# Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:04 AM UTC

| | | |
|---|---|---|
| PDB ID | : | 7BGL / pdb_00007bgl |
| EMDB ID | : | EMD-12183 |
| Title | : | Salmonella LP ring 26 mer refined in C26 map |
| Authors | : | Johnson, S.; Furlong, E.; Lea, S.M. |
| Deposited on | : | 2021-01-07 |
| Resolution | : | 2.20 Å(reported) |

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:

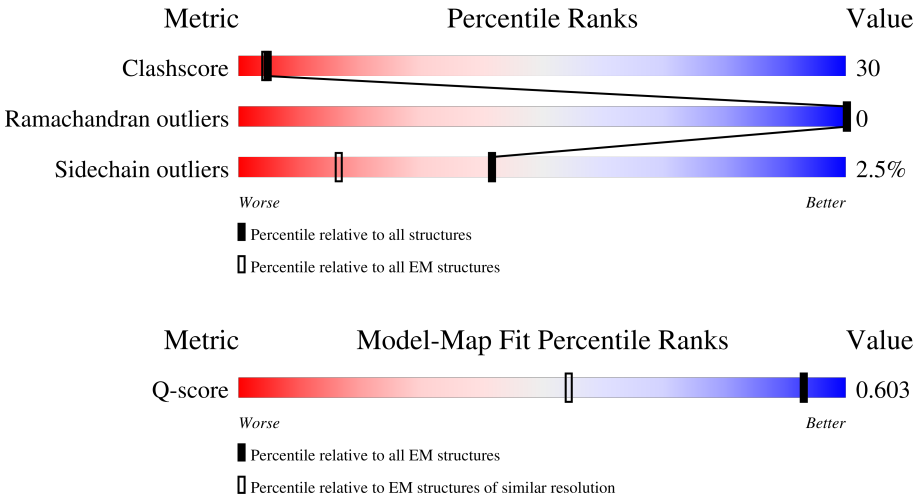
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 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 2.20 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 | 3184 ( 1.71 - 2.70 ) |

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 | 232 | 54% 36% • 9% |
| 1 | B | 232 | 54% 36% • 9% |
| 1 | C | 232 | 53% 37% • 9% |
| 1 | D | 232 | 54% 36% • 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | E | 232 | 54% 36% 9% |
| 1 | F | 232 | 53% 37% 9% |
| 1 | G | 232 | 54% 36% 9% |
| 1 | H | 232 | 53% 36% 9% |
| 1 | I | 232 | 54% 36% 9% |
| 1 | J | 232 | 54% 36% 9% |
| 1 | K | 232 | 53% 37% 9% |
| 1 | L | 232 | 54% 37% 9% |
| 1 | M | 232 | 53% 37% 9% |
| 1 | N | 232 | 53% 37% 9% |
| 1 | O | 232 | 53% 38% 9% |
| 1 | P | 232 | 53% 38% 9% |
| 1 | Q | 232 | 53% 37% 9% |
| 1 | R | 232 | 53% 37% 9% |
| 1 | S | 232 | 53% 37% 9% |
| 1 | T | 232 | 53% 37% 9% |
| 1 | U | 232 | 52% 38% 9% |
| 1 | V | 232 | 53% 37% 9% |
| 1 | W | 232 | 54% 36% 9% |
| 1 | X | 232 | 54% 35% 9% |
| 1 | Y | 232 | 54% 35% 9% |
| 1 | Z | 232 | 56% 34% 9% |
| 2 | a | 365 | 41% 42% 16% |
| 2 | b | 365 | 41% 42% 16% |
| 2 | c | 365 | 41% 42% 16% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | d | 365 | 42% 41% 16% |
| 2 | e | 365 | 42% 41% 16% |
| 2 | f | 365 | 40% 43% 16% |
| 2 | g | 365 | 42% 41% 16% |
| 2 | h | 365 | 42% 41% 16% |
| 2 | i | 365 | 42% 41% 16% |
| 2 | j | 365 | 42% 41% 16% |
| 2 | k | 365 | 42% 41% 16% |
| 2 | l | 365 | 41% 42% 16% |
| 2 | m | 365 | 41% 42% 16% |
| 2 | n | 365 | 40% 43% 16% |
| 2 | o | 365 | 41% 42% 16% |
| 2 | p | 365 | 41% 42% 16% |
| 2 | q | 365 | 40% 43% 16% |
| 2 | r | 365 | 41% 42% 16% |
| 2 | s | 365 | 41% 42% 16% |
| 2 | t | 365 | 42% 41% 16% |
| 2 | u | 365 | 42% 41% 16% |
| 2 | v | 365 | 41% 42% 16% |
| 2 | w | 365 | 41% 42% 16% |
| 2 | x | 365 | 41% 42% 16% |
| 2 | y | 365 | 43% 40% 16% |
| 2 | z | 365 | 41% 42% 16% |
| 3 | 1 | 111 | 74% 32% 44% 24% |
| 3 | 10 | 111 | 74% 31% 45% 24% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | 11 | 111 | 74% 31% 45% 24% |
| 3 | 12 | 111 | 74% 31% 45% 24% |
| 3 | 13 | 111 | 74% 31% 45% 24% |
| 3 | 14 | 111 | 74% 31% 45% 24% |
| 3 | 15 | 111 | 74% 31% 45% 24% |
| 3 | 16 | 111 | 74% 31% 45% 24% |
| 3 | 17 | 111 | 74% 32% 43% 24% |
| 3 | 18 | 111 | 74% 31% 45% 24% |
| 3 | 19 | 111 | 74% 31% 45% 24% |
| 3 | 2 | 111 | 74% 31% 45% 24% |
| 3 | 20 | 111 | 74% 31% 45% 24% |
| 3 | 21 | 111 | 74% 31% 45% 24% |
| 3 | 22 | 111 | 74% 31% 45% 24% |
| 3 | 23 | 111 | 74% 31% 45% 24% |
| 3 | 24 | 111 | 74% 30% 46% 24% |
| 3 | 25 | 111 | 74% 31% 45% 24% |
| 3 | 26 | 111 | 74% 31% 45% 24% |
| 3 | 3 | 111 | 74% 31% 45% 24% |
| 3 | 4 | 111 | 74% 31% 45% 24% |
| 3 | 5 | 111 | 74% 31% 45% 24% |
| 3 | 6 | 111 | 74% 31% 45% 24% |
| 3 | 7 | 111 | 74% 32% 44% 24% |
| 3 | 8 | 111 | 74% 31% 45% 24% |
| 3 | 9 | 111 | 74% 31% 45% 24% |

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 crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 4 | TLW | A | 301 | X | - | - | - |
| 4 | TLW | A | 303 | X | - | - | - |
| 4 | TLW | B | 302 | X | - | - | - |
| 4 | TLW | C | 302 | X | - | - | - |
| 4 | TLW | D | 302 | X | - | - | - |
| 4 | TLW | E | 302 | X | - | - | - |
| 4 | TLW | F | 302 | X | - | - | - |
| 4 | TLW | G | 302 | X | - | - | - |
| 4 | TLW | H | 302 | X | - | - | - |
| 4 | TLW | I | 302 | X | - | - | - |
| 4 | TLW | J | 302 | X | - | - | - |
| 4 | TLW | K | 302 | X | - | - | - |
| 4 | TLW | L | 302 | X | - | - | - |
| 4 | TLW | M | 302 | X | - | - | - |
| 4 | TLW | N | 302 | X | - | - | - |
| 4 | TLW | O | 302 | X | - | - | - |
| 4 | TLW | P | 302 | X | - | - | - |
| 4 | TLW | Q | 302 | X | - | - | - |
| 4 | TLW | R | 302 | X | - | - | - |
| 4 | TLW | S | 302 | X | - | - | - |
| 4 | TLW | T | 302 | X | - | - | - |
| 4 | TLW | U | 302 | X | - | - | - |
| 4 | TLW | V | 302 | X | - | - | - |
| 4 | TLW | W | 302 | X | - | - | - |
| 4 | TLW | X | 302 | X | - | - | - |
| 4 | TLW | Y | 302 | X | - | - | - |

# 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 126022 atoms, of which 5538 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 Flagellar L-ring protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | B | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | C | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | D | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | E | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | F | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | G | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | H | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | I | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | J | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | K | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | L | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | M | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | N | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | O | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | P | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | Q | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | R | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | S | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | T | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | U | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | V | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | W | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | X | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | Y | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |
| 1 | Z | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1581 | 985 | 282 | 310 | 4 | | |

- Molecule 2 is a protein called Flagellar P-ring protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | a | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | b | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | c | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | d | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | e | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | f | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | g | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | h | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | i | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | j | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | k | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | l | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | m | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | n | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | o | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | p | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | q | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | r | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | s | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | t | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | u | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | v | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | w | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | x | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | y | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |
| 2 | z | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2251 | 1378 | 409 | 451 | 13 | | |

- Molecule 3 is a protein called YecR.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 2 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 3 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | 4 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 5 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 6 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 7 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 8 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 9 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 10 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 11 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 12 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 13 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 14 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 15 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 16 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 17 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 18 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 19 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 20 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 21 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 22 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 23 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 24 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |

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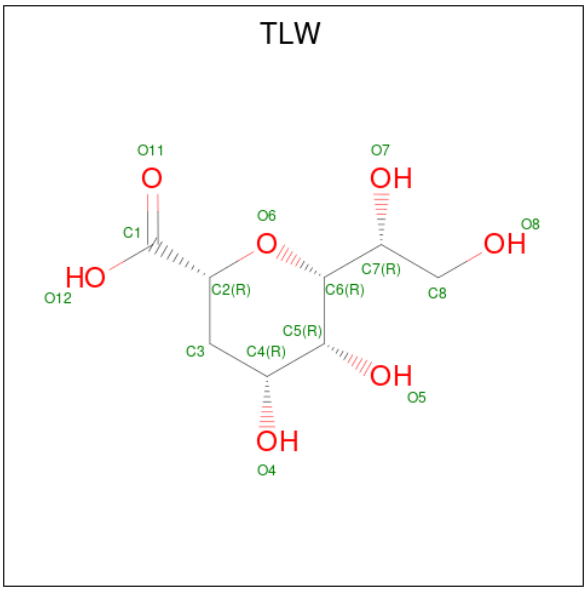
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | 25 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |
| 3 | 26 | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 647 | 401 | 114 | 126 | 6 | | |

- Molecule 4 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-4,5-bis(oxidanyl )oxane-2-carboxylic acid (CCD ID: TLW) (formula: $C_8H_{14}O_7$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 4 | A | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | A | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | B | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | C | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | D | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | E | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | F | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | G | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | H | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |

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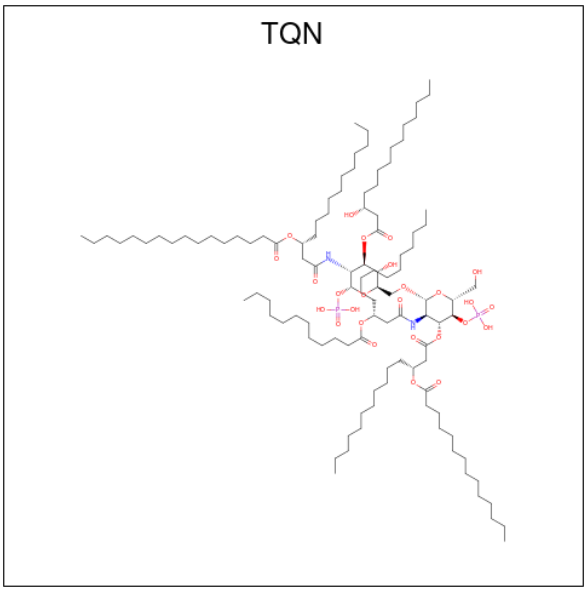
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 4 | I | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | J | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | K | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | L | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | M | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | N | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | O | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | P | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | Q | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | R | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | S | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | T | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | U | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | V | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | W | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | X | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |
| 4 | Y | 1 | Total | C | H | O | 0 |
| | | | 25 | 8 | 10 | 7 | |

- Molecule 5 is [(3 {R})-1-[[(2 {R},3 {R},4 {R},5 {S},6 {R})-6-[[(2 {R},3 {R},4 {R},5 {S},6 {R})-3-[[(3 {R})-3-dodecanoyloxytetradecanoyl]amino]-6-(hydroxymethyl)-5-phosphonooxy-4-[(3 {R})-3-tetradecanoyloxytetradecanoyl]oxy-oxan-2-yl]oxymethyl]-5-oxidanyl-4-[(3 {R})-3-oxidanyltetradecanoyl]oxy-2-phosphonooxy-oxan-3-yl]amino]-1-oxidanylidene-tetradecan-3-yl] hexadecanoate (CCD ID: TQN) (formula: $C_{110}H_{208}N_2O_{26}P_2$).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 5 | A | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | B | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | C | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | D | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | E | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | F | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | G | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | H | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | I | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | J | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | K | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | L | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | M | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | N | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |

*Continued on next page...*

*Continued from previous page...*

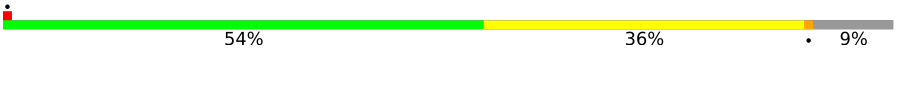
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 5 | O | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | P | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | Q | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | R | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | S | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | T | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | U | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | V | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | W | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | X | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | Y | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |
| 5 | Z | 1 | Total | C | H | N | O | P | 0 |
| | | | 343 | 110 | 203 | 2 | 26 | 2 | |

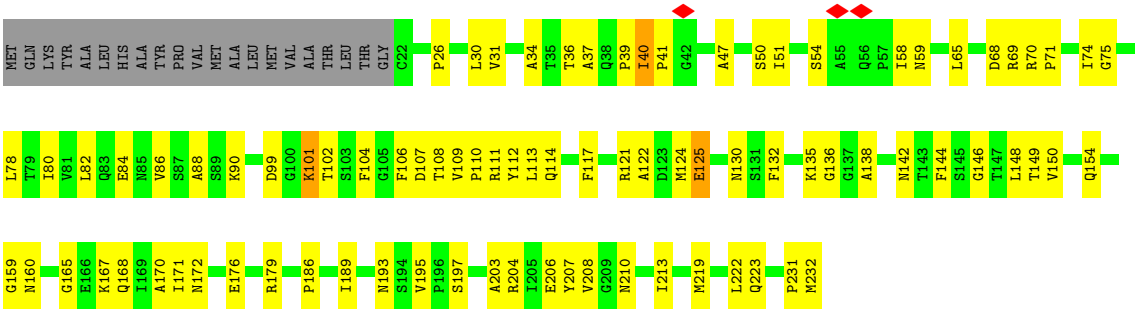
# 3 Residue-property plots (i)

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: Flagellar L-ring protein

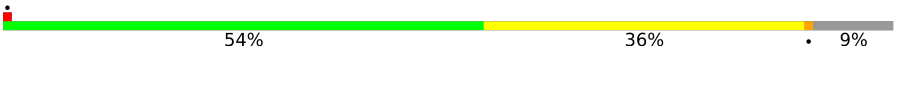
Chain A:

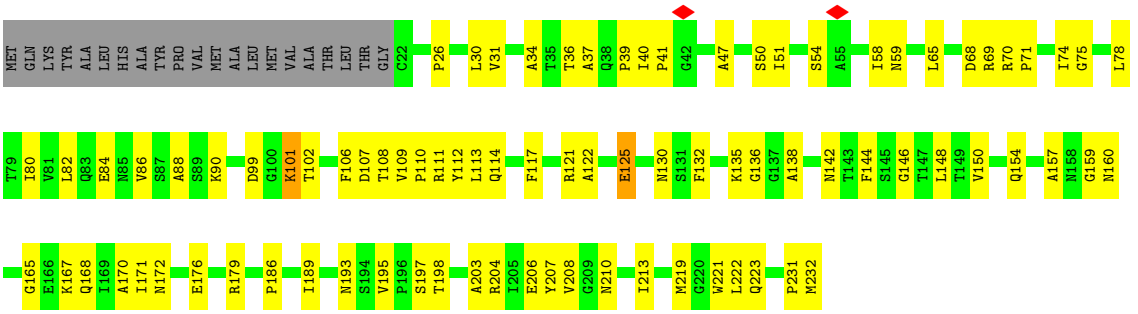



• Molecule 1: Flagellar L-ring protein

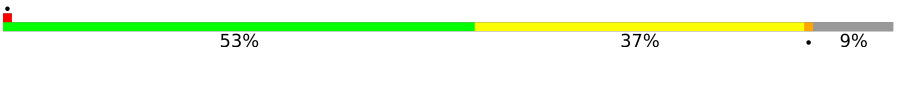
Chain B:

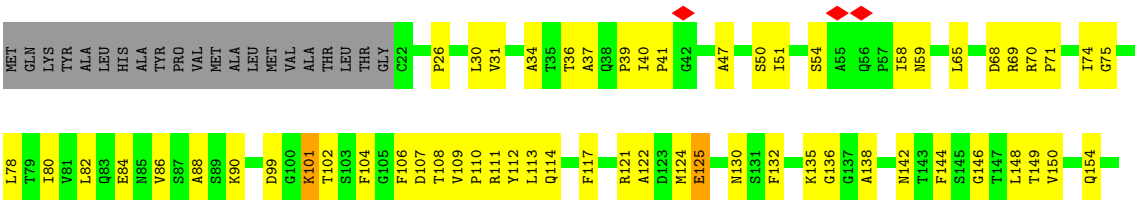



• Molecule 1: Flagellar L-ring protein

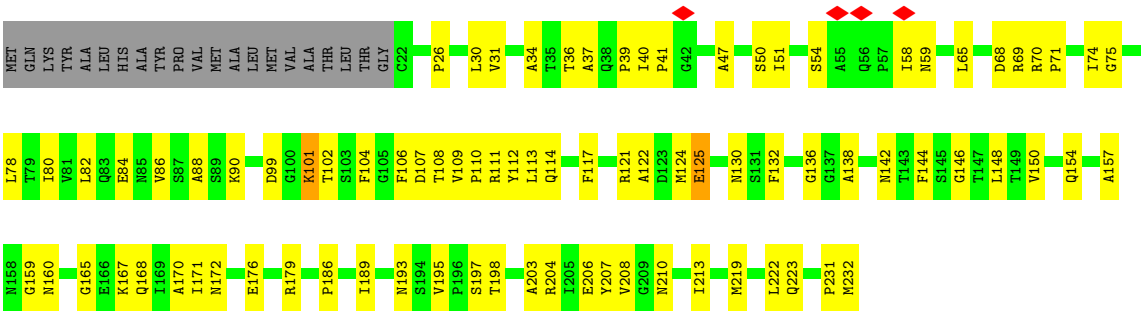
Chain C:



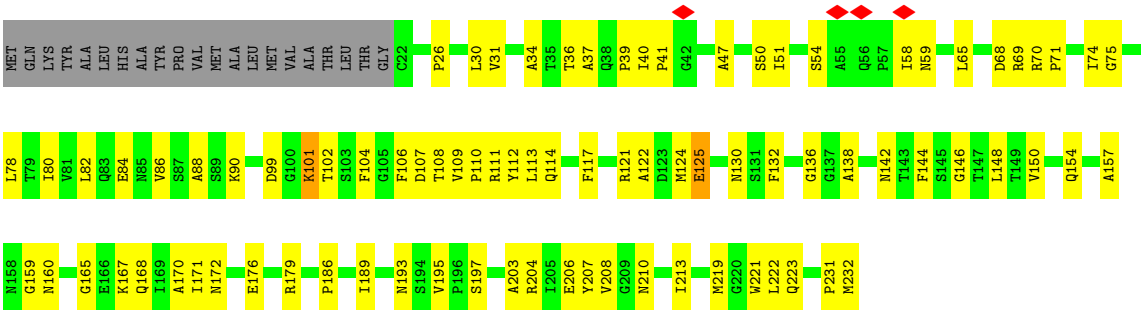
• Molecule 1: Flagellar L-ring protein

Chain D:



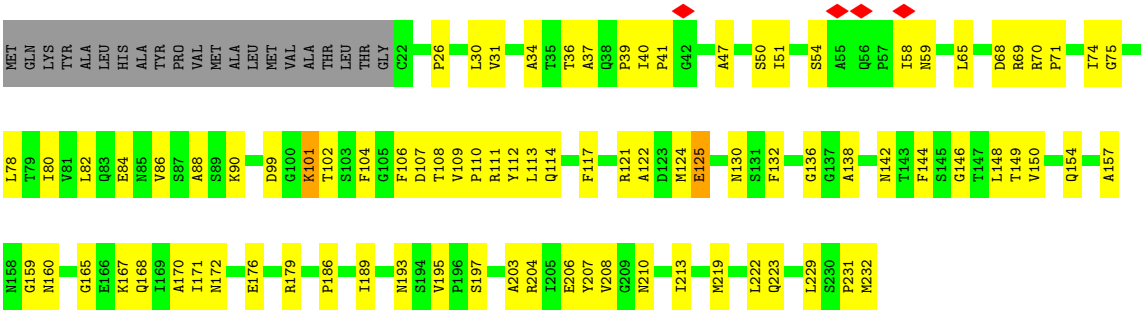

• Molecule 1: Flagellar L-ring protein

Chain E:



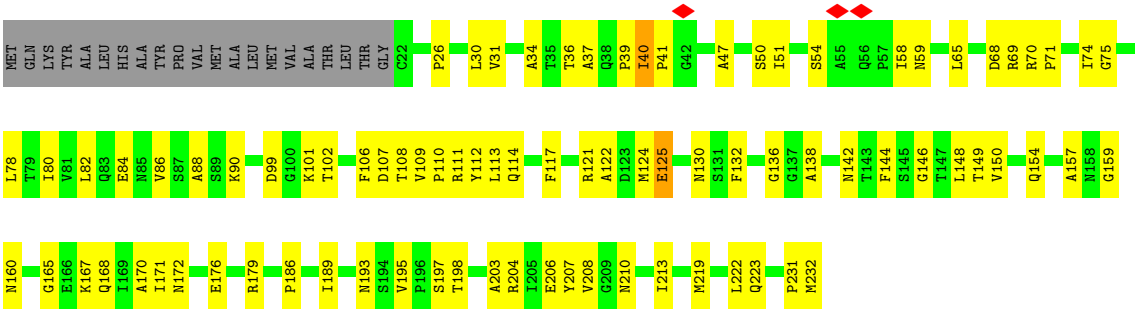

• Molecule 1: Flagellar L-ring protein

Chain F:



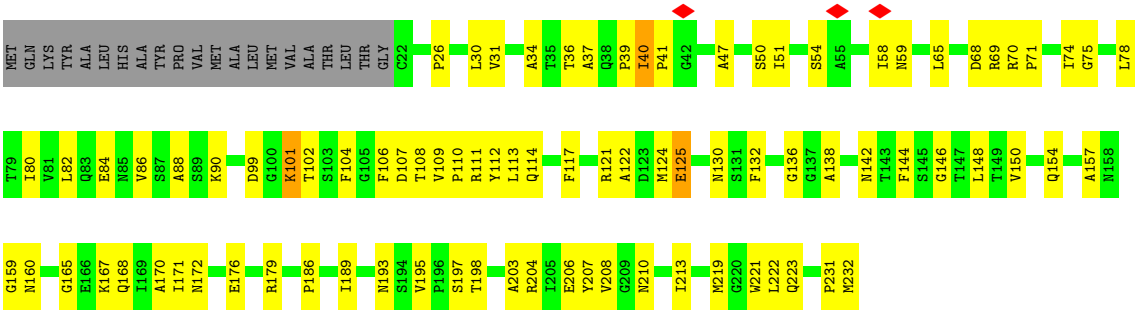

• Molecule 1: Flagellar L-ring protein

Chain G:



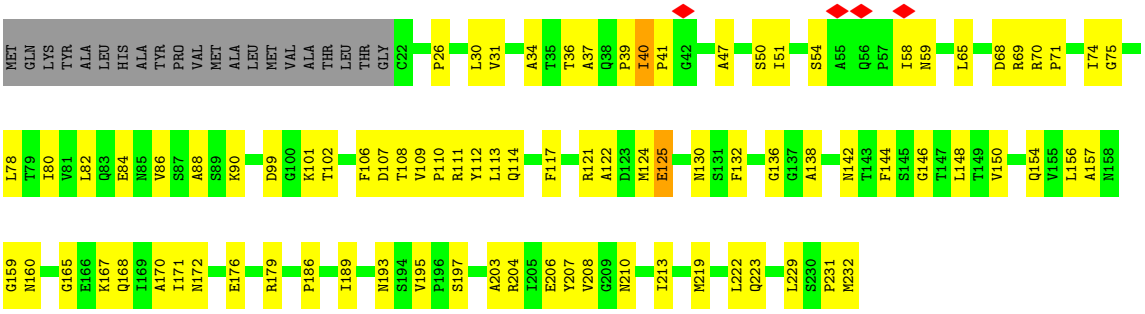
• Molecule 1: Flagellar L-ring protein

Chain H:



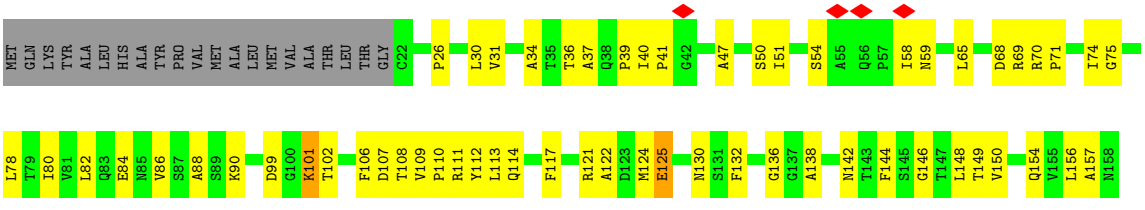
• Molecule 1: Flagellar L-ring protein

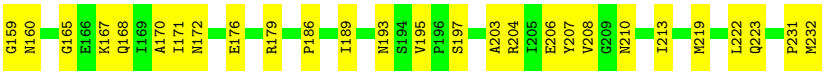
Chain I:



• Molecule 1: Flagellar L-ring protein

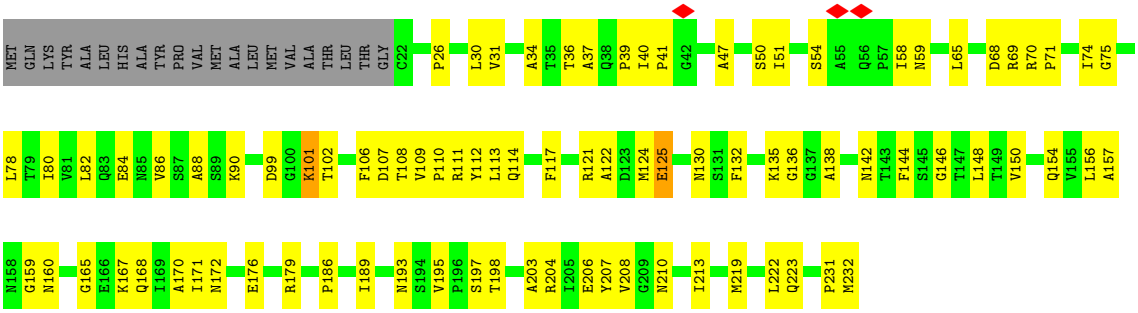
Chain J:





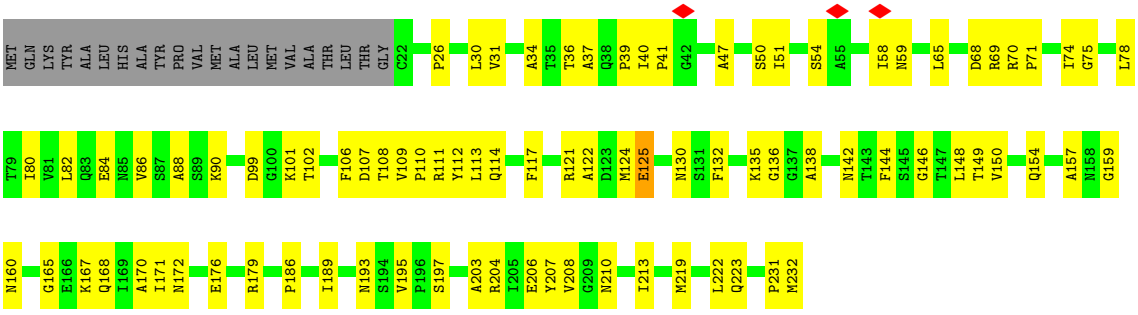

• Molecule 1: Flagellar L-ring protein

Chain K:



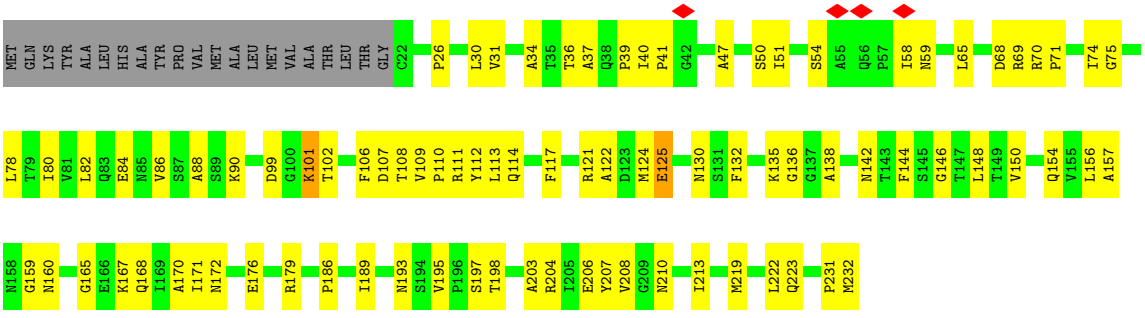

• Molecule 1: Flagellar L-ring protein

Chain L:



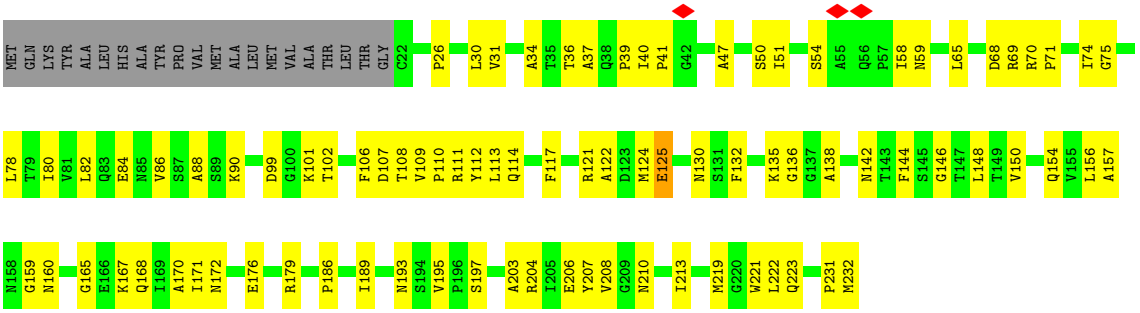

• Molecule 1: Flagellar L-ring protein

Chain M:



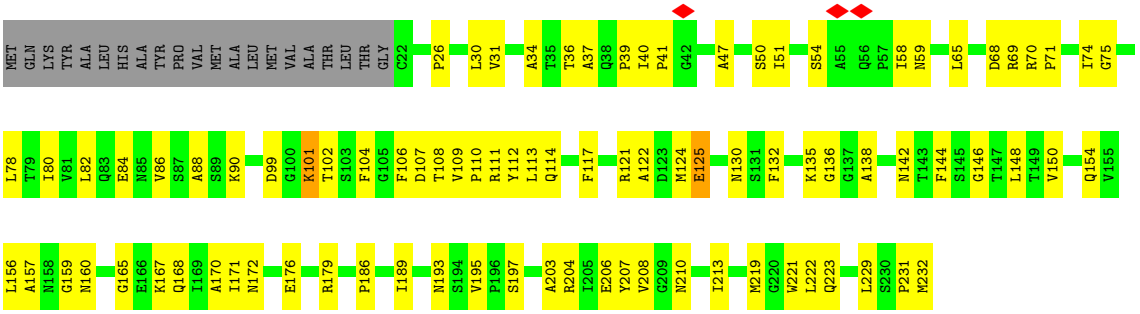

• Molecule 1: Flagellar L-ring protein

Chain N:



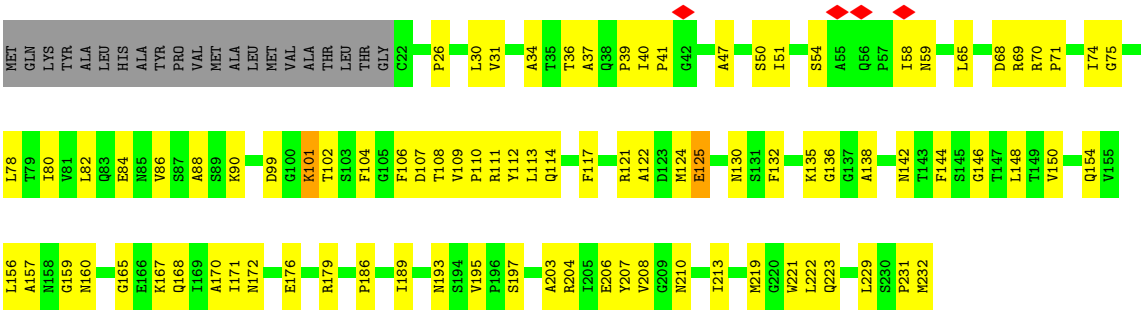
• Molecule 1: Flagellar L-ring protein

Chain O:



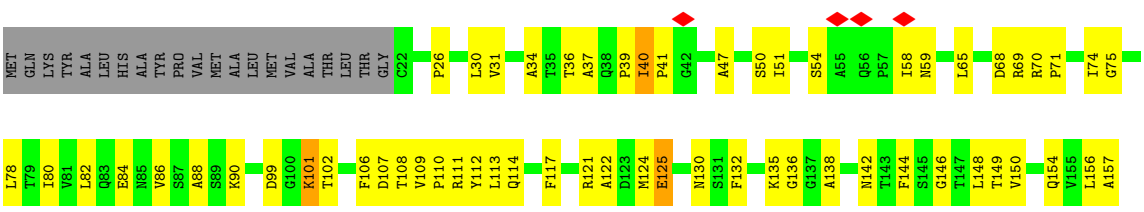
• Molecule 1: Flagellar L-ring protein

Chain P:



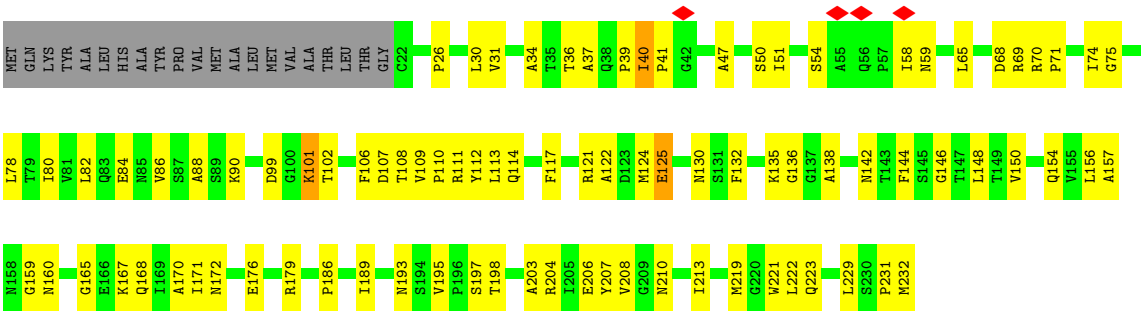
• Molecule 1: Flagellar L-ring protein

Chain Q:



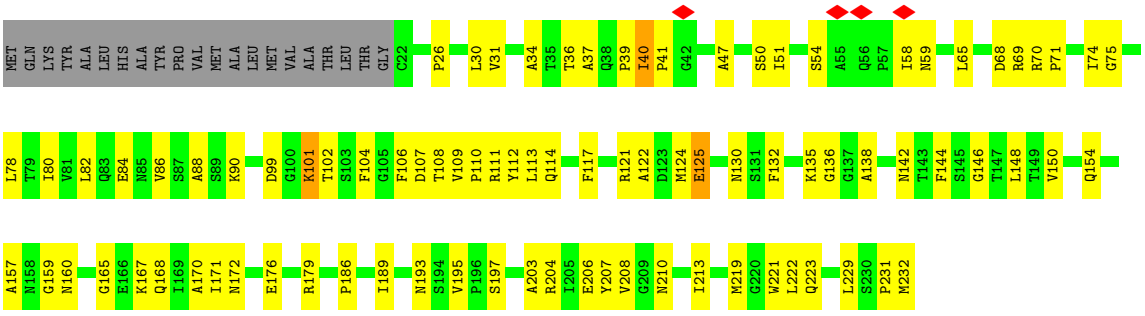
• Molecule 1: Flagellar L-ring protein

Chain R:



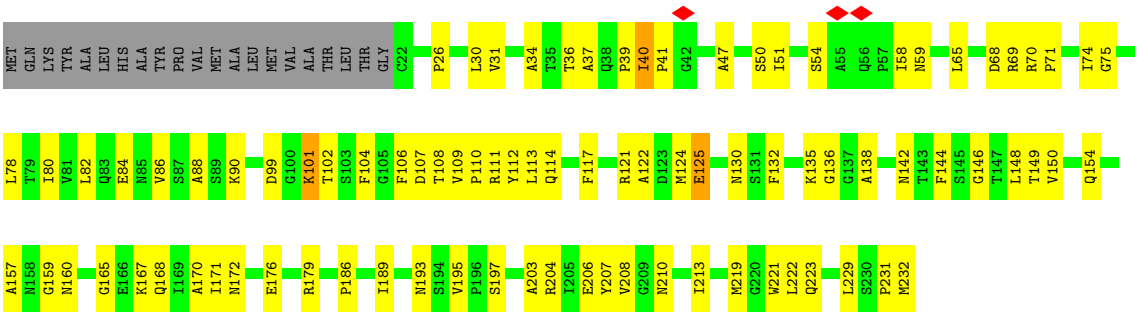

• Molecule 1: Flagellar L-ring protein

Chain S:



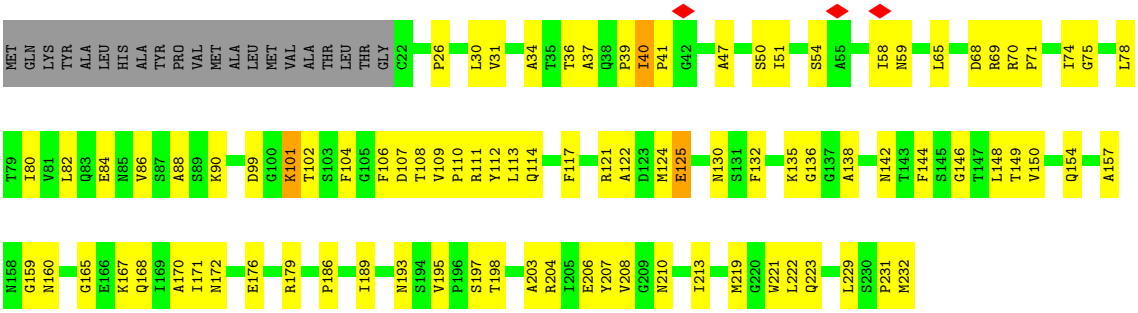

• Molecule 1: Flagellar L-ring protein

Chain T:



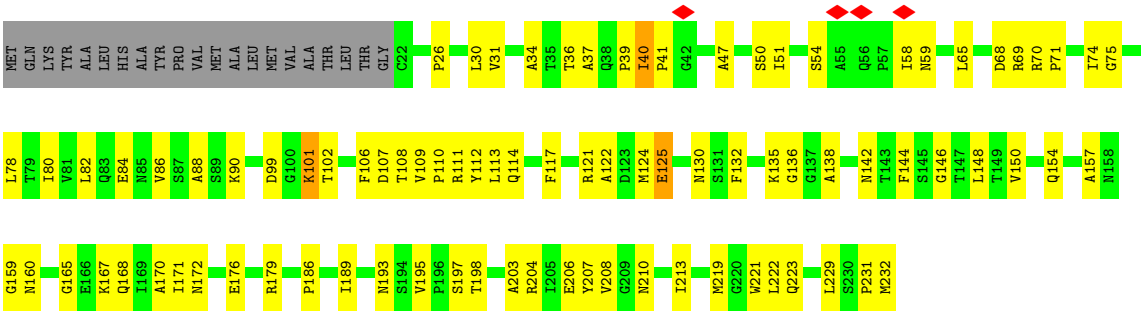

• Molecule 1: Flagellar L-ring protein

Chain U:



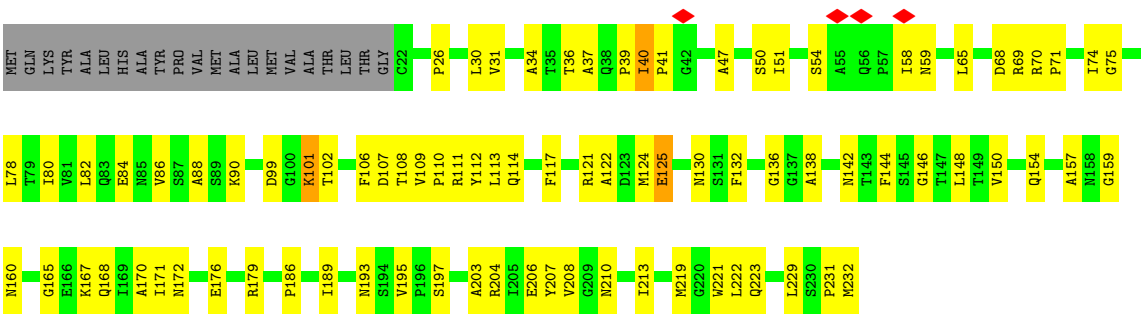
• Molecule 1: Flagellar L-ring protein

Chain V:



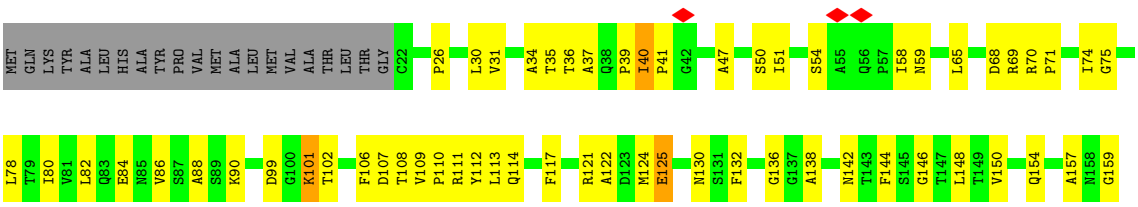
• Molecule 1: Flagellar L-ring protein

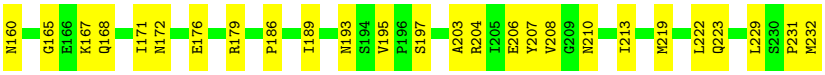
Chain W:



• Molecule 1: Flagellar L-ring protein

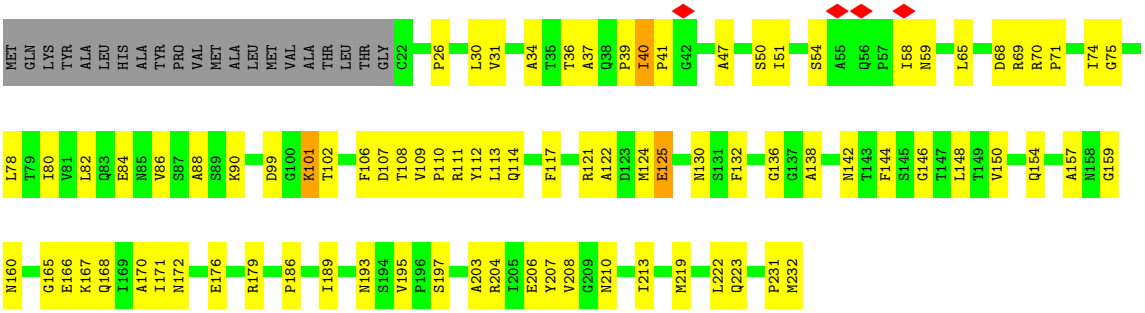
Chain X:





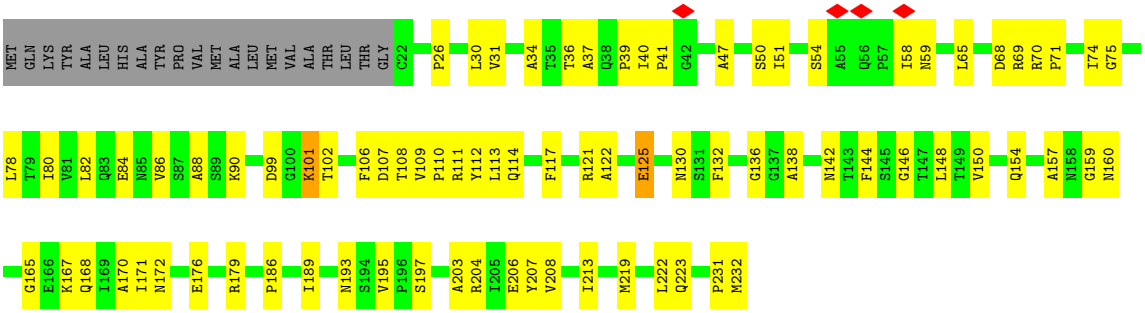
• Molecule 1: Flagellar L-ring protein

Chain Y:



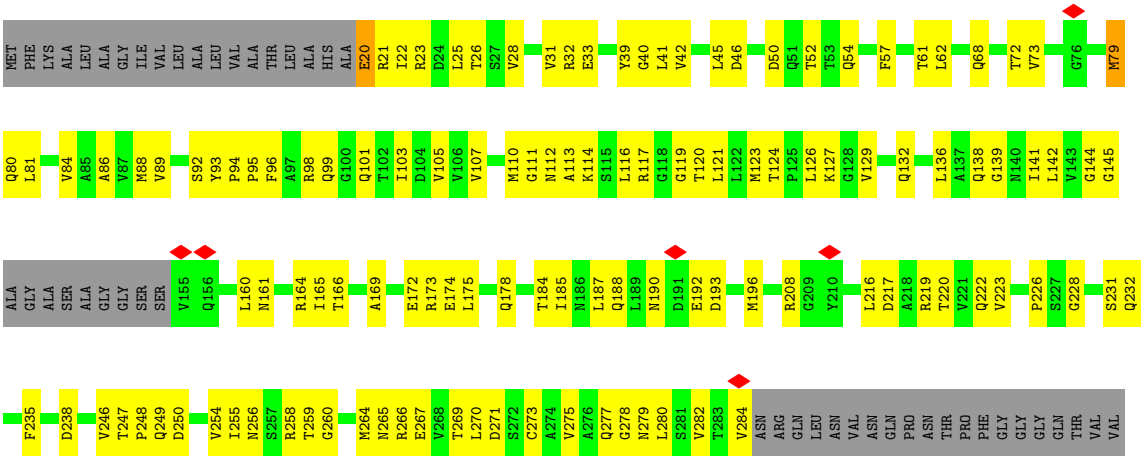
• Molecule 1: Flagellar L-ring protein

Chain Z:



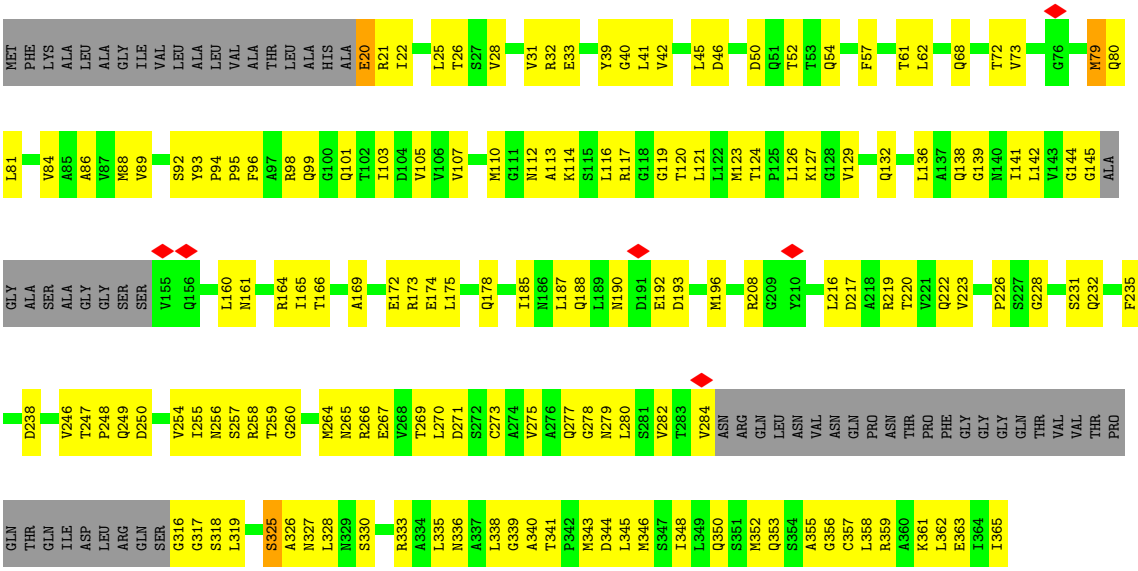
• Molecule 2: Flagellar P-ring protein

Chain a:



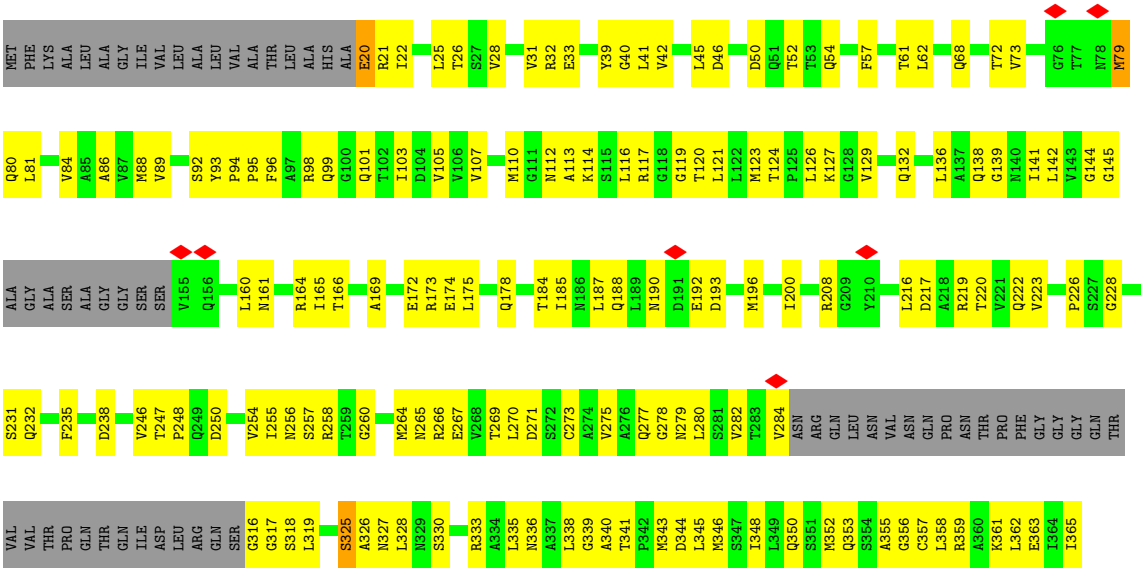
• Molecule 2: Flagellar P-ring protein

Chain b:



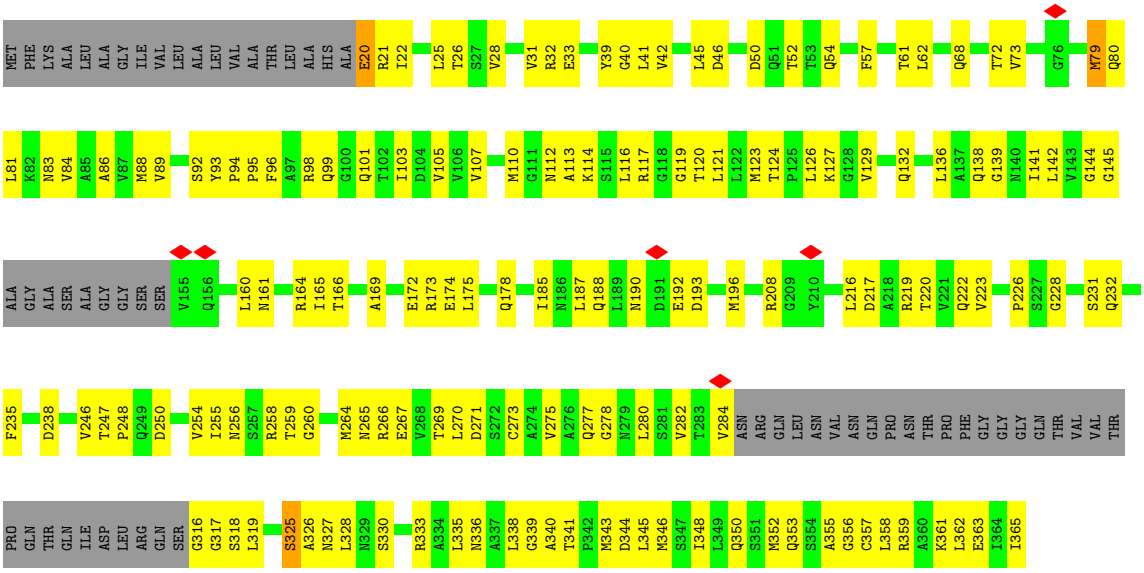
• Molecule 2: Flagellar P-ring protein

Chain c:



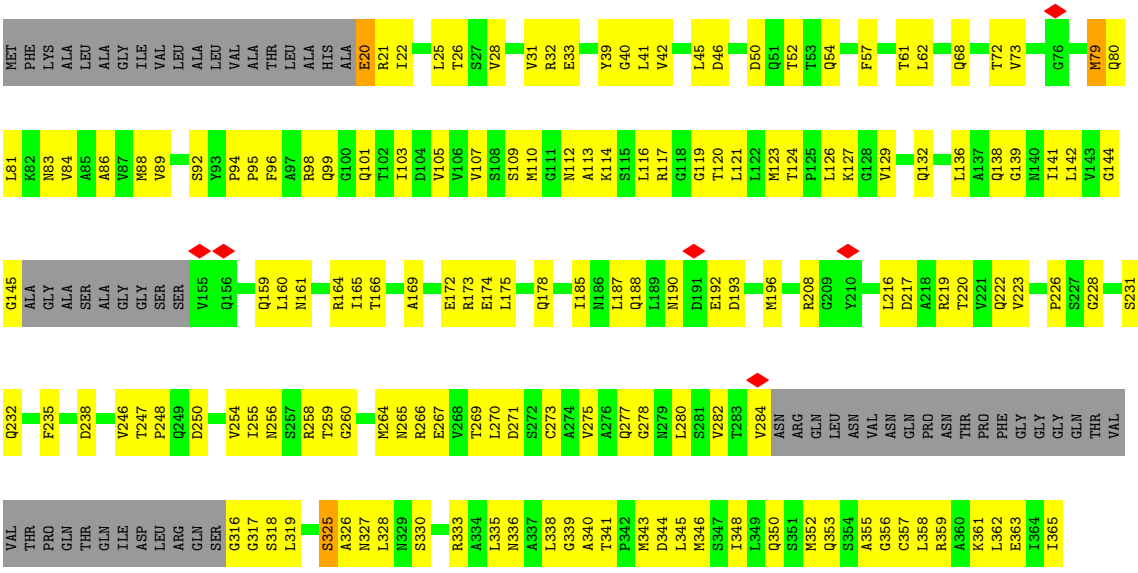
• Molecule 2: Flagellar P-ring protein

Chain d:



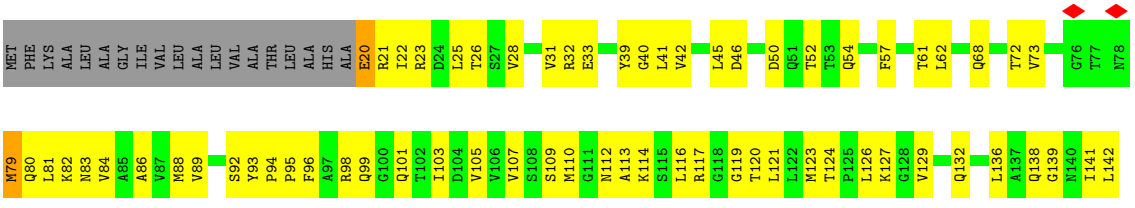
• Molecule 2: Flagellar P-ring protein

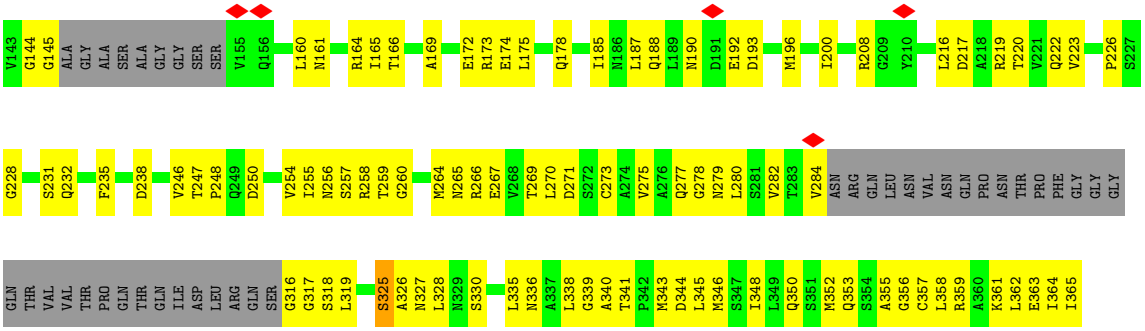
Chain e:



• Molecule 2: Flagellar P-ring protein

Chain f:



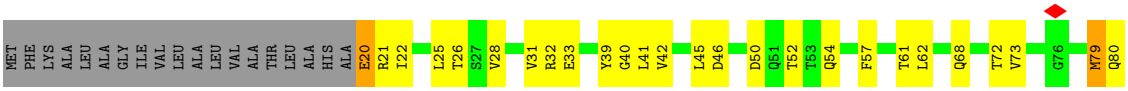


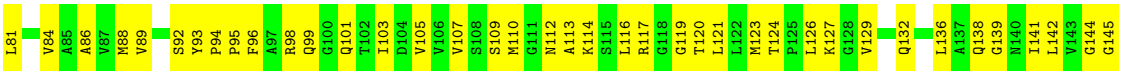


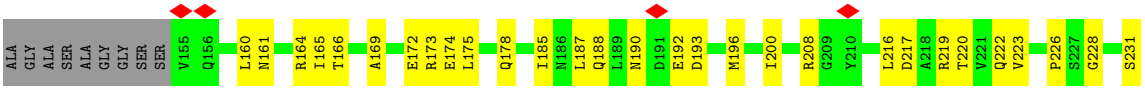


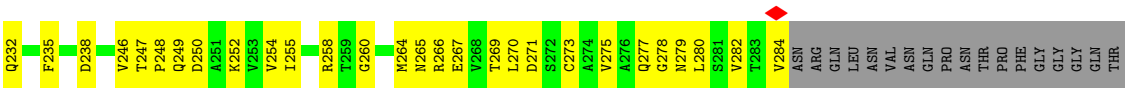
• Molecule 2: Flagellar P-ring protein

Chain g:



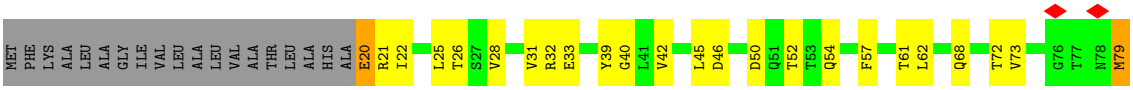


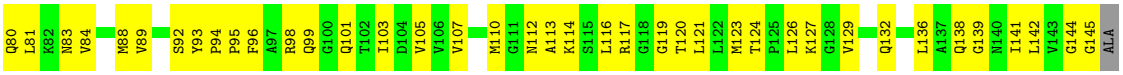


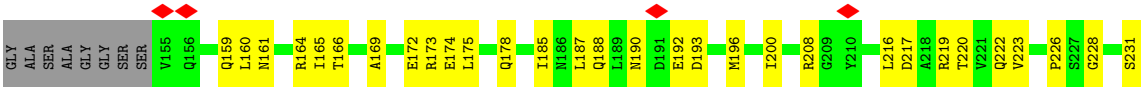


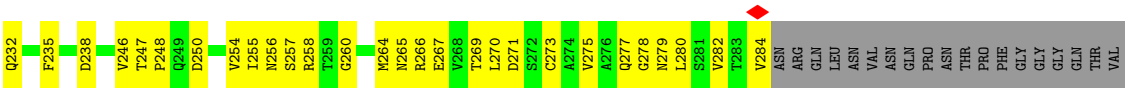
• Molecule 2: Flagellar P-ring protein

Chain h:



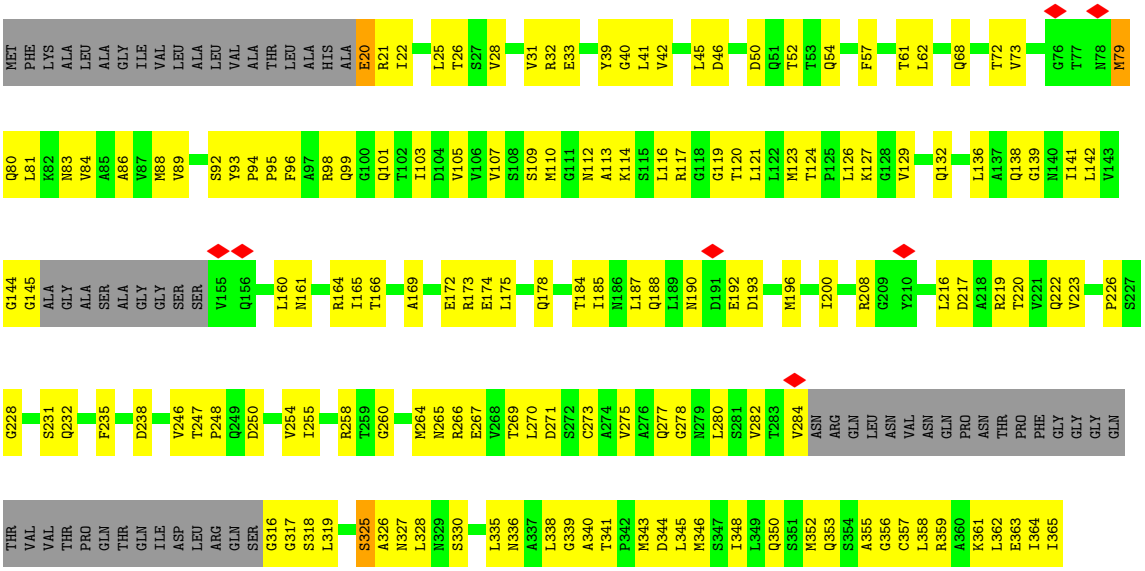






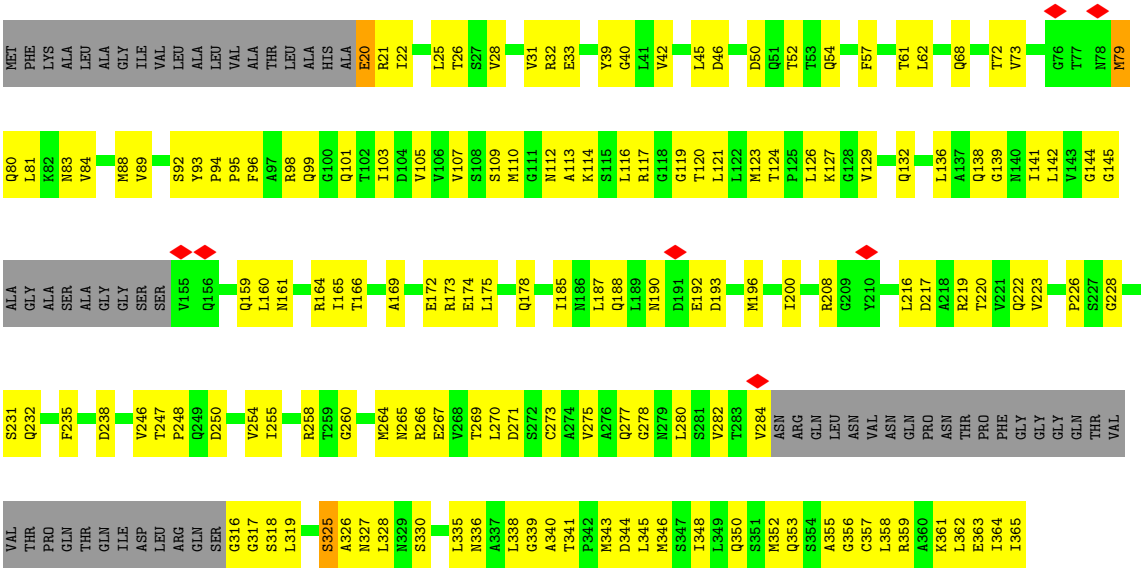
• Molecule 2: Flagellar P-ring protein

Chain i:



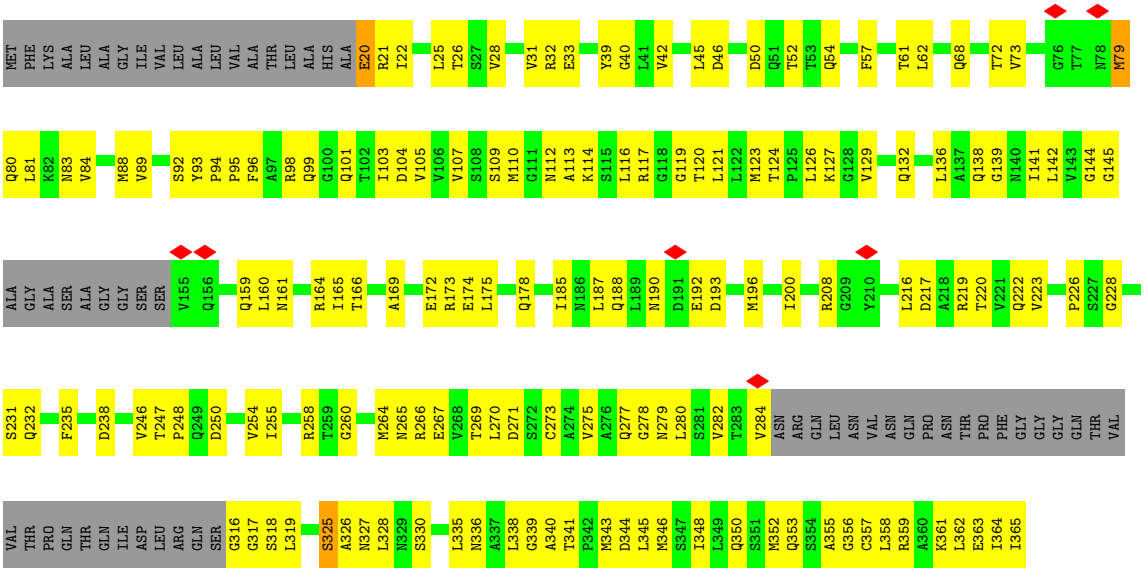
• Molecule 2: Flagellar P-ring protein

Chain j:



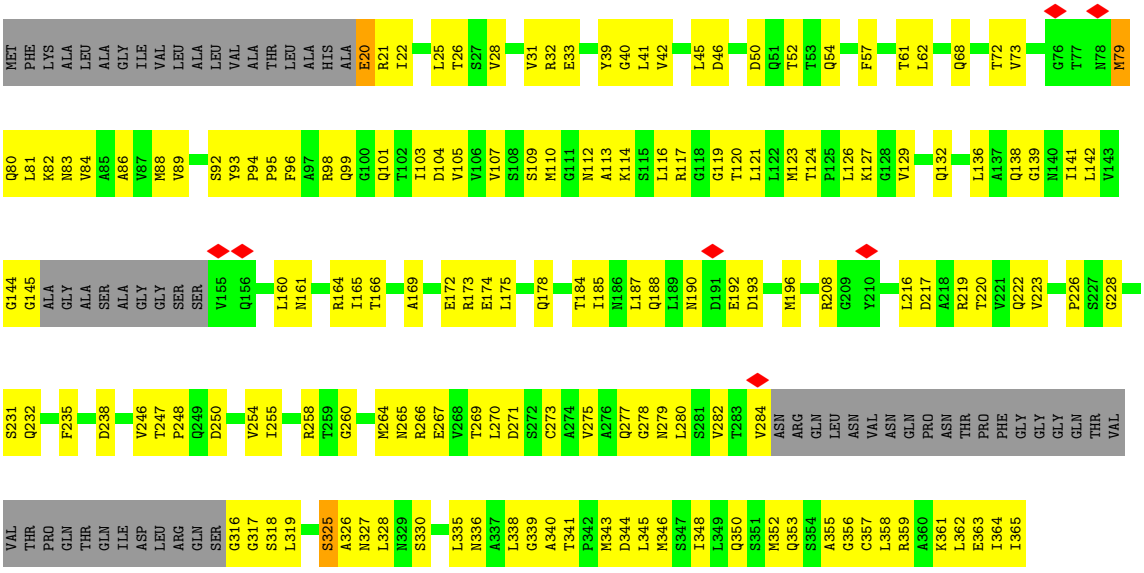
• Molecule 2: Flagellar P-ring protein

Chain k:



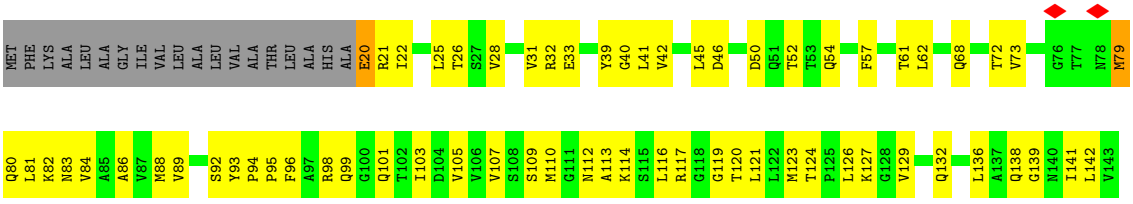
• Molecule 2: Flagellar P-ring protein

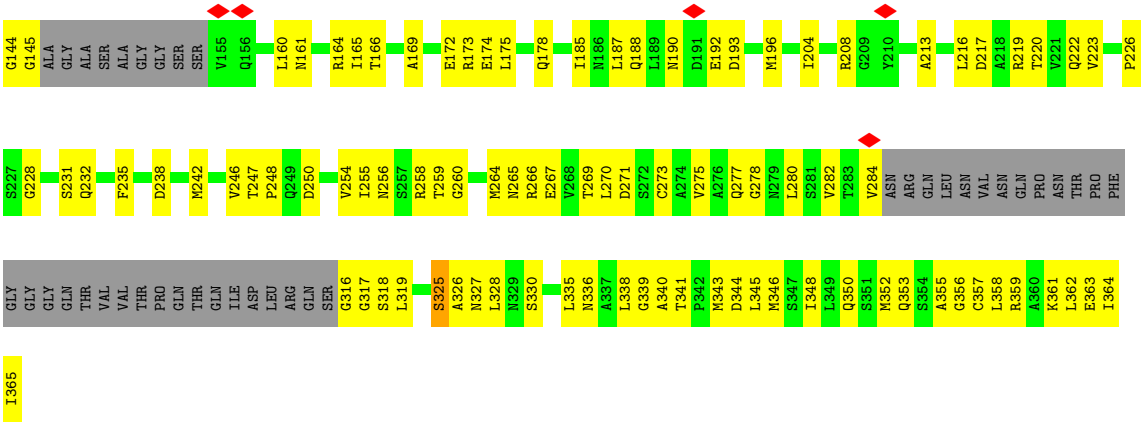
Chain l:



• Molecule 2: Flagellar P-ring protein

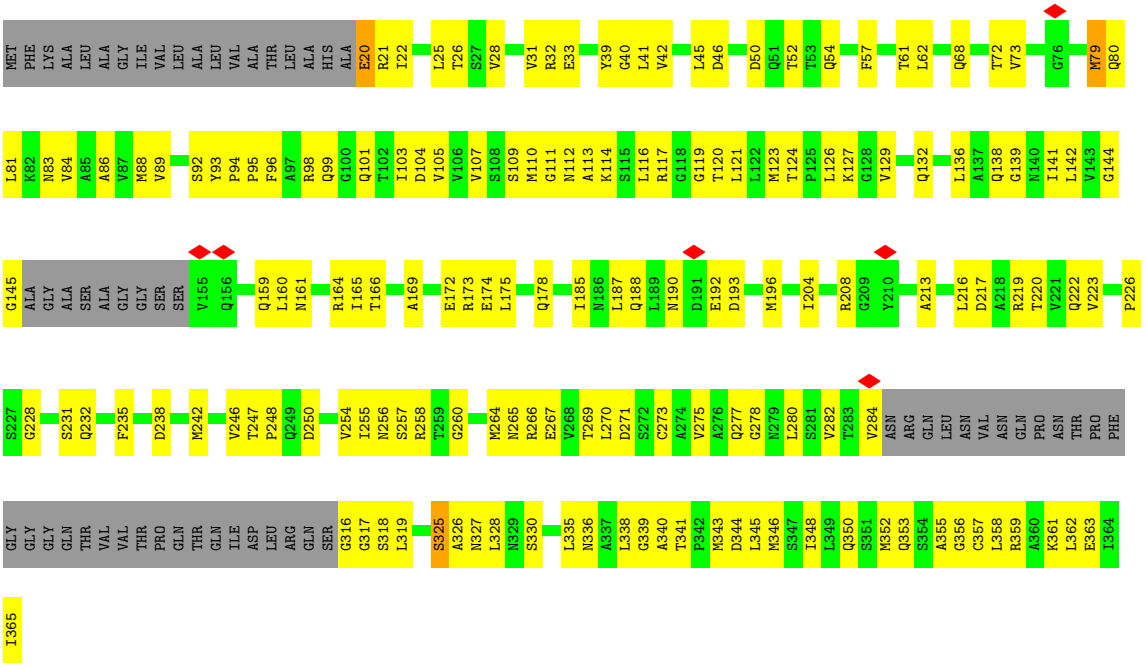
Chain m:





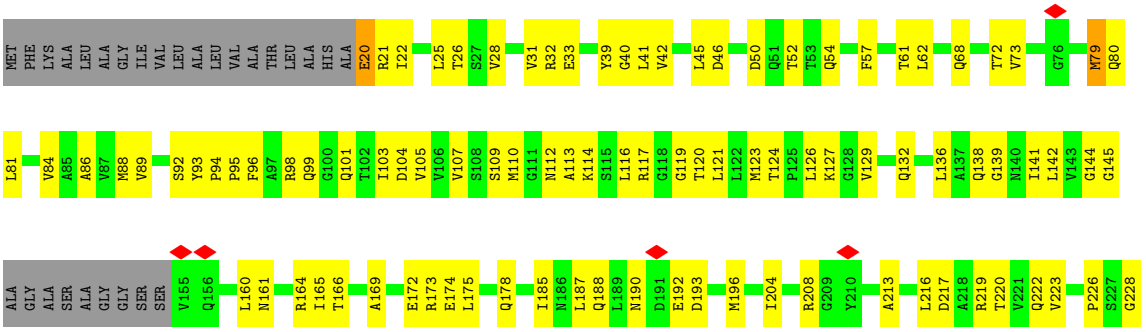

• Molecule 2: Flagellar P-ring protein

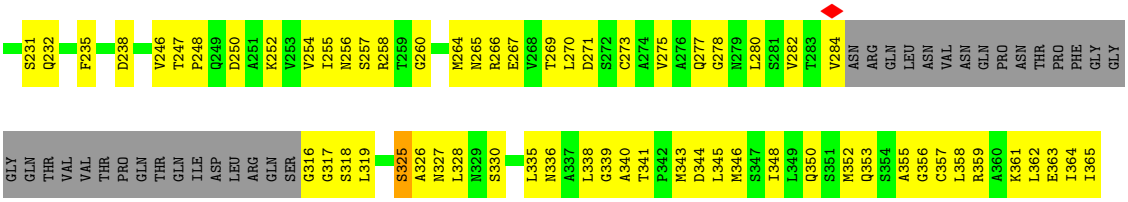
Chain n:




• Molecule 2: Flagellar P-ring protein

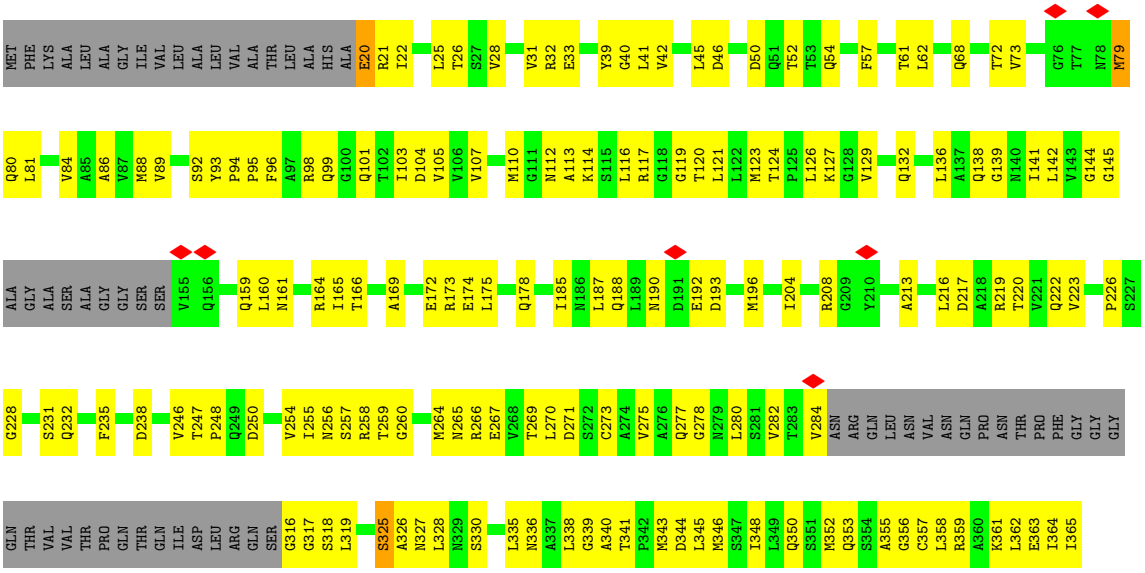
Chain o:





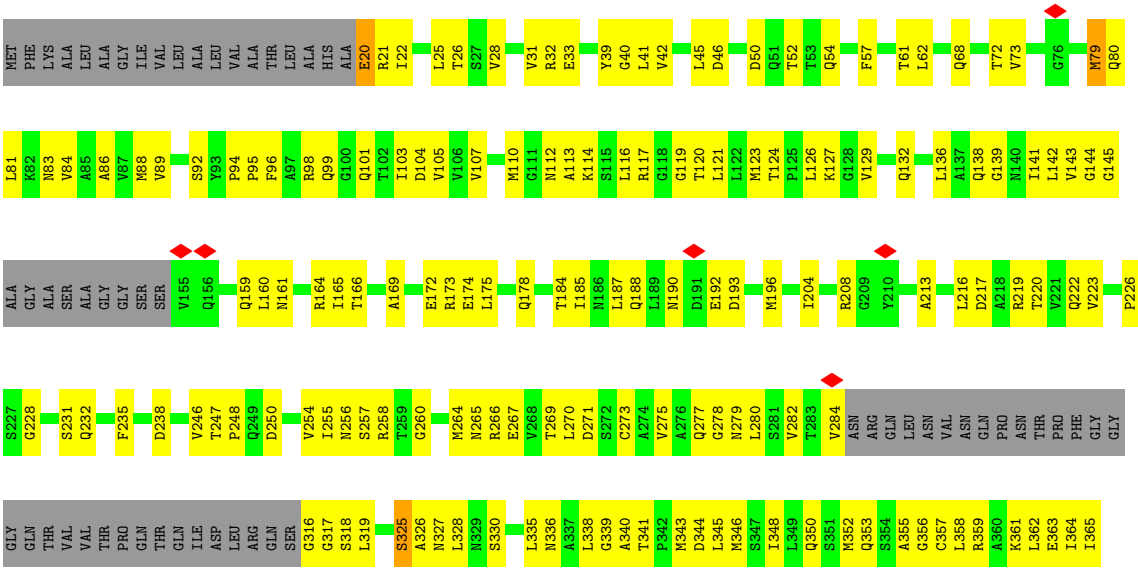
• Molecule 2: Flagellar P-ring protein

Chain p:



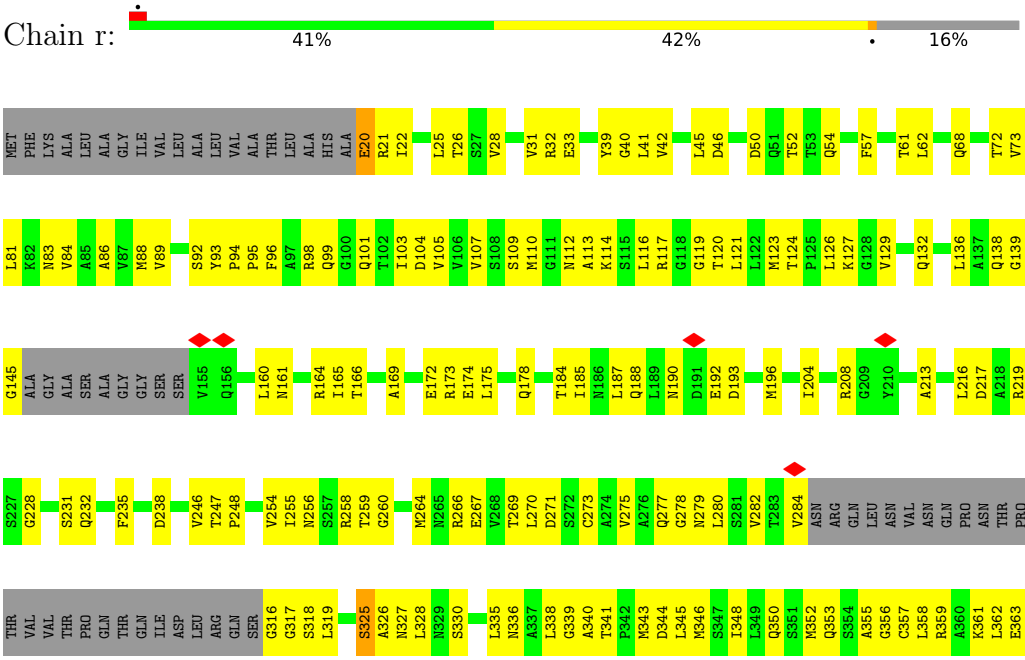
• Molecule 2: Flagellar P-ring protein

Chain q:



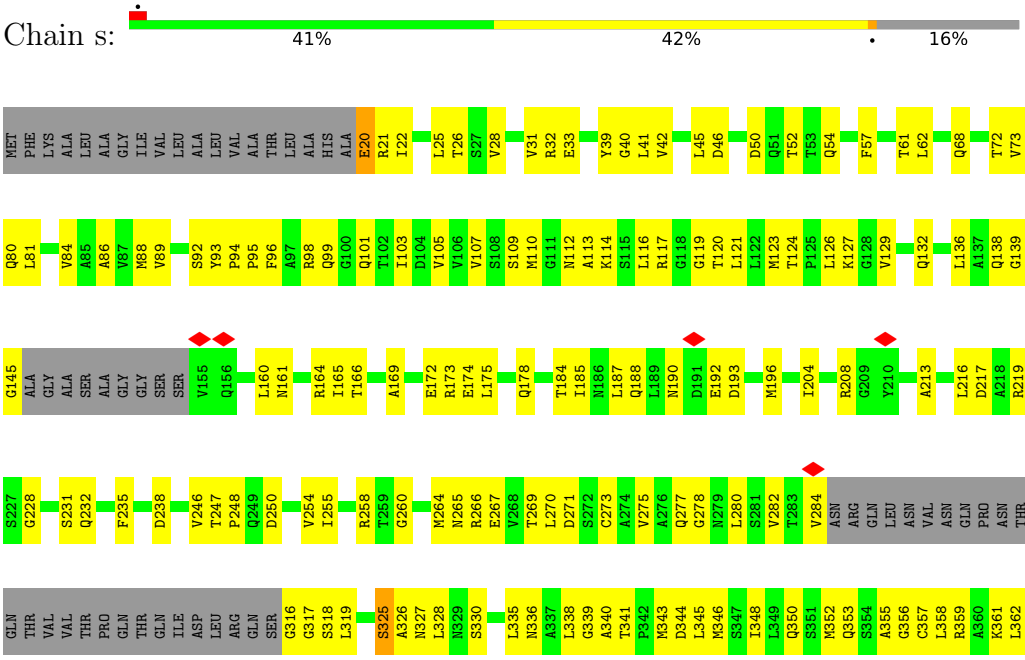
• Molecule 2: Flagellar P-ring protein

Chain r:



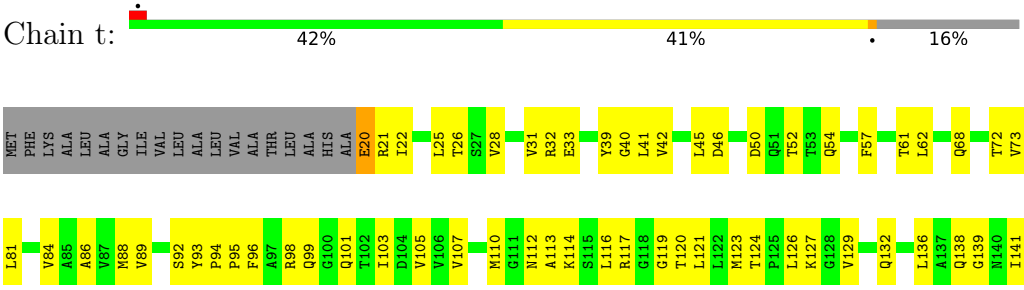

• Molecule 2: Flagellar P-ring protein

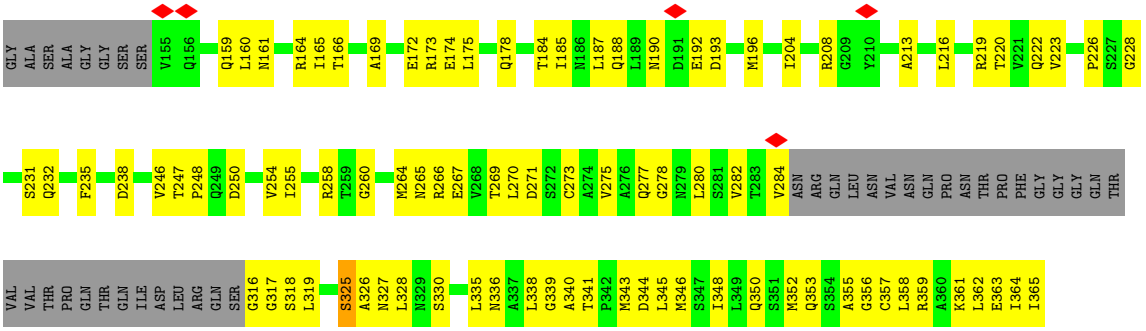
Chain s:




• Molecule 2: Flagellar P-ring protein

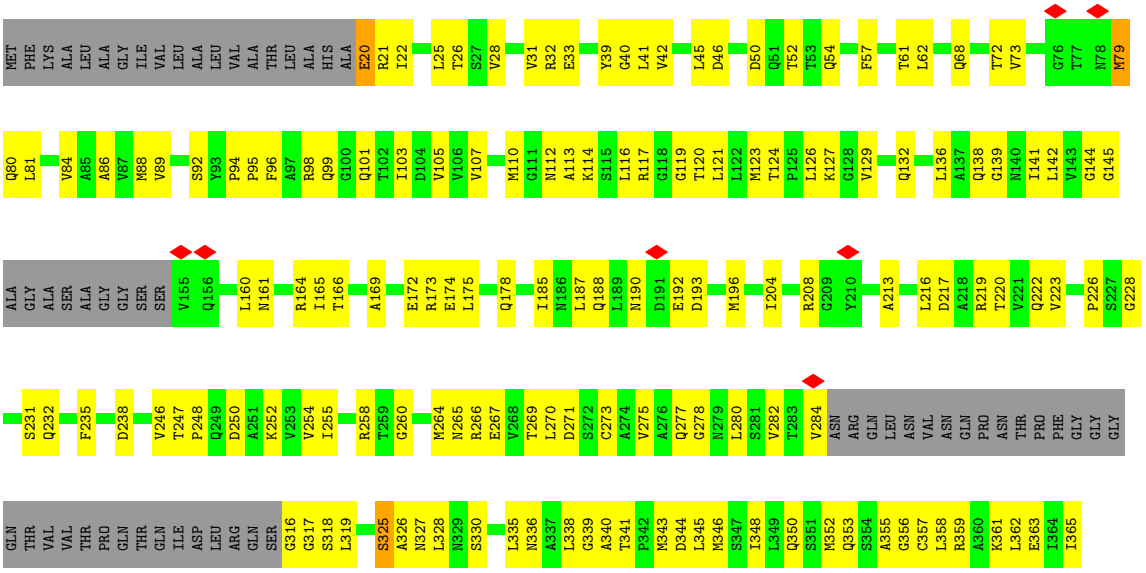
Chain t:





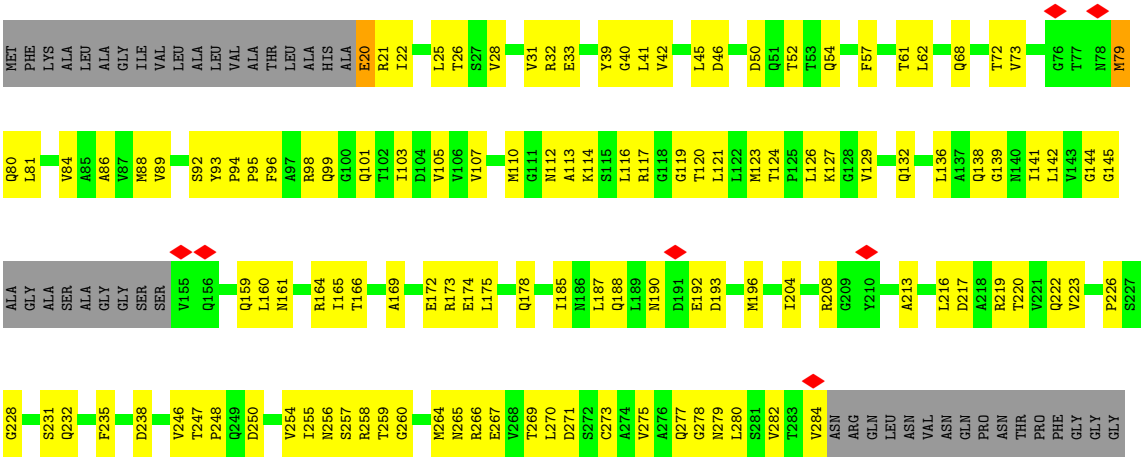
• Molecule 2: Flagellar P-ring protein

Chain u:



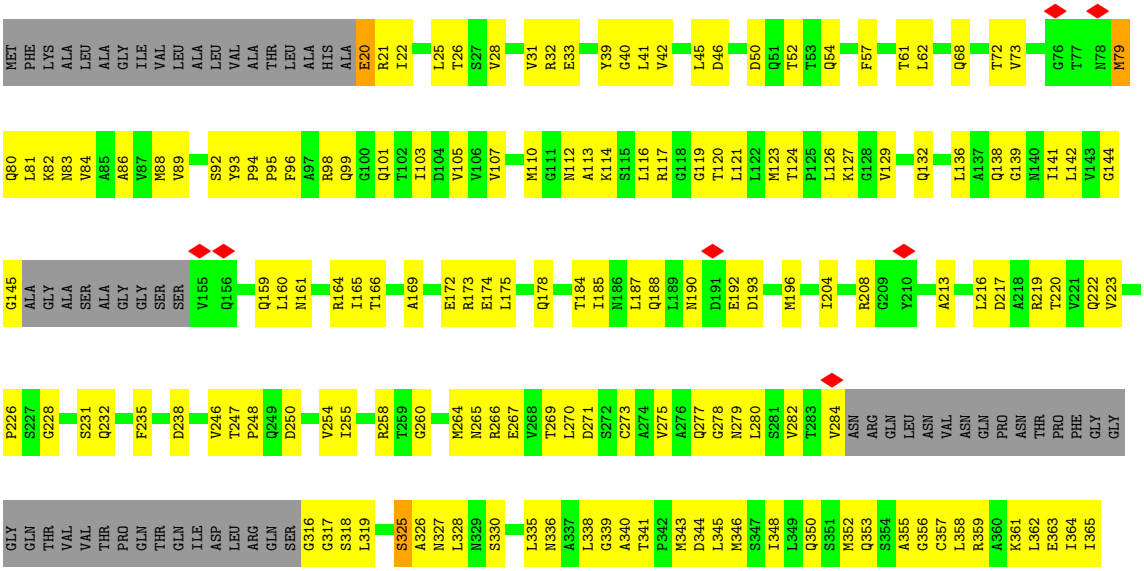
• Molecule 2: Flagellar P-ring protein

Chain v:



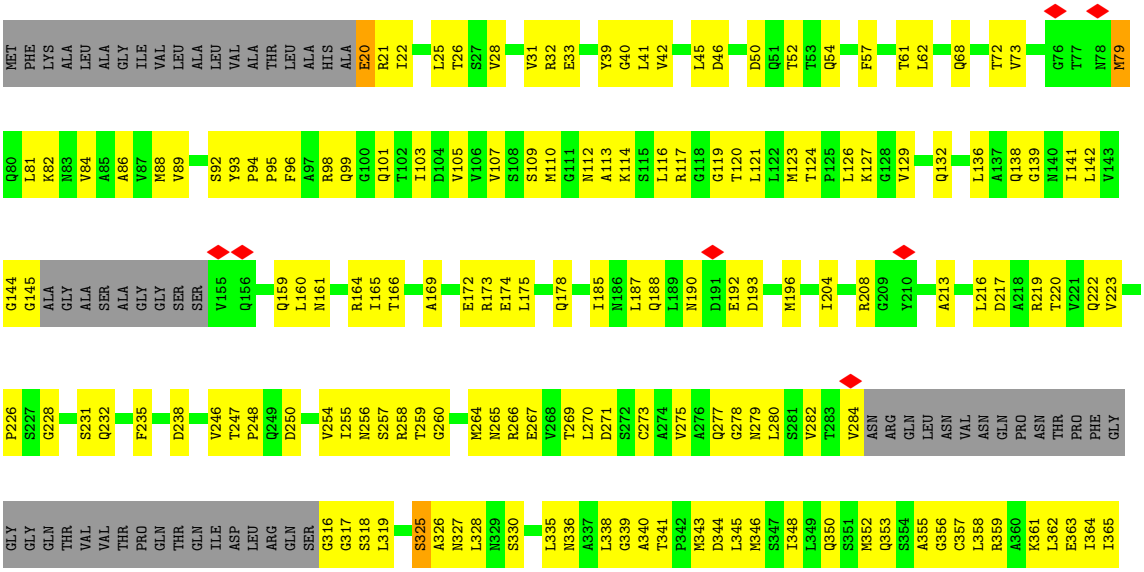
• Molecule 2: Flagellar P-ring protein

Chain w:



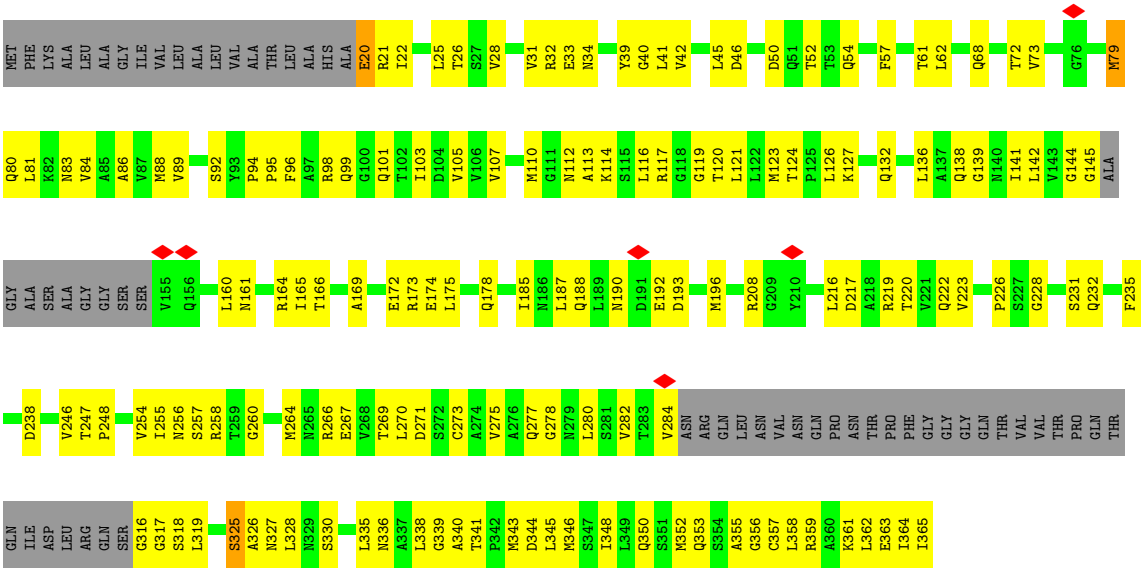
• Molecule 2: Flagellar P-ring protein

Chain x:



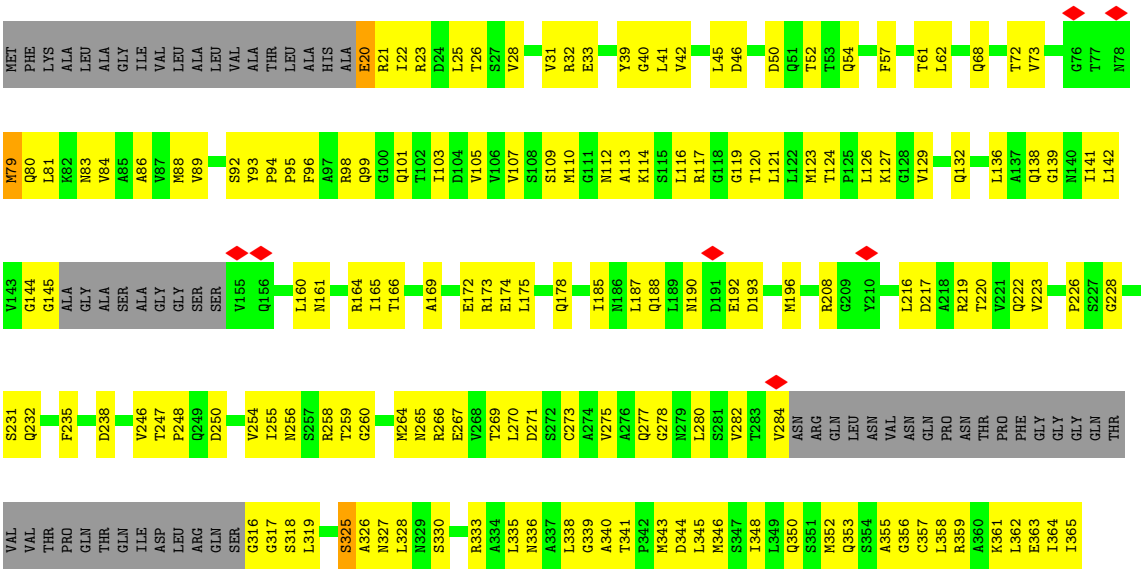
• Molecule 2: Flagellar P-ring protein

Chain y:



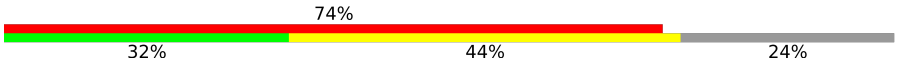
• Molecule 2: Flagellar P-ring protein

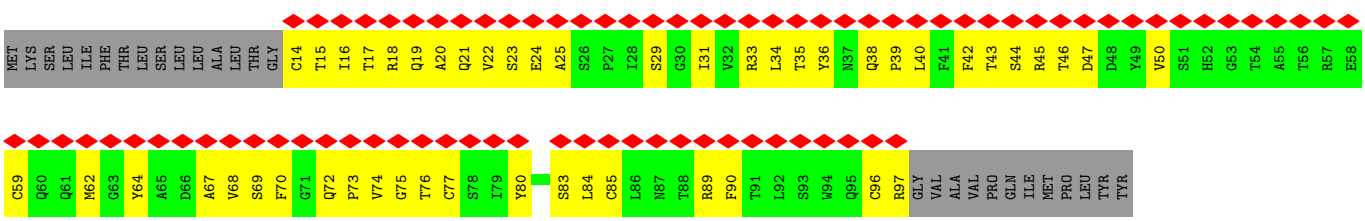
Chain z:



• Molecule 3: YecR

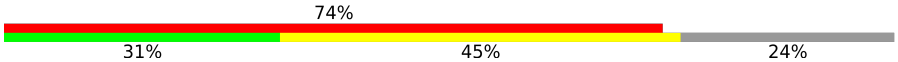
Chain 1:

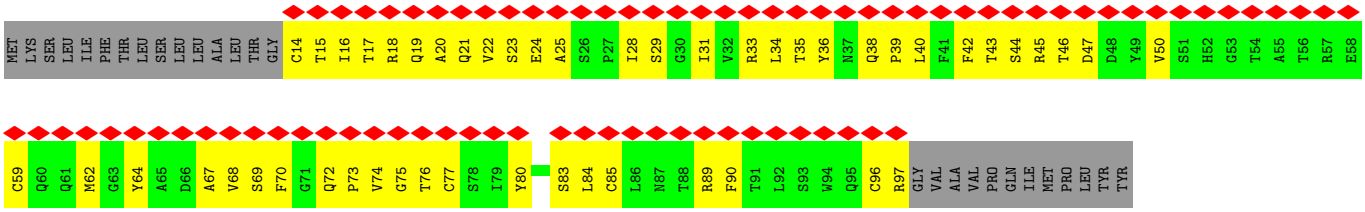


• Molecule 3: YecR

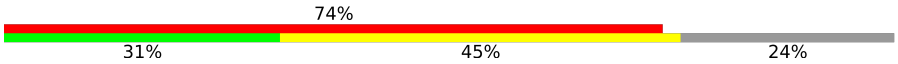
Chain 2:

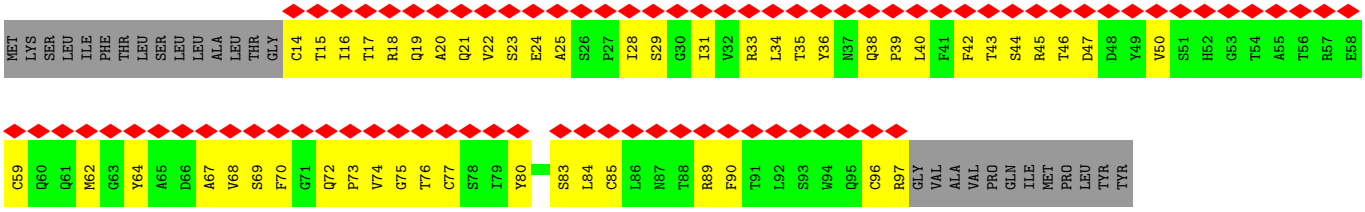



• Molecule 3: YecR

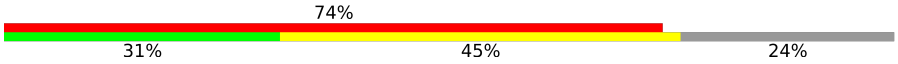
Chain 3:

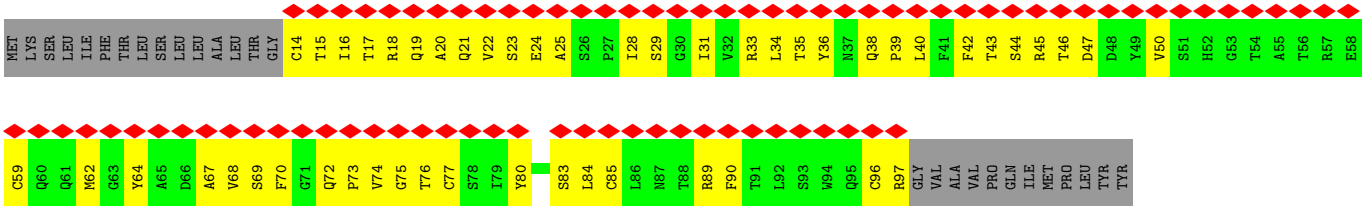



• Molecule 3: YecR

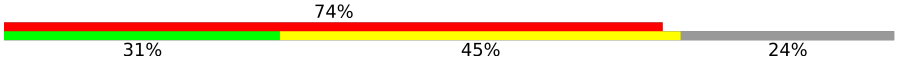
Chain 4:

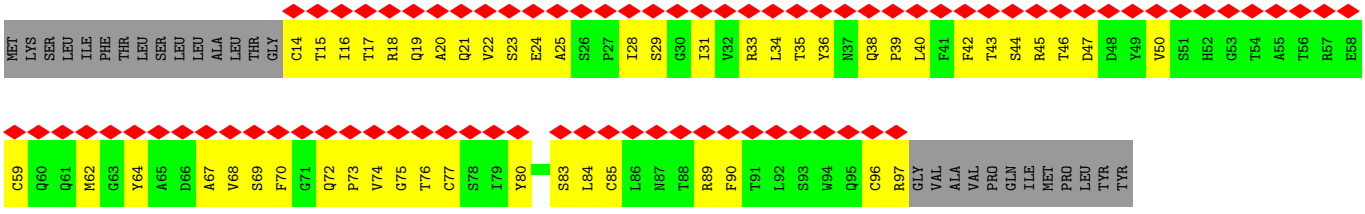



• Molecule 3: YecR

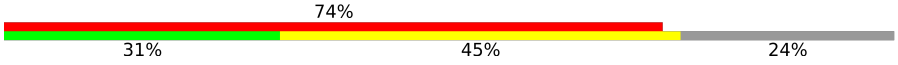
Chain 5:

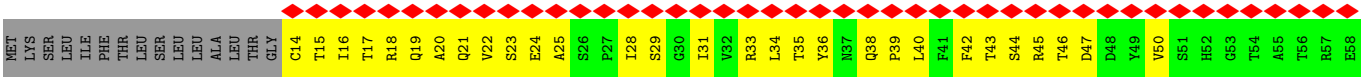


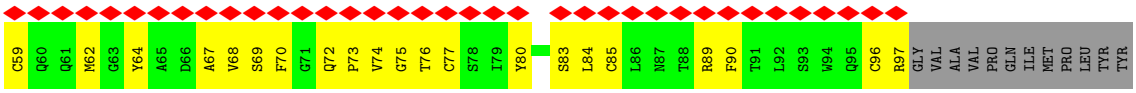




• Molecule 3: YecR

Chain 6:

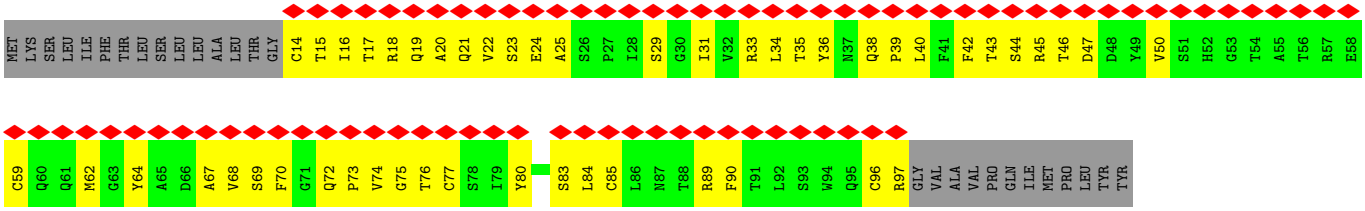




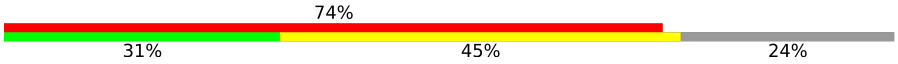

• Molecule 3: YecR

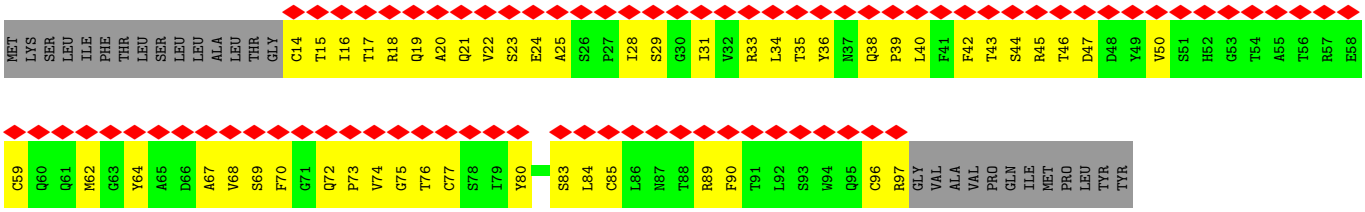
Chain 7:




• Molecule 3: YecR

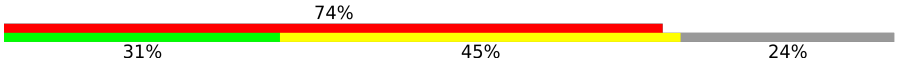
Chain 8:

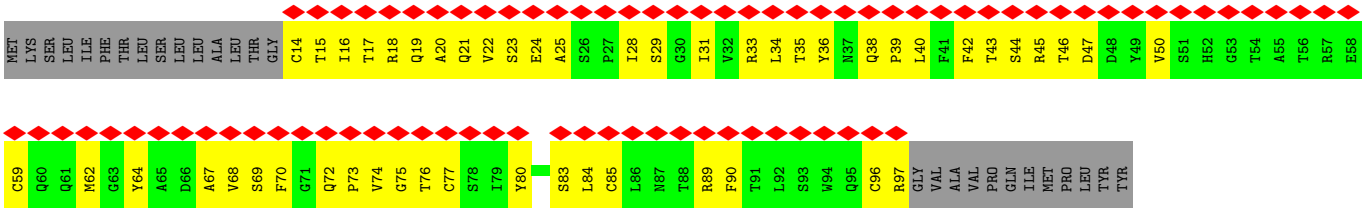



• Molecule 3: YecR

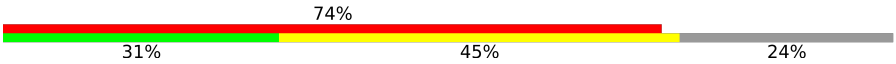
Chain 9:

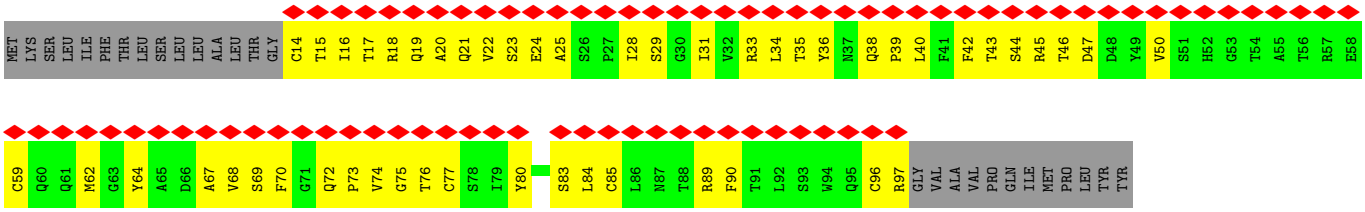



• Molecule 3: YecR

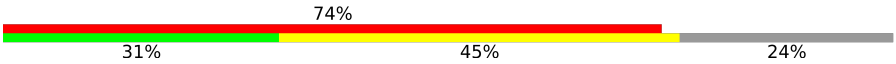
Chain 10:

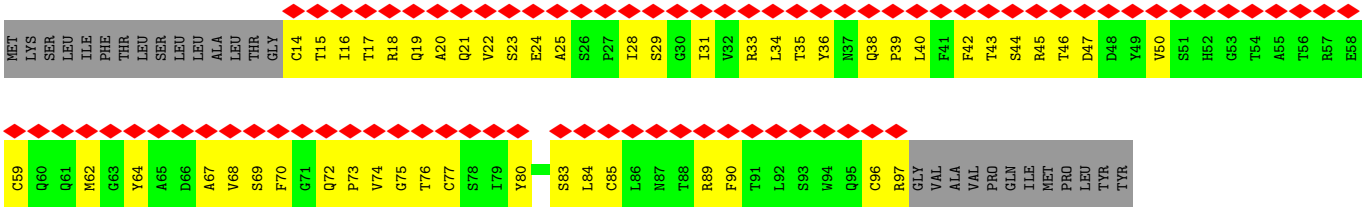



• Molecule 3: YecR

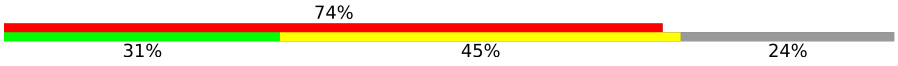
Chain 11:

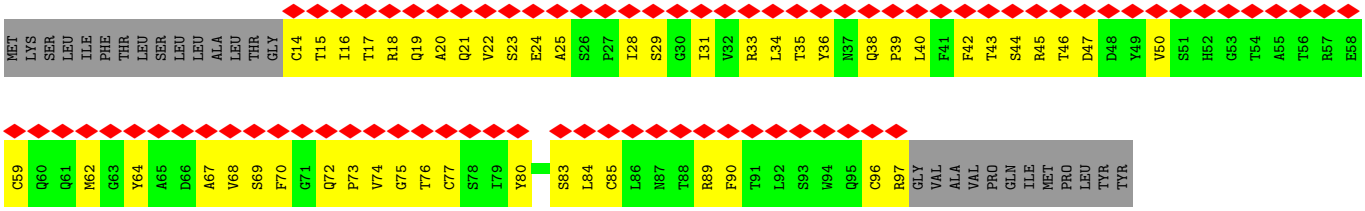





• Molecule 3: YecR

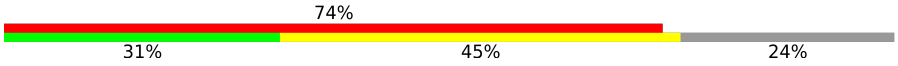
Chain 12:

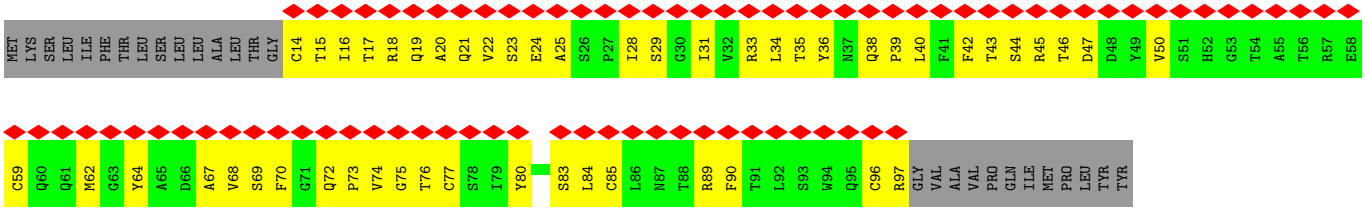



• Molecule 3: YecR

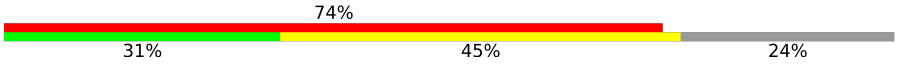
Chain 13:

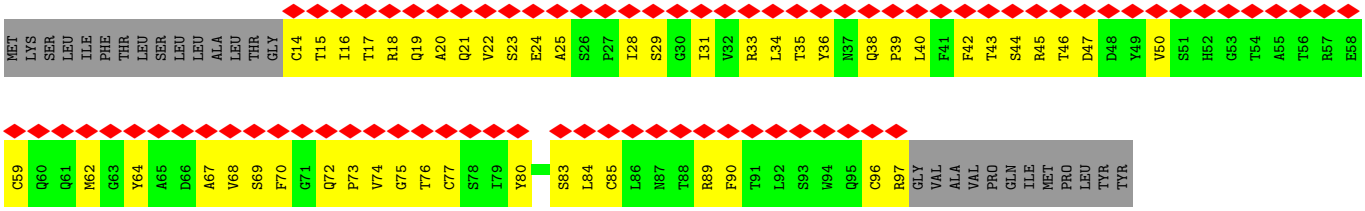



• Molecule 3: YecR

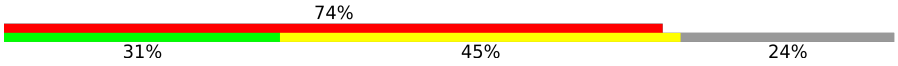
Chain 14:

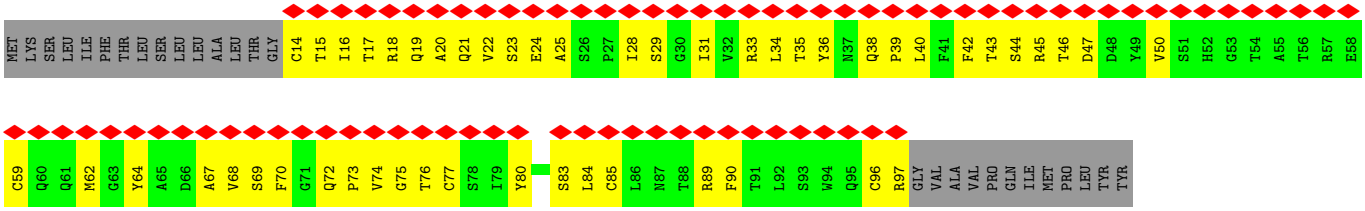



• Molecule 3: YecR

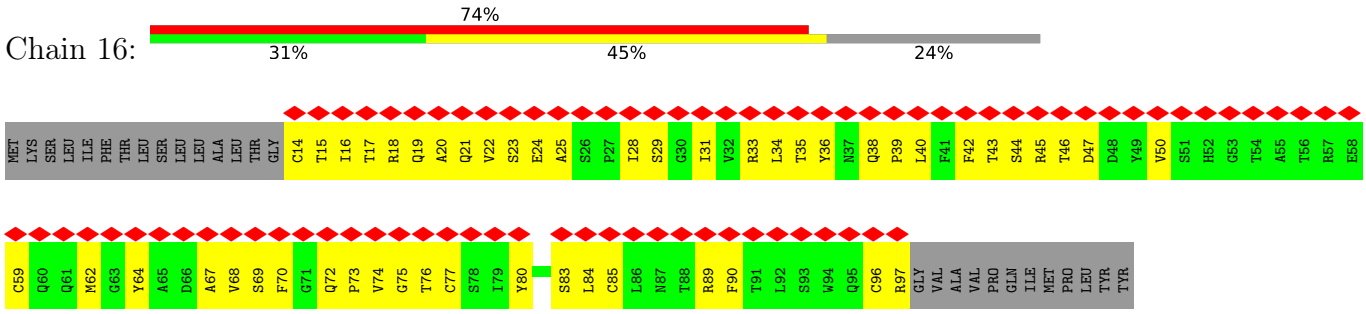
Chain 15:



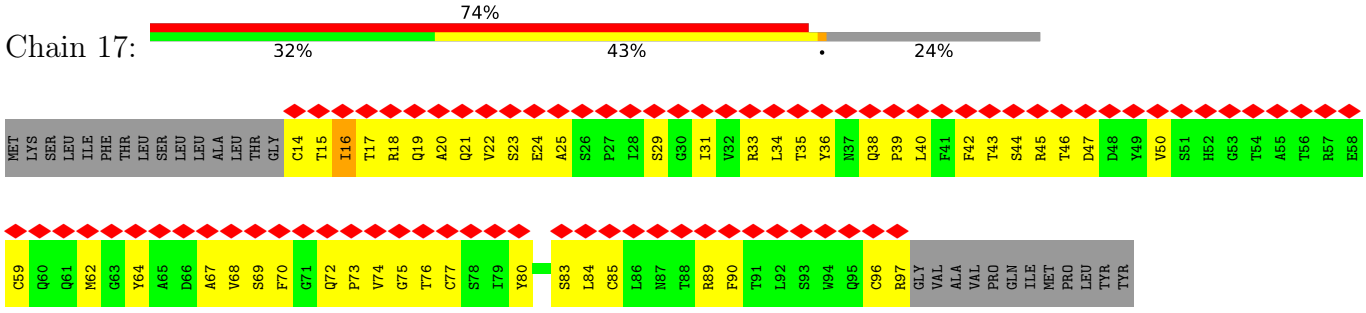
• Molecule 3: YecR

Chain 16:



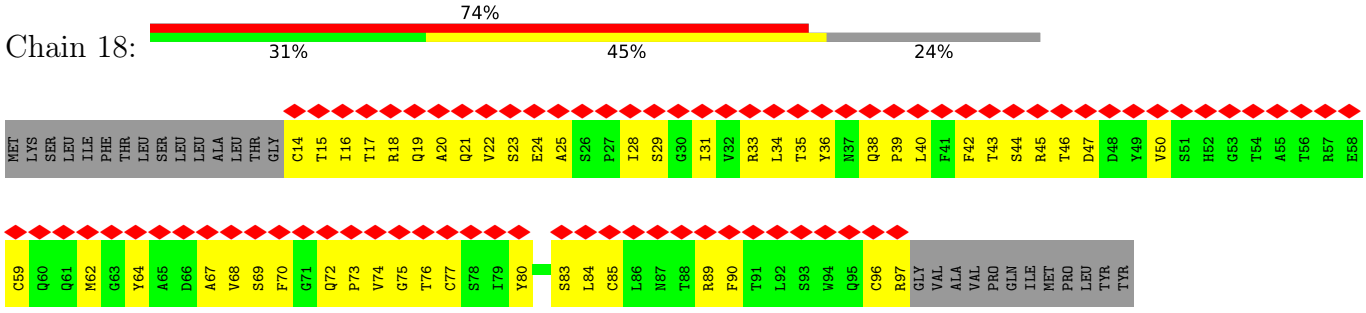

• Molecule 3: YecR

Chain 17:



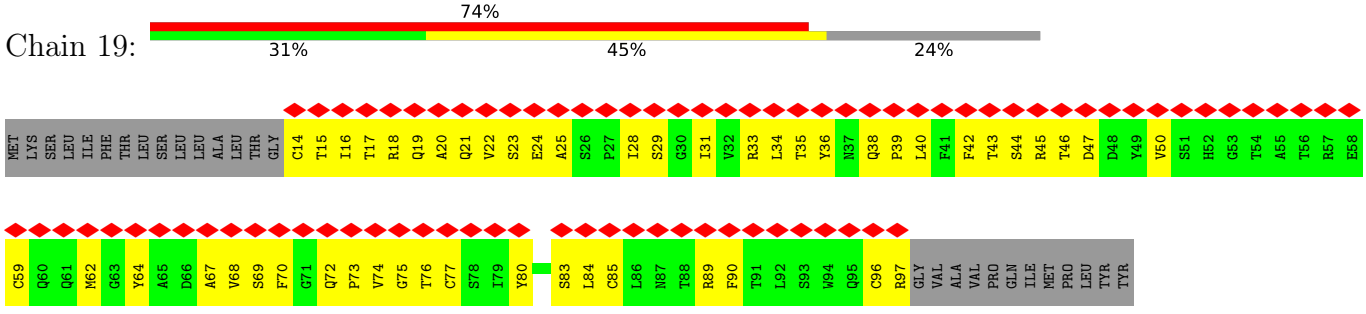

• Molecule 3: YecR

Chain 18:



