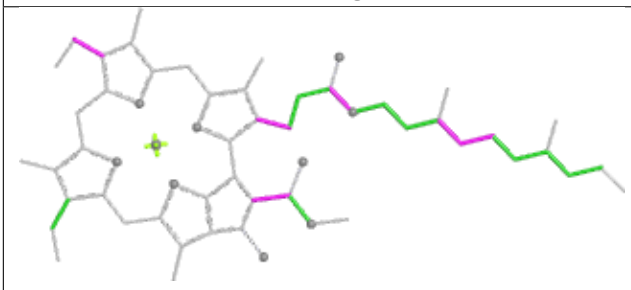
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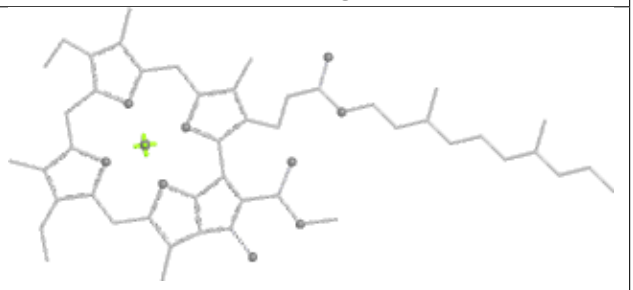
Bond lengths



Bond angles

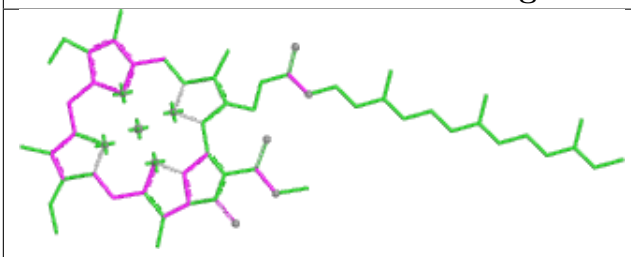


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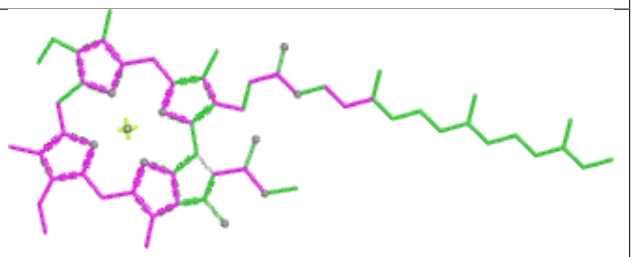


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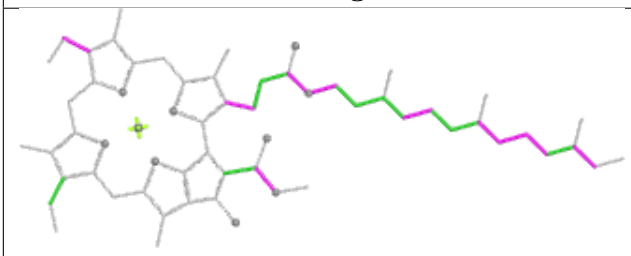
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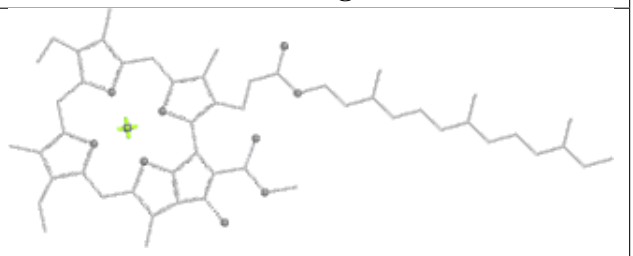
Bond lengths



Bond angles

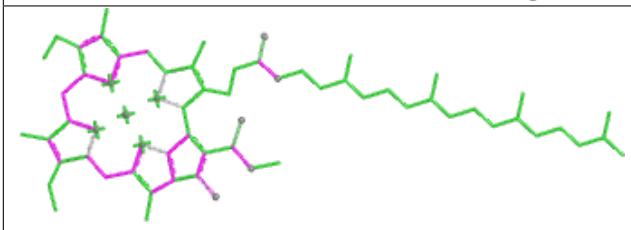


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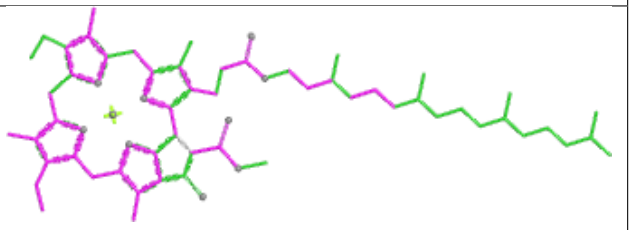


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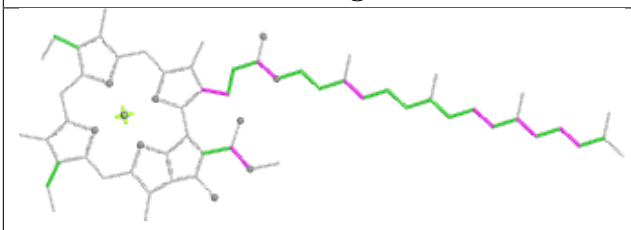
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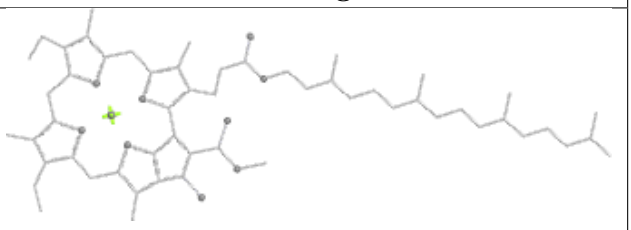
Bond lengths



Bond angles



Torsions

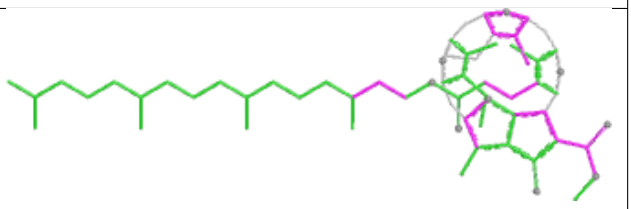


Rings

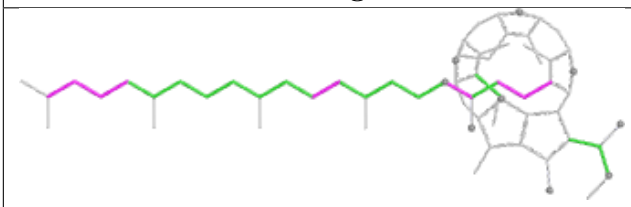
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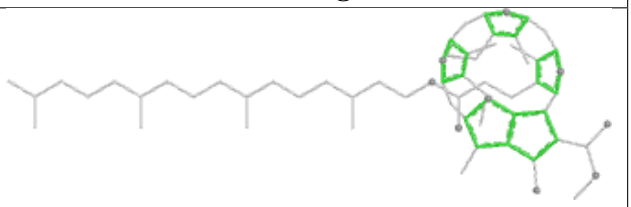
Bond lengths



Bond angles

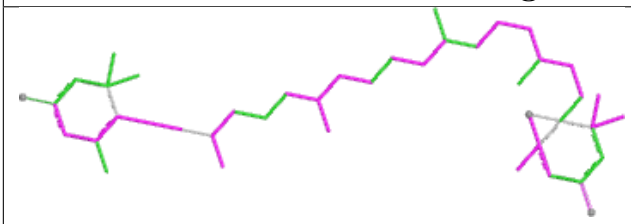


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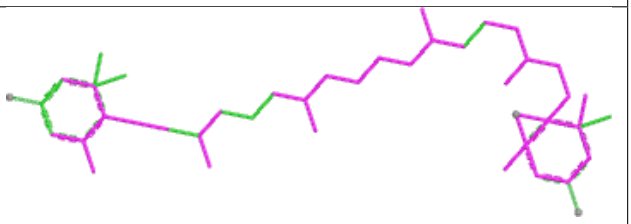


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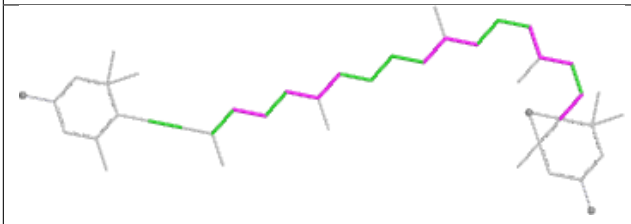
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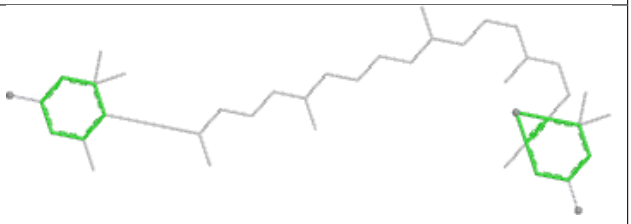
Bond lengths



Bond angles

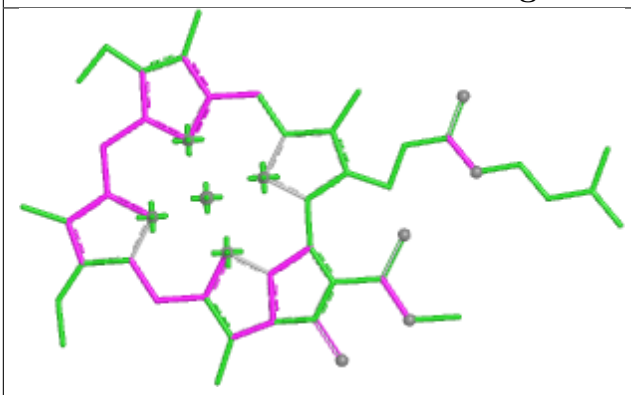


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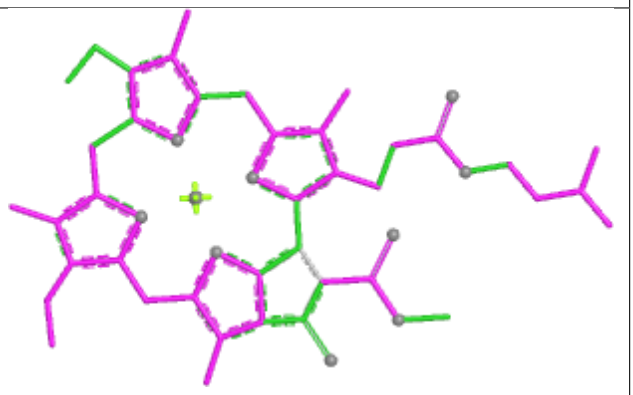


Rings

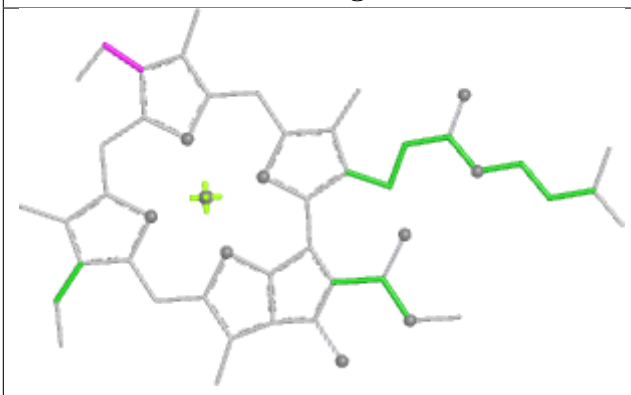
## Ligand CLA 32 208



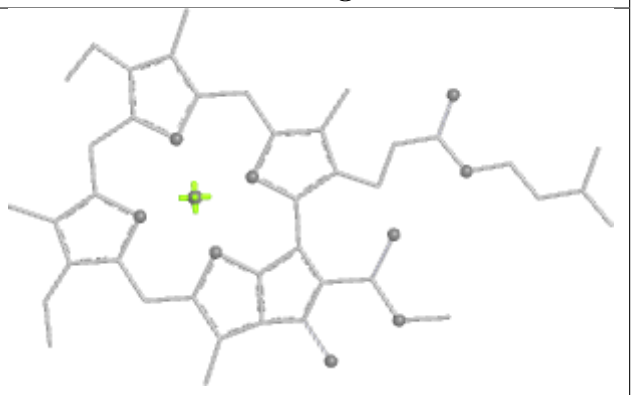
Bond lengths



Bond angles

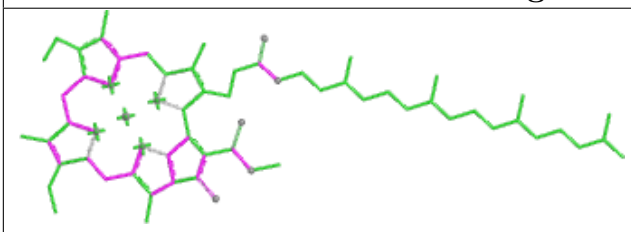


Torsions

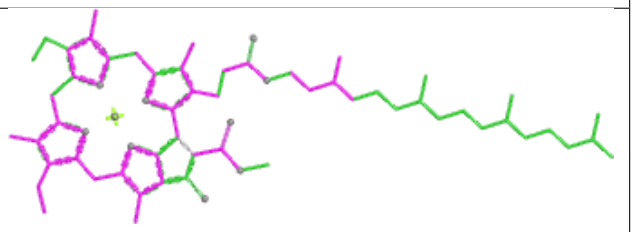


Rings

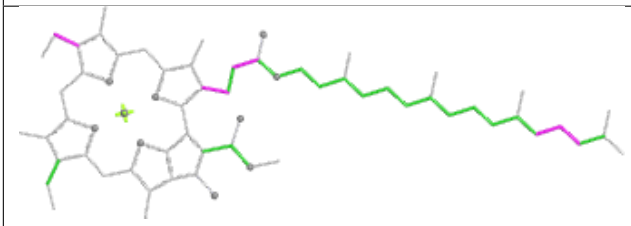
## Ligand CLA d 403



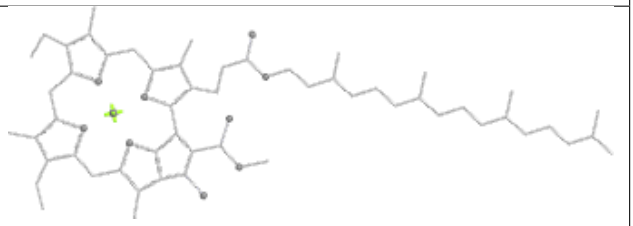
Bond lengths



Bond angles

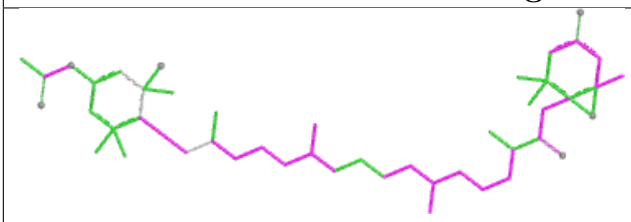


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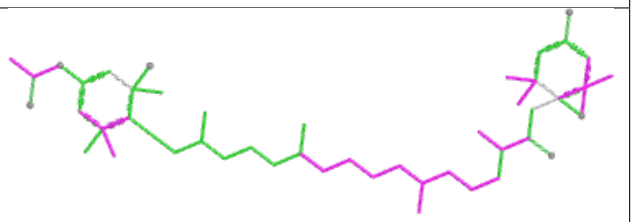


Rings

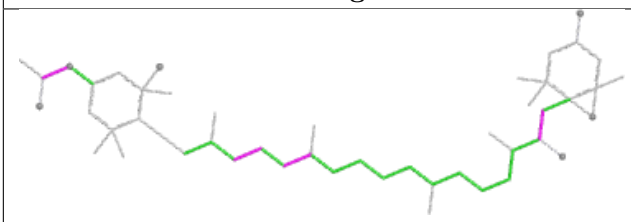
## Ligand A86 15 311



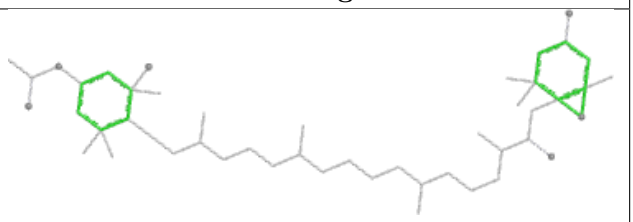
Bond lengths



Bond angles

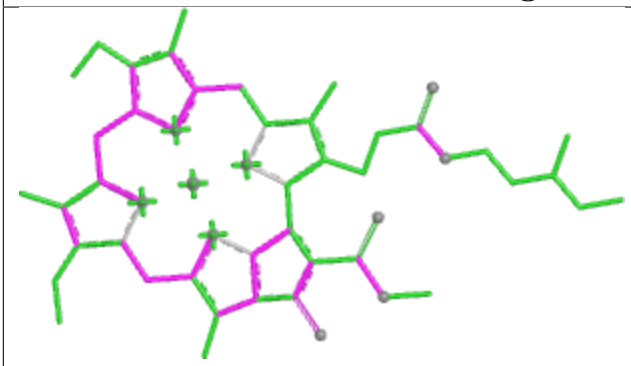


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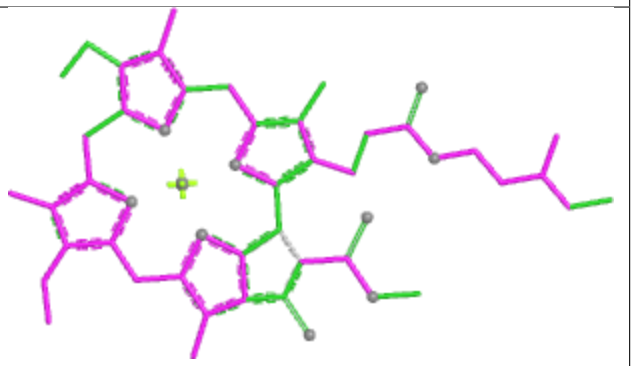


Rings

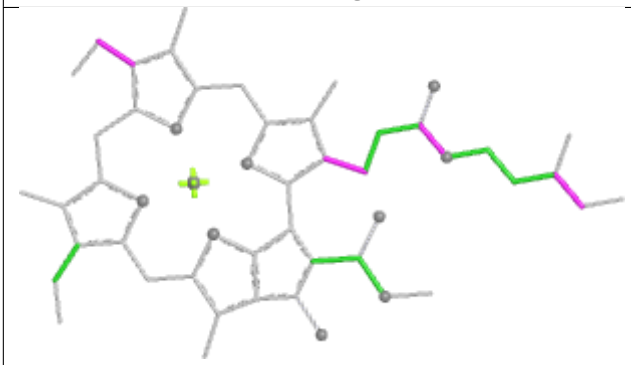
## Ligand CLA 19 305



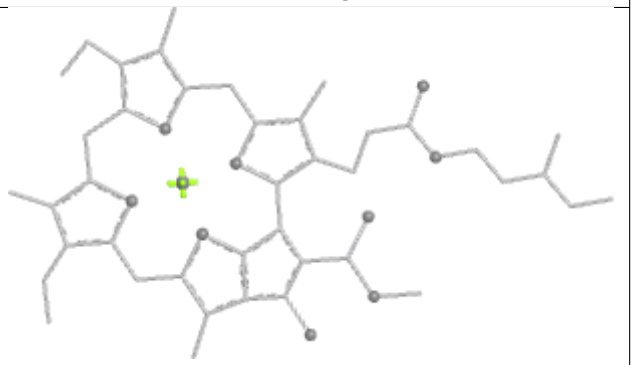
Bond lengths



Bond angles

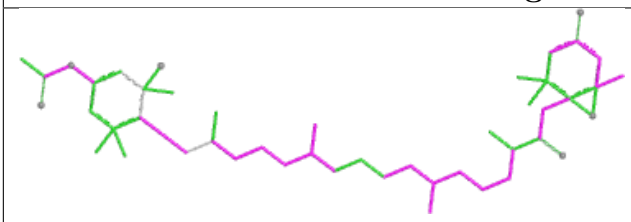


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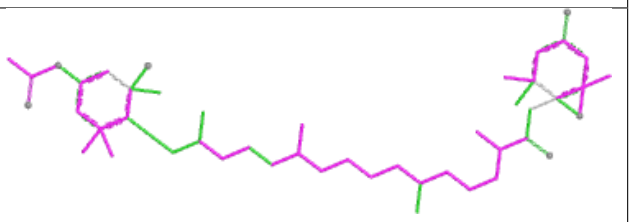


Rings

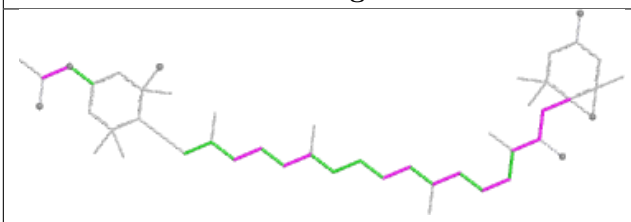
## Ligand A86 15 316



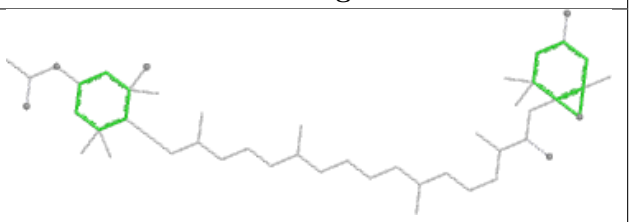
Bond lengths



Bond angles

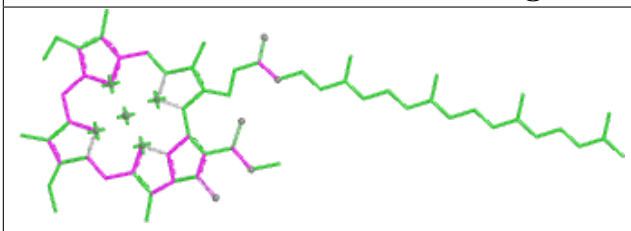


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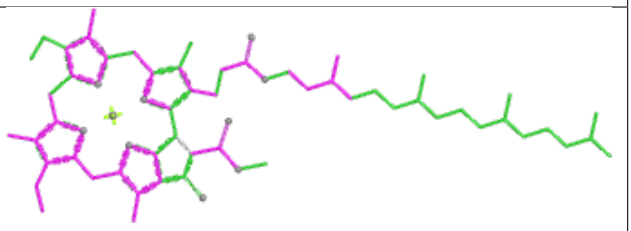


Rings

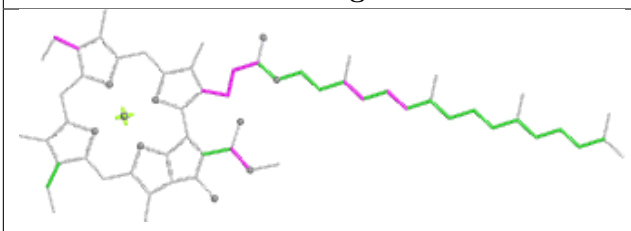
## Ligand CLA C 501



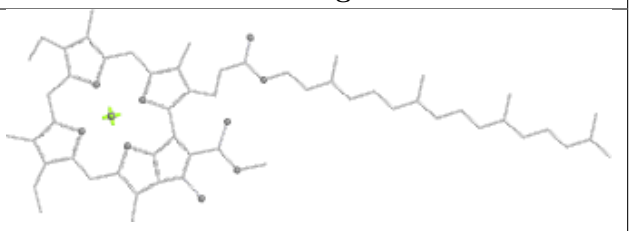
Bond lengths



Bond angles

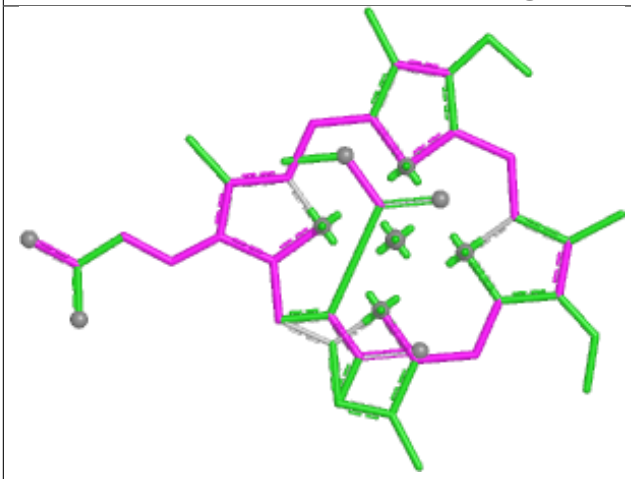


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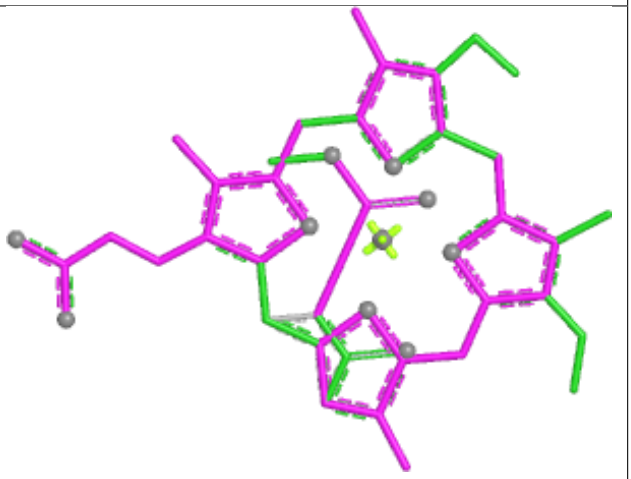


Rings

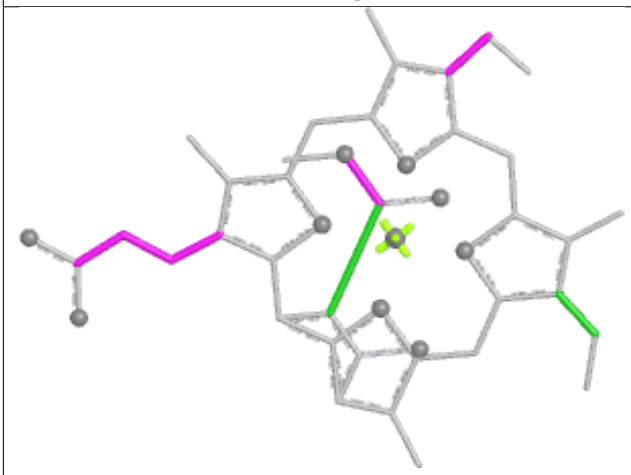
**Ligand KC1 11 306**



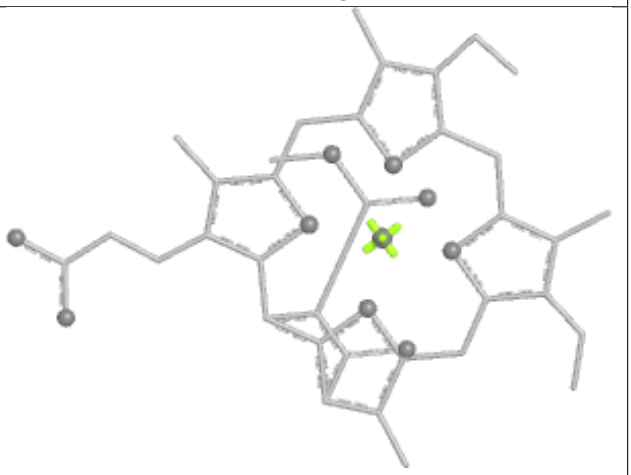
Bond lengths



Bond angles

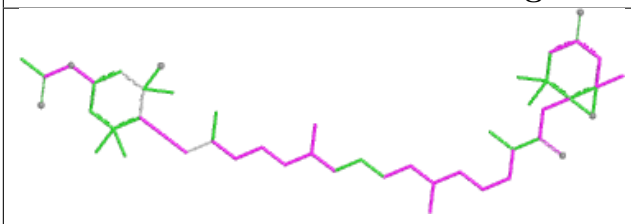


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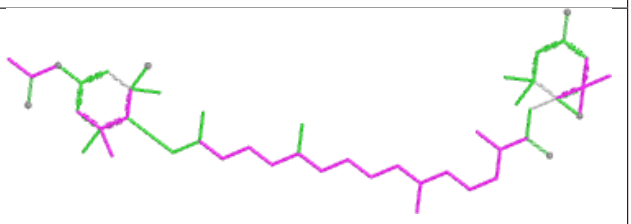


Rings

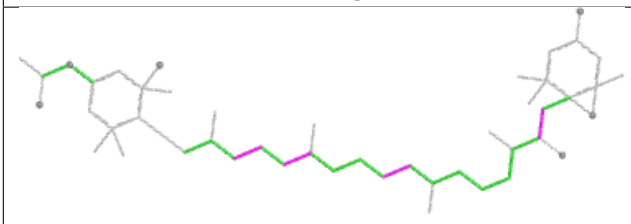
**Ligand A86 21 214**



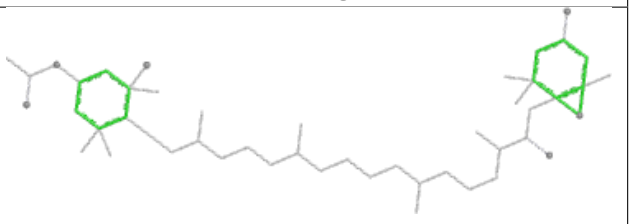
Bond lengths



Bond angles

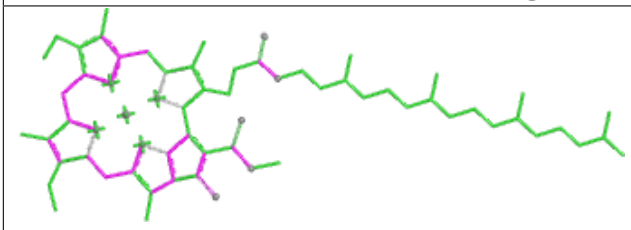


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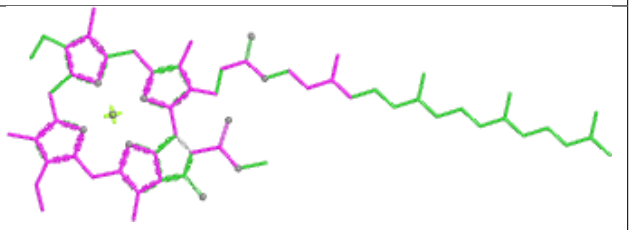


Rings

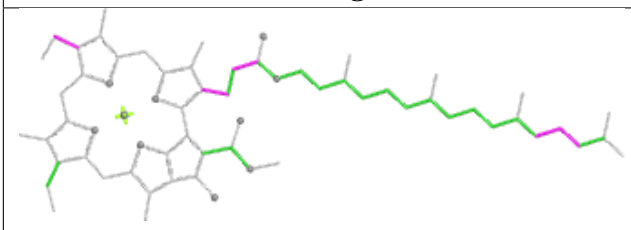
## Ligand CLA D 405



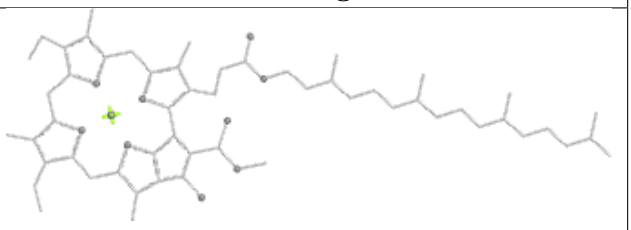
Bond lengths



Bond angles

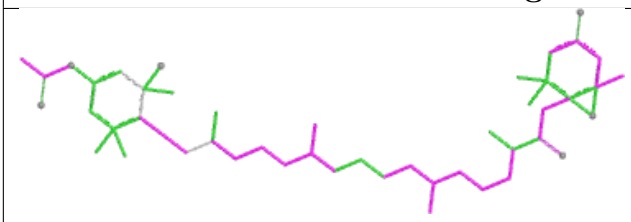


Torsions

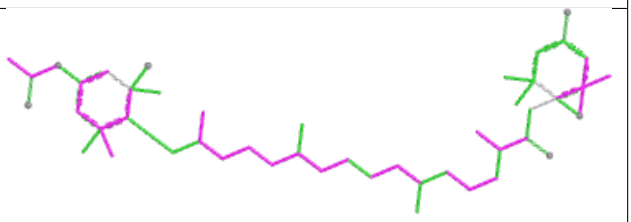


Rings

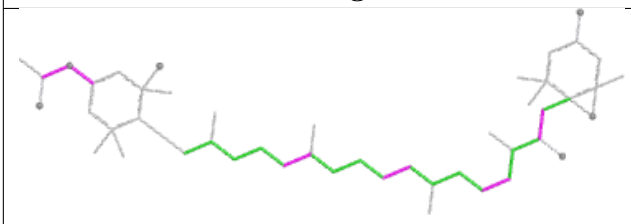
## Ligand A86 21 213



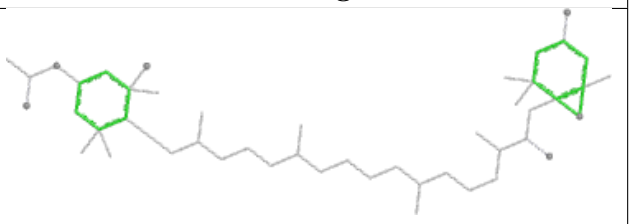
Bond lengths



Bond angles

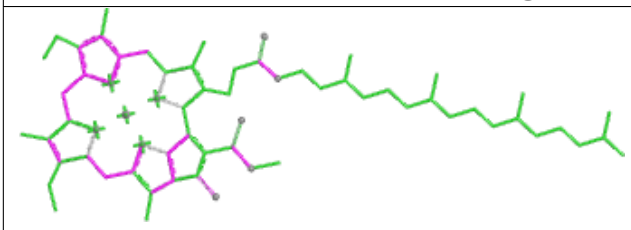


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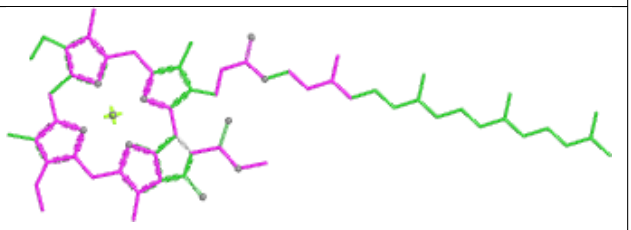


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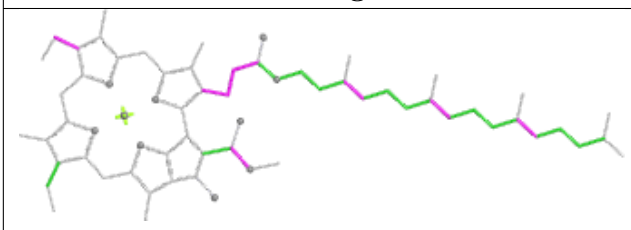
## Ligand CLA 18 202



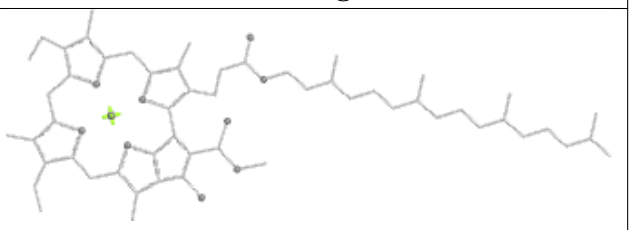
Bond lengths



Bond angles

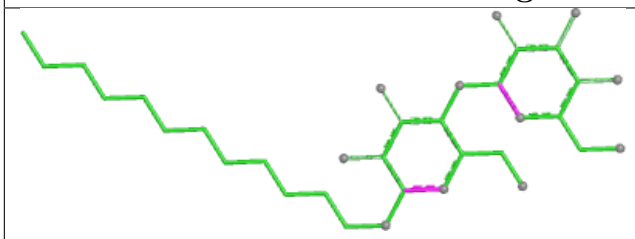


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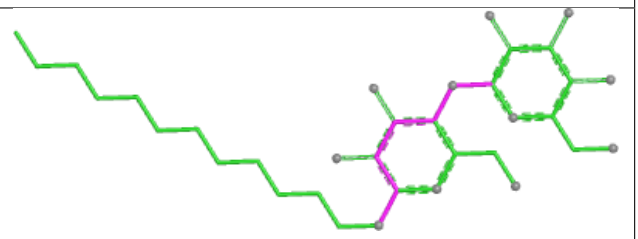


Rings

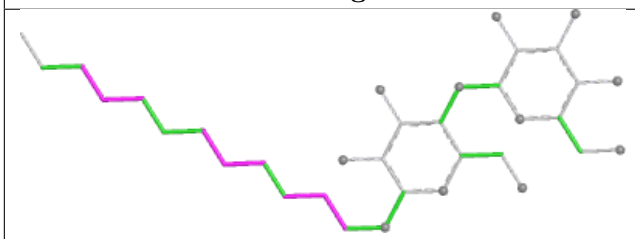
**Ligand LMU 19 315**



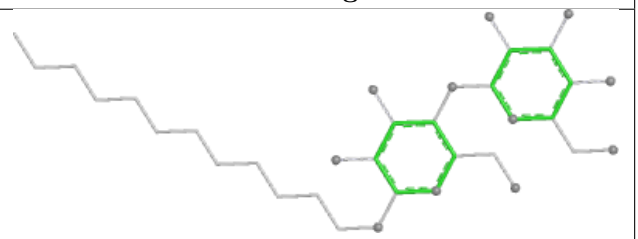
Bond lengths



Bond angles

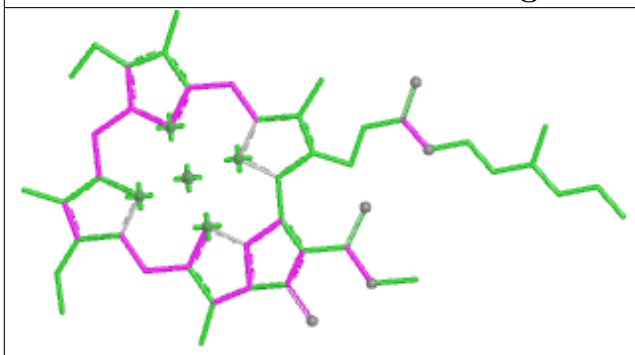


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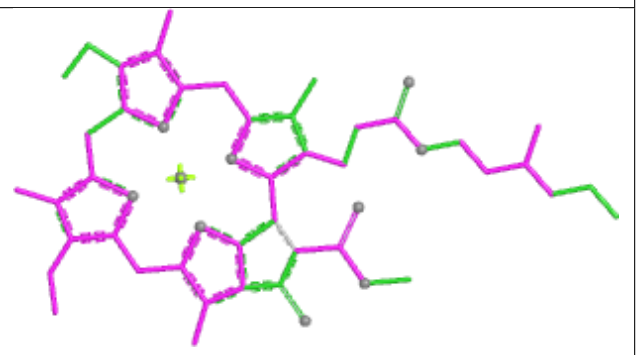


Rings

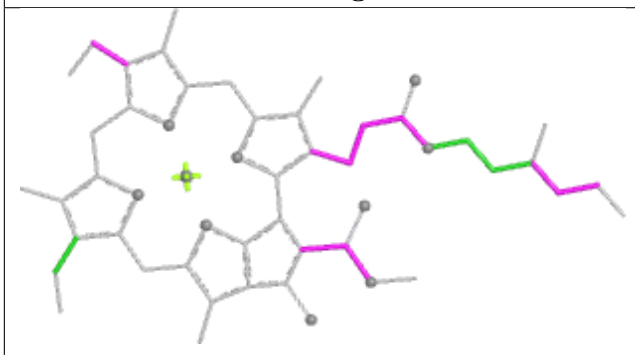
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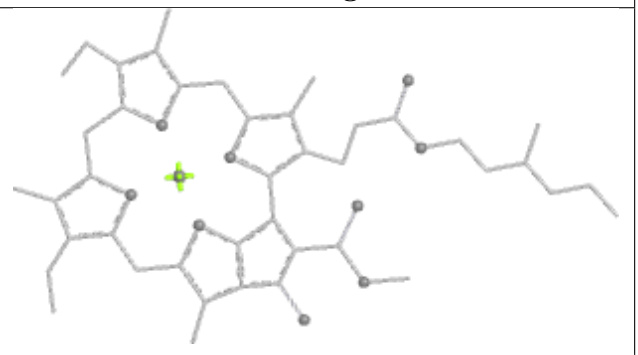
Bond lengths



Bond angles

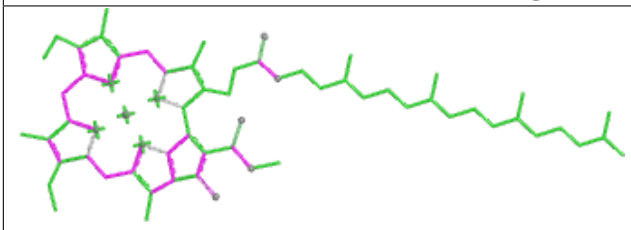


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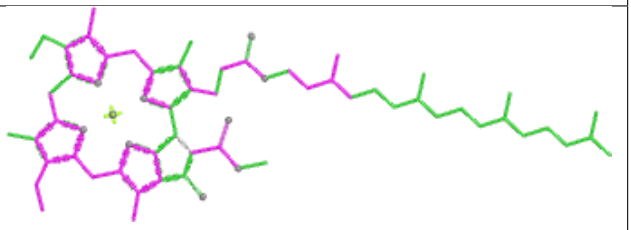


Rings

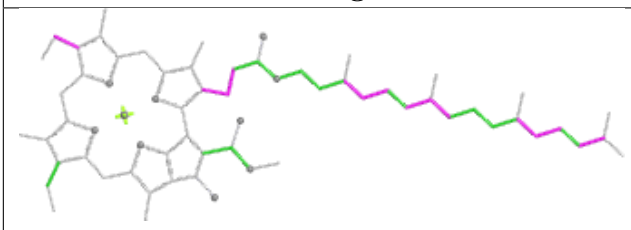
**Ligand CLA d 401**



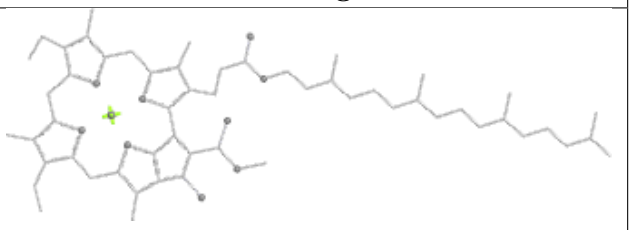
Bond lengths



Bond angles

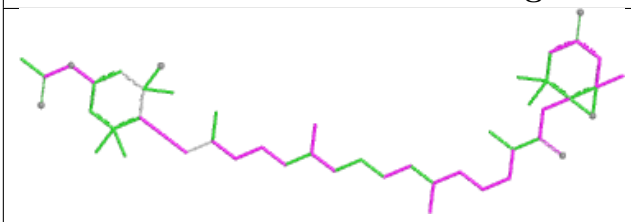


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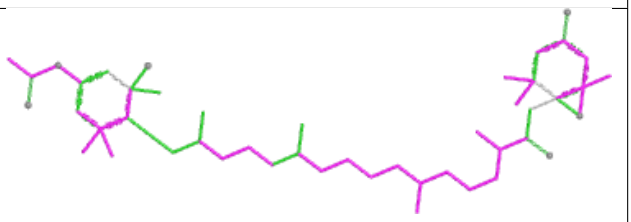


Rings

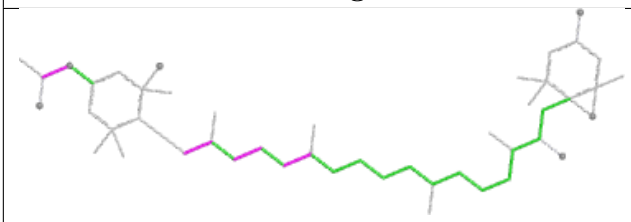
**Ligand A86 11 312**



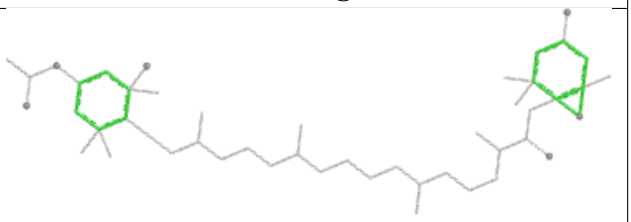
Bond lengths



Bond angles

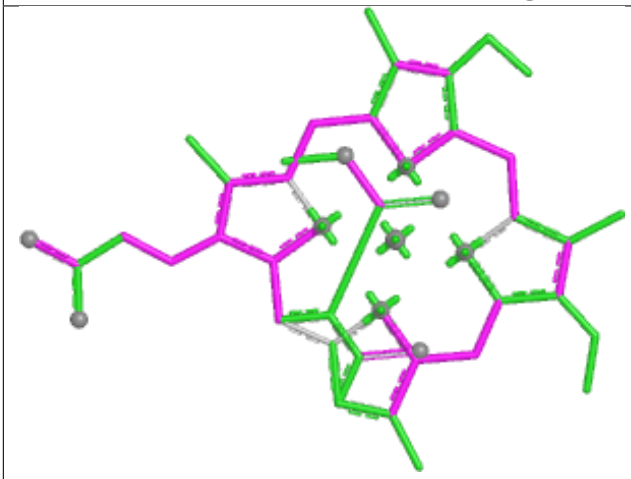


Torsions

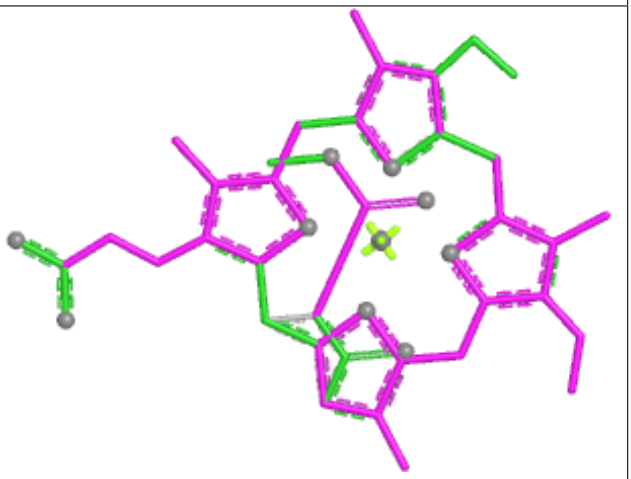


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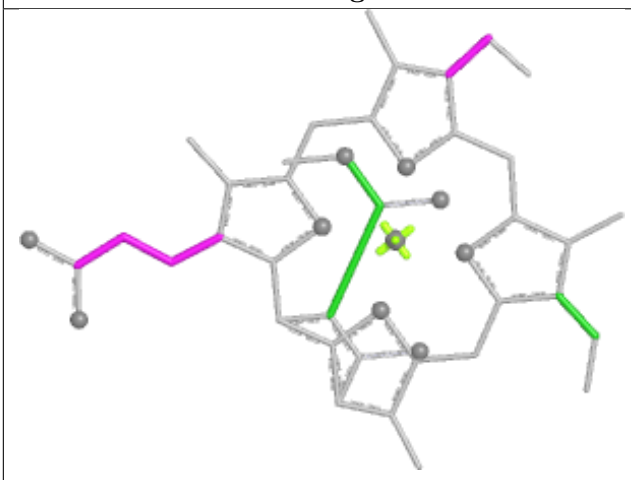
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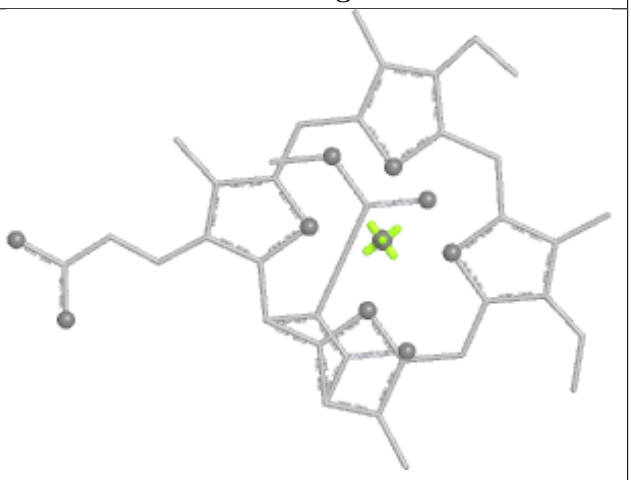
**Bond lengths**



**Bond angles**

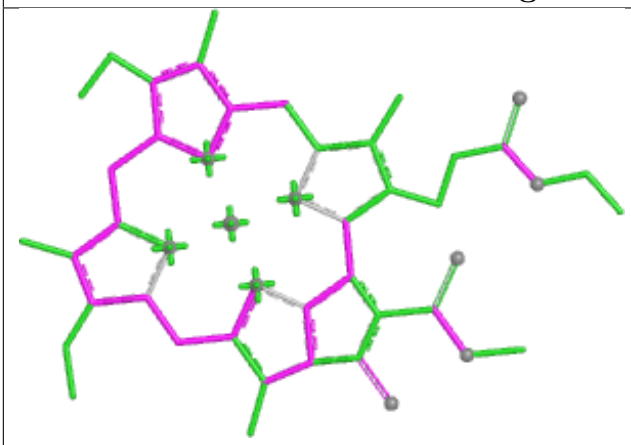


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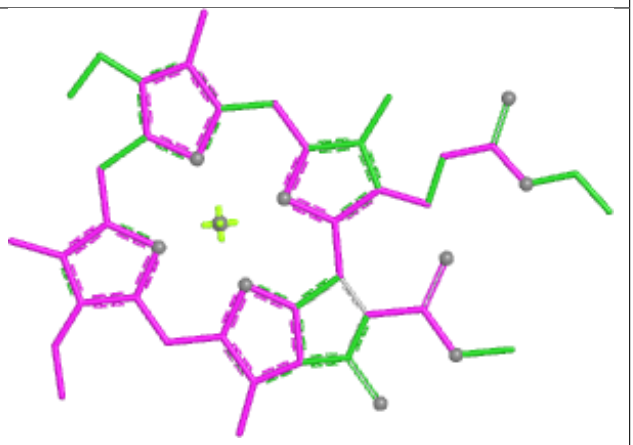


**Rings**

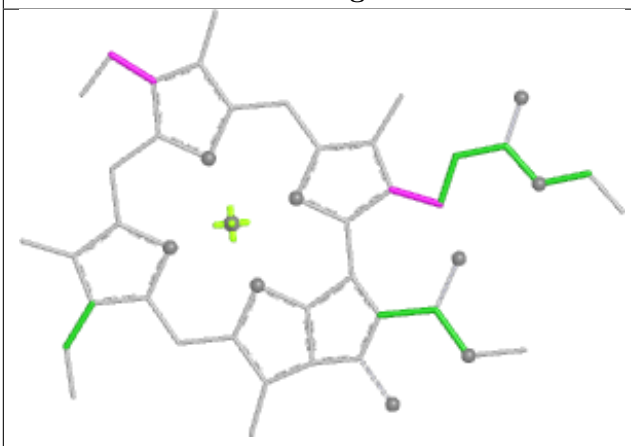
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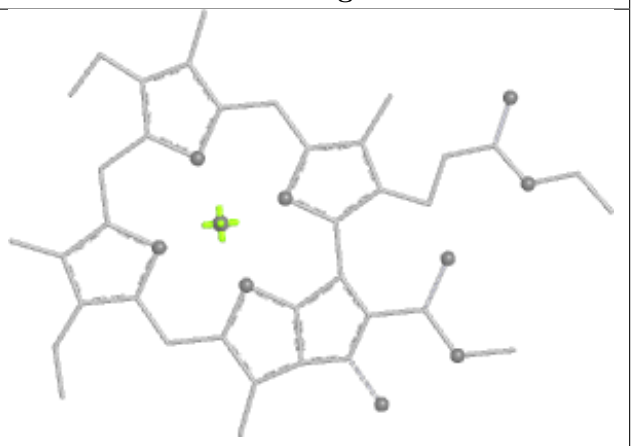
**Bond lengths**



**Bond angles**

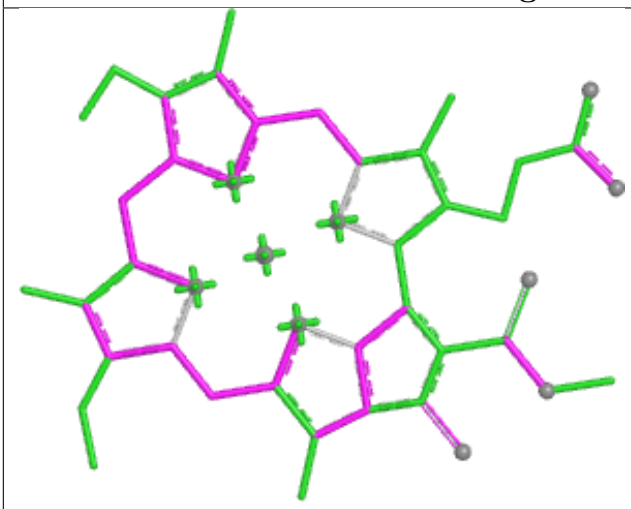


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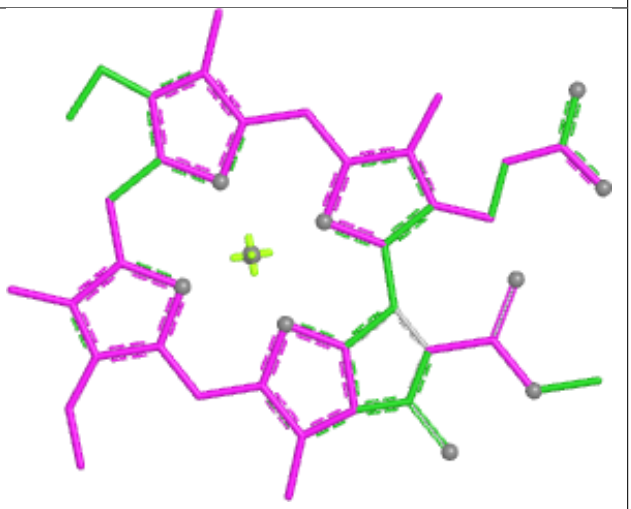


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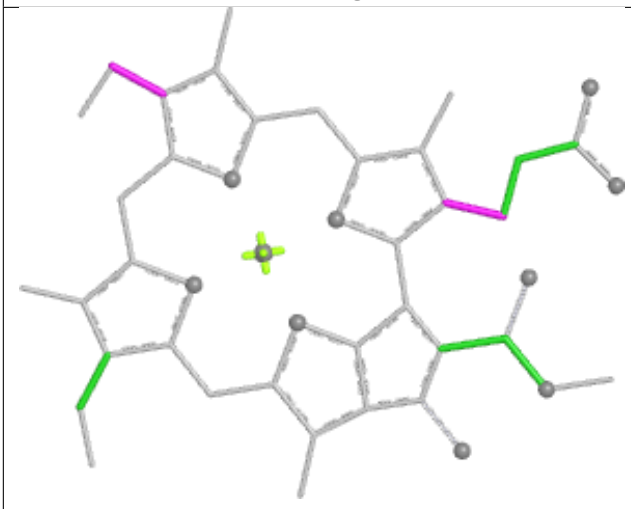
## Ligand CLA 11 305



Bond lengths



Bond angles

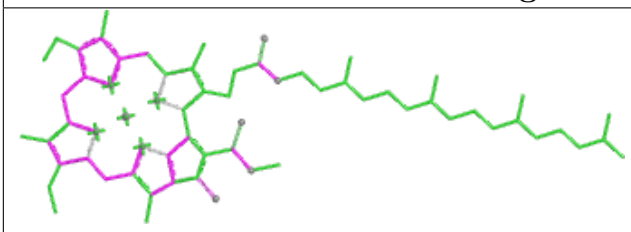


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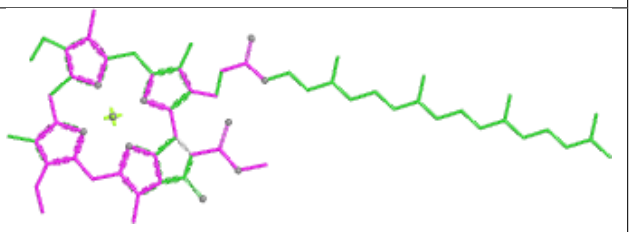


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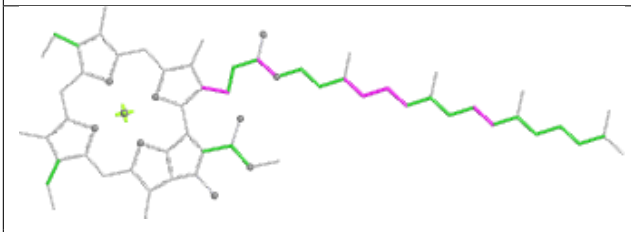
## Ligand CLA 33 308



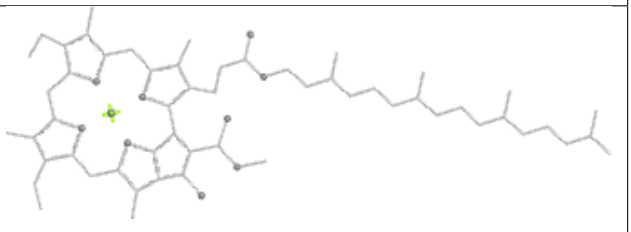
Bond lengths



Bond angles

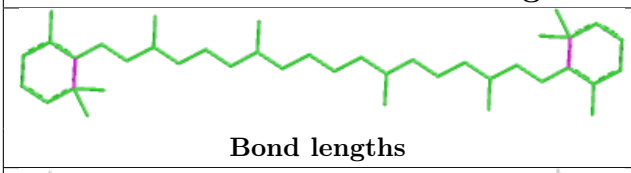


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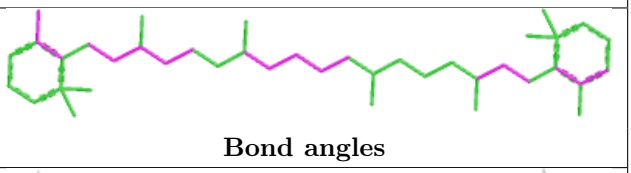


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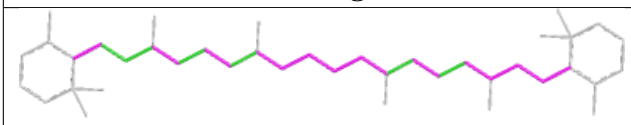
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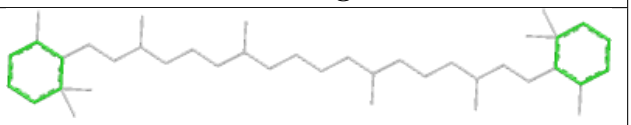
Bond lengths



Bond angles

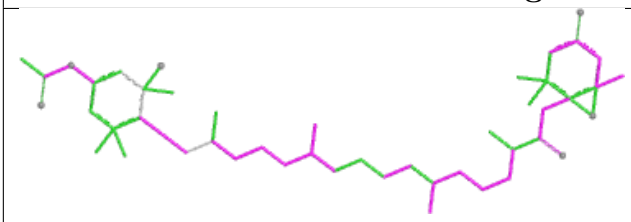


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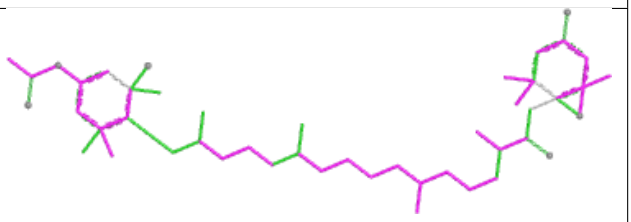


Rings

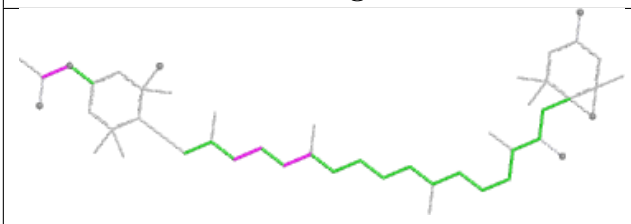
## Ligand A86 36 310



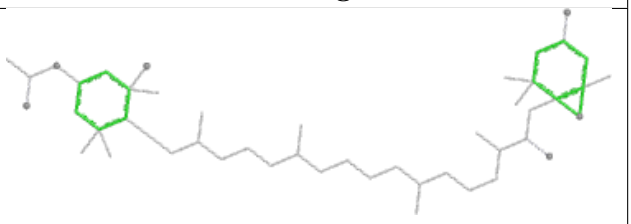
Bond lengths



Bond angles

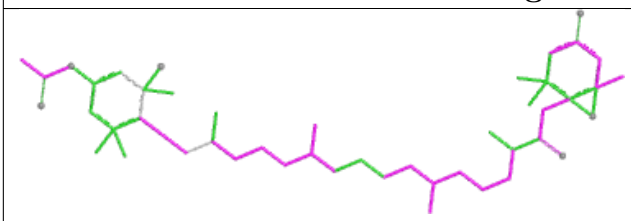


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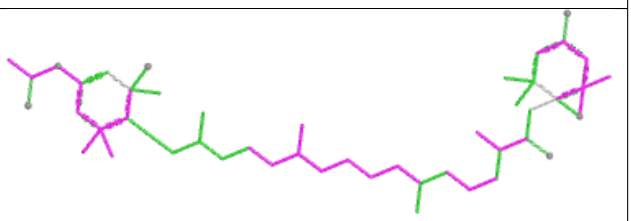


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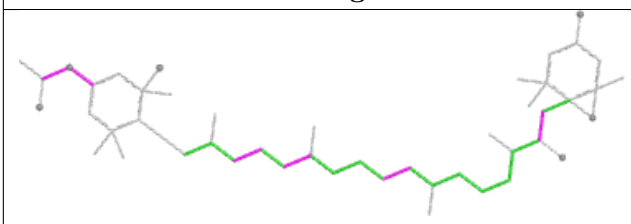
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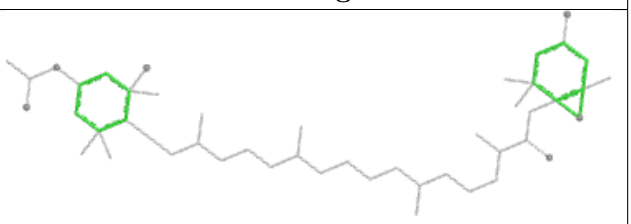
Bond lengths



Bond angles

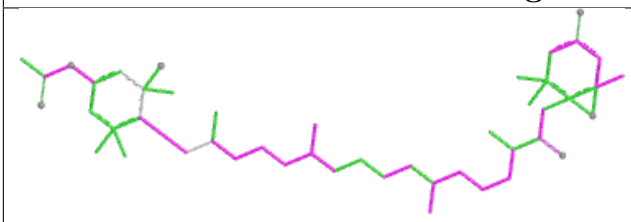


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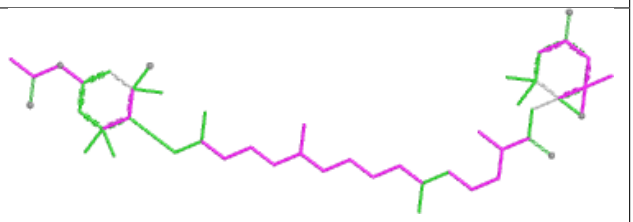


Rings

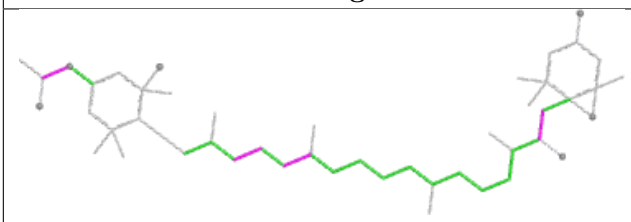
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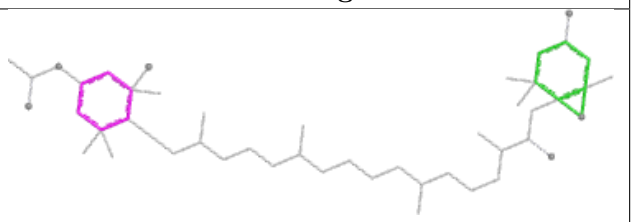
Bond lengths



Bond angles

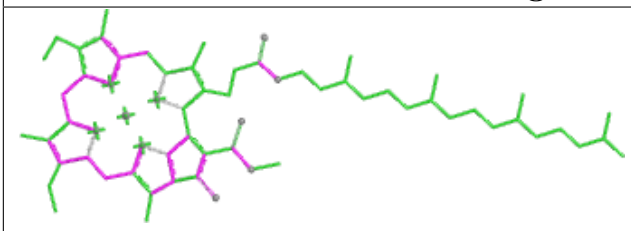


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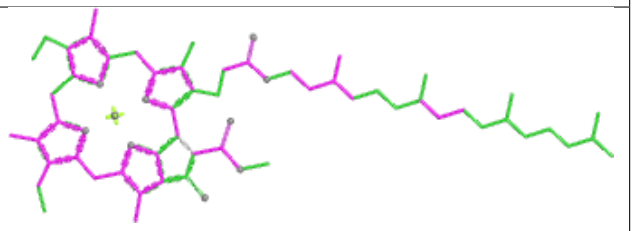


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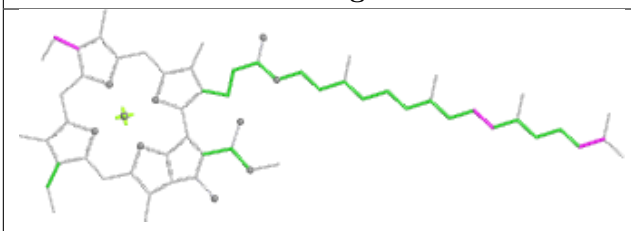
## Ligand CLA b 515



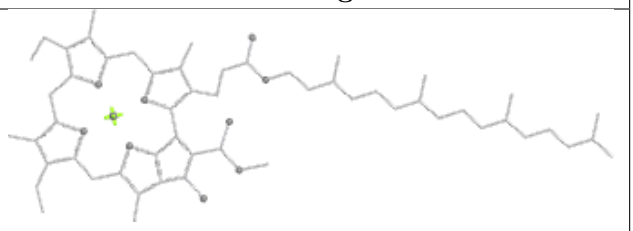
Bond lengths



Bond angles

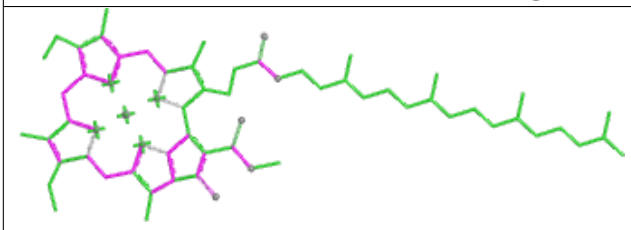


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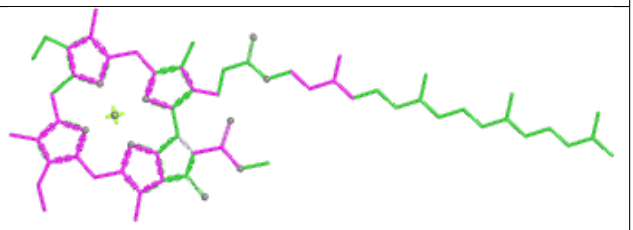


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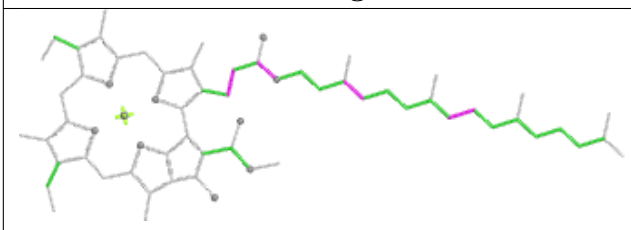
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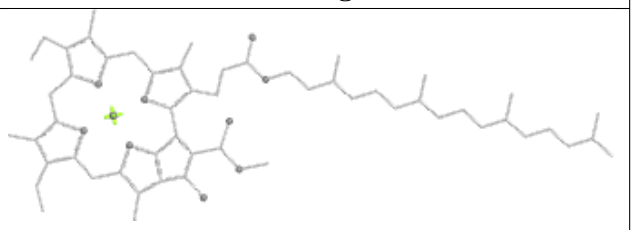
Bond lengths



Bond angles

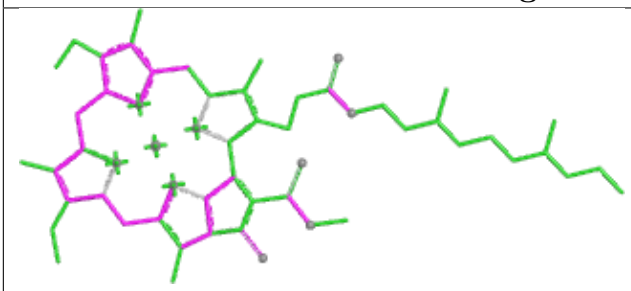


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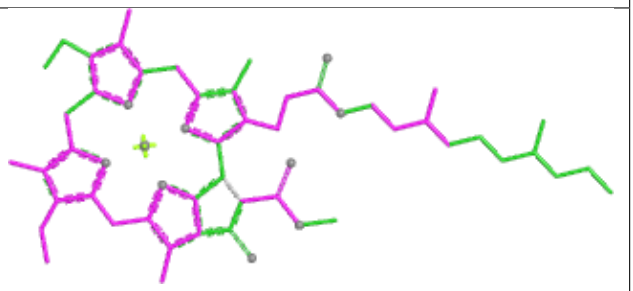


Rings

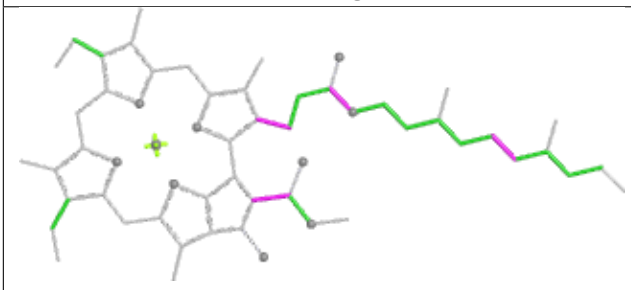
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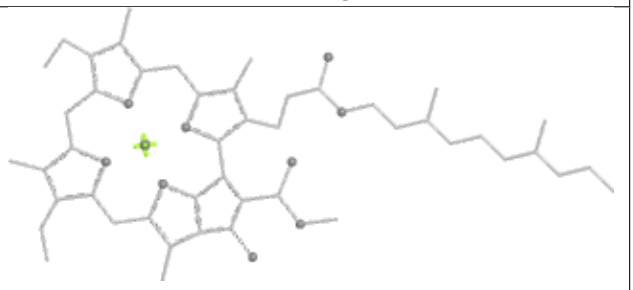
Bond lengths



Bond angles

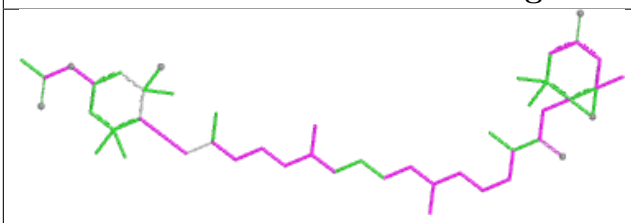


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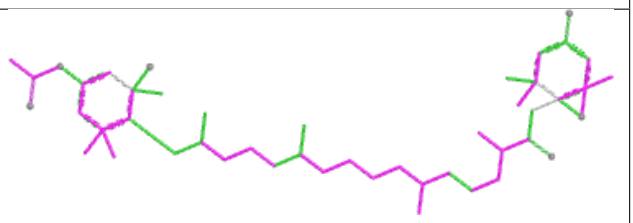


Rings

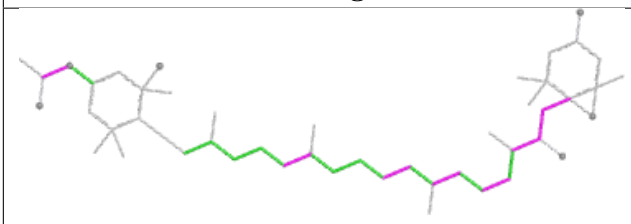
## Ligand A86 34 316



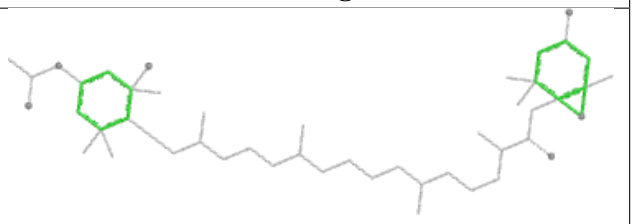
Bond lengths



Bond angles

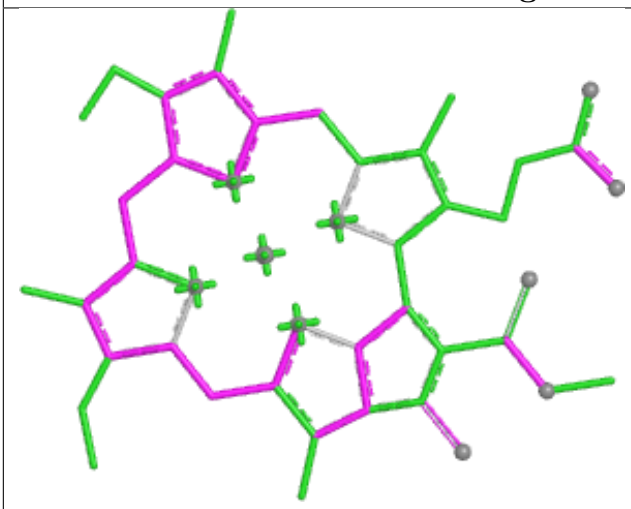


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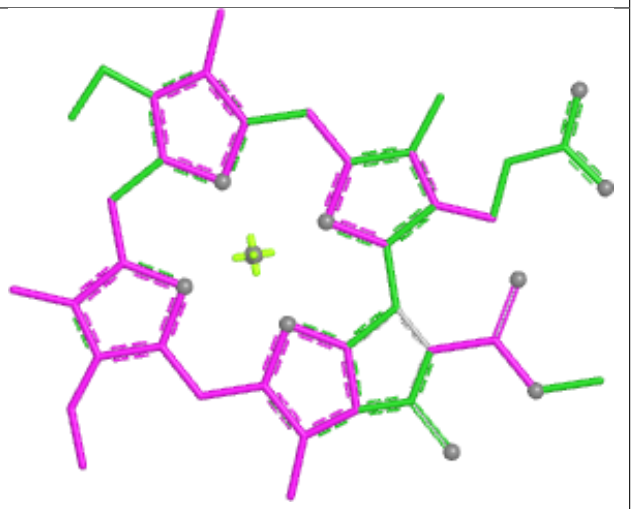


Rings

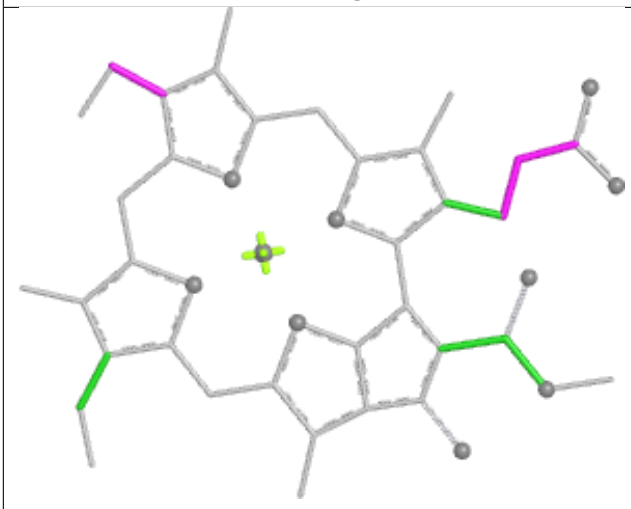
## Ligand CLA 35 305



Bond lengths



Bond angles

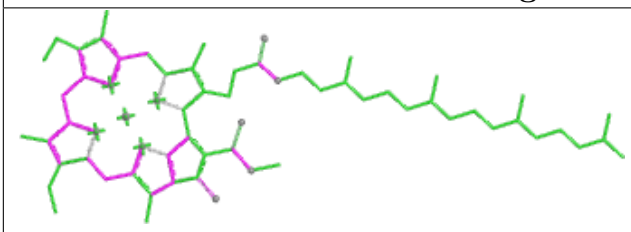


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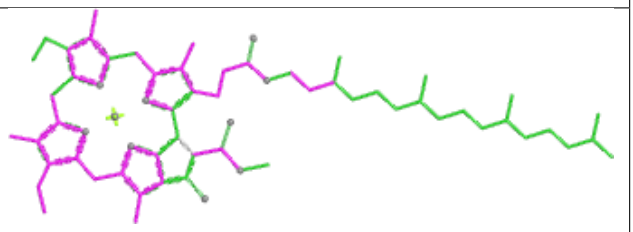


Rings

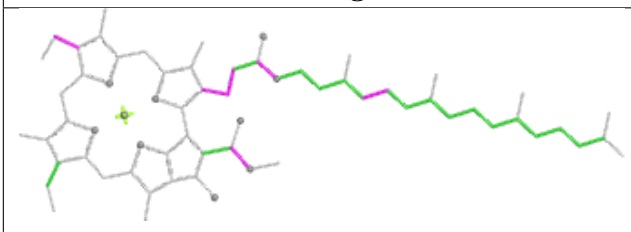
## Ligand CLA 19 301



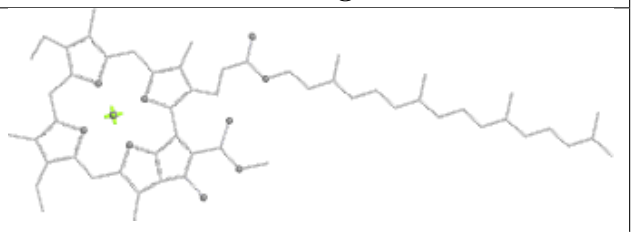
Bond lengths



Bond angles

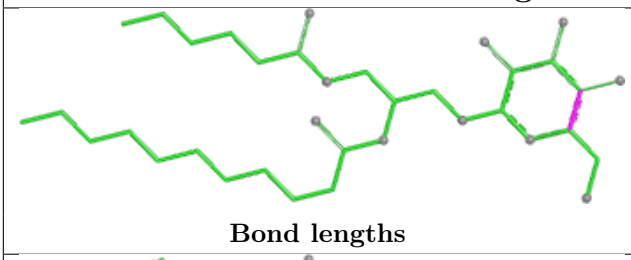


Torsions

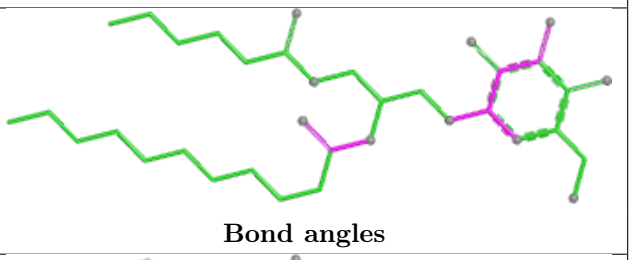


Rings

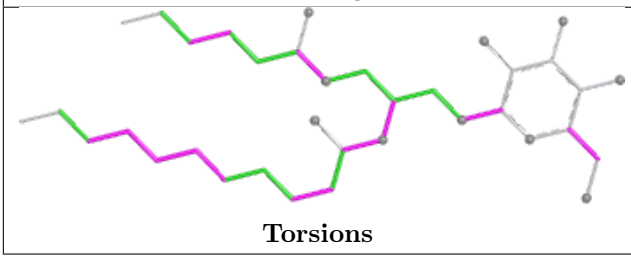
## Ligand LMG 36 314



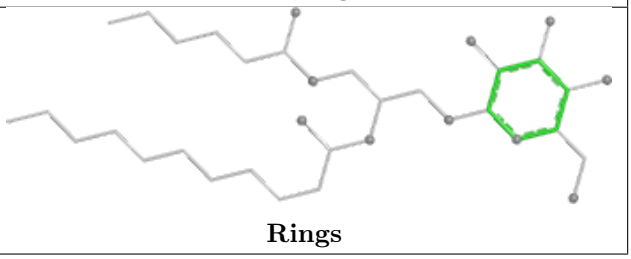
Bond lengths



Bond angles

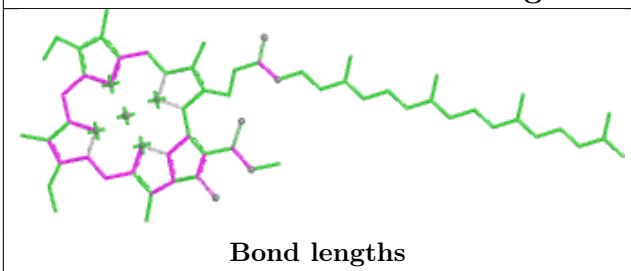


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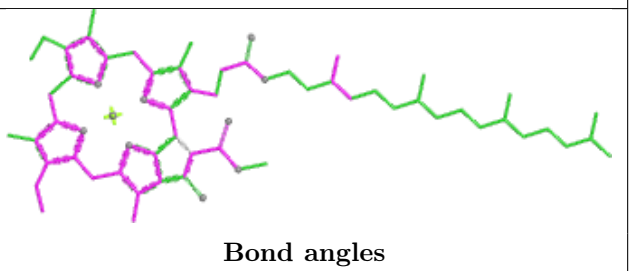


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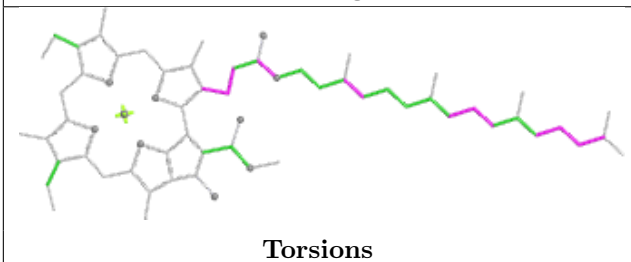
## Ligand CLA C 506



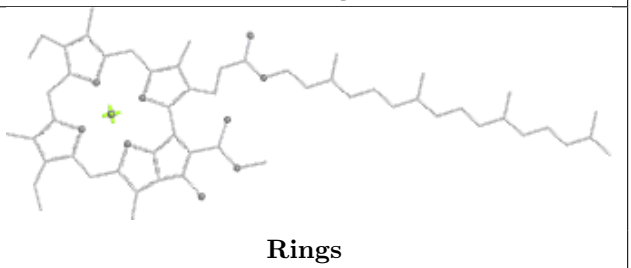
Bond lengths



Bond angles

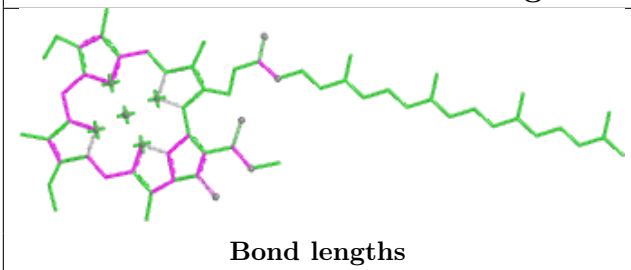


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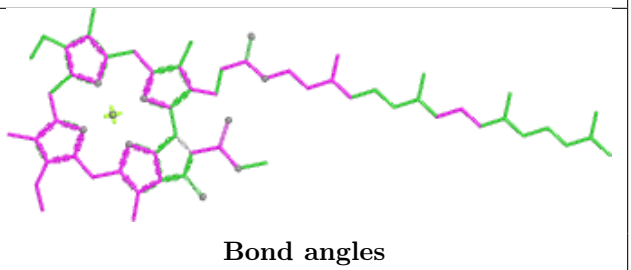


Rings

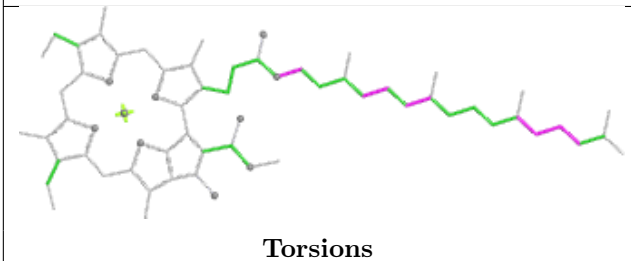
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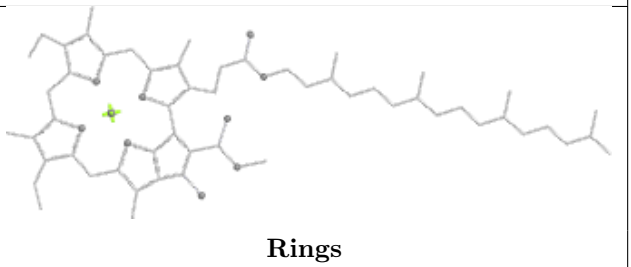
Bond lengths



Bond angles

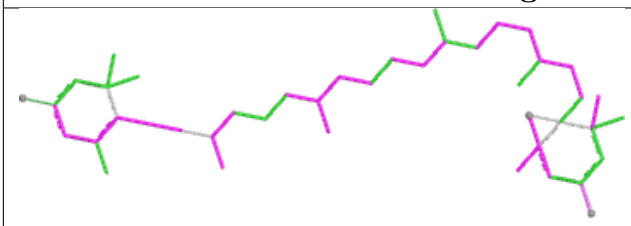


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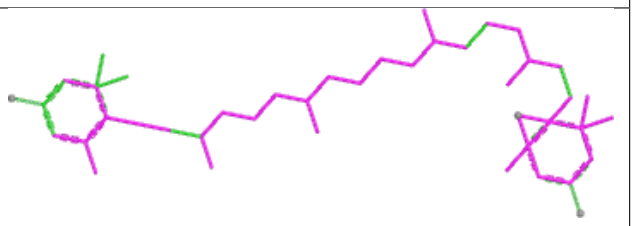


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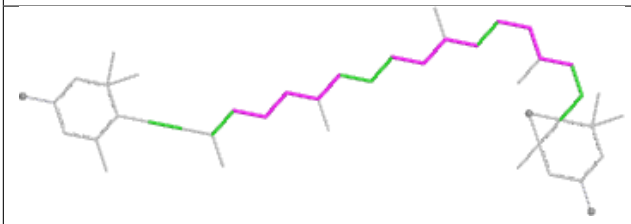
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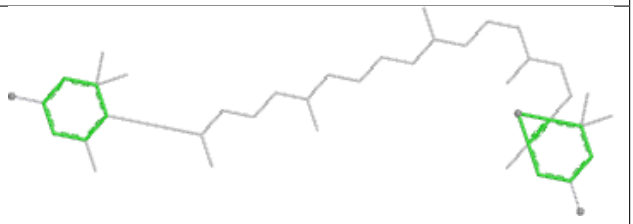
Bond lengths



Bond angles

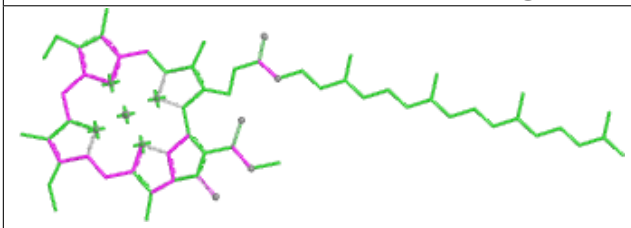


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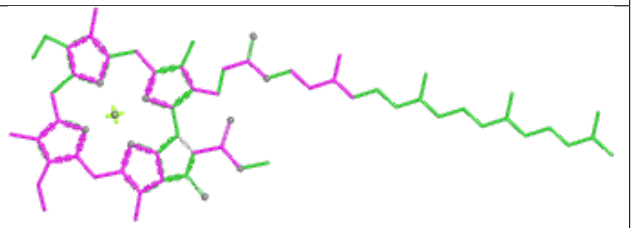


Rings

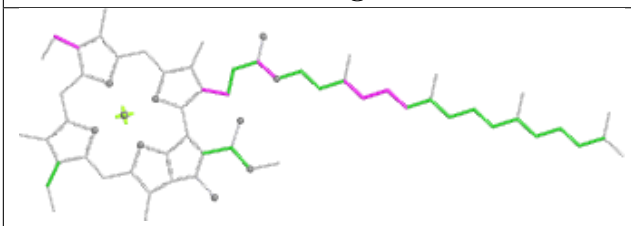
## Ligand CLA 39 310



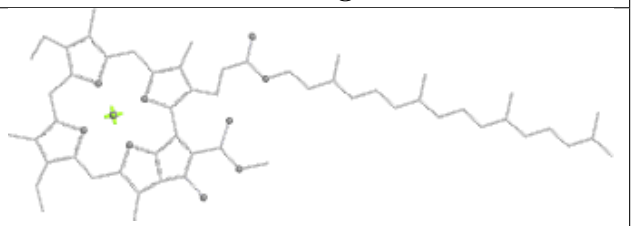
Bond lengths



Bond angles

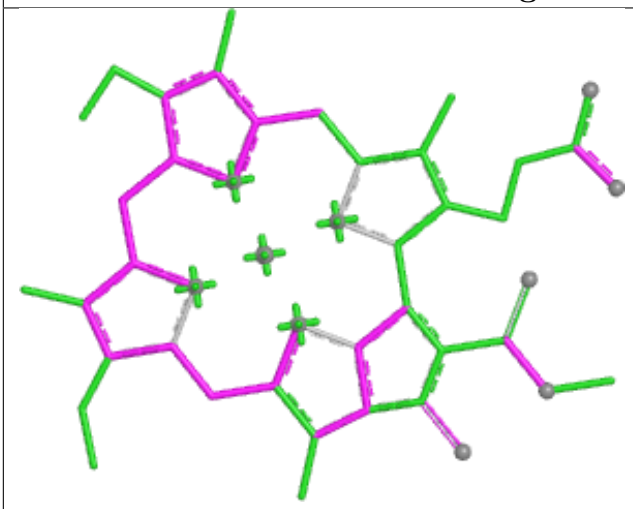


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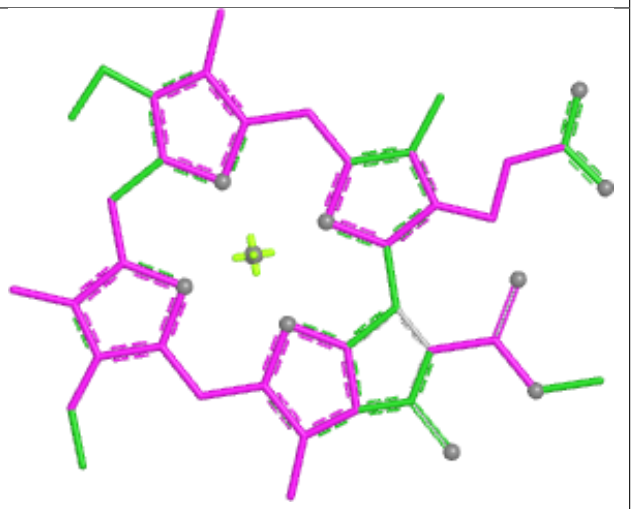


Rings

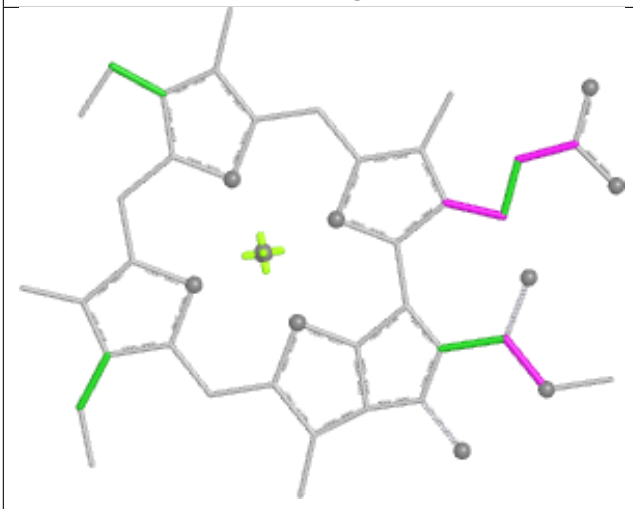
**Ligand CLA 36 309**



**Bond lengths**



**Bond angles**

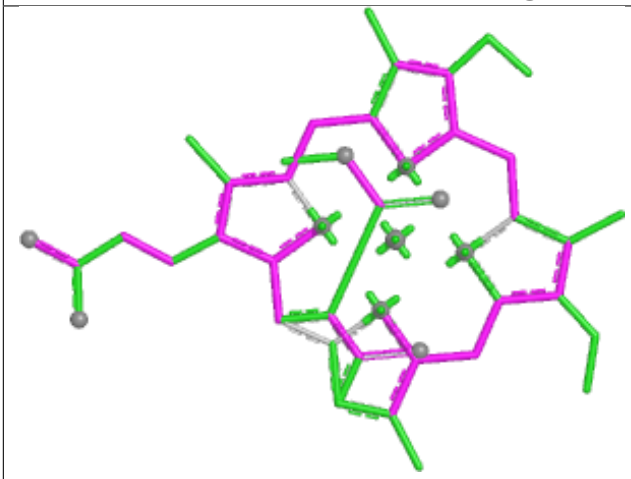


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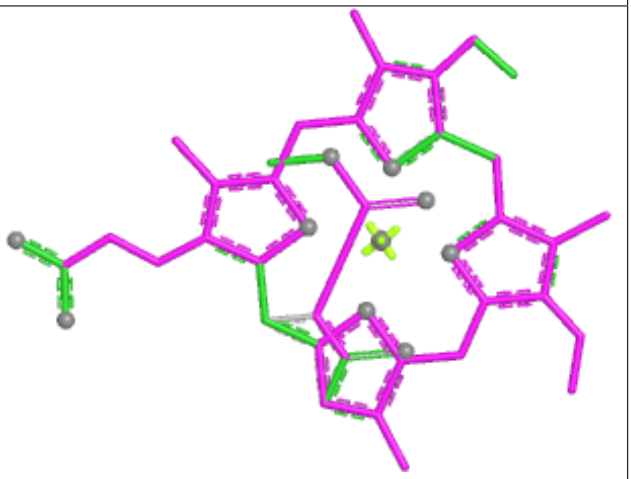


**Rings**

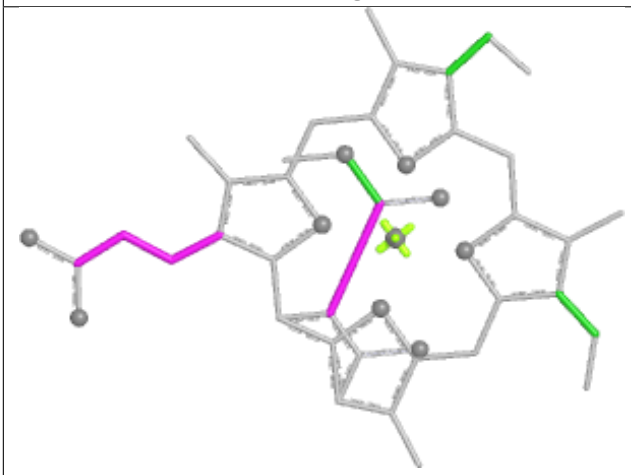
**Ligand KC1 12 211**



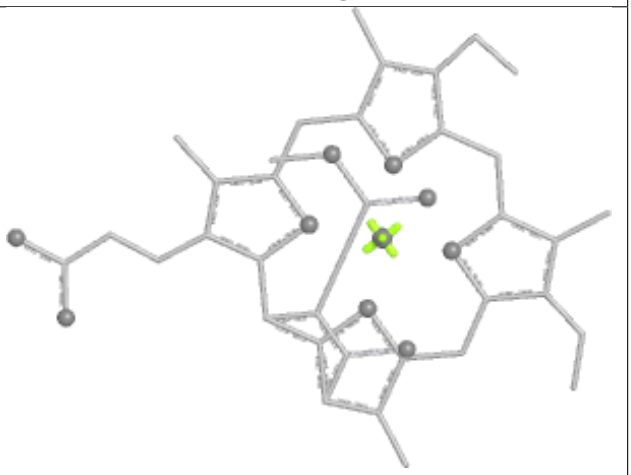
Bond lengths



Bond angles

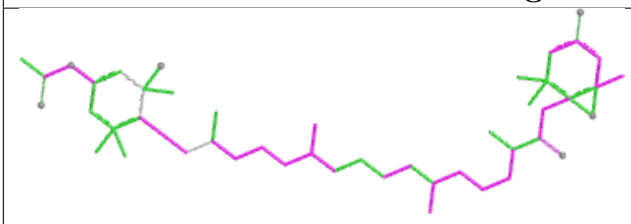


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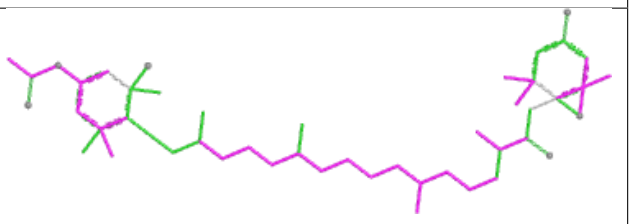


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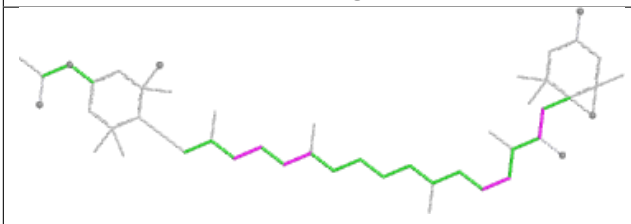
**Ligand A86 13 311**



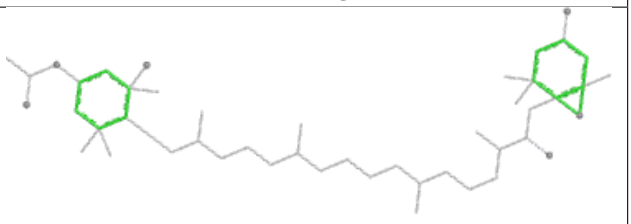
Bond lengths



Bond angles

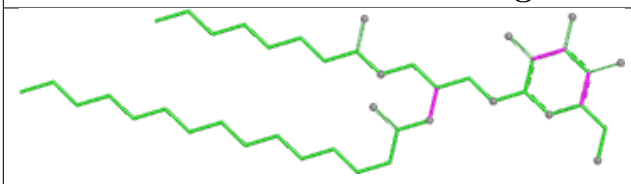


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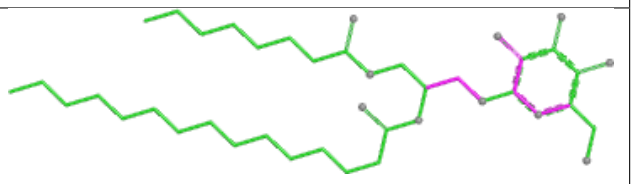


Rings

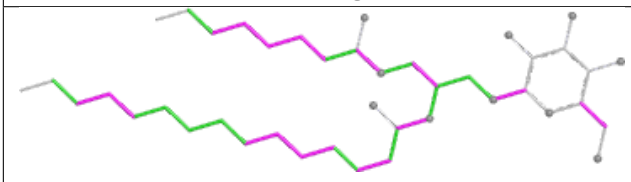
## Ligand LMG 11 316



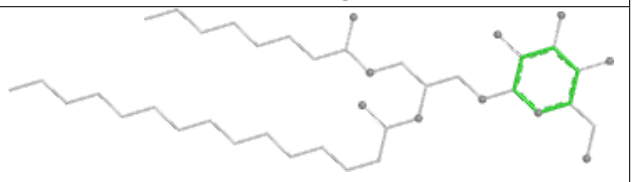
Bond lengths



Bond angles

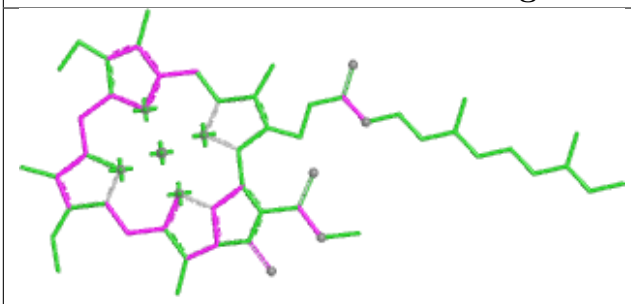


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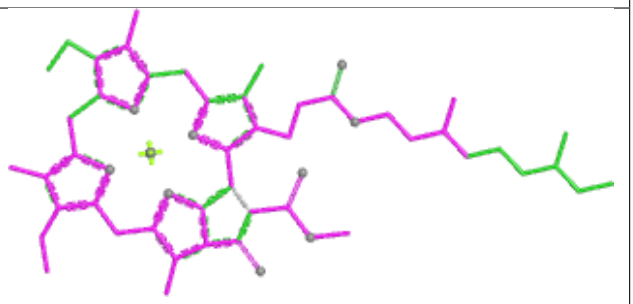


Rings

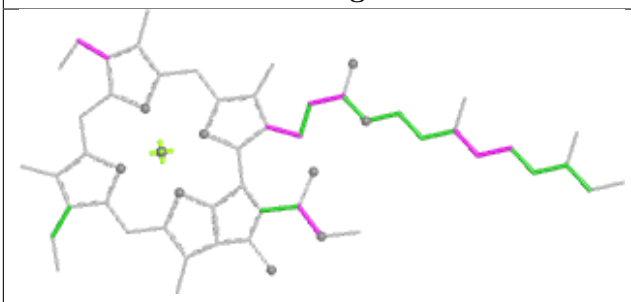
## Ligand CLA 20 303



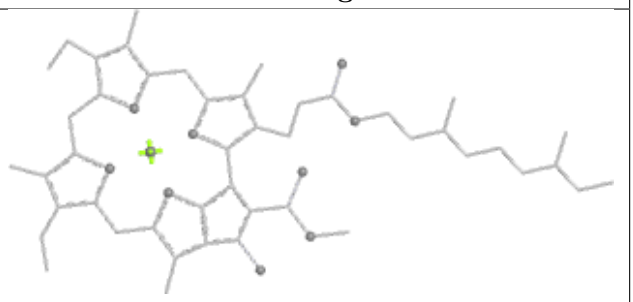
Bond lengths



Bond angles

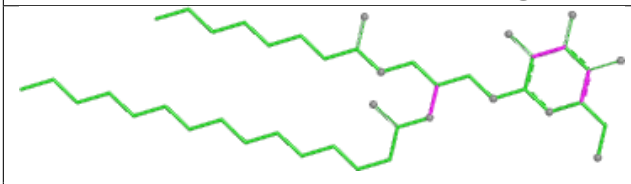


Torsions

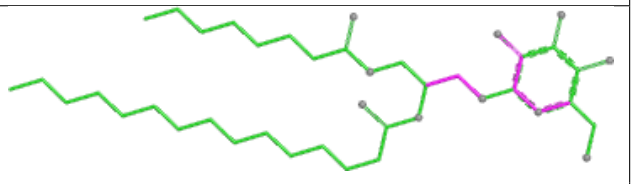


Rings

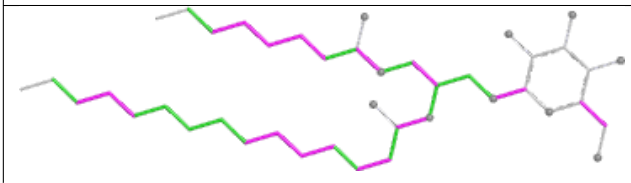
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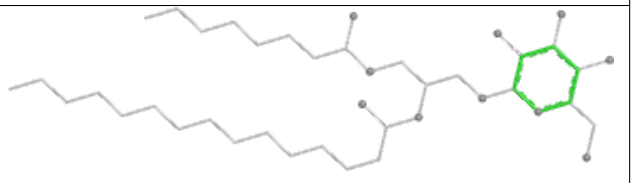
Bond lengths



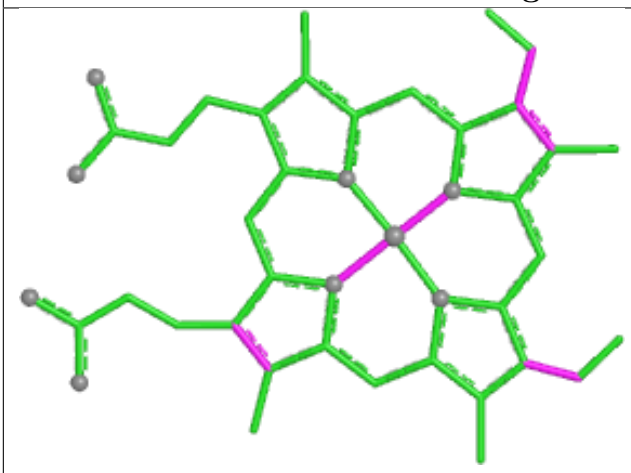
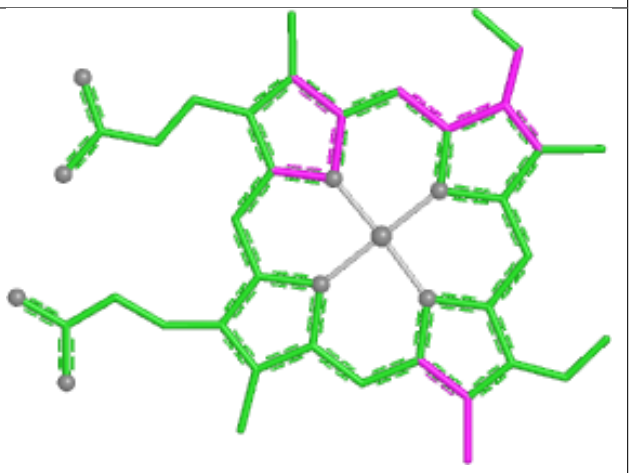
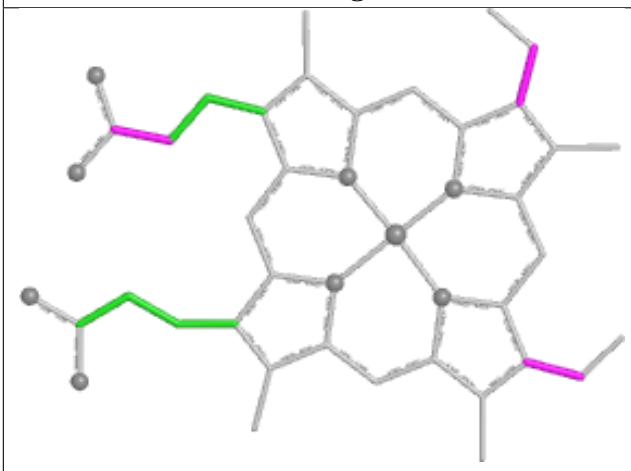
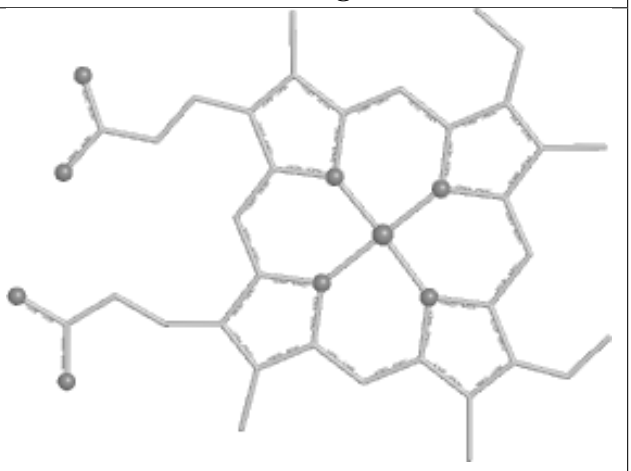
Bond angles