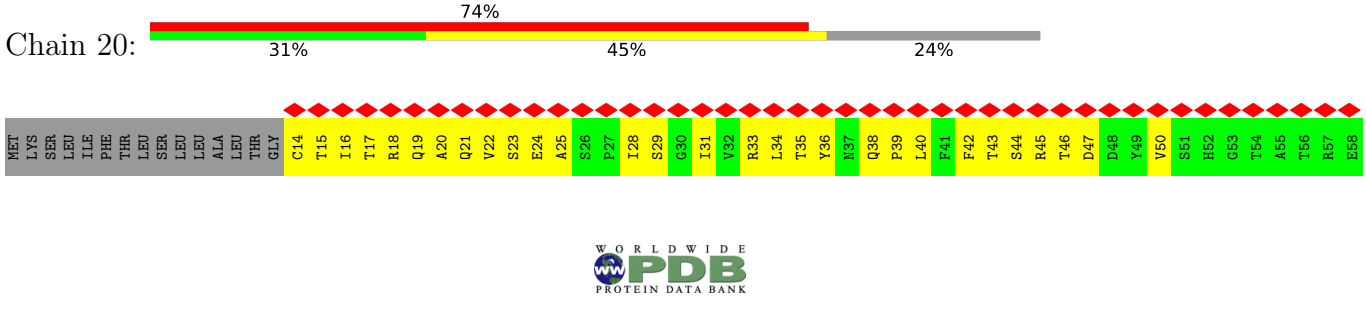

• Molecule 3: YecR

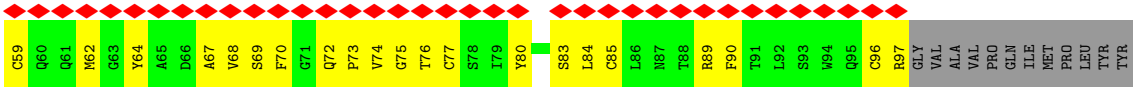
Chain 19:




• Molecule 3: YecR

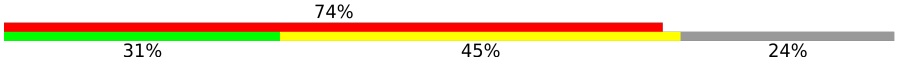
Chain 20:

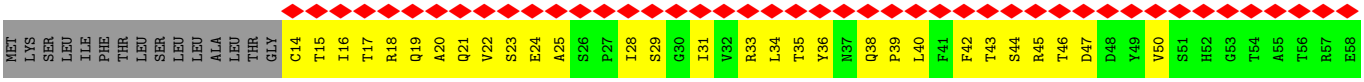


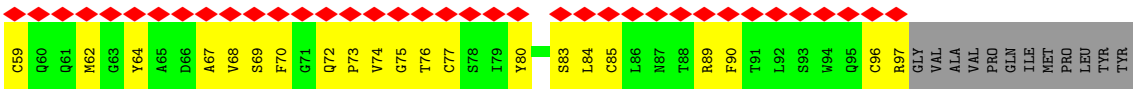



• Molecule 3: YecR

Chain 21:

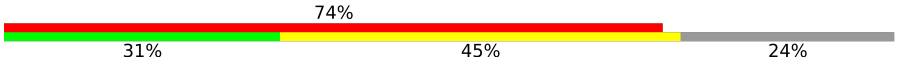


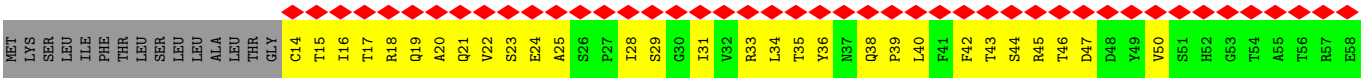



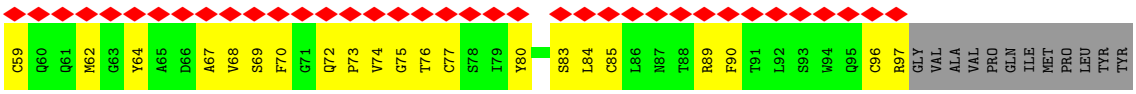




• Molecule 3: YecR

Chain 22:

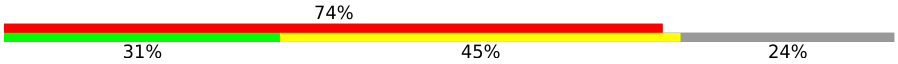


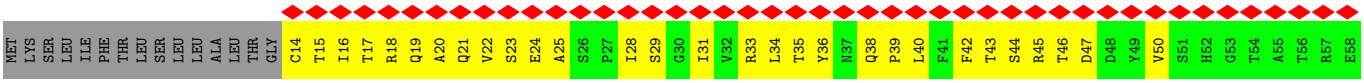



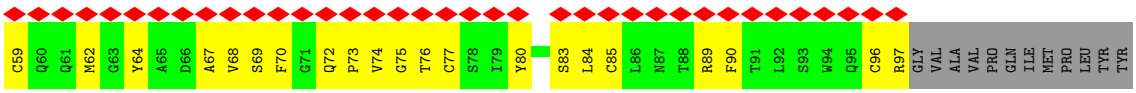




• Molecule 3: YecR

Chain 23:

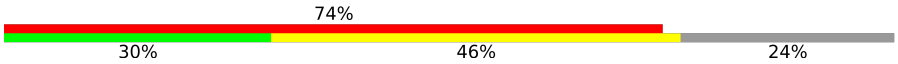


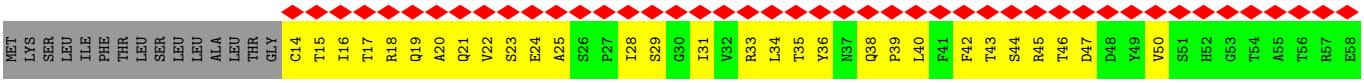



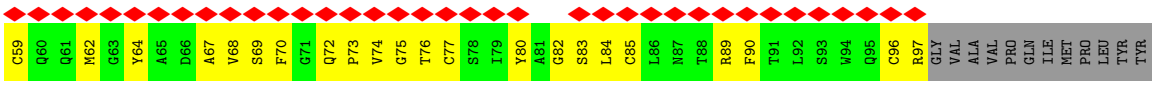




• Molecule 3: YecR

Chain 24:

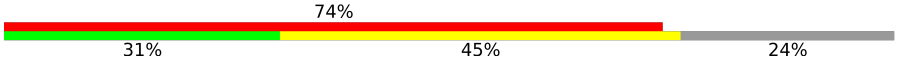


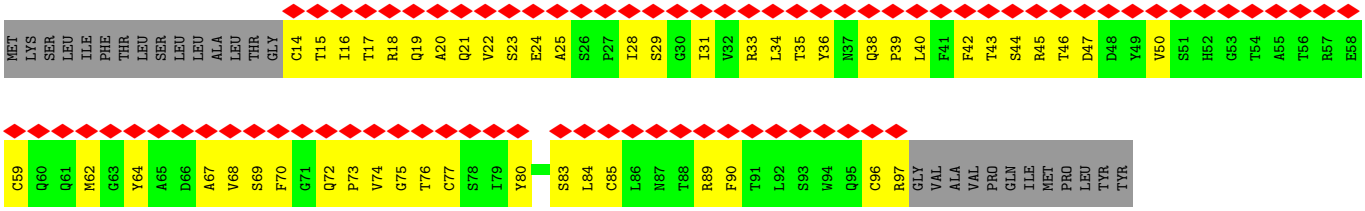



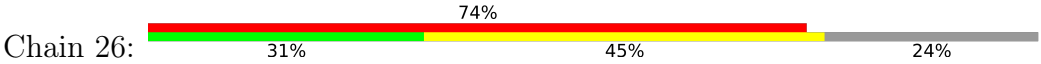

• Molecule 3: YecR

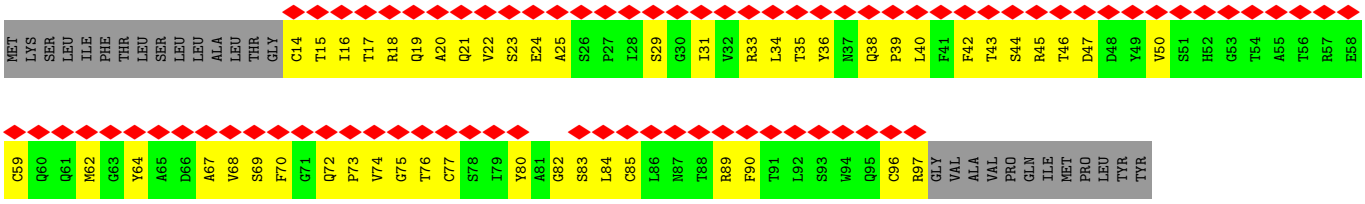
Chain 25:






• Molecule 3: YecR



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C26 | Depositor |
| Number of particles used | 31643 | 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 ($e^-/Å^2$) | 59 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.050 | Depositor |
| Minimum map value | -0.019 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.011 | Depositor |
| Map size (Å) | 359.424, 359.424, 359.424 | wwPDB |
| Map dimensions | 432, 432, 432 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.832, 0.832, 0.832 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TLW, TQN

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 | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | B | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | C | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | D | 0.11 | 0/1614 | 0.25 | 0/2194 |
| 1 | E | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | F | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | G | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | H | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | I | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | J | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | K | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | L | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | M | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | N | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | O | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | P | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | Q | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | R | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | S | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | T | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | U | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | V | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | W | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | X | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | Y | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 1 | Z | 0.11 | 0/1614 | 0.26 | 0/2194 |
| 2 | a | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | b | 0.10 | 0/2266 | 0.24 | 0/3071 |
| 2 | c | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | d | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | e | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | f | 0.10 | 0/2266 | 0.23 | 0/3071 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 2 | g | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | h | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | i | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | j | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | k | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | l | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | m | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | n | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | o | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | p | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | q | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | r | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | s | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | t | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | u | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | v | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | w | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | x | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 2 | y | 0.10 | 0/2266 | 0.24 | 0/3071 |
| 2 | z | 0.10 | 0/2266 | 0.23 | 0/3071 |
| 3 | 1 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 10 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 11 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 12 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 13 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 14 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 15 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 16 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 17 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 18 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 19 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 2 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 20 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 21 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 22 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 23 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 24 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 25 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 26 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 3 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 4 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 5 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 6 | 0.10 | 0/660 | 0.28 | 0/897 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 3 | 7 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 8 | 0.10 | 0/660 | 0.28 | 0/897 |
| 3 | 9 | 0.10 | 0/660 | 0.28 | 0/897 |
| All | All | 0.10 | 0/118040 | 0.25 | 0/160212 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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 | 1581 | 0 | 1534 | 109 | 0 |
| 1 | B | 1581 | 0 | 1534 | 108 | 0 |
| 1 | C | 1581 | 0 | 1534 | 109 | 0 |
| 1 | D | 1581 | 0 | 1534 | 105 | 0 |
| 1 | E | 1581 | 0 | 1534 | 107 | 0 |
| 1 | F | 1581 | 0 | 1534 | 108 | 0 |
| 1 | G | 1581 | 0 | 1534 | 108 | 0 |
| 1 | H | 1581 | 0 | 1534 | 108 | 0 |
| 1 | I | 1581 | 0 | 1534 | 106 | 0 |
| 1 | J | 1581 | 0 | 1534 | 106 | 0 |
| 1 | K | 1581 | 0 | 1534 | 106 | 0 |
| 1 | L | 1581 | 0 | 1534 | 104 | 0 |
| 1 | M | 1581 | 0 | 1534 | 108 | 0 |
| 1 | N | 1581 | 0 | 1534 | 104 | 0 |
| 1 | O | 1581 | 0 | 1534 | 107 | 0 |
| 1 | P | 1581 | 0 | 1534 | 109 | 0 |
| 1 | Q | 1581 | 0 | 1534 | 109 | 0 |
| 1 | R | 1581 | 0 | 1534 | 111 | 0 |
| 1 | S | 1581 | 0 | 1534 | 109 | 0 |
| 1 | T | 1581 | 0 | 1534 | 110 | 0 |
| 1 | U | 1581 | 0 | 1534 | 111 | 0 |
| 1 | V | 1581 | 0 | 1534 | 108 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | W | 1581 | 0 | 1534 | 107 | 0 |
| 1 | X | 1581 | 0 | 1534 | 105 | 0 |
| 1 | Y | 1581 | 0 | 1534 | 103 | 0 |
| 1 | Z | 1581 | 0 | 1534 | 102 | 0 |
| 2 | a | 2251 | 0 | 2289 | 182 | 0 |
| 2 | b | 2251 | 0 | 2289 | 180 | 0 |
| 2 | c | 2251 | 0 | 2289 | 178 | 0 |
| 2 | d | 2251 | 0 | 2289 | 182 | 0 |
| 2 | e | 2251 | 0 | 2289 | 178 | 0 |
| 2 | f | 2251 | 0 | 2289 | 186 | 0 |
| 2 | g | 2251 | 0 | 2289 | 179 | 0 |
| 2 | h | 2251 | 0 | 2289 | 178 | 0 |
| 2 | i | 2251 | 0 | 2289 | 181 | 0 |
| 2 | j | 2251 | 0 | 2289 | 180 | 0 |
| 2 | k | 2251 | 0 | 2289 | 183 | 0 |
| 2 | l | 2251 | 0 | 2289 | 183 | 0 |
| 2 | m | 2251 | 0 | 2289 | 186 | 0 |
| 2 | n | 2251 | 0 | 2289 | 184 | 0 |
| 2 | o | 2251 | 0 | 2289 | 181 | 0 |
| 2 | p | 2251 | 0 | 2289 | 183 | 0 |
| 2 | q | 2251 | 0 | 2289 | 183 | 0 |
| 2 | r | 2251 | 0 | 2289 | 186 | 0 |
| 2 | s | 2251 | 0 | 2289 | 182 | 0 |
| 2 | t | 2251 | 0 | 2289 | 177 | 0 |
| 2 | u | 2251 | 0 | 2289 | 178 | 0 |
| 2 | v | 2251 | 0 | 2289 | 183 | 0 |
| 2 | w | 2251 | 0 | 2289 | 186 | 0 |
| 2 | x | 2251 | 0 | 2289 | 184 | 0 |
| 2 | y | 2251 | 0 | 2289 | 181 | 0 |
| 2 | z | 2251 | 0 | 2289 | 185 | 0 |
| 3 | 1 | 647 | 0 | 616 | 49 | 0 |
| 3 | 10 | 647 | 0 | 616 | 49 | 0 |
| 3 | 11 | 647 | 0 | 616 | 49 | 0 |
| 3 | 12 | 647 | 0 | 616 | 49 | 0 |
| 3 | 13 | 647 | 0 | 616 | 49 | 0 |
| 3 | 14 | 647 | 0 | 616 | 50 | 0 |
| 3 | 15 | 647 | 0 | 616 | 50 | 0 |
| 3 | 16 | 647 | 0 | 616 | 50 | 0 |
| 3 | 17 | 647 | 0 | 616 | 50 | 0 |
| 3 | 18 | 647 | 0 | 616 | 50 | 0 |
| 3 | 19 | 647 | 0 | 616 | 51 | 0 |
| 3 | 2 | 647 | 0 | 616 | 49 | 0 |

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*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | 20 | 647 | 0 | 616 | 50 | 0 |
| 3 | 21 | 647 | 0 | 616 | 51 | 0 |
| 3 | 22 | 647 | 0 | 616 | 49 | 0 |
| 3 | 23 | 647 | 0 | 616 | 49 | 0 |
| 3 | 24 | 647 | 0 | 616 | 51 | 0 |
| 3 | 25 | 647 | 0 | 616 | 48 | 0 |
| 3 | 26 | 647 | 0 | 616 | 50 | 0 |
| 3 | 3 | 647 | 0 | 616 | 49 | 0 |
| 3 | 4 | 647 | 0 | 616 | 49 | 0 |
| 3 | 5 | 647 | 0 | 616 | 50 | 0 |
| 3 | 6 | 647 | 0 | 616 | 48 | 0 |
| 3 | 7 | 647 | 0 | 616 | 49 | 0 |
| 3 | 8 | 647 | 0 | 616 | 49 | 0 |
| 3 | 9 | 647 | 0 | 616 | 49 | 0 |
| 4 | A | 30 | 20 | 0 | 0 | 0 |
| 4 | B | 15 | 10 | 0 | 0 | 0 |
| 4 | C | 15 | 10 | 0 | 0 | 0 |
| 4 | D | 15 | 10 | 0 | 0 | 0 |
| 4 | E | 15 | 10 | 0 | 0 | 0 |
| 4 | F | 15 | 10 | 0 | 0 | 0 |
| 4 | G | 15 | 10 | 0 | 0 | 0 |
| 4 | H | 15 | 10 | 0 | 0 | 0 |
| 4 | I | 15 | 10 | 0 | 0 | 0 |
| 4 | J | 15 | 10 | 0 | 0 | 0 |
| 4 | K | 15 | 10 | 0 | 0 | 0 |
| 4 | L | 15 | 10 | 0 | 0 | 0 |
| 4 | M | 15 | 10 | 0 | 0 | 0 |
| 4 | N | 15 | 10 | 0 | 0 | 0 |
| 4 | O | 15 | 10 | 0 | 0 | 0 |
| 4 | P | 15 | 10 | 0 | 0 | 0 |
| 4 | Q | 15 | 10 | 0 | 0 | 0 |
| 4 | R | 15 | 10 | 0 | 0 | 0 |
| 4 | S | 15 | 10 | 0 | 0 | 0 |
| 4 | T | 15 | 10 | 0 | 0 | 0 |
| 4 | U | 15 | 10 | 0 | 0 | 0 |
| 4 | V | 15 | 10 | 0 | 0 | 0 |
| 4 | W | 15 | 10 | 0 | 0 | 0 |
| 4 | X | 15 | 10 | 0 | 0 | 0 |
| 4 | Y | 15 | 10 | 0 | 0 | 0 |
| 5 | A | 140 | 203 | 0 | 2 | 0 |
| 5 | B | 140 | 203 | 0 | 2 | 0 |
| 5 | C | 140 | 203 | 0 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 5 | D | 140 | 203 | 0 | 2 | 0 |
| 5 | E | 140 | 203 | 0 | 2 | 0 |
| 5 | F | 140 | 203 | 0 | 2 | 0 |
| 5 | G | 140 | 203 | 0 | 2 | 0 |
| 5 | H | 140 | 203 | 0 | 2 | 0 |
| 5 | I | 140 | 203 | 0 | 2 | 0 |
| 5 | J | 140 | 203 | 0 | 2 | 0 |
| 5 | K | 140 | 203 | 0 | 2 | 0 |
| 5 | L | 140 | 203 | 0 | 2 | 0 |
| 5 | M | 140 | 203 | 0 | 2 | 0 |
| 5 | N | 140 | 203 | 0 | 2 | 0 |
| 5 | O | 140 | 203 | 0 | 2 | 0 |
| 5 | P | 140 | 203 | 0 | 2 | 0 |
| 5 | Q | 140 | 203 | 0 | 2 | 0 |
| 5 | R | 140 | 203 | 0 | 2 | 0 |
| 5 | S | 140 | 203 | 0 | 2 | 0 |
| 5 | T | 140 | 203 | 0 | 2 | 0 |
| 5 | U | 140 | 203 | 0 | 2 | 0 |
| 5 | V | 140 | 203 | 0 | 2 | 0 |
| 5 | W | 140 | 203 | 0 | 2 | 0 |
| 5 | X | 140 | 203 | 0 | 2 | 0 |
| 5 | Y | 140 | 203 | 0 | 2 | 0 |
| 5 | Z | 140 | 203 | 0 | 2 | 0 |
| All | All | 120484 | 5538 | 115414 | 7070 | 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 30.

All (7070) 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) |
|---|---|---|---|
| 2:b:271:ASP:HB3 | 2:b:357:CYS:HA | 1.45 | 0.99 |
| 2:c:271:ASP:HB3 | 2:c:357:CYS:HA | 1.45 | 0.99 |
| 2:a:271:ASP:HB3 | 2:a:357:CYS:HA | 1.45 | 0.98 |
| 2:e:271:ASP:HB3 | 2:e:357:CYS:HA | 1.45 | 0.98 |
| 2:f:271:ASP:HB3 | 2:f:357:CYS:HA | 1.45 | 0.98 |
| 2:x:271:ASP:HB3 | 2:x:357:CYS:HA | 1.45 | 0.98 |
| 2:z:271:ASP:HB3 | 2:z:357:CYS:HA | 1.45 | 0.98 |
| 2:y:271:ASP:HB3 | 2:y:357:CYS:HA | 1.45 | 0.98 |
| 2:g:271:ASP:HB3 | 2:g:357:CYS:HA | 1.45 | 0.98 |
| 2:d:271:ASP:HB3 | 2:d:357:CYS:HA | 1.45 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:w:271:ASP:HB3 | 2:w:357:CYS:HA | 1.45 | 0.98 |
| 2:h:271:ASP:HB3 | 2:h:357:CYS:HA | 1.45 | 0.97 |
| 2:i:271:ASP:HB3 | 2:i:357:CYS:HA | 1.45 | 0.97 |
| 2:j:271:ASP:HB3 | 2:j:357:CYS:HA | 1.45 | 0.97 |
| 2:u:271:ASP:HB3 | 2:u:357:CYS:HA | 1.45 | 0.97 |
| 2:v:271:ASP:HB3 | 2:v:357:CYS:HA | 1.45 | 0.96 |
| 1:M:171:ILE:HD12 | 1:O:88:ALA:HB1 | 1.48 | 0.96 |
| 1:N:171:ILE:HD12 | 1:P:88:ALA:HB1 | 1.48 | 0.96 |
| 2:t:271:ASP:HB3 | 2:t:357:CYS:HA | 1.45 | 0.96 |
| 1:L:171:ILE:HD12 | 1:N:88:ALA:HB1 | 1.48 | 0.96 |
| 1:O:171:ILE:HD12 | 1:Q:88:ALA:HB1 | 1.48 | 0.95 |
| 2:k:271:ASP:HB3 | 2:k:357:CYS:HA | 1.45 | 0.95 |
| 2:o:271:ASP:HB3 | 2:o:357:CYS:HA | 1.45 | 0.95 |
| 2:m:271:ASP:HB3 | 2:m:357:CYS:HA | 1.45 | 0.95 |
| 2:l:271:ASP:HB3 | 2:l:357:CYS:HA | 1.45 | 0.95 |
| 2:q:271:ASP:HB3 | 2:q:357:CYS:HA | 1.45 | 0.95 |
| 2:r:271:ASP:HB3 | 2:r:357:CYS:HA | 1.45 | 0.95 |
| 2:s:271:ASP:HB3 | 2:s:357:CYS:HA | 1.45 | 0.95 |
| 1:I:171:ILE:HD12 | 1:K:88:ALA:HB1 | 1.48 | 0.95 |
| 2:n:271:ASP:HB3 | 2:n:357:CYS:HA | 1.45 | 0.95 |
| 2:p:271:ASP:HB3 | 2:p:357:CYS:HA | 1.45 | 0.95 |
| 1:J:171:ILE:HD12 | 1:L:88:ALA:HB1 | 1.49 | 0.95 |
| 1:K:171:ILE:HD12 | 1:M:88:ALA:HB1 | 1.49 | 0.95 |
| 1:B:88:ALA:HB1 | 1:Z:171:ILE:HD12 | 1.46 | 0.94 |
| 1:P:171:ILE:HD12 | 1:R:88:ALA:HB1 | 1.49 | 0.94 |
| 1:X:171:ILE:HD12 | 1:Z:88:ALA:HB1 | 1.48 | 0.94 |
| 1:H:171:ILE:HD12 | 1:J:88:ALA:HB1 | 1.48 | 0.94 |
| 1:Q:171:ILE:HD12 | 1:S:88:ALA:HB1 | 1.49 | 0.94 |
| 1:R:171:ILE:HD12 | 1:T:88:ALA:HB1 | 1.48 | 0.94 |
| 1:A:171:ILE:HD12 | 1:C:88:ALA:HB1 | 1.48 | 0.93 |
| 1:S:171:ILE:HD12 | 1:U:88:ALA:HB1 | 1.47 | 0.93 |
| 1:B:171:ILE:HD12 | 1:D:88:ALA:HB1 | 1.48 | 0.93 |
| 1:G:171:ILE:HD12 | 1:I:88:ALA:HB1 | 1.47 | 0.93 |
| 1:T:171:ILE:HD12 | 1:V:88:ALA:HB1 | 1.48 | 0.92 |
| 1:U:171:ILE:HD12 | 1:W:88:ALA:HB1 | 1.48 | 0.92 |
| 1:V:171:ILE:HD12 | 1:X:88:ALA:HB1 | 1.49 | 0.92 |
| 1:C:171:ILE:HD12 | 1:E:88:ALA:HB1 | 1.48 | 0.92 |
| 1:W:171:ILE:HD12 | 1:Y:88:ALA:HB1 | 1.48 | 0.92 |
| 1:D:171:ILE:HD12 | 1:F:88:ALA:HB1 | 1.49 | 0.92 |
| 1:F:171:ILE:HD12 | 1:H:88:ALA:HB1 | 1.47 | 0.92 |
| 1:E:171:ILE:HD12 | 1:G:88:ALA:HB1 | 1.48 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:y:46:ASP:HA | 2:z:161:ASN:HD22 | 1.34 | 0.91 |
| 2:i:270:LEU:HD11 | 2:i:352:MET:HE1 | 1.53 | 0.91 |
| 2:h:270:LEU:HD11 | 2:h:352:MET:HE1 | 1.53 | 0.91 |
| 2:j:270:LEU:HD11 | 2:j:352:MET:HE1 | 1.53 | 0.91 |
| 2:k:270:LEU:HD11 | 2:k:352:MET:HE1 | 1.53 | 0.90 |
| 2:g:270:LEU:HD11 | 2:g:352:MET:HE1 | 1.53 | 0.90 |
| 2:l:270:LEU:HD11 | 2:l:352:MET:HE1 | 1.53 | 0.90 |
| 2:f:270:LEU:HD11 | 2:f:352:MET:HE1 | 1.53 | 0.90 |
| 2:s:270:LEU:HD11 | 2:s:352:MET:HE1 | 1.53 | 0.89 |
| 2:m:270:LEU:HD11 | 2:m:352:MET:HE1 | 1.53 | 0.89 |
| 2:r:270:LEU:HD11 | 2:r:352:MET:HE1 | 1.53 | 0.89 |
| 2:t:270:LEU:HD11 | 2:t:352:MET:HE1 | 1.53 | 0.89 |
| 2:q:270:LEU:HD11 | 2:q:352:MET:HE1 | 1.53 | 0.89 |
| 1:A:88:ALA:HB1 | 1:Y:171:ILE:HD12 | 1.52 | 0.89 |
| 2:u:270:LEU:HD11 | 2:u:352:MET:HE1 | 1.53 | 0.89 |
| 2:e:270:LEU:HD11 | 2:e:352:MET:HE1 | 1.53 | 0.89 |
| 2:v:270:LEU:HD11 | 2:v:352:MET:HE1 | 1.53 | 0.88 |
| 3:6:22:VAL:HG22 | 3:6:34:LEU:HD22 | 1.56 | 0.88 |
| 3:23:22:VAL:HG22 | 3:23:34:LEU:HD22 | 1.56 | 0.88 |
| 2:n:270:LEU:HD11 | 2:n:352:MET:HE1 | 1.53 | 0.88 |
| 2:p:270:LEU:HD11 | 2:p:352:MET:HE1 | 1.54 | 0.88 |
| 3:7:22:VAL:HG22 | 3:7:34:LEU:HD22 | 1.56 | 0.88 |
| 3:24:22:VAL:HG22 | 3:24:34:LEU:HD22 | 1.56 | 0.88 |
| 2:w:270:LEU:HD11 | 2:w:352:MET:HE1 | 1.53 | 0.88 |
| 2:x:270:LEU:HD11 | 2:x:352:MET:HE1 | 1.53 | 0.88 |
| 3:10:22:VAL:HG22 | 3:10:34:LEU:HD22 | 1.56 | 0.88 |
| 3:11:22:VAL:HG22 | 3:11:34:LEU:HD22 | 1.56 | 0.88 |
| 3:20:22:VAL:HG22 | 3:20:34:LEU:HD22 | 1.56 | 0.88 |
| 3:2:22:VAL:HG22 | 3:2:34:LEU:HD22 | 1.56 | 0.88 |
| 3:5:22:VAL:HG22 | 3:5:34:LEU:HD22 | 1.56 | 0.88 |
| 3:19:22:VAL:HG22 | 3:19:34:LEU:HD22 | 1.56 | 0.88 |
| 3:9:22:VAL:HG22 | 3:9:34:LEU:HD22 | 1.56 | 0.88 |
| 3:1:22:VAL:HG22 | 3:1:34:LEU:HD22 | 1.56 | 0.88 |
| 2:y:270:LEU:HD11 | 2:y:352:MET:HE1 | 1.53 | 0.88 |
| 3:3:22:VAL:HG22 | 3:3:34:LEU:HD22 | 1.56 | 0.88 |
| 3:21:22:VAL:HG22 | 3:21:34:LEU:HD22 | 1.56 | 0.88 |
| 3:22:22:VAL:HG22 | 3:22:34:LEU:HD22 | 1.56 | 0.88 |
| 3:25:22:VAL:HG22 | 3:25:34:LEU:HD22 | 1.56 | 0.88 |
| 2:d:270:LEU:HD11 | 2:d:352:MET:HE1 | 1.53 | 0.88 |
| 2:o:270:LEU:HD11 | 2:o:352:MET:HE1 | 1.53 | 0.88 |
| 3:8:22:VAL:HG22 | 3:8:34:LEU:HD22 | 1.56 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:12:22:VAL:HG22 | 3:12:34:LEU:HD22 | 1.56 | 0.88 |
| 3:14:22:VAL:HG22 | 3:14:34:LEU:HD22 | 1.56 | 0.88 |
| 3:15:22:VAL:HG22 | 3:15:34:LEU:HD22 | 1.56 | 0.88 |
| 3:18:22:VAL:HG22 | 3:18:34:LEU:HD22 | 1.56 | 0.88 |
| 3:4:22:VAL:HG22 | 3:4:34:LEU:HD22 | 1.56 | 0.87 |
| 3:16:22:VAL:HG22 | 3:16:34:LEU:HD22 | 1.56 | 0.87 |
| 2:z:270:LEU:HD11 | 2:z:352:MET:HE1 | 1.53 | 0.87 |
| 3:13:22:VAL:HG22 | 3:13:34:LEU:HD22 | 1.56 | 0.87 |
| 3:26:22:VAL:HG22 | 3:26:34:LEU:HD22 | 1.56 | 0.87 |
| 2:a:270:LEU:HD11 | 2:a:352:MET:HE1 | 1.53 | 0.87 |
| 3:17:22:VAL:HG22 | 3:17:34:LEU:HD22 | 1.56 | 0.87 |
| 2:b:270:LEU:HD11 | 2:b:352:MET:HE1 | 1.53 | 0.87 |
| 2:c:270:LEU:HD11 | 2:c:352:MET:HE1 | 1.53 | 0.87 |
| 2:a:359:ARG:HB3 | 2:z:20:GLU:OE1 | 1.75 | 0.86 |
| 2:y:336:ASN:ND2 | 2:z:318:SER:O | 2.08 | 0.86 |
| 2:r:46:ASP:HA | 2:s:161:ASN:HD22 | 1.40 | 0.86 |
| 2:c:123:MET:HE1 | 2:c:136:LEU:HD22 | 1.58 | 0.86 |
| 2:d:123:MET:HE1 | 2:d:136:LEU:HD22 | 1.58 | 0.86 |
| 2:e:123:MET:HE1 | 2:e:136:LEU:HD22 | 1.58 | 0.86 |
| 2:f:123:MET:HE1 | 2:f:136:LEU:HD22 | 1.58 | 0.85 |
| 2:w:123:MET:HE1 | 2:w:136:LEU:HD22 | 1.58 | 0.85 |
| 2:b:123:MET:HE1 | 2:b:136:LEU:HD22 | 1.58 | 0.85 |
| 2:x:123:MET:HE1 | 2:x:136:LEU:HD22 | 1.58 | 0.85 |
| 2:a:20:GLU:OE1 | 2:b:359:ARG:HB3 | 1.77 | 0.85 |
| 2:j:123:MET:HE1 | 2:j:136:LEU:HD22 | 1.58 | 0.85 |
| 2:v:123:MET:HE1 | 2:v:136:LEU:HD22 | 1.58 | 0.85 |
| 2:d:46:ASP:HA | 2:e:161:ASN:HD22 | 1.42 | 0.85 |
| 2:k:123:MET:HE1 | 2:k:136:LEU:HD22 | 1.58 | 0.85 |
| 2:q:46:ASP:HA | 2:r:161:ASN:HD22 | 1.42 | 0.84 |
| 2:l:123:MET:HE1 | 2:l:136:LEU:HD22 | 1.58 | 0.84 |
| 2:a:123:MET:HE1 | 2:a:136:LEU:HD22 | 1.58 | 0.84 |
| 2:l:46:ASP:HA | 2:m:161:ASN:HD22 | 1.42 | 0.84 |
| 2:t:46:ASP:HA | 2:u:161:ASN:HD22 | 1.43 | 0.84 |
| 2:y:123:MET:HE1 | 2:y:136:LEU:HD22 | 1.58 | 0.84 |
| 2:f:46:ASP:HA | 2:g:161:ASN:HD22 | 1.42 | 0.84 |
| 2:g:123:MET:HE1 | 2:g:136:LEU:HD22 | 1.58 | 0.84 |
| 2:i:123:MET:HE1 | 2:i:136:LEU:HD22 | 1.58 | 0.84 |
| 2:w:46:ASP:HA | 2:x:161:ASN:HD22 | 1.42 | 0.84 |
| 2:u:123:MET:HE1 | 2:u:136:LEU:HD22 | 1.58 | 0.84 |
| 2:n:46:ASP:HA | 2:o:161:ASN:HD22 | 1.43 | 0.84 |
| 2:s:20:GLU:OE1 | 2:t:359:ARG:HB3 | 1.78 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:u:46:ASP:HA | 2:v:161:ASN:HD22 | 1.43 | 0.84 |
| 2:a:46:ASP:HA | 2:b:161:ASN:HD22 | 1.43 | 0.84 |
| 2:h:46:ASP:HA | 2:i:161:ASN:HD22 | 1.43 | 0.84 |
| 2:q:123:MET:HE1 | 2:q:136:LEU:HD22 | 1.58 | 0.84 |
| 2:c:46:ASP:HA | 2:d:161:ASN:HD22 | 1.43 | 0.83 |
| 2:g:20:GLU:OE1 | 2:h:359:ARG:HB3 | 1.78 | 0.83 |
| 2:o:46:ASP:HA | 2:p:161:ASN:HD22 | 1.43 | 0.83 |
| 2:p:123:MET:HE1 | 2:p:136:LEU:HD22 | 1.58 | 0.83 |
| 2:i:46:ASP:HA | 2:j:161:ASN:HD22 | 1.43 | 0.83 |
| 2:a:161:ASN:HD22 | 2:z:46:ASP:HA | 1.44 | 0.83 |
| 2:c:20:GLU:OE1 | 2:d:359:ARG:HB3 | 1.79 | 0.83 |
| 2:j:46:ASP:HA | 2:k:161:ASN:HD22 | 1.42 | 0.83 |
| 2:r:123:MET:HE1 | 2:r:136:LEU:HD22 | 1.58 | 0.83 |
| 2:v:46:ASP:HA | 2:w:161:ASN:HD22 | 1.42 | 0.83 |
| 2:g:46:ASP:HA | 2:h:161:ASN:HD22 | 1.43 | 0.83 |
| 2:h:123:MET:HE1 | 2:h:136:LEU:HD22 | 1.58 | 0.83 |
| 2:m:123:MET:HE1 | 2:m:136:LEU:HD22 | 1.58 | 0.83 |
| 2:s:141:ILE:HD13 | 2:s:165:ILE:HD11 | 1.61 | 0.83 |
| 2:z:123:MET:HE1 | 2:z:136:LEU:HD22 | 1.58 | 0.83 |
| 2:i:141:ILE:HD13 | 2:i:165:ILE:HD11 | 1.61 | 0.83 |
| 2:j:141:ILE:HD13 | 2:j:165:ILE:HD11 | 1.61 | 0.83 |
| 2:k:141:ILE:HD13 | 2:k:165:ILE:HD11 | 1.61 | 0.83 |
| 2:m:46:ASP:HA | 2:n:161:ASN:HD22 | 1.43 | 0.83 |
| 2:t:141:ILE:HD13 | 2:t:165:ILE:HD11 | 1.61 | 0.83 |
| 2:h:141:ILE:HD13 | 2:h:165:ILE:HD11 | 1.61 | 0.83 |
| 2:k:46:ASP:HA | 2:l:161:ASN:HD22 | 1.42 | 0.83 |
| 2:g:141:ILE:HD13 | 2:g:165:ILE:HD11 | 1.61 | 0.83 |
| 2:q:141:ILE:HD13 | 2:q:165:ILE:HD11 | 1.61 | 0.83 |
| 2:r:141:ILE:HD13 | 2:r:165:ILE:HD11 | 1.61 | 0.83 |
| 2:u:141:ILE:HD13 | 2:u:165:ILE:HD11 | 1.61 | 0.83 |
| 2:v:141:ILE:HD13 | 2:v:165:ILE:HD11 | 1.61 | 0.83 |
| 2:l:141:ILE:HD13 | 2:l:165:ILE:HD11 | 1.61 | 0.83 |
| 2:p:46:ASP:HA | 2:q:161:ASN:HD22 | 1.42 | 0.83 |
| 2:f:20:GLU:OE1 | 2:g:359:ARG:HB3 | 1.78 | 0.82 |
| 2:o:123:MET:HE1 | 2:o:136:LEU:HD22 | 1.58 | 0.82 |
| 2:w:141:ILE:HD13 | 2:w:165:ILE:HD11 | 1.61 | 0.82 |
| 2:e:141:ILE:HD13 | 2:e:165:ILE:HD11 | 1.61 | 0.82 |
| 2:l:32:ARG:NH1 | 2:l:33:GLU:O | 2.13 | 0.82 |
| 2:m:141:ILE:HD13 | 2:m:165:ILE:HD11 | 1.61 | 0.82 |
| 2:p:141:ILE:HD13 | 2:p:165:ILE:HD11 | 1.61 | 0.82 |
| 2:r:32:ARG:NH1 | 2:r:33:GLU:O | 2.13 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:s:32:ARG:NH1 | 2:s:33:GLU:O | 2.13 | 0.82 |
| 2:s:123:MET:HE1 | 2:s:136:LEU:HD22 | 1.58 | 0.82 |
| 2:b:46:ASP:HA | 2:c:161:ASN:HD22 | 1.43 | 0.82 |
| 2:b:141:ILE:HD13 | 2:b:165:ILE:HD11 | 1.61 | 0.82 |
| 2:c:141:ILE:HD13 | 2:c:165:ILE:HD11 | 1.61 | 0.82 |
| 2:d:141:ILE:HD13 | 2:d:165:ILE:HD11 | 1.61 | 0.82 |
| 2:f:141:ILE:HD13 | 2:f:165:ILE:HD11 | 1.61 | 0.82 |
| 2:m:20:GLU:OE1 | 2:n:359:ARG:HB3 | 1.78 | 0.82 |
| 2:t:123:MET:HE1 | 2:t:136:LEU:HD22 | 1.58 | 0.82 |
| 2:x:141:ILE:HD13 | 2:x:165:ILE:HD11 | 1.61 | 0.82 |
| 2:f:32:ARG:NH1 | 2:f:33:GLU:O | 2.13 | 0.82 |
| 2:m:32:ARG:NH1 | 2:m:33:GLU:O | 2.13 | 0.82 |
| 2:n:141:ILE:HD13 | 2:n:165:ILE:HD11 | 1.61 | 0.82 |
| 2:o:141:ILE:HD13 | 2:o:165:ILE:HD11 | 1.61 | 0.82 |
| 2:r:20:GLU:OE1 | 2:s:359:ARG:HB3 | 1.79 | 0.82 |
| 2:s:46:ASP:HA | 2:t:161:ASN:HD22 | 1.43 | 0.82 |
| 2:x:32:ARG:NH1 | 2:x:33:GLU:O | 2.13 | 0.82 |
| 2:y:32:ARG:NH1 | 2:y:33:GLU:O | 2.13 | 0.82 |
| 2:c:32:ARG:NH1 | 2:c:33:GLU:O | 2.13 | 0.82 |
| 2:g:32:ARG:NH1 | 2:g:33:GLU:O | 2.13 | 0.82 |
| 2:o:20:GLU:OE1 | 2:p:359:ARG:HB3 | 1.79 | 0.82 |
| 2:y:141:ILE:HD13 | 2:y:165:ILE:HD11 | 1.61 | 0.82 |
| 2:z:141:ILE:HD13 | 2:z:165:ILE:HD11 | 1.61 | 0.82 |
| 2:a:141:ILE:HD13 | 2:a:165:ILE:HD11 | 1.61 | 0.82 |
| 2:b:32:ARG:NH1 | 2:b:33:GLU:O | 2.13 | 0.82 |
| 2:k:32:ARG:NH1 | 2:k:33:GLU:O | 2.13 | 0.82 |
| 2:q:32:ARG:NH1 | 2:q:33:GLU:O | 2.13 | 0.82 |
| 2:z:32:ARG:NH1 | 2:z:33:GLU:O | 2.13 | 0.82 |
| 3:9:17:THR:OG1 | 3:9:43:THR:O | 1.98 | 0.82 |
| 3:21:17:THR:OG1 | 3:21:43:THR:O | 1.98 | 0.82 |
| 2:n:123:MET:HE1 | 2:n:136:LEU:HD22 | 1.58 | 0.82 |
| 2:s:226:PRO:HG2 | 2:s:231:SER:HB3 | 1.62 | 0.82 |
| 2:t:32:ARG:NH1 | 2:t:33:GLU:O | 2.13 | 0.82 |
| 3:20:17:THR:OG1 | 3:20:43:THR:O | 1.98 | 0.82 |
| 2:i:20:GLU:OE1 | 2:j:359:ARG:HB3 | 1.79 | 0.82 |
| 2:l:20:GLU:OE1 | 2:m:359:ARG:HB3 | 1.79 | 0.82 |
| 2:n:32:ARG:NH1 | 2:n:33:GLU:O | 2.13 | 0.82 |
| 2:t:226:PRO:HG2 | 2:t:231:SER:HB3 | 1.62 | 0.82 |
| 2:j:32:ARG:NH1 | 2:j:33:GLU:O | 2.13 | 0.82 |
| 2:o:226:PRO:HG2 | 2:o:231:SER:HB3 | 1.62 | 0.82 |
| 2:p:226:PRO:HG2 | 2:p:231:SER:HB3 | 1.62 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:u:20:GLU:OE1 | 2:v:359:ARG:HB3 | 1.79 | 0.82 |
| 2:w:32:ARG:NH1 | 2:w:33:GLU:O | 2.13 | 0.82 |
| 3:8:17:THR:OG1 | 3:8:43:THR:O | 1.98 | 0.82 |
| 3:10:17:THR:OG1 | 3:10:43:THR:O | 1.98 | 0.82 |
| 3:25:17:THR:OG1 | 3:25:43:THR:O | 1.98 | 0.82 |
| 2:p:336:ASN:ND2 | 2:q:318:SER:O | 2.13 | 0.81 |
| 2:r:226:PRO:HG2 | 2:r:231:SER:HB3 | 1.62 | 0.81 |
| 3:15:17:THR:OG1 | 3:15:43:THR:O | 1.98 | 0.81 |
| 3:26:17:THR:OG1 | 3:26:43:THR:O | 1.98 | 0.81 |
| 2:a:32:ARG:NH1 | 2:a:33:GLU:O | 2.13 | 0.81 |
| 2:d:336:ASN:ND2 | 2:e:318:SER:O | 2.13 | 0.81 |
| 2:e:46:ASP:HA | 2:f:161:ASN:HD22 | 1.42 | 0.81 |
| 2:i:32:ARG:NH1 | 2:i:33:GLU:O | 2.13 | 0.81 |
| 2:q:226:PRO:HG2 | 2:q:231:SER:HB3 | 1.62 | 0.81 |
| 2:w:226:PRO:HG2 | 2:w:231:SER:HB3 | 1.62 | 0.81 |
| 2:x:226:PRO:HG2 | 2:x:231:SER:HB3 | 1.62 | 0.81 |
| 3:4:17:THR:OG1 | 3:4:43:THR:O | 1.98 | 0.81 |
| 3:14:17:THR:OG1 | 3:14:43:THR:O | 1.98 | 0.81 |
| 2:e:32:ARG:NH1 | 2:e:33:GLU:O | 2.13 | 0.81 |
| 2:n:226:PRO:HG2 | 2:n:231:SER:HB3 | 1.62 | 0.81 |
| 2:p:32:ARG:NH1 | 2:p:33:GLU:O | 2.13 | 0.81 |
| 2:u:32:ARG:NH1 | 2:u:33:GLU:O | 2.13 | 0.81 |
| 2:u:226:PRO:HG2 | 2:u:231:SER:HB3 | 1.62 | 0.81 |
| 3:5:17:THR:OG1 | 3:5:43:THR:O | 1.98 | 0.81 |
| 3:19:17:THR:OG1 | 3:19:43:THR:O | 1.98 | 0.81 |
| 3:22:17:THR:OG1 | 3:22:43:THR:O | 1.98 | 0.81 |
| 2:d:20:GLU:OE1 | 2:e:359:ARG:HB3 | 1.81 | 0.81 |
| 2:d:32:ARG:NH1 | 2:d:33:GLU:O | 2.13 | 0.81 |
| 2:o:32:ARG:NH1 | 2:o:33:GLU:O | 2.13 | 0.81 |
| 2:v:226:PRO:HG2 | 2:v:231:SER:HB3 | 1.62 | 0.81 |
| 3:13:17:THR:OG1 | 3:13:43:THR:O | 1.98 | 0.81 |
| 3:16:17:THR:OG1 | 3:16:43:THR:O | 1.98 | 0.81 |
| 2:l:336:ASN:ND2 | 2:m:318:SER:O | 2.14 | 0.81 |
| 2:v:32:ARG:NH1 | 2:v:33:GLU:O | 2.13 | 0.81 |
| 2:y:226:PRO:HG2 | 2:y:231:SER:HB3 | 1.62 | 0.81 |
| 3:3:17:THR:OG1 | 3:3:43:THR:O | 1.98 | 0.81 |
| 3:24:17:THR:OG1 | 3:24:43:THR:O | 1.98 | 0.81 |
| 1:W:172:ASN:OD1 | 1:Y:138:ALA:HB1 | 1.81 | 0.81 |
| 2:l:226:PRO:HG2 | 2:l:231:SER:HB3 | 1.62 | 0.81 |
| 3:11:17:THR:OG1 | 3:11:43:THR:O | 1.98 | 0.81 |
| 3:1:17:THR:OG1 | 3:1:43:THR:O | 1.98 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:b:20:GLU:OE1 | 2:c:359:ARG:HB3 | 1.81 | 0.81 |
| 2:h:20:GLU:OE1 | 2:i:359:ARG:HB3 | 1.81 | 0.81 |
| 2:k:226:PRO:HG2 | 2:k:231:SER:HB3 | 1.62 | 0.81 |
| 2:m:226:PRO:HG2 | 2:m:231:SER:HB3 | 1.62 | 0.81 |
| 3:7:17:THR:OG1 | 3:7:43:THR:O | 1.98 | 0.81 |
| 2:a:175:LEU:HD11 | 1:Y:51:ILE:HG13 | 1.62 | 0.81 |
| 2:h:32:ARG:NH1 | 2:h:33:GLU:O | 2.13 | 0.81 |
| 2:v:20:GLU:OE1 | 2:w:359:ARG:HB3 | 1.81 | 0.81 |
| 2:a:226:PRO:HG2 | 2:a:231:SER:HB3 | 1.62 | 0.80 |
| 3:6:17:THR:OG1 | 3:6:43:THR:O | 1.98 | 0.80 |
| 2:f:336:ASN:ND2 | 2:g:318:SER:O | 2.13 | 0.80 |
| 2:j:226:PRO:HG2 | 2:j:231:SER:HB3 | 1.62 | 0.80 |
| 2:t:20:GLU:OE1 | 2:u:359:ARG:HB3 | 1.81 | 0.80 |
| 2:z:226:PRO:HG2 | 2:z:231:SER:HB3 | 1.62 | 0.80 |
| 3:17:17:THR:OG1 | 3:17:43:THR:O | 1.98 | 0.80 |
| 1:Y:167:LYS:HD3 | 1:Z:203:ALA:HB3 | 1.62 | 0.80 |
| 2:b:226:PRO:HG2 | 2:b:231:SER:HB3 | 1.62 | 0.80 |
| 3:12:17:THR:OG1 | 3:12:43:THR:O | 1.98 | 0.80 |
| 3:18:17:THR:OG1 | 3:18:43:THR:O | 1.98 | 0.80 |
| 2:r:336:ASN:ND2 | 2:s:318:SER:O | 2.12 | 0.80 |
| 2:y:20:GLU:OE1 | 2:z:359:ARG:HB3 | 1.82 | 0.80 |
| 3:23:17:THR:OG1 | 3:23:43:THR:O | 1.98 | 0.80 |
| 1:B:138:ALA:HB1 | 1:Z:172:ASN:OD1 | 1.82 | 0.80 |
| 2:a:267:GLU:OE1 | 2:z:21:ARG:NH1 | 2.13 | 0.80 |
| 2:c:226:PRO:HG2 | 2:c:231:SER:HB3 | 1.62 | 0.80 |
| 2:j:336:ASN:ND2 | 2:k:318:SER:O | 2.13 | 0.80 |
| 2:a:336:ASN:ND2 | 2:b:318:SER:O | 2.15 | 0.80 |
| 2:g:226:PRO:HG2 | 2:g:231:SER:HB3 | 1.62 | 0.80 |
| 2:h:336:ASN:ND2 | 2:i:318:SER:O | 2.15 | 0.80 |
| 2:p:20:GLU:OE1 | 2:q:359:ARG:HB3 | 1.81 | 0.80 |
| 2:w:20:GLU:OE1 | 2:x:359:ARG:HB3 | 1.82 | 0.80 |
| 2:f:226:PRO:HG2 | 2:f:231:SER:HB3 | 1.62 | 0.80 |
| 2:h:226:PRO:HG2 | 2:h:231:SER:HB3 | 1.62 | 0.80 |
| 2:i:226:PRO:HG2 | 2:i:231:SER:HB3 | 1.62 | 0.80 |
| 2:x:46:ASP:HA | 2:y:161:ASN:HD22 | 1.47 | 0.80 |
| 2:i:336:ASN:ND2 | 2:j:318:SER:O | 2.15 | 0.80 |
| 2:m:336:ASN:ND2 | 2:n:318:SER:O | 2.15 | 0.80 |
| 2:t:336:ASN:ND2 | 2:u:318:SER:O | 2.15 | 0.80 |
| 2:e:20:GLU:OE1 | 2:f:359:ARG:HB3 | 1.82 | 0.79 |
| 2:d:226:PRO:HG2 | 2:d:231:SER:HB3 | 1.62 | 0.79 |
| 2:e:226:PRO:HG2 | 2:e:231:SER:HB3 | 1.62 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:20:GLU:OE1 | 2:o:359:ARG:HB3 | 1.81 | 0.79 |
| 2:j:20:GLU:OE1 | 2:k:359:ARG:HB3 | 1.81 | 0.79 |
| 2:k:20:GLU:OE1 | 2:l:359:ARG:HB3 | 1.82 | 0.79 |
| 2:k:325:SER:HB3 | 2:k:330:SER:HB3 | 1.65 | 0.79 |
| 2:w:336:ASN:ND2 | 2:x:318:SER:O | 2.16 | 0.79 |
| 3:2:17:THR:OG1 | 3:2:43:THR:O | 1.98 | 0.79 |
| 2:c:336:ASN:ND2 | 2:d:318:SER:O | 2.15 | 0.79 |
| 2:z:175:LEU:HD11 | 1:X:51:ILE:HG13 | 1.63 | 0.79 |
| 1:M:82:LEU:HA | 1:M:197:SER:HB3 | 1.64 | 0.79 |
| 1:O:82:LEU:HA | 1:O:197:SER:HB3 | 1.64 | 0.79 |
| 2:h:325:SER:HB3 | 2:h:330:SER:HB3 | 1.65 | 0.79 |
| 3:16:68:VAL:HG21 | 3:16:97:ARG:HH21 | 1.48 | 0.79 |
| 1:N:82:LEU:HA | 1:N:197:SER:HB3 | 1.65 | 0.79 |
| 1:Q:82:LEU:HA | 1:Q:197:SER:HB3 | 1.64 | 0.79 |
| 2:i:325:SER:HB3 | 2:i:330:SER:HB3 | 1.65 | 0.79 |
| 2:j:325:SER:HB3 | 2:j:330:SER:HB3 | 1.65 | 0.79 |
| 2:k:336:ASN:ND2 | 2:l:318:SER:O | 2.16 | 0.79 |
| 2:m:21:ARG:NH1 | 2:n:267:GLU:OE1 | 2.16 | 0.79 |
| 2:n:325:SER:HB3 | 2:n:330:SER:HB3 | 1.65 | 0.79 |
| 1:L:82:LEU:HA | 1:L:197:SER:HB3 | 1.65 | 0.79 |
| 1:P:82:LEU:HA | 1:P:197:SER:HB3 | 1.65 | 0.79 |
| 2:f:325:SER:HB3 | 2:f:330:SER:HB3 | 1.65 | 0.79 |
| 2:l:21:ARG:NH1 | 2:m:267:GLU:OE1 | 2.16 | 0.79 |
| 2:m:325:SER:HB3 | 2:m:330:SER:HB3 | 1.65 | 0.79 |
| 1:J:82:LEU:HA | 1:J:197:SER:HB3 | 1.64 | 0.79 |
| 1:K:82:LEU:HA | 1:K:197:SER:HB3 | 1.65 | 0.79 |
| 2:b:336:ASN:ND2 | 2:c:318:SER:O | 2.15 | 0.79 |
| 2:e:325:SER:HB3 | 2:e:330:SER:HB3 | 1.65 | 0.79 |
| 2:q:20:GLU:OE1 | 2:r:359:ARG:HB3 | 1.82 | 0.79 |
| 1:R:82:LEU:HA | 1:R:197:SER:HB3 | 1.65 | 0.79 |
| 1:S:82:LEU:HA | 1:S:197:SER:HB3 | 1.65 | 0.79 |
| 1:T:82:LEU:HA | 1:T:197:SER:HB3 | 1.64 | 0.79 |
| 1:U:82:LEU:HA | 1:U:197:SER:HB3 | 1.64 | 0.79 |
| 2:l:325:SER:HB3 | 2:l:330:SER:HB3 | 1.65 | 0.79 |
| 3:14:68:VAL:HG21 | 3:14:97:ARG:HH21 | 1.48 | 0.79 |
| 5:G:301:TQN:C15 | 1:H:112:TYR:HB2 | 2.13 | 0.79 |
| 5:W:301:TQN:C15 | 1:X:112:TYR:HB2 | 2.13 | 0.79 |
| 5:Y:301:TQN:C15 | 1:Z:112:TYR:HB2 | 2.13 | 0.79 |
| 1:A:112:TYR:HB2 | 5:Z:301:TQN:C15 | 2.13 | 0.79 |
| 5:A:302:TQN:C15 | 1:B:112:TYR:HB2 | 2.13 | 0.79 |
| 2:e:336:ASN:ND2 | 2:f:318:SER:O | 2.16 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:u:21:ARG:NH1 | 2:v:267:GLU:OE1 | 2.16 | 0.79 |
| 2:u:336:ASN:ND2 | 2:v:318:SER:O | 2.15 | 0.79 |
| 5:V:301:TQN:C15 | 1:W:112:TYR:HB2 | 2.13 | 0.79 |
| 5:X:301:TQN:C15 | 1:Y:112:TYR:HB2 | 2.13 | 0.79 |
| 2:g:325:SER:HB3 | 2:g:330:SER:HB3 | 1.65 | 0.78 |
| 2:g:336:ASN:ND2 | 2:h:318:SER:O | 2.15 | 0.78 |
| 2:p:325:SER:HB3 | 2:p:330:SER:HB3 | 1.65 | 0.78 |
| 2:q:325:SER:HB3 | 2:q:330:SER:HB3 | 1.65 | 0.78 |
| 3:18:68:VAL:HG21 | 3:18:97:ARG:HH21 | 1.48 | 0.78 |
| 3:21:68:VAL:HG21 | 3:21:97:ARG:HH21 | 1.48 | 0.78 |
| 5:B:301:TQN:C15 | 1:C:112:TYR:HB2 | 2.13 | 0.78 |
| 1:I:82:LEU:HA | 1:I:197:SER:HB3 | 1.64 | 0.78 |
| 1:V:82:LEU:HA | 1:V:197:SER:HB3 | 1.65 | 0.78 |
| 2:c:325:SER:HB3 | 2:c:330:SER:HB3 | 1.65 | 0.78 |
| 2:q:336:ASN:ND2 | 2:r:318:SER:O | 2.16 | 0.78 |
| 2:r:21:ARG:NH1 | 2:s:267:GLU:OE1 | 2.15 | 0.78 |
| 2:s:21:ARG:NH1 | 2:t:267:GLU:OE1 | 2.16 | 0.78 |
| 2:b:325:SER:HB3 | 2:b:330:SER:HB3 | 1.65 | 0.78 |
| 2:f:21:ARG:NH1 | 2:g:267:GLU:OE1 | 2.14 | 0.78 |
| 2:l:175:LEU:HD11 | 1:J:51:ILE:HG13 | 1.65 | 0.78 |
| 2:o:325:SER:HB3 | 2:o:330:SER:HB3 | 1.65 | 0.78 |
| 5:C:301:TQN:C15 | 1:D:112:TYR:HB2 | 2.13 | 0.78 |
| 5:D:301:TQN:C15 | 1:E:112:TYR:HB2 | 2.13 | 0.78 |
| 5:U:301:TQN:C15 | 1:V:112:TYR:HB2 | 2.13 | 0.78 |
| 2:d:325:SER:HB3 | 2:d:330:SER:HB3 | 1.65 | 0.78 |
| 2:n:336:ASN:ND2 | 2:o:318:SER:O | 2.15 | 0.78 |
| 2:o:21:ARG:NH1 | 2:p:267:GLU:OE1 | 2.16 | 0.78 |
| 2:p:21:ARG:NH1 | 2:q:267:GLU:OE1 | 2.17 | 0.78 |
| 2:r:175:LEU:HD11 | 1:P:51:ILE:HG13 | 1.65 | 0.78 |
| 3:14:47:ASP:OD1 | 3:14:50:VAL:N | 2.13 | 0.78 |
| 3:19:68:VAL:HG21 | 3:19:97:ARG:HH21 | 1.48 | 0.78 |
| 1:H:82:LEU:HA | 1:H:197:SER:HB3 | 1.64 | 0.78 |
| 1:W:82:LEU:HA | 1:W:197:SER:HB3 | 1.65 | 0.78 |
| 2:a:21:ARG:NH1 | 2:b:267:GLU:OE1 | 2.15 | 0.78 |
| 3:1:68:VAL:HG21 | 3:1:97:ARG:HH21 | 1.48 | 0.78 |
| 2:c:21:ARG:NH1 | 2:d:267:GLU:OE1 | 2.16 | 0.78 |
| 3:11:68:VAL:HG21 | 3:11:97:ARG:HH21 | 1.48 | 0.78 |
| 5:E:301:TQN:C15 | 1:F:112:TYR:HB2 | 2.13 | 0.78 |
| 5:J:301:TQN:C15 | 1:K:112:TYR:HB2 | 2.13 | 0.78 |
| 5:T:301:TQN:C15 | 1:U:112:TYR:HB2 | 2.13 | 0.78 |
| 3:5:68:VAL:HG21 | 3:5:97:ARG:HH21 | 1.48 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:13:47:ASP:OD1 | 3:13:50:VAL:N | 2.13 | 0.78 |
| 1:X:82:LEU:HA | 1:X:197:SER:HB3 | 1.65 | 0.78 |
| 2:f:175:LEU:HD11 | 1:D:51:ILE:HG13 | 1.65 | 0.78 |
| 2:i:21:ARG:NH1 | 2:j:267:GLU:OE1 | 2.16 | 0.78 |
| 2:k:175:LEU:HD11 | 1:I:51:ILE:HG13 | 1.66 | 0.78 |
| 3:13:68:VAL:HG21 | 3:13:97:ARG:HH21 | 1.48 | 0.78 |
| 3:23:68:VAL:HG21 | 3:23:97:ARG:HH21 | 1.48 | 0.78 |
| 5:S:301:TQN:C15 | 1:T:112:TYR:HB2 | 2.13 | 0.78 |
| 2:r:325:SER:HB3 | 2:r:330:SER:HB3 | 1.65 | 0.78 |
| 2:x:20:GLU:OE1 | 2:y:359:ARG:HB3 | 1.83 | 0.78 |
| 3:9:68:VAL:HG21 | 3:9:97:ARG:HH21 | 1.48 | 0.78 |
| 1:G:82:LEU:HA | 1:G:197:SER:HB3 | 1.64 | 0.78 |
| 5:I:301:TQN:C15 | 1:J:112:TYR:HB2 | 2.13 | 0.78 |
| 5:R:301:TQN:C15 | 1:S:112:TYR:HB2 | 2.13 | 0.78 |
| 1:T:172:ASN:OD1 | 1:V:138:ALA:HB1 | 1.84 | 0.78 |
| 2:a:325:SER:HB3 | 2:a:330:SER:HB3 | 1.65 | 0.78 |
| 2:t:325:SER:HB3 | 2:t:330:SER:HB3 | 1.65 | 0.78 |
| 5:F:301:TQN:C15 | 1:G:112:TYR:HB2 | 2.13 | 0.78 |
| 1:A:172:ASN:OD1 | 1:C:138:ALA:HB1 | 1.83 | 0.78 |
| 2:s:325:SER:HB3 | 2:s:330:SER:HB3 | 1.65 | 0.78 |
| 2:x:175:LEU:HD11 | 1:V:51:ILE:HG13 | 1.65 | 0.78 |
| 3:12:68:VAL:HG21 | 3:12:97:ARG:HH21 | 1.48 | 0.78 |
| 5:L:301:TQN:C15 | 1:M:112:TYR:HB2 | 2.13 | 0.78 |
| 5:Q:301:TQN:C15 | 1:R:112:TYR:HB2 | 2.13 | 0.78 |
| 1:Y:82:LEU:HA | 1:Y:197:SER:HB3 | 1.65 | 0.78 |
| 2:g:21:ARG:NH1 | 2:h:267:GLU:OE1 | 2.16 | 0.77 |
| 5:H:301:TQN:C15 | 1:I:112:TYR:HB2 | 2.13 | 0.77 |
| 5:P:301:TQN:C15 | 1:Q:112:TYR:HB2 | 2.13 | 0.77 |
| 2:x:325:SER:HB3 | 2:x:330:SER:HB3 | 1.65 | 0.77 |
| 2:y:325:SER:HB3 | 2:y:330:SER:HB3 | 1.65 | 0.77 |
| 5:O:301:TQN:C15 | 1:P:112:TYR:HB2 | 2.13 | 0.77 |
| 1:Z:82:LEU:HA | 1:Z:197:SER:HB3 | 1.64 | 0.77 |
| 2:u:325:SER:HB3 | 2:u:330:SER:HB3 | 1.65 | 0.77 |
| 2:z:325:SER:HB3 | 2:z:330:SER:HB3 | 1.65 | 0.77 |
| 3:2:68:VAL:HG21 | 3:2:97:ARG:HH21 | 1.48 | 0.77 |
| 3:4:68:VAL:HG21 | 3:4:97:ARG:HH21 | 1.48 | 0.77 |
| 1:C:82:LEU:HA | 1:C:197:SER:HB3 | 1.64 | 0.77 |
| 5:K:301:TQN:C15 | 1:L:112:TYR:HB2 | 2.13 | 0.77 |
| 5:M:301:TQN:C15 | 1:N:112:TYR:HB2 | 2.13 | 0.77 |
| 5:N:301:TQN:C15 | 1:O:112:TYR:HB2 | 2.13 | 0.77 |
| 2:v:336:ASN:ND2 | 2:w:318:SER:O | 2.13 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:82:LEU:HA | 1:B:197:SER:HB3 | 1.65 | 0.77 |
| 1:F:82:LEU:HA | 1:F:197:SER:HB3 | 1.65 | 0.77 |
| 1:A:82:LEU:HA | 1:A:197:SER:HB3 | 1.64 | 0.77 |
| 2:d:21:ARG:NH1 | 2:e:267:GLU:OE1 | 2.17 | 0.77 |
| 3:23:47:ASP:OD1 | 3:23:50:VAL:N | 2.13 | 0.77 |
| 1:D:82:LEU:HA | 1:D:197:SER:HB3 | 1.65 | 0.77 |
| 2:g:175:LEU:HD11 | 1:E:51:ILE:HG13 | 1.66 | 0.77 |
| 2:p:26:THR:HG21 | 2:p:187:LEU:HB3 | 1.67 | 0.77 |
| 2:s:175:LEU:HD11 | 1:Q:51:ILE:HG13 | 1.67 | 0.77 |
| 2:t:21:ARG:NH1 | 2:u:267:GLU:OE1 | 2.18 | 0.77 |
| 2:v:325:SER:HB3 | 2:v:330:SER:HB3 | 1.65 | 0.77 |
| 3:15:47:ASP:OD1 | 3:15:50:VAL:N | 2.13 | 0.77 |
| 3:24:47:ASP:OD1 | 3:24:50:VAL:N | 2.13 | 0.77 |
| 1:S:172:ASN:OD1 | 1:U:138:ALA:HB1 | 1.84 | 0.77 |
| 2:o:26:THR:HG21 | 2:o:187:LEU:HB3 | 1.67 | 0.77 |
| 3:6:68:VAL:HG21 | 3:6:97:ARG:HH21 | 1.48 | 0.77 |
| 3:7:68:VAL:HG21 | 3:7:97:ARG:HH21 | 1.48 | 0.77 |
| 3:17:68:VAL:HG21 | 3:17:97:ARG:HH21 | 1.48 | 0.77 |
| 3:20:68:VAL:HG21 | 3:20:97:ARG:HH21 | 1.48 | 0.77 |
| 1:E:82:LEU:HA | 1:E:197:SER:HB3 | 1.65 | 0.77 |
| 1:U:172:ASN:OD1 | 1:W:138:ALA:HB1 | 1.85 | 0.77 |
| 3:22:47:ASP:OD1 | 3:22:50:VAL:N | 2.13 | 0.77 |
| 3:25:68:VAL:HG21 | 3:25:97:ARG:HH21 | 1.48 | 0.77 |
| 2:w:175:LEU:HD11 | 1:U:51:ILE:HG13 | 1.66 | 0.77 |
| 2:w:325:SER:HB3 | 2:w:330:SER:HB3 | 1.65 | 0.77 |
| 3:19:47:ASP:OD1 | 3:19:50:VAL:N | 2.13 | 0.77 |
| 2:k:26:THR:HG21 | 2:k:187:LEU:HB3 | 1.67 | 0.77 |
| 2:m:175:LEU:HD11 | 1:K:51:ILE:HG13 | 1.67 | 0.77 |
| 2:q:26:THR:HG21 | 2:q:187:LEU:HB3 | 1.67 | 0.77 |
| 2:q:175:LEU:HD11 | 1:O:51:ILE:HG13 | 1.66 | 0.77 |
| 2:a:318:SER:O | 2:z:336:ASN:ND2 | 2.15 | 0.76 |
| 2:i:175:LEU:HD11 | 1:G:51:ILE:HG13 | 1.68 | 0.76 |
| 2:j:193:ASP:HB3 | 2:j:196:MET:HB2 | 1.67 | 0.76 |
| 2:l:193:ASP:HB3 | 2:l:196:MET:HB2 | 1.67 | 0.76 |
| 3:8:47:ASP:OD1 | 3:8:50:VAL:N | 2.13 | 0.76 |
| 3:26:68:VAL:HG21 | 3:26:97:ARG:HH21 | 1.48 | 0.76 |
| 1:F:172:ASN:OD1 | 1:H:138:ALA:HB1 | 1.84 | 0.76 |
| 2:a:193:ASP:HB3 | 2:a:196:MET:HB2 | 1.67 | 0.76 |
| 2:j:175:LEU:HD11 | 1:H:51:ILE:HG13 | 1.68 | 0.76 |
| 2:k:193:ASP:HB3 | 2:k:196:MET:HB2 | 1.67 | 0.76 |
| 2:m:193:ASP:HB3 | 2:m:196:MET:HB2 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:z:193:ASP:HB3 | 2:z:196:MET:HB2 | 1.67 | 0.76 |
| 3:24:68:VAL:HG21 | 3:24:97:ARG:HH21 | 1.48 | 0.76 |
| 1:N:172:ASN:OD1 | 1:P:138:ALA:HB1 | 1.84 | 0.76 |
| 1:Q:172:ASN:OD1 | 1:S:138:ALA:HB1 | 1.85 | 0.76 |
| 1:V:172:ASN:OD1 | 1:X:138:ALA:HB1 | 1.86 | 0.76 |
| 2:b:193:ASP:HB3 | 2:b:196:MET:HB2 | 1.67 | 0.76 |
| 2:j:26:THR:HG21 | 2:j:187:LEU:HB3 | 1.67 | 0.76 |
| 2:y:193:ASP:HB3 | 2:y:196:MET:HB2 | 1.67 | 0.76 |
| 3:8:68:VAL:HG21 | 3:8:97:ARG:HH21 | 1.48 | 0.76 |
| 3:12:47:ASP:OD1 | 3:12:50:VAL:N | 2.13 | 0.76 |
| 2:f:121:LEU:HD11 | 2:f:124:THR:HG21 | 1.68 | 0.76 |
| 2:g:121:LEU:HD11 | 2:g:124:THR:HG21 | 1.68 | 0.76 |
| 2:i:193:ASP:HB3 | 2:i:196:MET:HB2 | 1.67 | 0.76 |
| 2:j:121:LEU:HD11 | 2:j:124:THR:HG21 | 1.68 | 0.76 |
| 2:l:26:THR:HG21 | 2:l:187:LEU:HB3 | 1.67 | 0.76 |
| 2:n:193:ASP:HB3 | 2:n:196:MET:HB2 | 1.67 | 0.76 |
| 2:o:336:ASN:ND2 | 2:p:318:SER:O | 2.15 | 0.76 |
| 2:r:121:LEU:HD11 | 2:r:124:THR:HG21 | 1.68 | 0.76 |
| 2:u:26:THR:HG21 | 2:u:187:LEU:HB3 | 1.67 | 0.76 |
| 2:w:193:ASP:HB3 | 2:w:196:MET:HB2 | 1.67 | 0.76 |
| 2:x:193:ASP:HB3 | 2:x:196:MET:HB2 | 1.67 | 0.76 |
| 3:15:68:VAL:HG21 | 3:15:97:ARG:HH21 | 1.48 | 0.76 |
| 1:O:172:ASN:OD1 | 1:Q:138:ALA:HB1 | 1.85 | 0.76 |
| 2:j:21:ARG:NH1 | 2:k:267:GLU:OE1 | 2.17 | 0.76 |
| 2:n:121:LEU:HD11 | 2:n:124:THR:HG21 | 1.68 | 0.76 |
| 2:o:121:LEU:HD11 | 2:o:124:THR:HG21 | 1.68 | 0.76 |
| 2:s:121:LEU:HD11 | 2:s:124:THR:HG21 | 1.68 | 0.76 |
| 2:t:26:THR:HG21 | 2:t:187:LEU:HB3 | 1.67 | 0.76 |
| 3:10:47:ASP:OD1 | 3:10:50:VAL:N | 2.13 | 0.76 |
| 2:c:193:ASP:HB3 | 2:c:196:MET:HB2 | 1.67 | 0.76 |
| 2:i:121:LEU:HD11 | 2:i:124:THR:HG21 | 1.68 | 0.76 |
| 2:k:121:LEU:HD11 | 2:k:124:THR:HG21 | 1.68 | 0.76 |
| 2:q:121:LEU:HD11 | 2:q:124:THR:HG21 | 1.68 | 0.76 |
| 2:y:21:ARG:NH1 | 2:z:267:GLU:OE1 | 2.17 | 0.76 |
| 3:11:47:ASP:OD1 | 3:11:50:VAL:N | 2.13 | 0.76 |
| 1:B:172:ASN:OD1 | 1:D:138:ALA:HB1 | 1.84 | 0.76 |
| 1:H:172:ASN:OD1 | 1:J:138:ALA:HB1 | 1.84 | 0.76 |
| 2:b:21:ARG:NH1 | 2:c:267:GLU:OE1 | 2.18 | 0.76 |
| 2:e:175:LEU:HD11 | 1:C:51:ILE:HG13 | 1.66 | 0.76 |
| 2:h:193:ASP:HB3 | 2:h:196:MET:HB2 | 1.67 | 0.76 |
| 2:n:21:ARG:NH1 | 2:o:267:GLU:OE1 | 2.18 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:26:THR:HG21 | 2:n:187:LEU:HB3 | 1.67 | 0.76 |
| 2:u:121:LEU:HD11 | 2:u:124:THR:HG21 | 1.68 | 0.76 |
| 2:u:193:ASP:HB3 | 2:u:196:MET:HB2 | 1.67 | 0.76 |
| 2:v:21:ARG:NH1 | 2:w:267:GLU:OE1 | 2.17 | 0.76 |
| 2:v:26:THR:HG21 | 2:v:187:LEU:HB3 | 1.67 | 0.76 |
| 2:v:193:ASP:HB3 | 2:v:196:MET:HB2 | 1.67 | 0.76 |
| 3:10:68:VAL:HG21 | 3:10:97:ARG:HH21 | 1.48 | 0.76 |
| 1:G:172:ASN:OD1 | 1:I:138:ALA:HB1 | 1.84 | 0.76 |
| 1:M:172:ASN:OD1 | 1:O:138:ALA:HB1 | 1.84 | 0.76 |
| 2:d:121:LEU:HD11 | 2:d:124:THR:HG21 | 1.68 | 0.76 |
| 2:h:21:ARG:NH1 | 2:i:267:GLU:OE1 | 2.18 | 0.76 |
| 2:h:121:LEU:HD11 | 2:h:124:THR:HG21 | 1.68 | 0.76 |
| 2:h:175:LEU:HD11 | 1:F:51:ILE:HG13 | 1.68 | 0.76 |
| 2:v:121:LEU:HD11 | 2:v:124:THR:HG21 | 1.68 | 0.76 |
| 1:E:172:ASN:OD1 | 1:G:138:ALA:HB1 | 1.84 | 0.76 |
| 2:c:121:LEU:HD11 | 2:c:124:THR:HG21 | 1.68 | 0.76 |
| 2:i:26:THR:HG21 | 2:i:187:LEU:HB3 | 1.67 | 0.76 |
| 2:m:121:LEU:HD11 | 2:m:124:THR:HG21 | 1.68 | 0.76 |
| 2:p:121:LEU:HD11 | 2:p:124:THR:HG21 | 1.68 | 0.76 |
| 3:3:68:VAL:HG21 | 3:3:97:ARG:HH21 | 1.48 | 0.76 |
| 1:C:172:ASN:OD1 | 1:E:138:ALA:HB1 | 1.85 | 0.76 |
| 1:L:172:ASN:OD1 | 1:N:138:ALA:HB1 | 1.84 | 0.76 |
| 2:a:121:LEU:HD11 | 2:a:124:THR:HG21 | 1.68 | 0.76 |
| 2:l:121:LEU:HD11 | 2:l:124:THR:HG21 | 1.68 | 0.76 |
| 2:o:193:ASP:HB3 | 2:o:196:MET:HB2 | 1.67 | 0.76 |
| 2:u:175:LEU:HD11 | 1:S:51:ILE:HG13 | 1.68 | 0.76 |
| 2:x:121:LEU:HD11 | 2:x:124:THR:HG21 | 1.68 | 0.76 |
| 3:18:47:ASP:OD1 | 3:18:50:VAL:N | 2.13 | 0.76 |
| 1:U:125:GLU:HB3 | 1:V:108:THR:HB | 1.68 | 0.76 |
| 2:b:26:THR:HG21 | 2:b:187:LEU:HB3 | 1.67 | 0.75 |
| 2:d:193:ASP:HB3 | 2:d:196:MET:HB2 | 1.67 | 0.75 |
| 2:e:121:LEU:HD11 | 2:e:124:THR:HG21 | 1.68 | 0.75 |
| 2:q:21:ARG:NH1 | 2:r:267:GLU:OE1 | 2.19 | 0.75 |
| 2:r:26:THR:HG21 | 2:r:187:LEU:HB3 | 1.67 | 0.75 |
| 2:s:193:ASP:HB3 | 2:s:196:MET:HB2 | 1.67 | 0.75 |
| 2:t:121:LEU:HD11 | 2:t:124:THR:HG21 | 1.68 | 0.75 |
| 2:t:175:LEU:HD11 | 1:R:51:ILE:HG13 | 1.68 | 0.75 |
| 2:t:193:ASP:HB3 | 2:t:196:MET:HB2 | 1.67 | 0.75 |
| 1:M:125:GLU:HB3 | 1:N:108:THR:HB | 1.68 | 0.75 |
| 1:P:172:ASN:OD1 | 1:R:138:ALA:HB1 | 1.85 | 0.75 |
| 1:Q:125:GLU:HB3 | 1:R:108:THR:HB | 1.69 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:179:ARG:HG3 | 1:T:206:GLU:HB3 | 1.69 | 0.75 |
| 1:Y:179:ARG:HG3 | 1:Y:206:GLU:HB3 | 1.69 | 0.75 |
| 2:s:26:THR:HG21 | 2:s:187:LEU:HB3 | 1.67 | 0.75 |
| 2:v:175:LEU:HD11 | 1:T:51:ILE:HG13 | 1.68 | 0.75 |
| 2:y:121:LEU:HD11 | 2:y:124:THR:HG21 | 1.68 | 0.75 |
| 3:2:47:ASP:OD1 | 3:2:50:VAL:N | 2.13 | 0.75 |
| 3:22:68:VAL:HG21 | 3:22:97:ARG:HH21 | 1.48 | 0.75 |
| 3:25:47:ASP:OD1 | 3:25:50:VAL:N | 2.13 | 0.75 |
| 1:R:172:ASN:OD1 | 1:T:138:ALA:HB1 | 1.85 | 0.75 |
| 1:S:179:ARG:HG3 | 1:S:206:GLU:HB3 | 1.68 | 0.75 |
| 1:Z:179:ARG:HG3 | 1:Z:206:GLU:HB3 | 1.68 | 0.75 |
| 1:A:108:THR:HB | 1:Z:125:GLU:HB3 | 1.68 | 0.75 |
| 2:c:26:THR:HG21 | 2:c:187:LEU:HB3 | 1.67 | 0.75 |
| 2:g:193:ASP:HB3 | 2:g:196:MET:HB2 | 1.67 | 0.75 |
| 2:w:26:THR:HG21 | 2:w:187:LEU:HB3 | 1.67 | 0.75 |
| 2:w:121:LEU:HD11 | 2:w:124:THR:HG21 | 1.68 | 0.75 |
| 2:z:121:LEU:HD11 | 2:z:124:THR:HG21 | 1.68 | 0.75 |
| 1:X:125:GLU:HB3 | 1:Y:108:THR:HB | 1.68 | 0.75 |
| 1:X:179:ARG:HG3 | 1:X:206:GLU:HB3 | 1.69 | 0.75 |
| 2:d:26:THR:HG21 | 2:d:187:LEU:HB3 | 1.67 | 0.75 |
| 2:e:26:THR:HG21 | 2:e:187:LEU:HB3 | 1.67 | 0.75 |
| 2:m:26:THR:HG21 | 2:m:187:LEU:HB3 | 1.67 | 0.75 |
| 2:x:21:ARG:NH1 | 2:y:267:GLU:OE1 | 2.19 | 0.75 |
| 2:x:336:ASN:ND2 | 2:y:318:SER:O | 2.18 | 0.75 |
| 2:z:26:THR:HG21 | 2:z:187:LEU:HB3 | 1.67 | 0.75 |
| 1:R:125:GLU:HB3 | 1:S:108:THR:HB | 1.69 | 0.75 |
| 2:a:26:THR:HG21 | 2:a:187:LEU:HB3 | 1.67 | 0.75 |
| 2:b:117:ARG:NH1 | 2:b:144:GLY:O | 2.20 | 0.75 |
| 2:p:193:ASP:HB3 | 2:p:196:MET:HB2 | 1.67 | 0.75 |
| 2:r:193:ASP:HB3 | 2:r:196:MET:HB2 | 1.67 | 0.75 |
| 1:W:125:GLU:HB3 | 1:X:108:THR:HB | 1.69 | 0.75 |
| 1:A:125:GLU:HB3 | 1:B:108:THR:HB | 1.68 | 0.75 |
| 3:1:47:ASP:OD1 | 3:1:50:VAL:N | 2.13 | 0.75 |
| 2:b:121:LEU:HD11 | 2:b:124:THR:HG21 | 1.68 | 0.75 |
| 2:f:117:ARG:NH1 | 2:f:144:GLY:O | 2.20 | 0.75 |
| 1:I:172:ASN:OD1 | 1:K:138:ALA:HB1 | 1.85 | 0.75 |
| 1:S:125:GLU:HB3 | 1:T:108:THR:HB | 1.68 | 0.75 |
| 1:T:125:GLU:HB3 | 1:U:108:THR:HB | 1.69 | 0.75 |
| 1:U:179:ARG:HG3 | 1:U:206:GLU:HB3 | 1.68 | 0.75 |
| 2:a:117:ARG:NH1 | 2:a:144:GLY:O | 2.20 | 0.75 |
| 2:e:117:ARG:NH1 | 2:e:144:GLY:O | 2.20 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:s:336:ASN:ND2 | 2:t:318:SER:O | 2.15 | 0.75 |
| 2:y:26:THR:HG21 | 2:y:187:LEU:HB3 | 1.67 | 0.75 |
| 1:D:172:ASN:OD1 | 1:F:138:ALA:HB1 | 1.85 | 0.75 |
| 1:J:172:ASN:OD1 | 1:L:138:ALA:HB1 | 1.85 | 0.75 |
| 1:K:172:ASN:OD1 | 1:M:138:ALA:HB1 | 1.85 | 0.75 |
| 1:N:125:GLU:HB3 | 1:O:108:THR:HB | 1.69 | 0.75 |
| 1:O:125:GLU:HB3 | 1:P:108:THR:HB | 1.69 | 0.75 |
| 2:e:193:ASP:HB3 | 2:e:196:MET:HB2 | 1.67 | 0.75 |
| 2:f:193:ASP:HB3 | 2:f:196:MET:HB2 | 1.67 | 0.75 |
| 1:B:136:GLY:HA3 | 1:Z:213:ILE:HG23 | 1.68 | 0.75 |
| 1:E:179:ARG:HG3 | 1:E:206:GLU:HB3 | 1.68 | 0.75 |
| 1:Q:30:LEU:HD23 | 1:Q:30:LEU:H | 1.52 | 0.75 |
| 2:c:117:ARG:NH1 | 2:c:144:GLY:O | 2.20 | 0.75 |
| 2:i:117:ARG:NH1 | 2:i:144:GLY:O | 2.20 | 0.75 |
| 2:x:117:ARG:NH1 | 2:x:144:GLY:O | 2.20 | 0.75 |
| 3:9:47:ASP:OD1 | 3:9:50:VAL:N | 2.13 | 0.75 |
| 3:16:47:ASP:OD1 | 3:16:50:VAL:N | 2.13 | 0.75 |
| 1:D:179:ARG:HG3 | 1:D:206:GLU:HB3 | 1.69 | 0.75 |
| 1:M:30:LEU:HD23 | 1:M:30:LEU:H | 1.52 | 0.75 |
| 1:N:30:LEU:HD23 | 1:N:30:LEU:H | 1.52 | 0.75 |
| 2:o:175:LEU:HD11 | 1:M:51:ILE:HG13 | 1.68 | 0.74 |
| 2:r:117:ARG:NH1 | 2:r:144:GLY:O | 2.20 | 0.74 |
| 3:26:47:ASP:OD1 | 3:26:50:VAL:N | 2.13 | 0.74 |
| 1:K:125:GLU:HB3 | 1:L:108:THR:HB | 1.69 | 0.74 |
| 1:O:30:LEU:HD23 | 1:O:30:LEU:H | 1.52 | 0.74 |
| 1:R:30:LEU:HD23 | 1:R:30:LEU:H | 1.52 | 0.74 |
| 1:R:179:ARG:HG3 | 1:R:206:GLU:HB3 | 1.69 | 0.74 |
| 2:j:117:ARG:NH1 | 2:j:144:GLY:O | 2.20 | 0.74 |
| 2:k:21:ARG:NH1 | 2:l:267:GLU:OE1 | 2.19 | 0.74 |
| 2:n:175:LEU:HD11 | 1:L:51:ILE:HG13 | 1.68 | 0.74 |
| 2:p:175:LEU:HD11 | 1:N:51:ILE:HG13 | 1.68 | 0.74 |
| 2:q:117:ARG:NH1 | 2:q:144:GLY:O | 2.20 | 0.74 |
| 2:q:193:ASP:HB3 | 2:q:196:MET:HB2 | 1.67 | 0.74 |
| 3:20:47:ASP:OD1 | 3:20:50:VAL:N | 2.13 | 0.74 |
| 1:B:125:GLU:HB3 | 1:C:108:THR:HB | 1.69 | 0.74 |
| 1:P:30:LEU:H | 1:P:30:LEU:HD23 | 1.52 | 0.74 |
| 1:A:179:ARG:HG3 | 1:A:206:GLU:HB3 | 1.68 | 0.74 |
| 2:f:26:THR:HG21 | 2:f:187:LEU:HB3 | 1.67 | 0.74 |
| 2:h:26:THR:HG21 | 2:h:187:LEU:HB3 | 1.67 | 0.74 |
| 2:n:117:ARG:NH1 | 2:n:144:GLY:O | 2.20 | 0.74 |
| 2:o:117:ARG:NH1 | 2:o:144:GLY:O | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:7:47:ASP:OD1 | 3:7:50:VAL:N | 2.13 | 0.74 |
| 1:C:179:ARG:HG3 | 1:C:206:GLU:HB3 | 1.69 | 0.74 |
| 1:L:125:GLU:HB3 | 1:M:108:THR:HB | 1.69 | 0.74 |
| 2:g:26:THR:HG21 | 2:g:187:LEU:HB3 | 1.67 | 0.74 |
| 2:g:117:ARG:NH1 | 2:g:144:GLY:O | 2.20 | 0.74 |
| 2:y:175:LEU:HD11 | 1:W:51:ILE:HG13 | 1.68 | 0.74 |
| 1:S:30:LEU:HD23 | 1:S:30:LEU:H | 1.52 | 0.74 |
| 1:W:179:ARG:HG3 | 1:W:206:GLU:HB3 | 1.69 | 0.74 |
| 2:e:21:ARG:NH1 | 2:f:267:GLU:OE1 | 2.19 | 0.74 |
| 2:t:117:ARG:NH1 | 2:t:144:GLY:O | 2.20 | 0.74 |
| 2:w:21:ARG:NH1 | 2:x:267:GLU:OE1 | 2.19 | 0.74 |
| 2:w:117:ARG:NH1 | 2:w:144:GLY:O | 2.20 | 0.74 |
| 2:y:117:ARG:NH1 | 2:y:144:GLY:O | 2.20 | 0.74 |
| 2:z:117:ARG:NH1 | 2:z:144:GLY:O | 2.20 | 0.74 |
| 1:C:125:GLU:HB3 | 1:D:108:THR:HB | 1.69 | 0.74 |
| 1:E:125:GLU:HB3 | 1:F:108:THR:HB | 1.69 | 0.74 |
| 1:F:179:ARG:HG3 | 1:F:206:GLU:HB3 | 1.69 | 0.74 |
| 1:N:179:ARG:HG3 | 1:N:206:GLU:HB3 | 1.69 | 0.74 |
| 1:T:30:LEU:HD23 | 1:T:30:LEU:H | 1.52 | 0.74 |
| 2:u:117:ARG:NH1 | 2:u:144:GLY:O | 2.20 | 0.74 |
| 1:M:179:ARG:HG3 | 1:M:206:GLU:HB3 | 1.68 | 0.74 |
| 1:O:179:ARG:HG3 | 1:O:206:GLU:HB3 | 1.69 | 0.74 |
| 1:U:30:LEU:HD23 | 1:U:30:LEU:H | 1.52 | 0.74 |
| 1:X:172:ASN:OD1 | 1:Z:138:ALA:HB1 | 1.87 | 0.74 |
| 2:d:117:ARG:NH1 | 2:d:144:GLY:O | 2.20 | 0.74 |
| 2:h:117:ARG:NH1 | 2:h:144:GLY:O | 2.20 | 0.74 |
| 2:x:26:THR:HG21 | 2:x:187:LEU:HB3 | 1.67 | 0.74 |
| 1:G:125:GLU:HB3 | 1:H:108:THR:HB | 1.69 | 0.74 |
| 1:H:125:GLU:HB3 | 1:I:108:THR:HB | 1.69 | 0.74 |
| 1:I:125:GLU:HB3 | 1:J:108:THR:HB | 1.69 | 0.74 |
| 1:L:30:LEU:HD23 | 1:L:30:LEU:H | 1.52 | 0.74 |
| 1:V:167:LYS:HD3 | 1:W:203:ALA:HB3 | 1.70 | 0.74 |
| 1:V:179:ARG:HG3 | 1:V:206:GLU:HB3 | 1.68 | 0.74 |
| 3:4:47:ASP:OD1 | 3:4:50:VAL:N | 2.13 | 0.74 |
| 1:V:125:GLU:HB3 | 1:W:108:THR:HB | 1.70 | 0.74 |
| 1:W:167:LYS:HD3 | 1:X:203:ALA:HB3 | 1.70 | 0.74 |
| 2:l:117:ARG:NH1 | 2:l:144:GLY:O | 2.20 | 0.74 |
| 2:m:117:ARG:NH1 | 2:m:144:GLY:O | 2.20 | 0.74 |
| 1:L:179:ARG:HG3 | 1:L:206:GLU:HB3 | 1.68 | 0.74 |
| 1:P:125:GLU:HB3 | 1:Q:108:THR:HB | 1.70 | 0.74 |
| 1:V:30:LEU:HD23 | 1:V:30:LEU:H | 1.52 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:d:175:LEU:HD11 | 1:B:51:ILE:HG13 | 1.68 | 0.73 |
| 2:k:117:ARG:NH1 | 2:k:144:GLY:O | 2.20 | 0.73 |
| 1:P:179:ARG:HG3 | 1:P:206:GLU:HB3 | 1.68 | 0.73 |
| 1:W:213:ILE:HG23 | 1:Y:136:GLY:HA3 | 1.70 | 0.73 |
| 2:s:117:ARG:NH1 | 2:s:144:GLY:O | 2.20 | 0.73 |
| 1:G:179:ARG:HG3 | 1:G:206:GLU:HB3 | 1.69 | 0.73 |
| 3:21:47:ASP:OD1 | 3:21:50:VAL:N | 2.13 | 0.73 |
| 1:B:179:ARG:HG3 | 1:B:206:GLU:HB3 | 1.68 | 0.73 |
| 1:K:30:LEU:HD23 | 1:K:30:LEU:H | 1.52 | 0.73 |
| 1:W:30:LEU:HD23 | 1:W:30:LEU:H | 1.52 | 0.73 |
| 1:F:30:LEU:HD23 | 1:F:30:LEU:H | 1.52 | 0.73 |
| 1:Q:179:ARG:HG3 | 1:Q:206:GLU:HB3 | 1.69 | 0.73 |
| 3:3:47:ASP:OD1 | 3:3:50:VAL:N | 2.13 | 0.73 |
| 3:6:47:ASP:OD1 | 3:6:50:VAL:N | 2.13 | 0.73 |
| 1:G:30:LEU:HD23 | 1:G:30:LEU:H | 1.52 | 0.73 |
| 1:A:51:ILE:HG13 | 2:c:175:LEU:HD11 | 1.69 | 0.73 |
| 2:p:117:ARG:NH1 | 2:p:144:GLY:O | 2.20 | 0.73 |
| 1:D:167:LYS:HD3 | 1:E:203:ALA:HB3 | 1.70 | 0.73 |
| 1:J:30:LEU:HD23 | 1:J:30:LEU:H | 1.52 | 0.73 |
| 1:K:179:ARG:HG3 | 1:K:206:GLU:HB3 | 1.69 | 0.73 |
| 1:S:213:ILE:HG23 | 1:U:136:GLY:HA3 | 1.71 | 0.73 |
| 1:X:30:LEU:HD23 | 1:X:30:LEU:H | 1.52 | 0.73 |
| 1:Y:30:LEU:HD23 | 1:Y:30:LEU:H | 1.52 | 0.73 |
| 1:Z:30:LEU:HD23 | 1:Z:30:LEU:H | 1.52 | 0.73 |
| 2:i:33:GLU:OE1 | 2:i:92:SER:OG | 2.07 | 0.73 |
| 2:w:33:GLU:OE1 | 2:w:92:SER:OG | 2.07 | 0.73 |
| 2:x:33:GLU:OE1 | 2:x:92:SER:OG | 2.07 | 0.73 |
| 3:5:47:ASP:OD1 | 3:5:50:VAL:N | 2.13 | 0.73 |
| 1:A:30:LEU:HD23 | 1:A:30:LEU:H | 1.52 | 0.73 |
| 1:B:30:LEU:HD23 | 1:B:30:LEU:H | 1.52 | 0.73 |
| 1:C:30:LEU:HD23 | 1:C:30:LEU:H | 1.52 | 0.73 |
| 1:D:30:LEU:HD23 | 1:D:30:LEU:H | 1.52 | 0.73 |
| 1:E:30:LEU:HD23 | 1:E:30:LEU:H | 1.52 | 0.73 |
| 1:J:125:GLU:HB3 | 1:K:108:THR:HB | 1.70 | 0.73 |
| 1:R:213:ILE:HG23 | 1:T:136:GLY:HA3 | 1.71 | 0.73 |
| 1:U:167:LYS:HD3 | 1:V:203:ALA:HB3 | 1.71 | 0.73 |
| 2:d:33:GLU:OE1 | 2:d:92:SER:OG | 2.07 | 0.73 |
| 2:j:33:GLU:OE1 | 2:j:92:SER:OG | 2.07 | 0.73 |
| 2:v:117:ARG:NH1 | 2:v:144:GLY:O | 2.20 | 0.73 |
| 1:B:167:LYS:HD3 | 1:C:203:ALA:HB3 | 1.71 | 0.73 |
| 2:c:33:GLU:OE1 | 2:c:92:SER:OG | 2.07 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:h:33:GLU:OE1 | 2:h:92:SER:OG | 2.07 | 0.73 |
| 1:E:167:LYS:HD3 | 1:F:203:ALA:HB3 | 1.70 | 0.73 |
| 1:H:30:LEU:H | 1:H:30:LEU:HD23 | 1.52 | 0.73 |
| 1:I:30:LEU:HD23 | 1:I:30:LEU:H | 1.52 | 0.73 |
| 1:I:179:ARG:HG3 | 1:I:206:GLU:HB3 | 1.69 | 0.73 |
| 1:T:213:ILE:HG23 | 1:V:136:GLY:HA3 | 1.71 | 0.73 |
| 1:A:213:ILE:HG23 | 1:C:136:GLY:HA3 | 1.70 | 0.72 |
| 2:s:33:GLU:OE1 | 2:s:92:SER:OG | 2.07 | 0.72 |
| 1:J:179:ARG:HG3 | 1:J:206:GLU:HB3 | 1.69 | 0.72 |
| 2:n:33:GLU:OE1 | 2:n:92:SER:OG | 2.07 | 0.72 |
| 2:y:33:GLU:OE1 | 2:y:92:SER:OG | 2.07 | 0.72 |
| 1:G:213:ILE:HG23 | 1:I:136:GLY:HA3 | 1.71 | 0.72 |
| 1:H:179:ARG:HG3 | 1:H:206:GLU:HB3 | 1.69 | 0.72 |
| 1:Q:167:LYS:HD3 | 1:R:203:ALA:HB3 | 1.70 | 0.72 |
| 2:r:33:GLU:OE1 | 2:r:92:SER:OG | 2.07 | 0.72 |
| 2:b:33:GLU:OE1 | 2:b:92:SER:OG | 2.07 | 0.72 |
| 2:e:33:GLU:OE1 | 2:e:92:SER:OG | 2.07 | 0.72 |
| 2:m:33:GLU:OE1 | 2:m:92:SER:OG | 2.07 | 0.72 |
| 2:v:33:GLU:OE1 | 2:v:92:SER:OG | 2.07 | 0.72 |
| 3:17:47:ASP:OD1 | 3:17:50:VAL:N | 2.13 | 0.72 |
| 1:D:125:GLU:HB3 | 1:E:108:THR:HB | 1.70 | 0.72 |
| 1:F:125:GLU:HB3 | 1:G:108:THR:HB | 1.70 | 0.72 |
| 1:R:167:LYS:HD3 | 1:S:203:ALA:HB3 | 1.70 | 0.72 |
| 1:T:167:LYS:HD3 | 1:U:203:ALA:HB3 | 1.70 | 0.72 |
| 2:t:33:GLU:OE1 | 2:t:92:SER:OG | 2.07 | 0.72 |
| 1:U:213:ILE:HG23 | 1:W:136:GLY:HA3 | 1.72 | 0.72 |
| 2:o:33:GLU:OE1 | 2:o:92:SER:OG | 2.07 | 0.72 |
| 1:C:167:LYS:HD3 | 1:D:203:ALA:HB3 | 1.71 | 0.72 |
| 1:F:167:LYS:HD3 | 1:G:203:ALA:HB3 | 1.70 | 0.72 |
| 2:k:33:GLU:OE1 | 2:k:92:SER:OG | 2.07 | 0.72 |
| 1:F:213:ILE:HG23 | 1:H:136:GLY:HA3 | 1.71 | 0.72 |
| 1:P:167:LYS:HD3 | 1:Q:203:ALA:HB3 | 1.70 | 0.72 |
| 2:g:33:GLU:OE1 | 2:g:92:SER:OG | 2.07 | 0.72 |
| 1:V:213:ILE:HG23 | 1:X:136:GLY:HA3 | 1.72 | 0.72 |
| 1:Q:213:ILE:HG23 | 1:S:136:GLY:HA3 | 1.71 | 0.72 |
| 1:S:167:LYS:HD3 | 1:T:203:ALA:HB3 | 1.71 | 0.72 |
| 2:a:33:GLU:OE1 | 2:a:92:SER:OG | 2.07 | 0.72 |
| 2:q:33:GLU:OE1 | 2:q:92:SER:OG | 2.07 | 0.72 |
| 2:f:33:GLU:OE1 | 2:f:92:SER:OG | 2.07 | 0.71 |
| 2:z:33:GLU:OE1 | 2:z:92:SER:OG | 2.07 | 0.71 |
| 3:12:72:GLN:HG2 | 3:12:73:PRO:HD2 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:213:ILE:HG23 | 1:J:136:GLY:HA3 | 1.71 | 0.71 |
| 1:J:167:LYS:HD3 | 1:K:203:ALA:HB3 | 1.70 | 0.71 |
| 1:A:167:LYS:HD3 | 1:B:203:ALA:HB3 | 1.72 | 0.71 |
| 2:l:33:GLU:OE1 | 2:l:92:SER:OG | 2.07 | 0.71 |
| 3:10:72:GLN:HG2 | 3:10:73:PRO:HD2 | 1.72 | 0.71 |
| 3:15:72:GLN:HG2 | 3:15:73:PRO:HD2 | 1.72 | 0.71 |
| 3:16:72:GLN:HG2 | 3:16:73:PRO:HD2 | 1.72 | 0.71 |
| 1:Y:125:GLU:HB3 | 1:Z:108:THR:HB | 1.73 | 0.71 |
| 3:11:72:GLN:HG2 | 3:11:73:PRO:HD2 | 1.73 | 0.71 |
| 3:13:72:GLN:HG2 | 3:13:73:PRO:HD2 | 1.72 | 0.71 |
| 3:17:72:GLN:HG2 | 3:17:73:PRO:HD2 | 1.72 | 0.71 |
| 2:x:345:LEU:HD21 | 2:y:319:LEU:HD22 | 1.72 | 0.71 |
| 2:u:33:GLU:OE1 | 2:u:92:SER:OG | 2.07 | 0.71 |
| 3:14:72:GLN:HG2 | 3:14:73:PRO:HD2 | 1.72 | 0.71 |
| 1:E:213:ILE:HG23 | 1:G:136:GLY:HA3 | 1.72 | 0.71 |
| 1:H:167:LYS:HD3 | 1:I:203:ALA:HB3 | 1.71 | 0.71 |
| 3:8:72:GLN:HG2 | 3:8:73:PRO:HD2 | 1.72 | 0.71 |
| 1:B:213:ILE:HG23 | 1:D:136:GLY:HA3 | 1.71 | 0.71 |
| 1:K:167:LYS:HD3 | 1:L:203:ALA:HB3 | 1.70 | 0.71 |
| 1:N:167:LYS:HD3 | 1:O:203:ALA:HB3 | 1.70 | 0.71 |
| 1:A:203:ALA:HB3 | 1:Z:167:LYS:HD3 | 1.73 | 0.71 |
| 3:9:72:GLN:HG2 | 3:9:73:PRO:HD2 | 1.72 | 0.71 |
| 1:E:179:ARG:HD2 | 1:E:206:GLU:OE1 | 1.91 | 0.71 |
| 1:F:179:ARG:HD2 | 1:F:206:GLU:OE1 | 1.91 | 0.71 |
| 1:I:167:LYS:HD3 | 1:J:203:ALA:HB3 | 1.71 | 0.71 |
| 1:O:167:LYS:HD3 | 1:P:203:ALA:HB3 | 1.71 | 0.71 |
| 1:A:138:ALA:HB1 | 1:Y:172:ASN:OD1 | 1.91 | 0.71 |
| 3:19:72:GLN:HG2 | 3:19:73:PRO:HD2 | 1.72 | 0.71 |
| 3:20:72:GLN:HG2 | 3:20:73:PRO:HD2 | 1.72 | 0.71 |
| 1:C:213:ILE:HG23 | 1:E:136:GLY:HA3 | 1.72 | 0.71 |
| 1:D:213:ILE:HG23 | 1:F:136:GLY:HA3 | 1.72 | 0.71 |
| 1:G:167:LYS:HD3 | 1:H:203:ALA:HB3 | 1.71 | 0.71 |
| 1:I:213:ILE:HG23 | 1:K:136:GLY:HA3 | 1.72 | 0.71 |
| 1:L:179:ARG:HD2 | 1:L:206:GLU:OE1 | 1.91 | 0.71 |
| 3:7:72:GLN:HG2 | 3:7:73:PRO:HD2 | 1.73 | 0.71 |
| 1:M:179:ARG:HD2 | 1:M:206:GLU:OE1 | 1.91 | 0.71 |
| 3:18:72:GLN:HG2 | 3:18:73:PRO:HD2 | 1.73 | 0.70 |
| 1:D:179:ARG:HD2 | 1:D:206:GLU:OE1 | 1.91 | 0.70 |
| 1:P:213:ILE:HG23 | 1:R:136:GLY:HA3 | 1.72 | 0.70 |
| 1:G:179:ARG:HD2 | 1:G:206:GLU:OE1 | 1.91 | 0.70 |
| 1:L:213:ILE:HG23 | 1:N:136:GLY:HA3 | 1.71 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:213:ILE:HG23 | 1:O:136:GLY:HA3 | 1.71 | 0.70 |
| 2:b:175:LEU:HD11 | 1:Z:51:ILE:HG13 | 1.72 | 0.70 |
| 3:6:72:GLN:HG2 | 3:6:73:PRO:HD2 | 1.73 | 0.70 |
| 1:K:179:ARG:HD2 | 1:K:206:GLU:OE1 | 1.91 | 0.70 |
| 1:N:179:ARG:HD2 | 1:N:206:GLU:OE1 | 1.91 | 0.70 |
| 3:21:72:GLN:HG2 | 3:21:73:PRO:HD2 | 1.72 | 0.70 |
| 2:p:33:GLU:OE1 | 2:p:92:SER:OG | 2.07 | 0.70 |
| 1:C:179:ARG:HD2 | 1:C:206:GLU:OE1 | 1.91 | 0.70 |
| 1:J:213:ILE:HG23 | 1:L:136:GLY:HA3 | 1.72 | 0.70 |
| 1:K:213:ILE:HG23 | 1:M:136:GLY:HA3 | 1.72 | 0.70 |
| 1:L:167:LYS:HD3 | 1:M:203:ALA:HB3 | 1.70 | 0.70 |
| 1:M:167:LYS:HD3 | 1:N:203:ALA:HB3 | 1.71 | 0.70 |
| 1:H:179:ARG:HD2 | 1:H:206:GLU:OE1 | 1.91 | 0.70 |
| 1:Y:179:ARG:HD2 | 1:Y:206:GLU:OE1 | 1.91 | 0.70 |
| 2:d:89:VAL:HG12 | 2:d:107:VAL:HG22 | 1.74 | 0.70 |
| 2:y:98:ARG:HG3 | 2:z:188:GLN:HG2 | 1.73 | 0.70 |
| 1:N:213:ILE:HG23 | 1:P:136:GLY:HA3 | 1.71 | 0.70 |
| 2:g:89:VAL:HG12 | 2:g:107:VAL:HG22 | 1.74 | 0.70 |
| 2:h:89:VAL:HG12 | 2:h:107:VAL:HG22 | 1.74 | 0.70 |
| 3:5:72:GLN:HG2 | 3:5:73:PRO:HD2 | 1.73 | 0.70 |
| 1:J:179:ARG:HD2 | 1:J:206:GLU:OE1 | 1.91 | 0.70 |
| 1:O:179:ARG:HD2 | 1:O:206:GLU:OE1 | 1.91 | 0.70 |
| 1:O:213:ILE:HG23 | 1:Q:136:GLY:HA3 | 1.72 | 0.70 |
| 1:P:179:ARG:HD2 | 1:P:206:GLU:OE1 | 1.91 | 0.70 |
| 1:Q:179:ARG:HD2 | 1:Q:206:GLU:OE1 | 1.91 | 0.70 |
| 1:X:179:ARG:HD2 | 1:X:206:GLU:OE1 | 1.91 | 0.70 |
| 1:X:213:ILE:HG23 | 1:Z:136:GLY:HA3 | 1.73 | 0.70 |
| 3:1:72:GLN:HG2 | 3:1:73:PRO:HD2 | 1.72 | 0.70 |
| 1:Z:179:ARG:HD2 | 1:Z:206:GLU:OE1 | 1.91 | 0.70 |
| 3:3:72:GLN:HG2 | 3:3:73:PRO:HD2 | 1.72 | 0.69 |
| 3:22:72:GLN:HG2 | 3:22:73:PRO:HD2 | 1.72 | 0.69 |
| 3:26:72:GLN:HG2 | 3:26:73:PRO:HD2 | 1.72 | 0.69 |
| 1:R:179:ARG:HD2 | 1:R:206:GLU:OE1 | 1.91 | 0.69 |
| 1:S:179:ARG:HD2 | 1:S:206:GLU:OE1 | 1.91 | 0.69 |
| 1:X:167:LYS:HD3 | 1:Y:203:ALA:HB3 | 1.74 | 0.69 |
| 3:2:72:GLN:HG2 | 3:2:73:PRO:HD2 | 1.72 | 0.69 |
| 3:4:72:GLN:HG2 | 3:4:73:PRO:HD2 | 1.72 | 0.69 |
| 3:25:72:GLN:HG2 | 3:25:73:PRO:HD2 | 1.72 | 0.69 |
| 1:T:179:ARG:HD2 | 1:T:206:GLU:OE1 | 1.91 | 0.69 |
| 1:V:179:ARG:HD2 | 1:V:206:GLU:OE1 | 1.91 | 0.69 |
| 3:23:72:GLN:HG2 | 3:23:73:PRO:HD2 | 1.72 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:24:72:GLN:HG2 | 3:24:73:PRO:HD2 | 1.72 | 0.69 |
| 1:I:179:ARG:HD2 | 1:I:206:GLU:OE1 | 1.91 | 0.69 |
| 1:U:179:ARG:HD2 | 1:U:206:GLU:OE1 | 1.91 | 0.69 |
| 1:W:179:ARG:HD2 | 1:W:206:GLU:OE1 | 1.91 | 0.69 |
| 2:c:89:VAL:HG12 | 2:c:107:VAL:HG22 | 1.74 | 0.69 |
| 1:B:179:ARG:HD2 | 1:B:206:GLU:OE1 | 1.91 | 0.69 |
| 1:A:179:ARG:HD2 | 1:A:206:GLU:OE1 | 1.91 | 0.69 |
| 2:e:89:VAL:HG12 | 2:e:107:VAL:HG22 | 1.74 | 0.69 |
| 2:k:89:VAL:HG12 | 2:k:107:VAL:HG22 | 1.74 | 0.69 |
| 2:z:89:VAL:HG12 | 2:z:107:VAL:HG22 | 1.74 | 0.69 |
| 2:s:89:VAL:HG12 | 2:s:107:VAL:HG22 | 1.74 | 0.69 |
| 2:u:258:ARG:NH2 | 2:u:365:ILE:O | 2.26 | 0.69 |
| 3:17:18:ARG:HE | 3:17:46:THR:HA | 1.58 | 0.69 |
| 3:21:18:ARG:HE | 3:21:46:THR:HA | 1.58 | 0.69 |
| 2:k:258:ARG:NH2 | 2:k:365:ILE:O | 2.26 | 0.69 |
| 2:l:89:VAL:HG12 | 2:l:107:VAL:HG22 | 1.74 | 0.69 |
| 2:p:258:ARG:NH2 | 2:p:365:ILE:O | 2.26 | 0.69 |
| 2:t:258:ARG:NH2 | 2:t:365:ILE:O | 2.26 | 0.69 |
| 2:u:89:VAL:HG12 | 2:u:107:VAL:HG22 | 1.74 | 0.69 |
| 3:14:18:ARG:HE | 3:14:46:THR:HA | 1.58 | 0.69 |
| 3:24:18:ARG:HE | 3:24:46:THR:HA | 1.58 | 0.69 |
| 1:L:86:VAL:HB | 1:L:142:ASN:OD1 | 1.93 | 0.69 |
| 1:V:86:VAL:HB | 1:V:142:ASN:OD1 | 1.93 | 0.69 |
| 1:W:86:VAL:HB | 1:W:142:ASN:OD1 | 1.93 | 0.69 |
| 1:Y:167:LYS:HD3 | 1:Z:203:ALA:CB | 2.23 | 0.69 |
| 2:m:258:ARG:NH2 | 2:m:365:ILE:O | 2.26 | 0.69 |
| 2:p:89:VAL:HG12 | 2:p:107:VAL:HG22 | 1.74 | 0.69 |
| 2:q:258:ARG:NH2 | 2:q:365:ILE:O | 2.26 | 0.69 |
| 3:2:18:ARG:HE | 3:2:46:THR:HA | 1.58 | 0.69 |
| 3:5:18:ARG:HE | 3:5:46:THR:HA | 1.58 | 0.69 |
| 3:7:18:ARG:HE | 3:7:46:THR:HA | 1.58 | 0.69 |
| 3:10:18:ARG:HE | 3:10:46:THR:HA | 1.58 | 0.69 |
| 1:M:86:VAL:HB | 1:M:142:ASN:OD1 | 1.93 | 0.69 |
| 1:U:86:VAL:HB | 1:U:142:ASN:OD1 | 1.93 | 0.69 |
| 1:X:86:VAL:HB | 1:X:142:ASN:OD1 | 1.93 | 0.69 |
| 2:a:89:VAL:HG12 | 2:a:107:VAL:HG22 | 1.74 | 0.68 |
| 3:1:18:ARG:HE | 3:1:46:THR:HA | 1.58 | 0.68 |
| 3:18:18:ARG:HE | 3:18:46:THR:HA | 1.58 | 0.68 |
| 1:E:86:VAL:HB | 1:E:142:ASN:OD1 | 1.93 | 0.68 |
| 1:G:86:VAL:HB | 1:G:142:ASN:OD1 | 1.93 | 0.68 |
| 1:K:86:VAL:HB | 1:K:142:ASN:OD1 | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:258:ARG:NH2 | 2:n:365:ILE:O | 2.26 | 0.68 |
| 2:x:258:ARG:NH2 | 2:x:365:ILE:O | 2.26 | 0.68 |
| 2:y:89:VAL:HG12 | 2:y:107:VAL:HG22 | 1.74 | 0.68 |
| 3:20:18:ARG:HE | 3:20:46:THR:HA | 1.58 | 0.68 |
| 1:D:86:VAL:HB | 1:D:142:ASN:OD1 | 1.93 | 0.68 |
| 1:F:86:VAL:HB | 1:F:142:ASN:OD1 | 1.93 | 0.68 |
| 1:T:86:VAL:HB | 1:T:142:ASN:OD1 | 1.93 | 0.68 |
| 1:Y:86:VAL:HB | 1:Y:142:ASN:OD1 | 1.93 | 0.68 |
| 2:h:258:ARG:NH2 | 2:h:365:ILE:O | 2.26 | 0.68 |
| 2:r:89:VAL:HG12 | 2:r:107:VAL:HG22 | 1.74 | 0.68 |
| 2:r:258:ARG:NH2 | 2:r:365:ILE:O | 2.26 | 0.68 |
| 2:s:258:ARG:NH2 | 2:s:365:ILE:O | 2.26 | 0.68 |
| 2:w:258:ARG:NH2 | 2:w:365:ILE:O | 2.26 | 0.68 |
| 3:15:18:ARG:HE | 3:15:46:THR:HA | 1.58 | 0.68 |
| 1:N:86:VAL:HB | 1:N:142:ASN:OD1 | 1.93 | 0.68 |
| 2:f:89:VAL:HG12 | 2:f:107:VAL:HG22 | 1.74 | 0.68 |
| 2:i:89:VAL:HG12 | 2:i:107:VAL:HG22 | 1.74 | 0.68 |
| 2:l:258:ARG:NH2 | 2:l:365:ILE:O | 2.26 | 0.68 |
| 1:S:86:VAL:HB | 1:S:142:ASN:OD1 | 1.93 | 0.68 |
| 2:n:89:VAL:HG12 | 2:n:107:VAL:HG22 | 1.74 | 0.68 |
| 2:q:89:VAL:HG12 | 2:q:107:VAL:HG22 | 1.74 | 0.68 |
| 2:z:258:ARG:NH2 | 2:z:365:ILE:O | 2.26 | 0.68 |
| 3:4:18:ARG:HE | 3:4:46:THR:HA | 1.58 | 0.68 |
| 3:8:18:ARG:HE | 3:8:46:THR:HA | 1.58 | 0.68 |
| 3:11:18:ARG:HE | 3:11:46:THR:HA | 1.58 | 0.68 |
| 3:12:18:ARG:HE | 3:12:46:THR:HA | 1.58 | 0.68 |
| 1:H:86:VAL:HB | 1:H:142:ASN:OD1 | 1.93 | 0.68 |
| 1:Z:86:VAL:HB | 1:Z:142:ASN:OD1 | 1.93 | 0.68 |
| 2:i:258:ARG:NH2 | 2:i:365:ILE:O | 2.26 | 0.68 |
| 2:j:89:VAL:HG12 | 2:j:107:VAL:HG22 | 1.74 | 0.68 |
| 2:j:258:ARG:NH2 | 2:j:365:ILE:O | 2.26 | 0.68 |
| 2:p:98:ARG:HG3 | 2:q:188:GLN:HG2 | 1.75 | 0.68 |
| 3:23:18:ARG:HE | 3:23:46:THR:HA | 1.58 | 0.68 |
| 1:R:86:VAL:HB | 1:R:142:ASN:OD1 | 1.93 | 0.68 |
| 2:w:89:VAL:HG12 | 2:w:107:VAL:HG22 | 1.74 | 0.68 |
| 3:3:18:ARG:HE | 3:3:46:THR:HA | 1.58 | 0.68 |
| 3:13:18:ARG:HE | 3:13:46:THR:HA | 1.58 | 0.68 |
| 3:26:18:ARG:HE | 3:26:46:THR:HA | 1.58 | 0.68 |
| 1:C:86:VAL:HB | 1:C:142:ASN:OD1 | 1.93 | 0.68 |
| 1:J:86:VAL:HB | 1:J:142:ASN:OD1 | 1.93 | 0.68 |
| 2:c:258:ARG:NH2 | 2:c:365:ILE:O | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:f:258:ARG:NH2 | 2:f:365:ILE:O | 2.26 | 0.68 |
| 2:l:172:GLU:OE1 | 2:l:172:GLU:HA | 1.94 | 0.68 |
| 2:v:172:GLU:OE1 | 2:v:172:GLU:HA | 1.94 | 0.68 |
| 3:9:18:ARG:HE | 3:9:46:THR:HA | 1.58 | 0.68 |
| 2:j:172:GLU:HA | 2:j:172:GLU:OE1 | 1.94 | 0.68 |
| 2:o:258:ARG:NH2 | 2:o:365:ILE:O | 2.26 | 0.68 |
| 2:v:89:VAL:HG12 | 2:v:107:VAL:HG22 | 1.74 | 0.68 |
| 2:y:172:GLU:OE1 | 2:y:172:GLU:HA | 1.94 | 0.68 |
| 3:6:18:ARG:HE | 3:6:46:THR:HA | 1.58 | 0.68 |
| 3:25:18:ARG:HE | 3:25:46:THR:HA | 1.58 | 0.68 |
| 1:B:86:VAL:HB | 1:B:142:ASN:OD1 | 1.93 | 0.68 |
| 1:A:86:VAL:HB | 1:A:142:ASN:OD1 | 1.93 | 0.68 |
| 2:b:172:GLU:HA | 2:b:172:GLU:OE1 | 1.94 | 0.68 |
| 2:i:172:GLU:OE1 | 2:i:172:GLU:HA | 1.94 | 0.68 |
| 2:v:258:ARG:NH2 | 2:v:365:ILE:O | 2.26 | 0.68 |
| 1:O:86:VAL:HB | 1:O:142:ASN:OD1 | 1.93 | 0.68 |
| 2:j:98:ARG:HG3 | 2:k:188:GLN:HG2 | 1.75 | 0.67 |
| 2:k:172:GLU:OE1 | 2:k:172:GLU:HA | 1.94 | 0.67 |
| 2:s:172:GLU:OE1 | 2:s:172:GLU:HA | 1.94 | 0.67 |
| 2:x:89:VAL:HG12 | 2:x:107:VAL:HG22 | 1.74 | 0.67 |
| 2:z:172:GLU:OE1 | 2:z:172:GLU:HA | 1.94 | 0.67 |
| 2:a:258:ARG:NH2 | 2:a:365:ILE:O | 2.26 | 0.67 |
| 2:c:172:GLU:OE1 | 2:c:172:GLU:HA | 1.94 | 0.67 |
| 2:e:258:ARG:NH2 | 2:e:365:ILE:O | 2.26 | 0.67 |
| 2:y:46:ASP:OD1 | 2:z:161:ASN:HB2 | 1.94 | 0.67 |
| 1:Q:86:VAL:HB | 1:Q:142:ASN:OD1 | 1.93 | 0.67 |
| 2:b:89:VAL:HG12 | 2:b:107:VAL:HG22 | 1.74 | 0.67 |
| 2:b:258:ARG:NH2 | 2:b:365:ILE:O | 2.26 | 0.67 |
| 2:f:172:GLU:OE1 | 2:f:172:GLU:HA | 1.94 | 0.67 |
| 2:m:89:VAL:HG12 | 2:m:107:VAL:HG22 | 1.74 | 0.67 |
| 2:o:172:GLU:OE1 | 2:o:172:GLU:HA | 1.94 | 0.67 |
| 2:p:172:GLU:OE1 | 2:p:172:GLU:HA | 1.94 | 0.67 |
| 2:t:89:VAL:HG12 | 2:t:107:VAL:HG22 | 1.74 | 0.67 |
| 3:16:18:ARG:HE | 3:16:46:THR:HA | 1.58 | 0.67 |
| 1:I:86:VAL:HB | 1:I:142:ASN:OD1 | 1.93 | 0.67 |
| 2:m:172:GLU:HA | 2:m:172:GLU:OE1 | 1.94 | 0.67 |
| 2:t:172:GLU:OE1 | 2:t:172:GLU:HA | 1.94 | 0.67 |
| 2:w:172:GLU:OE1 | 2:w:172:GLU:HA | 1.94 | 0.67 |
| 2:y:258:ARG:NH2 | 2:y:365:ILE:O | 2.26 | 0.67 |
| 3:22:18:ARG:HE | 3:22:46:THR:HA | 1.58 | 0.67 |
| 2:d:258:ARG:NH2 | 2:d:365:ILE:O | 2.26 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:r:98:ARG:HG3 | 2:s:188:GLN:HG2 | 1.76 | 0.67 |
| 2:o:89:VAL:HG12 | 2:o:107:VAL:HG22 | 1.74 | 0.67 |
| 2:e:172:GLU:OE1 | 2:e:172:GLU:HA | 1.94 | 0.67 |
| 2:x:98:ARG:HG3 | 2:y:188:GLN:HG2 | 1.76 | 0.67 |
| 1:P:86:VAL:HB | 1:P:142:ASN:OD1 | 1.93 | 0.67 |
| 1:A:136:GLY:HA3 | 1:Y:213:ILE:HG23 | 1.76 | 0.67 |
| 2:d:98:ARG:HG3 | 2:e:188:GLN:HG2 | 1.75 | 0.67 |
| 2:d:345:LEU:HD21 | 2:e:319:LEU:HD22 | 1.76 | 0.67 |
| 2:f:266:ARG:HA | 2:f:328:LEU:HD22 | 1.77 | 0.67 |
| 2:r:172:GLU:HA | 2:r:172:GLU:OE1 | 1.94 | 0.67 |
| 2:v:98:ARG:HG3 | 2:w:188:GLN:HG2 | 1.75 | 0.67 |
| 2:v:345:LEU:HD21 | 2:w:319:LEU:HD22 | 1.76 | 0.67 |
| 2:d:172:GLU:OE1 | 2:d:172:GLU:HA | 1.94 | 0.67 |
| 2:g:266:ARG:HA | 2:g:328:LEU:HD22 | 1.77 | 0.67 |
| 2:h:172:GLU:OE1 | 2:h:172:GLU:HA | 1.94 | 0.67 |
| 2:u:172:GLU:HA | 2:u:172:GLU:OE1 | 1.94 | 0.67 |
| 2:w:266:ARG:HA | 2:w:328:LEU:HD22 | 1.77 | 0.67 |
| 3:19:18:ARG:HE | 3:19:46:THR:HA | 1.58 | 0.67 |
| 2:h:266:ARG:HA | 2:h:328:LEU:HD22 | 1.77 | 0.67 |
| 2:u:266:ARG:HA | 2:u:328:LEU:HD22 | 1.77 | 0.67 |
| 2:v:266:ARG:HA | 2:v:328:LEU:HD22 | 1.77 | 0.67 |
| 2:y:88:MET:HG2 | 2:y:110:MET:HG3 | 1.77 | 0.67 |
| 2:e:266:ARG:HA | 2:e:328:LEU:HD22 | 1.77 | 0.66 |
| 2:g:258:ARG:NH2 | 2:g:365:ILE:O | 2.26 | 0.66 |
| 2:x:172:GLU:OE1 | 2:x:172:GLU:HA | 1.94 | 0.66 |
| 2:b:98:ARG:HG3 | 2:c:188:GLN:HG2 | 1.76 | 0.66 |
| 2:c:88:MET:HG2 | 2:c:110:MET:HG3 | 1.77 | 0.66 |
| 2:t:266:ARG:HA | 2:t:328:LEU:HD22 | 1.77 | 0.66 |
| 2:z:88:MET:HG2 | 2:z:110:MET:HG3 | 1.77 | 0.66 |
| 2:b:88:MET:HG2 | 2:b:110:MET:HG3 | 1.77 | 0.66 |
| 2:d:266:ARG:HA | 2:d:328:LEU:HD22 | 1.77 | 0.66 |
| 2:f:98:ARG:HG3 | 2:g:188:GLN:HG2 | 1.75 | 0.66 |
| 2:i:266:ARG:HA | 2:i:328:LEU:HD22 | 1.77 | 0.66 |
| 2:t:98:ARG:HG3 | 2:u:188:GLN:HG2 | 1.76 | 0.66 |
| 2:x:266:ARG:HA | 2:x:328:LEU:HD22 | 1.77 | 0.66 |
| 3:25:76:THR:HG21 | 1:Y:34:ALA:HA | 1.78 | 0.66 |
| 2:a:88:MET:HG2 | 2:a:110:MET:HG3 | 1.77 | 0.66 |
| 2:b:345:LEU:HD21 | 2:c:319:LEU:HD22 | 1.77 | 0.66 |
| 2:d:88:MET:HG2 | 2:d:110:MET:HG3 | 1.77 | 0.66 |
| 2:g:172:GLU:OE1 | 2:g:172:GLU:HA | 1.94 | 0.66 |
| 2:n:98:ARG:HG3 | 2:o:188:GLN:HG2 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:o:98:ARG:HG3 | 2:p:188:GLN:HG2 | 1.77 | 0.66 |
| 2:x:88:MET:HG2 | 2:x:110:MET:HG3 | 1.77 | 0.66 |
| 1:T:82:LEU:HD13 | 1:T:144:PHE:CD1 | 2.31 | 0.66 |
| 2:h:98:ARG:HG3 | 2:i:188:GLN:HG2 | 1.76 | 0.66 |
| 2:s:266:ARG:HA | 2:s:328:LEU:HD22 | 1.77 | 0.66 |
| 2:y:46:ASP:HA | 2:z:161:ASN:ND2 | 2.09 | 0.66 |
| 1:R:82:LEU:HD13 | 1:R:144:PHE:CD1 | 2.31 | 0.66 |
| 2:j:345:LEU:HD21 | 2:k:319:LEU:HD22 | 1.76 | 0.66 |
| 2:l:98:ARG:HG3 | 2:m:188:GLN:HG2 | 1.76 | 0.66 |
| 2:u:88:MET:HG2 | 2:u:110:MET:HG3 | 1.77 | 0.66 |
| 2:v:88:MET:HG2 | 2:v:110:MET:HG3 | 1.78 | 0.66 |
| 1:B:82:LEU:HD13 | 1:B:144:PHE:CD1 | 2.31 | 0.66 |
| 1:W:82:LEU:HD13 | 1:W:144:PHE:CD1 | 2.31 | 0.66 |
| 1:Y:82:LEU:HD13 | 1:Y:144:PHE:CD1 | 2.31 | 0.66 |
| 1:A:82:LEU:HD13 | 1:A:144:PHE:CD1 | 2.31 | 0.66 |
| 2:c:98:ARG:HG3 | 2:d:188:GLN:HG2 | 1.77 | 0.66 |
| 2:n:172:GLU:OE1 | 2:n:172:GLU:HA | 1.94 | 0.66 |
| 2:t:88:MET:HG2 | 2:t:110:MET:HG3 | 1.77 | 0.66 |
| 2:y:266:ARG:HA | 2:y:328:LEU:HD22 | 1.77 | 0.66 |
| 3:12:76:THR:HG21 | 1:L:34:ALA:HA | 1.78 | 0.66 |
| 3:24:76:THR:HG21 | 1:X:34:ALA:HA | 1.78 | 0.66 |
| 1:E:82:LEU:HD13 | 1:E:144:PHE:CD1 | 2.31 | 0.66 |
| 1:Q:82:LEU:HD13 | 1:Q:144:PHE:CD1 | 2.31 | 0.66 |
| 1:S:82:LEU:HD13 | 1:S:144:PHE:CD1 | 2.31 | 0.66 |
| 2:e:88:MET:HG2 | 2:e:110:MET:HG3 | 1.77 | 0.66 |
| 2:j:266:ARG:HA | 2:j:328:LEU:HD22 | 1.77 | 0.66 |
| 2:p:345:LEU:HD21 | 2:q:319:LEU:HD22 | 1.76 | 0.66 |
| 2:q:172:GLU:OE1 | 2:q:172:GLU:HA | 1.94 | 0.66 |
| 2:r:266:ARG:HA | 2:r:328:LEU:HD22 | 1.77 | 0.66 |
| 2:w:88:MET:HG2 | 2:w:110:MET:HG3 | 1.77 | 0.66 |
| 3:11:76:THR:HG21 | 1:K:34:ALA:HA | 1.78 | 0.66 |
| 3:16:76:THR:HG21 | 1:P:34:ALA:HA | 1.78 | 0.66 |
| 3:20:76:THR:HG21 | 1:T:34:ALA:HA | 1.78 | 0.66 |
| 1:O:37:ALA:HB1 | 1:P:74:ILE:HG22 | 1.78 | 0.66 |
| 2:c:266:ARG:HA | 2:c:328:LEU:HD22 | 1.77 | 0.66 |
| 2:n:345:LEU:HD21 | 2:o:319:LEU:HD22 | 1.77 | 0.66 |
| 2:q:98:ARG:HG3 | 2:r:188:GLN:HG2 | 1.77 | 0.66 |
| 3:15:76:THR:HG21 | 1:O:34:ALA:HA | 1.78 | 0.66 |
| 3:19:76:THR:HG21 | 1:S:34:ALA:HA | 1.78 | 0.66 |
| 3:21:76:THR:HG21 | 1:U:34:ALA:HA | 1.78 | 0.66 |
| 3:23:76:THR:HG21 | 1:W:34:ALA:HA | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:82:LEU:HD13 | 1:C:144:PHE:CD1 | 2.31 | 0.66 |
| 1:L:37:ALA:HB1 | 1:M:74:ILE:HG22 | 1.78 | 0.66 |
| 1:Z:82:LEU:HD13 | 1:Z:144:PHE:CD1 | 2.31 | 0.66 |
| 2:a:172:GLU:OE1 | 2:a:172:GLU:HA | 1.94 | 0.66 |
| 2:s:98:ARG:HG3 | 2:t:188:GLN:HG2 | 1.77 | 0.66 |
| 3:10:76:THR:HG21 | 1:J:34:ALA:HA | 1.78 | 0.66 |
| 1:D:82:LEU:HD13 | 1:D:144:PHE:CD1 | 2.31 | 0.66 |
| 1:O:82:LEU:HD13 | 1:O:144:PHE:CD1 | 2.31 | 0.66 |
| 1:P:82:LEU:HD13 | 1:P:144:PHE:CD1 | 2.31 | 0.66 |
| 1:V:82:LEU:HD13 | 1:V:144:PHE:CD1 | 2.31 | 0.66 |
| 2:c:345:LEU:HD21 | 2:d:319:LEU:HD22 | 1.78 | 0.65 |
| 2:f:88:MET:HG2 | 2:f:110:MET:HG3 | 1.77 | 0.65 |
| 2:g:88:MET:HG2 | 2:g:110:MET:HG3 | 1.77 | 0.65 |
| 2:i:98:ARG:HG3 | 2:j:188:GLN:HG2 | 1.77 | 0.65 |
| 2:k:266:ARG:HA | 2:k:328:LEU:HD22 | 1.77 | 0.65 |
| 2:u:98:ARG:HG3 | 2:v:188:GLN:HG2 | 1.77 | 0.65 |
| 3:8:76:THR:HG21 | 1:H:34:ALA:HA | 1.78 | 0.65 |
| 3:17:76:THR:HG21 | 1:Q:34:ALA:HA | 1.78 | 0.65 |
| 3:18:76:THR:HG21 | 1:R:34:ALA:HA | 1.78 | 0.65 |
| 1:H:82:LEU:HD13 | 1:H:144:PHE:CD1 | 2.31 | 0.65 |
| 1:N:82:LEU:HD13 | 1:N:144:PHE:CD1 | 2.31 | 0.65 |
| 1:U:82:LEU:HD13 | 1:U:144:PHE:CD1 | 2.31 | 0.65 |
| 2:q:266:ARG:HA | 2:q:328:LEU:HD22 | 1.77 | 0.65 |
| 2:w:98:ARG:HG3 | 2:x:188:GLN:HG2 | 1.77 | 0.65 |
| 2:w:345:LEU:HD21 | 2:x:319:LEU:HD22 | 1.78 | 0.65 |
| 2:z:266:ARG:HA | 2:z:328:LEU:HD22 | 1.77 | 0.65 |
| 3:2:76:THR:HG21 | 1:B:34:ALA:HA | 1.78 | 0.65 |
| 3:9:76:THR:HG21 | 1:I:34:ALA:HA | 1.78 | 0.65 |
| 3:13:76:THR:HG21 | 1:M:34:ALA:HA | 1.78 | 0.65 |
| 3:22:76:THR:HG21 | 1:V:34:ALA:HA | 1.78 | 0.65 |
| 1:K:82:LEU:HD13 | 1:K:144:PHE:CD1 | 2.31 | 0.65 |
| 1:P:37:ALA:HB1 | 1:Q:74:ILE:HG22 | 1.79 | 0.65 |
| 2:a:98:ARG:HG3 | 2:b:188:GLN:HG2 | 1.78 | 0.65 |
| 2:a:178:GLN:HG3 | 1:Y:47:ALA:O | 1.96 | 0.65 |
| 2:b:266:ARG:HA | 2:b:328:LEU:HD22 | 1.77 | 0.65 |
| 2:h:88:MET:HG2 | 2:h:110:MET:HG3 | 1.77 | 0.65 |
| 2:k:98:ARG:HG3 | 2:l:188:GLN:HG2 | 1.77 | 0.65 |
| 3:3:76:THR:HG21 | 1:C:34:ALA:HA | 1.78 | 0.65 |
| 3:7:76:THR:HG21 | 1:G:34:ALA:HA | 1.78 | 0.65 |
| 3:14:76:THR:HG21 | 1:N:34:ALA:HA | 1.78 | 0.65 |
| 1:G:82:LEU:HD13 | 1:G:144:PHE:CD1 | 2.31 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:k:345:LEU:HD21 | 2:l:319:LEU:HD22 | 1.78 | 0.65 |
| 3:6:76:THR:HG21 | 1:F:34:ALA:HA | 1.78 | 0.65 |
| 3:7:45:ARG:O | 3:7:45:ARG:HG2 | 1.97 | 0.65 |
| 3:10:45:ARG:HG2 | 3:10:45:ARG:O | 1.97 | 0.65 |
| 2:e:98:ARG:HG3 | 2:f:188:GLN:HG2 | 1.77 | 0.65 |
| 2:f:345:LEU:HD21 | 2:g:319:LEU:HD22 | 1.77 | 0.65 |
| 2:s:88:MET:HG2 | 2:s:110:MET:HG3 | 1.77 | 0.65 |
| 2:w:142:LEU:HD23 | 2:y:350:GLN:NE2 | 2.11 | 0.65 |
| 3:26:45:ARG:O | 3:26:45:ARG:HG2 | 1.97 | 0.65 |
| 1:L:82:LEU:HD13 | 1:L:144:PHE:CD1 | 2.31 | 0.65 |
| 2:m:88:MET:HG2 | 2:m:110:MET:HG3 | 1.77 | 0.65 |
| 2:q:88:MET:HG2 | 2:q:110:MET:HG3 | 1.77 | 0.65 |
| 3:4:45:ARG:O | 3:4:45:ARG:HG2 | 1.97 | 0.65 |
| 3:4:76:THR:HG21 | 1:D:34:ALA:HA | 1.78 | 0.65 |
| 3:23:45:ARG:O | 3:23:45:ARG:HG2 | 1.97 | 0.65 |
| 2:i:81:LEU:HD23 | 2:i:81:LEU:H | 1.62 | 0.65 |
| 2:l:88:MET:HG2 | 2:l:110:MET:HG3 | 1.77 | 0.65 |
| 2:l:345:LEU:HD21 | 2:m:319:LEU:HD22 | 1.78 | 0.65 |
| 2:p:266:ARG:HA | 2:p:328:LEU:HD22 | 1.77 | 0.65 |
| 2:r:81:LEU:H | 2:r:81:LEU:HD23 | 1.62 | 0.65 |
| 2:r:88:MET:HG2 | 2:r:110:MET:HG3 | 1.78 | 0.65 |
| 1:H:37:ALA:HB1 | 1:I:74:ILE:HG22 | 1.79 | 0.65 |
| 1:K:37:ALA:HB1 | 1:L:74:ILE:HG22 | 1.79 | 0.65 |
| 1:X:37:ALA:HB1 | 1:Y:74:ILE:HG22 | 1.77 | 0.65 |
| 3:1:45:ARG:O | 3:1:45:ARG:HG2 | 1.97 | 0.65 |
| 2:i:88:MET:HG2 | 2:i:110:MET:HG3 | 1.77 | 0.65 |
| 2:r:89:VAL:HG11 | 2:r:121:LEU:HD21 | 1.79 | 0.65 |
| 2:s:81:LEU:HD23 | 2:s:81:LEU:H | 1.62 | 0.65 |
| 2:v:89:VAL:HG11 | 2:v:121:LEU:HD21 | 1.79 | 0.65 |
| 2:w:89:VAL:HG11 | 2:w:121:LEU:HD21 | 1.79 | 0.65 |
| 3:3:45:ARG:HG2 | 3:3:45:ARG:O | 1.97 | 0.65 |
| 3:13:45:ARG:HG2 | 3:13:45:ARG:O | 1.97 | 0.65 |
| 3:16:45:ARG:HG2 | 3:16:45:ARG:O | 1.97 | 0.65 |
| 3:26:76:THR:HG21 | 1:Z:34:ALA:HA | 1.79 | 0.65 |
| 1:F:82:LEU:HD13 | 1:F:144:PHE:CD1 | 2.31 | 0.65 |
| 1:I:37:ALA:HB1 | 1:J:74:ILE:HG22 | 1.78 | 0.65 |
| 1:I:82:LEU:HD13 | 1:I:144:PHE:CD1 | 2.31 | 0.65 |
| 1:T:37:ALA:HB1 | 1:U:74:ILE:HG22 | 1.79 | 0.65 |
| 2:g:98:ARG:HG3 | 2:h:188:GLN:HG2 | 1.77 | 0.65 |
| 2:l:141:ILE:CD1 | 2:l:165:ILE:HD11 | 2.27 | 0.65 |
| 2:l:266:ARG:HA | 2:l:328:LEU:HD22 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:81:LEU:HD23 | 2:n:81:LEU:H | 1.62 | 0.65 |
| 2:p:88:MET:HG2 | 2:p:110:MET:HG3 | 1.77 | 0.65 |
| 2:q:345:LEU:HD21 | 2:r:319:LEU:HD22 | 1.78 | 0.65 |
| 3:5:76:THR:HG21 | 1:E:34:ALA:HA | 1.78 | 0.65 |
| 1:J:82:LEU:HD13 | 1:J:144:PHE:CD1 | 2.31 | 0.65 |
| 1:S:37:ALA:HB1 | 1:T:74:ILE:HG22 | 1.79 | 0.65 |
| 1:A:34:ALA:HA | 3:1:76:THR:HG21 | 1.79 | 0.65 |
| 2:a:89:VAL:HG11 | 2:a:121:LEU:HD21 | 1.79 | 0.65 |
| 2:a:266:ARG:HA | 2:a:328:LEU:HD22 | 1.77 | 0.65 |
| 2:d:81:LEU:HD23 | 2:d:81:LEU:H | 1.62 | 0.65 |
| 2:e:81:LEU:HD23 | 2:e:81:LEU:H | 1.62 | 0.65 |
| 2:h:345:LEU:HD21 | 2:i:319:LEU:HD22 | 1.77 | 0.65 |
| 2:j:81:LEU:HD23 | 2:j:81:LEU:H | 1.62 | 0.65 |
| 2:k:141:ILE:CD1 | 2:k:165:ILE:HD11 | 2.27 | 0.65 |
| 2:m:81:LEU:HD23 | 2:m:81:LEU:H | 1.62 | 0.65 |
| 2:m:98:ARG:HG3 | 2:n:188:GLN:HG2 | 1.77 | 0.65 |
| 2:m:141:ILE:CD1 | 2:m:165:ILE:HD11 | 2.27 | 0.65 |
| 2:q:89:VAL:HG11 | 2:q:121:LEU:HD21 | 1.79 | 0.65 |
| 2:s:89:VAL:HG11 | 2:s:121:LEU:HD21 | 1.79 | 0.65 |
| 2:t:345:LEU:HD21 | 2:u:319:LEU:HD22 | 1.77 | 0.65 |
| 2:u:89:VAL:HG11 | 2:u:121:LEU:HD21 | 1.79 | 0.65 |
| 2:z:89:VAL:HG11 | 2:z:121:LEU:HD21 | 1.79 | 0.65 |
| 3:20:45:ARG:O | 3:20:45:ARG:HG2 | 1.97 | 0.65 |
| 1:X:82:LEU:HD13 | 1:X:144:PHE:CD1 | 2.31 | 0.65 |
| 2:k:88:MET:HG2 | 2:k:110:MET:HG3 | 1.77 | 0.64 |
| 2:n:88:MET:HG2 | 2:n:110:MET:HG3 | 1.77 | 0.64 |
| 2:o:88:MET:HG2 | 2:o:110:MET:HG3 | 1.77 | 0.64 |
| 2:x:89:VAL:HG11 | 2:x:121:LEU:HD21 | 1.79 | 0.64 |
| 3:6:45:ARG:HG2 | 3:6:45:ARG:O | 1.97 | 0.64 |
| 3:11:45:ARG:O | 3:11:45:ARG:HG2 | 1.97 | 0.64 |
| 1:M:82:LEU:HD13 | 1:M:144:PHE:CD1 | 2.31 | 0.64 |
| 2:h:81:LEU:HD23 | 2:h:81:LEU:H | 1.62 | 0.64 |
| 2:n:141:ILE:CD1 | 2:n:165:ILE:HD11 | 2.27 | 0.64 |
| 2:o:81:LEU:HD23 | 2:o:81:LEU:H | 1.62 | 0.64 |
| 2:x:81:LEU:HD23 | 2:x:81:LEU:H | 1.62 | 0.64 |
| 2:y:89:VAL:HG11 | 2:y:121:LEU:HD21 | 1.79 | 0.64 |
| 3:14:45:ARG:O | 3:14:45:ARG:HG2 | 1.97 | 0.64 |
| 3:24:45:ARG:O | 3:24:45:ARG:HG2 | 1.97 | 0.64 |
| 2:b:89:VAL:HG11 | 2:b:121:LEU:HD21 | 1.79 | 0.64 |
| 2:e:345:LEU:HD21 | 2:f:319:LEU:HD22 | 1.78 | 0.64 |
| 2:j:88:MET:HG2 | 2:j:110:MET:HG3 | 1.77 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:j:141:ILE:CD1 | 2:j:165:ILE:HD11 | 2.27 | 0.64 |
| 2:o:266:ARG:HA | 2:o:328:LEU:HD22 | 1.77 | 0.64 |
| 3:15:45:ARG:O | 3:15:45:ARG:HG2 | 1.97 | 0.64 |
| 3:17:45:ARG:O | 3:17:45:ARG:HG2 | 1.97 | 0.64 |
| 1:C:37:ALA:HB1 | 1:D:74:ILE:HG22 | 1.78 | 0.64 |
| 2:c:81:LEU:HD23 | 2:c:81:LEU:H | 1.62 | 0.64 |
| 2:m:266:ARG:HA | 2:m:328:LEU:HD22 | 1.77 | 0.64 |
| 2:o:89:VAL:HG11 | 2:o:121:LEU:HD21 | 1.79 | 0.64 |
| 2:t:89:VAL:HG11 | 2:t:121:LEU:HD21 | 1.79 | 0.64 |
| 3:8:45:ARG:HG2 | 3:8:45:ARG:O | 1.97 | 0.64 |
| 3:9:45:ARG:O | 3:9:45:ARG:HG2 | 1.97 | 0.64 |
| 3:22:45:ARG:HG2 | 3:22:45:ARG:O | 1.97 | 0.64 |
| 1:M:37:ALA:HB1 | 1:N:74:ILE:HG22 | 1.79 | 0.64 |
| 2:a:188:GLN:HG2 | 2:z:98:ARG:HG3 | 1.79 | 0.64 |
| 2:n:89:VAL:HG11 | 2:n:121:LEU:HD21 | 1.79 | 0.64 |
| 2:o:141:ILE:CD1 | 2:o:165:ILE:HD11 | 2.27 | 0.64 |
| 2:p:89:VAL:HG11 | 2:p:121:LEU:HD21 | 1.79 | 0.64 |
| 2:t:81:LEU:HD23 | 2:t:81:LEU:H | 1.62 | 0.64 |
| 2:w:81:LEU:HD23 | 2:w:81:LEU:H | 1.62 | 0.64 |
| 1:D:37:ALA:HB1 | 1:E:74:ILE:HG22 | 1.78 | 0.64 |
| 1:G:37:ALA:HB1 | 1:H:74:ILE:HG22 | 1.79 | 0.64 |
| 1:L:82:LEU:HD12 | 1:L:146:GLY:CA | 2.28 | 0.64 |
| 1:N:37:ALA:HB1 | 1:O:74:ILE:HG22 | 1.79 | 0.64 |
| 1:U:82:LEU:HD12 | 1:U:146:GLY:CA | 2.28 | 0.64 |
| 1:Y:37:ALA:HB1 | 1:Z:74:ILE:HG22 | 1.80 | 0.64 |
| 2:i:345:LEU:HD21 | 2:j:319:LEU:HD22 | 1.78 | 0.64 |
| 2:t:141:ILE:CD1 | 2:t:165:ILE:HD11 | 2.27 | 0.64 |
| 2:y:81:LEU:HD23 | 2:y:81:LEU:H | 1.62 | 0.64 |
| 3:19:45:ARG:HG2 | 3:19:45:ARG:O | 1.97 | 0.64 |
| 3:25:45:ARG:HG2 | 3:25:45:ARG:O | 1.97 | 0.64 |
| 1:M:82:LEU:HD12 | 1:M:146:GLY:CA | 2.28 | 0.64 |
| 1:T:82:LEU:HD12 | 1:T:146:GLY:CA | 2.28 | 0.64 |
| 2:m:89:VAL:HG11 | 2:m:121:LEU:HD21 | 1.79 | 0.64 |
| 2:n:266:ARG:HA | 2:n:328:LEU:HD22 | 1.77 | 0.64 |
| 2:o:345:LEU:HD21 | 2:p:319:LEU:HD22 | 1.78 | 0.64 |
| 2:r:345:LEU:HD21 | 2:s:319:LEU:HD22 | 1.78 | 0.64 |
| 2:s:141:ILE:CD1 | 2:s:165:ILE:HD11 | 2.27 | 0.64 |
| 2:u:141:ILE:CD1 | 2:u:165:ILE:HD11 | 2.27 | 0.64 |
| 1:K:82:LEU:HD12 | 1:K:146:GLY:CA | 2.28 | 0.64 |
| 1:V:82:LEU:HD12 | 1:V:146:GLY:CA | 2.28 | 0.64 |
| 2:d:89:VAL:HG11 | 2:d:121:LEU:HD21 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:e:89:VAL:HG11 | 2:e:121:LEU:HD21 | 1.79 | 0.64 |
| 2:e:141:ILE:CD1 | 2:e:165:ILE:HD11 | 2.27 | 0.64 |
| 2:i:141:ILE:CD1 | 2:i:165:ILE:HD11 | 2.27 | 0.64 |
| 2:q:81:LEU:HD23 | 2:q:81:LEU:H | 1.62 | 0.64 |
| 1:R:82:LEU:HD12 | 1:R:146:GLY:CA | 2.28 | 0.64 |
| 2:c:89:VAL:HG11 | 2:c:121:LEU:HD21 | 1.79 | 0.64 |
| 2:d:141:ILE:CD1 | 2:d:165:ILE:HD11 | 2.27 | 0.64 |
| 2:f:81:LEU:HD23 | 2:f:81:LEU:H | 1.62 | 0.64 |
| 2:u:345:LEU:HD21 | 2:v:319:LEU:HD22 | 1.78 | 0.64 |
| 3:21:45:ARG:O | 3:21:45:ARG:HG2 | 1.97 | 0.64 |
| 1:N:82:LEU:HD12 | 1:N:146:GLY:CA | 2.28 | 0.64 |
| 1:Q:37:ALA:HB1 | 1:R:74:ILE:HG22 | 1.79 | 0.64 |
| 1:U:37:ALA:HB1 | 1:V:74:ILE:HG22 | 1.78 | 0.64 |
| 1:W:82:LEU:HD12 | 1:W:146:GLY:CA | 2.28 | 0.64 |
| 2:c:141:ILE:CD1 | 2:c:165:ILE:HD11 | 2.27 | 0.64 |
| 2:k:81:LEU:HD23 | 2:k:81:LEU:H | 1.62 | 0.64 |
| 2:v:81:LEU:HD23 | 2:v:81:LEU:H | 1.62 | 0.64 |
| 2:v:141:ILE:CD1 | 2:v:165:ILE:HD11 | 2.27 | 0.64 |
| 2:z:89:VAL:HG23 | 2:z:126:LEU:HD21 | 1.80 | 0.64 |
| 1:F:37:ALA:HB1 | 1:G:74:ILE:HG22 | 1.78 | 0.64 |
| 1:J:82:LEU:HD12 | 1:J:146:GLY:CA | 2.28 | 0.64 |
| 1:P:82:LEU:HD12 | 1:P:146:GLY:CA | 2.28 | 0.64 |
| 1:S:82:LEU:HD12 | 1:S:146:GLY:CA | 2.28 | 0.64 |
| 2:f:89:VAL:HG11 | 2:f:121:LEU:HD21 | 1.79 | 0.63 |
| 2:f:141:ILE:CD1 | 2:f:165:ILE:HD11 | 2.28 | 0.63 |
| 2:p:141:ILE:CD1 | 2:p:165:ILE:HD11 | 2.27 | 0.63 |
| 2:r:141:ILE:CD1 | 2:r:165:ILE:HD11 | 2.27 | 0.63 |
| 2:x:164:ARG:NH1 | 2:y:365:ILE:HG23 | 2.14 | 0.63 |
| 3:5:45:ARG:O | 3:5:45:ARG:HG2 | 1.97 | 0.63 |
| 3:12:45:ARG:O | 3:12:45:ARG:HG2 | 1.97 | 0.63 |
| 1:O:82:LEU:HD12 | 1:O:146:GLY:CA | 2.28 | 0.63 |
| 2:d:260:GLY:HA2 | 2:d:346:MET:HE1 | 1.81 | 0.63 |
| 2:l:89:VAL:HG11 | 2:l:121:LEU:HD21 | 1.79 | 0.63 |
| 2:w:89:VAL:HG23 | 2:w:126:LEU:HD21 | 1.81 | 0.63 |
| 2:x:89:VAL:HG23 | 2:x:126:LEU:HD21 | 1.81 | 0.63 |
| 3:2:45:ARG:O | 3:2:45:ARG:HG2 | 1.97 | 0.63 |
| 1:C:82:LEU:HD12 | 1:C:146:GLY:CA | 2.28 | 0.63 |
| 1:W:37:ALA:HB1 | 1:X:74:ILE:HG22 | 1.79 | 0.63 |
| 2:a:89:VAL:HG23 | 2:a:126:LEU:HD21 | 1.81 | 0.63 |
| 2:b:81:LEU:HD23 | 2:b:81:LEU:H | 1.62 | 0.63 |
| 2:b:89:VAL:HG23 | 2:b:126:LEU:HD21 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:g:81:LEU:H | 2:g:81:LEU:HD23 | 1.62 | 0.63 |
| 2:g:141:ILE:CD1 | 2:g:165:ILE:HD11 | 2.27 | 0.63 |
| 2:l:81:LEU:HD23 | 2:l:81:LEU:H | 1.62 | 0.63 |
| 2:v:89:VAL:HG23 | 2:v:126:LEU:HD21 | 1.81 | 0.63 |
| 2:y:89:VAL:HG23 | 2:y:126:LEU:HD21 | 1.81 | 0.63 |
| 2:z:81:LEU:H | 2:z:81:LEU:HD23 | 1.62 | 0.63 |
| 1:D:82:LEU:HD12 | 1:D:146:GLY:CA | 2.28 | 0.63 |
| 1:E:82:LEU:HD12 | 1:E:146:GLY:CA | 2.28 | 0.63 |
| 2:b:141:ILE:CD1 | 2:b:165:ILE:HD11 | 2.27 | 0.63 |
| 2:c:260:GLY:HA2 | 2:c:346:MET:HE1 | 1.81 | 0.63 |
| 2:h:141:ILE:CD1 | 2:h:165:ILE:HD11 | 2.27 | 0.63 |
| 2:i:89:VAL:HG11 | 2:i:121:LEU:HD21 | 1.79 | 0.63 |
| 2:w:141:ILE:CD1 | 2:w:165:ILE:HD11 | 2.27 | 0.63 |
| 2:y:345:LEU:HD21 | 2:z:319:LEU:HD22 | 1.79 | 0.63 |
| 1:J:37:ALA:HB1 | 1:K:74:ILE:HG22 | 1.79 | 0.63 |
| 1:X:82:LEU:HD12 | 1:X:146:GLY:CA | 2.28 | 0.63 |
| 2:a:260:GLY:HA2 | 2:a:346:MET:HE1 | 1.81 | 0.63 |
| 2:e:260:GLY:HA2 | 2:e:346:MET:HE1 | 1.81 | 0.63 |
| 2:h:89:VAL:HG11 | 2:h:121:LEU:HD21 | 1.79 | 0.63 |
| 2:i:260:GLY:HA2 | 2:i:346:MET:HE1 | 1.81 | 0.63 |
| 2:j:89:VAL:HG11 | 2:j:121:LEU:HD21 | 1.79 | 0.63 |
| 2:q:141:ILE:CD1 | 2:q:165:ILE:HD11 | 2.27 | 0.63 |
| 2:r:46:ASP:OD1 | 2:s:161:ASN:HB2 | 1.99 | 0.63 |
| 1:B:37:ALA:HB1 | 1:C:74:ILE:HG22 | 1.79 | 0.63 |
| 1:B:82:LEU:HD12 | 1:B:146:GLY:CA | 2.28 | 0.63 |
| 1:A:74:ILE:HG22 | 1:Z:37:ALA:HB1 | 1.79 | 0.63 |
| 2:c:89:VAL:HG23 | 2:c:126:LEU:HD21 | 1.81 | 0.63 |
| 2:g:89:VAL:HG11 | 2:g:121:LEU:HD21 | 1.79 | 0.63 |
| 2:g:142:LEU:HD23 | 2:i:350:GLN:NE2 | 2.14 | 0.63 |
| 2:h:260:GLY:HA2 | 2:h:346:MET:HE1 | 1.81 | 0.63 |
| 2:j:260:GLY:HA2 | 2:j:346:MET:HE1 | 1.81 | 0.63 |
| 2:k:89:VAL:HG11 | 2:k:121:LEU:HD21 | 1.79 | 0.63 |
| 2:v:196:MET:O | 2:v:196:MET:HE3 | 1.99 | 0.63 |
| 1:F:82:LEU:HD12 | 1:F:146:GLY:CA | 2.28 | 0.63 |
| 1:I:82:LEU:HD12 | 1:I:146:GLY:CA | 2.28 | 0.63 |
| 1:A:82:LEU:HD12 | 1:A:146:GLY:CA | 2.28 | 0.63 |
| 2:b:142:LEU:HD23 | 2:d:350:GLN:NE2 | 2.14 | 0.63 |
| 2:d:89:VAL:HG23 | 2:d:126:LEU:HD21 | 1.80 | 0.63 |
| 2:f:260:GLY:HA2 | 2:f:346:MET:HE1 | 1.81 | 0.63 |
| 2:g:260:GLY:HA2 | 2:g:346:MET:HE1 | 1.81 | 0.63 |
| 2:p:81:LEU:HD23 | 2:p:81:LEU:H | 1.62 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:t:142:LEU:HD23 | 2:v:350:GLN:NE2 | 2.14 | 0.63 |
| 2:u:89:VAL:HG23 | 2:u:126:LEU:HD21 | 1.81 | 0.63 |
| 2:z:260:GLY:HA2 | 2:z:346:MET:HE1 | 1.81 | 0.63 |
| 3:18:45:ARG:HG2 | 3:18:45:ARG:O | 1.97 | 0.63 |
| 1:R:37:ALA:HB1 | 1:S:74:ILE:HG22 | 1.80 | 0.63 |
| 2:a:141:ILE:CD1 | 2:a:165:ILE:HD11 | 2.27 | 0.63 |
| 2:b:260:GLY:HA2 | 2:b:346:MET:HE1 | 1.81 | 0.63 |
| 2:d:196:MET:HE3 | 2:d:196:MET:O | 1.99 | 0.63 |
| 2:l:260:GLY:HA2 | 2:l:346:MET:HE1 | 1.81 | 0.63 |
| 2:m:260:GLY:HA2 | 2:m:346:MET:HE1 | 1.81 | 0.63 |
| 2:s:142:LEU:HD23 | 2:u:350:GLN:NE2 | 2.14 | 0.63 |
| 2:u:81:LEU:HD23 | 2:u:81:LEU:H | 1.62 | 0.63 |
| 2:u:196:MET:O | 2:u:196:MET:HE3 | 1.99 | 0.63 |
| 3:22:18:ARG:NH2 | 3:22:45:ARG:O | 2.32 | 0.63 |
| 3:24:18:ARG:NH2 | 3:24:45:ARG:O | 2.32 | 0.63 |
| 1:Q:82:LEU:HD12 | 1:Q:146:GLY:CA | 2.28 | 0.63 |
| 2:c:196:MET:O | 2:c:196:MET:HE3 | 1.99 | 0.63 |
| 2:e:196:MET:O | 2:e:196:MET:HE3 | 1.99 | 0.63 |
| 2:j:196:MET:O | 2:j:196:MET:HE3 | 1.99 | 0.63 |
| 2:k:196:MET:O | 2:k:196:MET:HE3 | 1.99 | 0.63 |
| 2:k:260:GLY:HA2 | 2:k:346:MET:HE1 | 1.81 | 0.63 |
| 2:o:196:MET:HE3 | 2:o:196:MET:O | 1.99 | 0.63 |
| 2:w:196:MET:HE3 | 2:w:196:MET:O | 1.99 | 0.63 |
| 2:y:260:GLY:HA2 | 2:y:346:MET:HE1 | 1.81 | 0.63 |
| 3:20:18:ARG:NH2 | 3:20:45:ARG:O | 2.32 | 0.63 |
| 3:21:18:ARG:NH2 | 3:21:45:ARG:O | 2.32 | 0.63 |
| 3:26:18:ARG:NH2 | 3:26:45:ARG:O | 2.32 | 0.63 |
| 1:E:37:ALA:HB1 | 1:F:74:ILE:HG22 | 1.79 | 0.63 |
| 1:G:82:LEU:HD12 | 1:G:146:GLY:CA | 2.28 | 0.63 |
| 2:a:81:LEU:HD23 | 2:a:81:LEU:H | 1.62 | 0.62 |
| 2:a:345:LEU:HD21 | 2:b:319:LEU:HD22 | 1.80 | 0.62 |
| 2:a:365:ILE:HG23 | 2:z:164:ARG:NH1 | 2.14 | 0.62 |
| 2:b:196:MET:O | 2:b:196:MET:HE3 | 1.99 | 0.62 |
| 2:e:142:LEU:HD23 | 2:g:350:GLN:NE2 | 2.14 | 0.62 |
| 2:h:142:LEU:HD23 | 2:j:350:GLN:NE2 | 2.14 | 0.62 |
| 2:n:196:MET:O | 2:n:196:MET:HE3 | 1.99 | 0.62 |
| 2:p:196:MET:O | 2:p:196:MET:HE3 | 1.99 | 0.62 |
| 2:q:196:MET:O | 2:q:196:MET:HE3 | 1.99 | 0.62 |
| 2:t:89:VAL:HG23 | 2:t:126:LEU:HD21 | 1.81 | 0.62 |
| 2:u:123:MET:HE3 | 2:u:123:MET:C | 2.25 | 0.62 |
| 2:x:141:ILE:CD1 | 2:x:165:ILE:HD11 | 2.27 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:18:18:ARG:NH2 | 3:18:45:ARG:O | 2.32 | 0.62 |
| 3:19:18:ARG:NH2 | 3:19:45:ARG:O | 2.32 | 0.62 |
| 3:23:18:ARG:NH2 | 3:23:45:ARG:O | 2.32 | 0.62 |
| 3:25:18:ARG:NH2 | 3:25:45:ARG:O | 2.32 | 0.62 |
| 1:Y:82:LEU:HD12 | 1:Y:146:GLY:CA | 2.28 | 0.62 |
| 1:Z:82:LEU:HD12 | 1:Z:146:GLY:CA | 2.28 | 0.62 |
| 2:d:123:MET:C | 2:d:123:MET:HE3 | 2.25 | 0.62 |
| 2:f:196:MET:O | 2:f:196:MET:HE3 | 1.99 | 0.62 |
| 2:i:196:MET:O | 2:i:196:MET:HE3 | 1.99 | 0.62 |
| 2:j:142:LEU:HD23 | 2:l:350:GLN:NE2 | 2.14 | 0.62 |
| 2:k:89:VAL:HG23 | 2:k:126:LEU:HD21 | 1.81 | 0.62 |
| 2:k:123:MET:HE3 | 2:k:123:MET:C | 2.25 | 0.62 |
| 2:m:196:MET:O | 2:m:196:MET:HE3 | 1.99 | 0.62 |
| 2:s:123:MET:HE3 | 2:s:123:MET:C | 2.24 | 0.62 |
| 3:16:18:ARG:NH2 | 3:16:45:ARG:O | 2.32 | 0.62 |
| 3:1:18:ARG:NH2 | 3:1:45:ARG:O | 2.32 | 0.62 |
| 2:b:123:MET:C | 2:b:123:MET:HE3 | 2.24 | 0.62 |
| 2:e:89:VAL:HG23 | 2:e:126:LEU:HD21 | 1.81 | 0.62 |
| 2:j:89:VAL:HG23 | 2:j:126:LEU:HD21 | 1.81 | 0.62 |
| 2:j:123:MET:C | 2:j:123:MET:HE3 | 2.25 | 0.62 |
| 2:l:89:VAL:HG23 | 2:l:126:LEU:HD21 | 1.81 | 0.62 |
| 2:l:123:MET:C | 2:l:123:MET:HE3 | 2.25 | 0.62 |
| 2:l:142:LEU:HD23 | 2:n:350:GLN:NE2 | 2.14 | 0.62 |
| 2:n:260:GLY:HA2 | 2:n:346:MET:HE1 | 1.81 | 0.62 |
| 2:r:196:MET:O | 2:r:196:MET:HE3 | 1.99 | 0.62 |
| 2:s:196:MET:O | 2:s:196:MET:HE3 | 1.99 | 0.62 |
| 2:s:345:LEU:HD21 | 2:t:319:LEU:HD22 | 1.80 | 0.62 |
| 2:t:123:MET:C | 2:t:123:MET:HE3 | 2.24 | 0.62 |
| 2:u:164:ARG:NH1 | 2:v:365:ILE:HG23 | 2.15 | 0.62 |
| 2:x:196:MET:O | 2:x:196:MET:HE3 | 1.99 | 0.62 |
| 1:H:82:LEU:HD12 | 1:H:146:GLY:CA | 2.28 | 0.62 |
| 1:V:167:LYS:HD3 | 1:W:203:ALA:CB | 2.30 | 0.62 |
| 2:f:123:MET:HE3 | 2:f:123:MET:C | 2.25 | 0.62 |
| 2:i:123:MET:HE3 | 2:i:123:MET:C | 2.25 | 0.62 |
| 2:k:142:LEU:HD23 | 2:m:350:GLN:NE2 | 2.13 | 0.62 |
| 2:l:178:GLN:HG3 | 1:J:47:ALA:O | 2.00 | 0.62 |
| 2:l:196:MET:HE3 | 2:l:196:MET:O | 1.99 | 0.62 |
| 2:m:89:VAL:HG23 | 2:m:126:LEU:HD21 | 1.81 | 0.62 |
| 2:n:89:VAL:HG23 | 2:n:126:LEU:HD21 | 1.81 | 0.62 |
| 2:v:142:LEU:HD23 | 2:x:350:GLN:NE2 | 2.14 | 0.62 |
| 2:w:123:MET:C | 2:w:123:MET:HE3 | 2.25 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:w:260:GLY:HA2 | 2:w:346:MET:HE1 | 1.81 | 0.62 |
| 2:z:141:ILE:CD1 | 2:z:165:ILE:HD11 | 2.27 | 0.62 |
| 2:g:345:LEU:HD21 | 2:h:319:LEU:HD22 | 1.80 | 0.62 |
| 2:i:89:VAL:HG23 | 2:i:126:LEU:HD21 | 1.81 | 0.62 |
| 2:m:345:LEU:HD21 | 2:n:319:LEU:HD22 | 1.80 | 0.62 |
| 2:r:123:MET:C | 2:r:123:MET:HE3 | 2.25 | 0.62 |
| 2:r:178:GLN:HG3 | 1:P:47:ALA:O | 2.00 | 0.62 |
| 2:t:196:MET:HE3 | 2:t:196:MET:O | 1.99 | 0.62 |
| 2:v:260:GLY:HA2 | 2:v:346:MET:HE1 | 1.81 | 0.62 |
| 3:2:18:ARG:NH2 | 3:2:45:ARG:O | 2.32 | 0.62 |
| 3:3:18:ARG:NH2 | 3:3:45:ARG:O | 2.32 | 0.62 |
| 3:17:18:ARG:NH2 | 3:17:45:ARG:O | 2.32 | 0.62 |
| 1:V:37:ALA:HB1 | 1:W:74:ILE:HG22 | 1.79 | 0.62 |
| 2:x:260:GLY:HA2 | 2:x:346:MET:HE1 | 1.81 | 0.62 |
| 2:z:123:MET:C | 2:z:123:MET:HE3 | 2.25 | 0.62 |
| 3:14:18:ARG:NH2 | 3:14:45:ARG:O | 2.32 | 0.62 |
| 2:a:196:MET:O | 2:a:196:MET:HE3 | 1.99 | 0.62 |
| 2:b:350:GLN:NE2 | 2:z:142:LEU:HD23 | 2.14 | 0.62 |
| 2:h:123:MET:HE3 | 2:h:123:MET:C | 2.25 | 0.62 |
| 2:m:142:LEU:HD23 | 2:o:350:GLN:NE2 | 2.14 | 0.62 |
| 2:o:89:VAL:HG23 | 2:o:126:LEU:HD21 | 1.81 | 0.62 |
| 2:s:89:VAL:HG23 | 2:s:126:LEU:HD21 | 1.81 | 0.62 |
| 2:u:260:GLY:HA2 | 2:u:346:MET:HE1 | 1.81 | 0.62 |
| 2:y:123:MET:HE3 | 2:y:123:MET:C | 2.25 | 0.62 |
| 2:y:141:ILE:CD1 | 2:y:165:ILE:HD11 | 2.27 | 0.62 |
| 1:A:37:ALA:HB1 | 1:B:74:ILE:HG22 | 1.80 | 0.62 |
| 2:c:123:MET:HE3 | 2:c:123:MET:C | 2.25 | 0.62 |
| 2:d:46:ASP:OD1 | 2:e:161:ASN:HB2 | 2.00 | 0.62 |
| 2:e:46:ASP:OD1 | 2:f:161:ASN:HB2 | 1.99 | 0.62 |
| 2:f:178:GLN:HG3 | 1:D:47:ALA:O | 2.00 | 0.62 |
| 2:h:89:VAL:HG23 | 2:h:126:LEU:HD21 | 1.81 | 0.62 |
| 2:k:46:ASP:OD1 | 2:l:161:ASN:HB2 | 1.99 | 0.62 |
| 2:m:123:MET:HE3 | 2:m:123:MET:C | 2.25 | 0.62 |
| 2:p:46:ASP:OD1 | 2:q:161:ASN:HB2 | 2.00 | 0.62 |
| 2:q:123:MET:HE3 | 2:q:123:MET:C | 2.25 | 0.62 |
| 2:q:260:GLY:HA2 | 2:q:346:MET:HE1 | 1.81 | 0.62 |
| 2:t:46:ASP:OD1 | 2:u:161:ASN:HB2 | 2.00 | 0.62 |
| 2:v:46:ASP:OD1 | 2:w:161:ASN:HB2 | 2.00 | 0.62 |
| 2:z:178:GLN:HG3 | 1:X:47:ALA:O | 1.99 | 0.62 |
| 3:5:18:ARG:NH2 | 3:5:45:ARG:O | 2.32 | 0.62 |
| 3:10:18:ARG:NH2 | 3:10:45:ARG:O | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:W:167:LYS:HD3 | 1:X:203:ALA:CB | 2.30 | 0.62 |
| 2:a:123:MET:C | 2:a:123:MET:HE3 | 2.25 | 0.62 |
| 2:a:319:LEU:HD22 | 2:z:345:LEU:HD21 | 1.80 | 0.62 |
| 2:b:46:ASP:OD1 | 2:c:161:ASN:HB2 | 2.00 | 0.62 |
| 2:c:164:ARG:NH1 | 2:d:365:ILE:HG23 | 2.15 | 0.62 |
| 2:f:164:ARG:NH1 | 2:g:365:ILE:HG23 | 2.14 | 0.62 |
| 2:p:89:VAL:HG23 | 2:p:126:LEU:HD21 | 1.81 | 0.62 |
| 2:r:260:GLY:HA2 | 2:r:346:MET:HE1 | 1.81 | 0.62 |
| 3:7:18:ARG:NH2 | 3:7:45:ARG:O | 2.32 | 0.62 |
| 2:f:89:VAL:HG23 | 2:f:126:LEU:HD21 | 1.81 | 0.62 |
| 2:g:196:MET:HE3 | 2:g:196:MET:O | 1.99 | 0.62 |
| 2:h:196:MET:O | 2:h:196:MET:HE3 | 1.99 | 0.62 |
| 2:o:260:GLY:HA2 | 2:o:346:MET:HE1 | 1.81 | 0.62 |
| 2:p:260:GLY:HA2 | 2:p:346:MET:HE1 | 1.81 | 0.62 |
| 2:g:123:MET:C | 2:g:123:MET:HE3 | 2.25 | 0.61 |
| 2:n:142:LEU:HD23 | 2:p:350:GLN:NE2 | 2.14 | 0.61 |
| 2:p:123:MET:HE3 | 2:p:123:MET:C | 2.25 | 0.61 |
| 2:s:260:GLY:HA2 | 2:s:346:MET:HE1 | 1.81 | 0.61 |
| 2:t:260:GLY:HA2 | 2:t:346:MET:HE1 | 1.81 | 0.61 |
| 2:w:46:ASP:OD1 | 2:x:161:ASN:HB2 | 1.99 | 0.61 |
| 2:x:89:VAL:HG23 | 2:x:126:LEU:CD2 | 2.30 | 0.61 |
| 2:x:123:MET:HE3 | 2:x:123:MET:C | 2.25 | 0.61 |
| 2:y:196:MET:O | 2:y:196:MET:HE3 | 1.99 | 0.61 |
| 2:z:89:VAL:HG23 | 2:z:126:LEU:CD2 | 2.30 | 0.61 |
| 2:z:196:MET:HE3 | 2:z:196:MET:O | 1.99 | 0.61 |
| 3:9:18:ARG:NH2 | 3:9:45:ARG:O | 2.32 | 0.61 |
| 3:12:18:ARG:NH2 | 3:12:45:ARG:O | 2.32 | 0.61 |
| 2:a:164:ARG:NH1 | 2:b:365:ILE:HG23 | 2.15 | 0.61 |
| 2:c:89:VAL:HG23 | 2:c:126:LEU:CD2 | 2.30 | 0.61 |
| 2:g:89:VAL:HG23 | 2:g:126:LEU:HD21 | 1.81 | 0.61 |
| 2:n:123:MET:HE3 | 2:n:123:MET:C | 2.25 | 0.61 |
| 2:a:89:VAL:HG23 | 2:a:126:LEU:CD2 | 2.30 | 0.61 |
| 2:e:89:VAL:HG23 | 2:e:126:LEU:CD2 | 2.30 | 0.61 |
| 2:q:89:VAL:HG23 | 2:q:126:LEU:HD21 | 1.81 | 0.61 |
| 2:v:123:MET:HE3 | 2:v:123:MET:C | 2.25 | 0.61 |
| 2:w:196:MET:HE3 | 2:w:196:MET:CA | 2.31 | 0.61 |
| 2:y:196:MET:HE3 | 2:y:196:MET:CA | 2.31 | 0.61 |
| 3:4:18:ARG:NH2 | 3:4:45:ARG:O | 2.32 | 0.61 |
| 2:a:142:LEU:HD23 | 2:c:350:GLN:NE2 | 2.14 | 0.61 |
| 2:b:89:VAL:HG23 | 2:b:126:LEU:CD2 | 2.30 | 0.61 |
| 2:d:142:LEU:HD23 | 2:f:350:GLN:NE2 | 2.14 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:e:123:MET:HE3 | 2:e:123:MET:C | 2.25 | 0.61 |
| 2:s:196:MET:HE3 | 2:s:196:MET:CA | 2.31 | 0.61 |
| 2:u:196:MET:HE3 | 2:u:196:MET:CA | 2.31 | 0.61 |
| 3:15:18:ARG:NH2 | 3:15:45:ARG:O | 2.32 | 0.61 |
| 1:J:167:LYS:HD3 | 1:K:203:ALA:CB | 2.30 | 0.61 |
| 1:T:167:LYS:HD3 | 1:U:203:ALA:CB | 2.30 | 0.61 |
| 2:a:39:TYR:CE1 | 2:a:61:THR:HG21 | 2.36 | 0.61 |
| 2:b:39:TYR:CE1 | 2:b:61:THR:HG21 | 2.36 | 0.61 |
| 2:m:164:ARG:NH1 | 2:n:365:ILE:HG23 | 2.15 | 0.61 |
| 2:o:123:MET:C | 2:o:123:MET:HE3 | 2.25 | 0.61 |
| 2:q:142:LEU:HD23 | 2:s:350:GLN:NE2 | 2.15 | 0.61 |
| 2:r:142:LEU:HD23 | 2:t:350:GLN:NE2 | 2.15 | 0.61 |
| 2:s:164:ARG:NH1 | 2:t:365:ILE:HG23 | 2.15 | 0.61 |
| 2:y:89:VAL:HG23 | 2:y:126:LEU:CD2 | 2.30 | 0.61 |
| 3:8:18:ARG:NH2 | 3:8:45:ARG:O | 2.32 | 0.61 |
| 3:13:18:ARG:NH2 | 3:13:45:ARG:O | 2.32 | 0.61 |
| 1:U:167:LYS:HD3 | 1:V:203:ALA:CB | 2.31 | 0.61 |
| 2:a:196:MET:HE3 | 2:a:196:MET:CA | 2.31 | 0.61 |
| 3:1:77:CYS:HB3 | 3:1:80:TYR:HE1 | 1.66 | 0.61 |
| 2:d:39:TYR:CE1 | 2:d:61:THR:HG21 | 2.36 | 0.61 |
| 2:q:196:MET:HE3 | 2:q:196:MET:CA | 2.31 | 0.61 |
| 2:r:89:VAL:HG23 | 2:r:126:LEU:HD21 | 1.81 | 0.61 |
| 2:v:89:VAL:HG23 | 2:v:126:LEU:CD2 | 2.30 | 0.61 |
| 2:v:196:MET:HE3 | 2:v:196:MET:CA | 2.31 | 0.61 |
| 3:26:77:CYS:HB3 | 3:26:80:TYR:HE1 | 1.66 | 0.61 |
| 2:c:39:TYR:CE1 | 2:c:61:THR:HG21 | 2.36 | 0.61 |
| 2:l:46:ASP:OD1 | 2:m:161:ASN:HB2 | 2.00 | 0.61 |
| 2:n:46:ASP:OD1 | 2:o:161:ASN:HB2 | 2.00 | 0.61 |
| 2:p:142:LEU:HD23 | 2:r:350:GLN:NE2 | 2.14 | 0.61 |
| 2:x:178:GLN:HG3 | 1:V:47:ALA:O | 2.00 | 0.61 |
| 2:y:39:TYR:CE1 | 2:y:61:THR:HG21 | 2.36 | 0.61 |
| 3:6:47:ASP:OD2 | 3:6:50:VAL:HG23 | 2.01 | 0.61 |
| 3:25:77:CYS:HB3 | 3:25:80:TYR:HE1 | 1.66 | 0.61 |
| 1:D:167:LYS:HD3 | 1:E:203:ALA:CB | 2.30 | 0.61 |
| 2:g:46:ASP:OD1 | 2:h:161:ASN:HB2 | 2.00 | 0.61 |
| 2:i:164:ARG:NH1 | 2:j:365:ILE:HG23 | 2.15 | 0.61 |
| 2:o:164:ARG:NH1 | 2:p:365:ILE:HG23 | 2.15 | 0.61 |
| 2:v:39:TYR:CE1 | 2:v:61:THR:HG21 | 2.36 | 0.61 |
| 2:x:196:MET:HE3 | 2:x:196:MET:CA | 2.31 | 0.61 |
| 2:z:39:TYR:CE1 | 2:z:61:THR:HG21 | 2.36 | 0.61 |
| 3:3:47:ASP:OD2 | 3:3:50:VAL:HG23 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:6:18:ARG:NH2 | 3:6:45:ARG:O | 2.32 | 0.61 |
| 1:B:167:LYS:HD3 | 1:C:203:ALA:CB | 2.31 | 0.61 |
| 2:b:164:ARG:NH1 | 2:c:365:ILE:HG23 | 2.16 | 0.61 |
| 2:c:142:LEU:HD23 | 2:e:350:GLN:NE2 | 2.16 | 0.61 |
| 2:f:39:TYR:CE1 | 2:f:61:THR:HG21 | 2.36 | 0.61 |
| 2:g:39:TYR:CE1 | 2:g:61:THR:HG21 | 2.36 | 0.61 |
| 2:l:89:VAL:HG23 | 2:l:126:LEU:CD2 | 2.30 | 0.61 |
| 2:t:164:ARG:NH1 | 2:u:365:ILE:HG23 | 2.16 | 0.61 |
| 2:t:196:MET:HE3 | 2:t:196:MET:CA | 2.31 | 0.61 |
| 2:u:142:LEU:HD23 | 2:w:350:GLN:NE2 | 2.16 | 0.61 |
| 2:x:39:TYR:CE1 | 2:x:61:THR:HG21 | 2.36 | 0.61 |
| 3:2:77:CYS:HB3 | 3:2:80:TYR:HE1 | 1.66 | 0.61 |
| 3:7:47:ASP:OD2 | 3:7:50:VAL:HG23 | 2.01 | 0.61 |
| 3:16:77:CYS:HB3 | 3:16:80:TYR:HE1 | 1.66 | 0.61 |
| 3:17:77:CYS:HB3 | 3:17:80:TYR:HE1 | 1.66 | 0.61 |
| 3:24:77:CYS:HB3 | 3:24:80:TYR:HE1 | 1.66 | 0.61 |
| 1:K:167:LYS:HD3 | 1:L:203:ALA:CB | 2.30 | 0.61 |
| 1:P:167:LYS:HD3 | 1:Q:203:ALA:CB | 2.30 | 0.61 |
| 1:R:167:LYS:HD3 | 1:S:203:ALA:CB | 2.30 | 0.61 |
| 2:i:39:TYR:CE1 | 2:i:61:THR:HG21 | 2.36 | 0.61 |
| 2:i:46:ASP:OD1 | 2:j:161:ASN:HB2 | 2.01 | 0.61 |
| 2:o:196:MET:HE3 | 2:o:196:MET:CA | 2.31 | 0.61 |
| 2:q:46:ASP:OD1 | 2:r:161:ASN:HB2 | 1.99 | 0.61 |
| 2:q:178:GLN:HG3 | 1:O:47:ALA:O | 2.01 | 0.61 |
| 2:r:196:MET:HE3 | 2:r:196:MET:CA | 2.31 | 0.61 |
| 2:s:178:GLN:HG3 | 1:Q:47:ALA:O | 2.01 | 0.61 |
| 3:10:47:ASP:OD2 | 3:10:50:VAL:HG23 | 2.01 | 0.61 |
| 3:11:18:ARG:NH2 | 3:11:45:ARG:O | 2.32 | 0.61 |
| 3:15:77:CYS:HB3 | 3:15:80:TYR:HE1 | 1.66 | 0.61 |
| 3:20:47:ASP:OD2 | 3:20:50:VAL:HG23 | 2.01 | 0.61 |
| 1:Q:167:LYS:HD3 | 1:R:203:ALA:CB | 2.30 | 0.61 |
| 2:a:161:ASN:HB2 | 2:z:46:ASP:OD1 | 2.01 | 0.60 |
| 2:c:46:ASP:OD1 | 2:d:161:ASN:HB2 | 2.01 | 0.60 |
| 2:g:89:VAL:HG23 | 2:g:126:LEU:CD2 | 2.30 | 0.60 |
| 2:h:39:TYR:CE1 | 2:h:61:THR:HG21 | 2.36 | 0.60 |
| 2:j:89:VAL:HG23 | 2:j:126:LEU:CD2 | 2.30 | 0.60 |
| 2:n:89:VAL:HG23 | 2:n:126:LEU:CD2 | 2.30 | 0.60 |
| 2:p:196:MET:HE3 | 2:p:196:MET:CA | 2.31 | 0.60 |
| 2:s:101:GLN:HE22 | 2:t:219:ARG:HD3 | 1.66 | 0.60 |
| 3:5:47:ASP:OD2 | 3:5:50:VAL:HG23 | 2.01 | 0.60 |
| 3:14:77:CYS:HB3 | 3:14:80:TYR:HE1 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:18:77:CYS:HB3 | 3:18:80:TYR:HE1 | 1.66 | 0.60 |
| 1:C:58:ILE:HG13 | 1:C:59:ASN:H | 1.66 | 0.60 |
| 1:I:58:ILE:HG13 | 1:I:59:ASN:H | 1.66 | 0.60 |
| 1:S:167:LYS:HD3 | 1:T:203:ALA:CB | 2.31 | 0.60 |
| 2:a:46:ASP:OD1 | 2:b:161:ASN:HB2 | 2.01 | 0.60 |
| 2:a:219:ARG:HD3 | 2:z:101:GLN:HE22 | 1.66 | 0.60 |
| 2:c:196:MET:HE3 | 2:c:196:MET:CA | 2.31 | 0.60 |
| 2:h:89:VAL:HG23 | 2:h:126:LEU:CD2 | 2.30 | 0.60 |
| 2:k:89:VAL:HG23 | 2:k:126:LEU:CD2 | 2.30 | 0.60 |
| 2:m:178:GLN:HG3 | 1:K:47:ALA:O | 2.01 | 0.60 |
| 2:q:89:VAL:HG23 | 2:q:126:LEU:CD2 | 2.30 | 0.60 |
| 2:u:46:ASP:OD1 | 2:v:161:ASN:HB2 | 2.01 | 0.60 |
| 3:3:77:CYS:HB3 | 3:3:80:TYR:HE1 | 1.66 | 0.60 |
| 3:19:47:ASP:OD2 | 3:19:50:VAL:HG23 | 2.01 | 0.60 |
| 3:21:47:ASP:OD2 | 3:21:50:VAL:HG23 | 2.01 | 0.60 |
| 3:23:77:CYS:HB3 | 3:23:80:TYR:HE1 | 1.66 | 0.60 |
| 1:D:58:ILE:HG13 | 1:D:59:ASN:H | 1.67 | 0.60 |
| 1:H:58:ILE:HG13 | 1:H:59:ASN:H | 1.66 | 0.60 |
| 1:X:58:ILE:HG13 | 1:X:59:ASN:H | 1.66 | 0.60 |
| 2:h:164:ARG:NH1 | 2:i:365:ILE:HG23 | 2.16 | 0.60 |
| 2:i:89:VAL:HG23 | 2:i:126:LEU:CD2 | 2.30 | 0.60 |
| 2:j:39:TYR:CE1 | 2:j:61:THR:HG21 | 2.36 | 0.60 |
| 2:j:46:ASP:OD1 | 2:k:161:ASN:HB2 | 2.00 | 0.60 |
| 2:p:89:VAL:HG23 | 2:p:126:LEU:CD2 | 2.30 | 0.60 |
| 2:s:46:ASP:OD1 | 2:t:161:ASN:HB2 | 2.00 | 0.60 |
| 2:s:89:VAL:HG23 | 2:s:126:LEU:CD2 | 2.30 | 0.60 |
| 2:t:89:VAL:HG23 | 2:t:126:LEU:CD2 | 2.30 | 0.60 |
| 2:w:89:VAL:HG23 | 2:w:126:LEU:CD2 | 2.30 | 0.60 |
| 2:z:196:MET:HE3 | 2:z:196:MET:CA | 2.31 | 0.60 |
| 3:2:47:ASP:OD2 | 3:2:50:VAL:HG23 | 2.01 | 0.60 |
| 3:4:47:ASP:OD2 | 3:4:50:VAL:HG23 | 2.01 | 0.60 |
| 1:H:167:LYS:HD3 | 1:I:203:ALA:CB | 2.30 | 0.60 |
| 1:L:167:LYS:HD3 | 1:M:203:ALA:CB | 2.31 | 0.60 |
| 1:N:58:ILE:HG13 | 1:N:59:ASN:H | 1.67 | 0.60 |
| 1:Q:58:ILE:HG13 | 1:Q:59:ASN:H | 1.66 | 0.60 |
| 2:d:89:VAL:HG23 | 2:d:126:LEU:CD2 | 2.30 | 0.60 |
| 2:f:89:VAL:HG23 | 2:f:126:LEU:CD2 | 2.30 | 0.60 |
| 2:f:196:MET:HE3 | 2:f:196:MET:CA | 2.31 | 0.60 |
| 2:g:164:ARG:NH1 | 2:h:365:ILE:HG23 | 2.15 | 0.60 |
| 2:h:46:ASP:OD1 | 2:i:161:ASN:HB2 | 2.00 | 0.60 |
| 2:i:142:LEU:HD23 | 2:k:350:GLN:NE2 | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:j:164:ARG:NH1 | 2:k:365:ILE:HG23 | 2.16 | 0.60 |
| 2:n:271:ASP:CB | 2:n:357:CYS:HA | 2.28 | 0.60 |
| 2:o:89:VAL:HG23 | 2:o:126:LEU:CD2 | 2.30 | 0.60 |
| 2:q:101:GLN:HE22 | 2:r:219:ARG:HD3 | 1.67 | 0.60 |
| 2:r:89:VAL:HG23 | 2:r:126:LEU:CD2 | 2.30 | 0.60 |
| 2:s:39:TYR:CE1 | 2:s:61:THR:HG21 | 2.36 | 0.60 |
| 2:t:39:TYR:CE1 | 2:t:61:THR:HG21 | 2.36 | 0.60 |
| 2:u:39:TYR:CE1 | 2:u:61:THR:HG21 | 2.36 | 0.60 |
| 3:9:47:ASP:OD2 | 3:9:50:VAL:HG23 | 2.01 | 0.60 |
| 1:F:167:LYS:HD3 | 1:G:203:ALA:CB | 2.30 | 0.60 |
| 1:N:167:LYS:HD3 | 1:O:203:ALA:CB | 2.30 | 0.60 |
| 1:Y:58:ILE:HG13 | 1:Y:59:ASN:H | 1.66 | 0.60 |
| 2:e:101:GLN:HE22 | 2:f:219:ARG:HD3 | 1.67 | 0.60 |
| 2:f:46:ASP:OD1 | 2:g:161:ASN:HB2 | 2.01 | 0.60 |
| 2:g:196:MET:HE3 | 2:g:196:MET:CA | 2.31 | 0.60 |
| 2:k:39:TYR:CE1 | 2:k:61:THR:HG21 | 2.36 | 0.60 |
| 2:k:178:GLN:HG3 | 1:I:47:ALA:O | 2.01 | 0.60 |
| 2:l:39:TYR:CE1 | 2:l:61:THR:HG21 | 2.36 | 0.60 |
| 2:l:164:ARG:NH1 | 2:m:365:ILE:HG23 | 2.15 | 0.60 |
| 2:m:46:ASP:OD1 | 2:n:161:ASN:HB2 | 2.00 | 0.60 |
| 2:n:196:MET:HE3 | 2:n:196:MET:CA | 2.31 | 0.60 |
| 2:o:46:ASP:OD1 | 2:p:161:ASN:HB2 | 2.01 | 0.60 |
| 2:q:164:ARG:NH1 | 2:r:365:ILE:HG23 | 2.17 | 0.60 |
| 2:w:101:GLN:HE22 | 2:x:219:ARG:HD3 | 1.67 | 0.60 |
| 2:y:72:THR:OG1 | 1:Z:70:ARG:NH2 | 2.30 | 0.60 |
| 3:12:77:CYS:HB3 | 3:12:80:TYR:HE1 | 1.66 | 0.60 |
| 3:13:77:CYS:HB3 | 3:13:80:TYR:HE1 | 1.66 | 0.60 |
| 3:20:77:CYS:HB3 | 3:20:80:TYR:HE1 | 1.66 | 0.60 |
| 3:22:47:ASP:OD2 | 3:22:50:VAL:HG23 | 2.01 | 0.60 |
| 1:C:167:LYS:HD3 | 1:D:203:ALA:CB | 2.31 | 0.60 |
| 1:I:167:LYS:HD3 | 1:J:203:ALA:CB | 2.31 | 0.60 |
| 1:J:58:ILE:HG13 | 1:J:59:ASN:H | 1.66 | 0.60 |
| 1:T:58:ILE:HG13 | 1:T:59:ASN:H | 1.67 | 0.60 |
| 2:d:196:MET:HE3 | 2:d:196:MET:CA | 2.31 | 0.60 |
| 2:e:196:MET:HE3 | 2:e:196:MET:CA | 2.31 | 0.60 |
| 2:f:142:LEU:HD23 | 2:h:350:GLN:NE2 | 2.15 | 0.60 |
| 2:g:101:GLN:HE22 | 2:h:219:ARG:HD3 | 1.66 | 0.60 |
| 2:h:196:MET:HE3 | 2:h:196:MET:CA | 2.31 | 0.60 |
| 2:m:196:MET:HE3 | 2:m:196:MET:CA | 2.31 | 0.60 |
| 2:o:39:TYR:CE1 | 2:o:61:THR:HG21 | 2.36 | 0.60 |
| 2:r:164:ARG:NH1 | 2:s:365:ILE:HG23 | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:u:89:VAL:HG23 | 2:u:126:LEU:CD2 | 2.30 | 0.60 |
| 2:w:39:TYR:CE1 | 2:w:61:THR:HG21 | 2.36 | 0.60 |
| 3:18:47:ASP:OD2 | 3:18:50:VAL:HG23 | 2.01 | 0.60 |
| 3:19:77:CYS:HB3 | 3:19:80:TYR:HE1 | 1.66 | 0.60 |
| 3:21:77:CYS:HB3 | 3:21:80:TYR:HE1 | 1.66 | 0.60 |
| 1:B:58:ILE:HG13 | 1:B:59:ASN:H | 1.66 | 0.60 |
| 1:E:167:LYS:HD3 | 1:F:203:ALA:CB | 2.30 | 0.60 |
| 1:R:58:ILE:HG13 | 1:R:59:ASN:H | 1.66 | 0.60 |
| 2:e:39:TYR:CE1 | 2:e:61:THR:HG21 | 2.36 | 0.60 |
| 2:i:196:MET:HE3 | 2:i:196:MET:CA | 2.31 | 0.60 |
| 2:n:164:ARG:NH1 | 2:o:365:ILE:HG23 | 2.16 | 0.60 |
| 2:o:142:LEU:HD23 | 2:q:350:GLN:NE2 | 2.16 | 0.60 |
| 2:v:164:ARG:NH1 | 2:w:365:ILE:HG23 | 2.16 | 0.60 |
| 3:25:47:ASP:OD2 | 3:25:50:VAL:HG23 | 2.01 | 0.60 |
| 3:26:47:ASP:OD2 | 3:26:50:VAL:HG23 | 2.01 | 0.60 |
| 1:K:58:ILE:HG13 | 1:K:59:ASN:H | 1.67 | 0.60 |
| 1:W:58:ILE:HG13 | 1:W:59:ASN:H | 1.67 | 0.60 |
| 2:g:178:GLN:HG3 | 1:E:47:ALA:O | 2.02 | 0.60 |
| 2:p:164:ARG:NH1 | 2:q:365:ILE:HG23 | 2.16 | 0.60 |
| 3:4:77:CYS:HB3 | 3:4:80:TYR:HE1 | 1.66 | 0.60 |
| 3:8:47:ASP:OD2 | 3:8:50:VAL:HG23 | 2.01 | 0.60 |
| 3:10:72:GLN:CG | 3:10:73:PRO:HD2 | 2.32 | 0.60 |
| 3:11:47:ASP:OD2 | 3:11:50:VAL:HG23 | 2.01 | 0.60 |
| 1:U:58:ILE:HG13 | 1:U:59:ASN:H | 1.66 | 0.60 |
| 1:X:39:PRO:HB3 | 1:Y:75:GLY:HA3 | 1.84 | 0.60 |
| 2:h:271:ASP:CB | 2:h:357:CYS:HA | 2.28 | 0.60 |
| 2:j:196:MET:HE3 | 2:j:196:MET:CA | 2.31 | 0.60 |
| 2:k:164:ARG:NH1 | 2:l:365:ILE:HG23 | 2.17 | 0.60 |
| 2:m:39:TYR:CE1 | 2:m:61:THR:HG21 | 2.36 | 0.60 |
| 2:m:89:VAL:HG23 | 2:m:126:LEU:CD2 | 2.30 | 0.60 |
| 2:p:39:TYR:CE1 | 2:p:61:THR:HG21 | 2.36 | 0.60 |
| 2:r:39:TYR:CE1 | 2:r:61:THR:HG21 | 2.36 | 0.60 |
| 3:9:72:GLN:CG | 3:9:73:PRO:HD2 | 2.32 | 0.60 |
| 3:12:72:GLN:CG | 3:12:73:PRO:HD2 | 2.32 | 0.60 |
| 3:17:47:ASP:OD2 | 3:17:50:VAL:HG23 | 2.01 | 0.60 |
| 1:E:58:ILE:HG13 | 1:E:59:ASN:H | 1.66 | 0.60 |
| 1:M:167:LYS:HD3 | 1:N:203:ALA:CB | 2.31 | 0.60 |
| 1:O:58:ILE:HG13 | 1:O:59:ASN:H | 1.66 | 0.60 |
| 2:b:196:MET:HE3 | 2:b:196:MET:CA | 2.31 | 0.60 |
| 2:c:101:GLN:HE22 | 2:d:219:ARG:HD3 | 1.67 | 0.60 |
| 2:e:164:ARG:NH1 | 2:f:365:ILE:HG23 | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:k:196:MET:HE3 | 2:k:196:MET:CA | 2.31 | 0.60 |
| 2:q:39:TYR:CE1 | 2:q:61:THR:HG21 | 2.36 | 0.60 |
| 2:u:101:GLN:HE22 | 2:v:219:ARG:HD3 | 1.67 | 0.60 |
| 3:8:72:GLN:CG | 3:8:73:PRO:HD2 | 2.32 | 0.60 |
| 3:10:77:CYS:HB3 | 3:10:80:TYR:HE1 | 1.66 | 0.60 |
| 3:11:72:GLN:CG | 3:11:73:PRO:HD2 | 2.32 | 0.60 |
| 3:13:47:ASP:OD2 | 3:13:50:VAL:HG23 | 2.01 | 0.60 |
| 3:13:72:GLN:CG | 3:13:73:PRO:HD2 | 2.32 | 0.60 |
| 3:22:77:CYS:HB3 | 3:22:80:TYR:HE1 | 1.66 | 0.60 |
| 1:G:167:LYS:HD3 | 1:H:203:ALA:CB | 2.31 | 0.60 |
| 2:a:101:GLN:HE22 | 2:b:219:ARG:HD3 | 1.67 | 0.59 |
| 2:o:271:ASP:CB | 2:o:357:CYS:HA | 2.28 | 0.59 |
| 2:w:164:ARG:NH1 | 2:x:365:ILE:HG23 | 2.17 | 0.59 |
| 2:z:269:THR:HG22 | 2:z:326:ALA:O | 2.03 | 0.59 |
| 3:9:77:CYS:HB3 | 3:9:80:TYR:HE1 | 1.66 | 0.59 |
| 3:11:77:CYS:HB3 | 3:11:80:TYR:HE1 | 1.66 | 0.59 |
| 3:15:72:GLN:CG | 3:15:73:PRO:HD2 | 2.32 | 0.59 |
| 3:23:47:ASP:OD2 | 3:23:50:VAL:HG23 | 2.01 | 0.59 |
| 3:24:80:TYR:O | 1:X:26:PRO:HA | 2.02 | 0.59 |
| 2:u:269:THR:HG22 | 2:u:326:ALA:O | 2.03 | 0.59 |
| 3:5:77:CYS:HB3 | 3:5:80:TYR:HE1 | 1.66 | 0.59 |
| 3:7:72:GLN:CG | 3:7:73:PRO:HD2 | 2.32 | 0.59 |
| 3:8:77:CYS:HB3 | 3:8:80:TYR:HE1 | 1.66 | 0.59 |
| 3:8:80:TYR:O | 1:H:26:PRO:HA | 2.03 | 0.59 |
| 3:9:80:TYR:O | 1:I:26:PRO:HA | 2.03 | 0.59 |
| 3:14:47:ASP:OD2 | 3:14:50:VAL:HG23 | 2.01 | 0.59 |
| 3:14:72:GLN:CG | 3:14:73:PRO:HD2 | 2.32 | 0.59 |
| 1:G:58:ILE:HG13 | 1:G:59:ASN:H | 1.66 | 0.59 |
| 1:L:58:ILE:HG13 | 1:L:59:ASN:H | 1.66 | 0.59 |
| 1:O:167:LYS:HD3 | 1:P:203:ALA:CB | 2.31 | 0.59 |
| 1:V:58:ILE:HG13 | 1:V:59:ASN:H | 1.66 | 0.59 |
| 1:A:39:PRO:HB3 | 1:B:75:GLY:HA3 | 1.85 | 0.59 |
| 1:A:167:LYS:HD3 | 1:B:203:ALA:CB | 2.32 | 0.59 |
| 3:1:47:ASP:OD2 | 3:1:50:VAL:HG23 | 2.01 | 0.59 |
| 2:i:178:GLN:HG3 | 1:G:47:ALA:O | 2.03 | 0.59 |
| 2:l:196:MET:HE3 | 2:l:196:MET:CA | 2.31 | 0.59 |
| 2:s:269:THR:HG22 | 2:s:326:ALA:O | 2.03 | 0.59 |
| 3:6:72:GLN:CG | 3:6:73:PRO:HD2 | 2.32 | 0.59 |
| 3:16:72:GLN:CG | 3:16:73:PRO:HD2 | 2.32 | 0.59 |
| 3:23:80:TYR:O | 1:W:26:PRO:HA | 2.03 | 0.59 |
| 1:Z:58:ILE:HG13 | 1:Z:59:ASN:H | 1.66 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:75:GLY:HA3 | 1:Z:39:PRO:HB3 | 1.85 | 0.59 |
| 1:A:203:ALA:CB | 1:Z:167:LYS:HD3 | 2.33 | 0.59 |
| 2:b:269:THR:HG22 | 2:b:326:ALA:O | 2.03 | 0.59 |
| 2:e:178:GLN:HG3 | 1:C:47:ALA:O | 2.01 | 0.59 |
| 2:n:39:TYR:CE1 | 2:n:61:THR:HG21 | 2.36 | 0.59 |
| 2:x:269:THR:HG22 | 2:x:326:ALA:O | 2.02 | 0.59 |
| 3:5:72:GLN:CG | 3:5:73:PRO:HD2 | 2.32 | 0.59 |
| 3:7:77:CYS:HB3 | 3:7:80:TYR:HE1 | 1.66 | 0.59 |
| 3:12:47:ASP:OD2 | 3:12:50:VAL:HG23 | 2.01 | 0.59 |
| 3:15:80:TYR:O | 1:O:26:PRO:HA | 2.03 | 0.59 |
| 3:17:72:GLN:CG | 3:17:73:PRO:HD2 | 2.32 | 0.59 |
| 3:25:80:TYR:O | 1:Y:26:PRO:HA | 2.02 | 0.59 |
| 2:o:101:GLN:HE22 | 2:p:219:ARG:HD3 | 1.67 | 0.59 |
| 2:w:269:THR:HG22 | 2:w:326:ALA:O | 2.03 | 0.59 |
| 3:3:72:GLN:CG | 3:3:73:PRO:HD2 | 2.32 | 0.59 |
| 3:4:72:GLN:CG | 3:4:73:PRO:HD2 | 2.32 | 0.59 |
| 3:10:80:TYR:O | 1:J:26:PRO:HA | 2.03 | 0.59 |
| 3:15:47:ASP:OD2 | 3:15:50:VAL:HG23 | 2.01 | 0.59 |
| 3:22:80:TYR:O | 1:V:26:PRO:HA | 2.03 | 0.59 |
| 1:O:176:GLU:OE1 | 1:O:207:TYR:OH | 2.21 | 0.59 |
| 1:P:58:ILE:HG13 | 1:P:59:ASN:H | 1.66 | 0.59 |
| 1:S:176:GLU:OE1 | 1:S:207:TYR:OH | 2.21 | 0.59 |
| 2:b:101:GLN:HE22 | 2:c:219:ARG:HD3 | 1.68 | 0.59 |
| 2:j:178:GLN:HG3 | 1:H:47:ALA:O | 2.03 | 0.59 |
| 2:o:178:GLN:HG3 | 1:M:47:ALA:O | 2.03 | 0.59 |
| 2:p:178:GLN:HG3 | 1:N:47:ALA:O | 2.03 | 0.59 |
| 2:t:101:GLN:HE22 | 2:u:219:ARG:HD3 | 1.68 | 0.59 |
| 3:2:72:GLN:CG | 3:2:73:PRO:HD2 | 2.32 | 0.59 |
| 3:16:47:ASP:OD2 | 3:16:50:VAL:HG23 | 2.01 | 0.59 |
| 3:18:72:GLN:CG | 3:18:73:PRO:HD2 | 2.32 | 0.59 |
| 3:24:47:ASP:OD2 | 3:24:50:VAL:HG23 | 2.01 | 0.59 |
| 3:26:80:TYR:O | 1:Z:26:PRO:HA | 2.03 | 0.59 |
| 1:M:58:ILE:HG13 | 1:M:59:ASN:H | 1.66 | 0.59 |
| 1:M:176:GLU:OE1 | 1:M:207:TYR:OH | 2.21 | 0.59 |
| 2:i:101:GLN:HE22 | 2:j:219:ARG:HD3 | 1.67 | 0.59 |
| 2:p:271:ASP:CB | 2:p:357:CYS:HA | 2.28 | 0.59 |
| 3:14:80:TYR:O | 1:N:26:PRO:HA | 2.03 | 0.59 |
| 3:19:72:GLN:CG | 3:19:73:PRO:HD2 | 2.32 | 0.59 |
| 3:26:72:GLN:CG | 3:26:73:PRO:HD2 | 2.32 | 0.59 |
| 3:1:72:GLN:CG | 3:1:73:PRO:HD2 | 2.32 | 0.59 |
| 2:k:101:GLN:HE22 | 2:l:219:ARG:HD3 | 1.66 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:q:269:THR:HG22 | 2:q:326:ALA:O | 2.02 | 0.59 |
| 2:r:101:GLN:HE22 | 2:s:219:ARG:HD3 | 1.68 | 0.59 |
| 2:w:178:GLN:HG3 | 1:U:47:ALA:O | 2.01 | 0.59 |
| 3:6:80:TYR:O | 1:F:26:PRO:HA | 2.02 | 0.59 |
| 3:20:72:GLN:CG | 3:20:73:PRO:HD2 | 2.32 | 0.59 |
| 3:20:80:TYR:O | 1:T:26:PRO:HA | 2.03 | 0.59 |
| 3:25:72:GLN:CG | 3:25:73:PRO:HD2 | 2.32 | 0.59 |
| 1:E:160:ASN:HA | 1:E:186:PRO:HD3 | 1.85 | 0.59 |
| 1:H:223:GLN:HB2 | 1:I:232:MET:HG3 | 1.85 | 0.59 |
| 1:N:223:GLN:HB2 | 1:O:232:MET:HG3 | 1.85 | 0.59 |
| 1:T:176:GLU:OE1 | 1:T:207:TYR:OH | 2.21 | 0.59 |
| 2:c:269:THR:HG22 | 2:c:326:ALA:O | 2.02 | 0.59 |
| 2:h:101:GLN:HE22 | 2:i:219:ARG:HD3 | 1.68 | 0.59 |
| 2:x:101:GLN:HE22 | 2:y:219:ARG:HD3 | 1.68 | 0.59 |
| 2:y:353:GLN:HG3 | 2:y:362:LEU:HD22 | 1.85 | 0.59 |
| 3:6:77:CYS:HB3 | 3:6:80:TYR:HE1 | 1.66 | 0.59 |
| 3:7:80:TYR:O | 1:G:26:PRO:HA | 2.03 | 0.59 |
| 3:16:80:TYR:O | 1:P:26:PRO:HA | 2.03 | 0.59 |
| 3:21:80:TYR:O | 1:U:26:PRO:HA | 2.03 | 0.59 |
| 3:24:72:GLN:CG | 3:24:73:PRO:HD2 | 2.32 | 0.59 |
| 1:F:160:ASN:HA | 1:F:186:PRO:HD3 | 1.85 | 0.59 |
| 1:X:160:ASN:HA | 1:X:186:PRO:HD3 | 1.85 | 0.59 |
| 2:d:164:ARG:NH1 | 2:e:365:ILE:HG23 | 2.16 | 0.59 |
| 2:d:269:THR:HG22 | 2:d:326:ALA:O | 2.03 | 0.59 |
| 2:e:269:THR:HG22 | 2:e:326:ALA:O | 2.03 | 0.59 |
| 2:h:353:GLN:HG3 | 2:h:362:LEU:HD22 | 1.85 | 0.59 |
| 2:p:269:THR:HG22 | 2:p:326:ALA:O | 2.03 | 0.59 |
| 2:r:269:THR:HG22 | 2:r:326:ALA:O | 2.02 | 0.59 |
| 2:w:123:MET:HE3 | 2:w:123:MET:CA | 2.33 | 0.59 |
| 2:y:98:ARG:NH1 | 2:z:220:THR:OG1 | 2.35 | 0.59 |
| 3:11:80:TYR:O | 1:K:26:PRO:HA | 2.03 | 0.59 |
| 3:21:72:GLN:CG | 3:21:73:PRO:HD2 | 2.32 | 0.59 |
| 3:22:72:GLN:CG | 3:22:73:PRO:HD2 | 2.32 | 0.59 |
| 3:23:72:GLN:CG | 3:23:73:PRO:HD2 | 2.32 | 0.59 |
| 1:S:58:ILE:HG13 | 1:S:59:ASN:H | 1.66 | 0.59 |
| 1:W:176:GLU:OE1 | 1:W:207:TYR:OH | 2.21 | 0.59 |
| 2:g:123:MET:HE3 | 2:g:123:MET:CA | 2.33 | 0.58 |
| 2:h:123:MET:HE3 | 2:h:123:MET:CA | 2.33 | 0.58 |
| 2:i:123:MET:HE3 | 2:i:123:MET:CA | 2.33 | 0.58 |
| 2:i:269:THR:HG22 | 2:i:326:ALA:O | 2.03 | 0.58 |
| 2:i:353:GLN:HG3 | 2:i:362:LEU:HD22 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:l:269:THR:HG22 | 2:l:326:ALA:O | 2.02 | 0.58 |
| 2:l:353:GLN:HG3 | 2:l:362:LEU:HD22 | 1.85 | 0.58 |
| 2:x:353:GLN:HG3 | 2:x:362:LEU:HD22 | 1.85 | 0.58 |
| 3:17:80:TYR:O | 1:Q:26:PRO:HA | 2.03 | 0.58 |
| 1:D:160:ASN:HA | 1:D:186:PRO:HD3 | 1.85 | 0.58 |
| 1:F:58:ILE:HG13 | 1:F:59:ASN:H | 1.67 | 0.58 |
| 1:W:160:ASN:HA | 1:W:186:PRO:HD3 | 1.85 | 0.58 |
| 1:Y:160:ASN:HA | 1:Y:186:PRO:HD3 | 1.85 | 0.58 |
| 2:b:123:MET:HE3 | 2:b:123:MET:CA | 2.33 | 0.58 |
| 2:c:353:GLN:HG3 | 2:c:362:LEU:HD22 | 1.85 | 0.58 |
| 2:d:353:GLN:HG3 | 2:d:362:LEU:HD22 | 1.85 | 0.58 |
| 2:g:353:GLN:HG3 | 2:g:362:LEU:HD22 | 1.85 | 0.58 |
| 2:h:196:MET:HE3 | 2:h:196:MET:HA | 1.85 | 0.58 |
| 2:i:271:ASP:CB | 2:i:357:CYS:HA | 2.28 | 0.58 |
| 2:k:123:MET:HE3 | 2:k:123:MET:CA | 2.33 | 0.58 |
| 2:k:353:GLN:HG3 | 2:k:362:LEU:HD22 | 1.85 | 0.58 |
| 2:m:101:GLN:HE22 | 2:n:219:ARG:HD3 | 1.66 | 0.58 |
| 2:u:353:GLN:HG3 | 2:u:362:LEU:HD22 | 1.85 | 0.58 |
| 2:v:196:MET:HE3 | 2:v:196:MET:HA | 1.85 | 0.58 |
| 2:v:269:THR:HG22 | 2:v:326:ALA:O | 2.03 | 0.58 |
| 2:y:269:THR:HG22 | 2:y:326:ALA:O | 2.02 | 0.58 |
| 3:19:80:TYR:O | 1:S:26:PRO:HA | 2.03 | 0.58 |
| 1:B:223:GLN:HB2 | 1:C:232:MET:HG3 | 1.85 | 0.58 |
| 1:T:223:GLN:HB2 | 1:U:232:MET:HG3 | 1.85 | 0.58 |
| 1:A:58:ILE:HG13 | 1:A:59:ASN:H | 1.67 | 0.58 |
| 2:d:123:MET:HE3 | 2:d:123:MET:CA | 2.33 | 0.58 |
| 2:e:123:MET:HE3 | 2:e:123:MET:CA | 2.34 | 0.58 |
| 2:f:123:MET:HE3 | 2:f:123:MET:CA | 2.34 | 0.58 |