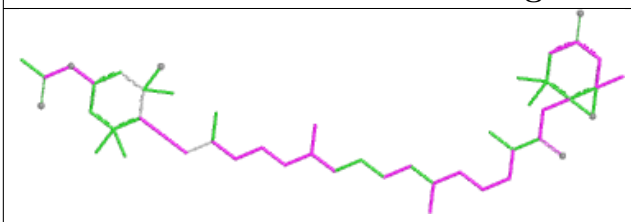
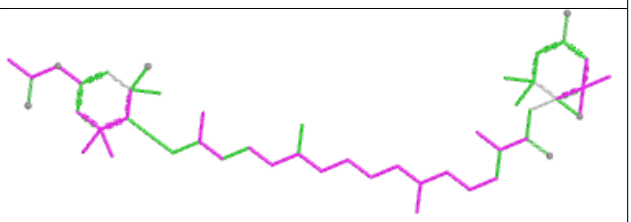
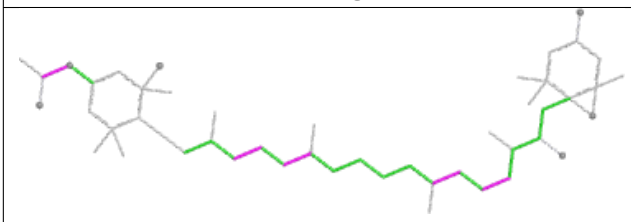
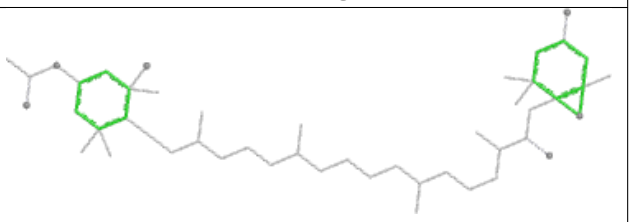


Torsions

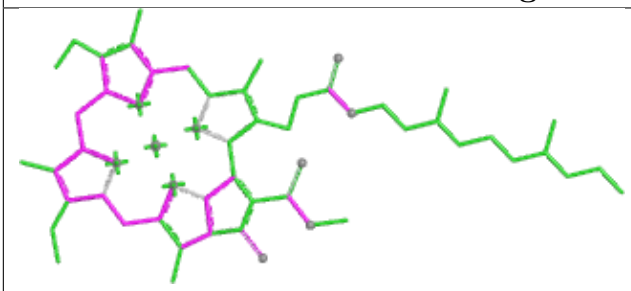


Rings

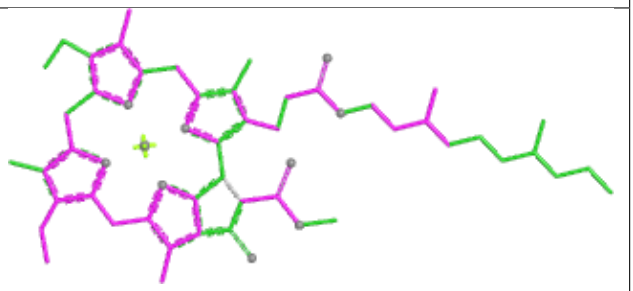
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|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand A86 37 310 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
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| Torsions | Rings |

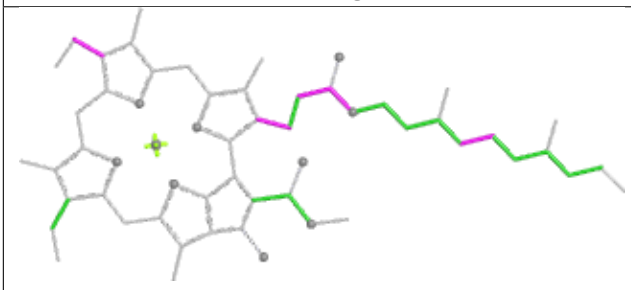
## Ligand CLA 21 202



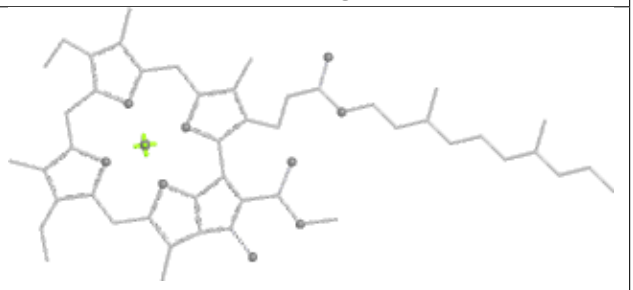
Bond lengths



Bond angles

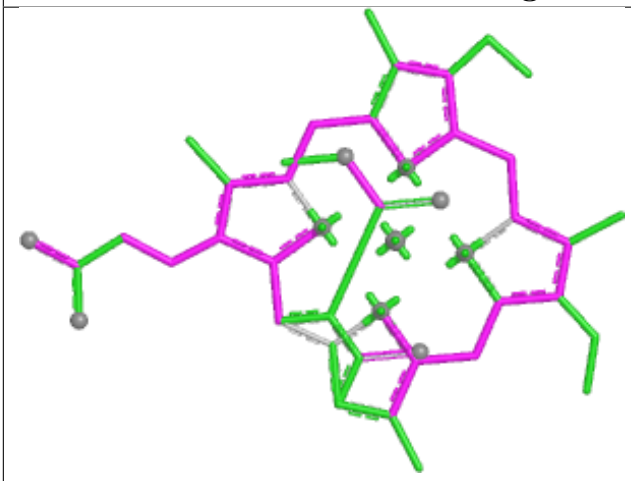


Torsions

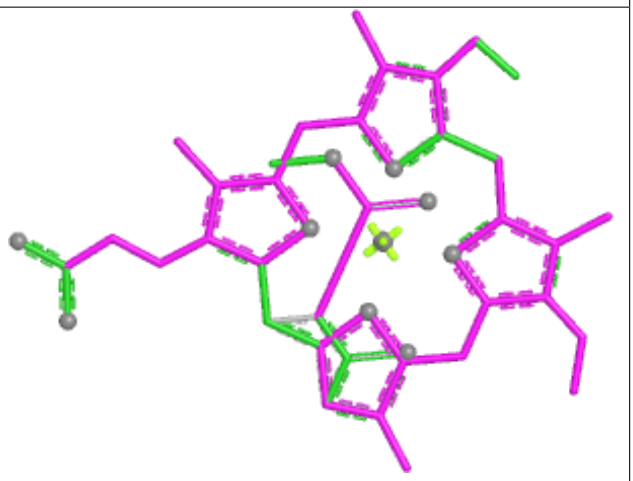


Rings

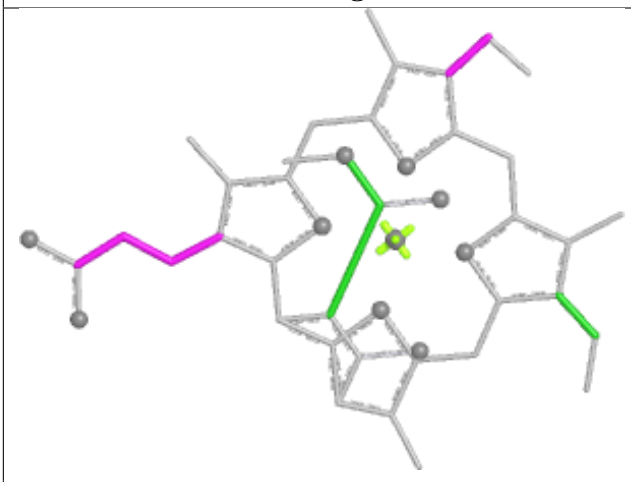
## Ligand KC1 33 302



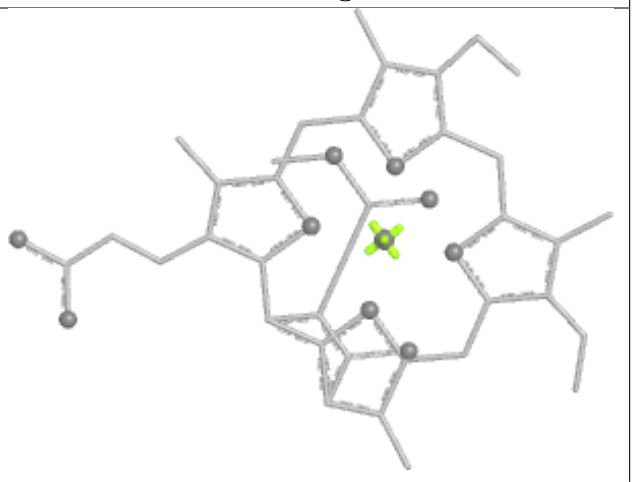
Bond lengths



Bond angles

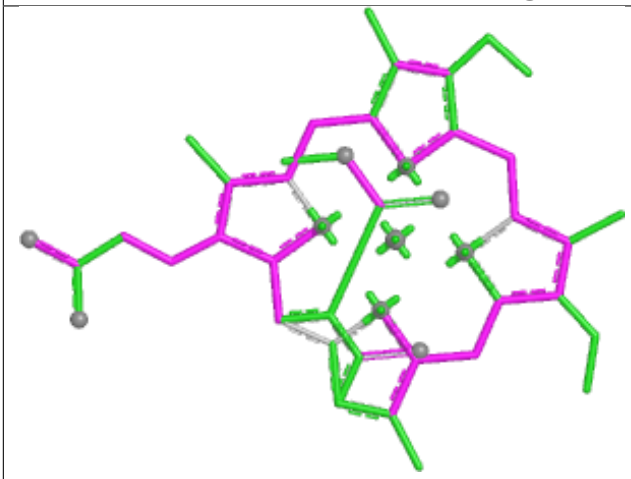


Torsions

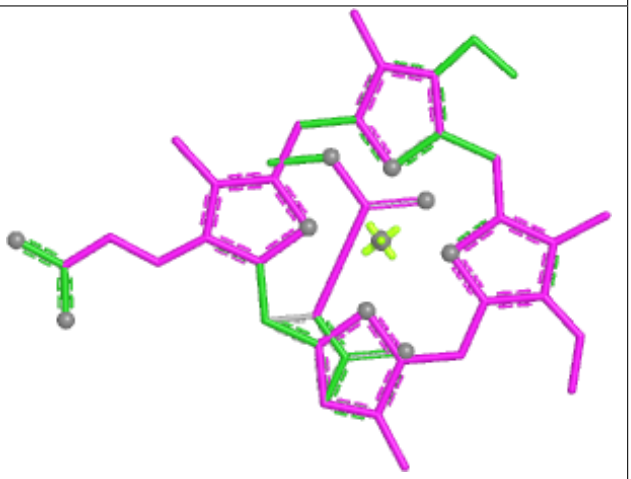


Rings

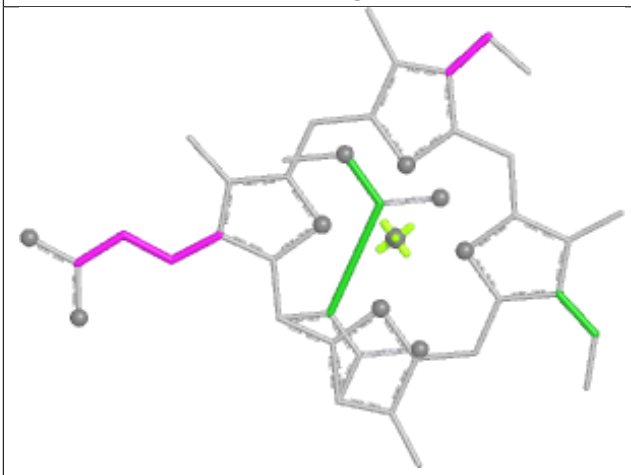
**Ligand KC1 35 306**



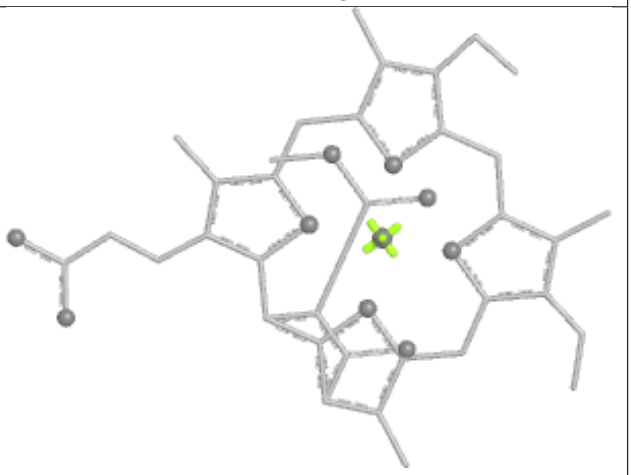
Bond lengths



Bond angles

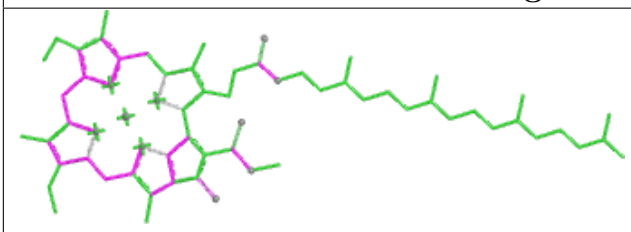


Torsions

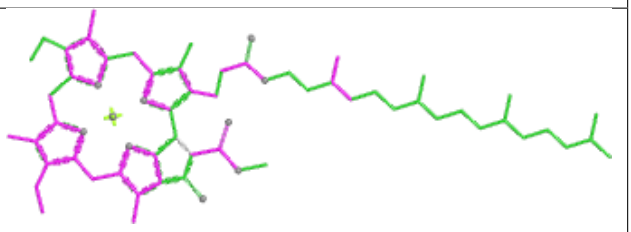


Rings

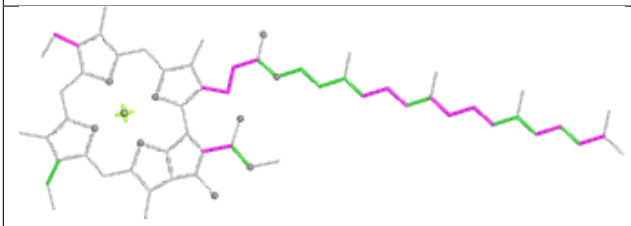
**Ligand CLA B 501**



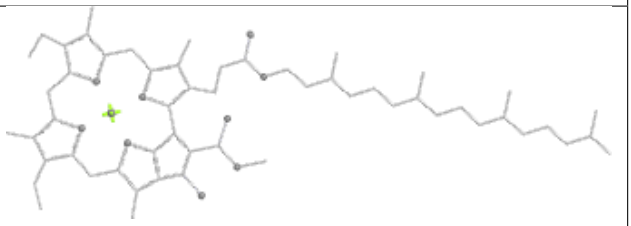
Bond lengths



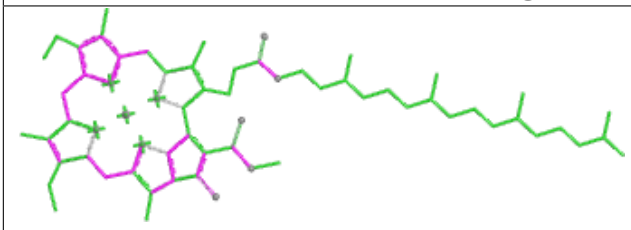
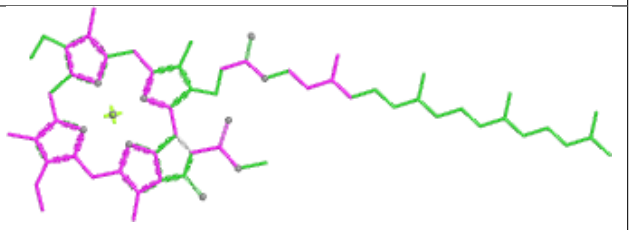
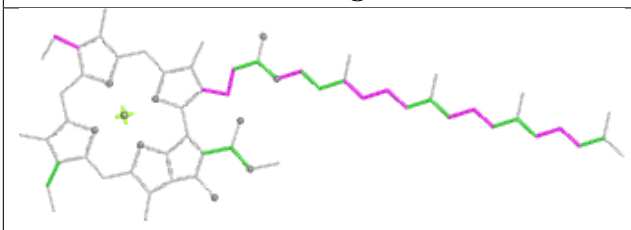
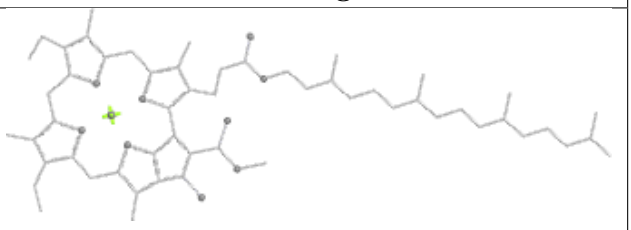
Bond angles

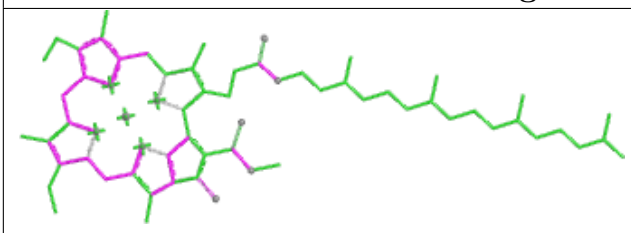
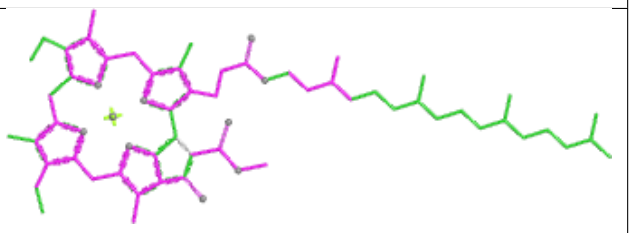
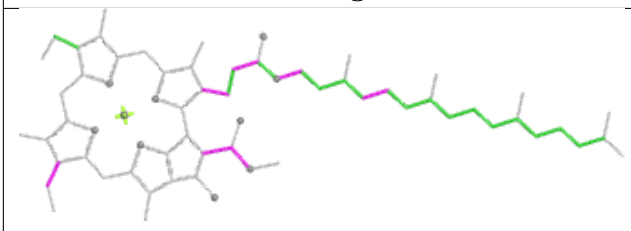
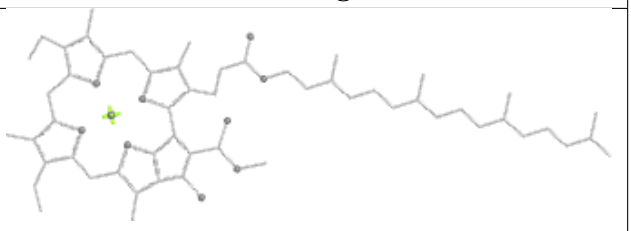


Torsions

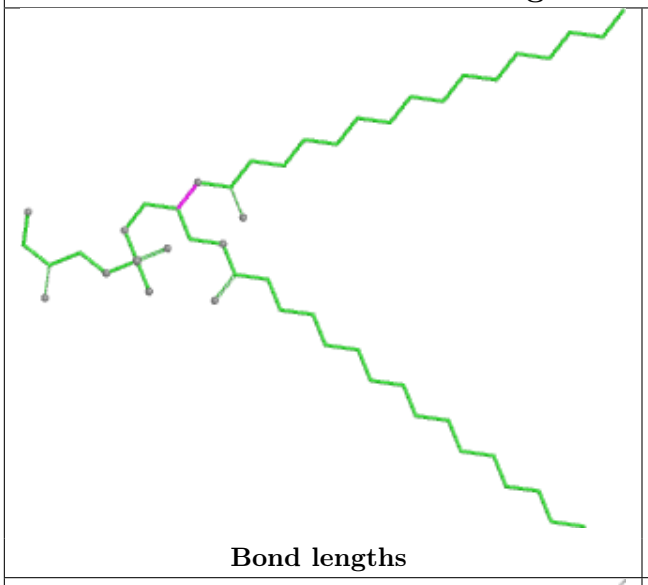


Rings

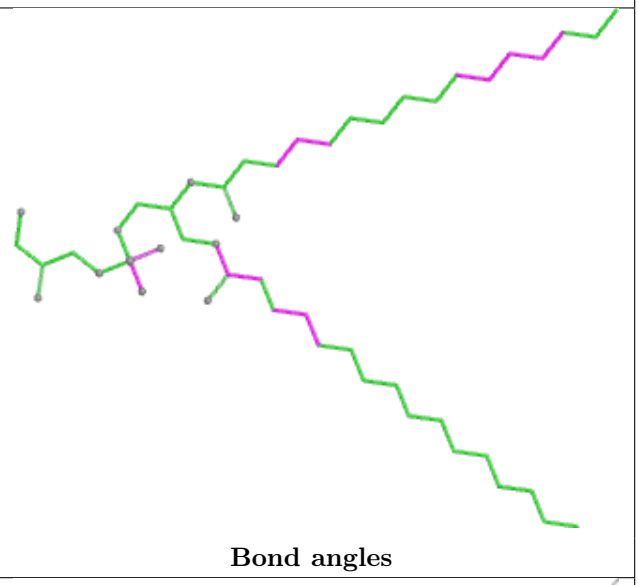
| Ligand CLA 32 204 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA 37 308 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

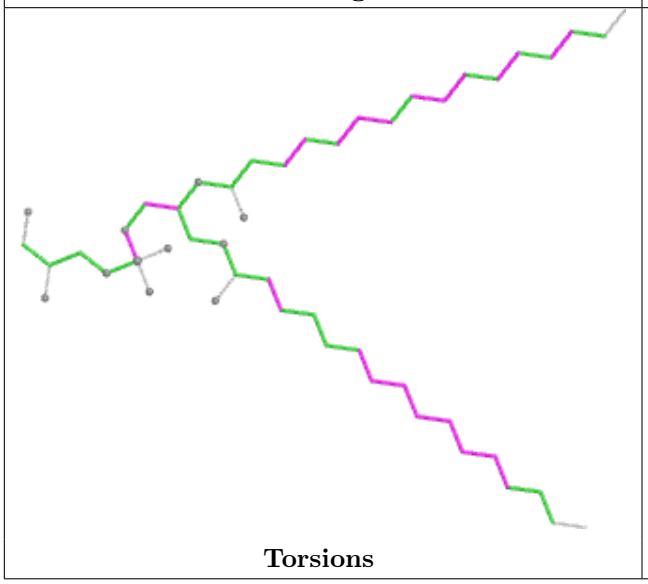
## Ligand LHG b 522



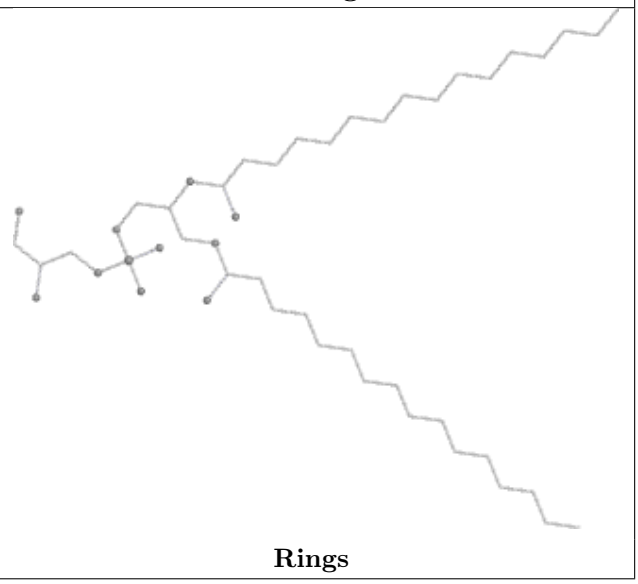
Bond lengths



Bond angles

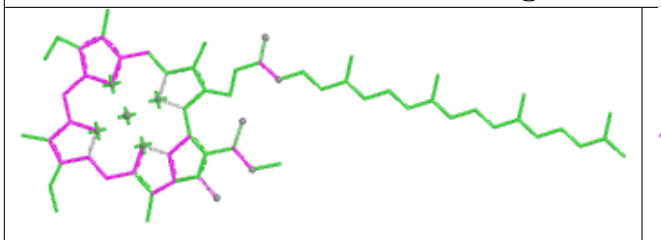


Torsions

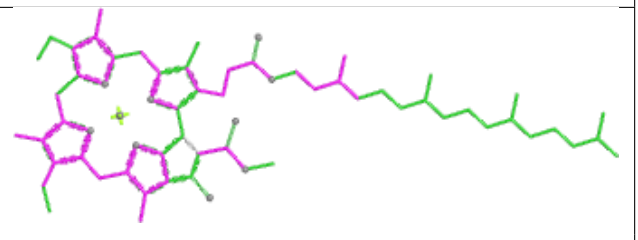


Rings

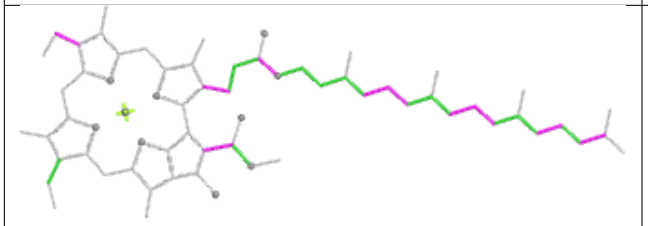
## Ligand CLA 19 303



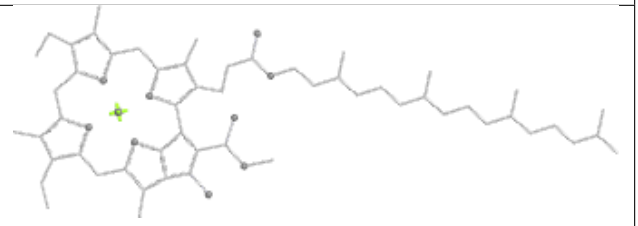
Bond lengths



Bond angles

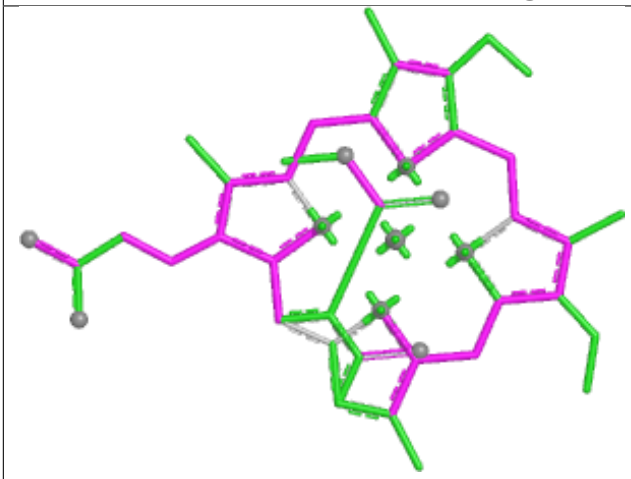


Torsions

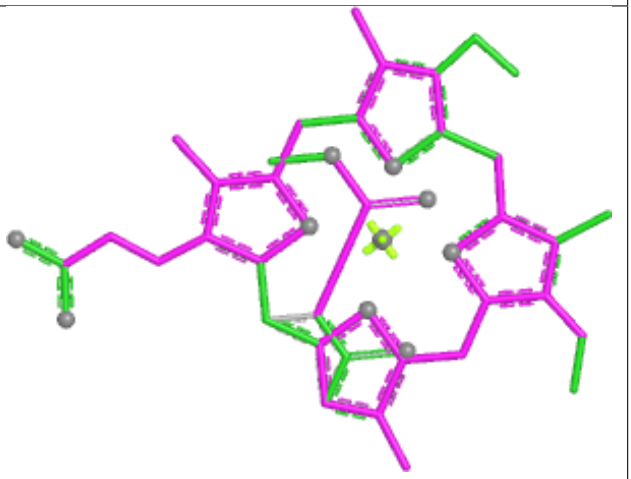


Rings

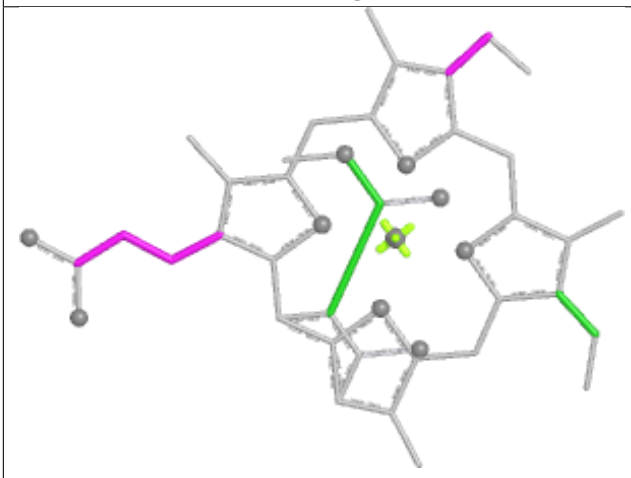
**Ligand KC1 36 305**



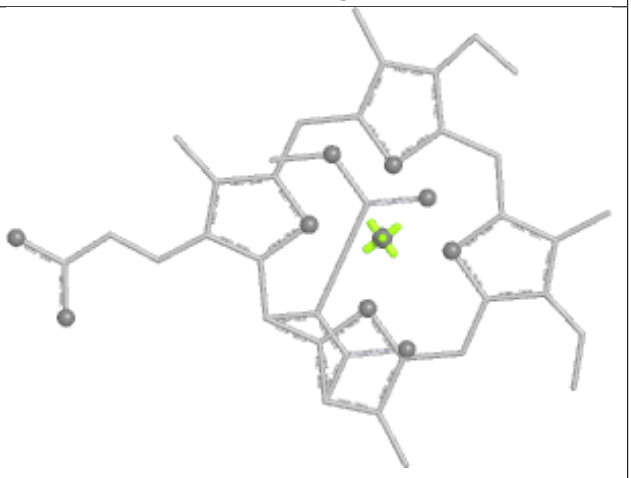
**Bond lengths**



**Bond angles**

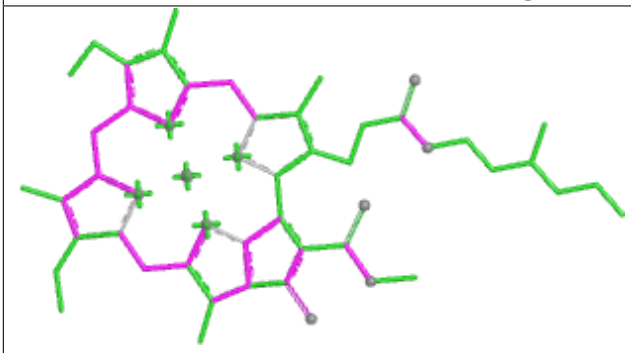


**Torsions**

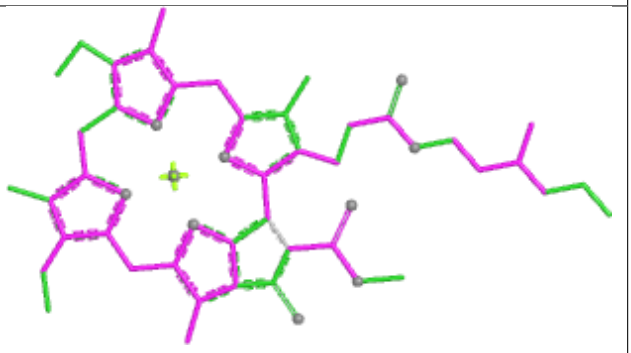


**Rings**

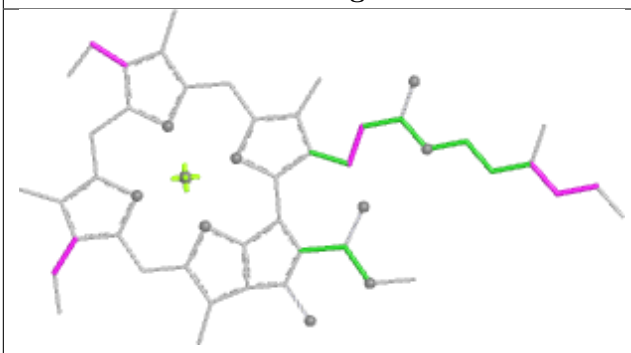
**Ligand CLA 31 308**



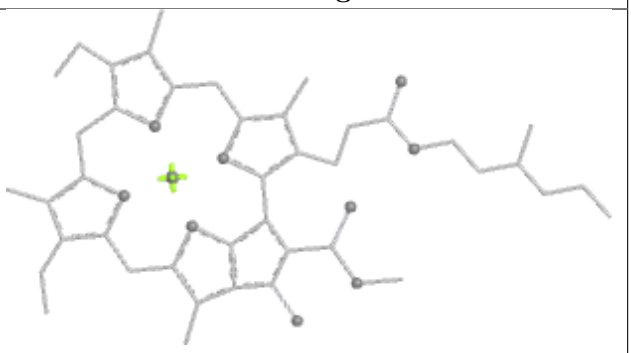
Bond lengths



Bond angles

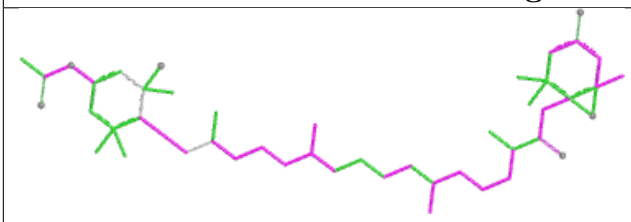


Torsions

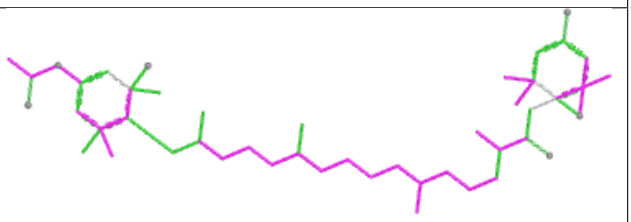


Rings

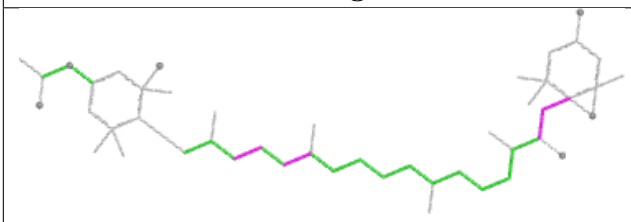
**Ligand A86 12 213**



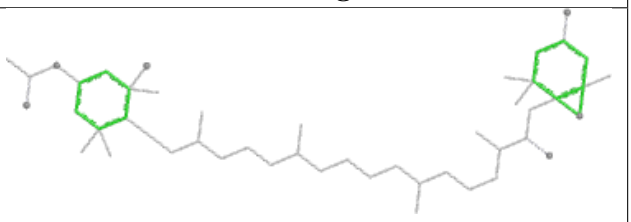
Bond lengths



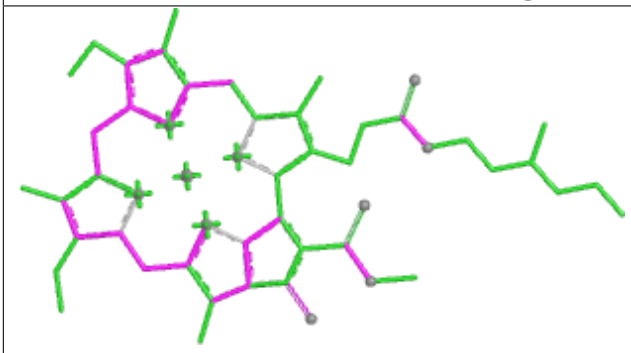
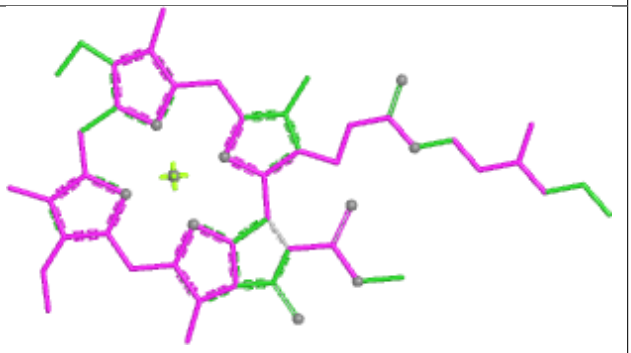
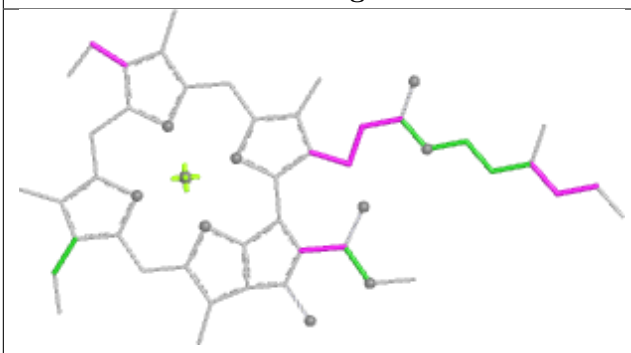
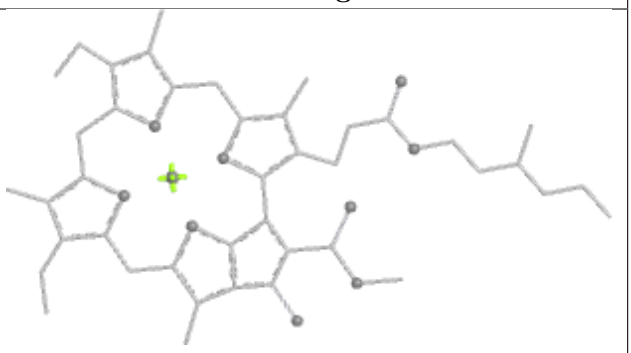
Bond angles

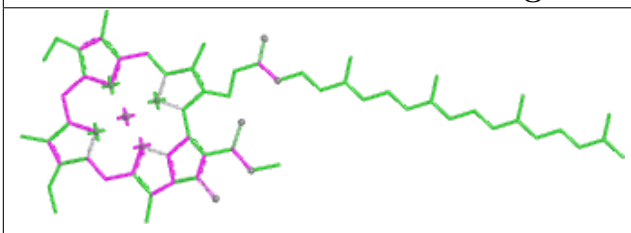
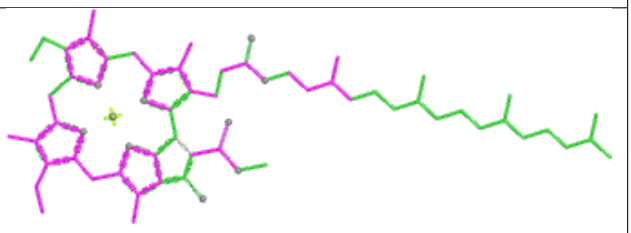
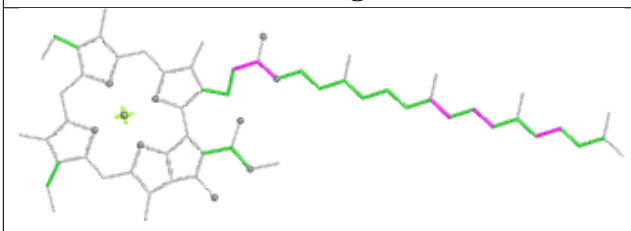
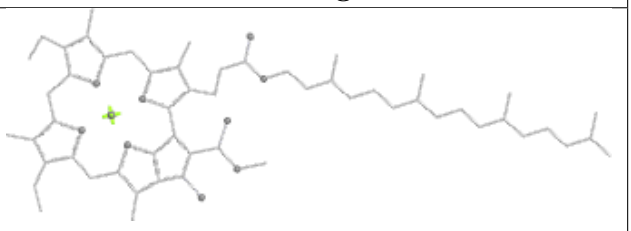


Torsions

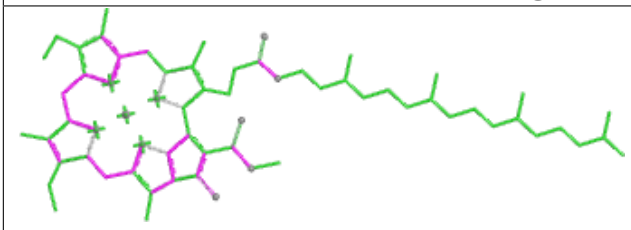


Rings

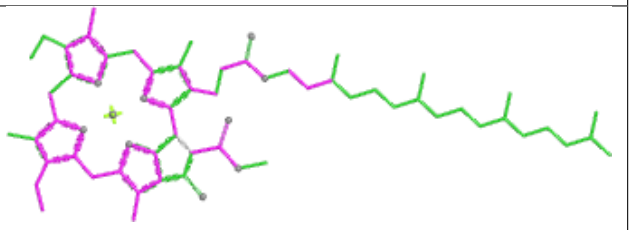
| Ligand CLA 17 307 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA B 512 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

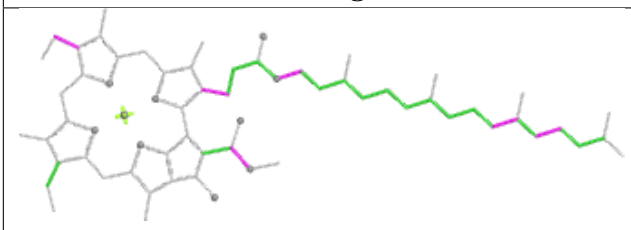
## Ligand CLA c 502



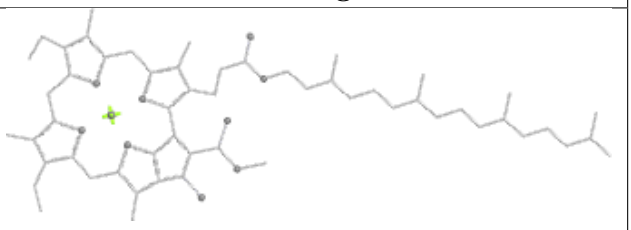
Bond lengths



Bond angles

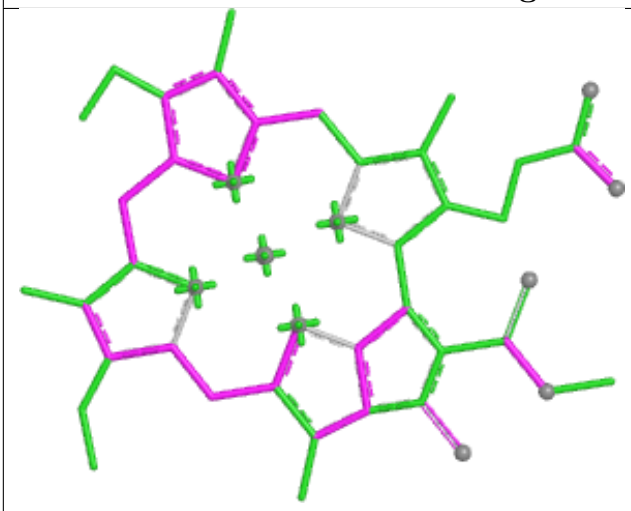


Torsions

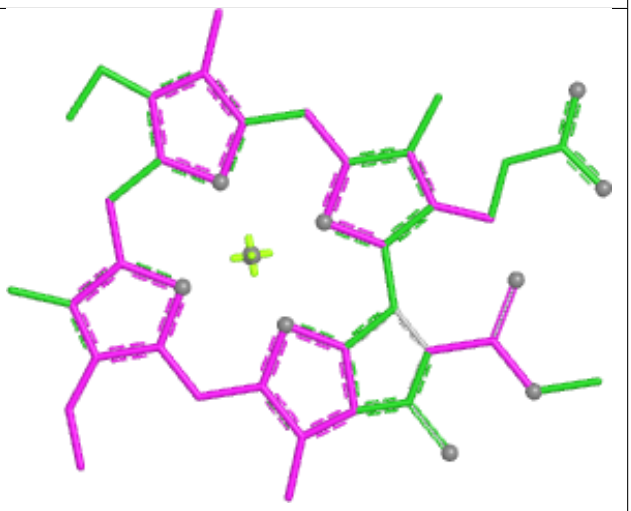


Rings

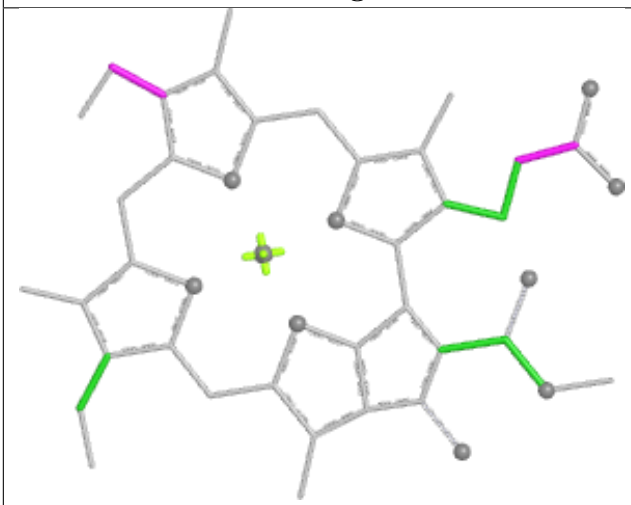
## Ligand CLA 34 310



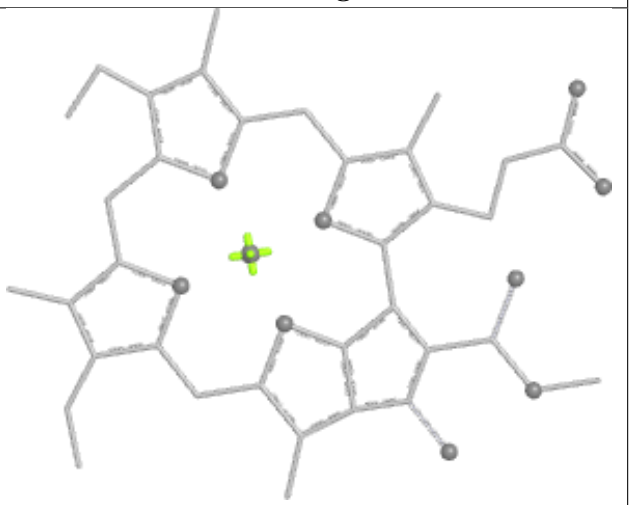
Bond lengths



Bond angles

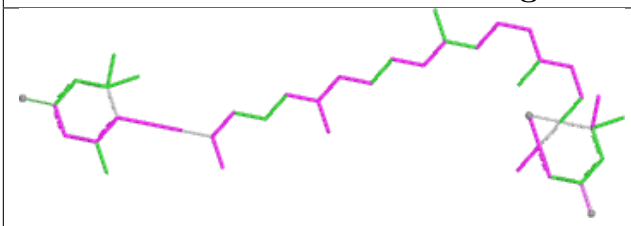


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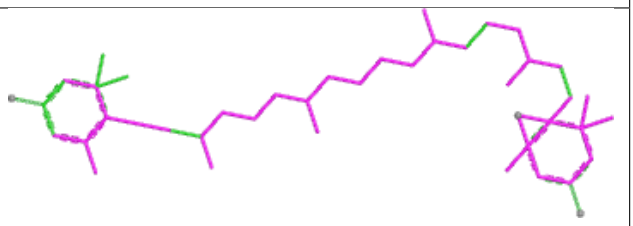


Rings

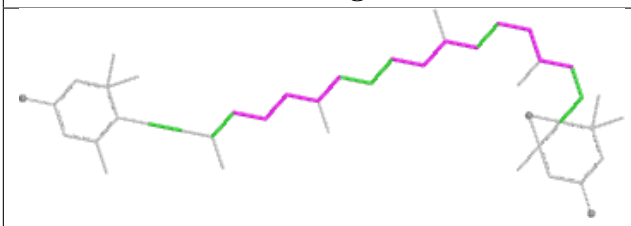
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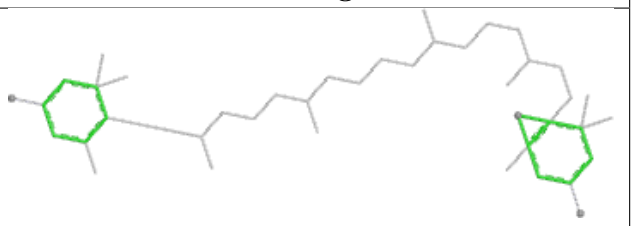
Bond lengths



Bond angles

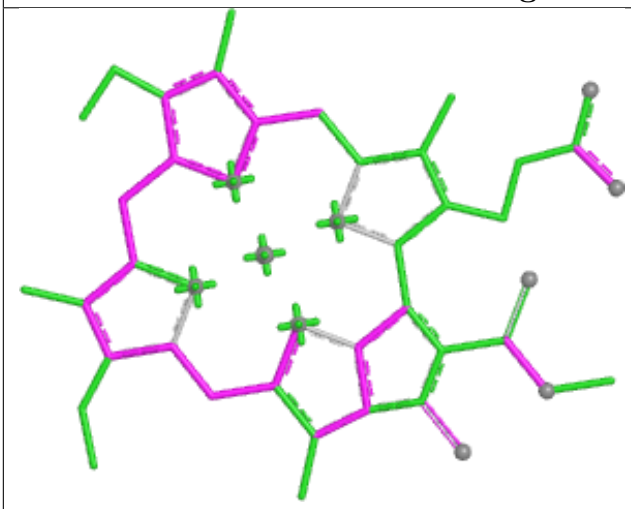


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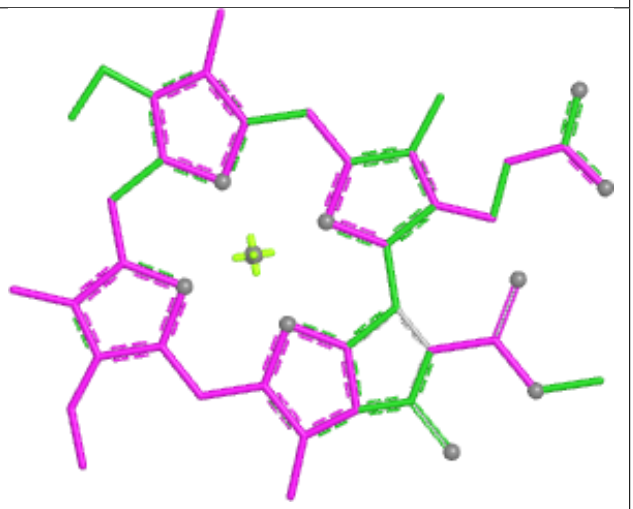


Rings

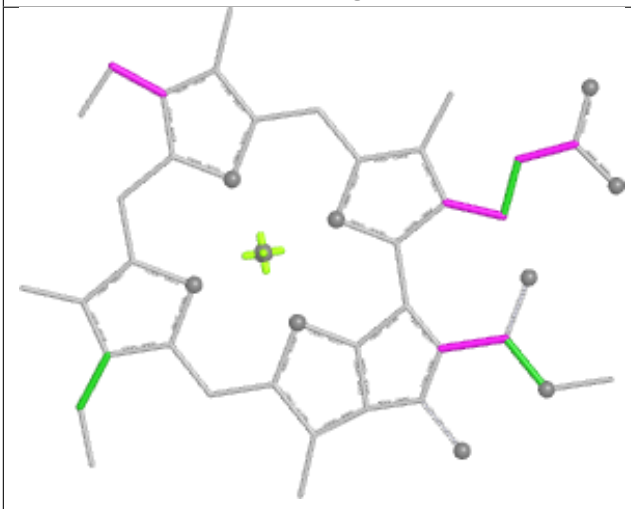
## Ligand CLA 40 209



Bond lengths



Bond angles

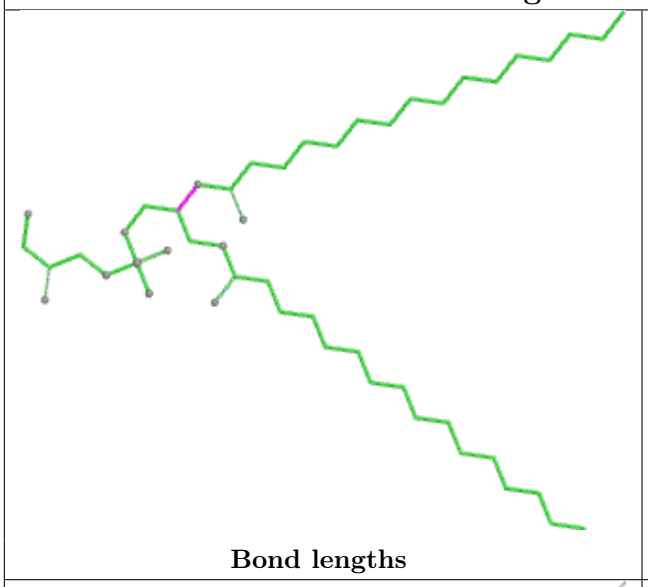


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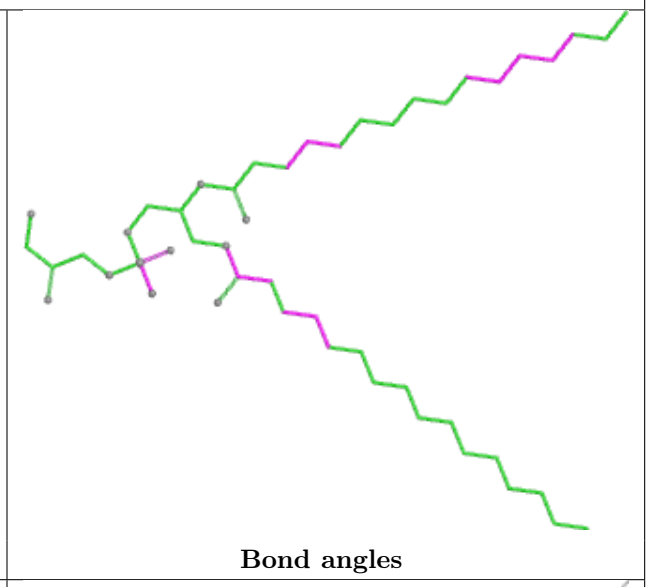


Rings

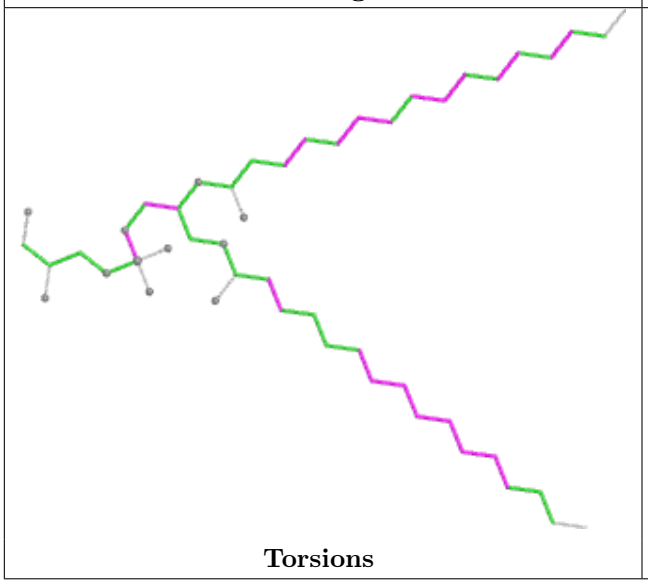
**Ligand LHG B 523**



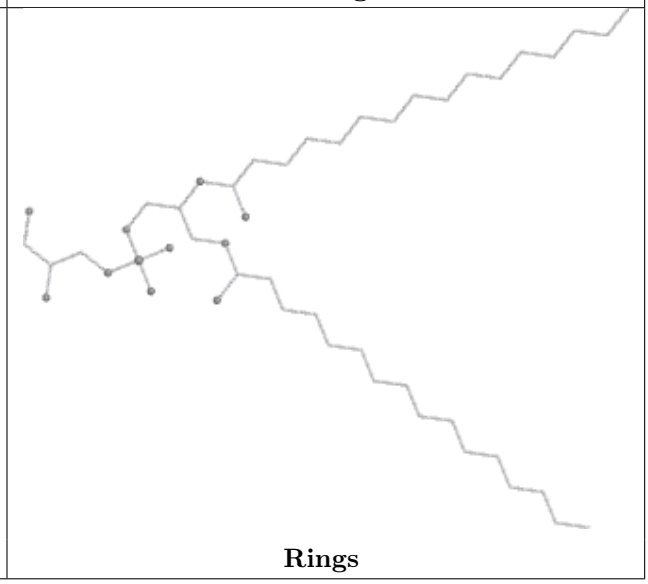
**Bond lengths**



**Bond angles**

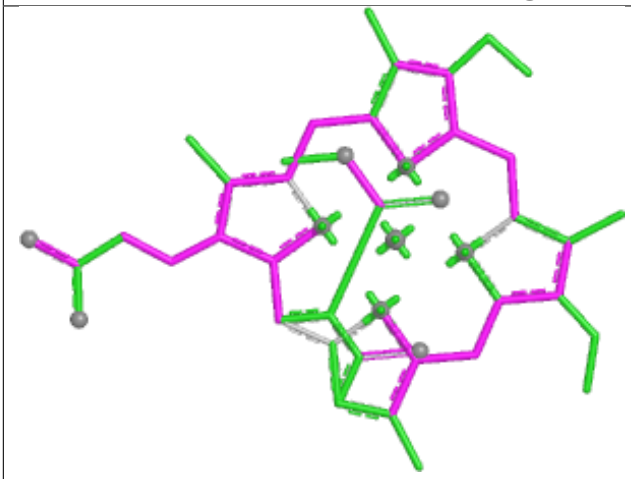


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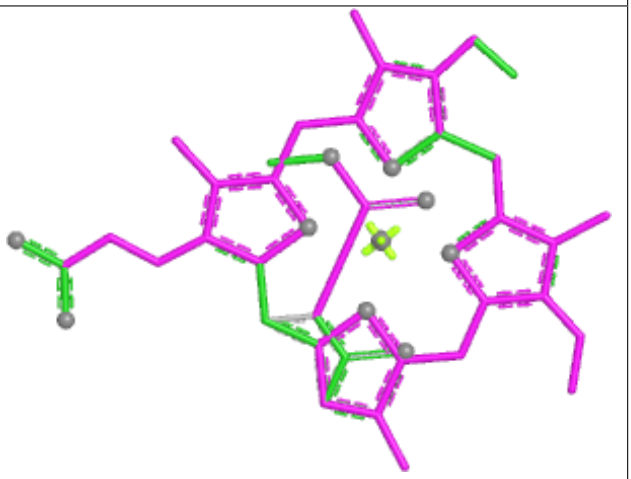


**Rings**

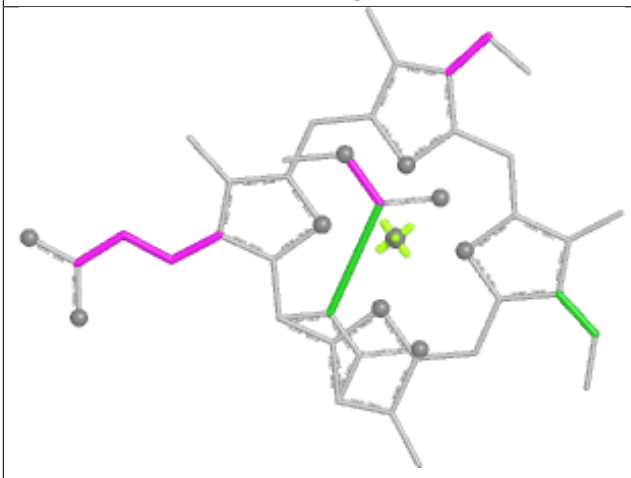
**Ligand KC1 40 204**



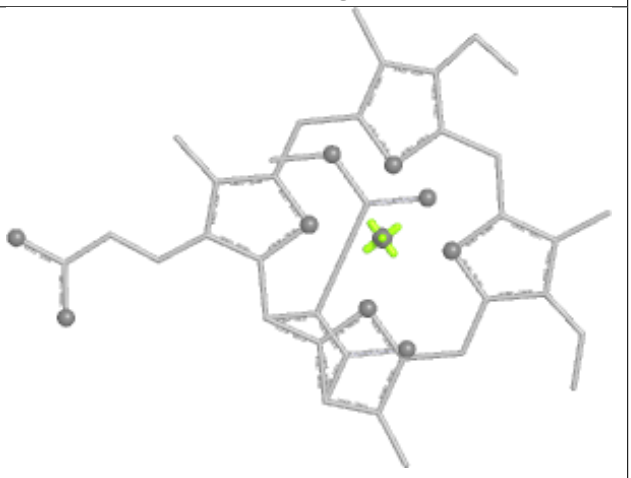
**Bond lengths**



**Bond angles**

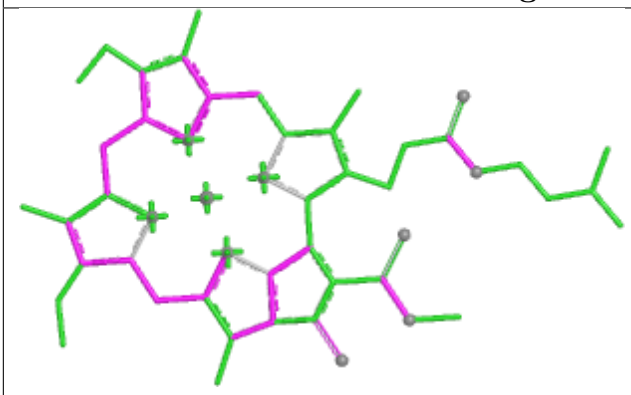


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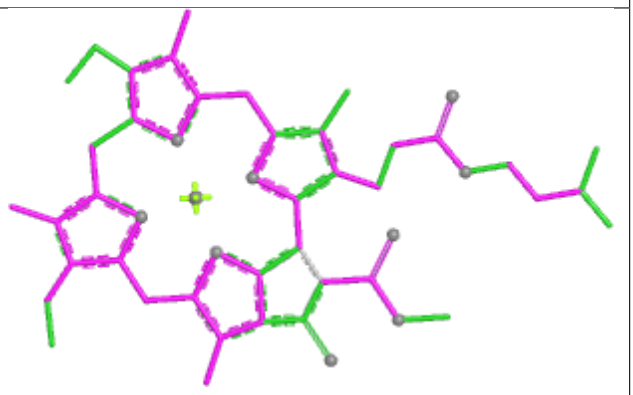


**Rings**

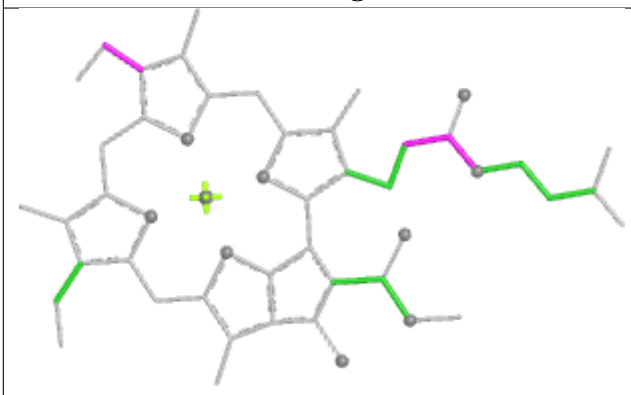
## Ligand CLA 20 306



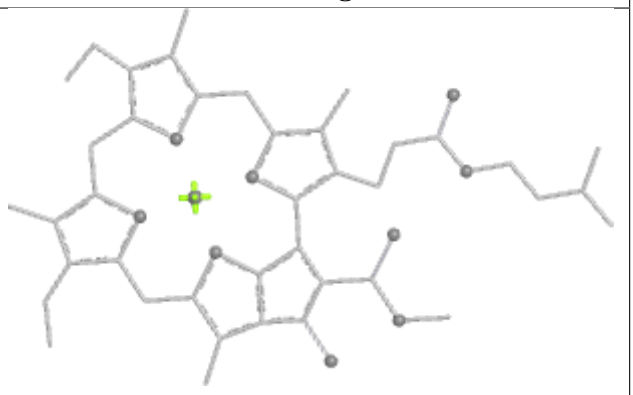
Bond lengths



Bond angles

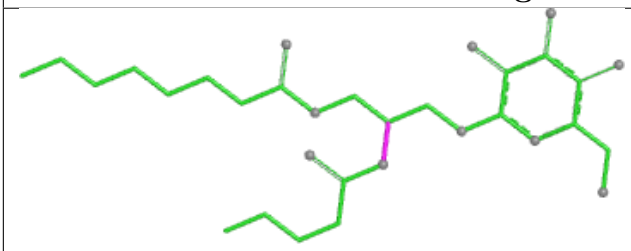


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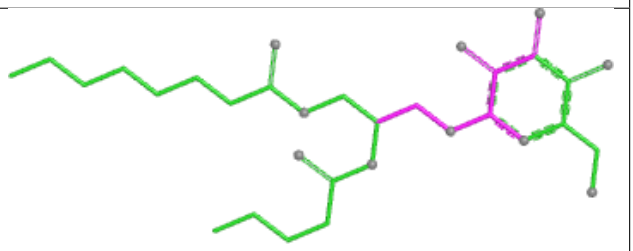


Rings

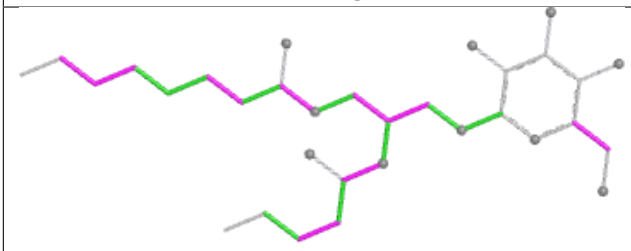
## Ligand LMG 11 317



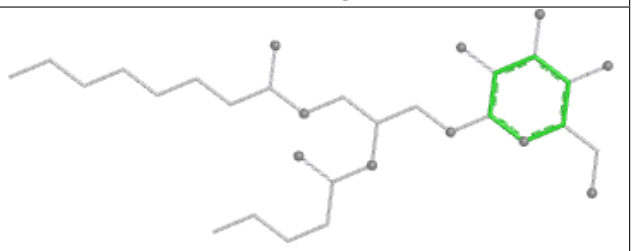
Bond lengths



Bond angles

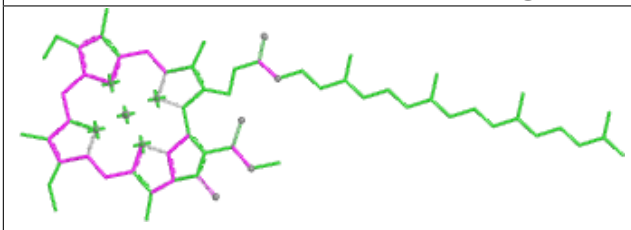


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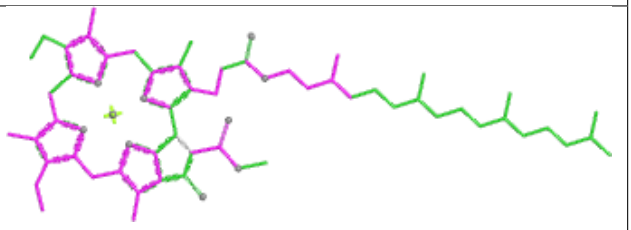


Rings

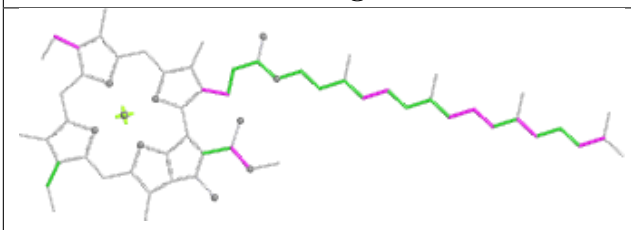
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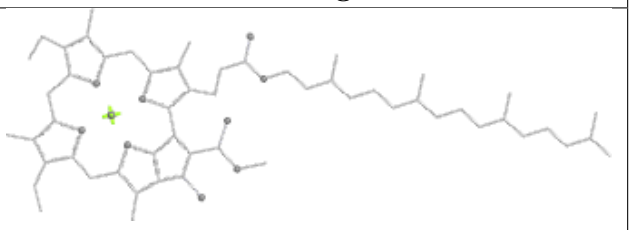
Bond lengths



Bond angles

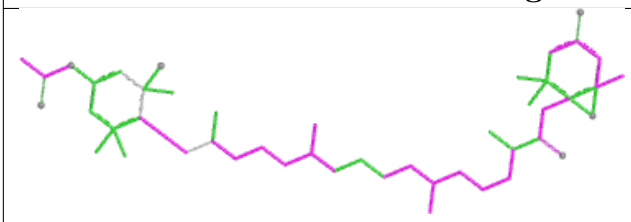


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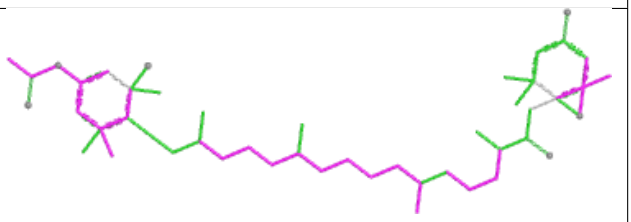


Rings

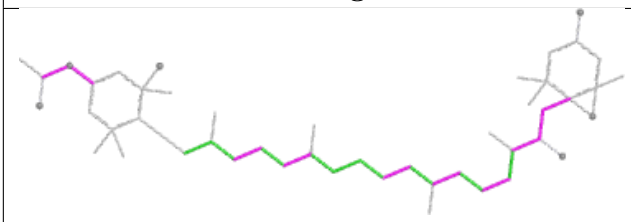
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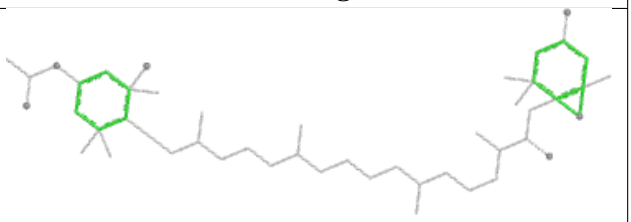
Bond lengths



Bond angles

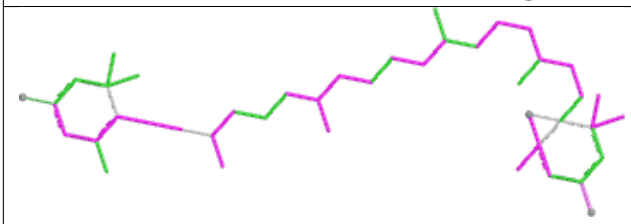


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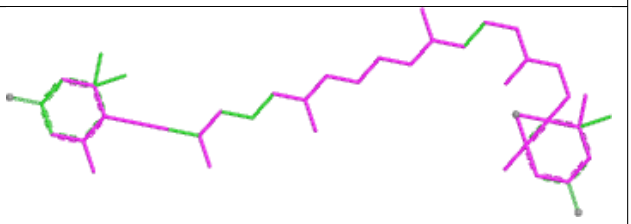


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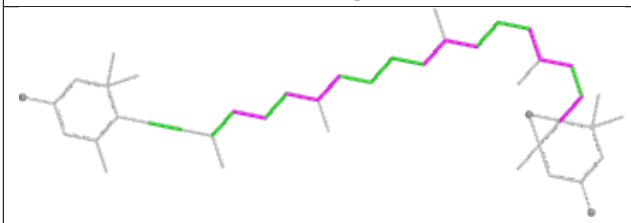
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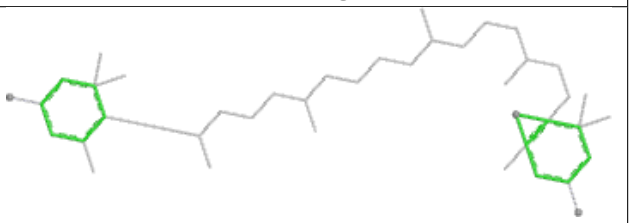
Bond lengths



Bond angles

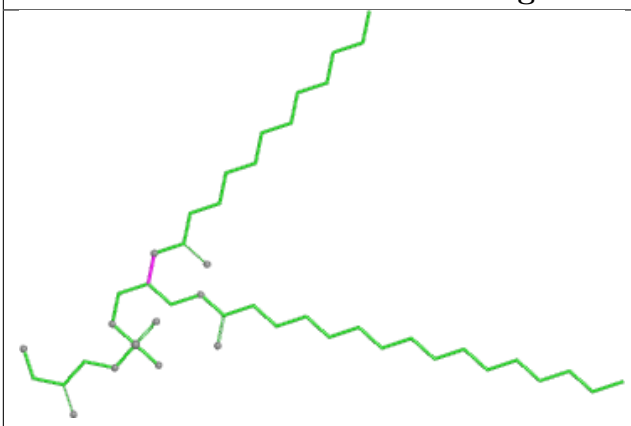


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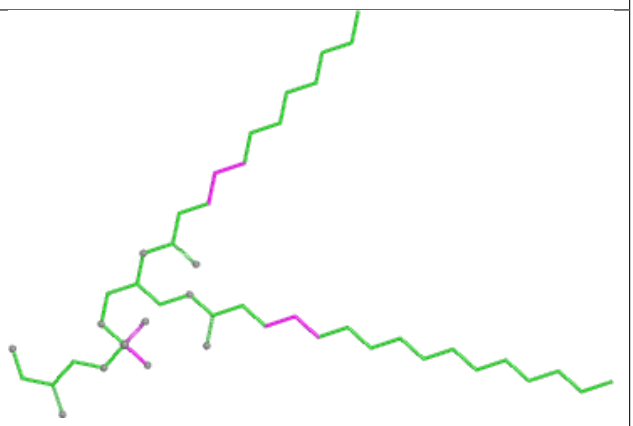


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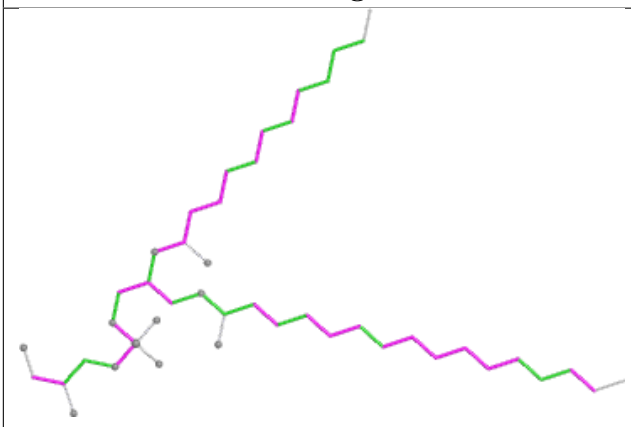
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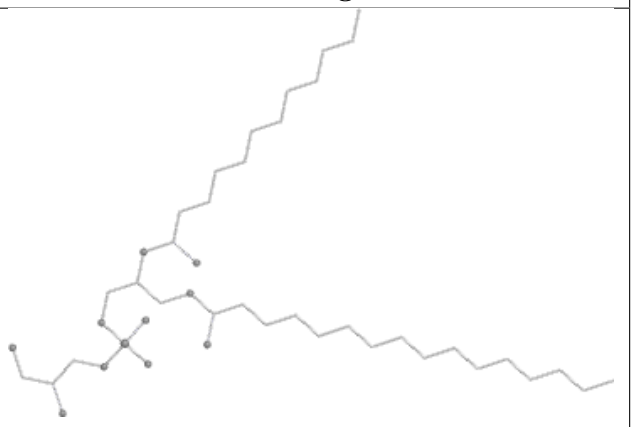
Bond lengths



Bond angles

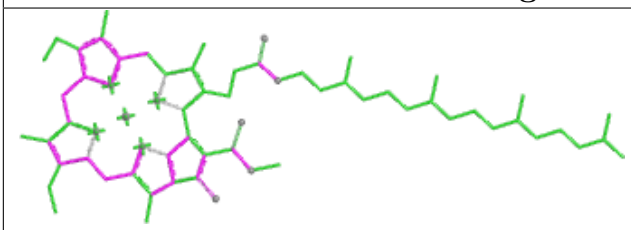


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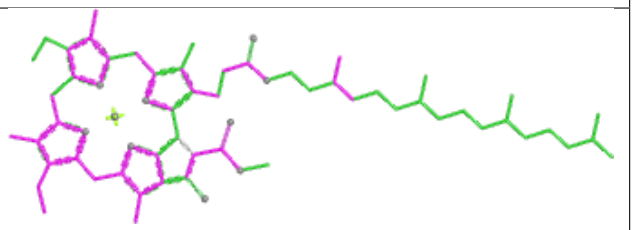


Rings

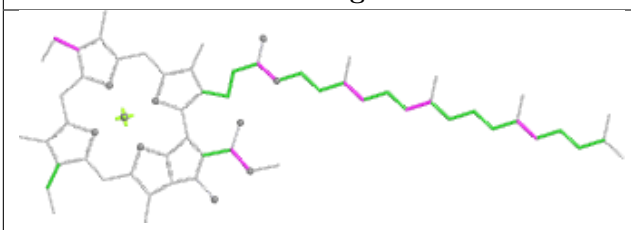
## Ligand CLA 19 302



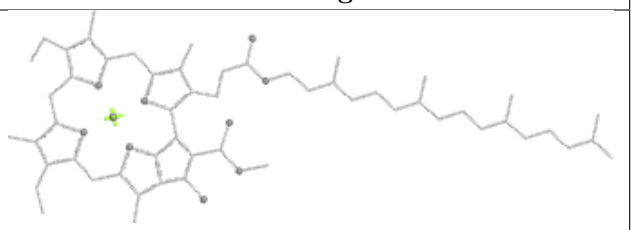
Bond lengths



Bond angles

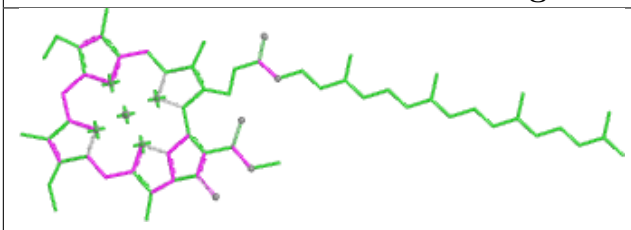


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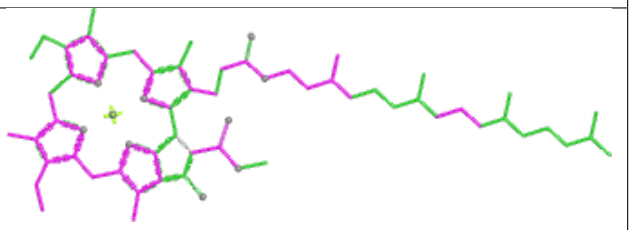


Rings

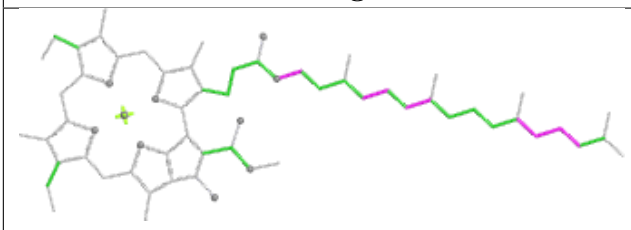
**Ligand CLA c 509**



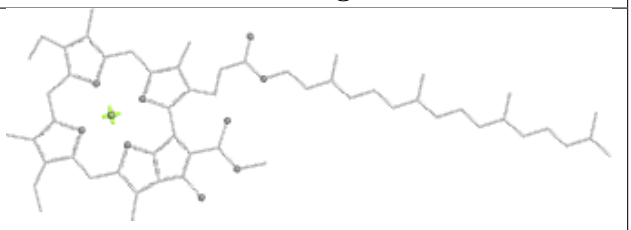
Bond lengths



Bond angles

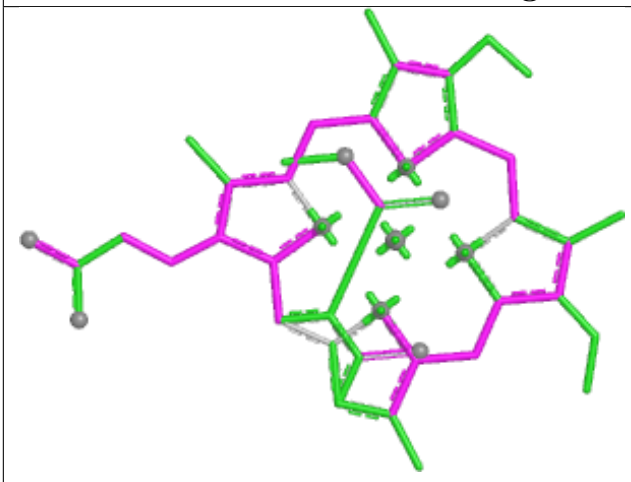


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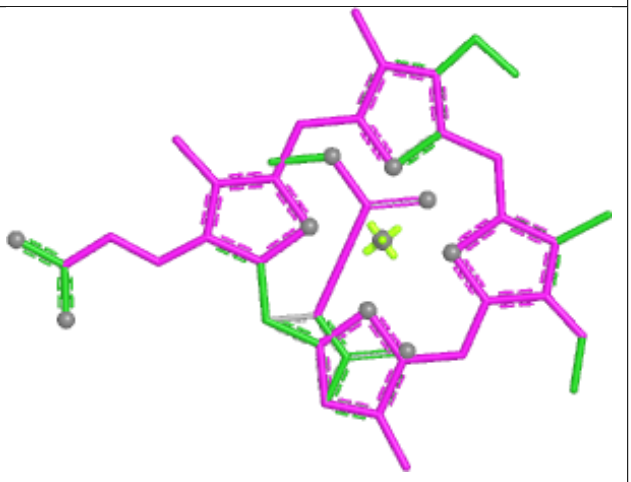


Rings

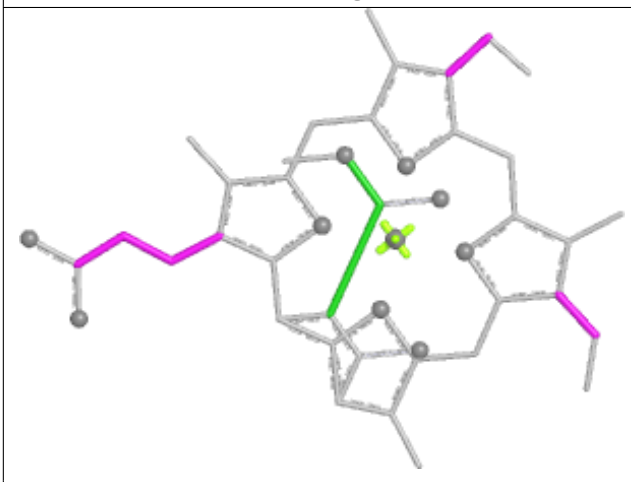
**Ligand KC1 37 305**



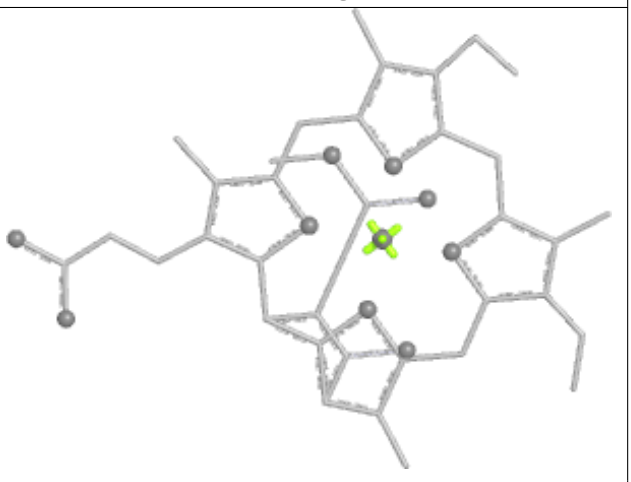
Bond lengths



Bond angles

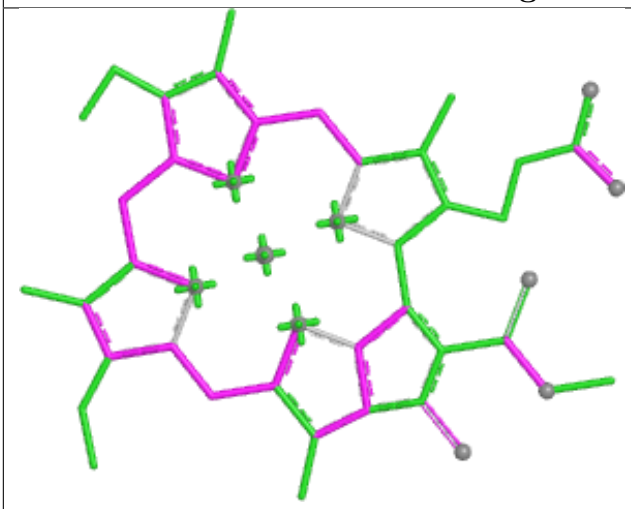


Torsions

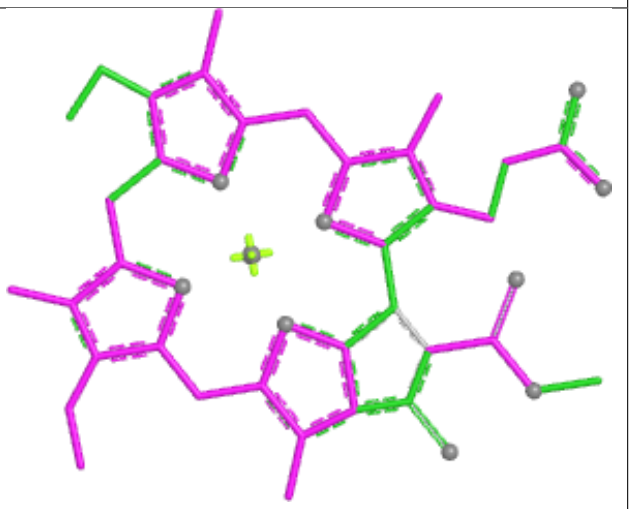


Rings

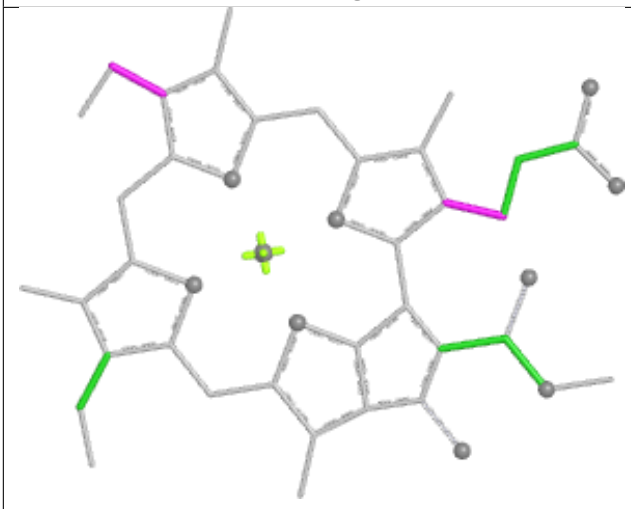
**Ligand CLA 31 306**



**Bond lengths**



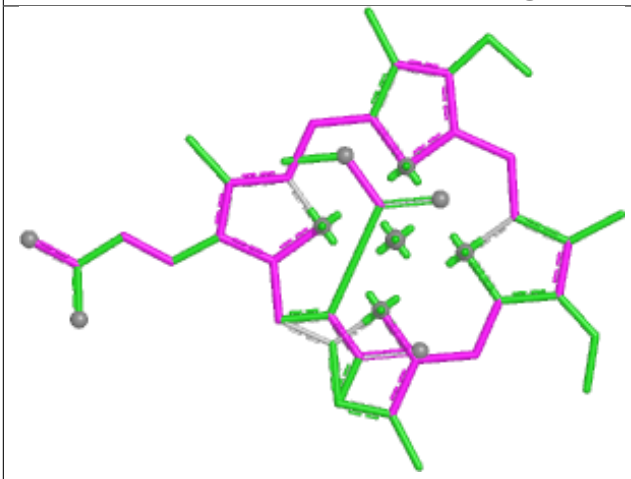
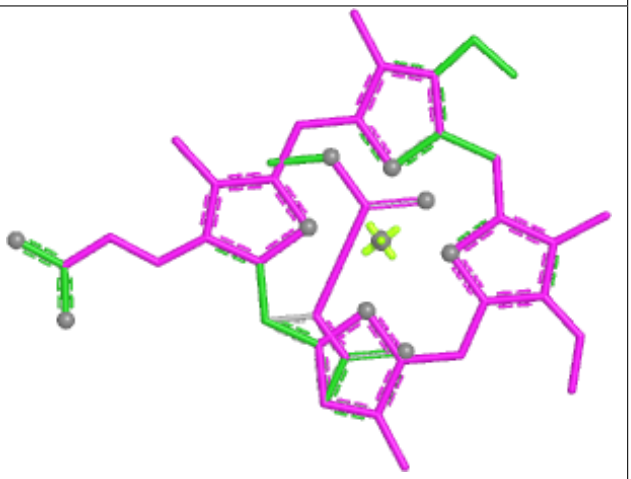
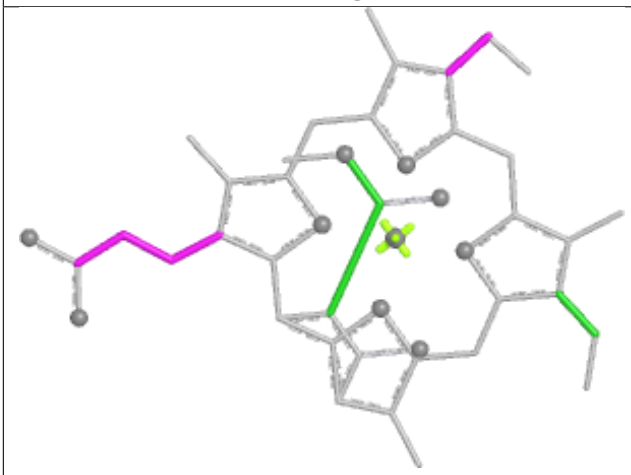
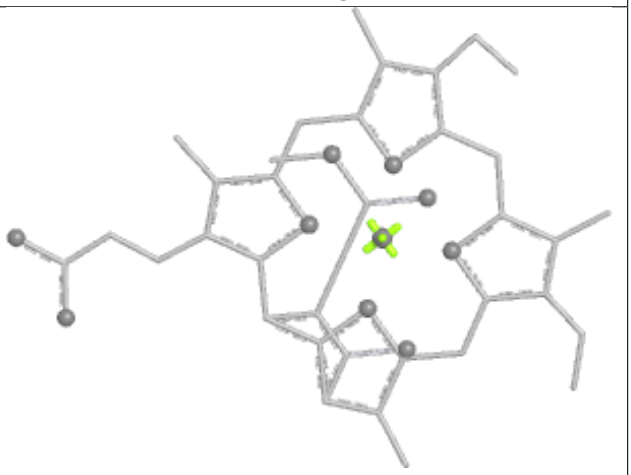
**Bond angles**

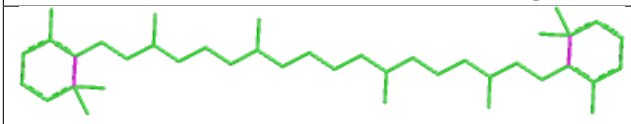
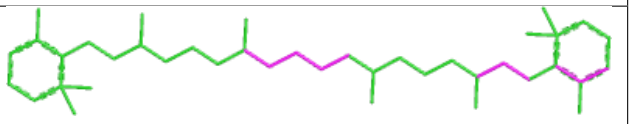
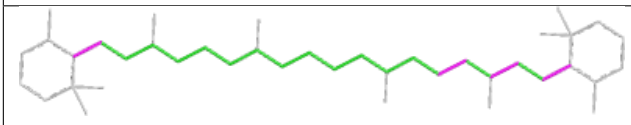
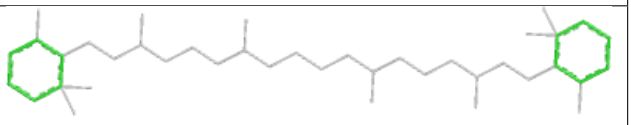


**Torsions**

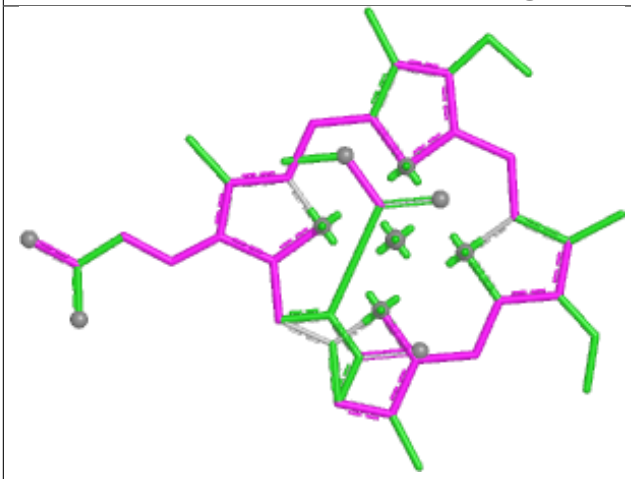


**Rings**

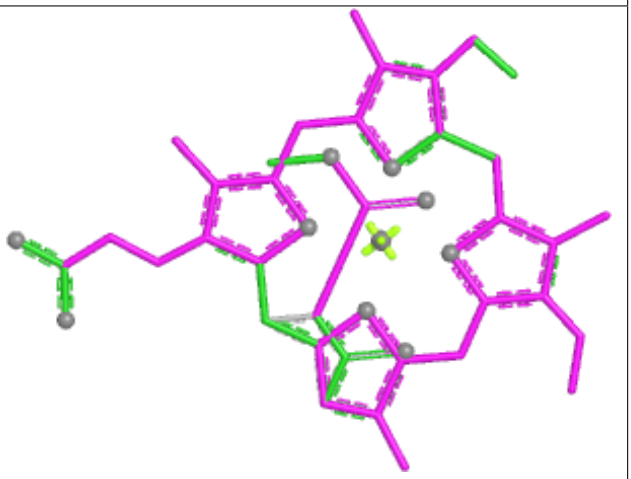
| Ligand KC1 34 309 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand BCR c 519 | |
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|  Bond lengths |  Bond angles |
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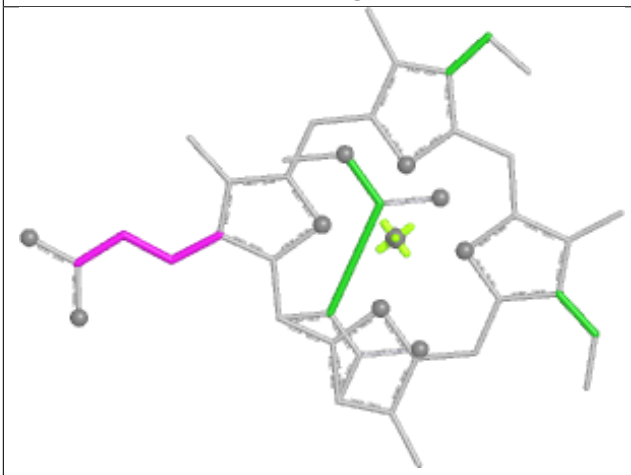
**Ligand KC1 13 309**



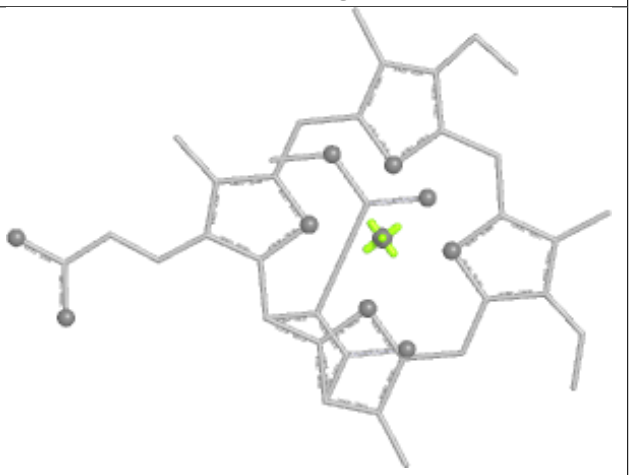
Bond lengths



Bond angles

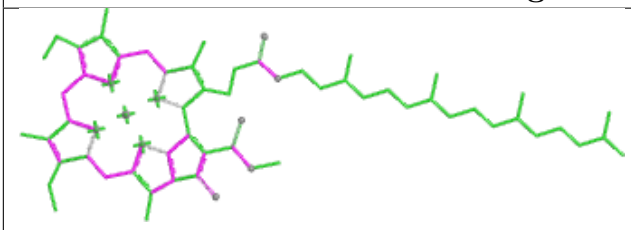


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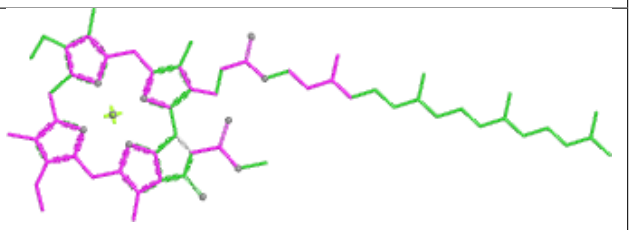


Rings

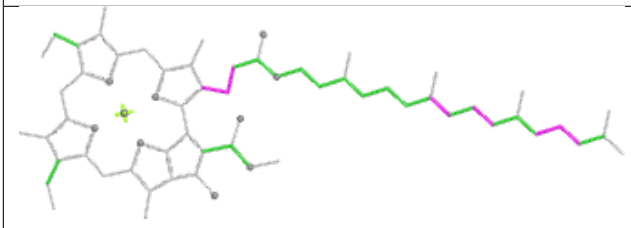
**Ligand CLA b 506**



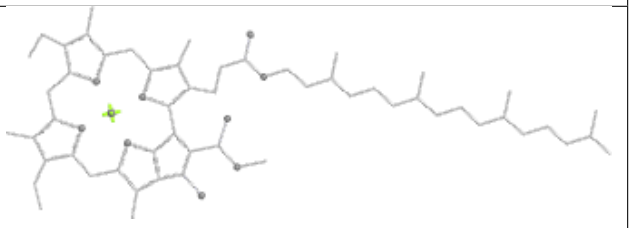
Bond lengths



Bond angles

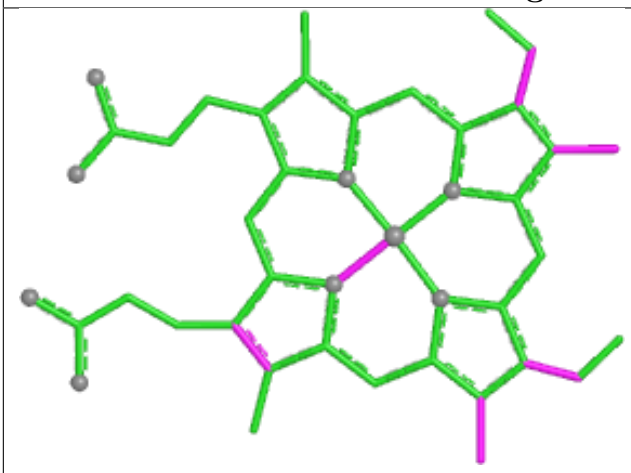


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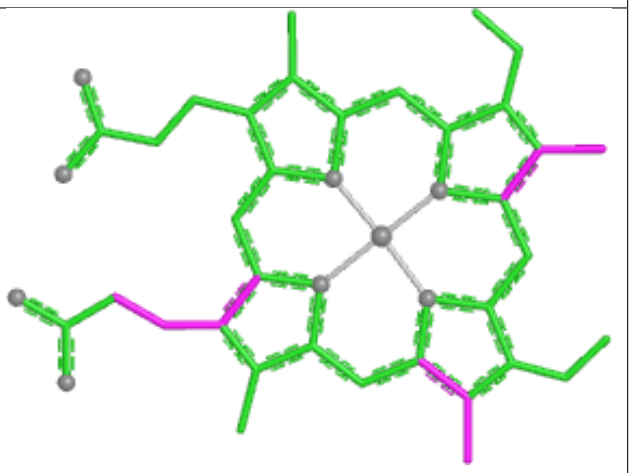


Rings

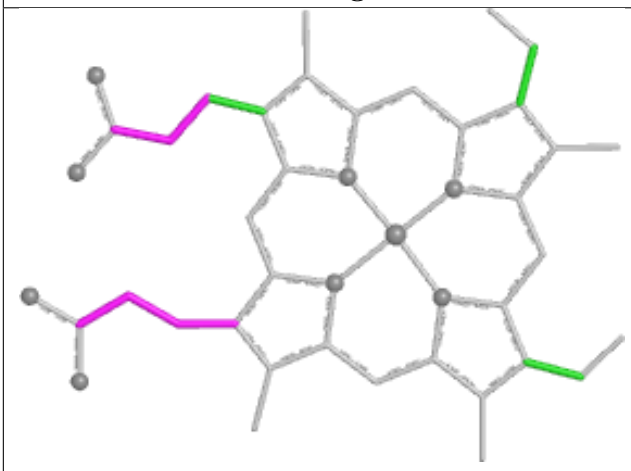
**Ligand HEM f 101**



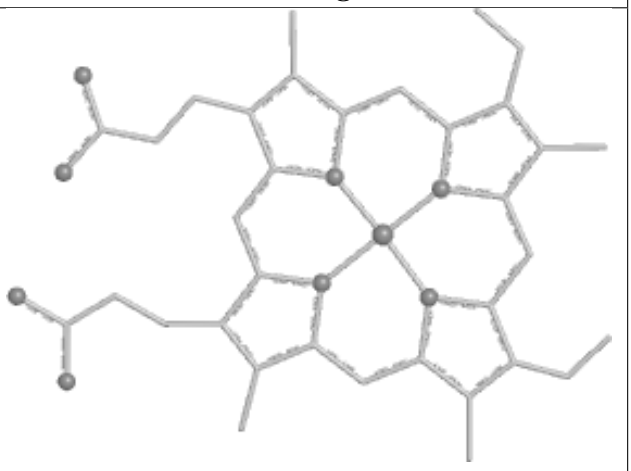
Bond lengths



Bond angles

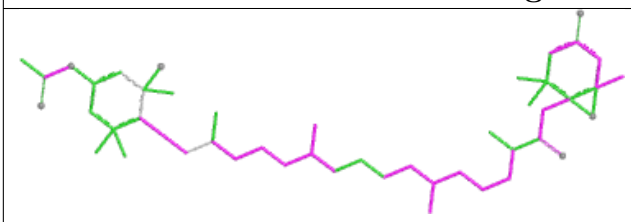


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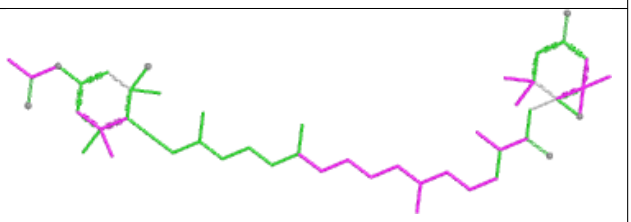


Rings

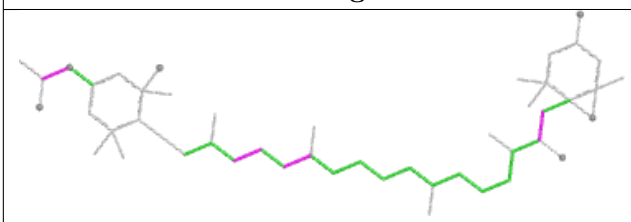
**Ligand A86 35 311**



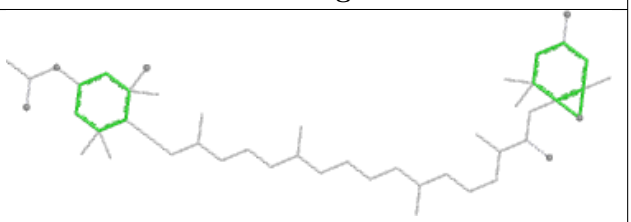
Bond lengths



Bond angles

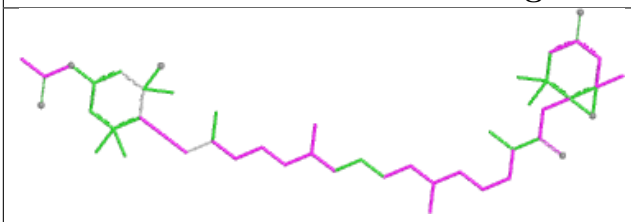


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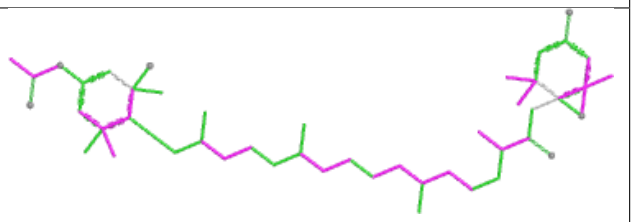


Rings

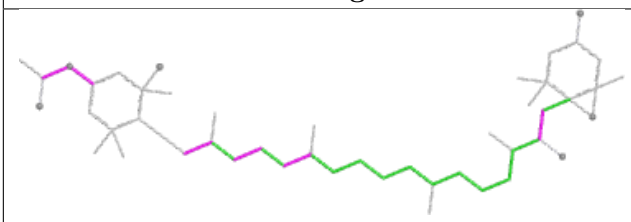
**Ligand A86 35 313**



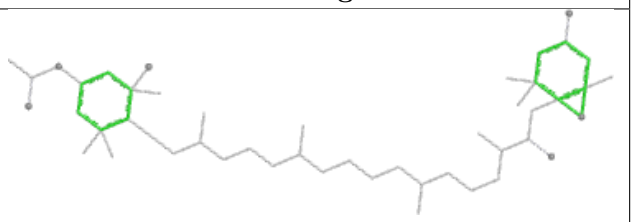
Bond lengths



Bond angles

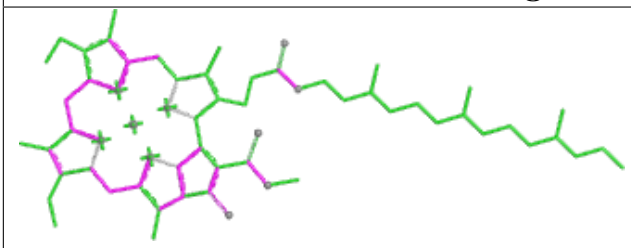


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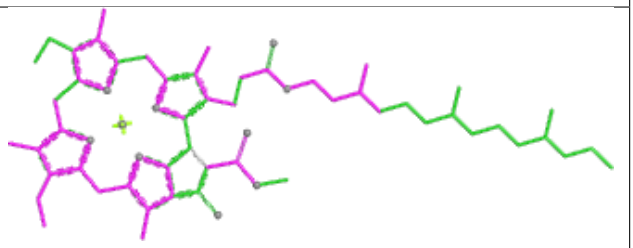


Rings

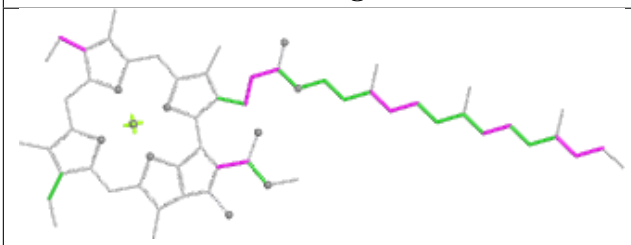
**Ligand CLA B 514**



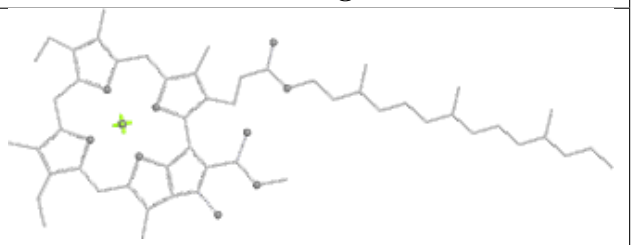
Bond lengths



Bond angles

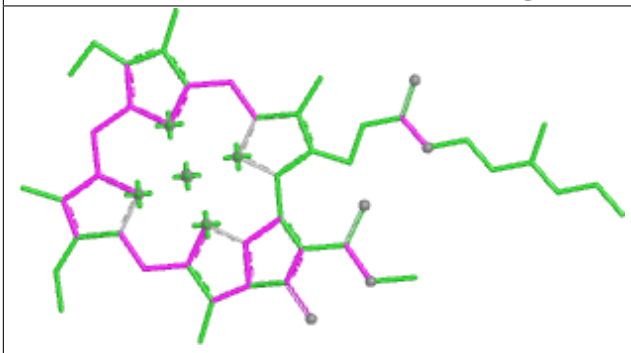


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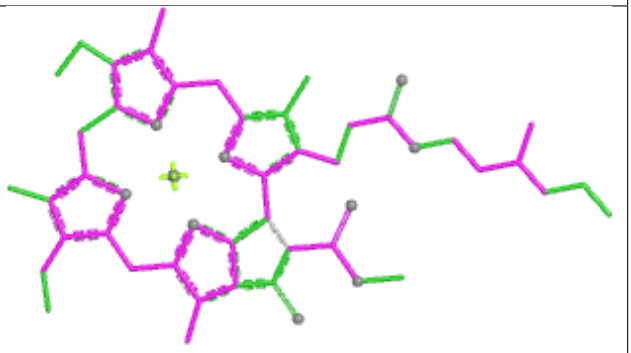


Rings

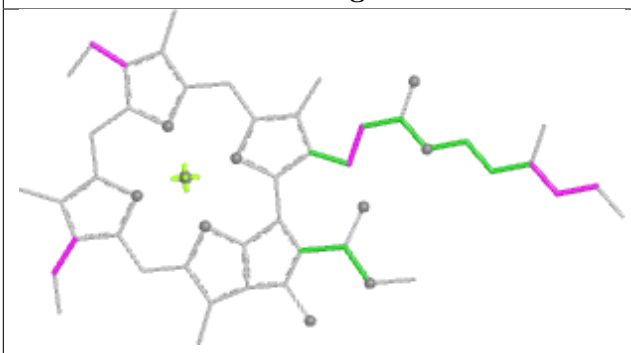
**Ligand CLA 11 307**



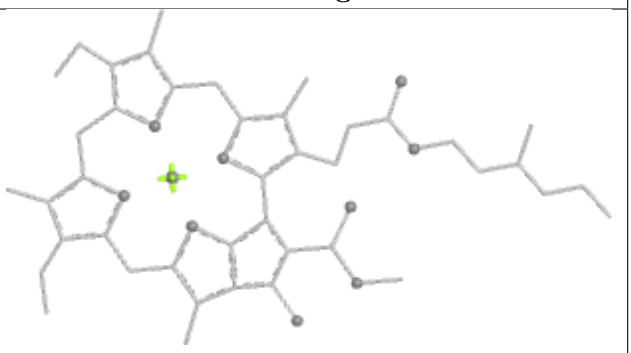
**Bond lengths**



**Bond angles**

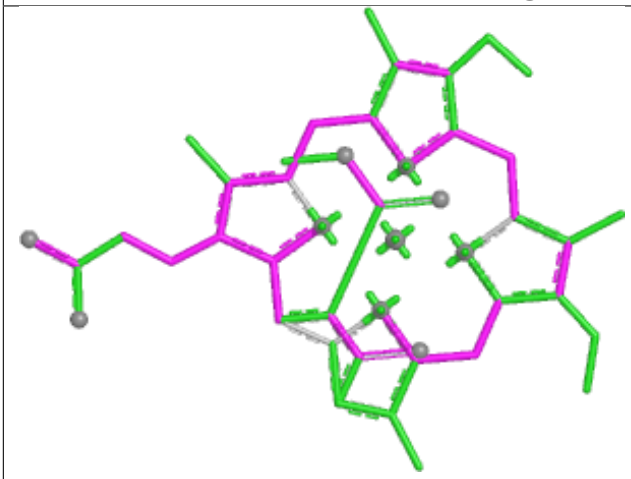


**Torsions**

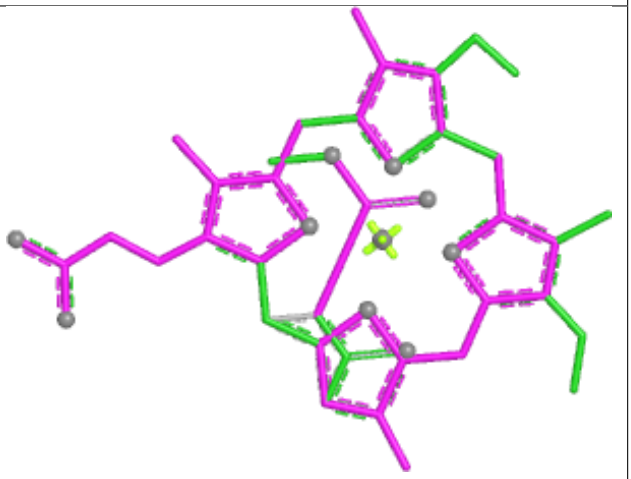


**Rings**

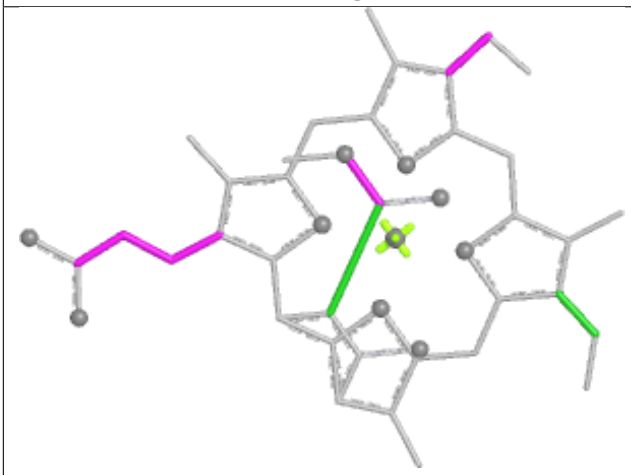
## Ligand KC1 31 307



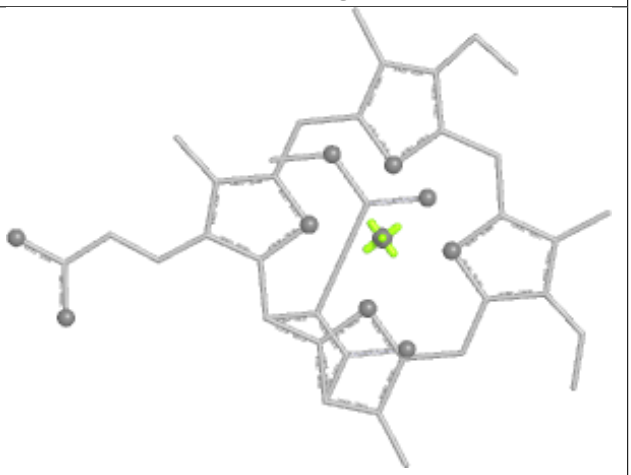
Bond lengths



Bond angles

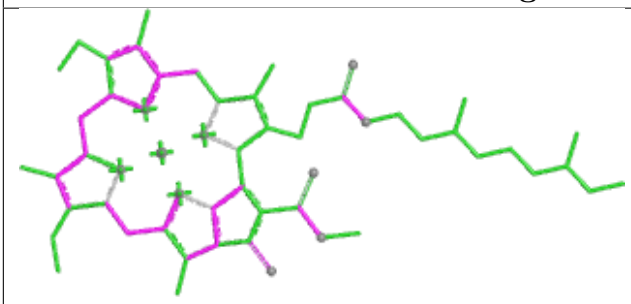


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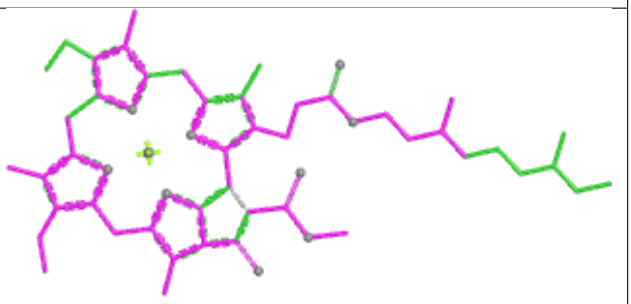


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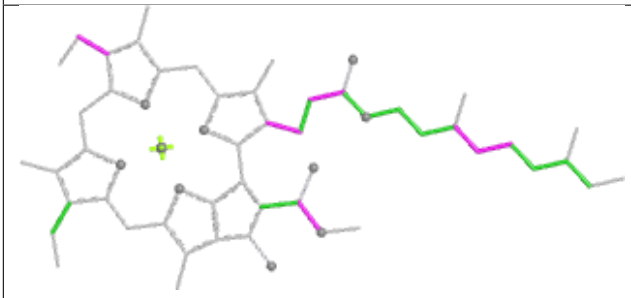
## Ligand CLA 40 205



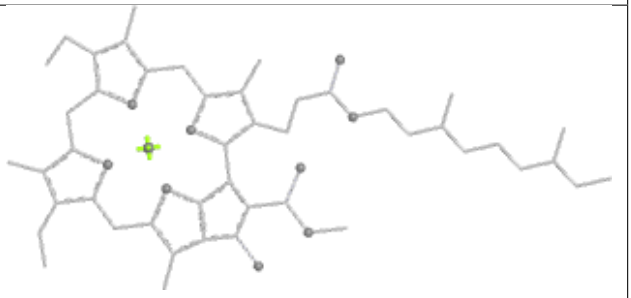
Bond lengths



Bond angles

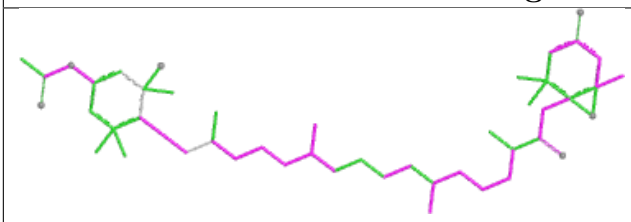


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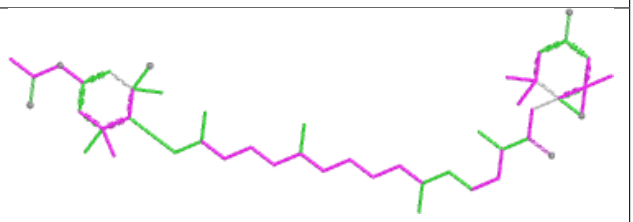


Rings

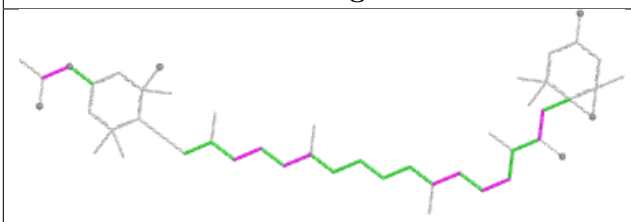
## Ligand A86 37 313



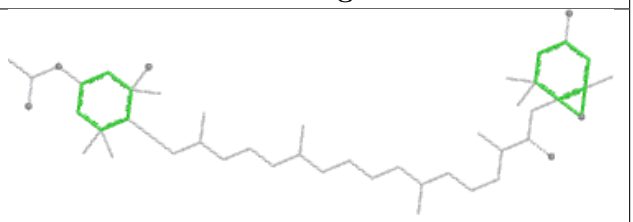
Bond lengths



Bond angles

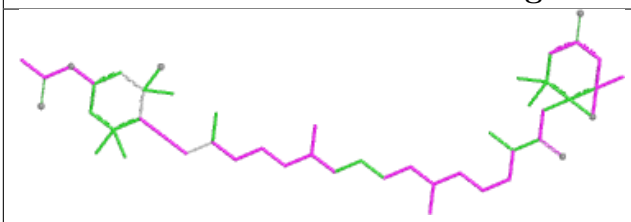


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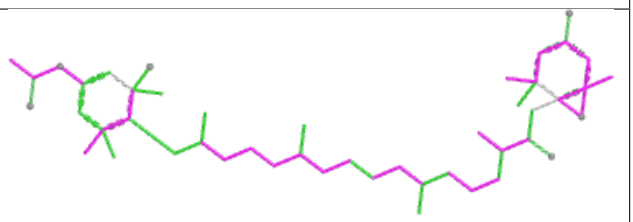


Rings

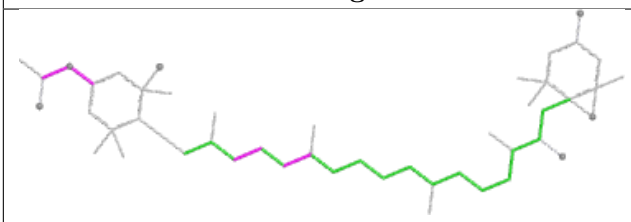
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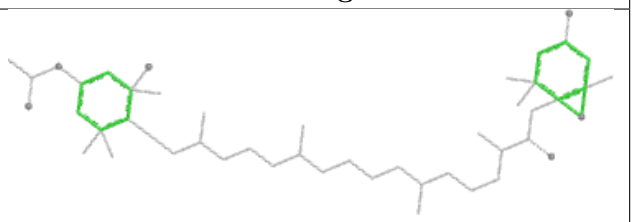
Bond lengths



Bond angles

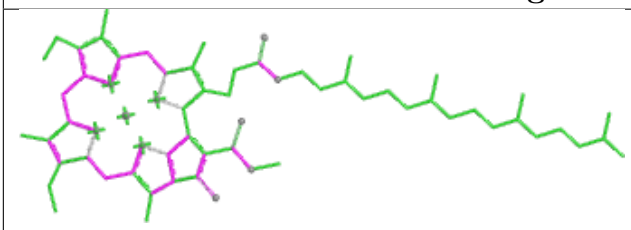


Torsions

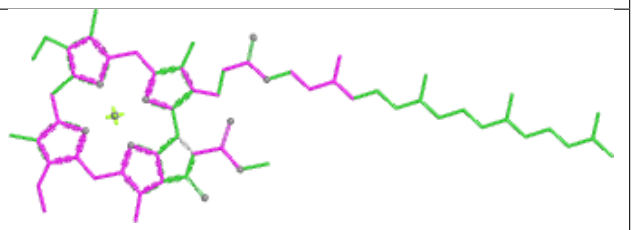


Rings

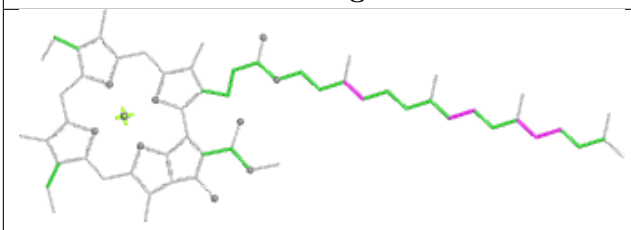
## Ligand CLA b 508



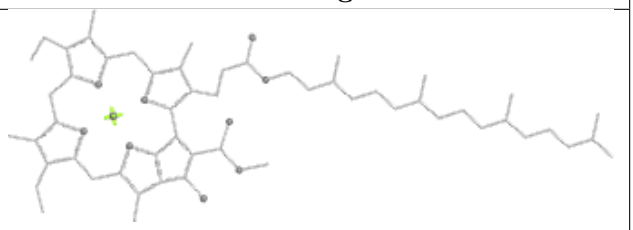
Bond lengths



Bond angles

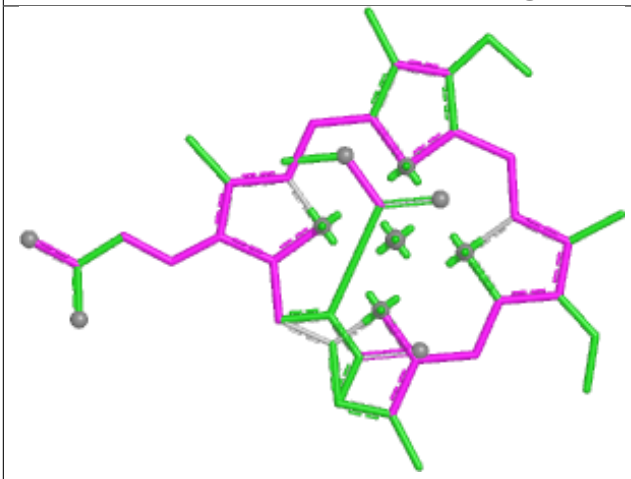


Torsions

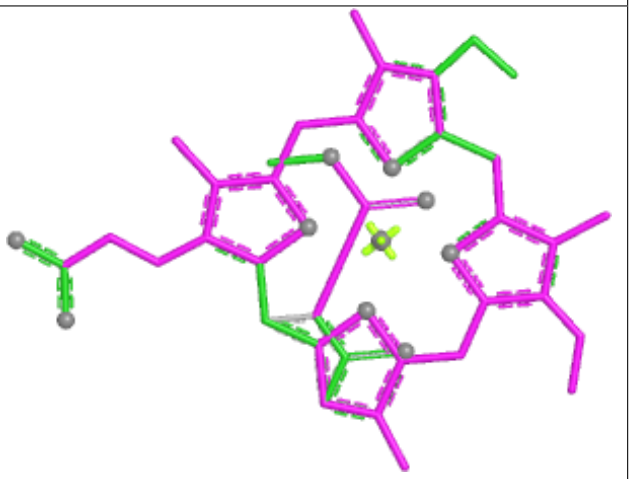


Rings

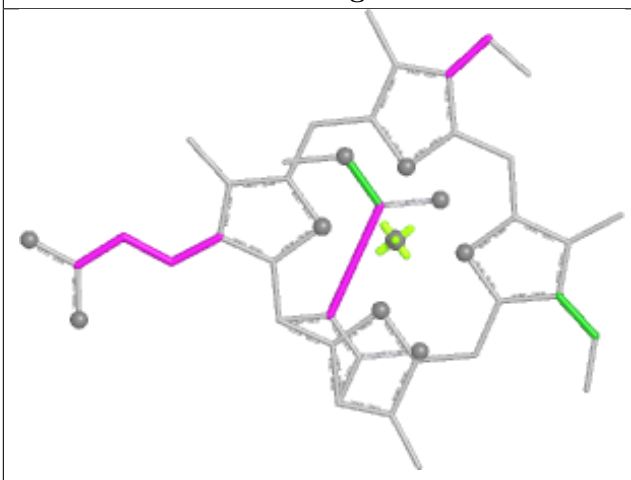
**Ligand KC1 15 309**



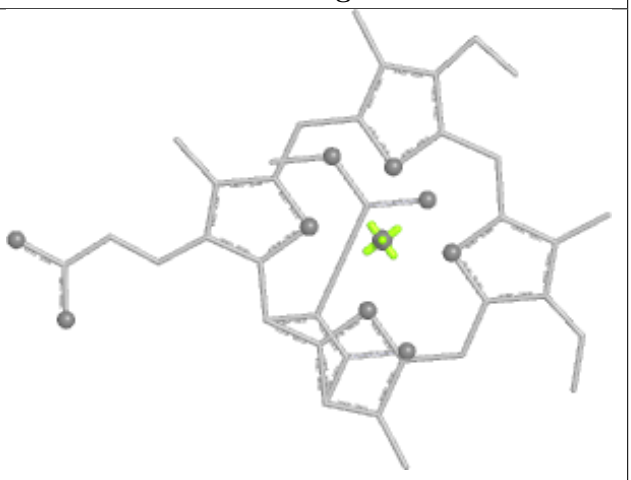
Bond lengths



Bond angles

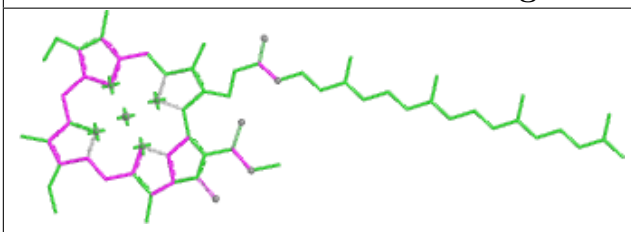


Torsions

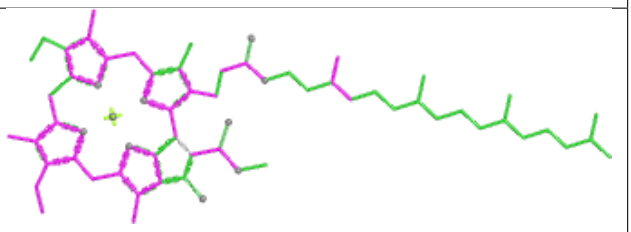


Rings

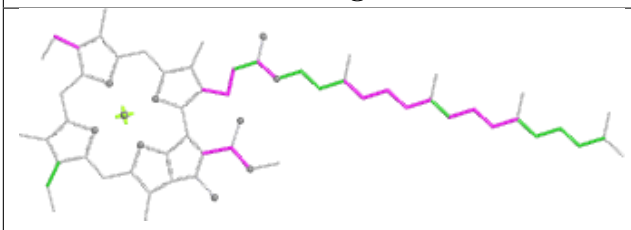
**Ligand CLA 34 302**



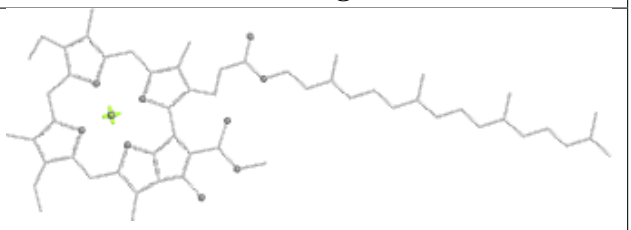
Bond lengths



Bond angles

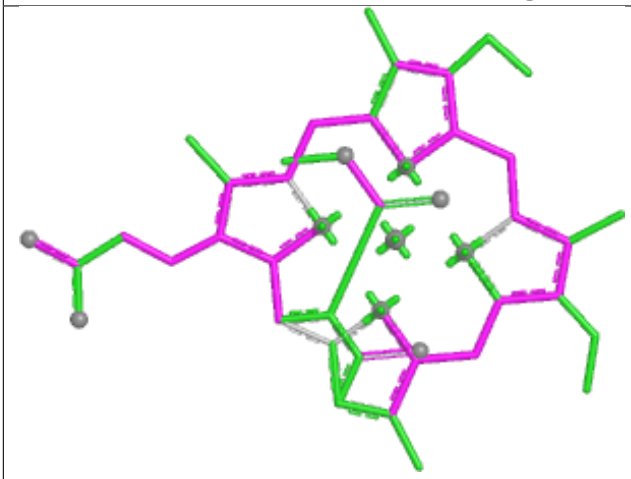


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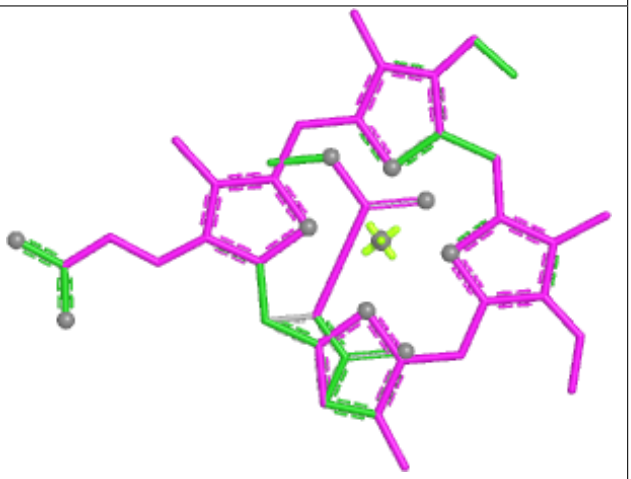


Rings

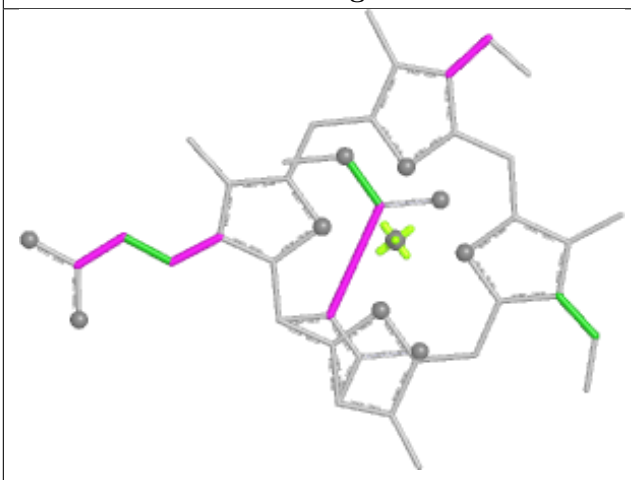
**Ligand KC1 41 207**



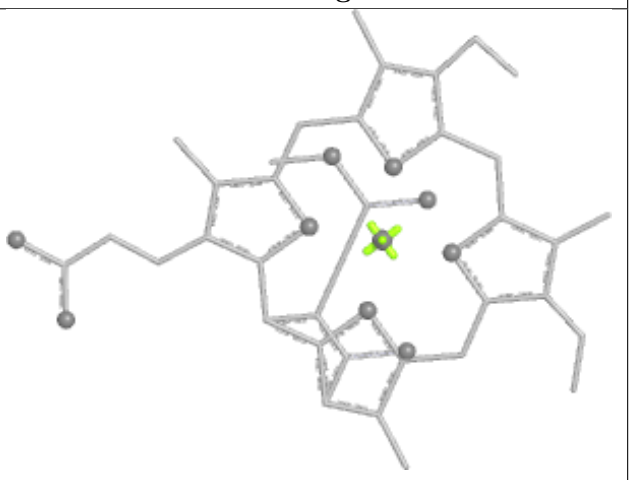
**Bond lengths**



**Bond angles**

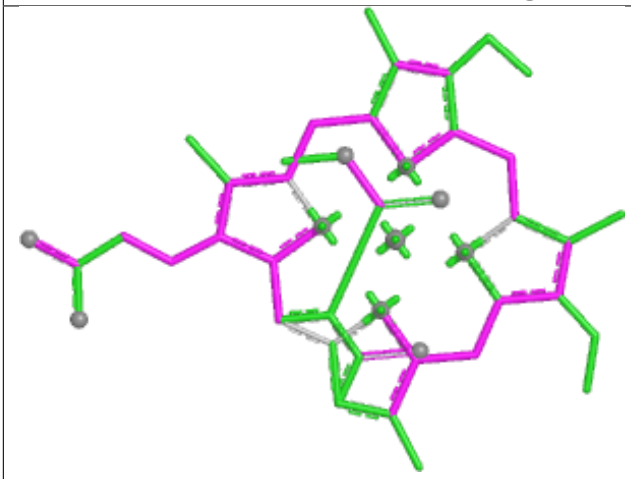


**Torsions**

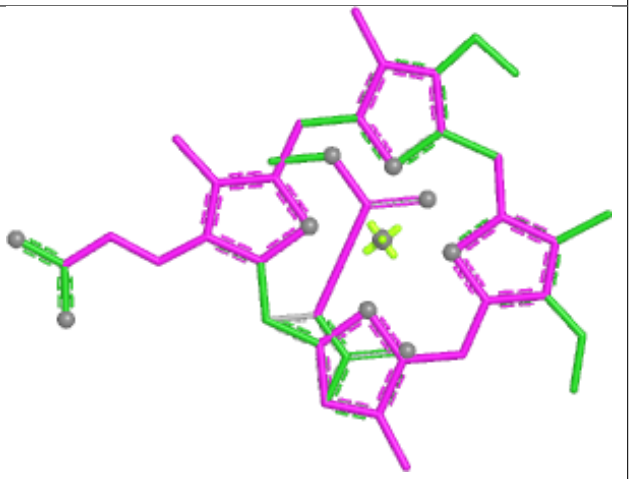


**Rings**

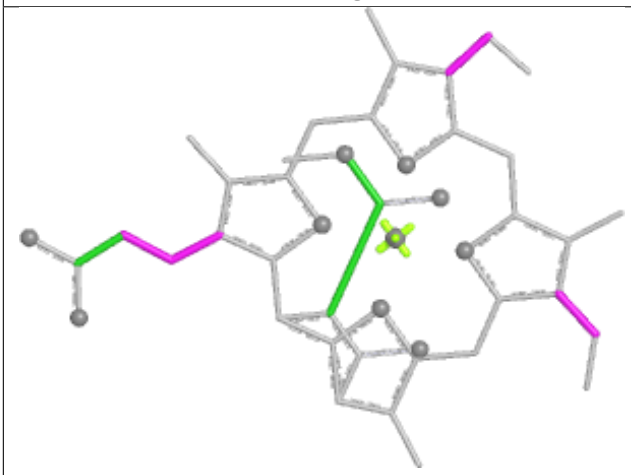
**Ligand KC1 14 304**



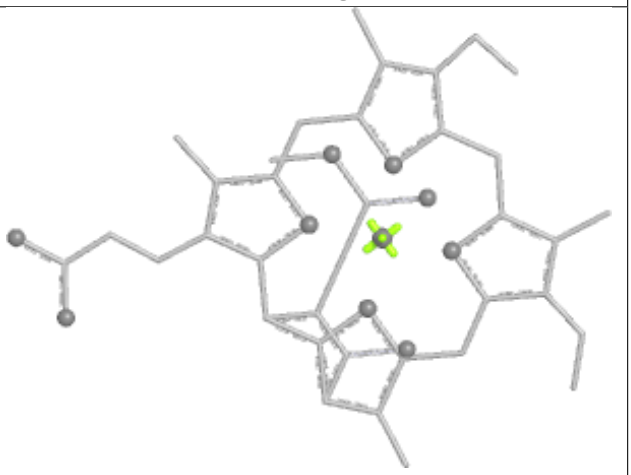
Bond lengths



Bond angles

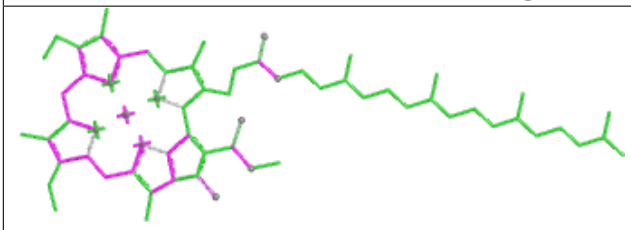


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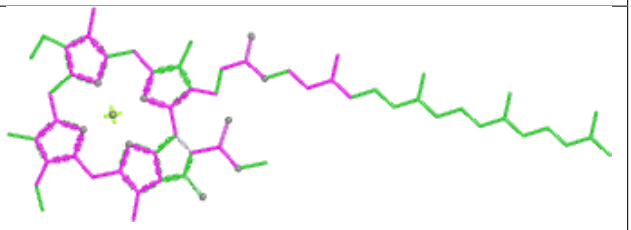


Rings

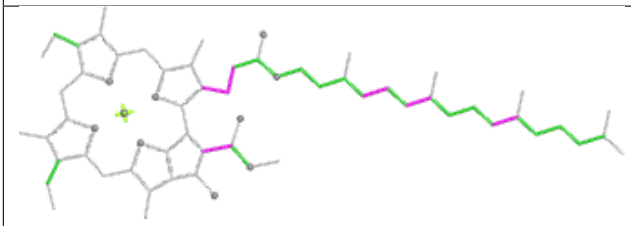
**Ligand CLA 32 205**



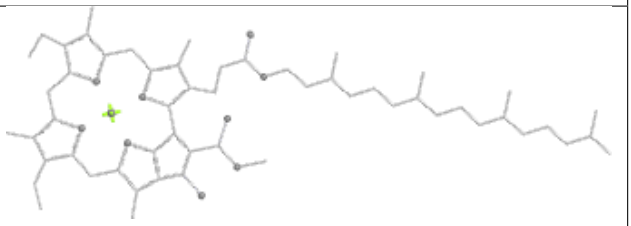
Bond lengths



Bond angles

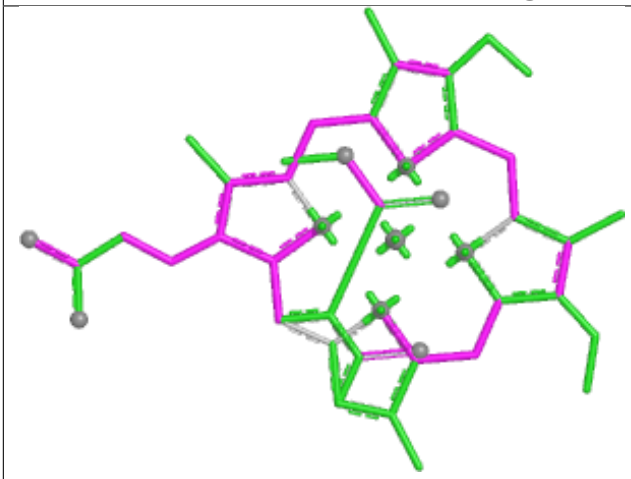


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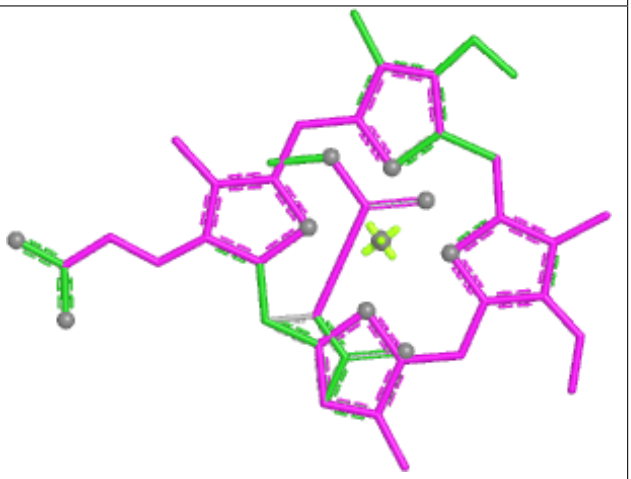


Rings

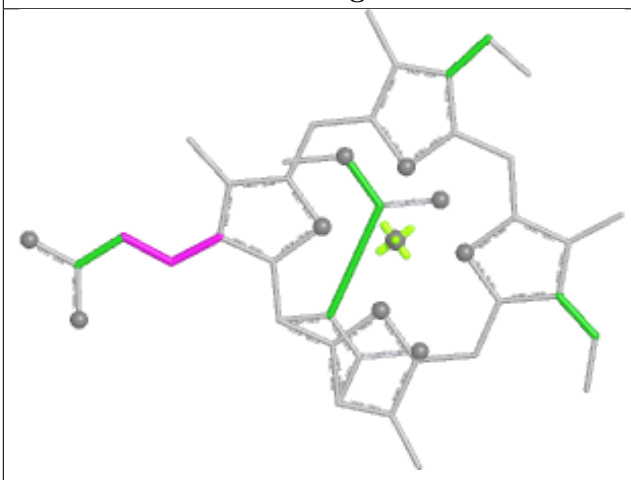
**Ligand KC1 31 303**



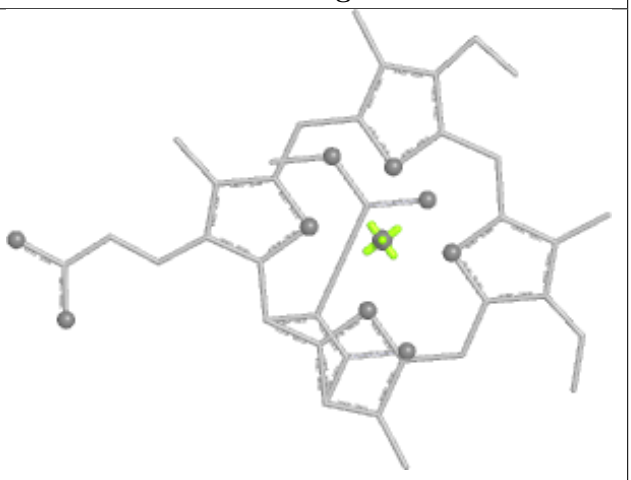
Bond lengths



Bond angles



Torsions

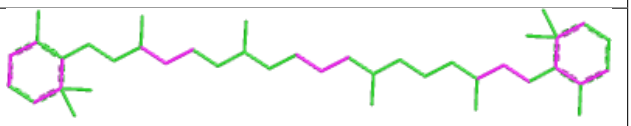


Rings

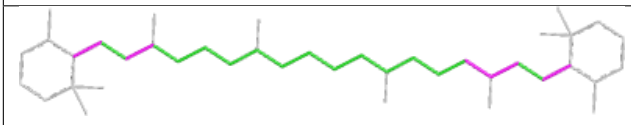
**Ligand BCR 5 101**



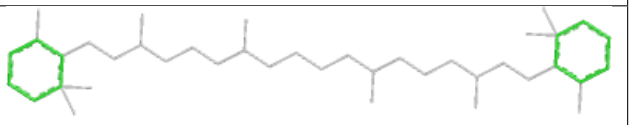
Bond lengths



Bond angles

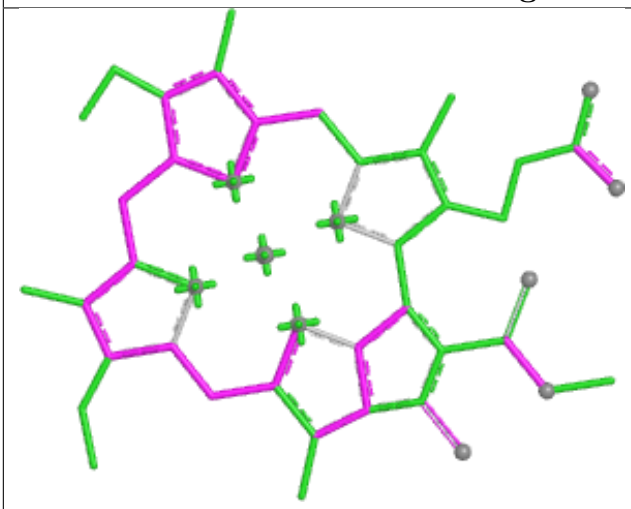


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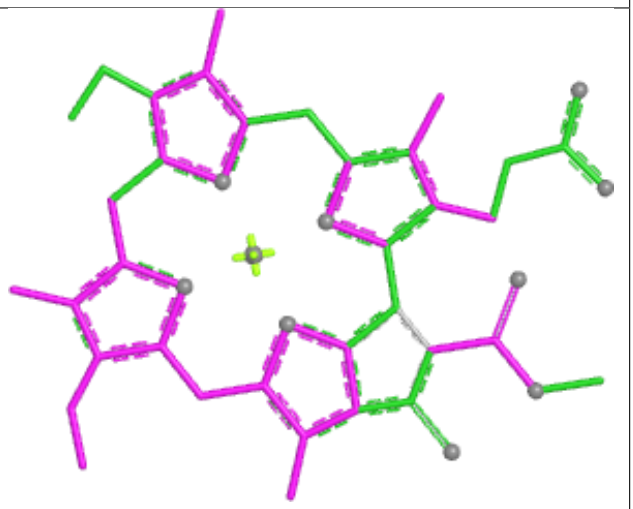


Rings

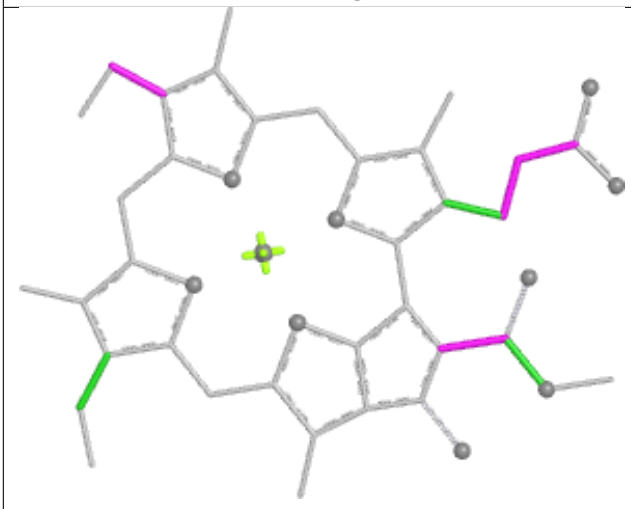
**Ligand CLA 38 206**



**Bond lengths**



**Bond angles**

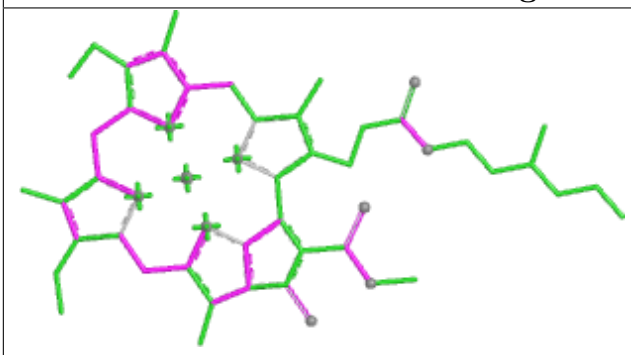


**Torsions**

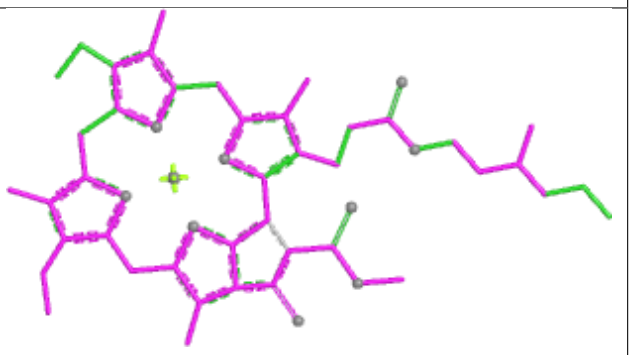


**Rings**

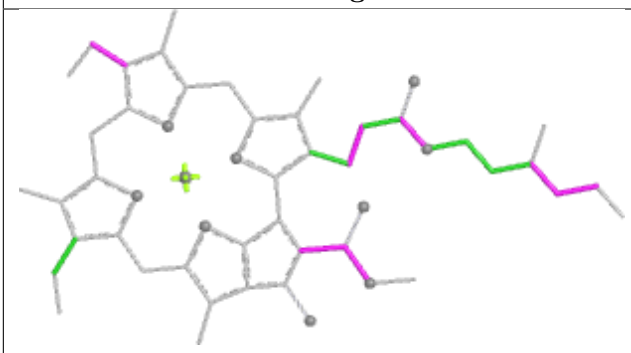
**Ligand CLA 13 307**



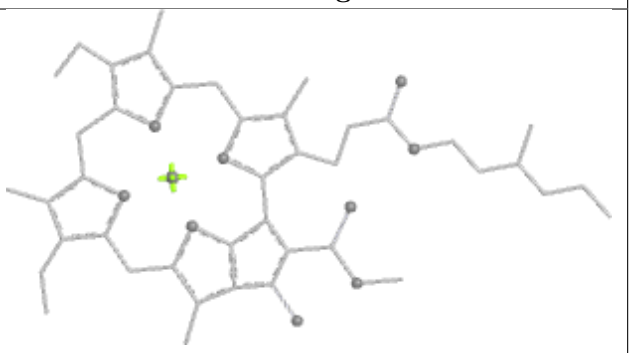
**Bond lengths**



**Bond angles**

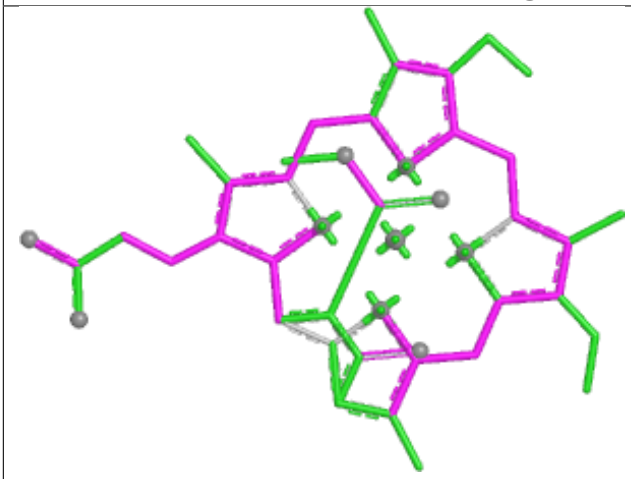


**Torsions**

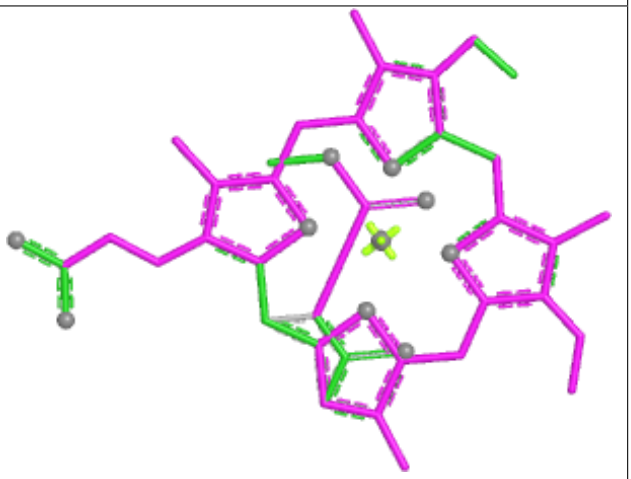


**Rings**

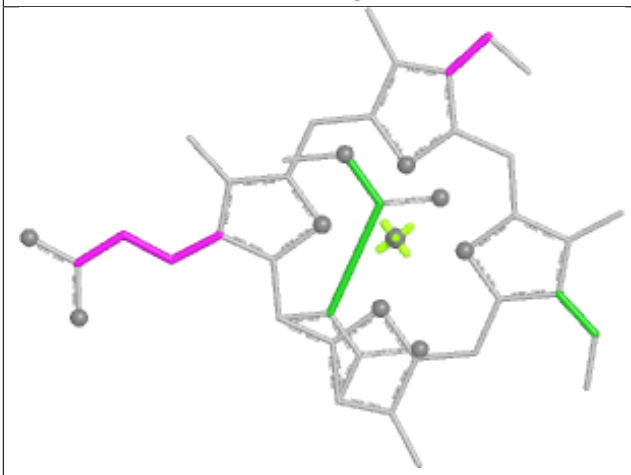
**Ligand KC1 13 302**



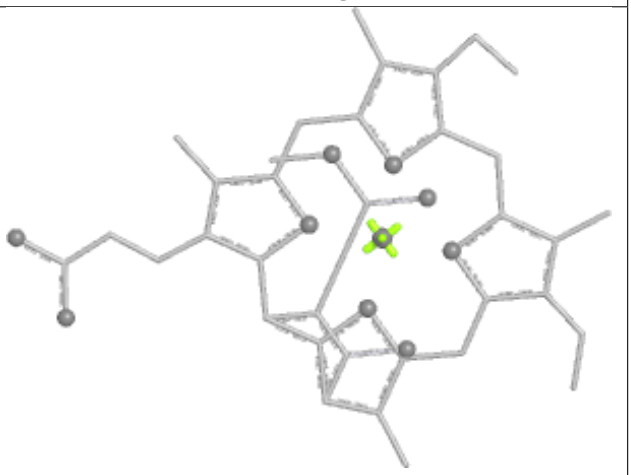
Bond lengths



Bond angles

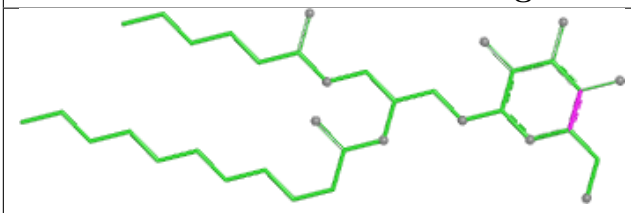


Torsions

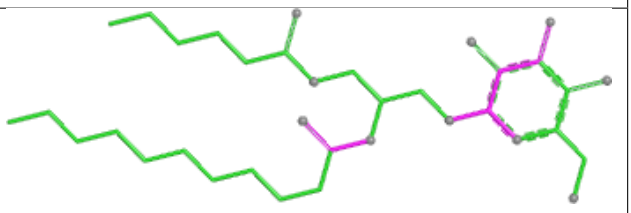


Rings

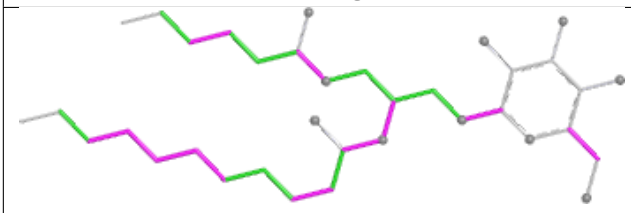
**Ligand LMG 16 316**



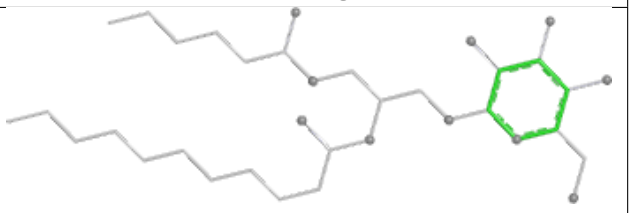
Bond lengths



Bond angles

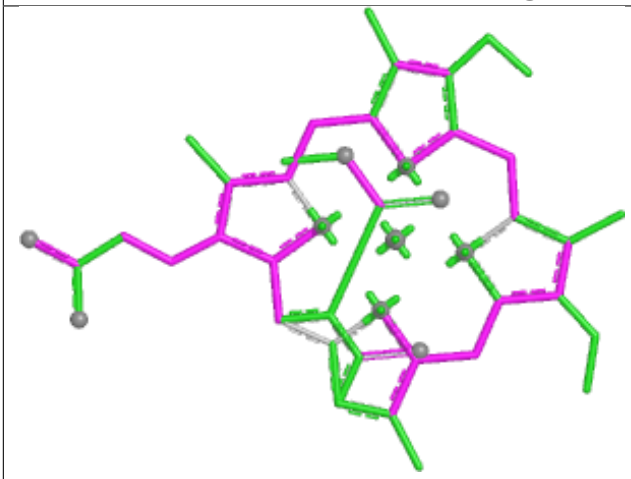


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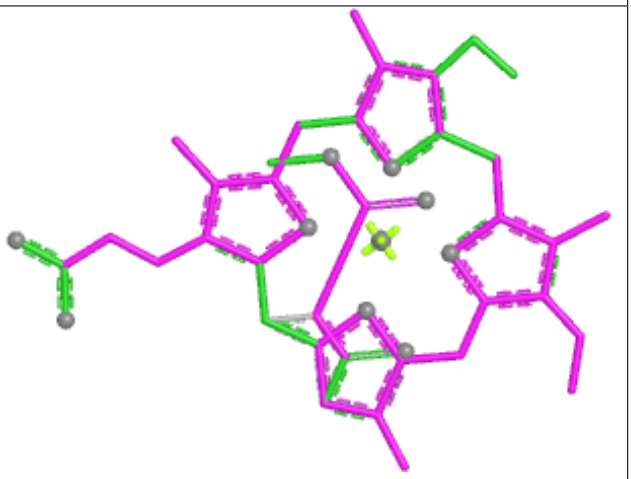


Rings

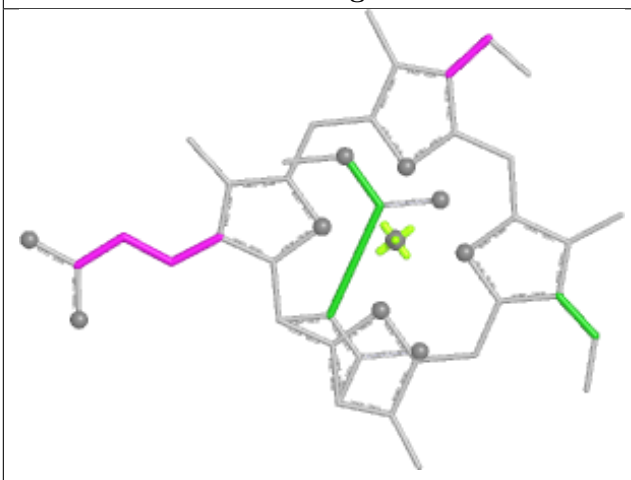
**Ligand KC1 35 302**



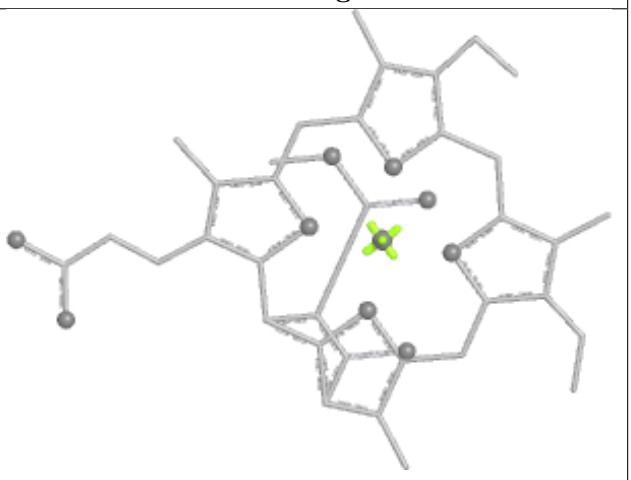
**Bond lengths**



**Bond angles**

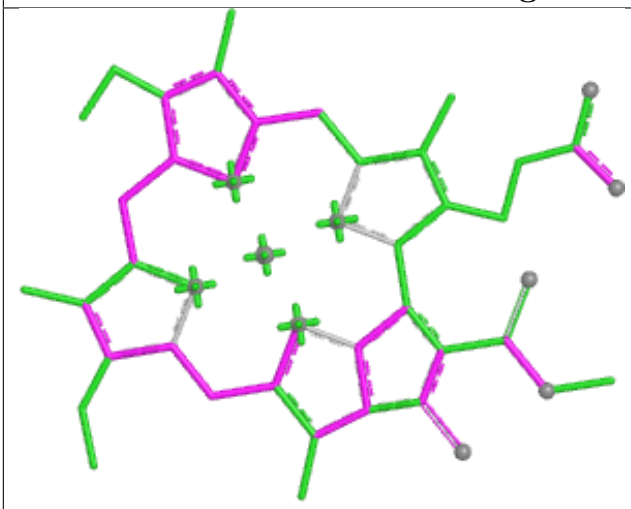


**Torsions**

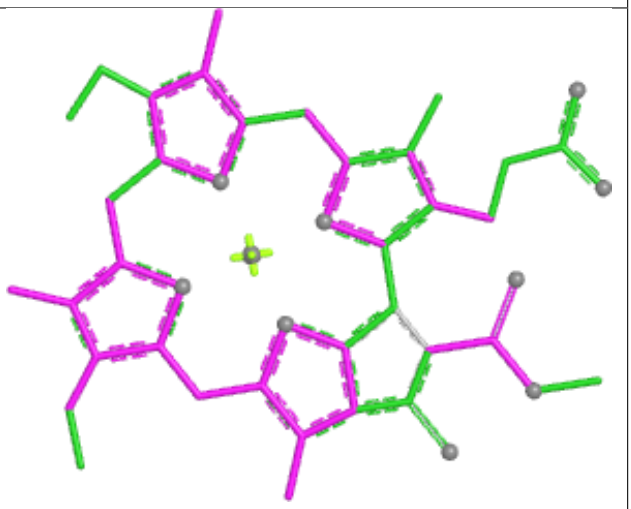


**Rings**

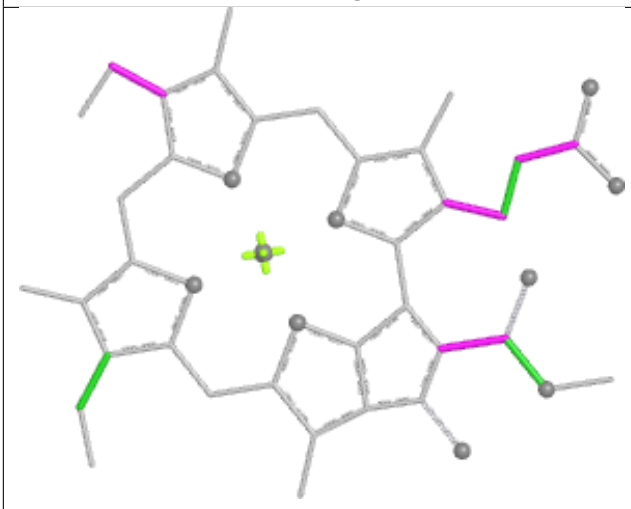
**Ligand CLA 19 304**



**Bond lengths**



**Bond angles**

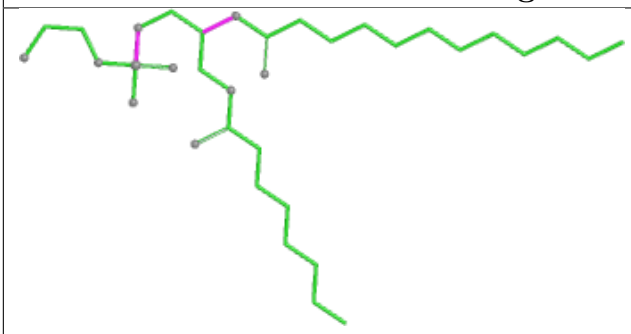


**Torsions**

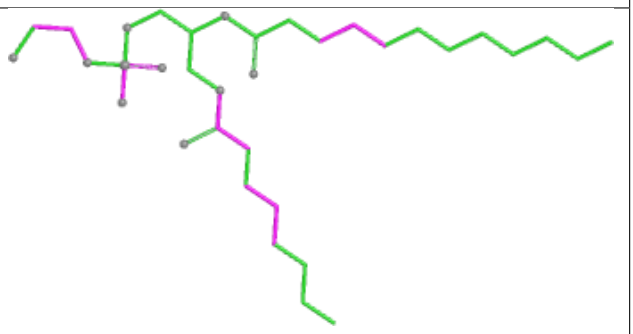


**Rings**

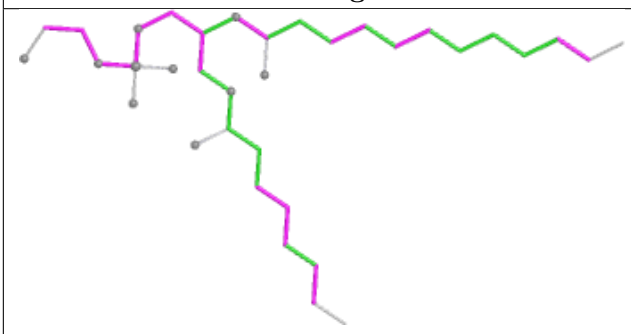
## Ligand LHG 21 201



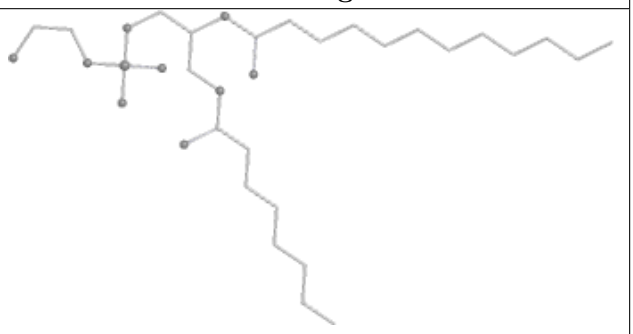
Bond lengths



Bond angles

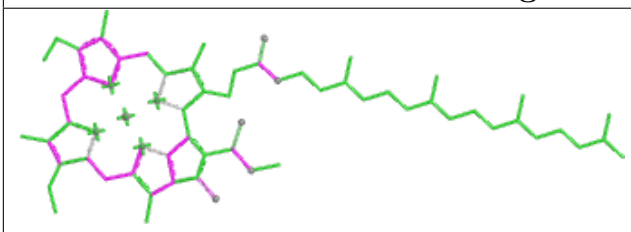


Torsions

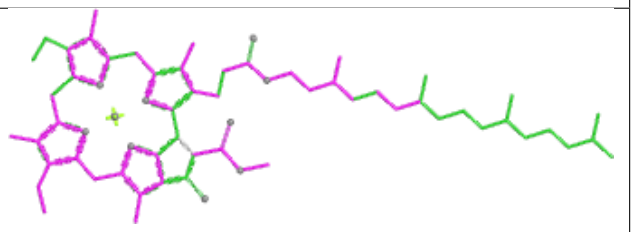


Rings

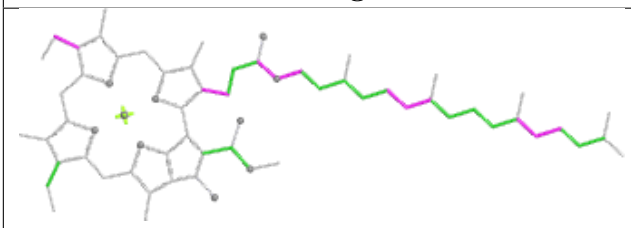
## Ligand CLA 14 308



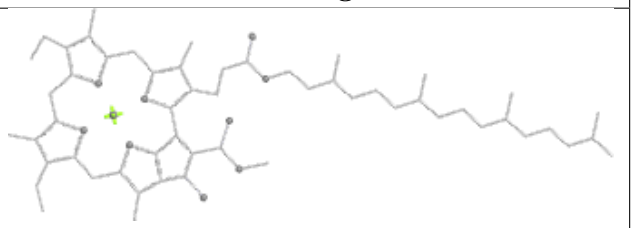
Bond lengths



Bond angles

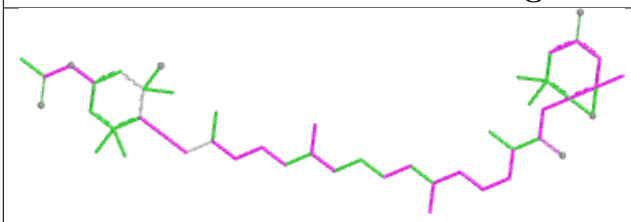


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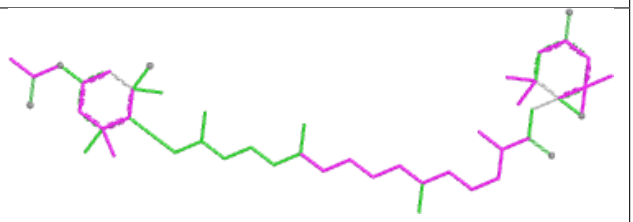


Rings

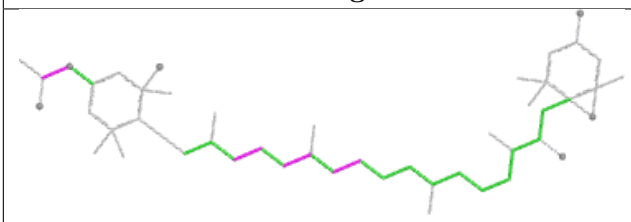
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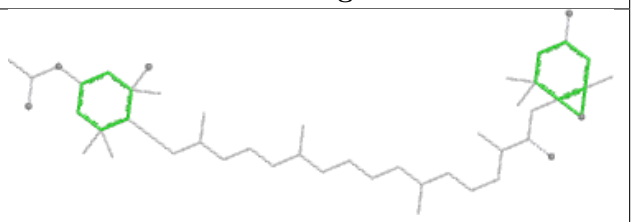
Bond lengths



Bond angles

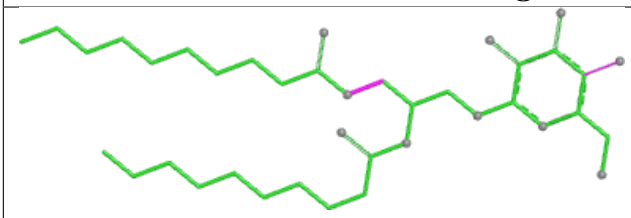


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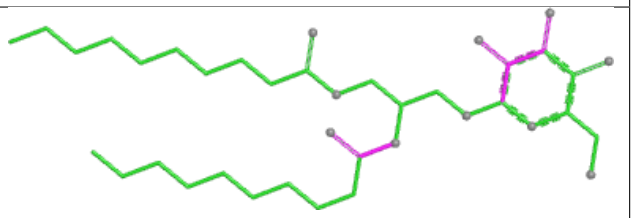


Rings

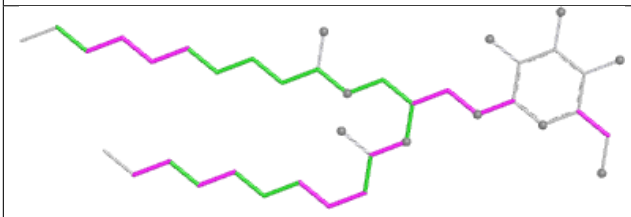
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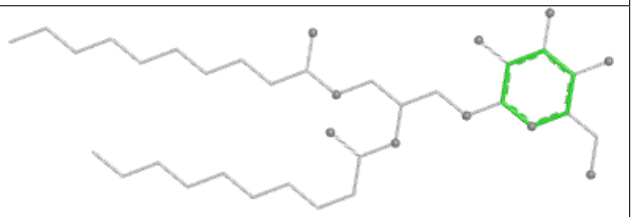
Bond lengths



Bond angles

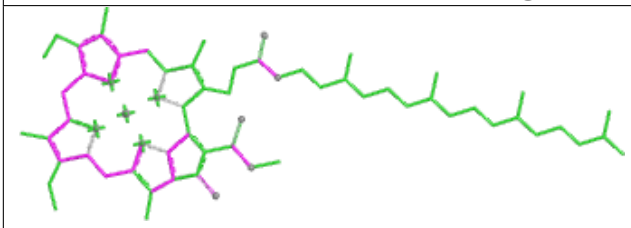


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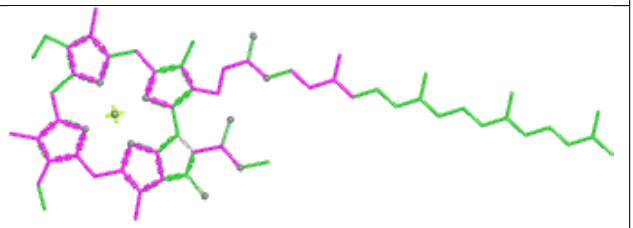


Rings

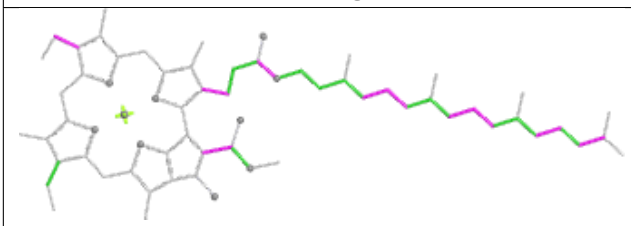
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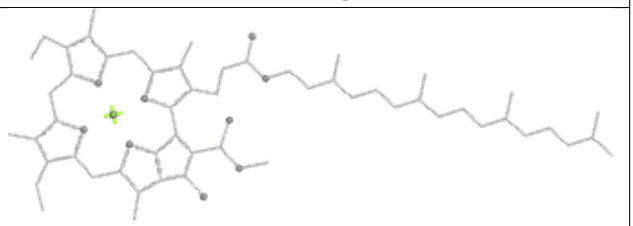
Bond lengths



Bond angles

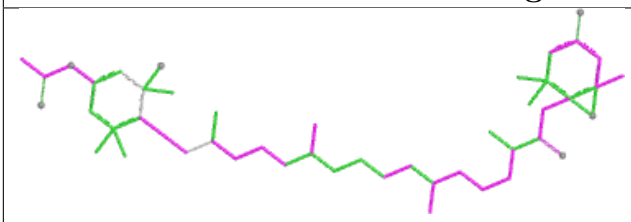


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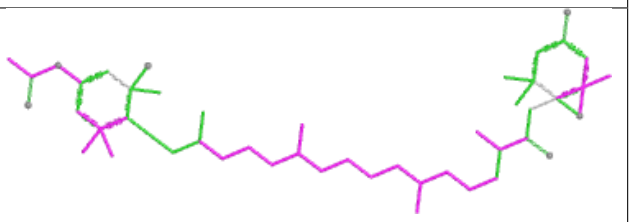


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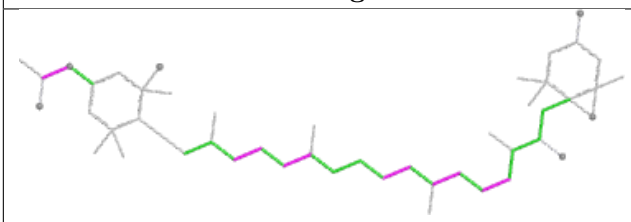
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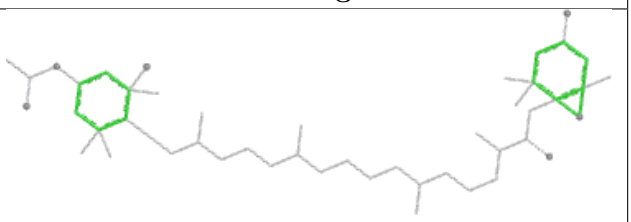
Bond lengths



Bond angles

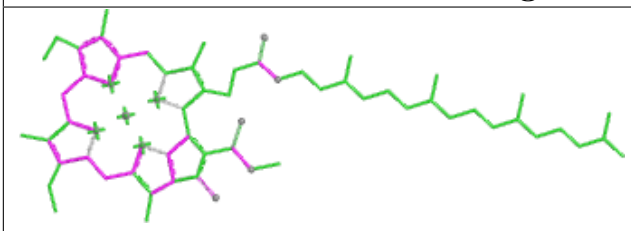


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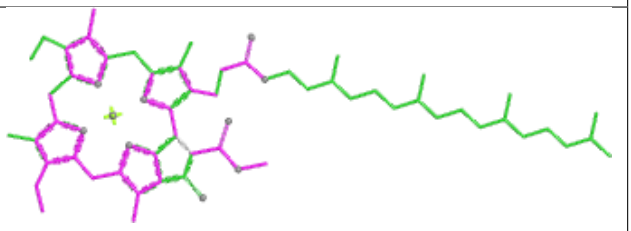


Rings

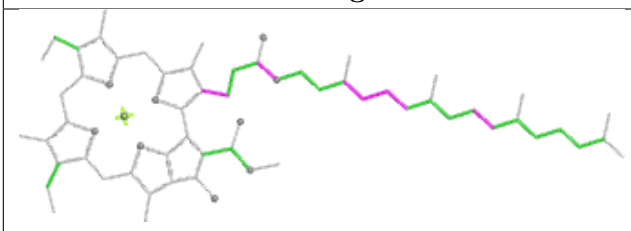
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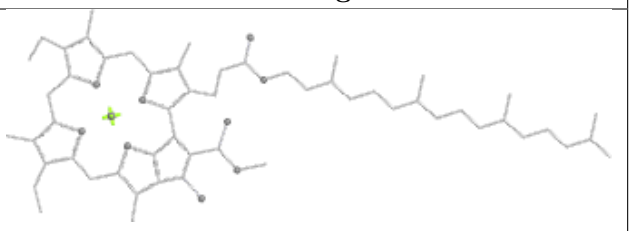
Bond lengths



Bond angles

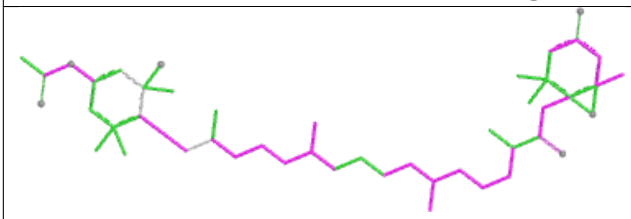


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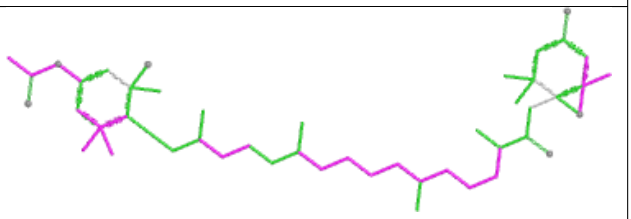


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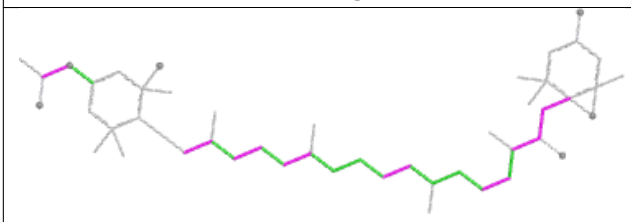
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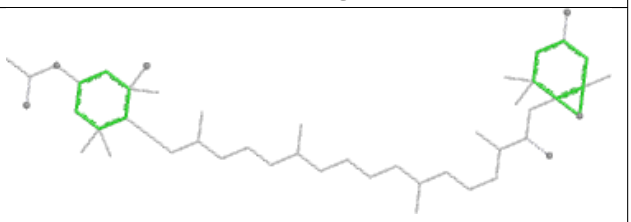
Bond lengths



Bond angles

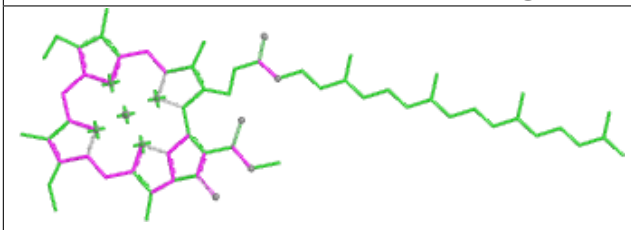


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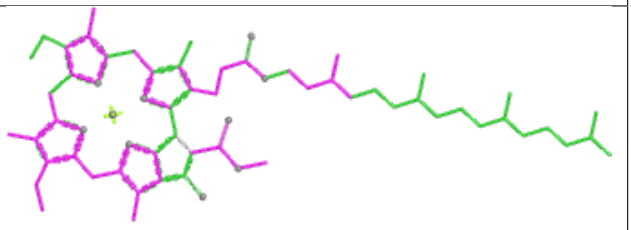


Rings

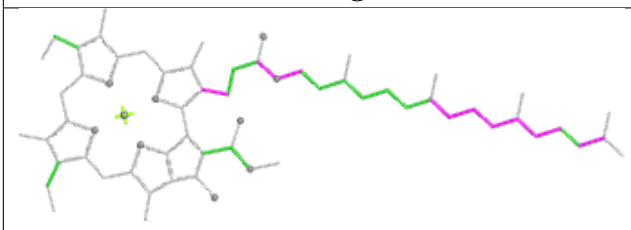
## Ligand CLA 32 202



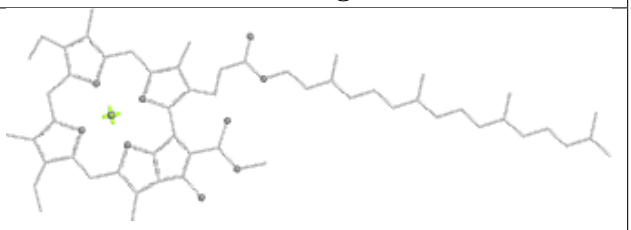
Bond lengths



Bond angles

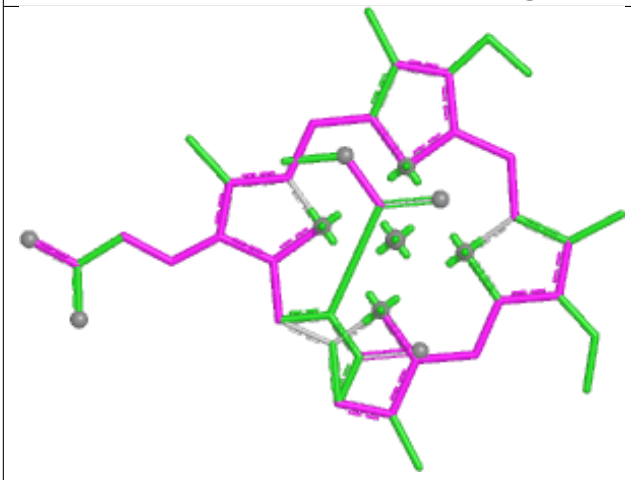


Torsions

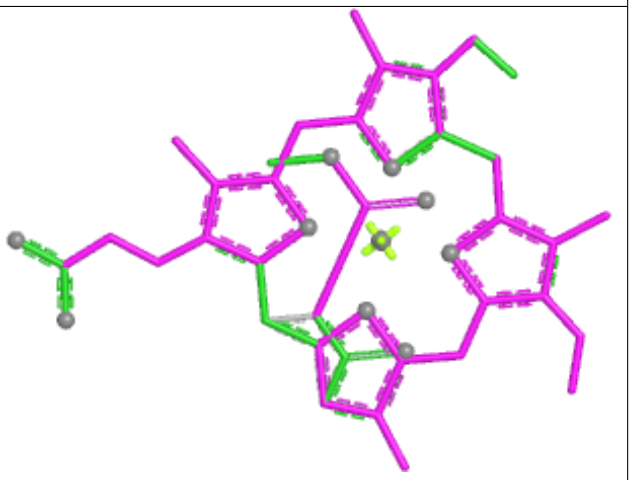


Rings

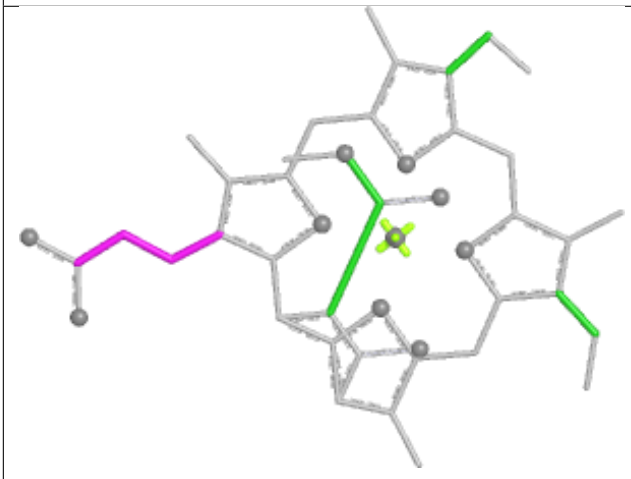
## Ligand KC1 33 309



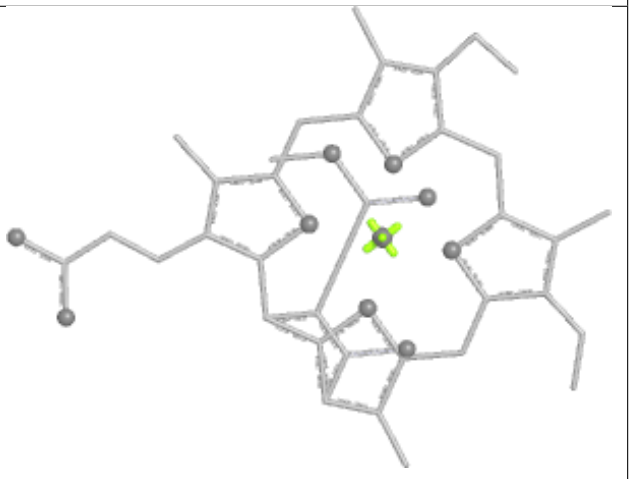
Bond lengths



Bond angles

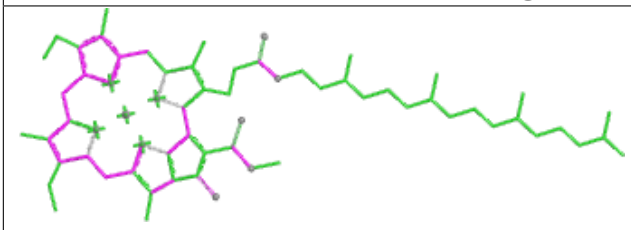


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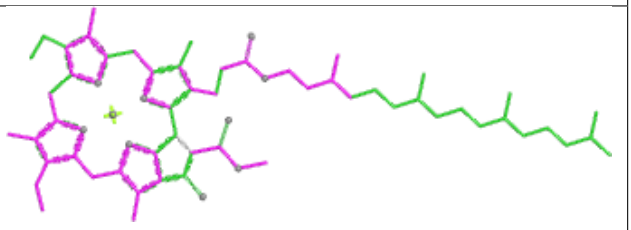


Rings

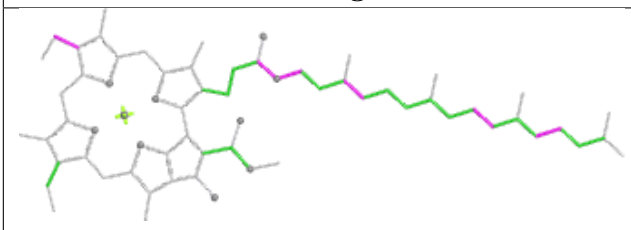
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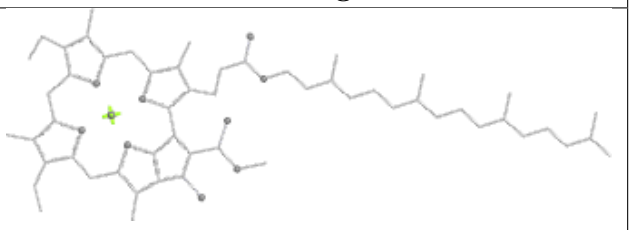
Bond lengths



Bond angles

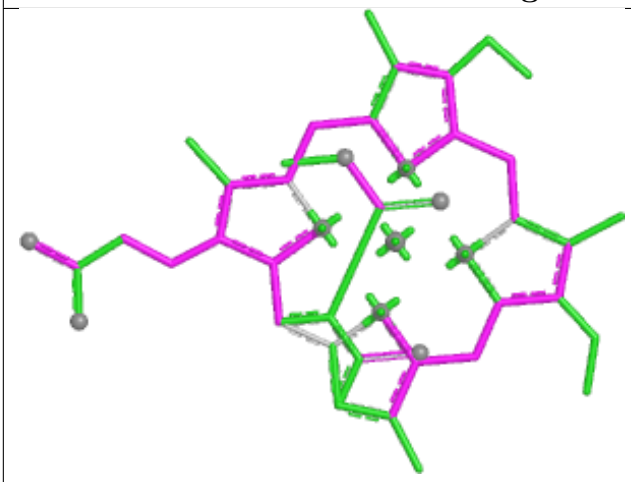


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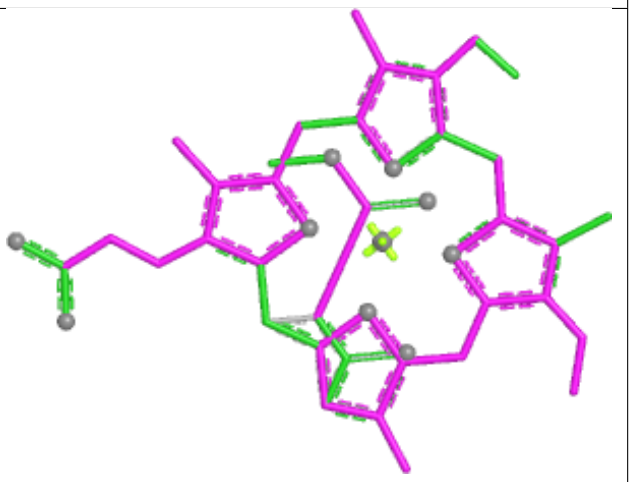


Rings

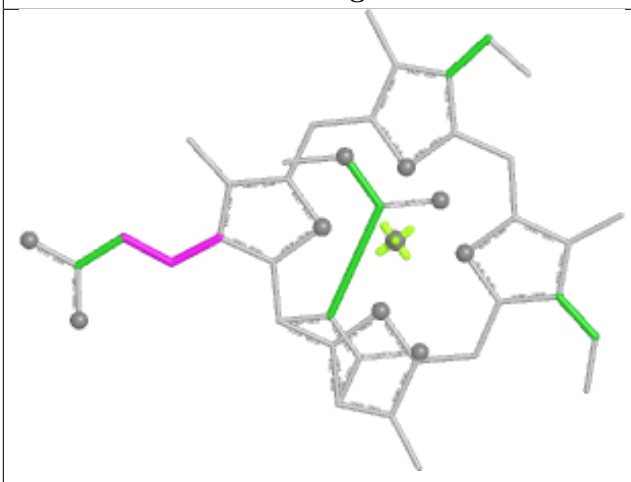
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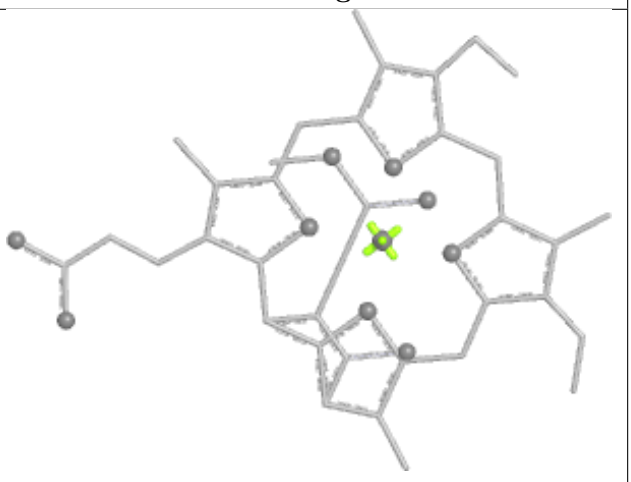
Bond lengths



Bond angles

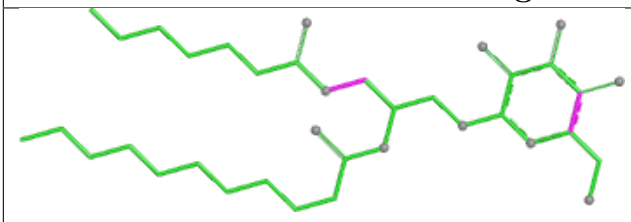


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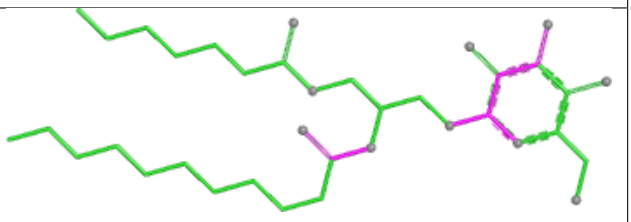


Rings

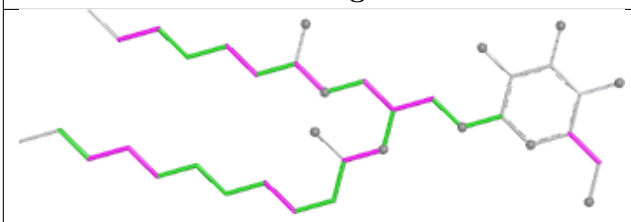
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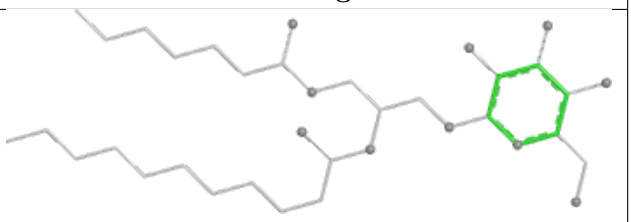
Bond lengths



Bond angles

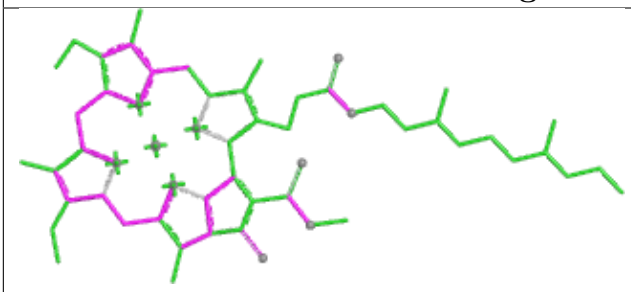


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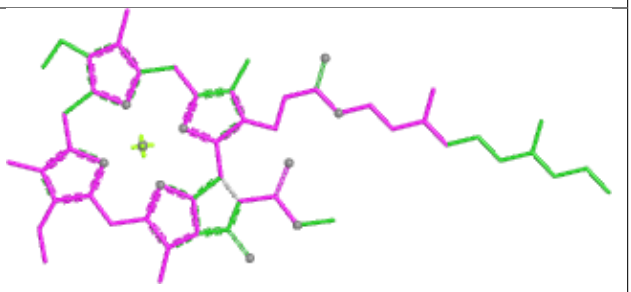


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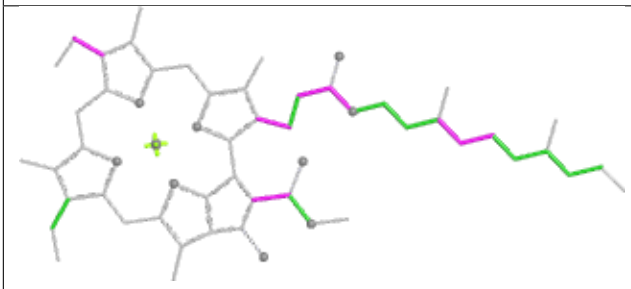
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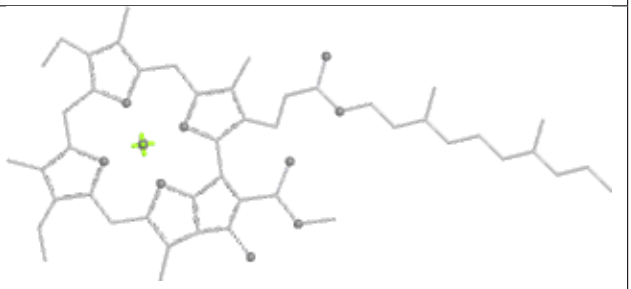
Bond lengths



Bond angles



Torsions



Rings

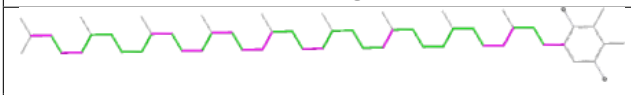
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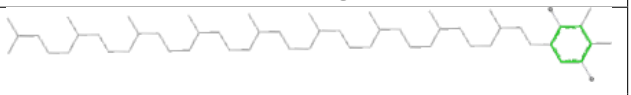
Bond lengths



Bond angles

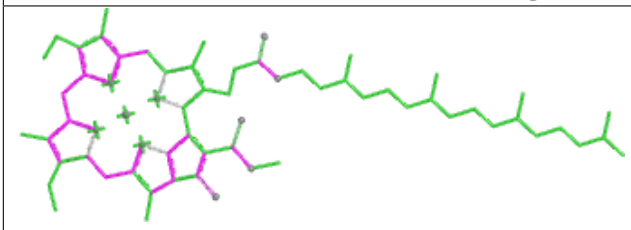


Torsions

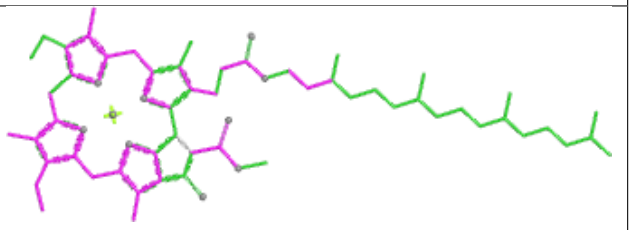


Rings

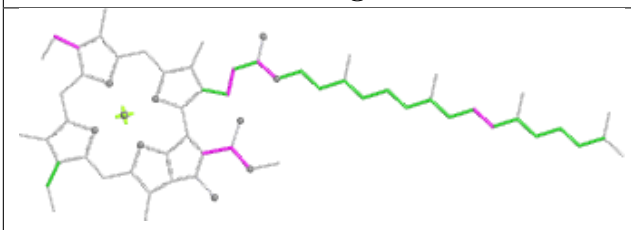
**Ligand CLA C 513**



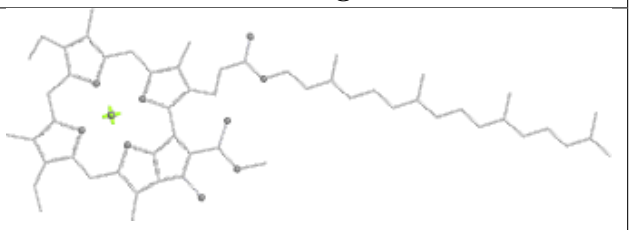
Bond lengths



Bond angles

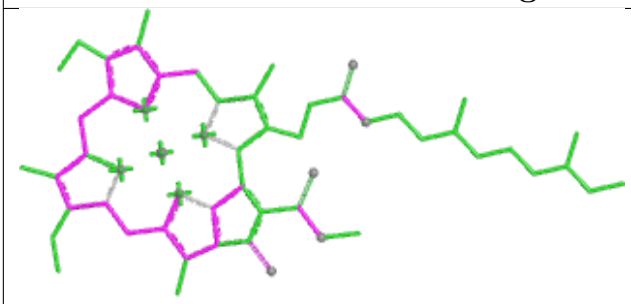


Torsions

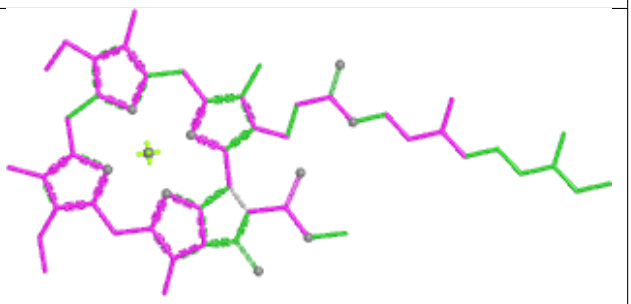


Rings

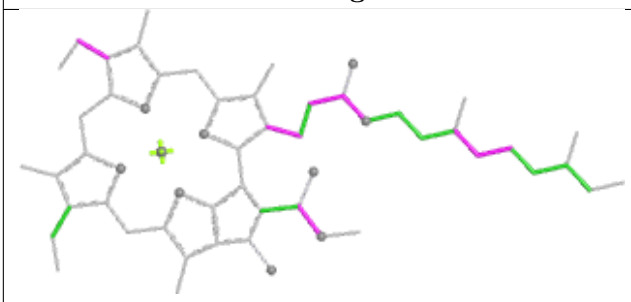
**Ligand CLA 40 203**



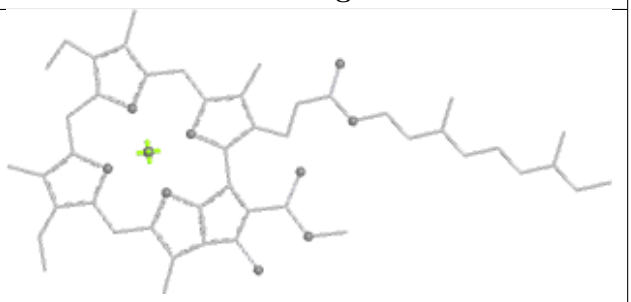
Bond lengths



Bond angles

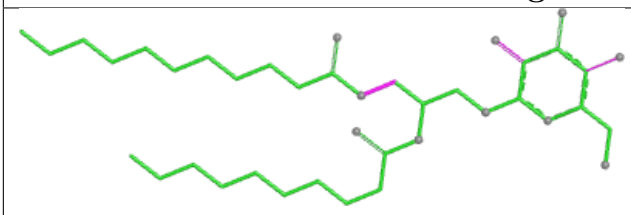


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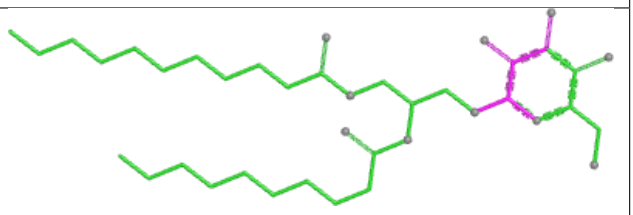


Rings

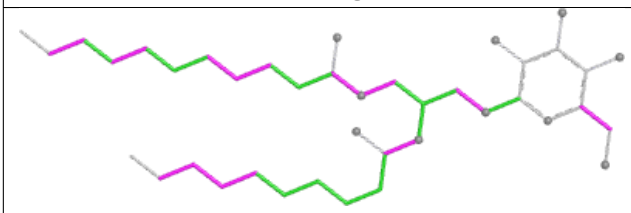
## Ligand LMG l 101



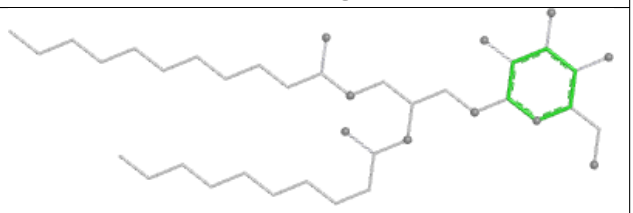
Bond lengths



Bond angles

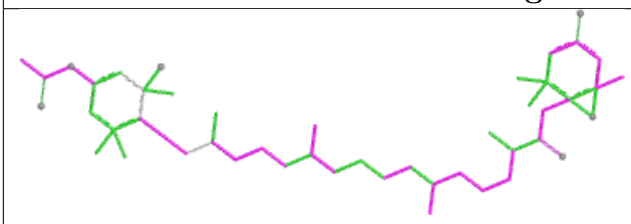


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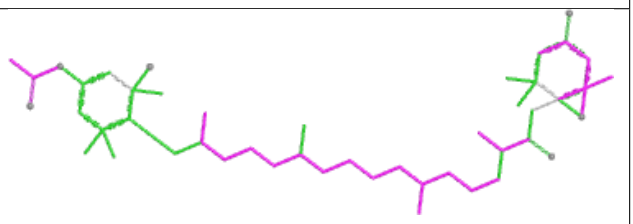


Rings

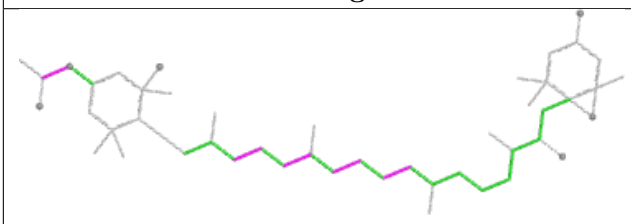
## Ligand A86 11 319



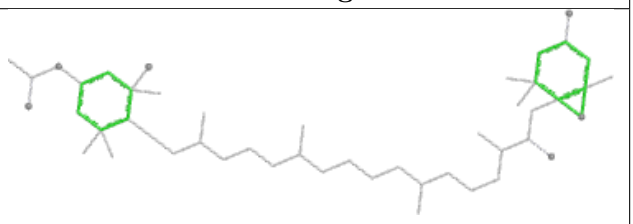
Bond lengths



Bond angles

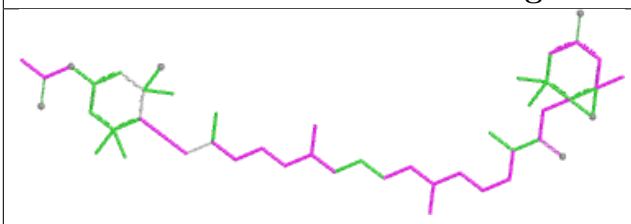


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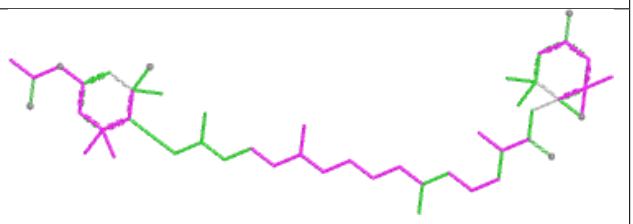


Rings

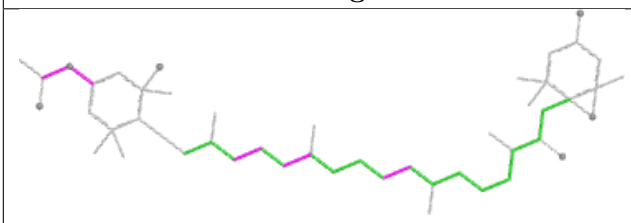
## Ligand A86 37 311



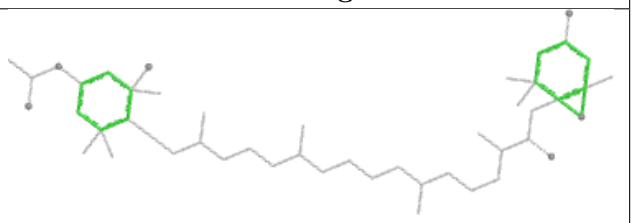
Bond lengths



Bond angles

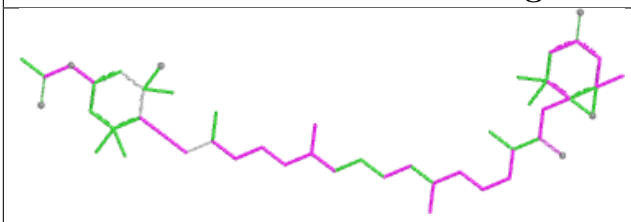


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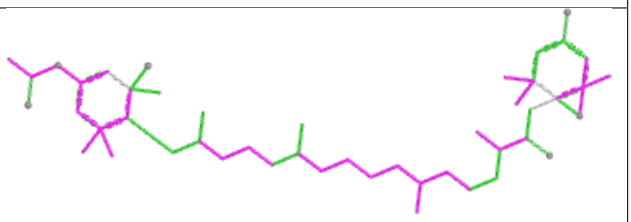


Rings

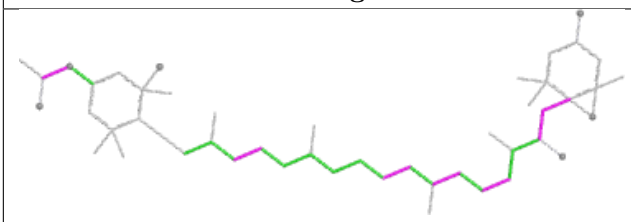
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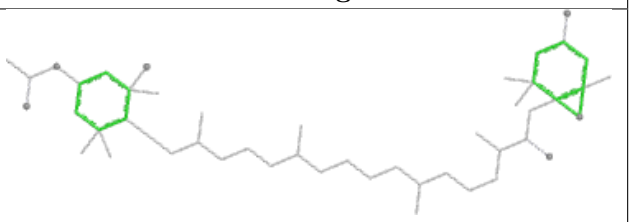
Bond lengths



Bond angles

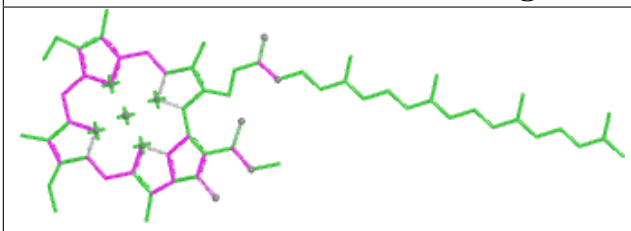


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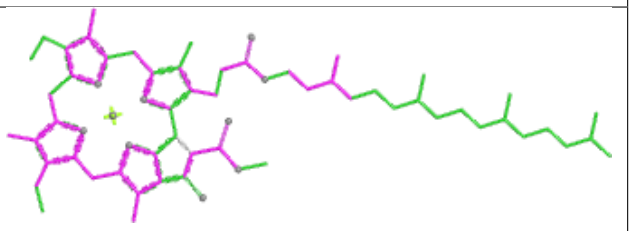


Rings

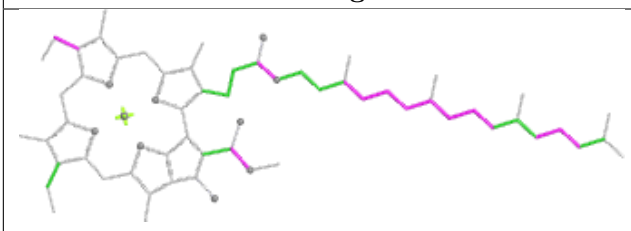
## Ligand CLA W 101



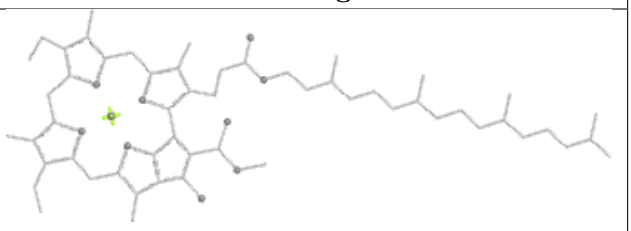
Bond lengths



Bond angles

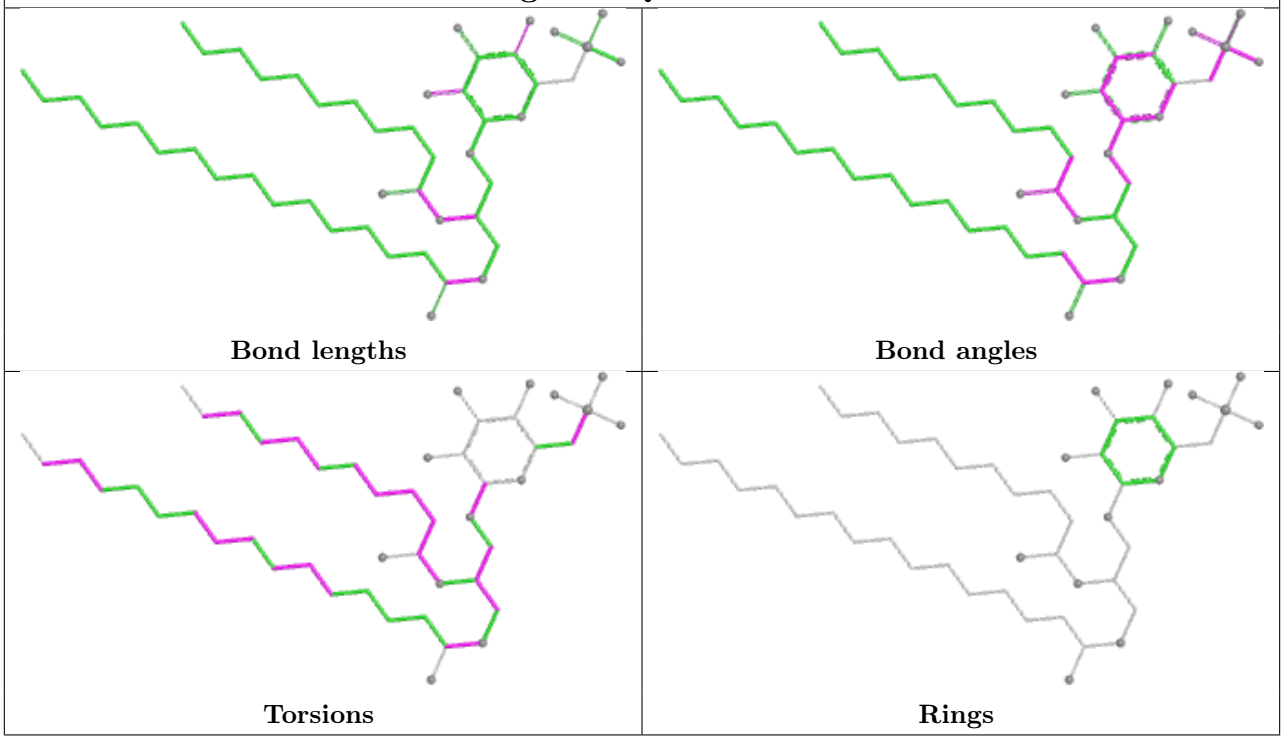


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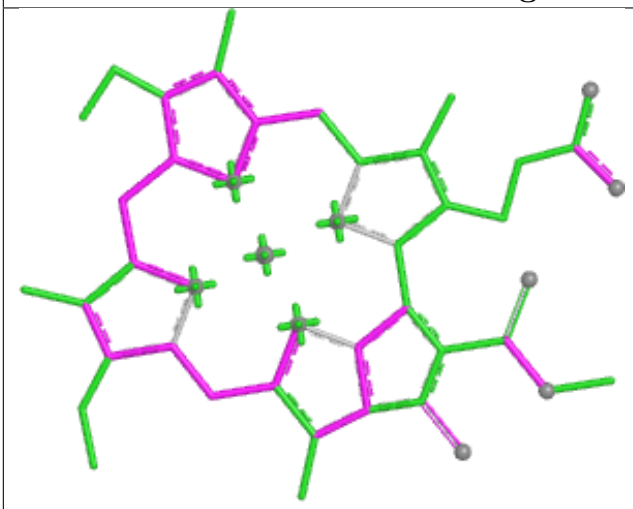


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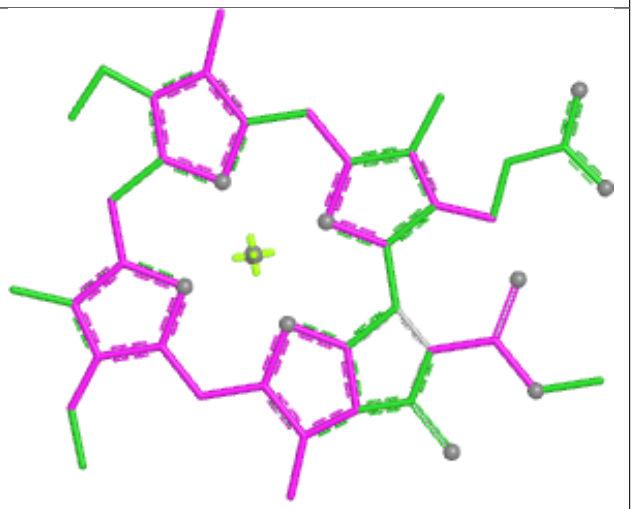
**Ligand SQD 17 301**



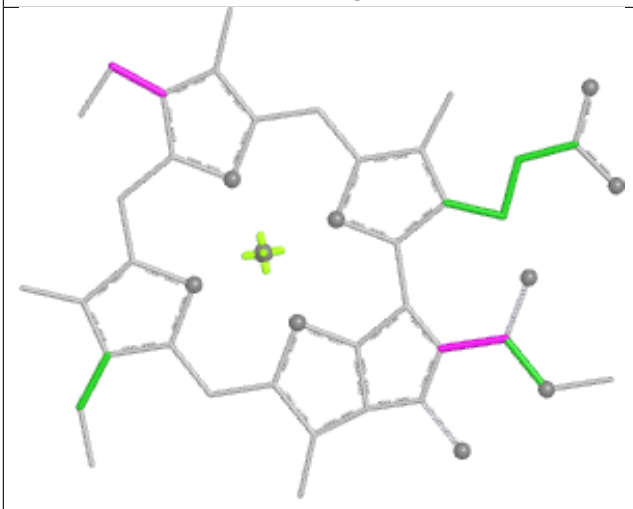
## Ligand CLA 18 211



Bond lengths



Bond angles

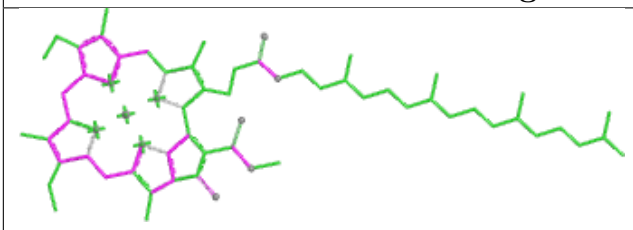


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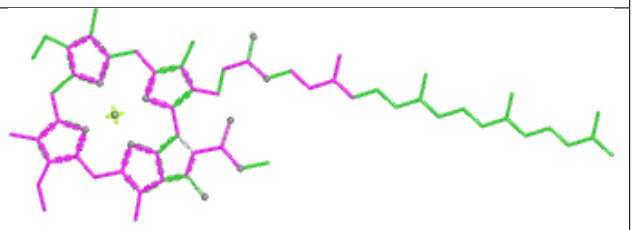