| 2:j:123:MET:HE3 | 2:j:123:MET:CA | 2.34 | 0.58 |
| 2:j:353:GLN:HG3 | 2:j:362:LEU:HD22 | 1.85 | 0.58 |
| 2:l:123:MET:HE3 | 2:l:123:MET:CA | 2.33 | 0.58 |
| 2:m:269:THR:HG22 | 2:m:326:ALA:O | 2.02 | 0.58 |
| 2:m:353:GLN:HG3 | 2:m:362:LEU:HD22 | 1.85 | 0.58 |
| 2:q:271:ASP:CB | 2:q:357:CYS:HA | 2.28 | 0.58 |
| 2:r:46:ASP:HA | 2:s:161:ASN:ND2 | 2.15 | 0.58 |
| 2:t:353:GLN:HG3 | 2:t:362:LEU:HD22 | 1.85 | 0.58 |
| 2:v:98:ARG:NH1 | 2:w:220:THR:OG1 | 2.36 | 0.58 |
| 2:v:353:GLN:HG3 | 2:v:362:LEU:HD22 | 1.85 | 0.58 |
| 2:y:178:GLN:HG3 | 1:W:47:ALA:O | 2.02 | 0.58 |
| 2:z:353:GLN:HG3 | 2:z:362:LEU:HD22 | 1.86 | 0.58 |
| 3:18:80:TYR:O | 1:R:26:PRO:HA | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:V:223:GLN:HB2 | 1:W:232:MET:HG3 | 1.86 | 0.58 |
| 1:A:232:MET:HG3 | 1:Z:223:GLN:HB2 | 1.85 | 0.58 |
| 2:a:123:MET:HE3 | 2:a:123:MET:CA | 2.33 | 0.58 |
| 2:a:353:GLN:HG3 | 2:a:362:LEU:HD22 | 1.85 | 0.58 |
| 2:b:353:GLN:HG3 | 2:b:362:LEU:HD22 | 1.85 | 0.58 |
| 2:c:123:MET:HE3 | 2:c:123:MET:CA | 2.33 | 0.58 |
| 2:h:269:THR:HG22 | 2:h:326:ALA:O | 2.02 | 0.58 |
| 2:i:196:MET:HE3 | 2:i:196:MET:HA | 1.85 | 0.58 |
| 2:i:269:THR:OG1 | 2:i:359:ARG:HB2 | 2.04 | 0.58 |
| 2:m:269:THR:OG1 | 2:m:359:ARG:HB2 | 2.03 | 0.58 |
| 2:r:353:GLN:HG3 | 2:r:362:LEU:HD22 | 1.85 | 0.58 |
| 2:u:123:MET:HE3 | 2:u:123:MET:CA | 2.33 | 0.58 |
| 2:x:46:ASP:OD1 | 2:y:161:ASN:HB2 | 2.04 | 0.58 |
| 2:z:123:MET:HE3 | 2:z:123:MET:CA | 2.33 | 0.58 |
| 3:2:80:TYR:O | 1:B:26:PRO:HA | 2.02 | 0.58 |
| 3:4:80:TYR:O | 1:D:26:PRO:HA | 2.03 | 0.58 |
| 1:G:160:ASN:HA | 1:G:186:PRO:HD3 | 1.85 | 0.58 |
| 1:L:176:GLU:OE1 | 1:L:207:TYR:OH | 2.21 | 0.58 |
| 1:W:223:GLN:HB2 | 1:X:232:MET:HG3 | 1.85 | 0.58 |
| 1:X:167:LYS:HD3 | 1:Y:203:ALA:CB | 2.34 | 0.58 |
| 2:c:192:GLU:OE1 | 2:c:192:GLU:N | 2.37 | 0.58 |
| 2:e:353:GLN:HG3 | 2:e:362:LEU:HD22 | 1.85 | 0.58 |
| 2:f:196:MET:HE3 | 2:f:196:MET:HA | 1.85 | 0.58 |
| 2:g:192:GLU:N | 2:g:192:GLU:OE1 | 2.37 | 0.58 |
| 2:g:196:MET:HE3 | 2:g:196:MET:HA | 1.85 | 0.58 |
| 2:g:269:THR:HG22 | 2:g:326:ALA:O | 2.02 | 0.58 |
| 2:l:192:GLU:N | 2:l:192:GLU:OE1 | 2.37 | 0.58 |
| 2:l:269:THR:OG1 | 2:l:359:ARG:HB2 | 2.03 | 0.58 |
| 2:n:101:GLN:HE22 | 2:o:219:ARG:HD3 | 1.68 | 0.58 |
| 2:n:269:THR:HG22 | 2:n:326:ALA:O | 2.03 | 0.58 |
| 2:o:269:THR:HG22 | 2:o:326:ALA:O | 2.02 | 0.58 |
| 2:p:98:ARG:NH1 | 2:q:220:THR:OG1 | 2.36 | 0.58 |
| 2:p:353:GLN:HG3 | 2:p:362:LEU:HD22 | 1.85 | 0.58 |
| 2:q:353:GLN:HG3 | 2:q:362:LEU:HD22 | 1.85 | 0.58 |
| 2:r:192:GLU:OE1 | 2:r:192:GLU:N | 2.37 | 0.58 |
| 2:r:196:MET:HE3 | 2:r:196:MET:HA | 1.85 | 0.58 |
| 2:s:196:MET:HE3 | 2:s:196:MET:HA | 1.85 | 0.58 |
| 2:s:353:GLN:HG3 | 2:s:362:LEU:HD22 | 1.85 | 0.58 |
| 2:t:123:MET:HE3 | 2:t:123:MET:CA | 2.33 | 0.58 |
| 2:u:196:MET:HE3 | 2:u:196:MET:HA | 1.85 | 0.58 |
| 2:v:178:GLN:HG3 | 1:T:47:ALA:O | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:w:353:GLN:HG3 | 2:w:362:LEU:HD22 | 1.85 | 0.58 |
| 2:y:192:GLU:OE1 | 2:y:192:GLU:N | 2.37 | 0.58 |
| 3:5:80:TYR:O | 1:E:26:PRO:HA | 2.03 | 0.58 |
| 1:G:223:GLN:HB2 | 1:H:232:MET:HG3 | 1.86 | 0.58 |
| 1:M:223:GLN:HB2 | 1:N:232:MET:HG3 | 1.86 | 0.58 |
| 1:A:223:GLN:HB2 | 1:B:232:MET:HG3 | 1.86 | 0.58 |
| 2:a:269:THR:HG22 | 2:a:326:ALA:O | 2.03 | 0.58 |
| 2:e:196:MET:HE3 | 2:e:196:MET:HA | 1.85 | 0.58 |
| 2:f:269:THR:HG22 | 2:f:326:ALA:O | 2.03 | 0.58 |
| 2:h:178:GLN:HG3 | 1:F:47:ALA:O | 2.04 | 0.58 |
| 2:m:123:MET:HE3 | 2:m:123:MET:CA | 2.33 | 0.58 |
| 2:n:353:GLN:HG3 | 2:n:362:LEU:HD22 | 1.85 | 0.58 |
| 2:t:196:MET:HE3 | 2:t:196:MET:HA | 1.85 | 0.58 |
| 2:x:269:THR:OG1 | 2:x:359:ARG:HB2 | 2.04 | 0.58 |
| 2:y:123:MET:HE3 | 2:y:123:MET:CA | 2.33 | 0.58 |
| 2:z:269:THR:OG1 | 2:z:359:ARG:HB2 | 2.03 | 0.58 |
| 3:7:70:PHE:CD1 | 1:G:41:PRO:HD3 | 2.39 | 0.58 |
| 3:12:80:TYR:O | 1:L:26:PRO:HA | 2.02 | 0.58 |
| 3:13:80:TYR:O | 1:M:26:PRO:HA | 2.03 | 0.58 |
| 3:25:70:PHE:CD1 | 1:Y:41:PRO:HD3 | 2.39 | 0.58 |
| 1:O:39:PRO:HB3 | 1:P:75:GLY:HA3 | 1.86 | 0.58 |
| 1:S:39:PRO:HB3 | 1:T:75:GLY:HA3 | 1.86 | 0.58 |
| 1:V:160:ASN:HA | 1:V:186:PRO:HD3 | 1.85 | 0.58 |
| 1:Z:160:ASN:HA | 1:Z:186:PRO:HD3 | 1.85 | 0.58 |
| 2:a:160:LEU:HD12 | 2:z:46:ASP:OD1 | 2.04 | 0.58 |
| 2:b:192:GLU:OE1 | 2:b:192:GLU:N | 2.37 | 0.58 |
| 2:d:101:GLN:HE22 | 2:e:219:ARG:HD3 | 1.69 | 0.58 |
| 2:d:196:MET:HE3 | 2:d:196:MET:HA | 1.85 | 0.58 |
| 2:f:353:GLN:HG3 | 2:f:362:LEU:HD22 | 1.85 | 0.58 |
| 2:h:192:GLU:OE1 | 2:h:192:GLU:N | 2.37 | 0.58 |
| 2:k:192:GLU:OE1 | 2:k:192:GLU:N | 2.37 | 0.58 |
| 2:m:192:GLU:OE1 | 2:m:192:GLU:N | 2.37 | 0.58 |
| 2:o:192:GLU:N | 2:o:192:GLU:OE1 | 2.37 | 0.58 |
| 2:o:353:GLN:HG3 | 2:o:362:LEU:HD22 | 1.85 | 0.58 |
| 2:u:269:THR:OG1 | 2:u:359:ARG:HB2 | 2.04 | 0.58 |
| 2:v:192:GLU:OE1 | 2:v:192:GLU:N | 2.37 | 0.58 |
| 2:w:196:MET:HE3 | 2:w:196:MET:HA | 1.85 | 0.58 |
| 2:x:123:MET:HE3 | 2:x:123:MET:CA | 2.34 | 0.58 |
| 1:C:160:ASN:HA | 1:C:186:PRO:HD3 | 1.85 | 0.58 |
| 1:Q:39:PRO:HB3 | 1:R:75:GLY:HA3 | 1.86 | 0.58 |
| 1:R:39:PRO:HB3 | 1:S:75:GLY:HA3 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:176:GLU:OE1 | 1:U:207:TYR:OH | 2.21 | 0.58 |
| 2:f:101:GLN:HE22 | 2:g:219:ARG:HD3 | 1.69 | 0.58 |
| 2:h:269:THR:OG1 | 2:h:359:ARG:HB2 | 2.04 | 0.58 |
| 2:j:196:MET:HE3 | 2:j:196:MET:HA | 1.85 | 0.58 |
| 2:n:123:MET:HE3 | 2:n:123:MET:CA | 2.33 | 0.58 |
| 2:q:196:MET:HE3 | 2:q:196:MET:HA | 1.85 | 0.58 |
| 2:r:123:MET:HE3 | 2:r:123:MET:CA | 2.33 | 0.58 |
| 2:t:178:GLN:HG3 | 1:R:47:ALA:O | 2.03 | 0.58 |
| 2:t:269:THR:HG22 | 2:t:326:ALA:O | 2.03 | 0.58 |
| 2:v:123:MET:HE3 | 2:v:123:MET:CA | 2.33 | 0.58 |
| 2:z:192:GLU:OE1 | 2:z:192:GLU:N | 2.37 | 0.58 |
| 1:K:176:GLU:OE1 | 1:K:207:TYR:OH | 2.21 | 0.58 |
| 1:U:39:PRO:HB3 | 1:V:75:GLY:HA3 | 1.86 | 0.58 |
| 1:V:176:GLU:OE1 | 1:V:207:TYR:OH | 2.21 | 0.58 |
| 1:A:26:PRO:HA | 3:1:80:TYR:O | 2.03 | 0.58 |
| 1:A:41:PRO:HD3 | 3:1:70:PHE:CD1 | 2.38 | 0.58 |
| 2:d:46:ASP:HA | 2:e:161:ASN:ND2 | 2.17 | 0.58 |
| 2:e:269:THR:OG1 | 2:e:359:ARG:HB2 | 2.04 | 0.58 |
| 2:f:46:ASP:HA | 2:g:161:ASN:ND2 | 2.17 | 0.58 |
| 2:f:46:ASP:OD1 | 2:g:160:LEU:HD12 | 2.04 | 0.58 |
| 2:l:196:MET:HE3 | 2:l:196:MET:HA | 1.85 | 0.58 |
| 2:p:101:GLN:HE22 | 2:q:219:ARG:HD3 | 1.69 | 0.58 |
| 2:p:192:GLU:OE1 | 2:p:192:GLU:N | 2.37 | 0.58 |
| 2:q:192:GLU:OE1 | 2:q:192:GLU:N | 2.37 | 0.58 |
| 2:s:192:GLU:OE1 | 2:s:192:GLU:N | 2.37 | 0.58 |
| 2:u:192:GLU:OE1 | 2:u:192:GLU:N | 2.37 | 0.58 |
| 2:x:142:LEU:HD23 | 2:z:350:GLN:NE2 | 2.18 | 0.58 |
| 3:4:70:PHE:CD1 | 1:D:41:PRO:HD3 | 2.39 | 0.58 |
| 3:10:70:PHE:CD1 | 1:J:41:PRO:HD3 | 2.39 | 0.58 |
| 1:H:160:ASN:HA | 1:H:186:PRO:HD3 | 1.85 | 0.58 |
| 1:K:160:ASN:HA | 1:K:186:PRO:HD3 | 1.85 | 0.58 |
| 1:L:160:ASN:HA | 1:L:186:PRO:HD3 | 1.85 | 0.58 |
| 1:M:39:PRO:HB3 | 1:N:75:GLY:HA3 | 1.86 | 0.58 |
| 1:R:160:ASN:HA | 1:R:186:PRO:HD3 | 1.85 | 0.58 |
| 1:W:39:PRO:HB3 | 1:X:75:GLY:HA3 | 1.86 | 0.58 |
| 2:f:192:GLU:OE1 | 2:f:192:GLU:N | 2.37 | 0.58 |
| 2:j:269:THR:OG1 | 2:j:359:ARG:HB2 | 2.03 | 0.58 |
| 2:l:98:ARG:NH1 | 2:m:220:THR:OG1 | 2.36 | 0.58 |
| 2:u:178:GLN:HG3 | 1:S:47:ALA:O | 2.03 | 0.58 |
| 2:w:269:THR:OG1 | 2:w:359:ARG:HB2 | 2.04 | 0.58 |
| 2:z:99:GLN:NE2 | 1:Y:50:SER:HB3 | 2.19 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:39:PRO:HB3 | 1:D:75:GLY:HA3 | 1.86 | 0.58 |
| 1:P:223:GLN:HB2 | 1:Q:232:MET:HG3 | 1.86 | 0.58 |
| 1:Q:160:ASN:HA | 1:Q:186:PRO:HD3 | 1.85 | 0.58 |
| 2:d:192:GLU:N | 2:d:192:GLU:OE1 | 2.37 | 0.57 |
| 2:d:271:ASP:CB | 2:d:357:CYS:HA | 2.28 | 0.57 |
| 2:j:269:THR:HG22 | 2:j:326:ALA:O | 2.03 | 0.57 |
| 2:k:196:MET:HE3 | 2:k:196:MET:HA | 1.85 | 0.57 |
| 2:o:123:MET:HE3 | 2:o:123:MET:CA | 2.34 | 0.57 |
| 2:p:123:MET:HE3 | 2:p:123:MET:CA | 2.33 | 0.57 |
| 2:p:269:THR:OG1 | 2:p:359:ARG:HB2 | 2.04 | 0.57 |
| 2:r:271:ASP:CB | 2:r:357:CYS:HA | 2.28 | 0.57 |
| 2:s:269:THR:OG1 | 2:s:359:ARG:HB2 | 2.04 | 0.57 |
| 2:v:101:GLN:HE22 | 2:w:219:ARG:HD3 | 1.69 | 0.57 |
| 2:y:196:MET:HE3 | 2:y:196:MET:HA | 1.85 | 0.57 |
| 3:3:80:TYR:O | 1:C:26:PRO:HA | 2.03 | 0.57 |
| 1:B:39:PRO:HB3 | 1:C:75:GLY:HA3 | 1.86 | 0.57 |
| 1:M:160:ASN:HA | 1:M:186:PRO:HD3 | 1.85 | 0.57 |
| 1:Q:223:GLN:HB2 | 1:R:232:MET:HG3 | 1.85 | 0.57 |
| 1:S:160:ASN:HA | 1:S:186:PRO:HD3 | 1.85 | 0.57 |
| 2:c:196:MET:HE3 | 2:c:196:MET:HA | 1.85 | 0.57 |
| 2:e:192:GLU:OE1 | 2:e:192:GLU:N | 2.37 | 0.57 |
| 2:i:192:GLU:N | 2:i:192:GLU:OE1 | 2.37 | 0.57 |
| 2:k:269:THR:HG22 | 2:k:326:ALA:O | 2.03 | 0.57 |
| 2:l:101:GLN:HE22 | 2:m:219:ARG:HD3 | 1.68 | 0.57 |
| 2:m:196:MET:HE3 | 2:m:196:MET:HA | 1.85 | 0.57 |
| 2:n:178:GLN:HG3 | 1:L:47:ALA:O | 2.04 | 0.57 |
| 2:q:269:THR:OG1 | 2:q:359:ARG:HB2 | 2.04 | 0.57 |
| 2:v:72:THR:OG1 | 1:W:70:ARG:NH2 | 2.37 | 0.57 |
| 2:v:269:THR:OG1 | 2:v:359:ARG:HB2 | 2.04 | 0.57 |
| 2:y:46:ASP:OD1 | 2:z:160:LEU:HD12 | 2.04 | 0.57 |
| 2:z:196:MET:HE3 | 2:z:196:MET:HA | 1.85 | 0.57 |
| 3:2:70:PHE:CD1 | 1:B:41:PRO:HD3 | 2.39 | 0.57 |
| 3:6:70:PHE:CD1 | 1:F:41:PRO:HD3 | 2.40 | 0.57 |
| 3:22:70:PHE:CD1 | 1:V:41:PRO:HD3 | 2.39 | 0.57 |
| 1:U:223:GLN:HB2 | 1:V:232:MET:HG3 | 1.87 | 0.57 |
| 1:A:160:ASN:HA | 1:A:186:PRO:HD3 | 1.85 | 0.57 |
| 2:a:192:GLU:N | 2:a:192:GLU:OE1 | 2.37 | 0.57 |
| 2:b:269:THR:OG1 | 2:b:359:ARG:HB2 | 2.04 | 0.57 |
| 2:d:72:THR:OG1 | 1:E:70:ARG:NH2 | 2.37 | 0.57 |
| 2:f:269:THR:OG1 | 2:f:359:ARG:HB2 | 2.03 | 0.57 |
| 2:g:46:ASP:HA | 2:h:161:ASN:ND2 | 2.18 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:192:GLU:OE1 | 2:n:192:GLU:N | 2.37 | 0.57 |
| 2:x:196:MET:HE3 | 2:x:196:MET:HA | 1.85 | 0.57 |
| 3:3:70:PHE:CD1 | 1:C:41:PRO:HD3 | 2.39 | 0.57 |
| 3:8:70:PHE:CD1 | 1:H:41:PRO:HD3 | 2.40 | 0.57 |
| 1:L:223:GLN:HB2 | 1:M:232:MET:HG3 | 1.86 | 0.57 |
| 1:N:39:PRO:HB3 | 1:O:75:GLY:HA3 | 1.86 | 0.57 |
| 2:c:269:THR:OG1 | 2:c:359:ARG:HB2 | 2.04 | 0.57 |
| 2:j:46:ASP:HA | 2:k:161:ASN:ND2 | 2.17 | 0.57 |
| 2:p:196:MET:HE3 | 2:p:196:MET:HA | 1.85 | 0.57 |
| 2:q:123:MET:HE3 | 2:q:123:MET:CA | 2.34 | 0.57 |
| 2:x:192:GLU:OE1 | 2:x:192:GLU:N | 2.37 | 0.57 |
| 3:11:70:PHE:CD1 | 1:K:41:PRO:HD3 | 2.39 | 0.57 |
| 3:16:24:GLU:HB3 | 3:16:33:ARG:HB2 | 1.87 | 0.57 |
| 3:20:24:GLU:HB3 | 3:20:33:ARG:HB2 | 1.87 | 0.57 |
| 3:21:24:GLU:HB3 | 3:21:33:ARG:HB2 | 1.87 | 0.57 |
| 3:24:70:PHE:CD1 | 1:X:41:PRO:HD3 | 2.39 | 0.57 |
| 3:26:70:PHE:CD1 | 1:Z:41:PRO:HD3 | 2.40 | 0.57 |
| 1:B:160:ASN:HA | 1:B:186:PRO:HD3 | 1.85 | 0.57 |
| 1:J:160:ASN:HA | 1:J:186:PRO:HD3 | 1.85 | 0.57 |
| 1:K:223:GLN:HB2 | 1:L:232:MET:HG3 | 1.86 | 0.57 |
| 1:L:39:PRO:HB3 | 1:M:75:GLY:HA3 | 1.86 | 0.57 |
| 1:S:223:GLN:HB2 | 1:T:232:MET:HG3 | 1.86 | 0.57 |
| 1:T:39:PRO:HB3 | 1:U:75:GLY:HA3 | 1.86 | 0.57 |
| 2:a:46:ASP:OD1 | 2:b:160:LEU:HD12 | 2.05 | 0.57 |
| 2:d:269:THR:OG1 | 2:d:359:ARG:HB2 | 2.03 | 0.57 |
| 2:h:46:ASP:HA | 2:i:161:ASN:ND2 | 2.18 | 0.57 |
| 2:h:98:ARG:NH1 | 2:i:220:THR:OG1 | 2.37 | 0.57 |
| 2:s:98:ARG:NH1 | 2:t:220:THR:OG1 | 2.37 | 0.57 |
| 2:w:192:GLU:N | 2:w:192:GLU:OE1 | 2.37 | 0.57 |
| 3:13:70:PHE:CD1 | 1:M:41:PRO:HD3 | 2.39 | 0.57 |
| 3:17:24:GLU:HB3 | 3:17:33:ARG:HB2 | 1.87 | 0.57 |
| 3:19:18:ARG:NE | 3:19:46:THR:HA | 2.20 | 0.57 |
| 3:22:18:ARG:NE | 3:22:46:THR:HA | 2.20 | 0.57 |
| 3:22:24:GLU:HB3 | 3:22:33:ARG:HB2 | 1.87 | 0.57 |
| 1:F:223:GLN:HB2 | 1:G:232:MET:HG3 | 1.86 | 0.57 |
| 1:I:39:PRO:HB3 | 1:J:75:GLY:HA3 | 1.86 | 0.57 |
| 1:K:39:PRO:HB3 | 1:L:75:GLY:HA3 | 1.86 | 0.57 |
| 1:O:223:GLN:HB2 | 1:P:232:MET:HG3 | 1.87 | 0.57 |
| 1:A:47:ALA:O | 2:c:178:GLN:HG3 | 2.04 | 0.57 |
| 2:a:196:MET:HE3 | 2:a:196:MET:HA | 1.85 | 0.57 |
| 2:a:269:THR:OG1 | 2:a:359:ARG:HB2 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:b:98:ARG:NH1 | 2:c:220:THR:OG1 | 2.37 | 0.57 |
| 2:j:192:GLU:OE1 | 2:j:192:GLU:N | 2.37 | 0.57 |
| 2:n:196:MET:HE3 | 2:n:196:MET:HA | 1.85 | 0.57 |
| 2:n:269:THR:OG1 | 2:n:359:ARG:HB2 | 2.03 | 0.57 |
| 2:s:123:MET:HE3 | 2:s:123:MET:CA | 2.33 | 0.57 |
| 3:13:24:GLU:HB3 | 3:13:33:ARG:HB2 | 1.87 | 0.57 |
| 3:19:70:PHE:CD1 | 1:S:41:PRO:HD3 | 2.39 | 0.57 |
| 3:23:28:ILE:O | 3:23:29:SER:OG | 2.21 | 0.57 |
| 3:23:70:PHE:CD1 | 1:W:41:PRO:HD3 | 2.39 | 0.57 |
| 3:24:24:GLU:HB3 | 3:24:33:ARG:HB2 | 1.87 | 0.57 |
| 3:25:24:GLU:HB3 | 3:25:33:ARG:HB2 | 1.87 | 0.57 |
| 1:E:39:PRO:HB3 | 1:F:75:GLY:HA3 | 1.86 | 0.57 |
| 1:E:223:GLN:HB2 | 1:F:232:MET:HG3 | 1.86 | 0.57 |
| 1:G:39:PRO:HB3 | 1:H:75:GLY:HA3 | 1.86 | 0.57 |
| 1:P:160:ASN:HA | 1:P:186:PRO:HD3 | 1.85 | 0.57 |
| 1:U:160:ASN:HA | 1:U:186:PRO:HD3 | 1.85 | 0.57 |
| 2:j:271:ASP:CB | 2:j:357:CYS:HA | 2.28 | 0.57 |
| 2:k:72:THR:OG1 | 1:L:70:ARG:NH2 | 2.37 | 0.57 |
| 2:n:72:THR:OG1 | 1:O:70:ARG:NH2 | 2.38 | 0.57 |
| 2:y:271:ASP:CB | 2:y:357:CYS:HA | 2.28 | 0.57 |
| 3:5:70:PHE:CD1 | 1:E:41:PRO:HD3 | 2.39 | 0.57 |
| 3:12:24:GLU:HB3 | 3:12:33:ARG:HB2 | 1.87 | 0.57 |
| 3:14:24:GLU:HB3 | 3:14:33:ARG:HB2 | 1.87 | 0.57 |
| 3:16:18:ARG:NE | 3:16:46:THR:HA | 2.20 | 0.57 |
| 3:18:24:GLU:HB3 | 3:18:33:ARG:HB2 | 1.87 | 0.57 |
| 3:19:24:GLU:HB3 | 3:19:33:ARG:HB2 | 1.87 | 0.57 |
| 3:21:70:PHE:CD1 | 1:U:41:PRO:HD3 | 2.39 | 0.57 |
| 3:26:24:GLU:HB3 | 3:26:33:ARG:HB2 | 1.87 | 0.57 |
| 1:R:223:GLN:HB2 | 1:S:232:MET:HG3 | 1.85 | 0.57 |
| 2:a:175:LEU:HD11 | 1:Y:51:ILE:CG1 | 2.34 | 0.57 |
| 2:d:46:ASP:OD1 | 2:e:160:LEU:HD12 | 2.05 | 0.57 |
| 2:e:20:GLU:OE2 | 2:e:246:VAL:HG21 | 2.05 | 0.57 |
| 2:k:269:THR:OG1 | 2:k:359:ARG:HB2 | 2.04 | 0.57 |
| 3:12:70:PHE:CD1 | 1:L:41:PRO:HD3 | 2.40 | 0.57 |
| 3:15:24:GLU:HB3 | 3:15:33:ARG:HB2 | 1.87 | 0.57 |
| 3:25:18:ARG:NE | 3:25:46:THR:HA | 2.20 | 0.57 |
| 3:26:18:ARG:NE | 3:26:46:THR:HA | 2.20 | 0.57 |
| 1:P:39:PRO:HB3 | 1:Q:75:GLY:HA3 | 1.87 | 0.57 |
| 2:a:105:VAL:HG22 | 2:a:165:ILE:HB | 1.87 | 0.57 |
| 2:b:105:VAL:HG22 | 2:b:165:ILE:HB | 1.87 | 0.57 |
| 2:b:196:MET:HE3 | 2:b:196:MET:HA | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:g:46:ASP:OD1 | 2:h:160:LEU:HD12 | 2.05 | 0.57 |
| 2:h:20:GLU:OE2 | 2:h:246:VAL:HG21 | 2.05 | 0.57 |
| 2:i:105:VAL:HG22 | 2:i:165:ILE:HB | 1.87 | 0.57 |
| 2:j:101:GLN:HE22 | 2:k:219:ARG:HD3 | 1.69 | 0.57 |
| 2:j:105:VAL:HG22 | 2:j:165:ILE:HB | 1.87 | 0.57 |
| 3:2:18:ARG:NE | 3:2:46:THR:HA | 2.20 | 0.57 |
| 3:11:24:GLU:HB3 | 3:11:33:ARG:HB2 | 1.87 | 0.57 |
| 3:16:70:PHE:CD1 | 1:P:41:PRO:HD3 | 2.39 | 0.57 |
| 3:17:70:PHE:CD1 | 1:Q:41:PRO:HD3 | 2.39 | 0.57 |
| 3:23:18:ARG:NE | 3:23:46:THR:HA | 2.20 | 0.57 |
| 3:23:24:GLU:HB3 | 3:23:33:ARG:HB2 | 1.87 | 0.57 |
| 1:I:223:GLN:HB2 | 1:J:232:MET:HG3 | 1.87 | 0.57 |
| 1:J:223:GLN:HB2 | 1:K:232:MET:HG3 | 1.86 | 0.57 |
| 1:T:160:ASN:HA | 1:T:186:PRO:HD3 | 1.85 | 0.57 |
| 1:V:39:PRO:HB3 | 1:W:75:GLY:HA3 | 1.87 | 0.57 |
| 2:a:350:GLN:NE2 | 2:y:142:LEU:HD23 | 2.18 | 0.57 |
| 3:1:24:GLU:HB3 | 3:1:33:ARG:HB2 | 1.87 | 0.57 |
| 2:c:46:ASP:HA | 2:d:161:ASN:ND2 | 2.18 | 0.57 |
| 2:d:178:GLN:HG3 | 1:B:47:ALA:O | 2.03 | 0.57 |
| 2:g:20:GLU:OE2 | 2:g:246:VAL:HG21 | 2.05 | 0.57 |
| 2:h:105:VAL:HG22 | 2:h:165:ILE:HB | 1.87 | 0.57 |
| 2:i:46:ASP:HA | 2:j:161:ASN:ND2 | 2.18 | 0.57 |
| 2:o:269:THR:OG1 | 2:o:359:ARG:HB2 | 2.04 | 0.57 |
| 2:r:46:ASP:OD1 | 2:s:160:LEU:HD12 | 2.04 | 0.57 |
| 2:r:72:THR:OG1 | 1:S:70:ARG:NH2 | 2.38 | 0.57 |
| 2:r:269:THR:OG1 | 2:r:359:ARG:HB2 | 2.04 | 0.57 |
| 2:y:20:GLU:OE2 | 2:y:246:VAL:HG21 | 2.05 | 0.57 |
| 2:y:247:THR:HB | 2:y:248:PRO:HD2 | 1.87 | 0.57 |
| 2:y:269:THR:OG1 | 2:y:359:ARG:HB2 | 2.03 | 0.57 |
| 3:20:18:ARG:NE | 3:20:46:THR:HA | 2.20 | 0.57 |
| 1:C:223:GLN:HB2 | 1:D:232:MET:HG3 | 1.86 | 0.57 |
| 1:H:39:PRO:HB3 | 1:I:75:GLY:HA3 | 1.86 | 0.57 |
| 2:b:20:GLU:OE2 | 2:b:246:VAL:HG21 | 2.05 | 0.56 |
| 2:f:98:ARG:NH1 | 2:g:220:THR:OG1 | 2.35 | 0.56 |
| 2:i:20:GLU:OE2 | 2:i:246:VAL:HG21 | 2.05 | 0.56 |
| 2:i:98:ARG:NH1 | 2:j:220:THR:OG1 | 2.36 | 0.56 |
| 2:o:196:MET:HE3 | 2:o:196:MET:HA | 1.85 | 0.56 |
| 2:t:192:GLU:N | 2:t:192:GLU:OE1 | 2.37 | 0.56 |
| 2:w:247:THR:HB | 2:w:248:PRO:HD2 | 1.87 | 0.56 |
| 2:z:20:GLU:OE2 | 2:z:246:VAL:HG21 | 2.05 | 0.56 |
| 2:z:105:VAL:HG22 | 2:z:165:ILE:HB | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:z:247:THR:HB | 2:z:248:PRO:HD2 | 1.87 | 0.56 |
| 3:2:24:GLU:HB3 | 3:2:33:ARG:HB2 | 1.87 | 0.56 |
| 3:3:24:GLU:HB3 | 3:3:33:ARG:HB2 | 1.87 | 0.56 |
| 3:9:24:GLU:HB3 | 3:9:33:ARG:HB2 | 1.87 | 0.56 |
| 3:9:70:PHE:CD1 | 1:I:41:PRO:HD3 | 2.39 | 0.56 |
| 3:13:28:ILE:O | 3:13:29:SER:OG | 2.21 | 0.56 |
| 1:N:160:ASN:HA | 1:N:186:PRO:HD3 | 1.85 | 0.56 |
| 2:e:98:ARG:NH1 | 2:f:220:THR:OG1 | 2.37 | 0.56 |
| 2:v:247:THR:HB | 2:v:248:PRO:HD2 | 1.87 | 0.56 |
| 3:8:24:GLU:HB3 | 3:8:33:ARG:HB2 | 1.87 | 0.56 |
| 3:14:70:PHE:CD1 | 1:N:41:PRO:HD3 | 2.40 | 0.56 |
| 1:D:223:GLN:HB2 | 1:E:232:MET:HG3 | 1.86 | 0.56 |
| 1:F:39:PRO:HB3 | 1:G:75:GLY:HA3 | 1.86 | 0.56 |
| 1:I:160:ASN:HA | 1:I:186:PRO:HD3 | 1.85 | 0.56 |
| 2:a:20:GLU:OE2 | 2:a:246:VAL:HG21 | 2.05 | 0.56 |
| 2:b:46:ASP:HA | 2:c:161:ASN:ND2 | 2.18 | 0.56 |
| 2:b:247:THR:HB | 2:b:248:PRO:HD2 | 1.87 | 0.56 |
| 2:c:105:VAL:HG22 | 2:c:165:ILE:HB | 1.87 | 0.56 |
| 2:f:20:GLU:OE2 | 2:f:246:VAL:HG21 | 2.05 | 0.56 |
| 2:j:20:GLU:OE2 | 2:j:246:VAL:HG21 | 2.05 | 0.56 |
| 2:k:105:VAL:HG22 | 2:k:165:ILE:HB | 1.87 | 0.56 |
| 2:s:271:ASP:CB | 2:s:357:CYS:HA | 2.28 | 0.56 |
| 2:t:247:THR:HB | 2:t:248:PRO:HD2 | 1.87 | 0.56 |
| 2:u:105:VAL:HG22 | 2:u:165:ILE:HB | 1.87 | 0.56 |
| 2:x:20:GLU:OE2 | 2:x:246:VAL:HG21 | 2.05 | 0.56 |
| 2:x:247:THR:HB | 2:x:248:PRO:HD2 | 1.87 | 0.56 |
| 3:3:18:ARG:NE | 3:3:46:THR:HA | 2.20 | 0.56 |
| 3:4:24:GLU:HB3 | 3:4:33:ARG:HB2 | 1.87 | 0.56 |
| 3:7:24:GLU:HB3 | 3:7:33:ARG:HB2 | 1.87 | 0.56 |
| 3:8:39:PRO:HB2 | 3:8:42:PHE:CD1 | 2.41 | 0.56 |
| 3:9:39:PRO:HB2 | 3:9:42:PHE:CD1 | 2.41 | 0.56 |
| 3:10:24:GLU:HB3 | 3:10:33:ARG:HB2 | 1.87 | 0.56 |
| 3:10:39:PRO:HB2 | 3:10:42:PHE:CD1 | 2.41 | 0.56 |
| 3:11:39:PRO:HB2 | 3:11:42:PHE:CD1 | 2.41 | 0.56 |
| 3:13:18:ARG:NE | 3:13:46:THR:HA | 2.20 | 0.56 |
| 3:14:39:PRO:HB2 | 3:14:42:PHE:CD1 | 2.41 | 0.56 |
| 3:15:70:PHE:CD1 | 1:O:41:PRO:HD3 | 2.39 | 0.56 |
| 3:16:39:PRO:HB2 | 3:16:42:PHE:CD1 | 2.41 | 0.56 |
| 3:17:18:ARG:NE | 3:17:46:THR:HA | 2.20 | 0.56 |
| 3:18:18:ARG:NE | 3:18:46:THR:HA | 2.20 | 0.56 |
| 3:21:18:ARG:NE | 3:21:46:THR:HA | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:39:PRO:HB3 | 1:E:75:GLY:HA3 | 1.87 | 0.56 |
| 1:Y:223:GLN:HB2 | 1:Z:232:MET:HG3 | 1.86 | 0.56 |
| 2:a:46:ASP:HA | 2:b:161:ASN:ND2 | 2.18 | 0.56 |
| 2:a:247:THR:HB | 2:a:248:PRO:HD2 | 1.87 | 0.56 |
| 3:1:39:PRO:HB2 | 3:1:42:PHE:CD1 | 2.41 | 0.56 |
| 2:o:105:VAL:HG22 | 2:o:165:ILE:HB | 1.87 | 0.56 |
| 2:p:46:ASP:OD1 | 2:q:160:LEU:HD12 | 2.05 | 0.56 |
| 2:t:269:THR:OG1 | 2:t:359:ARG:HB2 | 2.04 | 0.56 |
| 2:u:247:THR:HB | 2:u:248:PRO:HD2 | 1.87 | 0.56 |
| 2:v:105:VAL:HG22 | 2:v:165:ILE:HB | 1.87 | 0.56 |
| 3:5:18:ARG:NE | 3:5:46:THR:HA | 2.20 | 0.56 |
| 3:12:39:PRO:HB2 | 3:12:42:PHE:CD1 | 2.41 | 0.56 |
| 1:J:39:PRO:HB3 | 1:K:75:GLY:HA3 | 1.87 | 0.56 |
| 2:c:46:ASP:OD1 | 2:d:160:LEU:HD12 | 2.05 | 0.56 |
| 2:g:72:THR:OG1 | 1:H:70:ARG:NH2 | 2.39 | 0.56 |
| 2:g:105:VAL:HG22 | 2:g:165:ILE:HB | 1.87 | 0.56 |
| 2:g:269:THR:OG1 | 2:g:359:ARG:HB2 | 2.04 | 0.56 |
| 2:p:105:VAL:HG22 | 2:p:165:ILE:HB | 1.87 | 0.56 |
| 2:y:164:ARG:NH1 | 2:z:365:ILE:HG23 | 2.21 | 0.56 |
| 3:5:24:GLU:HB3 | 3:5:33:ARG:HB2 | 1.87 | 0.56 |
| 3:7:39:PRO:HB2 | 3:7:42:PHE:CD1 | 2.41 | 0.56 |
| 3:25:39:PRO:HB2 | 3:25:42:PHE:CD1 | 2.41 | 0.56 |
| 1:O:160:ASN:HA | 1:O:186:PRO:HD3 | 1.85 | 0.56 |
| 2:c:247:THR:HB | 2:c:248:PRO:HD2 | 1.87 | 0.56 |
| 2:d:105:VAL:HG22 | 2:d:165:ILE:HB | 1.87 | 0.56 |
| 2:k:46:ASP:HA | 2:l:161:ASN:ND2 | 2.18 | 0.56 |
| 2:l:20:GLU:OE2 | 2:l:246:VAL:HG21 | 2.05 | 0.56 |
| 2:s:247:THR:HB | 2:s:248:PRO:HD2 | 1.87 | 0.56 |
| 2:w:20:GLU:OE2 | 2:w:246:VAL:HG21 | 2.05 | 0.56 |
| 2:y:105:VAL:HG22 | 2:y:165:ILE:HB | 1.87 | 0.56 |
| 3:4:39:PRO:HB2 | 3:4:42:PHE:CD1 | 2.41 | 0.56 |
| 3:6:24:GLU:HB3 | 3:6:33:ARG:HB2 | 1.87 | 0.56 |
| 3:6:39:PRO:HB2 | 3:6:42:PHE:CD1 | 2.41 | 0.56 |
| 3:8:22:VAL:HG22 | 3:8:34:LEU:CD2 | 2.34 | 0.56 |
| 3:15:18:ARG:NE | 3:15:46:THR:HA | 2.20 | 0.56 |
| 3:20:70:PHE:CD1 | 1:T:41:PRO:HD3 | 2.39 | 0.56 |
| 2:d:20:GLU:OE2 | 2:d:246:VAL:HG21 | 2.05 | 0.56 |
| 2:h:72:THR:OG1 | 1:I:70:ARG:NH2 | 2.38 | 0.56 |
| 2:k:20:GLU:OE2 | 2:k:246:VAL:HG21 | 2.05 | 0.56 |
| 2:n:105:VAL:HG22 | 2:n:165:ILE:HB | 1.87 | 0.56 |
| 2:p:20:GLU:OE2 | 2:p:246:VAL:HG21 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:q:20:GLU:OE2 | 2:q:246:VAL:HG21 | 2.05 | 0.56 |
| 2:t:105:VAL:HG22 | 2:t:165:ILE:HB | 1.87 | 0.56 |
| 2:y:101:GLN:HE22 | 2:z:219:ARG:HD3 | 1.71 | 0.56 |
| 3:3:39:PRO:HB2 | 3:3:42:PHE:CD1 | 2.41 | 0.56 |
| 3:13:39:PRO:HB2 | 3:13:42:PHE:CD1 | 2.41 | 0.56 |
| 3:18:70:PHE:CD1 | 1:R:41:PRO:HD3 | 2.39 | 0.56 |
| 2:c:20:GLU:OE2 | 2:c:246:VAL:HG21 | 2.05 | 0.56 |
| 2:j:46:ASP:OD1 | 2:k:160:LEU:HD12 | 2.05 | 0.56 |
| 2:l:208:ARG:HH21 | 2:l:238:ASP:HB2 | 1.71 | 0.56 |
| 2:m:208:ARG:HH21 | 2:m:238:ASP:HB2 | 1.71 | 0.56 |
| 2:r:247:THR:HB | 2:r:248:PRO:HD2 | 1.87 | 0.56 |
| 2:t:98:ARG:NH1 | 2:u:220:THR:OG1 | 2.37 | 0.56 |
| 3:2:39:PRO:HB2 | 3:2:42:PHE:CD1 | 2.41 | 0.56 |
| 3:8:18:ARG:NE | 3:8:46:THR:HA | 2.20 | 0.56 |
| 3:9:22:VAL:HG22 | 3:9:34:LEU:CD2 | 2.34 | 0.56 |
| 3:10:18:ARG:NE | 3:10:46:THR:HA | 2.20 | 0.56 |
| 3:11:18:ARG:NE | 3:11:46:THR:HA | 2.20 | 0.56 |
| 3:18:23:SER:OG | 3:18:35:THR:HG23 | 2.06 | 0.56 |
| 3:18:39:PRO:HB2 | 3:18:42:PHE:CD1 | 2.41 | 0.56 |
| 3:19:23:SER:OG | 3:19:35:THR:HG23 | 2.06 | 0.56 |
| 3:20:23:SER:OG | 3:20:35:THR:HG23 | 2.06 | 0.56 |
| 3:21:23:SER:OG | 3:21:35:THR:HG23 | 2.06 | 0.56 |
| 3:23:39:PRO:HB2 | 3:23:42:PHE:CD1 | 2.41 | 0.56 |
| 2:d:247:THR:HB | 2:d:248:PRO:HD2 | 1.87 | 0.56 |
| 2:h:46:ASP:OD1 | 2:i:160:LEU:HD12 | 2.06 | 0.56 |
| 2:i:247:THR:HB | 2:i:248:PRO:HD2 | 1.87 | 0.56 |
| 2:k:208:ARG:HH21 | 2:k:238:ASP:HB2 | 1.71 | 0.56 |
| 2:l:46:ASP:OD1 | 2:m:160:LEU:HD12 | 2.05 | 0.56 |
| 2:m:98:ARG:NH1 | 2:n:220:THR:OG1 | 2.37 | 0.56 |
| 2:o:20:GLU:OE2 | 2:o:246:VAL:HG21 | 2.05 | 0.56 |
| 2:r:20:GLU:OE2 | 2:r:246:VAL:HG21 | 2.05 | 0.56 |
| 3:3:59:CYS:SG | 3:3:67:ALA:HB2 | 2.46 | 0.56 |
| 3:5:39:PRO:HB2 | 3:5:42:PHE:CD1 | 2.41 | 0.56 |
| 3:13:59:CYS:SG | 3:13:67:ALA:HB2 | 2.46 | 0.56 |
| 3:14:59:CYS:SG | 3:14:67:ALA:HB2 | 2.46 | 0.56 |
| 3:17:23:SER:OG | 3:17:35:THR:HG23 | 2.06 | 0.56 |
| 3:24:18:ARG:NE | 3:24:46:THR:HA | 2.20 | 0.56 |
| 3:24:59:CYS:SG | 3:24:67:ALA:HB2 | 2.46 | 0.56 |
| 3:25:59:CYS:SG | 3:25:67:ALA:HB2 | 2.46 | 0.56 |
| 3:26:59:CYS:SG | 3:26:67:ALA:HB2 | 2.46 | 0.56 |
| 1:O:80:ILE:HD13 | 1:O:195:VAL:HG13 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:80:ILE:HD13 | 1:P:195:VAL:HG13 | 1.88 | 0.56 |
| 1:X:223:GLN:HB2 | 1:Y:232:MET:HG3 | 1.87 | 0.56 |
| 3:1:59:CYS:SG | 3:1:67:ALA:HB2 | 2.46 | 0.56 |
| 2:e:247:THR:HB | 2:e:248:PRO:HD2 | 1.87 | 0.56 |
| 2:f:105:VAL:HG22 | 2:f:165:ILE:HB | 1.87 | 0.56 |
| 2:i:46:ASP:OD1 | 2:j:160:LEU:HD12 | 2.05 | 0.56 |
| 2:l:46:ASP:HA | 2:m:161:ASN:ND2 | 2.17 | 0.56 |
| 2:q:247:THR:HB | 2:q:248:PRO:HD2 | 1.87 | 0.56 |
| 2:w:72:THR:OG1 | 1:X:70:ARG:NH2 | 2.37 | 0.56 |
| 2:w:105:VAL:HG22 | 2:w:165:ILE:HB | 1.87 | 0.56 |
| 2:x:164:ARG:HD2 | 2:y:365:ILE:CG2 | 2.36 | 0.56 |
| 3:6:59:CYS:SG | 3:6:67:ALA:HB2 | 2.46 | 0.56 |
| 3:9:59:CYS:SG | 3:9:67:ALA:HB2 | 2.46 | 0.56 |
| 3:11:59:CYS:SG | 3:11:67:ALA:HB2 | 2.46 | 0.56 |
| 3:12:59:CYS:SG | 3:12:67:ALA:HB2 | 2.46 | 0.56 |
| 1:C:80:ILE:HD13 | 1:C:195:VAL:HG13 | 1.88 | 0.56 |
| 1:D:80:ILE:HD13 | 1:D:195:VAL:HG13 | 1.88 | 0.56 |
| 2:h:247:THR:HB | 2:h:248:PRO:HD2 | 1.87 | 0.55 |
| 2:k:271:ASP:CB | 2:k:357:CYS:HA | 2.28 | 0.55 |
| 2:m:247:THR:HB | 2:m:248:PRO:HD2 | 1.87 | 0.55 |
| 2:n:208:ARG:HH21 | 2:n:238:ASP:HB2 | 1.71 | 0.55 |
| 2:n:247:THR:HB | 2:n:248:PRO:HD2 | 1.87 | 0.55 |
| 2:o:46:ASP:OD1 | 2:p:160:LEU:HD12 | 2.06 | 0.55 |
| 2:q:105:VAL:HG22 | 2:q:165:ILE:HB | 1.87 | 0.55 |
| 2:s:20:GLU:OE2 | 2:s:246:VAL:HG21 | 2.05 | 0.55 |
| 2:s:46:ASP:OD1 | 2:t:160:LEU:HD12 | 2.05 | 0.55 |
| 2:v:46:ASP:OD1 | 2:w:160:LEU:HD12 | 2.05 | 0.55 |
| 3:10:22:VAL:HG22 | 3:10:34:LEU:CD2 | 2.34 | 0.55 |
| 3:15:59:CYS:SG | 3:15:67:ALA:HB2 | 2.46 | 0.55 |
| 3:21:39:PRO:HB2 | 3:21:42:PHE:CD1 | 2.41 | 0.55 |
| 3:23:59:CYS:SG | 3:23:67:ALA:HB2 | 2.46 | 0.55 |
| 3:26:39:PRO:HB2 | 3:26:42:PHE:CD1 | 2.41 | 0.55 |
| 1:V:80:ILE:HD13 | 1:V:195:VAL:HG13 | 1.88 | 0.55 |
| 1:W:80:ILE:HD13 | 1:W:195:VAL:HG13 | 1.88 | 0.55 |
| 2:a:161:ASN:ND2 | 2:z:46:ASP:HA | 2.18 | 0.55 |
| 3:1:18:ARG:NE | 3:1:46:THR:HA | 2.20 | 0.55 |
| 2:e:72:THR:OG1 | 1:F:70:ARG:NH2 | 2.37 | 0.55 |
| 2:e:271:ASP:CB | 2:e:357:CYS:HA | 2.28 | 0.55 |
| 2:l:105:VAL:HG22 | 2:l:165:ILE:HB | 1.87 | 0.55 |
| 2:n:20:GLU:OE2 | 2:n:246:VAL:HG21 | 2.05 | 0.55 |
| 2:o:26:THR:CG2 | 2:o:187:LEU:HB3 | 2.35 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:o:72:THR:OG1 | 1:P:70:ARG:NH2 | 2.38 | 0.55 |
| 3:2:59:CYS:SG | 3:2:67:ALA:HB2 | 2.46 | 0.55 |
| 3:9:18:ARG:NE | 3:9:46:THR:HA | 2.20 | 0.55 |
| 3:16:23:SER:OG | 3:16:35:THR:HG23 | 2.06 | 0.55 |
| 3:16:28:ILE:O | 3:16:29:SER:OG | 2.21 | 0.55 |
| 3:16:59:CYS:SG | 3:16:67:ALA:HB2 | 2.46 | 0.55 |
| 3:19:39:PRO:HB2 | 3:19:42:PHE:CD1 | 2.41 | 0.55 |
| 3:22:23:SER:OG | 3:22:35:THR:HG23 | 2.06 | 0.55 |
| 3:25:28:ILE:O | 3:25:29:SER:OG | 2.21 | 0.55 |
| 2:a:208:ARG:HH21 | 2:a:238:ASP:HB2 | 1.71 | 0.55 |
| 2:b:208:ARG:HH21 | 2:b:238:ASP:HB2 | 1.71 | 0.55 |
| 2:e:105:VAL:HG22 | 2:e:165:ILE:HB | 1.87 | 0.55 |
| 2:j:98:ARG:NH1 | 2:k:220:THR:OG1 | 2.36 | 0.55 |
| 2:j:208:ARG:HH21 | 2:j:238:ASP:HB2 | 1.71 | 0.55 |
| 2:n:26:THR:CG2 | 2:n:187:LEU:HB3 | 2.35 | 0.55 |
| 2:u:20:GLU:OE2 | 2:u:246:VAL:HG21 | 2.05 | 0.55 |
| 2:v:20:GLU:OE2 | 2:v:246:VAL:HG21 | 2.05 | 0.55 |
| 2:x:99:GLN:NE2 | 1:W:50:SER:HB3 | 2.21 | 0.55 |
| 3:2:28:ILE:O | 3:2:29:SER:OG | 2.21 | 0.55 |
| 3:7:18:ARG:NE | 3:7:46:THR:HA | 2.20 | 0.55 |
| 3:8:59:CYS:SG | 3:8:67:ALA:HB2 | 2.46 | 0.55 |
| 3:15:23:SER:OG | 3:15:35:THR:HG23 | 2.06 | 0.55 |
| 3:15:39:PRO:HB2 | 3:15:42:PHE:CD1 | 2.41 | 0.55 |
| 3:22:59:CYS:SG | 3:22:67:ALA:HB2 | 2.46 | 0.55 |
| 3:23:23:SER:OG | 3:23:35:THR:HG23 | 2.06 | 0.55 |
| 1:E:80:ILE:HD13 | 1:E:195:VAL:HG13 | 1.88 | 0.55 |
| 1:J:80:ILE:HD13 | 1:J:195:VAL:HG13 | 1.88 | 0.55 |
| 1:N:80:ILE:HD13 | 1:N:195:VAL:HG13 | 1.88 | 0.55 |
| 1:U:80:ILE:HD13 | 1:U:195:VAL:HG13 | 1.88 | 0.55 |
| 1:X:80:ILE:HD13 | 1:X:195:VAL:HG13 | 1.88 | 0.55 |
| 2:f:247:THR:HB | 2:f:248:PRO:HD2 | 1.87 | 0.55 |
| 2:m:26:THR:CG2 | 2:m:187:LEU:HB3 | 2.35 | 0.55 |
| 2:p:247:THR:HB | 2:p:248:PRO:HD2 | 1.87 | 0.55 |
| 3:4:18:ARG:NE | 3:4:46:THR:HA | 2.20 | 0.55 |
| 3:4:59:CYS:SG | 3:4:67:ALA:HB2 | 2.46 | 0.55 |
| 3:10:59:CYS:SG | 3:10:67:ALA:HB2 | 2.46 | 0.55 |
| 3:17:39:PRO:HB2 | 3:17:42:PHE:CD1 | 2.41 | 0.55 |
| 3:19:74:VAL:O | 3:19:90:PHE:HA | 2.07 | 0.55 |
| 3:22:28:ILE:O | 3:22:29:SER:OG | 2.21 | 0.55 |
| 3:24:39:PRO:HB2 | 3:24:42:PHE:CD1 | 2.41 | 0.55 |
| 1:I:80:ILE:HD13 | 1:I:195:VAL:HG13 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:176:GLU:OE1 | 1:J:207:TYR:OH | 2.21 | 0.55 |
| 1:Q:80:ILE:HD13 | 1:Q:195:VAL:HG13 | 1.88 | 0.55 |
| 2:c:98:ARG:NH1 | 2:d:220:THR:OG1 | 2.36 | 0.55 |
| 2:l:247:THR:HB | 2:l:248:PRO:HD2 | 1.87 | 0.55 |
| 2:o:208:ARG:HH21 | 2:o:238:ASP:HB2 | 1.71 | 0.55 |
| 2:p:26:THR:CG2 | 2:p:187:LEU:HB3 | 2.35 | 0.55 |
| 2:q:98:ARG:NH1 | 2:r:220:THR:OG1 | 2.37 | 0.55 |
| 2:s:105:VAL:HG22 | 2:s:165:ILE:HB | 1.87 | 0.55 |
| 2:u:166:THR:HG21 | 2:w:362:LEU:CD2 | 2.37 | 0.55 |
| 2:z:271:ASP:CB | 2:z:357:CYS:HA | 2.28 | 0.55 |
| 3:3:19:GLN:O | 3:3:21:GLN:NE2 | 2.40 | 0.55 |
| 3:6:74:VAL:O | 3:6:90:PHE:HA | 2.07 | 0.55 |
| 3:7:23:SER:OG | 3:7:35:THR:HG23 | 2.06 | 0.55 |
| 3:8:19:GLN:O | 3:8:21:GLN:NE2 | 2.40 | 0.55 |
| 3:8:23:SER:OG | 3:8:35:THR:HG23 | 2.06 | 0.55 |
| 3:11:22:VAL:HG22 | 3:11:34:LEU:CD2 | 2.34 | 0.55 |
| 3:12:74:VAL:O | 3:12:90:PHE:HA | 2.07 | 0.55 |
| 3:13:74:VAL:O | 3:13:90:PHE:HA | 2.07 | 0.55 |
| 3:17:59:CYS:SG | 3:17:67:ALA:HB2 | 2.46 | 0.55 |
| 3:20:39:PRO:HB2 | 3:20:42:PHE:CD1 | 2.41 | 0.55 |
| 3:20:74:VAL:O | 3:20:90:PHE:HA | 2.07 | 0.55 |
| 3:22:39:PRO:HB2 | 3:22:42:PHE:CD1 | 2.41 | 0.55 |
| 3:24:23:SER:OG | 3:24:35:THR:HG23 | 2.06 | 0.55 |
| 1:B:80:ILE:HD13 | 1:B:195:VAL:HG13 | 1.88 | 0.55 |
| 1:Y:176:GLU:OE1 | 1:Y:207:TYR:OH | 2.21 | 0.55 |
| 3:1:19:GLN:O | 3:1:21:GLN:NE2 | 2.40 | 0.55 |
| 2:i:208:ARG:HH21 | 2:i:238:ASP:HB2 | 1.70 | 0.55 |
| 2:j:247:THR:HB | 2:j:248:PRO:HD2 | 1.87 | 0.55 |
| 2:l:99:GLN:NE2 | 1:K:50:SER:HB3 | 2.21 | 0.55 |
| 2:m:105:VAL:HG22 | 2:m:165:ILE:HB | 1.87 | 0.55 |
| 2:o:166:THR:HG21 | 2:q:362:LEU:CD2 | 2.37 | 0.55 |
| 2:p:72:THR:OG1 | 1:Q:70:ARG:NH2 | 2.37 | 0.55 |
| 2:q:26:THR:CG2 | 2:q:187:LEU:HB3 | 2.35 | 0.55 |
| 2:r:99:GLN:NE2 | 1:Q:50:SER:HB3 | 2.21 | 0.55 |
| 2:t:271:ASP:CB | 2:t:357:CYS:HA | 2.28 | 0.55 |
| 2:x:105:VAL:HG22 | 2:x:165:ILE:HB | 1.87 | 0.55 |
| 3:6:19:GLN:O | 3:6:21:GLN:NE2 | 2.40 | 0.55 |
| 3:6:23:SER:OG | 3:6:35:THR:HG23 | 2.06 | 0.55 |
| 3:7:19:GLN:O | 3:7:21:GLN:NE2 | 2.40 | 0.55 |
| 3:12:18:ARG:NE | 3:12:46:THR:HA | 2.20 | 0.55 |
| 3:19:28:ILE:O | 3:19:29:SER:OG | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:80:ILE:HD13 | 1:T:195:VAL:HG13 | 1.88 | 0.55 |
| 2:a:271:ASP:CB | 2:a:357:CYS:HA | 2.28 | 0.55 |
| 2:m:20:GLU:OE2 | 2:m:246:VAL:HG21 | 2.05 | 0.55 |
| 2:t:20:GLU:OE2 | 2:t:246:VAL:HG21 | 2.05 | 0.55 |
| 2:t:208:ARG:HH21 | 2:t:238:ASP:HB2 | 1.71 | 0.55 |
| 2:v:208:ARG:HH21 | 2:v:238:ASP:HB2 | 1.71 | 0.55 |
| 2:z:175:LEU:HD11 | 1:X:51:ILE:CG1 | 2.36 | 0.55 |
| 3:5:59:CYS:SG | 3:5:67:ALA:HB2 | 2.46 | 0.55 |
| 3:5:74:VAL:O | 3:5:90:PHE:HA | 2.07 | 0.55 |
| 3:7:74:VAL:O | 3:7:90:PHE:HA | 2.07 | 0.55 |
| 3:9:23:SER:OG | 3:9:35:THR:HG23 | 2.06 | 0.55 |
| 3:11:19:GLN:O | 3:11:21:GLN:NE2 | 2.40 | 0.55 |
| 3:12:22:VAL:HG22 | 3:12:34:LEU:CD2 | 2.34 | 0.55 |
| 3:14:23:SER:OG | 3:14:35:THR:HG23 | 2.06 | 0.55 |
| 3:18:74:VAL:O | 3:18:90:PHE:HA | 2.07 | 0.55 |
| 3:24:74:VAL:O | 3:24:90:PHE:HA | 2.07 | 0.55 |
| 1:Y:80:ILE:HD13 | 1:Y:195:VAL:HG13 | 1.88 | 0.55 |
| 1:Z:176:GLU:OE1 | 1:Z:207:TYR:OH | 2.21 | 0.55 |
| 3:1:74:VAL:O | 3:1:90:PHE:HA | 2.07 | 0.55 |
| 2:f:114:LYS:O | 2:f:160:LEU:HD13 | 2.07 | 0.55 |
| 2:g:247:THR:HB | 2:g:248:PRO:HD2 | 1.87 | 0.55 |
| 2:l:26:THR:CG2 | 2:l:187:LEU:HB3 | 2.35 | 0.55 |
| 2:l:72:THR:OG1 | 1:M:70:ARG:NH2 | 2.38 | 0.55 |
| 2:o:247:THR:HB | 2:o:248:PRO:HD2 | 1.87 | 0.55 |
| 2:r:208:ARG:HH21 | 2:r:238:ASP:HB2 | 1.71 | 0.55 |
| 2:s:208:ARG:HH21 | 2:s:238:ASP:HB2 | 1.71 | 0.55 |
| 2:u:208:ARG:HH21 | 2:u:238:ASP:HB2 | 1.71 | 0.55 |
| 2:w:98:ARG:NH1 | 2:x:220:THR:OG1 | 2.37 | 0.55 |
| 2:x:208:ARG:HH21 | 2:x:238:ASP:HB2 | 1.71 | 0.55 |
| 2:z:208:ARG:HH21 | 2:z:238:ASP:HB2 | 1.71 | 0.55 |
| 3:4:19:GLN:O | 3:4:21:GLN:NE2 | 2.40 | 0.55 |
| 3:5:23:SER:OG | 3:5:35:THR:HG23 | 2.06 | 0.55 |
| 3:14:74:VAL:O | 3:14:90:PHE:HA | 2.07 | 0.55 |
| 3:21:59:CYS:SG | 3:21:67:ALA:HB2 | 2.47 | 0.55 |
| 3:21:74:VAL:O | 3:21:90:PHE:HA | 2.07 | 0.55 |
| 3:22:22:VAL:HG22 | 3:22:34:LEU:CD2 | 2.34 | 0.55 |
| 3:23:22:VAL:HG22 | 3:23:34:LEU:CD2 | 2.34 | 0.55 |
| 1:K:80:ILE:HD13 | 1:K:195:VAL:HG13 | 1.88 | 0.55 |
| 2:b:46:ASP:OD1 | 2:c:160:LEU:HD12 | 2.06 | 0.55 |
| 2:c:114:LYS:O | 2:c:160:LEU:HD13 | 2.07 | 0.55 |
| 2:c:208:ARG:HH21 | 2:c:238:ASP:HB2 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:k:99:GLN:NE2 | 1:J:50:SER:HB3 | 2.22 | 0.55 |
| 2:n:46:ASP:OD1 | 2:o:160:LEU:HD12 | 2.06 | 0.55 |
| 2:w:208:ARG:HH21 | 2:w:238:ASP:HB2 | 1.71 | 0.55 |
| 3:4:74:VAL:O | 3:4:90:PHE:HA | 2.07 | 0.55 |
| 3:5:28:ILE:O | 3:5:29:SER:OG | 2.21 | 0.55 |
| 3:7:59:CYS:SG | 3:7:67:ALA:HB2 | 2.46 | 0.55 |
| 3:10:19:GLN:O | 3:10:21:GLN:NE2 | 2.40 | 0.55 |
| 3:10:23:SER:OG | 3:10:35:THR:HG23 | 2.06 | 0.55 |
| 3:18:59:CYS:SG | 3:18:67:ALA:HB2 | 2.46 | 0.55 |
| 3:24:19:GLN:O | 3:24:21:GLN:NE2 | 2.40 | 0.55 |
| 3:24:22:VAL:HG22 | 3:24:34:LEU:CD2 | 2.34 | 0.55 |
| 3:25:22:VAL:HG22 | 3:25:34:LEU:CD2 | 2.34 | 0.55 |
| 3:25:23:SER:OG | 3:25:35:THR:HG23 | 2.06 | 0.55 |
| 1:H:80:ILE:HD13 | 1:H:195:VAL:HG13 | 1.88 | 0.55 |
| 1:H:176:GLU:OE1 | 1:H:207:TYR:OH | 2.21 | 0.55 |
| 1:M:219:MET:HE2 | 1:O:132:PHE:CB | 2.37 | 0.55 |
| 3:1:22:VAL:HG22 | 3:1:34:LEU:CD2 | 2.34 | 0.55 |
| 2:i:114:LYS:O | 2:i:160:LEU:HD13 | 2.07 | 0.55 |
| 2:m:46:ASP:OD1 | 2:n:160:LEU:HD12 | 2.05 | 0.55 |
| 2:p:208:ARG:HH21 | 2:p:238:ASP:HB2 | 1.71 | 0.55 |
| 2:q:99:GLN:NE2 | 1:P:50:SER:HB3 | 2.22 | 0.55 |
| 2:q:208:ARG:HH21 | 2:q:238:ASP:HB2 | 1.71 | 0.55 |
| 2:r:26:THR:CG2 | 2:r:187:LEU:HB3 | 2.35 | 0.55 |
| 2:s:46:ASP:HA | 2:t:161:ASN:ND2 | 2.18 | 0.55 |
| 2:u:45:LEU:HD22 | 2:u:116:LEU:HA | 1.89 | 0.55 |
| 2:u:46:ASP:OD1 | 2:v:160:LEU:HD12 | 2.05 | 0.55 |
| 2:v:45:LEU:HD22 | 2:v:116:LEU:HA | 1.89 | 0.55 |
| 2:w:114:LYS:O | 2:w:160:LEU:HD13 | 2.07 | 0.55 |
| 2:x:114:LYS:O | 2:x:160:LEU:HD13 | 2.07 | 0.55 |
| 2:x:271:ASP:CB | 2:x:357:CYS:HA | 2.28 | 0.55 |
| 2:z:114:LYS:O | 2:z:160:LEU:HD13 | 2.07 | 0.55 |
| 3:9:19:GLN:O | 3:9:21:GLN:NE2 | 2.40 | 0.55 |
| 3:11:74:VAL:O | 3:11:90:PHE:HA | 2.07 | 0.55 |
| 3:13:22:VAL:HG22 | 3:13:34:LEU:CD2 | 2.34 | 0.55 |
| 3:26:19:GLN:O | 3:26:21:GLN:NE2 | 2.40 | 0.55 |
| 3:26:22:VAL:HG22 | 3:26:34:LEU:CD2 | 2.34 | 0.55 |
| 2:b:271:ASP:CB | 2:b:357:CYS:HA | 2.28 | 0.54 |
| 2:f:166:THR:HG21 | 2:h:362:LEU:CD2 | 2.37 | 0.54 |
| 2:k:26:THR:CG2 | 2:k:187:LEU:HB3 | 2.35 | 0.54 |
| 2:m:46:ASP:HA | 2:n:161:ASN:ND2 | 2.18 | 0.54 |
| 2:s:72:THR:OG1 | 1:T:70:ARG:NH2 | 2.39 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:t:114:LYS:O | 2:t:160:LEU:HD13 | 2.07 | 0.54 |
| 2:y:83:ASN:ND2 | 2:z:109:SER:OG | 2.38 | 0.54 |
| 3:2:22:VAL:HG22 | 3:2:34:LEU:CD2 | 2.34 | 0.54 |
| 3:5:19:GLN:O | 3:5:21:GLN:NE2 | 2.40 | 0.54 |
| 3:11:23:SER:OG | 3:11:35:THR:HG23 | 2.06 | 0.54 |
| 3:13:23:SER:OG | 3:13:35:THR:HG23 | 2.06 | 0.54 |
| 3:14:18:ARG:NE | 3:14:46:THR:HA | 2.20 | 0.54 |
| 3:20:59:CYS:SG | 3:20:67:ALA:HB2 | 2.46 | 0.54 |
| 1:F:80:ILE:HD13 | 1:F:195:VAL:HG13 | 1.88 | 0.54 |
| 1:F:176:GLU:OE1 | 1:F:207:TYR:OH | 2.21 | 0.54 |
| 1:M:80:ILE:HD13 | 1:M:195:VAL:HG13 | 1.88 | 0.54 |
| 2:a:114:LYS:O | 2:a:160:LEU:HD13 | 2.07 | 0.54 |
| 2:f:208:ARG:HH21 | 2:f:238:ASP:HB2 | 1.71 | 0.54 |
| 2:h:208:ARG:HH21 | 2:h:238:ASP:HB2 | 1.71 | 0.54 |
| 2:n:98:ARG:NH1 | 2:o:220:THR:OG1 | 2.37 | 0.54 |
| 2:n:254:VAL:HG13 | 2:n:365:ILE:HG12 | 1.90 | 0.54 |
| 2:s:26:THR:CG2 | 2:s:187:LEU:HB3 | 2.35 | 0.54 |
| 2:t:45:LEU:HD22 | 2:t:116:LEU:HA | 1.89 | 0.54 |
| 2:u:114:LYS:O | 2:u:160:LEU:HD13 | 2.07 | 0.54 |
| 2:w:26:THR:CG2 | 2:w:187:LEU:HB3 | 2.35 | 0.54 |
| 2:w:45:LEU:HD22 | 2:w:116:LEU:HA | 1.89 | 0.54 |
| 2:y:208:ARG:HH21 | 2:y:238:ASP:HB2 | 1.71 | 0.54 |
| 3:2:74:VAL:O | 3:2:90:PHE:HA | 2.07 | 0.54 |
| 3:4:23:SER:OG | 3:4:35:THR:HG23 | 2.06 | 0.54 |
| 3:8:74:VAL:O | 3:8:90:PHE:HA | 2.07 | 0.54 |
| 3:13:19:GLN:O | 3:13:21:GLN:NE2 | 2.40 | 0.54 |
| 3:17:74:VAL:O | 3:17:90:PHE:HA | 2.07 | 0.54 |
| 3:21:22:VAL:HG22 | 3:21:34:LEU:CD2 | 2.34 | 0.54 |
| 1:J:68:ASP:O | 1:J:69:ARG:HG2 | 2.08 | 0.54 |
| 1:M:68:ASP:O | 1:M:69:ARG:HG2 | 2.08 | 0.54 |
| 1:P:219:MET:HE2 | 1:R:132:PHE:CB | 2.38 | 0.54 |
| 1:R:80:ILE:HD13 | 1:R:195:VAL:HG13 | 1.88 | 0.54 |
| 1:Z:68:ASP:O | 1:Z:69:ARG:HG2 | 2.08 | 0.54 |
| 1:Z:80:ILE:HD13 | 1:Z:195:VAL:HG13 | 1.88 | 0.54 |
| 2:e:46:ASP:OD1 | 2:f:160:LEU:HD12 | 2.07 | 0.54 |
| 2:e:166:THR:HG21 | 2:g:362:LEU:CD2 | 2.37 | 0.54 |
| 2:g:208:ARG:HH21 | 2:g:238:ASP:HB2 | 1.71 | 0.54 |
| 2:v:26:THR:CG2 | 2:v:187:LEU:HB3 | 2.35 | 0.54 |
| 2:v:46:ASP:HA | 2:w:161:ASN:ND2 | 2.17 | 0.54 |
| 2:w:99:GLN:NE2 | 1:V:50:SER:HB3 | 2.22 | 0.54 |
| 2:x:45:LEU:HD22 | 2:x:116:LEU:HA | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:74:VAL:O | 3:3:90:PHE:HA | 2.07 | 0.54 |
| 3:6:18:ARG:NE | 3:6:46:THR:HA | 2.20 | 0.54 |
| 3:14:22:VAL:HG22 | 3:14:34:LEU:CD2 | 2.34 | 0.54 |
| 3:15:74:VAL:O | 3:15:90:PHE:HA | 2.07 | 0.54 |
| 3:19:22:VAL:HG22 | 3:19:34:LEU:CD2 | 2.34 | 0.54 |
| 3:20:22:VAL:HG22 | 3:20:34:LEU:CD2 | 2.34 | 0.54 |
| 3:25:19:GLN:O | 3:25:21:GLN:NE2 | 2.40 | 0.54 |
| 3:26:23:SER:OG | 3:26:35:THR:HG23 | 2.06 | 0.54 |
| 1:N:68:ASP:O | 1:N:69:ARG:HG2 | 2.08 | 0.54 |
| 1:R:219:MET:HE2 | 1:T:132:PHE:CB | 2.38 | 0.54 |
| 1:S:80:ILE:HD13 | 1:S:195:VAL:HG13 | 1.88 | 0.54 |
| 1:V:68:ASP:O | 1:V:69:ARG:HG2 | 2.08 | 0.54 |
| 1:A:80:ILE:HD13 | 1:A:195:VAL:HG13 | 1.89 | 0.54 |
| 3:1:23:SER:OG | 3:1:35:THR:HG23 | 2.06 | 0.54 |
| 2:c:166:THR:HG21 | 2:e:362:LEU:CD2 | 2.37 | 0.54 |
| 2:c:271:ASP:CB | 2:c:357:CYS:HA | 2.28 | 0.54 |
| 2:d:114:LYS:O | 2:d:160:LEU:HD13 | 2.07 | 0.54 |
| 2:e:114:LYS:O | 2:e:160:LEU:HD13 | 2.07 | 0.54 |
| 2:e:208:ARG:HH21 | 2:e:238:ASP:HB2 | 1.71 | 0.54 |
| 2:r:105:VAL:HG22 | 2:r:165:ILE:HB | 1.87 | 0.54 |
| 2:x:26:THR:CG2 | 2:x:187:LEU:HB3 | 2.35 | 0.54 |
| 3:3:22:VAL:HG22 | 3:3:34:LEU:CD2 | 2.34 | 0.54 |
| 3:12:23:SER:OG | 3:12:35:THR:HG23 | 2.06 | 0.54 |
| 3:15:22:VAL:HG22 | 3:15:34:LEU:CD2 | 2.34 | 0.54 |
| 3:16:22:VAL:HG22 | 3:16:34:LEU:CD2 | 2.34 | 0.54 |
| 3:17:22:VAL:HG22 | 3:17:34:LEU:CD2 | 2.34 | 0.54 |
| 3:19:59:CYS:SG | 3:19:67:ALA:HB2 | 2.46 | 0.54 |
| 3:22:19:GLN:O | 3:22:21:GLN:NE2 | 2.40 | 0.54 |
| 3:22:74:VAL:O | 3:22:90:PHE:HA | 2.07 | 0.54 |
| 3:25:74:VAL:O | 3:25:90:PHE:HA | 2.07 | 0.54 |
| 1:I:176:GLU:OE1 | 1:I:207:TYR:OH | 2.21 | 0.54 |
| 1:O:68:ASP:O | 1:O:69:ARG:HG2 | 2.08 | 0.54 |
| 1:U:68:ASP:O | 1:U:69:ARG:HG2 | 2.08 | 0.54 |
| 1:W:68:ASP:O | 1:W:69:ARG:HG2 | 2.08 | 0.54 |
| 2:b:114:LYS:O | 2:b:160:LEU:HD13 | 2.07 | 0.54 |
| 2:j:114:LYS:O | 2:j:160:LEU:HD13 | 2.07 | 0.54 |
| 2:j:254:VAL:HG13 | 2:j:365:ILE:HG12 | 1.90 | 0.54 |
| 2:k:254:VAL:HG13 | 2:k:365:ILE:HG12 | 1.90 | 0.54 |
| 2:l:271:ASP:CB | 2:l:357:CYS:HA | 2.28 | 0.54 |
| 2:o:114:LYS:O | 2:o:160:LEU:HD13 | 2.07 | 0.54 |
| 2:w:46:ASP:HA | 2:x:161:ASN:ND2 | 2.18 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:w:271:ASP:CB | 2:w:357:CYS:HA | 2.28 | 0.54 |
| 2:y:26:THR:CG2 | 2:y:187:LEU:HB3 | 2.35 | 0.54 |
| 3:2:19:GLN:O | 3:2:21:GLN:NE2 | 2.40 | 0.54 |
| 3:3:23:SER:OG | 3:3:35:THR:HG23 | 2.06 | 0.54 |
| 3:10:74:VAL:O | 3:10:90:PHE:HA | 2.07 | 0.54 |
| 3:14:19:GLN:O | 3:14:21:GLN:NE2 | 2.40 | 0.54 |
| 3:18:22:VAL:HG22 | 3:18:34:LEU:CD2 | 2.34 | 0.54 |
| 1:C:68:ASP:O | 1:C:69:ARG:HG2 | 2.08 | 0.54 |
| 1:D:68:ASP:O | 1:D:69:ARG:HG2 | 2.08 | 0.54 |
| 1:G:68:ASP:O | 1:G:69:ARG:HG2 | 2.08 | 0.54 |
| 1:R:176:GLU:OE1 | 1:R:207:TYR:OH | 2.21 | 0.54 |
| 1:X:219:MET:HE2 | 1:Z:132:PHE:CB | 2.37 | 0.54 |
| 2:f:99:GLN:NE2 | 1:E:50:SER:HB3 | 2.21 | 0.54 |
| 2:g:114:LYS:O | 2:g:160:LEU:HD13 | 2.07 | 0.54 |
| 2:i:166:THR:HG21 | 2:k:362:LEU:CD2 | 2.37 | 0.54 |
| 2:j:26:THR:CG2 | 2:j:187:LEU:HB3 | 2.35 | 0.54 |
| 2:k:46:ASP:OD1 | 2:l:160:LEU:HD12 | 2.07 | 0.54 |
| 2:k:247:THR:HB | 2:k:248:PRO:HD2 | 1.87 | 0.54 |
| 2:l:114:LYS:O | 2:l:160:LEU:HD13 | 2.07 | 0.54 |
| 2:s:45:LEU:HD22 | 2:s:116:LEU:HA | 1.89 | 0.54 |
| 2:t:46:ASP:OD1 | 2:u:160:LEU:HD12 | 2.06 | 0.54 |
| 2:w:166:THR:HG21 | 2:y:362:LEU:CD2 | 2.37 | 0.54 |
| 2:z:26:THR:CG2 | 2:z:187:LEU:HB3 | 2.35 | 0.54 |
| 3:4:22:VAL:HG22 | 3:4:34:LEU:CD2 | 2.34 | 0.54 |
| 3:15:28:ILE:O | 3:15:29:SER:OG | 2.21 | 0.54 |
| 3:16:19:GLN:O | 3:16:21:GLN:NE2 | 2.40 | 0.54 |
| 3:16:74:VAL:O | 3:16:90:PHE:HA | 2.07 | 0.54 |
| 3:18:19:GLN:O | 3:18:21:GLN:NE2 | 2.40 | 0.54 |
| 1:E:68:ASP:O | 1:E:69:ARG:HG2 | 2.08 | 0.54 |
| 1:L:68:ASP:O | 1:L:69:ARG:HG2 | 2.08 | 0.54 |
| 1:N:219:MET:HE2 | 1:P:132:PHE:CB | 2.38 | 0.54 |
| 1:P:68:ASP:O | 1:P:69:ARG:HG2 | 2.08 | 0.54 |
| 1:X:68:ASP:O | 1:X:69:ARG:HG2 | 2.08 | 0.54 |
| 1:A:68:ASP:O | 1:A:69:ARG:HG2 | 2.08 | 0.54 |
| 2:d:208:ARG:HH21 | 2:d:238:ASP:HB2 | 1.71 | 0.54 |
| 2:g:254:VAL:HG13 | 2:g:365:ILE:HG12 | 1.90 | 0.54 |
| 2:h:114:LYS:O | 2:h:160:LEU:HD13 | 2.07 | 0.54 |
| 2:j:99:GLN:NE2 | 1:I:50:SER:HB3 | 2.22 | 0.54 |
| 2:m:114:LYS:O | 2:m:160:LEU:HD13 | 2.07 | 0.54 |
| 2:p:99:GLN:NE2 | 1:O:50:SER:HB3 | 2.22 | 0.54 |
| 2:q:46:ASP:OD1 | 2:r:160:LEU:HD12 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:q:114:LYS:O | 2:q:160:LEU:HD13 | 2.07 | 0.54 |
| 2:r:254:VAL:HG13 | 2:r:365:ILE:HG12 | 1.90 | 0.54 |
| 2:t:99:GLN:NE2 | 1:S:50:SER:HB3 | 2.23 | 0.54 |
| 2:u:99:GLN:NE2 | 1:T:50:SER:HB3 | 2.23 | 0.54 |
| 2:y:45:LEU:HD22 | 2:y:116:LEU:HA | 1.89 | 0.54 |
| 3:17:19:GLN:O | 3:17:21:GLN:NE2 | 2.40 | 0.54 |
| 3:23:74:VAL:O | 3:23:90:PHE:HA | 2.07 | 0.54 |
| 1:F:68:ASP:O | 1:F:69:ARG:HG2 | 2.08 | 0.54 |
| 1:K:68:ASP:O | 1:K:69:ARG:HG2 | 2.08 | 0.54 |
| 1:Q:68:ASP:O | 1:Q:69:ARG:HG2 | 2.08 | 0.54 |
| 1:T:68:ASP:O | 1:T:69:ARG:HG2 | 2.08 | 0.54 |
| 1:T:219:MET:HE2 | 1:V:132:PHE:CB | 2.38 | 0.54 |
| 1:Y:121:ARG:HA | 1:Z:111:ARG:HB2 | 1.90 | 0.54 |
| 2:a:26:THR:CG2 | 2:a:187:LEU:HB3 | 2.35 | 0.54 |
| 2:m:99:GLN:NE2 | 1:L:50:SER:HB3 | 2.22 | 0.54 |
| 2:n:45:LEU:HD22 | 2:n:116:LEU:HA | 1.89 | 0.54 |
| 2:n:46:ASP:HA | 2:o:161:ASN:ND2 | 2.18 | 0.54 |
| 2:n:99:GLN:NE2 | 1:M:50:SER:HB3 | 2.23 | 0.54 |
| 2:o:99:GLN:NE2 | 1:N:50:SER:HB3 | 2.23 | 0.54 |
| 2:o:254:VAL:HG13 | 2:o:365:ILE:HG12 | 1.90 | 0.54 |
| 2:t:166:THR:HG21 | 2:v:362:LEU:CD2 | 2.38 | 0.54 |
| 2:v:99:GLN:NE2 | 1:U:50:SER:HB3 | 2.22 | 0.54 |
| 2:w:46:ASP:OD1 | 2:x:160:LEU:HD12 | 2.07 | 0.54 |
| 3:2:23:SER:OG | 3:2:35:THR:HG23 | 2.06 | 0.54 |
| 3:19:19:GLN:O | 3:19:21:GLN:NE2 | 2.40 | 0.54 |
| 3:20:19:GLN:O | 3:20:21:GLN:NE2 | 2.40 | 0.54 |
| 3:21:19:GLN:O | 3:21:21:GLN:NE2 | 2.40 | 0.54 |
| 1:L:80:ILE:HD13 | 1:L:195:VAL:HG13 | 1.88 | 0.54 |
| 1:O:219:MET:HE2 | 1:Q:132:PHE:CB | 2.38 | 0.54 |
| 2:c:99:GLN:NE2 | 1:B:50:SER:HB3 | 2.23 | 0.54 |
| 2:d:99:GLN:NE2 | 1:C:50:SER:HB3 | 2.22 | 0.54 |
| 2:f:254:VAL:HG13 | 2:f:365:ILE:HG12 | 1.90 | 0.54 |
| 2:i:99:GLN:NE2 | 1:H:50:SER:HB3 | 2.23 | 0.54 |
| 2:l:166:THR:HG21 | 2:n:362:LEU:CD2 | 2.38 | 0.54 |
| 2:m:45:LEU:HD22 | 2:m:116:LEU:HA | 1.89 | 0.54 |
| 2:n:166:THR:HG21 | 2:p:362:LEU:CD2 | 2.38 | 0.54 |
| 2:r:45:LEU:HD22 | 2:r:116:LEU:HA | 1.89 | 0.54 |
| 2:s:123:MET:H | 2:s:138:GLN:HB2 | 1.73 | 0.54 |
| 2:t:26:THR:CG2 | 2:t:187:LEU:HB3 | 2.35 | 0.54 |
| 2:t:46:ASP:HA | 2:u:161:ASN:ND2 | 2.18 | 0.54 |
| 3:5:22:VAL:HG22 | 3:5:34:LEU:CD2 | 2.34 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:8:28:ILE:O | 3:8:29:SER:OG | 2.21 | 0.54 |
| 3:26:74:VAL:O | 3:26:90:PHE:HA | 2.07 | 0.54 |
| 1:B:121:ARG:HA | 1:C:111:ARG:HB2 | 1.90 | 0.54 |
| 1:B:132:PHE:CB | 1:Z:219:MET:HE2 | 2.37 | 0.54 |
| 1:G:80:ILE:HD13 | 1:G:195:VAL:HG13 | 1.88 | 0.54 |
| 2:b:26:THR:CG2 | 2:b:187:LEU:HB3 | 2.35 | 0.54 |
| 2:e:99:GLN:NE2 | 1:D:50:SER:HB3 | 2.22 | 0.54 |
| 2:f:45:LEU:HD22 | 2:f:116:LEU:HA | 1.89 | 0.54 |
| 2:g:45:LEU:HD22 | 2:g:116:LEU:HA | 1.89 | 0.54 |
| 2:k:114:LYS:O | 2:k:160:LEU:HD13 | 2.07 | 0.54 |
| 2:l:45:LEU:HD22 | 2:l:116:LEU:HA | 1.89 | 0.54 |
| 2:m:254:VAL:HG13 | 2:m:365:ILE:HG12 | 1.90 | 0.54 |
| 2:o:73:VAL:HG11 | 2:o:79:MET:HE1 | 1.90 | 0.54 |
| 2:p:114:LYS:O | 2:p:160:LEU:HD13 | 2.07 | 0.54 |
| 2:u:46:ASP:HA | 2:v:161:ASN:ND2 | 2.18 | 0.54 |
| 2:u:98:ARG:NH1 | 2:v:220:THR:OG1 | 2.36 | 0.54 |
| 2:y:101:GLN:NE2 | 2:z:188:GLN:HB3 | 2.23 | 0.54 |
| 3:9:74:VAL:O | 3:9:90:PHE:HA | 2.07 | 0.54 |
| 3:12:19:GLN:O | 3:12:21:GLN:NE2 | 2.40 | 0.54 |
| 3:23:19:GLN:O | 3:23:21:GLN:NE2 | 2.40 | 0.54 |
| 1:B:68:ASP:O | 1:B:69:ARG:HG2 | 2.08 | 0.54 |
| 1:V:219:MET:HE2 | 1:X:132:PHE:CB | 2.38 | 0.54 |
| 1:Y:68:ASP:O | 1:Y:69:ARG:HG2 | 2.08 | 0.54 |
| 2:b:166:THR:HG21 | 2:d:362:LEU:CD2 | 2.38 | 0.53 |
| 2:c:26:THR:CG2 | 2:c:187:LEU:HB3 | 2.35 | 0.53 |
| 2:c:123:MET:H | 2:c:138:GLN:HB2 | 1.73 | 0.53 |
| 2:i:26:THR:CG2 | 2:i:187:LEU:HB3 | 2.35 | 0.53 |
| 2:k:166:THR:HG21 | 2:m:362:LEU:CD2 | 2.38 | 0.53 |
| 2:o:45:LEU:HD22 | 2:o:116:LEU:HA | 1.89 | 0.53 |
| 2:q:254:VAL:HG13 | 2:q:365:ILE:HG12 | 1.90 | 0.53 |
| 2:r:73:VAL:HG11 | 2:r:79:MET:HE1 | 1.90 | 0.53 |
| 2:r:123:MET:H | 2:r:138:GLN:HB2 | 1.74 | 0.53 |
| 2:s:114:LYS:O | 2:s:160:LEU:HD13 | 2.07 | 0.53 |
| 2:w:73:VAL:HG11 | 2:w:79:MET:HE1 | 1.91 | 0.53 |
| 1:I:68:ASP:O | 1:I:69:ARG:HG2 | 2.08 | 0.53 |
| 1:S:68:ASP:O | 1:S:69:ARG:HG2 | 2.08 | 0.53 |
| 1:S:219:MET:HE2 | 1:U:132:PHE:CB | 2.37 | 0.53 |
| 1:X:121:ARG:HA | 1:Y:111:ARG:HB2 | 1.90 | 0.53 |
| 1:A:219:MET:HE2 | 1:C:132:PHE:CB | 2.38 | 0.53 |
| 2:d:26:THR:CG2 | 2:d:187:LEU:HB3 | 2.35 | 0.53 |
| 2:d:123:MET:H | 2:d:138:GLN:HB2 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:e:45:LEU:HD22 | 2:e:116:LEU:HA | 1.89 | 0.53 |
| 2:h:166:THR:HG21 | 2:j:362:LEU:CD2 | 2.38 | 0.53 |
| 2:i:72:THR:OG1 | 1:J:70:ARG:NH2 | 2.38 | 0.53 |
| 2:j:123:MET:H | 2:j:138:GLN:HB2 | 1.73 | 0.53 |
| 2:k:45:LEU:HD22 | 2:k:116:LEU:HA | 1.89 | 0.53 |
| 2:n:73:VAL:HG11 | 2:n:79:MET:HE1 | 1.91 | 0.53 |
| 2:p:46:ASP:HA | 2:q:161:ASN:ND2 | 2.17 | 0.53 |
| 2:s:254:VAL:HG13 | 2:s:365:ILE:HG12 | 1.90 | 0.53 |
| 2:t:73:VAL:HG11 | 2:t:79:MET:HE1 | 1.91 | 0.53 |
| 2:v:271:ASP:CB | 2:v:357:CYS:HA | 2.28 | 0.53 |
| 2:z:73:VAL:HG11 | 2:z:79:MET:HE1 | 1.91 | 0.53 |
| 3:15:19:GLN:O | 3:15:21:GLN:NE2 | 2.40 | 0.53 |
| 1:F:37:ALA:HB1 | 1:G:74:ILE:CG2 | 2.39 | 0.53 |
| 1:G:219:MET:HE2 | 1:I:132:PHE:CB | 2.37 | 0.53 |
| 1:K:219:MET:HE2 | 1:M:132:PHE:CB | 2.38 | 0.53 |
| 1:Q:219:MET:HE2 | 1:S:132:PHE:CB | 2.38 | 0.53 |
| 2:l:73:VAL:HG11 | 2:l:79:MET:HE1 | 1.91 | 0.53 |
| 2:p:45:LEU:HD22 | 2:p:116:LEU:HA | 1.89 | 0.53 |
| 2:q:73:VAL:HG11 | 2:q:79:MET:HE1 | 1.91 | 0.53 |
| 2:r:114:LYS:O | 2:r:160:LEU:HD13 | 2.07 | 0.53 |
| 2:t:72:THR:OG1 | 1:U:70:ARG:NH2 | 2.38 | 0.53 |
| 2:v:73:VAL:HG11 | 2:v:79:MET:HE1 | 1.91 | 0.53 |
| 2:x:73:VAL:HG11 | 2:x:79:MET:HE1 | 1.90 | 0.53 |
| 2:x:98:ARG:NH1 | 2:y:220:THR:OG1 | 2.35 | 0.53 |
| 2:x:123:MET:H | 2:x:138:GLN:HB2 | 1.74 | 0.53 |
| 2:y:73:VAL:HG11 | 2:y:79:MET:HE1 | 1.91 | 0.53 |
| 2:y:114:LYS:O | 2:y:160:LEU:HD13 | 2.07 | 0.53 |
| 2:z:45:LEU:HD22 | 2:z:116:LEU:HA | 1.89 | 0.53 |
| 1:L:219:MET:HE2 | 1:N:132:PHE:CB | 2.38 | 0.53 |
| 2:a:166:THR:HG21 | 2:c:362:LEU:CD2 | 2.39 | 0.53 |
| 2:h:45:LEU:HD22 | 2:h:116:LEU:HA | 1.89 | 0.53 |
| 2:h:254:VAL:HG13 | 2:h:365:ILE:HG12 | 1.90 | 0.53 |
| 2:i:123:MET:H | 2:i:138:GLN:HB2 | 1.73 | 0.53 |
| 2:j:45:LEU:HD22 | 2:j:116:LEU:HA | 1.89 | 0.53 |
| 2:k:73:VAL:HG11 | 2:k:79:MET:HE1 | 1.91 | 0.53 |
| 2:n:114:LYS:O | 2:n:160:LEU:HD13 | 2.07 | 0.53 |
| 2:p:73:VAL:HG11 | 2:p:79:MET:HE1 | 1.91 | 0.53 |
| 2:q:123:MET:H | 2:q:138:GLN:HB2 | 1.73 | 0.53 |
| 2:s:73:VAL:HG11 | 2:s:79:MET:HE1 | 1.90 | 0.53 |
| 2:u:73:VAL:HG11 | 2:u:79:MET:HE1 | 1.91 | 0.53 |
| 2:u:271:ASP:CB | 2:u:357:CYS:HA | 2.28 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:v:114:LYS:O | 2:v:160:LEU:HD13 | 2.07 | 0.53 |
| 2:w:123:MET:H | 2:w:138:GLN:HB2 | 1.73 | 0.53 |
| 2:y:99:GLN:NE2 | 1:X:50:SER:HB3 | 2.24 | 0.53 |
| 3:6:22:VAL:HG22 | 3:6:34:LEU:CD2 | 2.34 | 0.53 |
| 1:E:121:ARG:HA | 1:F:111:ARG:HB2 | 1.90 | 0.53 |
| 1:H:68:ASP:O | 1:H:69:ARG:HG2 | 2.08 | 0.53 |
| 1:U:219:MET:HE2 | 1:W:132:PHE:CB | 2.38 | 0.53 |
| 1:A:121:ARG:HA | 1:B:111:ARG:HB2 | 1.91 | 0.53 |
| 2:b:362:LEU:CD2 | 2:z:166:THR:HG21 | 2.38 | 0.53 |
| 2:c:45:LEU:HD22 | 2:c:116:LEU:HA | 1.89 | 0.53 |
| 2:e:26:THR:CG2 | 2:e:187:LEU:HB3 | 2.35 | 0.53 |
| 2:k:123:MET:H | 2:k:138:GLN:HB2 | 1.73 | 0.53 |
| 2:m:73:VAL:HG11 | 2:m:79:MET:HE1 | 1.91 | 0.53 |
| 2:q:45:LEU:HD22 | 2:q:116:LEU:HA | 1.89 | 0.53 |
| 2:q:164:ARG:HD2 | 2:r:365:ILE:CG2 | 2.39 | 0.53 |
| 2:y:123:MET:H | 2:y:138:GLN:HB2 | 1.74 | 0.53 |
| 1:D:219:MET:HE2 | 1:F:132:PHE:CB | 2.38 | 0.53 |
| 1:F:219:MET:HE2 | 1:H:132:PHE:CB | 2.38 | 0.53 |
| 1:I:219:MET:HE2 | 1:K:132:PHE:CB | 2.38 | 0.53 |
| 1:A:70:ARG:NH2 | 2:z:72:THR:OG1 | 2.41 | 0.53 |
| 2:e:123:MET:H | 2:e:138:GLN:HB2 | 1.74 | 0.53 |
| 2:f:271:ASP:CB | 2:f:357:CYS:HA | 2.28 | 0.53 |
| 2:l:254:VAL:HG13 | 2:l:365:ILE:HG12 | 1.90 | 0.53 |
| 2:m:264:MET:HE1 | 2:m:335:LEU:CD1 | 2.39 | 0.53 |
| 2:p:264:MET:HE1 | 2:p:335:LEU:CD1 | 2.39 | 0.53 |
| 2:u:26:THR:CG2 | 2:u:187:LEU:HB3 | 2.35 | 0.53 |
| 2:x:166:THR:HG21 | 2:z:362:LEU:CD2 | 2.38 | 0.53 |
| 1:C:37:ALA:HB1 | 1:D:74:ILE:CG2 | 2.39 | 0.53 |
| 1:I:37:ALA:HB1 | 1:J:74:ILE:CG2 | 2.39 | 0.53 |
| 1:T:121:ARG:HA | 1:U:111:ARG:HB2 | 1.90 | 0.53 |
| 1:W:121:ARG:HA | 1:X:111:ARG:HB2 | 1.90 | 0.53 |
| 1:X:37:ALA:HB1 | 1:Y:74:ILE:CG2 | 2.39 | 0.53 |
| 2:a:72:THR:OG1 | 1:B:70:ARG:NH2 | 2.39 | 0.53 |
| 2:a:73:VAL:HG11 | 2:a:79:MET:HE1 | 1.91 | 0.53 |
| 2:a:220:THR:OG1 | 2:z:98:ARG:NH1 | 2.38 | 0.53 |
| 2:b:73:VAL:HG11 | 2:b:79:MET:HE1 | 1.90 | 0.53 |
| 2:b:254:VAL:HG13 | 2:b:365:ILE:HG12 | 1.90 | 0.53 |
| 2:b:264:MET:HE1 | 2:b:335:LEU:CD1 | 2.39 | 0.53 |
| 2:d:45:LEU:HD22 | 2:d:116:LEU:HA | 1.89 | 0.53 |
| 2:e:264:MET:HE1 | 2:e:335:LEU:CD1 | 2.39 | 0.53 |
| 2:f:26:THR:CG2 | 2:f:187:LEU:HB3 | 2.35 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:g:99:GLN:NE2 | 1:F:50:SER:HB3 | 2.23 | 0.53 |
| 2:h:73:VAL:HG11 | 2:h:79:MET:HE1 | 1.91 | 0.53 |
| 2:i:45:LEU:HD22 | 2:i:116:LEU:HA | 1.89 | 0.53 |
| 2:i:254:VAL:HG13 | 2:i:365:ILE:HG12 | 1.90 | 0.53 |
| 2:n:123:MET:H | 2:n:138:GLN:HB2 | 1.74 | 0.53 |
| 2:o:46:ASP:HA | 2:p:161:ASN:ND2 | 2.18 | 0.53 |
| 2:u:264:MET:HE1 | 2:u:335:LEU:CD1 | 2.39 | 0.53 |
| 2:w:164:ARG:HD2 | 2:x:365:ILE:CG2 | 2.39 | 0.53 |
| 2:w:254:VAL:HG13 | 2:w:365:ILE:HG12 | 1.90 | 0.53 |
| 1:C:176:GLU:OE1 | 1:C:207:TYR:OH | 2.21 | 0.53 |
| 1:H:121:ARG:HA | 1:I:111:ARG:HB2 | 1.90 | 0.53 |
| 1:H:219:MET:HE2 | 1:J:132:PHE:CB | 2.38 | 0.53 |
| 1:J:219:MET:HE2 | 1:L:132:PHE:CB | 2.38 | 0.53 |
| 1:N:121:ARG:HA | 1:O:111:ARG:HB2 | 1.90 | 0.53 |
| 1:U:37:ALA:HB1 | 1:V:74:ILE:CG2 | 2.39 | 0.53 |
| 2:b:45:LEU:HD22 | 2:b:116:LEU:HA | 1.89 | 0.53 |
| 2:b:123:MET:H | 2:b:138:GLN:HB2 | 1.73 | 0.53 |
| 2:c:72:THR:OG1 | 1:D:70:ARG:NH2 | 2.38 | 0.53 |
| 2:c:73:VAL:HG11 | 2:c:79:MET:HE1 | 1.91 | 0.53 |
| 2:h:26:THR:CG2 | 2:h:187:LEU:HB3 | 2.35 | 0.53 |
| 2:h:99:GLN:NE2 | 1:G:50:SER:HB3 | 2.23 | 0.53 |
| 2:h:264:MET:HE1 | 2:h:335:LEU:CD1 | 2.39 | 0.53 |
| 2:i:73:VAL:HG11 | 2:i:79:MET:HE1 | 1.91 | 0.53 |
| 2:o:164:ARG:HD2 | 2:p:365:ILE:CG2 | 2.39 | 0.53 |
| 2:p:166:THR:HG21 | 2:r:362:LEU:CD2 | 2.39 | 0.53 |
| 2:s:264:MET:HE1 | 2:s:335:LEU:CD1 | 2.39 | 0.53 |
| 2:t:123:MET:H | 2:t:138:GLN:HB2 | 1.74 | 0.53 |
| 2:t:264:MET:HE1 | 2:t:335:LEU:CD1 | 2.39 | 0.53 |
| 2:u:164:ARG:HD2 | 2:v:365:ILE:CG2 | 2.39 | 0.53 |
| 2:v:52:THR:HG21 | 2:v:81:LEU:CD2 | 2.39 | 0.53 |
| 2:x:175:LEU:HD11 | 1:V:51:ILE:CG1 | 2.38 | 0.53 |
| 1:C:121:ARG:HA | 1:D:111:ARG:HB2 | 1.90 | 0.53 |
| 1:M:121:ARG:HA | 1:N:111:ARG:HB2 | 1.90 | 0.53 |
| 2:b:178:GLN:HG3 | 1:Z:47:ALA:O | 2.08 | 0.53 |
| 2:c:254:VAL:HG13 | 2:c:365:ILE:HG12 | 1.90 | 0.53 |
| 2:c:264:MET:HE1 | 2:c:335:LEU:CD1 | 2.39 | 0.53 |
| 2:d:73:VAL:HG11 | 2:d:79:MET:HE1 | 1.91 | 0.53 |
| 2:h:123:MET:H | 2:h:138:GLN:HB2 | 1.73 | 0.53 |
| 2:j:73:VAL:HG11 | 2:j:79:MET:HE1 | 1.91 | 0.53 |
| 2:j:264:MET:HE1 | 2:j:335:LEU:CD1 | 2.39 | 0.53 |
| 2:l:123:MET:H | 2:l:138:GLN:HB2 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:v:166:THR:HG21 | 2:x:362:LEU:CD2 | 2.39 | 0.53 |
| 2:v:254:VAL:HG13 | 2:v:365:ILE:HG12 | 1.90 | 0.53 |
| 2:v:264:MET:HE1 | 2:v:335:LEU:CD1 | 2.39 | 0.53 |
| 2:w:264:MET:HE1 | 2:w:335:LEU:CD1 | 2.39 | 0.53 |
| 2:x:52:THR:HG21 | 2:x:81:LEU:CD2 | 2.39 | 0.53 |
| 3:5:64:TYR:HB2 | 3:5:96:CYS:HB3 | 1.91 | 0.53 |
| 1:G:121:ARG:HA | 1:H:111:ARG:HB2 | 1.90 | 0.53 |
| 1:P:206:GLU:HG2 | 1:P:208:VAL:HG13 | 1.91 | 0.53 |
| 1:S:121:ARG:HA | 1:T:111:ARG:HB2 | 1.90 | 0.53 |
| 1:A:111:ARG:HB2 | 1:Z:121:ARG:HA | 1.91 | 0.53 |
| 2:a:45:LEU:HD22 | 2:a:116:LEU:HA | 1.89 | 0.53 |
| 2:a:254:VAL:HG13 | 2:a:365:ILE:HG12 | 1.90 | 0.53 |
| 2:b:72:THR:OG1 | 1:C:70:ARG:NH2 | 2.38 | 0.53 |
| 2:e:73:VAL:HG11 | 2:e:79:MET:HE1 | 1.91 | 0.53 |
| 2:g:73:VAL:HG11 | 2:g:79:MET:HE1 | 1.91 | 0.53 |
| 2:g:166:THR:HG21 | 2:i:362:LEU:CD2 | 2.39 | 0.53 |
| 2:j:166:THR:HG21 | 2:l:362:LEU:CD2 | 2.39 | 0.53 |
| 2:k:164:ARG:HD2 | 2:l:365:ILE:CG2 | 2.39 | 0.53 |
| 2:k:264:MET:HE1 | 2:k:335:LEU:CD1 | 2.39 | 0.53 |
| 2:o:264:MET:HE1 | 2:o:335:LEU:CD1 | 2.39 | 0.53 |
| 2:p:123:MET:H | 2:p:138:GLN:HB2 | 1.73 | 0.53 |
| 2:q:166:THR:HG21 | 2:s:362:LEU:CD2 | 2.39 | 0.53 |
| 2:r:264:MET:HE1 | 2:r:335:LEU:CD1 | 2.39 | 0.53 |
| 2:s:52:THR:HG21 | 2:s:81:LEU:CD2 | 2.39 | 0.53 |
| 2:s:99:GLN:NE2 | 1:R:50:SER:HB3 | 2.23 | 0.53 |
| 2:s:164:ARG:HD2 | 2:t:365:ILE:CG2 | 2.40 | 0.53 |
| 2:t:164:ARG:HD2 | 2:u:365:ILE:CG2 | 2.40 | 0.53 |
| 2:x:264:MET:HE1 | 2:x:335:LEU:CD1 | 2.39 | 0.53 |
| 2:y:264:MET:HE1 | 2:y:335:LEU:CD1 | 2.39 | 0.53 |
| 2:z:264:MET:HE1 | 2:z:335:LEU:CD1 | 2.39 | 0.53 |
| 3:7:22:VAL:HG22 | 3:7:34:LEU:CD2 | 2.34 | 0.53 |
| 3:7:64:TYR:HB2 | 3:7:96:CYS:HB3 | 1.91 | 0.53 |
| 1:B:219:MET:HE2 | 1:D:132:PHE:CB | 2.38 | 0.53 |
| 1:E:219:MET:HE2 | 1:G:132:PHE:CB | 2.38 | 0.53 |
| 1:K:121:ARG:HA | 1:L:111:ARG:HB2 | 1.90 | 0.53 |
| 1:O:37:ALA:HB1 | 1:P:74:ILE:CG2 | 2.39 | 0.53 |
| 1:O:121:ARG:HA | 1:P:111:ARG:HB2 | 1.90 | 0.53 |
| 1:Q:121:ARG:HA | 1:R:111:ARG:HB2 | 1.90 | 0.53 |
| 1:R:206:GLU:HG2 | 1:R:208:VAL:HG13 | 1.91 | 0.53 |
| 1:A:69:ARG:HG3 | 1:A:69:ARG:O | 2.10 | 0.52 |
| 2:d:98:ARG:NH1 | 2:e:220:THR:OG1 | 2.36 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:f:264:MET:HE1 | 2:f:335:LEU:CD1 | 2.39 | 0.52 |
| 2:m:271:ASP:CB | 2:m:357:CYS:HA | 2.28 | 0.52 |
| 2:w:52:THR:HG21 | 2:w:81:LEU:CD2 | 2.39 | 0.52 |
| 2:z:123:MET:H | 2:z:138:GLN:HB2 | 1.73 | 0.52 |
| 3:4:64:TYR:HB2 | 3:4:96:CYS:HB3 | 1.91 | 0.52 |
| 3:6:64:TYR:HB2 | 3:6:96:CYS:HB3 | 1.91 | 0.52 |
| 3:19:70:PHE:HD1 | 1:S:41:PRO:HD3 | 1.74 | 0.52 |
| 3:20:70:PHE:HD1 | 1:T:41:PRO:HD3 | 1.74 | 0.52 |
| 3:25:70:PHE:HD1 | 1:Y:41:PRO:HD3 | 1.74 | 0.52 |
| 1:D:37:ALA:HB1 | 1:E:74:ILE:CG2 | 2.39 | 0.52 |
| 1:L:206:GLU:HG2 | 1:L:208:VAL:HG13 | 1.91 | 0.52 |
| 1:N:206:GLU:HG2 | 1:N:208:VAL:HG13 | 1.91 | 0.52 |
| 1:R:68:ASP:O | 1:R:69:ARG:HG2 | 2.08 | 0.52 |
| 1:U:121:ARG:HA | 1:V:111:ARG:HB2 | 1.90 | 0.52 |
| 1:A:50:SER:HB3 | 2:b:99:GLN:NE2 | 2.24 | 0.52 |
| 2:a:98:ARG:NH1 | 2:b:220:THR:OG1 | 2.37 | 0.52 |
| 2:a:362:LEU:CD2 | 2:y:166:THR:HG21 | 2.39 | 0.52 |
| 2:e:254:VAL:HG13 | 2:e:365:ILE:HG12 | 1.90 | 0.52 |
| 2:g:26:THR:CG2 | 2:g:187:LEU:HB3 | 2.35 | 0.52 |
| 2:g:228:GLY:O | 2:g:232:GLN:HG3 | 2.10 | 0.52 |
| 2:g:264:MET:HE1 | 2:g:335:LEU:CD1 | 2.39 | 0.52 |
| 2:j:228:GLY:O | 2:j:232:GLN:HG3 | 2.10 | 0.52 |
| 2:m:72:THR:OG1 | 1:N:70:ARG:NH2 | 2.39 | 0.52 |
| 2:o:98:ARG:NH1 | 2:p:220:THR:OG1 | 2.36 | 0.52 |
| 2:o:123:MET:H | 2:o:138:GLN:HB2 | 1.73 | 0.52 |
| 2:p:254:VAL:HG13 | 2:p:365:ILE:HG12 | 1.90 | 0.52 |
| 2:q:46:ASP:HA | 2:r:161:ASN:ND2 | 2.18 | 0.52 |
| 2:q:52:THR:HG21 | 2:q:81:LEU:CD2 | 2.39 | 0.52 |
| 2:r:98:ARG:NH1 | 2:s:220:THR:OG1 | 2.37 | 0.52 |
| 2:r:166:THR:HG21 | 2:t:362:LEU:CD2 | 2.39 | 0.52 |
| 2:x:46:ASP:OD1 | 2:y:160:LEU:HD12 | 2.08 | 0.52 |
| 3:3:64:TYR:HB2 | 3:3:96:CYS:HB3 | 1.91 | 0.52 |
| 3:14:70:PHE:HD1 | 1:N:41:PRO:HD3 | 1.74 | 0.52 |
| 3:15:70:PHE:HD1 | 1:O:41:PRO:HD3 | 1.74 | 0.52 |
| 1:D:69:ARG:HG3 | 1:D:69:ARG:O | 2.09 | 0.52 |
| 1:E:69:ARG:HG3 | 1:E:69:ARG:O | 2.10 | 0.52 |
| 1:L:37:ALA:HB1 | 1:M:74:ILE:CG2 | 2.39 | 0.52 |
| 1:T:206:GLU:HG2 | 1:T:208:VAL:HG13 | 1.91 | 0.52 |
| 2:d:264:MET:HE1 | 2:d:335:LEU:CD1 | 2.39 | 0.52 |
| 2:e:228:GLY:O | 2:e:232:GLN:HG3 | 2.10 | 0.52 |
| 2:f:52:THR:HG21 | 2:f:81:LEU:CD2 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:f:72:THR:OG1 | 1:G:70:ARG:NH2 | 2.38 | 0.52 |
| 2:f:73:VAL:HG11 | 2:f:79:MET:HE1 | 1.91 | 0.52 |
| 2:f:228:GLY:O | 2:f:232:GLN:HG3 | 2.10 | 0.52 |
| 2:f:275:VAL:HG21 | 2:f:338:LEU:CD2 | 2.40 | 0.52 |
| 2:i:275:VAL:HG21 | 2:i:338:LEU:CD2 | 2.40 | 0.52 |
| 2:j:52:THR:HG21 | 2:j:81:LEU:CD2 | 2.39 | 0.52 |
| 2:k:98:ARG:NH1 | 2:l:220:THR:OG1 | 2.37 | 0.52 |
| 2:k:275:VAL:HG21 | 2:k:338:LEU:CD2 | 2.40 | 0.52 |
| 2:l:264:MET:HE1 | 2:l:335:LEU:CD1 | 2.39 | 0.52 |
| 2:l:275:VAL:HG21 | 2:l:338:LEU:CD2 | 2.40 | 0.52 |
| 2:m:166:THR:HG21 | 2:o:362:LEU:CD2 | 2.39 | 0.52 |
| 2:m:228:GLY:O | 2:m:232:GLN:HG3 | 2.10 | 0.52 |
| 2:m:275:VAL:HG21 | 2:m:338:LEU:CD2 | 2.40 | 0.52 |
| 2:n:164:ARG:HD2 | 2:o:365:ILE:CG2 | 2.40 | 0.52 |
| 2:n:264:MET:HE1 | 2:n:335:LEU:CD1 | 2.39 | 0.52 |
| 2:q:264:MET:HE1 | 2:q:335:LEU:CD1 | 2.39 | 0.52 |
| 2:u:52:THR:HG21 | 2:u:81:LEU:CD2 | 2.39 | 0.52 |
| 2:x:254:VAL:HG13 | 2:x:365:ILE:HG12 | 1.90 | 0.52 |
| 3:8:64:TYR:HB2 | 3:8:96:CYS:HB3 | 1.92 | 0.52 |
| 3:21:28:ILE:O | 3:21:29:SER:OG | 2.21 | 0.52 |
| 1:F:121:ARG:HA | 1:G:111:ARG:HB2 | 1.91 | 0.52 |
| 1:H:84:GLU:HG2 | 1:H:197:SER:OG | 2.10 | 0.52 |
| 1:N:84:GLU:HG2 | 1:N:197:SER:OG | 2.10 | 0.52 |
| 1:Q:84:GLU:HG2 | 1:Q:197:SER:OG | 2.10 | 0.52 |
| 1:V:37:ALA:HB1 | 1:W:74:ILE:CG2 | 2.39 | 0.52 |
| 2:d:166:THR:HG21 | 2:f:362:LEU:CD2 | 2.39 | 0.52 |
| 2:e:52:THR:HG21 | 2:e:81:LEU:CD2 | 2.39 | 0.52 |
| 2:f:123:MET:H | 2:f:138:GLN:HB2 | 1.73 | 0.52 |
| 2:g:52:THR:HG21 | 2:g:81:LEU:CD2 | 2.39 | 0.52 |
| 2:g:98:ARG:NH1 | 2:h:220:THR:OG1 | 2.37 | 0.52 |
| 2:g:271:ASP:CB | 2:g:357:CYS:HA | 2.28 | 0.52 |
| 2:g:275:VAL:HG21 | 2:g:338:LEU:CD2 | 2.40 | 0.52 |
| 2:h:275:VAL:HG21 | 2:h:338:LEU:CD2 | 2.40 | 0.52 |
| 2:i:228:GLY:O | 2:i:232:GLN:HG3 | 2.09 | 0.52 |
| 2:j:275:VAL:HG21 | 2:j:338:LEU:CD2 | 2.40 | 0.52 |
| 2:l:228:GLY:O | 2:l:232:GLN:HG3 | 2.10 | 0.52 |
| 2:m:123:MET:H | 2:m:138:GLN:HB2 | 1.73 | 0.52 |
| 2:n:275:VAL:HG21 | 2:n:338:LEU:CD2 | 2.40 | 0.52 |
| 2:t:52:THR:HG21 | 2:t:81:LEU:CD2 | 2.39 | 0.52 |
| 3:11:28:ILE:O | 3:11:29:SER:OG | 2.21 | 0.52 |
| 3:13:70:PHE:HD1 | 1:M:41:PRO:HD3 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:21:70:PHE:HD1 | 1:U:41:PRO:HD3 | 1.74 | 0.52 |
| 1:E:84:GLU:HG2 | 1:E:197:SER:OG | 2.10 | 0.52 |
| 1:H:69:ARG:O | 1:H:69:ARG:HG3 | 2.09 | 0.52 |
| 1:K:84:GLU:HG2 | 1:K:197:SER:OG | 2.10 | 0.52 |
| 2:a:99:GLN:NE2 | 1:Z:50:SER:HB3 | 2.24 | 0.52 |
| 2:d:228:GLY:O | 2:d:232:GLN:HG3 | 2.10 | 0.52 |
| 2:e:275:VAL:HG21 | 2:e:338:LEU:CD2 | 2.40 | 0.52 |
| 2:j:72:THR:OG1 | 1:K:70:ARG:NH2 | 2.37 | 0.52 |
| 2:m:164:ARG:HD2 | 2:n:365:ILE:CG2 | 2.40 | 0.52 |
| 2:o:275:VAL:HG21 | 2:o:338:LEU:CD2 | 2.40 | 0.52 |
| 2:s:166:THR:HG21 | 2:u:362:LEU:CD2 | 2.39 | 0.52 |
| 2:t:254:VAL:HG13 | 2:t:365:ILE:HG12 | 1.90 | 0.52 |
| 2:v:123:MET:H | 2:v:138:GLN:HB2 | 1.74 | 0.52 |
| 2:y:68:GLN:HG2 | 1:Y:65:LEU:HD23 | 1.92 | 0.52 |
| 2:z:52:THR:HG21 | 2:z:81:LEU:CD2 | 2.39 | 0.52 |
| 3:2:64:TYR:HB2 | 3:2:96:CYS:HB3 | 1.91 | 0.52 |
| 3:9:64:TYR:HB2 | 3:9:96:CYS:HB3 | 1.92 | 0.52 |
| 3:16:70:PHE:HD1 | 1:P:41:PRO:HD3 | 1.74 | 0.52 |
| 3:24:28:ILE:O | 3:24:29:SER:OG | 2.21 | 0.52 |
| 1:B:176:GLU:OE1 | 1:B:207:TYR:OH | 2.21 | 0.52 |
| 1:C:219:MET:HE2 | 1:E:132:PHE:CB | 2.38 | 0.52 |
| 1:G:84:GLU:HG2 | 1:G:197:SER:OG | 2.10 | 0.52 |
| 1:X:69:ARG:O | 1:X:69:ARG:HG3 | 2.10 | 0.52 |
| 1:Z:69:ARG:HG3 | 1:Z:69:ARG:O | 2.10 | 0.52 |
| 2:c:228:GLY:O | 2:c:232:GLN:HG3 | 2.09 | 0.52 |
| 2:c:275:VAL:HG21 | 2:c:338:LEU:CD2 | 2.40 | 0.52 |
| 2:d:275:VAL:HG21 | 2:d:338:LEU:CD2 | 2.40 | 0.52 |
| 2:h:52:THR:HG21 | 2:h:81:LEU:CD2 | 2.39 | 0.52 |
| 2:n:228:GLY:O | 2:n:232:GLN:HG3 | 2.10 | 0.52 |
| 2:o:52:THR:HG21 | 2:o:81:LEU:CD2 | 2.39 | 0.52 |
| 2:p:52:THR:HG21 | 2:p:81:LEU:CD2 | 2.39 | 0.52 |
| 2:y:52:THR:HG21 | 2:y:81:LEU:CD2 | 2.39 | 0.52 |
| 2:y:254:VAL:HG13 | 2:y:365:ILE:HG12 | 1.90 | 0.52 |
| 3:5:21:GLN:O | 3:5:34:LEU:HB3 | 2.10 | 0.52 |
| 3:9:25:ALA:HB1 | 3:9:62:MET:HE2 | 1.91 | 0.52 |
| 3:15:21:GLN:O | 3:15:34:LEU:HB3 | 2.10 | 0.52 |
| 3:23:21:GLN:O | 3:23:34:LEU:HB3 | 2.10 | 0.52 |
| 1:B:69:ARG:HG3 | 1:B:69:ARG:O | 2.10 | 0.52 |
| 1:B:84:GLU:HG2 | 1:B:197:SER:OG | 2.10 | 0.52 |
| 1:I:121:ARG:HA | 1:J:111:ARG:HB2 | 1.90 | 0.52 |
| 1:J:31:VAL:HB | 1:K:179:ARG:HD3 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:206:GLU:HG2 | 1:J:208:VAL:HG13 | 1.91 | 0.52 |
| 1:L:121:ARG:HA | 1:M:111:ARG:HB2 | 1.90 | 0.52 |
| 1:R:31:VAL:HB | 1:S:179:ARG:HD3 | 1.92 | 0.52 |
| 1:R:121:ARG:HA | 1:S:111:ARG:HB2 | 1.90 | 0.52 |
| 1:T:84:GLU:HG2 | 1:T:197:SER:OG | 2.10 | 0.52 |
| 1:W:69:ARG:HG3 | 1:W:69:ARG:O | 2.10 | 0.52 |
| 2:a:123:MET:H | 2:a:138:GLN:HB2 | 1.73 | 0.52 |
| 2:a:264:MET:HE1 | 2:a:335:LEU:CD1 | 2.39 | 0.52 |
| 2:a:365:ILE:CG2 | 2:z:164:ARG:HD2 | 2.40 | 0.52 |
| 2:p:275:VAL:HG21 | 2:p:338:LEU:CD2 | 2.40 | 0.52 |
| 2:u:254:VAL:HG13 | 2:u:365:ILE:HG12 | 1.90 | 0.52 |
| 2:v:68:GLN:HG2 | 1:V:65:LEU:HD23 | 1.92 | 0.52 |
| 3:9:21:GLN:O | 3:9:34:LEU:HB3 | 2.10 | 0.52 |
| 3:10:25:ALA:HB1 | 3:10:62:MET:HE2 | 1.92 | 0.52 |
| 3:10:70:PHE:HD1 | 1:J:41:PRO:HD3 | 1.74 | 0.52 |
| 3:18:21:GLN:O | 3:18:34:LEU:HB3 | 2.10 | 0.52 |
| 3:20:21:GLN:O | 3:20:34:LEU:HB3 | 2.10 | 0.52 |
| 1:D:84:GLU:HG2 | 1:D:197:SER:OG | 2.10 | 0.52 |
| 1:J:84:GLU:HG2 | 1:J:197:SER:OG | 2.10 | 0.52 |
| 1:K:37:ALA:HB1 | 1:L:74:ILE:CG2 | 2.39 | 0.52 |
| 1:N:31:VAL:HB | 1:O:179:ARG:HD3 | 1.92 | 0.52 |
| 1:S:37:ALA:HB1 | 1:T:74:ILE:CG2 | 2.40 | 0.52 |
| 1:V:206:GLU:HG2 | 1:V:208:VAL:HG13 | 1.91 | 0.52 |
| 1:Y:37:ALA:HB1 | 1:Z:74:ILE:CG2 | 2.39 | 0.52 |
| 1:Y:69:ARG:HG3 | 1:Y:69:ARG:O | 2.10 | 0.52 |
| 1:A:84:GLU:HG2 | 1:A:197:SER:OG | 2.10 | 0.52 |
| 1:A:132:PHE:CB | 1:Y:219:MET:HE2 | 2.39 | 0.52 |
| 1:A:179:ARG:HD3 | 1:Z:31:VAL:HB | 1.92 | 0.52 |
| 2:a:164:ARG:HD2 | 2:b:365:ILE:CG2 | 2.40 | 0.52 |
| 2:a:275:VAL:HG21 | 2:a:338:LEU:CD2 | 2.40 | 0.52 |
| 3:1:64:TYR:HB2 | 3:1:96:CYS:HB3 | 1.91 | 0.52 |
| 2:b:275:VAL:HG21 | 2:b:338:LEU:CD2 | 2.40 | 0.52 |
| 2:c:68:GLN:HG2 | 1:C:65:LEU:HD23 | 1.92 | 0.52 |
| 2:d:175:LEU:HD11 | 1:B:51:ILE:CG1 | 2.40 | 0.52 |
| 2:g:123:MET:H | 2:g:138:GLN:HB2 | 1.73 | 0.52 |
| 2:k:228:GLY:O | 2:k:232:GLN:HG3 | 2.10 | 0.52 |
| 2:l:52:THR:HG21 | 2:l:81:LEU:CD2 | 2.39 | 0.52 |
| 2:o:228:GLY:O | 2:o:232:GLN:HG3 | 2.10 | 0.52 |
| 2:u:123:MET:H | 2:u:138:GLN:HB2 | 1.74 | 0.52 |
| 2:z:254:VAL:HG13 | 2:z:365:ILE:HG12 | 1.90 | 0.52 |
| 3:8:25:ALA:HB1 | 3:8:62:MET:HE2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:10:64:TYR:HB2 | 3:10:96:CYS:HB3 | 1.92 | 0.52 |
| 3:12:21:GLN:O | 3:12:34:LEU:HB3 | 2.10 | 0.52 |
| 3:20:25:ALA:HB1 | 3:20:62:MET:HE2 | 1.92 | 0.52 |
| 3:25:25:ALA:HB1 | 3:25:62:MET:HE2 | 1.92 | 0.52 |
| 1:C:69:ARG:HG3 | 1:C:69:ARG:O | 2.10 | 0.52 |
| 1:H:37:ALA:HB1 | 1:I:74:ILE:CG2 | 2.40 | 0.52 |
| 1:P:31:VAL:HB | 1:Q:179:ARG:HD3 | 1.92 | 0.52 |
| 1:Z:84:GLU:HG2 | 1:Z:197:SER:OG | 2.10 | 0.52 |
| 3:1:21:GLN:O | 3:1:34:LEU:HB3 | 2.10 | 0.52 |
| 2:d:52:THR:HG21 | 2:d:81:LEU:CD2 | 2.39 | 0.52 |
| 2:h:228:GLY:O | 2:h:232:GLN:HG3 | 2.09 | 0.52 |
| 2:i:52:THR:HG21 | 2:i:81:LEU:CD2 | 2.39 | 0.52 |
| 2:n:52:THR:HG21 | 2:n:81:LEU:CD2 | 2.39 | 0.52 |
| 2:p:228:GLY:O | 2:p:232:GLN:HG3 | 2.09 | 0.52 |
| 2:q:72:THR:OG1 | 1:R:70:ARG:NH2 | 2.37 | 0.52 |
| 2:q:275:VAL:HG21 | 2:q:338:LEU:CD2 | 2.40 | 0.52 |
| 2:r:68:GLN:HG2 | 1:R:65:LEU:HD23 | 1.92 | 0.52 |
| 2:w:175:LEU:HD11 | 1:U:51:ILE:CG1 | 2.38 | 0.52 |
| 2:z:93:TYR:OH | 2:z:173:ARG:O | 2.25 | 0.52 |
| 3:2:21:GLN:O | 3:2:34:LEU:HB3 | 2.10 | 0.52 |
| 3:7:25:ALA:HB1 | 3:7:62:MET:HE2 | 1.92 | 0.52 |
| 3:11:25:ALA:HB1 | 3:11:62:MET:HE2 | 1.92 | 0.52 |
| 3:19:25:ALA:HB1 | 3:19:62:MET:HE2 | 1.92 | 0.52 |
| 3:24:25:ALA:HB1 | 3:24:62:MET:HE2 | 1.91 | 0.52 |
| 3:26:21:GLN:O | 3:26:34:LEU:HB3 | 2.10 | 0.52 |
| 3:26:25:ALA:HB1 | 3:26:62:MET:HE2 | 1.91 | 0.52 |
| 1:E:37:ALA:HB1 | 1:F:74:ILE:CG2 | 2.39 | 0.52 |
| 1:H:31:VAL:HB | 1:I:179:ARG:HD3 | 1.92 | 0.52 |
| 1:I:69:ARG:HG3 | 1:I:69:ARG:O | 2.09 | 0.52 |
| 1:L:84:GLU:HG2 | 1:L:197:SER:OG | 2.10 | 0.52 |
| 1:M:31:VAL:HB | 1:N:179:ARG:HD3 | 1.92 | 0.52 |
| 1:O:84:GLU:HG2 | 1:O:197:SER:OG | 2.10 | 0.52 |
| 1:X:206:GLU:HG2 | 1:X:208:VAL:HG13 | 1.91 | 0.52 |
| 1:Y:31:VAL:HB | 1:Z:179:ARG:HD3 | 1.92 | 0.52 |
| 1:Y:84:GLU:HG2 | 1:Y:197:SER:OG | 2.10 | 0.52 |
| 1:A:37:ALA:HB1 | 1:B:74:ILE:CG2 | 2.40 | 0.52 |
| 2:d:68:GLN:HG2 | 1:D:65:LEU:HD23 | 1.92 | 0.52 |
| 2:i:264:MET:HE1 | 2:i:335:LEU:CD1 | 2.39 | 0.52 |
| 2:l:164:ARG:HD2 | 2:m:365:ILE:CG2 | 2.40 | 0.52 |
| 2:u:68:GLN:HG2 | 1:U:65:LEU:HD23 | 1.92 | 0.52 |
| 2:x:254:VAL:CG2 | 2:y:355:ALA:HB2 | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:6:21:GLN:O | 3:6:34:LEU:HB3 | 2.10 | 0.52 |
| 3:8:21:GLN:O | 3:8:34:LEU:HB3 | 2.10 | 0.52 |
| 3:11:64:TYR:HB2 | 3:11:96:CYS:HB3 | 1.91 | 0.52 |
| 3:17:21:GLN:O | 3:17:34:LEU:HB3 | 2.10 | 0.52 |
| 1:B:31:VAL:HB | 1:C:179:ARG:HD3 | 1.92 | 0.52 |
| 1:G:37:ALA:HB1 | 1:H:74:ILE:CG2 | 2.40 | 0.52 |
| 1:J:37:ALA:HB1 | 1:K:74:ILE:CG2 | 2.39 | 0.52 |
| 1:M:84:GLU:HG2 | 1:M:197:SER:OG | 2.10 | 0.52 |
| 1:P:37:ALA:HB1 | 1:Q:74:ILE:CG2 | 2.39 | 0.52 |
| 1:R:84:GLU:HG2 | 1:R:197:SER:OG | 2.10 | 0.52 |
| 1:U:84:GLU:HG2 | 1:U:197:SER:OG | 2.10 | 0.52 |
| 1:V:31:VAL:HB | 1:W:179:ARG:HD3 | 1.92 | 0.52 |
| 1:Y:39:PRO:HB3 | 1:Z:75:GLY:HA3 | 1.92 | 0.52 |
| 1:Y:171:ILE:O | 1:Z:207:TYR:O | 2.27 | 0.52 |
| 2:a:52:THR:HG21 | 2:a:81:LEU:CD2 | 2.39 | 0.51 |
| 2:c:52:THR:HG21 | 2:c:81:LEU:CD2 | 2.39 | 0.51 |
| 2:d:254:VAL:HG13 | 2:d:365:ILE:HG12 | 1.90 | 0.51 |
| 2:i:164:ARG:HD2 | 2:j:365:ILE:CG2 | 2.39 | 0.51 |
| 2:m:52:THR:HG21 | 2:m:81:LEU:CD2 | 2.39 | 0.51 |
| 2:p:164:ARG:HD2 | 2:q:365:ILE:CG2 | 2.41 | 0.51 |
| 2:r:52:THR:HG21 | 2:r:81:LEU:CD2 | 2.39 | 0.51 |
| 2:r:275:VAL:HG21 | 2:r:338:LEU:CD2 | 2.40 | 0.51 |
| 2:v:164:ARG:HD2 | 2:w:365:ILE:CG2 | 2.40 | 0.51 |
| 2:z:68:GLN:HG2 | 1:Z:65:LEU:HD23 | 1.92 | 0.51 |
| 3:6:25:ALA:HB1 | 3:6:62:MET:HE2 | 1.92 | 0.51 |
| 3:10:21:GLN:O | 3:10:34:LEU:HB3 | 2.10 | 0.51 |
| 3:12:25:ALA:HB1 | 3:12:62:MET:HE2 | 1.92 | 0.51 |
| 3:13:21:GLN:O | 3:13:34:LEU:HB3 | 2.10 | 0.51 |
| 3:18:25:ALA:HB1 | 3:18:62:MET:HE2 | 1.91 | 0.51 |
| 3:18:70:PHE:HD1 | 1:R:41:PRO:HD3 | 1.74 | 0.51 |
| 3:21:21:GLN:O | 3:21:34:LEU:HB3 | 2.10 | 0.51 |
| 3:21:25:ALA:HB1 | 3:21:62:MET:HE2 | 1.92 | 0.51 |
| 3:24:70:PHE:HD1 | 1:X:41:PRO:HD3 | 1.74 | 0.51 |
| 3:25:21:GLN:O | 3:25:34:LEU:HB3 | 2.10 | 0.51 |
| 3:26:64:TYR:HB2 | 3:26:96:CYS:HB3 | 1.91 | 0.51 |
| 1:G:69:ARG:HG3 | 1:G:69:ARG:O | 2.10 | 0.51 |
| 1:T:31:VAL:HB | 1:U:179:ARG:HD3 | 1.92 | 0.51 |
| 1:W:37:ALA:HB1 | 1:X:74:ILE:CG2 | 2.39 | 0.51 |
| 1:W:84:GLU:HG2 | 1:W:197:SER:OG | 2.10 | 0.51 |
| 2:c:164:ARG:HD2 | 2:d:365:ILE:CG2 | 2.39 | 0.51 |
| 2:q:68:GLN:HG2 | 1:Q:65:LEU:HD23 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:r:175:LEU:HD11 | 1:P:51:ILE:CG1 | 2.38 | 0.51 |
| 3:3:21:GLN:O | 3:3:34:LEU:HB3 | 2.10 | 0.51 |
| 3:4:21:GLN:O | 3:4:34:LEU:HB3 | 2.10 | 0.51 |
| 3:9:70:PHE:HD1 | 1:I:41:PRO:HD3 | 1.74 | 0.51 |
| 3:11:70:PHE:HD1 | 1:K:41:PRO:HD3 | 1.74 | 0.51 |
| 3:17:70:PHE:HD1 | 1:Q:41:PRO:HD3 | 1.74 | 0.51 |
| 3:24:21:GLN:O | 3:24:34:LEU:HB3 | 2.10 | 0.51 |
| 1:P:84:GLU:HG2 | 1:P:197:SER:OG | 2.10 | 0.51 |
| 1:S:84:GLU:HG2 | 1:S:197:SER:OG | 2.10 | 0.51 |
| 1:V:84:GLU:HG2 | 1:V:197:SER:OG | 2.10 | 0.51 |
| 1:W:219:MET:HE2 | 1:Y:132:PHE:CB | 2.40 | 0.51 |
| 1:A:41:PRO:HD3 | 3:1:70:PHE:HD1 | 1.73 | 0.51 |
| 2:b:164:ARG:HD2 | 2:c:365:ILE:CG2 | 2.40 | 0.51 |
| 2:e:46:ASP:HA | 2:f:161:ASN:ND2 | 2.18 | 0.51 |
| 2:e:164:ARG:HD2 | 2:f:365:ILE:CG2 | 2.39 | 0.51 |
| 2:l:33:GLU:HG2 | 2:l:95:PRO:HD3 | 1.93 | 0.51 |
| 2:m:33:GLU:HG2 | 2:m:95:PRO:HD3 | 1.93 | 0.51 |
| 2:s:68:GLN:HG2 | 1:S:65:LEU:HD23 | 1.92 | 0.51 |
| 2:y:80:GLN:HB3 | 2:z:54:GLN:HB3 | 1.93 | 0.51 |
| 2:z:228:GLY:O | 2:z:232:GLN:HG3 | 2.09 | 0.51 |
| 2:z:275:VAL:HG21 | 2:z:338:LEU:CD2 | 2.40 | 0.51 |
| 3:13:25:ALA:HB1 | 3:13:62:MET:HE2 | 1.92 | 0.51 |
| 3:16:21:GLN:O | 3:16:34:LEU:HB3 | 2.10 | 0.51 |
| 3:22:70:PHE:HD1 | 1:V:41:PRO:HD3 | 1.74 | 0.51 |
| 1:B:37:ALA:HB1 | 1:C:74:ILE:CG2 | 2.40 | 0.51 |
| 1:F:69:ARG:HG3 | 1:F:69:ARG:O | 2.10 | 0.51 |
| 1:K:31:VAL:HB | 1:L:179:ARG:HD3 | 1.93 | 0.51 |
| 1:L:31:VAL:HB | 1:M:179:ARG:HD3 | 1.93 | 0.51 |
| 1:P:121:ARG:HA | 1:Q:111:ARG:HB2 | 1.91 | 0.51 |
| 1:Q:206:GLU:HG2 | 1:Q:208:VAL:HG13 | 1.91 | 0.51 |
| 1:S:31:VAL:HB | 1:T:179:ARG:HD3 | 1.92 | 0.51 |
| 1:T:69:ARG:HG3 | 1:T:69:ARG:O | 2.10 | 0.51 |
| 1:W:31:VAL:HB | 1:X:179:ARG:HD3 | 1.92 | 0.51 |
| 1:A:74:ILE:CG2 | 1:Z:37:ALA:HB1 | 2.40 | 0.51 |
| 2:b:327:ASN:OD1 | 2:b:330:SER:HB2 | 2.11 | 0.51 |
| 2:o:89:VAL:HG11 | 2:o:121:LEU:CD2 | 2.40 | 0.51 |
| 2:r:89:VAL:HG11 | 2:r:121:LEU:CD2 | 2.40 | 0.51 |
| 2:s:89:VAL:HG11 | 2:s:121:LEU:CD2 | 2.40 | 0.51 |
| 2:s:275:VAL:HG21 | 2:s:338:LEU:CD2 | 2.40 | 0.51 |
| 2:v:228:GLY:O | 2:v:232:GLN:HG3 | 2.10 | 0.51 |
| 2:w:68:GLN:HG2 | 1:W:65:LEU:HD23 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:5:25:ALA:HB1 | 3:5:62:MET:HE2 | 1.92 | 0.51 |
| 3:21:72:GLN:HG2 | 3:21:73:PRO:CD | 2.41 | 0.51 |
| 3:22:21:GLN:O | 3:22:34:LEU:HB3 | 2.10 | 0.51 |
| 3:22:72:GLN:HG2 | 3:22:73:PRO:CD | 2.41 | 0.51 |
| 3:23:25:ALA:HB1 | 3:23:62:MET:HE2 | 1.92 | 0.51 |
| 3:23:70:PHE:HD1 | 1:W:41:PRO:HD3 | 1.74 | 0.51 |
| 1:D:121:ARG:HA | 1:E:111:ARG:HB2 | 1.91 | 0.51 |
| 1:D:206:GLU:HG2 | 1:D:208:VAL:HG13 | 1.91 | 0.51 |
| 1:G:31:VAL:HB | 1:H:179:ARG:HD3 | 1.92 | 0.51 |
| 1:I:74:ILE:CD1 | 1:I:154:GLN:HA | 2.41 | 0.51 |
| 1:K:74:ILE:CD1 | 1:K:154:GLN:HA | 2.41 | 0.51 |
| 1:M:37:ALA:HB1 | 1:N:74:ILE:CG2 | 2.40 | 0.51 |
| 1:M:74:ILE:CD1 | 1:M:154:GLN:HA | 2.41 | 0.51 |
| 1:M:206:GLU:HG2 | 1:M:208:VAL:HG13 | 1.91 | 0.51 |
| 1:N:37:ALA:HB1 | 1:O:74:ILE:CG2 | 2.40 | 0.51 |
| 1:O:206:GLU:HG2 | 1:O:208:VAL:HG13 | 1.91 | 0.51 |
| 1:Q:31:VAL:HB | 1:R:179:ARG:HD3 | 1.93 | 0.51 |
| 1:A:31:VAL:HB | 1:B:179:ARG:HD3 | 1.92 | 0.51 |
| 1:A:65:LEU:HD23 | 2:a:68:GLN:HG2 | 1.92 | 0.51 |
| 2:a:327:ASN:OD1 | 2:a:330:SER:HB2 | 2.11 | 0.51 |
| 2:h:33:GLU:HG2 | 2:h:95:PRO:HD3 | 1.93 | 0.51 |
| 2:i:33:GLU:HG2 | 2:i:95:PRO:HD3 | 1.93 | 0.51 |
| 2:k:33:GLU:HG2 | 2:k:95:PRO:HD3 | 1.93 | 0.51 |
| 2:k:52:THR:HG21 | 2:k:81:LEU:CD2 | 2.39 | 0.51 |
| 2:m:89:VAL:HG11 | 2:m:121:LEU:CD2 | 2.40 | 0.51 |
| 2:n:33:GLU:HG2 | 2:n:95:PRO:HD3 | 1.93 | 0.51 |
| 2:p:33:GLU:HG2 | 2:p:95:PRO:HD3 | 1.93 | 0.51 |
| 2:t:327:ASN:OD1 | 2:t:330:SER:HB2 | 2.11 | 0.51 |
| 2:u:228:GLY:O | 2:u:232:GLN:HG3 | 2.10 | 0.51 |
| 2:v:216:LEU:HD11 | 2:v:222:GLN:HB2 | 1.93 | 0.51 |
| 2:w:327:ASN:OD1 | 2:w:330:SER:HB2 | 2.11 | 0.51 |
| 3:4:28:ILE:O | 3:4:29:SER:OG | 2.21 | 0.51 |
| 3:4:70:PHE:HD1 | 1:D:41:PRO:HD3 | 1.74 | 0.51 |
| 3:7:72:GLN:HG2 | 3:7:73:PRO:CD | 2.41 | 0.51 |
| 1:B:74:ILE:CD1 | 1:B:154:GLN:HA | 2.41 | 0.51 |
| 1:C:74:ILE:CD1 | 1:C:154:GLN:HA | 2.41 | 0.51 |
| 1:D:31:VAL:HB | 1:E:179:ARG:HD3 | 1.92 | 0.51 |
| 1:E:74:ILE:CD1 | 1:E:154:GLN:HA | 2.41 | 0.51 |
| 1:G:74:ILE:CD1 | 1:G:154:GLN:HA | 2.41 | 0.51 |
| 1:H:206:GLU:HG2 | 1:H:208:VAL:HG13 | 1.91 | 0.51 |
| 1:I:84:GLU:HG2 | 1:I:197:SER:OG | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:69:ARG:HG3 | 1:K:69:ARG:O | 2.09 | 0.51 |
| 1:L:69:ARG:HG3 | 1:L:69:ARG:O | 2.10 | 0.51 |
| 1:N:74:ILE:CD1 | 1:N:154:GLN:HA | 2.41 | 0.51 |
| 1:A:74:ILE:CD1 | 1:A:154:GLN:HA | 2.41 | 0.51 |
| 2:a:228:GLY:O | 2:a:232:GLN:HG3 | 2.09 | 0.51 |
| 3:1:25:ALA:HB1 | 3:1:62:MET:HE2 | 1.92 | 0.51 |
| 2:b:68:GLN:HG2 | 1:B:65:LEU:HD23 | 1.92 | 0.51 |
| 2:b:228:GLY:O | 2:b:232:GLN:HG3 | 2.09 | 0.51 |
| 2:c:327:ASN:OD1 | 2:c:330:SER:HB2 | 2.11 | 0.51 |
| 2:e:28:VAL:HB | 2:e:31:VAL:HG23 | 1.93 | 0.51 |
| 2:g:164:ARG:HD2 | 2:h:365:ILE:CG2 | 2.40 | 0.51 |
| 2:j:89:VAL:HG11 | 2:j:121:LEU:CD2 | 2.40 | 0.51 |
| 2:k:89:VAL:HG11 | 2:k:121:LEU:CD2 | 2.40 | 0.51 |
| 2:l:89:VAL:HG11 | 2:l:121:LEU:CD2 | 2.40 | 0.51 |
| 2:m:68:GLN:HG2 | 1:M:65:LEU:HD23 | 1.92 | 0.51 |
| 2:o:33:GLU:HG2 | 2:o:95:PRO:HD3 | 1.93 | 0.51 |
| 2:q:228:GLY:O | 2:q:232:GLN:HG3 | 2.10 | 0.51 |
| 2:t:275:VAL:HG21 | 2:t:338:LEU:CD2 | 2.40 | 0.51 |
| 2:u:216:LEU:HD11 | 2:u:222:GLN:HB2 | 1.93 | 0.51 |
| 2:u:327:ASN:OD1 | 2:u:330:SER:HB2 | 2.11 | 0.51 |
| 2:w:228:GLY:O | 2:w:232:GLN:HG3 | 2.10 | 0.51 |
| 2:y:275:VAL:HG21 | 2:y:338:LEU:CD2 | 2.40 | 0.51 |
| 2:z:216:LEU:HD11 | 2:z:222:GLN:HB2 | 1.93 | 0.51 |
| 3:7:21:GLN:O | 3:7:34:LEU:HB3 | 2.10 | 0.51 |
| 3:7:70:PHE:HD1 | 1:G:41:PRO:HD3 | 1.74 | 0.51 |
| 3:8:72:GLN:HG2 | 3:8:73:PRO:CD | 2.41 | 0.51 |
| 3:14:21:GLN:O | 3:14:34:LEU:HB3 | 2.10 | 0.51 |
| 3:14:25:ALA:HB1 | 3:14:62:MET:HE2 | 1.92 | 0.51 |
| 3:20:64:TYR:HB2 | 3:20:96:CYS:HB3 | 1.91 | 0.51 |
| 3:21:64:TYR:HB2 | 3:21:96:CYS:HB3 | 1.91 | 0.51 |
| 3:23:72:GLN:HG2 | 3:23:73:PRO:CD | 2.41 | 0.51 |
| 1:D:74:ILE:CD1 | 1:D:154:GLN:HA | 2.41 | 0.51 |
| 1:G:206:GLU:HG2 | 1:G:208:VAL:HG13 | 1.91 | 0.51 |
| 1:I:206:GLU:HG2 | 1:I:208:VAL:HG13 | 1.91 | 0.51 |
| 1:K:206:GLU:HG2 | 1:K:208:VAL:HG13 | 1.91 | 0.51 |
| 1:O:74:ILE:CD1 | 1:O:154:GLN:HA | 2.41 | 0.51 |
| 1:P:74:ILE:CD1 | 1:P:154:GLN:HA | 2.41 | 0.51 |
| 1:Q:37:ALA:HB1 | 1:R:74:ILE:CG2 | 2.39 | 0.51 |
| 1:Q:74:ILE:CD1 | 1:Q:154:GLN:HA | 2.41 | 0.51 |
| 1:Q:176:GLU:OE1 | 1:Q:207:TYR:OH | 2.21 | 0.51 |
| 1:S:206:GLU:HG2 | 1:S:208:VAL:HG13 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:37:ALA:HB1 | 1:U:74:ILE:CG2 | 2.40 | 0.51 |
| 1:A:90:LYS:HD3 | 1:Y:176:GLU:OE2 | 2.10 | 0.51 |
| 2:f:28:VAL:HB | 2:f:31:VAL:HG23 | 1.93 | 0.51 |
| 2:g:33:GLU:HG2 | 2:g:95:PRO:HD3 | 1.93 | 0.51 |
| 2:g:89:VAL:HG11 | 2:g:121:LEU:CD2 | 2.40 | 0.51 |
| 2:h:68:GLN:HG2 | 1:H:65:LEU:HD23 | 1.92 | 0.51 |
| 2:h:89:VAL:HG11 | 2:h:121:LEU:CD2 | 2.40 | 0.51 |
| 2:h:164:ARG:HD2 | 2:i:365:ILE:CG2 | 2.40 | 0.51 |
| 2:i:89:VAL:HG11 | 2:i:121:LEU:CD2 | 2.40 | 0.51 |
| 2:n:89:VAL:HG11 | 2:n:121:LEU:CD2 | 2.40 | 0.51 |
| 2:q:33:GLU:HG2 | 2:q:95:PRO:HD3 | 1.93 | 0.51 |
| 2:q:89:VAL:HG11 | 2:q:121:LEU:CD2 | 2.40 | 0.51 |
| 2:s:327:ASN:OD1 | 2:s:330:SER:HB2 | 2.11 | 0.51 |
| 2:x:275:VAL:HG21 | 2:x:338:LEU:CD2 | 2.40 | 0.51 |
| 2:y:175:LEU:HD11 | 1:W:51:ILE:CG1 | 2.39 | 0.51 |
| 2:z:327:ASN:OD1 | 2:z:330:SER:HB2 | 2.11 | 0.51 |
| 3:3:70:PHE:HD1 | 1:C:41:PRO:HD3 | 1.74 | 0.51 |
| 3:4:25:ALA:HB1 | 3:4:62:MET:HE2 | 1.92 | 0.51 |
| 3:5:70:PHE:HD1 | 1:E:41:PRO:HD3 | 1.74 | 0.51 |
| 3:9:72:GLN:HG2 | 3:9:73:PRO:CD | 2.41 | 0.51 |
| 3:12:64:TYR:HB2 | 3:12:96:CYS:HB3 | 1.91 | 0.51 |
| 3:17:64:TYR:HB2 | 3:17:96:CYS:HB3 | 1.91 | 0.51 |
| 3:18:64:TYR:HB2 | 3:18:96:CYS:HB3 | 1.91 | 0.51 |
| 3:19:64:TYR:HB2 | 3:19:96:CYS:HB3 | 1.91 | 0.51 |
| 3:22:25:ALA:HB1 | 3:22:62:MET:HE2 | 1.92 | 0.51 |
| 3:22:64:TYR:HB2 | 3:22:96:CYS:HB3 | 1.91 | 0.51 |
| 1:C:84:GLU:HG2 | 1:C:197:SER:OG | 2.10 | 0.51 |
| 1:E:206:GLU:HG2 | 1:E:208:VAL:HG13 | 1.91 | 0.51 |
| 1:F:74:ILE:HD13 | 1:F:154:GLN:HA | 1.93 | 0.51 |
| 1:F:84:GLU:HG2 | 1:F:197:SER:OG | 2.10 | 0.51 |
| 1:H:74:ILE:HD13 | 1:H:154:GLN:HA | 1.93 | 0.51 |
| 1:J:69:ARG:HG3 | 1:J:69:ARG:O | 2.10 | 0.51 |
| 1:J:121:ARG:HA | 1:K:111:ARG:HB2 | 1.91 | 0.51 |
| 1:R:37:ALA:HB1 | 1:S:74:ILE:CG2 | 2.41 | 0.51 |
| 1:X:84:GLU:HG2 | 1:X:197:SER:OG | 2.10 | 0.51 |
| 1:Z:74:ILE:CD1 | 1:Z:154:GLN:HA | 2.41 | 0.51 |
| 1:Z:206:GLU:HG2 | 1:Z:208:VAL:HG13 | 1.91 | 0.51 |
| 1:A:206:GLU:HG2 | 1:A:208:VAL:HG13 | 1.91 | 0.51 |
| 2:a:216:LEU:HD11 | 2:a:222:GLN:HB2 | 1.93 | 0.51 |
| 2:b:52:THR:HG21 | 2:b:81:LEU:CD2 | 2.39 | 0.51 |
| 2:f:254:VAL:CG2 | 2:g:355:ALA:HB2 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:g:68:GLN:HG2 | 1:G:65:LEU:HD23 | 1.92 | 0.51 |
| 2:j:33:GLU:HG2 | 2:j:95:PRO:HD3 | 1.93 | 0.51 |
| 2:j:164:ARG:HD2 | 2:k:365:ILE:CG2 | 2.40 | 0.51 |
| 2:k:32:ARG:HG2 | 2:k:32:ARG:HH11 | 1.76 | 0.51 |
| 2:t:228:GLY:O | 2:t:232:GLN:HG3 | 2.10 | 0.51 |
| 2:x:228:GLY:O | 2:x:232:GLN:HG3 | 2.09 | 0.51 |
| 3:12:70:PHE:HD1 | 1:L:41:PRO:HD3 | 1.75 | 0.51 |
| 3:17:25:ALA:HB1 | 3:17:62:MET:HE2 | 1.91 | 0.51 |
| 3:25:64:TYR:HB2 | 3:25:96:CYS:HB3 | 1.91 | 0.51 |
| 1:B:206:GLU:HG2 | 1:B:208:VAL:HG13 | 1.91 | 0.51 |
| 1:C:206:GLU:HG2 | 1:C:208:VAL:HG13 | 1.91 | 0.51 |
| 1:D:74:ILE:HD13 | 1:D:154:GLN:HA | 1.93 | 0.51 |
| 1:P:69:ARG:O | 1:P:69:ARG:HG3 | 2.10 | 0.51 |
| 1:Q:69:ARG:HG3 | 1:Q:69:ARG:O | 2.10 | 0.51 |
| 1:R:74:ILE:CD1 | 1:R:154:GLN:HA | 2.41 | 0.51 |
| 1:S:69:ARG:O | 1:S:69:ARG:HG3 | 2.10 | 0.51 |
| 1:U:69:ARG:HG3 | 1:U:69:ARG:O | 2.09 | 0.51 |
| 1:V:69:ARG:HG3 | 1:V:69:ARG:O | 2.10 | 0.51 |
| 1:Y:74:ILE:CD1 | 1:Y:154:GLN:HA | 2.41 | 0.51 |
| 1:Y:170:ALA:HB3 | 1:Z:206:GLU:HG3 | 1.92 | 0.51 |
| 2:b:28:VAL:HB | 2:b:31:VAL:HG23 | 1.93 | 0.51 |
| 2:c:28:VAL:HB | 2:c:31:VAL:HG23 | 1.93 | 0.51 |
| 2:d:28:VAL:HB | 2:d:31:VAL:HG23 | 1.93 | 0.51 |
| 2:d:327:ASN:OD1 | 2:d:330:SER:HB2 | 2.11 | 0.51 |
| 2:f:89:VAL:HG11 | 2:f:121:LEU:CD2 | 2.40 | 0.51 |
| 2:g:28:VAL:HB | 2:g:31:VAL:HG23 | 1.93 | 0.51 |
| 2:h:32:ARG:HG2 | 2:h:32:ARG:HH11 | 1.76 | 0.51 |
| 2:i:28:VAL:HB | 2:i:31:VAL:HG23 | 1.93 | 0.51 |
| 2:i:327:ASN:OD1 | 2:i:330:SER:HB2 | 2.11 | 0.51 |
| 2:j:28:VAL:HB | 2:j:31:VAL:HG23 | 1.93 | 0.51 |
| 2:k:28:VAL:HB | 2:k:31:VAL:HG23 | 1.93 | 0.51 |
| 2:l:28:VAL:HB | 2:l:31:VAL:HG23 | 1.93 | 0.51 |
| 2:n:68:GLN:HG2 | 1:N:65:LEU:HD23 | 1.92 | 0.51 |
| 2:r:327:ASN:OD1 | 2:r:330:SER:HB2 | 2.11 | 0.51 |
| 2:s:228:GLY:O | 2:s:232:GLN:HG3 | 2.10 | 0.51 |
| 2:v:275:VAL:HG21 | 2:v:338:LEU:CD2 | 2.40 | 0.51 |
| 2:v:327:ASN:OD1 | 2:v:330:SER:HB2 | 2.11 | 0.51 |
| 2:x:68:GLN:HG2 | 1:X:65:LEU:HD23 | 1.92 | 0.51 |
| 2:x:327:ASN:OD1 | 2:x:330:SER:HB2 | 2.11 | 0.51 |
| 3:11:21:GLN:O | 3:11:34:LEU:HB3 | 2.10 | 0.51 |
| 3:15:25:ALA:HB1 | 3:15:62:MET:HE2 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:16:64:TYR:HB2 | 3:16:96:CYS:HB3 | 1.91 | 0.51 |
| 3:24:72:GLN:HG2 | 3:24:73:PRO:CD | 2.41 | 0.51 |
| 1:C:74:ILE:HD13 | 1:C:154:GLN:HA | 1.93 | 0.51 |
| 1:E:74:ILE:HD13 | 1:E:154:GLN:HA | 1.93 | 0.51 |
| 1:G:74:ILE:HD13 | 1:G:154:GLN:HA | 1.93 | 0.51 |
| 1:I:74:ILE:HD13 | 1:I:154:GLN:HA | 1.93 | 0.51 |
| 1:J:74:ILE:HD13 | 1:J:154:GLN:HA | 1.93 | 0.51 |
| 1:M:69:ARG:HG3 | 1:M:69:ARG:O | 2.10 | 0.51 |
| 1:S:74:ILE:CD1 | 1:S:154:GLN:HA | 2.41 | 0.51 |
| 1:V:121:ARG:HA | 1:W:111:ARG:HB2 | 1.91 | 0.51 |
| 1:Y:130:ASN:CG | 1:Z:102:THR:HG22 | 2.36 | 0.51 |
| 2:b:362:LEU:HD21 | 2:z:166:THR:HG21 | 1.93 | 0.51 |
| 2:d:254:VAL:CG2 | 2:e:355:ALA:HB2 | 2.41 | 0.51 |
| 2:f:166:THR:HG21 | 2:h:362:LEU:HD21 | 1.93 | 0.51 |
| 2:h:28:VAL:HB | 2:h:31:VAL:HG23 | 1.93 | 0.51 |
| 2:l:327:ASN:OD1 | 2:l:330:SER:HB2 | 2.11 | 0.51 |
| 2:m:327:ASN:OD1 | 2:m:330:SER:HB2 | 2.11 | 0.51 |
| 2:n:32:ARG:HG2 | 2:n:32:ARG:HH11 | 1.76 | 0.51 |
| 2:p:89:VAL:HG11 | 2:p:121:LEU:CD2 | 2.40 | 0.51 |
| 2:q:32:ARG:HG2 | 2:q:32:ARG:HH11 | 1.76 | 0.51 |
| 2:q:175:LEU:HD11 | 1:O:51:ILE:CG1 | 2.38 | 0.51 |
| 2:t:216:LEU:HD11 | 2:t:222:GLN:HB2 | 1.93 | 0.51 |
| 2:u:275:VAL:HG21 | 2:u:338:LEU:CD2 | 2.40 | 0.51 |
| 2:y:216:LEU:HD11 | 2:y:222:GLN:HB2 | 1.93 | 0.51 |
| 3:8:70:PHE:HD1 | 1:H:41:PRO:HD3 | 1.74 | 0.51 |
| 3:10:72:GLN:HG2 | 3:10:73:PRO:CD | 2.41 | 0.51 |
| 1:I:31:VAL:HB | 1:J:179:ARG:HD3 | 1.93 | 0.51 |
| 1:O:31:VAL:HB | 1:P:179:ARG:HD3 | 1.93 | 0.51 |
| 1:U:206:GLU:HG2 | 1:U:208:VAL:HG13 | 1.91 | 0.51 |
| 2:c:89:VAL:HG11 | 2:c:121:LEU:CD2 | 2.40 | 0.50 |
| 2:e:89:VAL:HG11 | 2:e:121:LEU:CD2 | 2.40 | 0.50 |
| 2:g:284:VAL:HG21 | 2:g:316:GLY:HA2 | 1.93 | 0.50 |
| 2:h:280:LEU:HD11 | 2:h:340:ALA:HB2 | 1.93 | 0.50 |
| 2:i:68:GLN:HG2 | 1:I:65:LEU:HD23 | 1.92 | 0.50 |
| 2:l:175:LEU:HD11 | 1:J:51:ILE:CG1 | 2.37 | 0.50 |
| 2:r:33:GLU:HG2 | 2:r:95:PRO:HD3 | 1.93 | 0.50 |
| 2:r:164:ARG:HD2 | 2:s:365:ILE:CG2 | 2.42 | 0.50 |
| 2:t:32:ARG:HG2 | 2:t:32:ARG:HH11 | 1.76 | 0.50 |
| 2:v:89:VAL:HG11 | 2:v:121:LEU:CD2 | 2.40 | 0.50 |
| 2:v:254:VAL:CG2 | 2:w:355:ALA:HB2 | 2.42 | 0.50 |
| 2:x:89:VAL:HG11 | 2:x:121:LEU:CD2 | 2.40 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:y:327:ASN:OD1 | 2:y:330:SER:HB2 | 2.11 | 0.50 |
| 3:2:70:PHE:HD1 | 1:B:41:PRO:HD3 | 1.74 | 0.50 |
| 3:3:25:ALA:HB1 | 3:3:62:MET:HE2 | 1.92 | 0.50 |
| 3:6:70:PHE:HD1 | 1:F:41:PRO:HD3 | 1.74 | 0.50 |
| 3:14:28:ILE:O | 3:14:29:SER:OG | 2.21 | 0.50 |
| 3:23:64:TYR:HB2 | 3:23:96:CYS:HB3 | 1.92 | 0.50 |
| 1:B:74:ILE:HD13 | 1:B:154:GLN:HA | 1.93 | 0.50 |
| 1:E:31:VAL:HB | 1:F:179:ARG:HD3 | 1.92 | 0.50 |
| 1:F:31:VAL:HB | 1:G:179:ARG:HD3 | 1.93 | 0.50 |
| 1:K:74:ILE:HD13 | 1:K:154:GLN:HA | 1.93 | 0.50 |
| 1:L:74:ILE:CD1 | 1:L:154:GLN:HA | 2.41 | 0.50 |
| 1:N:69:ARG:HG3 | 1:N:69:ARG:O | 2.09 | 0.50 |
| 1:X:74:ILE:CD1 | 1:X:154:GLN:HA | 2.41 | 0.50 |
| 1:A:74:ILE:HD13 | 1:A:154:GLN:HA | 1.93 | 0.50 |
| 2:a:28:VAL:HB | 2:a:31:VAL:HG23 | 1.93 | 0.50 |
| 2:a:89:VAL:HG11 | 2:a:121:LEU:CD2 | 2.40 | 0.50 |
| 2:b:32:ARG:HG2 | 2:b:32:ARG:HH11 | 1.76 | 0.50 |
| 2:b:89:VAL:HG11 | 2:b:121:LEU:CD2 | 2.40 | 0.50 |
| 2:c:32:ARG:HG2 | 2:c:32:ARG:HH11 | 1.76 | 0.50 |
| 2:c:284:VAL:HG21 | 2:c:316:GLY:HA2 | 1.93 | 0.50 |
| 2:d:89:VAL:HG11 | 2:d:121:LEU:CD2 | 2.40 | 0.50 |
| 2:d:284:VAL:HG21 | 2:d:316:GLY:HA2 | 1.93 | 0.50 |
| 2:e:68:GLN:HG2 | 1:E:65:LEU:HD23 | 1.92 | 0.50 |
| 2:i:280:LEU:HD11 | 2:i:340:ALA:HB2 | 1.93 | 0.50 |
| 2:j:280:LEU:HD11 | 2:j:340:ALA:HB2 | 1.93 | 0.50 |
| 2:j:327:ASN:OD1 | 2:j:330:SER:HB2 | 2.11 | 0.50 |
| 2:y:228:GLY:O | 2:y:232:GLN:HG3 | 2.10 | 0.50 |
| 3:15:64:TYR:HB2 | 3:15:96:CYS:HB3 | 1.92 | 0.50 |
| 3:16:25:ALA:HB1 | 3:16:62:MET:HE2 | 1.92 | 0.50 |
| 3:24:83:SER:HA | 1:Y:210:ASN:ND2 | 2.25 | 0.50 |
| 3:25:72:GLN:HG2 | 3:25:73:PRO:CD | 2.41 | 0.50 |
| 1:F:74:ILE:CD1 | 1:F:154:GLN:HA | 2.41 | 0.50 |
| 1:F:206:GLU:HG2 | 1:F:208:VAL:HG13 | 1.91 | 0.50 |
| 1:U:31:VAL:HB | 1:V:179:ARG:HD3 | 1.93 | 0.50 |
| 1:Y:206:GLU:HG2 | 1:Y:208:VAL:HG13 | 1.91 | 0.50 |
| 2:b:216:LEU:HD11 | 2:b:222:GLN:HB2 | 1.93 | 0.50 |
| 2:f:33:GLU:HG2 | 2:f:95:PRO:HD3 | 1.93 | 0.50 |
| 2:g:280:LEU:HD11 | 2:g:340:ALA:HB2 | 1.93 | 0.50 |
| 2:k:280:LEU:HD11 | 2:k:340:ALA:HB2 | 1.93 | 0.50 |
| 2:l:280:LEU:HD11 | 2:l:340:ALA:HB2 | 1.93 | 0.50 |
| 2:m:28:VAL:HB | 2:m:31:VAL:HG23 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:280:LEU:HD11 | 2:n:340:ALA:HB2 | 1.93 | 0.50 |
| 2:p:216:LEU:HD11 | 2:p:222:GLN:HB2 | 1.93 | 0.50 |
| 2:p:254:VAL:CG2 | 2:q:355:ALA:HB2 | 2.41 | 0.50 |
| 2:t:89:VAL:HG11 | 2:t:121:LEU:CD2 | 2.40 | 0.50 |
| 2:v:175:LEU:HD11 | 1:T:51:ILE:CG1 | 2.40 | 0.50 |
| 2:w:62:LEU:HD13 | 2:w:81:LEU:HD11 | 1.94 | 0.50 |
| 2:w:216:LEU:HD11 | 2:w:222:GLN:HB2 | 1.93 | 0.50 |
| 2:y:89:VAL:HG11 | 2:y:121:LEU:CD2 | 2.40 | 0.50 |
| 2:y:328:LEU:HD21 | 2:z:273:CYS:HA | 1.93 | 0.50 |
| 2:z:89:VAL:HG11 | 2:z:121:LEU:CD2 | 2.40 | 0.50 |
| 3:2:25:ALA:HB1 | 3:2:62:MET:HE2 | 1.92 | 0.50 |
| 3:19:21:GLN:O | 3:19:34:LEU:HB3 | 2.10 | 0.50 |
| 3:24:64:TYR:HB2 | 3:24:96:CYS:HB3 | 1.91 | 0.50 |
| 1:L:74:ILE:HD13 | 1:L:154:GLN:HA | 1.93 | 0.50 |
| 1:T:74:ILE:CD1 | 1:T:154:GLN:HA | 2.41 | 0.50 |
| 1:V:58:ILE:HG13 | 1:V:59:ASN:N | 2.26 | 0.50 |
| 1:X:31:VAL:HB | 1:Y:179:ARG:HD3 | 1.94 | 0.50 |
| 2:e:32:ARG:HH11 | 2:e:32:ARG:HG2 | 1.76 | 0.50 |
| 2:e:33:GLU:HG2 | 2:e:95:PRO:HD3 | 1.93 | 0.50 |
| 2:e:255:ILE:HD12 | 2:e:362:LEU:HD12 | 1.94 | 0.50 |
| 2:f:255:ILE:HD12 | 2:f:362:LEU:HD12 | 1.94 | 0.50 |
| 2:f:280:LEU:HD11 | 2:f:340:ALA:HB2 | 1.93 | 0.50 |
| 2:h:284:VAL:HG21 | 2:h:316:GLY:HA2 | 1.93 | 0.50 |
| 2:m:280:LEU:HD11 | 2:m:340:ALA:HB2 | 1.93 | 0.50 |
| 2:o:32:ARG:HG2 | 2:o:32:ARG:HH11 | 1.76 | 0.50 |
| 2:o:216:LEU:HD11 | 2:o:222:GLN:HB2 | 1.93 | 0.50 |
| 2:p:280:LEU:HD11 | 2:p:340:ALA:HB2 | 1.93 | 0.50 |
| 2:q:216:LEU:HD11 | 2:q:222:GLN:HB2 | 1.93 | 0.50 |
| 2:q:327:ASN:OD1 | 2:q:330:SER:HB2 | 2.11 | 0.50 |
| 2:r:32:ARG:HG2 | 2:r:32:ARG:HH11 | 1.76 | 0.50 |
| 2:s:62:LEU:HD13 | 2:s:81:LEU:HD11 | 1.94 | 0.50 |
| 2:s:175:LEU:HD11 | 1:Q:51:ILE:CG1 | 2.39 | 0.50 |
| 2:s:275:VAL:HG21 | 2:s:338:LEU:HD21 | 1.94 | 0.50 |
| 2:u:62:LEU:HD13 | 2:u:81:LEU:HD11 | 1.94 | 0.50 |
| 2:u:89:VAL:HG11 | 2:u:121:LEU:CD2 | 2.40 | 0.50 |
| 2:v:62:LEU:HD13 | 2:v:81:LEU:HD11 | 1.94 | 0.50 |
| 2:w:32:ARG:HG2 | 2:w:32:ARG:HH11 | 1.76 | 0.50 |
| 2:w:89:VAL:HG11 | 2:w:121:LEU:CD2 | 2.40 | 0.50 |
| 2:w:275:VAL:HG21 | 2:w:338:LEU:CD2 | 2.40 | 0.50 |
| 3:14:64:TYR:HB2 | 3:14:96:CYS:HB3 | 1.91 | 0.50 |
| 3:26:70:PHE:HD1 | 1:Z:41:PRO:HD3 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:69:ARG:HG3 | 1:O:69:ARG:O | 2.10 | 0.50 |
| 1:T:58:ILE:HG13 | 1:T:59:ASN:N | 2.26 | 0.50 |
| 1:U:58:ILE:HG13 | 1:U:59:ASN:N | 2.26 | 0.50 |
| 1:W:74:ILE:CD1 | 1:W:154:GLN:HA | 2.41 | 0.50 |
| 1:Z:74:ILE:HD13 | 1:Z:154:GLN:HA | 1.93 | 0.50 |
| 2:a:62:LEU:HD13 | 2:a:81:LEU:HD11 | 1.94 | 0.50 |
| 2:e:280:LEU:HD11 | 2:e:340:ALA:HB2 | 1.93 | 0.50 |
| 2:e:327:ASN:OD1 | 2:e:330:SER:HB2 | 2.11 | 0.50 |
| 2:g:255:ILE:HD12 | 2:g:362:LEU:HD12 | 1.94 | 0.50 |
| 2:j:254:VAL:CG2 | 2:k:355:ALA:HB2 | 2.42 | 0.50 |
| 2:k:284:VAL:HG21 | 2:k:316:GLY:HA2 | 1.93 | 0.50 |
| 2:l:68:GLN:HG2 | 1:L:65:LEU:HD23 | 1.92 | 0.50 |
| 2:n:28:VAL:HB | 2:n:31:VAL:HG23 | 1.93 | 0.50 |
| 2:o:68:GLN:HG2 | 1:O:65:LEU:HD23 | 1.92 | 0.50 |
| 2:o:280:LEU:HD11 | 2:o:340:ALA:HB2 | 1.93 | 0.50 |
| 2:p:68:GLN:HG2 | 1:P:65:LEU:HD23 | 1.92 | 0.50 |
| 2:r:275:VAL:HG21 | 2:r:338:LEU:HD21 | 1.94 | 0.50 |
| 2:s:33:GLU:HG2 | 2:s:95:PRO:HD3 | 1.93 | 0.50 |
| 2:t:33:GLU:HG2 | 2:t:95:PRO:HD3 | 1.93 | 0.50 |
| 2:t:62:LEU:HD13 | 2:t:81:LEU:HD11 | 1.94 | 0.50 |
| 2:u:32:ARG:HH11 | 2:u:32:ARG:HG2 | 1.76 | 0.50 |
| 2:w:275:VAL:HG21 | 2:w:338:LEU:HD21 | 1.94 | 0.50 |
| 2:x:62:LEU:HD13 | 2:x:81:LEU:HD11 | 1.94 | 0.50 |
| 2:y:62:LEU:HD13 | 2:y:81:LEU:HD11 | 1.94 | 0.50 |
| 2:z:28:VAL:HB | 2:z:31:VAL:HG23 | 1.93 | 0.50 |
| 3:11:72:GLN:HG2 | 3:11:73:PRO:CD | 2.41 | 0.50 |
| 1:R:58:ILE:HG13 | 1:R:59:ASN:N | 2.26 | 0.50 |
| 1:S:58:ILE:HG13 | 1:S:59:ASN:N | 2.26 | 0.50 |
| 1:W:58:ILE:HG13 | 1:W:59:ASN:N | 2.26 | 0.50 |
| 1:W:206:GLU:HG2 | 1:W:208:VAL:HG13 | 1.91 | 0.50 |
| 1:X:58:ILE:HG13 | 1:X:59:ASN:N | 2.26 | 0.50 |
| 1:Y:58:ILE:HG13 | 1:Y:59:ASN:N | 2.26 | 0.50 |
| 1:Y:168:GLN:HG3 | 1:Z:204:ARG:NE | 2.27 | 0.50 |
| 2:b:62:LEU:HD13 | 2:b:81:LEU:HD11 | 1.94 | 0.50 |
| 2:c:62:LEU:HD13 | 2:c:81:LEU:HD11 | 1.94 | 0.50 |
| 2:d:33:GLU:HG2 | 2:d:95:PRO:HD3 | 1.93 | 0.50 |
| 2:d:93:TYR:OH | 2:d:173:ARG:O | 2.25 | 0.50 |
| 2:d:255:ILE:HD12 | 2:d:362:LEU:HD12 | 1.94 | 0.50 |
| 2:f:164:ARG:HD2 | 2:g:365:ILE:CG2 | 2.40 | 0.50 |
| 2:f:284:VAL:HG21 | 2:f:316:GLY:HA2 | 1.93 | 0.50 |
| 2:h:166:THR:HG21 | 2:j:362:LEU:HD21 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:h:255:ILE:HD12 | 2:h:362:LEU:HD12 | 1.94 | 0.50 |
| 2:k:327:ASN:OD1 | 2:k:330:SER:HB2 | 2.11 | 0.50 |
| 2:l:32:ARG:HG2 | 2:l:32:ARG:HH11 | 1.76 | 0.50 |
| 2:q:280:LEU:HD11 | 2:q:340:ALA:HB2 | 1.93 | 0.50 |
| 2:r:62:LEU:HD13 | 2:r:81:LEU:HD11 | 1.94 | 0.50 |
| 2:s:216:LEU:HD11 | 2:s:222:GLN:HB2 | 1.93 | 0.50 |
| 2:t:68:GLN:HG2 | 1:T:65:LEU:HD23 | 1.92 | 0.50 |
| 2:t:141:ILE:HD13 | 2:t:165:ILE:CD1 | 2.39 | 0.50 |
| 2:t:275:VAL:HG21 | 2:t:338:LEU:HD21 | 1.94 | 0.50 |
| 2:u:33:GLU:HG2 | 2:u:95:PRO:HD3 | 1.93 | 0.50 |
| 2:u:72:THR:OG1 | 1:V:70:ARG:NH2 | 2.38 | 0.50 |
| 2:u:255:ILE:HD12 | 2:u:362:LEU:HD12 | 1.94 | 0.50 |
| 2:v:275:VAL:HG21 | 2:v:338:LEU:HD21 | 1.94 | 0.50 |
| 2:x:32:ARG:HG2 | 2:x:32:ARG:HH11 | 1.76 | 0.50 |
| 2:y:33:GLU:HG2 | 2:y:95:PRO:HD3 | 1.93 | 0.50 |
| 2:z:32:ARG:HG2 | 2:z:32:ARG:HH11 | 1.76 | 0.50 |
| 2:z:62:LEU:HD13 | 2:z:81:LEU:HD11 | 1.94 | 0.50 |
| 2:z:284:VAL:HG21 | 2:z:316:GLY:HA2 | 1.93 | 0.50 |
| 3:13:64:TYR:HB2 | 3:13:96:CYS:HB3 | 1.92 | 0.50 |
| 3:15:47:ASP:CG | 3:15:50:VAL:H | 2.15 | 0.50 |
| 1:C:31:VAL:HB | 1:D:179:ARG:HD3 | 1.93 | 0.50 |
| 1:H:74:ILE:CD1 | 1:H:154:GLN:HA | 2.41 | 0.50 |
| 1:M:74:ILE:HD13 | 1:M:154:GLN:HA | 1.93 | 0.50 |
| 1:P:58:ILE:HG13 | 1:P:59:ASN:N | 2.26 | 0.50 |
| 1:Q:58:ILE:HG13 | 1:Q:59:ASN:N | 2.26 | 0.50 |
| 1:T:80:ILE:HD13 | 1:T:195:VAL:CG1 | 2.42 | 0.50 |
| 1:U:74:ILE:CD1 | 1:U:154:GLN:HA | 2.41 | 0.50 |
| 1:V:80:ILE:HD13 | 1:V:195:VAL:CG1 | 2.42 | 0.50 |
| 1:X:80:ILE:HD13 | 1:X:195:VAL:CG1 | 2.42 | 0.50 |
| 1:Z:58:ILE:HG13 | 1:Z:59:ASN:N | 2.26 | 0.50 |
| 2:c:33:GLU:HG2 | 2:c:95:PRO:HD3 | 1.93 | 0.50 |
| 2:j:32:ARG:HG2 | 2:j:32:ARG:HH11 | 1.76 | 0.50 |
| 2:j:93:TYR:OH | 2:j:173:ARG:O | 2.24 | 0.50 |
| 2:o:28:VAL:HB | 2:o:31:VAL:HG23 | 1.93 | 0.50 |
| 2:o:166:THR:HG21 | 2:q:362:LEU:HD21 | 1.94 | 0.50 |
| 2:o:275:VAL:HG21 | 2:o:338:LEU:HD21 | 1.94 | 0.50 |
| 2:p:327:ASN:OD1 | 2:p:330:SER:HB2 | 2.11 | 0.50 |
| 2:q:62:LEU:HD13 | 2:q:81:LEU:HD11 | 1.94 | 0.50 |
| 2:q:275:VAL:HG21 | 2:q:338:LEU:HD21 | 1.94 | 0.50 |
| 2:s:255:ILE:HD12 | 2:s:362:LEU:HD12 | 1.94 | 0.50 |
| 2:v:255:ILE:HD12 | 2:v:362:LEU:HD12 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:x:275:VAL:HG21 | 2:x:338:LEU:HD21 | 1.94 | 0.50 |
| 2:z:33:GLU:HG2 | 2:z:95:PRO:HD3 | 1.93 | 0.50 |
| 3:26:72:GLN:HG2 | 3:26:73:PRO:CD | 2.41 | 0.50 |
| 1:O:58:ILE:HG13 | 1:O:59:ASN:N | 2.26 | 0.50 |
| 1:Q:80:ILE:HD13 | 1:Q:195:VAL:CG1 | 2.42 | 0.50 |
| 1:V:74:ILE:CD1 | 1:V:154:GLN:HA | 2.41 | 0.50 |
| 1:Z:80:ILE:HD13 | 1:Z:195:VAL:CG1 | 2.42 | 0.50 |
| 1:A:58:ILE:HG13 | 1:A:59:ASN:N | 2.26 | 0.50 |
| 2:a:32:ARG:HG2 | 2:a:32:ARG:HH11 | 1.76 | 0.50 |
| 2:c:255:ILE:HD12 | 2:c:362:LEU:HD12 | 1.94 | 0.50 |
| 2:d:62:LEU:HD13 | 2:d:81:LEU:HD11 | 1.94 | 0.50 |
| 2:d:280:LEU:HD11 | 2:d:340:ALA:HB2 | 1.93 | 0.50 |
| 2:e:62:LEU:HD13 | 2:e:81:LEU:HD11 | 1.94 | 0.50 |
| 2:e:216:LEU:HD11 | 2:e:222:GLN:HB2 | 1.93 | 0.50 |
| 2:f:62:LEU:HD13 | 2:f:81:LEU:HD11 | 1.94 | 0.50 |
| 2:f:216:LEU:HD11 | 2:f:222:GLN:HB2 | 1.93 | 0.50 |
| 2:h:62:LEU:HD13 | 2:h:81:LEU:HD11 | 1.94 | 0.50 |
| 2:h:327:ASN:OD1 | 2:h:330:SER:HB2 | 2.11 | 0.50 |
| 2:i:32:ARG:HG2 | 2:i:32:ARG:HH11 | 1.76 | 0.50 |
| 2:i:217:ASP:OD1 | 2:i:219:ARG:N | 2.35 | 0.50 |
| 2:j:284:VAL:HG21 | 2:j:316:GLY:HA2 | 1.93 | 0.50 |
| 2:k:277:GLN:HB3 | 2:k:280:LEU:HD12 | 1.94 | 0.50 |
| 2:n:327:ASN:OD1 | 2:n:330:SER:HB2 | 2.11 | 0.50 |
| 2:q:255:ILE:HD12 | 2:q:362:LEU:HD12 | 1.94 | 0.50 |
| 2:r:228:GLY:O | 2:r:232:GLN:HG3 | 2.09 | 0.50 |
| 2:r:255:ILE:HD12 | 2:r:362:LEU:HD12 | 1.94 | 0.50 |
| 2:t:255:ILE:HD12 | 2:t:362:LEU:HD12 | 1.94 | 0.50 |
| 2:u:141:ILE:HD13 | 2:u:165:ILE:CD1 | 2.39 | 0.50 |
| 2:x:33:GLU:HG2 | 2:x:95:PRO:HD3 | 1.93 | 0.50 |
| 2:x:216:LEU:HD11 | 2:x:222:GLN:HB2 | 1.93 | 0.50 |
| 2:y:275:VAL:HG21 | 2:y:338:LEU:HD21 | 1.94 | 0.50 |
| 2:y:284:VAL:HG21 | 2:y:316:GLY:HA2 | 1.94 | 0.50 |
| 3:5:47:ASP:CG | 3:5:50:VAL:H | 2.14 | 0.50 |
| 3:12:72:GLN:HG2 | 3:12:73:PRO:CD | 2.41 | 0.50 |
| 1:B:58:ILE:HG13 | 1:B:59:ASN:N | 2.26 | 0.50 |
| 1:B:80:ILE:HD13 | 1:B:195:VAL:CG1 | 2.42 | 0.50 |
| 1:J:74:ILE:CD1 | 1:J:154:GLN:HA | 2.41 | 0.50 |
| 1:N:58:ILE:HG13 | 1:N:59:ASN:N | 2.26 | 0.50 |
| 1:N:74:ILE:HD13 | 1:N:154:GLN:HA | 1.93 | 0.50 |
| 1:P:80:ILE:HD13 | 1:P:195:VAL:CG1 | 2.42 | 0.50 |
| 1:R:80:ILE:HD13 | 1:R:195:VAL:CG1 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:80:ILE:HD13 | 1:U:195:VAL:CG1 | 2.42 | 0.50 |
| 1:W:82:LEU:O | 1:W:197:SER:OG | 2.28 | 0.50 |
| 1:Y:74:ILE:HD13 | 1:Y:154:GLN:HA | 1.93 | 0.50 |
| 1:Y:80:ILE:HD13 | 1:Y:195:VAL:CG1 | 2.42 | 0.50 |
| 2:c:277:GLN:HB3 | 2:c:280:LEU:HD12 | 1.94 | 0.50 |
| 2:f:32:ARG:HG2 | 2:f:32:ARG:HH11 | 1.76 | 0.50 |
| 2:f:327:ASN:OD1 | 2:f:330:SER:HB2 | 2.11 | 0.50 |
| 2:g:32:ARG:HG2 | 2:g:32:ARG:HH11 | 1.76 | 0.50 |
| 2:g:62:LEU:HD13 | 2:g:81:LEU:HD11 | 1.94 | 0.50 |
| 2:i:255:ILE:HD12 | 2:i:362:LEU:HD12 | 1.94 | 0.50 |
| 2:j:277:GLN:HB3 | 2:j:280:LEU:HD12 | 1.94 | 0.50 |
| 2:k:175:LEU:HD11 | 1:I:51:ILE:CG1 | 2.38 | 0.50 |
| 2:m:32:ARG:HH11 | 2:m:32:ARG:HG2 | 1.76 | 0.50 |
| 2:n:216:LEU:HD11 | 2:n:222:GLN:HB2 | 1.93 | 0.50 |
| 2:n:275:VAL:HG21 | 2:n:338:LEU:HD21 | 1.94 | 0.50 |
| 2:p:62:LEU:HD13 | 2:p:81:LEU:HD11 | 1.94 | 0.50 |
| 2:p:101:GLN:NE2 | 2:q:188:GLN:HB3 | 2.27 | 0.50 |
| 2:p:275:VAL:HG21 | 2:p:338:LEU:HD21 | 1.94 | 0.50 |
| 2:r:280:LEU:HD11 | 2:r:340:ALA:HB2 | 1.93 | 0.50 |
| 2:u:175:LEU:HD11 | 1:S:51:ILE:CG1 | 2.40 | 0.50 |
| 2:u:275:VAL:HG21 | 2:u:338:LEU:HD21 | 1.94 | 0.50 |
| 2:w:255:ILE:HD12 | 2:w:362:LEU:HD12 | 1.94 | 0.50 |
| 2:y:28:VAL:HB | 2:y:31:VAL:HG23 | 1.93 | 0.50 |
| 2:y:217:ASP:OD1 | 2:y:219:ARG:N | 2.35 | 0.50 |
| 1:C:58:ILE:HG13 | 1:C:59:ASN:N | 2.26 | 0.50 |
| 1:O:74:ILE:HD13 | 1:O:154:GLN:HA | 1.93 | 0.50 |
| 2:c:280:LEU:HD11 | 2:c:340:ALA:HB2 | 1.93 | 0.49 |
| 2:d:164:ARG:HD2 | 2:e:365:ILE:CG2 | 2.40 | 0.49 |
| 2:g:216:LEU:HD11 | 2:g:222:GLN:HB2 | 1.93 | 0.49 |
| 2:i:62:LEU:HD13 | 2:i:81:LEU:HD11 | 1.94 | 0.49 |
| 2:o:255:ILE:HD12 | 2:o:362:LEU:HD12 | 1.94 | 0.49 |
| 2:o:327:ASN:OD1 | 2:o:330:SER:HB2 | 2.11 | 0.49 |
| 2:p:255:ILE:HD12 | 2:p:362:LEU:HD12 | 1.94 | 0.49 |
| 2:r:216:LEU:HD11 | 2:r:222:GLN:HB2 | 1.93 | 0.49 |
| 2:v:32:ARG:HG2 | 2:v:32:ARG:HH11 | 1.76 | 0.49 |
| 2:v:33:GLU:HG2 | 2:v:95:PRO:HD3 | 1.93 | 0.49 |
| 2:y:254:VAL:CG2 | 2:z:355:ALA:HB2 | 2.42 | 0.49 |
| 1:D:58:ILE:HG13 | 1:D:59:ASN:N | 2.26 | 0.49 |
| 1:M:58:ILE:HG13 | 1:M:59:ASN:N | 2.26 | 0.49 |
| 1:P:74:ILE:HD13 | 1:P:154:GLN:HA | 1.93 | 0.49 |
| 1:Q:74:ILE:HD13 | 1:Q:154:GLN:HA | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:a:33:GLU:HG2 | 2:a:95:PRO:HD3 | 1.93 | 0.49 |
| 3:1:72:GLN:HG2 | 3:1:73:PRO:CD | 2.41 | 0.49 |
| 2:b:33:GLU:HG2 | 2:b:95:PRO:HD3 | 1.93 | 0.49 |
| 2:b:277:GLN:HB3 | 2:b:280:LEU:HD12 | 1.94 | 0.49 |
| 2:c:216:LEU:HD11 | 2:c:222:GLN:HB2 | 1.93 | 0.49 |
| 2:d:32:ARG:HG2 | 2:d:32:ARG:HH11 | 1.76 | 0.49 |
| 2:e:141:ILE:HD13 | 2:e:165:ILE:CD1 | 2.39 | 0.49 |
| 2:f:68:GLN:HG2 | 1:F:65:LEU:HD23 | 1.92 | 0.49 |
| 2:g:141:ILE:HD13 | 2:g:165:ILE:CD1 | 2.39 | 0.49 |
| 2:h:216:LEU:HD11 | 2:h:222:GLN:HB2 | 1.93 | 0.49 |
| 2:i:277:GLN:HB3 | 2:i:280:LEU:HD12 | 1.94 | 0.49 |
| 2:j:68:GLN:HG2 | 1:J:65:LEU:HD23 | 1.92 | 0.49 |
| 2:j:216:LEU:HD11 | 2:j:222:GLN:HB2 | 1.93 | 0.49 |
| 2:k:216:LEU:HD11 | 2:k:222:GLN:HB2 | 1.93 | 0.49 |
| 2:m:175:LEU:HD11 | 1:K:51:ILE:CG1 | 2.39 | 0.49 |
| 2:p:28:VAL:HB | 2:p:31:VAL:HG23 | 1.93 | 0.49 |
| 2:s:280:LEU:HD11 | 2:s:340:ALA:HB2 | 1.93 | 0.49 |
| 2:v:141:ILE:HD13 | 2:v:165:ILE:CD1 | 2.39 | 0.49 |
| 2:w:280:LEU:HD11 | 2:w:340:ALA:HB2 | 1.93 | 0.49 |
| 2:x:28:VAL:HB | 2:x:31:VAL:HG23 | 1.93 | 0.49 |
| 2:x:72:THR:OG1 | 1:Y:70:ARG:NH2 | 2.40 | 0.49 |
| 2:x:255:ILE:HD12 | 2:x:362:LEU:HD12 | 1.94 | 0.49 |
| 2:y:280:LEU:HD11 | 2:y:340:ALA:HB2 | 1.93 | 0.49 |
| 2:z:275:VAL:HG21 | 2:z:338:LEU:HD21 | 1.94 | 0.49 |
| 3:13:72:GLN:HG2 | 3:13:73:PRO:CD | 2.41 | 0.49 |
| 1:E:58:ILE:HG13 | 1:E:59:ASN:N | 2.26 | 0.49 |
| 1:L:58:ILE:HG13 | 1:L:59:ASN:N | 2.26 | 0.49 |
| 1:R:69:ARG:HG3 | 1:R:69:ARG:O | 2.10 | 0.49 |
| 1:X:74:ILE:HD13 | 1:X:154:GLN:HA | 1.93 | 0.49 |
| 1:A:80:ILE:HD13 | 1:A:195:VAL:CG1 | 2.42 | 0.49 |
| 2:a:275:VAL:HG21 | 2:a:338:LEU:HD21 | 1.94 | 0.49 |
| 2:b:255:ILE:HD12 | 2:b:362:LEU:HD12 | 1.94 | 0.49 |
| 2:b:284:VAL:HG21 | 2:b:316:GLY:HA2 | 1.93 | 0.49 |
| 2:d:277:GLN:HB3 | 2:d:280:LEU:HD12 | 1.94 | 0.49 |
| 2:e:166:THR:HG21 | 2:g:362:LEU:HD21 | 1.93 | 0.49 |
| 2:f:141:ILE:HD13 | 2:f:165:ILE:CD1 | 2.39 | 0.49 |
| 2:j:62:LEU:HD13 | 2:j:81:LEU:HD11 | 1.94 | 0.49 |
| 2:j:101:GLN:NE2 | 2:k:188:GLN:HB3 | 2.27 | 0.49 |
| 2:k:62:LEU:HD13 | 2:k:81:LEU:HD11 | 1.94 | 0.49 |
| 2:n:255:ILE:HD12 | 2:n:362:LEU:HD12 | 1.94 | 0.49 |
| 2:o:62:LEU:HD13 | 2:o:81:LEU:HD11 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:x:280:LEU:HD11 | 2:x:340:ALA:HB2 | 1.93 | 0.49 |
| 2:y:32:ARG:HG2 | 2:y:32:ARG:HH11 | 1.76 | 0.49 |
| 2:y:94:PRO:HB2 | 2:z:219:ARG:NH2 | 2.26 | 0.49 |
| 3:6:40:LEU:HG | 3:6:85:CYS:O | 2.13 | 0.49 |
| 3:12:40:LEU:HG | 3:12:85:CYS:O | 2.13 | 0.49 |
| 3:13:40:LEU:HG | 3:13:85:CYS:O | 2.13 | 0.49 |
| 1:F:58:ILE:HG13 | 1:F:59:ASN:N | 2.26 | 0.49 |
| 1:G:58:ILE:HG13 | 1:G:59:ASN:N | 2.26 | 0.49 |
| 1:S:74:ILE:HD13 | 1:S:154:GLN:HA | 1.93 | 0.49 |
| 1:S:80:ILE:HD13 | 1:S:195:VAL:CG1 | 2.42 | 0.49 |
| 2:d:141:ILE:HD13 | 2:d:165:ILE:CD1 | 2.39 | 0.49 |
| 2:g:101:GLN:NE2 | 2:h:219:ARG:HD3 | 2.27 | 0.49 |
| 2:i:166:THR:HG21 | 2:k:362:LEU:HD21 | 1.94 | 0.49 |
| 2:j:255:ILE:HD12 | 2:j:362:LEU:HD12 | 1.94 | 0.49 |
| 2:l:277:GLN:HB3 | 2:l:280:LEU:HD12 | 1.94 | 0.49 |
| 2:l:284:VAL:HG21 | 2:l:316:GLY:HA2 | 1.93 | 0.49 |
| 2:m:166:THR:HG21 | 2:o:362:LEU:HD21 | 1.94 | 0.49 |
| 2:m:275:VAL:HG21 | 2:m:338:LEU:HD21 | 1.94 | 0.49 |
| 2:p:32:ARG:HG2 | 2:p:32:ARG:HH11 | 1.76 | 0.49 |
| 2:t:280:LEU:HD11 | 2:t:340:ALA:HB2 | 1.93 | 0.49 |
| 2:v:280:LEU:HD11 | 2:v:340:ALA:HB2 | 1.93 | 0.49 |
| 2:w:28:VAL:HB | 2:w:31:VAL:HG23 | 1.93 | 0.49 |
| 2:w:33:GLU:HG2 | 2:w:95:PRO:HD3 | 1.93 | 0.49 |
| 3:5:40:LEU:HG | 3:5:85:CYS:O | 2.13 | 0.49 |
| 1:D:80:ILE:HD13 | 1:D:195:VAL:CG1 | 2.42 | 0.49 |
| 1:H:58:ILE:HG13 | 1:H:59:ASN:N | 2.26 | 0.49 |
| 1:K:58:ILE:HG13 | 1:K:59:ASN:N | 2.26 | 0.49 |
| 1:R:74:ILE:HD13 | 1:R:154:GLN:HA | 1.93 | 0.49 |
| 2:a:81:LEU:HD23 | 2:a:81:LEU:N | 2.28 | 0.49 |
| 2:b:275:VAL:HG21 | 2:b:338:LEU:HD21 | 1.94 | 0.49 |
| 2:b:280:LEU:HD11 | 2:b:340:ALA:HB2 | 1.93 | 0.49 |
| 2:d:136:LEU:HD12 | 2:d:172:GLU:OE2 | 2.13 | 0.49 |
| 2:e:101:GLN:NE2 | 2:f:219:ARG:HD3 | 2.27 | 0.49 |
| 2:g:327:ASN:OD1 | 2:g:330:SER:HB2 | 2.11 | 0.49 |
| 2:h:141:ILE:HD13 | 2:h:165:ILE:CD1 | 2.39 | 0.49 |
| 2:h:277:GLN:HB3 | 2:h:280:LEU:HD12 | 1.94 | 0.49 |