Rings

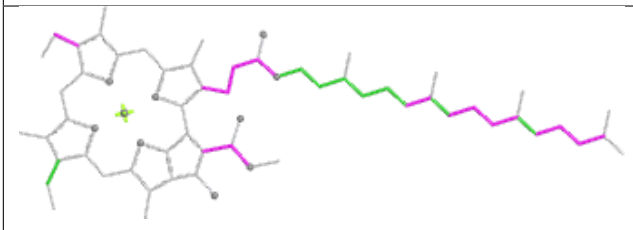
## Ligand CLA 31 301



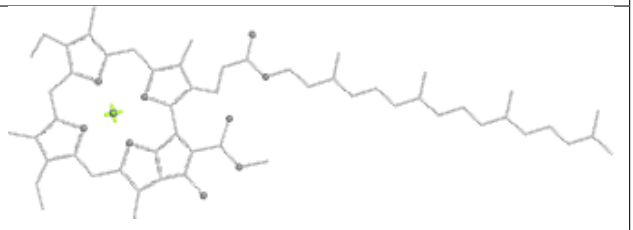
Bond lengths



Bond angles

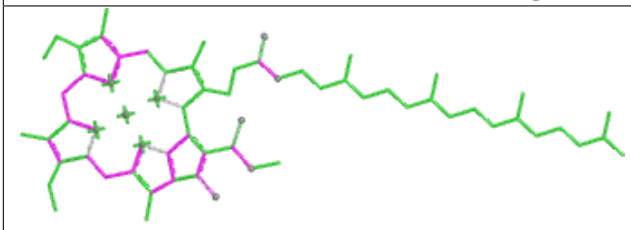


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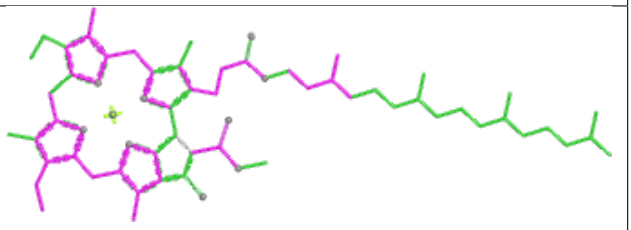


Rings

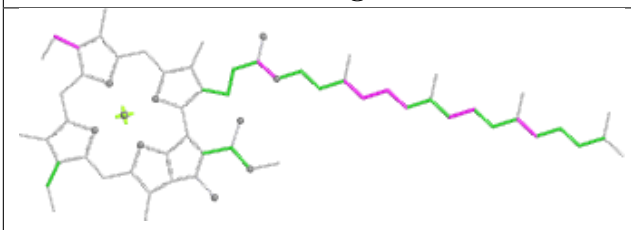
**Ligand CLA b 502**



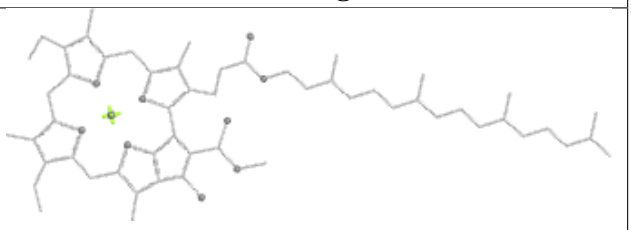
Bond lengths



Bond angles

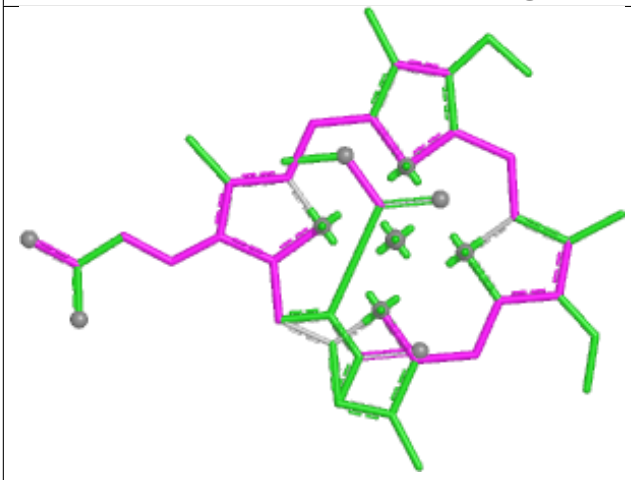


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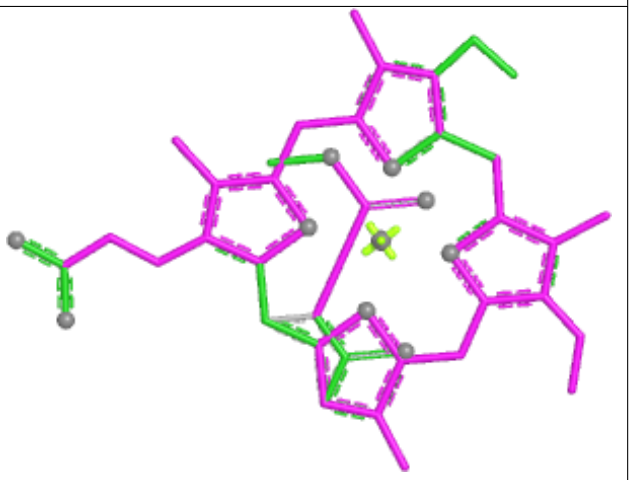


Rings

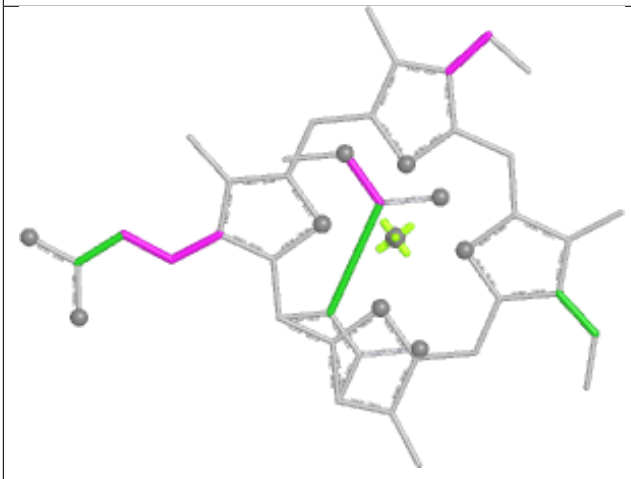
**Ligand KC1 33 306**



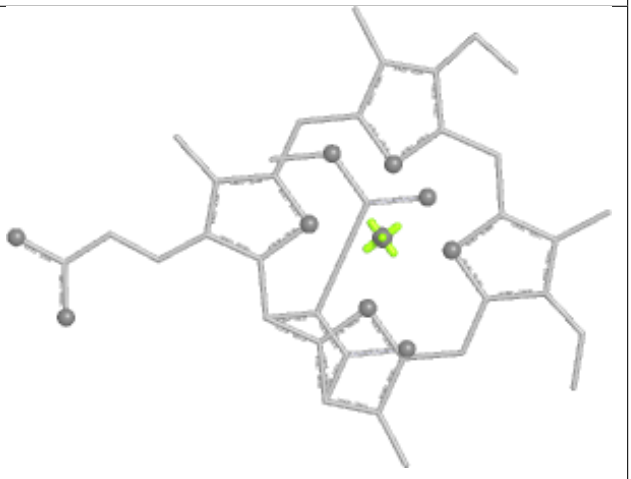
Bond lengths



Bond angles

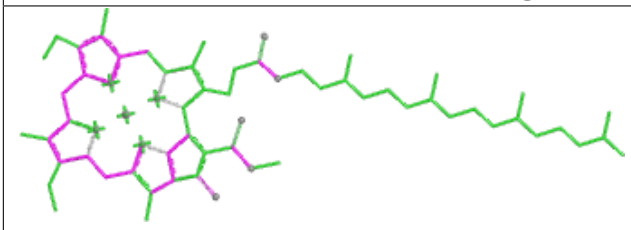


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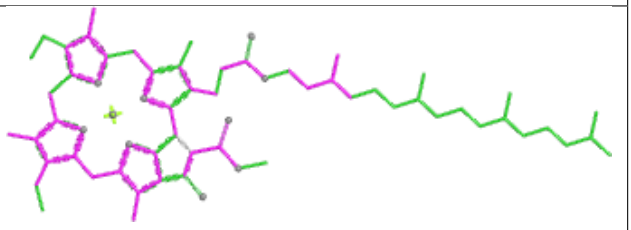


Rings

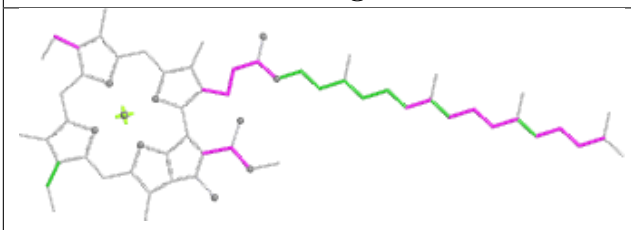
## Ligand CLA W 102



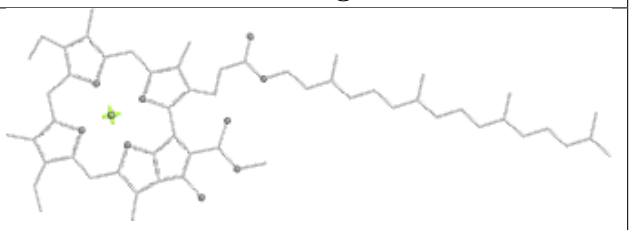
Bond lengths



Bond angles

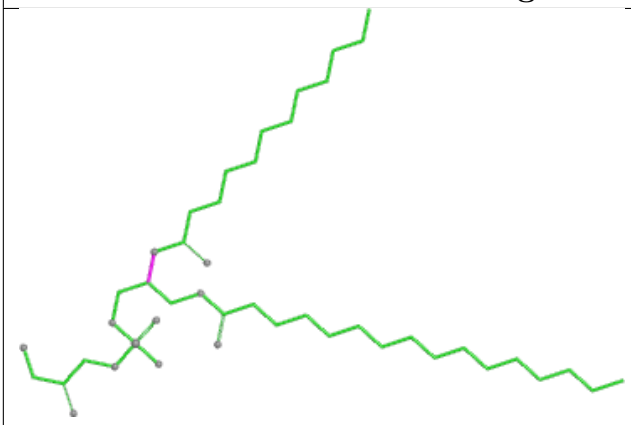


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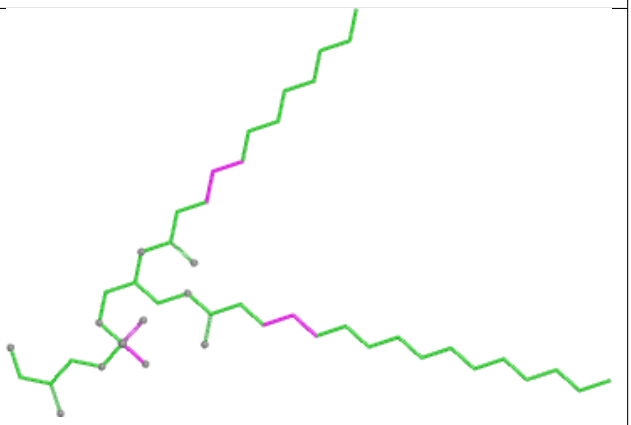


Rings

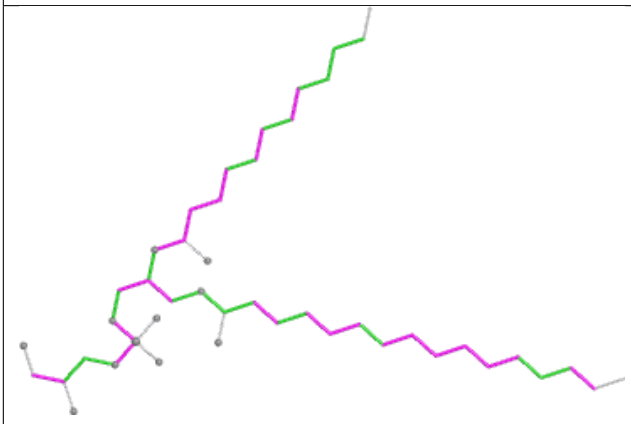
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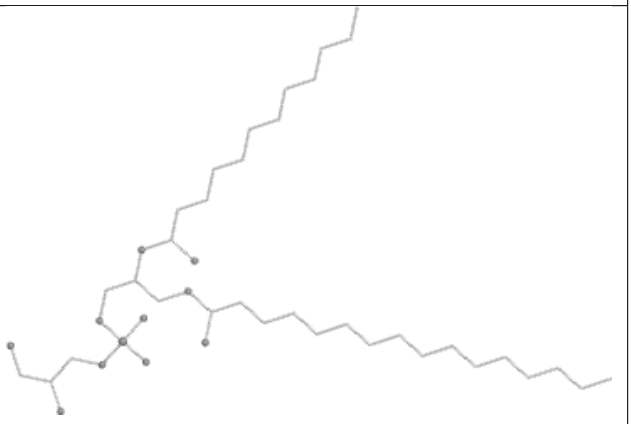
Bond lengths



Bond angles

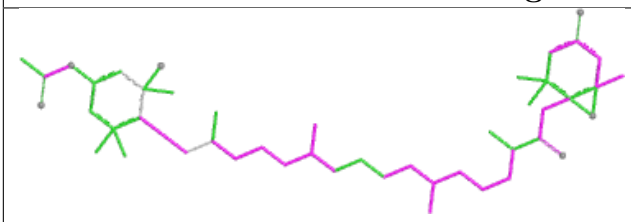


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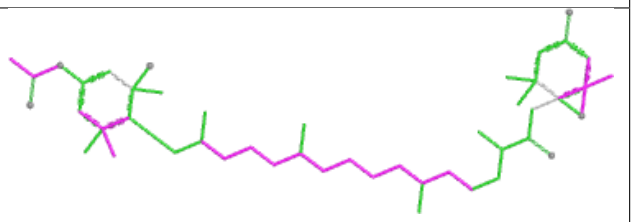


Rings

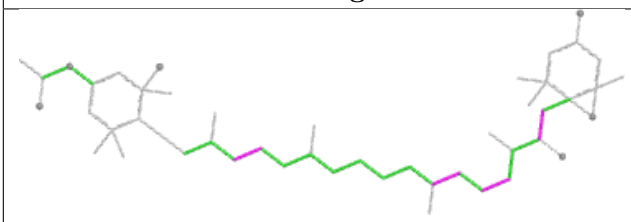
**Ligand A86 20 309**



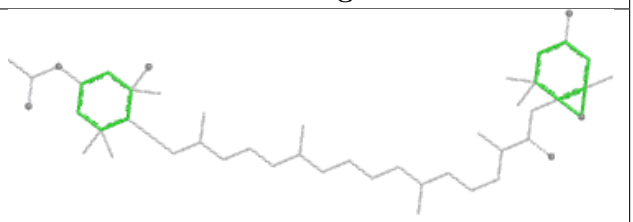
Bond lengths



Bond angles

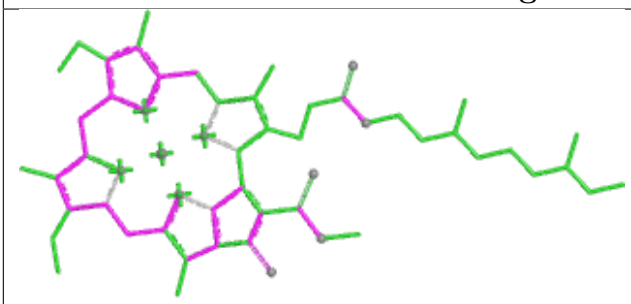


Torsions

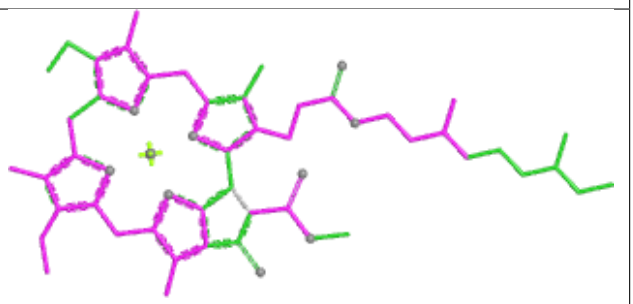


Rings

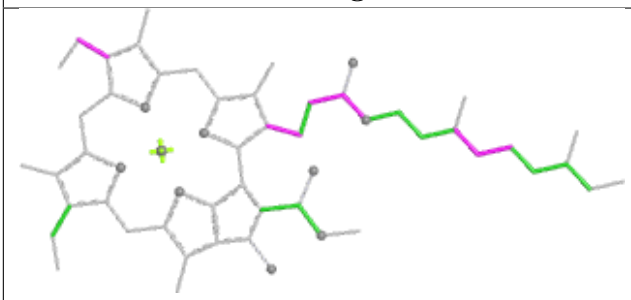
**Ligand CLA 18 204**



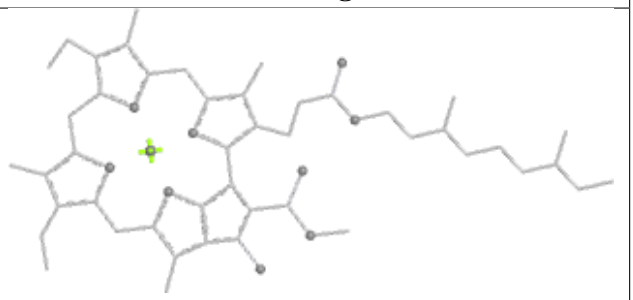
Bond lengths



Bond angles

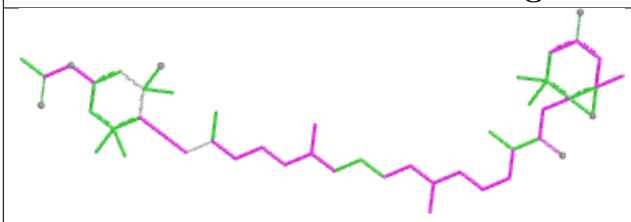


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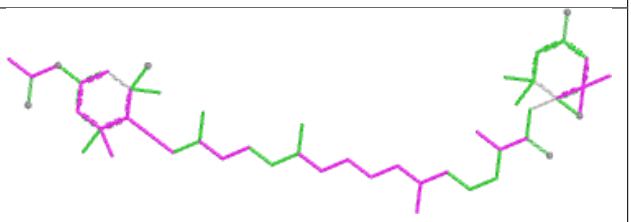


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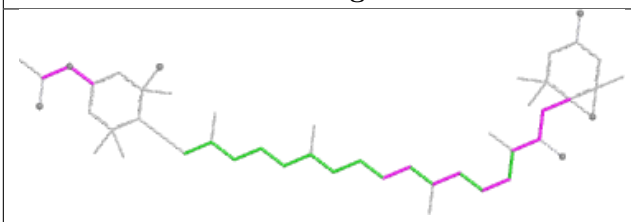
## Ligand A86 38 215



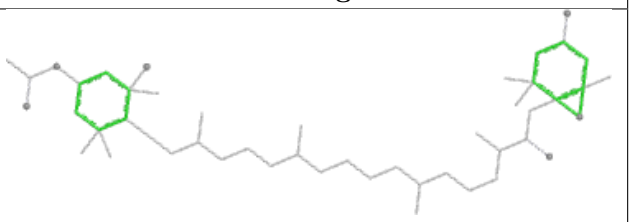
Bond lengths



Bond angles

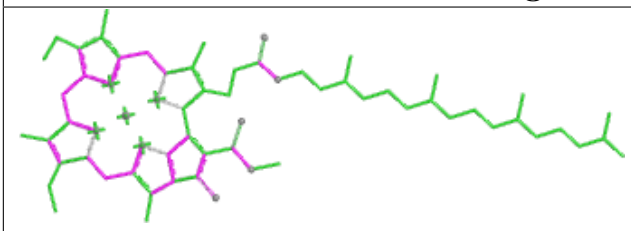


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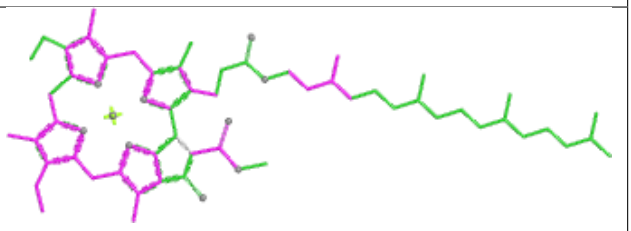


Rings

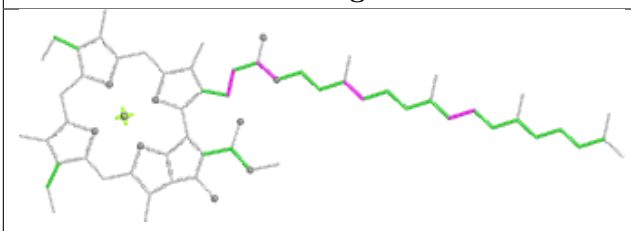
## Ligand CLA B 505



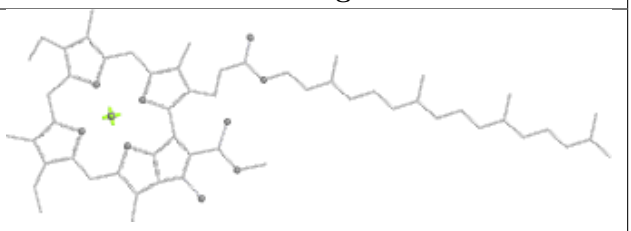
Bond lengths



Bond angles

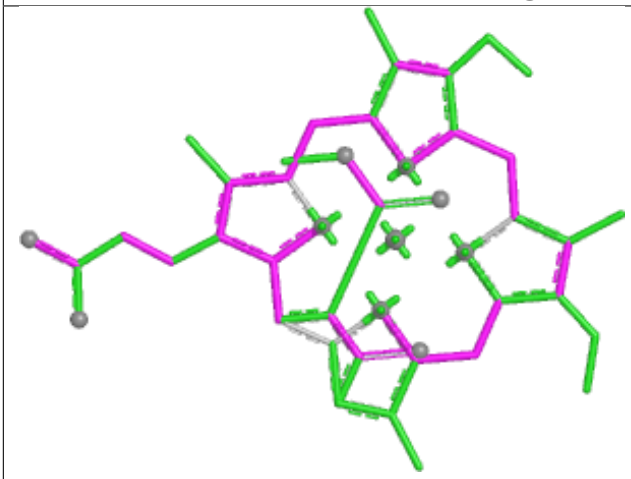


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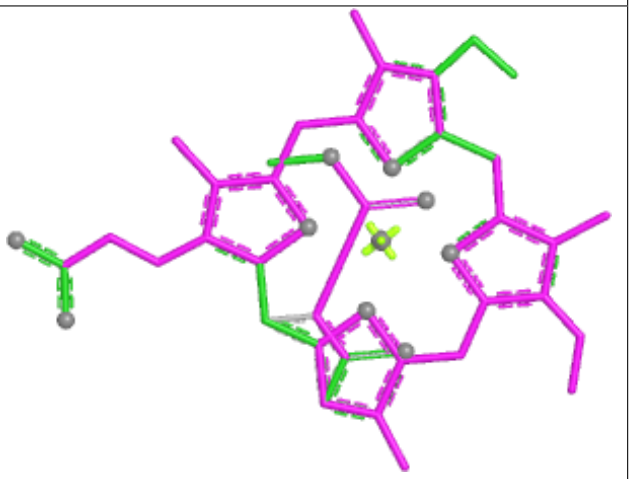


Rings

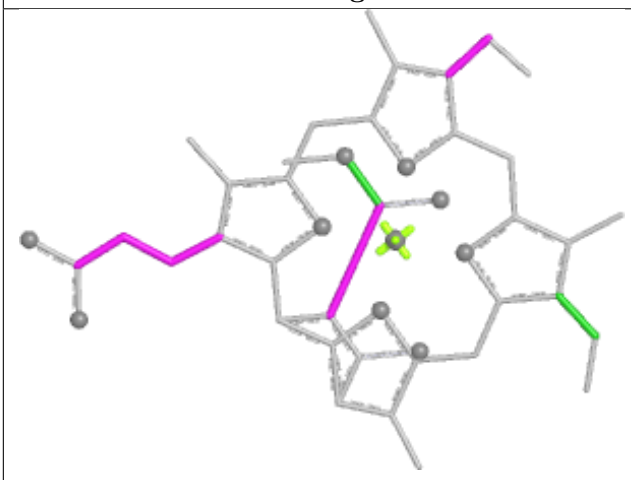
**Ligand KC1 31 309**



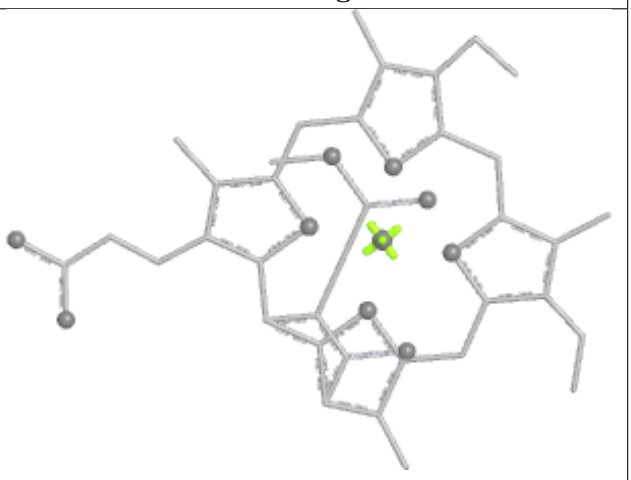
**Bond lengths**



**Bond angles**

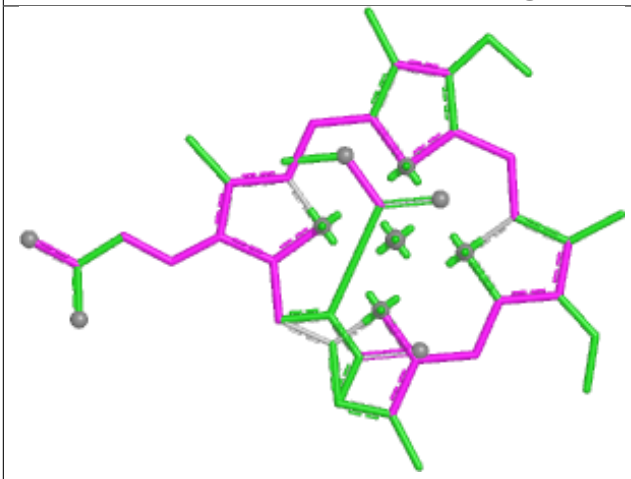


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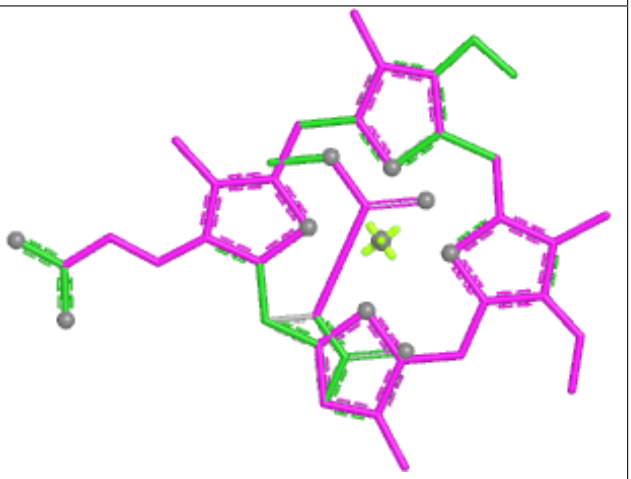


**Rings**

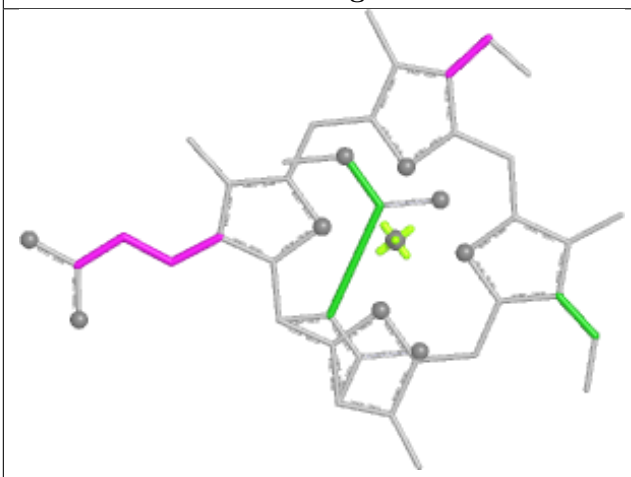
## Ligand KC1 40 206



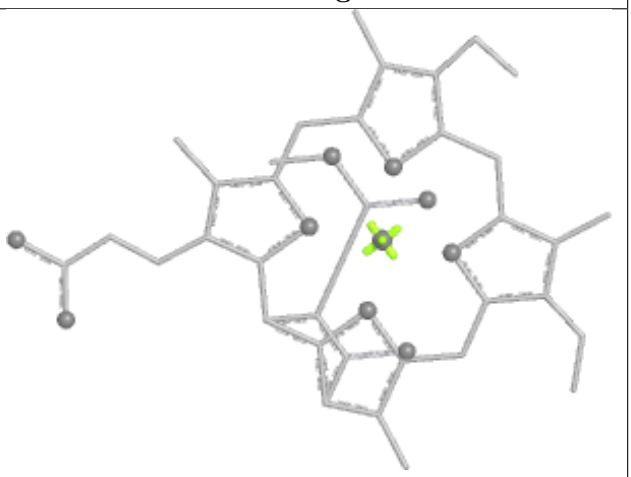
Bond lengths



Bond angles

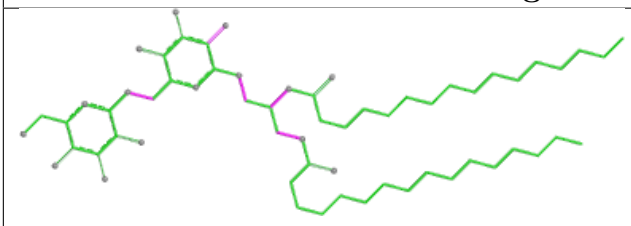


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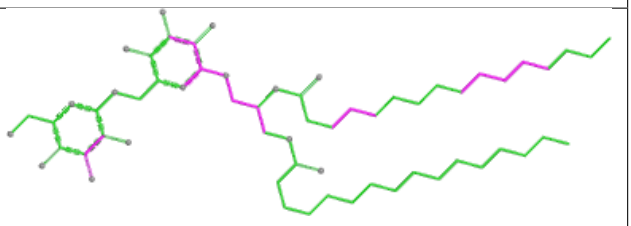


Rings

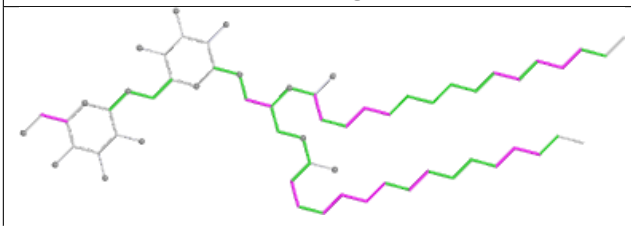
## Ligand DGD h 102



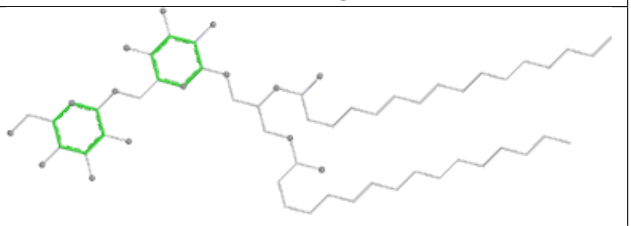
Bond lengths



Bond angles

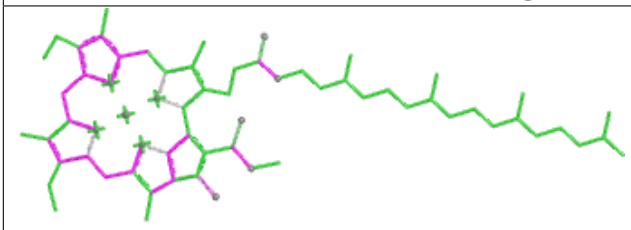


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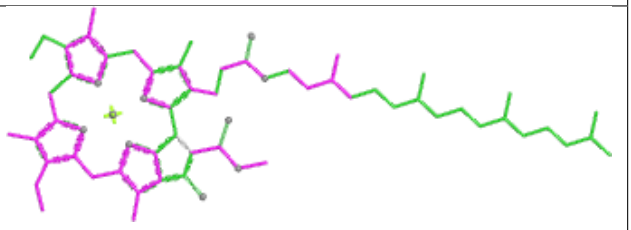


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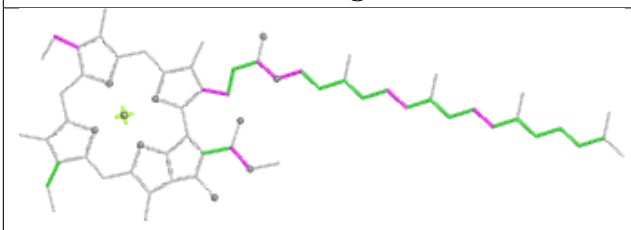
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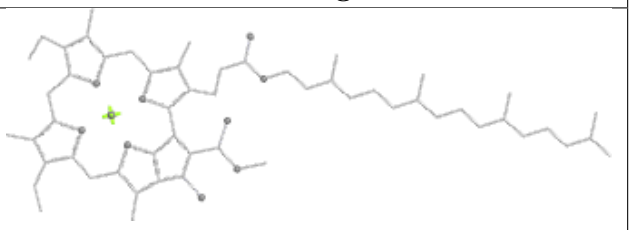
Bond lengths



Bond angles

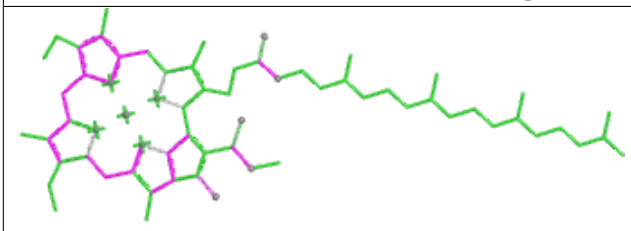


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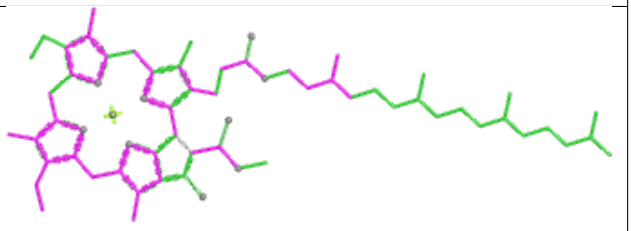


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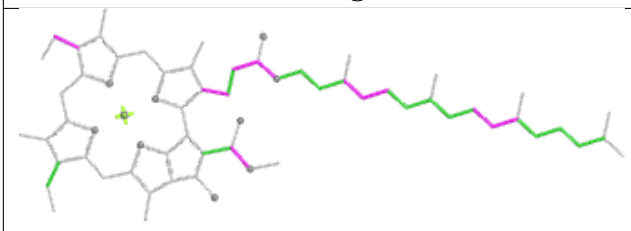
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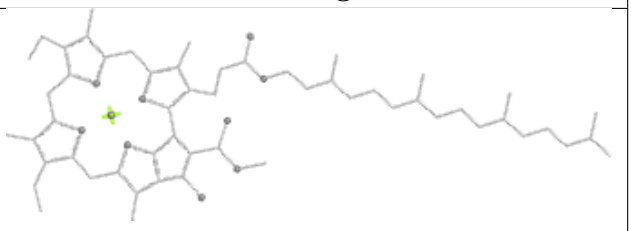
Bond lengths



Bond angles

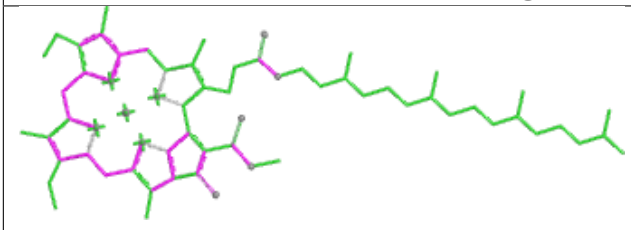


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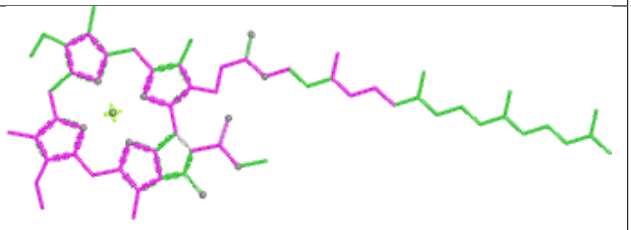


Rings

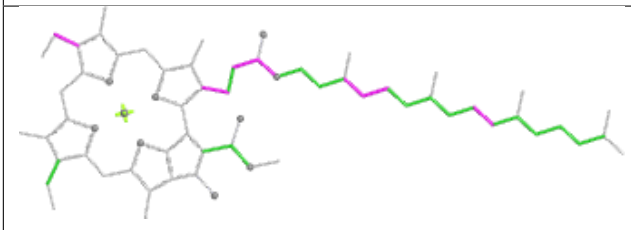
## Ligand CLA 31 304



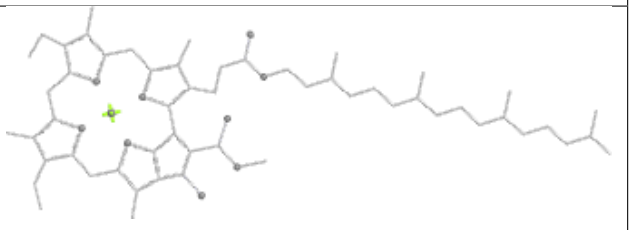
Bond lengths



Bond angles

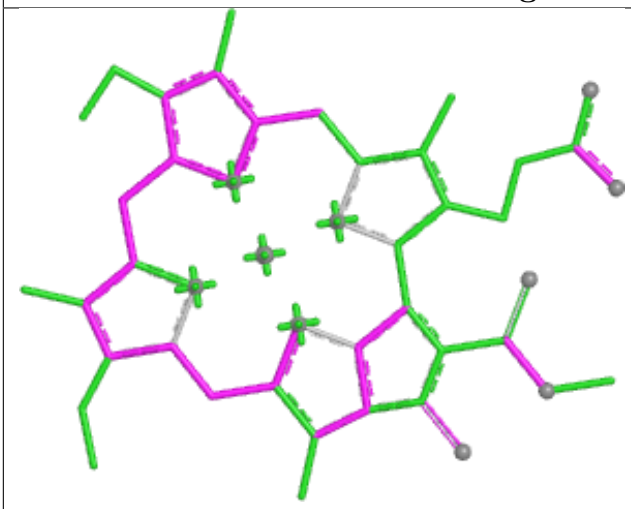


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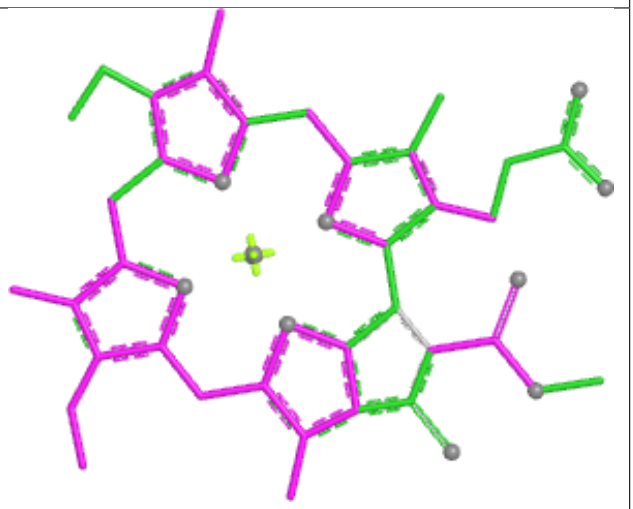


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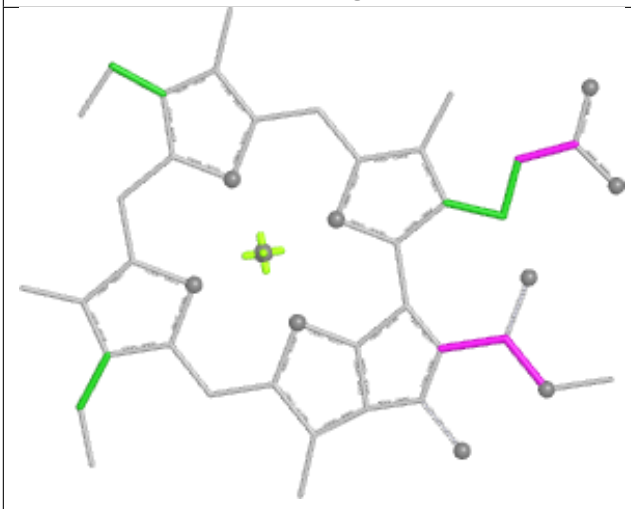
## Ligand CLA 21 209



Bond lengths



Bond angles

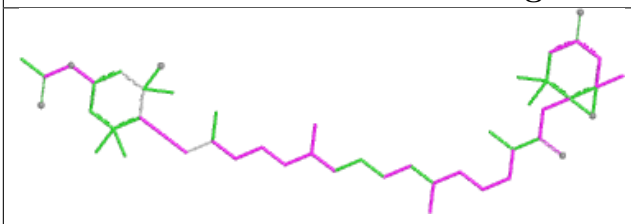


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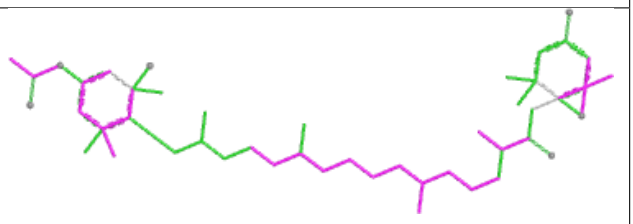


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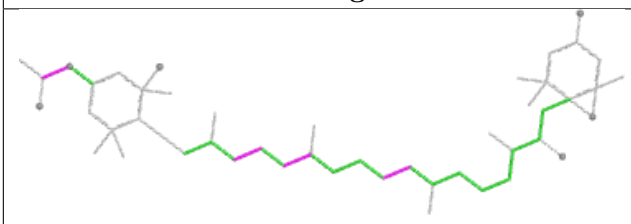
## Ligand A86 14 315



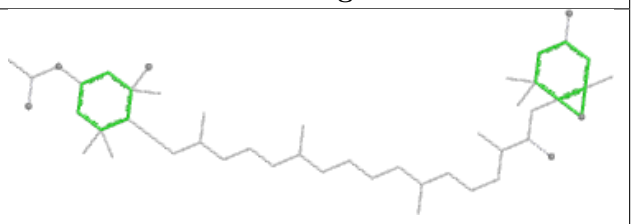
Bond lengths



Bond angles

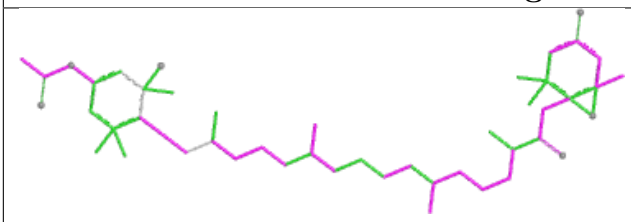


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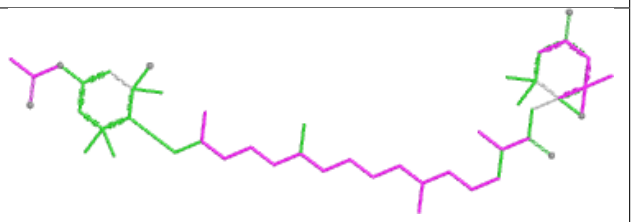


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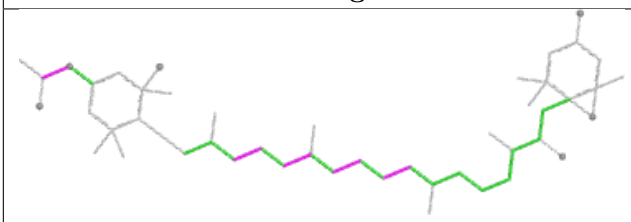
## Ligand A86 31 319



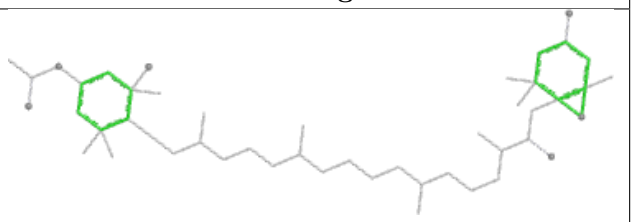
Bond lengths



Bond angles

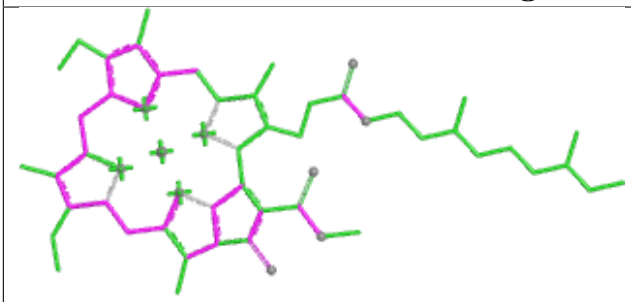


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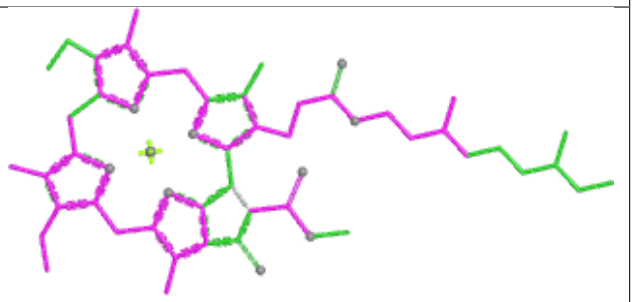


Rings

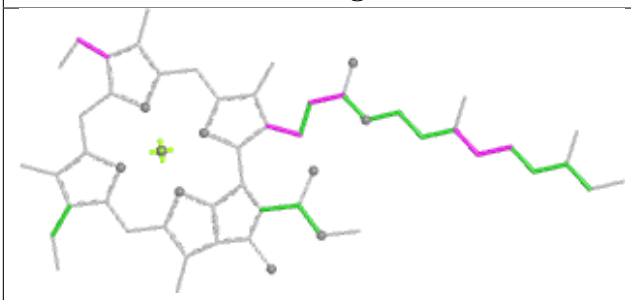
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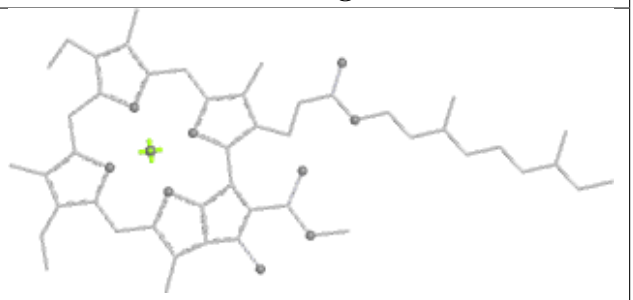
Bond lengths



Bond angles

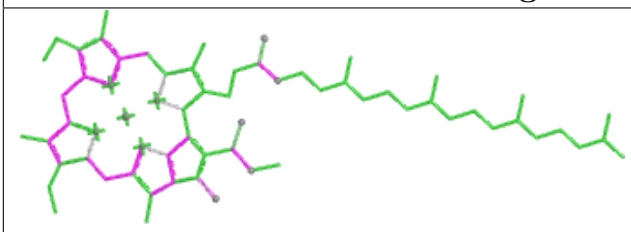


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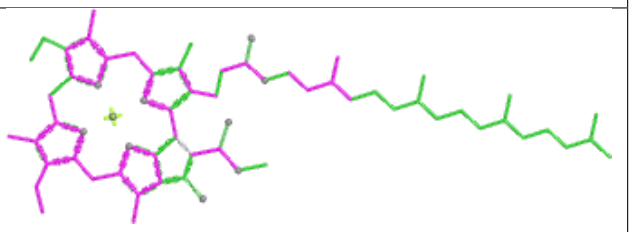


Rings

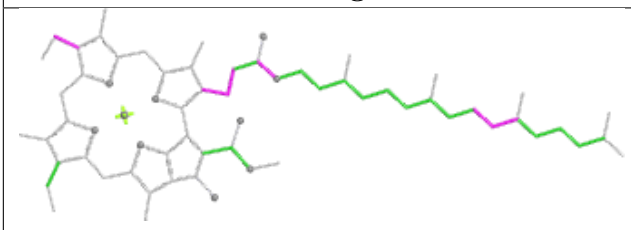
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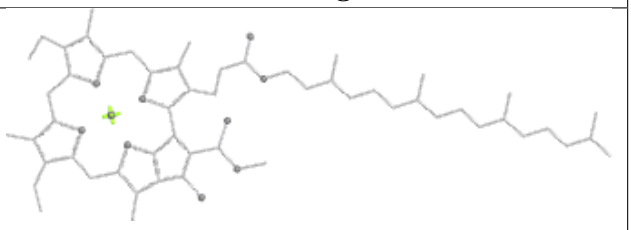
Bond lengths



Bond angles

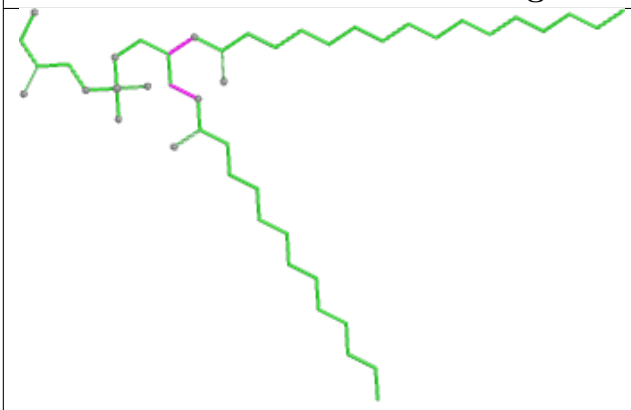


Torsions

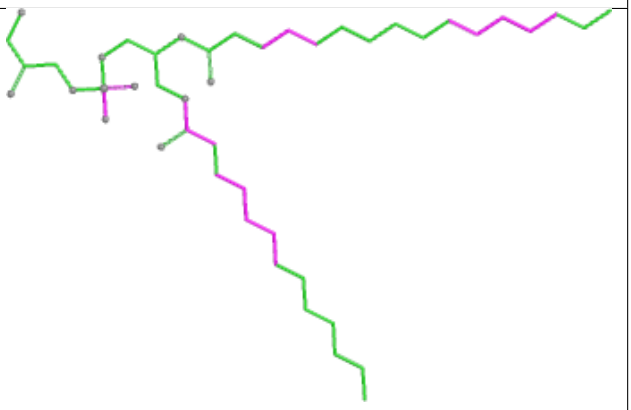


Rings

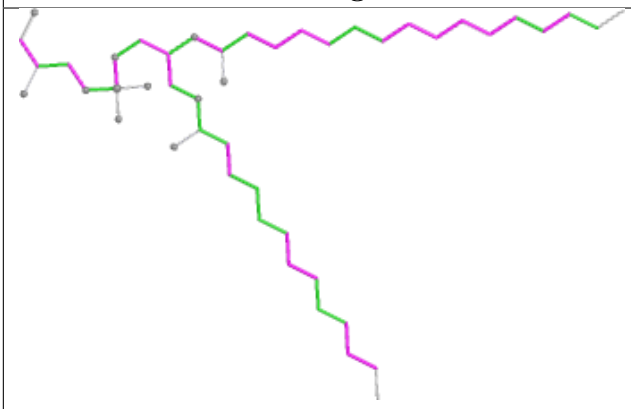
## Ligand LHG a 412



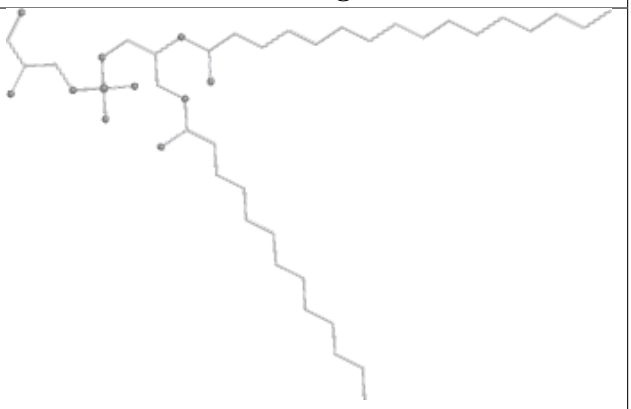
Bond lengths



Bond angles

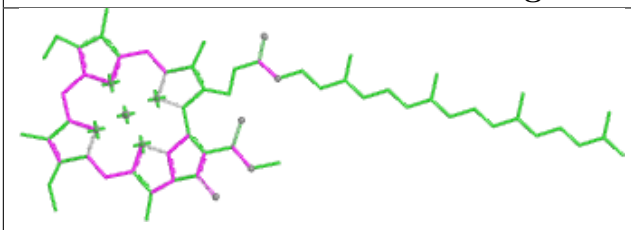


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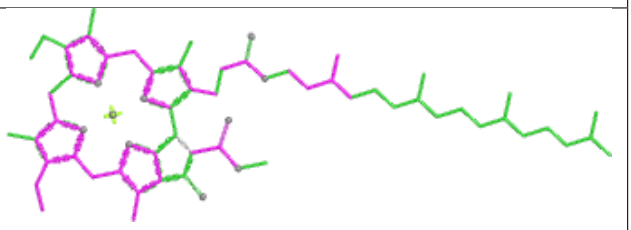


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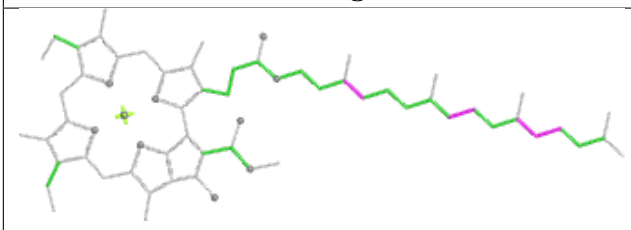
## Ligand CLA B 508



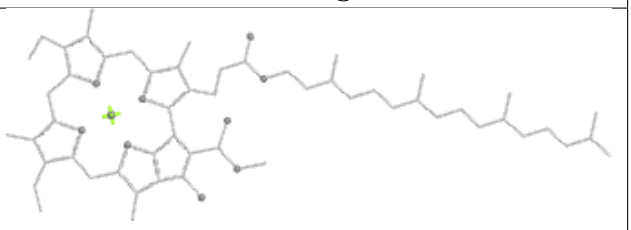
Bond lengths



Bond angles

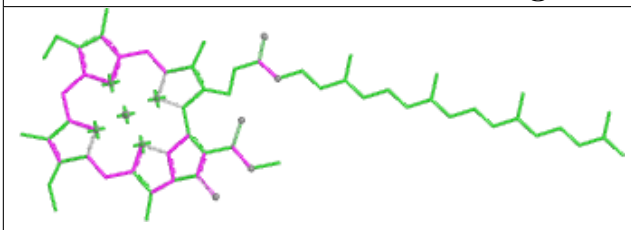


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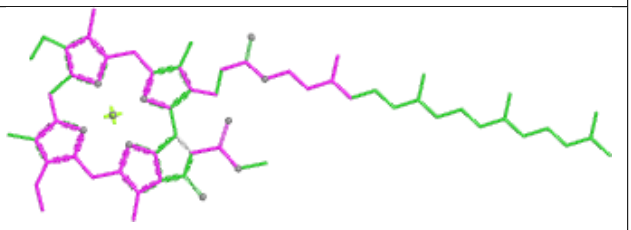


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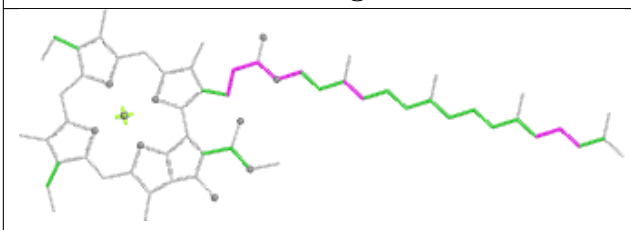
## Ligand CLA c 505



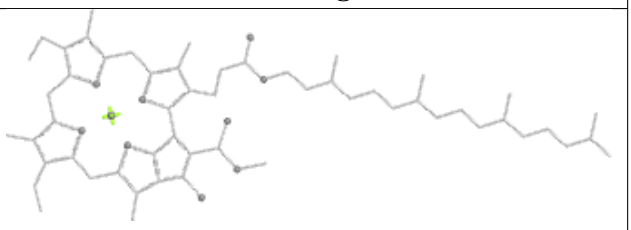
Bond lengths



Bond angles

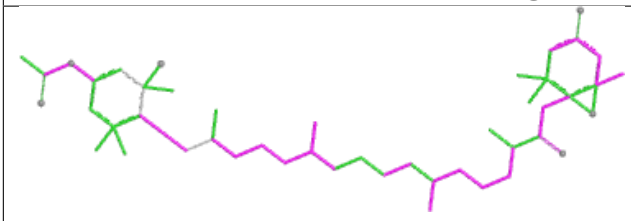


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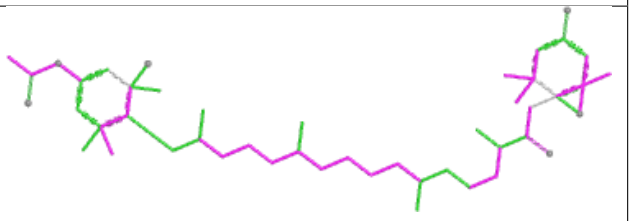


Rings

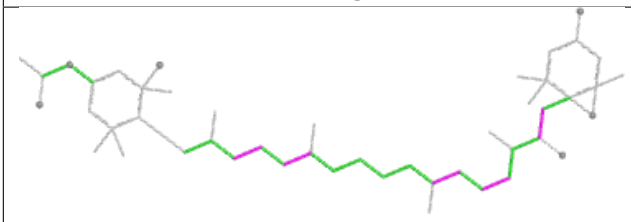
## Ligand A86 17 314



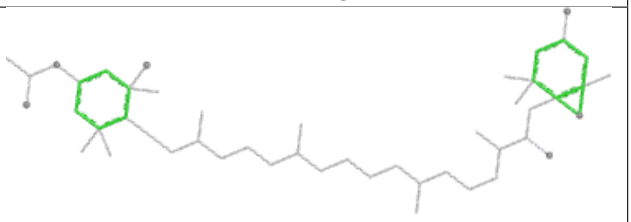
Bond lengths



Bond angles

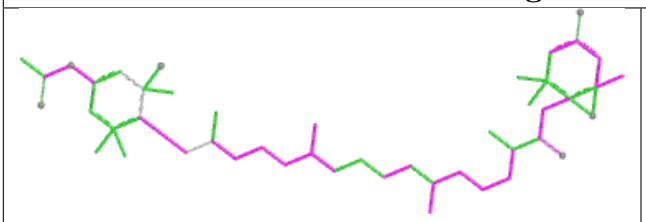


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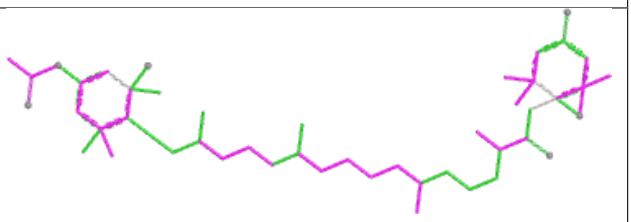


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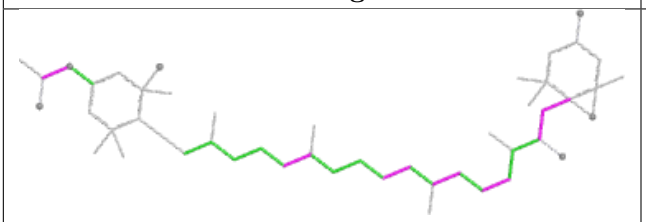
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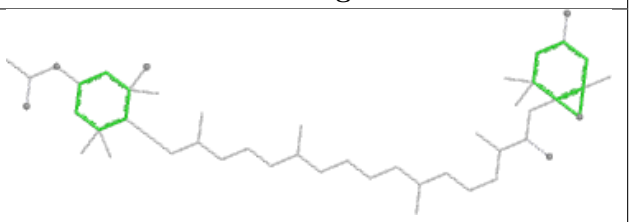
Bond lengths



Bond angles

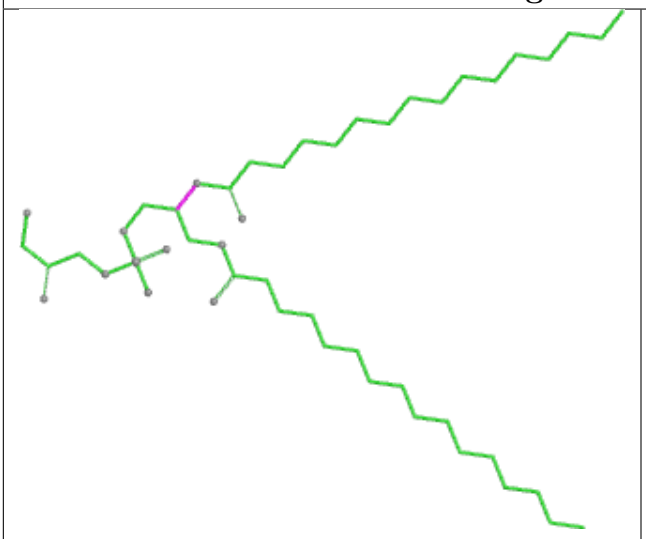


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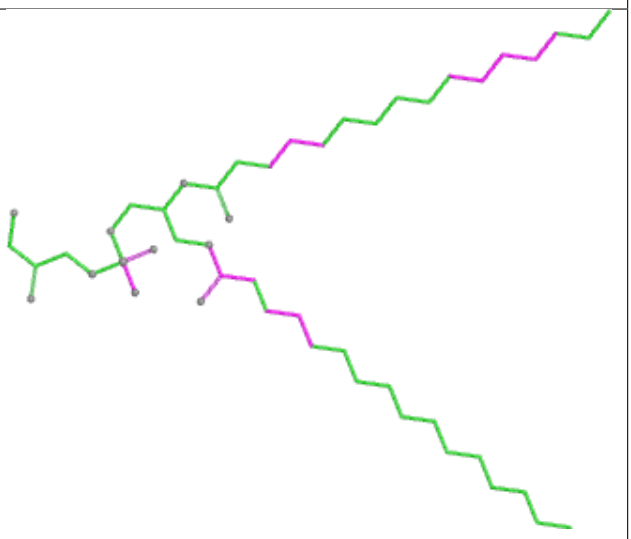


Rings

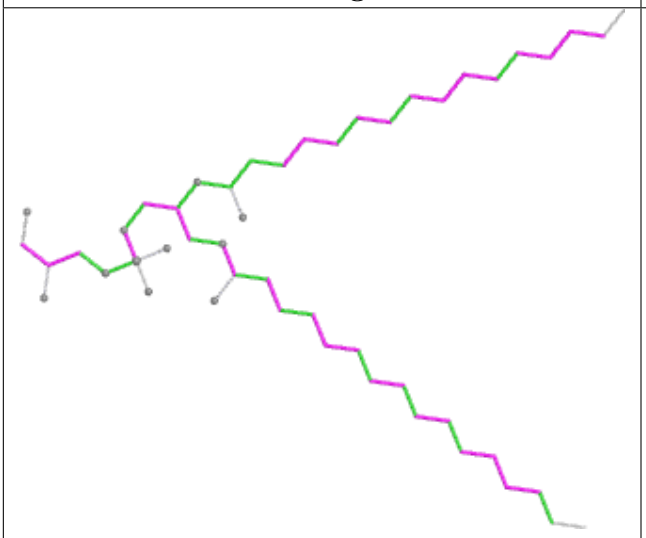
## Ligand LHG d 407



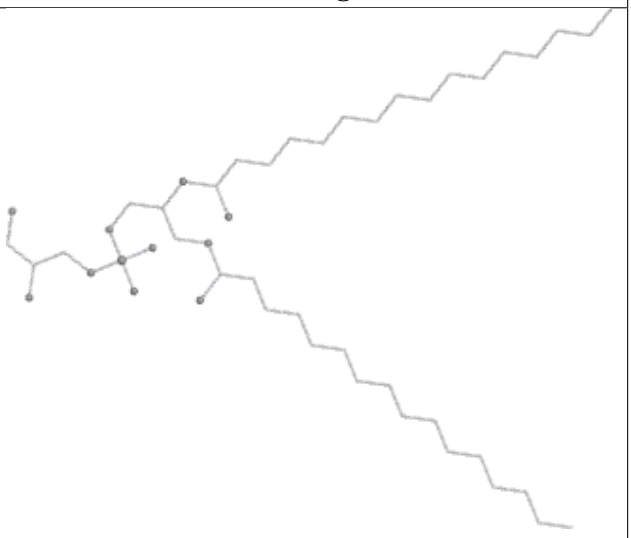
Bond lengths



Bond angles

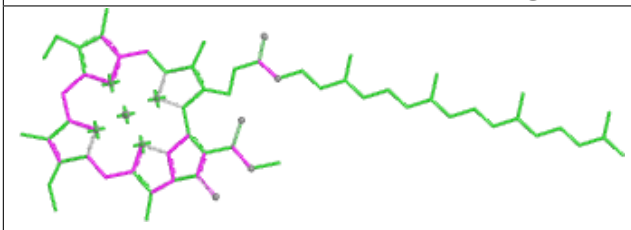


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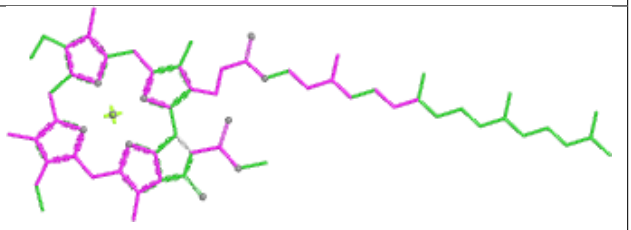


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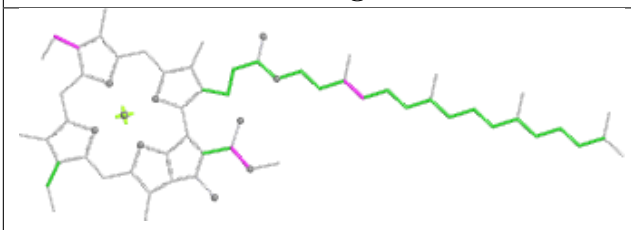
## Ligand CLA B 504



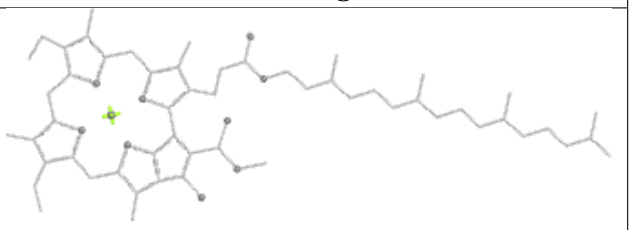
Bond lengths



Bond angles

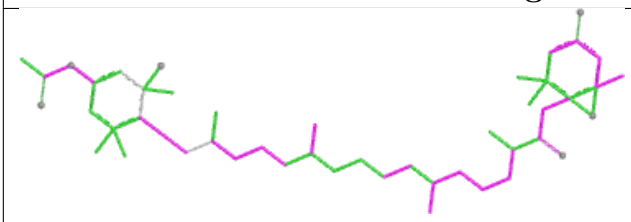


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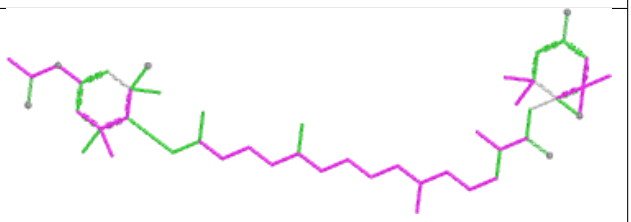


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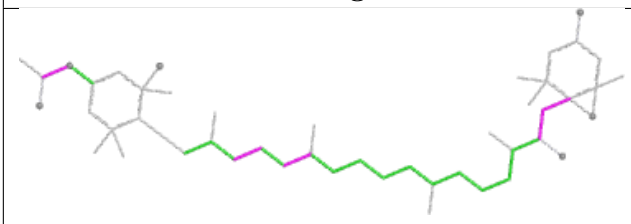
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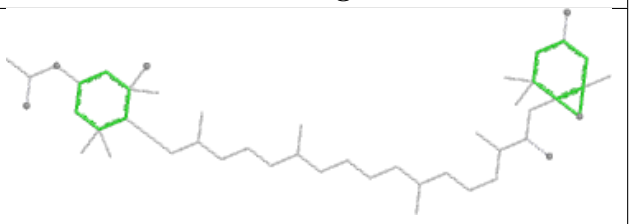
Bond lengths



Bond angles

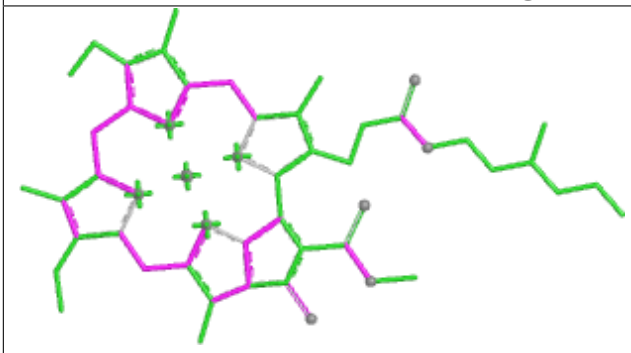


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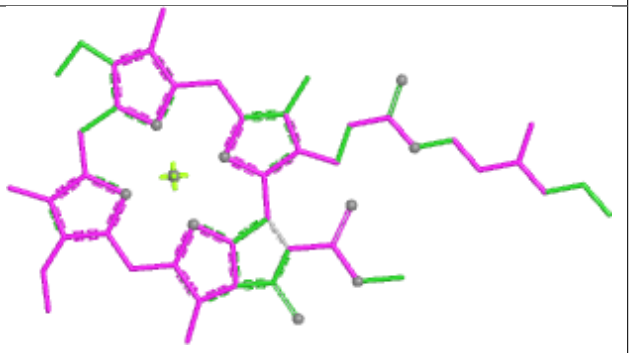


Rings

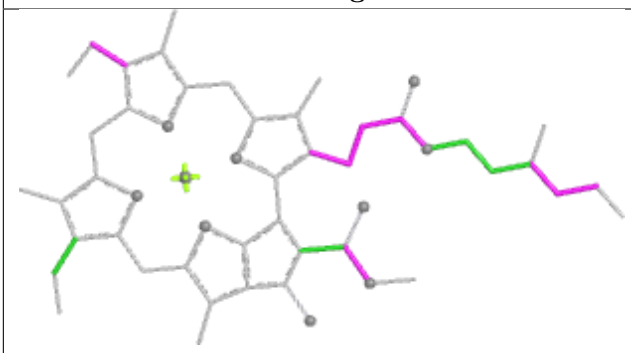
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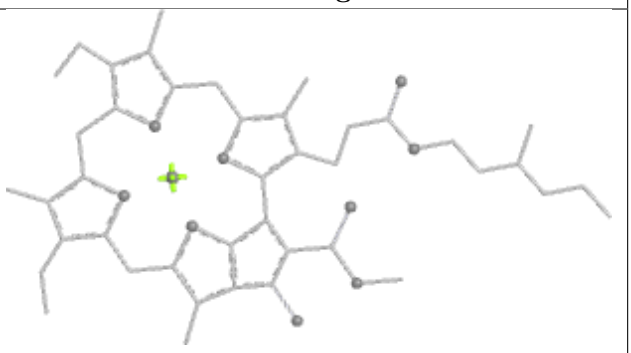
Bond lengths



Bond angles

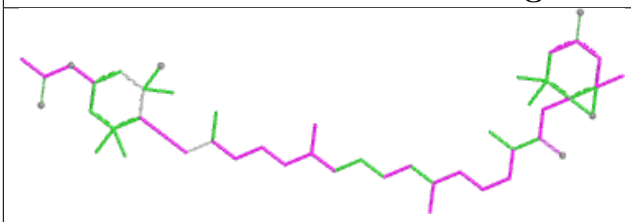


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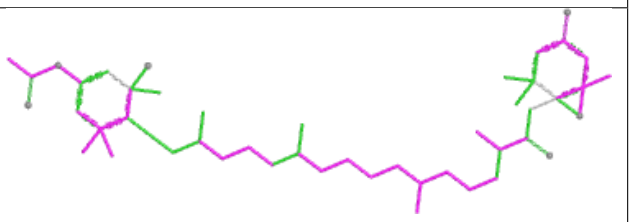


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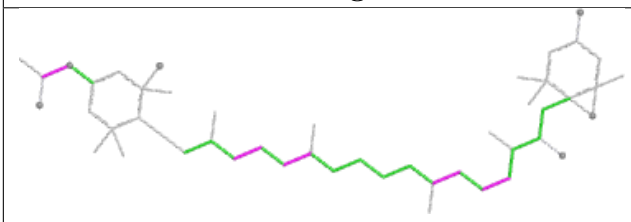
## Ligand A86 35 315



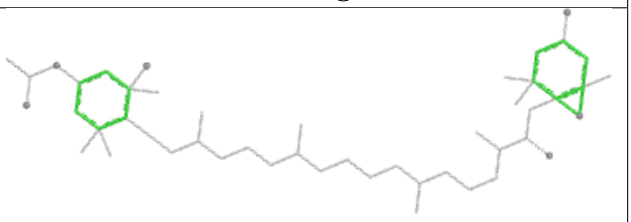
Bond lengths



Bond angles

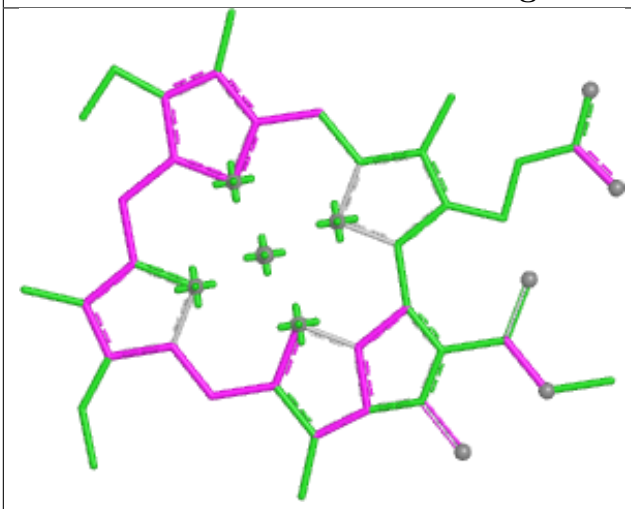


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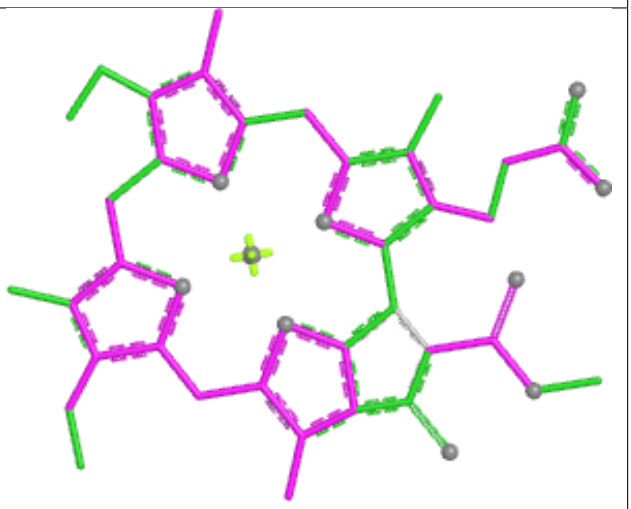


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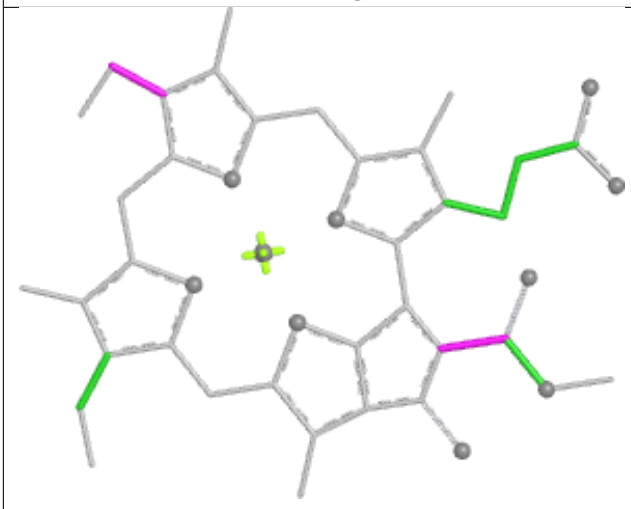
**Ligand CLA 15 310**



**Bond lengths**



**Bond angles**

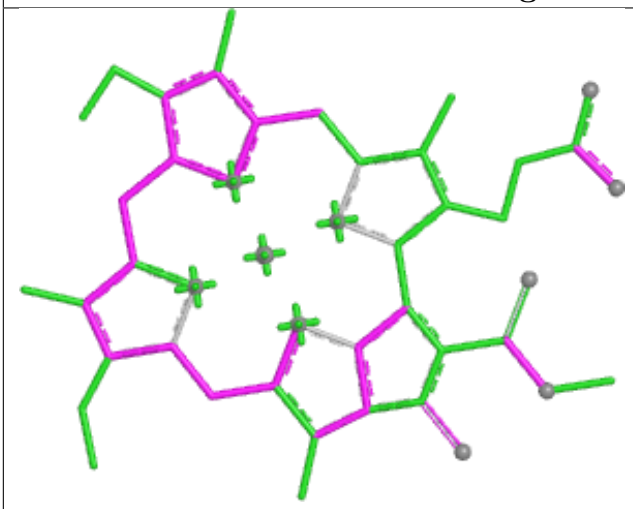


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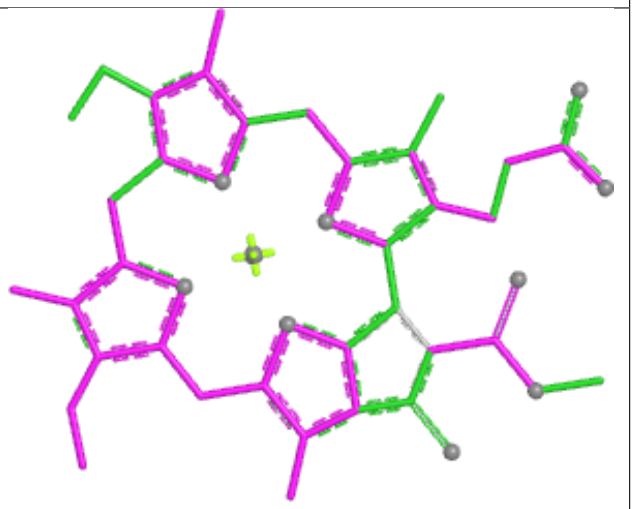


**Rings**

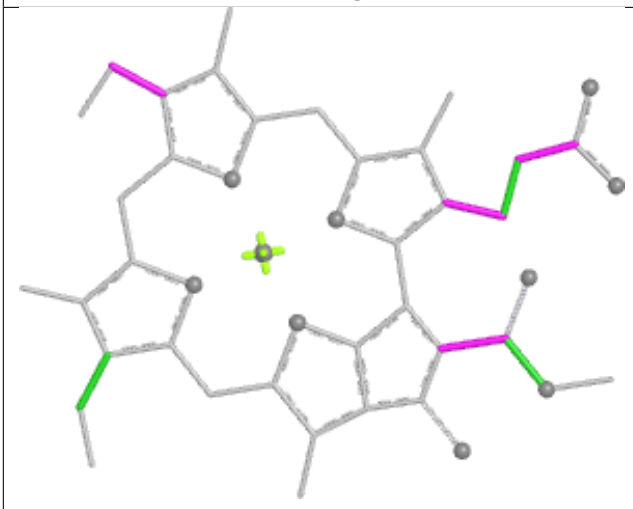
**Ligand CLA 20 307**



**Bond lengths**



**Bond angles**

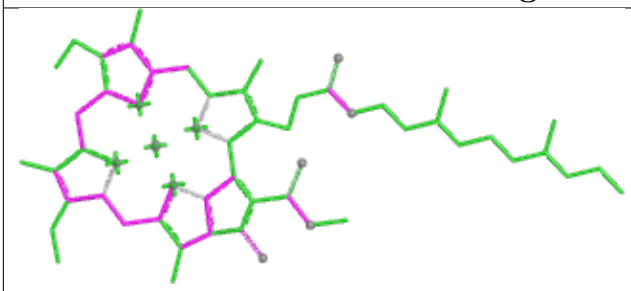


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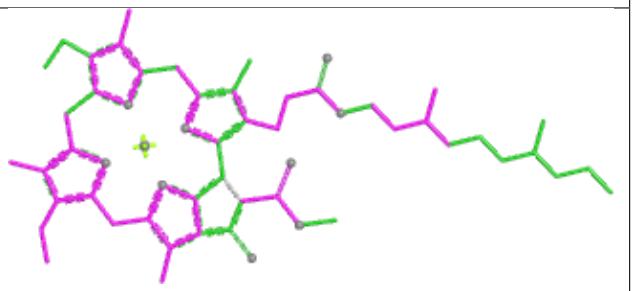


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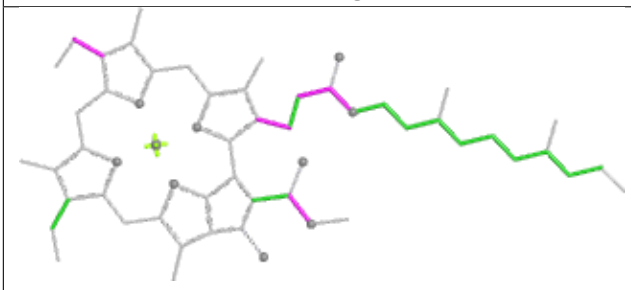
## Ligand CLA 16 303



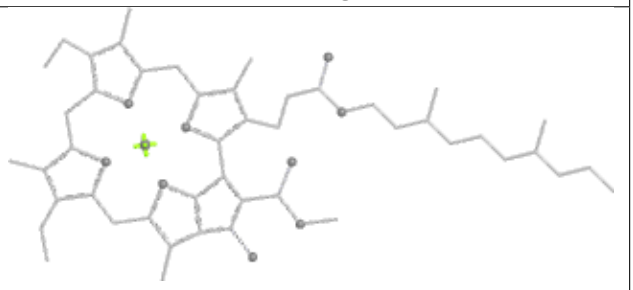
Bond lengths



Bond angles

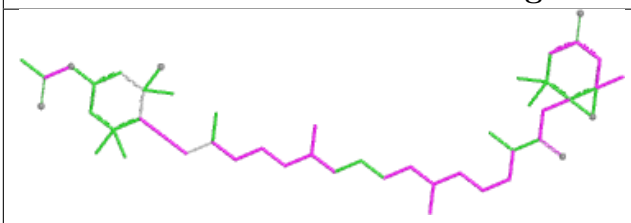


Torsions



Rings

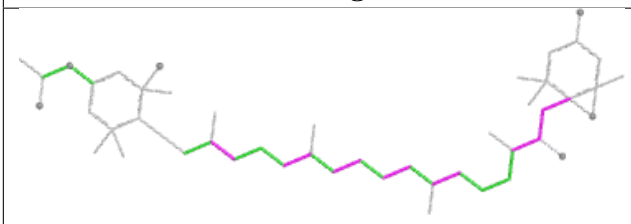
## Ligand A86 40 201



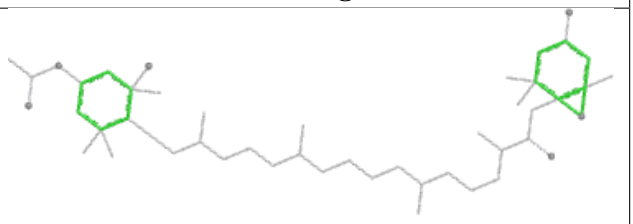
Bond lengths



Bond angles

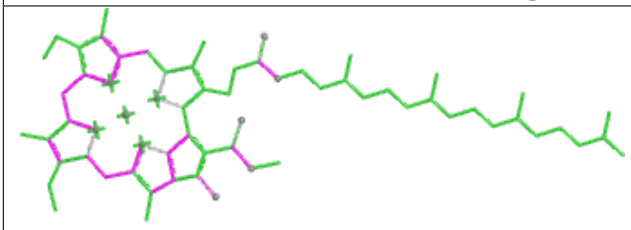


Torsions

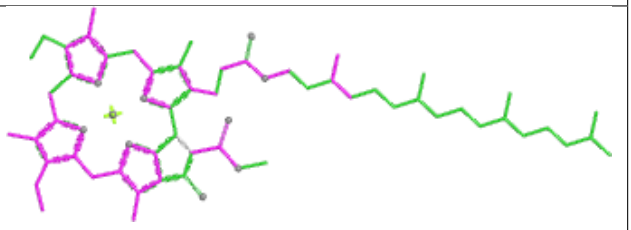


Rings

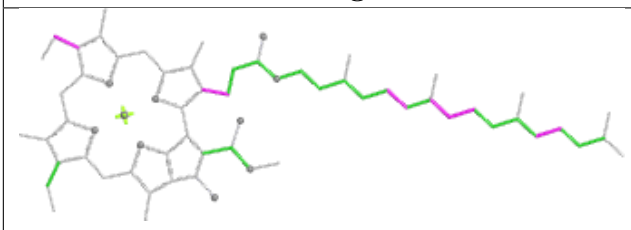
## Ligand CLA A 405



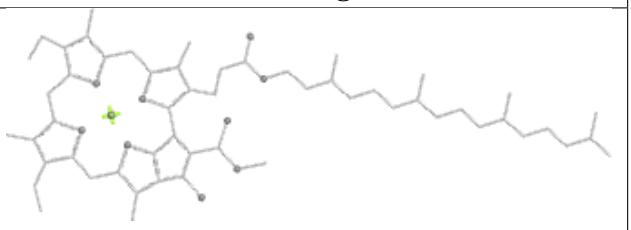
Bond lengths



Bond angles

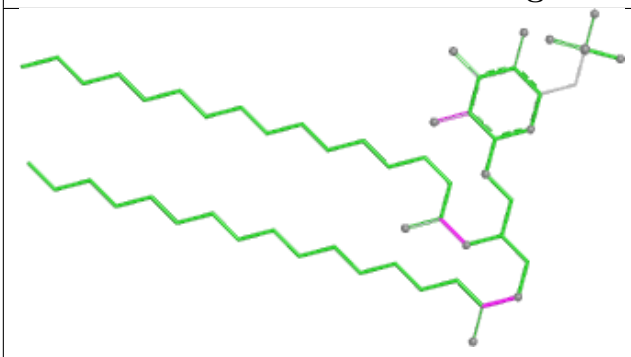


Torsions

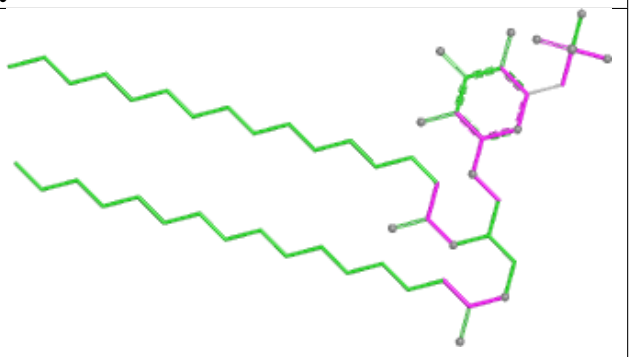


Rings

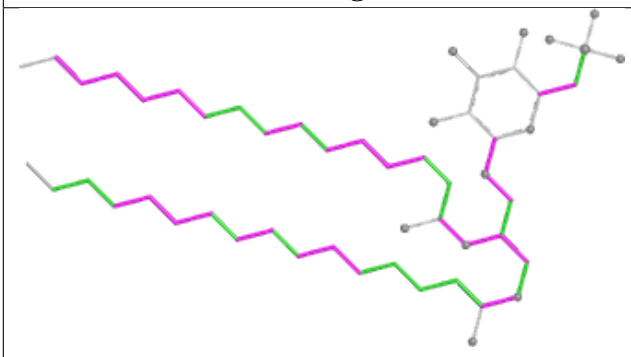
## Ligand SQD L 101



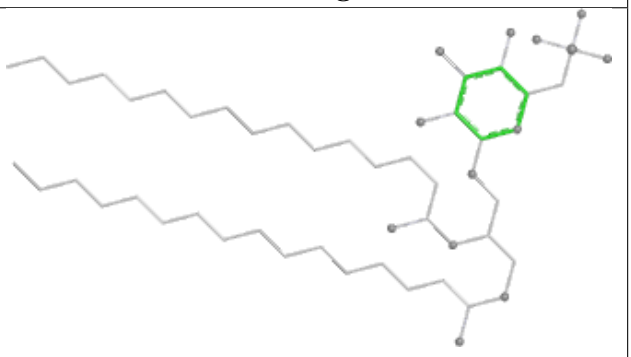
Bond lengths



Bond angles

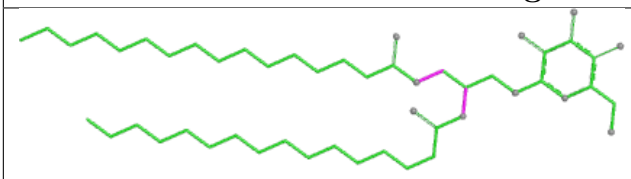


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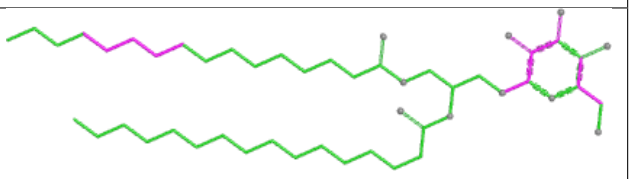


Rings

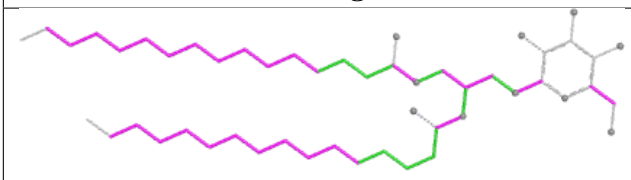
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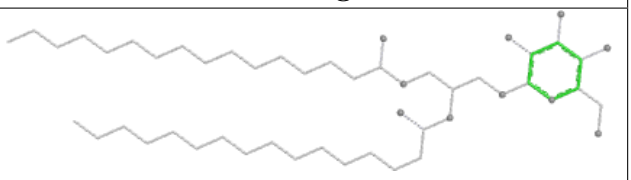
Bond lengths



Bond angles

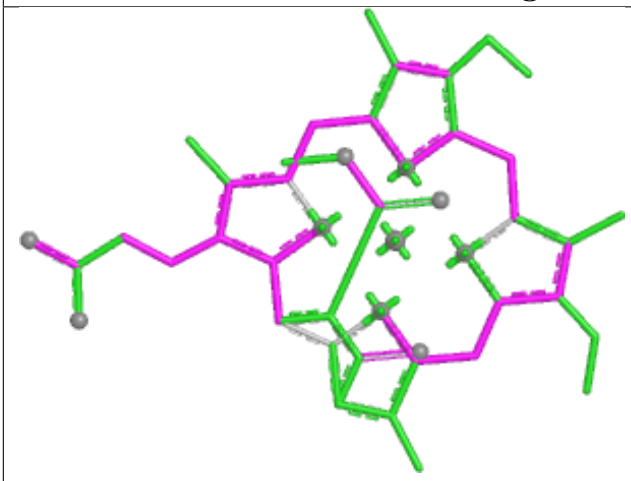


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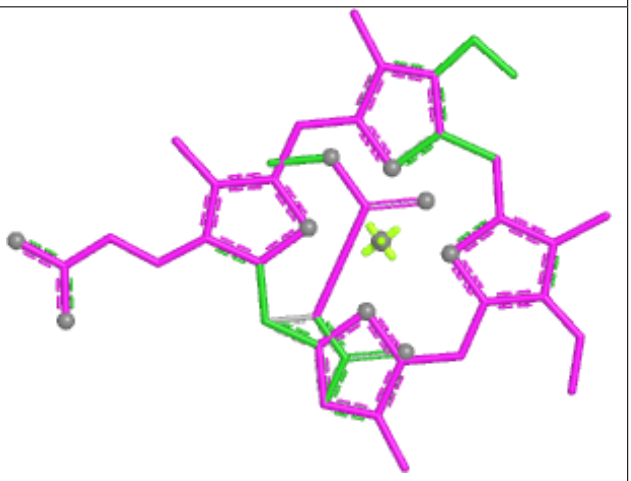


Rings

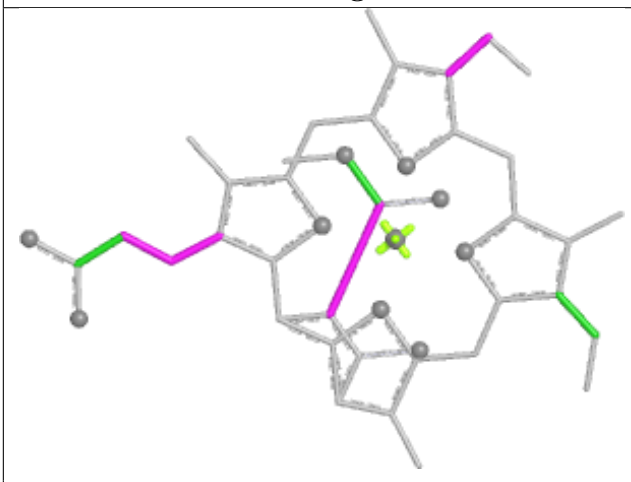
## Ligand KC1 14 306



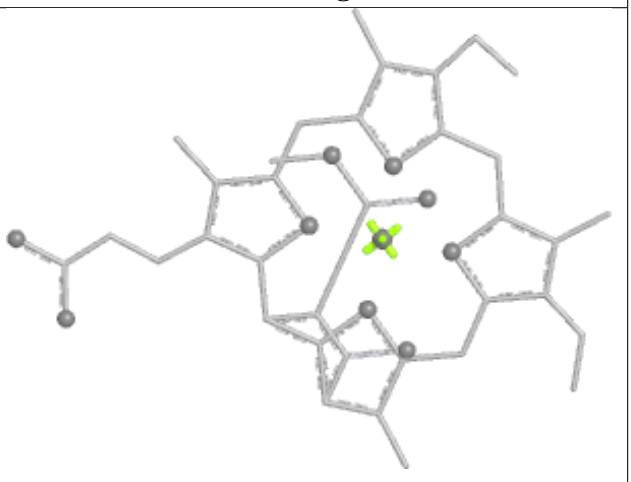
Bond lengths



Bond angles

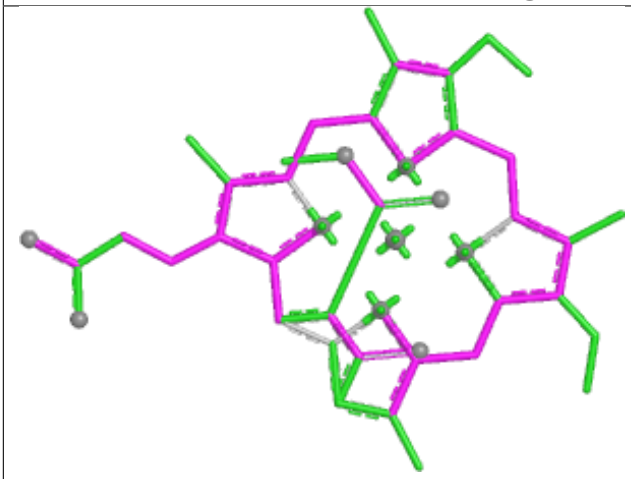


Torsions

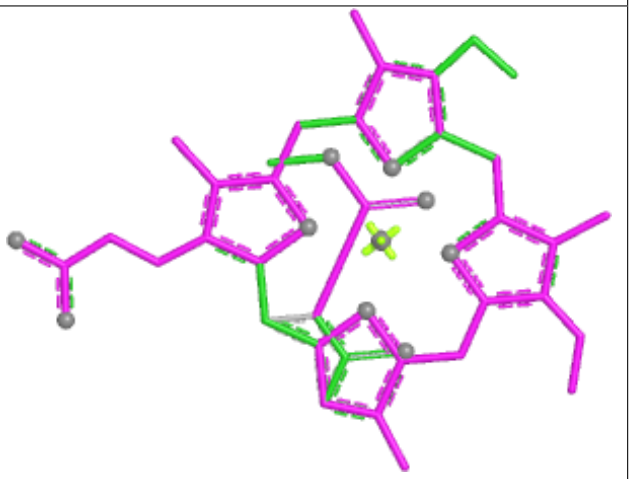


Rings

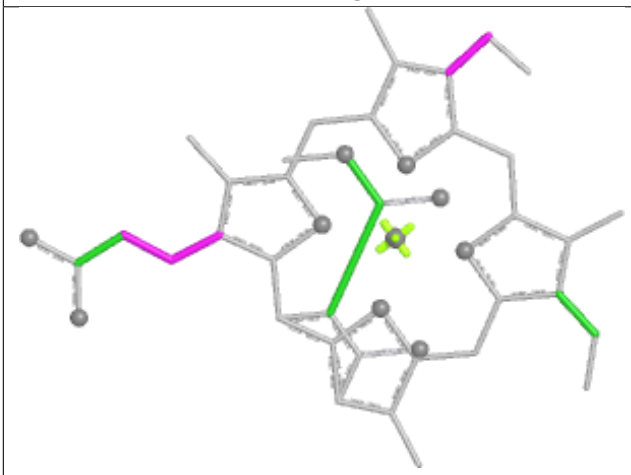
**Ligand KC1 16 308**



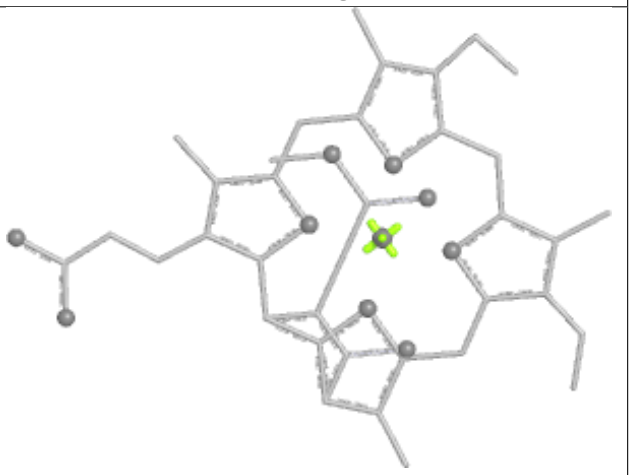
Bond lengths



Bond angles

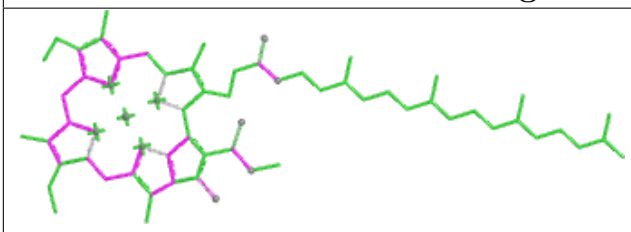


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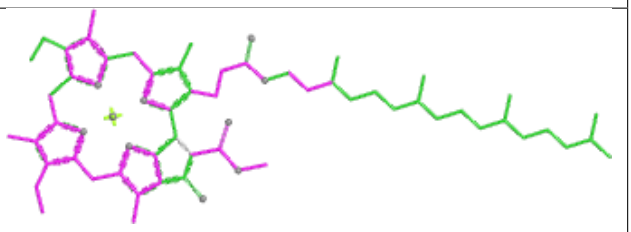


Rings

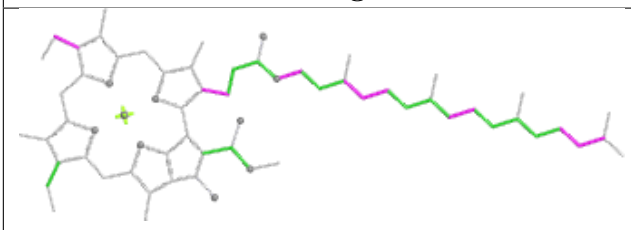
**Ligand CLA 16 301**



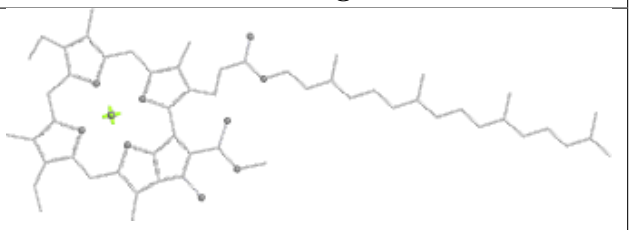
Bond lengths



Bond angles

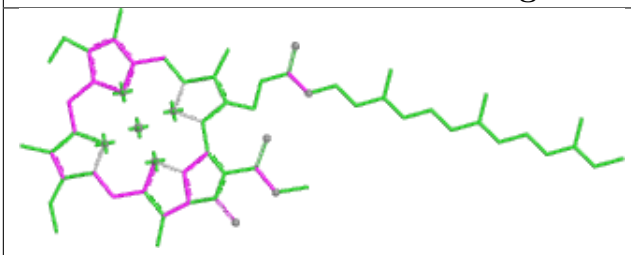


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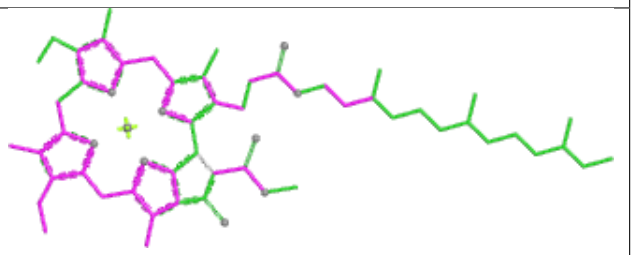


Rings

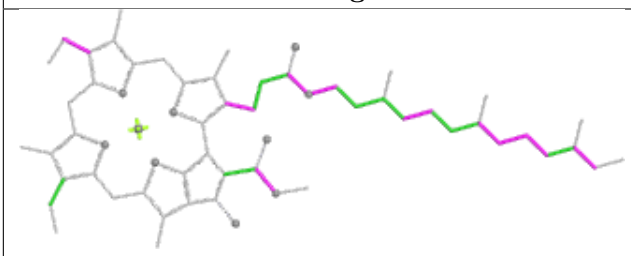
## Ligand CLA 36 307



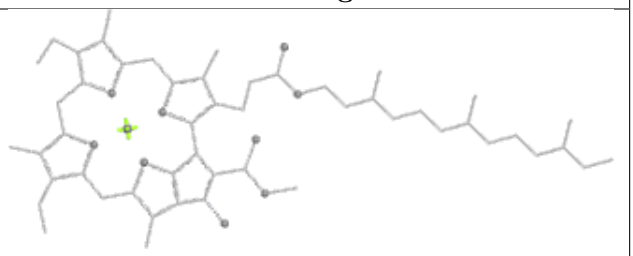
Bond lengths



Bond angles

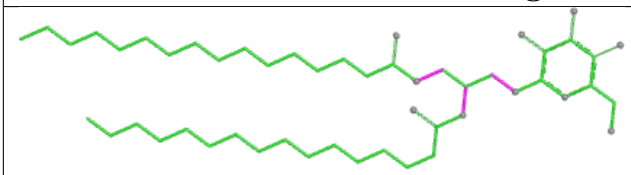


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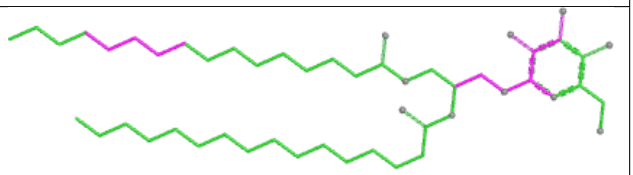


Rings

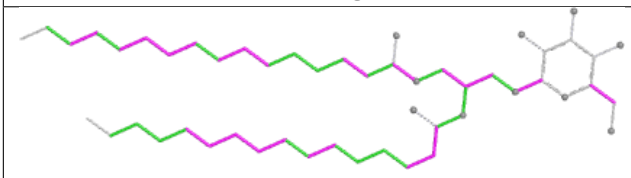
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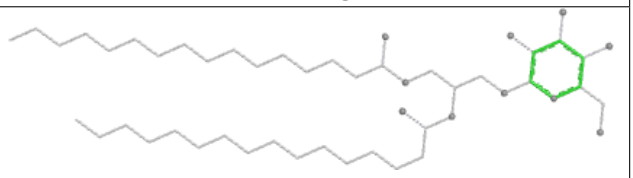
Bond lengths



Bond angles

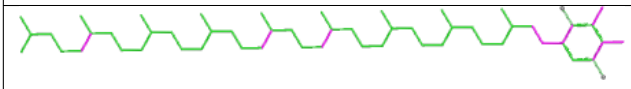


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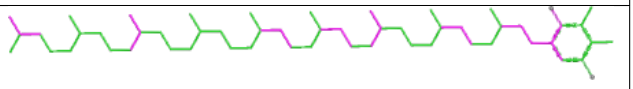


Rings

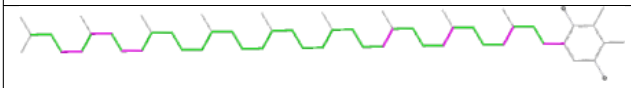
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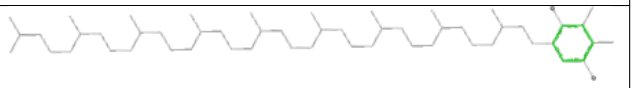
Bond lengths