| 2:k:68:GLN:HG2 | 1:K:65:LEU:HD23 | 1.92 | 0.49 |
| 2:k:166:THR:HG21 | 2:m:362:LEU:HD21 | 1.95 | 0.49 |
| 2:l:62:LEU:HD13 | 2:l:81:LEU:HD11 | 1.94 | 0.49 |
| 2:l:166:THR:HG21 | 2:n:362:LEU:HD21 | 1.94 | 0.49 |
| 2:p:277:GLN:HB3 | 2:p:280:LEU:HD12 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:q:28:VAL:HB | 2:q:31:VAL:HG23 | 1.93 | 0.49 |
| 2:q:42:VAL:O | 2:q:84:VAL:HA | 2.13 | 0.49 |
| 2:q:277:GLN:HB3 | 2:q:280:LEU:HD12 | 1.94 | 0.49 |
| 2:s:32:ARG:HG2 | 2:s:32:ARG:HH11 | 1.76 | 0.49 |
| 2:t:42:VAL:O | 2:t:84:VAL:HA | 2.13 | 0.49 |
| 2:v:28:VAL:HB | 2:v:31:VAL:HG23 | 1.93 | 0.49 |
| 2:w:101:GLN:NE2 | 2:x:219:ARG:HD3 | 2.27 | 0.49 |
| 2:y:136:LEU:HD12 | 2:y:172:GLU:OE2 | 2.13 | 0.49 |
| 2:z:136:LEU:HD12 | 2:z:172:GLU:OE2 | 2.13 | 0.49 |
| 1:I:58:ILE:HG13 | 1:I:59:ASN:N | 2.26 | 0.49 |
| 1:N:80:ILE:HD13 | 1:N:195:VAL:CG1 | 2.42 | 0.49 |
| 1:U:74:ILE:HD13 | 1:U:154:GLN:HA | 1.93 | 0.49 |
| 1:W:80:ILE:HD13 | 1:W:195:VAL:CG1 | 2.42 | 0.49 |
| 2:a:277:GLN:HB3 | 2:a:280:LEU:HD12 | 1.94 | 0.49 |
| 2:c:166:THR:HG21 | 2:e:362:LEU:HD21 | 1.94 | 0.49 |
| 2:d:216:LEU:HD11 | 2:d:222:GLN:HB2 | 1.93 | 0.49 |
| 2:h:254:VAL:CG2 | 2:i:355:ALA:HB2 | 2.43 | 0.49 |
| 2:i:42:VAL:O | 2:i:84:VAL:HA | 2.13 | 0.49 |
| 2:i:216:LEU:HD11 | 2:i:222:GLN:HB2 | 1.93 | 0.49 |
| 2:l:254:VAL:CG2 | 2:m:355:ALA:HB2 | 2.42 | 0.49 |
| 2:m:62:LEU:HD13 | 2:m:81:LEU:HD11 | 1.94 | 0.49 |
| 2:m:136:LEU:HD12 | 2:m:172:GLU:OE2 | 2.13 | 0.49 |
| 2:m:255:ILE:HD12 | 2:m:362:LEU:HD12 | 1.94 | 0.49 |
| 2:p:42:VAL:O | 2:p:84:VAL:HA | 2.13 | 0.49 |
| 2:p:175:LEU:HD11 | 1:N:51:ILE:CG1 | 2.40 | 0.49 |
| 2:r:28:VAL:HB | 2:r:31:VAL:HG23 | 1.93 | 0.49 |
| 2:s:28:VAL:HB | 2:s:31:VAL:HG23 | 1.93 | 0.49 |
| 2:s:42:VAL:O | 2:s:84:VAL:HA | 2.13 | 0.49 |
| 2:t:175:LEU:HD11 | 1:R:51:ILE:CG1 | 2.41 | 0.49 |
| 2:u:28:VAL:HB | 2:u:31:VAL:HG23 | 1.93 | 0.49 |
| 2:u:280:LEU:HD11 | 2:u:340:ALA:HB2 | 1.93 | 0.49 |
| 2:u:284:VAL:HG21 | 2:u:316:GLY:HA2 | 1.93 | 0.49 |
| 2:x:136:LEU:HD12 | 2:x:172:GLU:OE2 | 2.13 | 0.49 |
| 2:y:255:ILE:HD12 | 2:y:362:LEU:HD12 | 1.94 | 0.49 |
| 2:z:280:LEU:HD11 | 2:z:340:ALA:HB2 | 1.93 | 0.49 |
| 3:11:40:LEU:HG | 3:11:85:CYS:O | 2.13 | 0.49 |
| 3:14:40:LEU:HG | 3:14:85:CYS:O | 2.13 | 0.49 |
| 3:21:40:LEU:HG | 3:21:85:CYS:O | 2.13 | 0.49 |
| 3:24:40:LEU:HG | 3:24:85:CYS:O | 2.13 | 0.49 |
| 3:25:40:LEU:HG | 3:25:85:CYS:O | 2.13 | 0.49 |
| 3:26:40:LEU:HG | 3:26:85:CYS:O | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:58:ILE:HG13 | 1:J:59:ASN:N | 2.26 | 0.49 |
| 1:R:176:GLU:OE2 | 1:T:90:LYS:HD3 | 2.13 | 0.49 |
| 1:T:74:ILE:HD13 | 1:T:154:GLN:HA | 1.93 | 0.49 |
| 2:a:255:ILE:HD12 | 2:a:362:LEU:HD12 | 1.94 | 0.49 |
| 2:a:284:VAL:HG21 | 2:a:316:GLY:HA2 | 1.93 | 0.49 |
| 2:c:141:ILE:HD13 | 2:c:165:ILE:CD1 | 2.39 | 0.49 |
| 2:c:217:ASP:OD1 | 2:c:219:ARG:N | 2.35 | 0.49 |
| 2:e:136:LEU:HD12 | 2:e:172:GLU:OE2 | 2.13 | 0.49 |
| 2:e:277:GLN:HB3 | 2:e:280:LEU:HD12 | 1.94 | 0.49 |
| 2:f:217:ASP:OD1 | 2:f:219:ARG:N | 2.35 | 0.49 |
| 2:h:136:LEU:HD12 | 2:h:172:GLU:OE2 | 2.13 | 0.49 |
| 2:i:254:VAL:CG2 | 2:j:355:ALA:HB2 | 2.43 | 0.49 |
| 2:l:136:LEU:HD12 | 2:l:172:GLU:OE2 | 2.13 | 0.49 |
| 2:m:42:VAL:O | 2:m:84:VAL:HA | 2.13 | 0.49 |
| 2:m:216:LEU:HD11 | 2:m:222:GLN:HB2 | 1.93 | 0.49 |
| 2:n:166:THR:HG21 | 2:p:362:LEU:HD21 | 1.94 | 0.49 |
| 2:r:254:VAL:CG2 | 2:s:355:ALA:HB2 | 2.43 | 0.49 |
| 2:r:284:VAL:HG21 | 2:r:316:GLY:HA2 | 1.93 | 0.49 |
| 2:t:254:VAL:CG2 | 2:u:355:ALA:HB2 | 2.43 | 0.49 |
| 2:v:101:GLN:NE2 | 2:w:188:GLN:HB3 | 2.27 | 0.49 |
| 2:v:136:LEU:HD12 | 2:v:172:GLU:OE2 | 2.13 | 0.49 |
| 2:w:136:LEU:HD12 | 2:w:172:GLU:OE2 | 2.13 | 0.49 |
| 2:x:284:VAL:HG21 | 2:x:316:GLY:HA2 | 1.93 | 0.49 |
| 3:4:40:LEU:HG | 3:4:85:CYS:O | 2.13 | 0.49 |
| 3:7:40:LEU:HG | 3:7:85:CYS:O | 2.13 | 0.49 |
| 3:14:72:GLN:HG2 | 3:14:73:PRO:CD | 2.41 | 0.49 |
| 3:18:40:LEU:HG | 3:18:85:CYS:O | 2.13 | 0.49 |
| 1:Q:176:GLU:OE2 | 1:S:90:LYS:HD3 | 2.13 | 0.49 |
| 1:W:74:ILE:HD13 | 1:W:154:GLN:HA | 1.93 | 0.49 |
| 2:a:136:LEU:HD12 | 2:a:172:GLU:OE2 | 2.13 | 0.49 |
| 2:a:280:LEU:HD11 | 2:a:340:ALA:HB2 | 1.93 | 0.49 |
| 2:a:356:GLY:O | 2:a:358:LEU:N | 2.46 | 0.49 |
| 2:b:136:LEU:HD12 | 2:b:172:GLU:OE2 | 2.13 | 0.49 |
| 2:b:254:VAL:CG2 | 2:c:355:ALA:HB2 | 2.43 | 0.49 |
| 2:b:282:VAL:HG23 | 2:b:317:GLY:O | 2.13 | 0.49 |
| 2:b:356:GLY:O | 2:b:358:LEU:N | 2.46 | 0.49 |
| 2:c:356:GLY:O | 2:c:358:LEU:N | 2.46 | 0.49 |
| 2:d:101:GLN:NE2 | 2:e:188:GLN:HB3 | 2.27 | 0.49 |
| 2:e:284:VAL:HG21 | 2:e:316:GLY:HA2 | 1.93 | 0.49 |
| 2:f:96:PHE:O | 2:g:219:ARG:HD2 | 2.13 | 0.49 |
| 2:j:42:VAL:O | 2:j:84:VAL:HA | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:k:255:ILE:HD12 | 2:k:362:LEU:HD12 | 1.94 | 0.49 |
| 2:m:277:GLN:HB3 | 2:m:280:LEU:HD12 | 1.94 | 0.49 |
| 2:n:62:LEU:HD13 | 2:n:81:LEU:HD11 | 1.94 | 0.49 |
| 2:n:136:LEU:HD12 | 2:n:172:GLU:OE2 | 2.13 | 0.49 |
| 2:o:284:VAL:HG21 | 2:o:316:GLY:HA2 | 1.93 | 0.49 |
| 2:p:284:VAL:HG21 | 2:p:316:GLY:HA2 | 1.93 | 0.49 |
| 2:r:42:VAL:O | 2:r:84:VAL:HA | 2.13 | 0.49 |
| 2:t:282:VAL:HG23 | 2:t:317:GLY:O | 2.13 | 0.49 |
| 2:t:356:GLY:O | 2:t:358:LEU:N | 2.46 | 0.49 |
| 2:u:105:VAL:HG11 | 2:u:169:ALA:HB2 | 1.95 | 0.49 |
| 2:u:356:GLY:O | 2:u:358:LEU:N | 2.46 | 0.49 |
| 2:v:356:GLY:O | 2:v:358:LEU:N | 2.46 | 0.49 |
| 2:w:79:MET:HE2 | 2:w:79:MET:HB2 | 1.69 | 0.49 |
| 2:w:141:ILE:HD13 | 2:w:165:ILE:CD1 | 2.39 | 0.49 |
| 2:w:277:GLN:HB3 | 2:w:280:LEU:HD12 | 1.94 | 0.49 |
| 2:w:356:GLY:O | 2:w:358:LEU:N | 2.46 | 0.49 |
| 2:x:356:GLY:O | 2:x:358:LEU:N | 2.46 | 0.49 |
| 2:x:361:LYS:O | 2:x:361:LYS:HG3 | 2.13 | 0.49 |
| 2:y:356:GLY:O | 2:y:358:LEU:N | 2.46 | 0.49 |
| 2:z:81:LEU:HD23 | 2:z:81:LEU:N | 2.28 | 0.49 |
| 2:z:356:GLY:O | 2:z:358:LEU:N | 2.46 | 0.49 |
| 3:9:47:ASP:CG | 3:9:50:VAL:H | 2.14 | 0.49 |
| 3:21:47:ASP:CG | 3:21:50:VAL:H | 2.14 | 0.49 |
| 3:23:40:LEU:HG | 3:23:85:CYS:O | 2.13 | 0.49 |
| 1:I:80:ILE:HD13 | 1:I:195:VAL:CG1 | 2.42 | 0.49 |
| 1:K:80:ILE:HD13 | 1:K:195:VAL:CG1 | 2.42 | 0.49 |
| 1:M:80:ILE:HD13 | 1:M:195:VAL:CG1 | 2.42 | 0.49 |
| 1:V:74:ILE:HD13 | 1:V:154:GLN:HA | 1.93 | 0.49 |
| 2:a:361:LYS:O | 2:a:361:LYS:HG3 | 2.13 | 0.49 |
| 2:b:361:LYS:O | 2:b:361:LYS:HG3 | 2.13 | 0.49 |
| 2:c:136:LEU:HD12 | 2:c:172:GLU:OE2 | 2.13 | 0.49 |
| 2:c:208:ARG:NH2 | 2:c:238:ASP:OD2 | 2.46 | 0.49 |
| 2:c:275:VAL:HG21 | 2:c:338:LEU:HD21 | 1.94 | 0.49 |
| 2:c:282:VAL:HG23 | 2:c:317:GLY:O | 2.13 | 0.49 |
| 2:d:208:ARG:NH2 | 2:d:238:ASP:OD2 | 2.46 | 0.49 |
| 2:d:356:GLY:O | 2:d:358:LEU:N | 2.46 | 0.49 |
| 2:e:105:VAL:HG11 | 2:e:169:ALA:HB2 | 1.95 | 0.49 |
| 2:e:208:ARG:NH2 | 2:e:238:ASP:OD2 | 2.46 | 0.49 |
| 2:f:42:VAL:O | 2:f:84:VAL:HA | 2.13 | 0.49 |
| 2:f:105:VAL:HG11 | 2:f:169:ALA:HB2 | 1.95 | 0.49 |
| 2:g:105:VAL:HG11 | 2:g:169:ALA:HB2 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:h:101:GLN:NE2 | 2:i:188:GLN:HB3 | 2.28 | 0.49 |
| 2:i:101:GLN:NE2 | 2:j:219:ARG:HD3 | 2.28 | 0.49 |
| 2:i:141:ILE:HD13 | 2:i:165:ILE:CD1 | 2.39 | 0.49 |
| 2:k:136:LEU:HD12 | 2:k:172:GLU:OE2 | 2.13 | 0.49 |
| 2:k:275:VAL:HG21 | 2:k:338:LEU:HD21 | 1.94 | 0.49 |
| 2:k:361:LYS:O | 2:k:361:LYS:HG3 | 2.13 | 0.49 |
| 2:l:42:VAL:O | 2:l:84:VAL:HA | 2.13 | 0.49 |
| 2:l:275:VAL:HG21 | 2:l:338:LEU:HD21 | 1.94 | 0.49 |
| 2:o:136:LEU:HD12 | 2:o:172:GLU:OE2 | 2.13 | 0.49 |
| 2:r:141:ILE:HD13 | 2:r:165:ILE:CD1 | 2.39 | 0.49 |
| 2:r:208:ARG:NH2 | 2:r:238:ASP:OD2 | 2.46 | 0.49 |
| 2:r:277:GLN:HB3 | 2:r:280:LEU:HD12 | 1.94 | 0.49 |
| 2:s:105:VAL:HG11 | 2:s:169:ALA:HB2 | 1.95 | 0.49 |
| 2:s:282:VAL:HG23 | 2:s:317:GLY:O | 2.13 | 0.49 |
| 2:s:356:GLY:O | 2:s:358:LEU:N | 2.46 | 0.49 |
| 2:t:28:VAL:HB | 2:t:31:VAL:HG23 | 1.93 | 0.49 |
| 2:t:105:VAL:HG11 | 2:t:169:ALA:HB2 | 1.95 | 0.49 |
| 2:v:282:VAL:HG23 | 2:v:317:GLY:O | 2.13 | 0.49 |
| 2:x:42:VAL:O | 2:x:84:VAL:HA | 2.13 | 0.49 |
| 2:x:208:ARG:NH2 | 2:x:238:ASP:OD2 | 2.46 | 0.49 |
| 3:2:72:GLN:HG2 | 3:2:73:PRO:CD | 2.41 | 0.49 |
| 1:G:176:GLU:OE2 | 1:I:90:LYS:HD3 | 2.13 | 0.49 |
| 1:O:80:ILE:HD13 | 1:O:195:VAL:CG1 | 2.42 | 0.49 |
| 3:1:40:LEU:HG | 3:1:85:CYS:O | 2.13 | 0.49 |
| 2:b:208:ARG:NH2 | 2:b:238:ASP:OD2 | 2.46 | 0.49 |
| 2:e:356:GLY:O | 2:e:358:LEU:N | 2.46 | 0.49 |
| 2:g:42:VAL:O | 2:g:84:VAL:HA | 2.13 | 0.49 |
| 2:h:105:VAL:HG11 | 2:h:169:ALA:HB2 | 1.95 | 0.49 |
| 2:i:356:GLY:O | 2:i:358:LEU:N | 2.46 | 0.49 |
| 2:j:275:VAL:HG21 | 2:j:338:LEU:HD21 | 1.94 | 0.49 |
| 2:j:356:GLY:O | 2:j:358:LEU:N | 2.46 | 0.49 |
| 2:k:356:GLY:O | 2:k:358:LEU:N | 2.46 | 0.49 |
| 2:l:216:LEU:HD11 | 2:l:222:GLN:HB2 | 1.93 | 0.49 |
| 2:l:255:ILE:HD12 | 2:l:362:LEU:HD12 | 1.94 | 0.49 |
| 2:l:356:GLY:O | 2:l:358:LEU:N | 2.46 | 0.49 |
| 2:l:361:LYS:O | 2:l:361:LYS:HG3 | 2.13 | 0.49 |
| 2:m:208:ARG:NH2 | 2:m:238:ASP:OD2 | 2.46 | 0.49 |
| 2:n:254:VAL:CG2 | 2:o:355:ALA:HB2 | 2.43 | 0.49 |
| 2:o:42:VAL:CG1 | 2:o:119:GLY:HA3 | 2.43 | 0.49 |
| 2:o:42:VAL:O | 2:o:84:VAL:HA | 2.13 | 0.49 |
| 2:o:277:GLN:HB3 | 2:o:280:LEU:HD12 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:p:136:LEU:HD12 | 2:p:172:GLU:OE2 | 2.13 | 0.49 |
| 2:p:282:VAL:HG23 | 2:p:317:GLY:O | 2.13 | 0.49 |
| 2:q:282:VAL:HG23 | 2:q:317:GLY:O | 2.13 | 0.49 |
| 2:r:282:VAL:HG23 | 2:r:317:GLY:O | 2.13 | 0.49 |
| 2:r:356:GLY:O | 2:r:358:LEU:N | 2.46 | 0.49 |
| 2:v:105:VAL:HG11 | 2:v:169:ALA:HB2 | 1.95 | 0.49 |
| 2:v:277:GLN:HB3 | 2:v:280:LEU:HD12 | 1.94 | 0.49 |
| 2:w:42:VAL:O | 2:w:84:VAL:HA | 2.13 | 0.49 |
| 2:w:105:VAL:HG11 | 2:w:169:ALA:HB2 | 1.95 | 0.49 |
| 2:w:282:VAL:HG23 | 2:w:317:GLY:O | 2.13 | 0.49 |
| 2:x:217:ASP:OD1 | 2:x:219:ARG:N | 2.35 | 0.49 |
| 2:z:255:ILE:HD12 | 2:z:362:LEU:HD12 | 1.94 | 0.49 |
| 3:10:40:LEU:HG | 3:10:85:CYS:O | 2.13 | 0.49 |
| 3:14:47:ASP:CG | 3:14:50:VAL:H | 2.14 | 0.49 |
| 3:15:40:LEU:HG | 3:15:85:CYS:O | 2.13 | 0.49 |
| 3:17:40:LEU:HG | 3:17:85:CYS:O | 2.13 | 0.49 |
| 3:20:28:ILE:O | 3:20:29:SER:OG | 2.21 | 0.49 |
| 1:F:80:ILE:HD13 | 1:F:195:VAL:CG1 | 2.42 | 0.49 |
| 1:G:80:ILE:HD13 | 1:G:195:VAL:CG1 | 2.42 | 0.49 |
| 1:L:124:MET:HE3 | 1:L:124:MET:HB3 | 1.77 | 0.49 |
| 1:M:176:GLU:OE2 | 1:O:90:LYS:HD3 | 2.13 | 0.49 |
| 1:S:176:GLU:OE2 | 1:U:90:LYS:HD3 | 2.13 | 0.49 |
| 1:A:210:ASN:ND2 | 3:26:83:SER:HA | 2.28 | 0.48 |
| 2:a:123:MET:HE1 | 2:a:136:LEU:HB3 | 1.95 | 0.48 |
| 2:a:282:VAL:HG23 | 2:a:317:GLY:O | 2.13 | 0.48 |
| 2:b:141:ILE:HD13 | 2:b:165:ILE:CD1 | 2.39 | 0.48 |
| 2:d:105:VAL:HG11 | 2:d:169:ALA:HB2 | 1.95 | 0.48 |
| 2:e:42:VAL:O | 2:e:84:VAL:HA | 2.13 | 0.48 |
| 2:e:101:GLN:NE2 | 2:f:188:GLN:HB3 | 2.28 | 0.48 |
| 2:f:208:ARG:NH2 | 2:f:238:ASP:OD2 | 2.46 | 0.48 |
| 2:g:277:GLN:HB3 | 2:g:280:LEU:HD12 | 1.94 | 0.48 |
| 2:h:42:VAL:O | 2:h:84:VAL:HA | 2.13 | 0.48 |
| 2:h:275:VAL:HG21 | 2:h:338:LEU:HD21 | 1.94 | 0.48 |
| 2:h:282:VAL:HG23 | 2:h:317:GLY:O | 2.13 | 0.48 |
| 2:i:136:LEU:HD12 | 2:i:172:GLU:OE2 | 2.13 | 0.48 |
| 2:j:94:PRO:HB2 | 2:k:219:ARG:NH2 | 2.28 | 0.48 |
| 2:j:361:LYS:HG3 | 2:j:361:LYS:O | 2.13 | 0.48 |
| 2:k:101:GLN:NE2 | 2:l:188:GLN:HB3 | 2.28 | 0.48 |
| 2:k:101:GLN:NE2 | 2:l:219:ARG:HD3 | 2.27 | 0.48 |
| 2:l:208:ARG:NH2 | 2:l:238:ASP:OD2 | 2.46 | 0.48 |
| 2:m:42:VAL:CG1 | 2:m:119:GLY:HA3 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:m:356:GLY:O | 2:m:358:LEU:N | 2.46 | 0.48 |
| 2:o:175:LEU:HD11 | 1:M:51:ILE:CG1 | 2.40 | 0.48 |
| 2:o:282:VAL:HG23 | 2:o:317:GLY:O | 2.13 | 0.48 |
| 2:q:101:GLN:NE2 | 2:r:188:GLN:HB3 | 2.28 | 0.48 |
| 2:q:208:ARG:NH2 | 2:q:238:ASP:OD2 | 2.46 | 0.48 |
| 2:q:356:GLY:O | 2:q:358:LEU:N | 2.46 | 0.48 |
| 2:r:105:VAL:HG11 | 2:r:169:ALA:HB2 | 1.95 | 0.48 |
| 2:s:42:VAL:CG1 | 2:s:119:GLY:HA3 | 2.43 | 0.48 |
| 2:s:284:VAL:HG21 | 2:s:316:GLY:HA2 | 1.93 | 0.48 |
| 2:t:42:VAL:CG1 | 2:t:119:GLY:HA3 | 2.43 | 0.48 |
| 2:t:284:VAL:HG21 | 2:t:316:GLY:HA2 | 1.93 | 0.48 |
| 2:u:166:THR:HG21 | 2:w:362:LEU:HD21 | 1.94 | 0.48 |
| 2:u:282:VAL:HG23 | 2:u:317:GLY:O | 2.13 | 0.48 |
| 2:v:42:VAL:CG1 | 2:v:119:GLY:HA3 | 2.43 | 0.48 |
| 2:v:284:VAL:HG21 | 2:v:316:GLY:HA2 | 1.93 | 0.48 |
| 2:w:208:ARG:NH2 | 2:w:238:ASP:OD2 | 2.46 | 0.48 |
| 2:y:208:ARG:NH2 | 2:y:238:ASP:OD2 | 2.46 | 0.48 |
| 2:z:123:MET:HE1 | 2:z:136:LEU:HB3 | 1.95 | 0.48 |
| 3:10:28:ILE:O | 3:10:29:SER:OG | 2.21 | 0.48 |
| 3:15:72:GLN:HG2 | 3:15:73:PRO:CD | 2.41 | 0.48 |
| 3:22:40:LEU:HG | 3:22:85:CYS:O | 2.13 | 0.48 |
| 1:D:124:MET:HE3 | 1:D:124:MET:HB3 | 1.77 | 0.48 |
| 1:P:167:LYS:NZ | 1:Q:84:GLU:OE2 | 2.41 | 0.48 |
| 2:a:42:VAL:CG1 | 2:a:119:GLY:HA3 | 2.43 | 0.48 |
| 2:a:208:ARG:NH2 | 2:a:238:ASP:OD2 | 2.46 | 0.48 |
| 2:e:275:VAL:HG21 | 2:e:338:LEU:HD21 | 1.94 | 0.48 |
| 2:f:175:LEU:HD11 | 1:D:51:ILE:CG1 | 2.38 | 0.48 |
| 2:f:280:LEU:CD1 | 2:f:340:ALA:HB2 | 2.43 | 0.48 |
| 2:f:356:GLY:O | 2:f:358:LEU:N | 2.46 | 0.48 |
| 2:g:208:ARG:NH2 | 2:g:238:ASP:OD2 | 2.46 | 0.48 |
| 2:g:275:VAL:HG21 | 2:g:338:LEU:HD21 | 1.94 | 0.48 |
| 2:g:282:VAL:HG23 | 2:g:317:GLY:O | 2.13 | 0.48 |
| 2:i:105:VAL:HG11 | 2:i:169:ALA:HB2 | 1.95 | 0.48 |
| 2:j:136:LEU:HD12 | 2:j:172:GLU:OE2 | 2.13 | 0.48 |
| 2:m:280:LEU:CD1 | 2:m:340:ALA:HB2 | 2.43 | 0.48 |
| 2:m:282:VAL:HG23 | 2:m:317:GLY:O | 2.13 | 0.48 |
| 2:n:101:GLN:NE2 | 2:o:188:GLN:HB3 | 2.28 | 0.48 |
| 2:n:282:VAL:HG23 | 2:n:317:GLY:O | 2.13 | 0.48 |
| 2:o:81:LEU:HD23 | 2:o:81:LEU:N | 2.28 | 0.48 |
| 2:p:81:LEU:HD23 | 2:p:81:LEU:N | 2.28 | 0.48 |
| 2:p:361:LYS:O | 2:p:361:LYS:HG3 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:q:42:VAL:CG1 | 2:q:119:GLY:HA3 | 2.43 | 0.48 |
| 2:q:101:GLN:NE2 | 2:r:219:ARG:HD3 | 2.27 | 0.48 |
| 2:q:361:LYS:O | 2:q:361:LYS:HG3 | 2.13 | 0.48 |
| 2:s:208:ARG:NH2 | 2:s:238:ASP:OD2 | 2.46 | 0.48 |
| 2:t:280:LEU:CD1 | 2:t:340:ALA:HB2 | 2.43 | 0.48 |
| 2:u:42:VAL:O | 2:u:84:VAL:HA | 2.13 | 0.48 |
| 2:u:136:LEU:HD12 | 2:u:172:GLU:OE2 | 2.13 | 0.48 |
| 2:x:42:VAL:CG1 | 2:x:119:GLY:HA3 | 2.43 | 0.48 |
| 2:x:277:GLN:HB3 | 2:x:280:LEU:HD12 | 1.94 | 0.48 |
| 2:y:81:LEU:HD23 | 2:y:81:LEU:N | 2.28 | 0.48 |
| 2:y:361:LYS:O | 2:y:361:LYS:HG3 | 2.12 | 0.48 |
| 3:6:75:GLY:HA2 | 3:6:89:ARG:O | 2.14 | 0.48 |
| 3:20:40:LEU:HG | 3:20:85:CYS:O | 2.13 | 0.48 |
| 3:26:47:ASP:CG | 3:26:50:VAL:H | 2.14 | 0.48 |
| 1:C:80:ILE:HD13 | 1:C:195:VAL:CG1 | 2.42 | 0.48 |
| 1:E:80:ILE:HD13 | 1:E:195:VAL:CG1 | 2.42 | 0.48 |
| 1:V:124:MET:HE3 | 1:V:124:MET:HB3 | 1.77 | 0.48 |
| 2:a:42:VAL:O | 2:a:84:VAL:HA | 2.13 | 0.48 |
| 2:a:280:LEU:CD1 | 2:a:340:ALA:HB2 | 2.43 | 0.48 |
| 2:b:42:VAL:O | 2:b:84:VAL:HA | 2.13 | 0.48 |
| 2:b:166:THR:HG21 | 2:d:362:LEU:HD21 | 1.94 | 0.48 |
| 2:b:280:LEU:CD1 | 2:b:340:ALA:HB2 | 2.43 | 0.48 |
| 2:c:105:VAL:HG11 | 2:c:169:ALA:HB2 | 1.95 | 0.48 |
| 2:f:123:MET:HE1 | 2:f:136:LEU:HB3 | 1.95 | 0.48 |
| 2:g:136:LEU:HD12 | 2:g:172:GLU:OE2 | 2.13 | 0.48 |
| 2:h:101:GLN:NE2 | 2:i:219:ARG:HD3 | 2.28 | 0.48 |
| 2:h:280:LEU:CD1 | 2:h:340:ALA:HB2 | 2.43 | 0.48 |
| 2:i:275:VAL:HG21 | 2:i:338:LEU:HD21 | 1.94 | 0.48 |
| 2:i:284:VAL:HG21 | 2:i:316:GLY:HA2 | 1.93 | 0.48 |
| 2:j:282:VAL:HG23 | 2:j:317:GLY:O | 2.13 | 0.48 |
| 2:k:280:LEU:CD1 | 2:k:340:ALA:HB2 | 2.44 | 0.48 |
| 2:k:282:VAL:HG23 | 2:k:317:GLY:O | 2.13 | 0.48 |
| 2:l:282:VAL:HG23 | 2:l:317:GLY:O | 2.13 | 0.48 |
| 2:n:356:GLY:O | 2:n:358:LEU:N | 2.46 | 0.48 |
| 2:p:42:VAL:CG1 | 2:p:119:GLY:HA3 | 2.43 | 0.48 |
| 2:p:94:PRO:HB2 | 2:q:219:ARG:NH2 | 2.28 | 0.48 |
| 2:q:81:LEU:HD23 | 2:q:81:LEU:N | 2.28 | 0.48 |
| 2:q:136:LEU:HD12 | 2:q:172:GLU:OE2 | 2.13 | 0.48 |
| 2:r:280:LEU:CD1 | 2:r:340:ALA:HB2 | 2.43 | 0.48 |
| 2:s:136:LEU:HD12 | 2:s:172:GLU:OE2 | 2.13 | 0.48 |
| 2:s:280:LEU:CD1 | 2:s:340:ALA:HB2 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:x:105:VAL:HG11 | 2:x:169:ALA:HB2 | 1.95 | 0.48 |
| 3:8:40:LEU:HG | 3:8:85:CYS:O | 2.13 | 0.48 |
| 1:H:80:ILE:HD13 | 1:H:195:VAL:CG1 | 2.42 | 0.48 |
| 1:L:80:ILE:HD13 | 1:L:195:VAL:CG1 | 2.42 | 0.48 |
| 1:P:176:GLU:OE2 | 1:R:90:LYS:HD3 | 2.13 | 0.48 |
| 1:A:176:GLU:OE2 | 1:C:90:LYS:HD3 | 2.14 | 0.48 |
| 2:c:42:VAL:CG1 | 2:c:119:GLY:HA3 | 2.43 | 0.48 |
| 2:d:275:VAL:HG21 | 2:d:338:LEU:HD21 | 1.94 | 0.48 |
| 2:e:123:MET:HE1 | 2:e:136:LEU:HB3 | 1.95 | 0.48 |
| 2:f:275:VAL:HG21 | 2:f:338:LEU:HD21 | 1.94 | 0.48 |
| 2:f:277:GLN:HB3 | 2:f:280:LEU:HD12 | 1.94 | 0.48 |
| 2:g:81:LEU:HD23 | 2:g:81:LEU:N | 2.28 | 0.48 |
| 2:h:81:LEU:HD23 | 2:h:81:LEU:N | 2.28 | 0.48 |
| 2:h:208:ARG:NH2 | 2:h:238:ASP:OD2 | 2.46 | 0.48 |
| 2:h:356:GLY:O | 2:h:358:LEU:N | 2.46 | 0.48 |
| 2:j:105:VAL:HG11 | 2:j:169:ALA:HB2 | 1.95 | 0.48 |
| 2:k:42:VAL:CG1 | 2:k:119:GLY:HA3 | 2.43 | 0.48 |
| 2:n:42:VAL:O | 2:n:84:VAL:HA | 2.13 | 0.48 |
| 2:o:348:ILE:O | 2:o:352:MET:HG3 | 2.14 | 0.48 |
| 2:p:348:ILE:O | 2:p:352:MET:HG3 | 2.14 | 0.48 |
| 2:p:356:GLY:O | 2:p:358:LEU:N | 2.46 | 0.48 |
| 2:q:348:ILE:O | 2:q:352:MET:HG3 | 2.14 | 0.48 |
| 2:r:81:LEU:HD23 | 2:r:81:LEU:N | 2.28 | 0.48 |
| 2:r:101:GLN:NE2 | 2:s:188:GLN:HB3 | 2.28 | 0.48 |
| 2:r:348:ILE:O | 2:r:352:MET:HG3 | 2.14 | 0.48 |
| 2:t:166:THR:HG21 | 2:v:362:LEU:HD21 | 1.94 | 0.48 |
| 2:u:101:GLN:NE2 | 2:v:219:ARG:HD3 | 2.28 | 0.48 |
| 2:u:280:LEU:CD1 | 2:u:340:ALA:HB2 | 2.43 | 0.48 |
| 2:w:284:VAL:HG21 | 2:w:316:GLY:HA2 | 1.93 | 0.48 |
| 2:x:141:ILE:HD13 | 2:x:165:ILE:CD1 | 2.39 | 0.48 |
| 2:x:282:VAL:HG23 | 2:x:317:GLY:O | 2.13 | 0.48 |
| 2:y:42:VAL:CG1 | 2:y:119:GLY:HA3 | 2.43 | 0.48 |
| 2:z:208:ARG:NH2 | 2:z:238:ASP:OD2 | 2.46 | 0.48 |
| 3:2:75:GLY:HA2 | 3:2:89:ARG:O | 2.14 | 0.48 |
| 3:3:40:LEU:HG | 3:3:85:CYS:O | 2.13 | 0.48 |
| 1:Q:124:MET:HE3 | 1:Q:124:MET:HB3 | 1.77 | 0.48 |
| 3:1:75:GLY:HA2 | 3:1:89:ARG:O | 2.14 | 0.48 |
| 2:c:254:VAL:CG2 | 2:d:355:ALA:HB2 | 2.43 | 0.48 |
| 2:c:280:LEU:CD1 | 2:c:340:ALA:HB2 | 2.43 | 0.48 |
| 2:e:361:LYS:HG3 | 2:e:361:LYS:O | 2.13 | 0.48 |
| 2:f:282:VAL:HG23 | 2:f:317:GLY:O | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:g:356:GLY:O | 2:g:358:LEU:N | 2.46 | 0.48 |
| 2:i:280:LEU:CD1 | 2:i:340:ALA:HB2 | 2.43 | 0.48 |
| 2:j:141:ILE:HD13 | 2:j:165:ILE:CD1 | 2.39 | 0.48 |
| 2:k:105:VAL:HG11 | 2:k:169:ALA:HB2 | 1.95 | 0.48 |
| 2:k:208:ARG:NH2 | 2:k:238:ASP:OD2 | 2.46 | 0.48 |
| 2:m:284:VAL:HG21 | 2:m:316:GLY:HA2 | 1.93 | 0.48 |
| 2:n:81:LEU:HD23 | 2:n:81:LEU:N | 2.28 | 0.48 |
| 2:n:348:ILE:O | 2:n:352:MET:HG3 | 2.14 | 0.48 |
| 2:o:256:ASN:O | 2:o:257:SER:OG | 2.29 | 0.48 |
| 2:o:280:LEU:CD1 | 2:o:340:ALA:HB2 | 2.43 | 0.48 |
| 2:o:361:LYS:HG3 | 2:o:361:LYS:O | 2.13 | 0.48 |
| 2:p:208:ARG:NH2 | 2:p:238:ASP:OD2 | 2.46 | 0.48 |
| 2:s:277:GLN:HB3 | 2:s:280:LEU:HD12 | 1.94 | 0.48 |
| 2:s:348:ILE:O | 2:s:352:MET:HG3 | 2.14 | 0.48 |
| 2:w:361:LYS:HG3 | 2:w:361:LYS:O | 2.13 | 0.48 |
| 2:y:123:MET:HE1 | 2:y:136:LEU:HB3 | 1.95 | 0.48 |
| 2:z:42:VAL:CG1 | 2:z:119:GLY:HA3 | 2.43 | 0.48 |
| 2:z:280:LEU:CD1 | 2:z:340:ALA:HB2 | 2.43 | 0.48 |
| 3:7:75:GLY:HA2 | 3:7:89:ARG:O | 2.14 | 0.48 |
| 3:9:40:LEU:HG | 3:9:85:CYS:O | 2.13 | 0.48 |
| 1:N:176:GLU:OE1 | 1:N:207:TYR:OH | 2.21 | 0.48 |
| 1:V:176:GLU:OE2 | 1:X:90:LYS:HD3 | 2.13 | 0.48 |
| 1:X:176:GLU:OE2 | 1:Z:90:LYS:HD3 | 2.12 | 0.48 |
| 2:a:96:PHE:O | 2:b:219:ARG:HD2 | 2.14 | 0.48 |
| 2:a:141:ILE:HD13 | 2:a:165:ILE:CD1 | 2.39 | 0.48 |
| 2:a:254:VAL:HG13 | 2:a:365:ILE:CG1 | 2.44 | 0.48 |
| 2:d:280:LEU:CD1 | 2:d:340:ALA:HB2 | 2.43 | 0.48 |
| 2:d:282:VAL:HG23 | 2:d:317:GLY:O | 2.13 | 0.48 |
| 2:f:94:PRO:HB2 | 2:g:219:ARG:NH2 | 2.29 | 0.48 |
| 2:f:136:LEU:HD12 | 2:f:172:GLU:OE2 | 2.13 | 0.48 |
| 2:g:175:LEU:HD11 | 1:E:51:ILE:CG1 | 2.39 | 0.48 |
| 2:h:254:VAL:HG13 | 2:h:365:ILE:CG1 | 2.44 | 0.48 |
| 2:i:42:VAL:CG1 | 2:i:119:GLY:HA3 | 2.43 | 0.48 |
| 2:i:93:TYR:OH | 2:i:173:ARG:O | 2.24 | 0.48 |
| 2:i:282:VAL:HG23 | 2:i:317:GLY:O | 2.13 | 0.48 |
| 2:j:175:LEU:HD11 | 1:H:51:ILE:CG1 | 2.40 | 0.48 |
| 2:j:280:LEU:CD1 | 2:j:340:ALA:HB2 | 2.43 | 0.48 |
| 2:k:42:VAL:O | 2:k:84:VAL:HA | 2.13 | 0.48 |
| 2:m:81:LEU:HD23 | 2:m:81:LEU:N | 2.28 | 0.48 |
| 2:m:361:LYS:O | 2:m:361:LYS:HG3 | 2.13 | 0.48 |
| 2:n:42:VAL:CG1 | 2:n:119:GLY:HA3 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:208:ARG:NH2 | 2:n:238:ASP:OD2 | 2.46 | 0.48 |
| 2:o:356:GLY:O | 2:o:358:LEU:N | 2.46 | 0.48 |
| 2:q:254:VAL:HG13 | 2:q:365:ILE:CG1 | 2.44 | 0.48 |
| 2:q:254:VAL:CG2 | 2:r:355:ALA:HB2 | 2.44 | 0.48 |
| 2:q:280:LEU:CD1 | 2:q:340:ALA:HB2 | 2.43 | 0.48 |
| 2:r:42:VAL:CG1 | 2:r:119:GLY:HA3 | 2.43 | 0.48 |
| 2:r:361:LYS:HG3 | 2:r:361:LYS:O | 2.13 | 0.48 |
| 2:t:81:LEU:HD23 | 2:t:81:LEU:N | 2.28 | 0.48 |
| 2:t:136:LEU:HD12 | 2:t:172:GLU:OE2 | 2.13 | 0.48 |
| 2:t:208:ARG:NH2 | 2:t:238:ASP:OD2 | 2.46 | 0.48 |
| 2:u:277:GLN:HB3 | 2:u:280:LEU:HD12 | 1.94 | 0.48 |
| 2:u:361:LYS:HG3 | 2:u:361:LYS:O | 2.13 | 0.48 |
| 2:y:105:VAL:HG11 | 2:y:169:ALA:HB2 | 1.95 | 0.48 |
| 2:y:282:VAL:HG23 | 2:y:317:GLY:O | 2.13 | 0.48 |
| 2:z:277:GLN:HB3 | 2:z:280:LEU:HD12 | 1.94 | 0.48 |
| 3:2:40:LEU:HG | 3:2:85:CYS:O | 2.13 | 0.48 |
| 3:16:40:LEU:HG | 3:16:85:CYS:O | 2.13 | 0.48 |
| 3:16:72:GLN:HG2 | 3:16:73:PRO:CD | 2.41 | 0.48 |
| 3:19:40:LEU:HG | 3:19:85:CYS:O | 2.13 | 0.48 |
| 2:c:93:TYR:OH | 2:c:173:ARG:O | 2.24 | 0.48 |
| 2:c:254:VAL:HG13 | 2:c:365:ILE:CG1 | 2.44 | 0.48 |
| 2:e:42:VAL:CG1 | 2:e:119:GLY:HA3 | 2.43 | 0.48 |
| 2:f:81:LEU:HD23 | 2:f:81:LEU:N | 2.28 | 0.48 |
| 2:g:42:VAL:CG1 | 2:g:119:GLY:HA3 | 2.43 | 0.48 |
| 2:i:81:LEU:HD23 | 2:i:81:LEU:N | 2.28 | 0.48 |
| 2:i:208:ARG:NH2 | 2:i:238:ASP:OD2 | 2.46 | 0.48 |
| 2:i:361:LYS:O | 2:i:361:LYS:HG3 | 2.13 | 0.48 |
| 2:m:348:ILE:O | 2:m:352:MET:HG3 | 2.14 | 0.48 |
| 2:n:277:GLN:HB3 | 2:n:280:LEU:HD12 | 1.94 | 0.48 |
| 2:q:98:ARG:HA | 2:q:174:GLU:OE1 | 2.14 | 0.48 |
| 2:q:105:VAL:HG11 | 2:q:169:ALA:HB2 | 1.95 | 0.48 |
| 2:q:284:VAL:HG21 | 2:q:316:GLY:HA2 | 1.93 | 0.48 |
| 2:r:136:LEU:HD12 | 2:r:172:GLU:OE2 | 2.13 | 0.48 |
| 2:s:81:LEU:HD23 | 2:s:81:LEU:N | 2.28 | 0.48 |
| 2:t:93:TYR:OH | 2:t:173:ARG:O | 2.24 | 0.48 |
| 2:t:254:VAL:HG13 | 2:t:365:ILE:CG1 | 2.44 | 0.48 |
| 2:t:348:ILE:O | 2:t:352:MET:HG3 | 2.14 | 0.48 |
| 2:v:208:ARG:NH2 | 2:v:238:ASP:OD2 | 2.46 | 0.48 |
| 2:w:101:GLN:NE2 | 2:x:188:GLN:HB3 | 2.28 | 0.48 |
| 2:w:280:LEU:CD1 | 2:w:340:ALA:HB2 | 2.43 | 0.48 |
| 2:y:277:GLN:HB3 | 2:y:280:LEU:HD12 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:y:280:LEU:CD1 | 2:y:340:ALA:HB2 | 2.43 | 0.48 |
| 2:z:282:VAL:HG23 | 2:z:317:GLY:O | 2.13 | 0.48 |
| 3:3:28:ILE:O | 3:3:29:SER:OG | 2.21 | 0.48 |
| 3:3:72:GLN:HG2 | 3:3:73:PRO:CD | 2.41 | 0.48 |
| 3:19:75:GLY:HA2 | 3:19:89:ARG:O | 2.14 | 0.48 |
| 1:L:176:GLU:OE2 | 1:N:90:LYS:HD3 | 2.14 | 0.48 |
| 1:Z:101:LYS:HZ2 | 1:Z:101:LYS:HB3 | 1.79 | 0.48 |
| 2:b:123:MET:HE1 | 2:b:136:LEU:HB3 | 1.96 | 0.48 |
| 2:c:96:PHE:O | 2:d:219:ARG:HD2 | 2.14 | 0.48 |
| 2:c:98:ARG:HA | 2:c:174:GLU:OE1 | 2.14 | 0.48 |
| 2:c:101:GLN:NE2 | 2:d:219:ARG:HD3 | 2.28 | 0.48 |
| 2:c:361:LYS:HG3 | 2:c:361:LYS:O | 2.13 | 0.48 |
| 2:d:42:VAL:O | 2:d:84:VAL:HA | 2.13 | 0.48 |
| 2:d:123:MET:HE1 | 2:d:136:LEU:HB3 | 1.95 | 0.48 |
| 2:f:196:MET:HE3 | 2:f:196:MET:C | 2.39 | 0.48 |
| 2:g:123:MET:HE1 | 2:g:136:LEU:HB3 | 1.95 | 0.48 |
| 2:i:96:PHE:O | 2:j:219:ARG:HD2 | 2.14 | 0.48 |
| 2:i:98:ARG:HA | 2:i:174:GLU:OE1 | 2.14 | 0.48 |
| 2:j:254:VAL:HG13 | 2:j:365:ILE:CG1 | 2.44 | 0.48 |
| 2:k:254:VAL:HG13 | 2:k:365:ILE:CG1 | 2.44 | 0.48 |
| 2:l:42:VAL:CG1 | 2:l:119:GLY:HA3 | 2.43 | 0.48 |
| 2:l:98:ARG:HA | 2:l:174:GLU:OE1 | 2.14 | 0.48 |
| 2:l:105:VAL:HG11 | 2:l:169:ALA:HB2 | 1.95 | 0.48 |
| 2:n:175:LEU:HD11 | 1:L:51:ILE:CG1 | 2.40 | 0.48 |
| 2:n:284:VAL:HG21 | 2:n:316:GLY:HA2 | 1.94 | 0.48 |
| 2:o:93:TYR:OH | 2:o:173:ARG:O | 2.24 | 0.48 |
| 2:o:96:PHE:O | 2:p:219:ARG:HD2 | 2.14 | 0.48 |
| 2:s:93:TYR:OH | 2:s:173:ARG:O | 2.24 | 0.48 |
| 2:s:101:GLN:NE2 | 2:t:219:ARG:HD3 | 2.27 | 0.48 |
| 2:s:103:ILE:HG13 | 2:s:169:ALA:HB3 | 1.96 | 0.48 |
| 2:u:42:VAL:CG1 | 2:u:119:GLY:HA3 | 2.43 | 0.48 |
| 2:u:98:ARG:HA | 2:u:174:GLU:OE1 | 2.14 | 0.48 |
| 2:u:103:ILE:HG13 | 2:u:169:ALA:HB3 | 1.96 | 0.48 |
| 2:u:123:MET:HE1 | 2:u:136:LEU:HB3 | 1.95 | 0.48 |
| 2:u:254:VAL:HG13 | 2:u:365:ILE:CG1 | 2.44 | 0.48 |
| 2:u:254:VAL:CG2 | 2:v:355:ALA:HB2 | 2.43 | 0.48 |
| 2:u:348:ILE:O | 2:u:352:MET:HG3 | 2.14 | 0.48 |
| 2:v:42:VAL:O | 2:v:84:VAL:HA | 2.13 | 0.48 |
| 2:v:123:MET:HE1 | 2:v:136:LEU:HB3 | 1.95 | 0.48 |
| 2:v:280:LEU:CD1 | 2:v:340:ALA:HB2 | 2.43 | 0.48 |
| 2:x:81:LEU:HD23 | 2:x:81:LEU:N | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:x:94:PRO:HB2 | 2:y:219:ARG:NH2 | 2.28 | 0.48 |
| 2:x:96:PHE:O | 2:y:219:ARG:HD2 | 2.14 | 0.48 |
| 2:y:42:VAL:O | 2:y:84:VAL:HA | 2.13 | 0.48 |
| 2:y:98:ARG:HA | 2:y:174:GLU:OE1 | 2.14 | 0.48 |
| 3:20:75:GLY:HA2 | 3:20:89:ARG:O | 2.14 | 0.48 |
| 1:D:176:GLU:OE2 | 1:F:90:LYS:HD3 | 2.13 | 0.48 |
| 1:J:80:ILE:HD13 | 1:J:195:VAL:CG1 | 2.42 | 0.48 |
| 2:b:42:VAL:CG1 | 2:b:119:GLY:HA3 | 2.44 | 0.48 |
| 2:b:105:VAL:HG11 | 2:b:169:ALA:HB2 | 1.95 | 0.48 |
| 2:d:361:LYS:HG3 | 2:d:361:LYS:O | 2.12 | 0.48 |
| 2:e:254:VAL:CG2 | 2:f:355:ALA:HB2 | 2.44 | 0.48 |
| 2:f:101:GLN:NE2 | 2:g:188:GLN:HB3 | 2.29 | 0.48 |
| 2:f:254:VAL:HG13 | 2:f:365:ILE:CG1 | 2.44 | 0.48 |
| 2:h:42:VAL:CG1 | 2:h:119:GLY:HA3 | 2.43 | 0.48 |
| 2:j:42:VAL:CG1 | 2:j:119:GLY:HA3 | 2.43 | 0.48 |
| 2:l:348:ILE:O | 2:l:352:MET:HG3 | 2.14 | 0.48 |
| 2:m:96:PHE:O | 2:n:219:ARG:HD2 | 2.14 | 0.48 |
| 2:n:98:ARG:HA | 2:n:174:GLU:OE1 | 2.14 | 0.48 |
| 2:n:103:ILE:HG13 | 2:n:169:ALA:HB3 | 1.96 | 0.48 |
| 2:o:101:GLN:NE2 | 2:p:219:ARG:HD3 | 2.28 | 0.48 |
| 2:o:254:VAL:CG2 | 2:p:355:ALA:HB2 | 2.43 | 0.48 |
| 2:p:103:ILE:HG13 | 2:p:169:ALA:HB3 | 1.96 | 0.48 |
| 2:p:254:VAL:HG13 | 2:p:365:ILE:CG1 | 2.44 | 0.48 |
| 2:q:103:ILE:HG13 | 2:q:169:ALA:HB3 | 1.96 | 0.48 |
| 2:r:103:ILE:HG13 | 2:r:169:ALA:HB3 | 1.96 | 0.48 |
| 2:s:141:ILE:HD13 | 2:s:165:ILE:CD1 | 2.39 | 0.48 |
| 2:s:196:MET:HE3 | 2:s:196:MET:C | 2.39 | 0.48 |
| 2:t:103:ILE:HG13 | 2:t:169:ALA:HB3 | 1.96 | 0.48 |
| 2:t:361:LYS:O | 2:t:361:LYS:HG3 | 2.13 | 0.48 |
| 2:v:103:ILE:HG13 | 2:v:169:ALA:HB3 | 1.96 | 0.48 |
| 2:w:42:VAL:CG1 | 2:w:119:GLY:HA3 | 2.43 | 0.48 |
| 2:x:79:MET:HE2 | 2:x:79:MET:HB2 | 1.69 | 0.48 |
| 2:x:254:VAL:HG13 | 2:x:365:ILE:CG1 | 2.44 | 0.48 |
| 3:3:75:GLY:HA2 | 3:3:89:ARG:O | 2.14 | 0.48 |
| 3:5:75:GLY:HA2 | 3:5:89:ARG:O | 2.14 | 0.48 |
| 3:18:28:ILE:O | 3:18:29:SER:OG | 2.21 | 0.48 |
| 3:20:47:ASP:CG | 3:20:50:VAL:H | 2.14 | 0.48 |
| 3:21:75:GLY:HA2 | 3:21:89:ARG:O | 2.14 | 0.48 |
| 1:E:130:ASN:CG | 1:F:102:THR:HG22 | 2.39 | 0.48 |
| 1:J:109:VAL:HG21 | 1:J:117:PHE:O | 2.14 | 0.48 |
| 1:K:109:VAL:HG21 | 1:K:117:PHE:O | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:109:VAL:HG21 | 1:N:117:PHE:O | 2.14 | 0.48 |
| 1:O:109:VAL:HG21 | 1:O:117:PHE:O | 2.14 | 0.48 |
| 2:c:42:VAL:O | 2:c:84:VAL:HA | 2.13 | 0.48 |
| 2:c:196:MET:HE3 | 2:c:196:MET:C | 2.39 | 0.48 |
| 2:d:42:VAL:CG1 | 2:d:119:GLY:HA3 | 2.43 | 0.48 |
| 2:g:166:THR:HG21 | 2:i:362:LEU:HD21 | 1.95 | 0.48 |
| 2:g:280:LEU:CD1 | 2:g:340:ALA:HB2 | 2.43 | 0.48 |
| 2:h:256:ASN:O | 2:h:257:SER:OG | 2.29 | 0.48 |
| 2:i:175:LEU:HD11 | 1:G:51:ILE:CG1 | 2.40 | 0.48 |
| 2:j:208:ARG:NH2 | 2:j:238:ASP:OD2 | 2.46 | 0.48 |
| 2:k:254:VAL:CG2 | 2:l:355:ALA:HB2 | 2.44 | 0.48 |
| 2:k:348:ILE:O | 2:k:352:MET:HG3 | 2.13 | 0.48 |
| 2:l:81:LEU:HD23 | 2:l:81:LEU:N | 2.28 | 0.48 |
| 2:l:280:LEU:CD1 | 2:l:340:ALA:HB2 | 2.43 | 0.48 |
| 2:o:103:ILE:HG13 | 2:o:169:ALA:HB3 | 1.96 | 0.48 |
| 2:p:21:ARG:O | 2:p:25:LEU:HD22 | 2.14 | 0.48 |
| 2:p:280:LEU:CD1 | 2:p:340:ALA:HB2 | 2.43 | 0.48 |
| 2:q:21:ARG:O | 2:q:25:LEU:HD22 | 2.14 | 0.48 |
| 2:r:21:ARG:O | 2:r:25:LEU:HD22 | 2.14 | 0.48 |
| 2:r:196:MET:HE3 | 2:r:196:MET:C | 2.39 | 0.48 |
| 2:s:21:ARG:O | 2:s:25:LEU:HD22 | 2.14 | 0.48 |
| 2:s:361:LYS:O | 2:s:361:LYS:HG3 | 2.13 | 0.48 |
| 2:t:21:ARG:O | 2:t:25:LEU:HD22 | 2.14 | 0.48 |
| 2:t:98:ARG:HA | 2:t:174:GLU:OE1 | 2.14 | 0.48 |
| 2:v:96:PHE:O | 2:w:219:ARG:HD2 | 2.14 | 0.48 |
| 2:v:98:ARG:HA | 2:v:174:GLU:OE1 | 2.14 | 0.48 |
| 2:x:101:GLN:NE2 | 2:y:219:ARG:HD3 | 2.28 | 0.48 |
| 3:11:75:GLY:HA2 | 3:11:89:ARG:O | 2.14 | 0.48 |
| 3:17:22:VAL:HG13 | 3:17:34:LEU:HD23 | 1.96 | 0.48 |
| 3:17:72:GLN:HG2 | 3:17:73:PRO:CD | 2.41 | 0.48 |
| 3:17:75:GLY:HA2 | 3:17:89:ARG:O | 2.14 | 0.48 |
| 3:18:22:VAL:HG13 | 3:18:34:LEU:HD23 | 1.96 | 0.48 |
| 3:18:75:GLY:HA2 | 3:18:89:ARG:O | 2.14 | 0.48 |
| 3:22:75:GLY:HA2 | 3:22:89:ARG:O | 2.14 | 0.48 |
| 1:L:109:VAL:HG21 | 1:L:117:PHE:O | 2.14 | 0.48 |
| 1:Q:109:VAL:HG21 | 1:Q:117:PHE:O | 2.14 | 0.48 |
| 1:R:109:VAL:HG21 | 1:R:117:PHE:O | 2.14 | 0.48 |
| 1:A:159:GLY:O | 1:A:186:PRO:HG3 | 2.14 | 0.47 |
| 2:b:98:ARG:HA | 2:b:174:GLU:OE1 | 2.14 | 0.47 |
| 2:f:42:VAL:CG1 | 2:f:119:GLY:HA3 | 2.43 | 0.47 |
| 2:f:98:ARG:HA | 2:f:174:GLU:OE1 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:f:361:LYS:O | 2:f:361:LYS:HG3 | 2.13 | 0.47 |
| 2:g:196:MET:HE3 | 2:g:196:MET:C | 2.39 | 0.47 |
| 2:i:42:VAL:HA | 2:i:120:THR:O | 2.14 | 0.47 |
| 2:j:42:VAL:HA | 2:j:120:THR:O | 2.14 | 0.47 |
| 2:k:217:ASP:OD1 | 2:k:219:ARG:N | 2.35 | 0.47 |
| 2:l:103:ILE:HG13 | 2:l:169:ALA:HB3 | 1.96 | 0.47 |
| 2:m:103:ILE:HG13 | 2:m:169:ALA:HB3 | 1.96 | 0.47 |
| 2:m:254:VAL:HG13 | 2:m:365:ILE:CG1 | 2.44 | 0.47 |
| 2:o:21:ARG:O | 2:o:25:LEU:HD22 | 2.14 | 0.47 |
| 2:p:105:VAL:HG11 | 2:p:169:ALA:HB2 | 1.95 | 0.47 |
| 2:v:94:PRO:HB2 | 2:w:219:ARG:NH2 | 2.28 | 0.47 |
| 2:v:196:MET:HE3 | 2:v:196:MET:C | 2.39 | 0.47 |
| 2:w:103:ILE:HG13 | 2:w:169:ALA:HB3 | 1.96 | 0.47 |
| 2:w:254:VAL:CG2 | 2:x:355:ALA:HB2 | 2.44 | 0.47 |
| 2:x:101:GLN:NE2 | 2:y:188:GLN:HB3 | 2.29 | 0.47 |
| 2:x:196:MET:HE3 | 2:x:196:MET:C | 2.39 | 0.47 |
| 2:x:280:LEU:CD1 | 2:x:340:ALA:HB2 | 2.43 | 0.47 |
| 2:y:141:ILE:HD13 | 2:y:165:ILE:CD1 | 2.39 | 0.47 |
| 2:z:98:ARG:HA | 2:z:174:GLU:OE1 | 2.14 | 0.47 |
| 2:z:105:VAL:HG11 | 2:z:169:ALA:HB2 | 1.95 | 0.47 |
| 2:z:254:VAL:HG13 | 2:z:365:ILE:CG1 | 2.44 | 0.47 |
| 3:14:22:VAL:HG13 | 3:14:34:LEU:HD23 | 1.96 | 0.47 |
| 3:22:22:VAL:HG13 | 3:22:34:LEU:HD23 | 1.96 | 0.47 |
| 1:B:176:GLU:OE2 | 1:D:90:LYS:HD3 | 2.14 | 0.47 |
| 1:H:109:VAL:HG21 | 1:H:117:PHE:O | 2.14 | 0.47 |
| 1:H:176:GLU:OE2 | 1:J:90:LYS:HD3 | 2.14 | 0.47 |
| 1:I:109:VAL:HG21 | 1:I:117:PHE:O | 2.14 | 0.47 |
| 1:K:130:ASN:CG | 1:L:102:THR:HG22 | 2.39 | 0.47 |
| 1:S:109:VAL:HG21 | 1:S:117:PHE:O | 2.14 | 0.47 |
| 2:a:166:THR:HG21 | 2:c:362:LEU:HD21 | 1.94 | 0.47 |
| 2:b:101:GLN:NE2 | 2:c:188:GLN:HB3 | 2.28 | 0.47 |
| 2:e:81:LEU:HD23 | 2:e:81:LEU:N | 2.28 | 0.47 |
| 2:e:254:VAL:HG13 | 2:e:365:ILE:CG1 | 2.44 | 0.47 |
| 2:h:94:PRO:HB2 | 2:i:219:ARG:NH2 | 2.29 | 0.47 |
| 2:k:98:ARG:HA | 2:k:174:GLU:OE1 | 2.14 | 0.47 |
| 2:l:254:VAL:HG13 | 2:l:365:ILE:CG1 | 2.44 | 0.47 |
| 2:m:101:GLN:NE2 | 2:n:219:ARG:HD3 | 2.28 | 0.47 |
| 2:m:105:VAL:HG11 | 2:m:169:ALA:HB2 | 1.95 | 0.47 |
| 2:n:42:VAL:HA | 2:n:120:THR:O | 2.14 | 0.47 |
| 2:n:94:PRO:HB2 | 2:o:219:ARG:NH2 | 2.30 | 0.47 |
| 2:t:123:MET:HE1 | 2:t:136:LEU:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:u:21:ARG:O | 2:u:25:LEU:HD22 | 2.14 | 0.47 |
| 2:v:21:ARG:O | 2:v:25:LEU:HD22 | 2.14 | 0.47 |
| 2:v:254:VAL:HG13 | 2:v:365:ILE:CG1 | 2.44 | 0.47 |
| 2:v:348:ILE:O | 2:v:352:MET:HG3 | 2.14 | 0.47 |
| 2:x:98:ARG:HA | 2:x:174:GLU:OE1 | 2.14 | 0.47 |
| 2:y:196:MET:HE3 | 2:y:196:MET:C | 2.39 | 0.47 |
| 2:y:254:VAL:HG13 | 2:y:365:ILE:CG1 | 2.44 | 0.47 |
| 2:z:42:VAL:O | 2:z:84:VAL:HA | 2.13 | 0.47 |
| 2:z:141:ILE:HD13 | 2:z:165:ILE:CD1 | 2.39 | 0.47 |
| 2:z:361:LYS:HG3 | 2:z:361:LYS:O | 2.13 | 0.47 |
| 3:8:75:GLY:HA2 | 3:8:89:ARG:O | 2.14 | 0.47 |
| 3:10:75:GLY:HA2 | 3:10:89:ARG:O | 2.14 | 0.47 |
| 3:16:22:VAL:HG13 | 3:16:34:LEU:HD23 | 1.96 | 0.47 |
| 3:16:75:GLY:HA2 | 3:16:89:ARG:O | 2.14 | 0.47 |
| 3:18:72:GLN:HG2 | 3:18:73:PRO:CD | 2.41 | 0.47 |
| 3:19:22:VAL:HG13 | 3:19:34:LEU:HD23 | 1.96 | 0.47 |
| 3:23:75:GLY:HA2 | 3:23:89:ARG:O | 2.14 | 0.47 |
| 1:B:130:ASN:CG | 1:C:102:THR:HG22 | 2.40 | 0.47 |
| 1:J:176:GLU:OE2 | 1:L:90:LYS:HD3 | 2.13 | 0.47 |
| 1:K:176:GLU:OE2 | 1:M:90:LYS:HD3 | 2.14 | 0.47 |
| 1:P:109:VAL:HG21 | 1:P:117:PHE:O | 2.14 | 0.47 |
| 1:T:176:GLU:OE2 | 1:V:90:LYS:HD3 | 2.14 | 0.47 |
| 2:a:348:ILE:O | 2:a:352:MET:HG3 | 2.14 | 0.47 |
| 2:b:217:ASP:OD1 | 2:b:219:ARG:N | 2.35 | 0.47 |
| 2:d:94:PRO:HB2 | 2:e:219:ARG:NH2 | 2.28 | 0.47 |
| 2:d:196:MET:HE3 | 2:d:196:MET:C | 2.39 | 0.47 |
| 2:f:101:GLN:NE2 | 2:g:219:ARG:HD3 | 2.29 | 0.47 |
| 2:g:96:PHE:O | 2:h:219:ARG:HD2 | 2.14 | 0.47 |
| 2:g:98:ARG:HA | 2:g:174:GLU:OE1 | 2.14 | 0.47 |
| 2:g:254:VAL:CG2 | 2:h:355:ALA:HB2 | 2.45 | 0.47 |
| 2:i:196:MET:HE3 | 2:i:196:MET:C | 2.39 | 0.47 |
| 2:k:81:LEU:HD23 | 2:k:81:LEU:N | 2.28 | 0.47 |
| 2:k:141:ILE:HD13 | 2:k:165:ILE:CD1 | 2.39 | 0.47 |
| 2:n:196:MET:HE3 | 2:n:196:MET:C | 2.39 | 0.47 |
| 2:n:361:LYS:O | 2:n:361:LYS:HG3 | 2.13 | 0.47 |
| 2:o:98:ARG:HA | 2:o:174:GLU:OE1 | 2.14 | 0.47 |
| 2:q:196:MET:HE3 | 2:q:196:MET:C | 2.39 | 0.47 |
| 2:r:98:ARG:HA | 2:r:174:GLU:OE1 | 2.14 | 0.47 |
| 2:s:98:ARG:HA | 2:s:174:GLU:OE1 | 2.14 | 0.47 |
| 2:t:101:GLN:NE2 | 2:u:219:ARG:HD3 | 2.28 | 0.47 |
| 2:t:196:MET:HE3 | 2:t:196:MET:C | 2.39 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:w:42:VAL:HA | 2:w:120:THR:O | 2.14 | 0.47 |
| 2:w:166:THR:HG21 | 2:y:362:LEU:HD21 | 1.94 | 0.47 |
| 2:w:196:MET:HE3 | 2:w:196:MET:C | 2.39 | 0.47 |
| 2:w:348:ILE:O | 2:w:352:MET:HG3 | 2.14 | 0.47 |
| 2:x:42:VAL:HA | 2:x:120:THR:O | 2.14 | 0.47 |
| 2:x:93:TYR:OH | 2:x:173:ARG:O | 2.24 | 0.47 |
| 2:x:103:ILE:HG13 | 2:x:169:ALA:HB3 | 1.96 | 0.47 |
| 2:y:42:VAL:HA | 2:y:120:THR:O | 2.14 | 0.47 |
| 3:4:47:ASP:CG | 3:4:50:VAL:H | 2.14 | 0.47 |
| 3:13:22:VAL:HG13 | 3:13:34:LEU:HD23 | 1.96 | 0.47 |
| 3:14:36:TYR:HE2 | 3:14:44:SER:HG | 1.60 | 0.47 |
| 3:15:22:VAL:HG13 | 3:15:34:LEU:HD23 | 1.96 | 0.47 |
| 3:21:22:VAL:HG13 | 3:21:34:LEU:HD23 | 1.96 | 0.47 |
| 3:23:22:VAL:HG13 | 3:23:34:LEU:HD23 | 1.96 | 0.47 |
| 3:24:75:GLY:HA2 | 3:24:89:ARG:O | 2.14 | 0.47 |
| 3:26:75:GLY:HA2 | 3:26:89:ARG:O | 2.14 | 0.47 |
| 1:B:159:GLY:O | 1:B:186:PRO:HG3 | 2.14 | 0.47 |
| 1:C:159:GLY:O | 1:C:186:PRO:HG3 | 2.14 | 0.47 |
| 1:F:124:MET:HE3 | 1:F:124:MET:HB3 | 1.77 | 0.47 |
| 1:N:176:GLU:OE2 | 1:P:90:LYS:HD3 | 2.14 | 0.47 |
| 1:S:159:GLY:O | 1:S:186:PRO:HG3 | 2.14 | 0.47 |
| 1:T:159:GLY:O | 1:T:186:PRO:HG3 | 2.14 | 0.47 |
| 1:U:101:LYS:HB3 | 1:U:101:LYS:HZ2 | 1.80 | 0.47 |
| 1:Z:159:GLY:O | 1:Z:186:PRO:HG3 | 2.14 | 0.47 |
| 2:a:105:VAL:HG11 | 2:a:169:ALA:HB2 | 1.95 | 0.47 |
| 2:b:348:ILE:O | 2:b:352:MET:HG3 | 2.14 | 0.47 |
| 2:c:348:ILE:O | 2:c:352:MET:HG3 | 2.14 | 0.47 |
| 2:d:98:ARG:HA | 2:d:174:GLU:OE1 | 2.14 | 0.47 |
| 2:j:166:THR:HG21 | 2:l:362:LEU:HD21 | 1.96 | 0.47 |
| 2:k:103:ILE:HG13 | 2:k:169:ALA:HB3 | 1.96 | 0.47 |
| 2:m:42:VAL:HA | 2:m:120:THR:O | 2.14 | 0.47 |
| 2:m:196:MET:HE3 | 2:m:196:MET:C | 2.39 | 0.47 |
| 2:n:21:ARG:O | 2:n:25:LEU:HD22 | 2.14 | 0.47 |
| 2:o:208:ARG:NH2 | 2:o:238:ASP:OD2 | 2.46 | 0.47 |
| 2:q:166:THR:HG21 | 2:s:362:LEU:HD21 | 1.96 | 0.47 |
| 2:r:166:THR:HG21 | 2:t:362:LEU:HD21 | 1.95 | 0.47 |
| 2:r:254:VAL:HG13 | 2:r:365:ILE:CG1 | 2.44 | 0.47 |
| 2:s:254:VAL:CG2 | 2:t:355:ALA:HB2 | 2.45 | 0.47 |
| 2:u:196:MET:HE3 | 2:u:196:MET:C | 2.39 | 0.47 |
| 2:u:208:ARG:NH2 | 2:u:238:ASP:OD2 | 2.46 | 0.47 |
| 2:v:42:VAL:HA | 2:v:120:THR:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:w:98:ARG:HA | 2:w:174:GLU:OE1 | 2.14 | 0.47 |
| 2:w:123:MET:HE1 | 2:w:136:LEU:HB3 | 1.95 | 0.47 |
| 2:x:123:MET:HE1 | 2:x:136:LEU:HB3 | 1.95 | 0.47 |
| 2:x:353:GLN:HB2 | 2:x:358:LEU:HD23 | 1.97 | 0.47 |
| 2:z:348:ILE:O | 2:z:352:MET:HG3 | 2.14 | 0.47 |
| 3:4:72:GLN:HG2 | 3:4:73:PRO:CD | 2.41 | 0.47 |
| 3:6:83:SER:HA | 1:G:210:ASN:ND2 | 2.30 | 0.47 |
| 3:12:75:GLY:HA2 | 3:12:89:ARG:O | 2.14 | 0.47 |
| 1:B:90:LYS:HD3 | 1:Z:176:GLU:OE2 | 2.15 | 0.47 |
| 1:C:176:GLU:OE2 | 1:E:90:LYS:HD3 | 2.14 | 0.47 |
| 1:J:124:MET:HE3 | 1:J:124:MET:HB3 | 1.77 | 0.47 |
| 1:Q:130:ASN:CG | 1:R:102:THR:HG22 | 2.39 | 0.47 |
| 1:R:159:GLY:O | 1:R:186:PRO:HG3 | 2.14 | 0.47 |
| 1:R:171:ILE:HD12 | 1:T:88:ALA:CB | 2.34 | 0.47 |
| 1:U:109:VAL:HG21 | 1:U:117:PHE:O | 2.14 | 0.47 |
| 1:U:159:GLY:O | 1:U:186:PRO:HG3 | 2.14 | 0.47 |
| 1:U:176:GLU:OE2 | 1:W:90:LYS:HD3 | 2.14 | 0.47 |
| 1:A:102:THR:HG22 | 1:Z:130:ASN:CG | 2.40 | 0.47 |
| 2:a:254:VAL:CG2 | 2:b:355:ALA:HB2 | 2.45 | 0.47 |
| 2:c:353:GLN:HB2 | 2:c:358:LEU:HD23 | 1.96 | 0.47 |
| 2:d:96:PHE:O | 2:e:219:ARG:HD2 | 2.14 | 0.47 |
| 2:e:42:VAL:HA | 2:e:120:THR:O | 2.14 | 0.47 |
| 2:e:280:LEU:CD1 | 2:e:340:ALA:HB2 | 2.43 | 0.47 |
| 2:e:282:VAL:HG23 | 2:e:317:GLY:O | 2.13 | 0.47 |
| 2:i:254:VAL:HG13 | 2:i:365:ILE:CG1 | 2.44 | 0.47 |
| 2:j:103:ILE:HG13 | 2:j:169:ALA:HB3 | 1.96 | 0.47 |
| 2:j:196:MET:HE3 | 2:j:196:MET:C | 2.39 | 0.47 |
| 2:j:348:ILE:O | 2:j:352:MET:HG3 | 2.14 | 0.47 |
| 2:m:21:ARG:O | 2:m:25:LEU:HD22 | 2.14 | 0.47 |
| 2:n:101:GLN:NE2 | 2:o:219:ARG:HD3 | 2.28 | 0.47 |
| 2:n:105:VAL:HG11 | 2:n:169:ALA:HB2 | 1.95 | 0.47 |
| 2:o:123:MET:HE1 | 2:o:136:LEU:HB3 | 1.95 | 0.47 |
| 2:o:196:MET:HE3 | 2:o:196:MET:C | 2.39 | 0.47 |
| 2:p:98:ARG:HA | 2:p:174:GLU:OE1 | 2.14 | 0.47 |
| 2:r:96:PHE:O | 2:s:219:ARG:HD2 | 2.15 | 0.47 |
| 2:s:166:THR:HG21 | 2:u:362:LEU:HD21 | 1.95 | 0.47 |
| 2:t:277:GLN:HB3 | 2:t:280:LEU:HD12 | 1.94 | 0.47 |
| 2:u:42:VAL:HA | 2:u:120:THR:O | 2.14 | 0.47 |
| 2:w:21:ARG:O | 2:w:25:LEU:HD22 | 2.14 | 0.47 |
| 2:w:217:ASP:OD1 | 2:w:219:ARG:N | 2.35 | 0.47 |
| 2:w:353:GLN:HB2 | 2:w:358:LEU:HD23 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:y:103:ILE:HG13 | 2:y:169:ALA:HB3 | 1.96 | 0.47 |
| 2:z:42:VAL:HA | 2:z:120:THR:O | 2.14 | 0.47 |
| 2:z:196:MET:HE3 | 2:z:196:MET:C | 2.39 | 0.47 |
| 3:6:39:PRO:HD2 | 3:6:42:PHE:CB | 2.45 | 0.47 |
| 3:8:39:PRO:HD2 | 3:8:42:PHE:CB | 2.45 | 0.47 |
| 3:15:75:GLY:HA2 | 3:15:89:ARG:O | 2.14 | 0.47 |
| 1:D:159:GLY:O | 1:D:186:PRO:HG3 | 2.14 | 0.47 |
| 1:F:159:GLY:O | 1:F:186:PRO:HG3 | 2.14 | 0.47 |
| 1:F:176:GLU:OE2 | 1:H:90:LYS:HD3 | 2.15 | 0.47 |
| 1:G:159:GLY:O | 1:G:186:PRO:HG3 | 2.14 | 0.47 |
| 1:H:159:GLY:O | 1:H:186:PRO:HG3 | 2.14 | 0.47 |
| 1:Y:40:ILE:H | 1:Y:40:ILE:HG12 | 1.49 | 0.47 |
| 1:Y:159:GLY:O | 1:Y:186:PRO:HG3 | 2.14 | 0.47 |
| 2:a:219:ARG:HD3 | 2:z:101:GLN:NE2 | 2.27 | 0.47 |
| 2:b:103:ILE:HG13 | 2:b:169:ALA:HB3 | 1.96 | 0.47 |
| 2:b:175:LEU:HD11 | 1:Z:51:ILE:CG1 | 2.44 | 0.47 |
| 2:d:254:VAL:HG13 | 2:d:365:ILE:CG1 | 2.44 | 0.47 |
| 2:e:175:LEU:HD11 | 1:C:51:ILE:CG1 | 2.39 | 0.47 |
| 2:h:175:LEU:HD11 | 1:F:51:ILE:CG1 | 2.40 | 0.47 |
| 2:h:361:LYS:O | 2:h:361:LYS:HG3 | 2.13 | 0.47 |
| 2:j:98:ARG:HA | 2:j:174:GLU:OE1 | 2.14 | 0.47 |
| 2:k:123:MET:HE1 | 2:k:136:LEU:HB3 | 1.95 | 0.47 |
| 2:m:123:MET:HE1 | 2:m:136:LEU:HB3 | 1.95 | 0.47 |
| 2:m:254:VAL:CG2 | 2:n:355:ALA:HB2 | 2.45 | 0.47 |
| 2:n:254:VAL:HG13 | 2:n:365:ILE:CG1 | 2.44 | 0.47 |
| 2:o:42:VAL:HA | 2:o:120:THR:O | 2.14 | 0.47 |
| 2:o:101:GLN:NE2 | 2:p:188:GLN:HB3 | 2.30 | 0.47 |
| 2:p:123:MET:HE1 | 2:p:136:LEU:HB3 | 1.95 | 0.47 |
| 2:s:254:VAL:HG13 | 2:s:365:ILE:CG1 | 2.44 | 0.47 |
| 2:u:96:PHE:O | 2:v:219:ARG:HD2 | 2.14 | 0.47 |
| 2:x:348:ILE:O | 2:x:352:MET:HG3 | 2.14 | 0.47 |
| 3:9:83:SER:HA | 1:J:210:ASN:ND2 | 2.30 | 0.47 |
| 3:11:17:THR:O | 3:11:18:ARG:NE | 2.48 | 0.47 |
| 3:12:17:THR:O | 3:12:18:ARG:NE | 2.48 | 0.47 |
| 3:12:22:VAL:HG13 | 3:12:34:LEU:HD23 | 1.96 | 0.47 |
| 3:20:22:VAL:HG13 | 3:20:34:LEU:HD23 | 1.96 | 0.47 |
| 3:23:17:THR:O | 3:23:18:ARG:NE | 2.48 | 0.47 |
| 3:24:17:THR:O | 3:24:18:ARG:NE | 2.48 | 0.47 |
| 3:25:17:THR:O | 3:25:18:ARG:NE | 2.48 | 0.47 |
| 3:26:17:THR:O | 3:26:18:ARG:NE | 2.48 | 0.47 |
| 1:E:159:GLY:O | 1:E:186:PRO:HG3 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:159:GLY:O | 1:I:186:PRO:HG3 | 2.14 | 0.47 |
| 1:I:176:GLU:OE2 | 1:K:90:LYS:HD3 | 2.14 | 0.47 |
| 1:J:159:GLY:O | 1:J:186:PRO:HG3 | 2.14 | 0.47 |
| 1:Q:159:GLY:O | 1:Q:186:PRO:HG3 | 2.14 | 0.47 |
| 1:T:109:VAL:HG21 | 1:T:117:PHE:O | 2.14 | 0.47 |
| 1:V:159:GLY:O | 1:V:186:PRO:HG3 | 2.14 | 0.47 |
| 2:a:42:VAL:HA | 2:a:120:THR:O | 2.14 | 0.47 |
| 2:a:101:GLN:NE2 | 2:b:219:ARG:HD3 | 2.28 | 0.47 |
| 2:a:103:ILE:HG13 | 2:a:169:ALA:HB3 | 1.96 | 0.47 |
| 2:a:196:MET:HE3 | 2:a:196:MET:C | 2.39 | 0.47 |
| 2:a:219:ARG:HD2 | 2:z:96:PHE:O | 2.14 | 0.47 |
| 3:1:17:THR:O | 3:1:18:ARG:NE | 2.48 | 0.47 |
| 2:c:103:ILE:HG13 | 2:c:169:ALA:HB3 | 1.96 | 0.47 |
| 2:c:123:MET:HE1 | 2:c:136:LEU:HB3 | 1.95 | 0.47 |
| 2:d:42:VAL:HA | 2:d:120:THR:O | 2.14 | 0.47 |
| 2:d:103:ILE:HG13 | 2:d:169:ALA:HB3 | 1.96 | 0.47 |
| 2:d:166:THR:HG21 | 2:f:362:LEU:HD21 | 1.96 | 0.47 |
| 2:d:348:ILE:O | 2:d:352:MET:HG3 | 2.14 | 0.47 |
| 2:e:103:ILE:HG13 | 2:e:169:ALA:HB3 | 1.96 | 0.47 |
| 2:f:42:VAL:HA | 2:f:120:THR:O | 2.14 | 0.47 |
| 2:f:103:ILE:HG13 | 2:f:169:ALA:HB3 | 1.96 | 0.47 |
| 2:h:42:VAL:HA | 2:h:120:THR:O | 2.14 | 0.47 |
| 2:h:103:ILE:HG13 | 2:h:169:ALA:HB3 | 1.96 | 0.47 |
| 2:h:123:MET:HE1 | 2:h:136:LEU:HB3 | 1.96 | 0.47 |
| 2:h:348:ILE:O | 2:h:352:MET:HG3 | 2.14 | 0.47 |
| 2:i:94:PRO:HB2 | 2:j:219:ARG:NH2 | 2.30 | 0.47 |
| 2:i:101:GLN:NE2 | 2:j:188:GLN:HB3 | 2.30 | 0.47 |
| 2:i:348:ILE:O | 2:i:352:MET:HG3 | 2.14 | 0.47 |
| 2:j:96:PHE:O | 2:k:219:ARG:HD2 | 2.14 | 0.47 |
| 2:j:101:GLN:NE2 | 2:k:219:ARG:HD3 | 2.29 | 0.47 |
| 2:j:123:MET:HE1 | 2:j:136:LEU:HB3 | 1.95 | 0.47 |
| 2:k:21:ARG:O | 2:k:25:LEU:HD22 | 2.14 | 0.47 |
| 2:l:21:ARG:O | 2:l:25:LEU:HD22 | 2.14 | 0.47 |
| 2:l:94:PRO:HB2 | 2:m:219:ARG:NH2 | 2.29 | 0.47 |
| 2:l:96:PHE:O | 2:m:219:ARG:HD2 | 2.14 | 0.47 |
| 2:l:123:MET:HE1 | 2:l:136:LEU:HB3 | 1.95 | 0.47 |
| 2:n:280:LEU:CD1 | 2:n:340:ALA:HB2 | 2.43 | 0.47 |
| 2:o:94:PRO:HB2 | 2:p:219:ARG:NH2 | 2.30 | 0.47 |
| 2:o:105:VAL:HG11 | 2:o:169:ALA:HB2 | 1.95 | 0.47 |
| 2:p:96:PHE:O | 2:q:219:ARG:HD2 | 2.14 | 0.47 |
| 2:p:166:THR:HG21 | 2:r:362:LEU:HD21 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:s:123:MET:HE1 | 2:s:136:LEU:HB3 | 1.96 | 0.47 |
| 2:t:42:VAL:HA | 2:t:120:THR:O | 2.14 | 0.47 |
| 2:t:96:PHE:O | 2:u:219:ARG:HD2 | 2.15 | 0.47 |
| 2:t:101:GLN:NE2 | 2:u:188:GLN:HB3 | 2.28 | 0.47 |
| 2:v:361:LYS:O | 2:v:361:LYS:HG3 | 2.13 | 0.47 |
| 2:w:81:LEU:HD23 | 2:w:81:LEU:N | 2.28 | 0.47 |
| 2:w:254:VAL:HG13 | 2:w:365:ILE:CG1 | 2.44 | 0.47 |
| 2:x:21:ARG:O | 2:x:25:LEU:HD22 | 2.14 | 0.47 |
| 2:x:46:ASP:HA | 2:y:161:ASN:ND2 | 2.23 | 0.47 |
| 2:y:79:MET:HE2 | 2:y:79:MET:HB2 | 1.69 | 0.47 |
| 2:y:348:ILE:O | 2:y:352:MET:HG3 | 2.14 | 0.47 |
| 2:y:353:GLN:HB2 | 2:y:358:LEU:HD23 | 1.97 | 0.47 |
| 2:z:103:ILE:HG13 | 2:z:169:ALA:HB3 | 1.96 | 0.47 |
| 3:2:17:THR:O | 3:2:18:ARG:NE | 2.48 | 0.47 |
| 3:3:83:SER:HA | 1:D:210:ASN:ND2 | 2.30 | 0.47 |
| 3:4:39:PRO:HD2 | 3:4:42:PHE:CB | 2.45 | 0.47 |
| 3:5:77:CYS:HB3 | 3:5:80:TYR:CE1 | 2.48 | 0.47 |
| 3:6:77:CYS:HB3 | 3:6:80:TYR:CE1 | 2.48 | 0.47 |
| 3:7:77:CYS:HB3 | 3:7:80:TYR:CE1 | 2.48 | 0.47 |
| 3:9:17:THR:O | 3:9:18:ARG:NE | 2.48 | 0.47 |
| 3:10:17:THR:O | 3:10:18:ARG:NE | 2.48 | 0.47 |
| 3:13:17:THR:O | 3:13:18:ARG:NE | 2.48 | 0.47 |
| 3:17:39:PRO:HD2 | 3:17:42:PHE:CB | 2.45 | 0.47 |
| 3:21:17:THR:O | 3:21:18:ARG:NE | 2.48 | 0.47 |
| 3:22:17:THR:O | 3:22:18:ARG:NE | 2.48 | 0.47 |
| 3:25:22:VAL:HG13 | 3:25:34:LEU:HD23 | 1.96 | 0.47 |
| 1:E:109:VAL:HG21 | 1:E:117:PHE:O | 2.14 | 0.47 |
| 1:G:109:VAL:HG21 | 1:G:117:PHE:O | 2.14 | 0.47 |
| 1:H:124:MET:HE3 | 1:H:124:MET:HB3 | 1.77 | 0.47 |
| 1:H:130:ASN:CG | 1:I:102:THR:HG22 | 2.39 | 0.47 |
| 1:K:159:GLY:O | 1:K:186:PRO:HG3 | 2.14 | 0.47 |
| 1:O:176:GLU:OE2 | 1:Q:90:LYS:HD3 | 2.14 | 0.47 |
| 1:P:159:GLY:O | 1:P:186:PRO:HG3 | 2.14 | 0.47 |
| 1:R:130:ASN:CG | 1:S:102:THR:HG22 | 2.39 | 0.47 |
| 1:V:150:VAL:HG12 | 1:V:165:GLY:HA3 | 1.97 | 0.47 |
| 1:W:159:GLY:O | 1:W:186:PRO:HG3 | 2.14 | 0.47 |
| 1:X:159:GLY:O | 1:X:186:PRO:HG3 | 2.14 | 0.47 |
| 2:b:353:GLN:HB2 | 2:b:358:LEU:HD23 | 1.97 | 0.47 |
| 2:h:98:ARG:HA | 2:h:174:GLU:OE1 | 2.14 | 0.47 |
| 2:i:103:ILE:HG13 | 2:i:169:ALA:HB3 | 1.96 | 0.47 |
| 2:j:81:LEU:HD23 | 2:j:81:LEU:N | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:k:42:VAL:HA | 2:k:120:THR:O | 2.14 | 0.47 |
| 2:l:101:GLN:NE2 | 2:m:188:GLN:HB3 | 2.29 | 0.47 |
| 2:l:196:MET:HE3 | 2:l:196:MET:C | 2.39 | 0.47 |
| 2:p:328:LEU:HD21 | 2:q:273:CYS:HA | 1.97 | 0.47 |
| 2:r:123:MET:HE1 | 2:r:136:LEU:HB3 | 1.95 | 0.47 |
| 2:y:21:ARG:O | 2:y:25:LEU:HD22 | 2.14 | 0.47 |
| 3:3:17:THR:O | 3:3:18:ARG:NE | 2.48 | 0.47 |
| 3:3:39:PRO:HD2 | 3:3:42:PHE:CB | 2.45 | 0.47 |
| 3:4:75:GLY:HA2 | 3:4:89:ARG:O | 2.14 | 0.47 |
| 3:10:22:VAL:HG13 | 3:10:34:LEU:HD23 | 1.96 | 0.47 |
| 3:10:39:PRO:HD2 | 3:10:42:PHE:CB | 2.45 | 0.47 |
| 3:13:47:ASP:CG | 3:13:50:VAL:H | 2.14 | 0.47 |
| 3:14:17:THR:O | 3:14:18:ARG:NE | 2.48 | 0.47 |
| 3:19:39:PRO:HD2 | 3:19:42:PHE:CB | 2.45 | 0.47 |
| 3:19:72:GLN:HG2 | 3:19:73:PRO:CD | 2.41 | 0.47 |
| 3:20:17:THR:O | 3:20:18:ARG:NE | 2.48 | 0.47 |
| 3:24:22:VAL:HG13 | 3:24:34:LEU:HD23 | 1.96 | 0.47 |
| 3:26:22:VAL:HG13 | 3:26:34:LEU:HD23 | 1.96 | 0.47 |
| 1:D:130:ASN:CG | 1:E:102:THR:HG22 | 2.40 | 0.47 |
| 1:F:171:ILE:HD12 | 1:H:88:ALA:CB | 2.34 | 0.47 |
| 1:M:109:VAL:HG21 | 1:M:117:PHE:O | 2.14 | 0.47 |
| 1:S:130:ASN:CG | 1:T:102:THR:HG22 | 2.39 | 0.47 |
| 1:W:130:ASN:CG | 1:X:102:THR:HG22 | 2.39 | 0.47 |
| 1:W:150:VAL:HG12 | 1:W:165:GLY:HA3 | 1.97 | 0.47 |
| 1:X:150:VAL:HG12 | 1:X:165:GLY:HA3 | 1.97 | 0.47 |
| 1:Y:150:VAL:HG12 | 1:Y:165:GLY:HA3 | 1.97 | 0.47 |
| 2:a:21:ARG:O | 2:a:25:LEU:HD22 | 2.14 | 0.47 |
| 2:b:196:MET:HE3 | 2:b:196:MET:C | 2.39 | 0.47 |
| 2:d:353:GLN:HB2 | 2:d:358:LEU:HD23 | 1.96 | 0.47 |
| 2:e:98:ARG:HA | 2:e:174:GLU:OE1 | 2.14 | 0.47 |
| 2:e:196:MET:HE3 | 2:e:196:MET:C | 2.39 | 0.47 |
| 2:e:348:ILE:O | 2:e:352:MET:HG3 | 2.14 | 0.47 |
| 2:g:103:ILE:HG13 | 2:g:169:ALA:HB3 | 1.96 | 0.47 |
| 2:g:361:LYS:HG3 | 2:g:361:LYS:O | 2.13 | 0.47 |
| 2:j:21:ARG:O | 2:j:25:LEU:HD22 | 2.14 | 0.47 |
| 2:l:42:VAL:HA | 2:l:120:THR:O | 2.14 | 0.47 |
| 2:s:353:GLN:HB2 | 2:s:358:LEU:HD23 | 1.96 | 0.47 |
| 2:v:101:GLN:NE2 | 2:w:219:ARG:HD3 | 2.30 | 0.47 |
| 2:y:164:ARG:HD2 | 2:z:365:ILE:CG2 | 2.45 | 0.47 |
| 3:4:17:THR:O | 3:4:18:ARG:NE | 2.48 | 0.47 |
| 3:4:77:CYS:HB3 | 3:4:80:TYR:CE1 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:8:17:THR:O | 3:8:18:ARG:NE | 2.48 | 0.47 |
| 3:9:22:VAL:HG13 | 3:9:34:LEU:HD23 | 1.96 | 0.47 |
| 3:9:75:GLY:HA2 | 3:9:89:ARG:O | 2.14 | 0.47 |
| 3:11:22:VAL:HG13 | 3:11:34:LEU:HD23 | 1.96 | 0.47 |
| 3:14:75:GLY:HA2 | 3:14:89:ARG:O | 2.14 | 0.47 |
| 3:19:17:THR:O | 3:19:18:ARG:NE | 2.48 | 0.47 |
| 3:25:75:GLY:HA2 | 3:25:89:ARG:O | 2.14 | 0.47 |
| 1:G:130:ASN:CG | 1:H:102:THR:HG22 | 2.40 | 0.47 |
| 1:J:130:ASN:CG | 1:K:102:THR:HG22 | 2.40 | 0.47 |
| 1:N:130:ASN:CG | 1:O:102:THR:HG22 | 2.39 | 0.47 |
| 1:Y:222:LEU:HB2 | 1:Z:231:PRO:HB3 | 1.97 | 0.47 |
| 2:a:98:ARG:HA | 2:a:174:GLU:OE1 | 2.14 | 0.47 |
| 3:1:39:PRO:HD2 | 3:1:42:PHE:CB | 2.45 | 0.47 |
| 2:b:42:VAL:HA | 2:b:120:THR:O | 2.14 | 0.47 |
| 2:b:94:PRO:HB2 | 2:c:219:ARG:NH2 | 2.29 | 0.47 |
| 2:b:101:GLN:NE2 | 2:c:219:ARG:HD3 | 2.28 | 0.47 |
| 2:b:254:VAL:HG13 | 2:b:365:ILE:CG1 | 2.44 | 0.47 |
| 2:c:277:GLN:HG3 | 2:c:278:GLY:N | 2.30 | 0.47 |
| 2:d:101:GLN:NE2 | 2:e:219:ARG:HD3 | 2.29 | 0.47 |
| 2:g:348:ILE:O | 2:g:352:MET:HG3 | 2.14 | 0.47 |
| 2:k:94:PRO:HB2 | 2:l:219:ARG:NH2 | 2.30 | 0.47 |
| 2:l:353:GLN:HB2 | 2:l:358:LEU:HD23 | 1.96 | 0.47 |
| 2:n:120:THR:HG23 | 2:n:139:GLY:O | 2.15 | 0.47 |
| 2:n:123:MET:HE1 | 2:n:136:LEU:HB3 | 1.95 | 0.47 |
| 2:r:101:GLN:NE2 | 2:s:219:ARG:HD3 | 2.29 | 0.47 |
| 2:r:120:THR:HG23 | 2:r:139:GLY:O | 2.15 | 0.47 |
| 2:s:217:ASP:OD1 | 2:s:219:ARG:N | 2.35 | 0.47 |
| 2:t:94:PRO:HB2 | 2:u:219:ARG:NH2 | 2.29 | 0.47 |
| 2:u:120:THR:HG23 | 2:u:139:GLY:O | 2.15 | 0.47 |
| 2:v:338:LEU:HG | 2:v:338:LEU:O | 2.15 | 0.47 |
| 2:v:353:GLN:HB2 | 2:v:358:LEU:HD23 | 1.96 | 0.47 |
| 2:z:21:ARG:O | 2:z:25:LEU:HD22 | 2.14 | 0.47 |
| 3:3:77:CYS:HB3 | 3:3:80:TYR:CE1 | 2.48 | 0.47 |
| 3:5:39:PRO:HD2 | 3:5:42:PHE:CB | 2.45 | 0.47 |
| 3:7:83:SER:HA | 1:H:210:ASN:ND2 | 2.30 | 0.47 |
| 3:8:15:THR:HG23 | 3:8:43:THR:HG21 | 1.97 | 0.47 |
| 3:8:83:SER:HA | 1:I:210:ASN:ND2 | 2.30 | 0.47 |
| 3:11:77:CYS:HB3 | 3:11:80:TYR:CE1 | 2.48 | 0.47 |
| 3:12:77:CYS:HB3 | 3:12:80:TYR:CE1 | 2.48 | 0.47 |
| 3:15:17:THR:O | 3:15:18:ARG:NE | 2.48 | 0.47 |
| 3:16:15:THR:HG23 | 3:16:43:THR:HG21 | 1.98 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:20:39:PRO:HD2 | 3:20:42:PHE:CB | 2.45 | 0.47 |
| 3:21:39:PRO:HD2 | 3:21:42:PHE:CB | 2.45 | 0.47 |
| 3:21:83:SER:HA | 1:V:210:ASN:ND2 | 2.30 | 0.47 |
| 3:25:47:ASP:CG | 3:25:50:VAL:H | 2.14 | 0.47 |
| 1:E:176:GLU:OE2 | 1:G:90:LYS:HD3 | 2.14 | 0.47 |
| 1:J:150:VAL:HG12 | 1:J:165:GLY:HA3 | 1.97 | 0.47 |
| 1:L:159:GLY:O | 1:L:186:PRO:HG3 | 2.14 | 0.47 |
| 1:O:159:GLY:O | 1:O:186:PRO:HG3 | 2.14 | 0.47 |
| 1:S:171:ILE:HD12 | 1:U:88:ALA:CB | 2.34 | 0.47 |
| 1:T:130:ASN:CG | 1:U:102:THR:HG22 | 2.39 | 0.47 |
| 1:U:150:VAL:HG12 | 1:U:165:GLY:HA3 | 1.97 | 0.47 |
| 1:A:130:ASN:CG | 1:B:102:THR:HG22 | 2.41 | 0.46 |
| 1:A:150:VAL:HG12 | 1:A:165:GLY:HA3 | 1.97 | 0.46 |
| 3:1:22:VAL:HG13 | 3:1:34:LEU:HD23 | 1.96 | 0.46 |
| 2:d:81:LEU:HD23 | 2:d:81:LEU:N | 2.28 | 0.46 |
| 2:e:117:ARG:NH1 | 2:e:145:GLY:HA2 | 2.31 | 0.46 |
| 2:f:348:ILE:O | 2:f:352:MET:HG3 | 2.14 | 0.46 |
| 2:g:254:VAL:HG13 | 2:g:365:ILE:CG1 | 2.44 | 0.46 |
| 2:h:21:ARG:O | 2:h:25:LEU:HD22 | 2.14 | 0.46 |
| 2:i:21:ARG:O | 2:i:25:LEU:HD22 | 2.14 | 0.46 |
| 2:o:120:THR:HG23 | 2:o:139:GLY:O | 2.15 | 0.46 |
| 2:o:254:VAL:HG13 | 2:o:365:ILE:CG1 | 2.44 | 0.46 |
| 2:o:277:GLN:HG3 | 2:o:278:GLY:N | 2.31 | 0.46 |
| 2:p:196:MET:HE3 | 2:p:196:MET:C | 2.39 | 0.46 |
| 2:q:117:ARG:NH1 | 2:q:145:GLY:HA2 | 2.31 | 0.46 |
| 2:q:123:MET:HE1 | 2:q:136:LEU:HB3 | 1.95 | 0.46 |
| 2:r:79:MET:HE2 | 2:r:79:MET:HB2 | 1.69 | 0.46 |
| 2:r:328:LEU:HD21 | 2:s:273:CYS:HA | 1.97 | 0.46 |
| 2:r:353:GLN:HB2 | 2:r:358:LEU:HD23 | 1.96 | 0.46 |
| 2:s:42:VAL:HA | 2:s:120:THR:O | 2.14 | 0.46 |
| 2:x:166:THR:HG21 | 2:z:362:LEU:HD21 | 1.96 | 0.46 |
| 3:2:39:PRO:HD2 | 3:2:42:PHE:CB | 2.45 | 0.46 |
| 3:5:17:THR:O | 3:5:18:ARG:NE | 2.48 | 0.46 |
| 3:5:72:GLN:HG2 | 3:5:73:PRO:CD | 2.41 | 0.46 |
| 3:6:28:ILE:O | 3:6:29:SER:OG | 2.21 | 0.46 |
| 3:7:17:THR:O | 3:7:18:ARG:NE | 2.48 | 0.46 |
| 3:9:15:THR:HG23 | 3:9:43:THR:HG21 | 1.98 | 0.46 |
| 3:10:15:THR:HG23 | 3:10:43:THR:HG21 | 1.98 | 0.46 |
| 3:11:15:THR:HG23 | 3:11:43:THR:HG21 | 1.97 | 0.46 |
| 3:13:75:GLY:HA2 | 3:13:89:ARG:O | 2.14 | 0.46 |
| 3:14:15:THR:HG23 | 3:14:43:THR:HG21 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:15:15:THR:HG23 | 3:15:43:THR:HG21 | 1.98 | 0.46 |
| 3:15:39:PRO:HD2 | 3:15:42:PHE:CB | 2.45 | 0.46 |
| 3:17:15:THR:HG23 | 3:17:43:THR:HG21 | 1.97 | 0.46 |
| 3:18:17:THR:O | 3:18:18:ARG:NE | 2.48 | 0.46 |
| 3:19:47:ASP:CG | 3:19:50:VAL:H | 2.14 | 0.46 |
| 3:23:39:PRO:HD2 | 3:23:42:PHE:CB | 2.45 | 0.46 |
| 1:K:150:VAL:HG12 | 1:K:165:GLY:HA3 | 1.97 | 0.46 |
| 1:M:130:ASN:CG | 1:N:102:THR:HG22 | 2.39 | 0.46 |
| 1:M:150:VAL:HG12 | 1:M:165:GLY:HA3 | 1.97 | 0.46 |
| 1:V:109:VAL:HG21 | 1:V:117:PHE:O | 2.14 | 0.46 |
| 1:X:40:ILE:H | 1:X:40:ILE:HG12 | 1.49 | 0.46 |
| 1:X:109:VAL:HG21 | 1:X:117:PHE:O | 2.14 | 0.46 |
| 1:Z:109:VAL:HG21 | 1:Z:117:PHE:O | 2.14 | 0.46 |
| 1:Z:150:VAL:HG12 | 1:Z:165:GLY:HA3 | 1.97 | 0.46 |
| 1:A:109:VAL:HG21 | 1:A:117:PHE:O | 2.14 | 0.46 |
| 3:1:83:SER:HA | 1:B:210:ASN:ND2 | 2.30 | 0.46 |
| 2:c:21:ARG:O | 2:c:25:LEU:HD22 | 2.14 | 0.46 |
| 2:c:117:ARG:NH1 | 2:c:145:GLY:HA2 | 2.31 | 0.46 |
| 2:e:21:ARG:O | 2:e:25:LEU:HD22 | 2.14 | 0.46 |
| 2:e:94:PRO:HB2 | 2:f:219:ARG:NH2 | 2.30 | 0.46 |
| 2:e:277:GLN:HG3 | 2:e:278:GLY:N | 2.31 | 0.46 |
| 2:f:21:ARG:O | 2:f:25:LEU:HD22 | 2.14 | 0.46 |
| 2:g:21:ARG:O | 2:g:25:LEU:HD22 | 2.14 | 0.46 |
| 2:g:101:GLN:NE2 | 2:h:188:GLN:HB3 | 2.31 | 0.46 |
| 2:j:277:GLN:HG3 | 2:j:278:GLY:N | 2.30 | 0.46 |
| 2:j:353:GLN:HB2 | 2:j:358:LEU:HD23 | 1.96 | 0.46 |
| 2:l:141:ILE:HD13 | 2:l:165:ILE:CD1 | 2.39 | 0.46 |
| 2:m:98:ARG:HA | 2:m:174:GLU:OE1 | 2.14 | 0.46 |
| 2:m:353:GLN:HB2 | 2:m:358:LEU:HD23 | 1.96 | 0.46 |
| 2:o:117:ARG:NH1 | 2:o:145:GLY:HA2 | 2.31 | 0.46 |
| 2:q:94:PRO:HB2 | 2:r:219:ARG:NH2 | 2.30 | 0.46 |
| 2:q:277:GLN:HG3 | 2:q:278:GLY:N | 2.31 | 0.46 |
| 2:t:353:GLN:HB2 | 2:t:358:LEU:HD23 | 1.96 | 0.46 |
| 2:u:338:LEU:O | 2:u:338:LEU:HG | 2.15 | 0.46 |
| 2:v:120:THR:HG23 | 2:v:139:GLY:O | 2.15 | 0.46 |
| 2:v:328:LEU:HD21 | 2:w:273:CYS:HA | 1.97 | 0.46 |
| 3:5:83:SER:HA | 1:F:210:ASN:ND2 | 2.31 | 0.46 |
| 3:6:15:THR:HG23 | 3:6:43:THR:HG21 | 1.97 | 0.46 |
| 3:7:15:THR:HG23 | 3:7:43:THR:HG21 | 1.98 | 0.46 |
| 3:7:39:PRO:HD2 | 3:7:42:PHE:CB | 2.45 | 0.46 |
| 3:8:22:VAL:HG13 | 3:8:34:LEU:HD23 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:8:47:ASP:CG | 3:8:50:VAL:H | 2.14 | 0.46 |
| 3:10:77:CYS:HB3 | 3:10:80:TYR:CE1 | 2.48 | 0.46 |
| 3:13:15:THR:HG23 | 3:13:43:THR:HG21 | 1.97 | 0.46 |
| 3:16:17:THR:O | 3:16:18:ARG:NE | 2.48 | 0.46 |
| 3:18:15:THR:HG23 | 3:18:43:THR:HG21 | 1.98 | 0.46 |
| 3:18:39:PRO:HD2 | 3:18:42:PHE:CB | 2.45 | 0.46 |
| 3:20:83:SER:HA | 1:U:210:ASN:ND2 | 2.30 | 0.46 |
| 3:22:39:PRO:HD2 | 3:22:42:PHE:CB | 2.45 | 0.46 |
| 3:24:39:PRO:HD2 | 3:24:42:PHE:CB | 2.45 | 0.46 |
| 3:25:39:PRO:HD2 | 3:25:42:PHE:CB | 2.45 | 0.46 |
| 1:C:130:ASN:CG | 1:D:102:THR:HG22 | 2.41 | 0.46 |
| 1:E:112:TYR:CE1 | 1:E:113:LEU:HG | 2.51 | 0.46 |
| 1:I:40:ILE:H | 1:I:40:ILE:HG12 | 1.49 | 0.46 |
| 1:L:130:ASN:CG | 1:M:102:THR:HG22 | 2.40 | 0.46 |
| 1:L:150:VAL:HG12 | 1:L:165:GLY:HA3 | 1.97 | 0.46 |
| 1:T:150:VAL:HG12 | 1:T:165:GLY:HA3 | 1.97 | 0.46 |
| 1:V:101:LYS:HZ2 | 1:V:101:LYS:HB3 | 1.81 | 0.46 |
| 1:Y:121:ARG:HB3 | 1:Z:111:ARG:HB3 | 1.96 | 0.46 |
| 1:A:106:PHE:O | 1:A:107:ASP:HB2 | 2.16 | 0.46 |
| 2:a:117:ARG:NH1 | 2:a:145:GLY:HA2 | 2.30 | 0.46 |
| 2:a:340:ALA:HB1 | 2:a:344:ASP:HB2 | 1.98 | 0.46 |
| 2:a:355:ALA:HB2 | 2:z:254:VAL:CG2 | 2.45 | 0.46 |
| 2:b:21:ARG:O | 2:b:25:LEU:HD22 | 2.14 | 0.46 |
| 2:d:21:ARG:O | 2:d:25:LEU:HD22 | 2.14 | 0.46 |
| 2:g:117:ARG:NH1 | 2:g:145:GLY:HA2 | 2.31 | 0.46 |
| 2:h:96:PHE:O | 2:i:219:ARG:HD2 | 2.15 | 0.46 |
| 2:h:217:ASP:OD1 | 2:h:219:ARG:N | 2.35 | 0.46 |
| 2:h:277:GLN:HG3 | 2:h:278:GLY:N | 2.31 | 0.46 |
| 2:h:340:ALA:HB1 | 2:h:344:ASP:HB2 | 1.98 | 0.46 |
| 2:i:123:MET:HE1 | 2:i:136:LEU:HB3 | 1.95 | 0.46 |
| 2:i:353:GLN:HB2 | 2:i:358:LEU:HD23 | 1.97 | 0.46 |
| 2:j:338:LEU:O | 2:j:338:LEU:HG | 2.15 | 0.46 |
| 2:l:277:GLN:HG3 | 2:l:278:GLY:N | 2.30 | 0.46 |
| 2:m:101:GLN:NE2 | 2:n:188:GLN:HB3 | 2.31 | 0.46 |
| 2:m:117:ARG:NH1 | 2:m:145:GLY:HA2 | 2.31 | 0.46 |
| 2:p:120:THR:HG23 | 2:p:139:GLY:O | 2.15 | 0.46 |
| 2:w:338:LEU:HG | 2:w:338:LEU:O | 2.15 | 0.46 |
| 2:x:117:ARG:NH1 | 2:x:145:GLY:HA2 | 2.30 | 0.46 |
| 2:z:353:GLN:HB2 | 2:z:358:LEU:HD23 | 1.96 | 0.46 |
| 3:2:77:CYS:HB3 | 3:2:80:TYR:CE1 | 2.48 | 0.46 |
| 3:2:83:SER:HA | 1:C:210:ASN:ND2 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:12:15:THR:HG23 | 3:12:43:THR:HG21 | 1.98 | 0.46 |
| 3:19:83:SER:HA | 1:T:210:ASN:ND2 | 2.30 | 0.46 |
| 3:26:39:PRO:HD2 | 3:26:42:PHE:CB | 2.45 | 0.46 |
| 1:B:101:LYS:HB3 | 1:B:101:LYS:HZ2 | 1.81 | 0.46 |
| 1:B:109:VAL:HG21 | 1:B:117:PHE:O | 2.14 | 0.46 |
| 1:B:150:VAL:HG12 | 1:B:165:GLY:HA3 | 1.97 | 0.46 |
| 1:D:109:VAL:HG21 | 1:D:117:PHE:O | 2.14 | 0.46 |
| 1:F:106:PHE:O | 1:F:107:ASP:HB2 | 2.16 | 0.46 |
| 1:F:109:VAL:HG21 | 1:F:117:PHE:O | 2.14 | 0.46 |
| 1:G:82:LEU:HD12 | 1:G:146:GLY:HA3 | 1.97 | 0.46 |
| 1:I:71:PRO:HD2 | 1:I:189:ILE:HD13 | 1.98 | 0.46 |
| 1:J:71:PRO:HD2 | 1:J:189:ILE:HD13 | 1.98 | 0.46 |
| 1:N:110:PRO:O | 1:N:114:GLN:HG2 | 2.16 | 0.46 |
| 1:N:159:GLY:O | 1:N:186:PRO:HG3 | 2.14 | 0.46 |
| 1:Q:112:TYR:CE1 | 1:Q:113:LEU:HG | 2.51 | 0.46 |
| 1:S:112:TYR:CE1 | 1:S:113:LEU:HG | 2.51 | 0.46 |
| 1:S:150:VAL:HG12 | 1:S:165:GLY:HA3 | 1.97 | 0.46 |
| 1:T:101:LYS:HZ2 | 1:T:101:LYS:HB3 | 1.81 | 0.46 |
| 1:T:106:PHE:O | 1:T:107:ASP:HB2 | 2.16 | 0.46 |
| 1:Y:109:VAL:HG21 | 1:Y:117:PHE:O | 2.14 | 0.46 |
| 2:a:353:GLN:HB2 | 2:a:358:LEU:HD23 | 1.96 | 0.46 |
| 2:c:340:ALA:HB1 | 2:c:344:ASP:HB2 | 1.98 | 0.46 |
| 2:d:328:LEU:HD21 | 2:e:273:CYS:HA | 1.97 | 0.46 |
| 2:g:42:VAL:HA | 2:g:120:THR:O | 2.14 | 0.46 |
| 2:h:196:MET:HE3 | 2:h:196:MET:C | 2.39 | 0.46 |
| 2:i:338:LEU:HG | 2:i:338:LEU:O | 2.15 | 0.46 |
| 2:k:196:MET:HE3 | 2:k:196:MET:C | 2.39 | 0.46 |
| 2:k:353:GLN:HB2 | 2:k:358:LEU:HD23 | 1.96 | 0.46 |
| 2:l:105:VAL:CG1 | 2:l:169:ALA:HB2 | 2.46 | 0.46 |
| 2:p:101:GLN:NE2 | 2:q:219:ARG:HD3 | 2.29 | 0.46 |
| 2:p:217:ASP:OD1 | 2:p:219:ARG:N | 2.35 | 0.46 |
| 2:p:338:LEU:HG | 2:p:338:LEU:O | 2.15 | 0.46 |
| 2:q:120:THR:HG23 | 2:q:139:GLY:O | 2.15 | 0.46 |
| 2:v:117:ARG:NH1 | 2:v:145:GLY:HA2 | 2.31 | 0.46 |
| 2:x:277:GLN:HG3 | 2:x:278:GLY:N | 2.31 | 0.46 |
| 3:4:22:VAL:HG13 | 3:4:34:LEU:HD23 | 1.96 | 0.46 |
| 3:4:83:SER:HA | 1:E:210:ASN:ND2 | 2.31 | 0.46 |
| 3:6:17:THR:O | 3:6:18:ARG:NE | 2.48 | 0.46 |
| 3:15:83:SER:HA | 1:P:210:ASN:ND2 | 2.30 | 0.46 |
| 3:16:39:PRO:HD2 | 3:16:42:PHE:CB | 2.45 | 0.46 |
| 3:17:17:THR:O | 3:17:18:ARG:NE | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:23:83:SER:HA | 1:X:210:ASN:ND2 | 2.31 | 0.46 |
| 1:C:109:VAL:HG21 | 1:C:117:PHE:O | 2.14 | 0.46 |
| 1:C:112:TYR:CE1 | 1:C:113:LEU:HG | 2.51 | 0.46 |
| 1:F:82:LEU:HD12 | 1:F:146:GLY:HA3 | 1.98 | 0.46 |
| 1:F:110:PRO:O | 1:F:114:GLN:HG2 | 2.16 | 0.46 |
| 1:H:71:PRO:HD2 | 1:H:189:ILE:HD13 | 1.98 | 0.46 |
| 1:I:110:PRO:O | 1:I:114:GLN:HG2 | 2.16 | 0.46 |
| 1:I:150:VAL:HG12 | 1:I:165:GLY:HA3 | 1.97 | 0.46 |
| 1:K:110:PRO:O | 1:K:114:GLN:HG2 | 2.16 | 0.46 |
| 1:L:71:PRO:HD2 | 1:L:189:ILE:HD13 | 1.98 | 0.46 |
| 1:L:110:PRO:O | 1:L:114:GLN:HG2 | 2.16 | 0.46 |
| 1:N:106:PHE:O | 1:N:107:ASP:HB2 | 2.16 | 0.46 |
| 1:N:150:VAL:HG12 | 1:N:165:GLY:HA3 | 1.97 | 0.46 |
| 1:P:130:ASN:CG | 1:Q:102:THR:HG22 | 2.40 | 0.46 |
| 1:S:106:PHE:O | 1:S:107:ASP:HB2 | 2.16 | 0.46 |
| 1:U:106:PHE:O | 1:U:107:ASP:HB2 | 2.16 | 0.46 |
| 1:V:106:PHE:O | 1:V:107:ASP:HB2 | 2.16 | 0.46 |
| 1:V:112:TYR:CE1 | 1:V:113:LEU:HG | 2.51 | 0.46 |
| 1:W:112:TYR:CE1 | 1:W:113:LEU:HG | 2.51 | 0.46 |
| 1:X:101:LYS:HZ2 | 1:X:101:LYS:HB3 | 1.81 | 0.46 |
| 1:Z:106:PHE:O | 1:Z:107:ASP:HB2 | 2.16 | 0.46 |
| 2:b:96:PHE:O | 2:c:219:ARG:HD2 | 2.15 | 0.46 |
| 2:c:42:VAL:HA | 2:c:120:THR:O | 2.14 | 0.46 |
| 2:e:217:ASP:OD1 | 2:e:219:ARG:N | 2.35 | 0.46 |
| 2:f:340:ALA:HB1 | 2:f:344:ASP:HB2 | 1.98 | 0.46 |
| 2:h:338:LEU:HG | 2:h:338:LEU:O | 2.15 | 0.46 |
| 2:i:105:VAL:CG1 | 2:i:169:ALA:HB2 | 2.46 | 0.46 |
| 2:i:117:ARG:NH1 | 2:i:145:GLY:HA2 | 2.31 | 0.46 |
| 2:l:99:GLN:HE21 | 1:K:50:SER:HB3 | 1.81 | 0.46 |
| 2:m:105:VAL:CG1 | 2:m:169:ALA:HB2 | 2.46 | 0.46 |
| 2:n:105:VAL:CG1 | 2:n:169:ALA:HB2 | 2.46 | 0.46 |
| 2:n:123:MET:CE | 2:n:136:LEU:HD22 | 2.38 | 0.46 |
| 2:n:353:GLN:HB2 | 2:n:358:LEU:HD23 | 1.97 | 0.46 |
| 2:o:353:GLN:HB2 | 2:o:358:LEU:HD23 | 1.97 | 0.46 |
| 2:p:42:VAL:HA | 2:p:120:THR:O | 2.14 | 0.46 |
| 2:q:338:LEU:HG | 2:q:338:LEU:O | 2.15 | 0.46 |
| 2:r:42:VAL:HA | 2:r:120:THR:O | 2.14 | 0.46 |
| 2:r:319:LEU:HD12 | 2:r:319:LEU:HA | 1.80 | 0.46 |
| 2:s:117:ARG:NH1 | 2:s:145:GLY:HA2 | 2.31 | 0.46 |
| 2:s:120:THR:HG23 | 2:s:139:GLY:O | 2.15 | 0.46 |
| 2:t:338:LEU:HG | 2:t:338:LEU:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:u:94:PRO:HB2 | 2:v:219:ARG:NH2 | 2.30 | 0.46 |
| 2:v:166:THR:HG21 | 2:x:362:LEU:HD21 | 1.96 | 0.46 |
| 2:x:57:PHE:CE1 | 2:x:110:MET:HE2 | 2.51 | 0.46 |
| 3:2:22:VAL:HG13 | 3:2:34:LEU:HD23 | 1.96 | 0.46 |
| 3:5:15:THR:HG23 | 3:5:43:THR:HG21 | 1.98 | 0.46 |
| 3:5:22:VAL:HG13 | 3:5:34:LEU:HD23 | 1.96 | 0.46 |
| 3:12:39:PRO:HD2 | 3:12:42:PHE:CB | 2.45 | 0.46 |
| 3:13:77:CYS:HB3 | 3:13:80:TYR:CE1 | 2.48 | 0.46 |
| 3:14:39:PRO:HD2 | 3:14:42:PHE:CB | 2.45 | 0.46 |
| 3:19:15:THR:HG23 | 3:19:43:THR:HG21 | 1.98 | 0.46 |
| 1:F:130:ASN:CG | 1:G:102:THR:HG22 | 2.41 | 0.46 |
| 1:G:71:PRO:HD2 | 1:G:189:ILE:HD13 | 1.98 | 0.46 |
| 1:G:106:PHE:O | 1:G:107:ASP:HB2 | 2.16 | 0.46 |
| 1:J:171:ILE:O | 1:K:207:TYR:O | 2.34 | 0.46 |
| 1:K:71:PRO:HD2 | 1:K:189:ILE:HD13 | 1.98 | 0.46 |
| 1:L:112:TYR:CE1 | 1:L:113:LEU:HG | 2.51 | 0.46 |
| 1:M:71:PRO:HD2 | 1:M:189:ILE:HD13 | 1.98 | 0.46 |
| 1:M:159:GLY:O | 1:M:186:PRO:HG3 | 2.14 | 0.46 |
| 1:N:71:PRO:HD2 | 1:N:189:ILE:HD13 | 1.98 | 0.46 |
| 1:P:106:PHE:O | 1:P:107:ASP:HB2 | 2.16 | 0.46 |
| 1:Q:106:PHE:O | 1:Q:107:ASP:HB2 | 2.16 | 0.46 |
| 1:U:112:TYR:CE1 | 1:U:113:LEU:HG | 2.51 | 0.46 |
| 1:W:106:PHE:O | 1:W:107:ASP:HB2 | 2.16 | 0.46 |
| 1:W:110:PRO:O | 1:W:114:GLN:HG2 | 2.16 | 0.46 |
| 1:X:106:PHE:O | 1:X:107:ASP:HB2 | 2.16 | 0.46 |
| 1:X:112:TYR:CE1 | 1:X:113:LEU:HG | 2.51 | 0.46 |
| 1:Y:110:PRO:O | 1:Y:114:GLN:HG2 | 2.16 | 0.46 |
| 2:d:338:LEU:HG | 2:d:338:LEU:O | 2.15 | 0.46 |
| 2:e:120:THR:HG23 | 2:e:139:GLY:O | 2.15 | 0.46 |
| 2:e:338:LEU:O | 2:e:338:LEU:HG | 2.15 | 0.46 |
| 2:e:353:GLN:HB2 | 2:e:358:LEU:HD23 | 1.96 | 0.46 |
| 2:f:105:VAL:CG1 | 2:f:169:ALA:HB2 | 2.46 | 0.46 |
| 2:g:57:PHE:CE1 | 2:g:110:MET:HE2 | 2.51 | 0.46 |
| 2:g:277:GLN:HG3 | 2:g:278:GLY:N | 2.31 | 0.46 |
| 2:g:338:LEU:O | 2:g:338:LEU:HG | 2.15 | 0.46 |
| 2:h:40:GLY:HA3 | 2:h:124:THR:CG2 | 2.46 | 0.46 |
| 2:h:93:TYR:OH | 2:h:173:ARG:O | 2.24 | 0.46 |
| 2:j:340:ALA:HB1 | 2:j:344:ASP:HB2 | 1.98 | 0.46 |
| 2:k:105:VAL:CG1 | 2:k:169:ALA:HB2 | 2.46 | 0.46 |
| 2:k:117:ARG:NH1 | 2:k:145:GLY:HA2 | 2.31 | 0.46 |
| 2:k:120:THR:HG23 | 2:k:139:GLY:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:l:101:GLN:NE2 | 2:m:219:ARG:HD3 | 2.29 | 0.46 |
| 2:m:277:GLN:HG3 | 2:m:278:GLY:N | 2.31 | 0.46 |
| 2:n:277:GLN:HG3 | 2:n:278:GLY:N | 2.30 | 0.46 |
| 2:o:105:VAL:CG1 | 2:o:169:ALA:HB2 | 2.46 | 0.46 |
| 2:o:123:MET:CE | 2:o:136:LEU:HD22 | 2.38 | 0.46 |
| 2:o:338:LEU:O | 2:o:338:LEU:HG | 2.15 | 0.46 |
| 2:p:105:VAL:CG1 | 2:p:169:ALA:HB2 | 2.46 | 0.46 |
| 2:s:277:GLN:HG3 | 2:s:278:GLY:N | 2.30 | 0.46 |
| 2:x:99:GLN:HE21 | 1:W:50:SER:HB3 | 1.81 | 0.46 |
| 2:y:117:ARG:NH1 | 2:y:145:GLY:HA2 | 2.30 | 0.46 |
| 2:y:120:THR:HG23 | 2:y:139:GLY:O | 2.15 | 0.46 |
| 2:y:277:GLN:HG3 | 2:y:278:GLY:N | 2.31 | 0.46 |
| 2:y:340:ALA:HB1 | 2:y:344:ASP:HB2 | 1.98 | 0.46 |
| 2:z:57:PHE:CE1 | 2:z:110:MET:HE2 | 2.51 | 0.46 |
| 3:6:22:VAL:HG13 | 3:6:34:LEU:HD23 | 1.96 | 0.46 |
| 3:9:39:PRO:HD2 | 3:9:42:PHE:CB | 2.45 | 0.46 |
| 3:9:77:CYS:HB3 | 3:9:80:TYR:CE1 | 2.48 | 0.46 |
| 3:12:83:SER:HA | 1:M:210:ASN:ND2 | 2.30 | 0.46 |
| 3:20:15:THR:HG23 | 3:20:43:THR:HG21 | 1.98 | 0.46 |
| 3:20:72:GLN:HG2 | 3:20:73:PRO:CD | 2.41 | 0.46 |
| 1:E:106:PHE:O | 1:E:107:ASP:HB2 | 2.16 | 0.46 |
| 1:F:71:PRO:HD2 | 1:F:189:ILE:HD13 | 1.98 | 0.46 |
| 1:H:110:PRO:O | 1:H:114:GLN:HG2 | 2.16 | 0.46 |
| 1:H:150:VAL:HG12 | 1:H:165:GLY:HA3 | 1.97 | 0.46 |
| 1:I:130:ASN:CG | 1:J:102:THR:HG22 | 2.40 | 0.46 |
| 1:N:112:TYR:CE1 | 1:N:113:LEU:HG | 2.51 | 0.46 |
| 1:R:101:LYS:HZ2 | 1:R:101:LYS:HB3 | 1.81 | 0.46 |
| 1:R:106:PHE:O | 1:R:107:ASP:HB2 | 2.16 | 0.46 |
| 1:R:150:VAL:HG12 | 1:R:165:GLY:HA3 | 1.97 | 0.46 |
| 1:U:110:PRO:O | 1:U:114:GLN:HG2 | 2.16 | 0.46 |
| 1:Y:106:PHE:O | 1:Y:107:ASP:HB2 | 2.16 | 0.46 |
| 2:a:362:LEU:HD21 | 2:y:166:THR:HG21 | 1.96 | 0.46 |
| 3:1:77:CYS:HB3 | 3:1:80:TYR:CE1 | 2.48 | 0.46 |
| 2:e:57:PHE:CE1 | 2:e:110:MET:HE2 | 2.51 | 0.46 |
| 2:f:120:THR:HG23 | 2:f:139:GLY:O | 2.15 | 0.46 |
| 2:f:338:LEU:HG | 2:f:338:LEU:O | 2.15 | 0.46 |
| 2:g:40:GLY:HA3 | 2:g:124:THR:CG2 | 2.46 | 0.46 |
| 2:i:40:GLY:HA3 | 2:i:124:THR:CG2 | 2.46 | 0.46 |
| 2:j:40:GLY:HA3 | 2:j:124:THR:CG2 | 2.46 | 0.46 |
| 2:j:57:PHE:CE1 | 2:j:110:MET:HE2 | 2.51 | 0.46 |
| 2:m:57:PHE:CE1 | 2:m:110:MET:HE2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:57:PHE:CE1 | 2:n:110:MET:HE2 | 2.51 | 0.46 |
| 2:n:93:TYR:OH | 2:n:173:ARG:O | 2.24 | 0.46 |
| 2:r:105:VAL:CG1 | 2:r:169:ALA:HB2 | 2.46 | 0.46 |
| 2:s:96:PHE:O | 2:t:219:ARG:HD2 | 2.14 | 0.46 |
| 2:v:57:PHE:CE1 | 2:v:110:MET:HE2 | 2.51 | 0.46 |
| 2:v:340:ALA:HB1 | 2:v:344:ASP:HB2 | 1.98 | 0.46 |
| 3:3:22:VAL:HG13 | 3:3:34:LEU:HD23 | 1.96 | 0.46 |
| 3:7:22:VAL:HG13 | 3:7:34:LEU:HD23 | 1.96 | 0.46 |
| 1:C:150:VAL:HG12 | 1:C:165:GLY:HA3 | 1.97 | 0.46 |
| 1:D:176:GLU:OE1 | 1:D:207:TYR:OH | 2.21 | 0.46 |
| 1:G:112:TYR:CE1 | 1:G:113:LEU:HG | 2.51 | 0.46 |
| 1:H:82:LEU:HD12 | 1:H:146:GLY:HA3 | 1.98 | 0.46 |
| 1:J:112:TYR:CE1 | 1:J:113:LEU:HG | 2.51 | 0.46 |
| 1:M:106:PHE:O | 1:M:107:ASP:HB2 | 2.16 | 0.46 |
| 1:O:106:PHE:O | 1:O:107:ASP:HB2 | 2.16 | 0.46 |
| 1:O:110:PRO:O | 1:O:114:GLN:HG2 | 2.16 | 0.46 |
| 1:O:112:TYR:CE1 | 1:O:113:LEU:HG | 2.51 | 0.46 |
| 1:O:130:ASN:CG | 1:P:102:THR:HG22 | 2.40 | 0.46 |
| 1:O:150:VAL:HG12 | 1:O:165:GLY:HA3 | 1.97 | 0.46 |
| 1:T:124:MET:HE3 | 1:T:124:MET:HB3 | 1.77 | 0.46 |
| 1:A:110:PRO:O | 1:A:114:GLN:HG2 | 2.16 | 0.46 |
| 2:a:277:GLN:HG3 | 2:a:278:GLY:N | 2.31 | 0.46 |
| 2:c:57:PHE:CE1 | 2:c:110:MET:HE2 | 2.51 | 0.46 |
| 2:d:120:THR:HG23 | 2:d:139:GLY:O | 2.15 | 0.46 |
| 2:e:340:ALA:HB1 | 2:e:344:ASP:HB2 | 1.98 | 0.46 |
| 2:g:94:PRO:HB2 | 2:h:219:ARG:NH2 | 2.31 | 0.46 |
| 2:i:57:PHE:CE1 | 2:i:110:MET:HE2 | 2.51 | 0.46 |
| 2:l:57:PHE:CE1 | 2:l:110:MET:HE2 | 2.51 | 0.46 |
| 2:m:120:THR:HG23 | 2:m:139:GLY:O | 2.15 | 0.46 |
| 2:q:105:VAL:CG1 | 2:q:169:ALA:HB2 | 2.46 | 0.46 |
| 2:q:353:GLN:HB2 | 2:q:358:LEU:HD23 | 1.97 | 0.46 |
| 2:r:40:GLY:HA3 | 2:r:124:THR:CG2 | 2.46 | 0.46 |
| 2:r:99:GLN:HE21 | 1:Q:50:SER:HB3 | 1.81 | 0.46 |
| 2:s:40:GLY:HA3 | 2:s:124:THR:CG2 | 2.46 | 0.46 |
| 2:s:123:MET:CE | 2:s:136:LEU:HD22 | 2.38 | 0.46 |
| 2:t:40:GLY:HA3 | 2:t:124:THR:CG2 | 2.46 | 0.46 |
| 2:t:117:ARG:NH1 | 2:t:145:GLY:HA2 | 2.31 | 0.46 |
| 2:t:328:LEU:HD21 | 2:u:273:CYS:HA | 1.98 | 0.46 |
| 2:v:277:GLN:HG3 | 2:v:278:GLY:N | 2.31 | 0.46 |
| 2:x:340:ALA:HB1 | 2:x:344:ASP:HB2 | 1.98 | 0.46 |
| 2:z:117:ARG:NH1 | 2:z:145:GLY:HA2 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4:15:THR:HG23 | 3:4:43:THR:HG21 | 1.98 | 0.46 |
| 3:11:83:SER:HA | 1:L:210:ASN:ND2 | 2.31 | 0.46 |
| 1:C:110:PRO:O | 1:C:114:GLN:HG2 | 2.16 | 0.46 |
| 1:D:171:ILE:O | 1:E:207:TYR:O | 2.34 | 0.46 |
| 1:E:71:PRO:HD2 | 1:E:189:ILE:HD13 | 1.98 | 0.46 |
| 1:E:110:PRO:O | 1:E:114:GLN:HG2 | 2.16 | 0.46 |
| 1:H:112:TYR:CE1 | 1:H:113:LEU:HG | 2.51 | 0.46 |
| 1:K:106:PHE:O | 1:K:107:ASP:HB2 | 2.16 | 0.46 |
| 1:L:78:LEU:HD12 | 1:L:193:ASN:O | 2.16 | 0.46 |
| 1:O:71:PRO:HD2 | 1:O:189:ILE:HD13 | 1.98 | 0.46 |
| 1:O:78:LEU:HD12 | 1:O:193:ASN:O | 2.16 | 0.46 |
| 1:P:112:TYR:CE1 | 1:P:113:LEU:HG | 2.51 | 0.46 |
| 1:Q:110:PRO:O | 1:Q:114:GLN:HG2 | 2.16 | 0.46 |
| 1:S:110:PRO:O | 1:S:114:GLN:HG2 | 2.16 | 0.46 |
| 1:T:112:TYR:CE1 | 1:T:113:LEU:HG | 2.51 | 0.46 |
| 1:W:109:VAL:HG21 | 1:W:117:PHE:O | 2.14 | 0.46 |
| 1:Y:112:TYR:CE1 | 1:Y:113:LEU:HG | 2.51 | 0.46 |
| 2:a:217:ASP:OD1 | 2:a:219:ARG:N | 2.35 | 0.46 |
| 2:b:93:TYR:OH | 2:b:173:ARG:O | 2.24 | 0.46 |
| 2:c:101:GLN:NE2 | 2:d:188:GLN:HB3 | 2.30 | 0.46 |
| 2:f:277:GLN:HG3 | 2:f:278:GLY:N | 2.31 | 0.46 |
| 2:g:353:GLN:HB2 | 2:g:358:LEU:HD23 | 1.97 | 0.46 |
| 2:h:105:VAL:CG1 | 2:h:169:ALA:HB2 | 2.46 | 0.46 |
| 2:h:117:ARG:NH1 | 2:h:145:GLY:HA2 | 2.31 | 0.46 |
| 2:l:79:MET:HE2 | 2:l:79:MET:HB2 | 1.69 | 0.46 |
| 2:l:340:ALA:HB1 | 2:l:344:ASP:HB2 | 1.98 | 0.46 |
| 2:m:94:PRO:HB2 | 2:n:219:ARG:NH2 | 2.31 | 0.46 |
| 2:m:123:MET:CE | 2:m:136:LEU:HD22 | 2.38 | 0.46 |
| 2:n:96:PHE:O | 2:o:219:ARG:HD2 | 2.15 | 0.46 |
| 2:p:123:MET:CE | 2:p:136:LEU:HD22 | 2.38 | 0.46 |
| 2:p:353:GLN:HB2 | 2:p:358:LEU:HD23 | 1.96 | 0.46 |
| 2:q:40:GLY:HA3 | 2:q:124:THR:CG2 | 2.46 | 0.46 |
| 2:r:123:MET:CE | 2:r:136:LEU:HD22 | 2.38 | 0.46 |
| 2:r:338:LEU:O | 2:r:338:LEU:HG | 2.15 | 0.46 |
| 2:t:277:GLN:HG3 | 2:t:278:GLY:N | 2.31 | 0.46 |
| 2:t:340:ALA:HB1 | 2:t:344:ASP:HB2 | 1.98 | 0.46 |
| 2:u:40:GLY:HA3 | 2:u:124:THR:CG2 | 2.46 | 0.46 |
| 2:u:353:GLN:HB2 | 2:u:358:LEU:HD23 | 1.96 | 0.46 |
| 2:x:40:GLY:HA3 | 2:x:124:THR:CG2 | 2.46 | 0.46 |
| 2:z:40:GLY:HA3 | 2:z:124:THR:CG2 | 2.46 | 0.46 |
| 2:z:277:GLN:HG3 | 2:z:278:GLY:N | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:6:72:GLN:HG2 | 3:6:73:PRO:CD | 2.41 | 0.46 |
| 3:10:83:SER:HA | 1:K:210:ASN:ND2 | 2.31 | 0.46 |
| 3:11:39:PRO:HD2 | 3:11:42:PHE:CB | 2.45 | 0.46 |
| 3:17:83:SER:HA | 1:R:210:ASN:ND2 | 2.31 | 0.46 |
| 3:21:15:THR:HG23 | 3:21:43:THR:HG21 | 1.98 | 0.46 |
| 3:22:83:SER:HA | 1:W:210:ASN:ND2 | 2.31 | 0.46 |
| 1:B:106:PHE:O | 1:B:107:ASP:HB2 | 2.16 | 0.46 |
| 1:D:71:PRO:HD2 | 1:D:189:ILE:HD13 | 1.98 | 0.46 |
| 1:E:176:GLU:OE1 | 1:E:207:TYR:OH | 2.21 | 0.46 |
| 1:H:106:PHE:O | 1:H:107:ASP:HB2 | 2.16 | 0.46 |
| 1:K:78:LEU:HD12 | 1:K:193:ASN:O | 2.16 | 0.46 |
| 1:L:106:PHE:O | 1:L:107:ASP:HB2 | 2.16 | 0.46 |
| 1:R:78:LEU:HD12 | 1:R:193:ASN:O | 2.16 | 0.46 |
| 1:T:78:LEU:HD12 | 1:T:193:ASN:O | 2.16 | 0.46 |
| 1:U:78:LEU:HD12 | 1:U:193:ASN:O | 2.16 | 0.46 |
| 1:A:112:TYR:CE1 | 1:A:113:LEU:HG | 2.51 | 0.46 |
| 2:a:338:LEU:O | 2:a:338:LEU:HG | 2.15 | 0.46 |
| 2:d:340:ALA:HB1 | 2:d:344:ASP:HB2 | 1.98 | 0.46 |
| 2:f:40:GLY:HA3 | 2:f:124:THR:CG2 | 2.46 | 0.46 |
| 2:f:117:ARG:NH1 | 2:f:145:GLY:HA2 | 2.31 | 0.46 |
| 2:g:120:THR:HG23 | 2:g:139:GLY:O | 2.15 | 0.46 |
| 2:g:341:THR:OG1 | 2:g:343:MET:HE2 | 2.16 | 0.46 |
| 2:j:105:VAL:CG1 | 2:j:169:ALA:HB2 | 2.46 | 0.46 |
| 2:j:120:THR:HG23 | 2:j:139:GLY:O | 2.15 | 0.46 |
| 2:j:341:THR:OG1 | 2:j:343:MET:HE2 | 2.16 | 0.46 |
| 2:k:40:GLY:HA3 | 2:k:124:THR:CG2 | 2.46 | 0.46 |
| 2:k:57:PHE:CE1 | 2:k:110:MET:HE2 | 2.51 | 0.46 |
| 2:k:96:PHE:O | 2:l:219:ARG:HD2 | 2.16 | 0.46 |
| 2:m:352:MET:O | 2:m:356:GLY:O | 2.34 | 0.46 |
| 2:o:352:MET:O | 2:o:356:GLY:O | 2.34 | 0.46 |
| 2:q:42:VAL:HA | 2:q:120:THR:O | 2.14 | 0.46 |
| 2:q:352:MET:O | 2:q:356:GLY:O | 2.34 | 0.46 |
| 2:s:101:GLN:NE2 | 2:t:188:GLN:HB3 | 2.30 | 0.46 |
| 2:t:123:MET:CE | 2:t:136:LEU:HD22 | 2.38 | 0.46 |
| 2:u:57:PHE:CE1 | 2:u:110:MET:HE2 | 2.51 | 0.46 |
| 2:v:81:LEU:HD23 | 2:v:81:LEU:N | 2.28 | 0.46 |
| 2:w:340:ALA:HB1 | 2:w:344:ASP:HB2 | 1.98 | 0.46 |
| 2:x:120:THR:HG23 | 2:x:139:GLY:O | 2.15 | 0.46 |
| 2:y:46:ASP:OD1 | 2:z:161:ASN:N | 2.49 | 0.46 |
| 2:y:341:THR:OG1 | 2:y:343:MET:HE2 | 2.16 | 0.46 |
| 2:z:79:MET:HE2 | 2:z:79:MET:HB2 | 1.69 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:z:120:THR:HG23 | 2:z:139:GLY:O | 2.15 | 0.46 |
| 3:2:15:THR:HG23 | 3:2:43:THR:HG21 | 1.97 | 0.46 |
| 3:3:15:THR:HG23 | 3:3:43:THR:HG21 | 1.98 | 0.46 |
| 3:14:83:SER:HA | 1:O:210:ASN:ND2 | 2.30 | 0.46 |
| 3:22:15:THR:HG23 | 3:22:43:THR:HG21 | 1.98 | 0.46 |
| 3:23:15:THR:HG23 | 3:23:43:THR:HG21 | 1.97 | 0.46 |
| 1:C:101:LYS:HZ2 | 1:C:101:LYS:HB3 | 1.81 | 0.46 |
| 1:F:112:TYR:CE1 | 1:F:113:LEU:HG | 2.51 | 0.46 |
| 1:G:150:VAL:HG12 | 1:G:165:GLY:HA3 | 1.97 | 0.46 |
| 1:M:78:LEU:HD12 | 1:M:193:ASN:O | 2.16 | 0.46 |
| 1:O:148:LEU:HD13 | 1:O:167:LYS:HE2 | 1.99 | 0.46 |
| 1:S:148:LEU:HD13 | 1:S:167:LYS:HE2 | 1.98 | 0.46 |
| 1:T:148:LEU:HD13 | 1:T:167:LYS:HE2 | 1.99 | 0.46 |
| 1:Y:82:LEU:HD12 | 1:Y:146:GLY:HA3 | 1.97 | 0.46 |
| 1:Z:112:TYR:CE1 | 1:Z:113:LEU:HG | 2.51 | 0.46 |
| 3:1:15:THR:HG23 | 3:1:43:THR:HG21 | 1.98 | 0.45 |
| 2:b:40:GLY:HA3 | 2:b:124:THR:CG2 | 2.46 | 0.45 |
| 2:b:57:PHE:CE1 | 2:b:110:MET:HE2 | 2.51 | 0.45 |
| 2:b:277:GLN:HG3 | 2:b:278:GLY:N | 2.31 | 0.45 |
| 2:b:341:THR:OG1 | 2:b:343:MET:HE2 | 2.16 | 0.45 |
| 2:c:81:LEU:HD23 | 2:c:81:LEU:N | 2.28 | 0.45 |
| 2:c:94:PRO:HB2 | 2:d:219:ARG:NH2 | 2.30 | 0.45 |
| 2:c:338:LEU:O | 2:c:338:LEU:HG | 2.15 | 0.45 |
| 2:e:40:GLY:HA3 | 2:e:124:THR:CG2 | 2.46 | 0.45 |
| 2:f:353:GLN:HB2 | 2:f:358:LEU:HD23 | 1.96 | 0.45 |
| 2:h:57:PHE:CE1 | 2:h:110:MET:HE2 | 2.51 | 0.45 |
| 2:j:328:LEU:HD21 | 2:k:273:CYS:HA | 1.97 | 0.45 |
| 2:l:120:THR:HG23 | 2:l:139:GLY:O | 2.15 | 0.45 |
| 2:l:352:MET:O | 2:l:356:GLY:O | 2.34 | 0.45 |
| 2:m:341:THR:OG1 | 2:m:343:MET:HE2 | 2.16 | 0.45 |
| 2:n:256:ASN:O | 2:n:257:SER:OG | 2.29 | 0.45 |
| 2:n:328:LEU:HD21 | 2:o:273:CYS:HA | 1.98 | 0.45 |
| 2:o:57:PHE:CE1 | 2:o:110:MET:HE2 | 2.51 | 0.45 |
| 2:r:117:ARG:NH1 | 2:r:145:GLY:HA2 | 2.31 | 0.45 |
| 2:r:277:GLN:HG3 | 2:r:278:GLY:N | 2.30 | 0.45 |
| 2:s:105:VAL:CG1 | 2:s:169:ALA:HB2 | 2.46 | 0.45 |
| 2:t:57:PHE:CE1 | 2:t:110:MET:HE2 | 2.51 | 0.45 |
| 2:t:120:THR:HG23 | 2:t:139:GLY:O | 2.15 | 0.45 |
| 2:u:101:GLN:NE2 | 2:v:188:GLN:HB3 | 2.30 | 0.45 |
| 2:u:117:ARG:NH1 | 2:u:145:GLY:HA2 | 2.31 | 0.45 |
| 2:v:40:GLY:HA3 | 2:v:124:THR:CG2 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:v:99:GLN:HE21 | 1:U:50:SER:HB3 | 1.82 | 0.45 |
| 2:w:57:PHE:CE1 | 2:w:110:MET:HE2 | 2.51 | 0.45 |
| 2:w:94:PRO:HB2 | 2:x:219:ARG:NH2 | 2.30 | 0.45 |
| 2:w:328:LEU:HD21 | 2:x:273:CYS:HA | 1.98 | 0.45 |
| 2:z:338:LEU:O | 2:z:338:LEU:HG | 2.15 | 0.45 |
| 3:13:83:SER:HA | 1:N:210:ASN:ND2 | 2.30 | 0.45 |
| 1:D:150:VAL:HG12 | 1:D:165:GLY:HA3 | 1.97 | 0.45 |
| 1:H:171:ILE:O | 1:I:207:TYR:O | 2.35 | 0.45 |
| 1:J:78:LEU:HD12 | 1:J:193:ASN:O | 2.16 | 0.45 |
| 1:J:106:PHE:O | 1:J:107:ASP:HB2 | 2.16 | 0.45 |
| 1:K:112:TYR:CE1 | 1:K:113:LEU:HG | 2.51 | 0.45 |
| 1:K:171:ILE:O | 1:L:207:TYR:O | 2.34 | 0.45 |
| 1:L:148:LEU:HD13 | 1:L:167:LYS:HE2 | 1.98 | 0.45 |
| 1:L:167:LYS:NZ | 1:M:84:GLU:OE2 | 2.42 | 0.45 |
| 1:M:112:TYR:CE1 | 1:M:113:LEU:HG | 2.51 | 0.45 |
| 1:P:71:PRO:HD2 | 1:P:189:ILE:HD13 | 1.98 | 0.45 |
| 1:P:148:LEU:HD13 | 1:P:167:LYS:HE2 | 1.99 | 0.45 |
| 1:Q:150:VAL:HG12 | 1:Q:165:GLY:HA3 | 1.97 | 0.45 |
| 1:R:110:PRO:O | 1:R:114:GLN:HG2 | 2.16 | 0.45 |
| 1:R:167:LYS:NZ | 1:S:84:GLU:OE2 | 2.41 | 0.45 |
| 1:S:78:LEU:HD12 | 1:S:193:ASN:O | 2.16 | 0.45 |
| 1:A:82:LEU:HA | 1:A:197:SER:CB | 2.43 | 0.45 |
| 2:a:57:PHE:CE1 | 2:a:110:MET:HE2 | 2.51 | 0.45 |
| 2:b:328:LEU:HD21 | 2:c:273:CYS:HA | 1.98 | 0.45 |
| 2:c:120:THR:HG23 | 2:c:139:GLY:O | 2.15 | 0.45 |
| 2:e:96:PHE:O | 2:f:219:ARG:HD2 | 2.16 | 0.45 |
| 2:h:353:GLN:HB2 | 2:h:358:LEU:HD23 | 1.97 | 0.45 |
| 2:j:117:ARG:NH1 | 2:j:145:GLY:HA2 | 2.31 | 0.45 |
| 2:j:352:MET:O | 2:j:356:GLY:O | 2.34 | 0.45 |
| 2:l:40:GLY:HA3 | 2:l:124:THR:CG2 | 2.46 | 0.45 |
| 2:l:123:MET:CE | 2:l:136:LEU:HD22 | 2.38 | 0.45 |
| 2:m:40:GLY:HA3 | 2:m:124:THR:CG2 | 2.46 | 0.45 |
| 2:n:352:MET:O | 2:n:356:GLY:O | 2.34 | 0.45 |
| 2:p:57:PHE:CE1 | 2:p:110:MET:HE2 | 2.51 | 0.45 |
| 2:p:99:GLN:HE21 | 1:O:50:SER:HB3 | 1.82 | 0.45 |
| 2:q:123:MET:CE | 2:q:136:LEU:HD22 | 2.38 | 0.45 |
| 2:q:328:LEU:HD21 | 2:r:273:CYS:HA | 1.99 | 0.45 |
| 2:q:341:THR:OG1 | 2:q:343:MET:HE2 | 2.16 | 0.45 |
| 2:r:340:ALA:HB1 | 2:r:344:ASP:HB2 | 1.98 | 0.45 |
| 2:v:341:THR:OG1 | 2:v:343:MET:HE2 | 2.16 | 0.45 |
| 2:w:40:GLY:HA3 | 2:w:124:THR:CG2 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:w:120:THR:HG23 | 2:w:139:GLY:O | 2.15 | 0.45 |
| 3:2:15:THR:HG23 | 3:2:43:THR:CG2 | 2.47 | 0.45 |
| 3:8:15:THR:HG23 | 3:8:43:THR:CG2 | 2.47 | 0.45 |
| 3:9:15:THR:HG23 | 3:9:43:THR:CG2 | 2.47 | 0.45 |
| 3:10:15:THR:HG23 | 3:10:43:THR:CG2 | 2.47 | 0.45 |
| 3:13:39:PRO:HD2 | 3:13:42:PHE:CB | 2.45 | 0.45 |
| 3:14:77:CYS:HB3 | 3:14:80:TYR:CE1 | 2.48 | 0.45 |
| 3:16:83:SER:HA | 1:Q:210:ASN:ND2 | 2.31 | 0.45 |
| 3:18:83:SER:HA | 1:S:210:ASN:ND2 | 2.31 | 0.45 |
| 3:22:64:TYR:CB | 3:22:96:CYS:HB3 | 2.47 | 0.45 |
| 3:24:15:THR:HG23 | 3:24:43:THR:HG21 | 1.98 | 0.45 |
| 3:25:15:THR:HG23 | 3:25:43:THR:HG21 | 1.97 | 0.45 |
| 3:26:15:THR:HG23 | 3:26:43:THR:HG21 | 1.98 | 0.45 |
| 3:26:77:CYS:HB3 | 3:26:80:TYR:CE1 | 2.48 | 0.45 |
| 1:B:110:PRO:O | 1:B:114:GLN:HG2 | 2.16 | 0.45 |
| 1:B:112:TYR:CE1 | 1:B:113:LEU:HG | 2.51 | 0.45 |
| 1:E:171:ILE:O | 1:F:207:TYR:O | 2.34 | 0.45 |
| 1:F:171:ILE:O | 1:G:207:TYR:O | 2.35 | 0.45 |
| 1:H:101:LYS:HZ2 | 1:H:101:LYS:HB3 | 1.80 | 0.45 |
| 1:I:82:LEU:HD12 | 1:I:146:GLY:HA3 | 1.98 | 0.45 |
| 1:I:171:ILE:HD12 | 1:K:88:ALA:CB | 2.34 | 0.45 |
| 1:J:101:LYS:HB3 | 1:J:101:LYS:HZ2 | 1.81 | 0.45 |
| 1:N:78:LEU:HD12 | 1:N:193:ASN:O | 2.16 | 0.45 |
| 1:O:124:MET:HE3 | 1:O:124:MET:HB3 | 1.77 | 0.45 |
| 1:P:150:VAL:HG12 | 1:P:165:GLY:HA3 | 1.97 | 0.45 |
| 1:V:78:LEU:HD12 | 1:V:193:ASN:O | 2.16 | 0.45 |
| 1:W:148:LEU:HD13 | 1:W:167:LYS:HE2 | 1.99 | 0.45 |
| 1:X:148:LEU:HD13 | 1:X:167:LYS:HE2 | 1.98 | 0.45 |
| 2:c:105:VAL:CG1 | 2:c:169:ALA:HB2 | 2.46 | 0.45 |
| 2:e:341:THR:OG1 | 2:e:343:MET:HE2 | 2.16 | 0.45 |
| 2:g:105:VAL:CG1 | 2:g:169:ALA:HB2 | 2.46 | 0.45 |
| 2:i:277:GLN:HG3 | 2:i:278:GLY:N | 2.30 | 0.45 |
| 2:k:277:GLN:HG3 | 2:k:278:GLY:N | 2.30 | 0.45 |
| 2:k:352:MET:O | 2:k:356:GLY:O | 2.34 | 0.45 |
| 2:l:117:ARG:NH1 | 2:l:145:GLY:HA2 | 2.30 | 0.45 |
| 2:m:141:ILE:HD13 | 2:m:165:ILE:CD1 | 2.39 | 0.45 |
| 2:n:340:ALA:HB1 | 2:n:344:ASP:HB2 | 1.98 | 0.45 |
| 2:p:40:GLY:HA3 | 2:p:124:THR:CG2 | 2.46 | 0.45 |
| 2:p:340:ALA:HB1 | 2:p:344:ASP:HB2 | 1.98 | 0.45 |
| 2:r:94:PRO:HB2 | 2:s:219:ARG:NH2 | 2.30 | 0.45 |
| 2:s:57:PHE:CE1 | 2:s:110:MET:HE2 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:s:338:LEU:HG | 2:s:338:LEU:O | 2.15 | 0.45 |
| 2:s:341:THR:OG1 | 2:s:343:MET:HE2 | 2.16 | 0.45 |
| 2:t:105:VAL:CG1 | 2:t:169:ALA:HB2 | 2.46 | 0.45 |
| 2:t:341:THR:OG1 | 2:t:343:MET:HE2 | 2.17 | 0.45 |
| 2:w:341:THR:OG1 | 2:w:343:MET:HE2 | 2.16 | 0.45 |
| 2:x:338:LEU:HG | 2:x:338:LEU:O | 2.15 | 0.45 |
| 2:z:99:GLN:HE21 | 1:Y:50:SER:HB3 | 1.82 | 0.45 |
| 2:z:340:ALA:HB1 | 2:z:344:ASP:HB2 | 1.98 | 0.45 |
| 3:7:15:THR:HG23 | 3:7:43:THR:CG2 | 2.47 | 0.45 |
| 3:11:15:THR:HG23 | 3:11:43:THR:CG2 | 2.47 | 0.45 |
| 3:12:15:THR:HG23 | 3:12:43:THR:CG2 | 2.47 | 0.45 |
| 3:24:83:SER:HA | 1:Y:210:ASN:HD22 | 1.82 | 0.45 |
| 3:26:15:THR:HG23 | 3:26:43:THR:CG2 | 2.47 | 0.45 |
| 1:C:71:PRO:HD2 | 1:C:189:ILE:HD13 | 1.98 | 0.45 |
| 1:G:171:ILE:HD12 | 1:I:88:ALA:CB | 2.34 | 0.45 |
| 1:I:112:TYR:CE1 | 1:I:113:LEU:HG | 2.51 | 0.45 |
| 1:M:148:LEU:HD13 | 1:M:167:LYS:HE2 | 1.98 | 0.45 |
| 1:N:148:LEU:HD13 | 1:N:167:LYS:HE2 | 1.99 | 0.45 |
| 1:Q:148:LEU:HD13 | 1:Q:167:LYS:HE2 | 1.99 | 0.45 |
| 1:U:148:LEU:HD13 | 1:U:167:LYS:HE2 | 1.99 | 0.45 |
| 1:Z:82:LEU:HD12 | 1:Z:146:GLY:HA3 | 1.98 | 0.45 |
| 1:A:71:PRO:HD2 | 1:A:189:ILE:HD13 | 1.98 | 0.45 |
| 2:b:338:LEU:O | 2:b:338:LEU:HG | 2.15 | 0.45 |
| 2:d:105:VAL:CG1 | 2:d:169:ALA:HB2 | 2.46 | 0.45 |
| 2:d:341:THR:OG1 | 2:d:343:MET:HE2 | 2.16 | 0.45 |
| 2:e:105:VAL:CG1 | 2:e:169:ALA:HB2 | 2.46 | 0.45 |
| 2:h:120:THR:HG23 | 2:h:139:GLY:O | 2.15 | 0.45 |
| 2:j:99:GLN:HE21 | 1:I:50:SER:HB3 | 1.82 | 0.45 |
| 2:l:341:THR:OG1 | 2:l:343:MET:HE2 | 2.16 | 0.45 |
| 2:n:338:LEU:O | 2:n:338:LEU:HG | 2.15 | 0.45 |
| 2:p:117:ARG:NH1 | 2:p:145:GLY:HA2 | 2.31 | 0.45 |
| 2:p:341:THR:OG1 | 2:p:343:MET:HE2 | 2.17 | 0.45 |
| 2:p:352:MET:O | 2:p:356:GLY:O | 2.34 | 0.45 |
| 2:r:352:MET:O | 2:r:356:GLY:O | 2.34 | 0.45 |
| 2:s:352:MET:O | 2:s:356:GLY:O | 2.34 | 0.45 |
| 2:u:99:GLN:HE21 | 1:T:50:SER:HB3 | 1.82 | 0.45 |
| 2:u:105:VAL:CG1 | 2:u:169:ALA:HB2 | 2.46 | 0.45 |
| 2:u:123:MET:CE | 2:u:136:LEU:HD22 | 2.38 | 0.45 |
| 2:u:277:GLN:HG3 | 2:u:278:GLY:N | 2.30 | 0.45 |
| 2:u:341:THR:OG1 | 2:u:343:MET:HE2 | 2.16 | 0.45 |
| 2:w:96:PHE:O | 2:x:219:ARG:HD2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:y:96:PHE:O | 2:z:219:ARG:HD2 | 2.16 | 0.45 |
| 2:y:105:VAL:CG1 | 2:y:169:ALA:HB2 | 2.46 | 0.45 |
| 3:2:64:TYR:CB | 3:2:96:CYS:HB3 | 2.47 | 0.45 |
| 3:3:64:TYR:CB | 3:3:96:CYS:HB3 | 2.47 | 0.45 |
| 3:5:64:TYR:CB | 3:5:96:CYS:HB3 | 2.47 | 0.45 |
| 3:6:15:THR:HG23 | 3:6:43:THR:CG2 | 2.47 | 0.45 |
| 3:7:64:TYR:CB | 3:7:96:CYS:HB3 | 2.47 | 0.45 |
| 3:8:64:TYR:CB | 3:8:96:CYS:HB3 | 2.47 | 0.45 |
| 3:8:77:CYS:HB3 | 3:8:80:TYR:CE1 | 2.48 | 0.45 |
| 3:13:64:TYR:CB | 3:13:96:CYS:HB3 | 2.47 | 0.45 |
| 3:14:64:TYR:CB | 3:14:96:CYS:HB3 | 2.47 | 0.45 |
| 1:B:71:PRO:HD2 | 1:B:189:ILE:HD13 | 1.98 | 0.45 |
| 1:B:221:TRP:NE1 | 1:C:229:LEU:O | 2.39 | 0.45 |
| 1:D:106:PHE:O | 1:D:107:ASP:HB2 | 2.16 | 0.45 |
| 1:G:110:PRO:O | 1:G:114:GLN:HG2 | 2.16 | 0.45 |
| 1:I:78:LEU:HD12 | 1:I:193:ASN:O | 2.16 | 0.45 |
| 1:J:110:PRO:O | 1:J:114:GLN:HG2 | 2.16 | 0.45 |
| 1:K:148:LEU:HD13 | 1:K:167:LYS:HE2 | 1.99 | 0.45 |
| 1:M:101:LYS:HB3 | 1:M:101:LYS:HZ2 | 1.81 | 0.45 |
| 1:Q:71:PRO:HD2 | 1:Q:189:ILE:HD13 | 1.98 | 0.45 |
| 1:R:148:LEU:HD13 | 1:R:167:LYS:HE2 | 1.98 | 0.45 |
| 1:U:130:ASN:CG | 1:V:102:THR:HG22 | 2.40 | 0.45 |
| 1:V:148:LEU:HD13 | 1:V:167:LYS:HE2 | 1.99 | 0.45 |
| 1:Y:148:LEU:HD13 | 1:Y:167:LYS:HE2 | 1.98 | 0.45 |
| 2:a:105:VAL:CG1 | 2:a:169:ALA:HB2 | 2.46 | 0.45 |
| 3:1:64:TYR:CB | 3:1:96:CYS:HB3 | 2.47 | 0.45 |
| 2:b:105:VAL:CG1 | 2:b:169:ALA:HB2 | 2.46 | 0.45 |
| 2:b:117:ARG:NH1 | 2:b:145:GLY:HA2 | 2.31 | 0.45 |
| 2:d:40:GLY:HA3 | 2:d:124:THR:CG2 | 2.46 | 0.45 |
| 2:d:117:ARG:NH1 | 2:d:145:GLY:HA2 | 2.31 | 0.45 |
| 2:k:340:ALA:HB1 | 2:k:344:ASP:HB2 | 1.98 | 0.45 |
| 2:n:117:ARG:NH1 | 2:n:145:GLY:HA2 | 2.31 | 0.45 |
| 2:p:277:GLN:HG3 | 2:p:278:GLY:N | 2.30 | 0.45 |
| 2:q:57:PHE:CE1 | 2:q:110:MET:HE2 | 2.51 | 0.45 |
| 2:s:319:LEU:HD12 | 2:s:319:LEU:HA | 1.80 | 0.45 |
| 2:u:340:ALA:HB1 | 2:u:344:ASP:HB2 | 1.98 | 0.45 |
| 2:v:217:ASP:OD1 | 2:v:219:ARG:N | 2.35 | 0.45 |
| 2:w:117:ARG:NH1 | 2:w:145:GLY:HA2 | 2.31 | 0.45 |
| 2:x:105:VAL:CG1 | 2:x:169:ALA:HB2 | 2.46 | 0.45 |
| 2:z:105:VAL:CG1 | 2:z:169:ALA:HB2 | 2.46 | 0.45 |
| 3:4:15:THR:HG23 | 3:4:43:THR:CG2 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:13:15:THR:HG23 | 3:13:43:THR:CG2 | 2.47 | 0.45 |
| 3:17:15:THR:HG23 | 3:17:43:THR:CG2 | 2.47 | 0.45 |
| 3:19:15:THR:HG23 | 3:19:43:THR:CG2 | 2.47 | 0.45 |
| 3:21:64:TYR:CB | 3:21:96:CYS:HB3 | 2.47 | 0.45 |
| 3:22:15:THR:HG23 | 3:22:43:THR:CG2 | 2.47 | 0.45 |
| 3:23:64:TYR:CB | 3:23:96:CYS:HB3 | 2.47 | 0.45 |
| 3:24:15:THR:HG23 | 3:24:43:THR:CG2 | 2.47 | 0.45 |
| 1:D:110:PRO:O | 1:D:114:GLN:HG2 | 2.16 | 0.45 |
| 1:H:78:LEU:HD12 | 1:H:193:ASN:O | 2.16 | 0.45 |
| 1:I:106:PHE:O | 1:I:107:ASP:HB2 | 2.16 | 0.45 |
| 1:L:171:ILE:O | 1:M:207:TYR:O | 2.35 | 0.45 |
| 1:V:130:ASN:CG | 1:W:102:THR:HG22 | 2.40 | 0.45 |
| 1:V:171:ILE:O | 1:W:207:TYR:O | 2.34 | 0.45 |
| 1:Y:101:LYS:HZ2 | 1:Y:101:LYS:HB3 | 1.82 | 0.45 |
| 1:A:82:LEU:HD12 | 1:A:146:GLY:HA3 | 1.98 | 0.45 |
| 1:A:124:MET:HE3 | 1:A:124:MET:HB3 | 1.76 | 0.45 |
| 2:f:57:PHE:CE1 | 2:f:110:MET:HE2 | 2.51 | 0.45 |
| 2:f:99:GLN:HE21 | 1:E:50:SER:HB3 | 1.81 | 0.45 |
| 2:g:340:ALA:HB1 | 2:g:344:ASP:HB2 | 1.98 | 0.45 |
| 2:h:352:MET:O | 2:h:356:GLY:O | 2.34 | 0.45 |
| 2:i:352:MET:O | 2:i:356:GLY:O | 2.34 | 0.45 |
| 2:o:40:GLY:HA3 | 2:o:124:THR:CG2 | 2.46 | 0.45 |
| 2:o:99:GLN:HE21 | 1:N:50:SER:HB3 | 1.82 | 0.45 |
| 2:o:341:THR:OG1 | 2:o:343:MET:HE2 | 2.16 | 0.45 |
| 2:p:52:THR:HG21 | 2:p:81:LEU:HD23 | 1.99 | 0.45 |
| 2:q:96:PHE:O | 2:r:219:ARG:HD2 | 2.16 | 0.45 |
| 2:r:256:ASN:OD1 | 2:r:259:THR:OG1 | 2.10 | 0.45 |
| 2:t:352:MET:O | 2:t:356:GLY:O | 2.34 | 0.45 |
| 2:v:105:VAL:CG1 | 2:v:169:ALA:HB2 | 2.46 | 0.45 |
| 2:y:40:GLY:HA3 | 2:y:124:THR:CG2 | 2.46 | 0.45 |
| 2:y:57:PHE:CE1 | 2:y:110:MET:HE2 | 2.51 | 0.45 |
| 2:z:341:THR:OG1 | 2:z:343:MET:HE2 | 2.16 | 0.45 |
| 3:5:15:THR:HG23 | 3:5:43:THR:CG2 | 2.47 | 0.45 |
| 3:6:64:TYR:CB | 3:6:96:CYS:HB3 | 2.47 | 0.45 |
| 3:12:64:TYR:CB | 3:12:96:CYS:HB3 | 2.47 | 0.45 |
| 3:15:64:TYR:CB | 3:15:96:CYS:HB3 | 2.47 | 0.45 |
| 3:20:15:THR:HG23 | 3:20:43:THR:CG2 | 2.47 | 0.45 |
| 3:21:15:THR:HG23 | 3:21:43:THR:CG2 | 2.47 | 0.45 |
| 1:C:106:PHE:O | 1:C:107:ASP:HB2 | 2.16 | 0.45 |
| 1:D:112:TYR:CE1 | 1:D:113:LEU:HG | 2.51 | 0.45 |
| 1:E:150:VAL:HG12 | 1:E:165:GLY:HA3 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:150:VAL:HG12 | 1:F:165:GLY:HA3 | 1.97 | 0.45 |
| 1:J:148:LEU:HD13 | 1:J:167:LYS:HE2 | 1.99 | 0.45 |
| 1:J:170:ALA:HB3 | 1:K:206:GLU:HG3 | 1.98 | 0.45 |
| 1:N:171:ILE:O | 1:O:207:TYR:O | 2.35 | 0.45 |
| 1:P:171:ILE:O | 1:Q:207:TYR:O | 2.34 | 0.45 |
| 1:Q:78:LEU:HD12 | 1:Q:193:ASN:O | 2.16 | 0.45 |
| 1:R:112:TYR:CE1 | 1:R:113:LEU:HG | 2.51 | 0.45 |
| 1:W:78:LEU:HD12 | 1:W:193:ASN:O | 2.16 | 0.45 |
| 2:a:101:GLN:NE2 | 2:b:188:GLN:HB3 | 2.31 | 0.45 |
| 2:b:120:THR:HG23 | 2:b:139:GLY:O | 2.15 | 0.45 |
| 2:d:57:PHE:CE1 | 2:d:110:MET:HE2 | 2.51 | 0.45 |
| 2:h:192:GLU:HB2 | 2:h:219:ARG:HB2 | 1.99 | 0.45 |
| 2:h:341:THR:OG1 | 2:h:343:MET:HE2 | 2.16 | 0.45 |
| 2:i:340:ALA:HB1 | 2:i:344:ASP:HB2 | 1.98 | 0.45 |
| 2:i:341:THR:OG1 | 2:i:343:MET:HE2 | 2.16 | 0.45 |
| 2:m:340:ALA:HB1 | 2:m:344:ASP:HB2 | 1.98 | 0.45 |
| 2:o:52:THR:HG21 | 2:o:81:LEU:HD23 | 1.99 | 0.45 |
| 2:r:57:PHE:CE1 | 2:r:110:MET:HE2 | 2.51 | 0.45 |
| 2:r:80:GLN:HB3 | 2:s:54:GLN:HB3 | 1.99 | 0.45 |
| 2:t:52:THR:HG21 | 2:t:81:LEU:HD23 | 1.99 | 0.45 |
| 2:u:52:THR:HG21 | 2:u:81:LEU:HD23 | 1.99 | 0.45 |
| 2:w:105:VAL:CG1 | 2:w:169:ALA:HB2 | 2.46 | 0.45 |
| 2:x:341:THR:OG1 | 2:x:343:MET:HE2 | 2.16 | 0.45 |
| 2:y:338:LEU:HG | 2:y:338:LEU:O | 2.15 | 0.45 |
| 3:4:64:TYR:CB | 3:4:96:CYS:HB3 | 2.47 | 0.45 |
| 3:9:64:TYR:CB | 3:9:96:CYS:HB3 | 2.47 | 0.45 |
| 3:14:15:THR:HG23 | 3:14:43:THR:CG2 | 2.47 | 0.45 |
| 3:18:15:THR:HG23 | 3:18:43:THR:CG2 | 2.47 | 0.45 |
| 3:18:47:ASP:CG | 3:18:50:VAL:H | 2.14 | 0.45 |
| 3:20:64:TYR:CB | 3:20:96:CYS:HB3 | 2.47 | 0.45 |
| 3:24:64:TYR:CB | 3:24:96:CYS:HB3 | 2.47 | 0.45 |
| 3:25:77:CYS:HB3 | 3:25:80:TYR:CE1 | 2.48 | 0.45 |
| 1:C:78:LEU:HD12 | 1:C:193:ASN:O | 2.16 | 0.45 |
| 1:D:78:LEU:HD12 | 1:D:193:ASN:O | 2.16 | 0.45 |
| 1:D:168:GLN:HG3 | 1:E:204:ARG:NE | 2.32 | 0.45 |
| 1:G:171:ILE:O | 1:H:207:TYR:O | 2.35 | 0.45 |
| 1:H:121:ARG:HB3 | 1:I:111:ARG:HB3 | 1.99 | 0.45 |
| 1:M:82:LEU:HD12 | 1:M:146:GLY:HA3 | 1.97 | 0.45 |
| 1:M:110:PRO:O | 1:M:114:GLN:HG2 | 2.16 | 0.45 |
| 1:M:171:ILE:O | 1:N:207:TYR:O | 2.35 | 0.45 |
| 1:N:82:LEU:HD12 | 1:N:146:GLY:HA3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:82:LEU:HD12 | 1:U:146:GLY:HA3 | 1.97 | 0.45 |
| 1:Z:71:PRO:HD2 | 1:Z:189:ILE:HD13 | 1.98 | 0.45 |
| 1:Z:110:PRO:O | 1:Z:114:GLN:HG2 | 2.16 | 0.45 |
| 2:a:79:MET:HE2 | 2:a:79:MET:HB2 | 1.69 | 0.45 |
| 2:a:94:PRO:HB2 | 2:b:219:ARG:NH2 | 2.31 | 0.45 |
| 2:a:120:THR:HG23 | 2:a:139:GLY:O | 2.15 | 0.45 |
| 2:a:341:THR:OG1 | 2:a:343:MET:HE2 | 2.16 | 0.45 |
| 2:d:277:GLN:HG3 | 2:d:278:GLY:N | 2.31 | 0.45 |
| 2:g:352:MET:O | 2:g:356:GLY:O | 2.34 | 0.45 |
| 2:h:328:LEU:HD21 | 2:i:273:CYS:HA | 1.98 | 0.45 |
| 2:i:99:GLN:HE21 | 1:H:50:SER:HB3 | 1.82 | 0.45 |
| 2:i:192:GLU:HB2 | 2:i:219:ARG:HB2 | 1.99 | 0.45 |
| 2:l:328:LEU:HD21 | 2:m:273:CYS:HA | 1.99 | 0.45 |
| 2:m:217:ASP:OD1 | 2:m:219:ARG:N | 2.35 | 0.45 |
| 2:n:40:GLY:HA3 | 2:n:124:THR:CG2 | 2.46 | 0.45 |
| 2:p:93:TYR:OH | 2:p:173:ARG:O | 2.24 | 0.45 |
| 2:t:99:GLN:HE21 | 1:S:50:SER:HB3 | 1.82 | 0.45 |
| 2:v:256:ASN:OD1 | 2:v:259:THR:OG1 | 2.10 | 0.45 |
| 2:y:101:GLN:NE2 | 2:z:219:ARG:HD3 | 2.31 | 0.45 |
| 3:3:47:ASP:CG | 3:3:50:VAL:H | 2.14 | 0.45 |
| 3:11:47:ASP:CG | 3:11:50:VAL:HG23 | 2.42 | 0.45 |
| 3:23:15:THR:HG23 | 3:23:43:THR:CG2 | 2.47 | 0.45 |
| 3:23:47:ASP:CG | 3:23:50:VAL:HG23 | 2.42 | 0.45 |
| 1:B:82:LEU:HA | 1:B:197:SER:CB | 2.43 | 0.45 |
| 1:D:170:ALA:HB3 | 1:E:206:GLU:HG3 | 1.98 | 0.45 |
| 1:E:78:LEU:HD12 | 1:E:193:ASN:O | 2.16 | 0.45 |
| 1:H:170:ALA:HB3 | 1:I:206:GLU:HG3 | 1.99 | 0.45 |
| 1:J:82:LEU:HD12 | 1:J:146:GLY:HA3 | 1.97 | 0.45 |
| 1:K:121:ARG:HB3 | 1:L:111:ARG:HB3 | 1.99 | 0.45 |
| 1:P:78:LEU:HD12 | 1:P:193:ASN:O | 2.16 | 0.45 |
| 1:R:71:PRO:HD2 | 1:R:189:ILE:HD13 | 1.98 | 0.45 |
| 1:T:171:ILE:HD12 | 1:V:88:ALA:CB | 2.34 | 0.45 |
| 1:V:170:ALA:HB3 | 1:W:206:GLU:HG3 | 1.98 | 0.45 |
| 1:Y:71:PRO:HD2 | 1:Y:189:ILE:HD13 | 1.98 | 0.45 |
| 1:A:148:LEU:HD13 | 1:A:167:LYS:HE2 | 1.99 | 0.45 |
| 2:b:340:ALA:HB1 | 2:b:344:ASP:HB2 | 1.98 | 0.45 |
| 2:c:40:GLY:HA3 | 2:c:124:THR:CG2 | 2.46 | 0.45 |
| 2:f:328:LEU:HD21 | 2:g:273:CYS:HA | 1.99 | 0.45 |
| 2:k:99:GLN:HE21 | 1:J:50:SER:HB3 | 1.82 | 0.45 |
| 2:k:123:MET:CE | 2:k:136:LEU:HD22 | 2.38 | 0.45 |
| 2:k:338:LEU:O | 2:k:338:LEU:HG | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:l:338:LEU:O | 2:l:338:LEU:HG | 2.15 | 0.45 |
| 2:n:341:THR:OG1 | 2:n:343:MET:HE2 | 2.17 | 0.45 |
| 2:o:340:ALA:HB1 | 2:o:344:ASP:HB2 | 1.98 | 0.45 |
| 2:s:340:ALA:HB1 | 2:s:344:ASP:HB2 | 1.98 | 0.45 |
| 2:v:52:THR:HG21 | 2:v:81:LEU:HD23 | 1.99 | 0.45 |
| 2:w:52:THR:HG21 | 2:w:81:LEU:HD23 | 1.99 | 0.45 |
| 2:w:93:TYR:OH | 2:w:173:ARG:O | 2.24 | 0.45 |
| 2:x:52:THR:HG21 | 2:x:81:LEU:HD23 | 1.99 | 0.45 |
| 3:16:64:TYR:CB | 3:16:96:CYS:HB3 | 2.47 | 0.45 |
| 3:17:77:CYS:HB3 | 3:17:80:TYR:CE1 | 2.48 | 0.45 |
| 3:25:15:THR:HG23 | 3:25:43:THR:CG2 | 2.47 | 0.45 |
| 3:25:47:ASP:CG | 3:25:50:VAL:HG23 | 2.42 | 0.45 |
| 3:26:64:TYR:CB | 3:26:96:CYS:HB3 | 2.47 | 0.45 |
| 1:B:78:LEU:HD12 | 1:B:193:ASN:O | 2.16 | 0.45 |
| 1:B:148:LEU:HD13 | 1:B:167:LYS:HE2 | 1.99 | 0.45 |
| 1:B:222:LEU:HB2 | 1:C:231:PRO:HB3 | 1.99 | 0.45 |
| 1:F:148:LEU:HD13 | 1:F:167:LYS:HE2 | 1.98 | 0.45 |
| 1:G:148:LEU:HD13 | 1:G:167:LYS:HE2 | 1.99 | 0.45 |
| 1:H:148:LEU:HD13 | 1:H:167:LYS:HE2 | 1.99 | 0.45 |
| 1:I:171:ILE:O | 1:J:207:TYR:O | 2.35 | 0.45 |
| 1:J:82:LEU:HA | 1:J:197:SER:CB | 2.43 | 0.45 |
| 1:K:170:ALA:HB3 | 1:L:206:GLU:HG3 | 1.99 | 0.45 |
| 1:N:121:ARG:HB3 | 1:O:111:ARG:HB3 | 1.99 | 0.45 |
| 1:O:82:LEU:HD12 | 1:O:146:GLY:HA3 | 1.98 | 0.45 |
| 1:O:101:LYS:HZ2 | 1:O:101:LYS:HB3 | 1.81 | 0.45 |
| 1:P:110:PRO:O | 1:P:114:GLN:HG2 | 2.16 | 0.45 |
| 1:T:82:LEU:HD12 | 1:T:146:GLY:HA3 | 1.97 | 0.45 |
| 1:V:82:LEU:HD12 | 1:V:146:GLY:HA3 | 1.98 | 0.45 |
| 1:V:168:GLN:HG3 | 1:W:204:ARG:NE | 2.32 | 0.45 |
| 1:W:40:ILE:H | 1:W:40:ILE:HG12 | 1.49 | 0.45 |
| 1:W:71:PRO:HD2 | 1:W:189:ILE:HD13 | 1.98 | 0.45 |
| 1:X:71:PRO:HD2 | 1:X:189:ILE:HD13 | 1.98 | 0.45 |
| 2:b:352:MET:O | 2:b:356:GLY:O | 2.34 | 0.45 |
| 2:e:328:LEU:HD21 | 2:f:273:CYS:HA | 1.99 | 0.45 |
| 2:q:52:THR:HG21 | 2:q:81:LEU:HD23 | 1.99 | 0.45 |
| 2:r:341:THR:OG1 | 2:r:343:MET:HE2 | 2.16 | 0.45 |
| 2:r:359:ARG:N | 2:r:359:ARG:HD2 | 2.33 | 0.45 |
| 2:v:192:GLU:HB2 | 2:v:219:ARG:HB2 | 1.99 | 0.45 |
| 2:w:99:GLN:HE21 | 1:V:50:SER:HB3 | 1.82 | 0.45 |
| 2:x:192:GLU:HB2 | 2:x:219:ARG:HB2 | 1.99 | 0.45 |
| 2:y:52:THR:HG21 | 2:y:81:LEU:HD23 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:z:352:MET:O | 2:z:356:GLY:O | 2.34 | 0.45 |
| 3:15:15:THR:HG23 | 3:15:43:THR:CG2 | 2.47 | 0.45 |
| 3:16:15:THR:HG23 | 3:16:43:THR:CG2 | 2.47 | 0.45 |
| 3:16:77:CYS:HB3 | 3:16:80:TYR:CE1 | 2.48 | 0.45 |
| 1:B:171:ILE:O | 1:C:207:TYR:O | 2.35 | 0.45 |
| 1:C:148:LEU:HD13 | 1:C:167:LYS:HE2 | 1.98 | 0.45 |
| 1:H:222:LEU:HB2 | 1:I:231:PRO:HB3 | 1.99 | 0.45 |
| 1:I:148:LEU:HD13 | 1:I:167:LYS:HE2 | 1.99 | 0.45 |
| 1:J:222:LEU:HB2 | 1:K:231:PRO:HB3 | 2.00 | 0.45 |
| 1:L:82:LEU:HD12 | 1:L:146:GLY:HA3 | 1.97 | 0.45 |
| 1:Q:171:ILE:O | 1:R:207:TYR:O | 2.34 | 0.45 |
| 1:T:110:PRO:O | 1:T:114:GLN:HG2 | 2.16 | 0.45 |
| 1:T:168:GLN:HG3 | 1:U:204:ARG:NE | 2.32 | 0.45 |
| 1:V:71:PRO:HD2 | 1:V:189:ILE:HD13 | 1.98 | 0.45 |
| 1:V:110:PRO:O | 1:V:114:GLN:HG2 | 2.16 | 0.45 |
| 1:W:82:LEU:HD12 | 1:W:146:GLY:HA3 | 1.97 | 0.45 |
| 1:X:78:LEU:HD12 | 1:X:193:ASN:O | 2.16 | 0.45 |
| 1:Y:124:MET:HE3 | 1:Y:124:MET:HB3 | 1.77 | 0.45 |
| 1:A:78:LEU:HD12 | 1:A:193:ASN:O | 2.16 | 0.44 |
| 2:a:40:GLY:HA3 | 2:a:124:THR:CG2 | 2.46 | 0.44 |
| 3:1:15:THR:HG23 | 3:1:43:THR:CG2 | 2.47 | 0.44 |
| 2:e:83:ASN:ND2 | 2:f:109:SER:OG | 2.48 | 0.44 |
| 2:i:120:THR:HG23 | 2:i:139:GLY:O | 2.15 | 0.44 |
| 2:k:192:GLU:HB2 | 2:k:219:ARG:HB2 | 1.99 | 0.44 |
| 2:k:341:THR:OG1 | 2:k:343:MET:HE2 | 2.16 | 0.44 |
| 2:m:99:GLN:HE21 | 1:L:50:SER:HB3 | 1.82 | 0.44 |
| 2:n:52:THR:HG21 | 2:n:81:LEU:HD23 | 1.99 | 0.44 |
| 2:p:80:GLN:HB3 | 2:q:54:GLN:HB3 | 1.99 | 0.44 |
| 2:q:83:ASN:ND2 | 2:r:109:SER:OG | 2.48 | 0.44 |
| 2:q:340:ALA:HB1 | 2:q:344:ASP:HB2 | 1.98 | 0.44 |
| 2:r:52:THR:HG21 | 2:r:81:LEU:HD23 | 1.99 | 0.44 |
| 2:r:83:ASN:ND2 | 2:s:109:SER:OG | 2.47 | 0.44 |
| 2:s:94:PRO:HB2 | 2:t:219:ARG:NH2 | 2.31 | 0.44 |
| 2:t:192:GLU:HB2 | 2:t:219:ARG:HB2 | 1.99 | 0.44 |
| 2:t:359:ARG:N | 2:t:359:ARG:HD2 | 2.32 | 0.44 |
| 2:u:352:MET:O | 2:u:356:GLY:O | 2.34 | 0.44 |
| 2:u:353:GLN:CG | 2:u:362:LEU:HD22 | 2.48 | 0.44 |
| 2:v:80:GLN:HB3 | 2:w:54:GLN:HB3 | 2.00 | 0.44 |
| 2:v:123:MET:CE | 2:v:136:LEU:HD22 | 2.38 | 0.44 |
| 2:v:352:MET:O | 2:v:356:GLY:O | 2.34 | 0.44 |
| 2:v:353:GLN:CG | 2:v:362:LEU:HD22 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:x:142:LEU:HD22 | 2:z:364:ILE:CD1 | 2.47 | 0.44 |
| 3:10:64:TYR:CB | 3:10:96:CYS:HB3 | 2.47 | 0.44 |
| 3:11:64:TYR:CB | 3:11:96:CYS:HB3 | 2.47 | 0.44 |
| 3:12:47:ASP:CG | 3:12:50:VAL:H | 2.14 | 0.44 |
| 3:13:47:ASP:CG | 3:13:50:VAL:HG23 | 2.42 | 0.44 |
| 3:18:77:CYS:HB3 | 3:18:80:TYR:CE1 | 2.48 | 0.44 |
| 1:C:82:LEU:HA | 1:C:197:SER:CB | 2.43 | 0.44 |
| 1:E:170:ALA:HB3 | 1:F:206:GLU:HG3 | 1.99 | 0.44 |
| 1:N:222:LEU:HB2 | 1:O:231:PRO:HB3 | 1.99 | 0.44 |
| 1:P:82:LEU:HD12 | 1:P:146:GLY:HA3 | 1.98 | 0.44 |
| 1:Q:121:ARG:HB3 | 1:R:111:ARG:HB3 | 1.99 | 0.44 |
| 1:X:110:PRO:O | 1:X:114:GLN:HG2 | 2.16 | 0.44 |
| 1:Y:78:LEU:HD12 | 1:Y:193:ASN:O | 2.16 | 0.44 |
| 1:Z:148:LEU:HD13 | 1:Z:167:LYS:HE2 | 1.99 | 0.44 |
| 2:a:352:MET:O | 2:a:356:GLY:O | 2.34 | 0.44 |
| 2:a:364:ILE:CD1 | 2:y:142:LEU:HD22 | 2.46 | 0.44 |
| 3:1:36:TYR:CE2 | 3:1:90:PHE:HB2 | 2.53 | 0.44 |
| 2:c:352:MET:O | 2:c:356:GLY:O | 2.34 | 0.44 |
| 2:e:22:ILE:HA | 2:e:25:LEU:CD2 | 2.48 | 0.44 |
| 2:f:352:MET:O | 2:f:356:GLY:O | 2.34 | 0.44 |
| 2:g:192:GLU:HB2 | 2:g:219:ARG:HB2 | 1.99 | 0.44 |
| 2:j:192:GLU:HB2 | 2:j:219:ARG:HB2 | 1.99 | 0.44 |
| 2:l:192:GLU:HB2 | 2:l:219:ARG:HB2 | 1.99 | 0.44 |
| 2:q:256:ASN:O | 2:q:257:SER:OG | 2.29 | 0.44 |
| 2:s:22:ILE:HA | 2:s:25:LEU:CD2 | 2.48 | 0.44 |
| 2:t:353:GLN:CG | 2:t:362:LEU:HD22 | 2.47 | 0.44 |
| 2:w:359:ARG:N | 2:w:359:ARG:HD2 | 2.32 | 0.44 |
| 2:x:328:LEU:HD21 | 2:y:273:CYS:HA | 2.00 | 0.44 |
| 2:x:352:MET:O | 2:x:356:GLY:O | 2.34 | 0.44 |
| 2:y:352:MET:O | 2:y:356:GLY:O | 2.34 | 0.44 |
| 3:2:36:TYR:CE2 | 3:2:90:PHE:HB2 | 2.53 | 0.44 |
| 3:3:15:THR:HG23 | 3:3:43:THR:CG2 | 2.47 | 0.44 |
| 3:5:36:TYR:CE2 | 3:5:90:PHE:HB2 | 2.53 | 0.44 |
| 3:15:77:CYS:HB3 | 3:15:80:TYR:CE1 | 2.48 | 0.44 |
| 3:16:47:ASP:CG | 3:16:50:VAL:HG23 | 2.42 | 0.44 |
| 3:17:47:ASP:CG | 3:17:50:VAL:HG23 | 2.42 | 0.44 |
| 3:17:64:TYR:CB | 3:17:96:CYS:HB3 | 2.47 | 0.44 |
| 3:18:36:TYR:CE2 | 3:18:90:PHE:HB2 | 2.53 | 0.44 |
| 3:18:47:ASP:CG | 3:18:50:VAL:HG23 | 2.42 | 0.44 |
| 3:19:36:TYR:CE2 | 3:19:90:PHE:HB2 | 2.53 | 0.44 |
| 3:20:36:TYR:CE2 | 3:20:90:PHE:HB2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:24:47:ASP:CG | 3:24:50:VAL:H | 2.14 | 0.44 |
| 1:B:82:LEU:HD12 | 1:B:146:GLY:HA3 | 1.98 | 0.44 |
| 1:C:171:ILE:O | 1:D:207:TYR:O | 2.35 | 0.44 |
| 1:E:148:LEU:HD13 | 1:E:167:LYS:HE2 | 1.98 | 0.44 |
| 1:F:78:LEU:HD12 | 1:F:193:ASN:O | 2.16 | 0.44 |
| 1:H:40:ILE:H | 1:H:40:ILE:HG12 | 1.49 | 0.44 |
| 1:M:121:ARG:HB3 | 1:N:111:ARG:HB3 | 2.00 | 0.44 |
| 1:O:111:ARG:NH1 | 1:O:111:ARG:HG2 | 2.33 | 0.44 |
| 1:O:167:LYS:NZ | 1:P:84:GLU:OE2 | 2.43 | 0.44 |
| 1:S:71:PRO:HD2 | 1:S:189:ILE:HD13 | 1.98 | 0.44 |
| 1:S:82:LEU:HD12 | 1:S:146:GLY:HA3 | 1.98 | 0.44 |
| 1:T:111:ARG:NH1 | 1:T:111:ARG:HG2 | 2.33 | 0.44 |
| 1:U:71:PRO:HD2 | 1:U:189:ILE:HD13 | 1.98 | 0.44 |
| 1:Y:111:ARG:NH1 | 1:Y:111:ARG:HG2 | 2.33 | 0.44 |
| 3:1:47:ASP:CG | 3:1:50:VAL:HG23 | 2.42 | 0.44 |
| 2:b:22:ILE:HA | 2:b:25:LEU:CD2 | 2.48 | 0.44 |
| 2:c:341:THR:OG1 | 2:c:343:MET:HE2 | 2.16 | 0.44 |
| 2:d:22:ILE:HA | 2:d:25:LEU:CD2 | 2.48 | 0.44 |
| 2:d:352:MET:O | 2:d:356:GLY:O | 2.34 | 0.44 |
| 2:e:352:MET:O | 2:e:356:GLY:O | 2.34 | 0.44 |
| 2:k:328:LEU:HD21 | 2:l:273:CYS:HA | 1.98 | 0.44 |
| 2:m:192:GLU:HB2 | 2:m:219:ARG:HB2 | 1.99 | 0.44 |
| 2:n:22:ILE:HA | 2:n:25:LEU:CD2 | 2.48 | 0.44 |
| 2:n:353:GLN:CG | 2:n:362:LEU:HD22 | 2.48 | 0.44 |
| 2:p:359:ARG:HD2 | 2:p:359:ARG:N | 2.32 | 0.44 |
| 2:q:99:GLN:HE21 | 1:P:50:SER:HB3 | 1.82 | 0.44 |
| 2:w:277:GLN:HG3 | 2:w:278:GLY:N | 2.30 | 0.44 |
| 2:w:352:MET:O | 2:w:356:GLY:O | 2.34 | 0.44 |
| 2:w:353:GLN:CG | 2:w:362:LEU:HD22 | 2.48 | 0.44 |
| 3:3:36:TYR:CE2 | 3:3:90:PHE:HB2 | 2.53 | 0.44 |
| 3:6:47:ASP:CG | 3:6:50:VAL:HG23 | 2.42 | 0.44 |
| 3:19:64:TYR:CB | 3:19:96:CYS:HB3 | 2.47 | 0.44 |
| 3:20:47:ASP:CG | 3:20:50:VAL:HG23 | 2.42 | 0.44 |
| 3:24:77:CYS:HB3 | 3:24:80:TYR:CE1 | 2.48 | 0.44 |
| 1:B:157:ALA:HB1 | 1:Z:41:PRO:HA | 1.98 | 0.44 |
| 1:D:111:ARG:NH1 | 1:D:111:ARG:HG2 | 2.33 | 0.44 |
| 1:D:148:LEU:HD13 | 1:D:167:LYS:HE2 | 1.99 | 0.44 |
| 1:D:222:LEU:HB2 | 1:E:231:PRO:HB3 | 2.00 | 0.44 |
| 1:E:111:ARG:HG2 | 1:E:111:ARG:NH1 | 2.33 | 0.44 |
| 1:E:121:ARG:HB3 | 1:F:111:ARG:HB3 | 1.99 | 0.44 |
| 1:G:170:ALA:HB3 | 1:H:206:GLU:HG3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:111:ARG:HG2 | 1:P:111:ARG:NH1 | 2.33 | 0.44 |
| 1:P:168:GLN:HG3 | 1:Q:204:ARG:NE | 2.32 | 0.44 |
| 1:Z:111:ARG:NH1 | 1:Z:111:ARG:HG2 | 2.33 | 0.44 |
| 2:b:81:LEU:HD23 | 2:b:81:LEU:N | 2.28 | 0.44 |
| 2:d:192:GLU:HB2 | 2:d:219:ARG:HB2 | 1.99 | 0.44 |
| 2:e:192:GLU:HB2 | 2:e:219:ARG:HB2 | 1.99 | 0.44 |
| 2:f:22:ILE:HA | 2:f:25:LEU:CD2 | 2.48 | 0.44 |