Bond angles

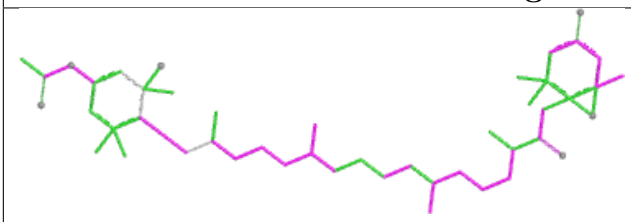


Torsions

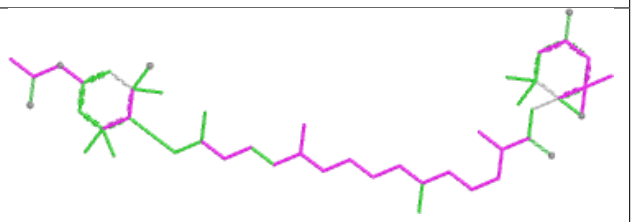


Rings

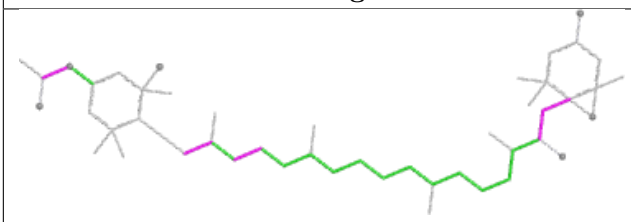
## Ligand A86 31 313



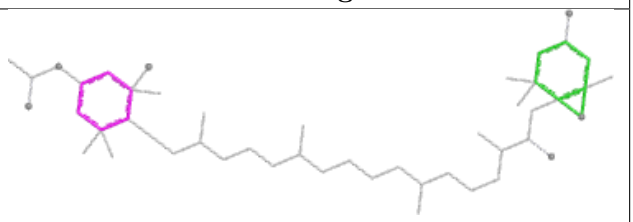
Bond lengths



Bond angles

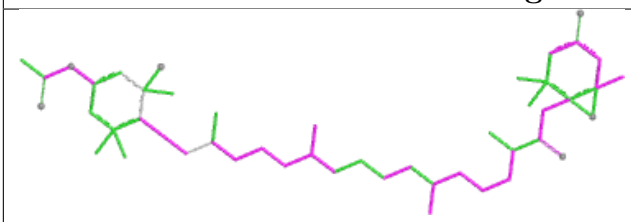


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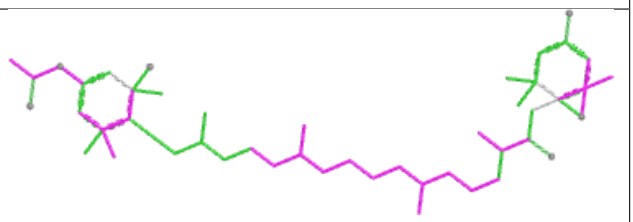


Rings

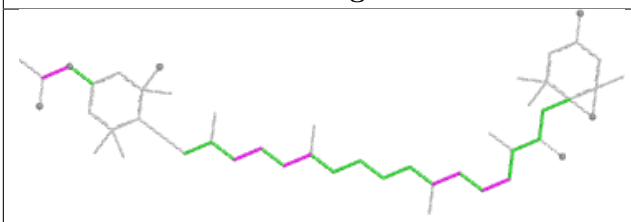
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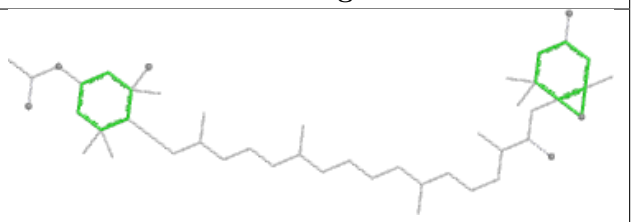
Bond lengths



Bond angles

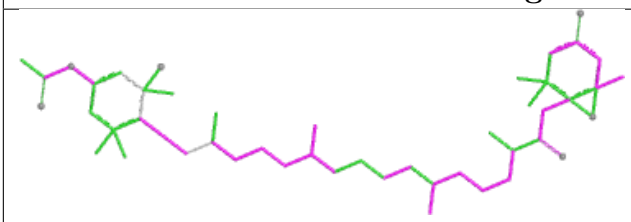


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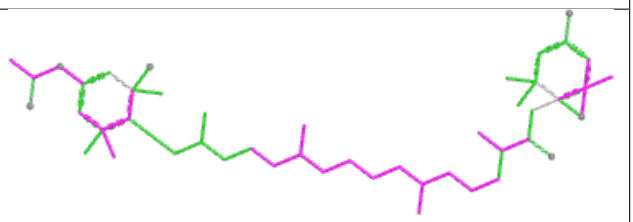


Rings

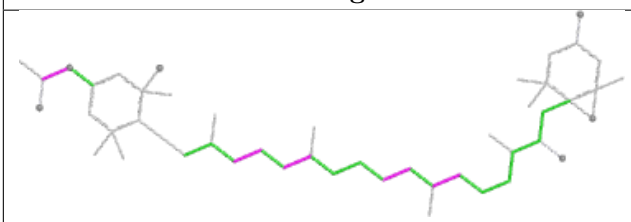
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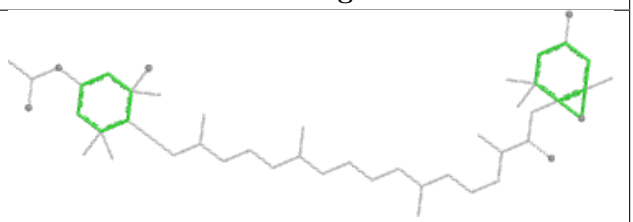
Bond lengths



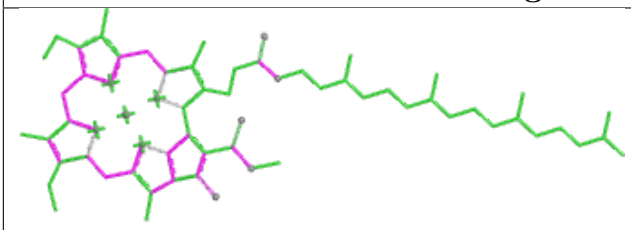
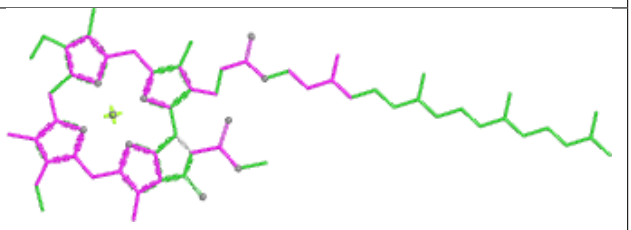
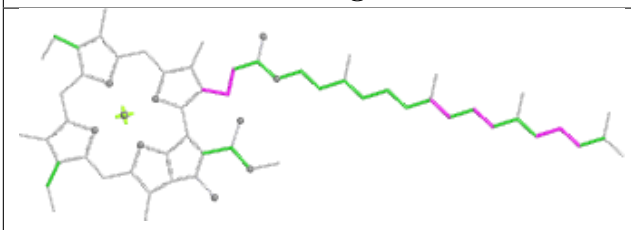
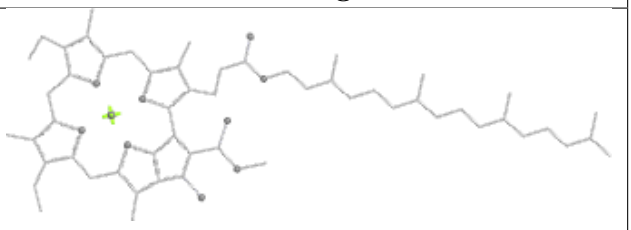
Bond angles

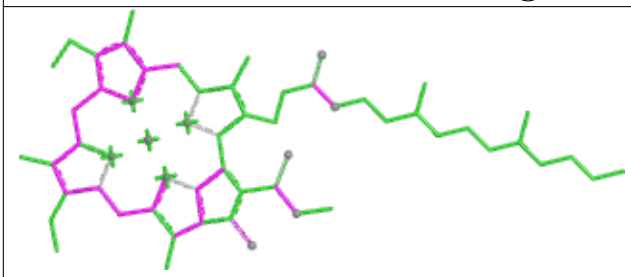
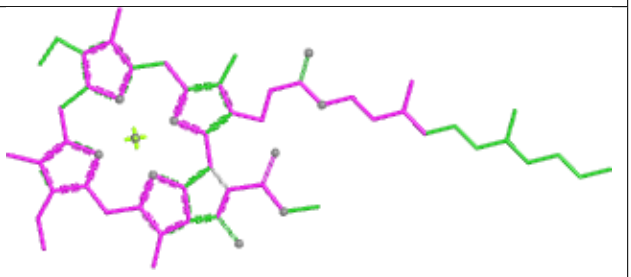
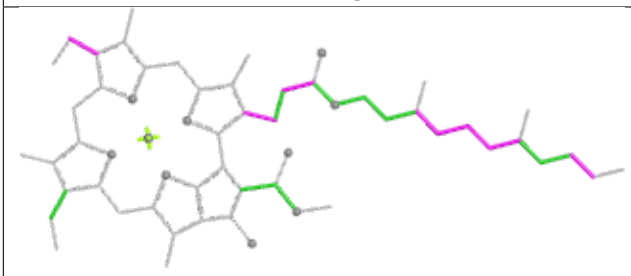
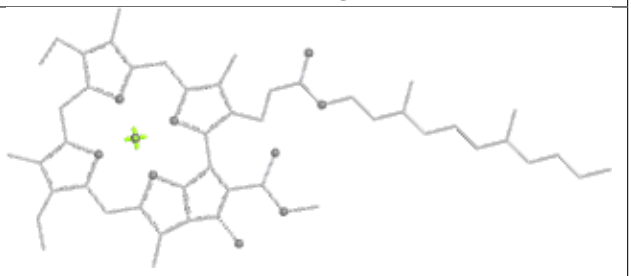


Torsions

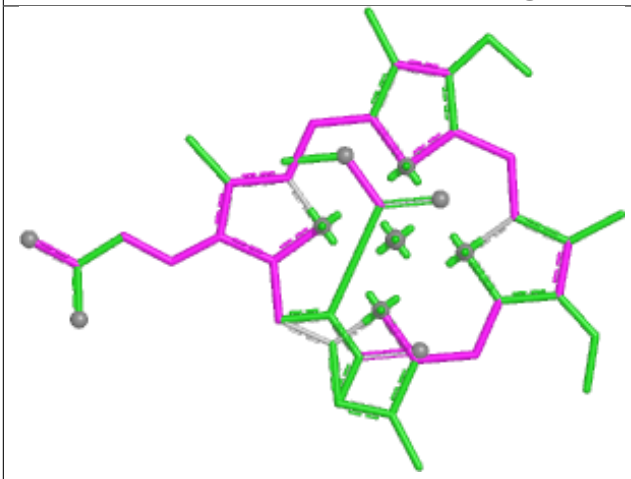


Rings

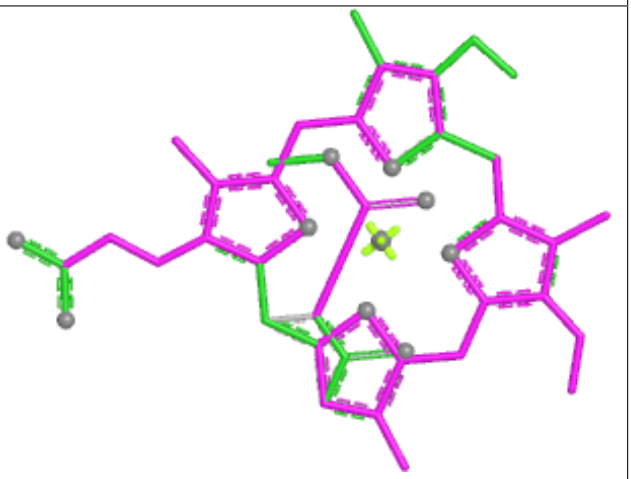
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|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 21 204 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

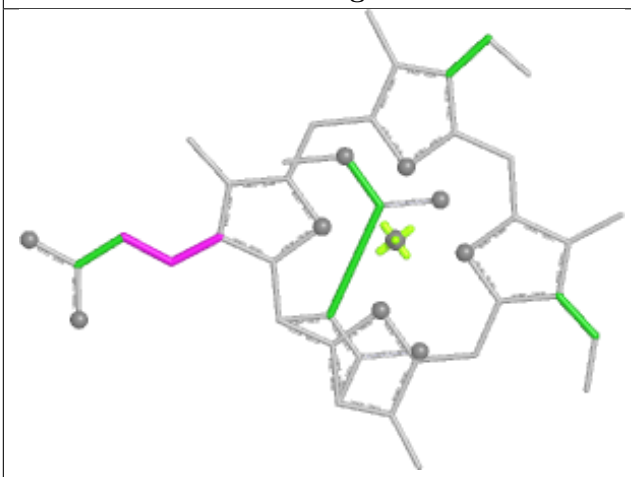
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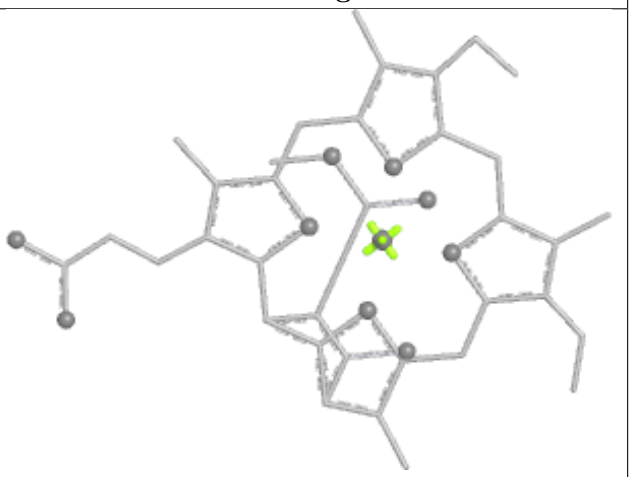
Bond lengths



Bond angles

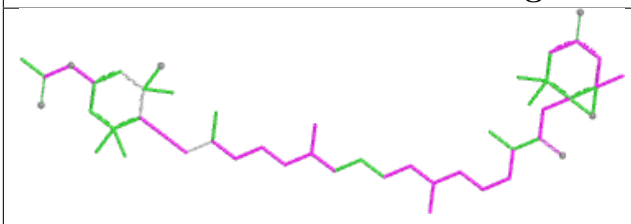


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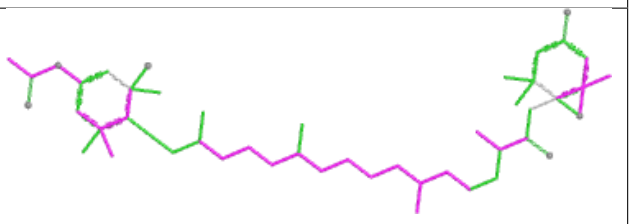


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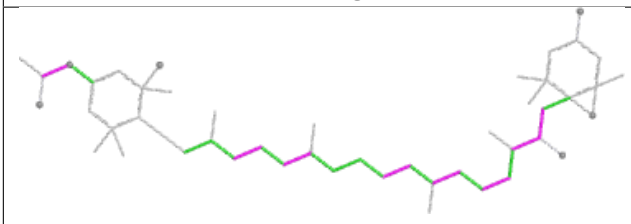
**Ligand A86 35 314**



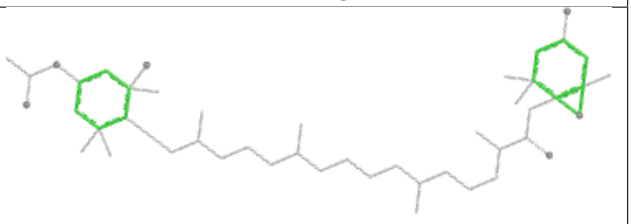
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Bond angles

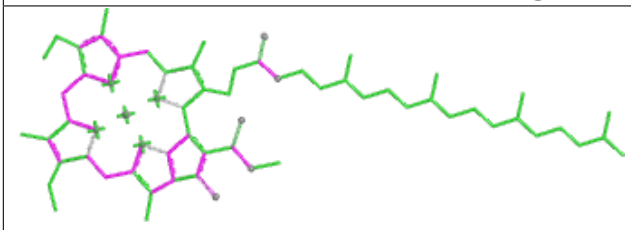


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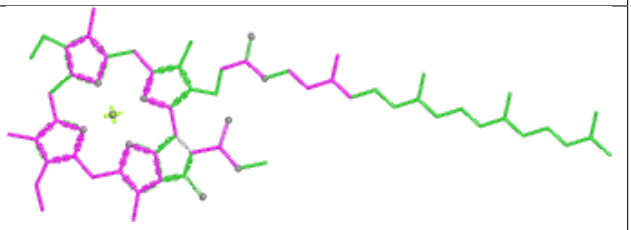


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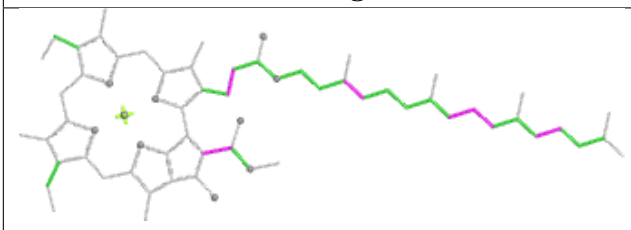
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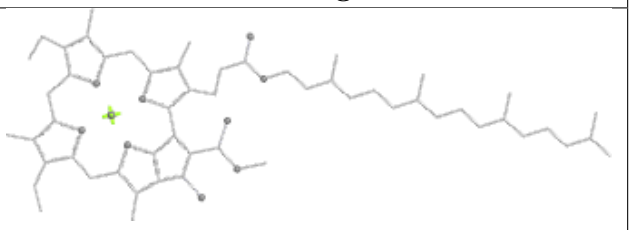
Bond lengths



Bond angles

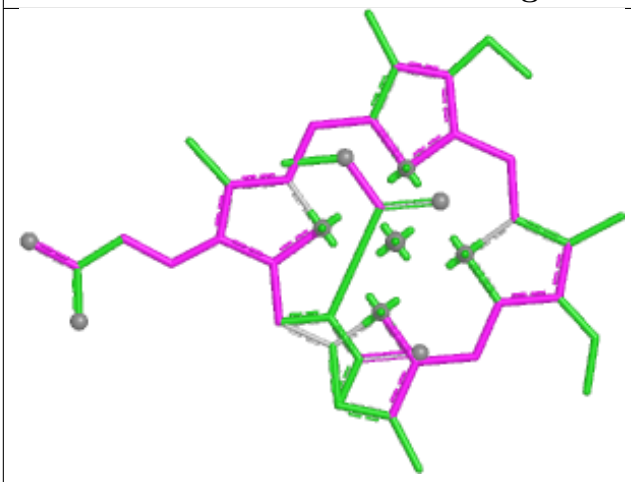


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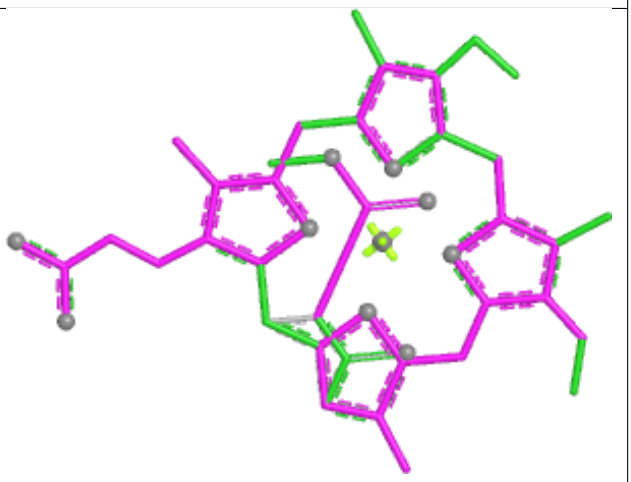


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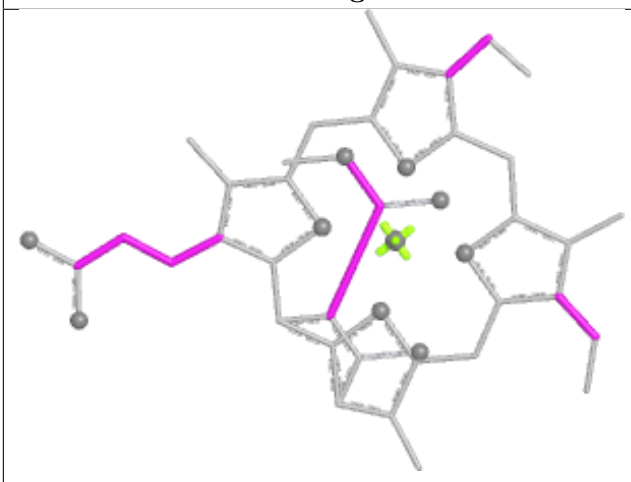
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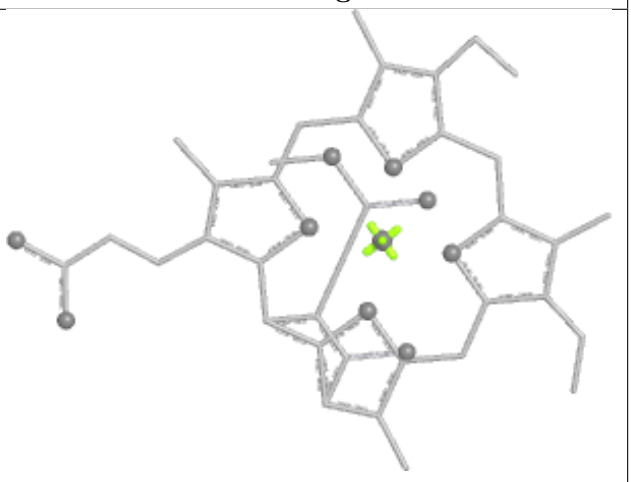
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Bond angles

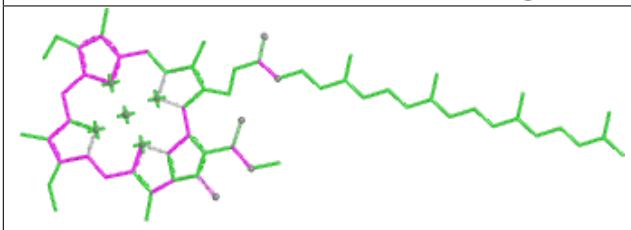


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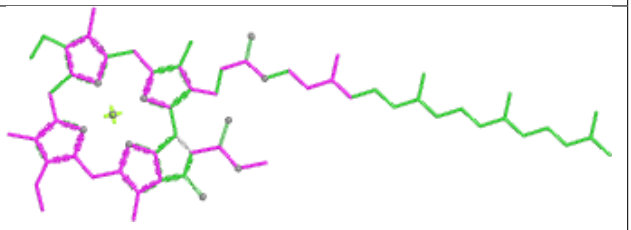


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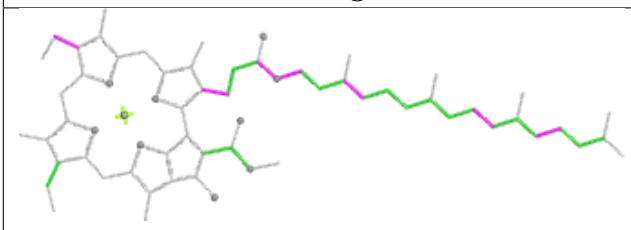
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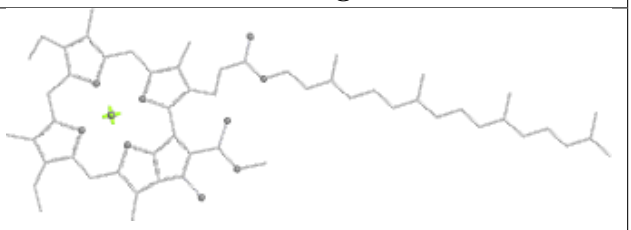
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Bond angles

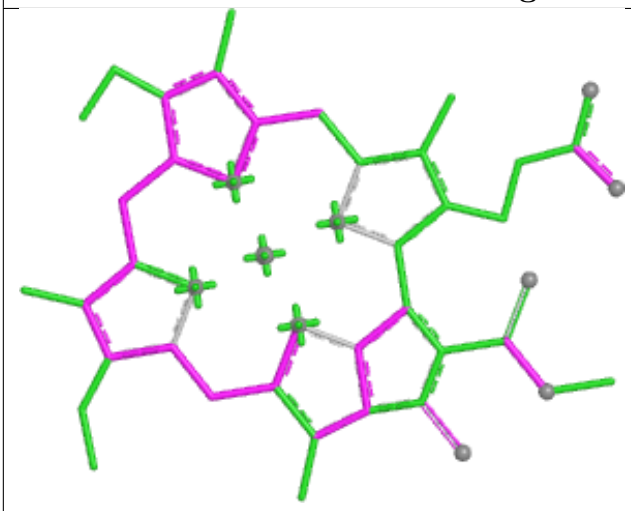


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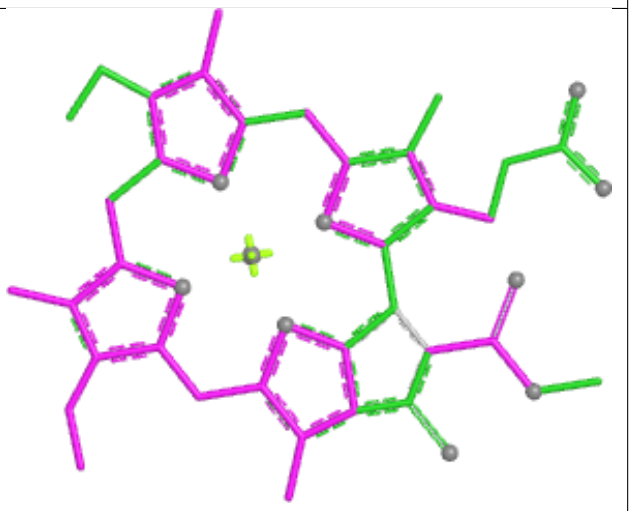


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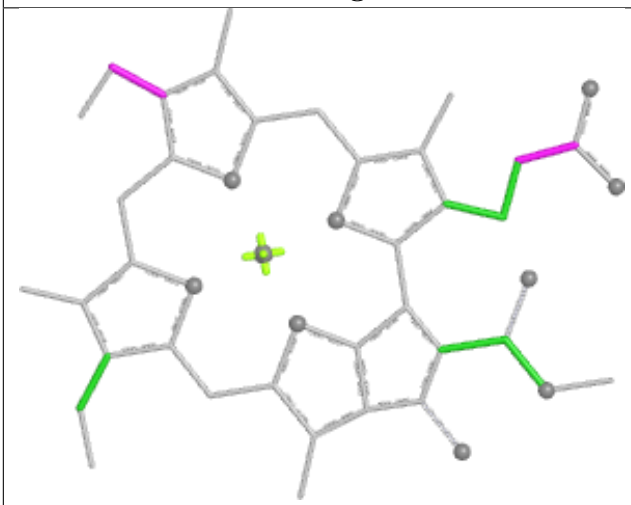
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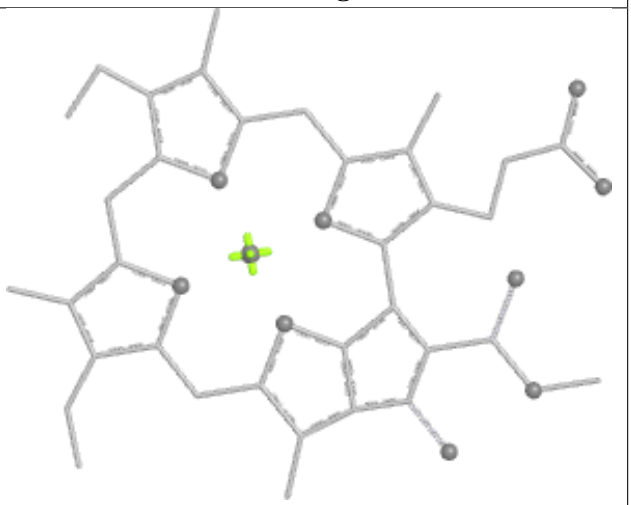
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Bond angles

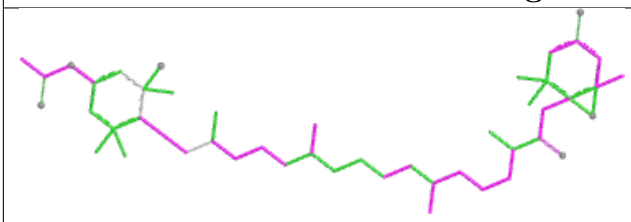


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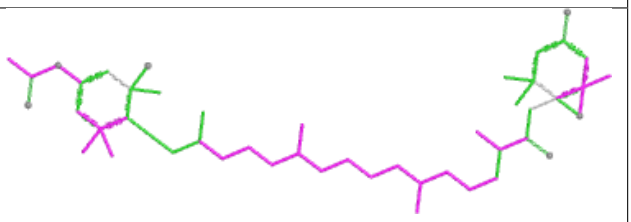


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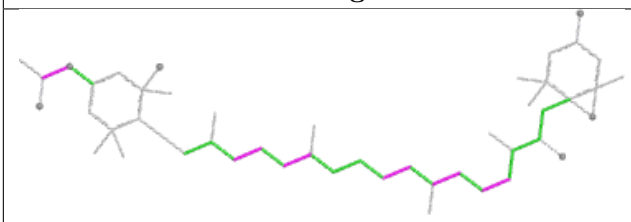
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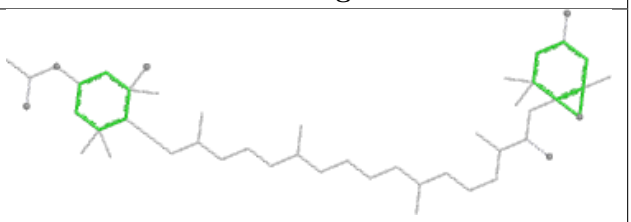
Bond lengths



Bond angles

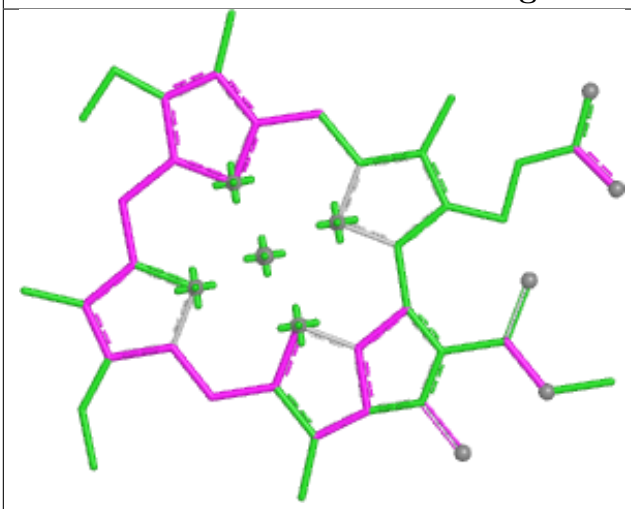


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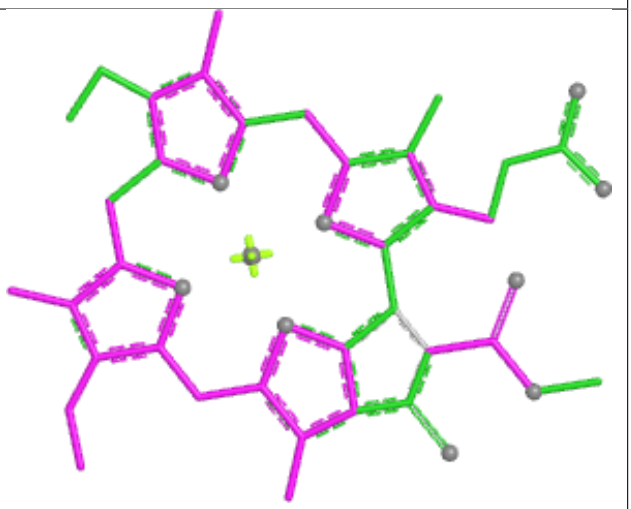


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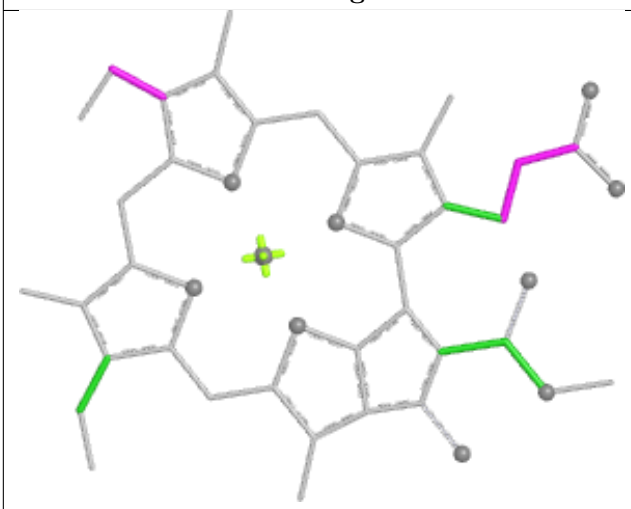
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Bond lengths



Bond angles

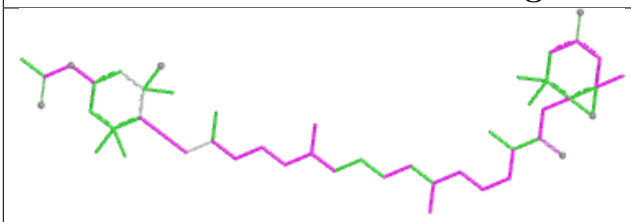


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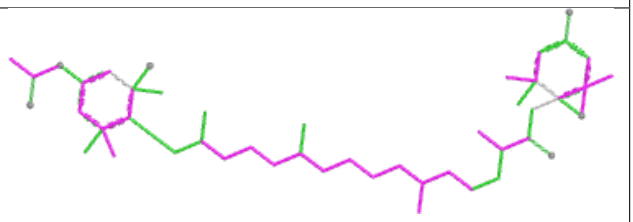


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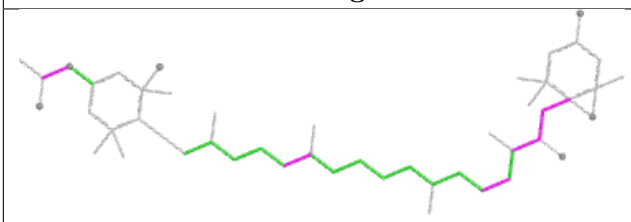
## Ligand A86 37 314



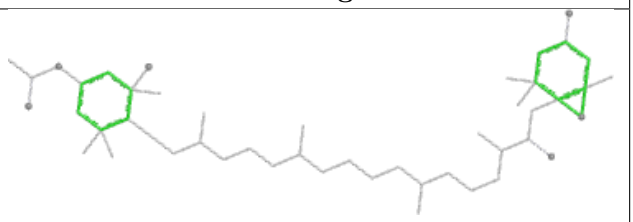
Bond lengths



Bond angles

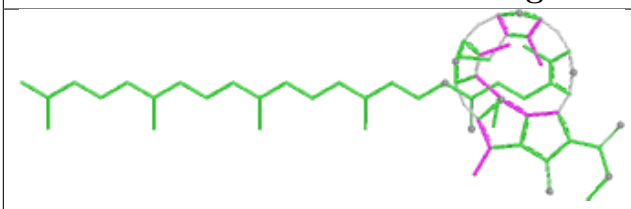


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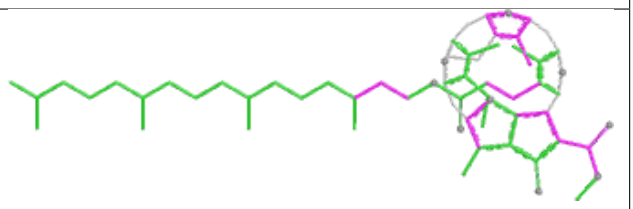


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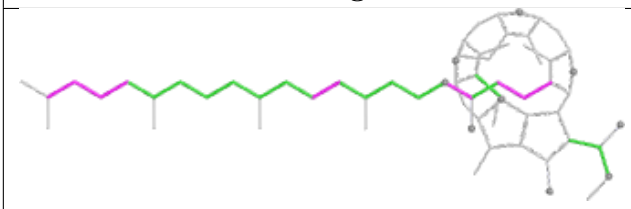
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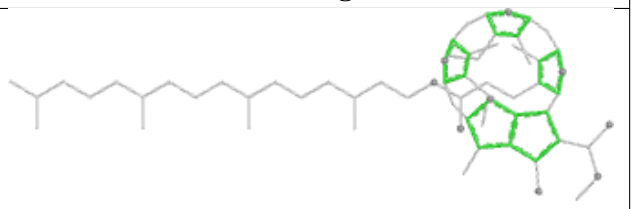
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Bond angles

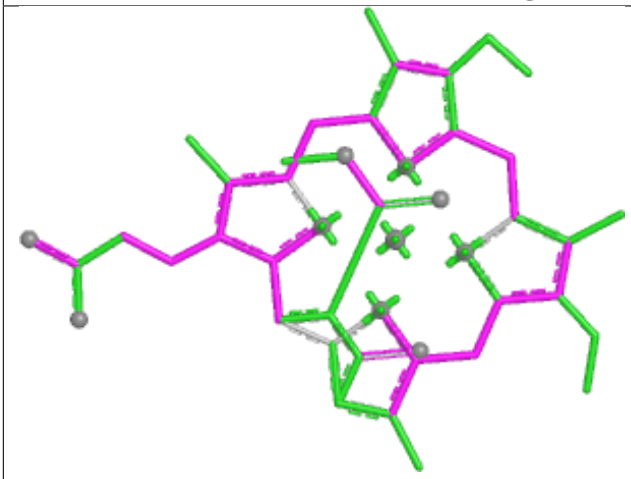


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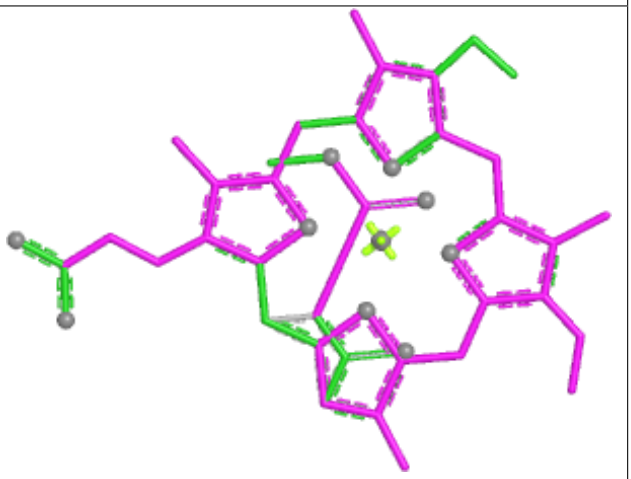


Rings

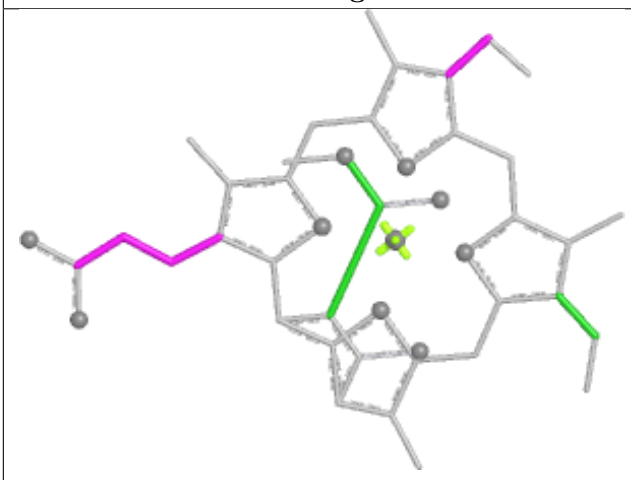
**Ligand KC1 37 302**



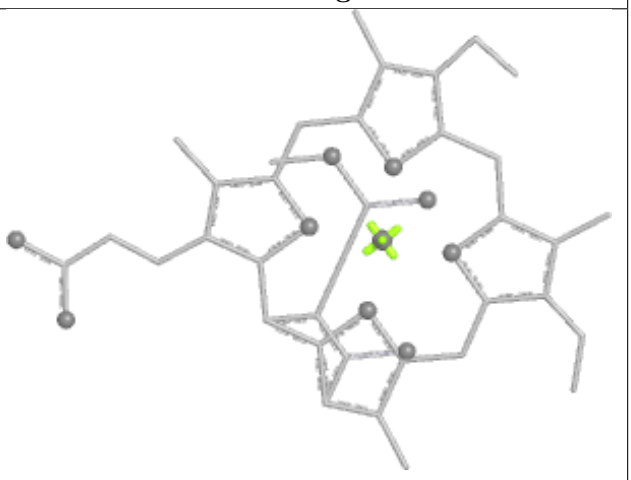
**Bond lengths**



**Bond angles**

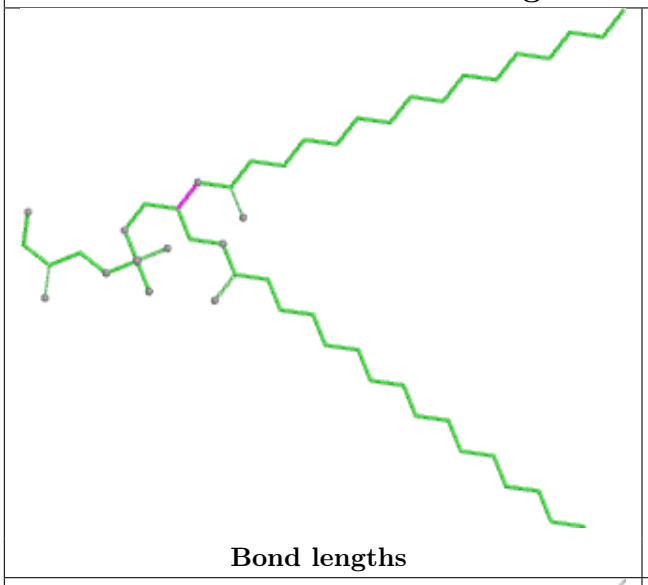


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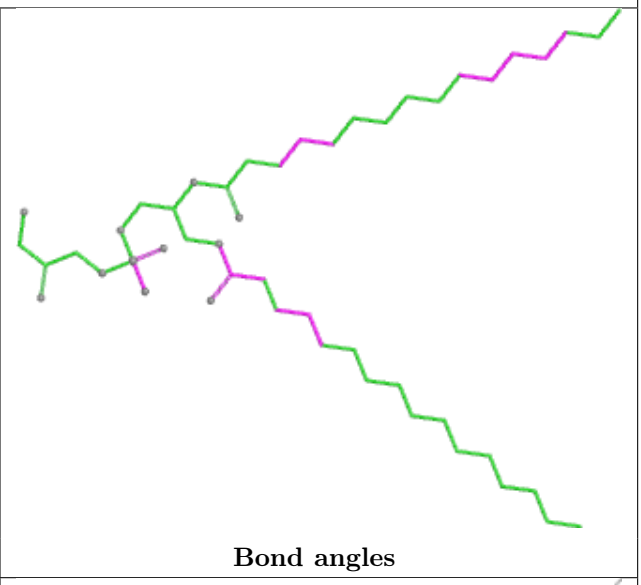


**Rings**

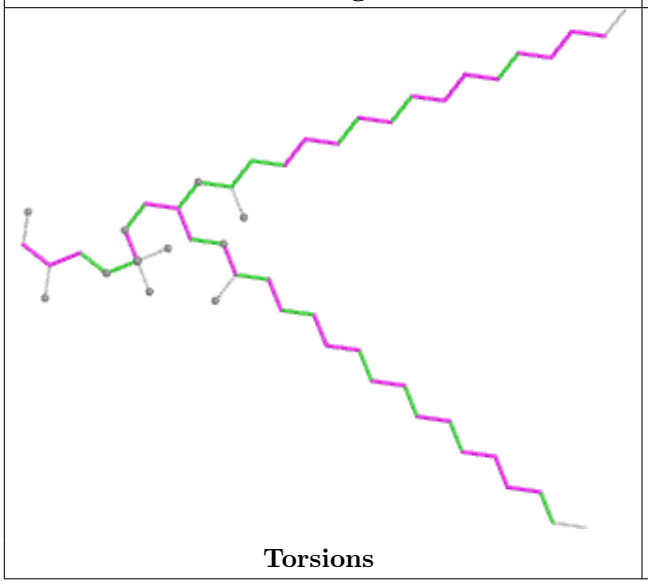
## Ligand LHG D 409



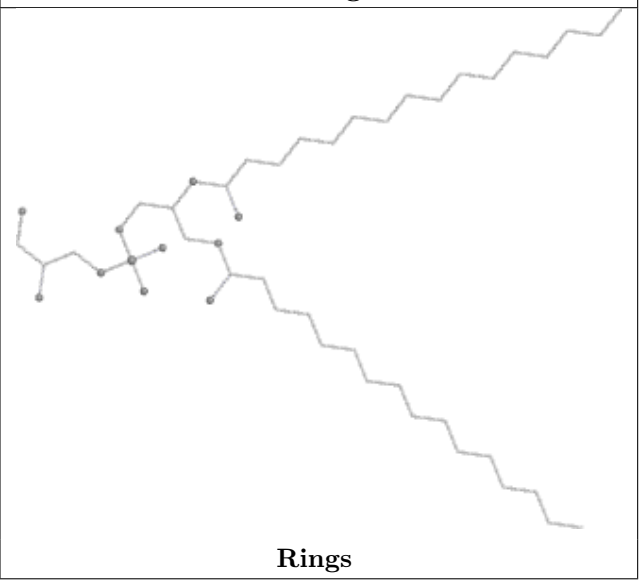
Bond lengths



Bond angles

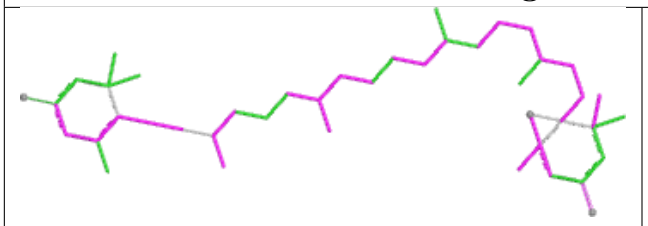


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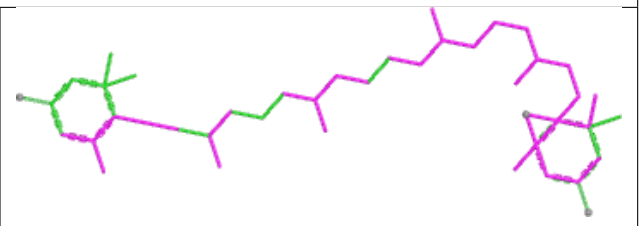


Rings

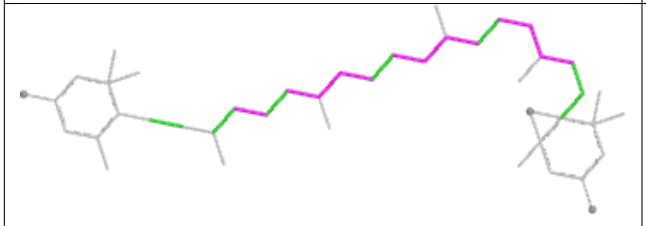
## Ligand DD6 21 216



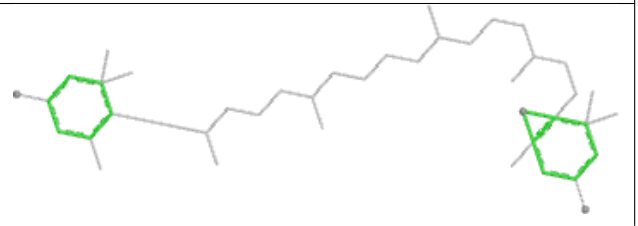
Bond lengths



Bond angles

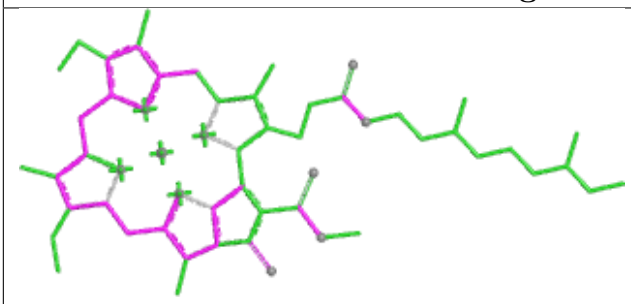


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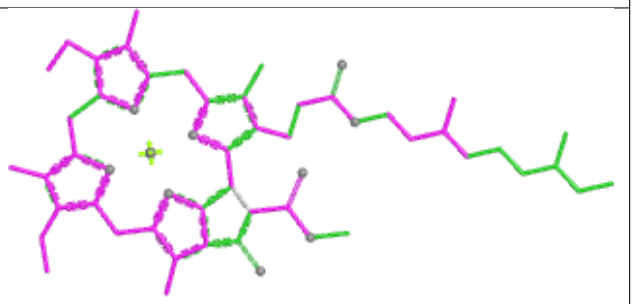


Rings

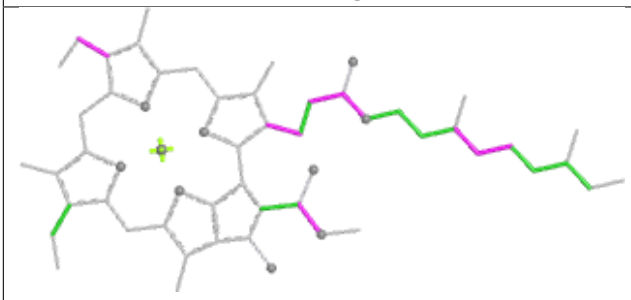
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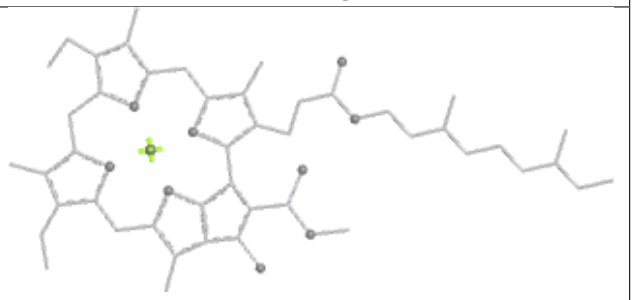
**Bond lengths**



**Bond angles**

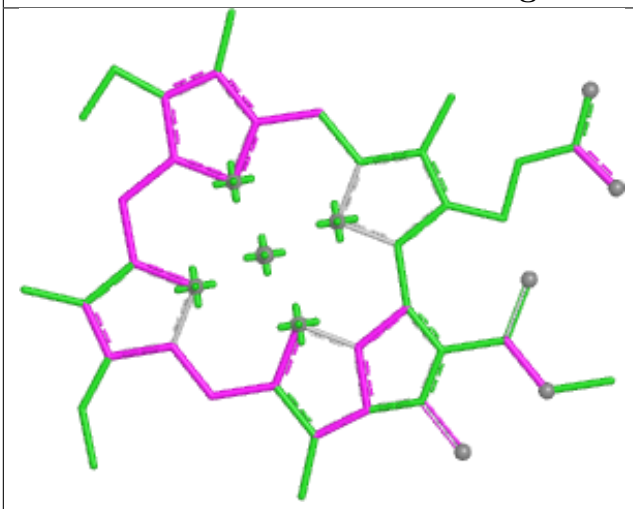


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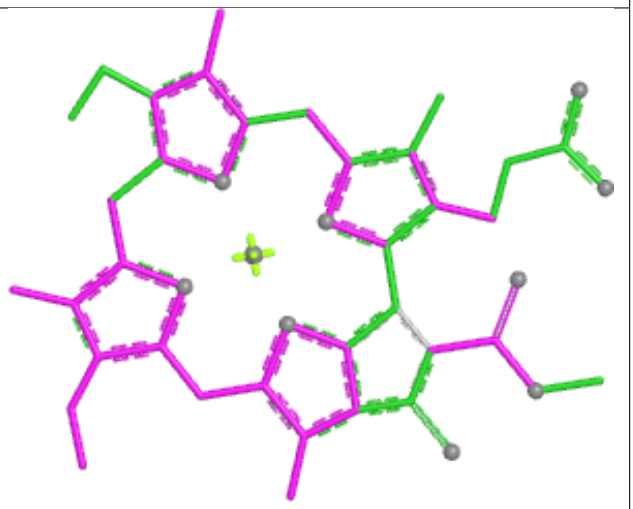


**Rings**

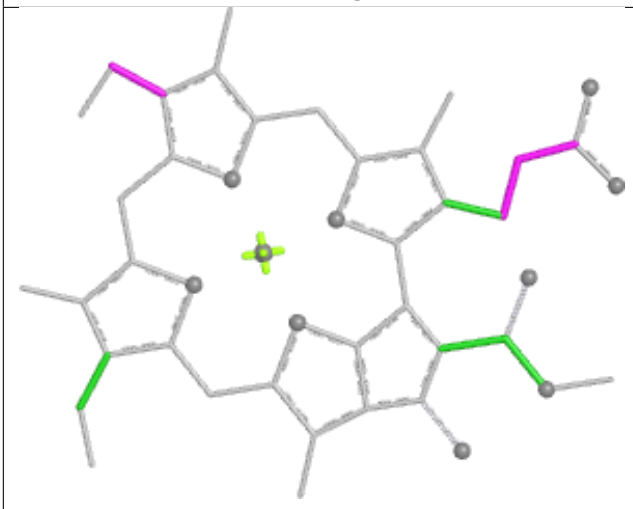
## Ligand CLA 39 309



Bond lengths



Bond angles

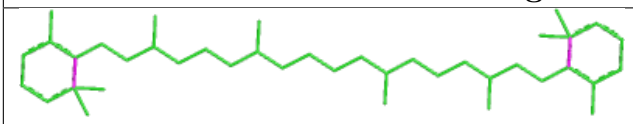


Torsions

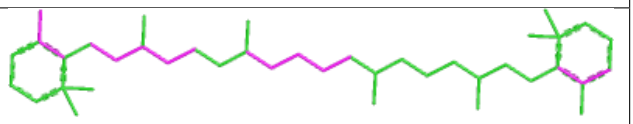


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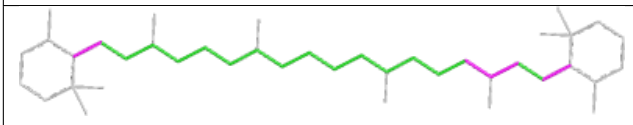
## Ligand BCR b 517



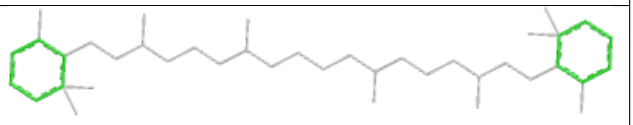
Bond lengths



Bond angles

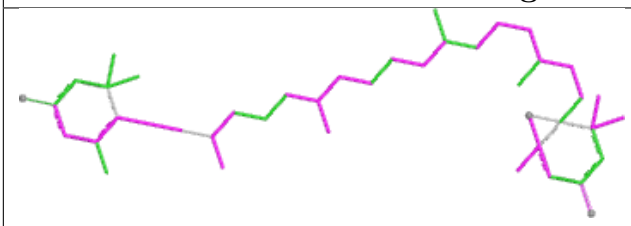


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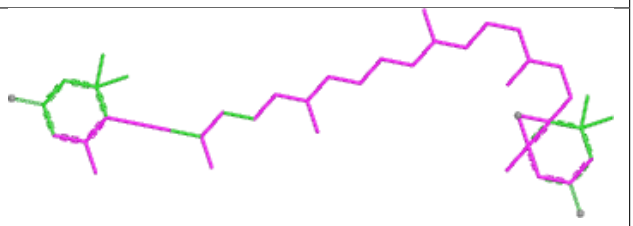


Rings

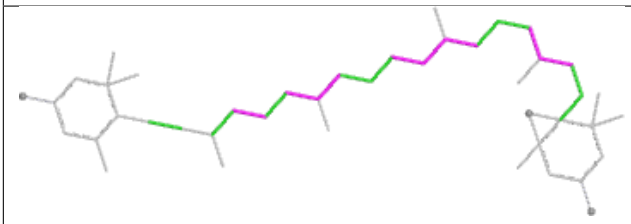
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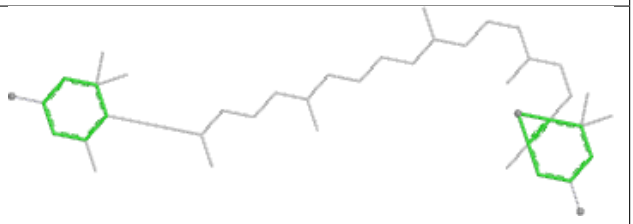
Bond lengths



Bond angles

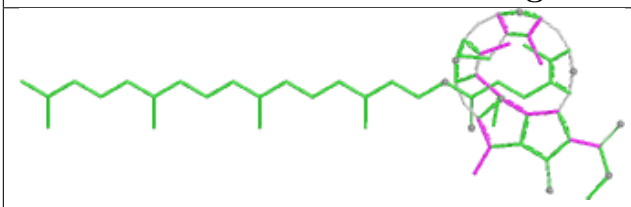


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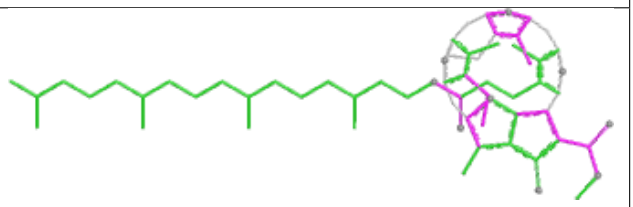


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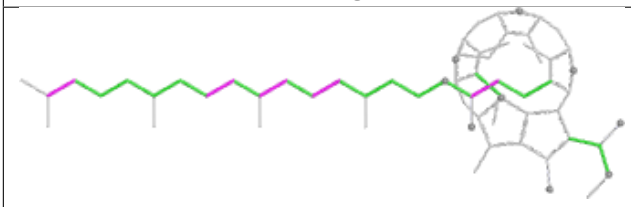
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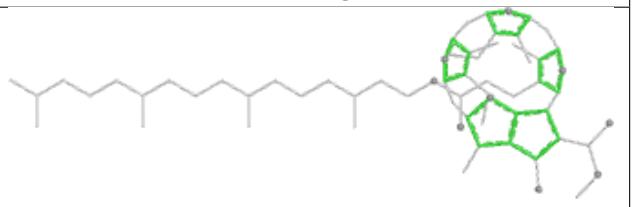
Bond lengths



Bond angles

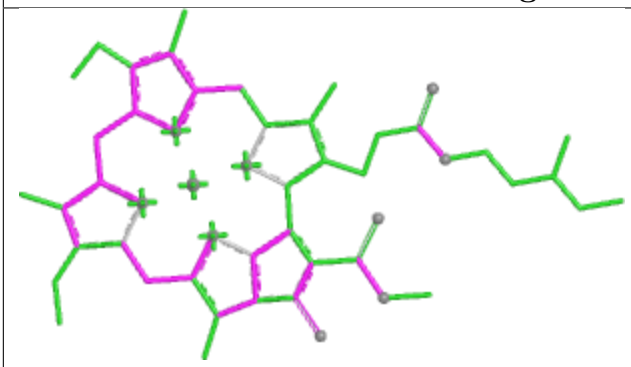


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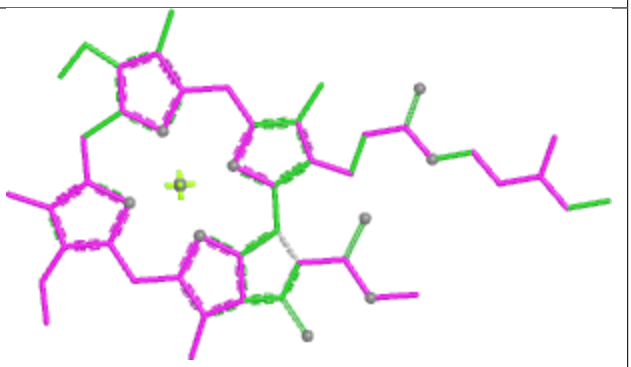


Rings

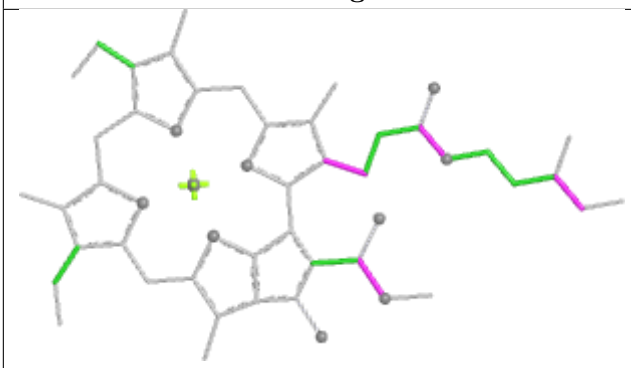
**Ligand CLA 11 310**



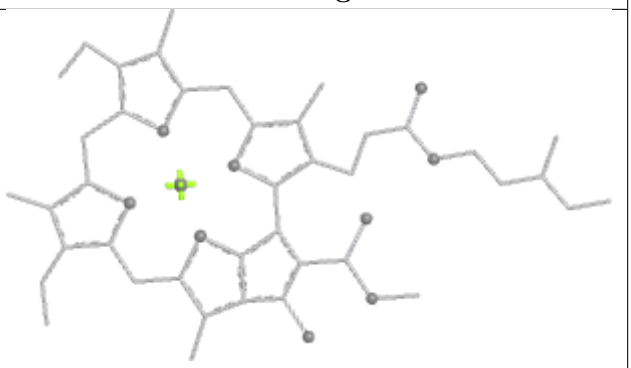
**Bond lengths**



**Bond angles**

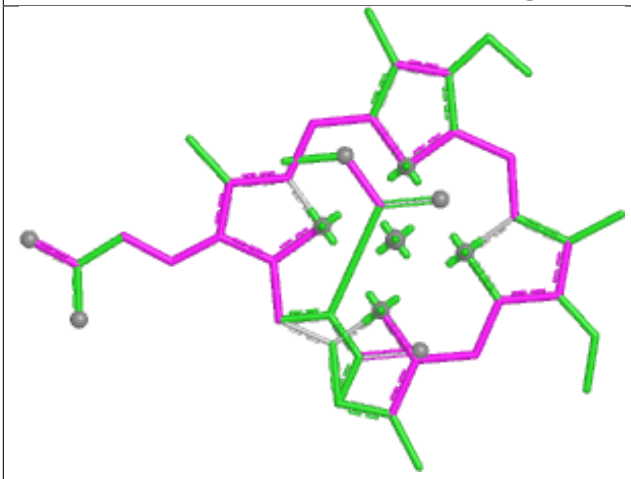


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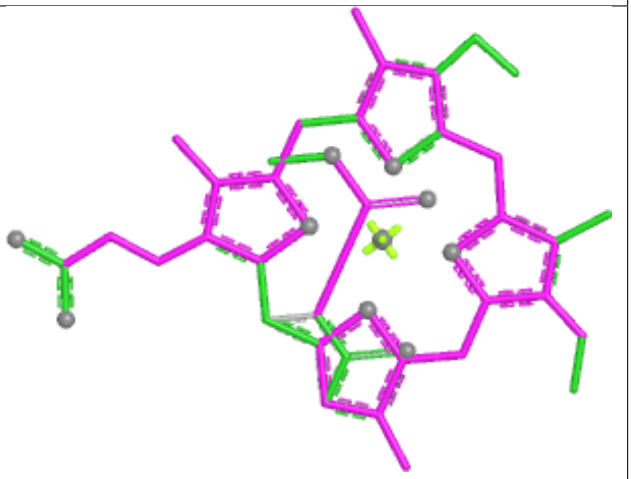


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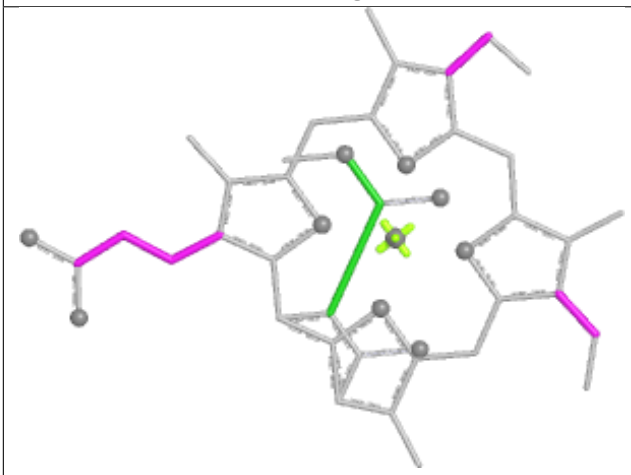
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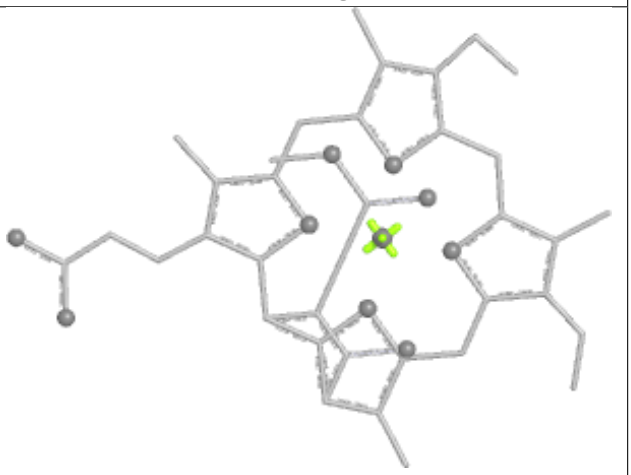
Bond lengths



Bond angles

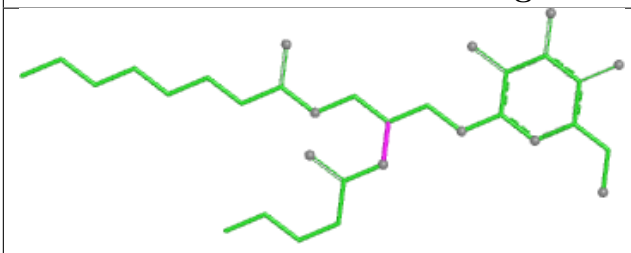


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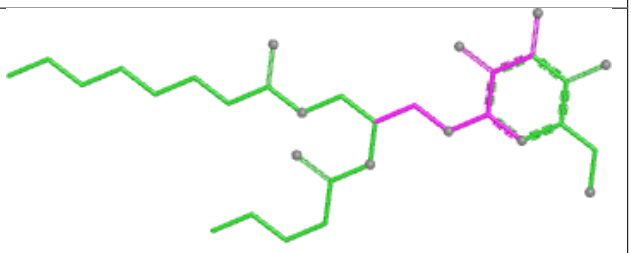


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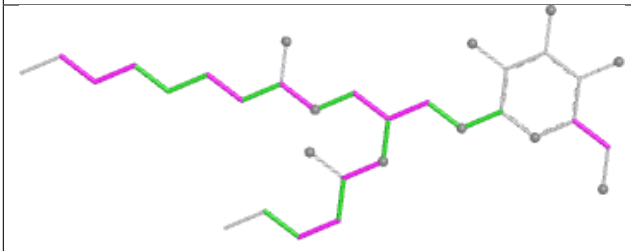
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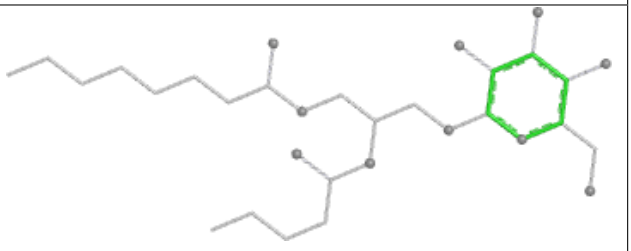
Bond lengths



Bond angles

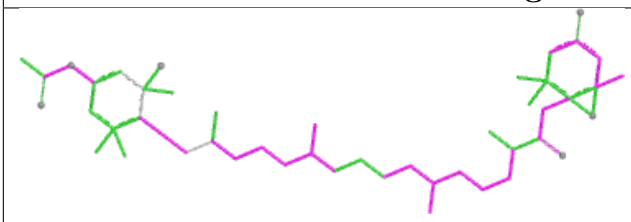


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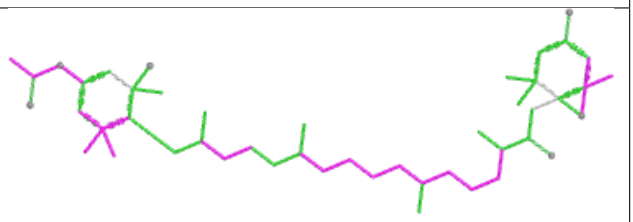


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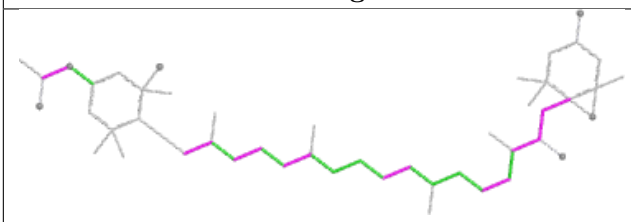
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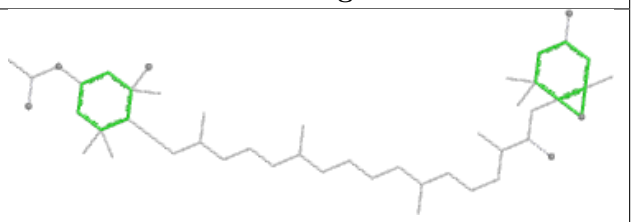
Bond lengths



Bond angles

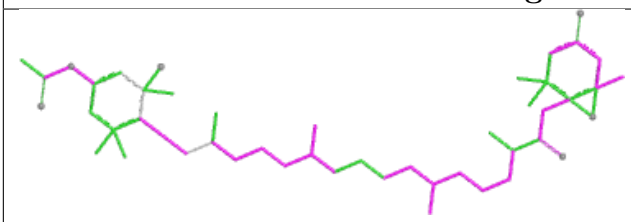


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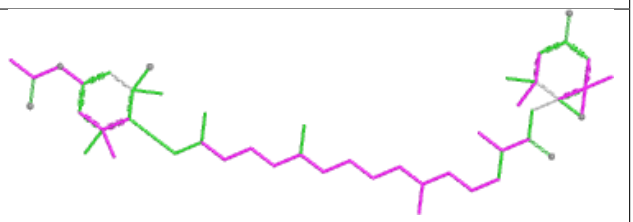


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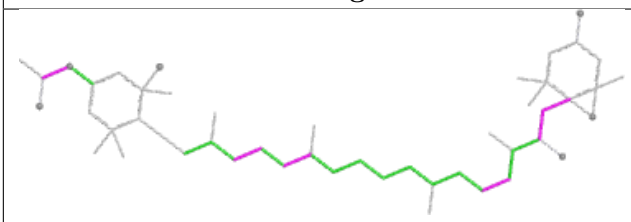
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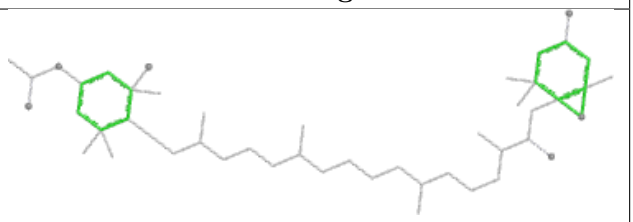
Bond lengths



Bond angles

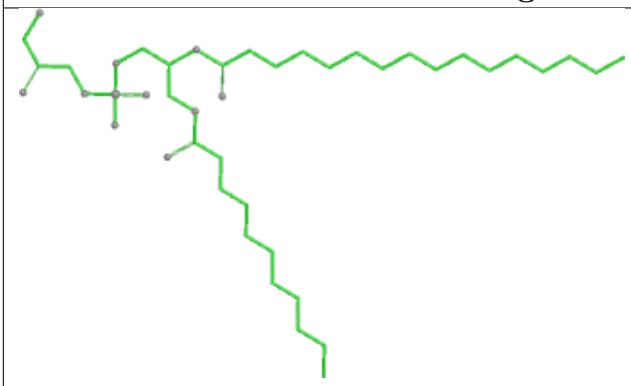


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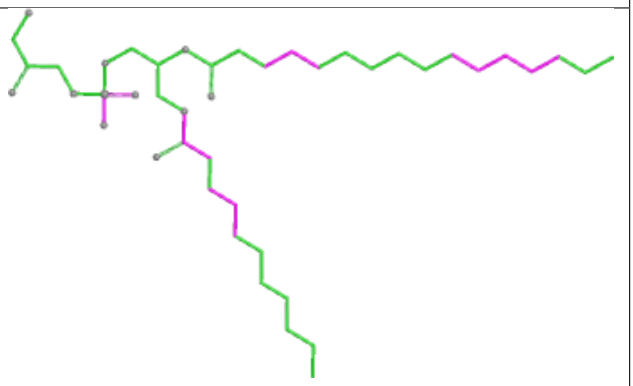


Rings

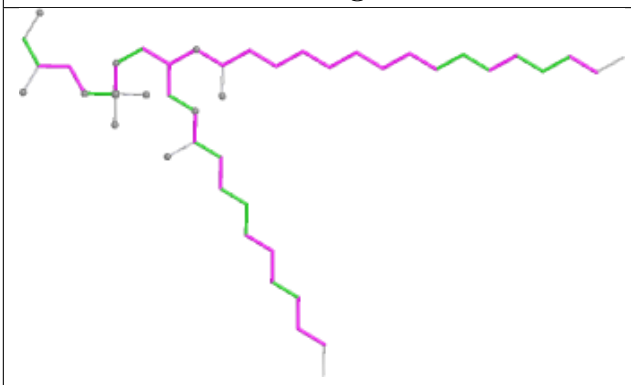
## Ligand LHG 17 316



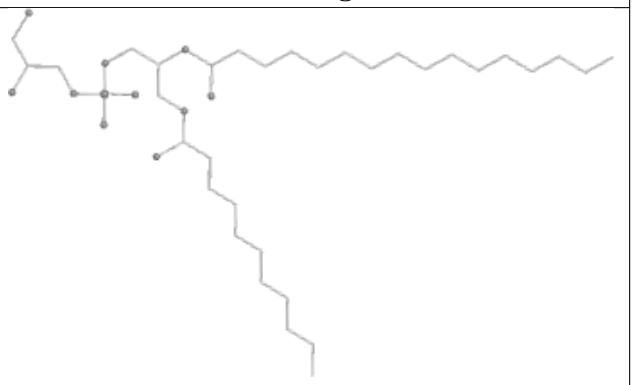
Bond lengths



Bond angles

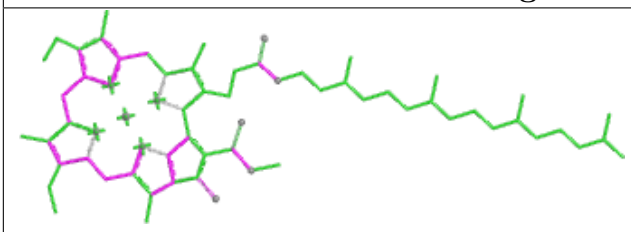


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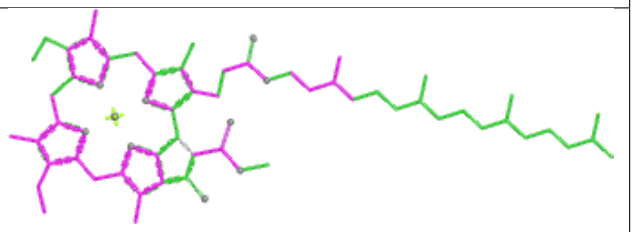


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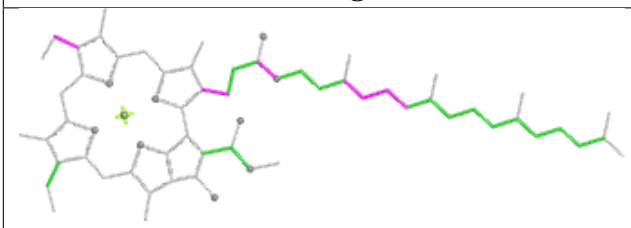
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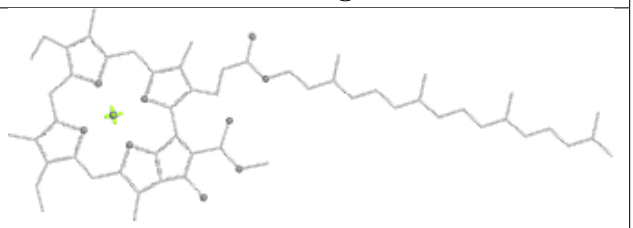
Bond lengths



Bond angles

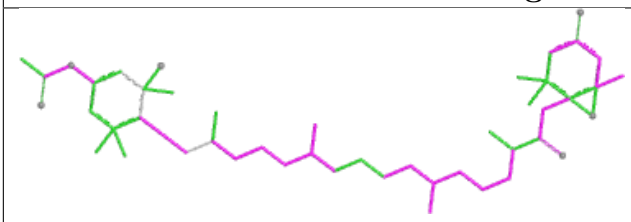


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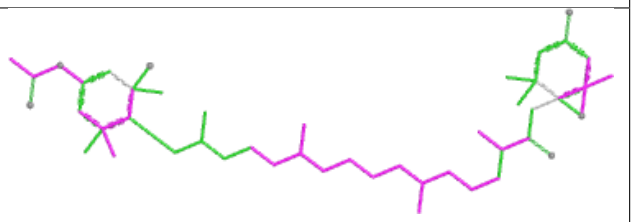


Rings

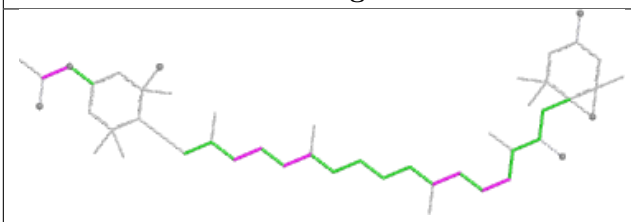
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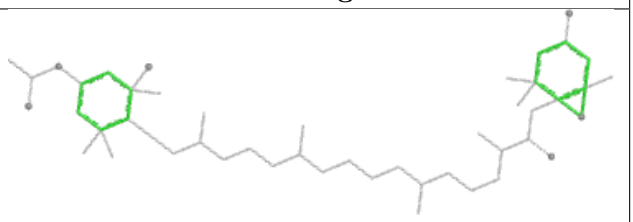
Bond lengths



Bond angles

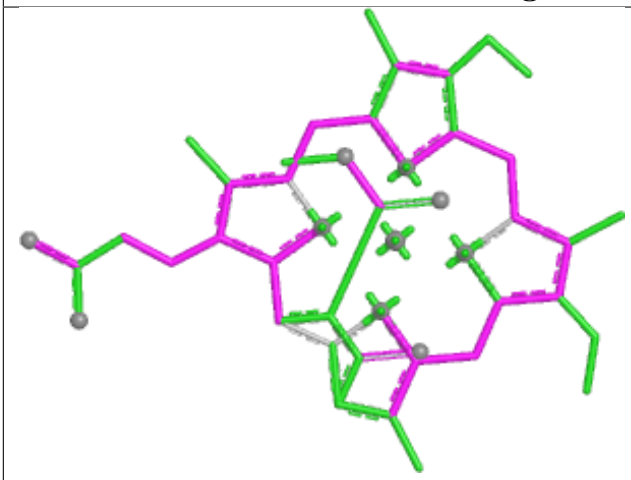


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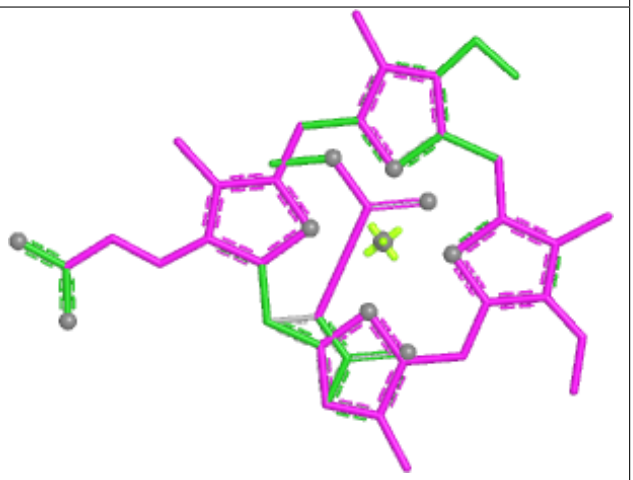


Rings

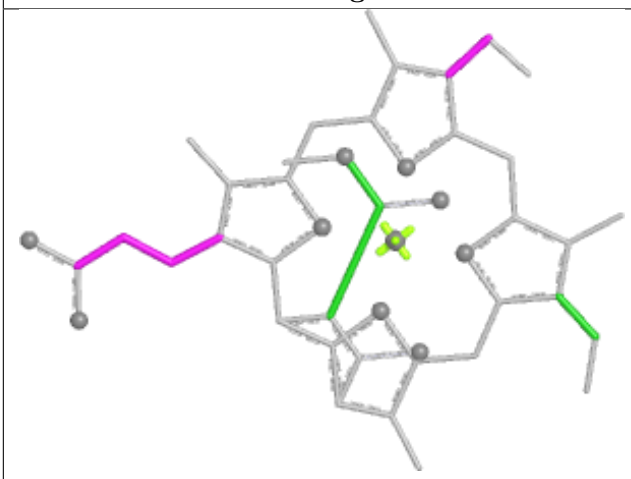
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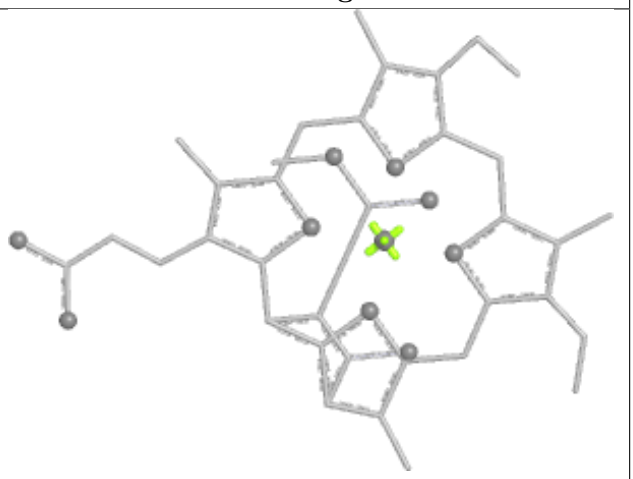
Bond lengths



Bond angles

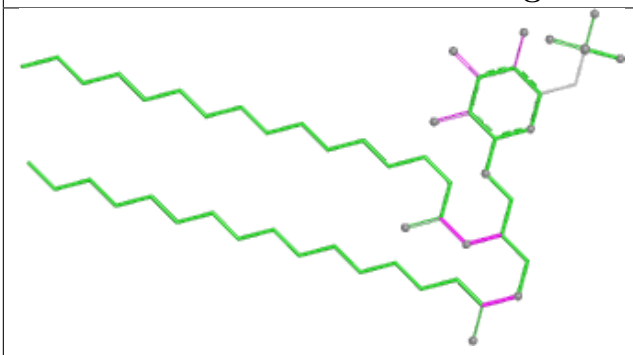


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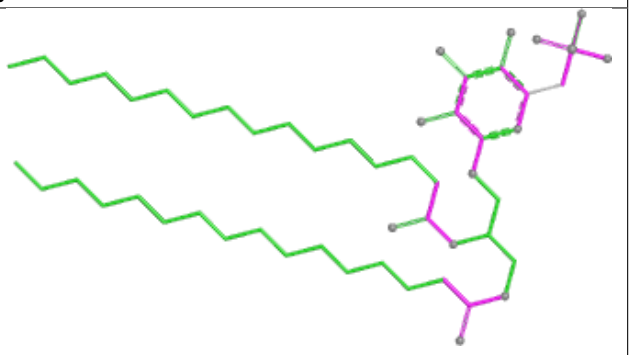


Rings

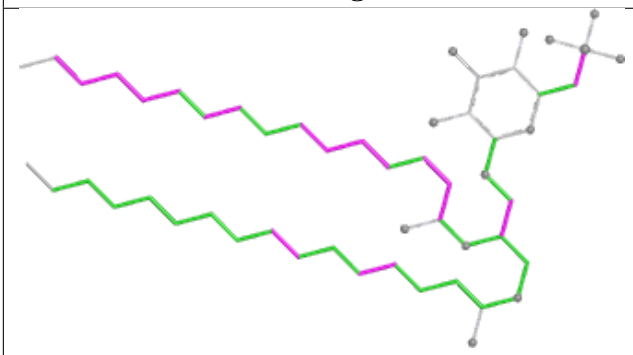
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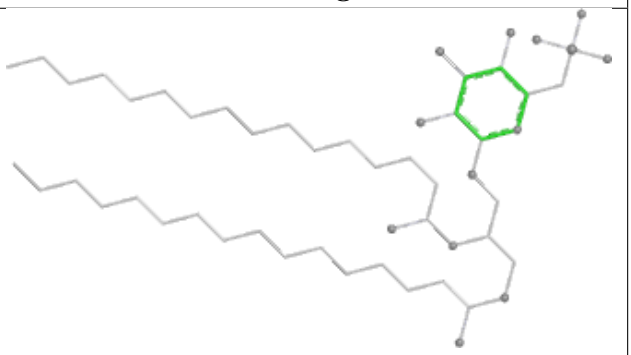
Bond lengths



Bond angles

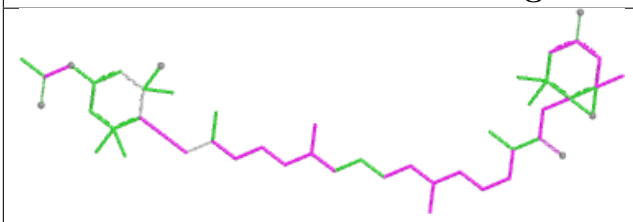


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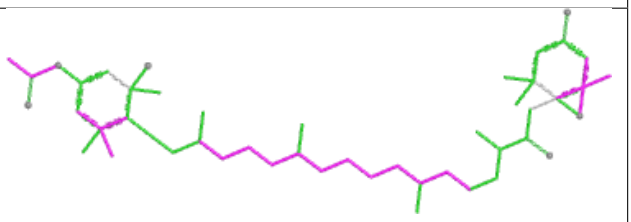


Rings

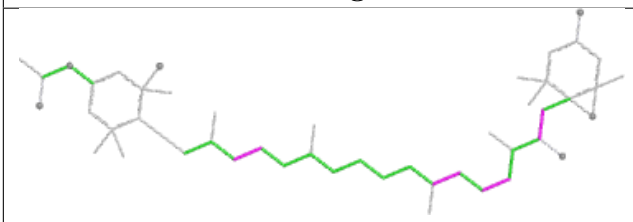
## Ligand A86 40 211



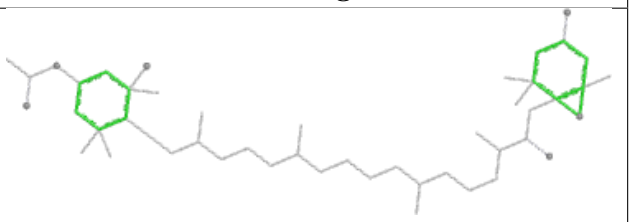
Bond lengths



Bond angles



Torsions

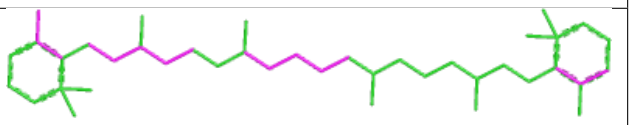


Rings

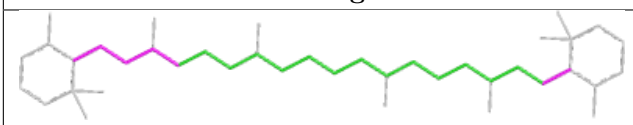
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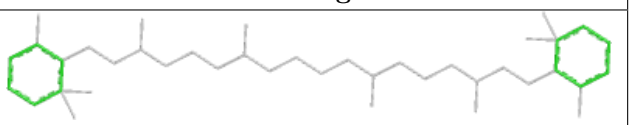
Bond lengths



Bond angles

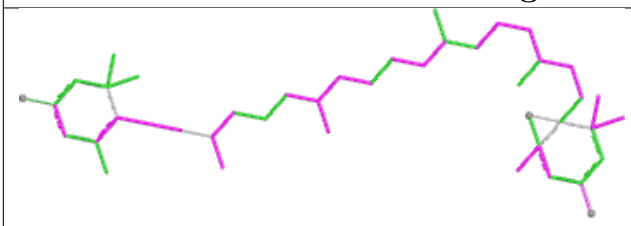


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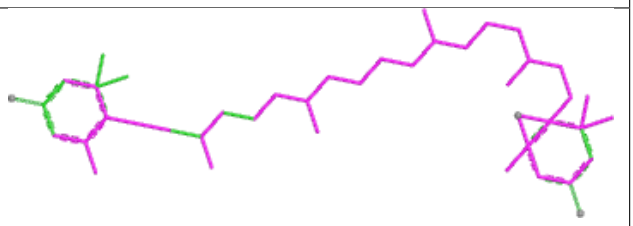


Rings

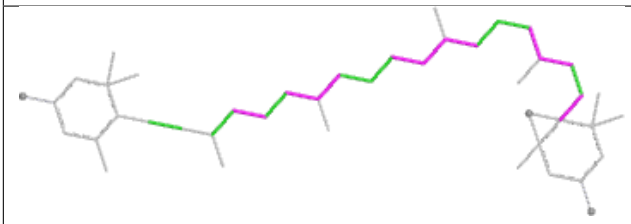
## Ligand DD6 39 312



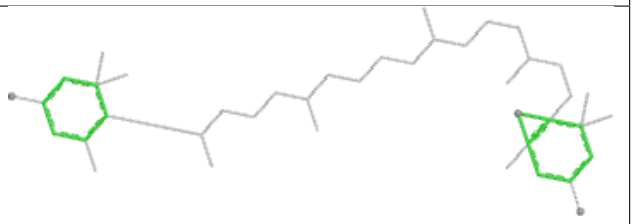
Bond lengths



Bond angles

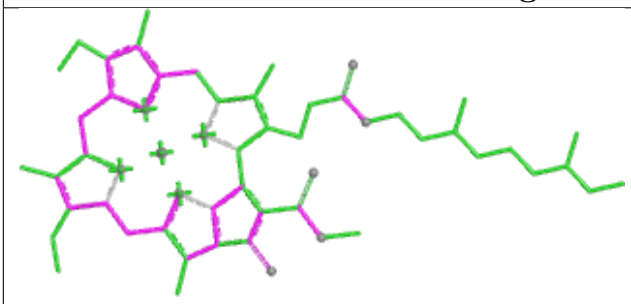


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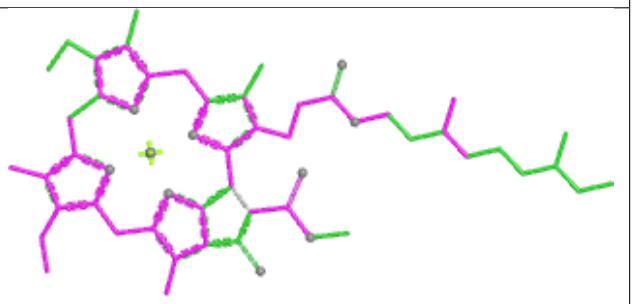


Rings

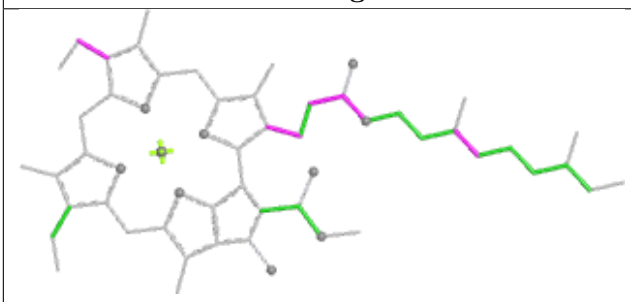
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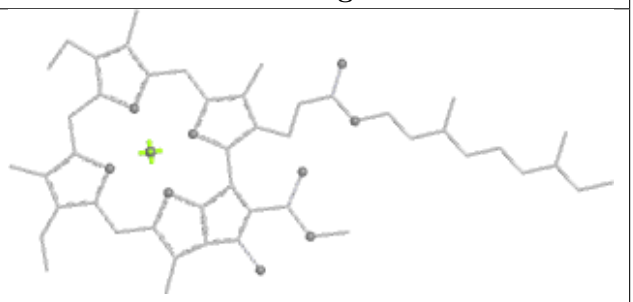
Bond lengths



Bond angles

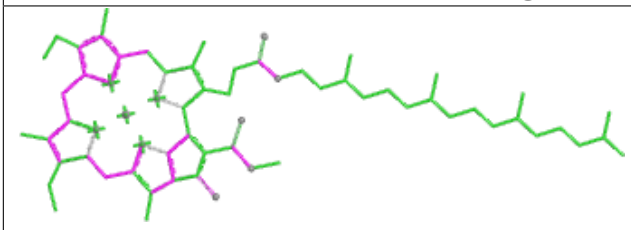


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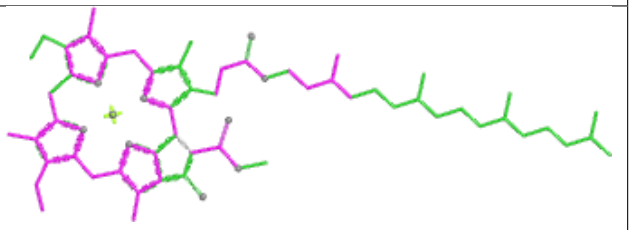


Rings

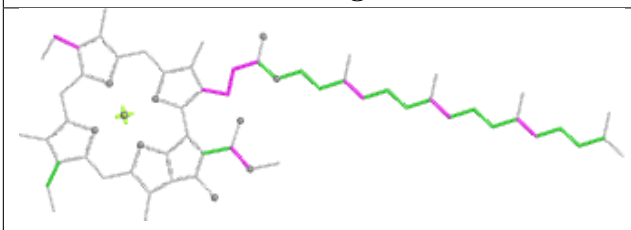
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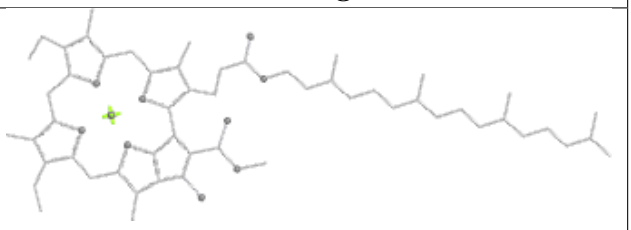
Bond lengths



Bond angles

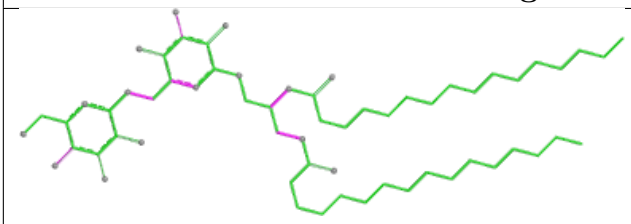


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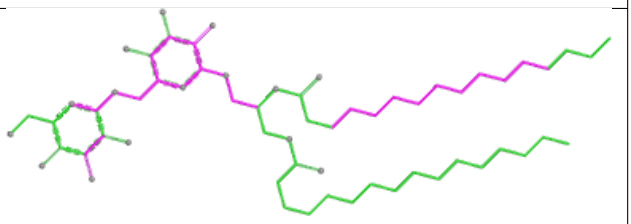


Rings

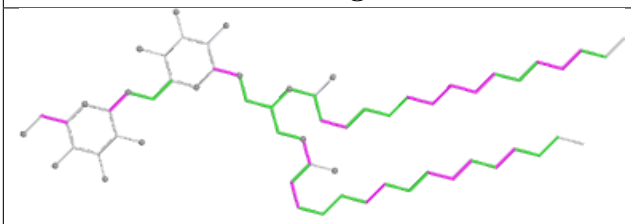
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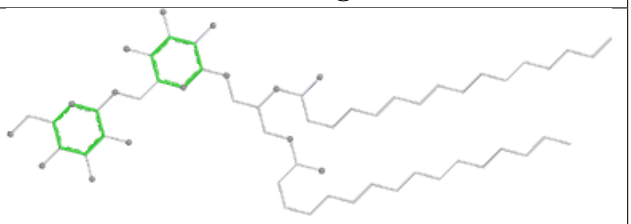
Bond lengths



Bond angles

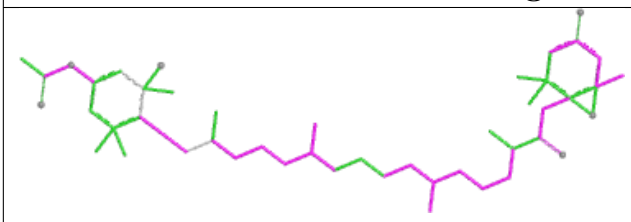


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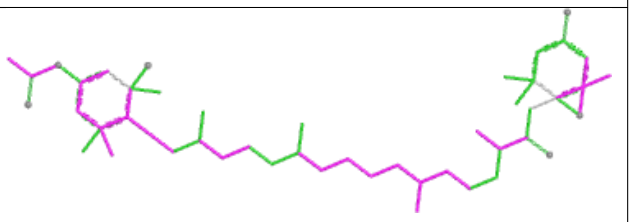


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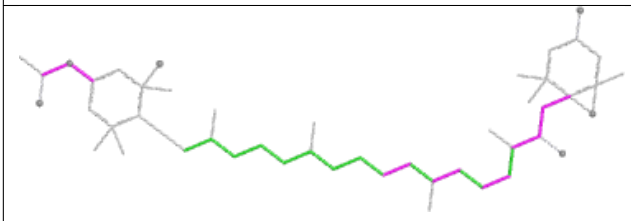
## Ligand A86 18 215



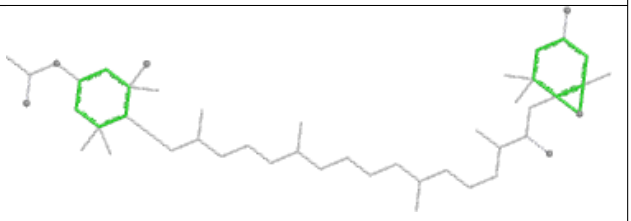
Bond lengths



Bond angles

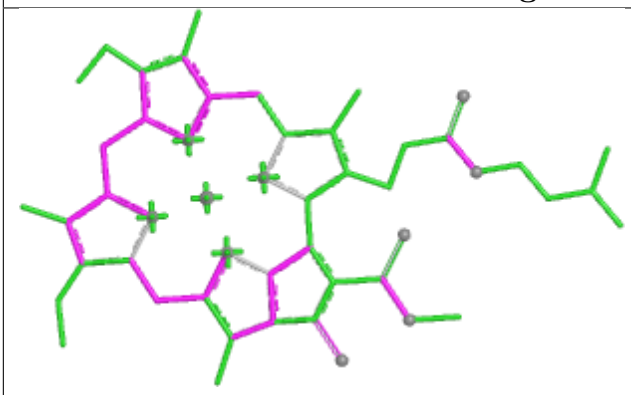


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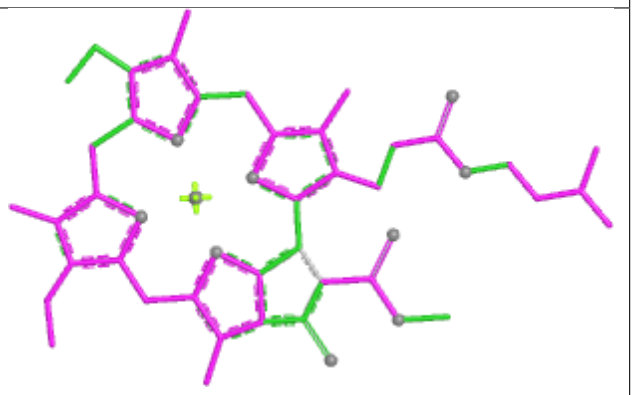


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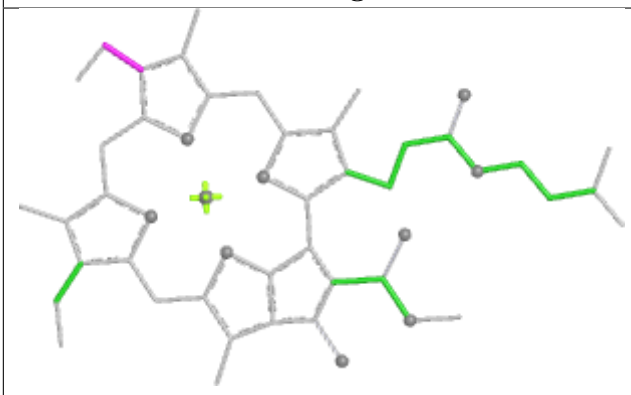
## Ligand CLA 12 207



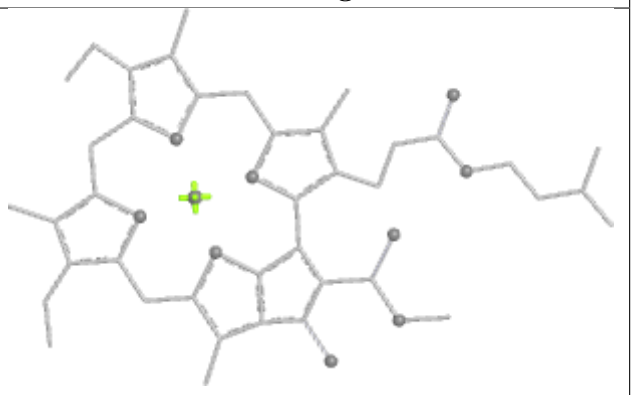
Bond lengths



Bond angles

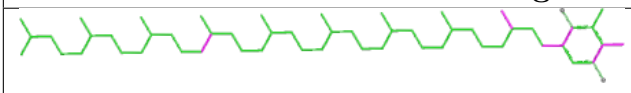


Torsions



Rings

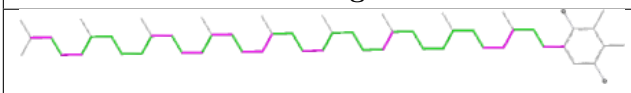
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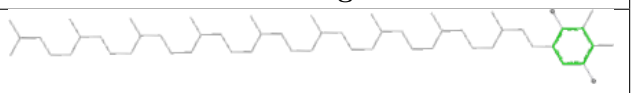
Bond lengths



Bond angles

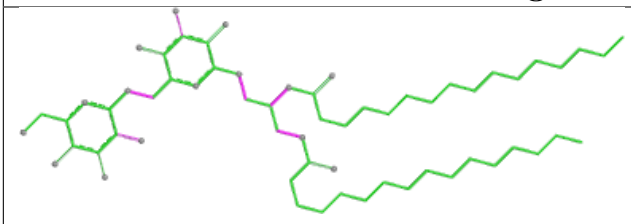


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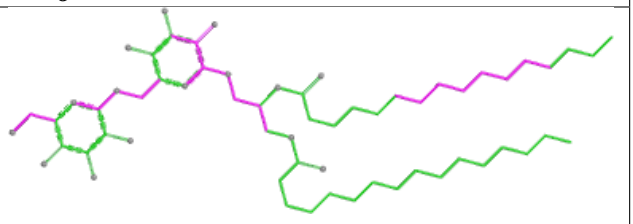


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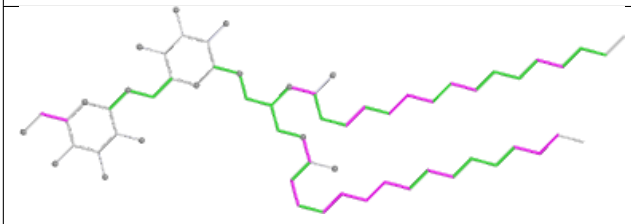
## Ligand DGD j 101



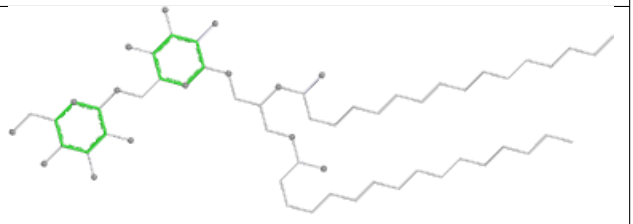
Bond lengths



Bond angles

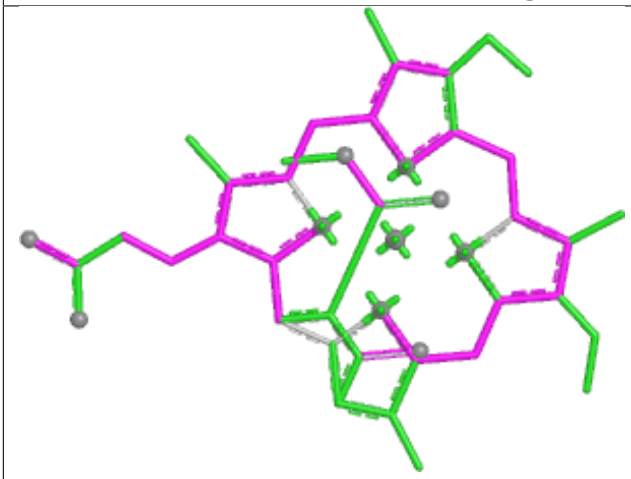


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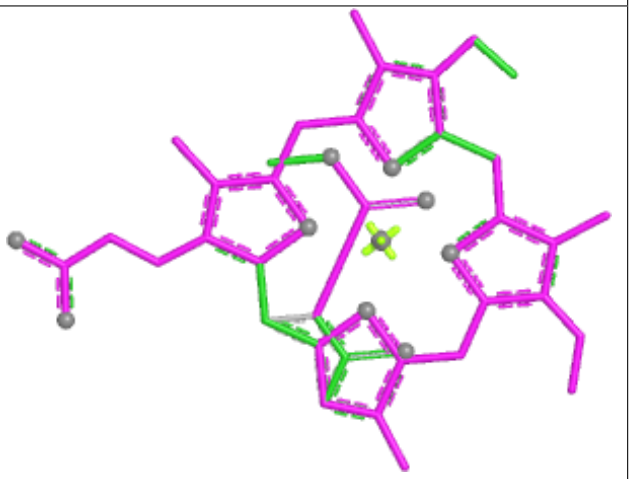


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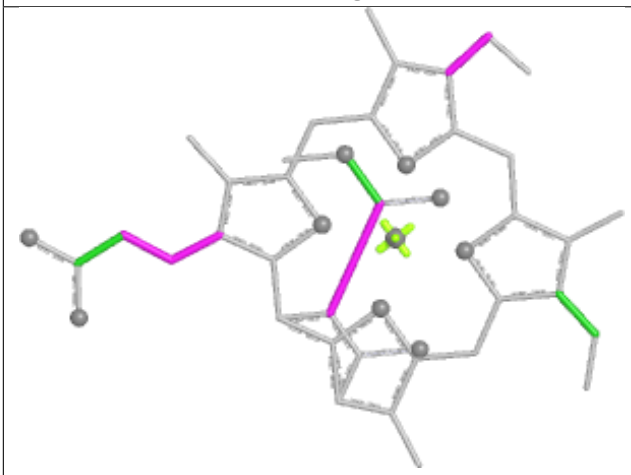
**Ligand KC1 18 207**



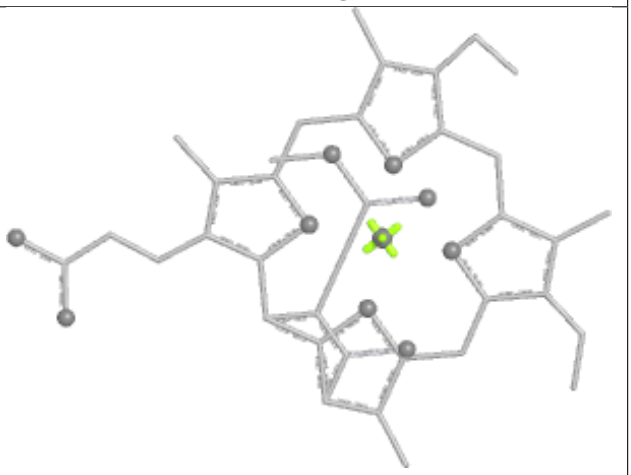
Bond lengths



Bond angles

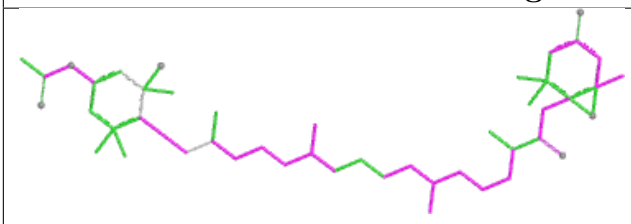


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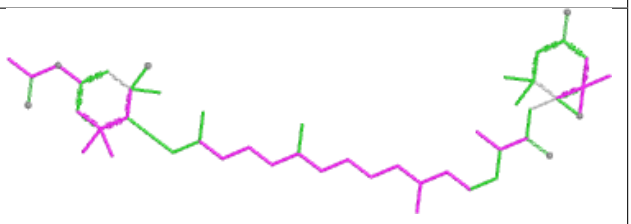


Rings

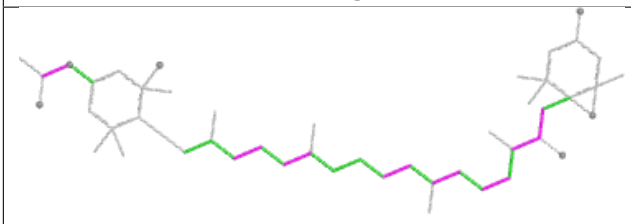
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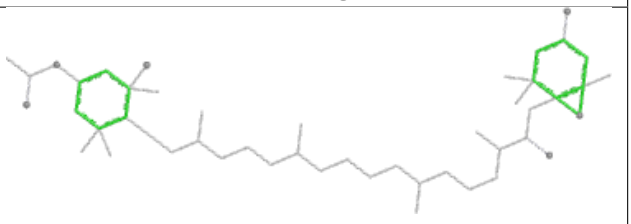
Bond lengths



Bond angles

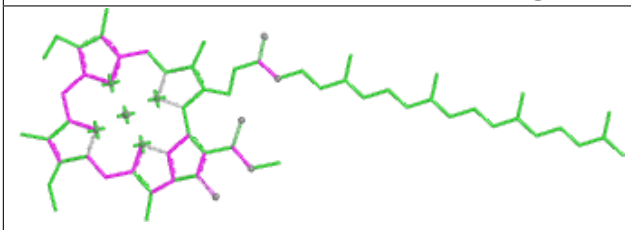


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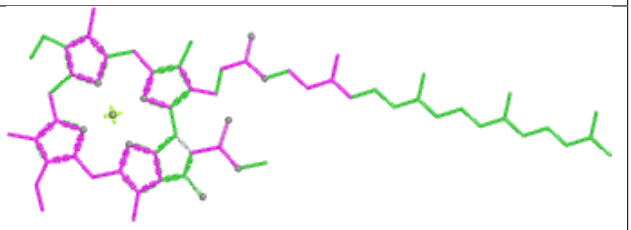


Rings

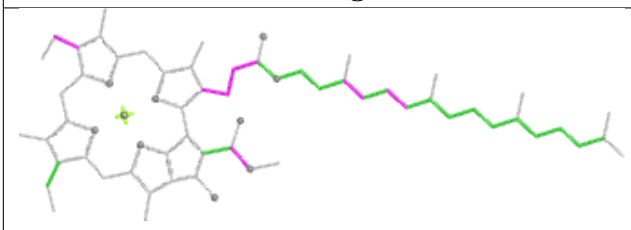
**Ligand CLA c 501**



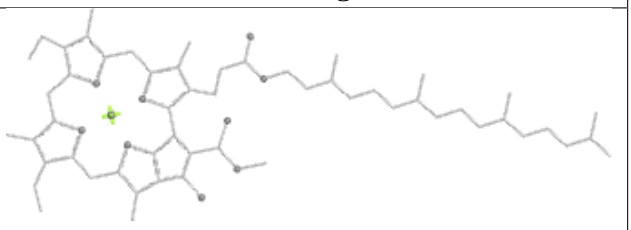
Bond lengths



Bond angles

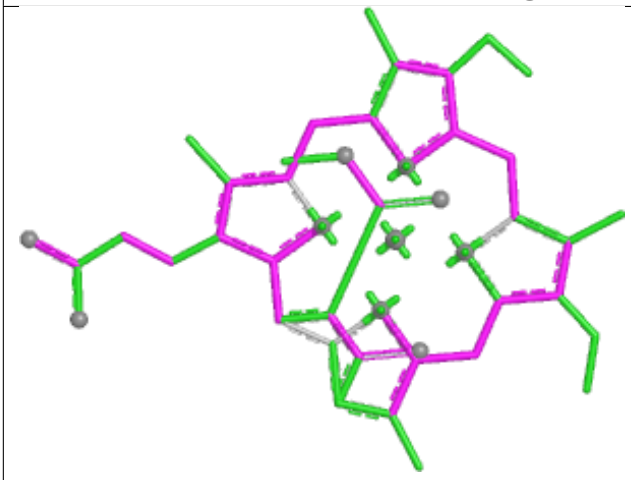


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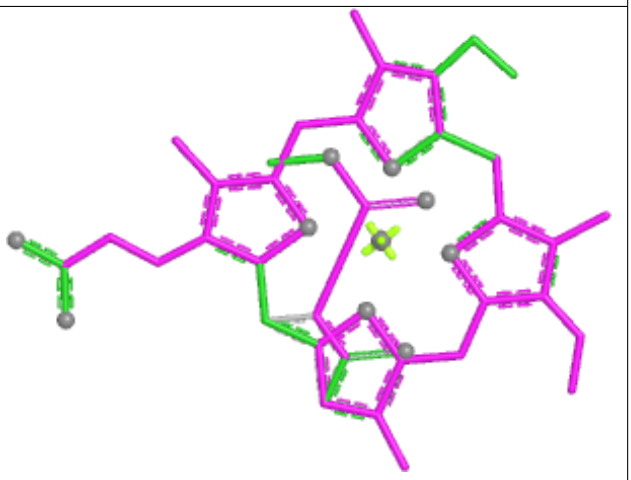


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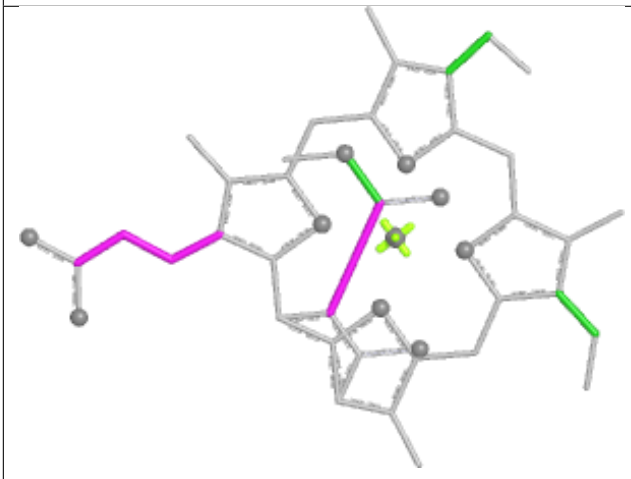
**Ligand KC1 32 212**



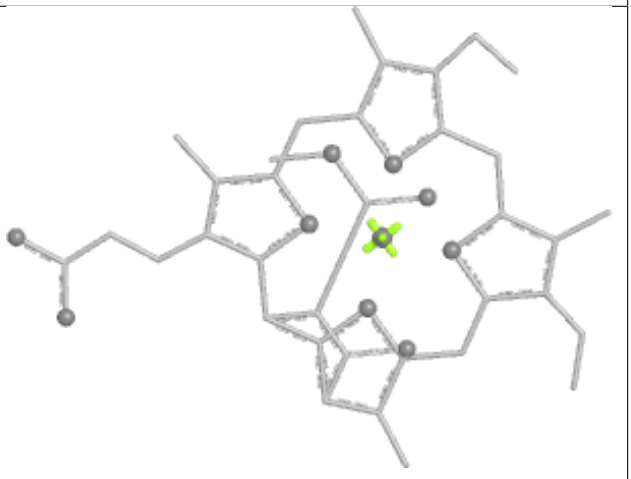
Bond lengths



Bond angles

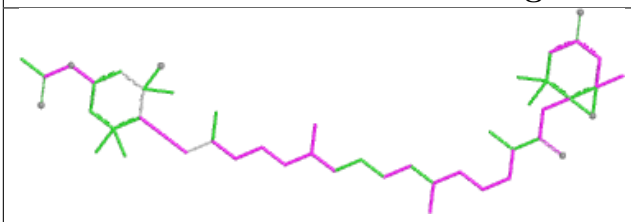


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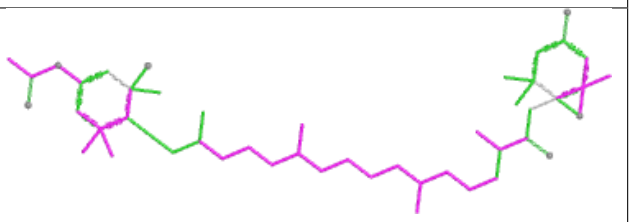


Rings

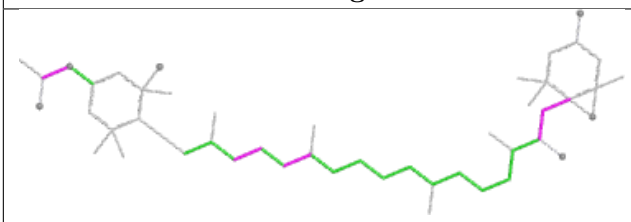
## Ligand A86 37 312



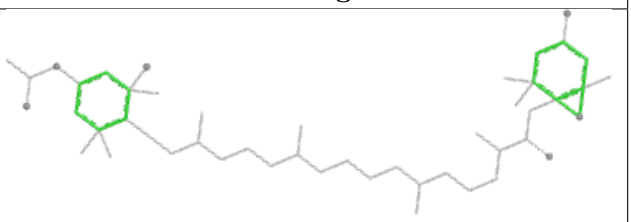
Bond lengths



Bond angles

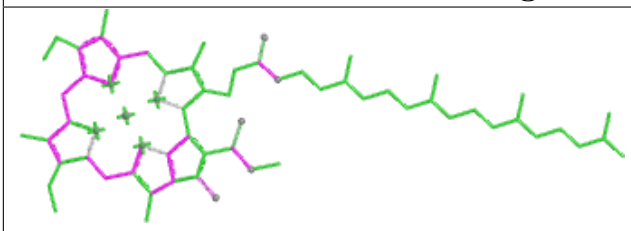


Torsions

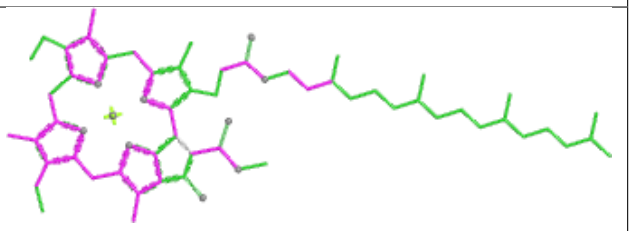


Rings

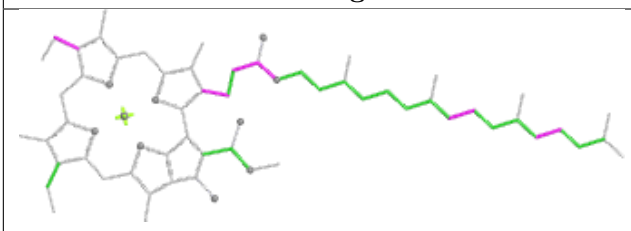
## Ligand CLA 15 301



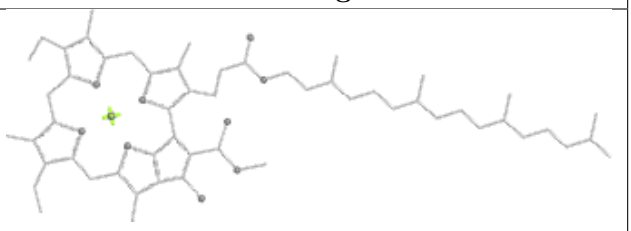
Bond lengths



Bond angles

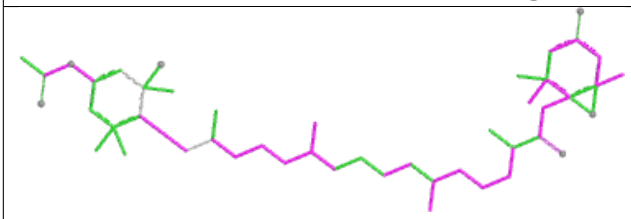


Torsions



Rings

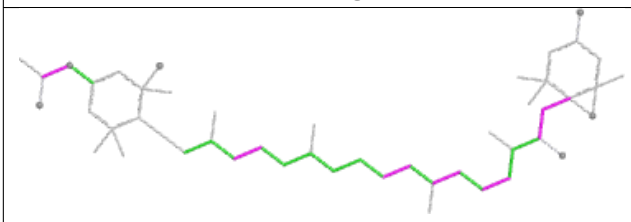
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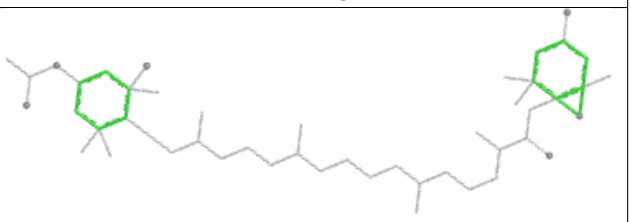
Bond lengths



Bond angles

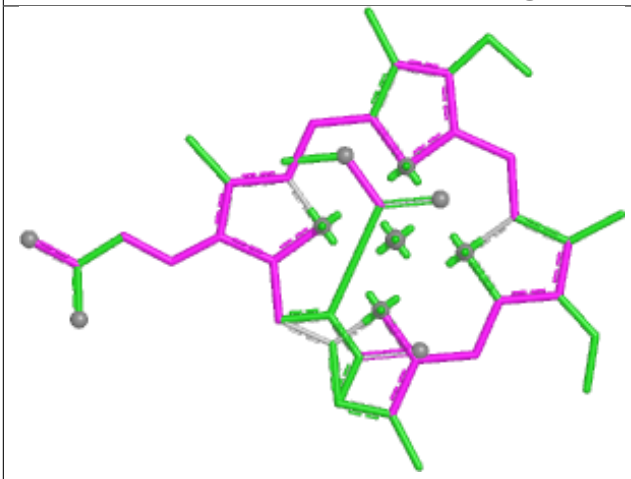


Torsions

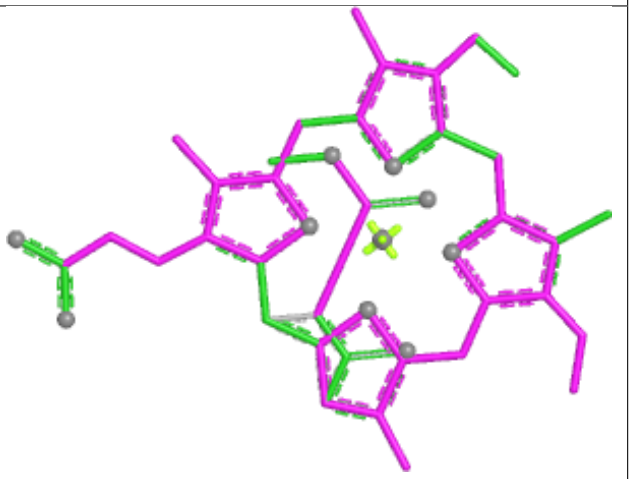


Rings

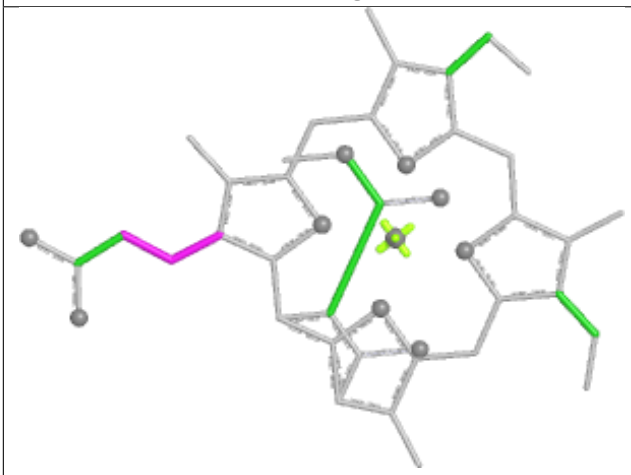
**Ligand KC1 16 302**



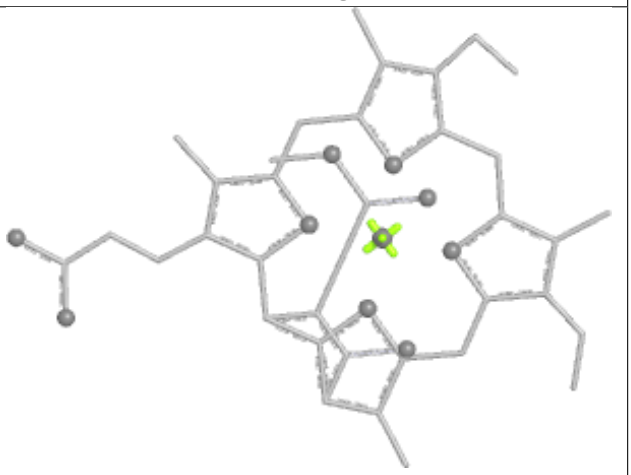
**Bond lengths**



**Bond angles**

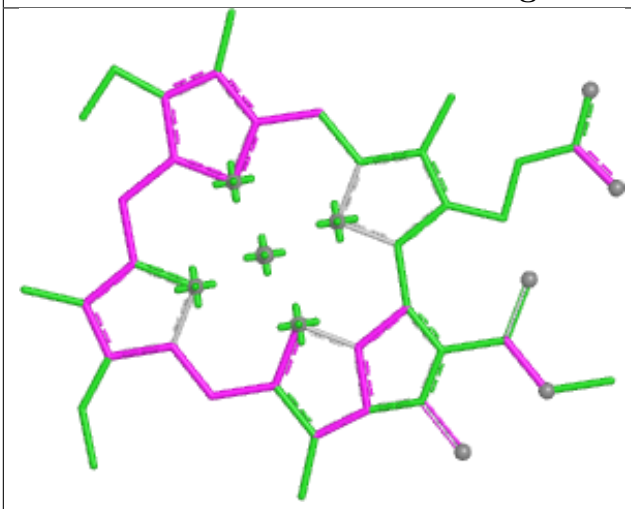


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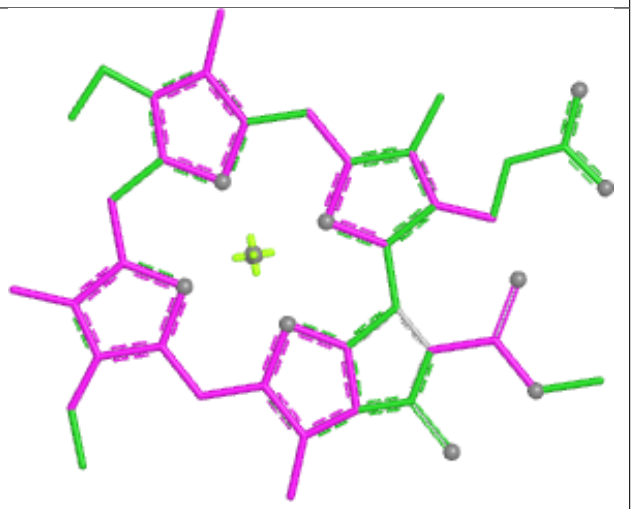


**Rings**

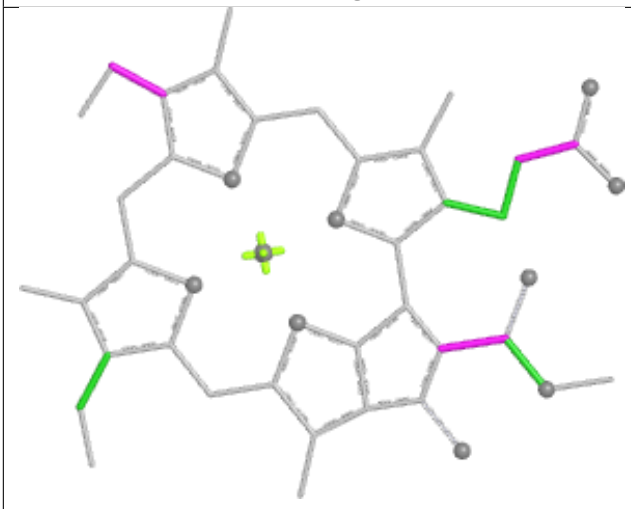
## Ligand CLA 21 210



Bond lengths



Bond angles

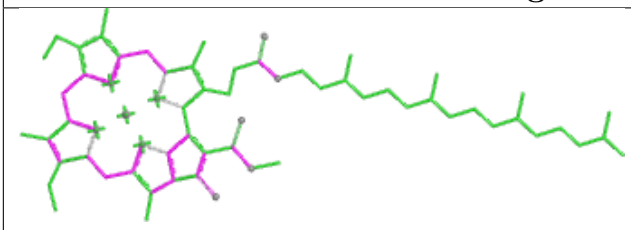


Torsions

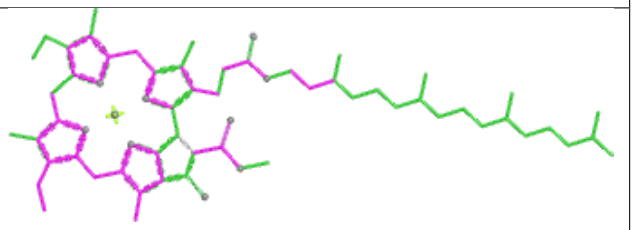


Rings

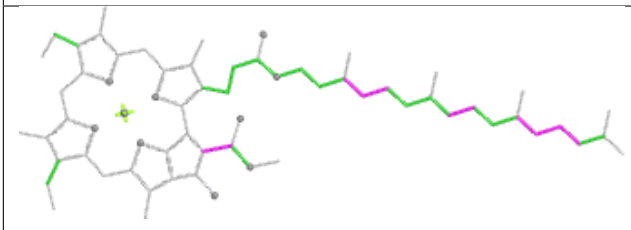
## Ligand CLA b 507



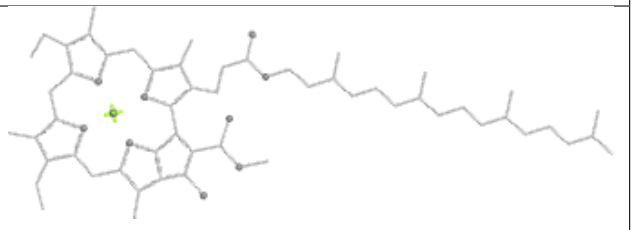
Bond lengths



Bond angles

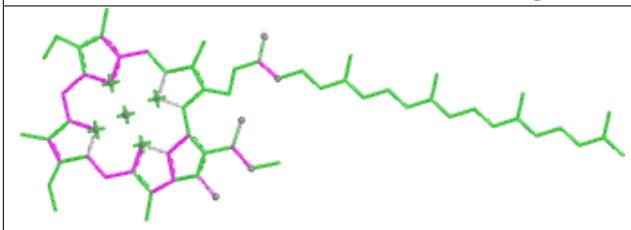


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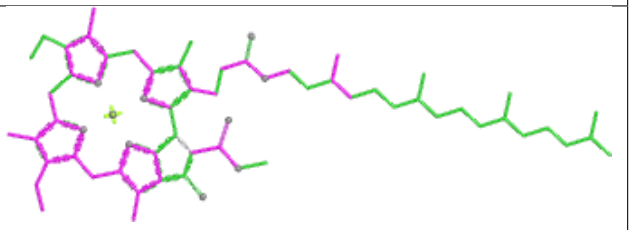


Rings

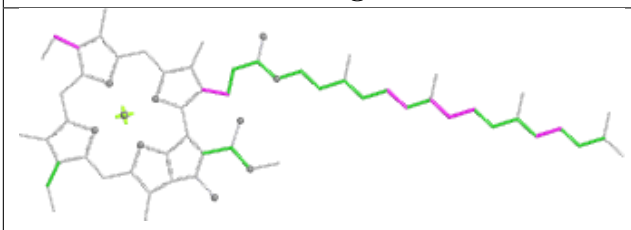
## Ligand CLA a 407



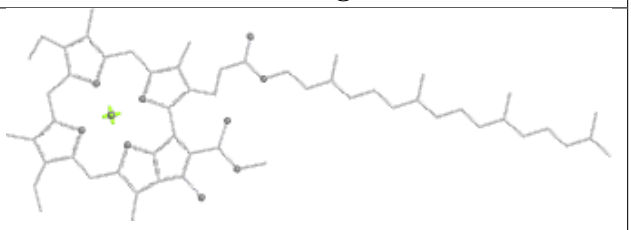
Bond lengths



Bond angles

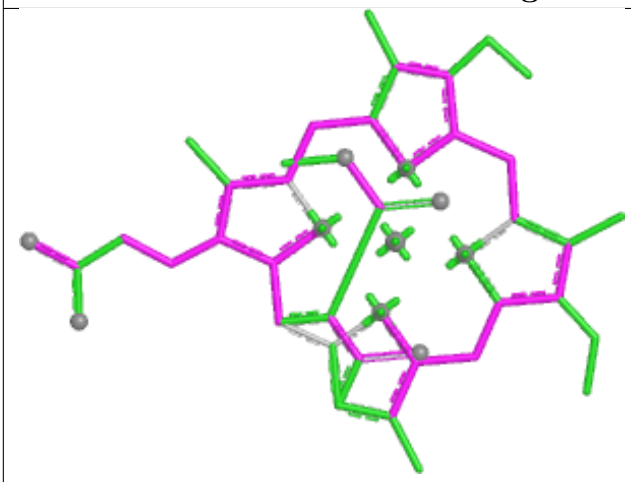


Torsions

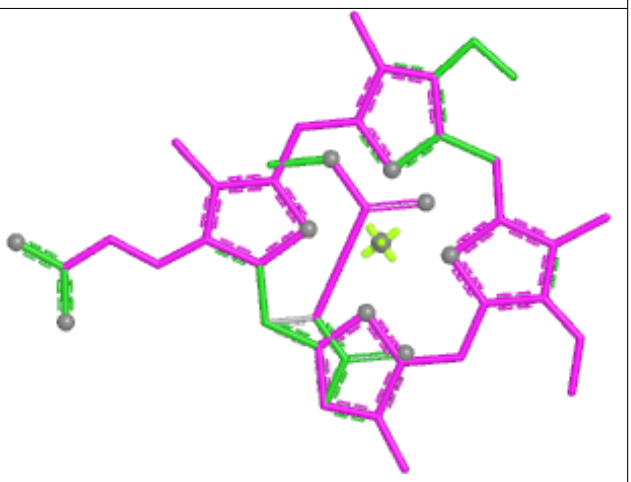


Rings

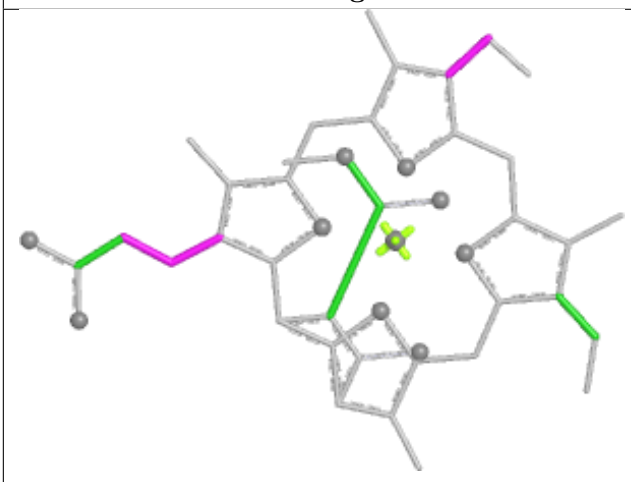
## Ligand KC1 37 307



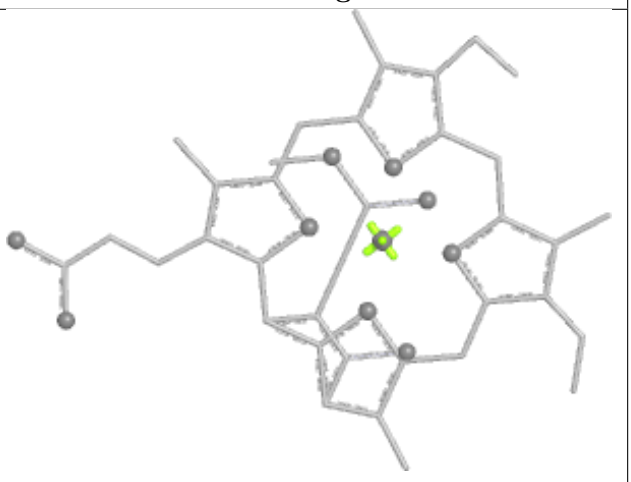
Bond lengths



Bond angles

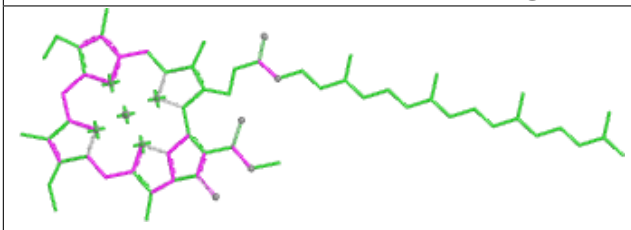


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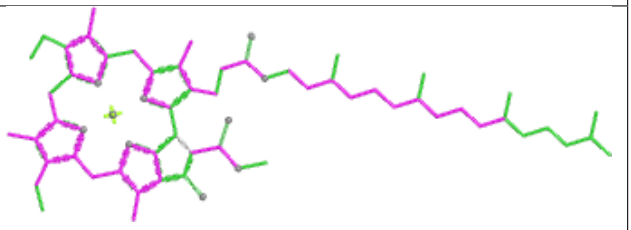


Rings

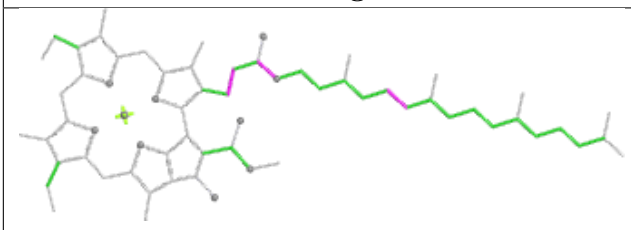
## Ligand CLA A 403



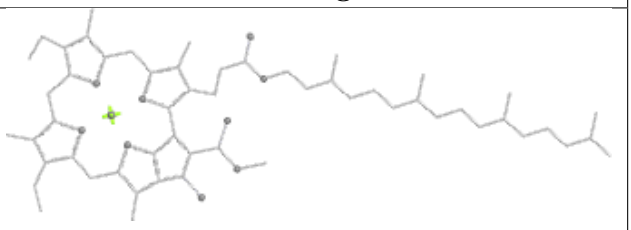
Bond lengths



Bond angles

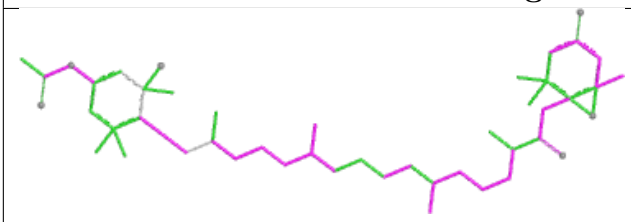


Torsions

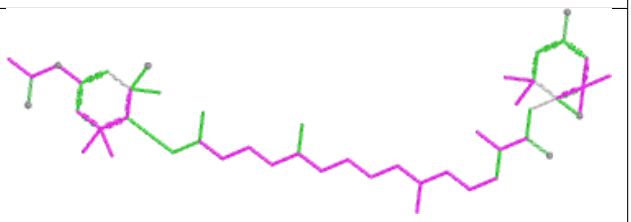


Rings

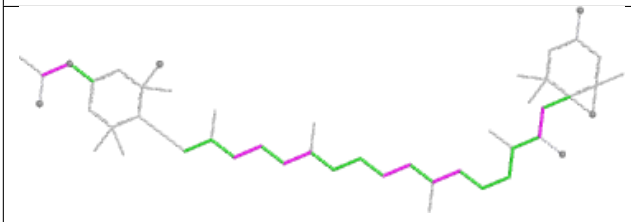
## Ligand A86 32 217



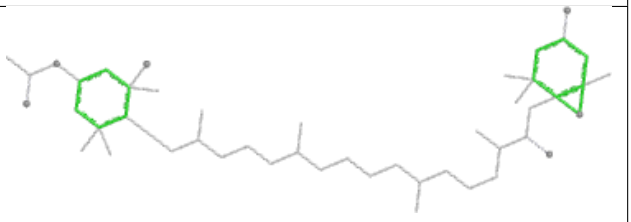
Bond lengths



Bond angles

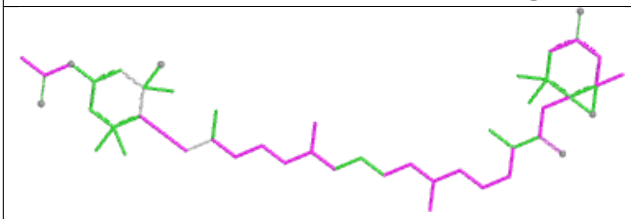


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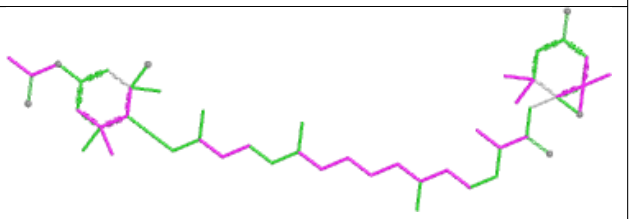


Rings

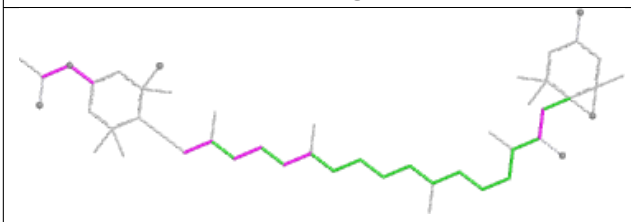
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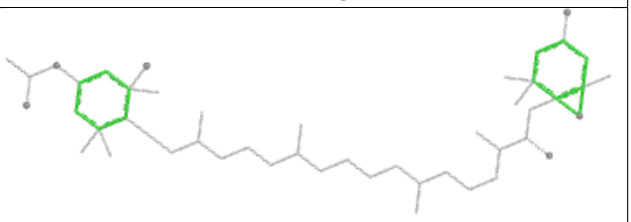
Bond lengths



Bond angles

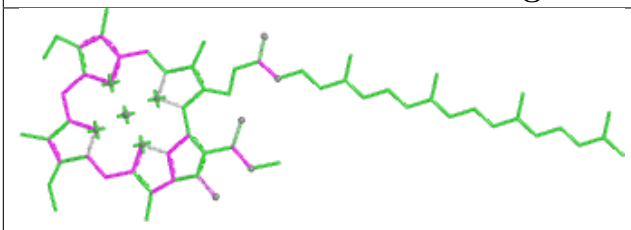


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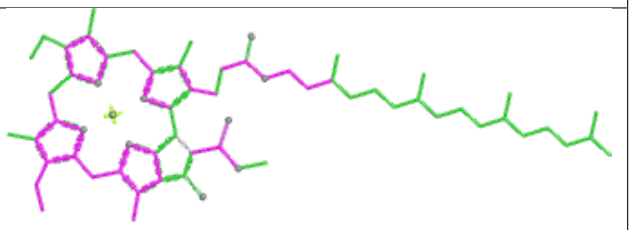


Rings

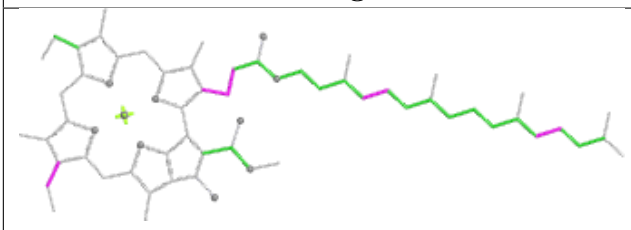
## Ligand CLA D 401



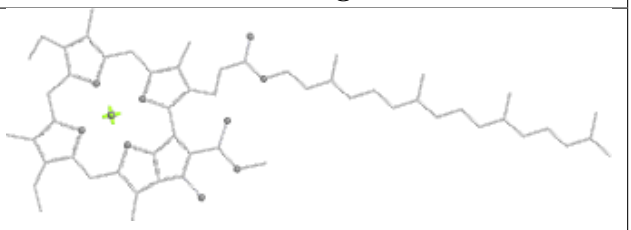
Bond lengths



Bond angles

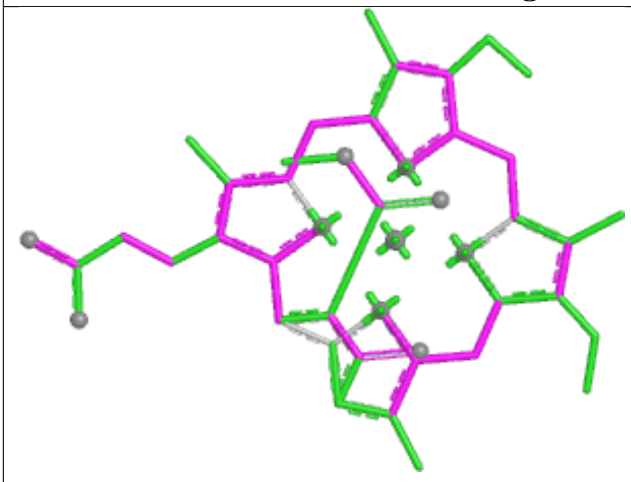


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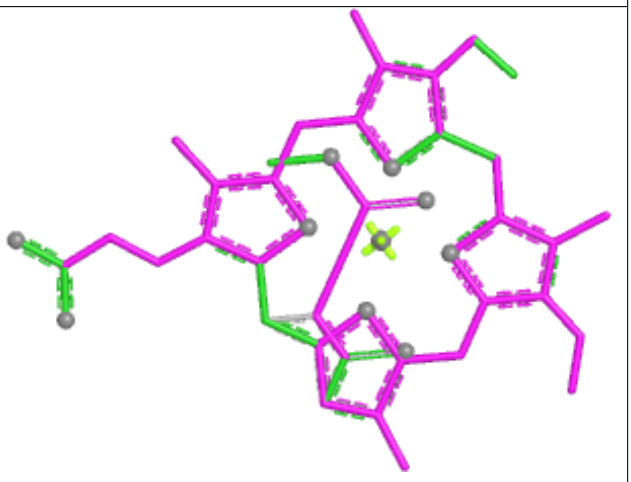


Rings

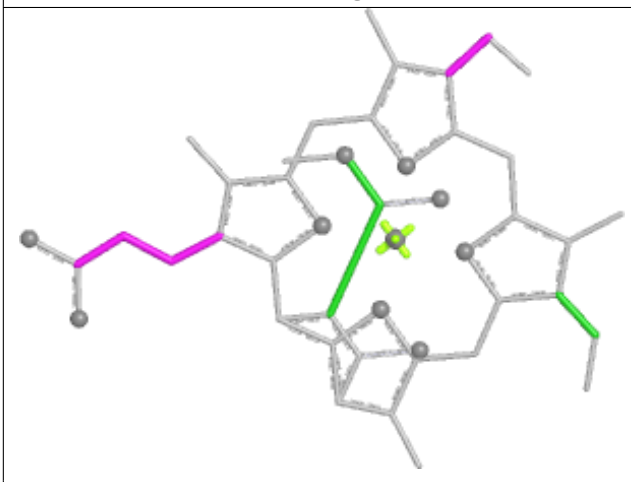
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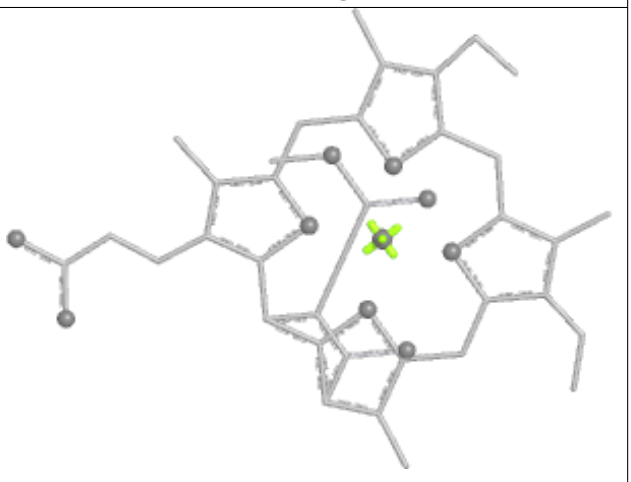
Bond lengths



Bond angles

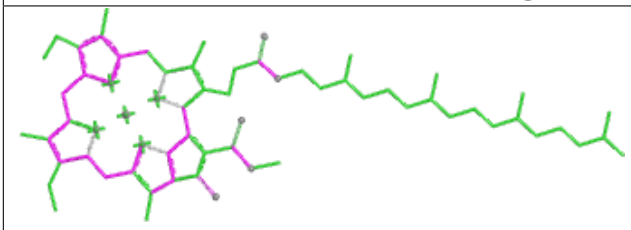


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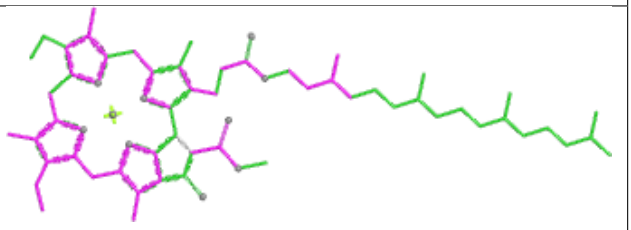


Rings

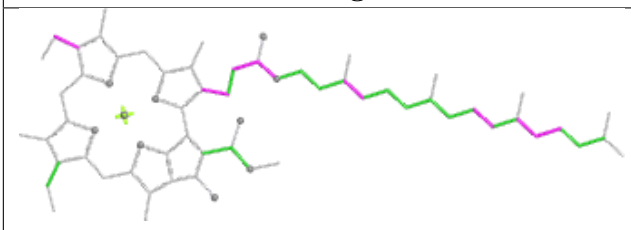
**Ligand CLA 41 208**



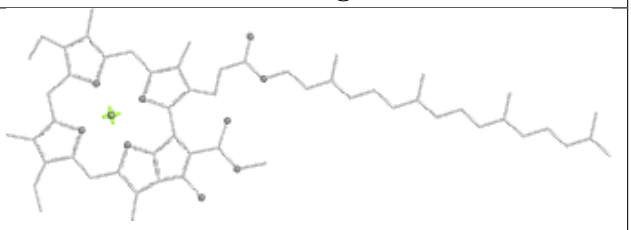
Bond lengths



Bond angles

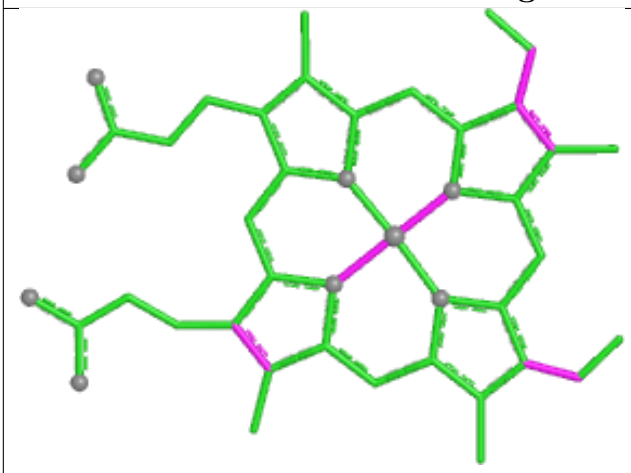


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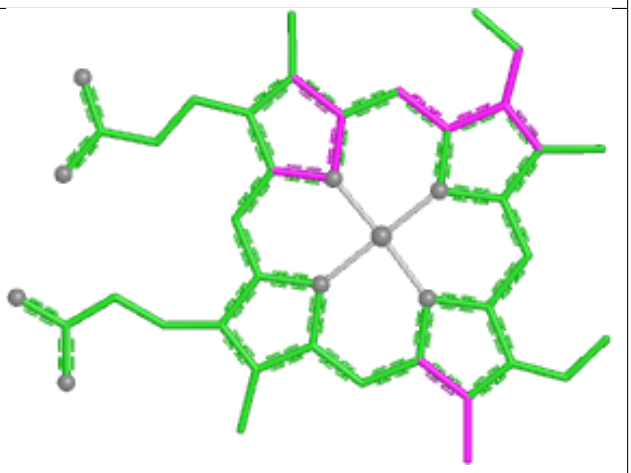


Rings

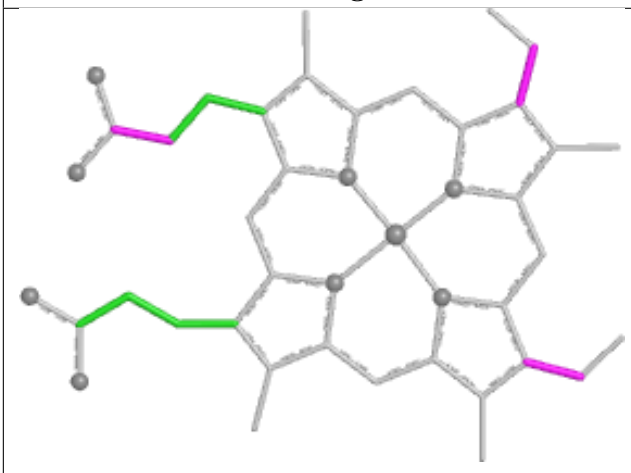
**Ligand HEM V 201**



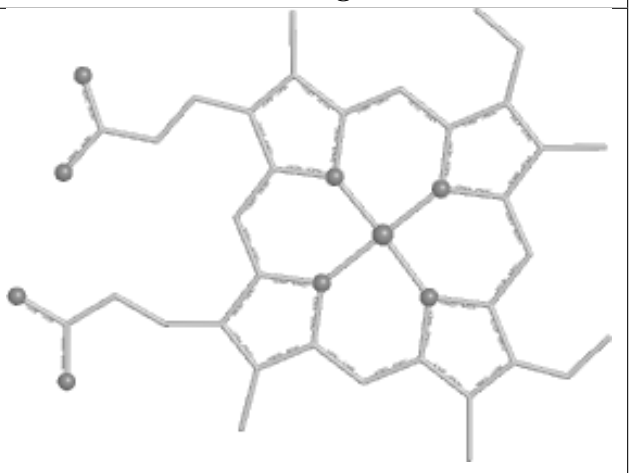
Bond lengths



Bond angles

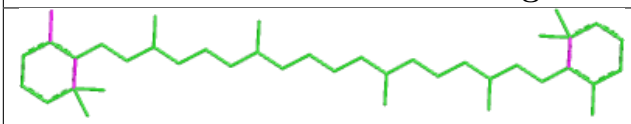


Torsions

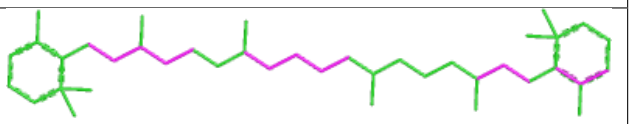


Rings

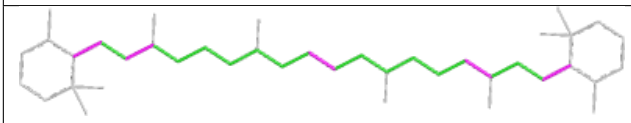
## Ligand BCR A 406



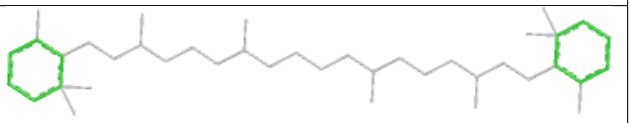
Bond lengths



Bond angles

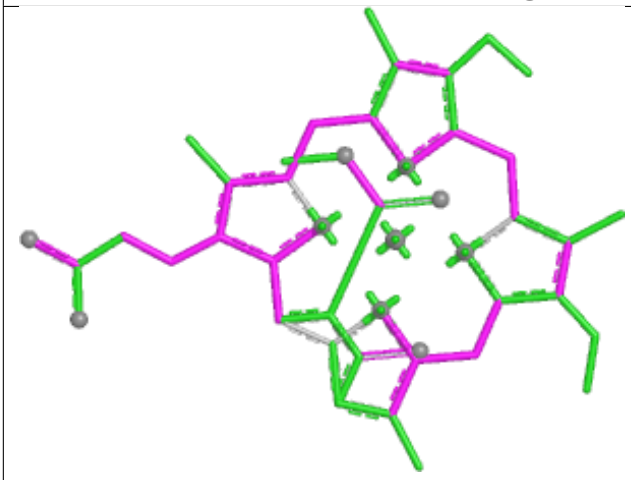


Torsions

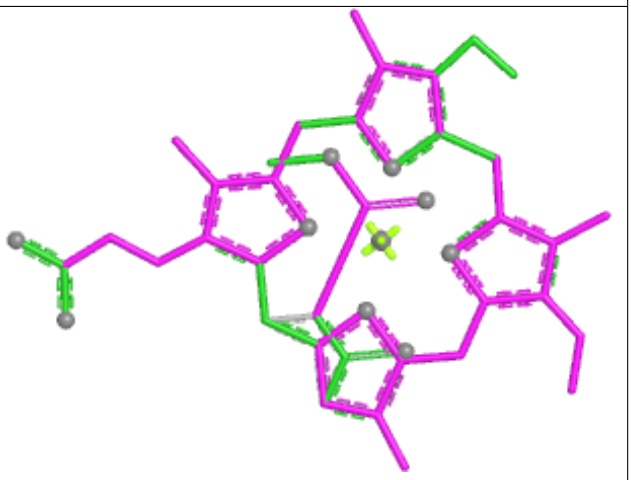


Rings

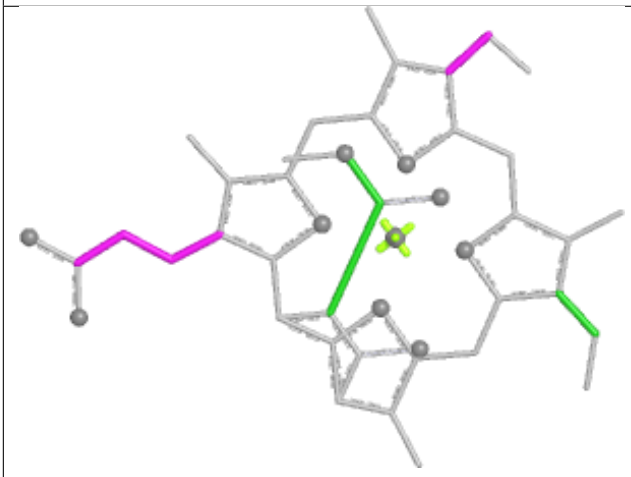
## Ligand KC1 33 304



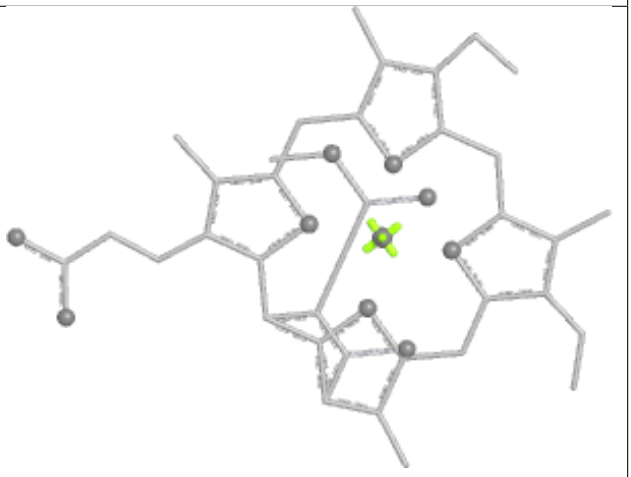
Bond lengths



Bond angles

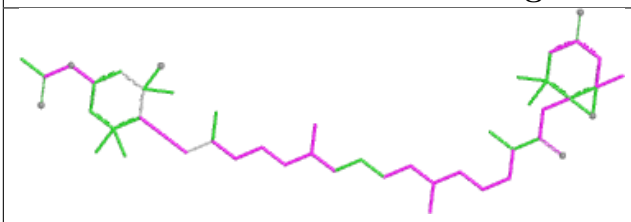


Torsions

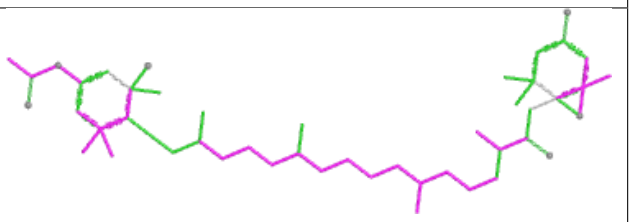


Rings

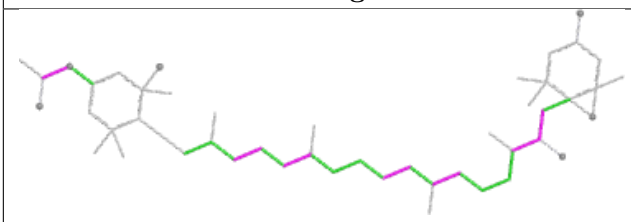
**Ligand A86 14 314**



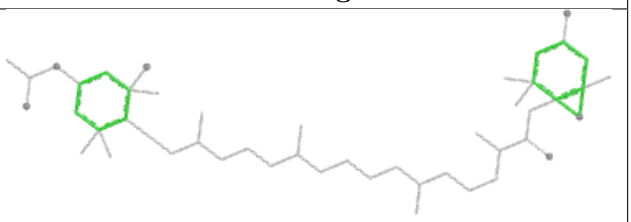
Bond lengths



Bond angles

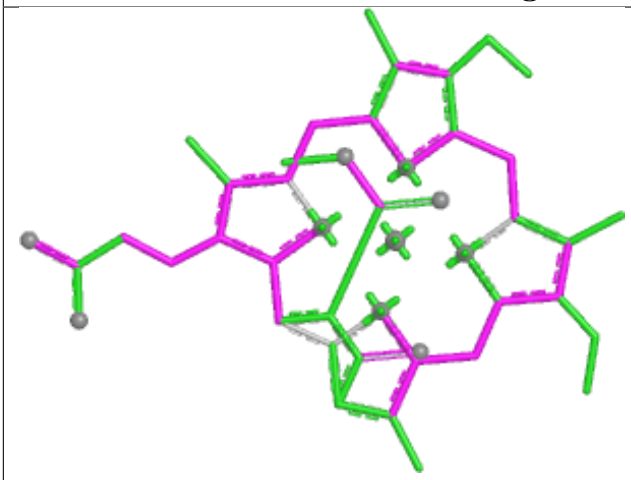


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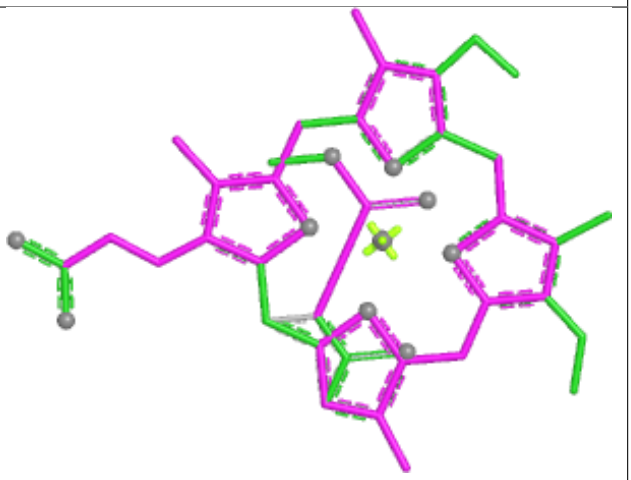


Rings

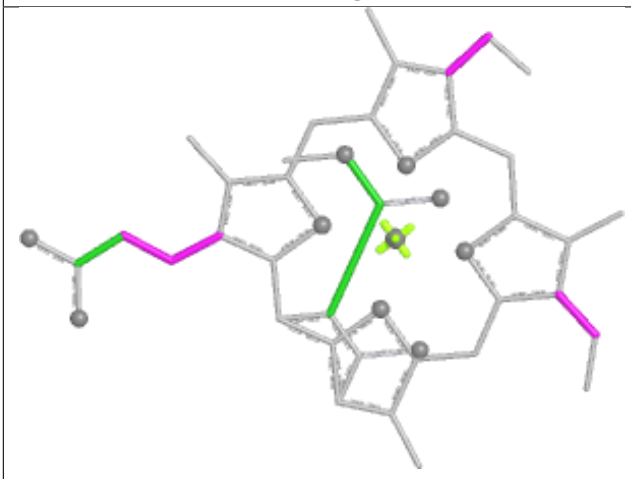
**Ligand KC1 34 304**



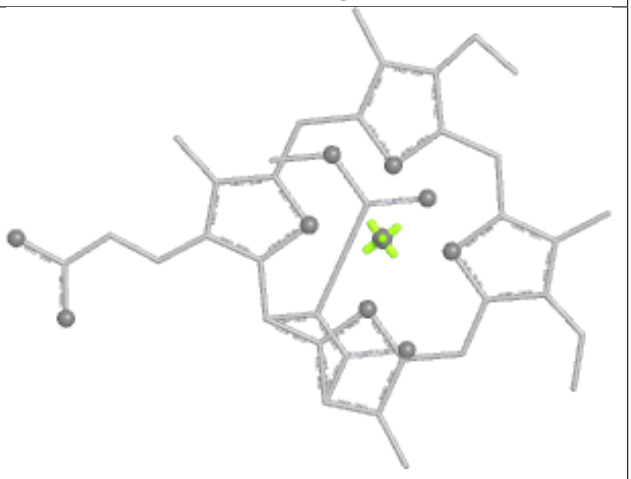
Bond lengths



Bond angles

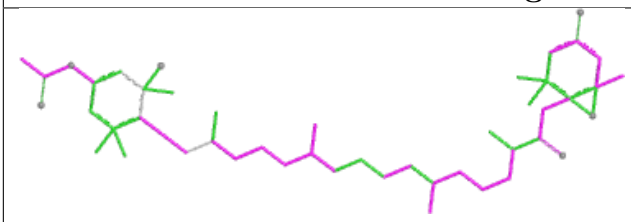


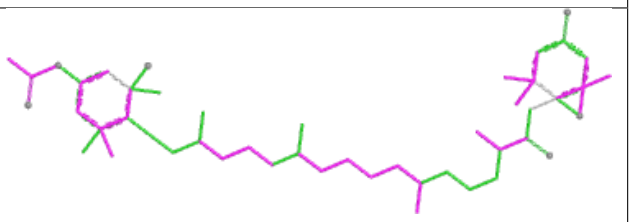
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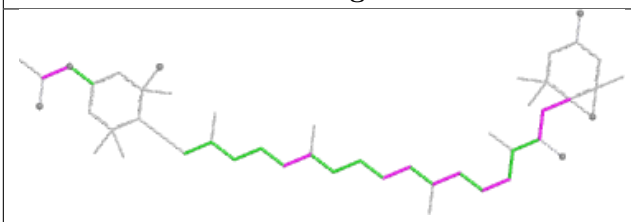


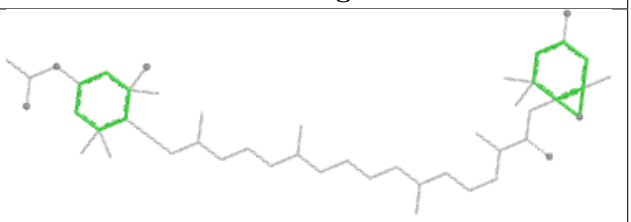
Rings

## Ligand A86 33 315

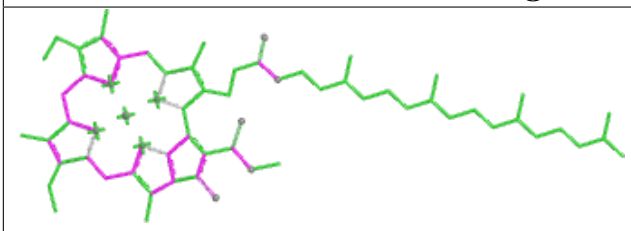

Bond lengths

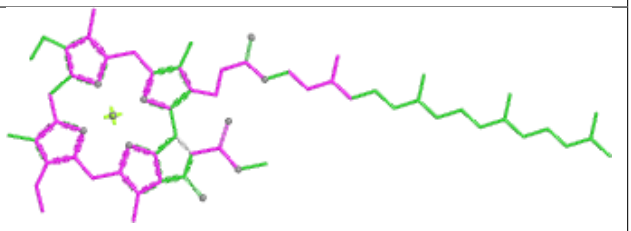

Bond angles

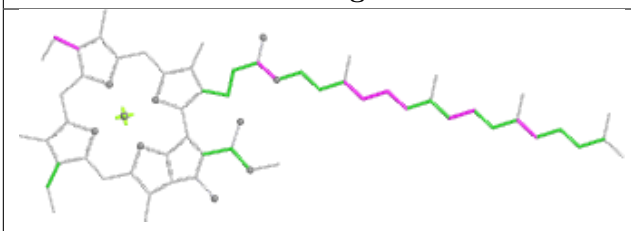

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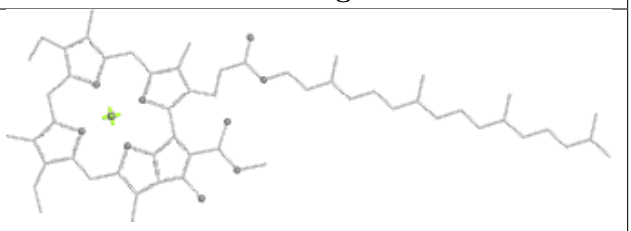

Rings

## Ligand CLA B 502

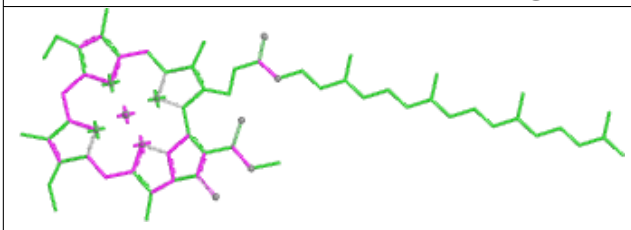

Bond lengths

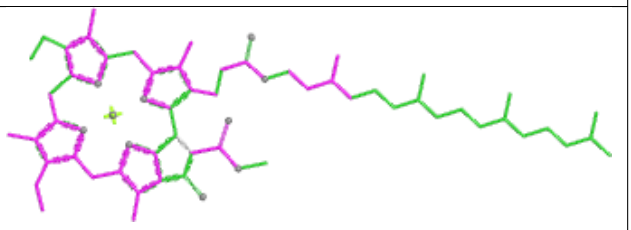

Bond angles

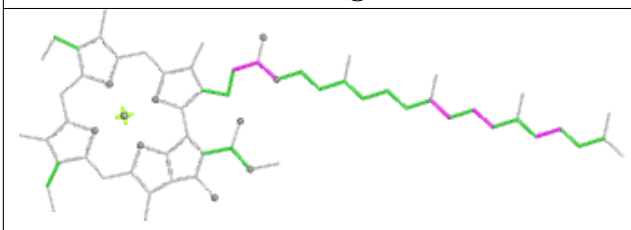

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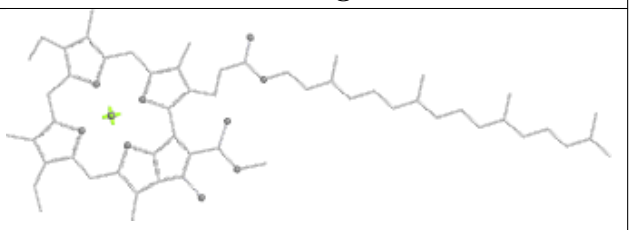

Rings

## Ligand CLA b 512

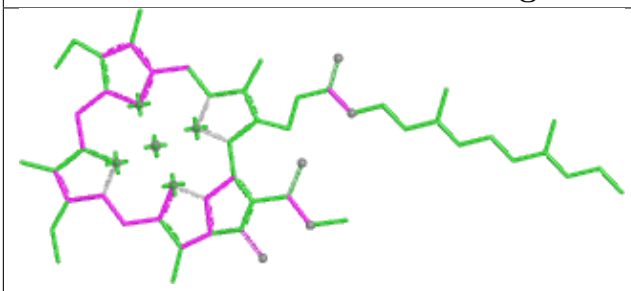

Bond lengths


Bond angles

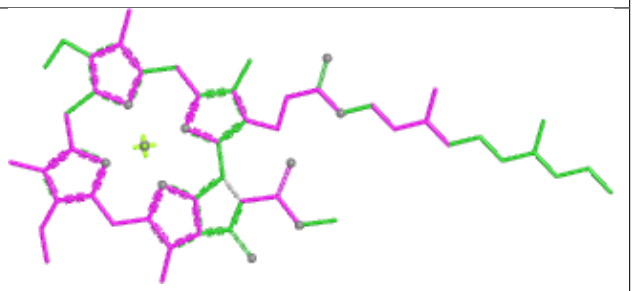

Torsions


Rings

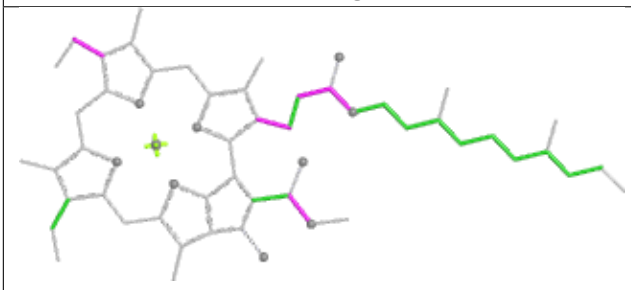
## Ligand CLA 36 303



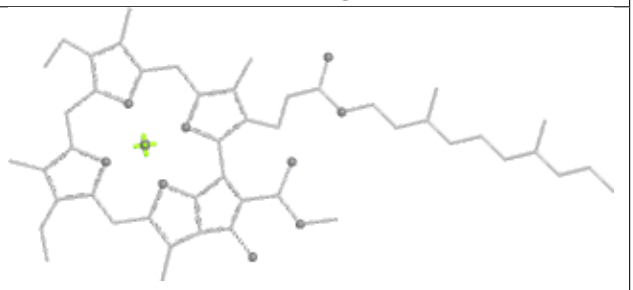
Bond lengths



Bond angles

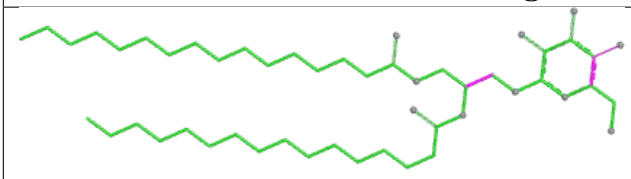


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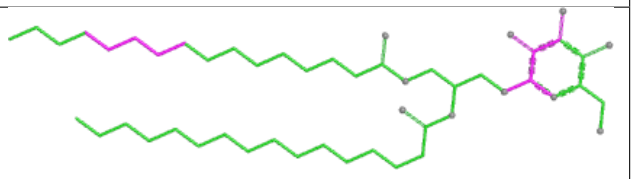


Rings

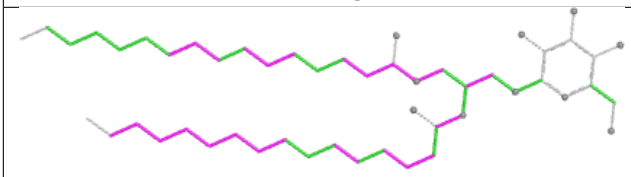
## Ligand LMG b 520



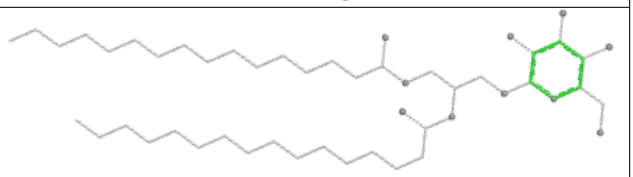
Bond lengths



Bond angles

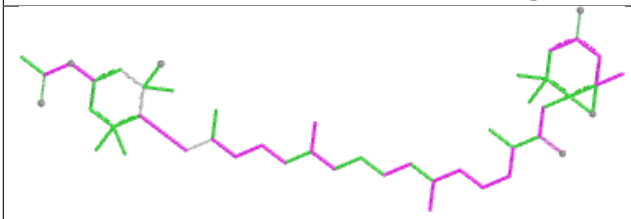


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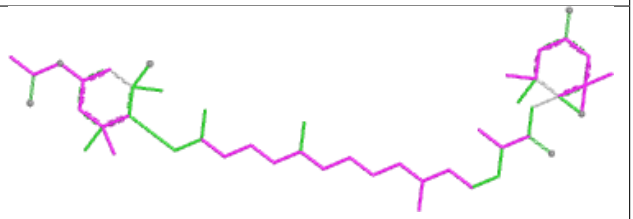


Rings

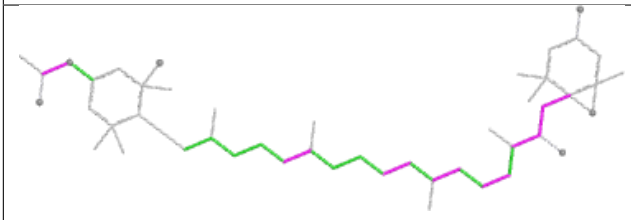
## Ligand A86 32 203



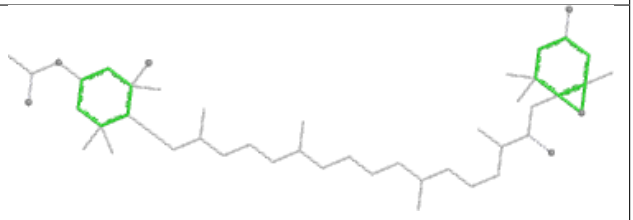
Bond lengths



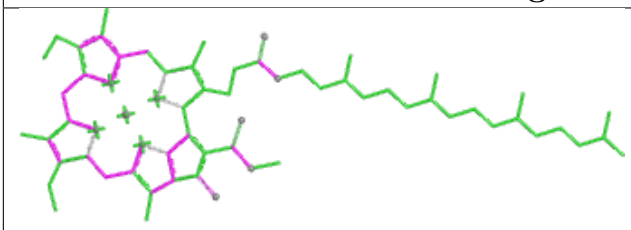
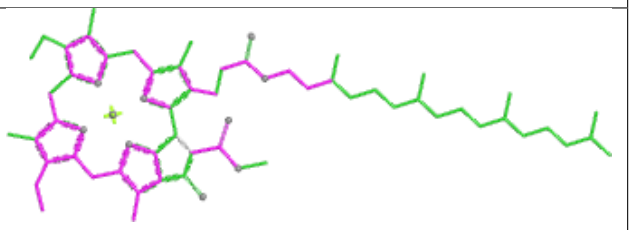
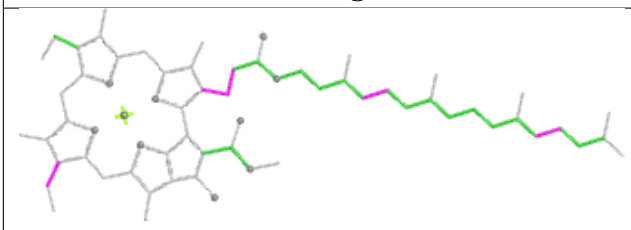
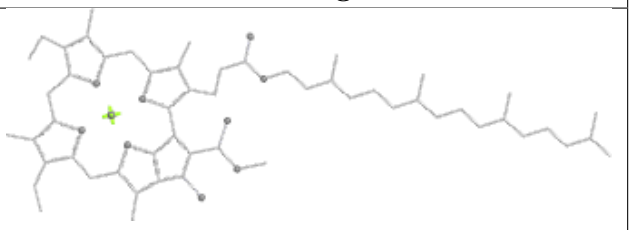
Bond angles

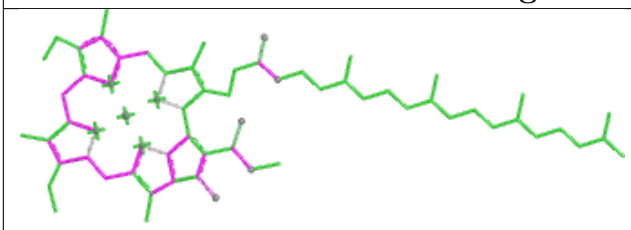
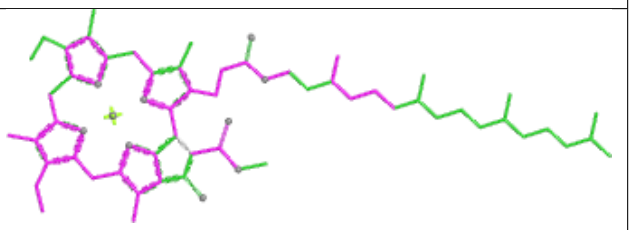
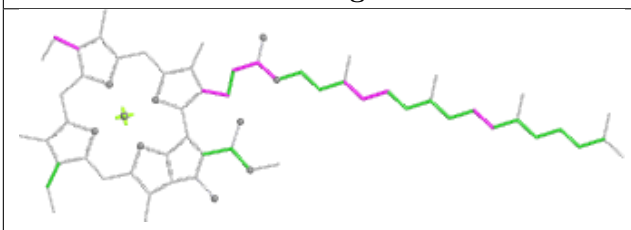
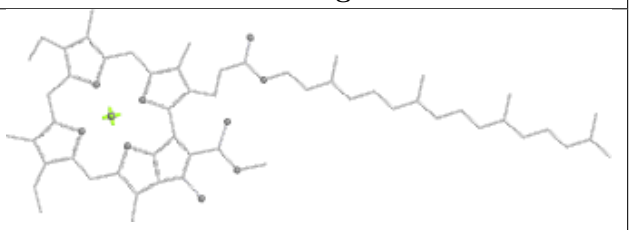


Torsions

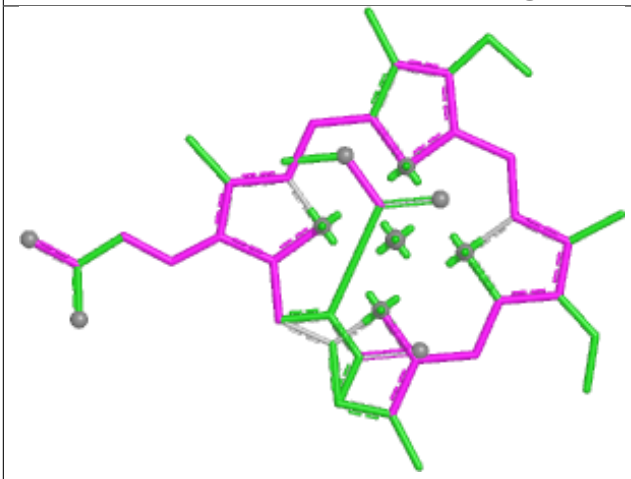


Rings

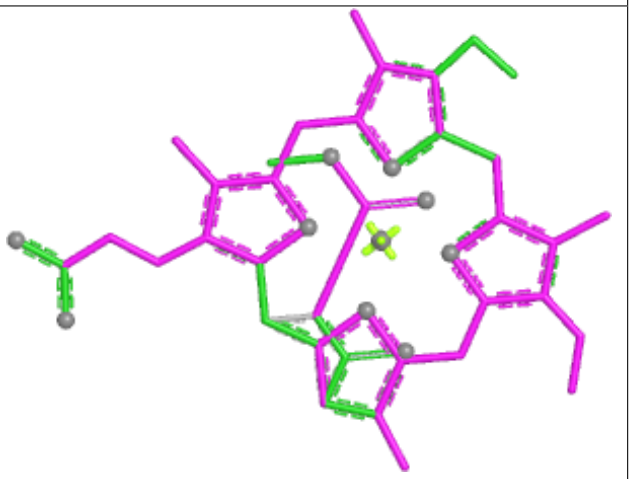
| Ligand CLA a 404 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 11 303 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

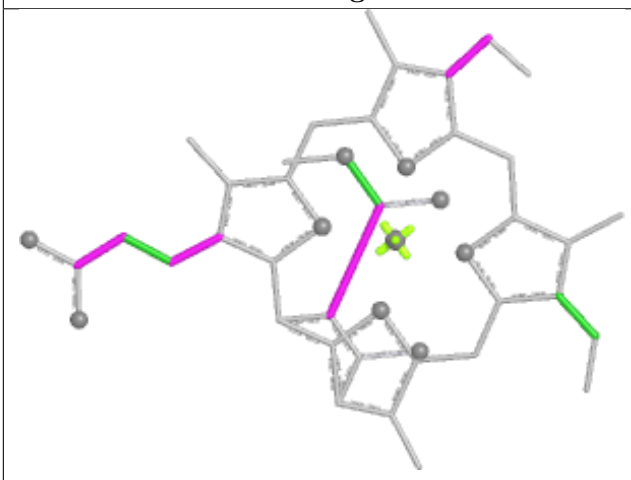
**Ligand KC1 21 207**



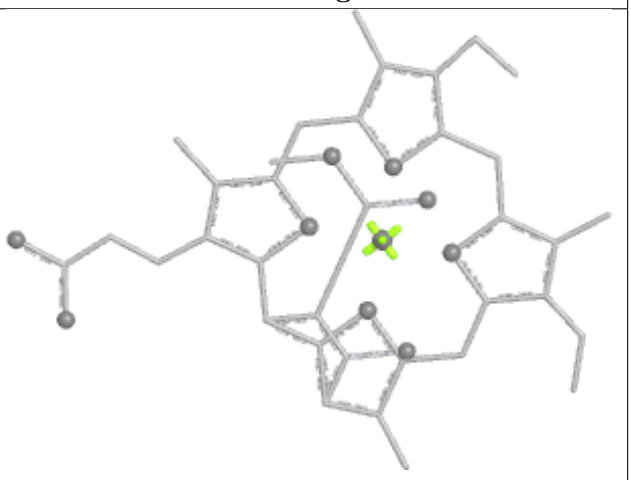
**Bond lengths**



**Bond angles**

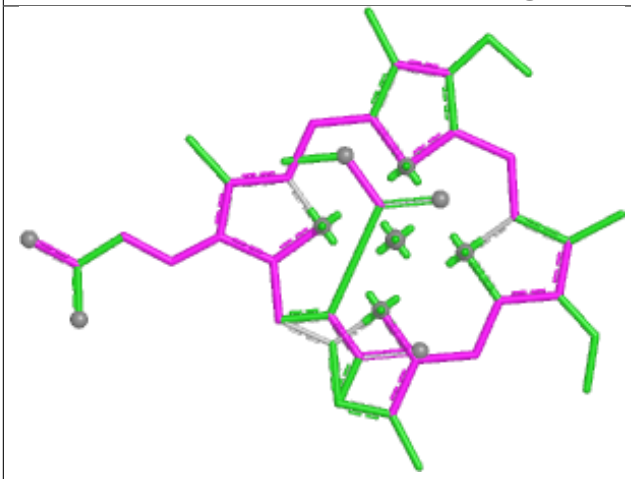


**Torsions**

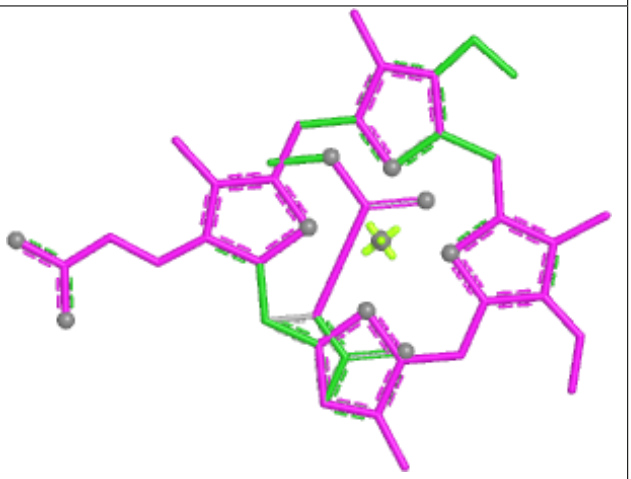


**Rings**

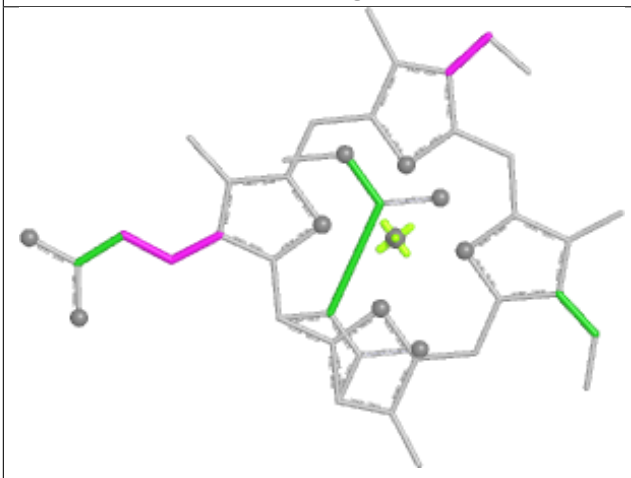
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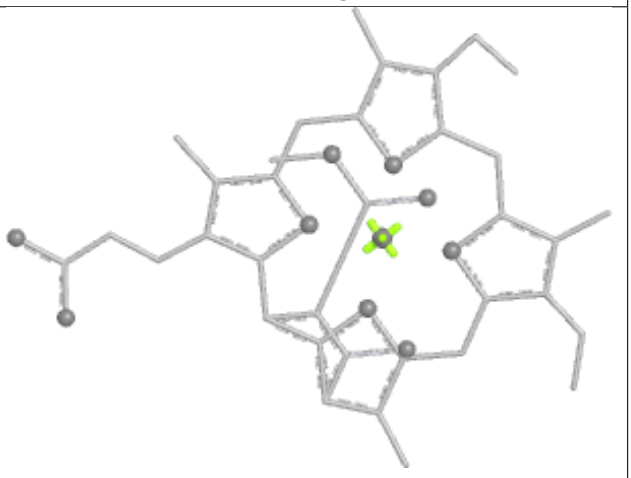
**Bond lengths**



**Bond angles**

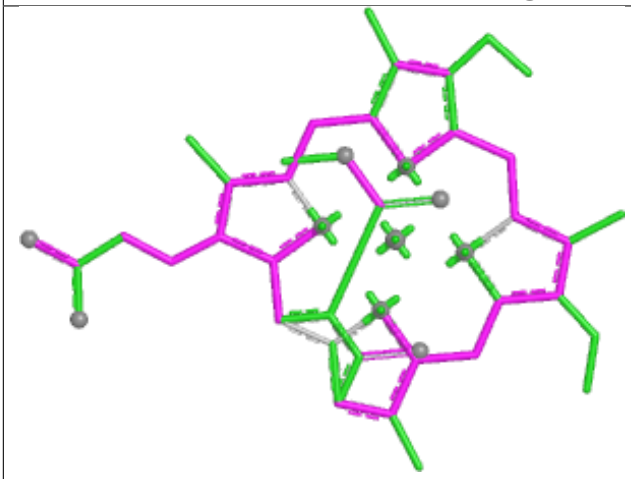


**Torsions**

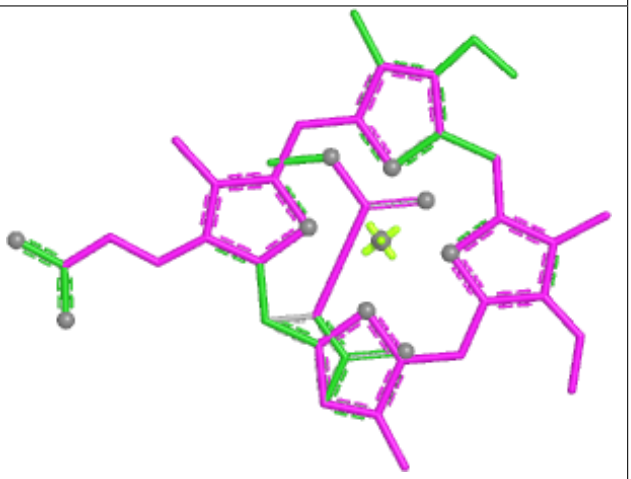


**Rings**

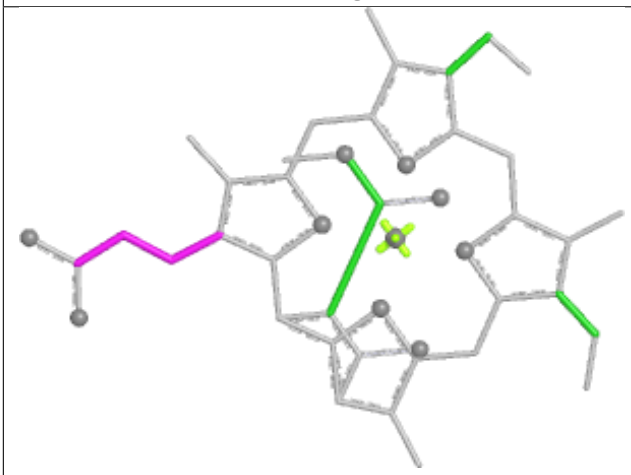
**Ligand KC1 21 203**



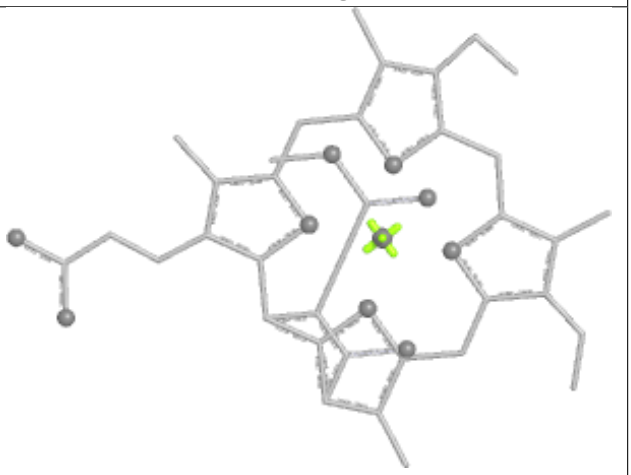
Bond lengths



Bond angles

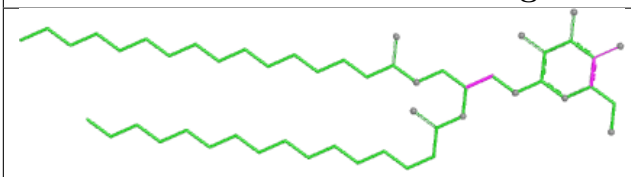


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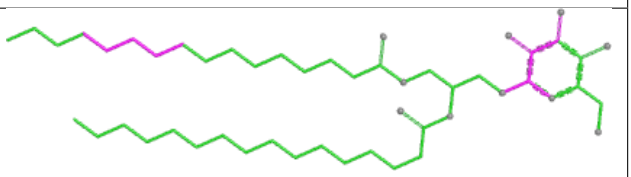


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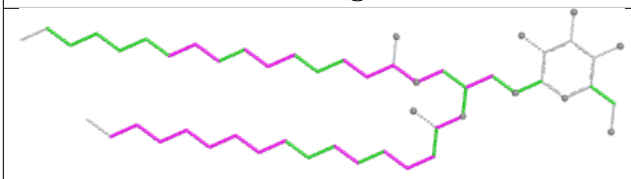
**Ligand LMG B 521**



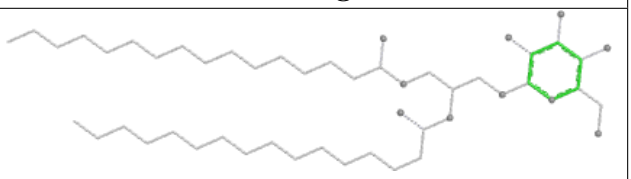
Bond lengths



Bond angles

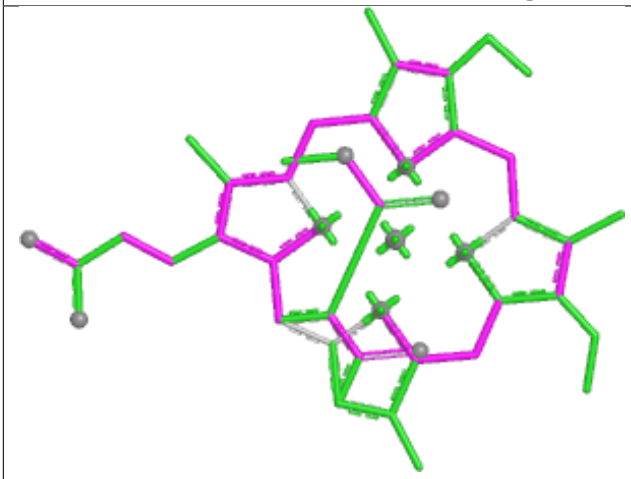


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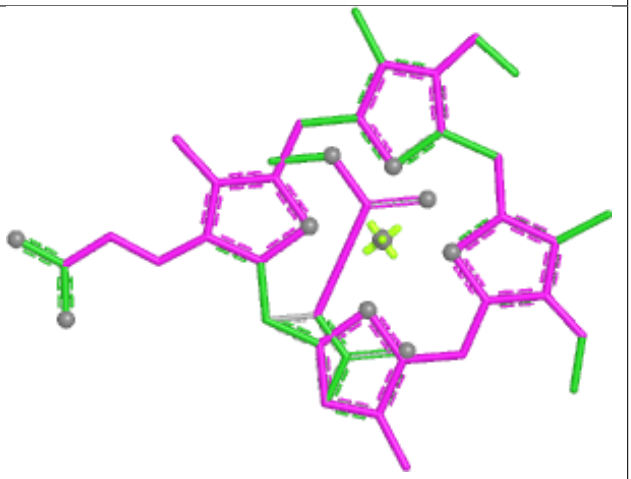


Rings

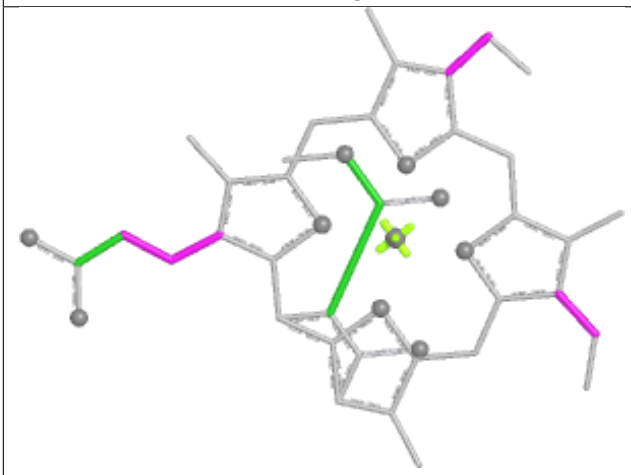
**Ligand KC1 12 206**



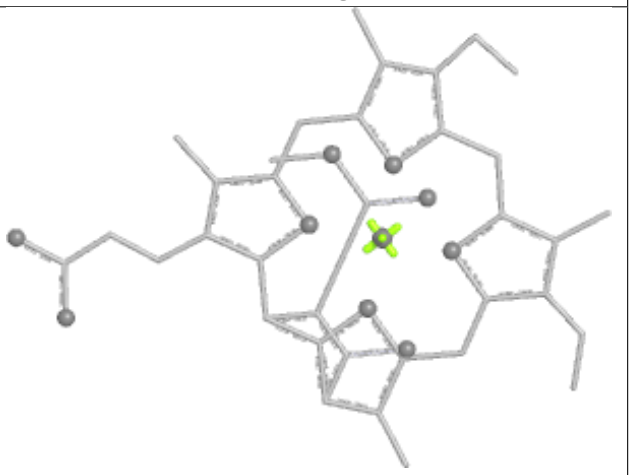
**Bond lengths**



**Bond angles**

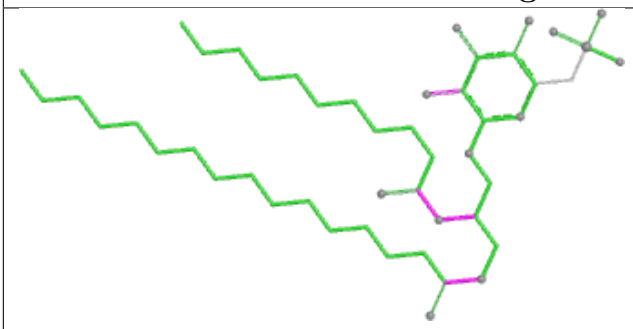


**Torsions**

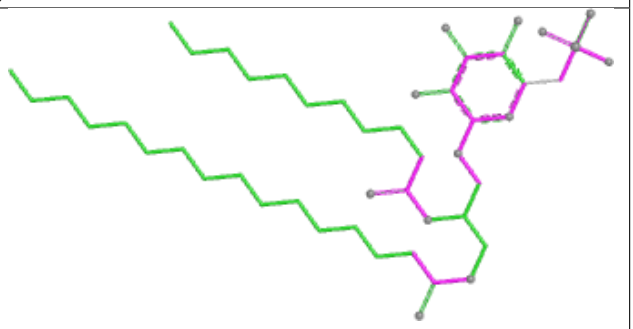


**Rings**

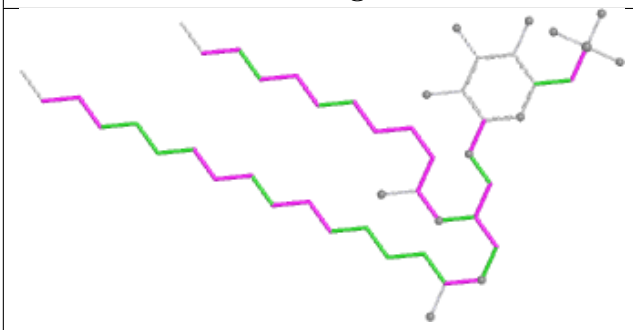
## Ligand SQD 36 315



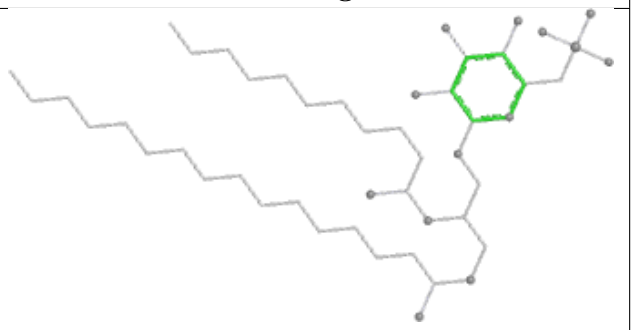
Bond lengths



Bond angles

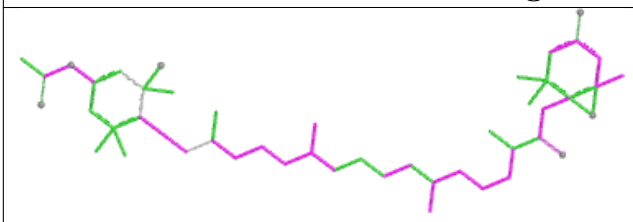


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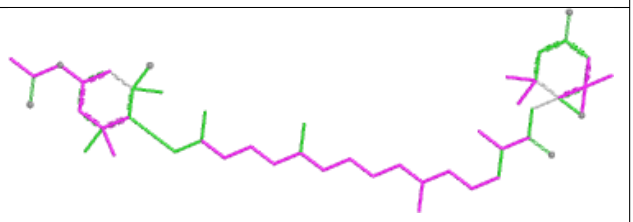


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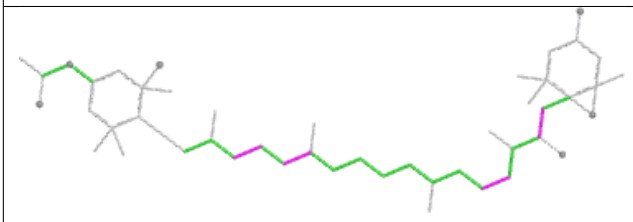
## Ligand A86 33 311



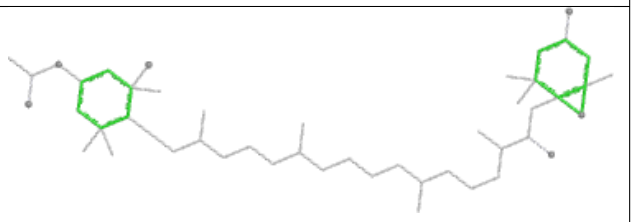
Bond lengths



Bond angles

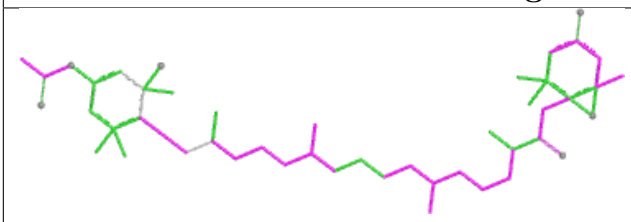


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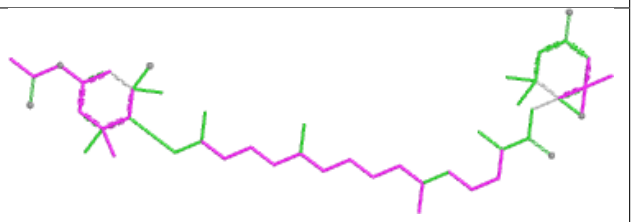


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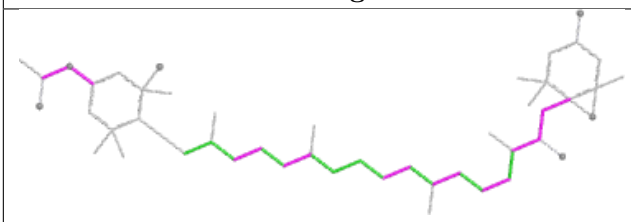
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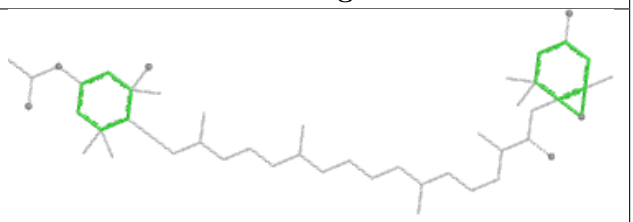
Bond lengths



Bond angles

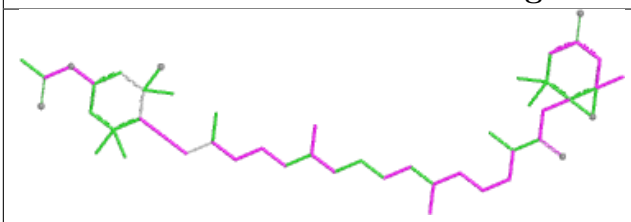


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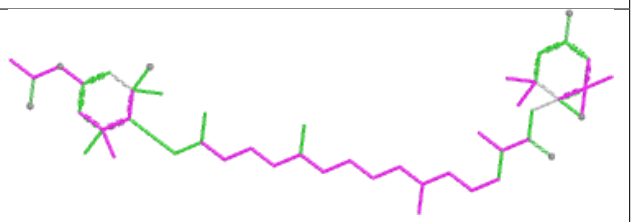


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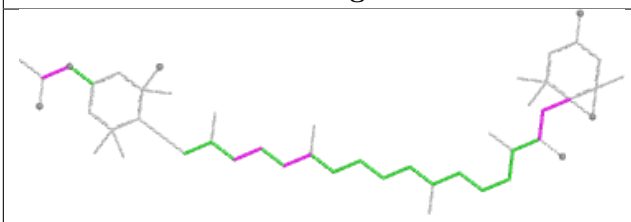
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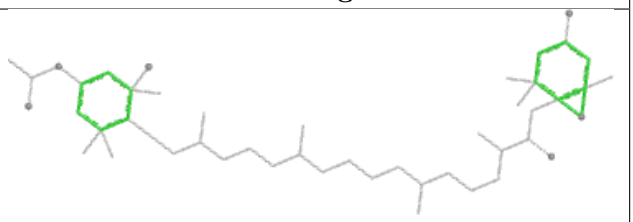
Bond lengths



Bond angles

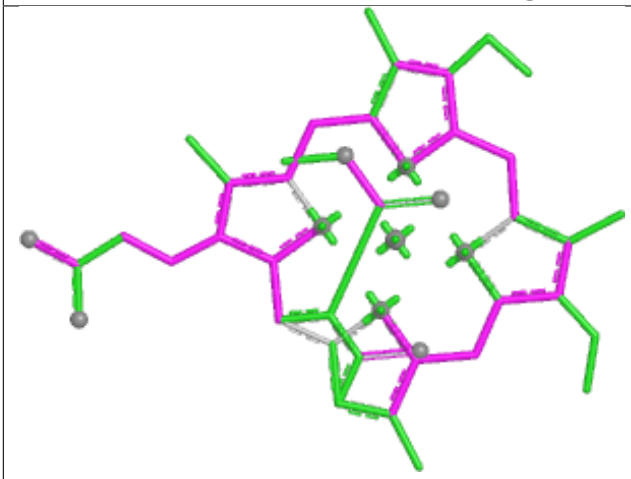


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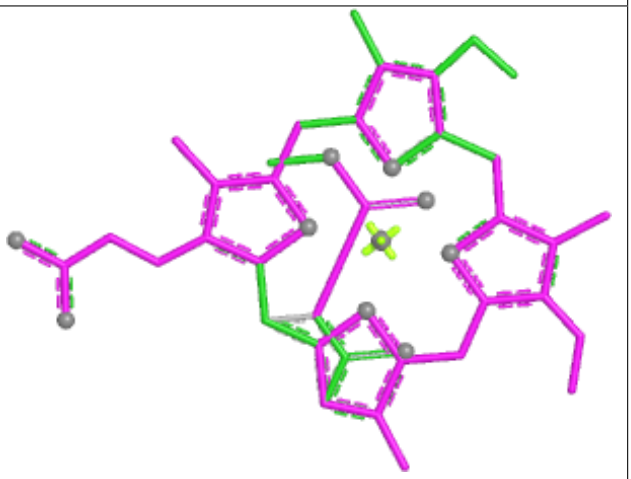


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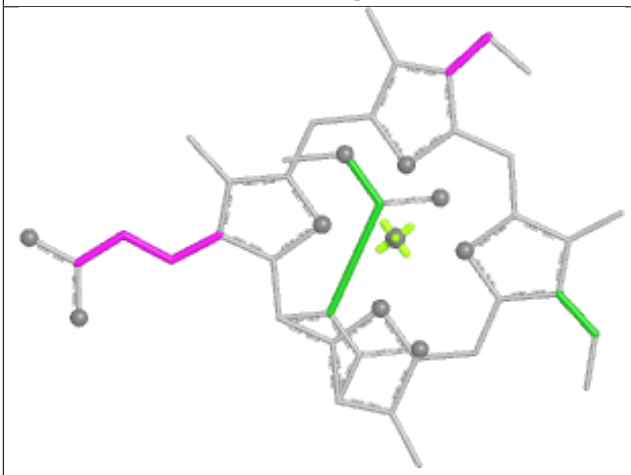
**Ligand KC1 16 304**



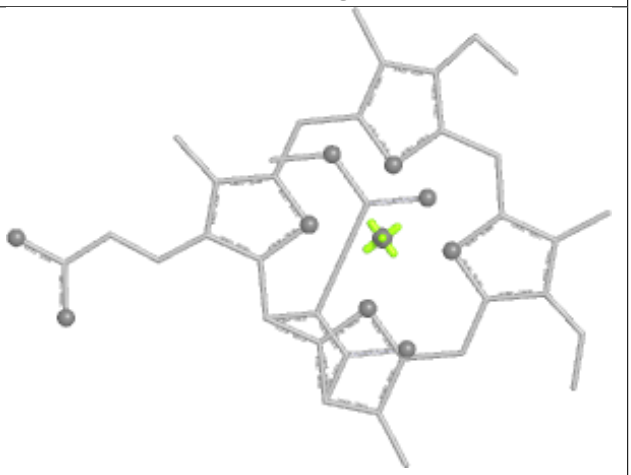
**Bond lengths**



**Bond angles**

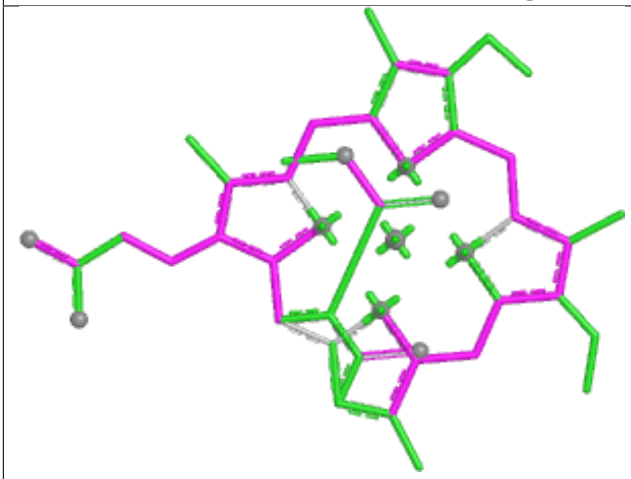


**Torsions**

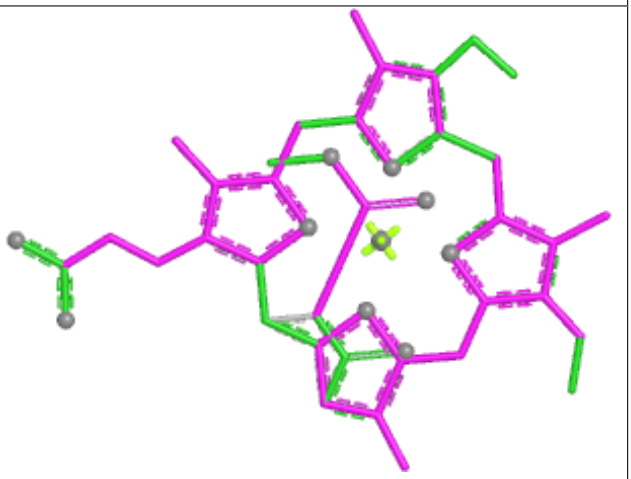


**Rings**

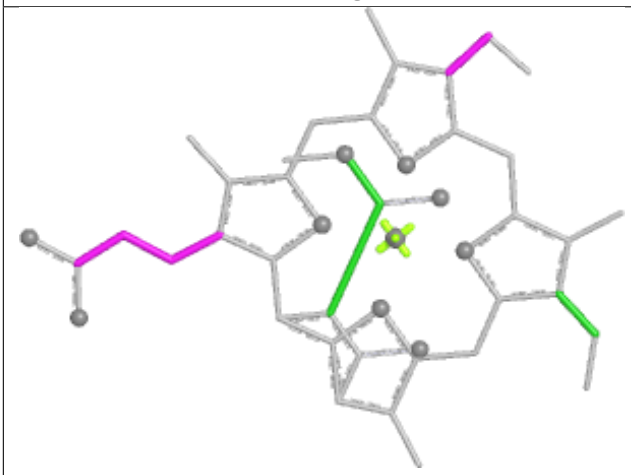
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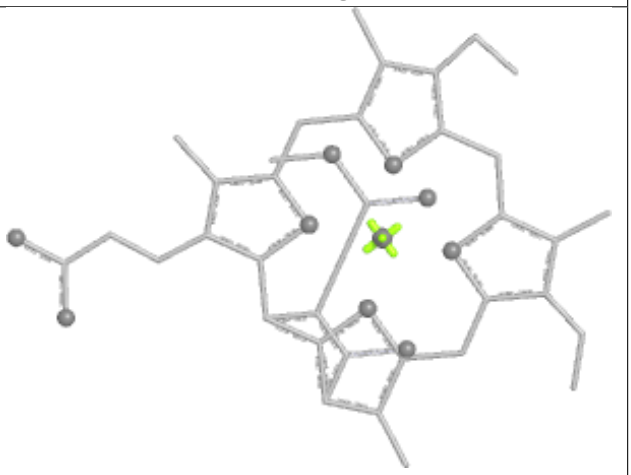
Bond lengths



Bond angles

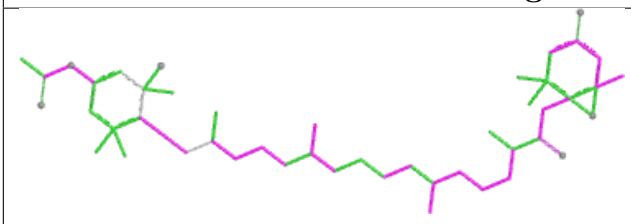


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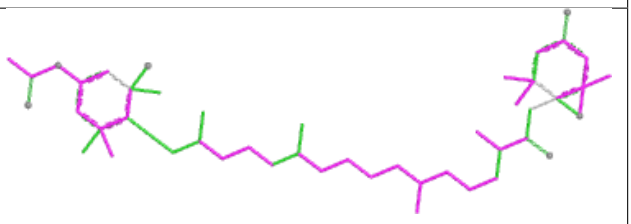