| 2:l:22:ILE:HA | 2:l:25:LEU:CD2 | 2.48 | 0.44 |
| 2:l:52:THR:HG21 | 2:l:81:LEU:HD23 | 1.99 | 0.44 |
| 2:m:22:ILE:HA | 2:m:25:LEU:CD2 | 2.48 | 0.44 |
| 2:m:353:GLN:CG | 2:m:362:LEU:HD22 | 2.48 | 0.44 |
| 2:m:359:ARG:N | 2:m:359:ARG:HD2 | 2.32 | 0.44 |
| 2:o:353:GLN:CG | 2:o:362:LEU:HD22 | 2.48 | 0.44 |
| 2:r:192:GLU:HB2 | 2:r:219:ARG:HB2 | 1.99 | 0.44 |
| 2:t:319:LEU:HD12 | 2:t:319:LEU:HA | 1.80 | 0.44 |
| 2:w:114:LYS:HD2 | 2:w:114:LYS:HA | 1.81 | 0.44 |
| 2:z:52:THR:HG21 | 2:z:81:LEU:HD23 | 1.99 | 0.44 |
| 3:2:47:ASP:CG | 3:2:50:VAL:HG23 | 2.42 | 0.44 |
| 3:15:36:TYR:CE2 | 3:15:90:PHE:HB2 | 2.53 | 0.44 |
| 3:21:36:TYR:CE2 | 3:21:90:PHE:HB2 | 2.53 | 0.44 |
| 3:25:64:TYR:CB | 3:25:96:CYS:HB3 | 2.47 | 0.44 |
| 3:26:36:TYR:CE2 | 3:26:90:PHE:HB2 | 2.53 | 0.44 |
| 3:26:47:ASP:CG | 3:26:50:VAL:HG23 | 2.42 | 0.44 |
| 1:C:124:MET:HE3 | 1:C:124:MET:HB3 | 1.77 | 0.44 |
| 1:E:168:GLN:HG3 | 1:F:204:ARG:NE | 2.32 | 0.44 |
| 1:L:121:ARG:HB3 | 1:M:111:ARG:HB3 | 2.00 | 0.44 |
| 1:L:170:ALA:HB3 | 1:M:206:GLU:HG3 | 1.99 | 0.44 |
| 1:O:171:ILE:O | 1:P:207:TYR:O | 2.35 | 0.44 |
| 1:Q:82:LEU:HD12 | 1:Q:146:GLY:HA3 | 1.98 | 0.44 |
| 1:S:168:GLN:HG3 | 1:T:204:ARG:NE | 2.33 | 0.44 |
| 2:a:219:ARG:NH2 | 2:z:94:PRO:HB2 | 2.32 | 0.44 |
| 2:c:22:ILE:HA | 2:c:25:LEU:CD2 | 2.48 | 0.44 |
| 2:f:192:GLU:HB2 | 2:f:219:ARG:HB2 | 1.99 | 0.44 |
| 2:f:196:MET:HA | 2:f:196:MET:CE | 2.47 | 0.44 |
| 2:f:341:THR:OG1 | 2:f:343:MET:HE2 | 2.16 | 0.44 |
| 2:k:52:THR:HG21 | 2:k:81:LEU:HD23 | 1.99 | 0.44 |
| 2:m:52:THR:HG21 | 2:m:81:LEU:HD23 | 1.99 | 0.44 |
| 2:n:141:ILE:HD13 | 2:n:165:ILE:CD1 | 2.39 | 0.44 |
| 2:o:328:LEU:HD21 | 2:p:273:CYS:HA | 2.00 | 0.44 |
| 2:o:359:ARG:N | 2:o:359:ARG:HD2 | 2.33 | 0.44 |
| 2:u:22:ILE:HA | 2:u:25:LEU:CD2 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:u:328:LEU:HD21 | 2:v:273:CYS:HA | 2.00 | 0.44 |
| 2:y:359:ARG:HD2 | 2:y:359:ARG:N | 2.33 | 0.44 |
| 2:z:22:ILE:HA | 2:z:25:LEU:CD2 | 2.48 | 0.44 |
| 2:z:192:GLU:HB2 | 2:z:219:ARG:HB2 | 1.99 | 0.44 |
| 3:19:47:ASP:CG | 3:19:50:VAL:HG23 | 2.42 | 0.44 |
| 1:B:132:PHE:HB3 | 1:Z:219:MET:HE2 | 1.99 | 0.44 |
| 1:E:222:LEU:HB2 | 1:F:231:PRO:HB3 | 2.00 | 0.44 |
| 1:F:168:GLN:HG3 | 1:G:204:ARG:NE | 2.32 | 0.44 |
| 1:I:121:ARG:HB3 | 1:J:111:ARG:HB3 | 2.00 | 0.44 |
| 1:K:82:LEU:HD12 | 1:K:146:GLY:HA3 | 1.98 | 0.44 |
| 1:M:41:PRO:HA | 1:O:157:ALA:HB1 | 2.00 | 0.44 |
| 1:N:82:LEU:HD13 | 1:N:144:PHE:CE1 | 2.53 | 0.44 |
| 1:N:168:GLN:HG3 | 1:O:204:ARG:NE | 2.32 | 0.44 |
| 1:O:82:LEU:HD13 | 1:O:144:PHE:CE1 | 2.53 | 0.44 |
| 1:P:82:LEU:HD13 | 1:P:144:PHE:CE1 | 2.53 | 0.44 |
| 1:Q:82:LEU:HD13 | 1:Q:144:PHE:CE1 | 2.53 | 0.44 |
| 1:Q:101:LYS:HZ2 | 1:Q:101:LYS:HB3 | 1.83 | 0.44 |
| 1:S:111:ARG:HG2 | 1:S:111:ARG:NH1 | 2.33 | 0.44 |
| 1:T:71:PRO:HD2 | 1:T:189:ILE:HD13 | 1.98 | 0.44 |
| 1:T:170:ALA:HB3 | 1:U:206:GLU:HG3 | 1.99 | 0.44 |
| 1:T:222:LEU:HB2 | 1:U:231:PRO:HB3 | 1.99 | 0.44 |
| 1:U:111:ARG:HA | 1:U:111:ARG:HD3 | 1.90 | 0.44 |
| 1:V:222:LEU:HB2 | 1:W:231:PRO:HB3 | 2.00 | 0.44 |
| 1:W:101:LYS:HZ2 | 1:W:101:LYS:HB3 | 1.83 | 0.44 |
| 1:X:82:LEU:HD12 | 1:X:146:GLY:HA3 | 1.98 | 0.44 |
| 1:Z:78:LEU:HD12 | 1:Z:193:ASN:O | 2.16 | 0.44 |
| 1:A:41:PRO:HA | 1:C:157:ALA:HB1 | 1.99 | 0.44 |
| 1:A:171:ILE:HD12 | 1:C:88:ALA:CB | 2.34 | 0.44 |
| 2:g:22:ILE:HA | 2:g:25:LEU:CD2 | 2.48 | 0.44 |
| 2:h:99:GLN:HE21 | 1:G:50:SER:HB3 | 1.82 | 0.44 |
| 2:j:123:MET:CE | 2:j:136:LEU:HD22 | 2.38 | 0.44 |
| 2:k:22:ILE:HA | 2:k:25:LEU:CD2 | 2.48 | 0.44 |
| 2:k:114:LYS:HD2 | 2:k:114:LYS:HA | 1.81 | 0.44 |
| 2:l:353:GLN:CG | 2:l:362:LEU:HD22 | 2.48 | 0.44 |
| 2:n:192:GLU:HB2 | 2:n:219:ARG:HB2 | 1.99 | 0.44 |
| 2:o:22:ILE:HA | 2:o:25:LEU:CD2 | 2.48 | 0.44 |
| 2:p:22:ILE:HA | 2:p:25:LEU:CD2 | 2.48 | 0.44 |
| 2:p:353:GLN:CG | 2:p:362:LEU:HD22 | 2.48 | 0.44 |
| 2:q:22:ILE:HA | 2:q:25:LEU:CD2 | 2.48 | 0.44 |
| 2:s:196:MET:HA | 2:s:196:MET:CE | 2.47 | 0.44 |
| 2:u:81:LEU:HD23 | 2:u:81:LEU:N | 2.28 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:u:359:ARG:N | 2:u:359:ARG:HD2 | 2.33 | 0.44 |
| 2:x:353:GLN:CG | 2:x:362:LEU:HD22 | 2.47 | 0.44 |
| 2:z:217:ASP:OD1 | 2:z:219:ARG:N | 2.35 | 0.44 |
| 3:7:47:ASP:CG | 3:7:50:VAL:HG23 | 2.42 | 0.44 |
| 3:8:47:ASP:CG | 3:8:50:VAL:HG23 | 2.42 | 0.44 |
| 3:19:77:CYS:HB3 | 3:19:80:TYR:CE1 | 2.48 | 0.44 |
| 3:22:36:TYR:CE2 | 3:22:90:PHE:HB2 | 2.53 | 0.44 |
| 1:D:101:LYS:HZ2 | 1:D:101:LYS:HB3 | 1.83 | 0.44 |
| 1:G:78:LEU:HD12 | 1:G:193:ASN:O | 2.16 | 0.44 |
| 1:G:121:ARG:HB3 | 1:H:111:ARG:HB3 | 2.00 | 0.44 |
| 1:H:111:ARG:HG2 | 1:H:111:ARG:NH1 | 2.33 | 0.44 |
| 1:J:168:GLN:HG3 | 1:K:204:ARG:NE | 2.32 | 0.44 |
| 1:K:222:LEU:HB2 | 1:L:231:PRO:HB3 | 2.00 | 0.44 |
| 1:L:111:ARG:NH1 | 1:L:111:ARG:HG2 | 2.33 | 0.44 |
| 1:M:82:LEU:HD13 | 1:M:144:PHE:CE1 | 2.52 | 0.44 |
| 1:M:170:ALA:HB3 | 1:N:206:GLU:HG3 | 1.99 | 0.44 |
| 1:N:170:ALA:HB3 | 1:O:206:GLU:HG3 | 1.99 | 0.44 |
| 1:P:121:ARG:HB3 | 1:Q:111:ARG:HB3 | 2.00 | 0.44 |
| 1:P:170:ALA:HB3 | 1:Q:206:GLU:HG3 | 1.99 | 0.44 |
| 1:R:82:LEU:HD13 | 1:R:144:PHE:CE1 | 2.53 | 0.44 |
| 1:R:168:GLN:HG3 | 1:S:204:ARG:NE | 2.33 | 0.44 |
| 1:R:171:ILE:O | 1:S:207:TYR:O | 2.35 | 0.44 |
| 1:U:111:ARG:HG2 | 1:U:111:ARG:NH1 | 2.33 | 0.44 |
| 1:U:168:GLN:HG3 | 1:V:204:ARG:NE | 2.33 | 0.44 |
| 1:W:168:GLN:HG3 | 1:X:204:ARG:NE | 2.32 | 0.44 |
| 1:W:222:LEU:HB2 | 1:X:231:PRO:HB3 | 2.00 | 0.44 |
| 1:A:111:ARG:NH1 | 1:A:111:ARG:HG2 | 2.33 | 0.44 |
| 2:c:52:THR:HG21 | 2:c:81:LEU:HD23 | 1.99 | 0.44 |
| 2:c:328:LEU:HD21 | 2:d:273:CYS:HA | 2.00 | 0.44 |
| 2:d:80:GLN:HB3 | 2:e:54:GLN:HB3 | 1.99 | 0.44 |
| 2:d:99:GLN:HE21 | 1:C:50:SER:HB3 | 1.82 | 0.44 |
| 2:f:256:ASN:OD1 | 2:f:259:THR:OG1 | 2.10 | 0.44 |
| 2:l:83:ASN:ND2 | 2:m:109:SER:OG | 2.48 | 0.44 |
| 2:m:338:LEU:O | 2:m:338:LEU:HG | 2.15 | 0.44 |
| 2:o:192:GLU:HB2 | 2:o:219:ARG:HB2 | 1.99 | 0.44 |
| 2:r:127:LYS:HA | 2:r:132:GLN:O | 2.18 | 0.44 |
| 2:s:79:MET:HE2 | 2:s:79:MET:HB2 | 1.69 | 0.44 |
| 2:s:328:LEU:HD21 | 2:t:273:CYS:HA | 2.00 | 0.44 |
| 2:t:22:ILE:HA | 2:t:25:LEU:CD2 | 2.48 | 0.44 |
| 2:v:22:ILE:HA | 2:v:25:LEU:CD2 | 2.48 | 0.44 |
| 2:v:359:ARG:HD2 | 2:v:359:ARG:N | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:x:101:GLN:OE1 | 2:y:219:ARG:HD3 | 2.18 | 0.44 |
| 2:y:136:LEU:HD13 | 2:z:129:VAL:HG11 | 1.99 | 0.44 |
| 2:y:319:LEU:HD12 | 2:y:319:LEU:HA | 1.80 | 0.44 |
| 3:3:47:ASP:CG | 3:3:50:VAL:HG23 | 2.42 | 0.44 |
| 3:4:36:TYR:CE2 | 3:4:90:PHE:HB2 | 2.53 | 0.44 |
| 3:6:70:PHE:CD1 | 3:6:70:PHE:C | 2.96 | 0.44 |
| 3:8:70:PHE:CD1 | 3:8:70:PHE:C | 2.96 | 0.44 |
| 3:9:28:ILE:O | 3:9:29:SER:OG | 2.21 | 0.44 |
| 3:9:47:ASP:CG | 3:9:50:VAL:HG23 | 2.42 | 0.44 |
| 3:13:36:TYR:CE2 | 3:13:90:PHE:HB2 | 2.53 | 0.44 |
| 3:15:47:ASP:CG | 3:15:50:VAL:HG23 | 2.42 | 0.44 |
| 3:16:36:TYR:CE2 | 3:16:90:PHE:HB2 | 2.53 | 0.44 |
| 3:17:36:TYR:CE2 | 3:17:90:PHE:HB2 | 2.53 | 0.44 |
| 3:18:64:TYR:CB | 3:18:96:CYS:HB3 | 2.47 | 0.44 |
| 3:23:36:TYR:CE2 | 3:23:90:PHE:HB2 | 2.53 | 0.44 |
| 3:24:82:GLY:O | 1:Y:210:ASN:ND2 | 2.50 | 0.44 |
| 1:B:106:PHE:C | 1:B:108:THR:H | 2.26 | 0.44 |
| 1:D:82:LEU:HD13 | 1:D:144:PHE:CE1 | 2.53 | 0.44 |
| 1:F:170:ALA:HB3 | 1:G:206:GLU:HG3 | 1.99 | 0.44 |
| 1:G:106:PHE:C | 1:G:108:THR:H | 2.26 | 0.44 |
| 1:I:106:PHE:C | 1:I:108:THR:H | 2.26 | 0.44 |
| 1:I:170:ALA:HB3 | 1:J:206:GLU:HG3 | 2.00 | 0.44 |
| 1:Q:168:GLN:HG3 | 1:R:204:ARG:NE | 2.32 | 0.44 |
| 1:S:82:LEU:HD13 | 1:S:144:PHE:CE1 | 2.53 | 0.44 |
| 1:T:121:ARG:HB3 | 1:U:111:ARG:HB3 | 1.99 | 0.44 |
| 1:W:170:ALA:HB3 | 1:X:206:GLU:HG3 | 1.99 | 0.44 |
| 1:W:171:ILE:O | 1:X:207:TYR:O | 2.34 | 0.44 |
| 1:X:111:ARG:HG2 | 1:X:111:ARG:NH1 | 2.33 | 0.44 |
| 2:a:188:GLN:HB3 | 2:z:101:GLN:NE2 | 2.33 | 0.44 |
| 2:d:89:VAL:HG21 | 2:d:124:THR:OG1 | 2.18 | 0.44 |
| 2:f:80:GLN:HB3 | 2:g:54:GLN:HB3 | 1.99 | 0.44 |
| 2:g:196:MET:HA | 2:g:196:MET:CE | 2.47 | 0.44 |
| 2:j:80:GLN:HB3 | 2:k:54:GLN:HB3 | 2.00 | 0.44 |
| 2:j:127:LYS:HA | 2:j:132:GLN:O | 2.18 | 0.44 |
| 2:k:127:LYS:HA | 2:k:132:GLN:O | 2.18 | 0.44 |
| 2:q:127:LYS:HA | 2:q:132:GLN:O | 2.18 | 0.44 |
| 2:s:127:LYS:HA | 2:s:132:GLN:O | 2.18 | 0.44 |
| 2:w:22:ILE:HA | 2:w:25:LEU:CD2 | 2.48 | 0.44 |
| 2:x:22:ILE:HA | 2:x:25:LEU:CD2 | 2.48 | 0.44 |
| 3:7:36:TYR:CE2 | 3:7:90:PHE:HB2 | 2.53 | 0.44 |
| 3:22:47:ASP:CG | 3:22:50:VAL:HG23 | 2.42 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:25:36:TYR:CE2 | 3:25:90:PHE:HB2 | 2.53 | 0.44 |
| 3:25:38:GLN:HG2 | 3:25:44:SER:HB3 | 2.00 | 0.44 |
| 1:C:82:LEU:HD12 | 1:C:146:GLY:HA3 | 1.97 | 0.44 |
| 1:E:82:LEU:HD13 | 1:E:144:PHE:CE1 | 2.53 | 0.44 |
| 1:F:82:LEU:HD13 | 1:F:144:PHE:CE1 | 2.53 | 0.44 |
| 1:J:121:ARG:HB3 | 1:K:111:ARG:HB3 | 2.00 | 0.44 |
| 1:K:111:ARG:HG2 | 1:K:111:ARG:NH1 | 2.33 | 0.44 |
| 1:L:82:LEU:HD13 | 1:L:144:PHE:CE1 | 2.53 | 0.44 |
| 1:M:106:PHE:C | 1:M:108:THR:H | 2.26 | 0.44 |
| 1:O:135:LYS:HB2 | 1:O:135:LYS:HE2 | 1.73 | 0.44 |
| 1:P:222:LEU:HB2 | 1:Q:231:PRO:HB3 | 2.00 | 0.44 |
| 1:R:82:LEU:HD12 | 1:R:146:GLY:HA3 | 1.98 | 0.44 |
| 1:S:171:ILE:O | 1:T:207:TYR:O | 2.35 | 0.44 |
| 1:T:82:LEU:HD13 | 1:T:144:PHE:CE1 | 2.53 | 0.44 |
| 1:Z:82:LEU:HD13 | 1:Z:144:PHE:CE1 | 2.53 | 0.44 |
| 1:A:82:LEU:HD13 | 1:A:144:PHE:CE1 | 2.53 | 0.44 |
| 2:c:89:VAL:HG21 | 2:c:124:THR:OG1 | 2.18 | 0.44 |
| 2:c:127:LYS:HA | 2:c:132:GLN:O | 2.18 | 0.44 |
| 2:d:127:LYS:HA | 2:d:132:GLN:O | 2.18 | 0.44 |
| 2:f:250:ASP:O | 2:f:265:ASN:ND2 | 2.51 | 0.44 |
| 2:g:93:TYR:OH | 2:g:173:ARG:O | 2.24 | 0.44 |
| 2:h:83:ASN:ND2 | 2:i:109:SER:OG | 2.48 | 0.44 |
| 2:j:22:ILE:HA | 2:j:25:LEU:CD2 | 2.48 | 0.44 |
| 2:j:89:VAL:HG21 | 2:j:124:THR:OG1 | 2.18 | 0.44 |
| 2:m:328:LEU:HD21 | 2:n:273:CYS:HA | 2.00 | 0.44 |
| 2:o:89:VAL:HG21 | 2:o:124:THR:OG1 | 2.18 | 0.44 |
| 2:p:192:GLU:HB2 | 2:p:219:ARG:HB2 | 1.99 | 0.44 |
| 2:s:52:THR:HG21 | 2:s:81:LEU:HD23 | 1.99 | 0.44 |
| 2:s:99:GLN:HE21 | 1:R:50:SER:HB3 | 1.83 | 0.44 |
| 2:t:89:VAL:HG21 | 2:t:124:THR:OG1 | 2.18 | 0.44 |
| 2:u:89:VAL:HG21 | 2:u:124:THR:OG1 | 2.18 | 0.44 |
| 2:u:192:GLU:HB2 | 2:u:219:ARG:HB2 | 1.99 | 0.44 |
| 2:v:173:ARG:HH12 | 1:U:54:SER:HB2 | 1.83 | 0.44 |
| 2:w:89:VAL:HG21 | 2:w:124:THR:OG1 | 2.18 | 0.44 |
| 2:w:123:MET:CE | 2:w:136:LEU:HD22 | 2.38 | 0.44 |
| 2:w:192:GLU:HB2 | 2:w:219:ARG:HB2 | 1.99 | 0.44 |
| 2:x:89:VAL:HG21 | 2:x:124:THR:OG1 | 2.18 | 0.44 |
| 2:y:89:VAL:HG21 | 2:y:124:THR:OG1 | 2.18 | 0.44 |
| 3:4:70:PHE:CD1 | 3:4:70:PHE:C | 2.96 | 0.44 |
| 3:8:36:TYR:CE2 | 3:8:90:PHE:HB2 | 2.53 | 0.44 |
| 3:10:36:TYR:CE2 | 3:10:90:PHE:HB2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:18:70:PHE:CD1 | 3:18:70:PHE:C | 2.96 | 0.44 |
| 3:23:70:PHE:CD1 | 3:23:70:PHE:C | 2.96 | 0.44 |
| 3:23:77:CYS:HB3 | 3:23:80:TYR:CE1 | 2.48 | 0.44 |
| 1:B:121:ARG:HB3 | 1:C:111:ARG:HB3 | 1.99 | 0.44 |
| 1:C:106:PHE:C | 1:C:108:THR:H | 2.26 | 0.44 |
| 1:C:111:ARG:HG2 | 1:C:111:ARG:NH1 | 2.33 | 0.44 |
| 1:C:168:GLN:HG3 | 1:D:204:ARG:NE | 2.33 | 0.44 |
| 1:D:121:ARG:HB3 | 1:E:111:ARG:HB3 | 2.00 | 0.44 |
| 1:F:106:PHE:C | 1:F:108:THR:H | 2.26 | 0.44 |
| 1:F:219:MET:HE2 | 1:H:132:PHE:HB3 | 2.00 | 0.44 |
| 1:H:171:ILE:HD12 | 1:J:88:ALA:CB | 2.34 | 0.44 |
| 1:I:111:ARG:NH1 | 1:I:111:ARG:HG2 | 2.33 | 0.44 |
| 1:J:171:ILE:HD12 | 1:L:88:ALA:CB | 2.35 | 0.44 |
| 1:L:106:PHE:C | 1:L:108:THR:H | 2.26 | 0.44 |
| 1:N:106:PHE:C | 1:N:108:THR:H | 2.26 | 0.44 |
| 1:N:111:ARG:NH1 | 1:N:111:ARG:HG2 | 2.33 | 0.44 |
| 1:N:135:LYS:HE2 | 1:N:135:LYS:HB2 | 1.73 | 0.44 |
| 1:O:121:ARG:HB3 | 1:P:111:ARG:HB3 | 2.00 | 0.44 |
| 1:R:106:PHE:C | 1:R:108:THR:H | 2.26 | 0.44 |
| 1:R:170:ALA:HB3 | 1:S:206:GLU:HG3 | 1.99 | 0.44 |
| 1:U:171:ILE:O | 1:V:207:TYR:O | 2.35 | 0.44 |
| 1:X:82:LEU:HD13 | 1:X:144:PHE:CE1 | 2.53 | 0.44 |
| 1:Y:82:LEU:HD13 | 1:Y:144:PHE:CE1 | 2.53 | 0.44 |
| 1:A:231:PRO:HB3 | 1:Z:222:LEU:HB2 | 2.00 | 0.43 |
| 2:a:127:LYS:HA | 2:a:132:GLN:O | 2.18 | 0.43 |
| 2:a:328:LEU:HD21 | 2:b:273:CYS:HA | 2.00 | 0.43 |
| 3:1:38:GLN:HG2 | 3:1:44:SER:HB3 | 2.00 | 0.43 |
| 2:b:127:LYS:HA | 2:b:132:GLN:O | 2.18 | 0.43 |
| 2:c:99:GLN:HE21 | 1:B:50:SER:HB3 | 1.82 | 0.43 |
| 2:c:192:GLU:HB2 | 2:c:219:ARG:HB2 | 1.99 | 0.43 |
| 2:c:250:ASP:O | 2:c:265:ASN:ND2 | 2.51 | 0.43 |
| 2:g:99:GLN:HE21 | 1:F:50:SER:HB3 | 1.82 | 0.43 |
| 2:i:22:ILE:HA | 2:i:25:LEU:CD2 | 2.48 | 0.43 |
| 2:i:89:VAL:HG21 | 2:i:124:THR:OG1 | 2.18 | 0.43 |
| 2:i:127:LYS:HA | 2:i:132:GLN:O | 2.18 | 0.43 |
| 2:j:142:LEU:HD22 | 2:l:364:ILE:CD1 | 2.48 | 0.43 |
| 2:k:83:ASN:ND2 | 2:l:109:SER:OG | 2.48 | 0.43 |
| 2:k:359:ARG:N | 2:k:359:ARG:HD2 | 2.32 | 0.43 |
| 2:l:127:LYS:HA | 2:l:132:GLN:O | 2.18 | 0.43 |
| 2:m:93:TYR:OH | 2:m:173:ARG:O | 2.24 | 0.43 |
| 2:m:127:LYS:HA | 2:m:132:GLN:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:99:GLN:HE21 | 1:M:50:SER:HB3 | 1.82 | 0.43 |
| 2:n:359:ARG:HD2 | 2:n:359:ARG:N | 2.32 | 0.43 |
| 2:p:127:LYS:HA | 2:p:132:GLN:O | 2.18 | 0.43 |
| 2:q:89:VAL:HG21 | 2:q:124:THR:OG1 | 2.18 | 0.43 |
| 2:q:359:ARG:N | 2:q:359:ARG:HD2 | 2.32 | 0.43 |
| 2:r:22:ILE:HA | 2:r:25:LEU:CD2 | 2.48 | 0.43 |
| 2:r:89:VAL:HG21 | 2:r:124:THR:OG1 | 2.18 | 0.43 |
| 2:s:89:VAL:HG21 | 2:s:124:THR:OG1 | 2.18 | 0.43 |
| 2:v:89:VAL:HG21 | 2:v:124:THR:OG1 | 2.18 | 0.43 |
| 2:y:192:GLU:HB2 | 2:y:219:ARG:HB2 | 1.99 | 0.43 |
| 2:z:89:VAL:HG21 | 2:z:124:THR:OG1 | 2.18 | 0.43 |
| 2:z:127:LYS:HA | 2:z:132:GLN:O | 2.18 | 0.43 |
| 3:9:36:TYR:CE2 | 3:9:90:PHE:HB2 | 2.53 | 0.43 |
| 3:10:70:PHE:CD1 | 3:10:70:PHE:C | 2.96 | 0.43 |
| 3:11:36:TYR:CE2 | 3:11:90:PHE:HB2 | 2.53 | 0.43 |
| 3:12:36:TYR:CE2 | 3:12:90:PHE:HB2 | 2.53 | 0.43 |
| 3:21:70:PHE:CD1 | 3:21:70:PHE:C | 2.96 | 0.43 |
| 3:26:38:GLN:HG2 | 3:26:44:SER:HB3 | 2.00 | 0.43 |
| 1:C:149:THR:OG1 | 1:D:198:THR:O | 2.35 | 0.43 |
| 1:F:111:ARG:NH1 | 1:F:111:ARG:HG2 | 2.33 | 0.43 |
| 1:F:121:ARG:HB3 | 1:G:111:ARG:HB3 | 2.00 | 0.43 |
| 1:G:82:LEU:HD13 | 1:G:144:PHE:CE1 | 2.53 | 0.43 |
| 1:K:82:LEU:HA | 1:K:197:SER:CB | 2.43 | 0.43 |
| 1:K:82:LEU:HD13 | 1:K:144:PHE:CE1 | 2.53 | 0.43 |
| 1:M:222:LEU:HB2 | 1:N:231:PRO:HB3 | 2.00 | 0.43 |
| 1:O:168:GLN:HG3 | 1:P:204:ARG:NE | 2.33 | 0.43 |
| 1:Q:90:LYS:HE2 | 1:Q:138:ALA:HB3 | 2.00 | 0.43 |
| 1:Q:170:ALA:HB3 | 1:R:206:GLU:HG3 | 1.99 | 0.43 |
| 1:Q:222:LEU:HB2 | 1:R:231:PRO:HB3 | 2.00 | 0.43 |
| 1:S:101:LYS:HZ2 | 1:S:101:LYS:HB3 | 1.83 | 0.43 |
| 1:U:82:LEU:HD13 | 1:U:144:PHE:CE1 | 2.53 | 0.43 |
| 1:U:170:ALA:HB3 | 1:V:206:GLU:HG3 | 2.00 | 0.43 |
| 1:W:176:GLU:OE2 | 1:Y:90:LYS:HD3 | 2.18 | 0.43 |
| 2:a:89:VAL:HG21 | 2:a:124:THR:OG1 | 2.18 | 0.43 |
| 2:b:79:MET:HE2 | 2:b:79:MET:HB2 | 1.69 | 0.43 |
| 2:d:353:GLN:CG | 2:d:362:LEU:HD22 | 2.47 | 0.43 |
| 2:e:127:LYS:HA | 2:e:132:GLN:O | 2.18 | 0.43 |
| 2:f:83:ASN:ND2 | 2:g:109:SER:OG | 2.48 | 0.43 |
| 2:h:22:ILE:HA | 2:h:25:LEU:CD2 | 2.48 | 0.43 |
| 2:i:250:ASP:O | 2:i:265:ASN:ND2 | 2.51 | 0.43 |
| 2:k:89:VAL:HG21 | 2:k:124:THR:OG1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:p:89:VAL:HG21 | 2:p:124:THR:OG1 | 2.18 | 0.43 |
| 2:x:159:GLN:CB | 2:y:258:ARG:HG2 | 2.48 | 0.43 |
| 2:y:99:GLN:HE21 | 1:X:50:SER:HB3 | 1.82 | 0.43 |
| 2:y:353:GLN:CG | 2:y:362:LEU:HD22 | 2.47 | 0.43 |
| 3:2:38:GLN:HG2 | 3:2:44:SER:HB3 | 2.00 | 0.43 |
| 3:10:47:ASP:CG | 3:10:50:VAL:HG23 | 2.42 | 0.43 |
| 3:19:36:TYR:HE2 | 3:19:44:SER:HG | 1.64 | 0.43 |
| 3:20:70:PHE:CD1 | 3:20:70:PHE:C | 2.96 | 0.43 |
| 3:24:38:GLN:HG2 | 3:24:44:SER:HB3 | 2.00 | 0.43 |
| 1:C:121:ARG:HB3 | 1:D:111:ARG:HB3 | 2.00 | 0.43 |
| 1:D:82:LEU:HA | 1:D:197:SER:CB | 2.43 | 0.43 |
| 1:F:222:LEU:HB2 | 1:G:231:PRO:HB3 | 2.00 | 0.43 |
| 1:L:168:GLN:HG3 | 1:M:204:ARG:NE | 2.32 | 0.43 |
| 1:M:90:LYS:HE2 | 1:M:138:ALA:HB3 | 2.01 | 0.43 |
| 1:N:90:LYS:HE2 | 1:N:138:ALA:HB3 | 2.01 | 0.43 |
| 1:Q:111:ARG:NH1 | 1:Q:111:ARG:HG2 | 2.33 | 0.43 |
| 1:R:111:ARG:NH1 | 1:R:111:ARG:HG2 | 2.33 | 0.43 |
| 1:R:121:ARG:HB3 | 1:S:111:ARG:HB3 | 2.00 | 0.43 |
| 1:S:41:PRO:HA | 1:U:157:ALA:HB1 | 2.00 | 0.43 |
| 1:T:171:ILE:O | 1:U:207:TYR:O | 2.34 | 0.43 |
| 1:A:84:GLU:OE2 | 1:Z:167:LYS:NZ | 2.41 | 0.43 |
| 1:A:106:PHE:C | 1:A:108:THR:H | 2.26 | 0.43 |
| 2:a:89:VAL:CG2 | 2:a:126:LEU:HD21 | 2.48 | 0.43 |
| 2:b:89:VAL:HG21 | 2:b:124:THR:OG1 | 2.18 | 0.43 |
| 2:b:89:VAL:CG2 | 2:b:126:LEU:HD21 | 2.48 | 0.43 |
| 2:b:192:GLU:HB2 | 2:b:219:ARG:HB2 | 1.99 | 0.43 |
| 2:d:52:THR:HG21 | 2:d:81:LEU:HD23 | 1.99 | 0.43 |
| 2:d:217:ASP:OD1 | 2:d:219:ARG:N | 2.35 | 0.43 |
| 2:e:89:VAL:HG21 | 2:e:124:THR:OG1 | 2.18 | 0.43 |
| 2:e:353:GLN:CG | 2:e:362:LEU:HD22 | 2.48 | 0.43 |
| 2:f:52:THR:HG21 | 2:f:81:LEU:HD23 | 1.99 | 0.43 |
| 2:g:52:THR:HG21 | 2:g:81:LEU:HD23 | 1.99 | 0.43 |
| 2:h:196:MET:HA | 2:h:196:MET:CE | 2.47 | 0.43 |
| 2:j:83:ASN:ND2 | 2:k:109:SER:OG | 2.47 | 0.43 |
| 2:n:89:VAL:HG21 | 2:n:124:THR:OG1 | 2.18 | 0.43 |
| 2:q:353:GLN:CG | 2:q:362:LEU:HD22 | 2.48 | 0.43 |
| 2:s:192:GLU:HB2 | 2:s:219:ARG:HB2 | 1.99 | 0.43 |
| 2:t:114:LYS:HA | 2:t:114:LYS:HD2 | 1.81 | 0.43 |
| 2:x:127:LYS:HA | 2:x:132:GLN:O | 2.18 | 0.43 |
| 2:x:173:ARG:HH12 | 1:W:54:SER:HB2 | 1.83 | 0.43 |
| 2:y:22:ILE:HA | 2:y:25:LEU:CD2 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:y:127:LYS:HA | 2:y:132:GLN:O | 2.18 | 0.43 |
| 3:11:70:PHE:CD1 | 3:11:70:PHE:C | 2.96 | 0.43 |
| 3:16:70:PHE:CD1 | 3:16:70:PHE:C | 2.96 | 0.43 |
| 3:24:47:ASP:CG | 3:24:50:VAL:HG23 | 2.42 | 0.43 |
| 1:B:82:LEU:HD13 | 1:B:144:PHE:CE1 | 2.53 | 0.43 |
| 1:G:219:MET:HE2 | 1:I:132:PHE:HB3 | 2.00 | 0.43 |
| 1:G:222:LEU:HB2 | 1:H:231:PRO:HB3 | 2.00 | 0.43 |
| 1:I:168:GLN:HG3 | 1:J:204:ARG:NE | 2.33 | 0.43 |
| 1:J:106:PHE:C | 1:J:108:THR:H | 2.26 | 0.43 |
| 1:L:41:PRO:HA | 1:N:157:ALA:HB1 | 2.00 | 0.43 |
| 1:L:90:LYS:HE2 | 1:L:138:ALA:HB3 | 2.01 | 0.43 |
| 1:N:171:ILE:O | 1:N:172:ASN:HB3 | 2.19 | 0.43 |
| 1:O:90:LYS:HE2 | 1:O:138:ALA:HB3 | 2.01 | 0.43 |
| 1:P:90:LYS:HE2 | 1:P:138:ALA:HB3 | 2.01 | 0.43 |
| 1:P:171:ILE:O | 1:P:172:ASN:HB3 | 2.19 | 0.43 |
| 1:R:90:LYS:HE2 | 1:R:138:ALA:HB3 | 2.01 | 0.43 |
| 1:R:171:ILE:O | 1:R:172:ASN:HB3 | 2.19 | 0.43 |
| 1:R:222:LEU:HB2 | 1:S:231:PRO:HB3 | 2.00 | 0.43 |
| 1:S:106:PHE:C | 1:S:108:THR:H | 2.26 | 0.43 |
| 1:S:124:MET:HB3 | 1:S:124:MET:HE3 | 1.76 | 0.43 |
| 1:T:90:LYS:HE2 | 1:T:138:ALA:HB3 | 2.01 | 0.43 |
| 1:T:221:TRP:NE1 | 1:U:229:LEU:O | 2.39 | 0.43 |
| 1:V:171:ILE:HD12 | 1:X:88:ALA:CB | 2.35 | 0.43 |
| 1:W:106:PHE:C | 1:W:108:THR:H | 2.26 | 0.43 |
| 2:a:52:THR:HG21 | 2:a:81:LEU:HD23 | 1.99 | 0.43 |
| 2:a:359:ARG:N | 2:a:359:ARG:HD2 | 2.32 | 0.43 |
| 2:f:127:LYS:HA | 2:f:132:GLN:O | 2.18 | 0.43 |
| 2:f:359:ARG:HD2 | 2:f:359:ARG:N | 2.32 | 0.43 |
| 2:i:328:LEU:HD21 | 2:j:273:CYS:HA | 1.99 | 0.43 |
| 2:l:80:GLN:HB3 | 2:m:54:GLN:HB3 | 2.00 | 0.43 |
| 2:r:173:ARG:HH12 | 1:Q:54:SER:HB2 | 1.83 | 0.43 |
| 2:s:359:ARG:N | 2:s:359:ARG:HD2 | 2.32 | 0.43 |
| 2:z:250:ASP:O | 2:z:265:ASN:ND2 | 2.51 | 0.43 |
| 3:4:29:SER:OG | 3:4:31:ILE:HG12 | 2.19 | 0.43 |
| 3:4:47:ASP:CG | 3:4:50:VAL:HG23 | 2.42 | 0.43 |
| 3:7:47:ASP:CG | 3:7:50:VAL:H | 2.14 | 0.43 |
| 3:9:29:SER:OG | 3:9:31:ILE:HG12 | 2.19 | 0.43 |
| 3:9:70:PHE:CD1 | 3:9:70:PHE:C | 2.96 | 0.43 |
| 3:14:47:ASP:CG | 3:14:50:VAL:HG23 | 2.42 | 0.43 |
| 3:15:29:SER:OG | 3:15:31:ILE:HG12 | 2.19 | 0.43 |
| 3:19:70:PHE:CD1 | 3:19:70:PHE:C | 2.96 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:20:77:CYS:HB3 | 3:20:80:TYR:CE1 | 2.48 | 0.43 |
| 3:23:38:GLN:HG2 | 3:23:44:SER:HB3 | 2.00 | 0.43 |
| 3:25:70:PHE:CD1 | 3:25:70:PHE:C | 2.96 | 0.43 |
| 1:B:168:GLN:HG3 | 1:C:204:ARG:NE | 2.32 | 0.43 |
| 1:C:82:LEU:HD13 | 1:C:144:PHE:CE1 | 2.53 | 0.43 |
| 1:F:101:LYS:HZ2 | 1:F:101:LYS:HB3 | 1.83 | 0.43 |
| 1:G:111:ARG:NH1 | 1:G:111:ARG:HG2 | 2.33 | 0.43 |
| 1:J:82:LEU:HD13 | 1:J:144:PHE:CE1 | 2.53 | 0.43 |
| 1:K:168:GLN:HG3 | 1:L:204:ARG:NE | 2.32 | 0.43 |
| 1:L:171:ILE:O | 1:L:172:ASN:HB3 | 2.19 | 0.43 |
| 1:R:41:PRO:HA | 1:T:157:ALA:HB1 | 2.00 | 0.43 |
| 1:S:90:LYS:HE2 | 1:S:138:ALA:HB3 | 2.01 | 0.43 |
| 1:S:135:LYS:HE2 | 1:S:135:LYS:HB2 | 1.73 | 0.43 |
| 1:S:170:ALA:HB3 | 1:T:206:GLU:HG3 | 1.99 | 0.43 |
| 1:T:171:ILE:O | 1:T:172:ASN:HB3 | 2.19 | 0.43 |
| 1:U:90:LYS:HE2 | 1:U:138:ALA:HB3 | 2.01 | 0.43 |
| 1:V:40:ILE:H | 1:V:40:ILE:HG12 | 1.49 | 0.43 |
| 1:V:111:ARG:NH1 | 1:V:111:ARG:HG2 | 2.33 | 0.43 |
| 1:X:106:PHE:C | 1:X:108:THR:H | 2.26 | 0.43 |
| 2:a:192:GLU:HB2 | 2:a:219:ARG:HB2 | 1.99 | 0.43 |
| 2:f:173:ARG:HH12 | 1:E:54:SER:HB2 | 1.83 | 0.43 |
| 2:f:353:GLN:CG | 2:f:362:LEU:HD22 | 2.48 | 0.43 |
| 2:h:52:THR:HG21 | 2:h:81:LEU:HD23 | 1.99 | 0.43 |
| 2:h:359:ARG:N | 2:h:359:ARG:HD2 | 2.32 | 0.43 |
| 2:i:52:THR:HG21 | 2:i:81:LEU:HD23 | 1.99 | 0.43 |
| 2:j:217:ASP:OD1 | 2:j:219:ARG:N | 2.35 | 0.43 |
| 2:k:101:GLN:OE1 | 2:l:219:ARG:HD3 | 2.19 | 0.43 |
| 2:k:343:MET:SD | 2:k:343:MET:N | 2.91 | 0.43 |
| 2:m:79:MET:HE2 | 2:m:79:MET:HB2 | 1.69 | 0.43 |
| 2:n:127:LYS:HA | 2:n:132:GLN:O | 2.18 | 0.43 |
| 2:p:142:LEU:HD22 | 2:r:364:ILE:CD1 | 2.48 | 0.43 |
| 2:q:192:GLU:HB2 | 2:q:219:ARG:HB2 | 1.99 | 0.43 |
| 2:t:127:LYS:HA | 2:t:132:GLN:O | 2.18 | 0.43 |
| 2:v:142:LEU:HD22 | 2:x:364:ILE:CD1 | 2.48 | 0.43 |
| 3:3:38:GLN:HG2 | 3:3:44:SER:HB3 | 2.00 | 0.43 |
| 3:3:70:PHE:CD1 | 3:3:70:PHE:C | 2.96 | 0.43 |
| 3:5:47:ASP:CG | 3:5:50:VAL:HG23 | 2.42 | 0.43 |
| 3:13:70:PHE:CD1 | 3:13:70:PHE:C | 2.96 | 0.43 |
| 3:14:29:SER:OG | 3:14:31:ILE:HG12 | 2.19 | 0.43 |
| 3:14:36:TYR:CE2 | 3:14:90:PHE:HB2 | 2.53 | 0.43 |
| 3:22:47:ASP:CG | 3:22:50:VAL:H | 2.14 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:22:70:PHE:CD1 | 3:22:70:PHE:C | 2.96 | 0.43 |
| 3:24:36:TYR:CE2 | 3:24:90:PHE:HB2 | 2.53 | 0.43 |
| 1:B:170:ALA:HB3 | 1:C:206:GLU:HG3 | 1.99 | 0.43 |
| 1:C:170:ALA:HB3 | 1:D:206:GLU:HG3 | 2.00 | 0.43 |
| 1:H:221:TRP:NE1 | 1:I:229:LEU:O | 2.39 | 0.43 |
| 1:I:82:LEU:HD13 | 1:I:144:PHE:CE1 | 2.53 | 0.43 |
| 1:K:90:LYS:HE2 | 1:K:138:ALA:HB3 | 2.01 | 0.43 |
| 1:M:111:ARG:HG2 | 1:M:111:ARG:NH1 | 2.33 | 0.43 |
| 1:M:168:GLN:HG3 | 1:N:204:ARG:NE | 2.33 | 0.43 |
| 1:O:106:PHE:C | 1:O:108:THR:H | 2.26 | 0.43 |
| 1:P:82:LEU:HA | 1:P:197:SER:CB | 2.43 | 0.43 |
| 1:S:121:ARG:HB3 | 1:T:111:ARG:HB3 | 2.00 | 0.43 |
| 1:V:82:LEU:HD13 | 1:V:144:PHE:CE1 | 2.53 | 0.43 |
| 1:V:171:ILE:O | 1:V:172:ASN:HB3 | 2.19 | 0.43 |
| 1:W:111:ARG:NH1 | 1:W:111:ARG:HG2 | 2.33 | 0.43 |
| 1:A:88:ALA:CB | 1:Y:171:ILE:HD12 | 2.37 | 0.43 |
| 1:A:171:ILE:O | 1:B:207:TYR:O | 2.36 | 0.43 |
| 2:a:22:ILE:HA | 2:a:25:LEU:CD2 | 2.48 | 0.43 |
| 2:a:273:CYS:HA | 2:z:328:LEU:HD21 | 2.01 | 0.43 |
| 2:a:364:ILE:HD12 | 2:y:142:LEU:HD22 | 2.01 | 0.43 |
| 2:c:359:ARG:HD2 | 2:c:359:ARG:N | 2.32 | 0.43 |
| 2:e:52:THR:HG21 | 2:e:81:LEU:HD23 | 1.99 | 0.43 |
| 2:g:353:GLN:CG | 2:g:362:LEU:HD22 | 2.47 | 0.43 |
| 2:h:89:VAL:HG21 | 2:h:124:THR:OG1 | 2.18 | 0.43 |
| 2:p:173:ARG:HH12 | 1:O:54:SER:HB2 | 1.83 | 0.43 |
| 2:t:173:ARG:HH12 | 1:S:54:SER:HB2 | 1.84 | 0.43 |
| 3:2:70:PHE:CD1 | 3:2:70:PHE:C | 2.96 | 0.43 |
| 3:3:29:SER:OG | 3:3:31:ILE:HG12 | 2.19 | 0.43 |
| 3:6:36:TYR:CE2 | 3:6:90:PHE:HB2 | 2.53 | 0.43 |
| 3:10:29:SER:OG | 3:10:31:ILE:HG12 | 2.19 | 0.43 |
| 3:11:38:GLN:HG2 | 3:11:44:SER:HB3 | 2.00 | 0.43 |
| 3:12:38:GLN:HG2 | 3:12:44:SER:HB3 | 2.00 | 0.43 |
| 3:13:38:GLN:HG2 | 3:13:44:SER:HB3 | 2.00 | 0.43 |
| 3:14:38:GLN:HG2 | 3:14:44:SER:HB3 | 2.00 | 0.43 |
| 3:22:38:GLN:HG2 | 3:22:44:SER:HB3 | 2.00 | 0.43 |
| 1:D:106:PHE:C | 1:D:108:THR:H | 2.26 | 0.43 |
| 1:E:106:PHE:C | 1:E:108:THR:H | 2.26 | 0.43 |
| 1:E:219:MET:HE2 | 1:G:132:PHE:HB3 | 2.01 | 0.43 |
| 1:H:30:LEU:HD21 | 1:I:206:GLU:HG3 | 2.01 | 0.43 |
| 1:H:82:LEU:HD13 | 1:H:144:PHE:CE1 | 2.53 | 0.43 |
| 1:H:168:GLN:HG3 | 1:I:204:ARG:NE | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:90:LYS:HE2 | 1:J:138:ALA:HB3 | 2.01 | 0.43 |
| 1:M:124:MET:HE3 | 1:M:124:MET:HB3 | 1.76 | 0.43 |
| 1:M:135:LYS:HB2 | 1:M:135:LYS:HE2 | 1.73 | 0.43 |
| 1:P:106:PHE:C | 1:P:108:THR:H | 2.26 | 0.43 |
| 1:P:135:LYS:HE2 | 1:P:135:LYS:HB2 | 1.73 | 0.43 |
| 1:Q:106:PHE:C | 1:Q:108:THR:H | 2.26 | 0.43 |
| 1:U:121:ARG:HB3 | 1:V:111:ARG:HB3 | 2.00 | 0.43 |
| 1:W:121:ARG:HB3 | 1:X:111:ARG:HB3 | 1.99 | 0.43 |
| 1:X:219:MET:HE2 | 1:Z:132:PHE:HB3 | 2.00 | 0.43 |
| 2:a:93:TYR:OH | 2:a:173:ARG:O | 2.24 | 0.43 |
| 2:a:129:VAL:HG11 | 2:z:136:LEU:HD13 | 2.01 | 0.43 |
| 2:a:136:LEU:HD13 | 2:b:129:VAL:HG11 | 2.01 | 0.43 |
| 3:1:70:PHE:CD1 | 3:1:70:PHE:C | 2.96 | 0.43 |
| 2:c:89:VAL:CG2 | 2:c:126:LEU:HD21 | 2.48 | 0.43 |
| 2:d:173:ARG:HH12 | 1:C:54:SER:HB2 | 1.83 | 0.43 |
| 2:e:359:ARG:N | 2:e:359:ARG:HD2 | 2.32 | 0.43 |
| 2:h:127:LYS:HA | 2:h:132:GLN:O | 2.18 | 0.43 |
| 2:i:123:MET:CE | 2:i:136:LEU:HD22 | 2.38 | 0.43 |
| 2:j:250:ASP:O | 2:j:265:ASN:ND2 | 2.51 | 0.43 |
| 2:l:173:ARG:HH12 | 1:K:54:SER:HB2 | 1.83 | 0.43 |
| 2:l:250:ASP:O | 2:l:265:ASN:ND2 | 2.52 | 0.43 |
| 2:n:80:GLN:HB3 | 2:o:54:GLN:HB3 | 2.01 | 0.43 |
| 2:n:217:ASP:OD1 | 2:n:219:ARG:N | 2.35 | 0.43 |
| 2:r:208:ARG:HG3 | 2:r:235:PHE:CZ | 2.54 | 0.43 |
| 2:u:173:ARG:HH12 | 1:T:54:SER:HB2 | 1.84 | 0.43 |
| 2:w:50:ASP:OD1 | 2:w:113:ALA:N | 2.52 | 0.43 |
| 2:w:127:LYS:HA | 2:w:132:GLN:O | 2.18 | 0.43 |
| 2:y:336:ASN:HD22 | 2:y:336:ASN:HA | 1.66 | 0.43 |
| 3:5:70:PHE:CD1 | 3:5:70:PHE:C | 2.96 | 0.43 |
| 3:12:47:ASP:CG | 3:12:50:VAL:HG23 | 2.42 | 0.43 |
| 3:12:70:PHE:CD1 | 3:12:70:PHE:C | 2.96 | 0.43 |
| 3:16:29:SER:OG | 3:16:31:ILE:HG12 | 2.19 | 0.43 |
| 3:17:47:ASP:CG | 3:17:50:VAL:H | 2.14 | 0.43 |
| 1:B:111:ARG:HG2 | 1:B:111:ARG:NH1 | 2.33 | 0.43 |
| 1:E:221:TRP:NE1 | 1:F:229:LEU:O | 2.39 | 0.43 |
| 1:G:168:GLN:HG3 | 1:H:204:ARG:NE | 2.33 | 0.43 |
| 1:I:90:LYS:HE2 | 1:I:138:ALA:HB3 | 2.01 | 0.43 |
| 1:J:171:ILE:O | 1:J:172:ASN:HB3 | 2.19 | 0.43 |
| 1:L:222:LEU:HB2 | 1:M:231:PRO:HB3 | 2.01 | 0.43 |
| 1:N:124:MET:HE3 | 1:N:124:MET:HB3 | 1.77 | 0.43 |
| 1:Q:82:LEU:HA | 1:Q:197:SER:CB | 2.43 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:219:MET:HE2 | 1:U:132:PHE:HB3 | 2.00 | 0.43 |
| 1:S:222:LEU:HB2 | 1:T:231:PRO:HB3 | 2.00 | 0.43 |
| 1:T:106:PHE:C | 1:T:108:THR:H | 2.26 | 0.43 |
| 1:V:90:LYS:HE2 | 1:V:138:ALA:HB3 | 2.01 | 0.43 |
| 1:W:82:LEU:HD13 | 1:W:144:PHE:CE1 | 2.53 | 0.43 |
| 1:X:90:LYS:HE2 | 1:X:138:ALA:HB3 | 2.00 | 0.43 |
| 1:A:51:ILE:CG1 | 2:c:175:LEU:HD11 | 2.41 | 0.43 |
| 1:A:204:ARG:NE | 1:Z:168:GLN:HG3 | 2.34 | 0.43 |
| 2:a:50:ASP:OD1 | 2:a:113:ALA:N | 2.52 | 0.43 |
| 2:b:136:LEU:HD13 | 2:c:129:VAL:HG11 | 2.01 | 0.43 |
| 2:b:280:LEU:HD22 | 2:b:339:GLY:O | 2.19 | 0.43 |
| 2:b:359:ARG:N | 2:b:359:ARG:HD2 | 2.33 | 0.43 |
| 2:d:208:ARG:HG3 | 2:d:235:PHE:CZ | 2.54 | 0.43 |
| 2:f:89:VAL:HG21 | 2:f:124:THR:OG1 | 2.18 | 0.43 |
| 2:g:250:ASP:O | 2:g:265:ASN:ND2 | 2.52 | 0.43 |
| 2:g:328:LEU:HD21 | 2:h:273:CYS:HA | 2.00 | 0.43 |
| 2:j:52:THR:HG21 | 2:j:81:LEU:HD23 | 1.99 | 0.43 |
| 2:l:89:VAL:HG21 | 2:l:124:THR:OG1 | 2.18 | 0.43 |
| 2:n:208:ARG:HG3 | 2:n:235:PHE:CZ | 2.54 | 0.43 |
| 2:o:217:ASP:OD1 | 2:o:219:ARG:N | 2.35 | 0.43 |
| 2:r:93:TYR:OH | 2:r:173:ARG:O | 2.24 | 0.43 |
| 2:r:353:GLN:CG | 2:r:362:LEU:HD22 | 2.47 | 0.43 |
| 2:u:208:ARG:HG3 | 2:u:235:PHE:CZ | 2.54 | 0.43 |
| 2:v:172:GLU:OE1 | 2:v:172:GLU:CA | 2.66 | 0.43 |
| 2:v:208:ARG:HG3 | 2:v:235:PHE:CZ | 2.54 | 0.43 |
| 2:w:101:GLN:OE1 | 2:x:219:ARG:HD3 | 2.19 | 0.43 |
| 2:x:114:LYS:HD2 | 2:x:114:LYS:HA | 1.81 | 0.43 |
| 2:x:123:MET:CE | 2:x:136:LEU:HD22 | 2.38 | 0.43 |
| 2:x:280:LEU:HD22 | 2:x:339:GLY:O | 2.19 | 0.43 |
| 2:x:359:ARG:HD2 | 2:x:359:ARG:N | 2.32 | 0.43 |
| 2:z:359:ARG:N | 2:z:359:ARG:HD2 | 2.32 | 0.43 |
| 3:7:70:PHE:CD1 | 3:7:70:PHE:C | 2.96 | 0.43 |
| 3:8:29:SER:OG | 3:8:31:ILE:HG12 | 2.19 | 0.43 |
| 3:10:38:GLN:HG2 | 3:10:44:SER:HB3 | 2.00 | 0.43 |
| 3:10:69:SER:O | 3:10:70:PHE:CD2 | 2.72 | 0.43 |
| 3:15:38:GLN:HG2 | 3:15:44:SER:HB3 | 2.00 | 0.43 |
| 3:21:47:ASP:CG | 3:21:50:VAL:HG23 | 2.42 | 0.43 |
| 3:22:77:CYS:HB3 | 3:22:80:TYR:CE1 | 2.49 | 0.43 |
| 3:25:29:SER:OG | 3:25:31:ILE:HG12 | 2.19 | 0.43 |
| 1:B:135:LYS:HE2 | 1:B:135:LYS:HB2 | 1.73 | 0.43 |
| 1:B:171:ILE:O | 1:B:172:ASN:HB3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:219:MET:HE2 | 1:F:132:PHE:HB3 | 2.01 | 0.43 |
| 1:E:171:ILE:O | 1:E:172:ASN:HB3 | 2.19 | 0.43 |
| 1:G:41:PRO:HA | 1:I:157:ALA:HB1 | 2.00 | 0.43 |
| 1:H:106:PHE:C | 1:H:108:THR:H | 2.26 | 0.43 |
| 1:H:219:MET:HE2 | 1:J:132:PHE:HB3 | 2.01 | 0.43 |
| 1:I:222:LEU:HB2 | 1:J:231:PRO:HB3 | 2.01 | 0.43 |
| 1:J:149:THR:OG1 | 1:K:198:THR:O | 2.35 | 0.43 |
| 1:K:106:PHE:C | 1:K:108:THR:H | 2.26 | 0.43 |
| 1:N:41:PRO:HA | 1:P:157:ALA:HB1 | 2.01 | 0.43 |
| 1:O:170:ALA:HB3 | 1:P:206:GLU:HG3 | 2.00 | 0.43 |
| 1:P:221:TRP:NE1 | 1:Q:229:LEU:O | 2.39 | 0.43 |
| 1:T:149:THR:OG1 | 1:U:198:THR:O | 2.35 | 0.43 |
| 1:T:219:MET:HE2 | 1:V:132:PHE:HB3 | 2.01 | 0.43 |
| 1:U:219:MET:HE2 | 1:W:132:PHE:HB3 | 2.01 | 0.43 |
| 1:V:106:PHE:C | 1:V:108:THR:H | 2.26 | 0.43 |
| 1:V:219:MET:HE2 | 1:X:132:PHE:HB3 | 2.01 | 0.43 |
| 1:W:90:LYS:HE2 | 1:W:138:ALA:HB3 | 2.01 | 0.43 |
| 1:W:124:MET:HE3 | 1:W:124:MET:HB3 | 1.77 | 0.43 |
| 1:X:171:ILE:O | 1:X:172:ASN:HB3 | 2.19 | 0.43 |
| 2:d:359:ARG:N | 2:d:359:ARG:HD2 | 2.32 | 0.43 |
| 2:e:101:GLN:OE1 | 2:f:219:ARG:HD3 | 2.19 | 0.43 |
| 2:g:127:LYS:HA | 2:g:132:GLN:O | 2.18 | 0.43 |
| 2:g:136:LEU:HD13 | 2:h:129:VAL:HG11 | 2.01 | 0.43 |
| 2:g:208:ARG:HG3 | 2:g:235:PHE:CZ | 2.54 | 0.43 |
| 2:i:208:ARG:HG3 | 2:i:235:PHE:CZ | 2.54 | 0.43 |
| 2:i:359:ARG:N | 2:i:359:ARG:HD2 | 2.32 | 0.43 |
| 2:k:50:ASP:OD1 | 2:k:113:ALA:N | 2.52 | 0.43 |
| 2:l:50:ASP:OD1 | 2:l:113:ALA:N | 2.52 | 0.43 |
| 2:l:280:LEU:HD22 | 2:l:339:GLY:O | 2.19 | 0.43 |
| 2:o:127:LYS:HA | 2:o:132:GLN:O | 2.18 | 0.43 |
| 2:r:217:ASP:OD1 | 2:r:219:ARG:N | 2.35 | 0.43 |
| 2:s:80:GLN:HB3 | 2:t:54:GLN:HB3 | 2.01 | 0.43 |
| 2:t:50:ASP:OD1 | 2:t:113:ALA:N | 2.52 | 0.43 |
| 2:u:80:GLN:HB3 | 2:v:54:GLN:HB3 | 2.01 | 0.43 |
| 2:u:319:LEU:HD12 | 2:u:319:LEU:HA | 1.80 | 0.43 |
| 2:y:208:ARG:HG3 | 2:y:235:PHE:CZ | 2.54 | 0.43 |
| 3:2:29:SER:OG | 3:2:31:ILE:HG12 | 2.19 | 0.43 |
| 3:5:29:SER:OG | 3:5:31:ILE:HG12 | 2.19 | 0.43 |
| 3:5:69:SER:O | 3:5:70:PHE:CD2 | 2.72 | 0.43 |
| 3:11:29:SER:OG | 3:11:31:ILE:HG12 | 2.19 | 0.43 |
| 3:14:70:PHE:CD1 | 3:14:70:PHE:C | 2.96 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:16:38:GLN:HG2 | 3:16:44:SER:HB3 | 2.00 | 0.43 |
| 1:D:82:LEU:HD12 | 1:D:146:GLY:HA3 | 1.97 | 0.43 |
| 1:E:124:MET:HE3 | 1:E:124:MET:HB3 | 1.77 | 0.43 |
| 1:G:30:LEU:HD21 | 1:H:206:GLU:HG3 | 2.01 | 0.43 |
| 1:J:111:ARG:HG2 | 1:J:111:ARG:NH1 | 2.33 | 0.43 |
| 1:R:135:LYS:HE2 | 1:R:135:LYS:HB2 | 1.73 | 0.43 |
| 1:Y:90:LYS:HE2 | 1:Y:138:ALA:HB3 | 2.01 | 0.43 |
| 1:Z:90:LYS:HE2 | 1:Z:138:ALA:HB3 | 2.01 | 0.43 |
| 1:A:90:LYS:HE2 | 1:A:138:ALA:HB3 | 2.01 | 0.43 |
| 3:1:69:SER:O | 3:1:70:PHE:CD2 | 2.72 | 0.43 |
| 2:c:101:GLN:OE1 | 2:d:219:ARG:HD3 | 2.19 | 0.43 |
| 2:c:353:GLN:CG | 2:c:362:LEU:HD22 | 2.48 | 0.43 |
| 2:d:250:ASP:O | 2:d:265:ASN:ND2 | 2.51 | 0.43 |
| 2:h:353:GLN:CG | 2:h:362:LEU:HD22 | 2.48 | 0.43 |
| 2:i:89:VAL:CG2 | 2:i:126:LEU:HD21 | 2.48 | 0.43 |
| 2:i:353:GLN:CG | 2:i:362:LEU:HD22 | 2.48 | 0.43 |
| 2:k:280:LEU:HD22 | 2:k:339:GLY:O | 2.19 | 0.43 |
| 2:m:89:VAL:HG21 | 2:m:124:THR:OG1 | 2.18 | 0.43 |
| 2:m:250:ASP:O | 2:m:265:ASN:ND2 | 2.51 | 0.43 |
| 2:o:80:GLN:HB3 | 2:p:54:GLN:HB3 | 2.01 | 0.43 |
| 2:o:141:ILE:HD13 | 2:o:165:ILE:CD1 | 2.39 | 0.43 |
| 2:q:208:ARG:HG3 | 2:q:235:PHE:CZ | 2.54 | 0.43 |
| 2:s:50:ASP:OD1 | 2:s:113:ALA:N | 2.52 | 0.43 |
| 2:t:280:LEU:HD22 | 2:t:339:GLY:O | 2.19 | 0.43 |
| 2:u:127:LYS:HA | 2:u:132:GLN:O | 2.18 | 0.43 |
| 2:v:127:LYS:HA | 2:v:132:GLN:O | 2.18 | 0.43 |
| 2:v:250:ASP:O | 2:v:265:ASN:ND2 | 2.51 | 0.43 |
| 2:z:50:ASP:OD1 | 2:z:113:ALA:N | 2.52 | 0.43 |
| 2:z:319:LEU:HD12 | 2:z:319:LEU:HA | 1.80 | 0.43 |
| 3:4:38:GLN:HG2 | 3:4:44:SER:HB3 | 2.00 | 0.43 |
| 3:6:69:SER:O | 3:6:70:PHE:CD2 | 2.72 | 0.43 |
| 3:9:38:GLN:HG2 | 3:9:44:SER:HB3 | 2.00 | 0.43 |
| 3:9:69:SER:O | 3:9:70:PHE:CD2 | 2.72 | 0.43 |
| 3:13:69:SER:O | 3:13:70:PHE:CD2 | 2.72 | 0.43 |
| 3:14:22:VAL:HG13 | 3:14:34:LEU:CD2 | 2.49 | 0.43 |
| 3:14:69:SER:O | 3:14:70:PHE:CD2 | 2.72 | 0.43 |
| 3:15:70:PHE:CD1 | 3:15:70:PHE:C | 2.96 | 0.43 |
| 3:17:70:PHE:CD1 | 3:17:70:PHE:C | 2.96 | 0.43 |
| 3:20:29:SER:OG | 3:20:31:ILE:HG12 | 2.19 | 0.43 |
| 3:21:38:GLN:HG2 | 3:21:44:SER:HB3 | 2.00 | 0.43 |
| 1:C:104:PHE:CZ | 1:Z:231:PRO:HG2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:219:MET:HE2 | 1:E:132:PHE:HB3 | 2.01 | 0.43 |
| 1:E:82:LEU:HD12 | 1:E:146:GLY:HA3 | 1.97 | 0.43 |
| 1:G:171:ILE:O | 1:G:172:ASN:HB3 | 2.19 | 0.43 |
| 1:H:90:LYS:HE2 | 1:H:138:ALA:HB3 | 2.01 | 0.43 |
| 1:O:222:LEU:HB2 | 1:P:231:PRO:HB3 | 2.01 | 0.43 |
| 1:V:121:ARG:HB3 | 1:W:111:ARG:HB3 | 2.00 | 0.43 |
| 1:W:111:ARG:HA | 1:W:111:ARG:HD3 | 1.90 | 0.43 |
| 1:Y:171:ILE:O | 1:Y:172:ASN:HB3 | 2.19 | 0.43 |
| 1:A:207:TYR:O | 1:Z:171:ILE:O | 2.36 | 0.42 |
| 1:A:222:LEU:HB2 | 1:B:231:PRO:HB3 | 2.02 | 0.42 |
| 3:1:29:SER:OG | 3:1:31:ILE:HG12 | 2.19 | 0.42 |
| 2:b:208:ARG:HG3 | 2:b:235:PHE:CZ | 2.54 | 0.42 |
| 2:b:353:GLN:CG | 2:b:362:LEU:HD22 | 2.48 | 0.42 |
| 2:d:50:ASP:OD1 | 2:d:113:ALA:N | 2.52 | 0.42 |
| 2:d:89:VAL:CG2 | 2:d:126:LEU:HD21 | 2.48 | 0.42 |
| 2:e:280:LEU:HD22 | 2:e:339:GLY:O | 2.19 | 0.42 |
| 2:f:256:ASN:O | 2:f:257:SER:OG | 2.28 | 0.42 |
| 2:f:280:LEU:HD22 | 2:f:339:GLY:O | 2.19 | 0.42 |
| 2:g:359:ARG:N | 2:g:359:ARG:HD2 | 2.32 | 0.42 |
| 2:h:114:LYS:HA | 2:h:114:LYS:HD2 | 1.81 | 0.42 |
| 2:h:136:LEU:HD13 | 2:i:129:VAL:HG11 | 2.01 | 0.42 |
| 2:j:50:ASP:OD1 | 2:j:113:ALA:N | 2.52 | 0.42 |
| 2:j:280:LEU:HD22 | 2:j:339:GLY:O | 2.19 | 0.42 |
| 2:j:359:ARG:N | 2:j:359:ARG:HD2 | 2.32 | 0.42 |
| 2:m:208:ARG:HG3 | 2:m:235:PHE:CZ | 2.54 | 0.42 |
| 2:m:280:LEU:HD22 | 2:m:339:GLY:O | 2.19 | 0.42 |
| 2:r:136:LEU:HD13 | 2:s:129:VAL:HG11 | 2.00 | 0.42 |
| 2:t:22:ILE:O | 2:t:25:LEU:HD23 | 2.19 | 0.42 |
| 2:t:80:GLN:HB3 | 2:u:54:GLN:HB3 | 2.01 | 0.42 |
| 2:u:101:GLN:OE1 | 2:v:219:ARG:HD3 | 2.19 | 0.42 |
| 2:w:250:ASP:O | 2:w:265:ASN:ND2 | 2.51 | 0.42 |
| 2:x:50:ASP:OD1 | 2:x:113:ALA:N | 2.52 | 0.42 |
| 2:y:280:LEU:HD22 | 2:y:339:GLY:O | 2.19 | 0.42 |
| 2:z:208:ARG:HG3 | 2:z:235:PHE:CZ | 2.54 | 0.42 |
| 2:z:280:LEU:HD22 | 2:z:339:GLY:O | 2.19 | 0.42 |
| 2:z:353:GLN:CG | 2:z:362:LEU:HD22 | 2.48 | 0.42 |
| 3:2:69:SER:O | 3:2:70:PHE:CD2 | 2.72 | 0.42 |
| 3:16:22:VAL:HG13 | 3:16:34:LEU:CD2 | 2.49 | 0.42 |
| 3:17:38:GLN:HG2 | 3:17:44:SER:HB3 | 2.00 | 0.42 |
| 3:21:39:PRO:HD2 | 3:21:42:PHE:HB2 | 2.01 | 0.42 |
| 3:22:39:PRO:HD2 | 3:22:42:PHE:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:23:22:VAL:HG13 | 3:23:34:LEU:CD2 | 2.49 | 0.42 |
| 3:24:29:SER:OG | 3:24:31:ILE:HG12 | 2.19 | 0.42 |
| 3:26:29:SER:OG | 3:26:31:ILE:HG12 | 2.19 | 0.42 |
| 1:B:90:LYS:HE2 | 1:B:138:ALA:HB3 | 2.01 | 0.42 |
| 1:E:82:LEU:HA | 1:E:197:SER:CB | 2.43 | 0.42 |
| 5:G:301:TQN:C14 | 1:H:112:TYR:HB2 | 2.49 | 0.42 |
| 5:H:301:TQN:C14 | 1:I:112:TYR:HB2 | 2.49 | 0.42 |
| 1:Q:171:ILE:O | 1:Q:172:ASN:HB3 | 2.19 | 0.42 |
| 5:Q:301:TQN:C14 | 1:R:112:TYR:HB2 | 2.49 | 0.42 |
| 1:S:171:ILE:O | 1:S:172:ASN:HB3 | 2.19 | 0.42 |
| 1:U:171:ILE:HD12 | 1:W:88:ALA:CB | 2.34 | 0.42 |
| 1:V:135:LYS:HE2 | 1:V:135:LYS:HB2 | 1.73 | 0.42 |
| 1:X:130:ASN:CG | 1:Y:102:THR:HG22 | 2.44 | 0.42 |
| 5:X:301:TQN:C14 | 1:Y:112:TYR:HB2 | 2.49 | 0.42 |
| 1:Y:106:PHE:C | 1:Y:108:THR:H | 2.26 | 0.42 |
| 5:Y:301:TQN:C14 | 1:Z:112:TYR:HB2 | 2.49 | 0.42 |
| 1:A:206:GLU:HG3 | 1:Z:30:LEU:HD21 | 2.00 | 0.42 |
| 1:A:210:ASN:HD22 | 3:26:83:SER:HA | 1.84 | 0.42 |
| 2:a:280:LEU:HD22 | 2:a:339:GLY:O | 2.19 | 0.42 |
| 2:b:52:THR:HG21 | 2:b:81:LEU:HD23 | 1.99 | 0.42 |
| 2:b:80:GLN:HB3 | 2:c:54:GLN:HB3 | 2.01 | 0.42 |
| 2:c:22:ILE:O | 2:c:25:LEU:HD23 | 2.19 | 0.42 |
| 2:c:79:MET:HE2 | 2:c:79:MET:HB2 | 1.69 | 0.42 |
| 2:d:22:ILE:O | 2:d:25:LEU:HD23 | 2.19 | 0.42 |
| 2:d:114:LYS:HA | 2:d:114:LYS:HD2 | 1.81 | 0.42 |
| 2:e:99:GLN:HE21 | 1:D:50:SER:HB3 | 1.82 | 0.42 |
| 2:f:50:ASP:OD1 | 2:f:113:ALA:N | 2.52 | 0.42 |
| 2:f:136:LEU:HD13 | 2:g:129:VAL:HG11 | 2.02 | 0.42 |
| 2:f:208:ARG:HG3 | 2:f:235:PHE:CZ | 2.54 | 0.42 |
| 2:g:217:ASP:OD1 | 2:g:219:ARG:N | 2.35 | 0.42 |
| 2:h:123:MET:HE3 | 2:h:123:MET:HA | 2.02 | 0.42 |
| 2:i:101:GLN:OE1 | 2:j:219:ARG:HD3 | 2.19 | 0.42 |
| 2:i:185:ILE:O | 2:i:223:VAL:HG22 | 2.20 | 0.42 |
| 2:j:173:ARG:HH12 | 1:I:54:SER:HB2 | 1.83 | 0.42 |
| 2:l:343:MET:SD | 2:l:343:MET:N | 2.91 | 0.42 |
| 2:m:80:GLN:HB3 | 2:n:54:GLN:HB3 | 2.01 | 0.42 |
| 2:m:185:ILE:O | 2:m:223:VAL:HG22 | 2.19 | 0.42 |
| 2:n:280:LEU:HD22 | 2:n:339:GLY:O | 2.19 | 0.42 |
| 2:o:208:ARG:HG3 | 2:o:235:PHE:CZ | 2.54 | 0.42 |
| 2:p:50:ASP:OD1 | 2:p:113:ALA:N | 2.52 | 0.42 |
| 2:s:172:GLU:OE1 | 2:s:172:GLU:CA | 2.66 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:u:22:ILE:O | 2:u:25:LEU:HD23 | 2.19 | 0.42 |
| 2:u:280:LEU:HD22 | 2:u:339:GLY:O | 2.19 | 0.42 |
| 2:u:343:MET:SD | 2:u:343:MET:N | 2.91 | 0.42 |
| 2:v:185:ILE:O | 2:v:223:VAL:HG22 | 2.20 | 0.42 |
| 2:v:280:LEU:HD22 | 2:v:339:GLY:O | 2.19 | 0.42 |
| 2:w:80:GLN:HB3 | 2:x:54:GLN:HB3 | 2.02 | 0.42 |
| 2:y:173:ARG:HH12 | 1:X:54:SER:HB2 | 1.83 | 0.42 |
| 3:8:38:GLN:HG2 | 3:8:44:SER:HB3 | 2.00 | 0.42 |
| 3:13:29:SER:OG | 3:13:31:ILE:HG12 | 2.19 | 0.42 |
| 3:15:22:VAL:HG13 | 3:15:34:LEU:CD2 | 2.49 | 0.42 |
| 3:19:29:SER:OG | 3:19:31:ILE:HG12 | 2.19 | 0.42 |
| 3:20:39:PRO:HD2 | 3:20:42:PHE:HB2 | 2.01 | 0.42 |
| 3:21:22:VAL:HG13 | 3:21:34:LEU:CD2 | 2.50 | 0.42 |
| 3:23:39:PRO:HD2 | 3:23:42:PHE:HB2 | 2.02 | 0.42 |
| 3:24:22:VAL:HG13 | 3:24:34:LEU:CD2 | 2.49 | 0.42 |
| 3:24:70:PHE:CD1 | 3:24:70:PHE:C | 2.96 | 0.42 |
| 1:B:219:MET:HE2 | 1:D:132:PHE:HB3 | 2.01 | 0.42 |
| 1:C:90:LYS:HE2 | 1:C:138:ALA:HB3 | 2.01 | 0.42 |
| 1:C:222:LEU:HB2 | 1:D:231:PRO:HB3 | 2.01 | 0.42 |
| 1:D:171:ILE:O | 1:D:172:ASN:HB3 | 2.19 | 0.42 |
| 1:H:171:ILE:O | 1:H:172:ASN:HB3 | 2.19 | 0.42 |
| 1:I:171:ILE:O | 1:I:172:ASN:HB3 | 2.19 | 0.42 |
| 1:I:219:MET:HE2 | 1:K:132:PHE:HB3 | 2.01 | 0.42 |
| 5:I:301:TQN:C14 | 1:J:112:TYR:HB2 | 2.49 | 0.42 |
| 1:K:171:ILE:HD12 | 1:M:88:ALA:CB | 2.35 | 0.42 |
| 1:K:171:ILE:O | 1:K:172:ASN:HB3 | 2.19 | 0.42 |
| 1:M:171:ILE:O | 1:M:172:ASN:HB3 | 2.19 | 0.42 |
| 1:O:41:PRO:HA | 1:Q:157:ALA:HB1 | 2.01 | 0.42 |
| 1:O:171:ILE:O | 1:O:172:ASN:HB3 | 2.19 | 0.42 |
| 5:O:301:TQN:C14 | 1:P:112:TYR:HB2 | 2.49 | 0.42 |
| 5:P:301:TQN:C14 | 1:Q:112:TYR:HB2 | 2.49 | 0.42 |
| 1:R:82:LEU:HA | 1:R:197:SER:CB | 2.43 | 0.42 |
| 1:R:124:MET:HE3 | 1:R:124:MET:HB3 | 1.77 | 0.42 |
| 1:S:221:TRP:NE1 | 1:T:229:LEU:O | 2.40 | 0.42 |
| 1:T:41:PRO:HA | 1:V:157:ALA:HB1 | 2.01 | 0.42 |
| 1:A:112:TYR:HB2 | 5:Z:301:TQN:C14 | 2.49 | 0.42 |
| 1:A:168:GLN:HG3 | 1:B:204:ARG:NE | 2.34 | 0.42 |
| 2:a:123:MET:HE3 | 2:a:123:MET:HA | 2.02 | 0.42 |
| 2:a:185:ILE:O | 2:a:223:VAL:HG22 | 2.20 | 0.42 |
| 2:b:22:ILE:O | 2:b:25:LEU:HD23 | 2.19 | 0.42 |
| 2:b:50:ASP:OD1 | 2:b:113:ALA:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:b:256:ASN:O | 2:b:257:SER:OG | 2.28 | 0.42 |
| 2:e:22:ILE:O | 2:e:25:LEU:HD23 | 2.19 | 0.42 |
| 2:e:50:ASP:OD1 | 2:e:113:ALA:N | 2.52 | 0.42 |
| 2:e:185:ILE:O | 2:e:223:VAL:HG22 | 2.20 | 0.42 |
| 2:g:89:VAL:HG21 | 2:g:124:THR:OG1 | 2.18 | 0.42 |
| 2:i:83:ASN:ND2 | 2:j:109:SER:OG | 2.49 | 0.42 |
| 2:i:280:LEU:HD22 | 2:i:339:GLY:O | 2.19 | 0.42 |
| 2:j:89:VAL:CG2 | 2:j:126:LEU:HD21 | 2.48 | 0.42 |
| 2:k:208:ARG:HG3 | 2:k:235:PHE:CZ | 2.54 | 0.42 |
| 2:l:101:GLN:OE1 | 2:m:219:ARG:HD3 | 2.19 | 0.42 |
| 2:l:136:LEU:HD13 | 2:m:129:VAL:HG11 | 2.01 | 0.42 |
| 2:l:359:ARG:N | 2:l:359:ARG:HD2 | 2.33 | 0.42 |
| 2:m:50:ASP:OD1 | 2:m:113:ALA:N | 2.52 | 0.42 |
| 2:m:136:LEU:HD13 | 2:n:129:VAL:HG11 | 2.01 | 0.42 |
| 2:o:101:GLN:OE1 | 2:p:219:ARG:HD3 | 2.19 | 0.42 |
| 2:o:250:ASP:O | 2:o:265:ASN:ND2 | 2.51 | 0.42 |
| 2:q:80:GLN:HB3 | 2:r:54:GLN:HB3 | 2.02 | 0.42 |
| 2:s:89:VAL:CG2 | 2:s:126:LEU:HD21 | 2.48 | 0.42 |
| 2:s:208:ARG:HG3 | 2:s:235:PHE:CZ | 2.54 | 0.42 |
| 2:v:50:ASP:OD1 | 2:v:113:ALA:N | 2.52 | 0.42 |
| 2:w:280:LEU:HD22 | 2:w:339:GLY:O | 2.19 | 0.42 |
| 2:x:123:MET:HE3 | 2:x:123:MET:HA | 2.02 | 0.42 |
| 2:y:22:ILE:O | 2:y:25:LEU:HD23 | 2.19 | 0.42 |
| 2:y:185:ILE:O | 2:y:223:VAL:HG22 | 2.20 | 0.42 |
| 2:z:196:MET:HA | 2:z:196:MET:CE | 2.48 | 0.42 |
| 3:4:69:SER:O | 3:4:70:PHE:CD2 | 2.72 | 0.42 |
| 3:6:29:SER:OG | 3:6:31:ILE:HG12 | 2.19 | 0.42 |
| 3:11:69:SER:O | 3:11:70:PHE:CD2 | 2.72 | 0.42 |
| 3:15:39:PRO:HD2 | 3:15:42:PHE:HB2 | 2.01 | 0.42 |
| 3:17:39:PRO:HD2 | 3:17:42:PHE:HB2 | 2.01 | 0.42 |
| 3:19:22:VAL:HG13 | 3:19:34:LEU:CD2 | 2.49 | 0.42 |
| 3:19:39:PRO:HD2 | 3:19:42:PHE:HB2 | 2.02 | 0.42 |
| 3:22:22:VAL:HG13 | 3:22:34:LEU:CD2 | 2.49 | 0.42 |
| 3:23:47:ASP:CG | 3:23:50:VAL:H | 2.14 | 0.42 |
| 3:25:22:VAL:HG13 | 3:25:34:LEU:CD2 | 2.49 | 0.42 |
| 3:25:39:PRO:HD2 | 3:25:42:PHE:HB2 | 2.01 | 0.42 |
| 3:26:22:VAL:HG13 | 3:26:34:LEU:CD2 | 2.49 | 0.42 |
| 1:B:171:ILE:HD12 | 1:D:88:ALA:CB | 2.34 | 0.42 |
| 1:C:171:ILE:O | 1:C:172:ASN:HB3 | 2.19 | 0.42 |
| 1:D:30:LEU:HD21 | 1:E:206:GLU:HG3 | 2.01 | 0.42 |
| 5:F:301:TQN:C14 | 1:G:112:TYR:HB2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:90:LYS:HE2 | 1:G:138:ALA:HB3 | 2.01 | 0.42 |
| 1:J:30:LEU:HD21 | 1:K:206:GLU:HG3 | 2.01 | 0.42 |
| 1:L:82:LEU:HA | 1:L:197:SER:CB | 2.43 | 0.42 |
| 1:M:167:LYS:NZ | 1:N:84:GLU:OE2 | 2.42 | 0.42 |
| 5:R:301:TQN:C14 | 1:S:112:TYR:HB2 | 2.49 | 0.42 |
| 1:U:40:ILE:H | 1:U:40:ILE:HG12 | 1.49 | 0.42 |
| 1:U:106:PHE:C | 1:U:108:THR:H | 2.26 | 0.42 |
| 5:W:301:TQN:C14 | 1:X:112:TYR:HB2 | 2.49 | 0.42 |
| 1:Z:106:PHE:C | 1:Z:108:THR:H | 2.26 | 0.42 |
| 1:Z:171:ILE:O | 1:Z:172:ASN:HB3 | 2.19 | 0.42 |
| 1:A:101:LYS:HZ2 | 1:A:101:LYS:HB3 | 1.84 | 0.42 |
| 2:a:250:ASP:O | 2:a:265:ASN:ND2 | 2.51 | 0.42 |
| 2:b:123:MET:HE3 | 2:b:123:MET:HA | 2.02 | 0.42 |
| 2:c:280:LEU:HD22 | 2:c:339:GLY:O | 2.19 | 0.42 |
| 2:d:142:LEU:HD22 | 2:f:364:ILE:CD1 | 2.48 | 0.42 |
| 2:e:114:LYS:HA | 2:e:114:LYS:HD2 | 1.81 | 0.42 |
| 2:e:123:MET:HE3 | 2:e:123:MET:HA | 2.02 | 0.42 |
| 2:f:114:LYS:HA | 2:f:114:LYS:HD2 | 1.81 | 0.42 |
| 2:f:185:ILE:O | 2:f:223:VAL:HG22 | 2.20 | 0.42 |
| 2:g:173:ARG:HH12 | 1:F:54:SER:HB2 | 1.84 | 0.42 |
| 2:h:22:ILE:O | 2:h:25:LEU:HD23 | 2.19 | 0.42 |
| 2:i:196:MET:HA | 2:i:196:MET:CE | 2.48 | 0.42 |
| 2:j:208:ARG:HG3 | 2:j:235:PHE:CZ | 2.54 | 0.42 |
| 2:l:208:ARG:HG3 | 2:l:235:PHE:CZ | 2.54 | 0.42 |
| 2:m:22:ILE:O | 2:m:25:LEU:HD23 | 2.19 | 0.42 |
| 2:m:173:ARG:HH12 | 1:L:54:SER:HB2 | 1.84 | 0.42 |
| 2:n:22:ILE:O | 2:n:25:LEU:HD23 | 2.19 | 0.42 |
| 2:n:101:GLN:OE1 | 2:o:219:ARG:HD3 | 2.20 | 0.42 |
| 2:o:22:ILE:O | 2:o:25:LEU:HD23 | 2.19 | 0.42 |
| 2:p:185:ILE:O | 2:p:223:VAL:HG22 | 2.20 | 0.42 |
| 2:p:250:ASP:O | 2:p:265:ASN:ND2 | 2.51 | 0.42 |
| 2:q:101:GLN:OE1 | 2:r:219:ARG:HD3 | 2.19 | 0.42 |
| 2:q:185:ILE:O | 2:q:223:VAL:HG22 | 2.20 | 0.42 |
| 2:q:280:LEU:HD22 | 2:q:339:GLY:O | 2.19 | 0.42 |
| 2:s:280:LEU:HD22 | 2:s:339:GLY:O | 2.19 | 0.42 |
| 2:t:89:VAL:CG2 | 2:t:126:LEU:HD21 | 2.48 | 0.42 |
| 2:v:136:LEU:HD13 | 2:w:129:VAL:HG11 | 2.01 | 0.42 |
| 2:w:54:GLN:HB2 | 2:w:112:ASN:HD21 | 1.85 | 0.42 |
| 2:w:173:ARG:HH12 | 1:V:54:SER:HB2 | 1.84 | 0.42 |
| 2:x:22:ILE:O | 2:x:25:LEU:HD23 | 2.19 | 0.42 |
| 2:x:256:ASN:O | 2:x:257:SER:OG | 2.29 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:z:54:GLN:HB2 | 2:z:112:ASN:HD21 | 1.85 | 0.42 |
| 3:5:38:GLN:HG2 | 3:5:44:SER:HB3 | 2.00 | 0.42 |
| 3:7:29:SER:OG | 3:7:31:ILE:HG12 | 2.19 | 0.42 |
| 3:13:39:PRO:HD2 | 3:13:42:PHE:HB2 | 2.01 | 0.42 |
| 3:14:39:PRO:HD2 | 3:14:42:PHE:HB2 | 2.01 | 0.42 |
| 3:17:22:VAL:HG13 | 3:17:34:LEU:CD2 | 2.50 | 0.42 |
| 3:18:38:GLN:HG2 | 3:18:44:SER:HB3 | 2.00 | 0.42 |
| 3:18:39:PRO:HD2 | 3:18:42:PHE:HB2 | 2.02 | 0.42 |
| 3:20:83:SER:O | 3:20:84:LEU:HD23 | 2.20 | 0.42 |
| 3:21:29:SER:OG | 3:21:31:ILE:HG12 | 2.19 | 0.42 |
| 3:21:77:CYS:HB3 | 3:21:80:TYR:CE1 | 2.48 | 0.42 |
| 3:23:29:SER:OG | 3:23:31:ILE:HG12 | 2.19 | 0.42 |
| 3:23:83:SER:O | 3:23:84:LEU:HD23 | 2.20 | 0.42 |
| 3:24:39:PRO:HD2 | 3:24:42:PHE:HB2 | 2.02 | 0.42 |
| 3:26:70:PHE:CD1 | 3:26:70:PHE:C | 2.96 | 0.42 |
| 1:D:90:LYS:HE2 | 1:D:138:ALA:HB3 | 2.01 | 0.42 |
| 1:F:30:LEU:HD21 | 1:G:206:GLU:HG3 | 2.01 | 0.42 |
| 1:J:167:LYS:NZ | 1:K:84:GLU:OE2 | 2.42 | 0.42 |
| 1:A:219:MET:HE2 | 1:C:132:PHE:HB3 | 2.00 | 0.42 |
| 2:a:22:ILE:O | 2:a:25:LEU:HD23 | 2.19 | 0.42 |
| 2:a:80:GLN:HB3 | 2:b:54:GLN:HB3 | 2.02 | 0.42 |
| 3:1:83:SER:O | 3:1:84:LEU:HD23 | 2.20 | 0.42 |
| 2:d:101:GLN:OE1 | 2:e:219:ARG:HD3 | 2.20 | 0.42 |
| 2:d:185:ILE:O | 2:d:223:VAL:HG22 | 2.20 | 0.42 |
| 2:e:208:ARG:HG3 | 2:e:235:PHE:CZ | 2.54 | 0.42 |
| 2:f:22:ILE:O | 2:f:25:LEU:HD23 | 2.19 | 0.42 |
| 2:f:101:GLN:OE1 | 2:g:219:ARG:HD3 | 2.20 | 0.42 |
| 2:g:50:ASP:OD1 | 2:g:113:ALA:N | 2.52 | 0.42 |
| 2:h:80:GLN:HB3 | 2:i:54:GLN:HB3 | 2.01 | 0.42 |
| 2:h:173:ARG:HH12 | 1:G:54:SER:HB2 | 1.84 | 0.42 |
| 2:h:280:LEU:HD22 | 2:h:339:GLY:O | 2.19 | 0.42 |
| 2:i:284:VAL:CG2 | 2:i:316:GLY:HA2 | 2.50 | 0.42 |
| 2:k:123:MET:HE3 | 2:k:123:MET:HA | 2.01 | 0.42 |
| 2:l:22:ILE:O | 2:l:25:LEU:HD23 | 2.19 | 0.42 |
| 2:l:319:LEU:HD12 | 2:l:319:LEU:HA | 1.80 | 0.42 |
| 2:n:83:ASN:ND2 | 2:o:109:SER:OG | 2.48 | 0.42 |
| 2:p:22:ILE:O | 2:p:25:LEU:HD23 | 2.19 | 0.42 |
| 2:p:280:LEU:HD22 | 2:p:339:GLY:O | 2.19 | 0.42 |
| 2:q:50:ASP:OD1 | 2:q:113:ALA:N | 2.52 | 0.42 |
| 2:r:54:GLN:HB2 | 2:r:112:ASN:HD21 | 1.85 | 0.42 |
| 2:r:89:VAL:CG2 | 2:r:126:LEU:HD21 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:s:22:ILE:O | 2:s:25:LEU:HD23 | 2.19 | 0.42 |
| 2:s:185:ILE:O | 2:s:223:VAL:HG22 | 2.20 | 0.42 |
| 2:s:250:ASP:O | 2:s:265:ASN:ND2 | 2.52 | 0.42 |
| 2:t:208:ARG:HG3 | 2:t:235:PHE:CZ | 2.54 | 0.42 |
| 2:u:217:ASP:OD1 | 2:u:219:ARG:N | 2.35 | 0.42 |
| 2:v:343:MET:SD | 2:v:343:MET:N | 2.91 | 0.42 |
| 2:x:208:ARG:HG3 | 2:x:235:PHE:CZ | 2.54 | 0.42 |
| 3:7:38:GLN:HG2 | 3:7:44:SER:HB3 | 2.00 | 0.42 |
| 3:8:39:PRO:HD2 | 3:8:42:PHE:HB2 | 2.01 | 0.42 |
| 3:9:39:PRO:HD2 | 3:9:42:PHE:HB2 | 2.01 | 0.42 |
| 3:10:39:PRO:HD2 | 3:10:42:PHE:HB2 | 2.01 | 0.42 |
| 3:11:39:PRO:HD2 | 3:11:42:PHE:HB2 | 2.01 | 0.42 |
| 3:15:69:SER:O | 3:15:70:PHE:CD2 | 2.72 | 0.42 |
| 3:16:39:PRO:HD2 | 3:16:42:PHE:HB2 | 2.02 | 0.42 |
| 3:17:69:SER:O | 3:17:70:PHE:CD2 | 2.72 | 0.42 |
| 3:22:29:SER:OG | 3:22:31:ILE:HG12 | 2.19 | 0.42 |
| 3:24:69:SER:O | 3:24:70:PHE:CD2 | 2.72 | 0.42 |
| 3:24:83:SER:O | 3:24:84:LEU:HD23 | 2.20 | 0.42 |
| 3:26:39:PRO:HD2 | 3:26:42:PHE:HB2 | 2.01 | 0.42 |
| 1:B:30:LEU:HD21 | 1:C:206:GLU:HG3 | 2.01 | 0.42 |
| 1:E:90:LYS:HE2 | 1:E:138:ALA:HB3 | 2.01 | 0.42 |
| 1:F:41:PRO:HA | 1:H:157:ALA:HB1 | 2.00 | 0.42 |
| 1:G:40:ILE:H | 1:G:40:ILE:HG12 | 1.49 | 0.42 |
| 1:L:171:ILE:HD12 | 1:N:88:ALA:CB | 2.34 | 0.42 |
| 5:N:301:TQN:C14 | 1:O:112:TYR:HB2 | 2.49 | 0.42 |
| 1:Q:135:LYS:HE2 | 1:Q:135:LYS:HB2 | 1.73 | 0.42 |
| 1:R:219:MET:HE2 | 1:T:132:PHE:HB3 | 2.01 | 0.42 |
| 1:U:171:ILE:O | 1:U:172:ASN:HB3 | 2.19 | 0.42 |
| 1:U:222:LEU:HB2 | 1:V:231:PRO:HB3 | 2.01 | 0.42 |
| 1:W:219:MET:HE2 | 1:Y:132:PHE:HB3 | 2.02 | 0.42 |
| 5:A:302:TQN:C14 | 1:B:112:TYR:HB2 | 2.49 | 0.42 |
| 2:a:54:GLN:HB3 | 2:z:80:GLN:HB3 | 2.02 | 0.42 |
| 2:c:208:ARG:HG3 | 2:c:235:PHE:CZ | 2.54 | 0.42 |
| 2:d:123:MET:HE3 | 2:d:123:MET:HA | 2.02 | 0.42 |
| 2:e:54:GLN:HB2 | 2:e:112:ASN:HD21 | 1.85 | 0.42 |
| 2:g:114:LYS:HA | 2:g:114:LYS:HD2 | 1.81 | 0.42 |
| 2:h:54:GLN:HB2 | 2:h:112:ASN:HD21 | 1.85 | 0.42 |
| 2:h:185:ILE:O | 2:h:223:VAL:HG22 | 2.19 | 0.42 |
| 2:i:80:GLN:HB3 | 2:j:54:GLN:HB3 | 2.01 | 0.42 |
| 2:j:101:GLN:OE1 | 2:k:219:ARG:HD3 | 2.20 | 0.42 |
| 2:k:89:VAL:CG2 | 2:k:126:LEU:HD21 | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:l:114:LYS:HA | 2:l:114:LYS:HD2 | 1.81 | 0.42 |
| 2:l:185:ILE:O | 2:l:223:VAL:HG22 | 2.20 | 0.42 |
| 2:n:136:LEU:HD13 | 2:o:129:VAL:HG11 | 2.01 | 0.42 |
| 2:o:173:ARG:HH12 | 1:N:54:SER:HB2 | 1.84 | 0.42 |
| 2:o:280:LEU:HD22 | 2:o:339:GLY:O | 2.19 | 0.42 |
| 2:q:89:VAL:CG2 | 2:q:126:LEU:HD21 | 2.48 | 0.42 |
| 2:q:159:GLN:CB | 2:r:258:ARG:HG2 | 2.50 | 0.42 |
| 2:s:353:GLN:CG | 2:s:362:LEU:HD22 | 2.48 | 0.42 |
| 2:t:185:ILE:O | 2:t:223:VAL:HG22 | 2.20 | 0.42 |
| 2:u:123:MET:HE3 | 2:u:123:MET:HA | 2.02 | 0.42 |
| 2:v:256:ASN:O | 2:v:257:SER:OG | 2.29 | 0.42 |
| 2:z:22:ILE:O | 2:z:25:LEU:HD23 | 2.19 | 0.42 |
| 3:2:22:VAL:HG13 | 3:2:34:LEU:CD2 | 2.49 | 0.42 |
| 3:7:39:PRO:HD2 | 3:7:42:PHE:HB2 | 2.01 | 0.42 |
| 3:11:20:ALA:HA | 3:11:36:TYR:HB3 | 2.02 | 0.42 |
| 3:12:29:SER:OG | 3:12:31:ILE:HG12 | 2.19 | 0.42 |
| 3:17:29:SER:OG | 3:17:31:ILE:HG12 | 2.19 | 0.42 |
| 3:19:38:GLN:HG2 | 3:19:44:SER:HB3 | 2.00 | 0.42 |
| 3:22:20:ALA:HA | 3:22:36:TYR:HB3 | 2.02 | 0.42 |
| 3:23:20:ALA:HA | 3:23:36:TYR:HB3 | 2.02 | 0.42 |
| 1:B:41:PRO:HA | 1:D:157:ALA:HB1 | 2.01 | 0.42 |
| 1:E:30:LEU:HD21 | 1:F:206:GLU:HG3 | 2.02 | 0.42 |
| 5:E:301:TQN:C14 | 1:F:112:TYR:HB2 | 2.49 | 0.42 |
| 1:F:90:LYS:HE2 | 1:F:138:ALA:HB3 | 2.01 | 0.42 |
| 1:G:149:THR:OG1 | 1:H:198:THR:O | 2.34 | 0.42 |
| 1:H:30:LEU:HD21 | 1:I:206:GLU:CG | 2.50 | 0.42 |
| 5:J:301:TQN:C14 | 1:K:112:TYR:HB2 | 2.49 | 0.42 |
| 1:R:30:LEU:H | 1:R:30:LEU:CD2 | 2.29 | 0.42 |
| 5:V:301:TQN:C14 | 1:W:112:TYR:HB2 | 2.49 | 0.42 |
| 1:X:168:GLN:HG3 | 1:Y:204:ARG:NE | 2.35 | 0.42 |
| 1:A:171:ILE:O | 1:A:172:ASN:HB3 | 2.19 | 0.42 |
| 1:A:206:GLU:HG3 | 1:Z:170:ALA:HB3 | 2.01 | 0.42 |
| 2:b:101:GLN:OE1 | 2:c:219:ARG:HD3 | 2.20 | 0.42 |
| 2:b:185:ILE:O | 2:b:223:VAL:HG22 | 2.20 | 0.42 |
| 2:c:54:GLN:HB2 | 2:c:112:ASN:HD21 | 1.85 | 0.42 |
| 2:c:80:GLN:HB3 | 2:d:54:GLN:HB3 | 2.01 | 0.42 |
| 2:d:280:LEU:HD22 | 2:d:339:GLY:O | 2.19 | 0.42 |
| 2:e:89:VAL:CG2 | 2:e:126:LEU:HD21 | 2.48 | 0.42 |
| 2:g:22:ILE:O | 2:g:25:LEU:HD23 | 2.19 | 0.42 |
| 2:i:50:ASP:OD1 | 2:i:113:ALA:N | 2.52 | 0.42 |
| 2:i:173:ARG:HH12 | 1:H:54:SER:HB2 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:j:185:ILE:O | 2:j:223:VAL:HG22 | 2.20 | 0.42 |
| 2:k:22:ILE:O | 2:k:25:LEU:HD23 | 2.19 | 0.42 |
| 2:k:136:LEU:HD13 | 2:l:129:VAL:HG11 | 2.02 | 0.42 |
| 2:m:54:GLN:HB2 | 2:m:112:ASN:HD21 | 1.85 | 0.42 |
| 2:m:101:GLN:OE1 | 2:n:219:ARG:HD3 | 2.20 | 0.42 |
| 2:m:123:MET:HE3 | 2:m:123:MET:HA | 2.02 | 0.42 |
| 2:n:343:MET:SD | 2:n:343:MET:N | 2.91 | 0.42 |
| 2:s:114:LYS:HA | 2:s:114:LYS:HD2 | 1.81 | 0.42 |
| 2:s:123:MET:HE3 | 2:s:123:MET:HA | 2.02 | 0.42 |
| 2:t:32:ARG:H | 2:t:95:PRO:HB3 | 1.85 | 0.42 |
| 2:u:50:ASP:OD1 | 2:u:113:ALA:N | 2.52 | 0.42 |
| 2:u:54:GLN:HB2 | 2:u:112:ASN:HD21 | 1.85 | 0.42 |
| 2:u:89:VAL:CG2 | 2:u:126:LEU:HD21 | 2.48 | 0.42 |
| 2:v:123:MET:HE3 | 2:v:123:MET:HA | 2.02 | 0.42 |
| 2:w:208:ARG:HG3 | 2:w:235:PHE:CZ | 2.54 | 0.42 |
| 2:x:185:ILE:O | 2:x:223:VAL:HG22 | 2.20 | 0.42 |
| 3:2:47:ASP:CG | 3:2:50:VAL:H | 2.14 | 0.42 |
| 3:6:20:ALA:HA | 3:6:36:TYR:HB3 | 2.02 | 0.42 |
| 3:6:38:GLN:HG2 | 3:6:44:SER:HB3 | 2.00 | 0.42 |
| 3:6:39:PRO:HD2 | 3:6:42:PHE:HB2 | 2.01 | 0.42 |
| 3:8:69:SER:O | 3:8:70:PHE:CD2 | 2.72 | 0.42 |
| 3:9:20:ALA:HA | 3:9:36:TYR:HB3 | 2.02 | 0.42 |
| 3:10:20:ALA:HA | 3:10:36:TYR:HB3 | 2.02 | 0.42 |
| 3:12:22:VAL:HG13 | 3:12:34:LEU:CD2 | 2.50 | 0.42 |
| 3:12:39:PRO:HD2 | 3:12:42:PHE:HB2 | 2.02 | 0.42 |
| 3:19:20:ALA:HA | 3:19:36:TYR:HB3 | 2.02 | 0.42 |
| 3:20:38:GLN:HG2 | 3:20:44:SER:HB3 | 2.00 | 0.42 |
| 3:26:69:SER:O | 3:26:70:PHE:CD2 | 2.72 | 0.42 |
| 1:C:117:PHE:HD1 | 1:C:122:ALA:CB | 2.33 | 0.42 |
| 1:G:167:LYS:NZ | 1:H:84:GLU:OE2 | 2.42 | 0.42 |
| 1:I:117:PHE:HD1 | 1:I:122:ALA:CB | 2.33 | 0.42 |
| 1:J:219:MET:HE2 | 1:L:132:PHE:HB3 | 2.01 | 0.42 |
| 1:L:135:LYS:HB2 | 1:L:135:LYS:HE2 | 1.73 | 0.42 |
| 1:P:111:ARG:HA | 1:P:111:ARG:HD3 | 1.90 | 0.42 |
| 1:S:82:LEU:HA | 1:S:197:SER:CB | 2.43 | 0.42 |
| 5:S:301:TQN:C14 | 1:T:112:TYR:HB2 | 2.49 | 0.42 |
| 1:T:30:LEU:HD21 | 1:U:206:GLU:HG3 | 2.01 | 0.42 |
| 1:T:135:LYS:HB2 | 1:T:135:LYS:HE2 | 1.73 | 0.42 |
| 1:U:41:PRO:HA | 1:W:157:ALA:HB1 | 2.01 | 0.42 |
| 1:V:30:LEU:HD21 | 1:W:206:GLU:HG3 | 2.01 | 0.42 |
| 1:A:117:PHE:HD1 | 1:A:122:ALA:CB | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:a:208:ARG:HG3 | 2:a:235:PHE:CZ | 2.54 | 0.42 |
| 2:a:353:GLN:CG | 2:a:362:LEU:HD22 | 2.47 | 0.42 |
| 2:b:54:GLN:HB2 | 2:b:112:ASN:HD21 | 1.85 | 0.42 |
| 2:c:50:ASP:OD1 | 2:c:113:ALA:N | 2.52 | 0.42 |
| 2:c:185:ILE:O | 2:c:223:VAL:HG22 | 2.20 | 0.42 |
| 2:d:344:ASP:OD1 | 2:d:344:ASP:N | 2.53 | 0.42 |
| 2:e:284:VAL:CG2 | 2:e:316:GLY:HA2 | 2.50 | 0.42 |
| 2:g:123:MET:HE3 | 2:g:123:MET:HA | 2.02 | 0.42 |
| 2:h:208:ARG:HG3 | 2:h:235:PHE:CZ | 2.54 | 0.42 |
| 2:i:344:ASP:OD1 | 2:i:344:ASP:N | 2.53 | 0.42 |
| 2:j:54:GLN:HB2 | 2:j:112:ASN:HD21 | 1.85 | 0.42 |
| 2:m:83:ASN:ND2 | 2:n:109:SER:OG | 2.50 | 0.42 |
| 2:n:185:ILE:O | 2:n:223:VAL:HG22 | 2.20 | 0.42 |
| 2:o:54:GLN:HB2 | 2:o:112:ASN:HD21 | 1.85 | 0.42 |
| 2:q:22:ILE:O | 2:q:25:LEU:HD23 | 2.19 | 0.42 |
| 2:q:54:GLN:HB2 | 2:q:112:ASN:HD21 | 1.85 | 0.42 |
| 2:r:32:ARG:H | 2:r:95:PRO:HB3 | 1.85 | 0.42 |
| 2:s:32:ARG:H | 2:s:95:PRO:HB3 | 1.85 | 0.42 |
| 2:t:54:GLN:HB2 | 2:t:112:ASN:HD21 | 1.85 | 0.42 |
| 2:t:136:LEU:HD13 | 2:u:129:VAL:HG11 | 2.01 | 0.42 |
| 2:t:343:MET:SD | 2:t:343:MET:N | 2.91 | 0.42 |
| 2:u:32:ARG:H | 2:u:95:PRO:HB3 | 1.85 | 0.42 |
| 2:u:344:ASP:OD1 | 2:u:344:ASP:N | 2.53 | 0.42 |
| 2:v:22:ILE:O | 2:v:25:LEU:HD23 | 2.19 | 0.42 |
| 2:v:101:GLN:OE1 | 2:w:219:ARG:HD3 | 2.20 | 0.42 |
| 2:x:336:ASN:HD22 | 2:x:336:ASN:HA | 1.66 | 0.42 |
| 2:y:123:MET:HE3 | 2:y:123:MET:HA | 2.02 | 0.42 |
| 2:y:123:MET:CE | 2:y:136:LEU:HD22 | 2.38 | 0.42 |
| 2:y:344:ASP:OD1 | 2:y:344:ASP:N | 2.53 | 0.42 |
| 2:z:344:ASP:N | 2:z:344:ASP:OD1 | 2.53 | 0.42 |
| 3:5:20:ALA:HA | 3:5:36:TYR:HB3 | 2.02 | 0.42 |
| 3:7:69:SER:O | 3:7:70:PHE:CD2 | 2.72 | 0.42 |
| 3:12:28:ILE:O | 3:12:29:SER:OG | 2.21 | 0.42 |
| 3:12:69:SER:O | 3:12:70:PHE:CD2 | 2.72 | 0.42 |
| 3:13:22:VAL:HG13 | 3:13:34:LEU:CD2 | 2.50 | 0.42 |
| 3:14:20:ALA:HA | 3:14:36:TYR:HB3 | 2.02 | 0.42 |
| 3:16:69:SER:O | 3:16:70:PHE:CD2 | 2.72 | 0.42 |
| 3:18:20:ALA:HA | 3:18:36:TYR:HB3 | 2.02 | 0.42 |
| 3:18:22:VAL:HG13 | 3:18:34:LEU:CD2 | 2.50 | 0.42 |
| 3:18:69:SER:O | 3:18:70:PHE:CD2 | 2.72 | 0.42 |
| 3:19:83:SER:O | 3:19:84:LEU:HD23 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:21:20:ALA:HA | 3:21:36:TYR:HB3 | 2.02 | 0.42 |
| 3:21:83:SER:O | 3:21:84:LEU:HD23 | 2.20 | 0.42 |
| 3:26:83:SER:O | 3:26:84:LEU:HD23 | 2.20 | 0.42 |
| 1:B:117:PHE:HD1 | 1:B:122:ALA:CB | 2.33 | 0.42 |
| 1:D:41:PRO:HA | 1:F:157:ALA:HB1 | 2.01 | 0.42 |
| 1:D:117:PHE:HD1 | 1:D:122:ALA:CB | 2.33 | 0.42 |
| 1:F:30:LEU:H | 1:F:30:LEU:CD2 | 2.29 | 0.42 |
| 1:G:124:MET:HE3 | 1:G:124:MET:HB3 | 1.76 | 0.42 |
| 5:M:301:TQN:C14 | 1:N:112:TYR:HB2 | 2.49 | 0.42 |
| 1:N:30:LEU:HD21 | 1:O:206:GLU:HG3 | 2.01 | 0.42 |
| 1:N:117:PHE:HD1 | 1:N:122:ALA:CB | 2.33 | 0.42 |
| 1:Q:221:TRP:NE1 | 1:R:229:LEU:O | 2.39 | 0.42 |
| 1:W:171:ILE:O | 1:W:172:ASN:HB3 | 2.19 | 0.42 |
| 1:Y:117:PHE:HD1 | 1:Y:122:ALA:CB | 2.33 | 0.42 |
| 1:Z:117:PHE:HD1 | 1:Z:122:ALA:CB | 2.33 | 0.42 |
| 1:A:170:ALA:HB3 | 1:B:206:GLU:HG3 | 2.01 | 0.42 |
| 3:1:39:PRO:HD2 | 3:1:42:PHE:HB2 | 2.01 | 0.42 |
| 2:c:114:LYS:HD2 | 2:c:114:LYS:HA | 1.81 | 0.42 |
| 2:c:173:ARG:HH12 | 1:B:54:SER:HB2 | 1.84 | 0.42 |
| 2:e:136:LEU:HD13 | 2:f:129:VAL:HG11 | 2.02 | 0.42 |
| 2:e:344:ASP:OD1 | 2:e:344:ASP:N | 2.53 | 0.42 |
| 2:f:54:GLN:HB2 | 2:f:112:ASN:HD21 | 1.85 | 0.42 |
| 2:g:101:GLN:OE1 | 2:h:219:ARG:HD3 | 2.20 | 0.42 |
| 2:g:280:LEU:HD22 | 2:g:339:GLY:O | 2.19 | 0.42 |
| 2:h:123:MET:CE | 2:h:136:LEU:HD22 | 2.38 | 0.42 |
| 2:j:123:MET:HE3 | 2:j:123:MET:HA | 2.02 | 0.42 |
| 2:j:136:LEU:HD13 | 2:k:129:VAL:HG11 | 2.01 | 0.42 |
| 2:j:353:GLN:CG | 2:j:362:LEU:HD22 | 2.48 | 0.42 |
| 2:k:54:GLN:HB2 | 2:k:112:ASN:HD21 | 1.85 | 0.42 |
| 2:k:196:MET:HA | 2:k:196:MET:CE | 2.47 | 0.42 |
| 2:k:353:GLN:CG | 2:k:362:LEU:HD22 | 2.48 | 0.42 |
| 2:l:217:ASP:OD1 | 2:l:219:ARG:N | 2.35 | 0.42 |
| 2:n:50:ASP:OD1 | 2:n:113:ALA:N | 2.52 | 0.42 |
| 2:p:89:VAL:CG2 | 2:p:126:LEU:HD21 | 2.48 | 0.42 |
| 2:p:123:MET:HE3 | 2:p:123:MET:HA | 2.02 | 0.42 |
| 2:p:344:ASP:OD1 | 2:p:344:ASP:N | 2.53 | 0.42 |
| 2:r:50:ASP:OD1 | 2:r:113:ALA:N | 2.52 | 0.42 |
| 2:s:173:ARG:HH12 | 1:R:54:SER:HB2 | 1.85 | 0.42 |
| 2:t:250:ASP:O | 2:t:265:ASN:ND2 | 2.51 | 0.42 |
| 2:v:344:ASP:OD1 | 2:v:344:ASP:N | 2.53 | 0.42 |
| 3:3:69:SER:O | 3:3:70:PHE:CD2 | 2.72 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:4:39:PRO:HD2 | 3:4:42:PHE:HB2 | 2.01 | 0.42 |
| 3:5:39:PRO:HD2 | 3:5:42:PHE:HB2 | 2.02 | 0.42 |
| 3:9:22:VAL:HG13 | 3:9:34:LEU:CD2 | 2.49 | 0.42 |
| 3:11:22:VAL:HG13 | 3:11:34:LEU:CD2 | 2.50 | 0.42 |
| 3:13:20:ALA:HA | 3:13:36:TYR:HB3 | 2.02 | 0.42 |
| 3:15:20:ALA:HA | 3:15:36:TYR:HB3 | 2.02 | 0.42 |
| 3:18:29:SER:OG | 3:18:31:ILE:HG12 | 2.19 | 0.42 |
| 3:19:69:SER:O | 3:19:70:PHE:CD2 | 2.72 | 0.42 |
| 3:20:20:ALA:HA | 3:20:36:TYR:HB3 | 2.02 | 0.42 |
| 3:21:69:SER:O | 3:21:70:PHE:CD2 | 2.72 | 0.42 |
| 3:23:69:SER:O | 3:23:70:PHE:CD2 | 2.72 | 0.42 |
| 3:25:69:SER:O | 3:25:70:PHE:CD2 | 2.72 | 0.42 |
| 1:C:41:PRO:HA | 1:E:157:ALA:HB1 | 2.01 | 0.42 |
| 1:E:117:PHE:HD1 | 1:E:122:ALA:CB | 2.33 | 0.42 |
| 1:F:171:ILE:O | 1:F:172:ASN:HB3 | 2.19 | 0.42 |
| 1:G:117:PHE:HD1 | 1:G:122:ALA:CB | 2.33 | 0.42 |
| 1:I:30:LEU:HD21 | 1:J:206:GLU:HG3 | 2.02 | 0.42 |
| 1:K:41:PRO:HA | 1:M:157:ALA:HB1 | 2.01 | 0.42 |
| 1:K:117:PHE:HD1 | 1:K:122:ALA:CB | 2.33 | 0.42 |
| 1:P:41:PRO:HA | 1:R:157:ALA:HB1 | 2.01 | 0.42 |
| 1:X:117:PHE:HD1 | 1:X:122:ALA:CB | 2.33 | 0.42 |
| 1:X:222:LEU:HB2 | 1:Y:231:PRO:HB3 | 2.02 | 0.42 |
| 1:A:206:GLU:CG | 1:Z:30:LEU:HD21 | 2.50 | 0.42 |
| 1:A:210:ASN:ND2 | 3:26:82:GLY:O | 2.53 | 0.42 |
| 3:1:20:ALA:HA | 3:1:36:TYR:HB3 | 2.02 | 0.42 |
| 2:e:80:GLN:HB3 | 2:f:54:GLN:HB3 | 2.02 | 0.42 |
| 2:e:173:ARG:HH12 | 1:D:54:SER:HB2 | 1.85 | 0.42 |
| 2:f:284:VAL:CG2 | 2:f:316:GLY:HA2 | 2.50 | 0.42 |
| 2:g:80:GLN:HB3 | 2:h:54:GLN:HB3 | 2.01 | 0.42 |
| 2:h:50:ASP:OD1 | 2:h:113:ALA:N | 2.52 | 0.42 |
| 2:h:101:GLN:OE1 | 2:i:219:ARG:HD3 | 2.20 | 0.42 |
| 2:h:284:VAL:CG2 | 2:h:316:GLY:HA2 | 2.50 | 0.42 |
| 2:i:54:GLN:HB2 | 2:i:112:ASN:HD21 | 1.85 | 0.42 |
| 2:i:114:LYS:HA | 2:i:114:LYS:HD2 | 1.81 | 0.42 |
| 2:j:22:ILE:O | 2:j:25:LEU:HD23 | 2.19 | 0.42 |
| 2:j:284:VAL:CG2 | 2:j:316:GLY:HA2 | 2.50 | 0.42 |
| 2:k:159:GLN:CB | 2:l:258:ARG:HG2 | 2.50 | 0.42 |
| 2:l:54:GLN:HB2 | 2:l:112:ASN:HD21 | 1.85 | 0.42 |
| 2:m:256:ASN:OD1 | 2:m:259:THR:OG1 | 2.10 | 0.42 |
| 2:m:284:VAL:CG2 | 2:m:316:GLY:HA2 | 2.50 | 0.42 |
| 2:n:54:GLN:HB2 | 2:n:112:ASN:HD21 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:173:ARG:HH12 | 1:M:54:SER:HB2 | 1.84 | 0.42 |
| 2:p:101:GLN:OE1 | 2:q:219:ARG:HD3 | 2.20 | 0.42 |
| 2:p:172:GLU:OE1 | 2:p:172:GLU:CA | 2.66 | 0.42 |
| 2:q:173:ARG:HH12 | 1:P:54:SER:HB2 | 1.85 | 0.42 |
| 2:r:123:MET:HE3 | 2:r:123:MET:HA | 2.02 | 0.42 |
| 2:t:344:ASP:N | 2:t:344:ASP:OD1 | 2.53 | 0.42 |
| 2:v:89:VAL:CG2 | 2:v:126:LEU:HD21 | 2.48 | 0.42 |
| 2:w:159:GLN:CB | 2:x:258:ARG:HG2 | 2.50 | 0.42 |
| 2:w:185:ILE:O | 2:w:223:VAL:HG22 | 2.20 | 0.42 |
| 2:x:142:LEU:HD22 | 2:z:364:ILE:HD12 | 2.02 | 0.42 |
| 2:y:50:ASP:OD1 | 2:y:113:ALA:N | 2.52 | 0.42 |
| 2:y:114:LYS:HD2 | 2:y:114:LYS:HA | 1.81 | 0.42 |
| 3:2:20:ALA:HA | 3:2:36:TYR:HB3 | 2.02 | 0.42 |
| 3:4:20:ALA:HA | 3:4:36:TYR:HB3 | 2.02 | 0.42 |
| 3:4:83:SER:O | 3:4:84:LEU:HD23 | 2.20 | 0.42 |
| 3:7:20:ALA:HA | 3:7:36:TYR:HB3 | 2.02 | 0.42 |
| 3:8:20:ALA:HA | 3:8:36:TYR:HB3 | 2.02 | 0.42 |
| 3:10:83:SER:O | 3:10:84:LEU:HD23 | 2.20 | 0.42 |
| 3:17:20:ALA:HA | 3:17:36:TYR:HB3 | 2.02 | 0.42 |
| 3:20:69:SER:O | 3:20:70:PHE:CD2 | 2.72 | 0.42 |
| 3:22:69:SER:O | 3:22:70:PHE:CD2 | 2.72 | 0.42 |
| 3:22:83:SER:O | 3:22:84:LEU:HD23 | 2.20 | 0.42 |
| 3:24:20:ALA:HA | 3:24:36:TYR:HB3 | 2.02 | 0.42 |
| 1:F:117:PHE:HD1 | 1:F:122:ALA:CB | 2.33 | 0.42 |
| 5:K:301:TQN:C14 | 1:L:112:TYR:HB2 | 2.49 | 0.42 |
| 1:L:149:THR:OG1 | 1:M:198:THR:O | 2.35 | 0.42 |
| 1:P:30:LEU:HD21 | 1:Q:206:GLU:HG3 | 2.01 | 0.42 |
| 1:P:117:PHE:HD1 | 1:P:122:ALA:CB | 2.33 | 0.42 |
| 1:Q:41:PRO:HA | 1:S:157:ALA:HB1 | 2.00 | 0.42 |
| 1:R:30:LEU:HD21 | 1:S:206:GLU:HG3 | 2.01 | 0.42 |
| 5:T:301:TQN:C14 | 1:U:112:TYR:HB2 | 2.49 | 0.42 |
| 1:X:30:LEU:HD21 | 1:Y:206:GLU:HG3 | 2.01 | 0.42 |
| 2:a:99:GLN:HE21 | 1:Z:50:SER:HB3 | 1.83 | 0.41 |
| 2:a:319:LEU:HD12 | 2:a:319:LEU:HA | 1.80 | 0.41 |
| 2:a:344:ASP:OD1 | 2:a:344:ASP:N | 2.53 | 0.41 |
| 2:d:32:ARG:H | 2:d:95:PRO:HB3 | 1.85 | 0.41 |
| 2:d:136:LEU:HD13 | 2:e:129:VAL:HG11 | 2.01 | 0.41 |
| 2:f:344:ASP:OD1 | 2:f:344:ASP:N | 2.53 | 0.41 |
| 2:g:185:ILE:O | 2:g:223:VAL:HG22 | 2.20 | 0.41 |
| 2:j:114:LYS:HA | 2:j:114:LYS:HD2 | 1.81 | 0.41 |
| 2:j:343:MET:SD | 2:j:343:MET:N | 2.91 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:k:250:ASP:O | 2:k:265:ASN:ND2 | 2.51 | 0.41 |
| 2:l:284:VAL:CG2 | 2:l:316:GLY:HA2 | 2.50 | 0.41 |
| 2:m:343:MET:SD | 2:m:343:MET:N | 2.91 | 0.41 |
| 2:o:50:ASP:OD1 | 2:o:113:ALA:N | 2.52 | 0.41 |
| 2:o:343:MET:SD | 2:o:343:MET:N | 2.91 | 0.41 |
| 2:p:54:GLN:HB2 | 2:p:112:ASN:HD21 | 1.85 | 0.41 |
| 2:p:208:ARG:HG3 | 2:p:235:PHE:CZ | 2.54 | 0.41 |
| 2:q:32:ARG:H | 2:q:95:PRO:HB3 | 1.85 | 0.41 |
| 2:q:142:LEU:HD22 | 2:s:364:ILE:CD1 | 2.50 | 0.41 |
| 2:q:250:ASP:O | 2:q:265:ASN:ND2 | 2.51 | 0.41 |
| 2:r:22:ILE:O | 2:r:25:LEU:HD23 | 2.19 | 0.41 |
| 2:r:280:LEU:HD22 | 2:r:339:GLY:O | 2.19 | 0.41 |
| 2:r:343:MET:SD | 2:r:343:MET:N | 2.91 | 0.41 |
| 2:s:136:LEU:HD13 | 2:t:129:VAL:HG11 | 2.01 | 0.41 |
| 2:t:101:GLN:OE1 | 2:u:219:ARG:HD3 | 2.20 | 0.41 |
| 2:v:32:ARG:H | 2:v:95:PRO:HB3 | 1.85 | 0.41 |
| 2:v:196:MET:HA | 2:v:196:MET:CE | 2.47 | 0.41 |
| 2:w:32:ARG:H | 2:w:95:PRO:HB3 | 1.85 | 0.41 |
| 2:x:54:GLN:HB2 | 2:x:112:ASN:HD21 | 1.85 | 0.41 |
| 2:x:250:ASP:O | 2:x:265:ASN:ND2 | 2.51 | 0.41 |
| 2:y:328:LEU:CD2 | 2:z:273:CYS:HA | 2.50 | 0.41 |
| 2:z:185:ILE:O | 2:z:223:VAL:HG22 | 2.20 | 0.41 |
| 3:2:83:SER:O | 3:2:84:LEU:HD23 | 2.20 | 0.41 |
| 3:3:39:PRO:HD2 | 3:3:42:PHE:HB2 | 2.01 | 0.41 |
| 3:5:83:SER:O | 3:5:84:LEU:HD23 | 2.20 | 0.41 |
| 3:6:22:VAL:HG13 | 3:6:34:LEU:CD2 | 2.49 | 0.41 |
| 3:7:22:VAL:HG13 | 3:7:34:LEU:CD2 | 2.49 | 0.41 |
| 3:11:83:SER:O | 3:11:84:LEU:HD23 | 2.20 | 0.41 |
| 3:20:22:VAL:HG13 | 3:20:34:LEU:CD2 | 2.50 | 0.41 |
| 3:26:20:ALA:HA | 3:26:36:TYR:HB3 | 2.02 | 0.41 |
| 5:B:301:TQN:C14 | 1:C:112:TYR:HB2 | 2.49 | 0.41 |
| 1:D:30:LEU:HD21 | 1:E:206:GLU:CG | 2.50 | 0.41 |
| 1:H:41:PRO:HA | 1:J:157:ALA:HB1 | 2.01 | 0.41 |
| 1:Q:219:MET:HE2 | 1:S:132:PHE:HB3 | 2.01 | 0.41 |
| 1:S:30:LEU:H | 1:S:30:LEU:CD2 | 2.29 | 0.41 |
| 1:T:82:LEU:HA | 1:T:197:SER:CB | 2.43 | 0.41 |
| 1:V:117:PHE:HD1 | 1:V:122:ALA:CB | 2.33 | 0.41 |
| 1:V:221:TRP:NE1 | 1:W:229:LEU:O | 2.39 | 0.41 |
| 1:W:30:LEU:HD21 | 1:X:206:GLU:HG3 | 2.01 | 0.41 |
| 1:W:117:PHE:HD1 | 1:W:122:ALA:CB | 2.33 | 0.41 |
| 1:X:171:ILE:HD12 | 1:Z:88:ALA:CB | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:30:LEU:HD21 | 1:Z:206:GLU:CG | 2.50 | 0.41 |
| 1:A:30:LEU:HD21 | 1:B:206:GLU:HG3 | 2.01 | 0.41 |
| 1:A:54:SER:HB2 | 2:b:173:ARG:HH12 | 1.84 | 0.41 |
| 2:a:256:ASN:OD1 | 2:a:259:THR:OG1 | 2.10 | 0.41 |
| 2:c:344:ASP:OD1 | 2:c:344:ASP:N | 2.53 | 0.41 |
| 2:e:32:ARG:H | 2:e:95:PRO:HB3 | 1.85 | 0.41 |
| 2:f:32:ARG:H | 2:f:95:PRO:HB3 | 1.85 | 0.41 |
| 2:g:32:ARG:H | 2:g:95:PRO:HB3 | 1.85 | 0.41 |
| 2:i:22:ILE:O | 2:i:25:LEU:HD23 | 2.19 | 0.41 |
| 2:k:80:GLN:HB3 | 2:l:54:GLN:HB3 | 2.02 | 0.41 |
| 2:l:89:VAL:CG2 | 2:l:126:LEU:HD21 | 2.48 | 0.41 |
| 2:o:252:LYS:HB2 | 2:o:252:LYS:HE3 | 1.89 | 0.41 |
| 2:q:217:ASP:OD1 | 2:q:219:ARG:N | 2.35 | 0.41 |
| 2:q:343:MET:SD | 2:q:343:MET:N | 2.91 | 0.41 |
| 2:u:185:ILE:O | 2:u:223:VAL:HG22 | 2.19 | 0.41 |
| 2:v:93:TYR:OH | 2:v:173:ARG:O | 2.24 | 0.41 |
| 2:w:136:LEU:HD13 | 2:x:129:VAL:HG11 | 2.02 | 0.41 |
| 2:z:114:LYS:HD2 | 2:z:114:LYS:HA | 1.81 | 0.41 |
| 3:4:22:VAL:HG13 | 3:4:34:LEU:CD2 | 2.49 | 0.41 |
| 3:11:47:ASP:CG | 3:11:50:VAL:H | 2.14 | 0.41 |
| 3:12:20:ALA:HA | 3:12:36:TYR:HB3 | 2.02 | 0.41 |
| 3:12:83:SER:O | 3:12:84:LEU:HD23 | 2.20 | 0.41 |
| 3:16:20:ALA:HA | 3:16:36:TYR:HB3 | 2.02 | 0.41 |
| 3:16:83:SER:O | 3:16:84:LEU:HD23 | 2.20 | 0.41 |
| 5:D:301:TQN:C14 | 1:E:112:TYR:HB2 | 2.49 | 0.41 |
| 1:G:30:LEU:HD21 | 1:H:206:GLU:CG | 2.51 | 0.41 |
| 1:H:117:PHE:HD1 | 1:H:122:ALA:CB | 2.33 | 0.41 |
| 1:K:124:MET:HB3 | 1:K:124:MET:HE3 | 1.77 | 0.41 |
| 5:L:301:TQN:C14 | 1:M:112:TYR:HB2 | 2.49 | 0.41 |
| 1:P:219:MET:HE2 | 1:R:132:PHE:HB3 | 2.01 | 0.41 |
| 1:T:40:ILE:H | 1:T:40:ILE:HG12 | 1.49 | 0.41 |
| 1:U:117:PHE:HD1 | 1:U:122:ALA:CB | 2.33 | 0.41 |
| 1:X:41:PRO:HA | 1:Z:157:ALA:HB1 | 2.01 | 0.41 |
| 1:Y:111:ARG:HA | 1:Y:111:ARG:HD3 | 1.90 | 0.41 |
| 1:A:111:ARG:HB3 | 1:Z:121:ARG:HB3 | 2.01 | 0.41 |
| 2:b:196:MET:HA | 2:b:196:MET:CE | 2.48 | 0.41 |
| 2:c:32:ARG:H | 2:c:95:PRO:HB3 | 1.85 | 0.41 |
| 2:c:136:LEU:HD13 | 2:d:129:VAL:HG11 | 2.02 | 0.41 |
| 2:d:83:ASN:ND2 | 2:e:109:SER:OG | 2.47 | 0.41 |
| 2:d:284:VAL:CG2 | 2:d:316:GLY:HA2 | 2.50 | 0.41 |
| 2:g:54:GLN:HB2 | 2:g:112:ASN:HD21 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:h:32:ARG:H | 2:h:95:PRO:HB3 | 1.85 | 0.41 |
| 2:i:32:ARG:H | 2:i:95:PRO:HB3 | 1.85 | 0.41 |
| 2:l:82:LYS:HE2 | 2:l:82:LYS:HB3 | 1.96 | 0.41 |
| 2:l:93:TYR:OH | 2:l:173:ARG:O | 2.24 | 0.41 |
| 2:m:344:ASP:N | 2:m:344:ASP:OD1 | 2.53 | 0.41 |
| 2:n:123:MET:HE3 | 2:n:123:MET:HA | 2.02 | 0.41 |
| 2:n:250:ASP:O | 2:n:265:ASN:ND2 | 2.51 | 0.41 |
| 2:o:185:ILE:O | 2:o:223:VAL:HG22 | 2.20 | 0.41 |
| 2:q:41:LEU:HD23 | 2:q:86:ALA:HA | 2.03 | 0.41 |
| 2:r:41:LEU:HD23 | 2:r:86:ALA:HA | 2.03 | 0.41 |
| 2:s:41:LEU:HD23 | 2:s:86:ALA:HA | 2.03 | 0.41 |
| 2:s:101:GLN:OE1 | 2:t:219:ARG:HD3 | 2.20 | 0.41 |
| 2:t:41:LEU:HD23 | 2:t:86:ALA:HA | 2.03 | 0.41 |
| 2:t:79:MET:HE2 | 2:t:79:MET:HB2 | 1.69 | 0.41 |
| 2:u:41:LEU:HD23 | 2:u:86:ALA:HA | 2.03 | 0.41 |
| 2:v:41:LEU:HD23 | 2:v:86:ALA:HA | 2.03 | 0.41 |
| 2:v:319:LEU:HD12 | 2:v:319:LEU:HA | 1.80 | 0.41 |
| 2:w:22:ILE:O | 2:w:25:LEU:HD23 | 2.19 | 0.41 |
| 2:w:142:LEU:HD22 | 2:y:364:ILE:CD1 | 2.50 | 0.41 |
| 2:y:54:GLN:HB2 | 2:y:112:ASN:HD21 | 1.85 | 0.41 |
| 3:3:20:ALA:HA | 3:3:36:TYR:HB3 | 2.02 | 0.41 |
| 3:5:22:VAL:HG13 | 3:5:34:LEU:CD2 | 2.49 | 0.41 |
| 3:9:83:SER:O | 3:9:84:LEU:HD23 | 2.20 | 0.41 |
| 3:18:83:SER:O | 3:18:84:LEU:HD23 | 2.20 | 0.41 |
| 1:F:82:LEU:HA | 1:F:197:SER:CB | 2.43 | 0.41 |
| 1:G:111:ARG:HA | 1:G:111:ARG:HD3 | 1.90 | 0.41 |
| 1:J:30:LEU:HD21 | 1:K:206:GLU:CG | 2.50 | 0.41 |
| 1:K:30:LEU:HD21 | 1:L:206:GLU:HG3 | 2.02 | 0.41 |
| 1:L:117:PHE:HD1 | 1:L:122:ALA:CB | 2.33 | 0.41 |
| 1:M:117:PHE:HD1 | 1:M:122:ALA:CB | 2.33 | 0.41 |
| 1:R:221:TRP:NE1 | 1:S:229:LEU:O | 2.40 | 0.41 |
| 1:S:30:LEU:HD21 | 1:T:206:GLU:HG3 | 2.01 | 0.41 |
| 1:U:124:MET:HE3 | 1:U:124:MET:HB3 | 1.77 | 0.41 |
| 5:U:301:TQN:C14 | 1:V:112:TYR:HB2 | 2.49 | 0.41 |
| 1:V:41:PRO:HA | 1:X:157:ALA:HB1 | 2.01 | 0.41 |
| 1:X:35:THR:HG21 | 1:Y:166:GLU:HB2 | 2.02 | 0.41 |
| 1:X:111:ARG:HA | 1:X:111:ARG:HD3 | 1.90 | 0.41 |
| 1:X:121:ARG:HB3 | 1:Y:111:ARG:HB3 | 2.01 | 0.41 |
| 2:a:173:ARG:HH12 | 1:Z:54:SER:HB2 | 1.84 | 0.41 |
| 2:b:32:ARG:H | 2:b:95:PRO:HB3 | 1.85 | 0.41 |
| 2:b:344:ASP:N | 2:b:344:ASP:OD1 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:g:284:VAL:CG2 | 2:g:316:GLY:HA2 | 2.50 | 0.41 |
| 2:h:250:ASP:O | 2:h:265:ASN:ND2 | 2.51 | 0.41 |
| 2:j:32:ARG:H | 2:j:95:PRO:HB3 | 1.85 | 0.41 |
| 2:j:344:ASP:N | 2:j:344:ASP:OD1 | 2.53 | 0.41 |
| 2:k:32:ARG:H | 2:k:95:PRO:HB3 | 1.85 | 0.41 |
| 2:k:284:VAL:CG2 | 2:k:316:GLY:HA2 | 2.50 | 0.41 |
| 2:p:41:LEU:HD23 | 2:p:86:ALA:HA | 2.03 | 0.41 |
| 2:u:136:LEU:HD13 | 2:v:129:VAL:HG11 | 2.02 | 0.41 |
| 2:v:284:VAL:CG2 | 2:v:316:GLY:HA2 | 2.50 | 0.41 |
| 2:w:41:LEU:HD23 | 2:w:86:ALA:HA | 2.03 | 0.41 |
| 2:w:196:MET:HA | 2:w:196:MET:CE | 2.48 | 0.41 |
| 2:x:32:ARG:H | 2:x:95:PRO:HB3 | 1.85 | 0.41 |
| 2:y:256:ASN:O | 2:y:257:SER:OG | 2.28 | 0.41 |
| 3:2:39:PRO:HD2 | 3:2:42:PHE:HB2 | 2.02 | 0.41 |
| 3:3:83:SER:O | 3:3:84:LEU:HD23 | 2.20 | 0.41 |
| 3:8:22:VAL:HG13 | 3:8:34:LEU:CD2 | 2.50 | 0.41 |
| 3:8:83:SER:O | 3:8:84:LEU:HD23 | 2.20 | 0.41 |
| 3:17:83:SER:O | 3:17:84:LEU:HD23 | 2.20 | 0.41 |
| 3:25:20:ALA:HA | 3:25:36:TYR:HB3 | 2.02 | 0.41 |
| 1:E:111:ARG:HA | 1:E:111:ARG:HD3 | 1.90 | 0.41 |
| 1:M:30:LEU:HD21 | 1:N:206:GLU:HG3 | 2.01 | 0.41 |
| 1:T:117:PHE:HD1 | 1:T:122:ALA:CB | 2.33 | 0.41 |
| 1:A:50:SER:HB3 | 2:b:99:GLN:HE21 | 1.83 | 0.41 |
| 1:A:121:ARG:HB3 | 1:B:111:ARG:HB3 | 2.01 | 0.41 |
| 1:A:231:PRO:HG2 | 1:D:104:PHE:CZ | 2.56 | 0.41 |
| 2:a:101:GLN:OE1 | 2:b:219:ARG:HD3 | 2.20 | 0.41 |
| 2:a:330:SER:OG | 2:a:333:ARG:NH1 | 2.54 | 0.41 |
| 3:1:22:VAL:HG13 | 3:1:34:LEU:CD2 | 2.50 | 0.41 |
| 2:b:284:VAL:CG2 | 2:b:316:GLY:HA2 | 2.50 | 0.41 |
| 2:b:330:SER:OG | 2:b:333:ARG:NH1 | 2.54 | 0.41 |
| 2:d:79:MET:HE2 | 2:d:79:MET:HB2 | 1.69 | 0.41 |
| 2:d:256:ASN:OD1 | 2:d:259:THR:OG1 | 2.10 | 0.41 |
| 2:e:159:GLN:CB | 2:f:258:ARG:HG2 | 2.50 | 0.41 |
| 2:f:123:MET:CE | 2:f:136:LEU:HD22 | 2.38 | 0.41 |
| 2:g:252:LYS:HB2 | 2:g:252:LYS:HE3 | 1.89 | 0.41 |
| 2:h:344:ASP:OD1 | 2:h:344:ASP:N | 2.53 | 0.41 |
| 2:k:142:LEU:HD22 | 2:m:364:ILE:CD1 | 2.51 | 0.41 |
| 2:t:159:GLN:CB | 2:u:258:ARG:HG2 | 2.51 | 0.41 |
| 2:u:196:MET:HA | 2:u:196:MET:CE | 2.48 | 0.41 |
| 2:w:336:ASN:HD22 | 2:w:336:ASN:HA | 1.66 | 0.41 |
| 2:x:41:LEU:HD23 | 2:x:86:ALA:HA | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:x:344:ASP:OD1 | 2:x:344:ASP:N | 2.53 | 0.41 |
| 2:z:330:SER:OG | 2:z:333:ARG:NH1 | 2.54 | 0.41 |
| 3:5:36:TYR:HE2 | 3:5:44:SER:HG | 1.66 | 0.41 |
| 3:10:22:VAL:HG13 | 3:10:34:LEU:CD2 | 2.49 | 0.41 |
| 1:B:30:LEU:HD21 | 1:C:206:GLU:CG | 2.50 | 0.41 |
| 1:C:30:LEU:HD21 | 1:D:206:GLU:HG3 | 2.02 | 0.41 |
| 1:C:135:LYS:HB2 | 1:C:135:LYS:HE2 | 1.73 | 0.41 |
| 1:F:30:LEU:HD21 | 1:G:206:GLU:CG | 2.51 | 0.41 |
| 1:J:117:PHE:HD1 | 1:J:122:ALA:CB | 2.33 | 0.41 |
| 1:M:171:ILE:HD12 | 1:O:88:ALA:CB | 2.34 | 0.41 |
| 1:N:30:LEU:HD21 | 1:O:206:GLU:CG | 2.50 | 0.41 |
| 1:O:219:MET:HE2 | 1:Q:132:PHE:HB3 | 2.01 | 0.41 |
| 1:R:117:PHE:HD1 | 1:R:122:ALA:CB | 2.33 | 0.41 |
| 1:S:117:PHE:HD1 | 1:S:122:ALA:CB | 2.33 | 0.41 |
| 1:T:30:LEU:HD21 | 1:U:206:GLU:CG | 2.50 | 0.41 |
| 1:A:111:ARG:HA | 1:A:111:ARG:HD3 | 1.90 | 0.41 |
| 2:a:249:GLN:O | 2:z:23:ARG:NH1 | 2.53 | 0.41 |
| 2:e:256:ASN:OD1 | 2:e:259:THR:OG1 | 2.10 | 0.41 |
| 2:f:89:VAL:CG2 | 2:f:126:LEU:HD21 | 2.48 | 0.41 |
| 2:f:93:TYR:OH | 2:f:173:ARG:O | 2.24 | 0.41 |
| 2:f:123:MET:HE3 | 2:f:123:MET:HA | 2.02 | 0.41 |
| 2:i:123:MET:HE3 | 2:i:123:MET:HA | 2.02 | 0.41 |
| 2:i:142:LEU:HD22 | 2:k:364:ILE:CD1 | 2.51 | 0.41 |
| 2:k:173:ARG:HH12 | 1:J:54:SER:HB2 | 1.85 | 0.41 |
| 2:m:196:MET:HA | 2:m:196:MET:CE | 2.48 | 0.41 |
| 2:o:142:LEU:HD22 | 2:q:364:ILE:CD1 | 2.50 | 0.41 |
| 2:o:344:ASP:OD1 | 2:o:344:ASP:N | 2.53 | 0.41 |
| 2:p:32:ARG:H | 2:p:95:PRO:HB3 | 1.85 | 0.41 |
| 2:p:136:LEU:HD13 | 2:q:129:VAL:HG11 | 2.01 | 0.41 |
| 2:q:123:MET:HE1 | 2:q:136:LEU:CD2 | 2.42 | 0.41 |
| 2:q:344:ASP:OD1 | 2:q:344:ASP:N | 2.53 | 0.41 |
| 2:s:343:MET:SD | 2:s:343:MET:N | 2.91 | 0.41 |
| 2:t:284:VAL:CG2 | 2:t:316:GLY:HA2 | 2.50 | 0.41 |
| 2:w:82:LYS:HE2 | 2:w:82:LYS:HB3 | 1.96 | 0.41 |
| 2:w:123:MET:HE3 | 2:w:123:MET:HA | 2.02 | 0.41 |
| 2:w:343:MET:SD | 2:w:343:MET:N | 2.91 | 0.41 |
| 2:y:41:LEU:HD23 | 2:y:86:ALA:HA | 2.03 | 0.41 |
| 2:y:101:GLN:OE1 | 2:z:219:ARG:HD3 | 2.20 | 0.41 |
| 2:z:41:LEU:HD23 | 2:z:86:ALA:HA | 2.03 | 0.41 |
| 2:z:123:MET:HE3 | 2:z:123:MET:HA | 2.02 | 0.41 |
| 3:13:83:SER:O | 3:13:84:LEU:HD23 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:111:ARG:HA | 1:C:111:ARG:HD3 | 1.90 | 0.41 |
| 1:F:167:LYS:NZ | 1:G:84:GLU:OE2 | 2.42 | 0.41 |
| 1:I:124:MET:HE3 | 1:I:124:MET:HB3 | 1.77 | 0.41 |
| 1:J:41:PRO:HA | 1:L:157:ALA:HB1 | 2.01 | 0.41 |
| 1:K:101:LYS:HZ2 | 1:K:101:LYS:HB3 | 1.86 | 0.41 |
| 1:L:219:MET:HE2 | 1:N:132:PHE:HB3 | 2.01 | 0.41 |
| 1:M:82:LEU:HA | 1:M:197:SER:CB | 2.43 | 0.41 |
| 1:P:30:LEU:HD21 | 1:Q:206:GLU:CG | 2.50 | 0.41 |
| 1:T:30:LEU:H | 1:T:30:LEU:CD2 | 2.29 | 0.41 |
| 1:U:30:LEU:HD21 | 1:V:206:GLU:HG3 | 2.02 | 0.41 |
| 1:V:30:LEU:HD21 | 1:W:206:GLU:CG | 2.50 | 0.41 |
| 1:A:135:LYS:HE2 | 1:A:135:LYS:HB2 | 1.73 | 0.41 |
| 2:a:32:ARG:H | 2:a:95:PRO:HB3 | 1.85 | 0.41 |
| 2:c:330:SER:OG | 2:c:333:ARG:NH1 | 2.54 | 0.41 |
| 2:d:270:LEU:CD1 | 2:d:352:MET:HE1 | 2.39 | 0.41 |
| 2:e:123:MET:CE | 2:e:136:LEU:HD22 | 2.38 | 0.41 |
| 2:g:123:MET:CE | 2:g:136:LEU:HD22 | 2.38 | 0.41 |
| 2:i:172:GLU:OE1 | 2:i:172:GLU:CA | 2.66 | 0.41 |
| 2:k:344:ASP:OD1 | 2:k:344:ASP:N | 2.53 | 0.41 |
| 2:m:242:MET:HE3 | 2:m:242:MET:HB3 | 1.96 | 0.41 |
| 2:o:41:LEU:HD23 | 2:o:86:ALA:HA | 2.03 | 0.41 |
| 2:o:284:VAL:CG2 | 2:o:316:GLY:HA2 | 2.50 | 0.41 |
| 2:p:141:ILE:HD13 | 2:p:165:ILE:CD1 | 2.39 | 0.41 |
| 2:p:284:VAL:CG2 | 2:p:316:GLY:HA2 | 2.50 | 0.41 |
| 2:s:344:ASP:OD1 | 2:s:344:ASP:N | 2.53 | 0.41 |
| 2:w:89:VAL:CG2 | 2:w:126:LEU:HD21 | 2.48 | 0.41 |
| 2:w:344:ASP:N | 2:w:344:ASP:OD1 | 2.53 | 0.41 |
| 3:3:22:VAL:HG13 | 3:3:34:LEU:CD2 | 2.49 | 0.41 |
| 5:C:301:TQN:C14 | 1:D:112:TYR:HB2 | 2.49 | 0.41 |
| 1:G:30:LEU:H | 1:G:30:LEU:CD2 | 2.29 | 0.41 |
| 1:I:111:ARG:HA | 1:I:111:ARG:HD3 | 1.90 | 0.41 |
| 1:L:30:LEU:HD21 | 1:M:206:GLU:HG3 | 2.01 | 0.41 |
| 1:L:231:PRO:HG2 | 1:O:104:PHE:CZ | 2.56 | 0.41 |
| 1:Q:30:LEU:HD21 | 1:R:206:GLU:HG3 | 2.01 | 0.41 |
| 1:U:82:LEU:HA | 1:U:197:SER:CB | 2.43 | 0.41 |
| 1:U:149:THR:OG1 | 1:V:198:THR:O | 2.35 | 0.41 |
| 1:A:104:PHE:CZ | 1:X:231:PRO:HG2 | 2.55 | 0.41 |
| 1:A:149:THR:OG1 | 1:B:198:THR:O | 2.33 | 0.41 |
| 2:a:284:VAL:CG2 | 2:a:316:GLY:HA2 | 2.50 | 0.41 |
| 2:d:123:MET:CE | 2:d:136:LEU:HD22 | 2.38 | 0.41 |
| 2:e:250:ASP:O | 2:e:265:ASN:ND2 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:h:159:GLN:CB | 2:i:258:ARG:HG2 | 2.51 | 0.41 |
| 2:i:136:LEU:HD13 | 2:j:129:VAL:HG11 | 2.02 | 0.41 |
| 2:k:185:ILE:O | 2:k:223:VAL:HG22 | 2.20 | 0.41 |
| 2:l:32:ARG:H | 2:l:95:PRO:HB3 | 1.85 | 0.41 |
| 2:n:284:VAL:CG2 | 2:n:316:GLY:HA2 | 2.50 | 0.41 |
| 2:p:123:MET:HE1 | 2:p:136:LEU:CD2 | 2.42 | 0.41 |
| 2:r:123:MET:HE1 | 2:r:136:LEU:CD2 | 2.42 | 0.41 |
| 2:s:284:VAL:CG2 | 2:s:316:GLY:HA2 | 2.50 | 0.41 |
| 2:w:172:GLU:OE1 | 2:w:172:GLU:CA | 2.66 | 0.41 |
| 2:x:196:MET:HA | 2:x:196:MET:CE | 2.48 | 0.41 |
| 2:x:259:THR:O | 2:y:277:GLN:NE2 | 2.54 | 0.41 |
| 2:y:32:ARG:H | 2:y:95:PRO:HB3 | 1.85 | 0.41 |
| 2:y:34:ASN:HB3 | 1:W:51:ILE:HD12 | 2.03 | 0.41 |
| 2:y:284:VAL:CG2 | 2:y:316:GLY:HA2 | 2.50 | 0.41 |
| 2:z:172:GLU:OE1 | 2:z:172:GLU:CA | 2.66 | 0.41 |
| 3:25:83:SER:O | 3:25:84:LEU:HD23 | 2.20 | 0.41 |
| 1:F:149:THR:OG1 | 1:G:198:THR:O | 2.35 | 0.41 |
| 1:K:219:MET:HE2 | 1:M:132:PHE:HB3 | 2.01 | 0.41 |
| 1:M:219:MET:HE2 | 1:O:132:PHE:HB3 | 2.00 | 0.41 |
| 1:N:219:MET:HE2 | 1:P:132:PHE:HB3 | 2.01 | 0.41 |
| 1:P:124:MET:HE3 | 1:P:124:MET:HB3 | 1.77 | 0.41 |
| 1:Q:117:PHE:HD1 | 1:Q:122:ALA:CB | 2.33 | 0.41 |
| 1:S:30:LEU:HD21 | 1:T:206:GLU:CG | 2.51 | 0.41 |
| 2:a:41:LEU:HD23 | 2:a:86:ALA:HA | 2.03 | 0.41 |
| 2:a:54:GLN:HB2 | 2:a:112:ASN:HD21 | 1.85 | 0.41 |
| 2:a:123:MET:CE | 2:a:136:LEU:HD22 | 2.38 | 0.41 |
| 2:a:219:ARG:HD3 | 2:z:101:GLN:OE1 | 2.21 | 0.41 |
| 2:b:41:LEU:HD23 | 2:b:86:ALA:HA | 2.03 | 0.41 |
| 2:b:123:MET:CE | 2:b:136:LEU:HD22 | 2.38 | 0.41 |
| 2:c:123:MET:CE | 2:c:136:LEU:HD22 | 2.38 | 0.41 |
| 2:d:54:GLN:HB2 | 2:d:112:ASN:HD21 | 1.85 | 0.41 |
| 2:d:330:SER:OG | 2:d:333:ARG:NH1 | 2.54 | 0.41 |
| 2:f:23:ARG:NH1 | 2:g:249:GLN:O | 2.54 | 0.41 |
| 2:f:82:LYS:HE2 | 2:f:82:LYS:HB3 | 1.96 | 0.41 |
| 2:j:159:GLN:CB | 2:k:258:ARG:HG2 | 2.51 | 0.41 |
| 2:k:319:LEU:HD12 | 2:k:319:LEU:HA | 1.80 | 0.41 |
| 2:m:32:ARG:H | 2:m:95:PRO:HB3 | 1.85 | 0.41 |
| 2:m:89:VAL:CG2 | 2:m:126:LEU:HD21 | 2.48 | 0.41 |
| 2:m:142:LEU:HD22 | 2:o:364:ILE:CD1 | 2.51 | 0.41 |
| 2:m:172:GLU:OE1 | 2:m:172:GLU:CA | 2.66 | 0.41 |
| 2:n:41:LEU:HD23 | 2:n:86:ALA:HA | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:159:GLN:CB | 2:o:258:ARG:HG2 | 2.51 | 0.41 |
| 2:o:32:ARG:H | 2:o:95:PRO:HB3 | 1.85 | 0.41 |
| 2:o:123:MET:HE3 | 2:o:123:MET:HA | 2.02 | 0.41 |
| 2:o:136:LEU:HD13 | 2:p:129:VAL:HG11 | 2.02 | 0.41 |
| 2:p:104:ASP:OD1 | 2:p:166:THR:HA | 2.21 | 0.41 |
| 2:p:159:GLN:CB | 2:q:258:ARG:HG2 | 2.51 | 0.41 |
| 2:p:256:ASN:O | 2:p:257:SER:OG | 2.28 | 0.41 |
| 2:q:123:MET:HE3 | 2:q:123:MET:HA | 2.02 | 0.41 |
| 2:q:284:VAL:CG2 | 2:q:316:GLY:HA2 | 2.50 | 0.41 |
| 2:r:185:ILE:O | 2:r:223:VAL:HG22 | 2.20 | 0.41 |
| 2:s:54:GLN:HB2 | 2:s:112:ASN:HD21 | 1.85 | 0.41 |
| 2:v:54:GLN:HB2 | 2:v:112:ASN:HD21 | 1.85 | 0.41 |
| 2:v:336:ASN:HD22 | 2:v:336:ASN:HA | 1.66 | 0.41 |
| 2:w:284:VAL:CG2 | 2:w:316:GLY:HA2 | 2.50 | 0.41 |
| 2:y:196:MET:HA | 2:y:196:MET:CE | 2.48 | 0.41 |
| 2:z:123:MET:CE | 2:z:136:LEU:HD22 | 2.38 | 0.41 |
| 2:z:284:VAL:CG2 | 2:z:316:GLY:HA2 | 2.50 | 0.41 |
| 3:6:83:SER:O | 3:6:84:LEU:HD23 | 2.20 | 0.41 |
| 3:7:83:SER:O | 3:7:84:LEU:HD23 | 2.20 | 0.41 |
| 3:15:83:SER:O | 3:15:84:LEU:HD23 | 2.20 | 0.41 |
| 3:16:47:ASP:CG | 3:16:50:VAL:H | 2.14 | 0.41 |
| 1:B:88:ALA:CB | 1:Z:171:ILE:HD12 | 2.33 | 0.41 |
| 1:E:30:LEU:HD21 | 1:F:206:GLU:CG | 2.51 | 0.41 |
| 1:E:41:PRO:HA | 1:G:157:ALA:HB1 | 2.01 | 0.41 |
| 1:I:41:PRO:HA | 1:K:157:ALA:HB1 | 2.01 | 0.41 |
| 1:O:30:LEU:HD21 | 1:P:206:GLU:HG3 | 2.02 | 0.41 |
| 1:P:231:PRO:HG2 | 1:S:104:PHE:CZ | 2.56 | 0.41 |
| 1:Q:30:LEU:HD21 | 1:R:206:GLU:CG | 2.51 | 0.41 |
| 1:Q:231:PRO:HG2 | 1:T:104:PHE:CZ | 2.55 | 0.41 |
| 1:R:30:LEU:HD21 | 1:S:206:GLU:CG | 2.50 | 0.41 |
| 1:R:231:PRO:HG2 | 1:U:104:PHE:CZ | 2.55 | 0.41 |
| 1:S:40:ILE:H | 1:S:40:ILE:HG12 | 1.49 | 0.41 |
| 1:U:135:LYS:HE2 | 1:U:135:LYS:HB2 | 1.73 | 0.41 |
| 1:W:30:LEU:HD21 | 1:X:206:GLU:CG | 2.51 | 0.41 |
| 1:W:221:TRP:NE1 | 1:X:229:LEU:O | 2.39 | 0.41 |
| 1:A:30:LEU:HD21 | 1:B:206:GLU:CG | 2.51 | 0.41 |
| 2:c:172:GLU:OE1 | 2:c:172:GLU:CA | 2.66 | 0.41 |
| 2:c:284:VAL:CG2 | 2:c:316:GLY:HA2 | 2.50 | 0.41 |
| 2:f:196:MET:O | 2:f:200:ILE:HG12 | 2.21 | 0.41 |
| 2:j:196:MET:O | 2:j:200:ILE:HG12 | 2.21 | 0.41 |
| 2:n:344:ASP:OD1 | 2:n:344:ASP:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:o:104:ASP:OD1 | 2:o:166:THR:HA | 2.21 | 0.41 |
| 2:o:123:MET:HE1 | 2:o:136:LEU:CD2 | 2.42 | 0.41 |
| 2:p:142:LEU:HD22 | 2:r:364:ILE:HD12 | 2.03 | 0.41 |
| 2:p:343:MET:SD | 2:p:343:MET:N | 2.91 | 0.41 |
| 2:q:104:ASP:OD1 | 2:q:166:THR:HA | 2.21 | 0.41 |
| 2:q:136:LEU:HD13 | 2:r:129:VAL:HG11 | 2.02 | 0.41 |
| 2:r:344:ASP:OD1 | 2:r:344:ASP:N | 2.53 | 0.41 |
| 2:t:204:ILE:HG21 | 2:t:213:ALA:HB2 | 2.03 | 0.41 |
| 2:v:159:GLN:CB | 2:w:258:ARG:HG2 | 2.51 | 0.41 |
| 2:x:284:VAL:CG2 | 2:x:316:GLY:HA2 | 2.50 | 0.41 |
| 2:z:32:ARG:H | 2:z:95:PRO:HB3 | 1.85 | 0.41 |
| 2:z:173:ARG:HH12 | 1:Y:54:SER:HB2 | 1.86 | 0.41 |
| 2:z:256:ASN:OD1 | 2:z:259:THR:OG1 | 2.10 | 0.41 |
| 1:M:231:PRO:HG2 | 1:P:104:PHE:CZ | 2.56 | 0.41 |
| 1:O:117:PHE:HD1 | 1:O:122:ALA:CB | 2.33 | 0.41 |
| 1:O:221:TRP:NE1 | 1:P:229:LEU:O | 2.41 | 0.41 |
| 1:Q:149:THR:OG1 | 1:R:198:THR:O | 2.36 | 0.41 |
| 1:U:221:TRP:NE1 | 1:V:229:LEU:O | 2.41 | 0.41 |
| 2:a:111:GLY:O | 2:z:83:ASN:HB2 | 2.20 | 0.40 |
| 2:b:319:LEU:HD12 | 2:b:319:LEU:HA | 1.80 | 0.40 |
| 2:c:123:MET:HE3 | 2:c:123:MET:HA | 2.02 | 0.40 |
| 2:c:256:ASN:O | 2:c:257:SER:OG | 2.28 | 0.40 |
| 2:d:142:LEU:HD22 | 2:f:364:ILE:HD12 | 2.03 | 0.40 |
| 2:d:196:MET:HA | 2:d:196:MET:CE | 2.47 | 0.40 |
| 2:f:278:GLY:O | 2:f:279:ASN:HB2 | 2.21 | 0.40 |
| 2:g:196:MET:O | 2:g:200:ILE:HG12 | 2.21 | 0.40 |
| 2:g:278:GLY:O | 2:g:279:ASN:HB2 | 2.21 | 0.40 |
| 2:g:344:ASP:N | 2:g:344:ASP:OD1 | 2.53 | 0.40 |
| 2:j:142:LEU:HD22 | 2:l:364:ILE:HD12 | 2.03 | 0.40 |
| 2:m:41:LEU:HD23 | 2:m:86:ALA:HA | 2.03 | 0.40 |
| 2:n:79:MET:HE2 | 2:n:79:MET:HB2 | 1.69 | 0.40 |
| 2:r:104:ASP:OD1 | 2:r:166:THR:HA | 2.21 | 0.40 |
| 2:s:123:MET:HE1 | 2:s:136:LEU:CD2 | 2.42 | 0.40 |
| 2:t:123:MET:HE3 | 2:t:123:MET:HA | 2.02 | 0.40 |
| 2:u:204:ILE:HG21 | 2:u:213:ALA:HB2 | 2.04 | 0.40 |
| 2:w:278:GLY:O | 2:w:279:ASN:HB2 | 2.22 | 0.40 |
| 2:x:278:GLY:O | 2:x:279:ASN:HB2 | 2.21 | 0.40 |
| 1:B:101:LYS:O | 1:B:101:LYS:NZ | 2.54 | 0.40 |
| 1:D:167:LYS:NZ | 1:E:84:GLU:OE2 | 2.42 | 0.40 |
| 1:I:30:LEU:HD21 | 1:J:206:GLU:CG | 2.51 | 0.40 |
| 1:K:135:LYS:HB2 | 1:K:135:LYS:HE2 | 1.73 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:30:LEU:HD21 | 1:N:206:GLU:CG | 2.51 | 0.40 |
| 1:U:30:LEU:H | 1:U:30:LEU:CD2 | 2.29 | 0.40 |
| 3:1:83:SER:HA | 1:B:210:ASN:HD22 | 1.87 | 0.40 |
| 2:c:41:LEU:HD23 | 2:c:86:ALA:HA | 2.03 | 0.40 |
| 2:d:41:LEU:HD23 | 2:d:86:ALA:HA | 2.03 | 0.40 |
| 2:e:330:SER:OG | 2:e:333:ARG:NH1 | 2.54 | 0.40 |
| 2:f:172:GLU:OE1 | 2:f:172:GLU:CA | 2.66 | 0.40 |
| 2:g:142:LEU:HD22 | 2:i:364:ILE:CD1 | 2.51 | 0.40 |
| 2:l:344:ASP:OD1 | 2:l:344:ASP:N | 2.53 | 0.40 |
| 2:m:114:LYS:HA | 2:m:114:LYS:HD2 | 1.81 | 0.40 |
| 2:n:104:ASP:OD1 | 2:n:166:THR:HA | 2.21 | 0.40 |
| 2:o:196:MET:HA | 2:o:196:MET:CE | 2.48 | 0.40 |
| 2:o:204:ILE:HG21 | 2:o:213:ALA:HB2 | 2.04 | 0.40 |
| 2:p:204:ILE:HG21 | 2:p:213:ALA:HB2 | 2.03 | 0.40 |
| 2:r:101:GLN:OE1 | 2:s:219:ARG:HD3 | 2.21 | 0.40 |
| 2:r:284:VAL:CG2 | 2:r:316:GLY:HA2 | 2.50 | 0.40 |
| 2:u:142:LEU:HD22 | 2:w:364:ILE:CD1 | 2.50 | 0.40 |
| 2:u:250:ASP:O | 2:u:265:ASN:ND2 | 2.51 | 0.40 |
| 2:u:252:LYS:HB2 | 2:u:252:LYS:HE3 | 1.89 | 0.40 |
| 2:v:204:ILE:HG21 | 2:v:213:ALA:HB2 | 2.04 | 0.40 |
| 2:v:278:GLY:O | 2:v:279:ASN:HB2 | 2.21 | 0.40 |
| 2:w:204:ILE:HG21 | 2:w:213:ALA:HB2 | 2.04 | 0.40 |
| 3:10:47:ASP:CG | 3:10:50:VAL:H | 2.14 | 0.40 |
| 3:17:64:TYR:HB2 | 3:17:96:CYS:CB | 2.51 | 0.40 |
| 1:C:171:ILE:HD12 | 1:E:88:ALA:CB | 2.34 | 0.40 |
| 1:E:101:LYS:O | 1:E:101:LYS:NZ | 2.55 | 0.40 |
| 1:J:156:LEU:HD12 | 1:J:160:ASN:HB2 | 2.03 | 0.40 |
| 1:N:221:TRP:NE1 | 1:O:229:LEU:O | 2.39 | 0.40 |
| 1:R:40:ILE:H | 1:R:40:ILE:HG12 | 1.49 | 0.40 |
| 1:X:113:LEU:HD23 | 1:X:113:LEU:HA | 1.95 | 0.40 |
| 1:X:124:MET:HE3 | 1:X:124:MET:HB3 | 1.77 | 0.40 |
| 2:a:278:GLY:O | 2:a:279:ASN:HB2 | 2.21 | 0.40 |
| 2:b:114:LYS:HD2 | 2:b:114:LYS:HA | 1.81 | 0.40 |
| 2:b:250:ASP:O | 2:b:265:ASN:ND2 | 2.51 | 0.40 |
| 2:b:278:GLY:O | 2:b:279:ASN:HB2 | 2.22 | 0.40 |
| 2:d:259:THR:O | 2:e:277:GLN:NE2 | 2.55 | 0.40 |
| 2:e:41:LEU:HD23 | 2:e:86:ALA:HA | 2.03 | 0.40 |
| 2:f:41:LEU:HD23 | 2:f:86:ALA:HA | 2.03 | 0.40 |
| 2:k:278:GLY:O | 2:k:279:ASN:HB2 | 2.21 | 0.40 |
| 2:l:104:ASP:OD1 | 2:l:166:THR:HA | 2.21 | 0.40 |
| 2:l:123:MET:HE3 | 2:l:123:MET:HA | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:n:204:ILE:HG21 | 2:n:213:ALA:HB2 | 2.04 | 0.40 |
| 2:p:259:THR:O | 2:q:277:GLN:NE2 | 2.54 | 0.40 |
| 2:s:204:ILE:HG21 | 2:s:213:ALA:HB2 | 2.04 | 0.40 |
| 2:u:336:ASN:HD22 | 2:u:336:ASN:HA | 1.66 | 0.40 |
| 2:v:259:THR:O | 2:w:277:GLN:NE2 | 2.55 | 0.40 |
| 2:x:89:VAL:CG2 | 2:x:126:LEU:HD21 | 2.48 | 0.40 |
| 2:x:204:ILE:HG21 | 2:x:213:ALA:HB2 | 2.04 | 0.40 |
| 3:7:70:PHE:CD1 | 1:G:40:ILE:HA | 2.57 | 0.40 |
| 3:14:83:SER:O | 3:14:84:LEU:HD23 | 2.20 | 0.40 |
| 3:18:64:TYR:HB2 | 3:18:96:CYS:CB | 2.51 | 0.40 |
| 3:21:64:TYR:HB2 | 3:21:96:CYS:CB | 2.51 | 0.40 |
| 1:D:101:LYS:NZ | 1:D:101:LYS:O | 2.55 | 0.40 |
| 1:F:101:LYS:O | 1:F:101:LYS:NZ | 2.55 | 0.40 |
| 1:G:82:LEU:HA | 1:G:197:SER:CB | 2.43 | 0.40 |
| 1:H:167:LYS:NZ | 1:I:84:GLU:OE2 | 2.42 | 0.40 |
| 1:N:156:LEU:HD12 | 1:N:160:ASN:HB2 | 2.04 | 0.40 |
| 1:P:101:LYS:HZ2 | 1:P:101:LYS:HB3 | 1.87 | 0.40 |
| 1:V:82:LEU:HA | 1:V:197:SER:CB | 2.43 | 0.40 |
| 1:W:41:PRO:HA | 1:Y:157:ALA:HB1 | 2.01 | 0.40 |
| 1:Y:30:LEU:HD21 | 1:Z:206:GLU:HG3 | 2.03 | 0.40 |
| 1:Y:101:LYS:O | 1:Y:101:LYS:NZ | 2.55 | 0.40 |
| 1:A:40:ILE:HA | 3:1:70:PHE:CD1 | 2.57 | 0.40 |
| 2:a:23:ARG:NH1 | 2:b:249:GLN:O | 2.55 | 0.40 |
| 2:a:31:VAL:HG12 | 2:a:95:PRO:HG3 | 2.04 | 0.40 |
| 2:b:256:ASN:OD1 | 2:b:259:THR:OG1 | 2.10 | 0.40 |
| 2:c:196:MET:O | 2:c:200:ILE:HG12 | 2.21 | 0.40 |
| 2:e:31:VAL:HG12 | 2:e:95:PRO:HG3 | 2.04 | 0.40 |
| 2:g:41:LEU:HD23 | 2:g:86:ALA:HA | 2.03 | 0.40 |
| 2:i:196:MET:O | 2:i:200:ILE:HG12 | 2.21 | 0.40 |
| 2:l:278:GLY:O | 2:l:279:ASN:HB2 | 2.22 | 0.40 |
| 2:m:83:ASN:HB2 | 2:n:111:GLY:O | 2.22 | 0.40 |
| 2:m:319:LEU:HA | 2:m:319:LEU:HD12 | 1.80 | 0.40 |
| 2:n:32:ARG:H | 2:n:95:PRO:HB3 | 1.85 | 0.40 |
| 2:n:89:VAL:CG2 | 2:n:126:LEU:HD21 | 2.48 | 0.40 |
| 2:n:142:LEU:HD22 | 2:p:364:ILE:CD1 | 2.52 | 0.40 |
| 2:n:242:MET:HE3 | 2:n:242:MET:HB3 | 1.96 | 0.40 |
| 2:q:117:ARG:HA | 2:q:143:VAL:HG21 | 2.04 | 0.40 |
| 2:q:204:ILE:HG21 | 2:q:213:ALA:HB2 | 2.04 | 0.40 |
| 2:r:117:ARG:HA | 2:r:143:VAL:HG21 | 2.03 | 0.40 |
| 2:r:142:LEU:HD22 | 2:t:364:ILE:CD1 | 2.51 | 0.40 |
| 2:r:204:ILE:HG21 | 2:r:213:ALA:HB2 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:r:278:GLY:O | 2:r:279:ASN:HB2 | 2.21 | 0.40 |
| 2:w:83:ASN:ND2 | 2:x:109:SER:OG | 2.48 | 0.40 |
| 3:17:16:ILE:H | 3:17:16:ILE:HG12 | 1.83 | 0.40 |
| 3:19:64:TYR:HB2 | 3:19:96:CYS:CB | 2.51 | 0.40 |
| 3:20:64:TYR:HB2 | 3:20:96:CYS:CB | 2.51 | 0.40 |
| 1:K:156:LEU:HD12 | 1:K:160:ASN:HB2 | 2.04 | 0.40 |
| 1:M:156:LEU:HD12 | 1:M:160:ASN:HB2 | 2.04 | 0.40 |
| 1:O:30:LEU:HD21 | 1:P:206:GLU:CG | 2.51 | 0.40 |
| 1:O:156:LEU:HD12 | 1:O:160:ASN:HB2 | 2.04 | 0.40 |
| 1:P:156:LEU:HD12 | 1:P:160:ASN:HB2 | 2.04 | 0.40 |
| 1:Q:156:LEU:HD12 | 1:Q:160:ASN:HB2 | 2.03 | 0.40 |
| 1:R:156:LEU:HD12 | 1:R:160:ASN:HB2 | 2.04 | 0.40 |
| 2:c:278:GLY:O | 2:c:279:ASN:HB2 | 2.21 | 0.40 |
| 2:d:31:VAL:HG12 | 2:d:95:PRO:HG3 | 2.04 | 0.40 |
| 2:f:31:VAL:HG12 | 2:f:95:PRO:HG3 | 2.04 | 0.40 |
| 2:g:89:VAL:CG2 | 2:g:126:LEU:HD21 | 2.48 | 0.40 |
| 2:h:31:VAL:HG12 | 2:h:95:PRO:HG3 | 2.04 | 0.40 |
| 2:h:142:LEU:HD22 | 2:j:364:ILE:CD1 | 2.51 | 0.40 |
| 2:h:196:MET:O | 2:h:200:ILE:HG12 | 2.21 | 0.40 |
| 2:h:278:GLY:O | 2:h:279:ASN:HB2 | 2.21 | 0.40 |
| 2:i:31:VAL:HG12 | 2:i:95:PRO:HG3 | 2.04 | 0.40 |
| 2:i:41:LEU:HD23 | 2:i:86:ALA:HA | 2.03 | 0.40 |
| 2:j:31:VAL:HG12 | 2:j:95:PRO:HG3 | 2.04 | 0.40 |
| 2:k:93:TYR:OH | 2:k:173:ARG:O | 2.24 | 0.40 |
| 2:k:104:ASP:OD1 | 2:k:166:THR:HA | 2.21 | 0.40 |
| 2:k:196:MET:O | 2:k:200:ILE:HG12 | 2.21 | 0.40 |
| 2:l:41:LEU:HD23 | 2:l:86:ALA:HA | 2.03 | 0.40 |
| 2:m:82:LYS:HE2 | 2:m:82:LYS:HB3 | 1.96 | 0.40 |
| 2:m:204:ILE:HG21 | 2:m:213:ALA:HB2 | 2.04 | 0.40 |
| 2:n:88:MET:HE3 | 2:n:88:MET:HB3 | 1.98 | 0.40 |
| 2:n:123:MET:HE1 | 2:n:136:LEU:CD2 | 2.42 | 0.40 |
| 2:p:270:LEU:CD1 | 2:p:352:MET:HE1 | 2.39 | 0.40 |
| 2:q:278:GLY:O | 2:q:279:ASN:HB2 | 2.21 | 0.40 |
| 2:q:336:ASN:HD22 | 2:q:336:ASN:HA | 1.66 | 0.40 |
| 2:r:114:LYS:HA | 2:r:114:LYS:HD2 | 1.81 | 0.40 |
| 2:s:117:ARG:HA | 2:s:143:VAL:HG21 | 2.04 | 0.40 |
| 2:u:284:VAL:CG2 | 2:u:316:GLY:HA2 | 2.50 | 0.40 |
| 2:x:82:LYS:HE2 | 2:x:82:LYS:HB3 | 1.96 | 0.40 |
| 2:z:31:VAL:HG12 | 2:z:95:PRO:HG3 | 2.04 | 0.40 |
| 3:15:64:TYR:HB2 | 3:15:96:CYS:CB | 2.51 | 0.40 |
| 3:16:64:TYR:HB2 | 3:16:96:CYS:CB | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:21:83:SER:HA | 1:V:210:ASN:HD22 | 1.87 | 0.40 |
| 1:B:231:PRO:HG2 | 1:E:104:PHE:CZ | 2.57 | 0.40 |
| 1:C:101:LYS:O | 1:C:101:LYS:NZ | 2.55 | 0.40 |
| 1:C:231:PRO:HG2 | 1:F:104:PHE:CZ | 2.57 | 0.40 |
| 1:E:231:PRO:HG2 | 1:H:104:PHE:CZ | 2.56 | 0.40 |
| 1:I:156:LEU:HD12 | 1:I:160:ASN:HB2 | 2.04 | 0.40 |
| 1:Q:40:ILE:H | 1:Q:40:ILE:HG12 | 1.49 | 0.40 |
| 1:X:30:LEU:HD21 | 1:Y:206:GLU:CG | 2.52 | 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 | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | B | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | C | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | D | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | E | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | F | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | G | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | H | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | I | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | J | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | K | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | L | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | M | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | N | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | O | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | P | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | Q | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | R | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | S | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | T | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | U | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | V | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | W | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | X | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | Y | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 1 | Z | 209/232 (90%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 2 | a | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | b | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | c | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | d | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | e | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | f | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | g | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | h | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | i | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | j | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | k | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | l | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | m | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | n | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | o | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | p | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | q | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | r | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | s | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | t | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | u | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | v | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | w | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | x | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | y | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 2 | z | 300/365 (82%) | 287 (96%) | 13 (4%) | 0 | 100 | 100 |
| 3 | 1 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 10 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 11 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 12 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 13 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 14 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 15 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 16 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 17 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 18 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 19 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 2 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 20 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 21 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 22 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 23 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 24 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 25 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 26 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 3 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 4 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 5 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 6 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | 7 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 8 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| 3 | 9 | 82/111 (74%) | 68 (83%) | 14 (17%) | 0 | 100 | 100 |
| All | All | 15366/18408 (84%) | 14248 (93%) | 1118 (7%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | B | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | C | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | D | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | E | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | F | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | G | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | H | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | I | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | J | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | K | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | L | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | M | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | N | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | O | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | P | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | Q | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | R | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | S | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | T | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | U | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | V | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | W | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | X | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | Y | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 1 | Z | 170/186 (91%) | 165 (97%) | 5 (3%) | 37 | 51 |
| 2 | a | 251/294 (85%) | 245 (98%) | 6 (2%) | 43 | 58 |
| 2 | b | 193/294 (66%) | 188 (97%) | 5 (3%) | 40 | 55 |
| 2 | c | 251/294 (85%) | 245 (98%) | 6 (2%) | 43 | 58 |
| 2 | d | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | e | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | f | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | g | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | h | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | i | 251/294 (85%) | 245 (98%) | 6 (2%) | 43 | 58 |
| 2 | j | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | k | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | l | 251/294 (85%) | 245 (98%) | 6 (2%) | 43 | 58 |
| 2 | m | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | n | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | o | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | p | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | q | 251/294 (85%) | 245 (98%) | 6 (2%) | 43 | 58 |
| 2 | r | 251/294 (85%) | 245 (98%) | 6 (2%) | 43 | 58 |
| 2 | s | 251/294 (85%) | 245 (98%) | 6 (2%) | 43 | 58 |
| 2 | t | 251/294 (85%) | 245 (98%) | 6 (2%) | 43 | 58 |
| 2 | u | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | v | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | w | 251/294 (85%) | 245 (98%) | 6 (2%) | 43 | 58 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 2 | x | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | y | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 2 | z | 251/294 (85%) | 246 (98%) | 5 (2%) | 48 | 64 |
| 3 | 1 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 10 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 11 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 12 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 13 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 14 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 15 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 16 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 17 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 18 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 19 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 2 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 20 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 21 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 22 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 23 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 24 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 25 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 26 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 3 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 4 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 5 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 6 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 7 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 8 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| 3 | 9 | 72/95 (76%) | 70 (97%) | 2 (3%) | 38 | 52 |
| All | All | 12760/14950 (85%) | 12439 (98%) | 321 (2%) | 42 | 56 |

All (321) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 36 | THR |
| 1 | A | 40 | ILE |
| 1 | A | 99 | ASP |
| 1 | A | 101 | LYS |
| 1 | A | 125 | GLU |
| 2 | a | 20 | GLU |
| 2 | a | 79 | MET |
| 2 | a | 184 | THR |
| 2 | a | 190 | ASN |
| 2 | a | 325 | SER |
| 2 | a | 363 | GLU |
| 3 | 1 | 14 | CYS |
| 3 | 1 | 16 | ILE |
| 2 | b | 20 | GLU |
| 2 | b | 79 | MET |
| 2 | b | 190 | ASN |
| 2 | b | 325 | SER |
| 2 | b | 363 | GLU |
| 2 | c | 20 | GLU |
| 2 | c | 79 | MET |
| 2 | c | 184 | THR |
| 2 | c | 190 | ASN |
| 2 | c | 325 | SER |
| 2 | c | 363 | GLU |
| 2 | d | 20 | GLU |
| 2 | d | 79 | MET |
| 2 | d | 190 | ASN |
| 2 | d | 325 | SER |
| 2 | d | 363 | GLU |
| 2 | e | 20 | GLU |
| 2 | e | 79 | MET |
| 2 | e | 190 | ASN |
| 2 | e | 325 | SER |
| 2 | e | 363 | GLU |
| 2 | f | 20 | GLU |
| 2 | f | 79 | MET |
| 2 | f | 190 | ASN |
| 2 | f | 325 | SER |
| 2 | f | 363 | GLU |
| 2 | g | 20 | GLU |
| 2 | g | 79 | MET |
| 2 | g | 190 | ASN |
| 2 | g | 325 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | g | 363 | GLU |
| 2 | h | 20 | GLU |
| 2 | h | 79 | MET |
| 2 | h | 190 | ASN |
| 2 | h | 325 | SER |
| 2 | h | 363 | GLU |
| 2 | i | 20 | GLU |
| 2 | i | 79 | MET |
| 2 | i | 184 | THR |
| 2 | i | 190 | ASN |
| 2 | i | 325 | SER |
| 2 | i | 363 | GLU |
| 2 | j | 20 | GLU |
| 2 | j | 79 | MET |
| 2 | j | 190 | ASN |
| 2 | j | 325 | SER |
| 2 | j | 363 | GLU |
| 2 | k | 20 | GLU |
| 2 | k | 79 | MET |
| 2 | k | 190 | ASN |
| 2 | k | 325 | SER |
| 2 | k | 363 | GLU |
| 2 | l | 20 | GLU |
| 2 | l | 79 | MET |
| 2 | l | 184 | THR |
| 2 | l | 190 | ASN |
| 2 | l | 325 | SER |
| 2 | l | 363 | GLU |
| 2 | m | 20 | GLU |
| 2 | m | 79 | MET |
| 2 | m | 190 | ASN |
| 2 | m | 325 | SER |
| 2 | m | 363 | GLU |
| 2 | n | 20 | GLU |
| 2 | n | 79 | MET |
| 2 | n | 190 | ASN |
| 2 | n | 325 | SER |
| 2 | n | 363 | GLU |
| 2 | o | 20 | GLU |
| 2 | o | 79 | MET |
| 2 | o | 190 | ASN |
| 2 | o | 325 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | o | 363 | GLU |
| 2 | p | 20 | GLU |
| 2 | p | 79 | MET |
| 2 | p | 190 | ASN |
| 2 | p | 325 | SER |
| 2 | p | 363 | GLU |
| 2 | q | 20 | GLU |
| 2 | q | 79 | MET |
| 2 | q | 184 | THR |
| 2 | q | 190 | ASN |
| 2 | q | 325 | SER |
| 2 | q | 363 | GLU |
| 2 | r | 20 | GLU |
| 2 | r | 79 | MET |
| 2 | r | 184 | THR |
| 2 | r | 190 | ASN |
| 2 | r | 325 | SER |
| 2 | r | 363 | GLU |
| 2 | s | 20 | GLU |
| 2 | s | 79 | MET |
| 2 | s | 184 | THR |
| 2 | s | 190 | ASN |
| 2 | s | 325 | SER |
| 2 | s | 363 | GLU |
| 2 | t | 20 | GLU |
| 2 | t | 79 | MET |
| 2 | t | 184 | THR |
| 2 | t | 190 | ASN |
| 2 | t | 325 | SER |
| 2 | t | 363 | GLU |
| 2 | u | 20 | GLU |
| 2 | u | 79 | MET |
| 2 | u | 190 | ASN |
| 2 | u | 325 | SER |
| 2 | u | 363 | GLU |
| 2 | v | 20 | GLU |
| 2 | v | 79 | MET |
| 2 | v | 190 | ASN |
| 2 | v | 325 | SER |
| 2 | v | 363 | GLU |
| 2 | w | 20 | GLU |
| 2 | w | 79 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | w | 184 | THR |
| 2 | w | 190 | ASN |
| 2 | w | 325 | SER |
| 2 | w | 363 | GLU |
| 2 | x | 20 | GLU |
| 2 | x | 79 | MET |
| 2 | x | 190 | ASN |
| 2 | x | 325 | SER |
| 2 | x | 363 | GLU |
| 2 | y | 20 | GLU |
| 2 | y | 79 | MET |
| 2 | y | 190 | ASN |
| 2 | y | 325 | SER |
| 2 | y | 363 | GLU |
| 2 | z | 20 | GLU |
| 2 | z | 79 | MET |
| 2 | z | 190 | ASN |
| 2 | z | 325 | SER |
| 2 | z | 363 | GLU |
| 3 | 2 | 14 | CYS |
| 3 | 2 | 16 | ILE |
| 3 | 3 | 14 | CYS |
| 3 | 3 | 16 | ILE |
| 3 | 4 | 14 | CYS |
| 3 | 4 | 16 | ILE |
| 3 | 5 | 14 | CYS |
| 3 | 5 | 16 | ILE |
| 3 | 6 | 14 | CYS |
| 3 | 6 | 16 | ILE |
| 3 | 7 | 14 | CYS |
| 3 | 7 | 16 | ILE |
| 3 | 8 | 14 | CYS |
| 3 | 8 | 16 | ILE |
| 3 | 9 | 14 | CYS |
| 3 | 9 | 16 | ILE |
| 3 | 10 | 14 | CYS |
| 3 | 10 | 16 | ILE |
| 3 | 11 | 14 | CYS |
| 3 | 11 | 16 | ILE |
| 3 | 12 | 14 | CYS |
| 3 | 12 | 16 | ILE |
| 3 | 13 | 14 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 13 | 16 | ILE |
| 3 | 14 | 14 | CYS |
| 3 | 14 | 16 | ILE |
| 3 | 15 | 14 | CYS |
| 3 | 15 | 16 | ILE |
| 3 | 16 | 14 | CYS |
| 3 | 16 | 16 | ILE |
| 3 | 17 | 14 | CYS |
| 3 | 17 | 16 | ILE |
| 3 | 18 | 14 | CYS |
| 3 | 18 | 16 | ILE |
| 3 | 19 | 14 | CYS |
| 3 | 19 | 16 | ILE |
| 3 | 20 | 14 | CYS |
| 3 | 20 | 16 | ILE |
| 3 | 21 | 14 | CYS |
| 3 | 21 | 16 | ILE |
| 3 | 22 | 14 | CYS |
| 3 | 22 | 16 | ILE |
| 3 | 23 | 14 | CYS |
| 3 | 23 | 16 | ILE |
| 3 | 24 | 14 | CYS |
| 3 | 24 | 16 | ILE |
| 3 | 25 | 14 | CYS |
| 3 | 25 | 16 | ILE |
| 3 | 26 | 14 | CYS |
| 3 | 26 | 16 | ILE |
| 1 | B | 36 | THR |
| 1 | B | 40 | ILE |
| 1 | B | 99 | ASP |
| 1 | B | 101 | LYS |
| 1 | B | 125 | GLU |
| 1 | C | 36 | THR |
| 1 | C | 40 | ILE |
| 1 | C | 99 | ASP |
| 1 | C | 101 | LYS |
| 1 | C | 125 | GLU |
| 1 | D | 36 | THR |
| 1 | D | 40 | ILE |
| 1 | D | 99 | ASP |
| 1 | D | 101 | LYS |
| 1 | D | 125 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 36 | THR |
| 1 | E | 40 | ILE |
| 1 | E | 99 | ASP |
| 1 | E | 101 | LYS |
| 1 | E | 125 | GLU |
| 1 | F | 36 | THR |
| 1 | F | 40 | ILE |
| 1 | F | 99 | ASP |
| 1 | F | 101 | LYS |
| 1 | F | 125 | GLU |
| 1 | G | 36 | THR |
| 1 | G | 40 | ILE |
| 1 | G | 99 | ASP |
| 1 | G | 101 | LYS |
| 1 | G | 125 | GLU |
| 1 | H | 36 | THR |
| 1 | H | 40 | ILE |
| 1 | H | 99 | ASP |
| 1 | H | 101 | LYS |
| 1 | H | 125 | GLU |
| 1 | I | 36 | THR |
| 1 | I | 40 | ILE |
| 1 | I | 99 | ASP |
| 1 | I | 101 | LYS |
| 1 | I | 125 | GLU |
| 1 | J | 36 | THR |
| 1 | J | 40 | ILE |
| 1 | J | 99 | ASP |
| 1 | J | 101 | LYS |
| 1 | J | 125 | GLU |
| 1 | K | 36 | THR |
| 1 | K | 40 | ILE |
| 1 | K | 99 | ASP |
| 1 | K | 101 | LYS |
| 1 | K | 125 | GLU |
| 1 | L | 36 | THR |
| 1 | L | 40 | ILE |
| 1 | L | 99 | ASP |
| 1 | L | 101 | LYS |
| 1 | L | 125 | GLU |
| 1 | M | 36 | THR |
| 1 | M | 40 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 99 | ASP |
| 1 | M | 101 | LYS |
| 1 | M | 125 | GLU |
| 1 | N | 36 | THR |
| 1 | N | 40 | ILE |
| 1 | N | 99 | ASP |
| 1 | N | 101 | LYS |
| 1 | N | 125 | GLU |
| 1 | O | 36 | THR |
| 1 | O | 40 | ILE |
| 1 | O | 99 | ASP |
| 1 | O | 101 | LYS |
| 1 | O | 125 | GLU |
| 1 | P | 36 | THR |
| 1 | P | 40 | ILE |
| 1 | P | 99 | ASP |
| 1 | P | 101 | LYS |
| 1 | P | 125 | GLU |
| 1 | Q | 36 | THR |
| 1 | Q | 40 | ILE |
| 1 | Q | 99 | ASP |
| 1 | Q | 101 | LYS |
| 1 | Q | 125 | GLU |
| 1 | R | 36 | THR |
| 1 | R | 40 | ILE |
| 1 | R | 99 | ASP |
| 1 | R | 101 | LYS |
| 1 | R | 125 | GLU |
| 1 | S | 36 | THR |
| 1 | S | 40 | ILE |
| 1 | S | 99 | ASP |
| 1 | S | 101 | LYS |
| 1 | S | 125 | GLU |
| 1 | T | 36 | THR |
| 1 | T | 40 | ILE |
| 1 | T | 99 | ASP |
| 1 | T | 101 | LYS |
| 1 | T | 125 | GLU |
| 1 | U | 36 | THR |
| 1 | U | 40 | ILE |
| 1 | U | 99 | ASP |
| 1 | U | 101 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | U | 125 | GLU |
| 1 | V | 36 | THR |
| 1 | V | 40 | ILE |
| 1 | V | 99 | ASP |
| 1 | V | 101 | LYS |
| 1 | V | 125 | GLU |
| 1 | W | 36 | THR |
| 1 | W | 40 | ILE |
| 1 | W | 99 | ASP |
| 1 | W | 101 | LYS |
| 1 | W | 125 | GLU |
| 1 | X | 36 | THR |
| 1 | X | 40 | ILE |
| 1 | X | 99 | ASP |
| 1 | X | 101 | LYS |
| 1 | X | 125 | GLU |
| 1 | Y | 36 | THR |
| 1 | Y | 40 | ILE |
| 1 | Y | 99 | ASP |
| 1 | Y | 101 | LYS |
| 1 | Y | 125 | GLU |
| 1 | Z | 36 | THR |
| 1 | Z | 40 | ILE |
| 1 | Z | 99 | ASP |
| 1 | Z | 101 | LYS |
| 1 | Z | 125 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (232) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 210 | ASN |
| 1 | A | 223 | GLN |
| 2 | a | 78 | ASN |
| 2 | a | 99 | GLN |
| 2 | a | 159 | GLN |
| 2 | a | 161 | ASN |
| 2 | a | 183 | ASN |
| 2 | a | 198 | GLN |
| 2 | a | 350 | GLN |
| 2 | b | 78 | ASN |
| 2 | b | 99 | GLN |
| 2 | b | 159 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | b | 161 | ASN |
| 2 | b | 183 | ASN |
| 2 | b | 198 | GLN |
| 2 | c | 78 | ASN |
| 2 | c | 99 | GLN |
| 2 | c | 159 | GLN |
| 2 | c | 161 | ASN |
| 2 | c | 183 | ASN |
| 2 | c | 198 | GLN |
| 2 | c | 350 | GLN |
| 2 | d | 78 | ASN |
| 2 | d | 99 | GLN |
| 2 | d | 159 | GLN |
| 2 | d | 161 | ASN |
| 2 | d | 183 | ASN |
| 2 | d | 198 | GLN |
| 2 | d | 350 | GLN |
| 2 | e | 78 | ASN |
| 2 | e | 99 | GLN |
| 2 | e | 159 | GLN |
| 2 | e | 161 | ASN |
| 2 | e | 183 | ASN |
| 2 | e | 198 | GLN |
| 2 | e | 350 | GLN |
| 2 | f | 78 | ASN |
| 2 | f | 99 | GLN |
| 2 | f | 159 | GLN |
| 2 | f | 161 | ASN |
| 2 | f | 183 | ASN |
| 2 | f | 198 | GLN |
| 2 | f | 350 | GLN |
| 2 | g | 78 | ASN |
| 2 | g | 99 | GLN |
| 2 | g | 159 | GLN |
| 2 | g | 161 | ASN |
| 2 | g | 183 | ASN |
| 2 | g | 198 | GLN |
| 2 | g | 350 | GLN |
| 2 | h | 78 | ASN |
| 2 | h | 99 | GLN |
| 2 | h | 159 | GLN |
| 2 | h | 161 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | h | 183 | ASN |
| 2 | h | 198 | GLN |
| 2 | h | 350 | GLN |
| 2 | i | 78 | ASN |
| 2 | i | 99 | GLN |
| 2 | i | 159 | GLN |
| 2 | i | 161 | ASN |
| 2 | i | 183 | ASN |
| 2 | i | 198 | GLN |
| 2 | i | 350 | GLN |
| 2 | j | 78 | ASN |
| 2 | j | 99 | GLN |
| 2 | j | 159 | GLN |
| 2 | j | 161 | ASN |
| 2 | j | 183 | ASN |
| 2 | j | 198 | GLN |
| 2 | j | 350 | GLN |
| 2 | k | 78 | ASN |
| 2 | k | 159 | GLN |
| 2 | k | 161 | ASN |
| 2 | k | 183 | ASN |
| 2 | k | 198 | GLN |
| 2 | k | 350 | GLN |
| 2 | l | 78 | ASN |
| 2 | l | 99 | GLN |
| 2 | l | 159 | GLN |
| 2 | l | 161 | ASN |
| 2 | l | 183 | ASN |
| 2 | l | 198 | GLN |
| 2 | l | 350 | GLN |
| 2 | m | 78 | ASN |
| 2 | m | 99 | GLN |
| 2 | m | 159 | GLN |
| 2 | m | 161 | ASN |
| 2 | m | 183 | ASN |
| 2 | m | 198 | GLN |
| 2 | m | 350 | GLN |
| 2 | n | 78 | ASN |
| 2 | n | 99 | GLN |
| 2 | n | 159 | GLN |
| 2 | n | 161 | ASN |
| 2 | n | 183 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | n | 198 | GLN |
| 2 | n | 350 | GLN |
| 2 | o | 78 | ASN |
| 2 | o | 99 | GLN |
| 2 | o | 159 | GLN |
| 2 | o | 161 | ASN |
| 2 | o | 183 | ASN |
| 2 | o | 198 | GLN |
| 2 | o | 350 | GLN |
| 2 | p | 78 | ASN |
| 2 | p | 99 | GLN |
| 2 | p | 159 | GLN |
| 2 | p | 161 | ASN |
| 2 | p | 183 | ASN |
| 2 | p | 198 | GLN |
| 2 | p | 350 | GLN |
| 2 | q | 78 | ASN |
| 2 | q | 99 | GLN |
| 2 | q | 159 | GLN |
| 2 | q | 161 | ASN |
| 2 | q | 183 | ASN |
| 2 | q | 198 | GLN |
| 2 | q | 350 | GLN |
| 2 | r | 78 | ASN |
| 2 | r | 99 | GLN |
| 2 | r | 159 | GLN |
| 2 | r | 161 | ASN |
| 2 | r | 183 | ASN |
| 2 | r | 198 | GLN |
| 2 | r | 350 | GLN |
| 2 | s | 78 | ASN |
| 2 | s | 99 | GLN |
| 2 | s | 159 | GLN |
| 2 | s | 161 | ASN |
| 2 | s | 183 | ASN |
| 2 | s | 198 | GLN |
| 2 | s | 350 | GLN |
| 2 | t | 78 | ASN |
| 2 | t | 99 | GLN |
| 2 | t | 159 | GLN |
| 2 | t | 161 | ASN |
| 2 | t | 183 | ASN |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | t | 198 | GLN |
| 2 | t | 350 | GLN |
| 2 | u | 78 | ASN |
| 2 | u | 99 | GLN |
| 2 | u | 159 | GLN |
| 2 | u | 161 | ASN |
| 2 | u | 183 | ASN |
| 2 | u | 198 | GLN |
| 2 | u | 350 | GLN |
| 2 | v | 78 | ASN |
| 2 | v | 99 | GLN |
| 2 | v | 159 | GLN |
| 2 | v | 161 | ASN |
| 2 | v | 183 | ASN |
| 2 | v | 198 | GLN |
| 2 | w | 78 | ASN |
| 2 | w | 159 | GLN |
| 2 | w | 161 | ASN |
| 2 | w | 183 | ASN |
| 2 | w | 198 | GLN |
| 2 | x | 78 | ASN |
| 2 | x | 159 | GLN |
| 2 | x | 161 | ASN |
| 2 | x | 183 | ASN |
| 2 | x | 198 | GLN |
| 2 | x | 199 | GLN |
| 2 | x | 350 | GLN |
| 2 | y | 78 | ASN |
| 2 | y | 159 | GLN |
| 2 | y | 161 | ASN |
| 2 | y | 183 | ASN |
| 2 | y | 198 | GLN |
| 2 | y | 350 | GLN |
| 2 | z | 78 | ASN |
| 2 | z | 99 | GLN |
| 2 | z | 161 | ASN |
| 2 | z | 183 | ASN |
| 2 | z | 198 | GLN |
| 1 | B | 210 | ASN |
| 1 | B | 223 | GLN |
| 1 | C | 210 | ASN |
| 1 | C | 223 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 210 | ASN |
| 1 | D | 223 | GLN |
| 1 | E | 210 | ASN |
| 1 | E | 223 | GLN |
| 1 | F | 210 | ASN |
| 1 | F | 223 | GLN |
| 1 | G | 210 | ASN |
| 1 | G | 223 | GLN |
| 1 | H | 210 | ASN |
| 1 | H | 223 | GLN |
| 1 | I | 210 | ASN |
| 1 | I | 218 | ASN |
| 1 | I | 223 | GLN |
| 1 | J | 210 | ASN |
| 1 | J | 223 | GLN |
| 1 | K | 210 | ASN |
| 1 | K | 223 | GLN |
| 1 | L | 210 | ASN |
| 1 | L | 218 | ASN |
| 1 | L | 223 | GLN |
| 1 | M | 210 | ASN |
| 1 | M | 223 | GLN |
| 1 | N | 210 | ASN |
| 1 | N | 223 | GLN |
| 1 | O | 210 | ASN |
| 1 | O | 223 | GLN |
| 1 | P | 210 | ASN |
| 1 | P | 223 | GLN |
| 1 | Q | 210 | ASN |
| 1 | Q | 223 | GLN |
| 1 | R | 210 | ASN |
| 1 | R | 223 | GLN |
| 1 | S | 210 | ASN |
| 1 | S | 223 | GLN |
| 1 | T | 210 | ASN |
| 1 | T | 223 | GLN |
| 1 | U | 210 | ASN |
| 1 | U | 218 | ASN |
| 1 | U | 223 | GLN |
| 1 | V | 210 | ASN |
| 1 | V | 218 | ASN |
| 1 | V | 223 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | W | 210 | ASN |
| 1 | W | 223 | GLN |
| 1 | X | 210 | ASN |
| 1 | X | 218 | ASN |
| 1 | X | 223 | GLN |
| 1 | Y | 210 | ASN |
| 1 | Y | 223 | GLN |
| 1 | Z | 210 | ASN |
| 1 | Z | 218 | ASN |
| 1 | Z | 223 | GLN |