Rings

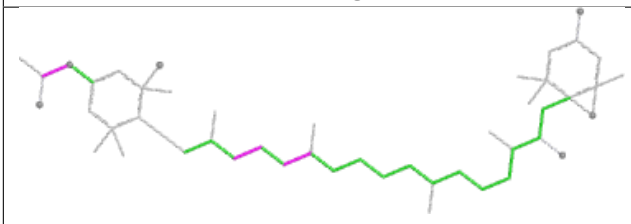
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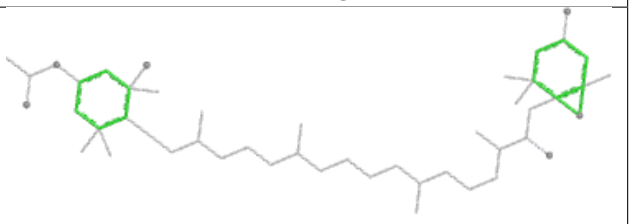
Bond lengths



Bond angles

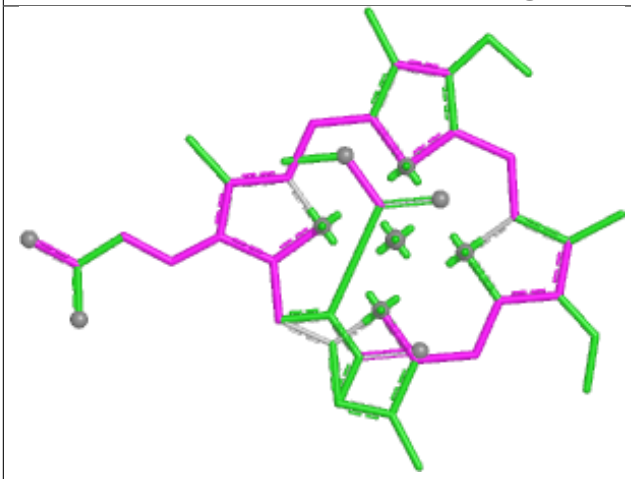


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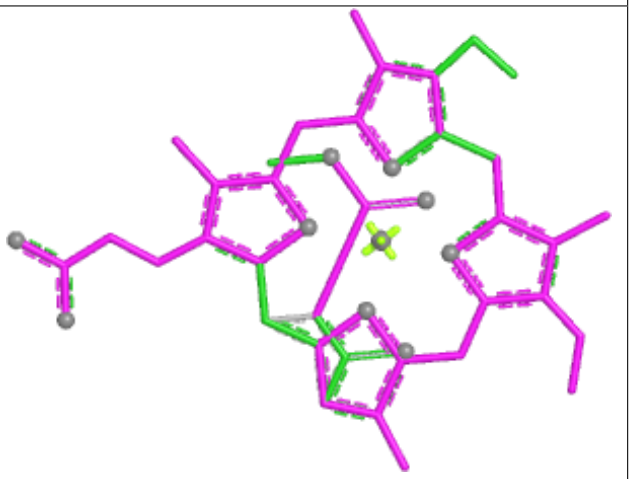


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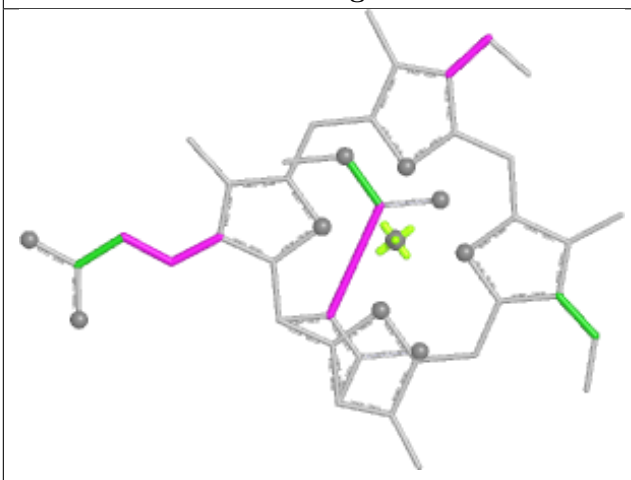
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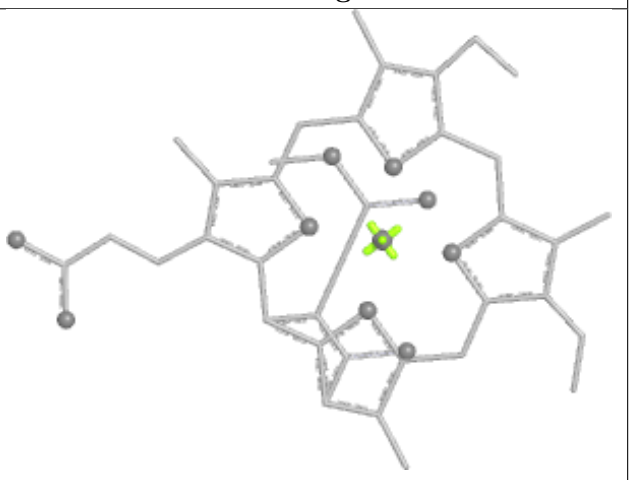
**Bond lengths**



**Bond angles**

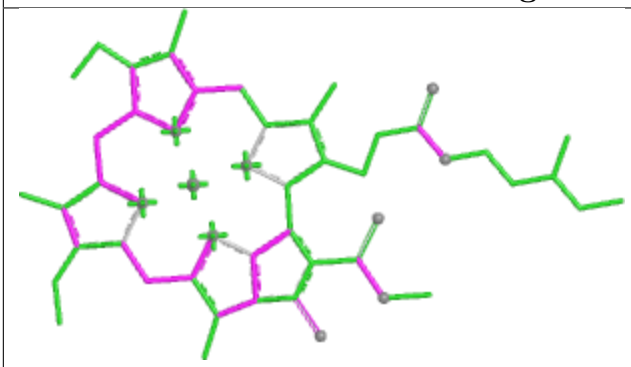


**Torsions**

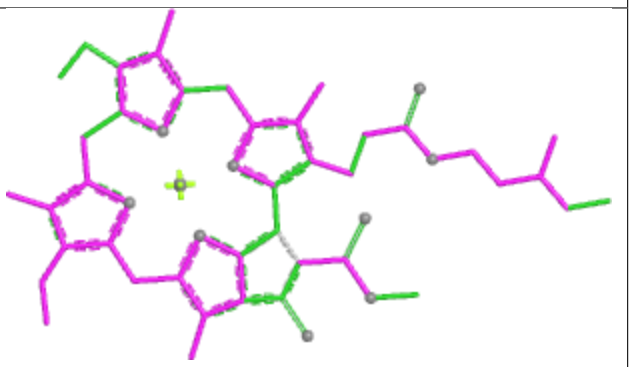


**Rings**

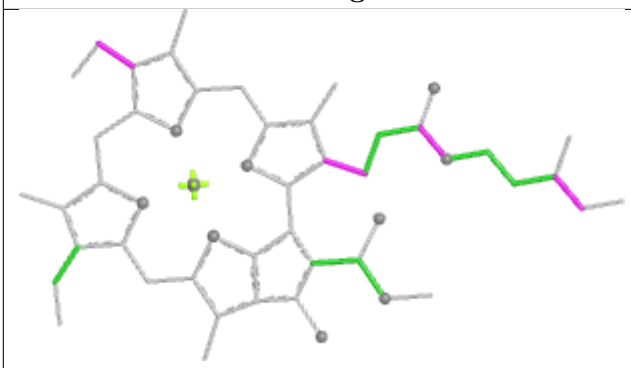
## Ligand CLA 39 305



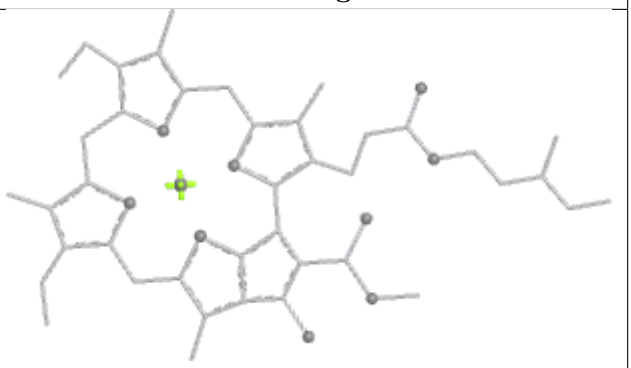
Bond lengths



Bond angles

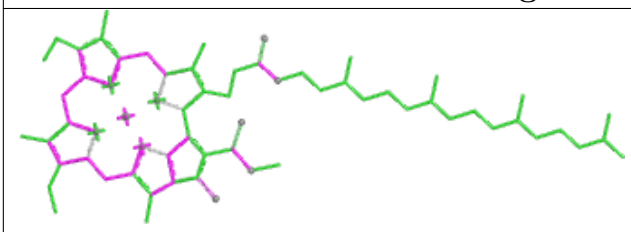


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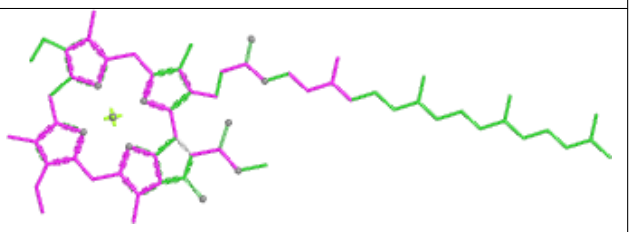


Rings

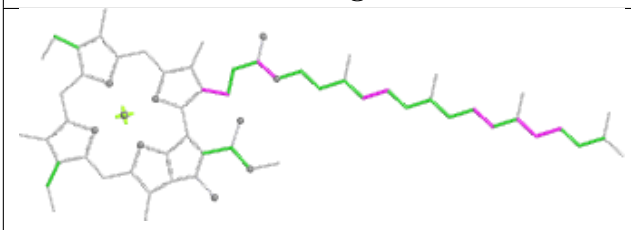
## Ligand CLA 39 307



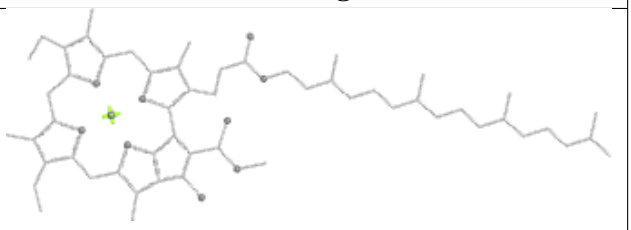
Bond lengths



Bond angles

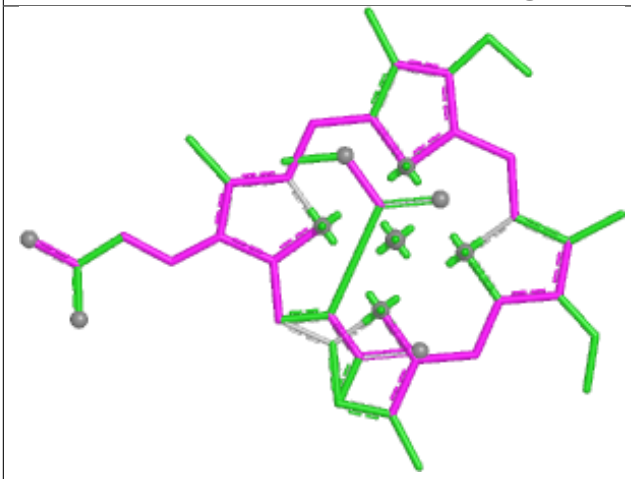


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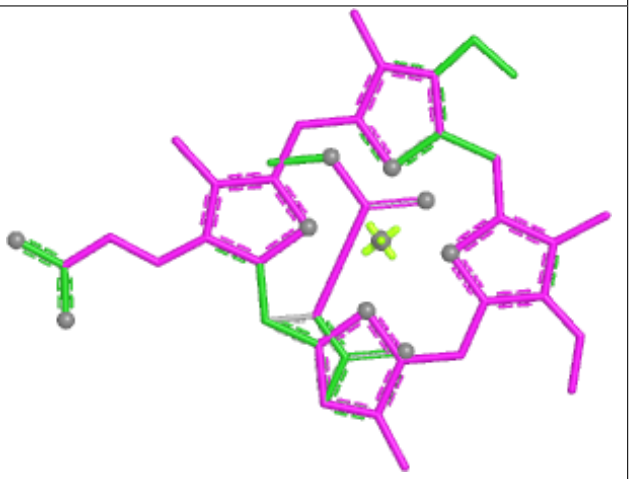


Rings

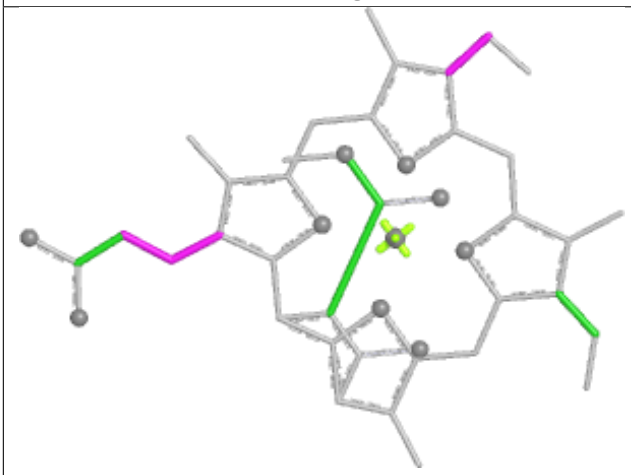
**Ligand KC1 17 308**



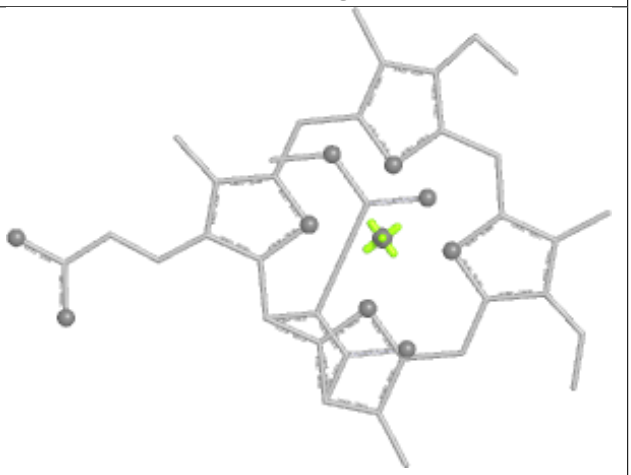
**Bond lengths**



**Bond angles**

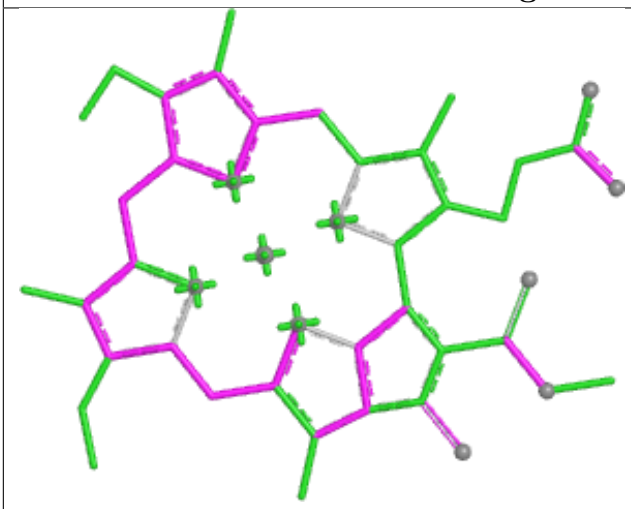


**Torsions**

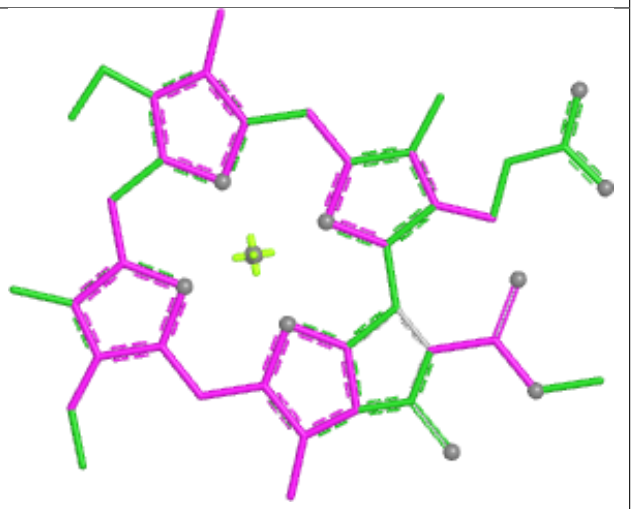


**Rings**

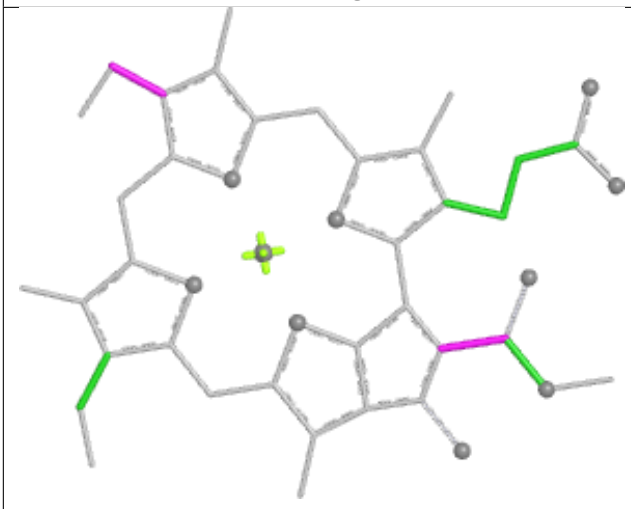
**Ligand CLA 38 211**



**Bond lengths**



**Bond angles**

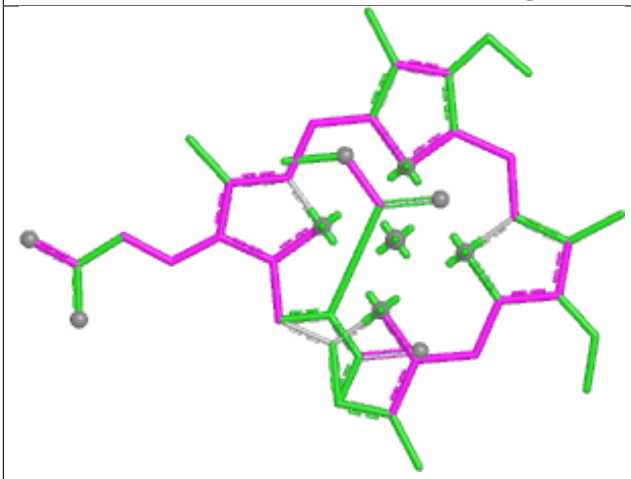


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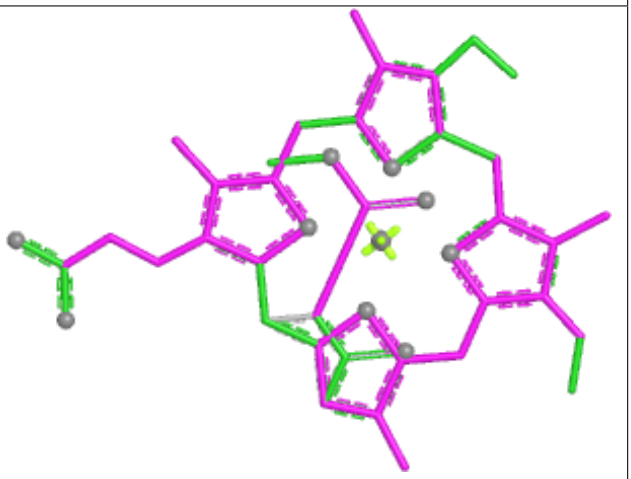


**Rings**

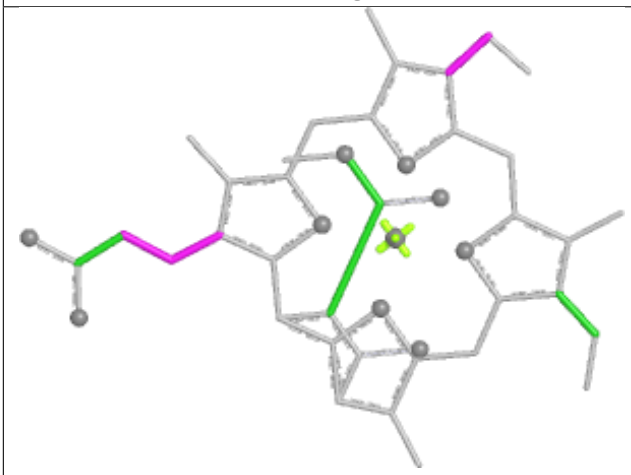
## Ligand KC1 11 304



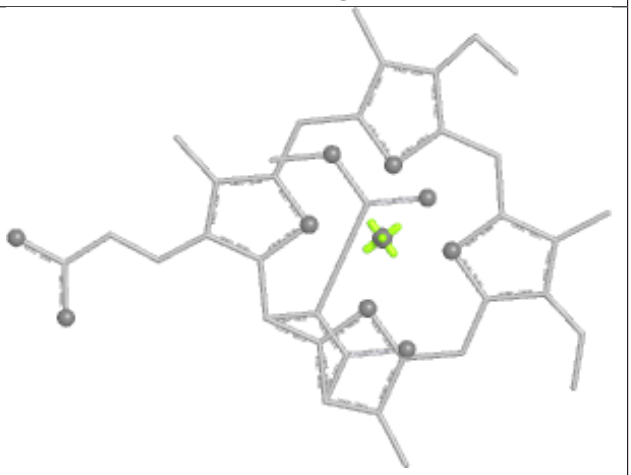
Bond lengths



Bond angles

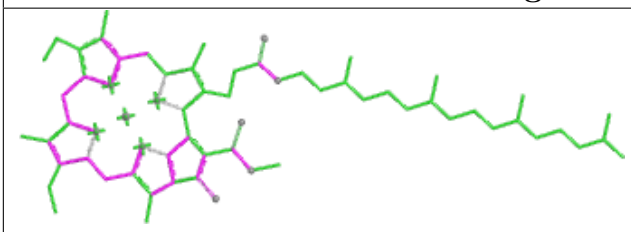


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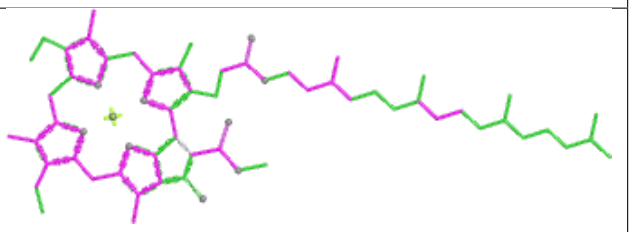


Rings

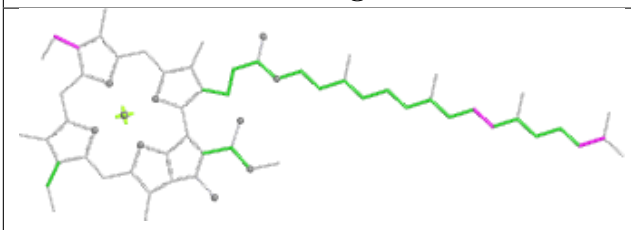
## Ligand CLA B 515



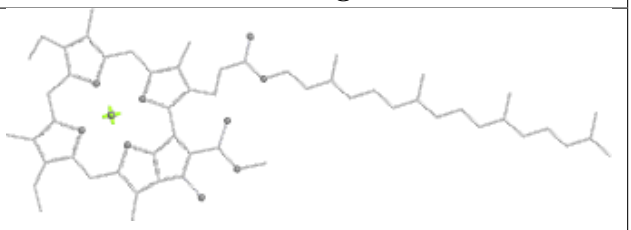
Bond lengths



Bond angles

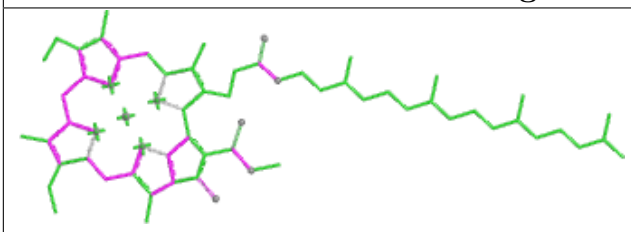


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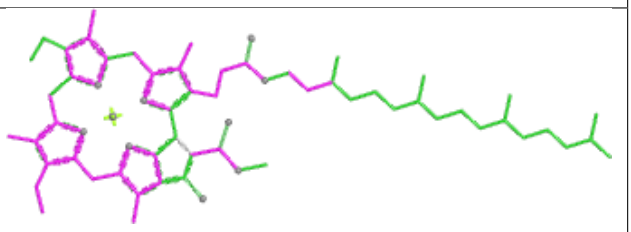


Rings

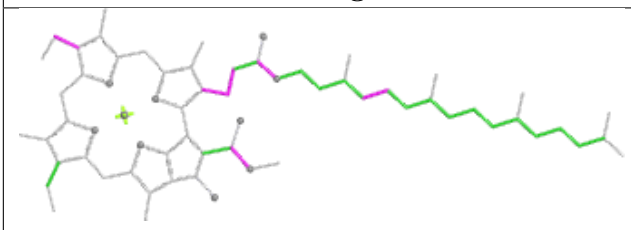
## Ligand CLA 39 301



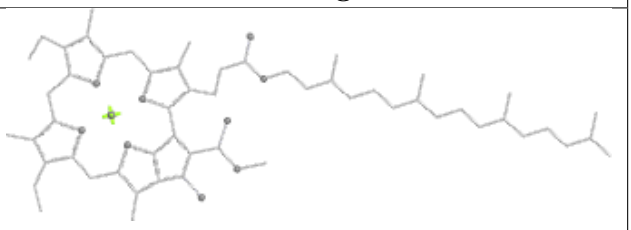
Bond lengths



Bond angles

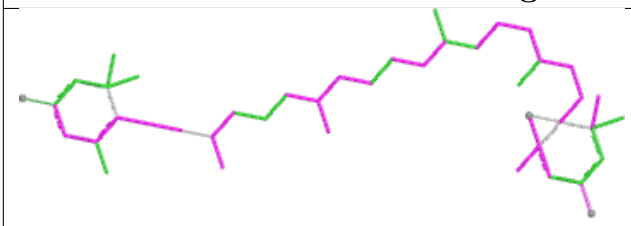


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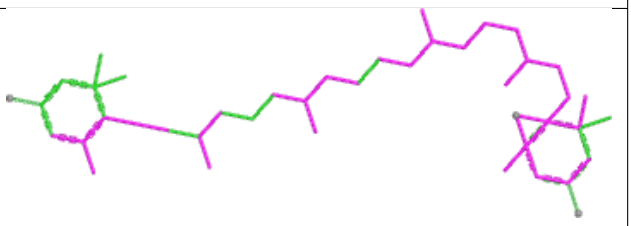


Rings

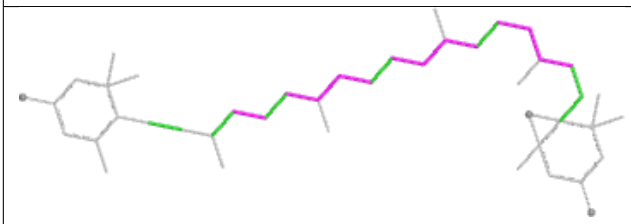
## Ligand DD6 41 216



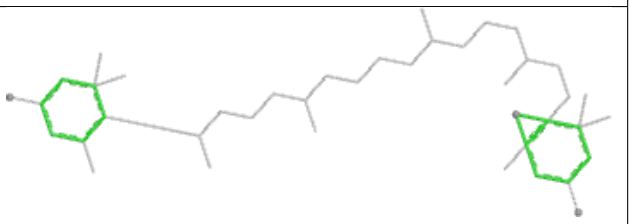
Bond lengths



Bond angles

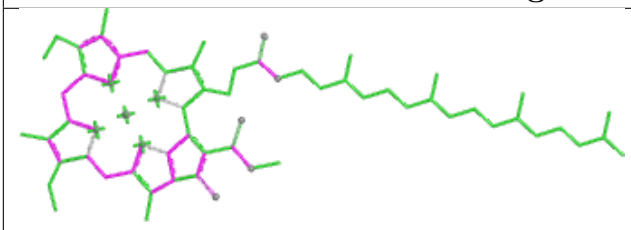


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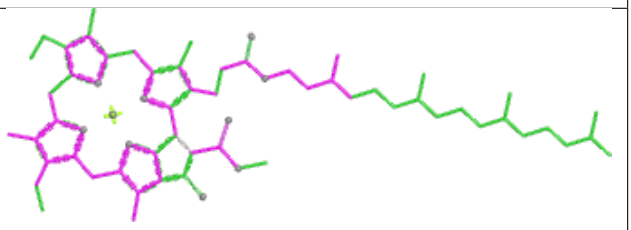


Rings

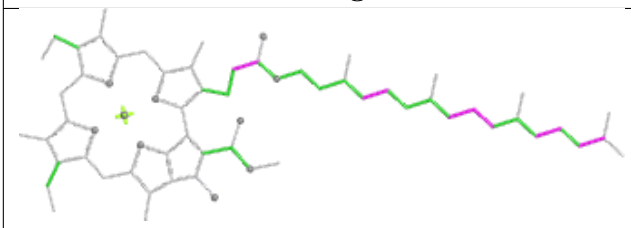
## Ligand CLA b 513



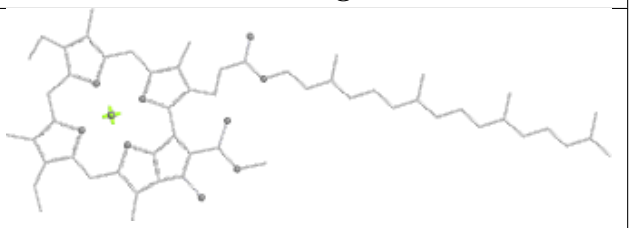
Bond lengths



Bond angles

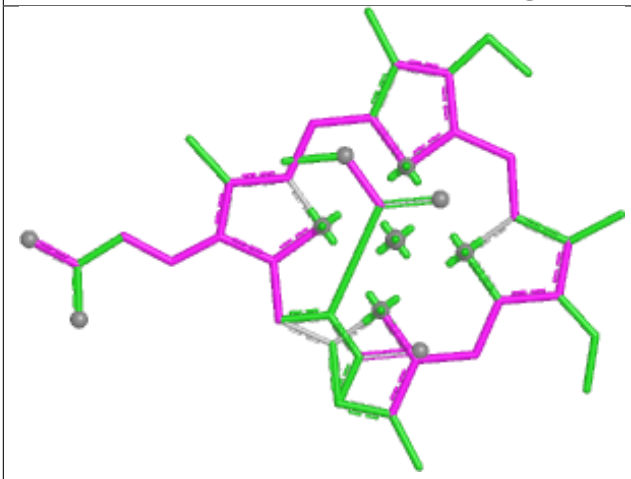


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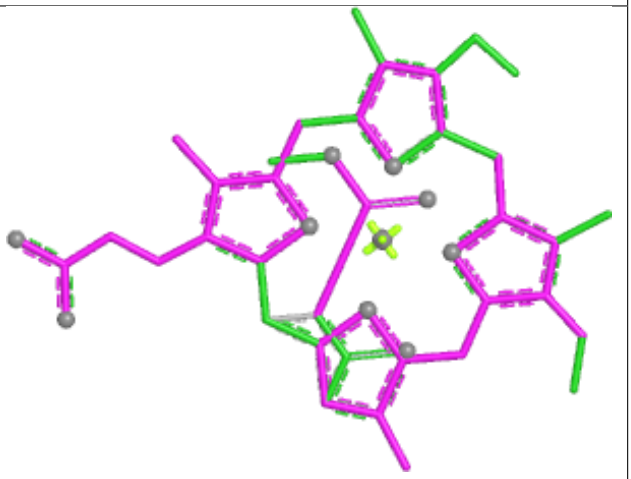


Rings

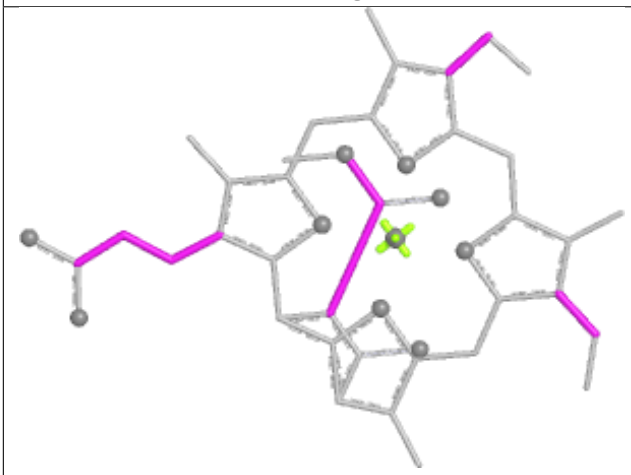
**Ligand KC1 20 305**



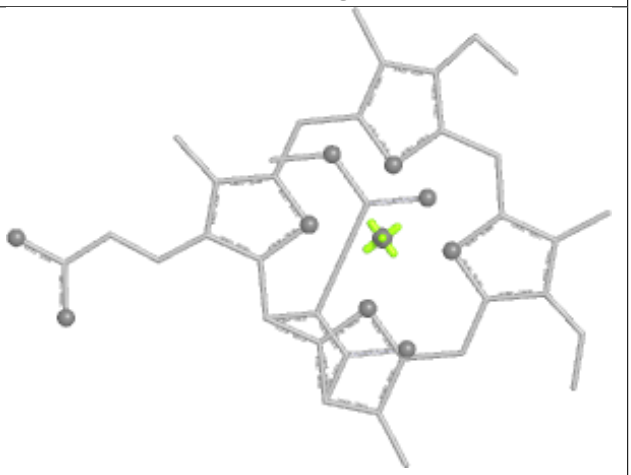
Bond lengths



Bond angles

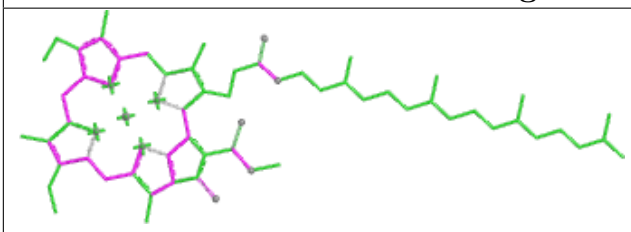


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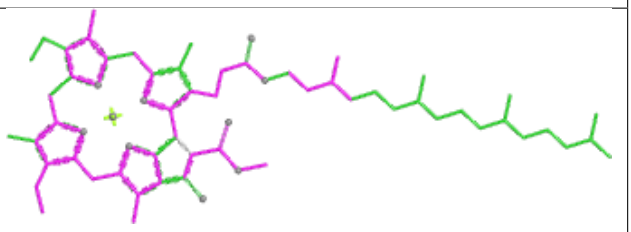


Rings

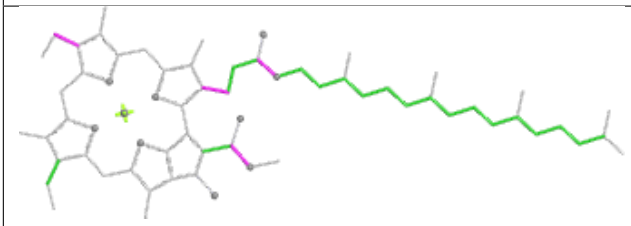
**Ligand CLA 38 203**



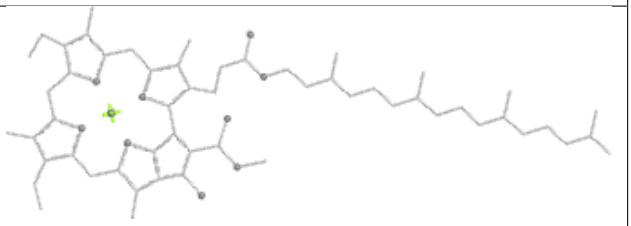
Bond lengths



Bond angles

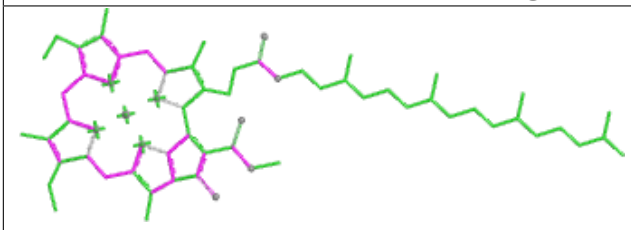


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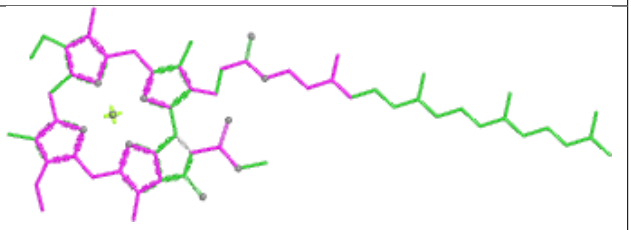


Rings

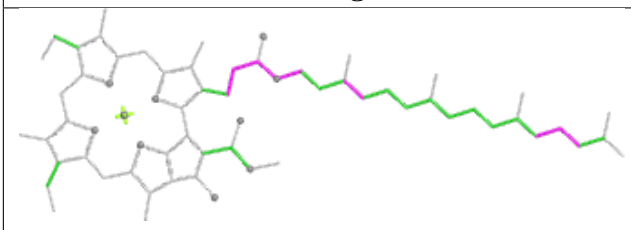
## Ligand CLA C 505



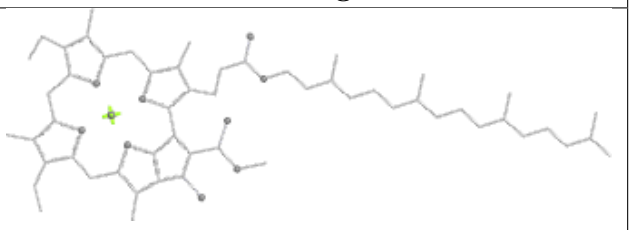
Bond lengths



Bond angles

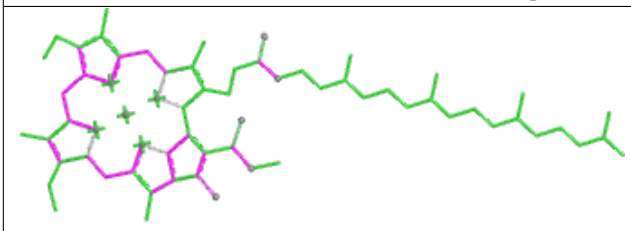


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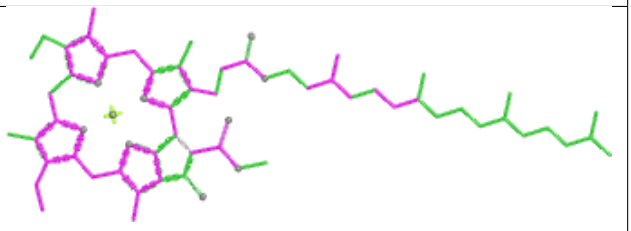


Rings

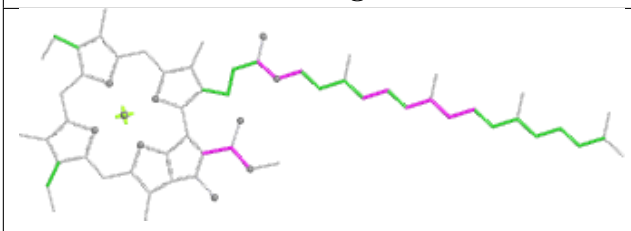
## Ligand CLA B 516



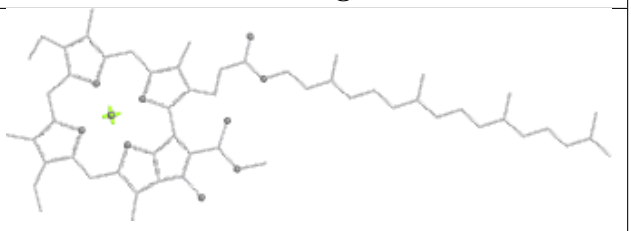
Bond lengths



Bond angles

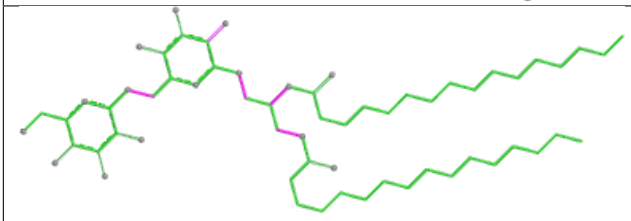


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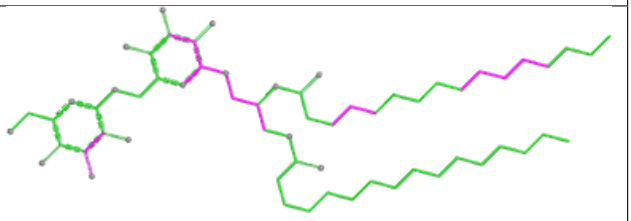


Rings

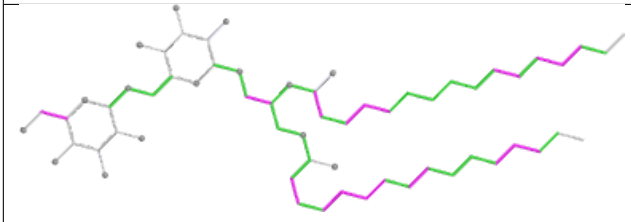
## Ligand DGD H 102



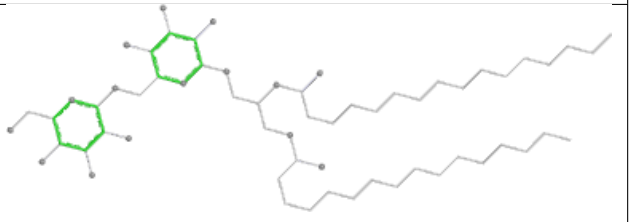
Bond lengths



Bond angles

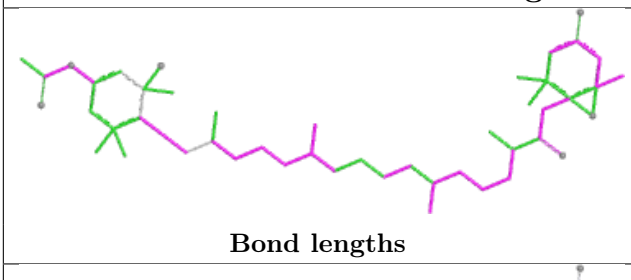


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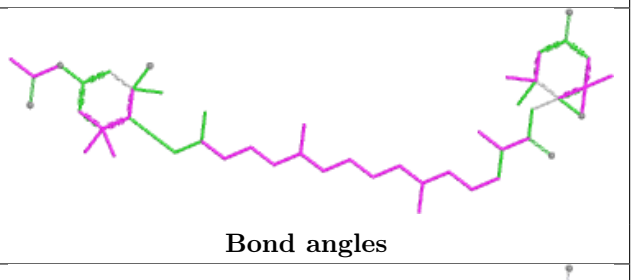


Rings

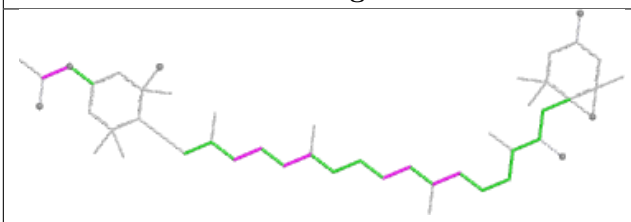
**Ligand A86 17 320**



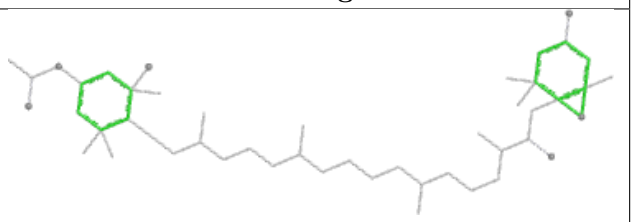
Bond lengths



Bond angles

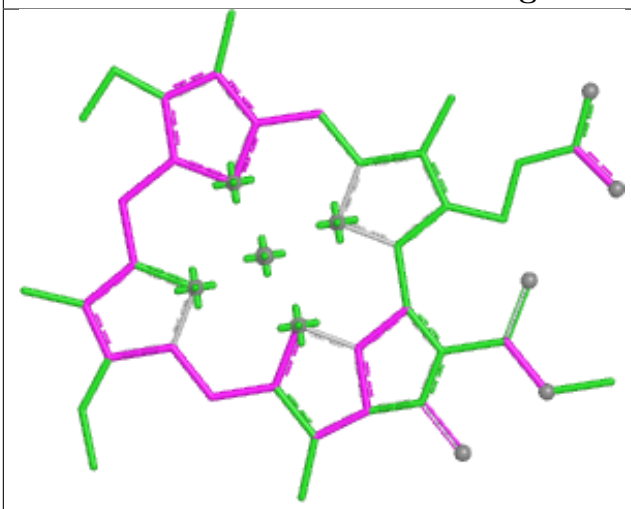


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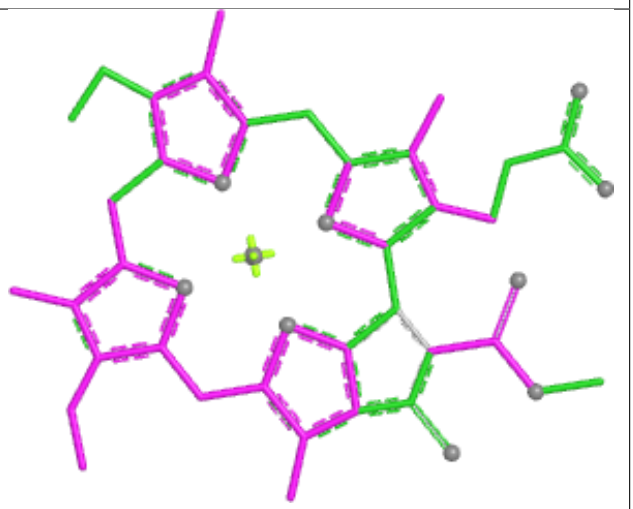


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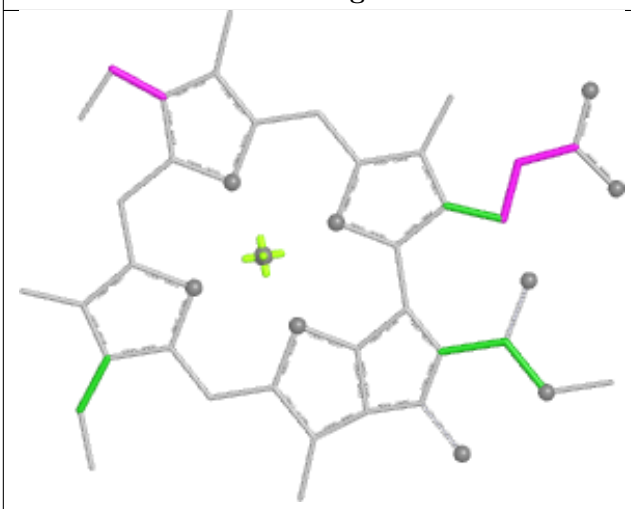
**Ligand CLA 18 206**



Bond lengths



Bond angles

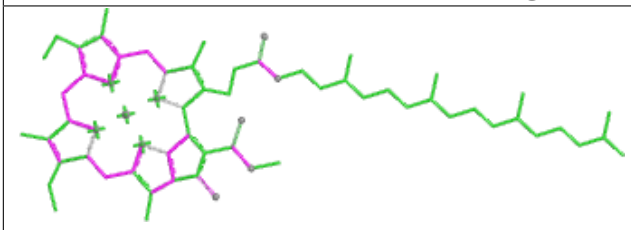


Torsions

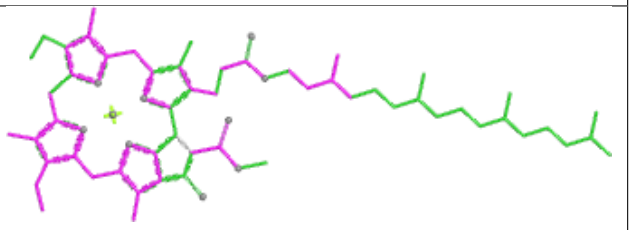


Rings

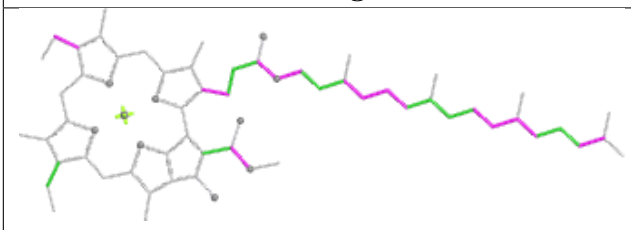
## Ligand CLA D 406



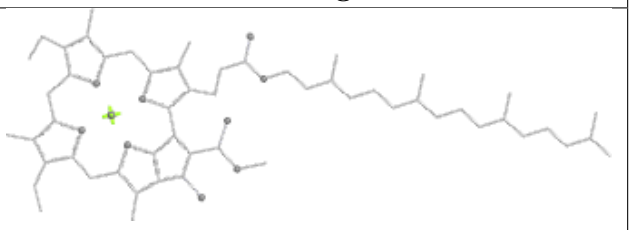
Bond lengths



Bond angles

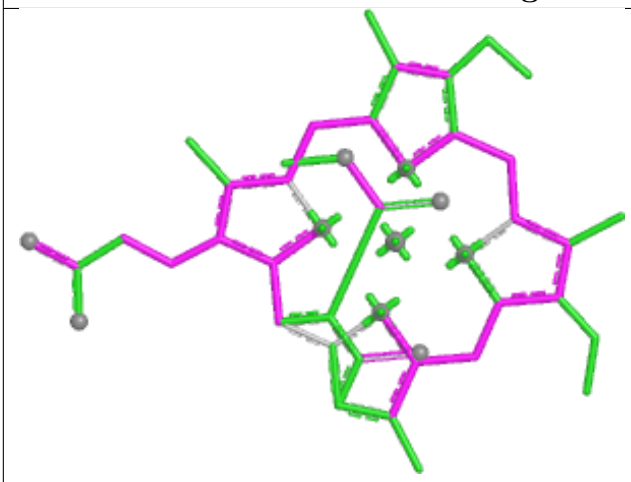


Torsions

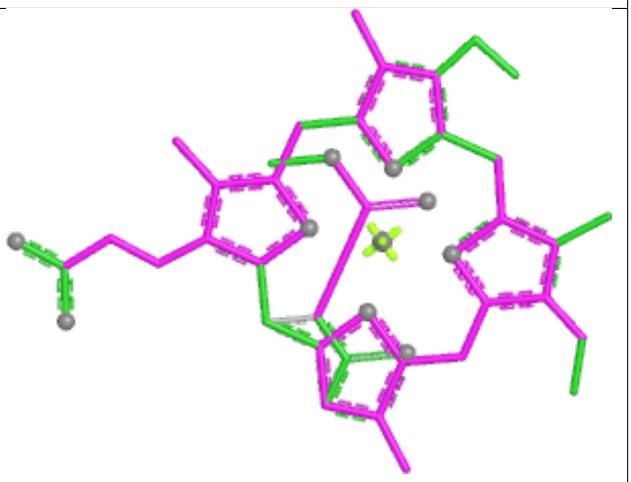


Rings

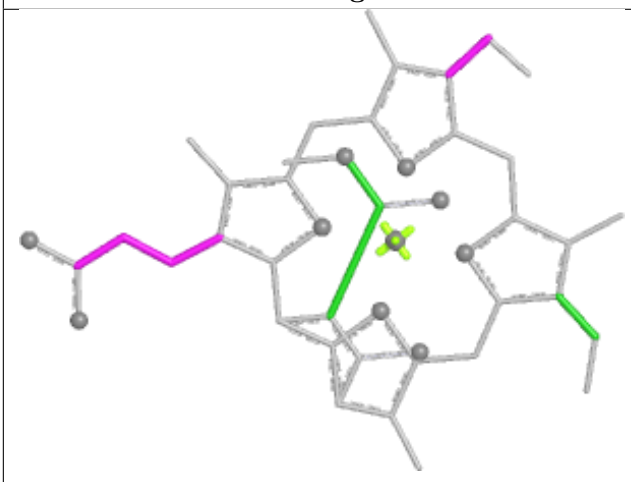
## Ligand KC1 16 305



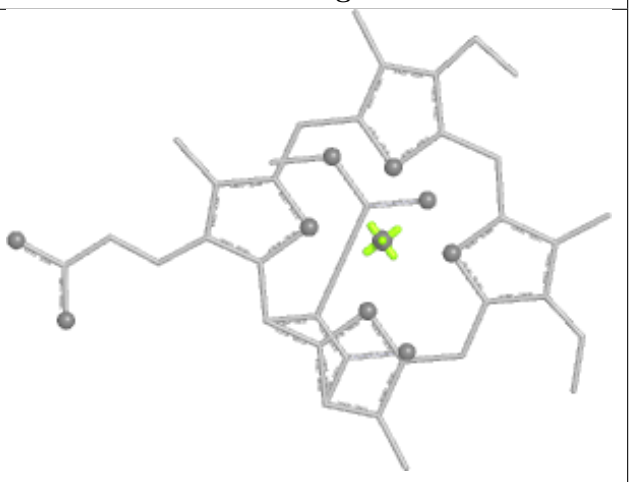
Bond lengths



Bond angles

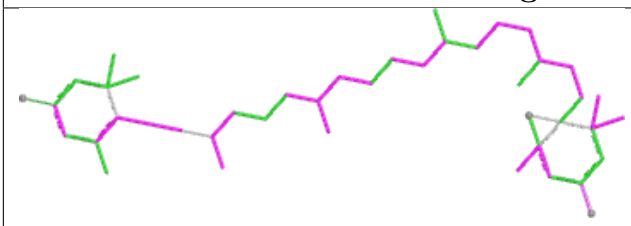


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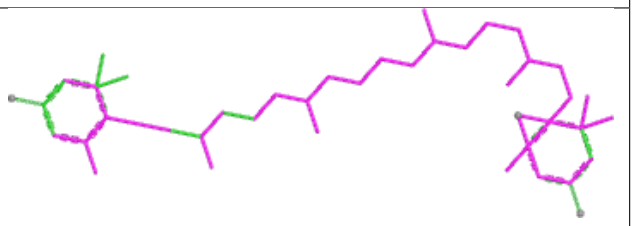


Rings

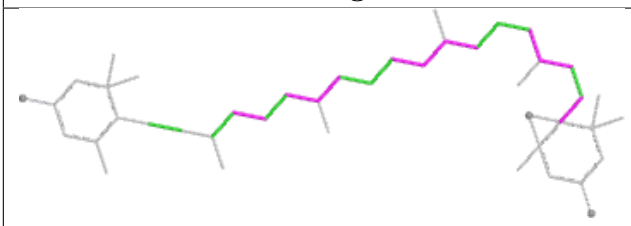
## Ligand DD6 19 312



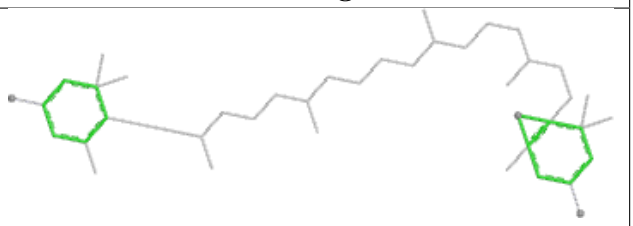
Bond lengths



Bond angles

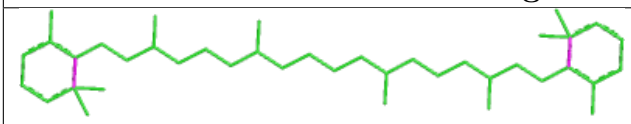


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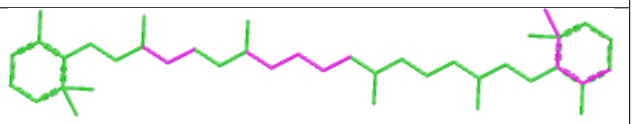


Rings

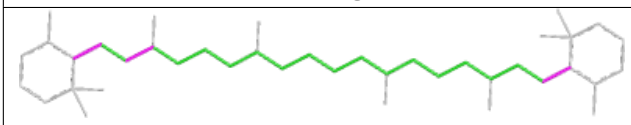
## Ligand BCR B 518



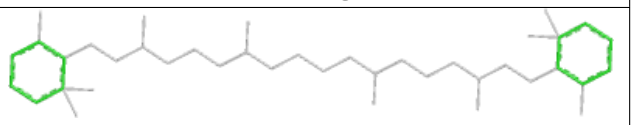
Bond lengths



Bond angles

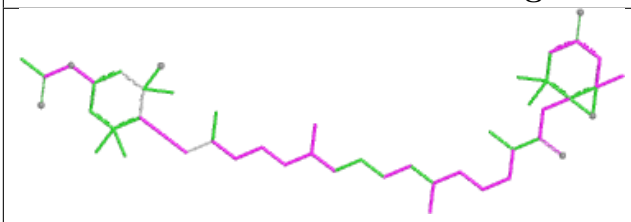


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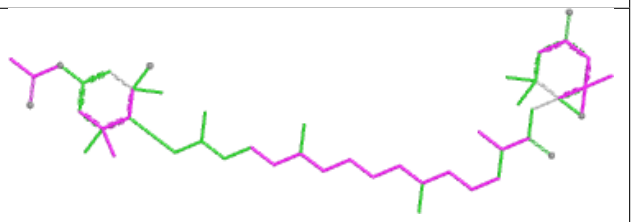


Rings

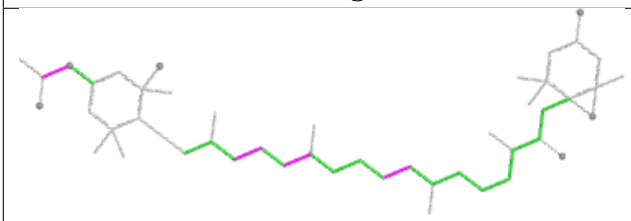
## Ligand A86 31 315



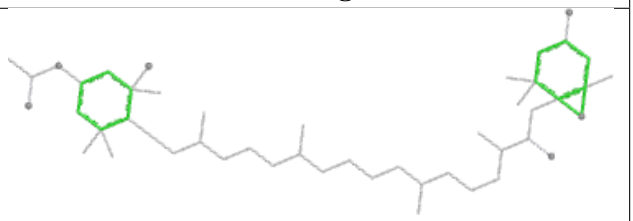
Bond lengths



Bond angles

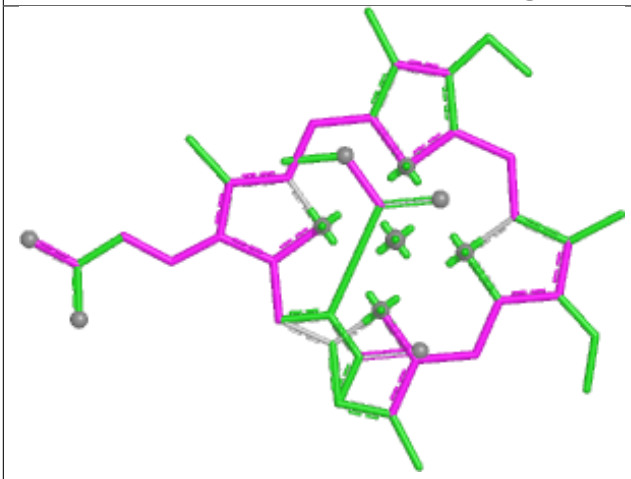


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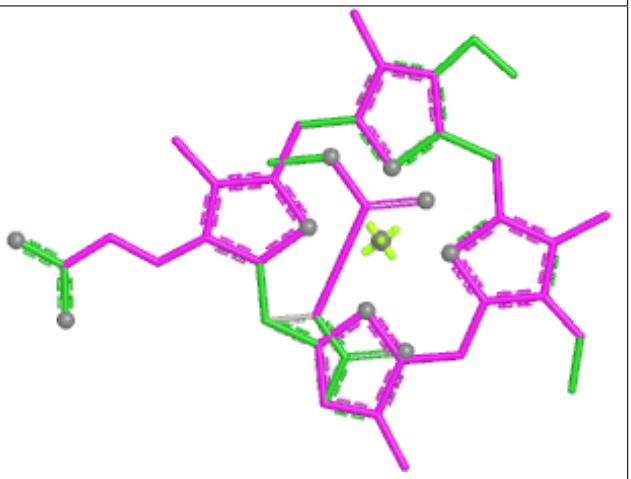


Rings

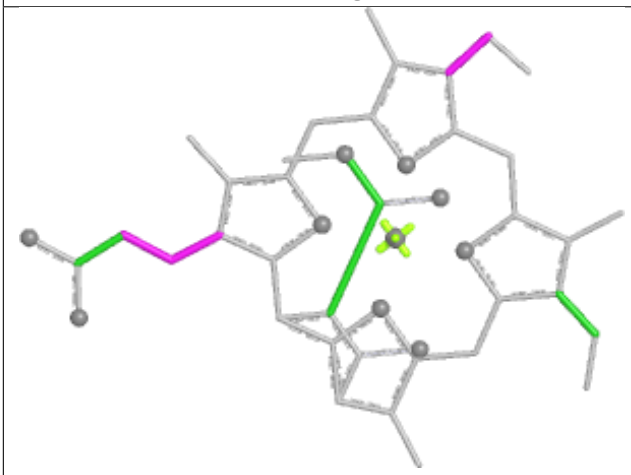
**Ligand KC1 31 305**



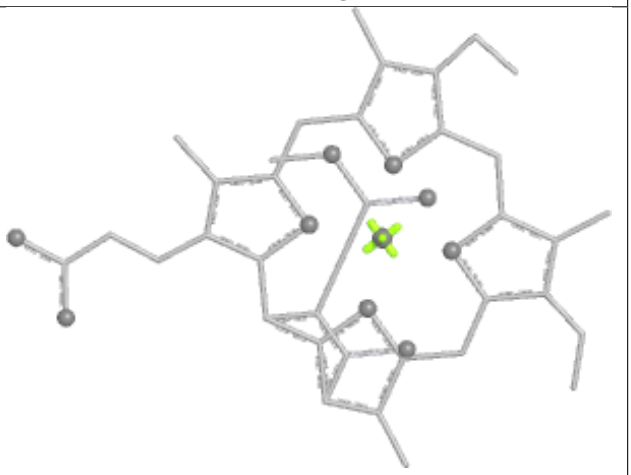
Bond lengths



Bond angles

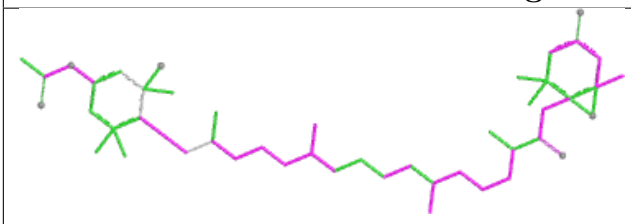


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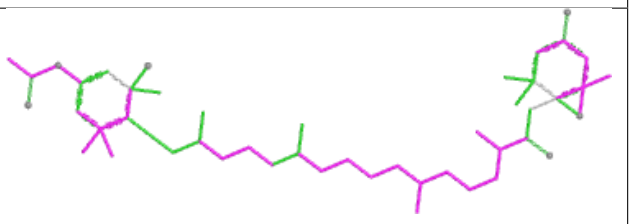


Rings

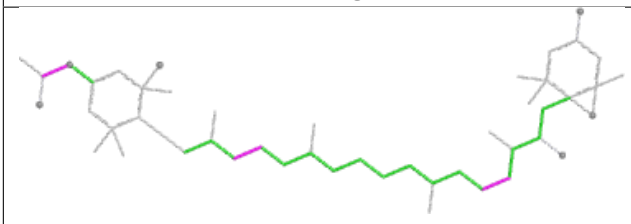
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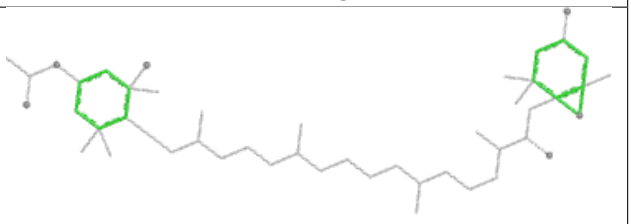
Bond lengths



Bond angles

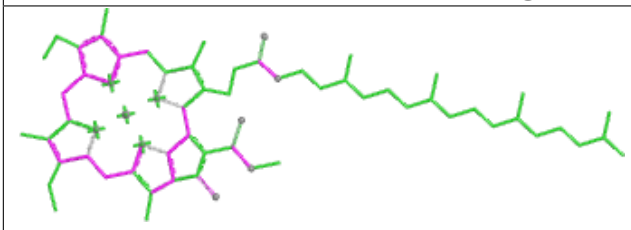


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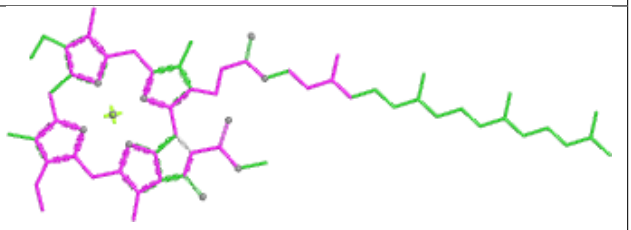


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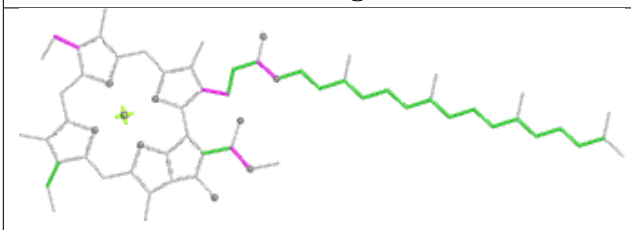
## Ligand CLA 18 203



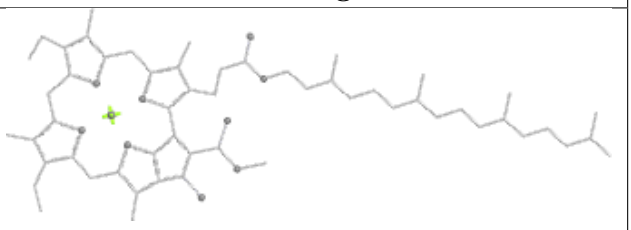
Bond lengths



Bond angles

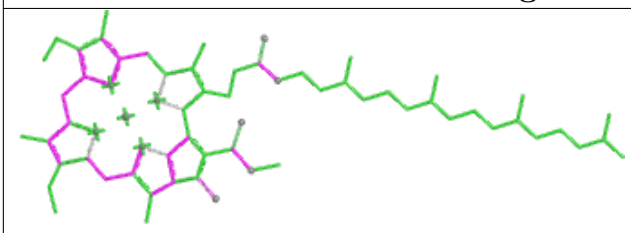


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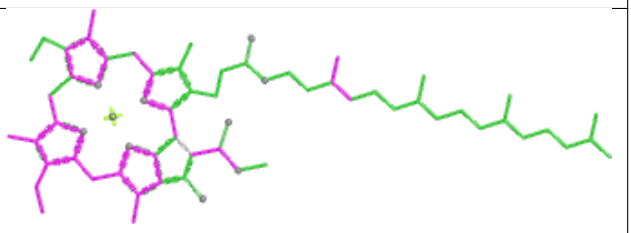


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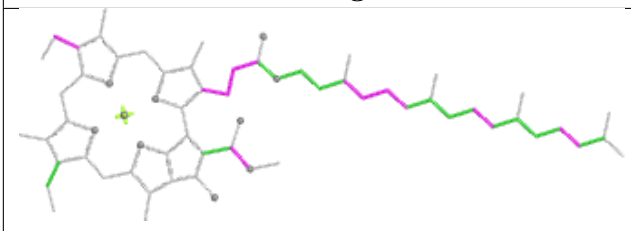
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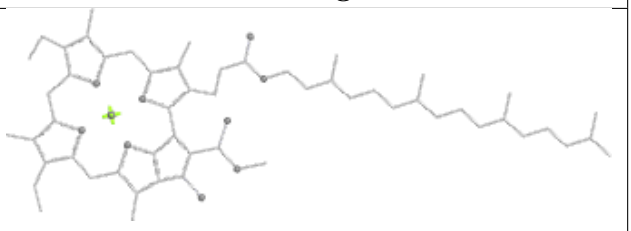
Bond lengths



Bond angles

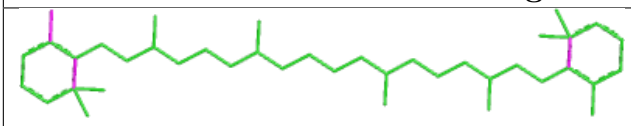


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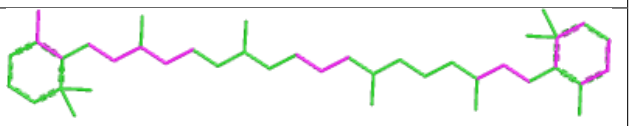


Rings

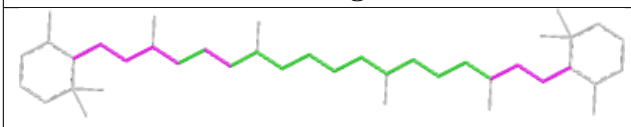
## Ligand BCR d 405



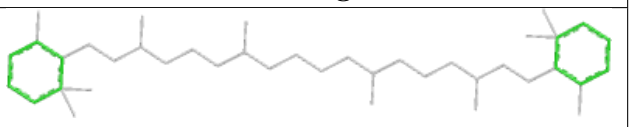
Bond lengths



Bond angles

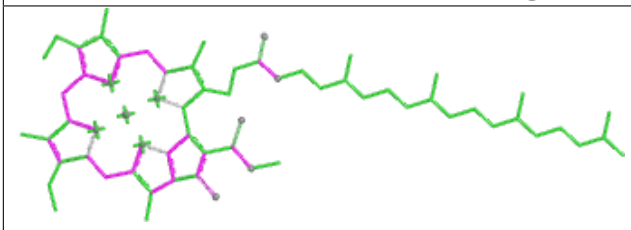


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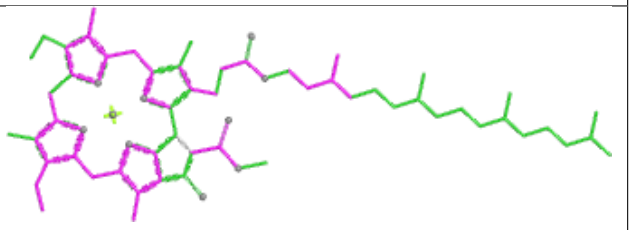


Rings

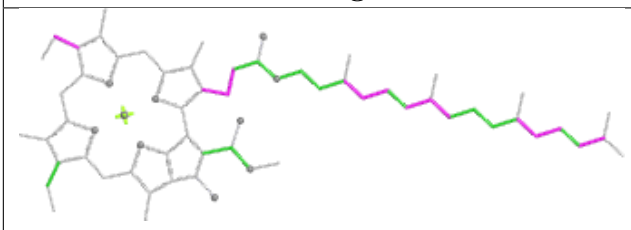
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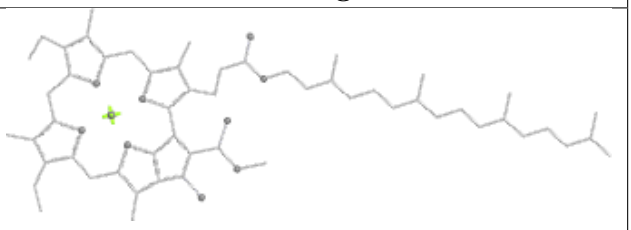
Bond lengths



Bond angles

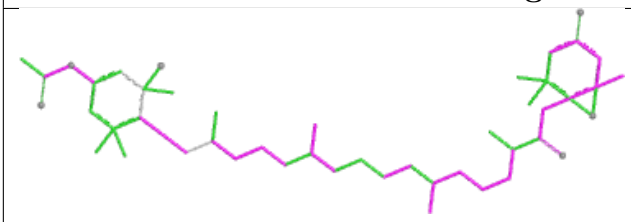


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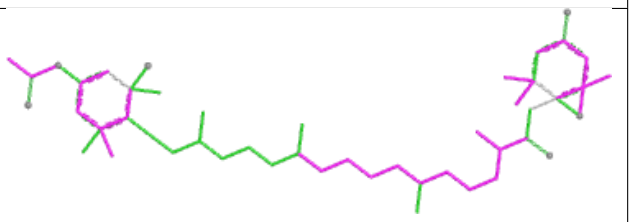


Rings

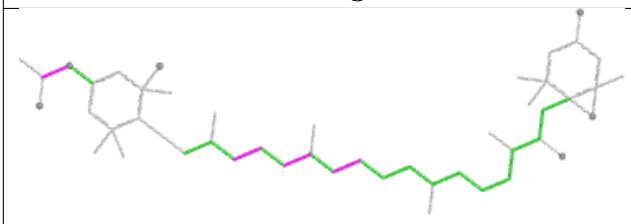
## Ligand A86 11 311



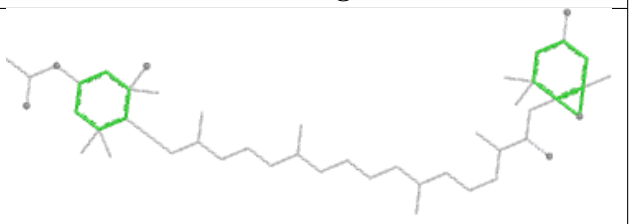
Bond lengths



Bond angles

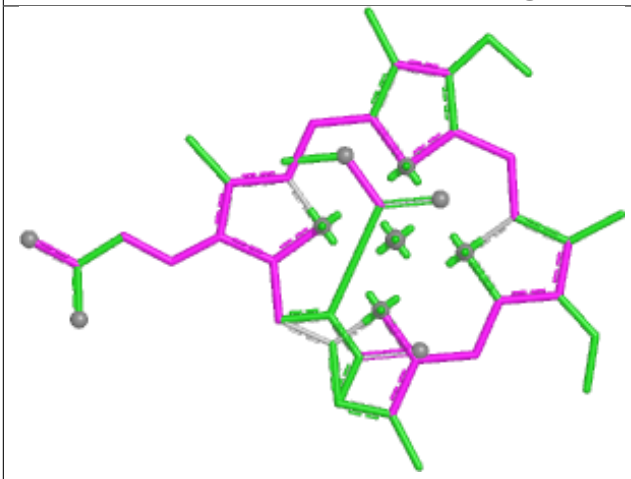


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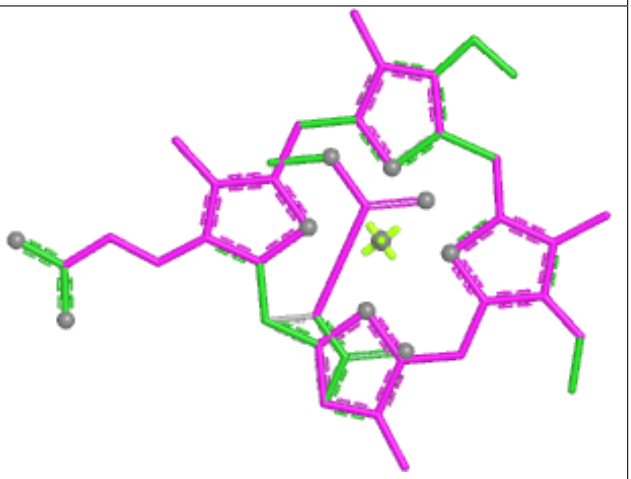


Rings

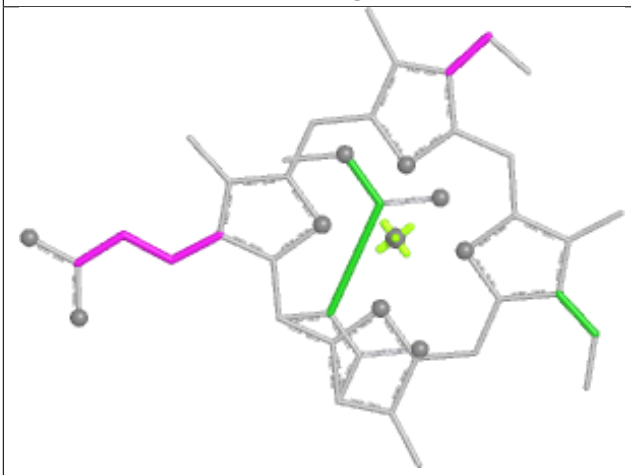
**Ligand KC1 20 304**



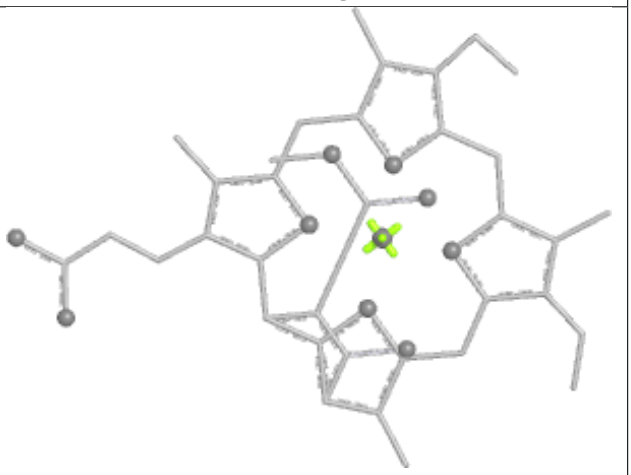
Bond lengths



Bond angles

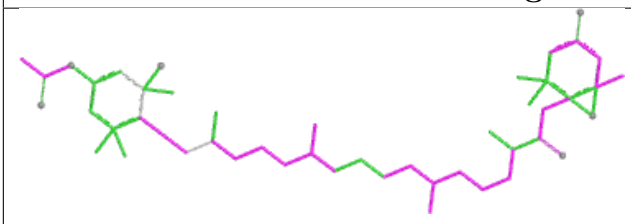


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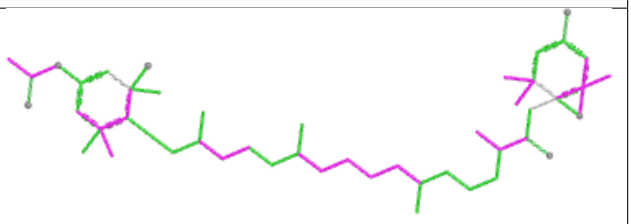


Rings

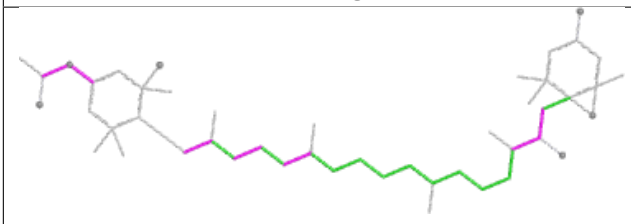
**Ligand A86 12 215**



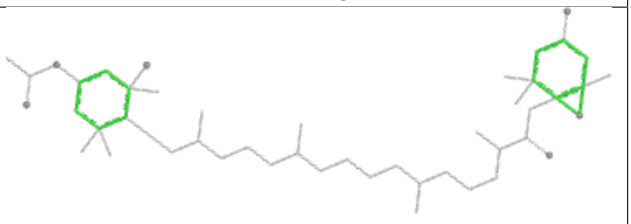
Bond lengths



Bond angles

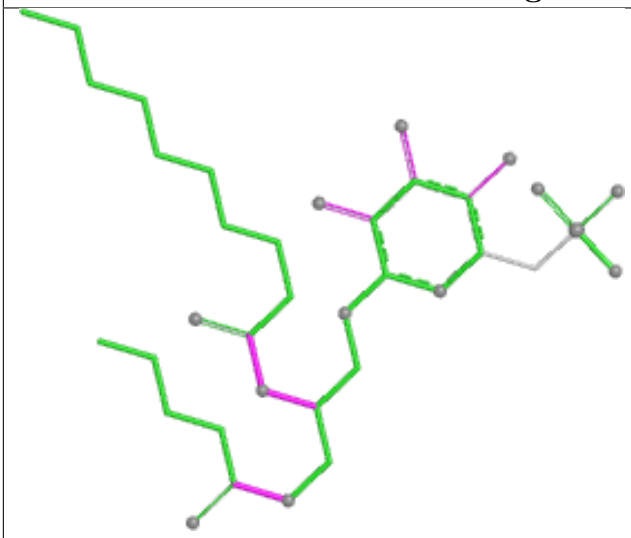


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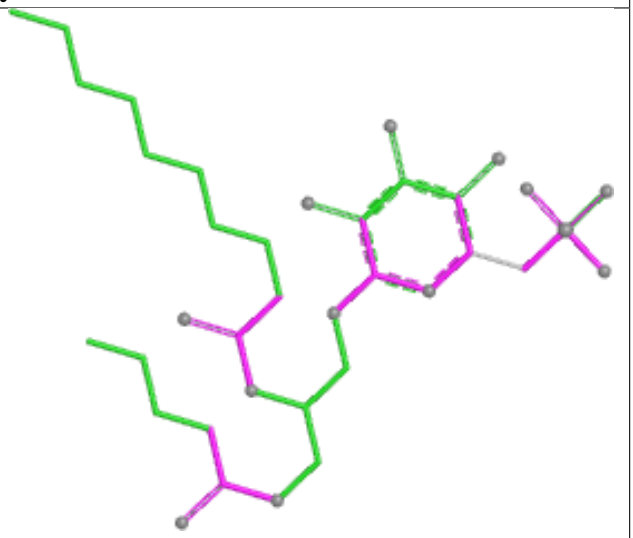


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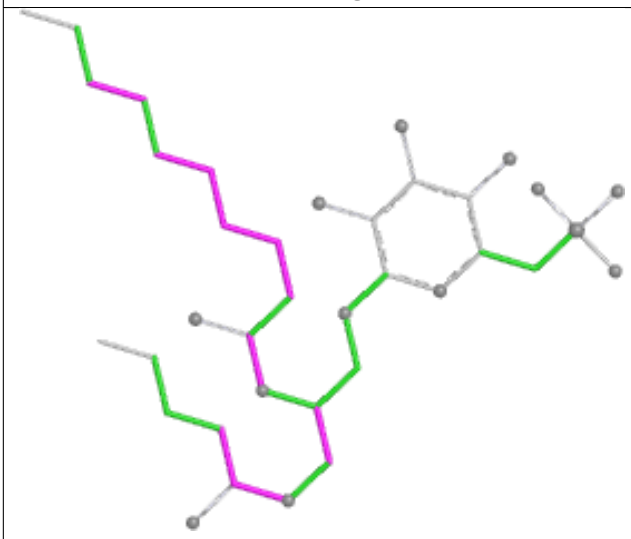
## Ligand SQD B 522



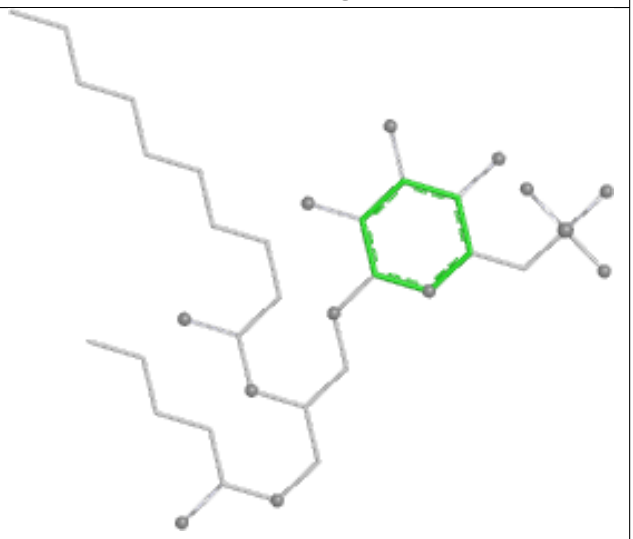
Bond lengths



Bond angles

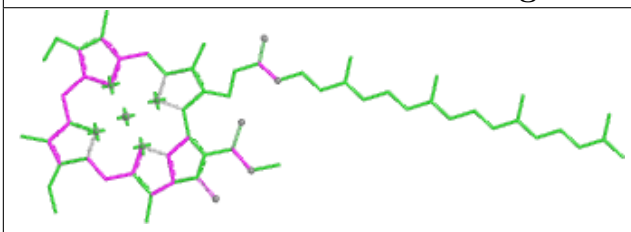


Torsions

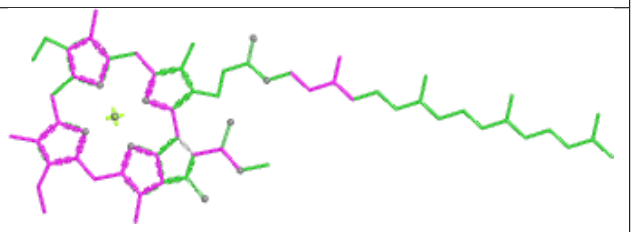


Rings

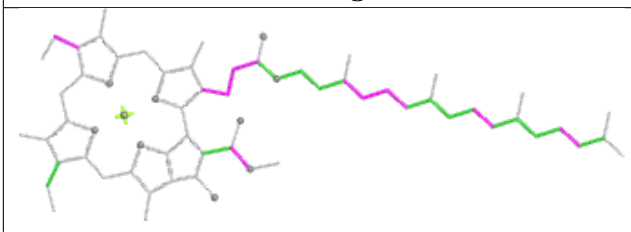
## Ligand CLA 13 301



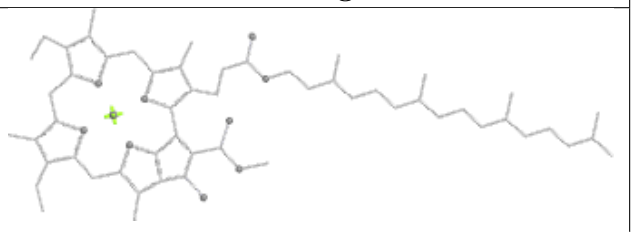
Bond lengths



Bond angles

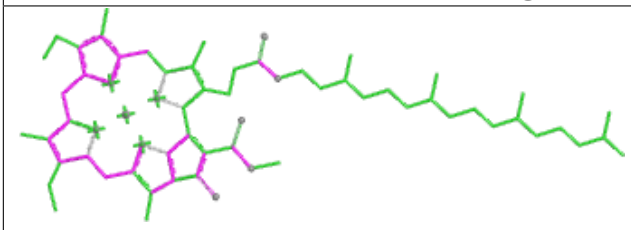


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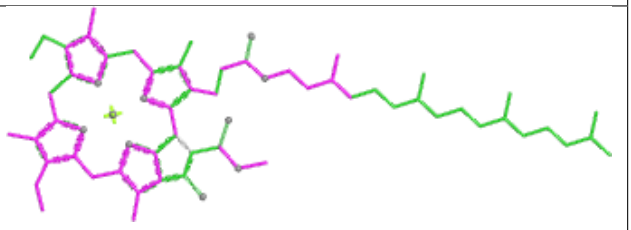


Rings

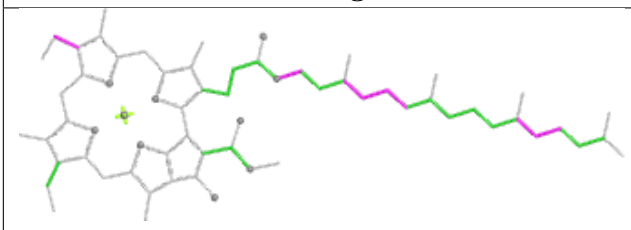
## Ligand CLA 35 308



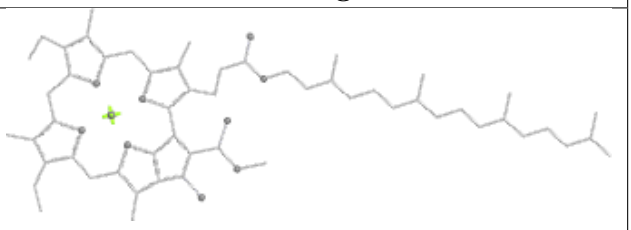
Bond lengths



Bond angles

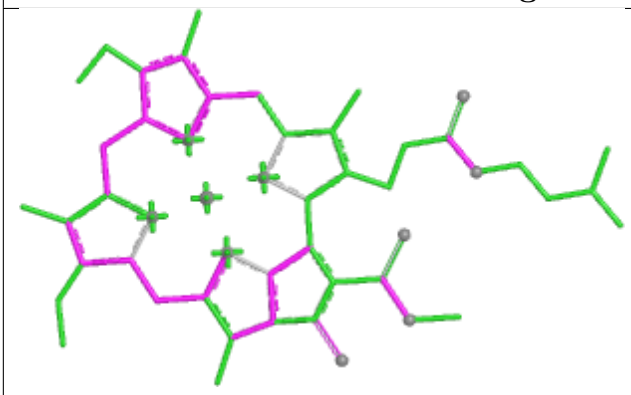


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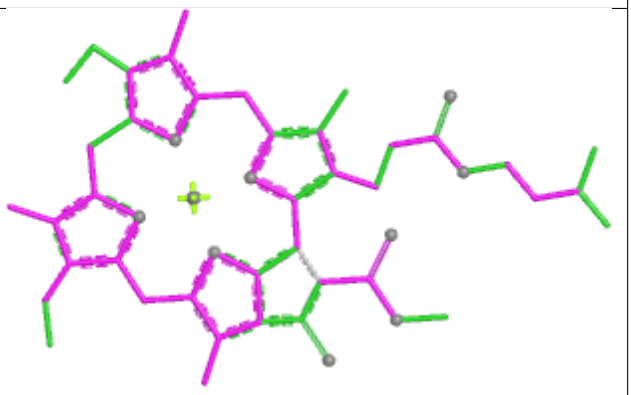


Rings

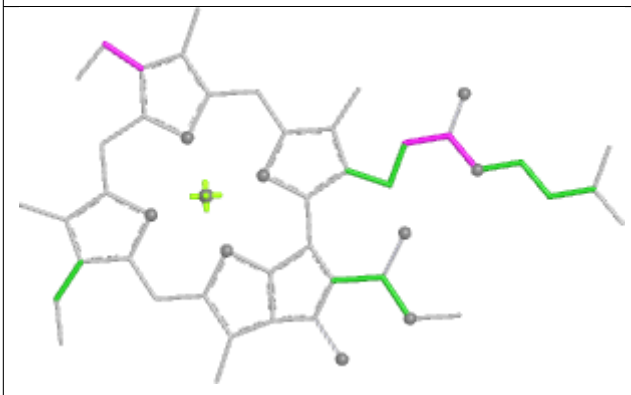
## Ligand CLA 40 208



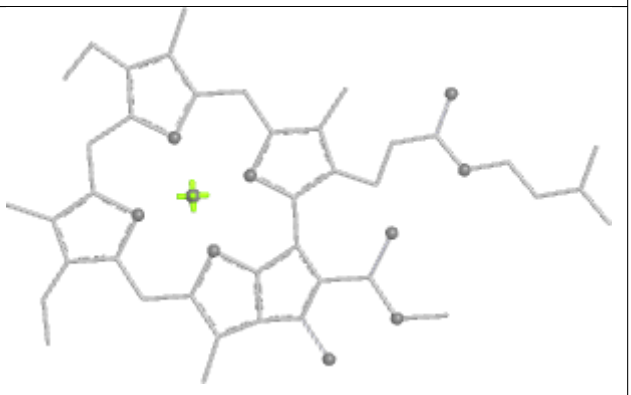
Bond lengths



Bond angles

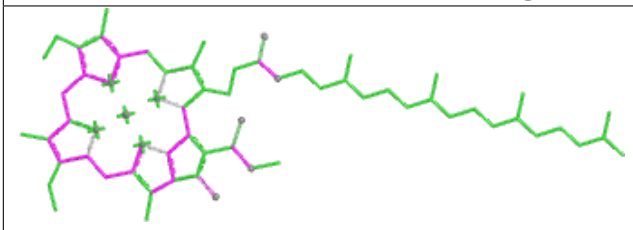


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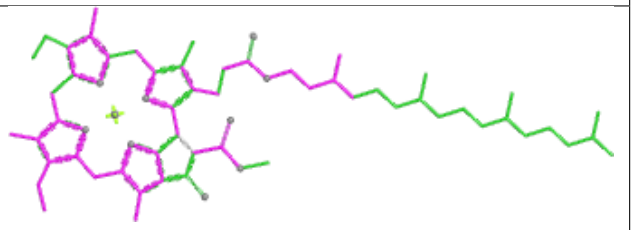


Rings

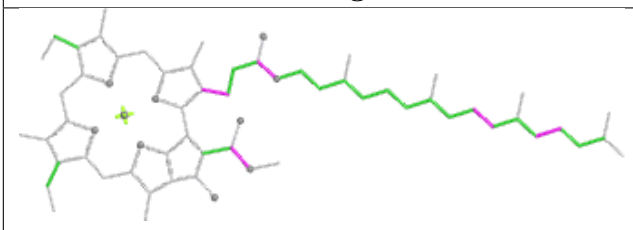
## Ligand CLA 18 201



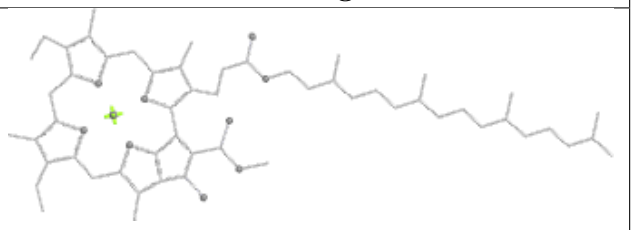
Bond lengths



Bond angles

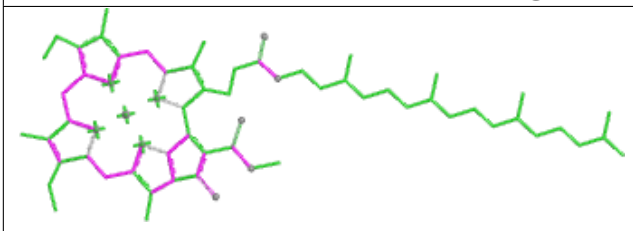


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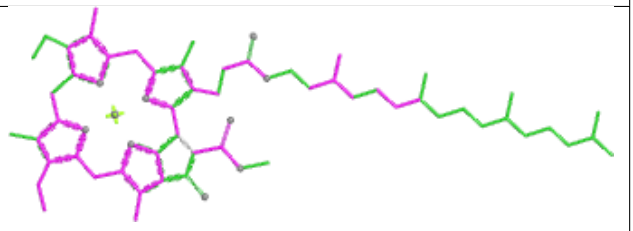


Rings

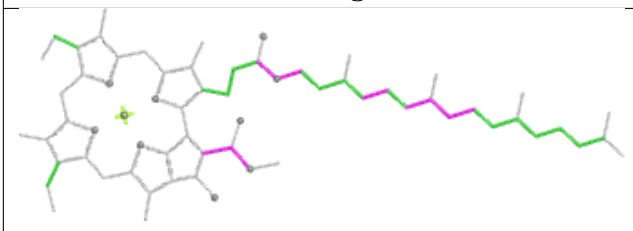
## Ligand CLA b 516



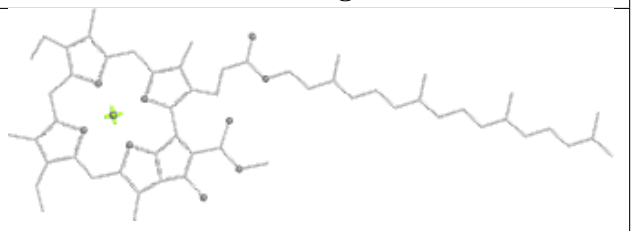
Bond lengths



Bond angles

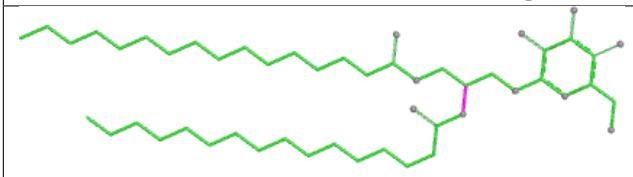


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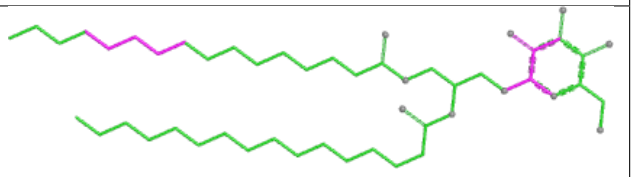


Rings

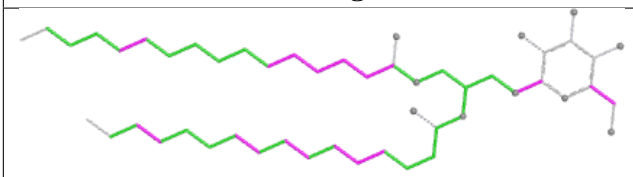
## Ligand LMG B 520



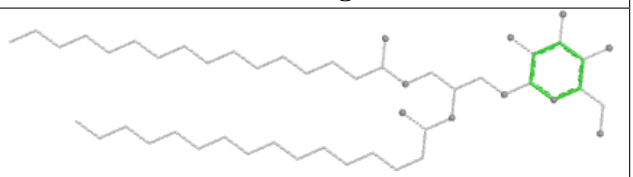
Bond lengths



Bond angles

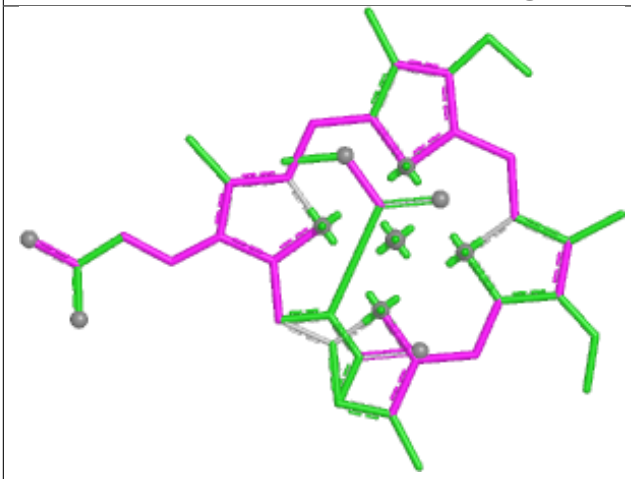


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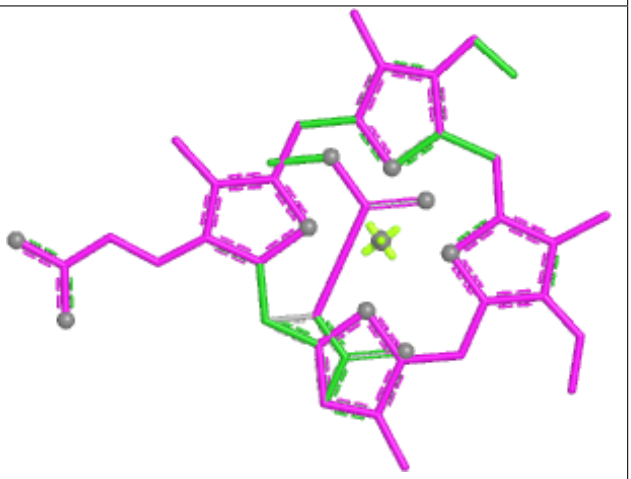


Rings

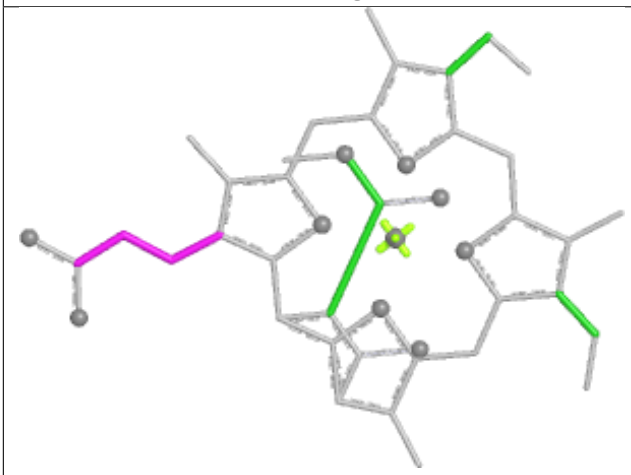
**Ligand KC1 39 308**



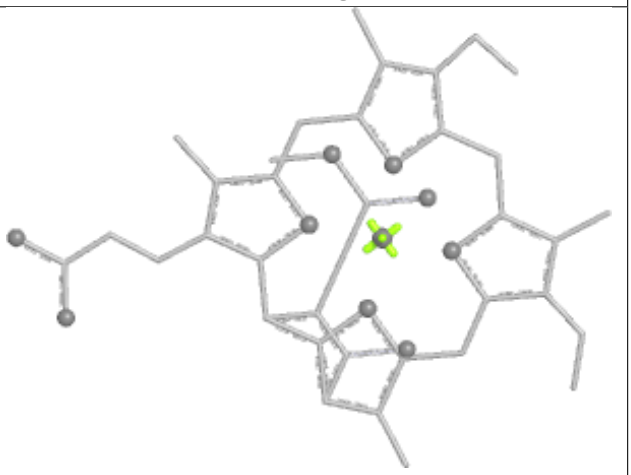
**Bond lengths**



**Bond angles**

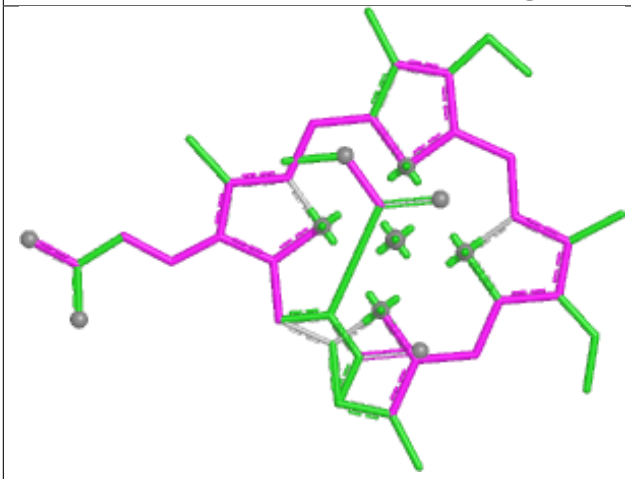


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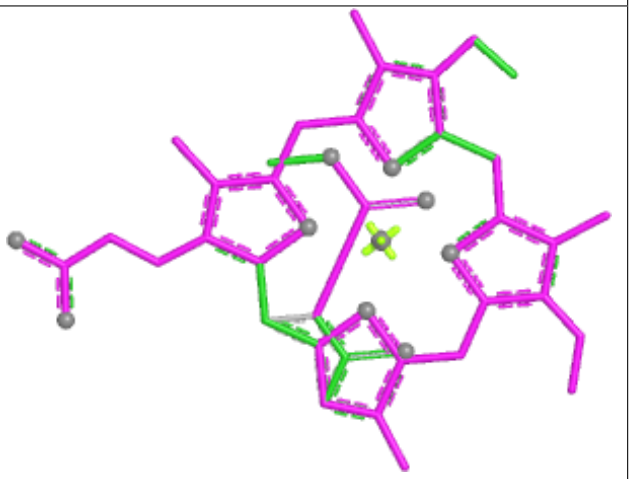


**Rings**

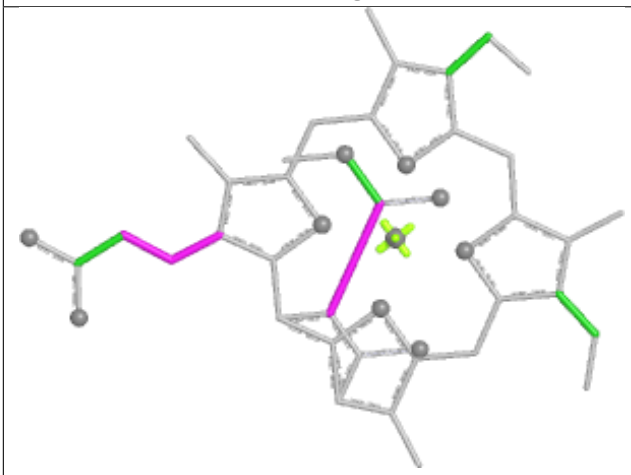
**Ligand KC1 38 207**



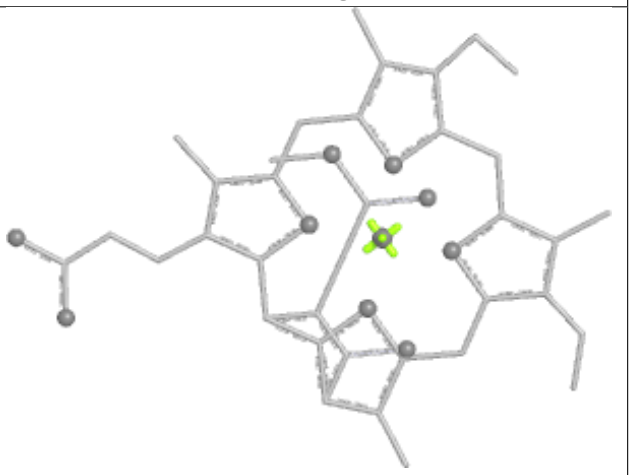
**Bond lengths**



**Bond angles**

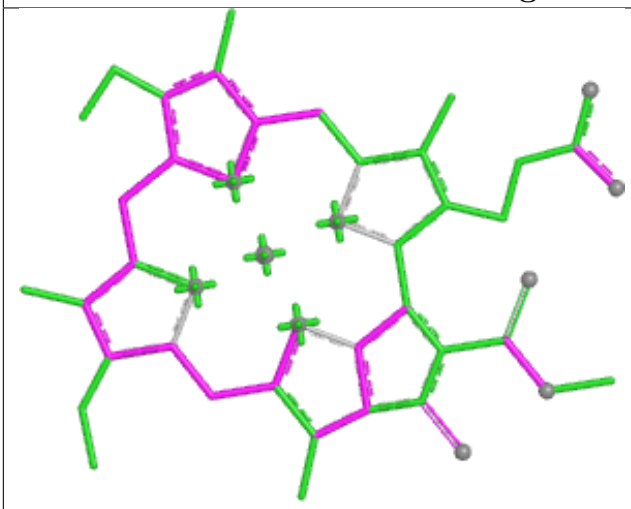


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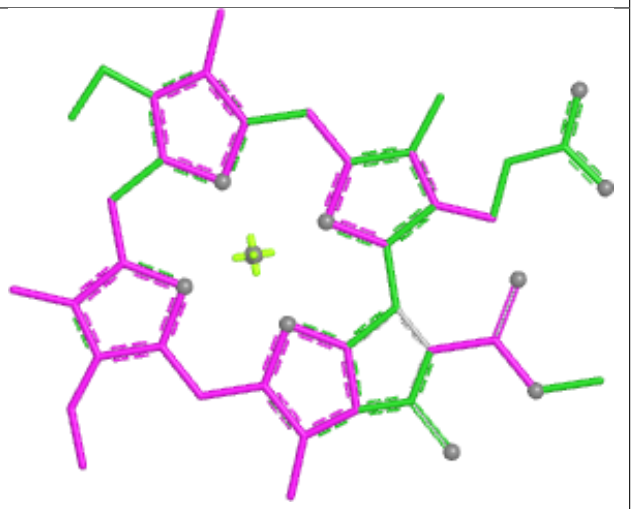


**Rings**

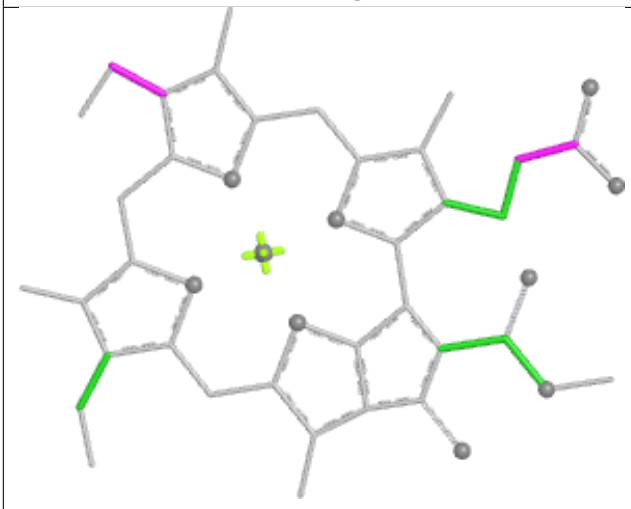
## Ligand CLA 33 305



Bond lengths



Bond angles

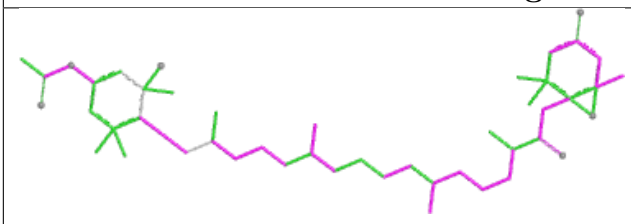


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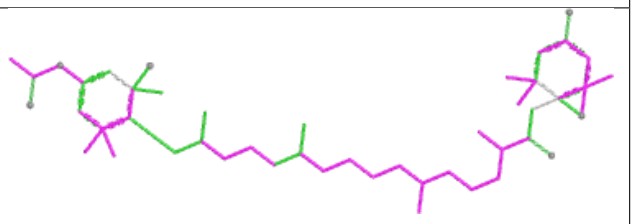


Rings

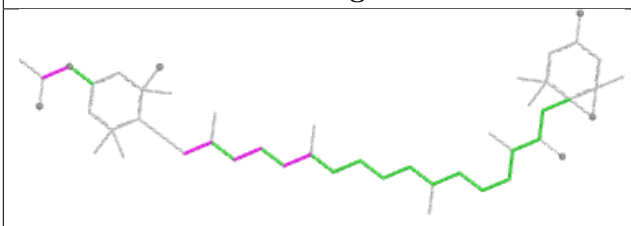
## Ligand A86 31 312



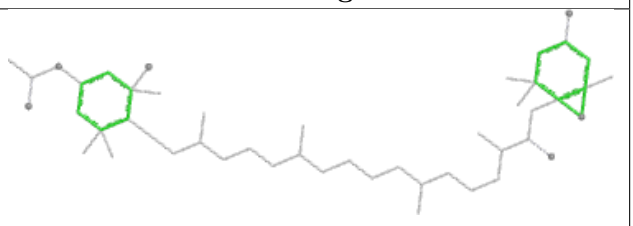
Bond lengths



Bond angles

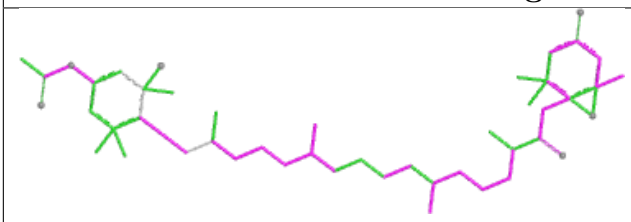


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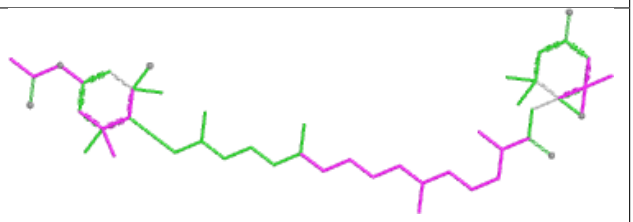


Rings

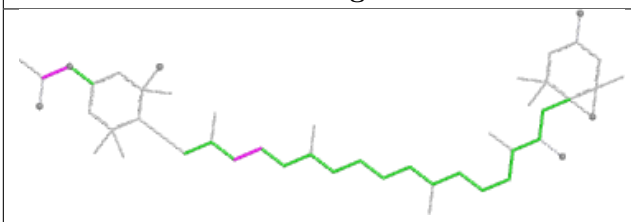
**Ligand A86 32 215**



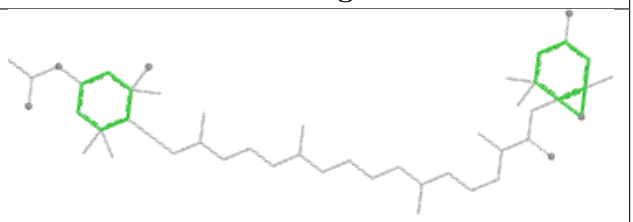
Bond lengths



Bond angles

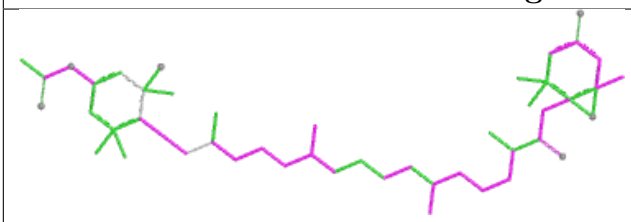


Torsions

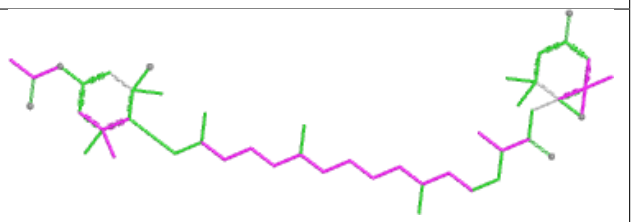


Rings

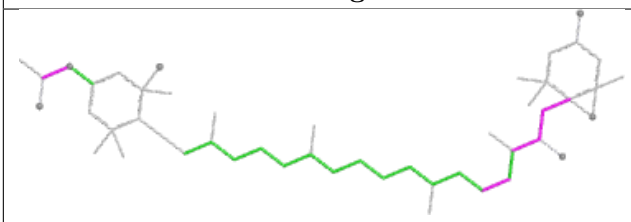
**Ligand A86 16 314**



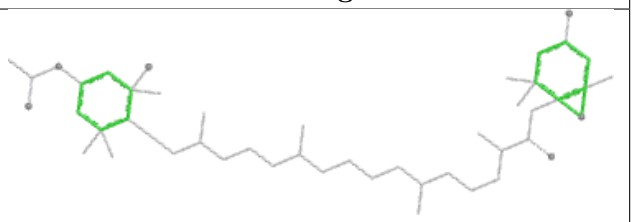
Bond lengths



Bond angles

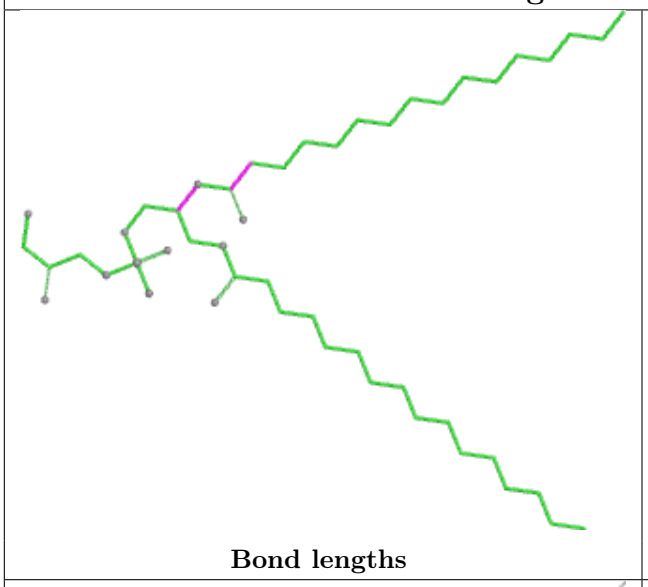


Torsions

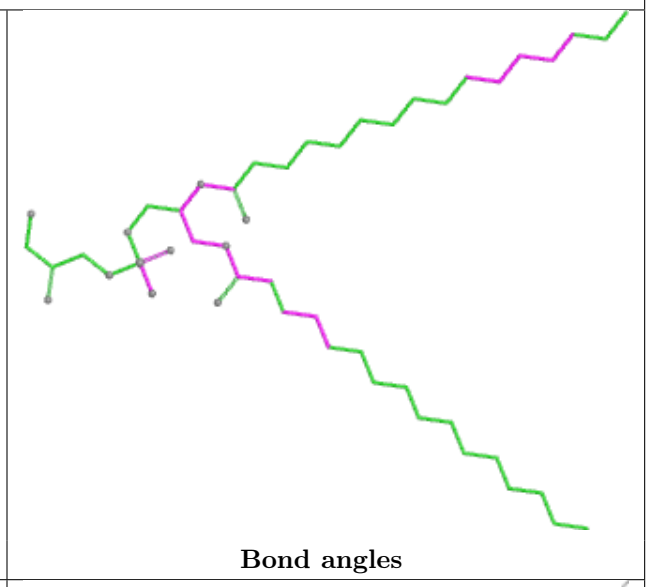


Rings

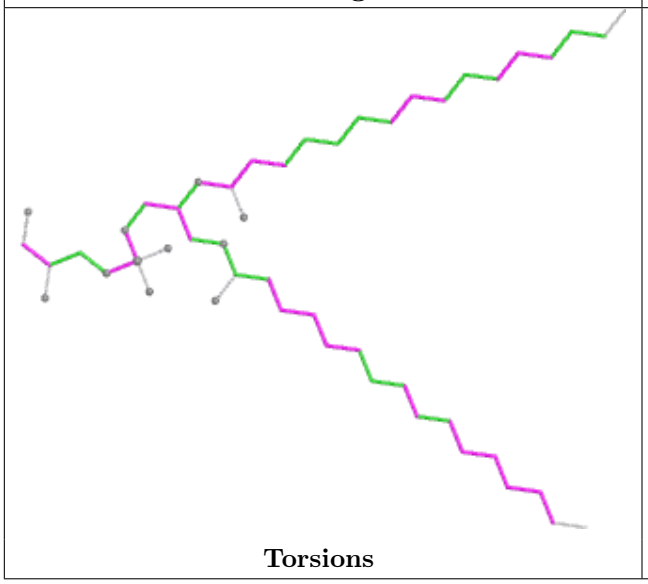
## Ligand LHG d 408



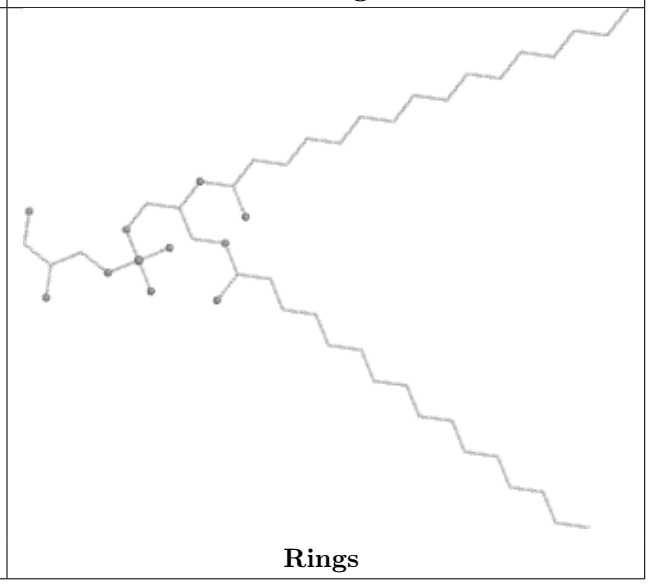
Bond lengths



Bond angles

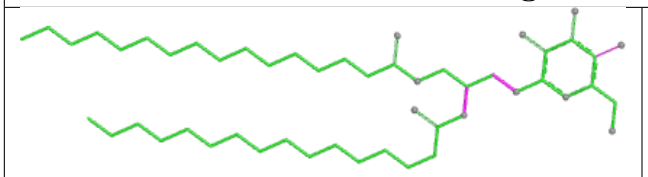


Torsions

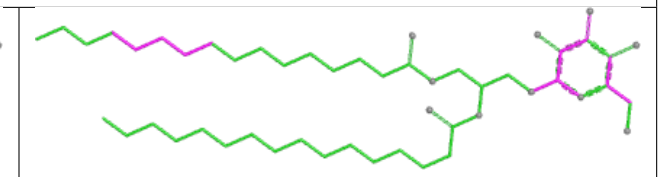


Rings

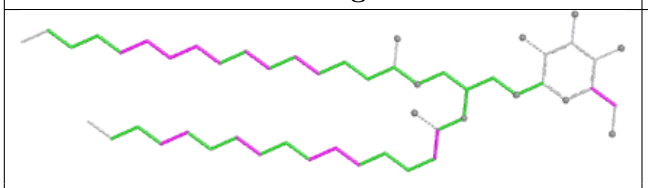
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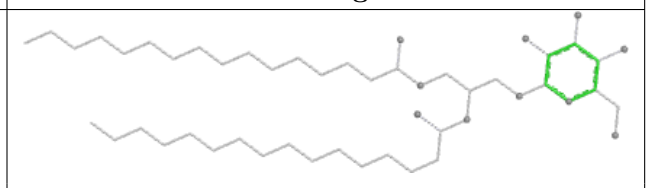
Bond lengths



Bond angles

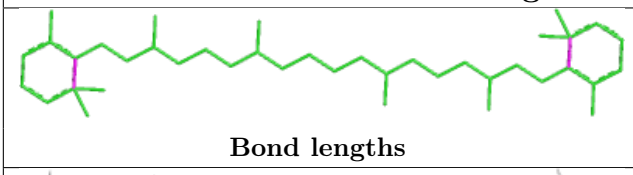


Torsions

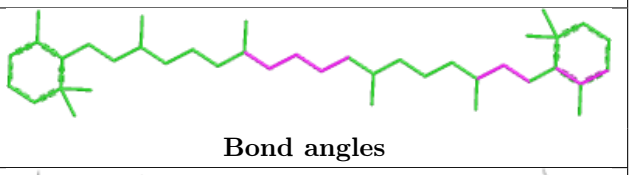


Rings

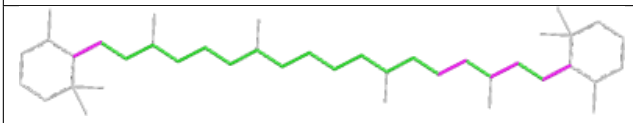
## Ligand BCR C 519



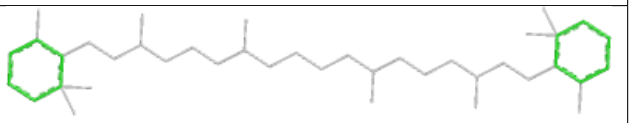
Bond lengths



Bond angles

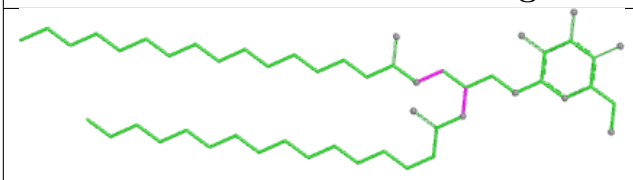


Torsions

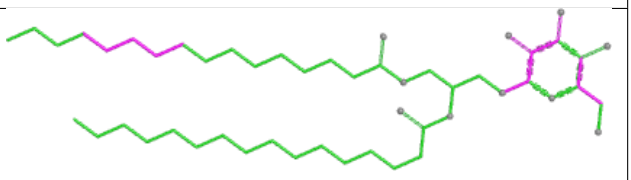


Rings

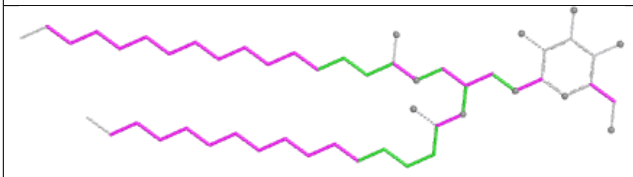
## Ligand LMG A 408



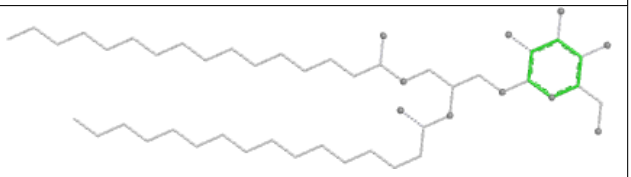
Bond lengths



Bond angles

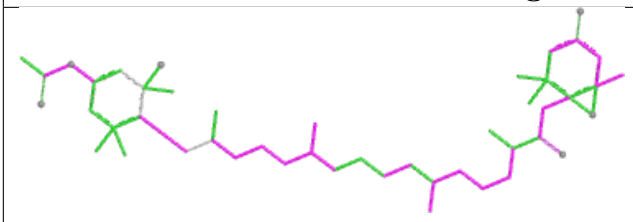


Torsions



Rings

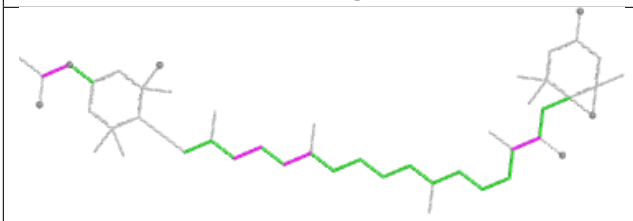
## Ligand A86 31 314



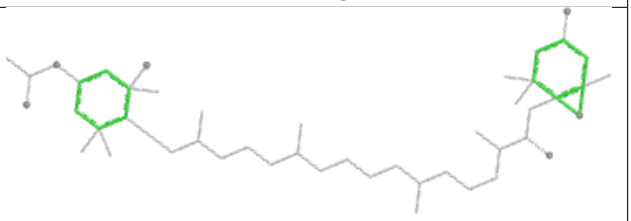
Bond lengths



Bond angles

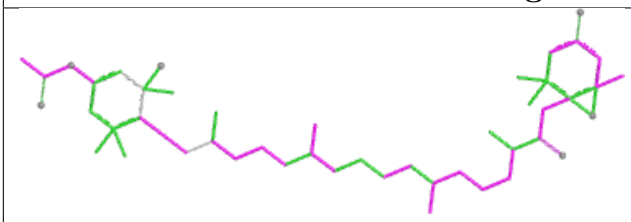


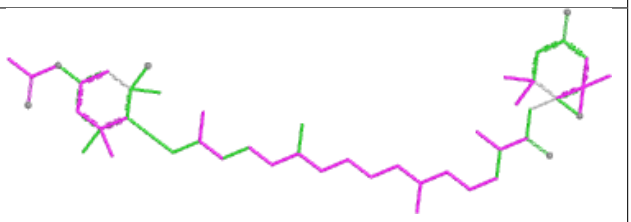
Torsions

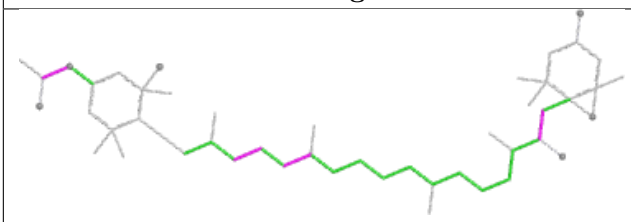


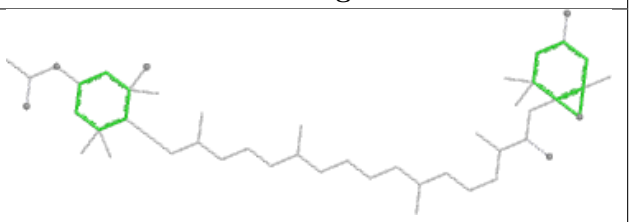
Rings

## Ligand A86 39 311

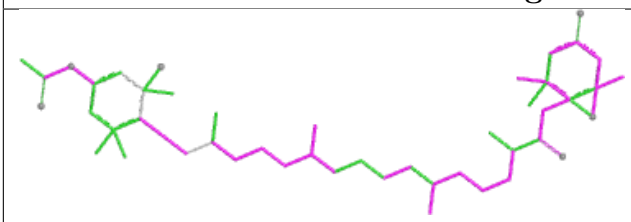

Bond lengths

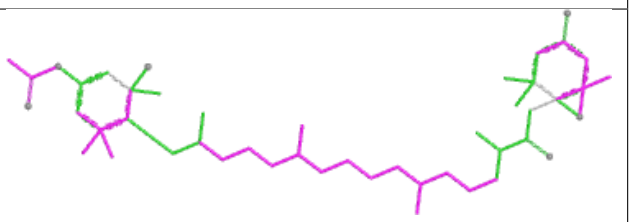

Bond angles

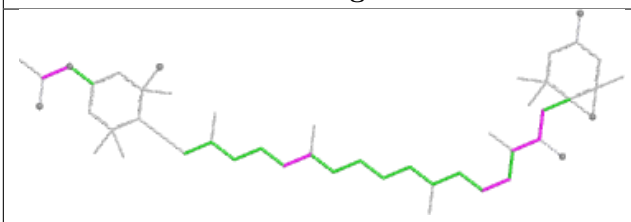

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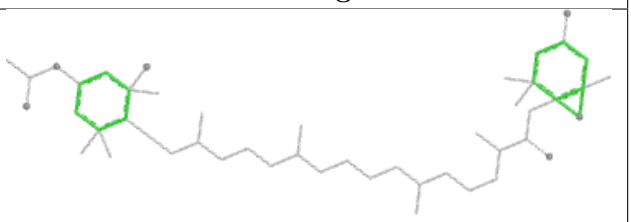

Rings

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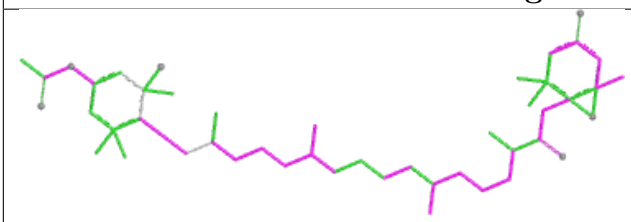

Bond lengths

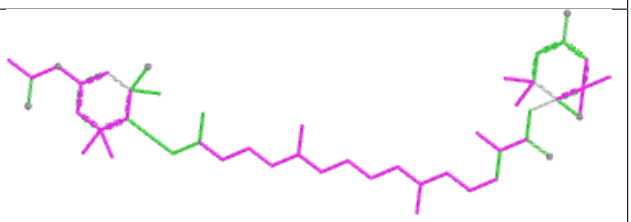

Bond angles

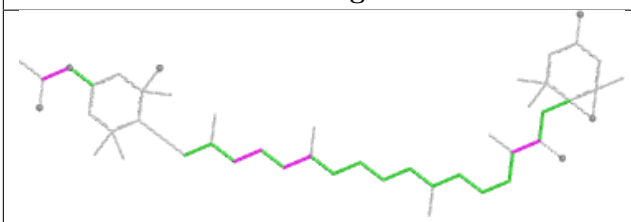

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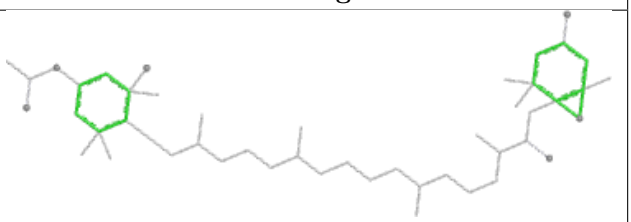

Rings

## Ligand A86 11 314

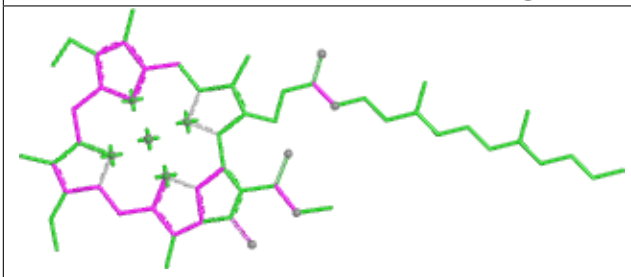

Bond lengths


Bond angles

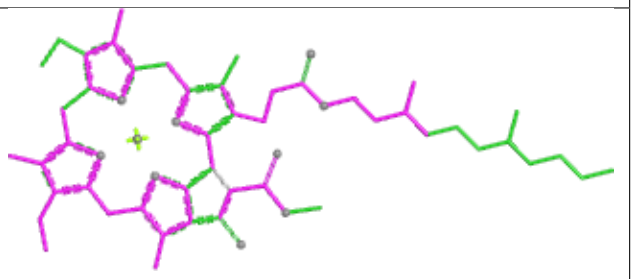

Torsions


Rings

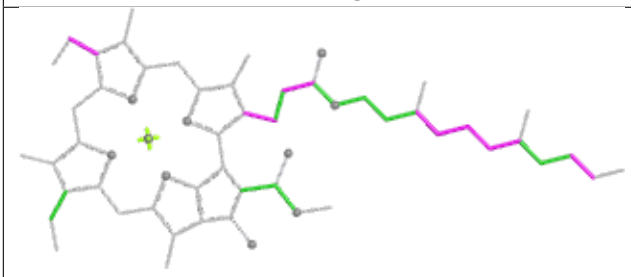
## Ligand CLA 41 204



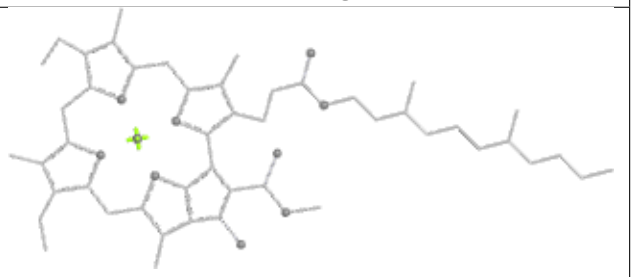
Bond lengths



Bond angles

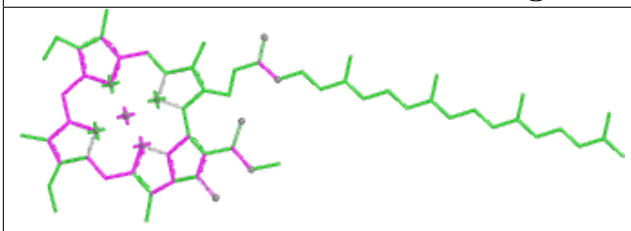


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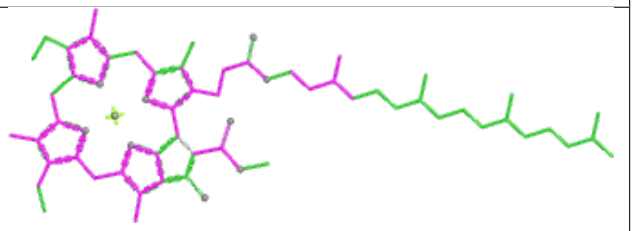


Rings

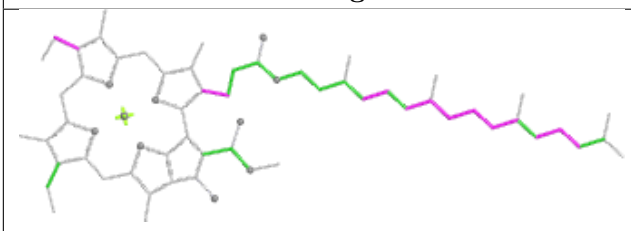
## Ligand CLA b 523



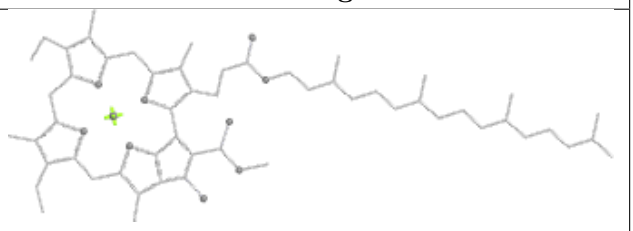
Bond lengths



Bond angles

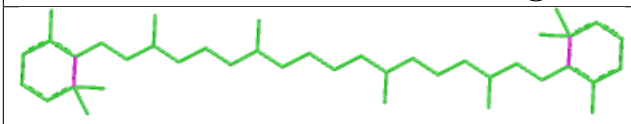


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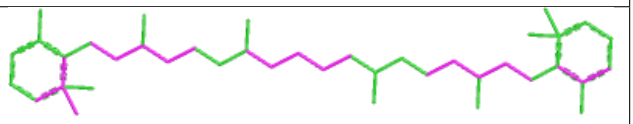


Rings

## Ligand BCR c 514



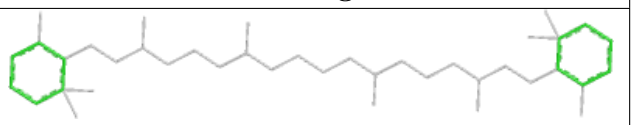
Bond lengths



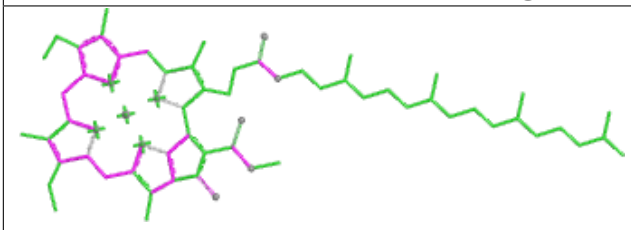
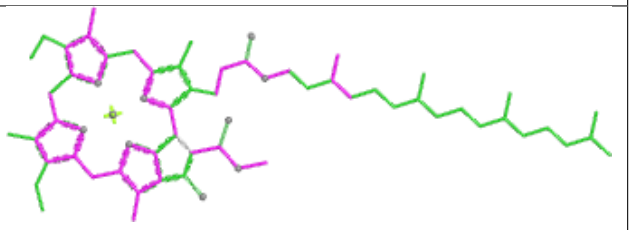
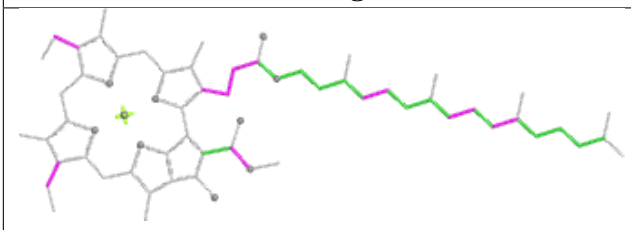
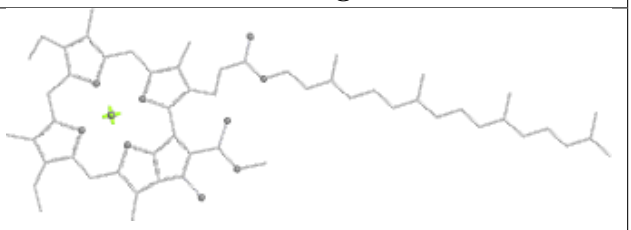
Bond angles

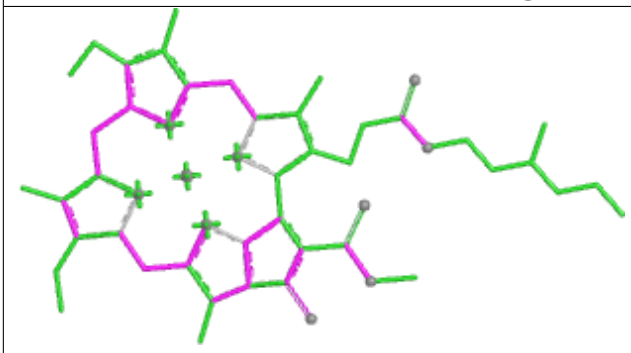
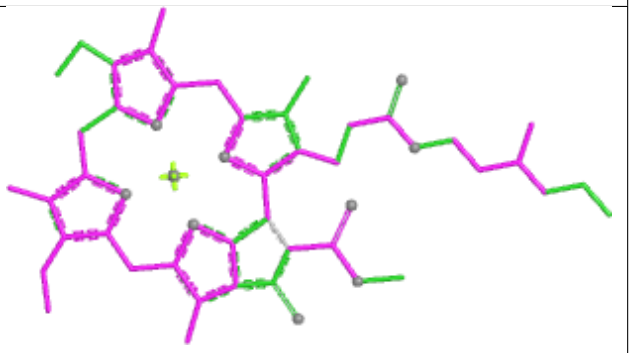
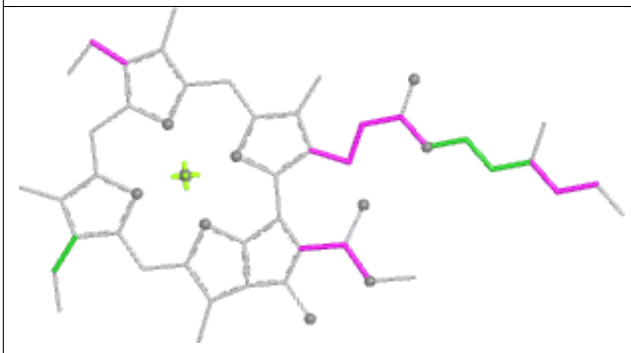
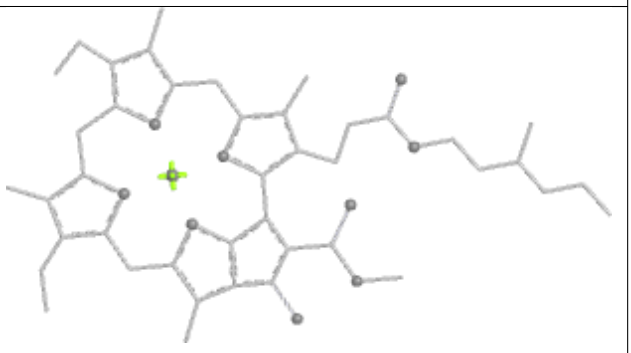


Torsions

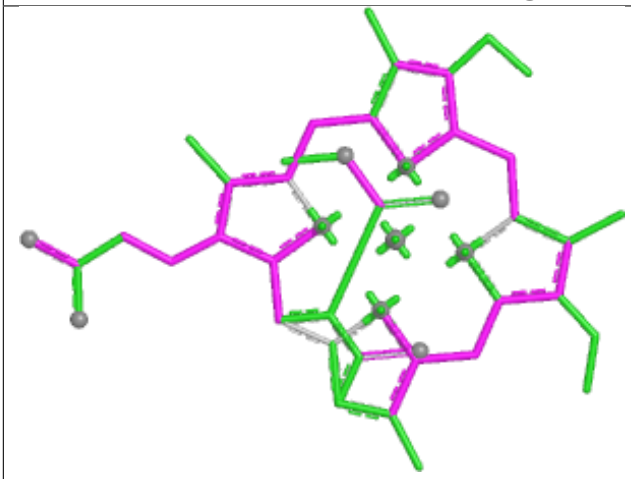


Rings

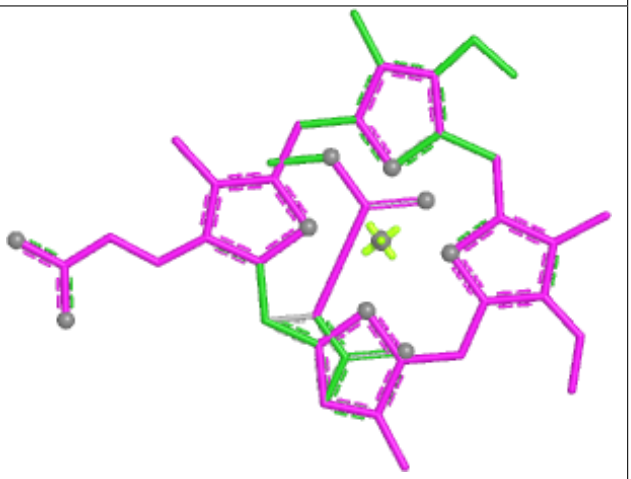
| Ligand CLA 37 301 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

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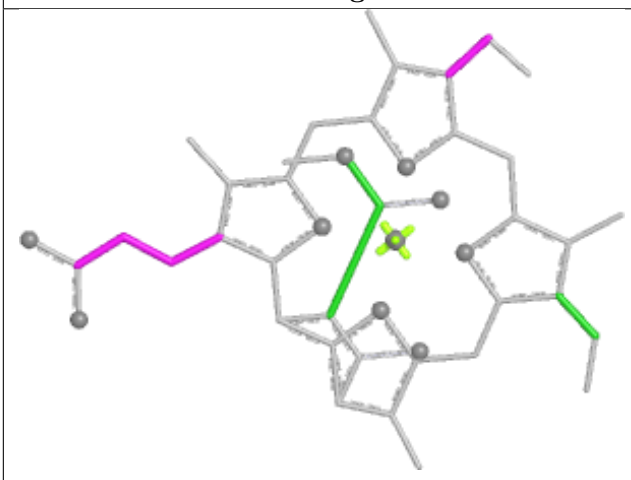
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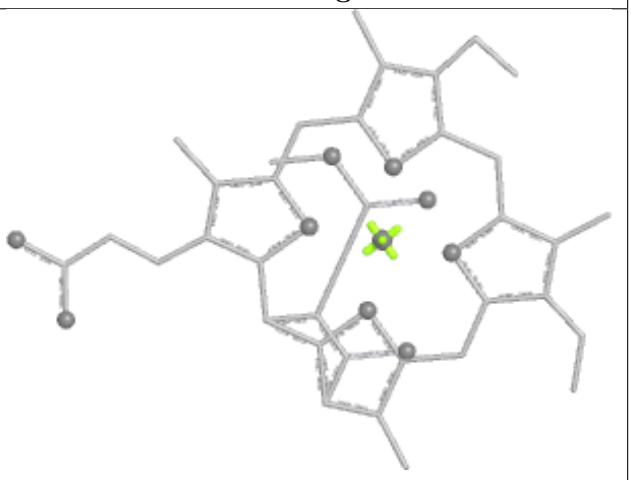
Bond lengths



Bond angles

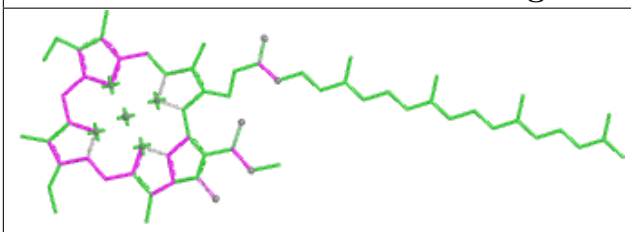


Torsions

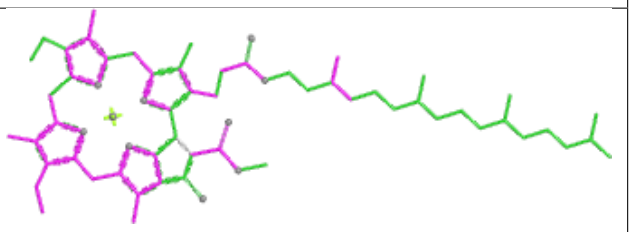


Rings

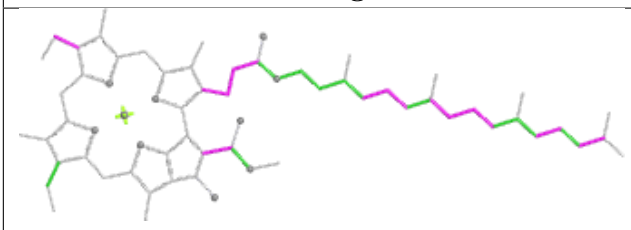
## Ligand CLA b 501



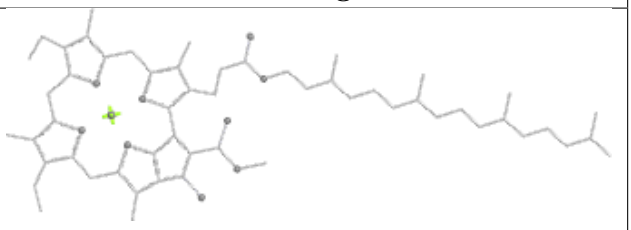
Bond lengths



Bond angles

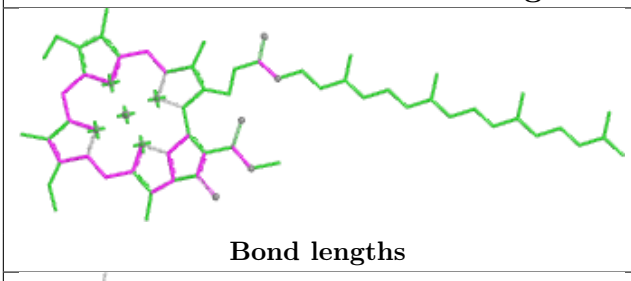


Torsions

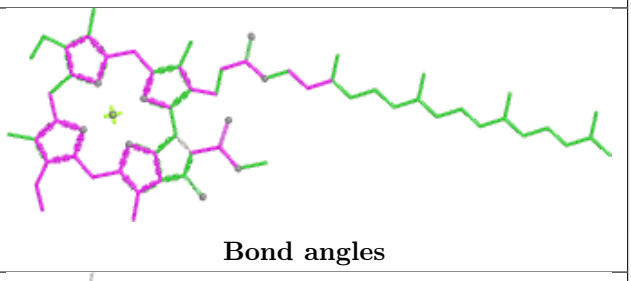


Rings

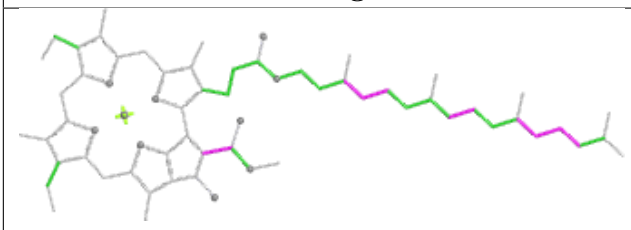
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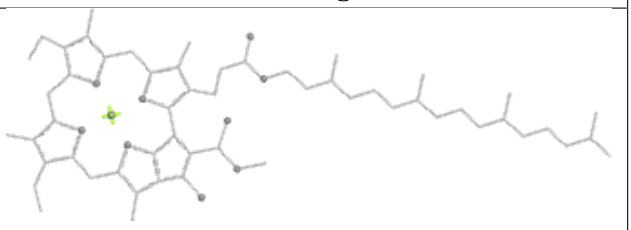
Bond lengths



Bond angles

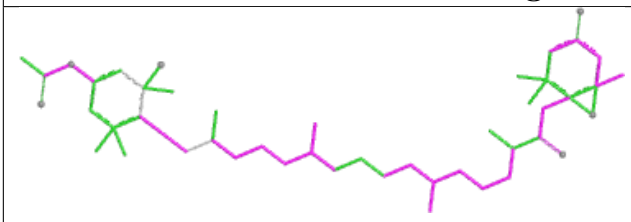


Torsions

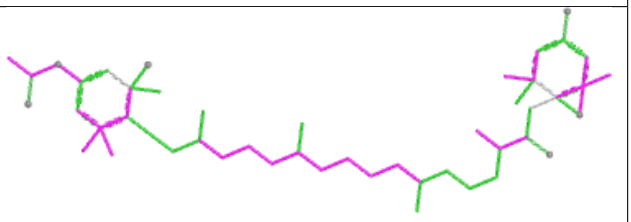


Rings

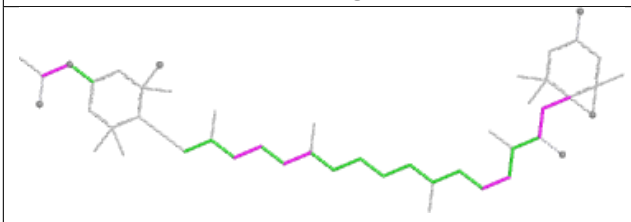
## Ligand A86 13 314



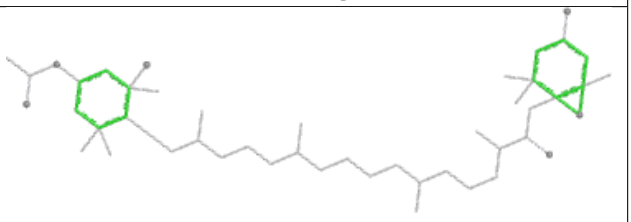
Bond lengths



Bond angles

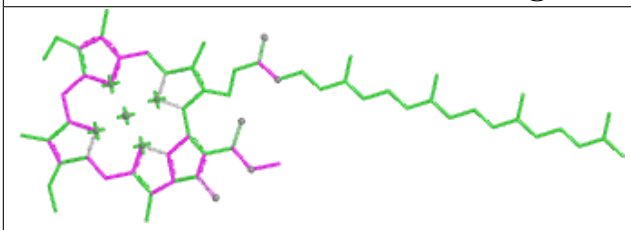


Torsions

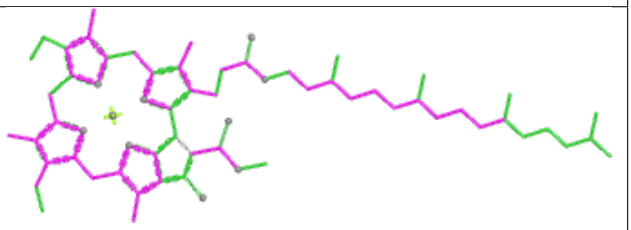


Rings

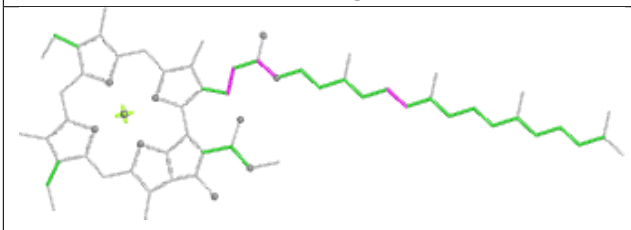
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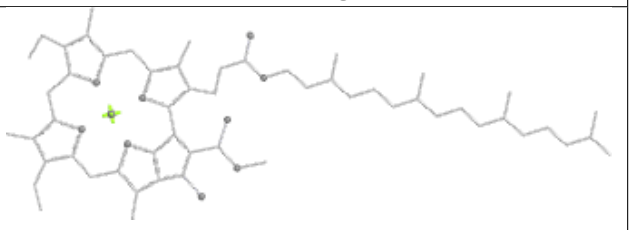
Bond lengths



Bond angles

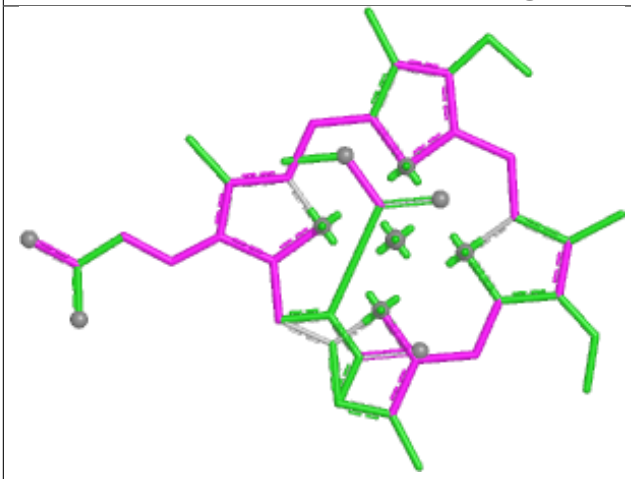


Torsions

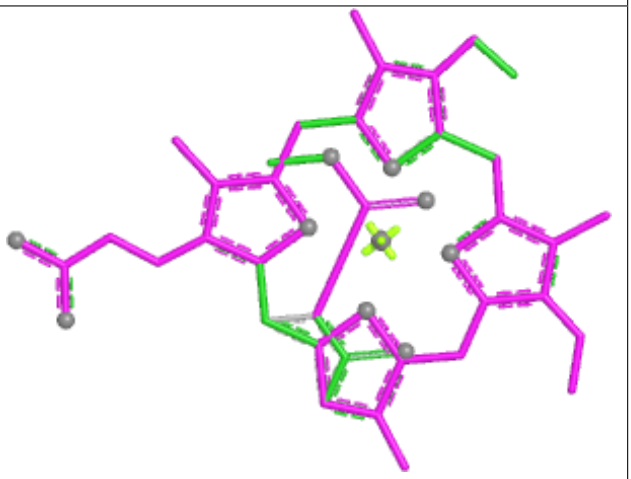


Rings

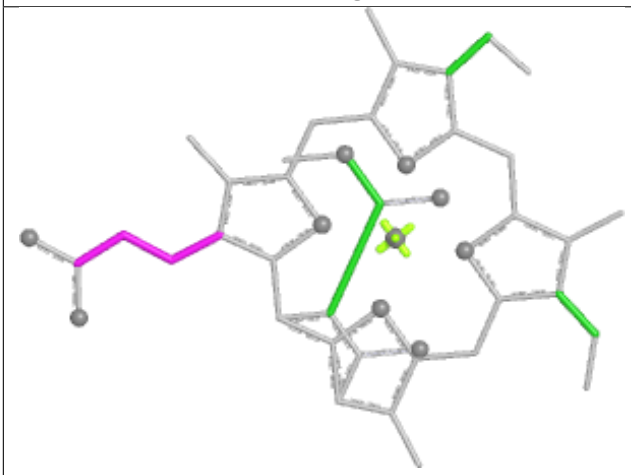
**Ligand KC1 19 308**



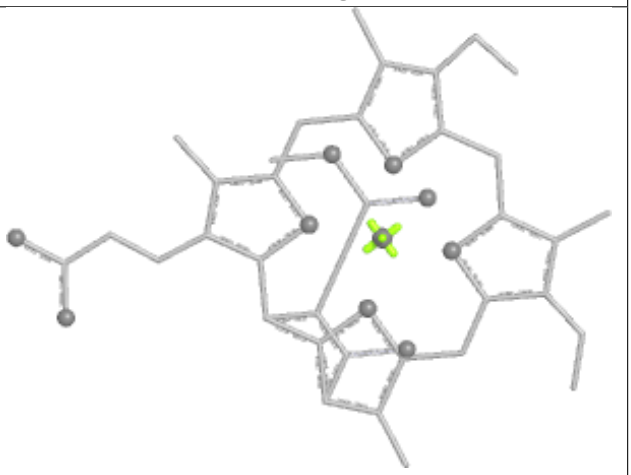
Bond lengths



Bond angles

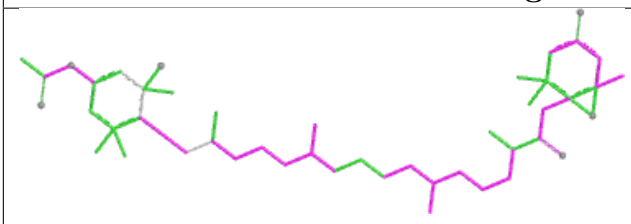


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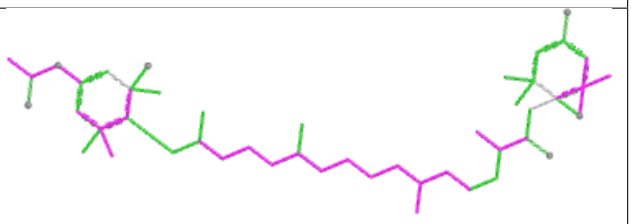


Rings

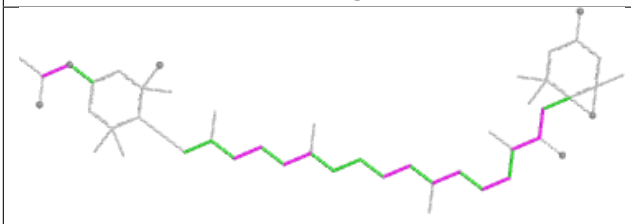
**Ligand A86 15 314**



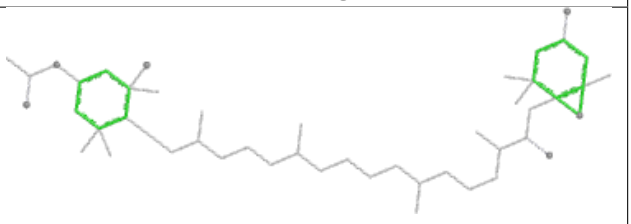
Bond lengths



Bond angles

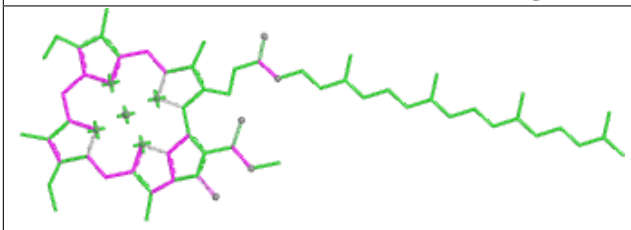


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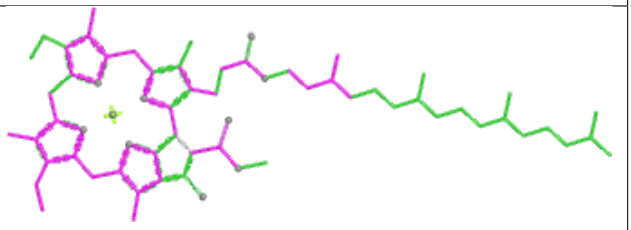


Rings

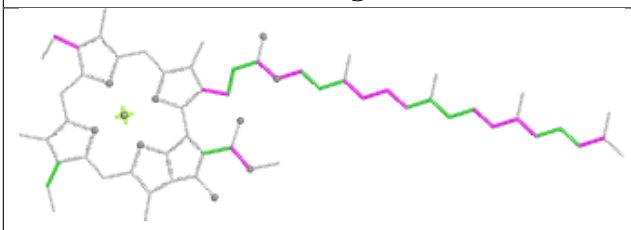
## Ligand CLA d 404



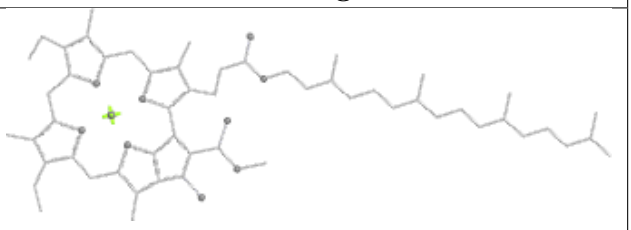
Bond lengths



Bond angles

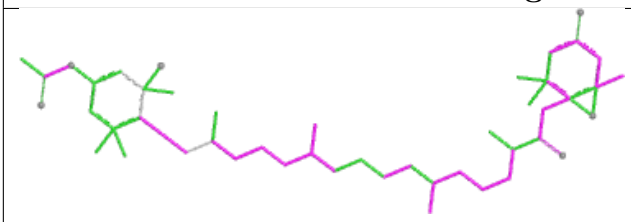


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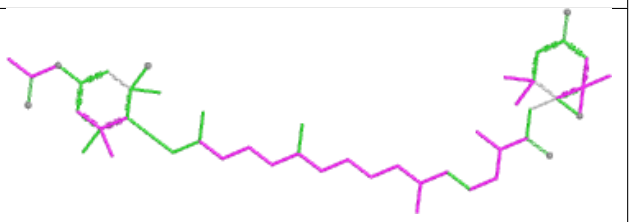


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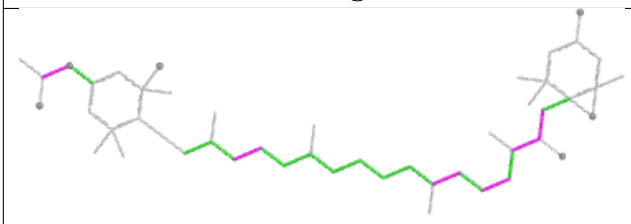
## Ligand A86 17 310



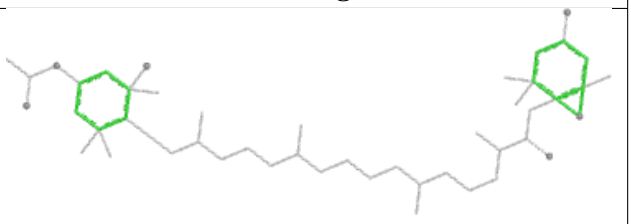
Bond lengths



Bond angles

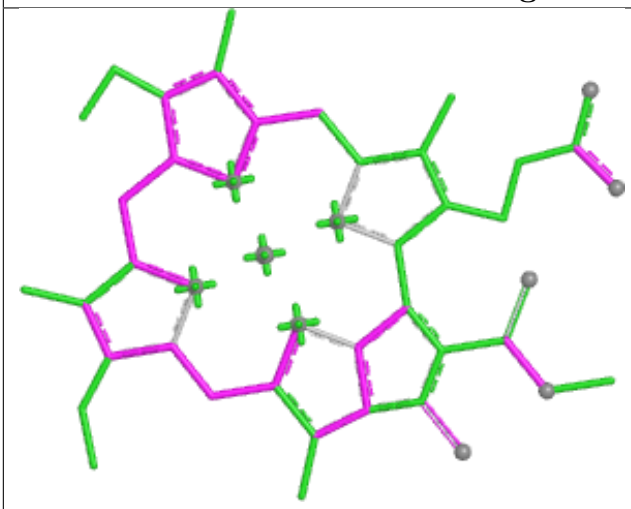


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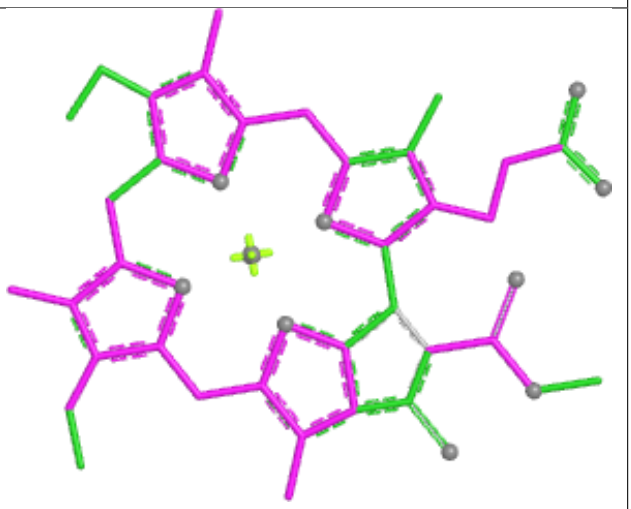


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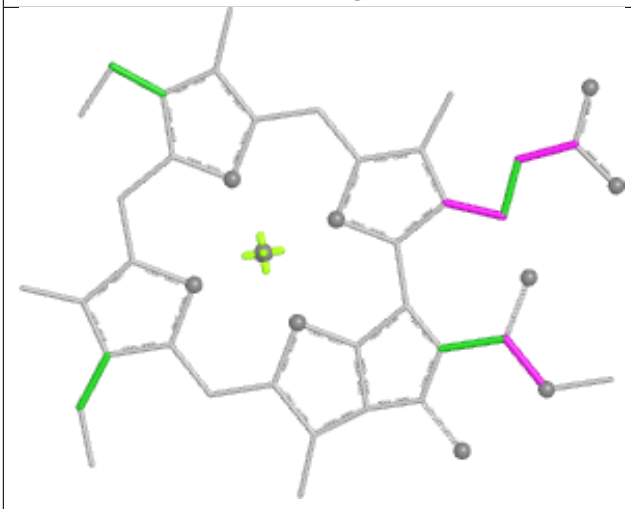
**Ligand CLA 16 309**



**Bond lengths**



**Bond angles**

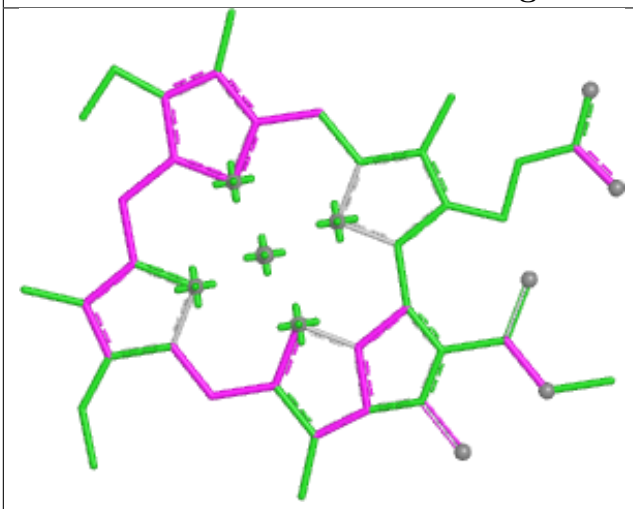


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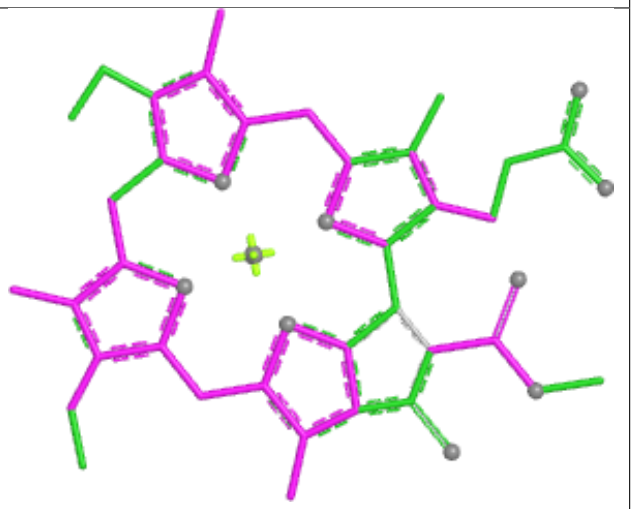


**Rings**

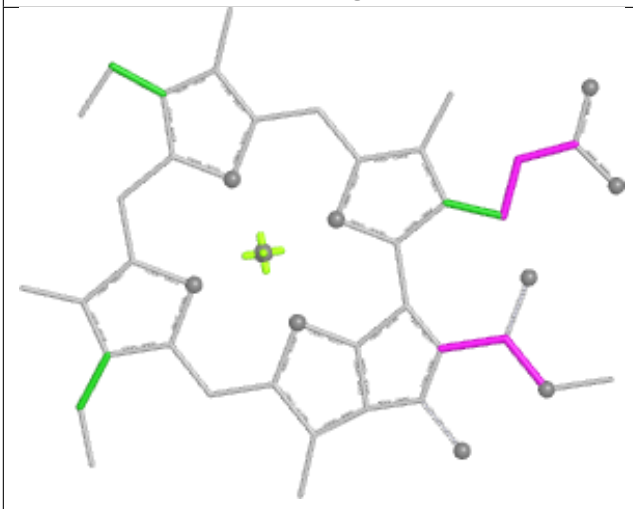
## Ligand CLA 32 213



Bond lengths



Bond angles

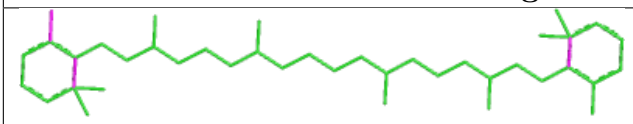


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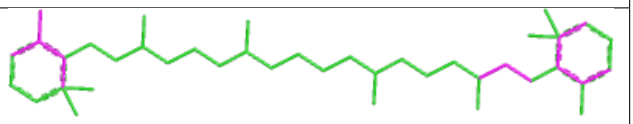


Rings

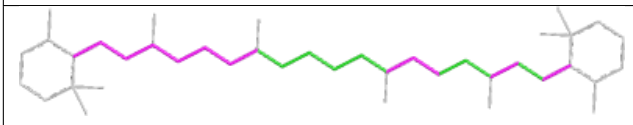
## Ligand BCR K 101



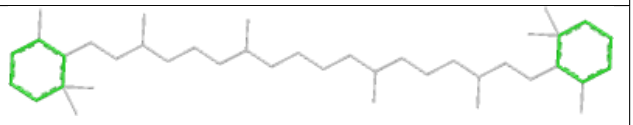
Bond lengths



Bond angles

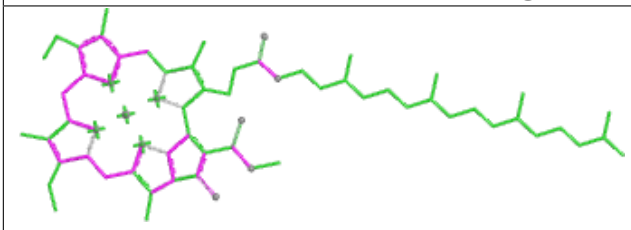


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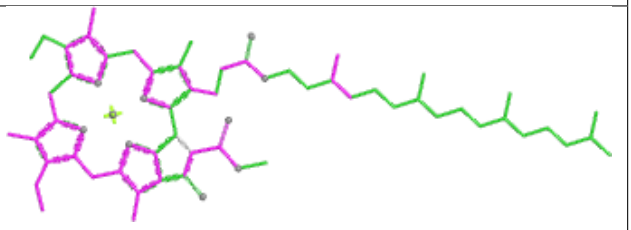


Rings

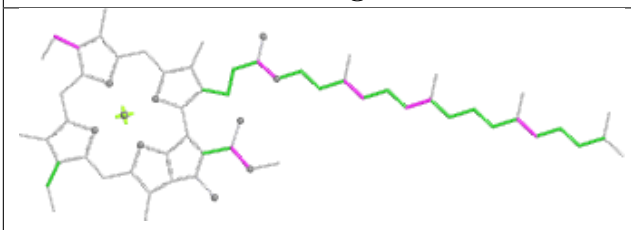
## Ligand CLA 39 302



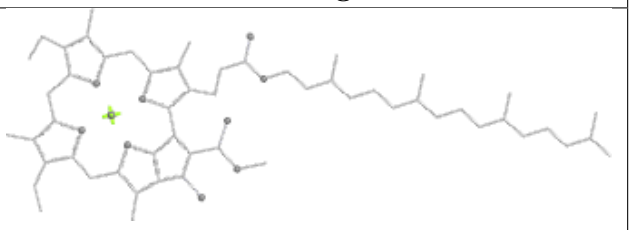
Bond lengths



Bond angles

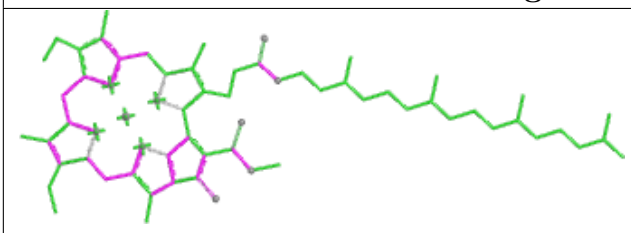


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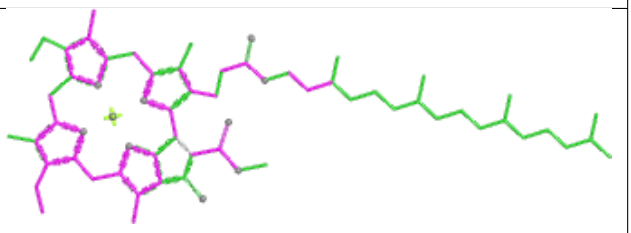


Rings

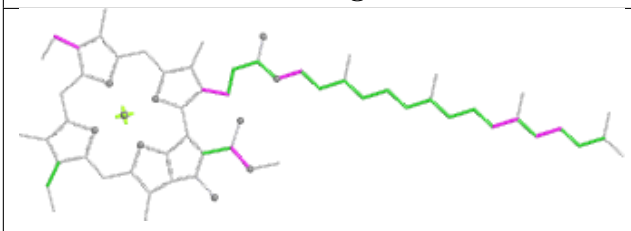
## Ligand CLA C 502



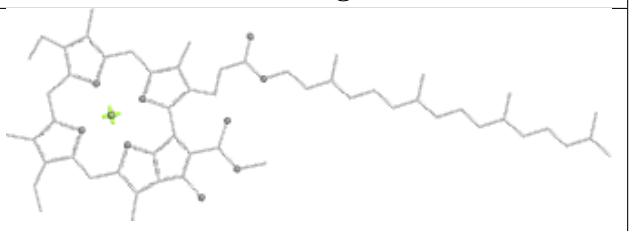
Bond lengths



Bond angles

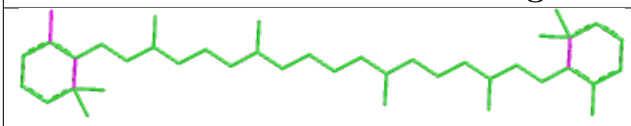


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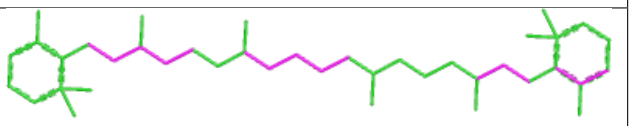


Rings

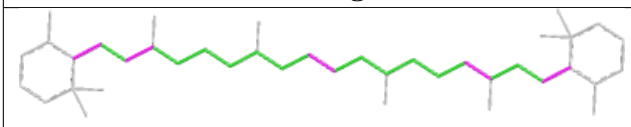
## Ligand BCR a 408



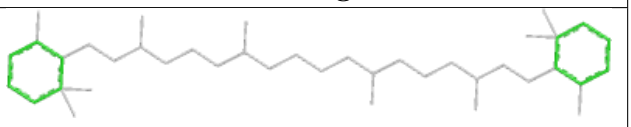
Bond lengths



Bond angles

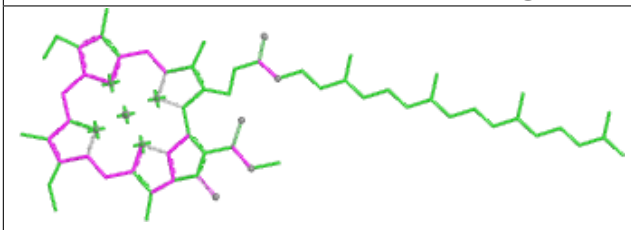


Torsions

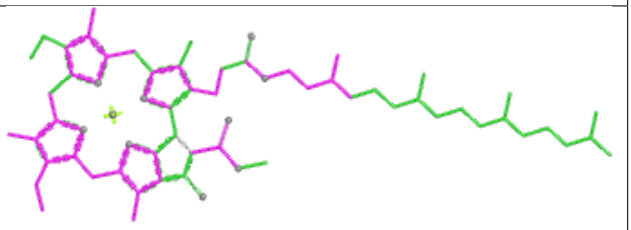


Rings

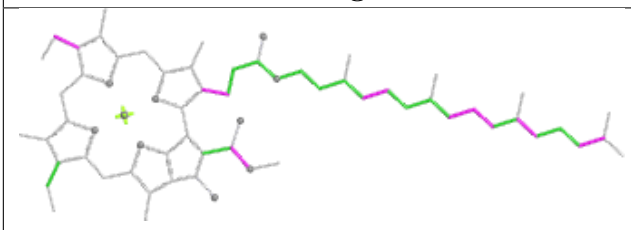
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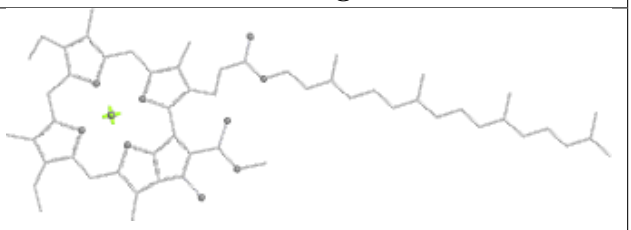
Bond lengths



Bond angles

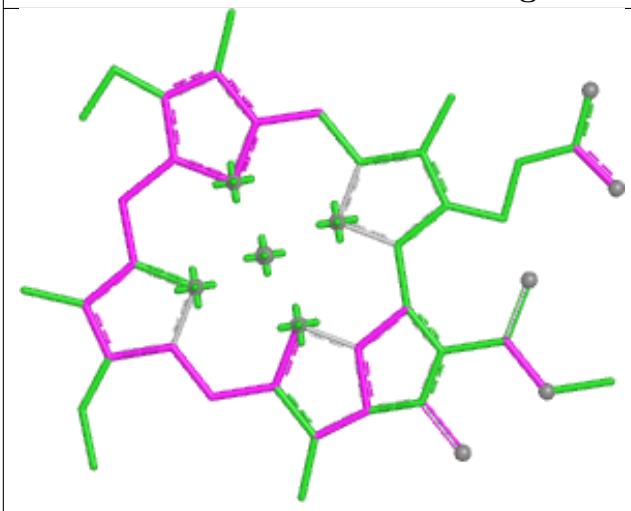


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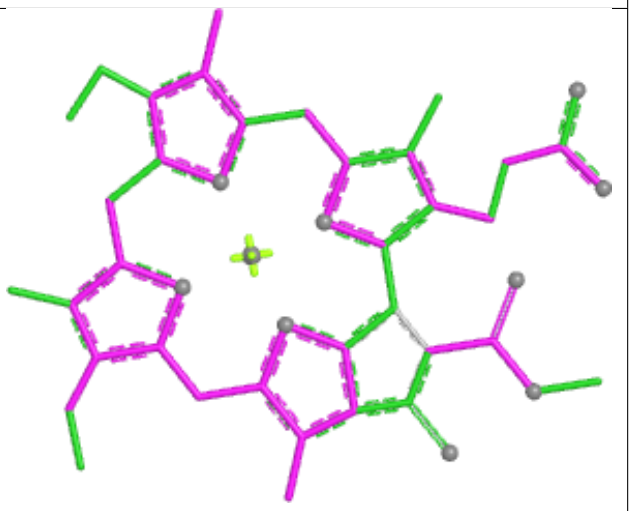


Rings

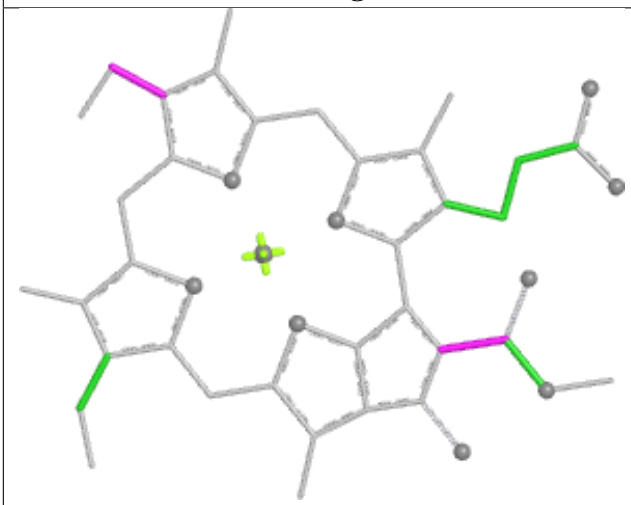
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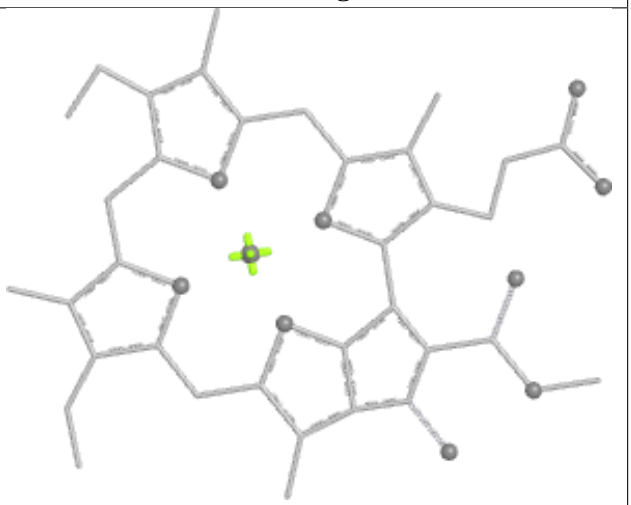
Bond lengths



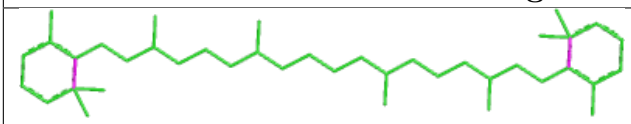
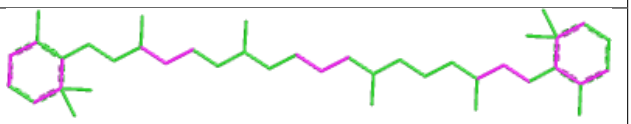
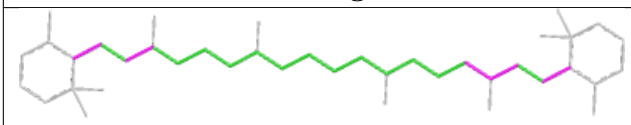
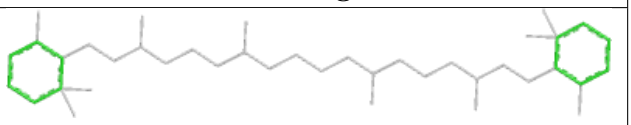
Bond angles



Torsions



Rings

| Ligand BCR 0 101 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

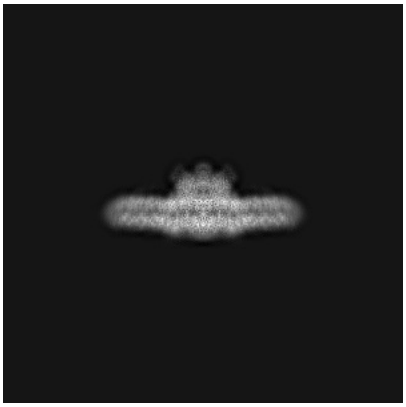
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31905. These allow visual inspection of the internal detail of the map and identification of artifacts.

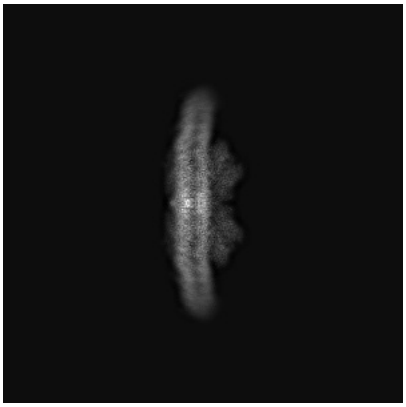
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

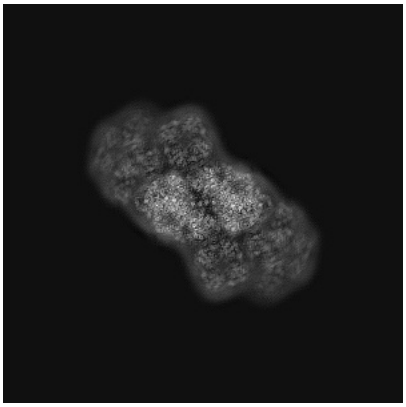
### 6.1.1 Primary map



X



Y

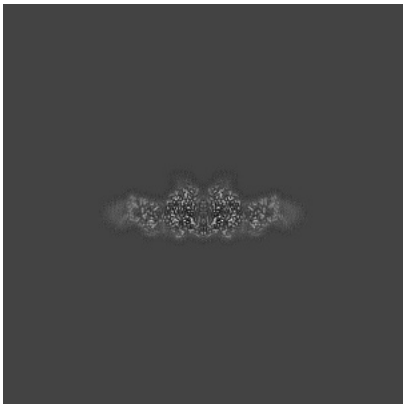


Z

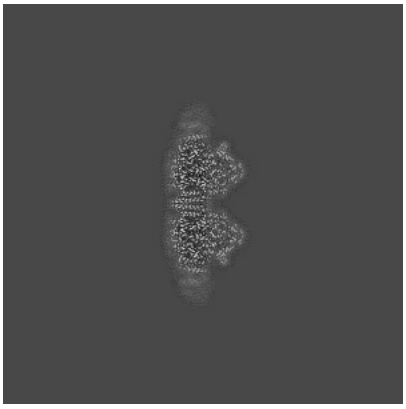
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

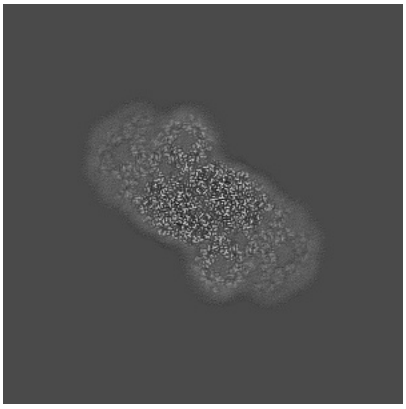
### 6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

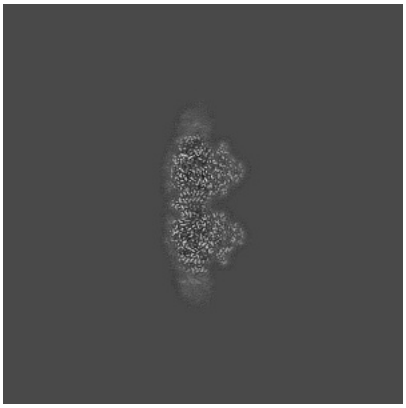
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

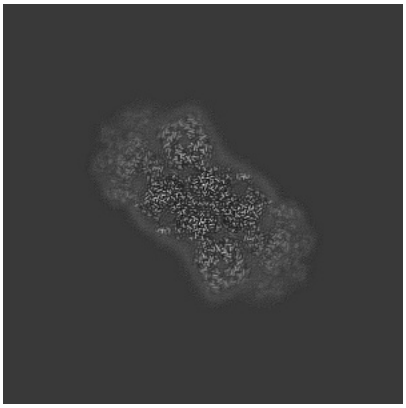
### 6.3.1 Primary map



X Index: 252



Y Index: 257

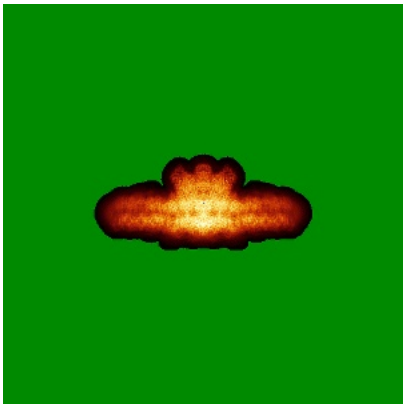


Z Index: 234

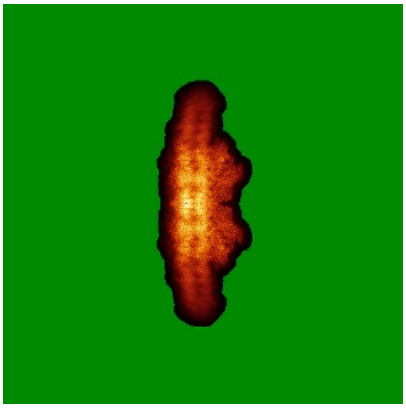
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

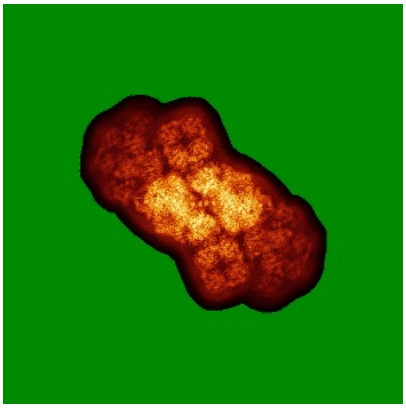
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

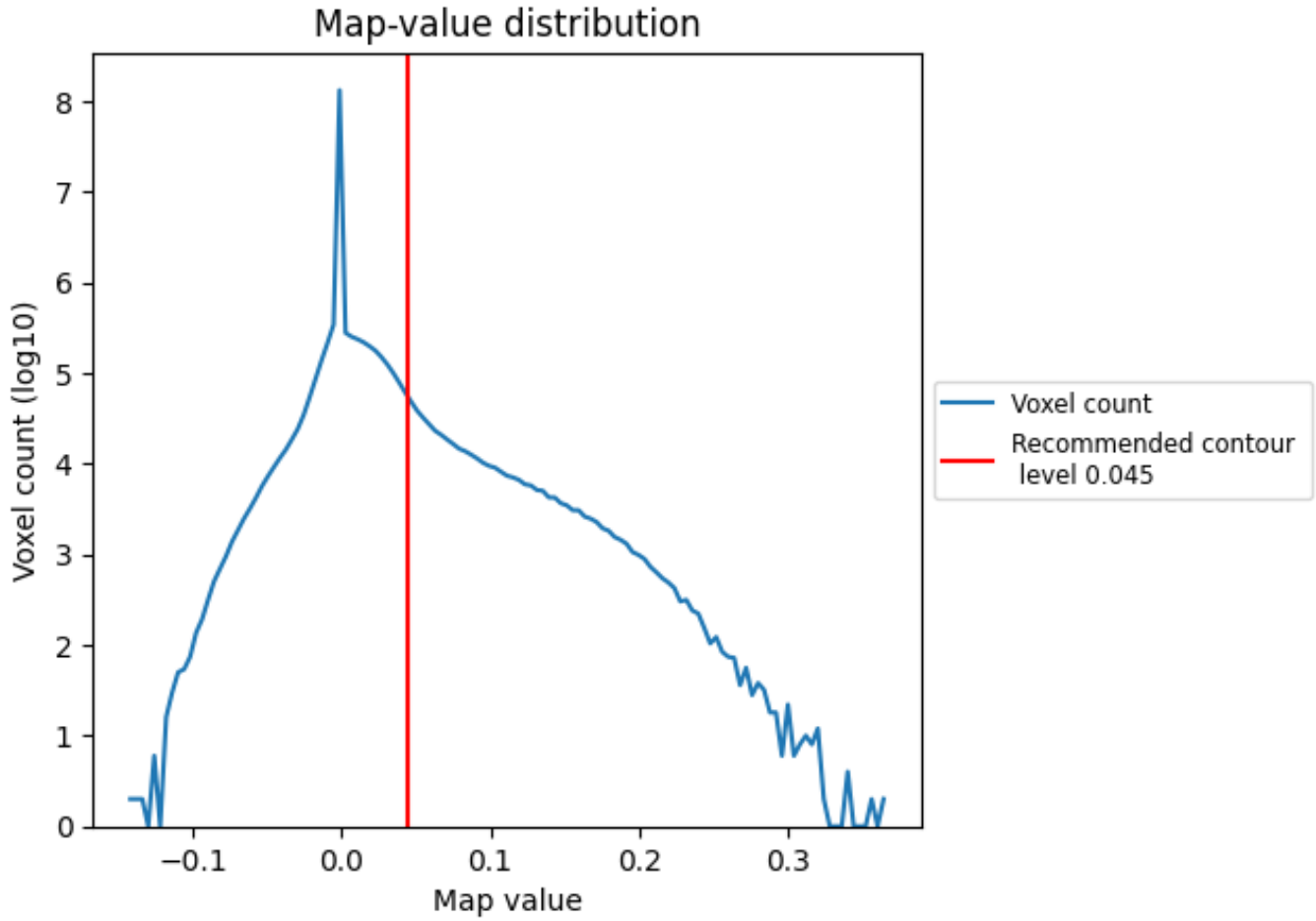
## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

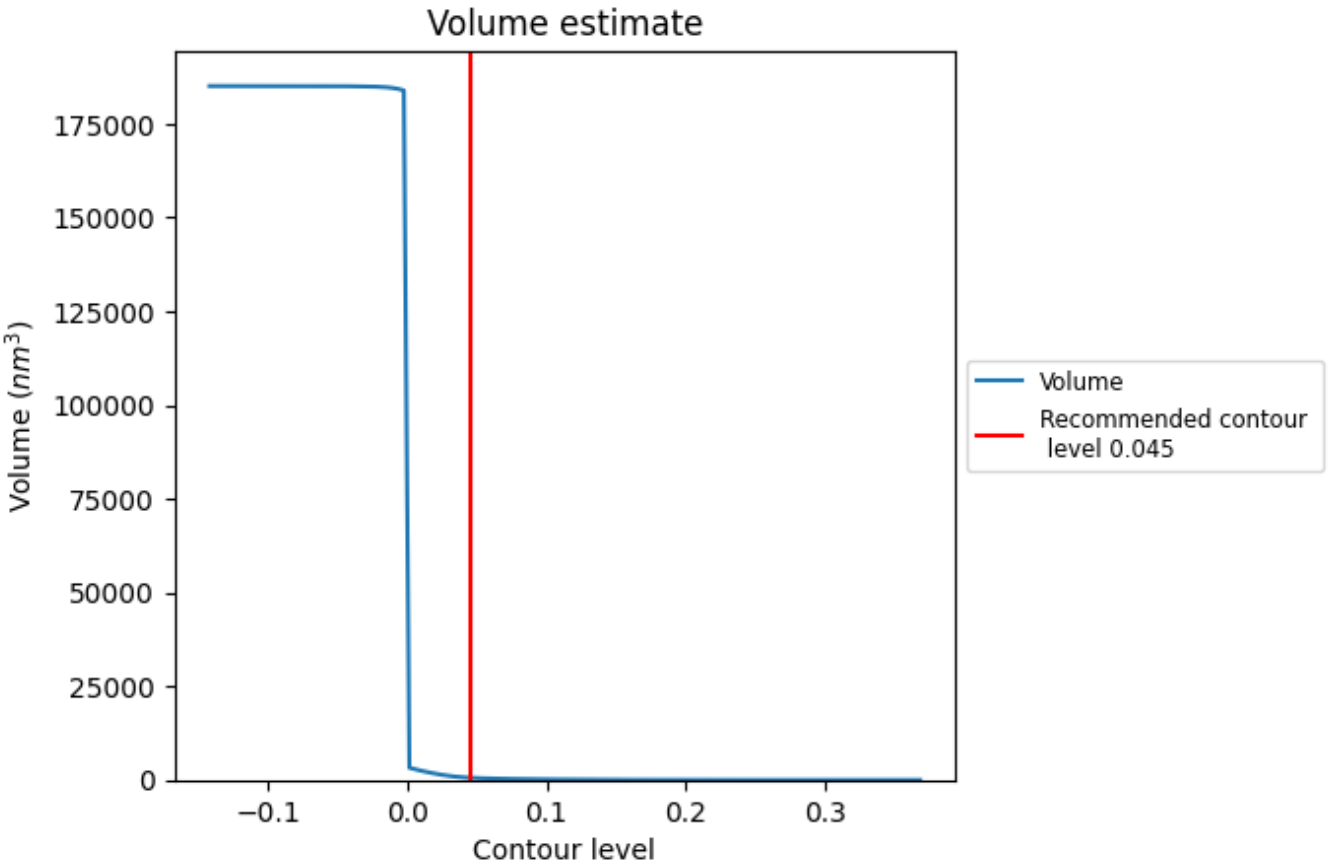
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

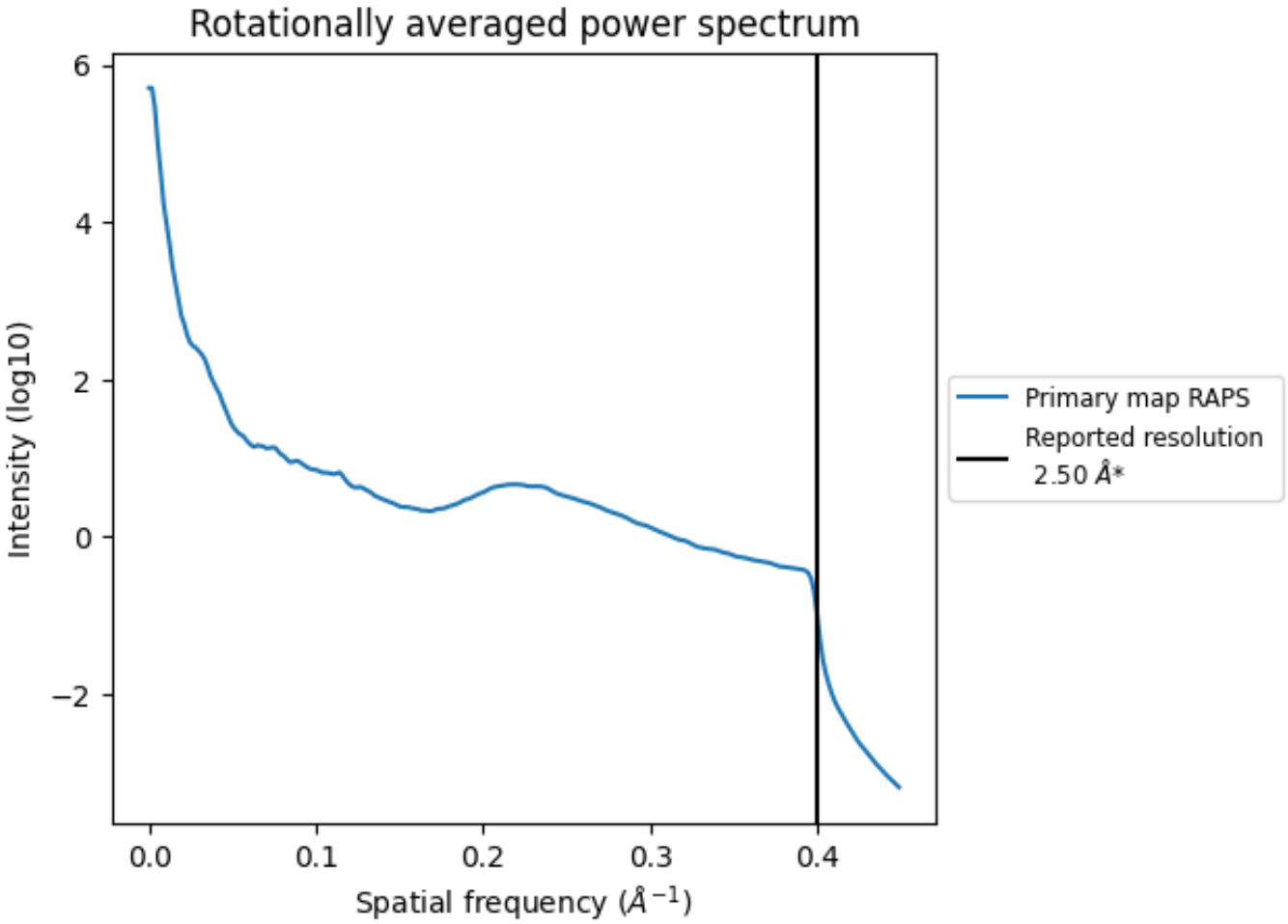
## 7.2 Volume estimate




The volume at the recommended contour level is 588 $nm^3$; this corresponds to an approximate mass of 532 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

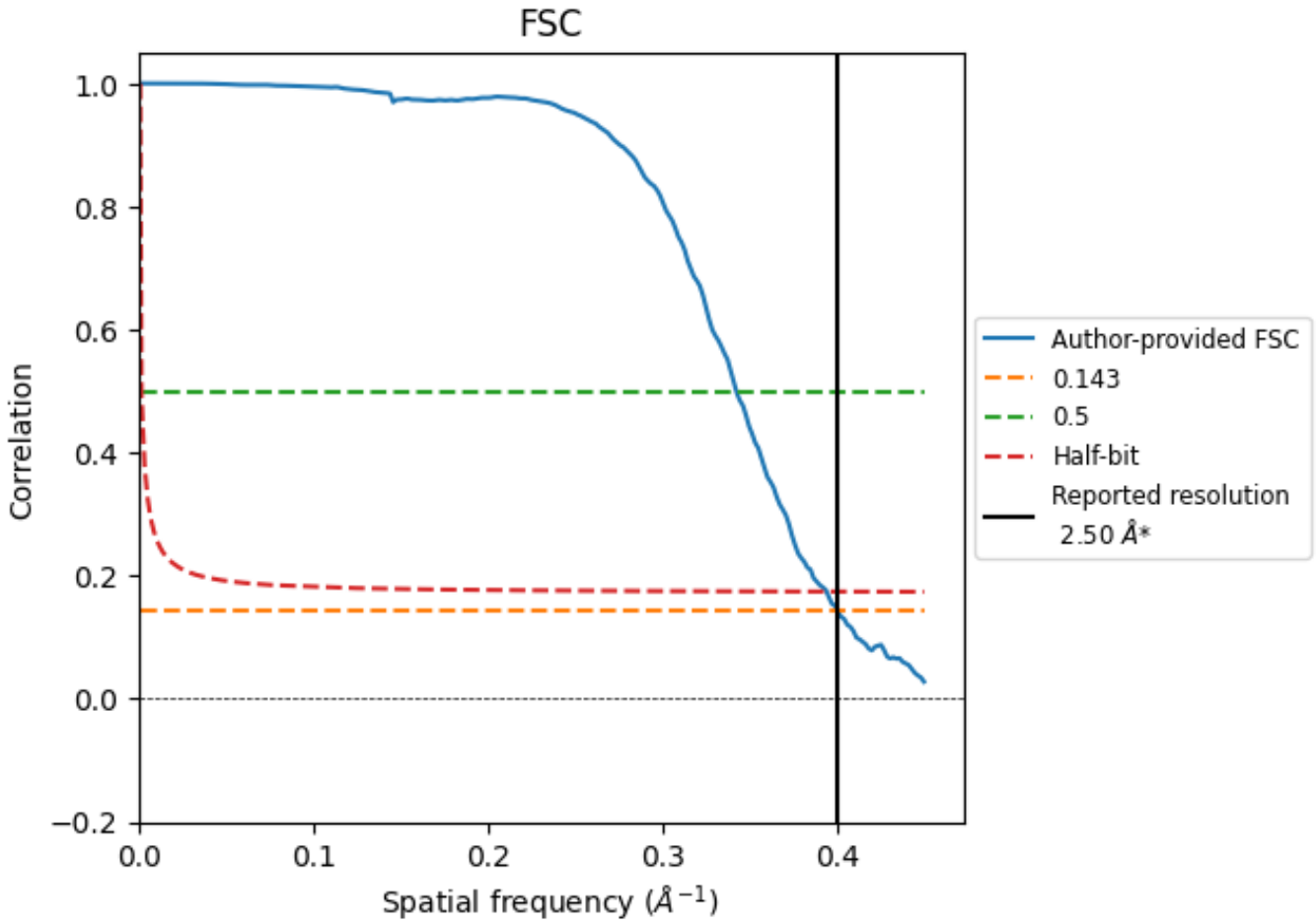



*Reported resolution corresponds to spatial frequency of 0.400 $Å^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.400 Å$^{-1}$

## 8.2 Resolution estimates (i)

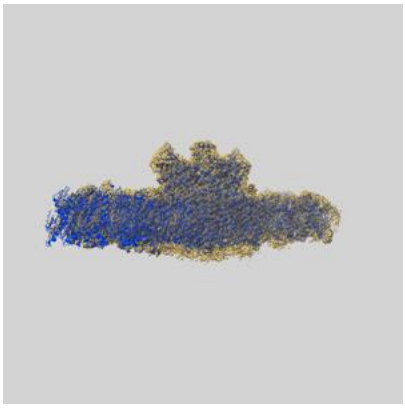
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.50 | - | - |
| Author-provided FSC curve | 2.50 | 2.92 | 2.54 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

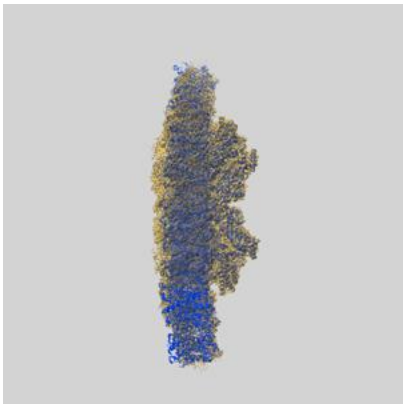
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31905 and PDB model 7VD5. Per-residue inclusion information can be found in section 3 on page 51.

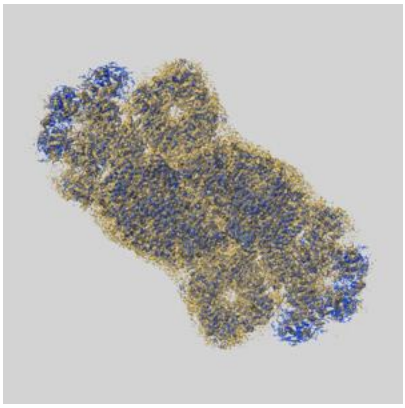
## 9.1 Map-model overlay



X



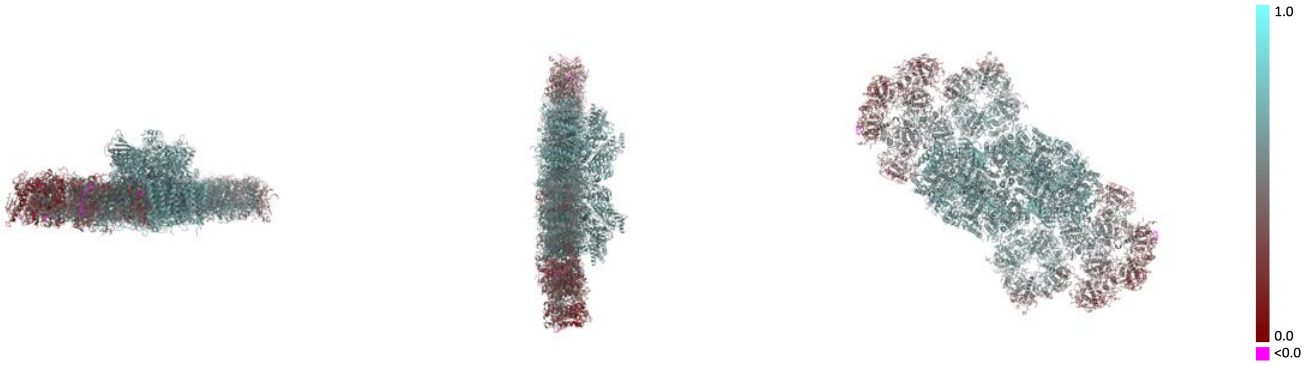
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

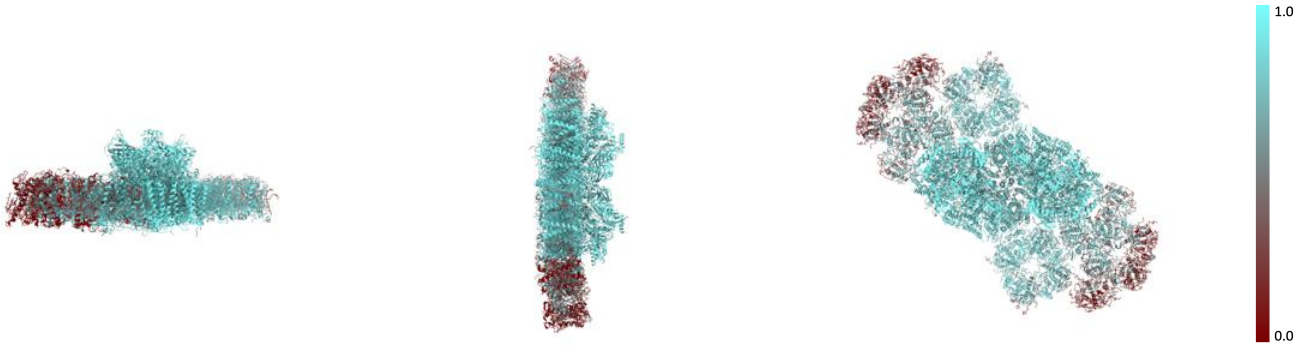
## 9.2 Q-score mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

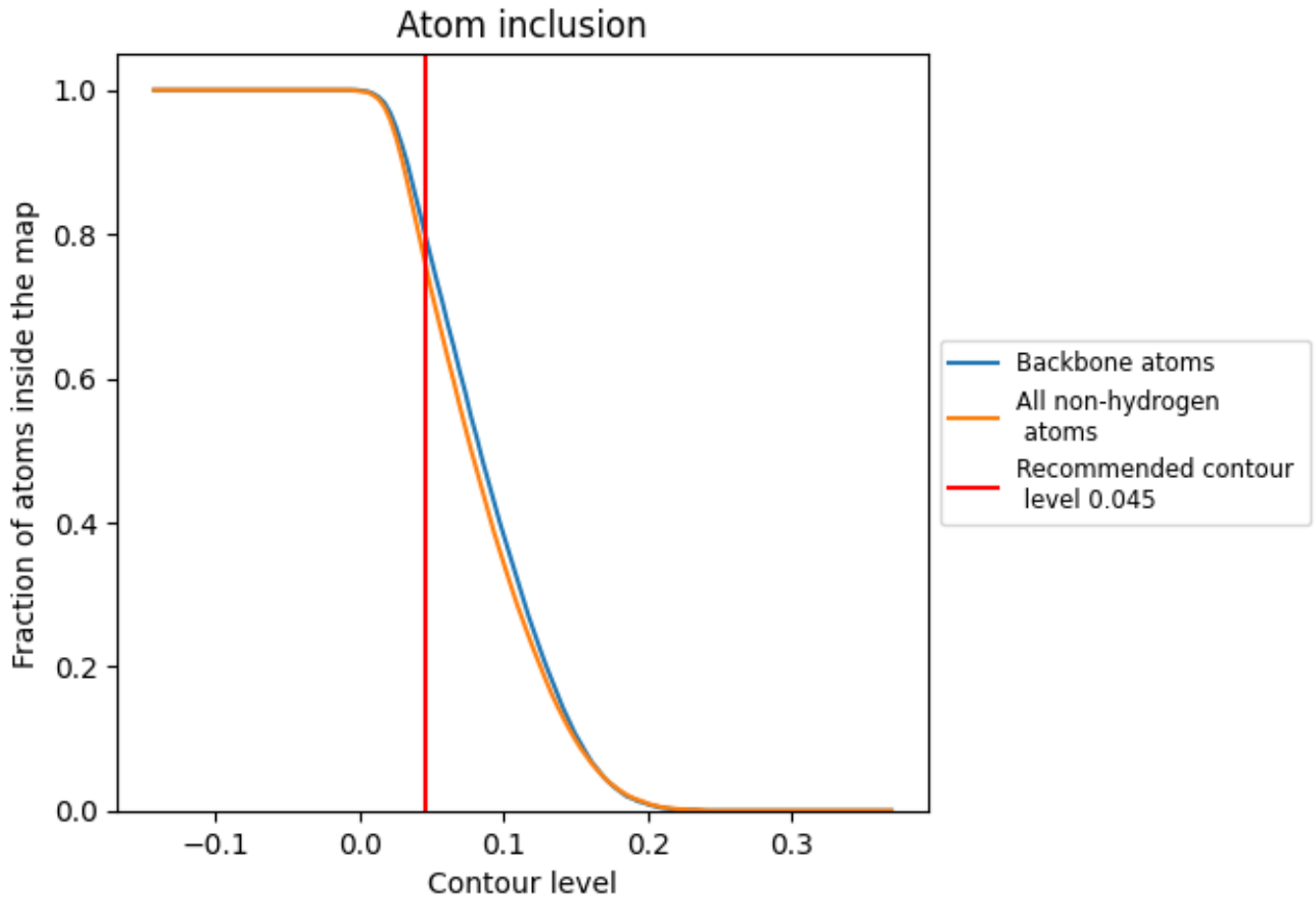
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

## 9.4 Atom inclusion (i)




At the recommended contour level, 80% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7640 | 0.5430 |
| 0 | 0.9590 | 0.6360 |
| 1 | 0.9330 | 0.6130 |
| 11 | 0.8820 | 0.6000 |
| 12 | 0.8680 | 0.5780 |
| 13 | 0.7230 | 0.4570 |
| 14 | 0.7450 | 0.4800 |
| 15 | 0.2430 | 0.2840 |
| 16 | 0.6780 | 0.4740 |
| 17 | 0.5850 | 0.4350 |
| 18 | 0.2380 | 0.2830 |
| 19 | 0.7830 | 0.5510 |
| 20 | 0.5020 | 0.3420 |
| 21 | 0.1260 | 0.2530 |
| 31 | 0.8690 | 0.5900 |
| 32 | 0.8710 | 0.5790 |
| 33 | 0.7220 | 0.4550 |
| 34 | 0.7460 | 0.4770 |
| 35 | 0.2400 | 0.2850 |
| 36 | 0.6890 | 0.4790 |
| 37 | 0.5830 | 0.4360 |
| 38 | 0.2400 | 0.2860 |
| 39 | 0.7830 | 0.5490 |
| 40 | 0.4820 | 0.3370 |
| 41 | 0.1300 | 0.2520 |
| 5 | 0.9590 | 0.6400 |
| 6 | 0.9330 | 0.6080 |
| A | 0.9630 | 0.6690 |
| B | 0.9350 | 0.6540 |
| C | 0.9440 | 0.6550 |
| D | 0.9420 | 0.6620 |
| E | 0.9020 | 0.6110 |
| F | 0.9200 | 0.5950 |
| H | 0.9340 | 0.6390 |
| I | 0.9540 | 0.6560 |




*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| J | 0.8940 | 0.6380 |
| K | 0.9200 | 0.6260 |
| L | 0.8900 | 0.6400 |
| M | 0.8590 | 0.6400 |
| O | 0.8830 | 0.6120 |
| Q | 0.8670 | 0.5980 |
| T | 0.9100 | 0.6520 |
| U | 0.9070 | 0.6120 |
| V | 0.9320 | 0.6200 |
| W | 0.8070 | 0.5830 |
| X | 0.8380 | 0.5580 |
| Y | 0.8270 | 0.5920 |
| Z | 0.8640 | 0.5670 |
| a | 0.9630 | 0.6680 |
| b | 0.9370 | 0.6550 |
| c | 0.9430 | 0.6530 |
| d | 0.9390 | 0.6610 |
| e | 0.8920 | 0.6110 |
| f | 0.9200 | 0.5950 |
| h | 0.9390 | 0.6350 |
| i | 0.9540 | 0.6570 |
| j | 0.8870 | 0.6360 |
| k | 0.9360 | 0.6190 |
| l | 0.9480 | 0.6530 |
| m | 0.8630 | 0.6410 |
| o | 0.8870 | 0.6120 |
| q | 0.8730 | 0.6000 |
| t | 0.9100 | 0.6570 |
| u | 0.9070 | 0.6140 |
| v | 0.9300 | 0.6220 |
| w | 0.8520 | 0.6140 |
| x | 0.8220 | 0.5620 |
| y | 0.8410 | 0.6050 |
| z | 0.8720 | 0.5650 |