#### 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

52 ligands are modelled in this entry.

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 | $\#\|Z\| > 2$ |
| 5 | TQN | G | 301 | - | 140,141,141 | 1.71 | 28 (20%) | 162,169,169 | 1.38 | 14 (8%) |
| 4 | TLW | F | 302 | - | 15,15,15 | 1.10 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 5 | TQN | U | 301 | - | 140,141,141 | 1.70 | 27 (19%) | 162,169,169 | 1.38 | 14 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 5 | TQN | H | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 13 (8%) |
| 4 | TLW | R | 302 | - | 15,15,15 | 1.08 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 4 | TLW | K | 302 | - | 15,15,15 | 1.09 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 4 | TLW | I | 302 | - | 15,15,15 | 1.10 | 1 (6%) | 17,21,21 | 2.26 | 3 (17%) |
| 5 | TQN | W | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 13 (8%) |
| 5 | TQN | O | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 14 (8%) |
| 5 | TQN | L | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 14 (8%) |
| 4 | TLW | P | 302 | - | 15,15,15 | 1.09 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 5 | TQN | D | 301 | - | 140,141,141 | 1.71 | 27 (19%) | 162,169,169 | 1.38 | 14 (8%) |
| 5 | TQN | F | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 13 (8%) |
| 4 | TLW | M | 302 | - | 15,15,15 | 1.08 | 0 | 17,21,21 | 2.25 | 3 (17%) |
| 4 | TLW | Q | 302 | - | 15,15,15 | 1.09 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 4 | TLW | G | 302 | - | 15,15,15 | 1.09 | 0 | 17,21,21 | 2.26 | 3 (17%) |
| 4 | TLW | Y | 302 | - | 15,15,15 | 1.09 | 0 | 17,21,21 | 2.25 | 3 (17%) |
| 4 | TLW | U | 302 | - | 15,15,15 | 1.09 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 4 | TLW | E | 302 | - | 15,15,15 | 1.08 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 5 | TQN | I | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.39 | 14 (8%) |
| 4 | TLW | S | 302 | - | 15,15,15 | 1.09 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 4 | TLW | J | 302 | - | 15,15,15 | 1.09 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 5 | TQN | M | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 15 (9%) |
| 4 | TLW | A | 301 | - | 15,15,15 | 1.09 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 5 | TQN | Q | 301 | - | 140,141,141 | 1.70 | 27 (19%) | 162,169,169 | 1.38 | 14 (8%) |
| 4 | TLW | T | 302 | - | 15,15,15 | 1.08 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 5 | TQN | N | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 14 (8%) |
| 5 | TQN | Y | 301 | - | 140,141,141 | 1.70 | 27 (19%) | 162,169,169 | 1.38 | 13 (8%) |
| 4 | TLW | V | 302 | - | 15,15,15 | 1.09 | 0 | 17,21,21 | 2.25 | 3 (17%) |
| 5 | TQN | Z | 301 | - | 140,141,141 | 1.70 | 27 (19%) | 162,169,169 | 1.38 | 14 (8%) |
| 4 | TLW | D | 302 | - | 15,15,15 | 1.08 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 4 | TLW | C | 302 | - | 15,15,15 | 1.08 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 5 | TQN | E | 301 | - | 140,141,141 | 1.70 | 27 (19%) | 162,169,169 | 1.38 | 13 (8%) |
| 5 | TQN | S | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 13 (8%) |
| 4 | TLW | B | 302 | - | 15,15,15 | 1.08 | 0 | 17,21,21 | 2.26 | 3 (17%) |
| 5 | TQN | A | 302 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 13 (8%) |
| 4 | TLW | A | 303 | - | 15,15,15 | 1.10 | 1 (6%) | 17,21,21 | 2.26 | 3 (17%) |
| 4 | TLW | X | 302 | - | 15,15,15 | 1.08 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 5 | TQN | K | 301 | - | 140,141,141 | 1.70 | 27 (19%) | 162,169,169 | 1.38 | 14 (8%) |
| 5 | TQN | T | 301 | - | 140,141,141 | 1.70 | 27 (19%) | 162,169,169 | 1.38 | 13 (8%) |
| 5 | TQN | B | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 14 (8%) |
| 5 | TQN | V | 301 | - | 140,141,141 | 1.71 | 28 (20%) | 162,169,169 | 1.38 | 14 (8%) |
| 5 | TQN | R | 301 | - | 140,141,141 | 1.70 | 27 (19%) | 162,169,169 | 1.38 | 14 (8%) |
| 5 | TQN | C | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 14 (8%) |
| 5 | TQN | X | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 13 (8%) |
| 5 | TQN | J | 301 | - | 140,141,141 | 1.71 | 28 (20%) | 162,169,169 | 1.38 | 13 (8%) |
| 4 | TLW | H | 302 | - | 15,15,15 | 1.08 | 1 (6%) | 17,21,21 | 2.26 | 3 (17%) |
| 4 | TLW | N | 302 | - | 15,15,15 | 1.08 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 4 | TLW | W | 302 | - | 15,15,15 | 1.08 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 4 | TLW | O | 302 | - | 15,15,15 | 1.09 | 1 (6%) | 17,21,21 | 2.25 | 3 (17%) |
| 5 | TQN | P | 301 | - | 140,141,141 | 1.70 | 28 (20%) | 162,169,169 | 1.38 | 14 (8%) |
| 4 | TLW | L | 302 | - | 15,15,15 | 1.09 | 0 | 17,21,21 | 2.25 | 3 (17%) |

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 |
|---|---|---|---|---|---|---|---|
| 5 | TQN | G | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | F | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | U | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | H | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | R | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | K | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | I | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | W | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | O | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | L | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | P | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | D | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | F | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | M | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | Q | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 4 | TLW | G | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | Y | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | U | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | E | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | I | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | S | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | J | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | M | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | A | 301 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | Q | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | T | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | N | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | Y | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | V | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | Z | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | D | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | C | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | E | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | S | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | B | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | A | 302 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | A | 303 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | X | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | K | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | T | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | B | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | V | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | R | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | C | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | X | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 5 | TQN | J | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | H | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | N | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 4 | TLW | W | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 4 | TLW | O | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |
| 5 | TQN | P | 301 | - | - | 53/143/184/184 | 0/2/2/2 |
| 4 | TLW | L | 302 | - | 1/1/6/6 | 5/10/26/26 | 0/1/1/1 |

All (739) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | G | 301 | TQN | C51-NB2 | 7.96 | 1.50 | 1.34 |
| 5 | M | 301 | TQN | C51-NB2 | 7.96 | 1.50 | 1.34 |
| 5 | O | 301 | TQN | C51-NB2 | 7.96 | 1.50 | 1.34 |
| 5 | R | 301 | TQN | C51-NB2 | 7.95 | 1.50 | 1.34 |
| 5 | J | 301 | TQN | C51-NB2 | 7.95 | 1.50 | 1.34 |
| 5 | H | 301 | TQN | C51-NB2 | 7.95 | 1.50 | 1.34 |
| 5 | C | 301 | TQN | C51-NB2 | 7.94 | 1.50 | 1.34 |
| 5 | L | 301 | TQN | C51-NB2 | 7.94 | 1.50 | 1.34 |
| 5 | U | 301 | TQN | C51-NB2 | 7.94 | 1.50 | 1.34 |
| 5 | Y | 301 | TQN | C51-NB2 | 7.94 | 1.50 | 1.34 |
| 5 | A | 302 | TQN | C51-NB2 | 7.94 | 1.50 | 1.34 |
| 5 | D | 301 | TQN | C51-NB2 | 7.94 | 1.50 | 1.34 |
| 5 | Q | 301 | TQN | C51-NB2 | 7.94 | 1.50 | 1.34 |
| 5 | F | 301 | TQN | C51-NB2 | 7.93 | 1.50 | 1.34 |
| 5 | S | 301 | TQN | C51-NB2 | 7.93 | 1.50 | 1.34 |
| 5 | X | 301 | TQN | C51-NB2 | 7.93 | 1.50 | 1.34 |
| 5 | P | 301 | TQN | C51-NB2 | 7.92 | 1.50 | 1.34 |
| 5 | W | 301 | TQN | C51-NB2 | 7.92 | 1.50 | 1.34 |
| 5 | I | 301 | TQN | C51-NB2 | 7.92 | 1.50 | 1.34 |
| 5 | V | 301 | TQN | C51-NB2 | 7.92 | 1.50 | 1.34 |
| 5 | Z | 301 | TQN | C51-NB2 | 7.91 | 1.50 | 1.34 |
| 5 | T | 301 | TQN | C51-NB2 | 7.91 | 1.50 | 1.34 |
| 5 | E | 301 | TQN | C51-NB2 | 7.91 | 1.50 | 1.34 |
| 5 | B | 301 | TQN | C51-NB2 | 7.91 | 1.50 | 1.34 |
| 5 | K | 301 | TQN | C51-NB2 | 7.90 | 1.50 | 1.34 |
| 5 | N | 301 | TQN | C51-NB2 | 7.90 | 1.50 | 1.34 |
| 5 | T | 301 | TQN | C11-NA2 | 7.78 | 1.50 | 1.34 |
| 5 | J | 301 | TQN | C11-NA2 | 7.76 | 1.50 | 1.34 |
| 5 | P | 301 | TQN | C11-NA2 | 7.76 | 1.50 | 1.34 |
| 5 | G | 301 | TQN | C11-NA2 | 7.76 | 1.50 | 1.34 |
| 5 | O | 301 | TQN | C11-NA2 | 7.76 | 1.50 | 1.34 |
| 5 | Q | 301 | TQN | C11-NA2 | 7.76 | 1.50 | 1.34 |
| 5 | I | 301 | TQN | C11-NA2 | 7.75 | 1.50 | 1.34 |
| 5 | U | 301 | TQN | C11-NA2 | 7.75 | 1.50 | 1.34 |
| 5 | Z | 301 | TQN | C11-NA2 | 7.75 | 1.50 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | R | 301 | TQN | C11-NA2 | 7.74 | 1.50 | 1.34 |
| 5 | A | 302 | TQN | C11-NA2 | 7.74 | 1.50 | 1.34 |
| 5 | K | 301 | TQN | C11-NA2 | 7.74 | 1.50 | 1.34 |
| 5 | C | 301 | TQN | C11-NA2 | 7.74 | 1.50 | 1.34 |
| 5 | V | 301 | TQN | C11-NA2 | 7.74 | 1.50 | 1.34 |
| 5 | N | 301 | TQN | C11-NA2 | 7.73 | 1.50 | 1.34 |
| 5 | B | 301 | TQN | C11-NA2 | 7.73 | 1.50 | 1.34 |
| 5 | H | 301 | TQN | C11-NA2 | 7.73 | 1.50 | 1.34 |
| 5 | D | 301 | TQN | C11-NA2 | 7.73 | 1.50 | 1.34 |
| 5 | X | 301 | TQN | C11-NA2 | 7.73 | 1.50 | 1.34 |
| 5 | Y | 301 | TQN | C11-NA2 | 7.72 | 1.50 | 1.34 |
| 5 | W | 301 | TQN | C11-NA2 | 7.72 | 1.50 | 1.34 |
| 5 | M | 301 | TQN | C11-NA2 | 7.72 | 1.50 | 1.34 |
| 5 | F | 301 | TQN | C11-NA2 | 7.72 | 1.50 | 1.34 |
| 5 | S | 301 | TQN | C11-NA2 | 7.72 | 1.50 | 1.34 |
| 5 | L | 301 | TQN | C11-NA2 | 7.71 | 1.50 | 1.34 |
| 5 | E | 301 | TQN | C11-NA2 | 7.69 | 1.50 | 1.34 |
| 5 | O | 301 | TQN | OB6-CB6 | -5.56 | 1.19 | 1.42 |
| 5 | J | 301 | TQN | OB6-CB6 | -5.56 | 1.19 | 1.42 |
| 5 | B | 301 | TQN | OB6-CB6 | -5.56 | 1.19 | 1.42 |
| 5 | C | 301 | TQN | OB6-CB6 | -5.56 | 1.19 | 1.42 |
| 5 | V | 301 | TQN | OB6-CB6 | -5.56 | 1.19 | 1.42 |
| 5 | G | 301 | TQN | OB6-CB6 | -5.56 | 1.19 | 1.42 |
| 5 | D | 301 | TQN | OB6-CB6 | -5.55 | 1.19 | 1.42 |
| 5 | W | 301 | TQN | OB6-CB6 | -5.55 | 1.19 | 1.42 |
| 5 | X | 301 | TQN | OB6-CB6 | -5.55 | 1.19 | 1.42 |
| 5 | E | 301 | TQN | OB6-CB6 | -5.55 | 1.19 | 1.42 |
| 5 | K | 301 | TQN | OB6-CB6 | -5.55 | 1.19 | 1.42 |
| 5 | F | 301 | TQN | OB6-CB6 | -5.54 | 1.19 | 1.42 |
| 5 | P | 301 | TQN | OB6-CB6 | -5.54 | 1.19 | 1.42 |
| 5 | Y | 301 | TQN | OB6-CB6 | -5.54 | 1.19 | 1.42 |
| 5 | S | 301 | TQN | OB6-CB6 | -5.54 | 1.19 | 1.42 |
| 5 | A | 302 | TQN | OB6-CB6 | -5.54 | 1.19 | 1.42 |
| 5 | N | 301 | TQN | OB6-CB6 | -5.54 | 1.19 | 1.42 |
| 5 | T | 301 | TQN | OB6-CB6 | -5.54 | 1.19 | 1.42 |
| 5 | Q | 301 | TQN | OB6-CB6 | -5.54 | 1.19 | 1.42 |
| 5 | H | 301 | TQN | OB6-CB6 | -5.54 | 1.19 | 1.42 |
| 5 | U | 301 | TQN | OB6-CB6 | -5.54 | 1.19 | 1.42 |
| 5 | L | 301 | TQN | OB6-CB6 | -5.53 | 1.19 | 1.42 |
| 5 | R | 301 | TQN | OB6-CB6 | -5.53 | 1.19 | 1.42 |
| 5 | M | 301 | TQN | OB6-CB6 | -5.53 | 1.19 | 1.42 |
| 5 | I | 301 | TQN | OB6-CB6 | -5.53 | 1.19 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | Z | 301 | TQN | OB6-CB6 | -5.53 | 1.19 | 1.42 |
| 5 | L | 301 | TQN | CA2-NA2 | 4.11 | 1.52 | 1.45 |
| 5 | M | 301 | TQN | CA2-NA2 | 4.09 | 1.52 | 1.45 |
| 5 | W | 301 | TQN | CA2-NA2 | 4.09 | 1.52 | 1.45 |
| 5 | U | 301 | TQN | CA2-NA2 | 4.09 | 1.52 | 1.45 |
| 5 | E | 301 | TQN | CA2-NA2 | 4.09 | 1.52 | 1.45 |
| 5 | N | 301 | TQN | CA2-NA2 | 4.08 | 1.52 | 1.45 |
| 5 | V | 301 | TQN | CA2-NA2 | 4.07 | 1.52 | 1.45 |
| 5 | G | 301 | TQN | CA2-NA2 | 4.06 | 1.52 | 1.45 |
| 5 | T | 301 | TQN | CA2-NA2 | 4.06 | 1.52 | 1.45 |
| 5 | Y | 301 | TQN | CA2-NA2 | 4.06 | 1.52 | 1.45 |
| 5 | B | 301 | TQN | CA2-NA2 | 4.05 | 1.52 | 1.45 |
| 5 | J | 301 | TQN | CA2-NA2 | 4.05 | 1.52 | 1.45 |
| 5 | D | 301 | TQN | CA2-NA2 | 4.05 | 1.52 | 1.45 |
| 5 | H | 301 | TQN | CA2-NA2 | 4.05 | 1.52 | 1.45 |
| 5 | R | 301 | TQN | CA2-NA2 | 4.05 | 1.52 | 1.45 |
| 5 | A | 302 | TQN | CA2-NA2 | 4.04 | 1.52 | 1.45 |
| 5 | Z | 301 | TQN | CA2-NA2 | 4.04 | 1.52 | 1.45 |
| 5 | X | 301 | TQN | CA2-NA2 | 4.04 | 1.52 | 1.45 |
| 5 | Q | 301 | TQN | CA2-NA2 | 4.04 | 1.52 | 1.45 |
| 5 | K | 301 | TQN | CA2-NA2 | 4.04 | 1.52 | 1.45 |
| 5 | F | 301 | TQN | CA2-NA2 | 4.03 | 1.52 | 1.45 |
| 5 | S | 301 | TQN | CA2-NA2 | 4.03 | 1.52 | 1.45 |
| 5 | P | 301 | TQN | CA2-NA2 | 4.03 | 1.52 | 1.45 |
| 5 | O | 301 | TQN | CA2-NA2 | 4.02 | 1.52 | 1.45 |
| 5 | I | 301 | TQN | CA2-NA2 | 4.01 | 1.52 | 1.45 |
| 5 | C | 301 | TQN | CA2-NA2 | 3.99 | 1.52 | 1.45 |
| 5 | F | 301 | TQN | OB3-C71 | 3.77 | 1.44 | 1.34 |
| 5 | P | 301 | TQN | OB3-C71 | 3.75 | 1.44 | 1.34 |
| 5 | X | 301 | TQN | OB3-C71 | 3.75 | 1.44 | 1.34 |
| 5 | V | 301 | TQN | OB3-C71 | 3.74 | 1.44 | 1.34 |
| 5 | E | 301 | TQN | OB3-C71 | 3.74 | 1.44 | 1.34 |
| 5 | Z | 301 | TQN | OB3-C71 | 3.74 | 1.44 | 1.34 |
| 5 | J | 301 | TQN | OB3-C71 | 3.74 | 1.44 | 1.34 |
| 5 | G | 301 | TQN | OB3-C71 | 3.73 | 1.44 | 1.34 |
| 5 | L | 301 | TQN | OB3-C71 | 3.73 | 1.44 | 1.34 |
| 5 | Y | 301 | TQN | OB3-C71 | 3.73 | 1.44 | 1.34 |
| 5 | D | 301 | TQN | OB3-C71 | 3.73 | 1.44 | 1.34 |
| 5 | Q | 301 | TQN | OB3-C71 | 3.73 | 1.44 | 1.34 |
| 5 | I | 301 | TQN | OB3-C71 | 3.73 | 1.44 | 1.34 |
| 5 | W | 301 | TQN | OB3-C71 | 3.73 | 1.44 | 1.34 |
| 5 | B | 301 | TQN | OB3-C71 | 3.73 | 1.44 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | O | 301 | TQN | OB3-C71 | 3.73 | 1.44 | 1.34 |
| 5 | A | 302 | TQN | OB3-C71 | 3.72 | 1.44 | 1.34 |
| 5 | N | 301 | TQN | OB3-C71 | 3.72 | 1.44 | 1.34 |
| 5 | C | 301 | TQN | OB3-C71 | 3.72 | 1.44 | 1.34 |
| 5 | K | 301 | TQN | OB3-C71 | 3.72 | 1.44 | 1.34 |
| 5 | M | 301 | TQN | OB3-C71 | 3.72 | 1.44 | 1.34 |
| 5 | S | 301 | TQN | OB3-C71 | 3.72 | 1.44 | 1.34 |
| 5 | R | 301 | TQN | OB3-C71 | 3.72 | 1.44 | 1.34 |
| 5 | T | 301 | TQN | OB3-C71 | 3.71 | 1.44 | 1.34 |
| 5 | H | 301 | TQN | OB3-C71 | 3.71 | 1.44 | 1.34 |
| 5 | U | 301 | TQN | OB3-C71 | 3.71 | 1.44 | 1.34 |
| 5 | E | 301 | TQN | C12-C11 | 3.51 | 1.59 | 1.51 |
| 5 | J | 301 | TQN | C12-C11 | 3.51 | 1.59 | 1.51 |
| 5 | V | 301 | TQN | C12-C11 | 3.50 | 1.59 | 1.51 |
| 5 | M | 301 | TQN | C12-C11 | 3.49 | 1.59 | 1.51 |
| 5 | C | 301 | TQN | C12-C11 | 3.49 | 1.59 | 1.51 |
| 5 | G | 301 | TQN | C12-C11 | 3.48 | 1.59 | 1.51 |
| 5 | N | 301 | TQN | C12-C11 | 3.48 | 1.59 | 1.51 |
| 5 | Z | 301 | TQN | C12-C11 | 3.48 | 1.59 | 1.51 |
| 5 | V | 301 | TQN | CA1-CA2 | -3.48 | 1.47 | 1.53 |
| 5 | A | 302 | TQN | C12-C11 | 3.48 | 1.59 | 1.51 |
| 5 | G | 301 | TQN | CA1-CA2 | -3.48 | 1.47 | 1.53 |
| 5 | Y | 301 | TQN | C12-C11 | 3.48 | 1.59 | 1.51 |
| 5 | N | 301 | TQN | O53-C61 | 3.48 | 1.44 | 1.34 |
| 5 | M | 301 | TQN | CA1-CA2 | -3.48 | 1.47 | 1.53 |
| 5 | Z | 301 | TQN | CA1-CA2 | -3.48 | 1.47 | 1.53 |
| 5 | A | 302 | TQN | CA1-CA2 | -3.48 | 1.47 | 1.53 |
| 5 | E | 301 | TQN | CA1-CA2 | -3.48 | 1.47 | 1.53 |
| 5 | S | 301 | TQN | C12-C11 | 3.48 | 1.59 | 1.51 |
| 5 | F | 301 | TQN | O53-C61 | 3.48 | 1.44 | 1.34 |
| 5 | C | 301 | TQN | O53-C61 | 3.48 | 1.44 | 1.34 |
| 5 | Q | 301 | TQN | CA1-CA2 | -3.48 | 1.47 | 1.53 |
| 5 | P | 301 | TQN | CA1-CA2 | -3.48 | 1.47 | 1.53 |
| 5 | H | 301 | TQN | O53-C61 | 3.48 | 1.44 | 1.34 |
| 5 | K | 301 | TQN | CA1-CA2 | -3.47 | 1.47 | 1.53 |
| 5 | Y | 301 | TQN | CA1-CA2 | -3.47 | 1.47 | 1.53 |
| 5 | I | 301 | TQN | C12-C11 | 3.47 | 1.59 | 1.51 |
| 5 | X | 301 | TQN | O53-C61 | 3.47 | 1.44 | 1.34 |
| 5 | U | 301 | TQN | O53-C61 | 3.47 | 1.44 | 1.34 |
| 5 | V | 301 | TQN | O53-C61 | 3.47 | 1.44 | 1.34 |
| 5 | T | 301 | TQN | O53-C61 | 3.47 | 1.44 | 1.34 |
| 5 | L | 301 | TQN | C12-C11 | 3.47 | 1.59 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | R | 301 | TQN | C12-C11 | 3.47 | 1.59 | 1.51 |
| 5 | W | 301 | TQN | C12-C11 | 3.47 | 1.59 | 1.51 |
| 5 | X | 301 | TQN | C12-C11 | 3.47 | 1.59 | 1.51 |
| 5 | T | 301 | TQN | CA1-CA2 | -3.47 | 1.47 | 1.53 |
| 5 | B | 301 | TQN | O53-C61 | 3.47 | 1.44 | 1.34 |
| 5 | N | 301 | TQN | CA1-CA2 | -3.47 | 1.47 | 1.53 |
| 5 | F | 301 | TQN | C12-C11 | 3.47 | 1.59 | 1.51 |
| 5 | E | 301 | TQN | O53-C61 | 3.47 | 1.44 | 1.34 |
| 5 | L | 301 | TQN | O53-C61 | 3.47 | 1.44 | 1.34 |
| 5 | R | 301 | TQN | O53-C61 | 3.47 | 1.44 | 1.34 |
| 5 | Y | 301 | TQN | O53-C61 | 3.47 | 1.44 | 1.34 |
| 5 | I | 301 | TQN | O53-C61 | 3.47 | 1.44 | 1.34 |
| 5 | B | 301 | TQN | C12-C11 | 3.46 | 1.59 | 1.51 |
| 5 | O | 301 | TQN | C12-C11 | 3.46 | 1.59 | 1.51 |
| 5 | A | 302 | TQN | O53-C61 | 3.46 | 1.44 | 1.34 |
| 5 | J | 301 | TQN | CA1-CA2 | -3.46 | 1.47 | 1.53 |
| 5 | W | 301 | TQN | CA1-CA2 | -3.46 | 1.47 | 1.53 |
| 5 | J | 301 | TQN | O53-C61 | 3.46 | 1.44 | 1.34 |
| 5 | P | 301 | TQN | C12-C11 | 3.46 | 1.59 | 1.51 |
| 5 | L | 301 | TQN | CA1-CA2 | -3.46 | 1.47 | 1.53 |
| 5 | T | 301 | TQN | C12-C11 | 3.46 | 1.59 | 1.51 |
| 5 | U | 301 | TQN | C12-C11 | 3.45 | 1.59 | 1.51 |
| 5 | D | 301 | TQN | O53-C61 | 3.45 | 1.44 | 1.34 |
| 5 | Q | 301 | TQN | O53-C61 | 3.45 | 1.44 | 1.34 |
| 5 | O | 301 | TQN | O53-C61 | 3.45 | 1.44 | 1.34 |
| 5 | H | 301 | TQN | C12-C11 | 3.45 | 1.59 | 1.51 |
| 5 | D | 301 | TQN | C12-C11 | 3.44 | 1.59 | 1.51 |
| 5 | Q | 301 | TQN | C12-C11 | 3.44 | 1.59 | 1.51 |
| 5 | P | 301 | TQN | O53-C61 | 3.44 | 1.44 | 1.34 |
| 5 | K | 301 | TQN | O53-C61 | 3.44 | 1.44 | 1.34 |
| 5 | K | 301 | TQN | C12-C11 | 3.44 | 1.59 | 1.51 |
| 5 | G | 301 | TQN | O53-C61 | 3.44 | 1.44 | 1.34 |
| 5 | M | 301 | TQN | O53-C61 | 3.43 | 1.44 | 1.34 |
| 5 | Z | 301 | TQN | O53-C61 | 3.43 | 1.44 | 1.34 |
| 5 | S | 301 | TQN | O53-C61 | 3.43 | 1.44 | 1.34 |
| 5 | W | 301 | TQN | O53-C61 | 3.43 | 1.44 | 1.34 |
| 5 | C | 301 | TQN | CA1-CA2 | -3.43 | 1.47 | 1.53 |
| 5 | S | 301 | TQN | CA1-CA2 | -3.42 | 1.47 | 1.53 |
| 5 | B | 301 | TQN | CA1-CA2 | -3.42 | 1.47 | 1.53 |
| 5 | O | 301 | TQN | CA1-CA2 | -3.42 | 1.47 | 1.53 |
| 5 | R | 301 | TQN | CA1-CA2 | -3.42 | 1.47 | 1.53 |
| 5 | D | 301 | TQN | CA1-CA2 | -3.42 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | X | 301 | TQN | CA1-CA2 | -3.41 | 1.47 | 1.53 |
| 5 | H | 301 | TQN | CA1-CA2 | -3.41 | 1.47 | 1.53 |
| 5 | I | 301 | TQN | CA1-CA2 | -3.41 | 1.47 | 1.53 |
| 5 | U | 301 | TQN | CA1-CA2 | -3.41 | 1.47 | 1.53 |
| 5 | F | 301 | TQN | CA1-CA2 | -3.41 | 1.47 | 1.53 |
| 5 | S | 301 | TQN | O73-C73 | -3.39 | 1.38 | 1.46 |
| 5 | D | 301 | TQN | O73-C73 | -3.39 | 1.38 | 1.46 |
| 5 | X | 301 | TQN | O73-C73 | -3.39 | 1.38 | 1.46 |
| 5 | W | 301 | TQN | O73-C73 | -3.38 | 1.38 | 1.46 |
| 5 | M | 301 | TQN | O73-C73 | -3.38 | 1.38 | 1.46 |
| 5 | Z | 301 | TQN | O73-C73 | -3.38 | 1.38 | 1.46 |
| 5 | V | 301 | TQN | O73-C73 | -3.38 | 1.38 | 1.46 |
| 5 | C | 301 | TQN | O73-C73 | -3.38 | 1.38 | 1.46 |
| 5 | Y | 301 | TQN | O73-C73 | -3.38 | 1.38 | 1.46 |
| 5 | A | 302 | TQN | O73-C73 | -3.37 | 1.38 | 1.46 |
| 5 | B | 301 | TQN | O73-C73 | -3.37 | 1.38 | 1.46 |
| 5 | P | 301 | TQN | O73-C73 | -3.37 | 1.38 | 1.46 |
| 5 | J | 301 | TQN | O73-C73 | -3.36 | 1.38 | 1.46 |
| 5 | K | 301 | TQN | O73-C73 | -3.36 | 1.38 | 1.46 |
| 5 | I | 301 | TQN | O73-C73 | -3.35 | 1.38 | 1.46 |
| 5 | N | 301 | TQN | O73-C73 | -3.35 | 1.38 | 1.46 |
| 5 | E | 301 | TQN | O73-C73 | -3.35 | 1.38 | 1.46 |
| 5 | Q | 301 | TQN | O73-C73 | -3.35 | 1.38 | 1.46 |
| 5 | F | 301 | TQN | O73-C73 | -3.35 | 1.38 | 1.46 |
| 5 | R | 301 | TQN | O73-C73 | -3.34 | 1.38 | 1.46 |
| 5 | O | 301 | TQN | O73-C73 | -3.34 | 1.38 | 1.46 |
| 5 | G | 301 | TQN | O73-C73 | -3.34 | 1.38 | 1.46 |
| 5 | T | 301 | TQN | O73-C73 | -3.34 | 1.38 | 1.46 |
| 5 | L | 301 | TQN | O73-C73 | -3.34 | 1.38 | 1.46 |
| 5 | H | 301 | TQN | O73-C73 | -3.32 | 1.38 | 1.46 |
| 5 | U | 301 | TQN | O73-C73 | -3.32 | 1.38 | 1.46 |
| 5 | O | 301 | TQN | OA3-CA3 | -3.14 | 1.40 | 1.44 |
| 5 | A | 302 | TQN | OA3-CA3 | -3.14 | 1.40 | 1.44 |
| 5 | K | 301 | TQN | OA3-CA3 | -3.14 | 1.40 | 1.44 |
| 5 | I | 301 | TQN | OA3-CA3 | -3.13 | 1.40 | 1.44 |
| 5 | R | 301 | TQN | OA3-CA3 | -3.13 | 1.40 | 1.44 |
| 5 | G | 301 | TQN | OA3-CA3 | -3.13 | 1.40 | 1.44 |
| 5 | B | 301 | TQN | OA3-CA3 | -3.12 | 1.40 | 1.44 |
| 5 | D | 301 | TQN | OA3-CA3 | -3.10 | 1.40 | 1.44 |
| 5 | U | 301 | TQN | OA3-CA3 | -3.08 | 1.40 | 1.44 |
| 5 | L | 301 | TQN | OA3-CA3 | -3.07 | 1.40 | 1.44 |
| 5 | E | 301 | TQN | OA3-CA3 | -3.07 | 1.40 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | H | 301 | TQN | OA3-CA3 | -3.07 | 1.40 | 1.44 |
| 5 | C | 301 | TQN | OA3-CA3 | -3.07 | 1.40 | 1.44 |
| 5 | J | 301 | TQN | OA3-CA3 | -3.07 | 1.40 | 1.44 |
| 5 | M | 301 | TQN | OA3-CA3 | -3.07 | 1.40 | 1.44 |
| 5 | W | 301 | TQN | OA3-CA3 | -3.07 | 1.40 | 1.44 |
| 5 | V | 301 | TQN | OA3-CA3 | -3.07 | 1.40 | 1.44 |
| 5 | Q | 301 | TQN | OA3-CA3 | -3.06 | 1.40 | 1.44 |
| 5 | S | 301 | TQN | OA3-CA3 | -3.06 | 1.40 | 1.44 |
| 5 | X | 301 | TQN | OA3-CA3 | -3.06 | 1.40 | 1.44 |
| 5 | Y | 301 | TQN | OA3-CA3 | -3.06 | 1.40 | 1.44 |
| 5 | Z | 301 | TQN | OA3-CA3 | -3.06 | 1.40 | 1.44 |
| 5 | T | 301 | TQN | OA3-CA3 | -3.05 | 1.40 | 1.44 |
| 5 | P | 301 | TQN | OA3-CA3 | -3.05 | 1.40 | 1.44 |
| 5 | F | 301 | TQN | OA3-CA3 | -3.05 | 1.40 | 1.44 |
| 5 | N | 301 | TQN | OA3-CA3 | -3.05 | 1.40 | 1.44 |
| 5 | M | 301 | TQN | O53-C53 | -2.93 | 1.39 | 1.46 |
| 5 | Z | 301 | TQN | O53-C53 | -2.93 | 1.39 | 1.46 |
| 5 | Y | 301 | TQN | O53-C53 | -2.92 | 1.39 | 1.46 |
| 5 | E | 301 | TQN | O53-C53 | -2.92 | 1.39 | 1.46 |
| 5 | C | 301 | TQN | O53-C53 | -2.92 | 1.39 | 1.46 |
| 5 | P | 301 | TQN | O53-C53 | -2.92 | 1.39 | 1.46 |
| 5 | A | 302 | TQN | O53-C53 | -2.92 | 1.39 | 1.46 |
| 5 | N | 301 | TQN | O53-C53 | -2.92 | 1.39 | 1.46 |
| 5 | V | 301 | TQN | O53-C53 | -2.92 | 1.39 | 1.46 |
| 5 | H | 301 | TQN | O53-C53 | -2.92 | 1.39 | 1.46 |
| 5 | G | 301 | TQN | O53-C53 | -2.91 | 1.39 | 1.46 |
| 5 | T | 301 | TQN | O53-C53 | -2.91 | 1.39 | 1.46 |
| 5 | J | 301 | TQN | O53-C53 | -2.91 | 1.39 | 1.46 |
| 5 | X | 301 | TQN | PB-OB4 | 2.91 | 1.64 | 1.59 |
| 5 | D | 301 | TQN | O53-C53 | -2.91 | 1.39 | 1.46 |
| 5 | Q | 301 | TQN | O53-C53 | -2.91 | 1.39 | 1.46 |
| 5 | H | 301 | TQN | PB-OB4 | 2.91 | 1.64 | 1.59 |
| 5 | B | 301 | TQN | O53-C53 | -2.90 | 1.39 | 1.46 |
| 5 | O | 301 | TQN | O53-C53 | -2.90 | 1.39 | 1.46 |
| 5 | L | 301 | TQN | PB-OB4 | 2.90 | 1.64 | 1.59 |
| 5 | R | 301 | TQN | O53-C53 | -2.90 | 1.39 | 1.46 |
| 5 | L | 301 | TQN | O53-C53 | -2.90 | 1.39 | 1.46 |
| 5 | Z | 301 | TQN | PB-OB4 | 2.90 | 1.64 | 1.59 |
| 5 | U | 301 | TQN | O53-C53 | -2.89 | 1.39 | 1.46 |
| 5 | B | 301 | TQN | PB-OB4 | 2.89 | 1.64 | 1.59 |
| 5 | G | 301 | TQN | PB-OB4 | 2.89 | 1.64 | 1.59 |
| 5 | F | 301 | TQN | O53-C53 | -2.89 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | X | 301 | TQN | O53-C53 | -2.89 | 1.39 | 1.46 |
| 5 | K | 301 | TQN | O53-C53 | -2.89 | 1.39 | 1.46 |
| 5 | I | 301 | TQN | O53-C53 | -2.89 | 1.39 | 1.46 |
| 5 | S | 301 | TQN | O53-C53 | -2.89 | 1.39 | 1.46 |
| 5 | W | 301 | TQN | O53-C53 | -2.88 | 1.39 | 1.46 |
| 5 | V | 301 | TQN | PB-OB4 | 2.88 | 1.64 | 1.59 |
| 5 | D | 301 | TQN | PB-OB4 | 2.88 | 1.64 | 1.59 |
| 5 | R | 301 | TQN | PB-OB4 | 2.88 | 1.64 | 1.59 |
| 5 | C | 301 | TQN | PB-OB4 | 2.88 | 1.64 | 1.59 |
| 5 | P | 301 | TQN | PB-OB4 | 2.88 | 1.64 | 1.59 |
| 5 | S | 301 | TQN | PB-OB4 | 2.88 | 1.64 | 1.59 |
| 5 | T | 301 | TQN | PB-OB4 | 2.87 | 1.64 | 1.59 |
| 5 | J | 301 | TQN | PB-OB4 | 2.87 | 1.64 | 1.59 |
| 5 | W | 301 | TQN | PB-OB4 | 2.87 | 1.64 | 1.59 |
| 5 | N | 301 | TQN | O13-C21 | 2.87 | 1.42 | 1.34 |
| 5 | C | 301 | TQN | O13-C21 | 2.87 | 1.42 | 1.34 |
| 5 | A | 302 | TQN | PB-OB4 | 2.87 | 1.64 | 1.59 |
| 5 | K | 301 | TQN | PB-OB4 | 2.87 | 1.64 | 1.59 |
| 5 | K | 301 | TQN | O13-C21 | 2.87 | 1.42 | 1.34 |
| 5 | Y | 301 | TQN | PB-OB4 | 2.86 | 1.64 | 1.59 |
| 5 | D | 301 | TQN | O13-C21 | 2.86 | 1.42 | 1.34 |
| 5 | Q | 301 | TQN | O13-C21 | 2.86 | 1.42 | 1.34 |
| 5 | U | 301 | TQN | PB-OB4 | 2.86 | 1.64 | 1.59 |
| 5 | Z | 301 | TQN | O13-C21 | 2.86 | 1.42 | 1.34 |
| 5 | M | 301 | TQN | PB-OB4 | 2.86 | 1.64 | 1.59 |
| 5 | X | 301 | TQN | O13-C21 | 2.85 | 1.42 | 1.34 |
| 5 | E | 301 | TQN | PB-OB4 | 2.85 | 1.64 | 1.59 |
| 5 | Q | 301 | TQN | PB-OB4 | 2.85 | 1.64 | 1.59 |
| 5 | T | 301 | TQN | O13-C21 | 2.85 | 1.42 | 1.34 |
| 5 | O | 301 | TQN | PB-OB4 | 2.85 | 1.64 | 1.59 |
| 5 | H | 301 | TQN | O13-C21 | 2.85 | 1.42 | 1.34 |
| 5 | U | 301 | TQN | O13-C21 | 2.84 | 1.42 | 1.34 |
| 5 | E | 301 | TQN | O13-C21 | 2.84 | 1.42 | 1.34 |
| 5 | R | 301 | TQN | O13-C21 | 2.84 | 1.42 | 1.34 |
| 5 | M | 301 | TQN | O13-C21 | 2.84 | 1.42 | 1.34 |
| 5 | V | 301 | TQN | O13-C21 | 2.84 | 1.42 | 1.34 |
| 5 | F | 301 | TQN | PB-OB4 | 2.84 | 1.64 | 1.59 |
| 5 | J | 301 | TQN | O13-C21 | 2.84 | 1.42 | 1.34 |
| 5 | W | 301 | TQN | O13-C21 | 2.84 | 1.42 | 1.34 |
| 5 | I | 301 | TQN | PB-OB4 | 2.84 | 1.64 | 1.59 |
| 5 | F | 301 | TQN | O13-C21 | 2.84 | 1.42 | 1.34 |
| 5 | N | 301 | TQN | PB-OB4 | 2.84 | 1.64 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | L | 301 | TQN | O13-C21 | 2.84 | 1.42 | 1.34 |
| 5 | Y | 301 | TQN | O13-C21 | 2.84 | 1.42 | 1.34 |
| 5 | I | 301 | TQN | O13-C21 | 2.83 | 1.42 | 1.34 |
| 5 | S | 301 | TQN | O13-C21 | 2.83 | 1.42 | 1.34 |
| 5 | G | 301 | TQN | O13-C21 | 2.83 | 1.42 | 1.34 |
| 5 | B | 301 | TQN | O13-C21 | 2.83 | 1.42 | 1.34 |
| 5 | A | 302 | TQN | O13-C21 | 2.83 | 1.42 | 1.34 |
| 5 | O | 301 | TQN | O13-C21 | 2.83 | 1.42 | 1.34 |
| 5 | P | 301 | TQN | O13-C21 | 2.83 | 1.42 | 1.34 |
| 5 | A | 302 | TQN | C72-C71 | 2.82 | 1.56 | 1.50 |
| 5 | J | 301 | TQN | C72-C71 | 2.82 | 1.56 | 1.50 |
| 5 | K | 301 | TQN | C72-C71 | 2.82 | 1.56 | 1.50 |
| 5 | G | 301 | TQN | C72-C71 | 2.82 | 1.56 | 1.50 |
| 5 | B | 301 | TQN | C72-C71 | 2.81 | 1.56 | 1.50 |
| 5 | E | 301 | TQN | C72-C71 | 2.81 | 1.56 | 1.50 |
| 5 | R | 301 | TQN | C72-C71 | 2.81 | 1.56 | 1.50 |
| 5 | S | 301 | TQN | C72-C71 | 2.81 | 1.56 | 1.50 |
| 5 | O | 301 | TQN | C72-C71 | 2.81 | 1.56 | 1.50 |
| 5 | L | 301 | TQN | C72-C71 | 2.81 | 1.56 | 1.50 |
| 5 | H | 301 | TQN | C72-C71 | 2.80 | 1.56 | 1.50 |
| 5 | X | 301 | TQN | C72-C71 | 2.80 | 1.56 | 1.50 |
| 5 | D | 301 | TQN | C72-C71 | 2.80 | 1.56 | 1.50 |
| 5 | Q | 301 | TQN | C72-C71 | 2.80 | 1.56 | 1.50 |
| 5 | C | 301 | TQN | C72-C71 | 2.79 | 1.56 | 1.50 |
| 5 | P | 301 | TQN | C72-C71 | 2.79 | 1.56 | 1.50 |
| 5 | N | 301 | TQN | C72-C71 | 2.79 | 1.56 | 1.50 |
| 5 | U | 301 | TQN | C72-C71 | 2.79 | 1.56 | 1.50 |
| 5 | V | 301 | TQN | C72-C71 | 2.79 | 1.56 | 1.50 |
| 5 | I | 301 | TQN | C72-C71 | 2.79 | 1.56 | 1.50 |
| 5 | Y | 301 | TQN | C72-C71 | 2.77 | 1.56 | 1.50 |
| 5 | W | 301 | TQN | C72-C71 | 2.77 | 1.56 | 1.50 |
| 5 | M | 301 | TQN | C72-C71 | 2.77 | 1.56 | 1.50 |
| 5 | Z | 301 | TQN | C72-C71 | 2.77 | 1.56 | 1.50 |
| 5 | T | 301 | TQN | C72-C71 | 2.77 | 1.56 | 1.50 |
| 5 | F | 301 | TQN | C72-C71 | 2.77 | 1.56 | 1.50 |
| 5 | D | 301 | TQN | PA-OA1 | 2.62 | 1.64 | 1.59 |
| 5 | S | 301 | TQN | PA-OA1 | 2.62 | 1.64 | 1.59 |
| 5 | I | 301 | TQN | PA-OA1 | 2.62 | 1.64 | 1.59 |
| 5 | B | 301 | TQN | PA-OA1 | 2.61 | 1.64 | 1.59 |
| 5 | R | 301 | TQN | PA-OA1 | 2.61 | 1.64 | 1.59 |
| 5 | J | 301 | TQN | PA-OA1 | 2.61 | 1.64 | 1.59 |
| 5 | G | 301 | TQN | PA-OA1 | 2.60 | 1.64 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | Q | 301 | TQN | PA-OA1 | 2.59 | 1.64 | 1.59 |
| 5 | Z | 301 | TQN | PA-OA1 | 2.59 | 1.64 | 1.59 |
| 5 | U | 301 | TQN | PA-OA1 | 2.58 | 1.64 | 1.59 |
| 5 | T | 301 | TQN | PA-OA1 | 2.58 | 1.64 | 1.59 |
| 5 | F | 301 | TQN | PA-OA1 | 2.58 | 1.64 | 1.59 |
| 5 | V | 301 | TQN | PA-OA1 | 2.58 | 1.64 | 1.59 |
| 5 | A | 302 | TQN | PA-OA1 | 2.58 | 1.64 | 1.59 |
| 5 | P | 301 | TQN | PA-OA1 | 2.58 | 1.64 | 1.59 |
| 5 | K | 301 | TQN | PA-OA1 | 2.57 | 1.64 | 1.59 |
| 5 | X | 301 | TQN | PA-OA1 | 2.57 | 1.64 | 1.59 |
| 5 | E | 301 | TQN | PA-OA1 | 2.56 | 1.64 | 1.59 |
| 5 | W | 301 | TQN | PA-OA1 | 2.56 | 1.64 | 1.59 |
| 5 | L | 301 | TQN | PA-OA1 | 2.56 | 1.64 | 1.59 |
| 5 | I | 301 | TQN | CB2-NB2 | 2.56 | 1.49 | 1.45 |
| 5 | V | 301 | TQN | CB2-NB2 | 2.56 | 1.49 | 1.45 |
| 5 | P | 301 | TQN | CB2-NB2 | 2.55 | 1.49 | 1.45 |
| 5 | M | 301 | TQN | PA-OA1 | 2.55 | 1.64 | 1.59 |
| 5 | D | 301 | TQN | CB2-NB2 | 2.55 | 1.49 | 1.45 |
| 5 | N | 301 | TQN | PA-OA1 | 2.55 | 1.64 | 1.59 |
| 5 | W | 301 | TQN | CB2-NB2 | 2.55 | 1.49 | 1.45 |
| 5 | Y | 301 | TQN | PA-OA1 | 2.55 | 1.64 | 1.59 |
| 5 | B | 301 | TQN | CB2-NB2 | 2.55 | 1.49 | 1.45 |
| 5 | A | 302 | TQN | CB2-NB2 | 2.55 | 1.49 | 1.45 |
| 5 | H | 301 | TQN | PA-OA1 | 2.54 | 1.64 | 1.59 |
| 5 | U | 301 | TQN | CB2-NB2 | 2.54 | 1.49 | 1.45 |
| 5 | C | 301 | TQN | PA-OA1 | 2.54 | 1.64 | 1.59 |
| 5 | Z | 301 | TQN | CB2-NB2 | 2.54 | 1.49 | 1.45 |
| 5 | K | 301 | TQN | CB2-NB2 | 2.53 | 1.49 | 1.45 |
| 5 | X | 301 | TQN | CB2-NB2 | 2.53 | 1.49 | 1.45 |
| 5 | O | 301 | TQN | PA-OA1 | 2.53 | 1.64 | 1.59 |
| 5 | C | 301 | TQN | CB2-NB2 | 2.52 | 1.49 | 1.45 |
| 5 | J | 301 | TQN | CB2-NB2 | 2.52 | 1.49 | 1.45 |
| 5 | Q | 301 | TQN | CB2-NB2 | 2.52 | 1.49 | 1.45 |
| 5 | L | 301 | TQN | CB2-NB2 | 2.52 | 1.49 | 1.45 |
| 5 | Y | 301 | TQN | CB2-NB2 | 2.52 | 1.49 | 1.45 |
| 5 | T | 301 | TQN | CB2-NB2 | 2.51 | 1.49 | 1.45 |
| 5 | M | 301 | TQN | CB2-NB2 | 2.50 | 1.49 | 1.45 |
| 5 | O | 301 | TQN | CB2-NB2 | 2.49 | 1.49 | 1.45 |
| 5 | S | 301 | TQN | CB2-NB2 | 2.49 | 1.49 | 1.45 |
| 5 | N | 301 | TQN | CB2-NB2 | 2.49 | 1.49 | 1.45 |
| 5 | G | 301 | TQN | CB2-NB2 | 2.49 | 1.49 | 1.45 |
| 5 | H | 301 | TQN | CB2-NB2 | 2.48 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | F | 301 | TQN | CB2-NB2 | 2.48 | 1.49 | 1.45 |
| 5 | E | 301 | TQN | CB2-NB2 | 2.47 | 1.49 | 1.45 |
| 5 | R | 301 | TQN | CB2-NB2 | 2.47 | 1.49 | 1.45 |
| 5 | Y | 301 | TQN | C52-C51 | 2.44 | 1.56 | 1.51 |
| 5 | I | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | V | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | K | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | X | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | Q | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | C | 301 | TQN | O73-C81 | 2.43 | 1.41 | 1.34 |
| 5 | F | 301 | TQN | O73-C81 | 2.43 | 1.41 | 1.34 |
| 5 | P | 301 | TQN | O73-C81 | 2.43 | 1.41 | 1.34 |
| 5 | E | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | G | 301 | TQN | O73-C81 | 2.43 | 1.41 | 1.34 |
| 5 | T | 301 | TQN | O73-C81 | 2.43 | 1.41 | 1.34 |
| 5 | S | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | G | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | T | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | Z | 301 | TQN | O73-C81 | 2.43 | 1.41 | 1.34 |
| 5 | E | 301 | TQN | O73-C81 | 2.43 | 1.41 | 1.34 |
| 5 | K | 301 | TQN | O73-C81 | 2.43 | 1.41 | 1.34 |
| 5 | X | 301 | TQN | O73-C81 | 2.43 | 1.41 | 1.34 |
| 5 | B | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | C | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | M | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | P | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | Z | 301 | TQN | C52-C51 | 2.43 | 1.56 | 1.51 |
| 5 | L | 301 | TQN | C52-C51 | 2.42 | 1.56 | 1.51 |
| 5 | N | 301 | TQN | O73-C81 | 2.42 | 1.41 | 1.34 |
| 5 | H | 301 | TQN | C52-C51 | 2.42 | 1.56 | 1.51 |
| 5 | U | 301 | TQN | C52-C51 | 2.42 | 1.56 | 1.51 |
| 5 | A | 302 | TQN | C52-C51 | 2.42 | 1.56 | 1.51 |
| 5 | N | 301 | TQN | C52-C51 | 2.42 | 1.56 | 1.51 |
| 5 | Y | 301 | TQN | O73-C81 | 2.42 | 1.41 | 1.34 |
| 5 | O | 301 | TQN | O73-C81 | 2.42 | 1.41 | 1.34 |
| 5 | Q | 301 | TQN | O73-C81 | 2.42 | 1.41 | 1.34 |
| 5 | O | 301 | TQN | C52-C51 | 2.41 | 1.56 | 1.51 |
| 5 | R | 301 | TQN | C52-C51 | 2.41 | 1.56 | 1.51 |
| 5 | D | 301 | TQN | C52-C51 | 2.41 | 1.56 | 1.51 |
| 5 | F | 301 | TQN | C52-C51 | 2.41 | 1.56 | 1.51 |
| 5 | J | 301 | TQN | C52-C51 | 2.41 | 1.56 | 1.51 |
| 5 | W | 301 | TQN | C52-C51 | 2.41 | 1.56 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | S | 301 | TQN | O73-C81 | 2.40 | 1.41 | 1.34 |
| 5 | V | 301 | TQN | O73-C81 | 2.40 | 1.41 | 1.34 |
| 5 | B | 301 | TQN | O73-C81 | 2.40 | 1.41 | 1.34 |
| 5 | W | 301 | TQN | O73-C81 | 2.40 | 1.41 | 1.34 |
| 5 | J | 301 | TQN | O73-C81 | 2.40 | 1.41 | 1.34 |
| 5 | A | 302 | TQN | O73-C81 | 2.40 | 1.41 | 1.34 |
| 5 | L | 301 | TQN | O73-C81 | 2.40 | 1.41 | 1.34 |
| 5 | D | 301 | TQN | O73-C81 | 2.40 | 1.41 | 1.34 |
| 5 | M | 301 | TQN | O73-C81 | 2.39 | 1.41 | 1.34 |
| 5 | R | 301 | TQN | O73-C81 | 2.39 | 1.41 | 1.34 |
| 5 | H | 301 | TQN | O73-C81 | 2.39 | 1.41 | 1.34 |
| 5 | I | 301 | TQN | O73-C81 | 2.39 | 1.41 | 1.34 |
| 5 | U | 301 | TQN | O73-C81 | 2.39 | 1.41 | 1.34 |
| 5 | S | 301 | TQN | OA3-C31 | 2.36 | 1.40 | 1.34 |
| 5 | T | 301 | TQN | OA3-C31 | 2.36 | 1.40 | 1.34 |
| 5 | G | 301 | TQN | OA3-C31 | 2.35 | 1.40 | 1.34 |
| 5 | D | 301 | TQN | OA3-C31 | 2.35 | 1.40 | 1.34 |
| 5 | W | 301 | TQN | OA3-C31 | 2.35 | 1.40 | 1.34 |
| 5 | K | 301 | TQN | OA3-C31 | 2.35 | 1.40 | 1.34 |
| 5 | R | 301 | TQN | OA3-C31 | 2.35 | 1.40 | 1.34 |
| 5 | N | 301 | TQN | OA3-C31 | 2.35 | 1.40 | 1.34 |
| 5 | A | 302 | TQN | OA3-C31 | 2.35 | 1.40 | 1.34 |
| 5 | M | 301 | TQN | OA3-C31 | 2.35 | 1.40 | 1.34 |
| 5 | P | 301 | TQN | OA3-C31 | 2.35 | 1.40 | 1.34 |
| 5 | H | 301 | TQN | OA3-C31 | 2.34 | 1.40 | 1.34 |
| 5 | U | 301 | TQN | OA3-C31 | 2.34 | 1.40 | 1.34 |
| 5 | Y | 301 | TQN | OA3-C31 | 2.34 | 1.40 | 1.34 |
| 5 | B | 301 | TQN | OA3-C31 | 2.34 | 1.40 | 1.34 |
| 5 | O | 301 | TQN | OA3-C31 | 2.34 | 1.40 | 1.34 |
| 5 | F | 301 | TQN | OA3-C31 | 2.34 | 1.40 | 1.34 |
| 5 | I | 301 | TQN | OA3-C31 | 2.34 | 1.40 | 1.34 |
| 5 | L | 301 | TQN | OA3-C31 | 2.33 | 1.40 | 1.34 |
| 5 | E | 301 | TQN | OA3-C31 | 2.33 | 1.40 | 1.34 |
| 5 | R | 301 | TQN | PA-OP7 | -2.33 | 1.46 | 1.54 |
| 5 | Z | 301 | TQN | OA3-C31 | 2.33 | 1.40 | 1.34 |
| 5 | X | 301 | TQN | OA3-C31 | 2.33 | 1.40 | 1.34 |
| 5 | E | 301 | TQN | PA-OP7 | -2.33 | 1.46 | 1.54 |
| 5 | D | 301 | TQN | PA-OP7 | -2.33 | 1.46 | 1.54 |
| 5 | F | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | S | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | Y | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | V | 301 | TQN | OA3-C31 | 2.32 | 1.40 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | Q | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | J | 301 | TQN | OA3-C31 | 2.32 | 1.40 | 1.34 |
| 5 | G | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | H | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | J | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | U | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | I | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | V | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | X | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | K | 301 | TQN | PA-OP7 | -2.32 | 1.46 | 1.54 |
| 5 | C | 301 | TQN | OA3-C31 | 2.31 | 1.40 | 1.34 |
| 5 | B | 301 | TQN | PA-OP7 | -2.31 | 1.46 | 1.54 |
| 5 | C | 301 | TQN | PA-OP7 | -2.31 | 1.46 | 1.54 |
| 5 | O | 301 | TQN | PA-OP7 | -2.31 | 1.46 | 1.54 |
| 5 | P | 301 | TQN | PA-OP7 | -2.31 | 1.46 | 1.54 |
| 5 | Z | 301 | TQN | PA-OP7 | -2.31 | 1.46 | 1.54 |
| 5 | L | 301 | TQN | PA-OP7 | -2.31 | 1.46 | 1.54 |
| 5 | M | 301 | TQN | PA-OP7 | -2.31 | 1.46 | 1.54 |
| 5 | W | 301 | TQN | PB-OP2 | -2.31 | 1.46 | 1.54 |
| 5 | A | 302 | TQN | PA-OP7 | -2.31 | 1.46 | 1.54 |
| 5 | N | 301 | TQN | PA-OP7 | -2.31 | 1.46 | 1.54 |
| 5 | W | 301 | TQN | PA-OP7 | -2.31 | 1.46 | 1.54 |
| 5 | Q | 301 | TQN | OA3-C31 | 2.30 | 1.40 | 1.34 |
| 5 | P | 301 | TQN | PB-OP2 | -2.30 | 1.46 | 1.54 |
| 5 | M | 301 | TQN | PB-OP2 | -2.30 | 1.46 | 1.54 |
| 5 | S | 301 | TQN | PB-OP2 | -2.30 | 1.46 | 1.54 |
| 5 | T | 301 | TQN | PA-OP7 | -2.30 | 1.46 | 1.54 |
| 5 | I | 301 | TQN | PB-OP2 | -2.29 | 1.46 | 1.54 |
| 5 | J | 301 | TQN | PB-OP2 | -2.29 | 1.46 | 1.54 |
| 5 | D | 301 | TQN | PB-OP2 | -2.29 | 1.46 | 1.54 |
| 5 | H | 301 | TQN | PB-OP2 | -2.29 | 1.46 | 1.54 |
| 5 | X | 301 | TQN | PB-OP2 | -2.29 | 1.46 | 1.54 |
| 5 | L | 301 | TQN | PB-OP2 | -2.29 | 1.46 | 1.54 |
| 5 | T | 301 | TQN | PB-OP2 | -2.29 | 1.46 | 1.54 |
| 5 | U | 301 | TQN | PB-OP2 | -2.29 | 1.46 | 1.54 |
| 5 | F | 301 | TQN | O51-C51 | -2.29 | 1.18 | 1.23 |
| 5 | G | 301 | TQN | O51-C51 | -2.29 | 1.18 | 1.23 |
| 5 | P | 301 | TQN | O51-C51 | -2.28 | 1.18 | 1.23 |
| 5 | R | 301 | TQN | PB-OP2 | -2.28 | 1.46 | 1.54 |
| 5 | Z | 301 | TQN | PB-OP2 | -2.28 | 1.46 | 1.54 |
| 5 | A | 302 | TQN | PB-OP2 | -2.28 | 1.46 | 1.54 |
| 5 | Y | 301 | TQN | PB-OP2 | -2.28 | 1.46 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | B | 301 | TQN | PB-OP2 | -2.28 | 1.46 | 1.54 |
| 5 | K | 301 | TQN | PB-OP2 | -2.28 | 1.46 | 1.54 |
| 5 | O | 301 | TQN | PB-OP2 | -2.28 | 1.46 | 1.54 |
| 5 | O | 301 | TQN | O51-C51 | -2.28 | 1.18 | 1.23 |
| 5 | V | 301 | TQN | PB-OP2 | -2.28 | 1.46 | 1.54 |
| 5 | G | 301 | TQN | PB-OP2 | -2.27 | 1.46 | 1.54 |
| 5 | E | 301 | TQN | PB-OP2 | -2.27 | 1.46 | 1.54 |
| 5 | M | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | J | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | R | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | W | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | N | 301 | TQN | PB-OP2 | -2.27 | 1.46 | 1.54 |
| 5 | H | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | U | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | Q | 301 | TQN | PB-OP2 | -2.27 | 1.46 | 1.54 |
| 5 | F | 301 | TQN | PB-OP2 | -2.27 | 1.46 | 1.54 |
| 5 | A | 302 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | N | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | K | 301 | TQN | O13-C13 | -2.27 | 1.41 | 1.46 |
| 5 | D | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | Q | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | X | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | I | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | V | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | Y | 301 | TQN | O51-C51 | -2.27 | 1.18 | 1.23 |
| 5 | C | 301 | TQN | PB-OP2 | -2.26 | 1.46 | 1.54 |
| 5 | Z | 301 | TQN | O51-C51 | -2.26 | 1.18 | 1.23 |
| 5 | L | 301 | TQN | O51-C51 | -2.26 | 1.18 | 1.23 |
| 5 | C | 301 | TQN | O51-C51 | -2.25 | 1.18 | 1.23 |
| 5 | E | 301 | TQN | O51-C51 | -2.25 | 1.18 | 1.23 |
| 5 | K | 301 | TQN | O51-C51 | -2.25 | 1.18 | 1.23 |
| 5 | B | 301 | TQN | O51-C51 | -2.25 | 1.18 | 1.23 |
| 5 | J | 301 | TQN | O11-C11 | -2.24 | 1.18 | 1.23 |
| 5 | T | 301 | TQN | O51-C51 | -2.24 | 1.18 | 1.23 |
| 5 | Z | 301 | TQN | PB-OP3 | -2.24 | 1.46 | 1.54 |
| 5 | F | 301 | TQN | PB-OP3 | -2.24 | 1.46 | 1.54 |
| 5 | T | 301 | TQN | O13-C13 | -2.23 | 1.41 | 1.46 |
| 5 | D | 301 | TQN | O13-C13 | -2.23 | 1.41 | 1.46 |
| 5 | Y | 301 | TQN | O11-C11 | -2.23 | 1.18 | 1.23 |
| 5 | O | 301 | TQN | PB-OP3 | -2.23 | 1.46 | 1.54 |
| 5 | K | 301 | TQN | O11-C11 | -2.22 | 1.18 | 1.23 |
| 5 | N | 301 | TQN | O13-C13 | -2.22 | 1.41 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | F | 301 | TQN | O11-C11 | -2.22 | 1.18 | 1.23 |
| 5 | S | 301 | TQN | O11-C11 | -2.22 | 1.18 | 1.23 |
| 5 | H | 301 | TQN | PB-OP3 | -2.22 | 1.46 | 1.54 |
| 5 | M | 301 | TQN | PB-OP3 | -2.22 | 1.46 | 1.54 |
| 5 | W | 301 | TQN | PB-OP3 | -2.22 | 1.46 | 1.54 |
| 5 | Q | 301 | TQN | O13-C13 | -2.22 | 1.41 | 1.46 |
| 5 | T | 301 | TQN | PB-OP3 | -2.22 | 1.46 | 1.54 |
| 5 | E | 301 | TQN | O13-C13 | -2.22 | 1.41 | 1.46 |
| 5 | J | 301 | TQN | O13-C13 | -2.22 | 1.41 | 1.46 |
| 5 | R | 301 | TQN | PB-OP3 | -2.22 | 1.46 | 1.54 |
| 5 | Y | 301 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | V | 301 | TQN | O13-C13 | -2.21 | 1.41 | 1.46 |
| 5 | N | 301 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | E | 301 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | Q | 301 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | H | 301 | TQN | O11-C11 | -2.21 | 1.18 | 1.23 |
| 5 | U | 301 | TQN | O11-C11 | -2.21 | 1.18 | 1.23 |
| 5 | A | 302 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | A | 302 | TQN | O11-C11 | -2.21 | 1.18 | 1.23 |
| 5 | N | 301 | TQN | O11-C11 | -2.21 | 1.18 | 1.23 |
| 5 | C | 301 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | P | 301 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | X | 301 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | S | 301 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | G | 301 | TQN | O13-C13 | -2.21 | 1.41 | 1.46 |
| 5 | B | 301 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | C | 301 | TQN | O13-C13 | -2.21 | 1.41 | 1.46 |
| 5 | D | 301 | TQN | O11-C11 | -2.21 | 1.18 | 1.23 |
| 5 | Q | 301 | TQN | O11-C11 | -2.21 | 1.18 | 1.23 |
| 5 | G | 301 | TQN | O11-C11 | -2.21 | 1.18 | 1.23 |
| 5 | C | 301 | TQN | O11-C11 | -2.21 | 1.18 | 1.23 |
| 5 | V | 301 | TQN | PB-OP3 | -2.21 | 1.46 | 1.54 |
| 5 | B | 301 | TQN | O11-C11 | -2.21 | 1.18 | 1.23 |
| 5 | O | 301 | TQN | O11-C11 | -2.21 | 1.18 | 1.23 |
| 5 | M | 301 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | Z | 301 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | T | 301 | TQN | O11-C11 | -2.20 | 1.18 | 1.23 |
| 5 | W | 301 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | U | 301 | TQN | PB-OP3 | -2.20 | 1.46 | 1.54 |
| 5 | P | 301 | TQN | O11-C11 | -2.20 | 1.18 | 1.23 |
| 5 | I | 301 | TQN | PB-OP3 | -2.20 | 1.46 | 1.54 |
| 5 | J | 301 | TQN | PB-OP3 | -2.20 | 1.46 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | T | 301 | TQN | PA-OP6 | -2.20 | 1.46 | 1.54 |
| 5 | B | 301 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | O | 301 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | D | 301 | TQN | PA-OP6 | -2.20 | 1.46 | 1.54 |
| 5 | L | 301 | TQN | PB-OP3 | -2.20 | 1.46 | 1.54 |
| 5 | R | 301 | TQN | PA-OP6 | -2.20 | 1.46 | 1.54 |
| 5 | S | 301 | TQN | O51-C51 | -2.20 | 1.18 | 1.23 |
| 5 | L | 301 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | G | 301 | TQN | PB-OP3 | -2.20 | 1.46 | 1.54 |
| 5 | A | 302 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | H | 301 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | U | 301 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | E | 301 | TQN | O11-C11 | -2.20 | 1.18 | 1.23 |
| 5 | R | 301 | TQN | O11-C11 | -2.20 | 1.18 | 1.23 |
| 5 | Y | 301 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | K | 301 | TQN | PB-OP3 | -2.20 | 1.46 | 1.54 |
| 5 | X | 301 | TQN | PA-OP6 | -2.20 | 1.46 | 1.54 |
| 5 | L | 301 | TQN | PA-OP6 | -2.20 | 1.46 | 1.54 |
| 5 | F | 301 | TQN | O13-C13 | -2.20 | 1.41 | 1.46 |
| 5 | X | 301 | TQN | O11-C11 | -2.20 | 1.18 | 1.23 |
| 5 | S | 301 | TQN | O13-C13 | -2.19 | 1.41 | 1.46 |
| 5 | D | 301 | TQN | PB-OP3 | -2.19 | 1.46 | 1.54 |
| 5 | I | 301 | TQN | O13-C13 | -2.19 | 1.41 | 1.46 |
| 5 | R | 301 | TQN | O13-C13 | -2.19 | 1.41 | 1.46 |
| 5 | P | 301 | TQN | O13-C13 | -2.19 | 1.41 | 1.46 |
| 5 | M | 301 | TQN | PA-OP6 | -2.19 | 1.46 | 1.54 |
| 5 | X | 301 | TQN | O13-C13 | -2.19 | 1.41 | 1.46 |
| 5 | M | 301 | TQN | O11-C11 | -2.19 | 1.18 | 1.23 |
| 5 | Z | 301 | TQN | O11-C11 | -2.19 | 1.18 | 1.23 |
| 5 | U | 301 | TQN | PA-OP6 | -2.19 | 1.46 | 1.54 |
| 5 | A | 302 | TQN | PA-OP6 | -2.19 | 1.46 | 1.54 |
| 5 | J | 301 | TQN | PA-OP6 | -2.19 | 1.46 | 1.54 |
| 5 | W | 301 | TQN | PA-OP6 | -2.19 | 1.46 | 1.54 |
| 5 | S | 301 | TQN | PA-OP6 | -2.19 | 1.46 | 1.54 |
| 5 | B | 301 | TQN | PA-OP6 | -2.18 | 1.46 | 1.54 |
| 5 | O | 301 | TQN | PA-OP6 | -2.18 | 1.46 | 1.54 |
| 5 | N | 301 | TQN | PA-OP6 | -2.18 | 1.46 | 1.54 |
| 5 | Z | 301 | TQN | PA-OP6 | -2.18 | 1.46 | 1.54 |
| 5 | L | 301 | TQN | O11-C11 | -2.18 | 1.18 | 1.23 |
| 5 | I | 301 | TQN | PA-OP6 | -2.18 | 1.46 | 1.54 |
| 5 | G | 301 | TQN | PA-OP6 | -2.18 | 1.46 | 1.54 |
| 5 | K | 301 | TQN | PA-OP6 | -2.18 | 1.46 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | C | 301 | TQN | PA-OP6 | -2.18 | 1.46 | 1.54 |
| 5 | P | 301 | TQN | PA-OP6 | -2.18 | 1.46 | 1.54 |
| 5 | Y | 301 | TQN | PA-OP6 | -2.18 | 1.46 | 1.54 |
| 5 | F | 301 | TQN | PA-OP6 | -2.17 | 1.46 | 1.54 |
| 5 | W | 301 | TQN | O11-C11 | -2.17 | 1.19 | 1.23 |
| 5 | V | 301 | TQN | PA-OP6 | -2.17 | 1.46 | 1.54 |
| 5 | V | 301 | TQN | O11-C11 | -2.17 | 1.19 | 1.23 |
| 5 | I | 301 | TQN | O11-C11 | -2.17 | 1.19 | 1.23 |
| 5 | Q | 301 | TQN | PA-OP6 | -2.17 | 1.46 | 1.54 |
| 5 | E | 301 | TQN | PA-OP6 | -2.17 | 1.46 | 1.54 |
| 5 | H | 301 | TQN | PA-OP6 | -2.16 | 1.46 | 1.54 |
| 4 | I | 302 | TLW | O6-C6 | -2.07 | 1.40 | 1.44 |
| 5 | H | 301 | TQN | C62-C61 | 2.06 | 1.56 | 1.50 |
| 5 | V | 301 | TQN | C62-C61 | 2.06 | 1.56 | 1.50 |
| 5 | B | 301 | TQN | C62-C61 | 2.06 | 1.56 | 1.50 |
| 4 | O | 302 | TLW | O6-C6 | -2.06 | 1.40 | 1.44 |
| 5 | F | 301 | TQN | C62-C61 | 2.05 | 1.56 | 1.50 |
| 4 | F | 302 | TLW | O6-C6 | -2.05 | 1.40 | 1.44 |
| 5 | D | 301 | TQN | C62-C61 | 2.05 | 1.56 | 1.50 |
| 5 | Q | 301 | TQN | C62-C61 | 2.05 | 1.56 | 1.50 |
| 5 | K | 301 | TQN | C62-C61 | 2.05 | 1.56 | 1.50 |
| 5 | E | 301 | TQN | C62-C61 | 2.05 | 1.56 | 1.50 |
| 5 | S | 301 | TQN | C62-C61 | 2.05 | 1.56 | 1.50 |
| 4 | K | 302 | TLW | O6-C6 | -2.05 | 1.40 | 1.44 |
| 5 | Z | 301 | TQN | C62-C61 | 2.05 | 1.56 | 1.50 |
| 4 | Q | 302 | TLW | O6-C6 | -2.05 | 1.40 | 1.44 |
| 4 | U | 302 | TLW | O6-C6 | -2.05 | 1.40 | 1.44 |
| 5 | N | 301 | TQN | C62-C61 | 2.05 | 1.56 | 1.50 |
| 4 | A | 301 | TLW | O6-C6 | -2.05 | 1.40 | 1.44 |
| 5 | C | 301 | TQN | C62-C61 | 2.04 | 1.56 | 1.50 |
| 5 | P | 301 | TQN | C62-C61 | 2.04 | 1.56 | 1.50 |
| 4 | A | 303 | TLW | O6-C6 | -2.04 | 1.40 | 1.44 |
| 4 | N | 302 | TLW | O6-C6 | -2.04 | 1.40 | 1.44 |
| 5 | O | 301 | TQN | C62-C61 | 2.04 | 1.56 | 1.50 |
| 5 | U | 301 | TQN | C62-C61 | 2.04 | 1.56 | 1.50 |
| 4 | T | 302 | TLW | O6-C6 | -2.03 | 1.40 | 1.44 |
| 5 | M | 301 | TQN | C62-C61 | 2.03 | 1.56 | 1.50 |
| 5 | G | 301 | TQN | C62-C61 | 2.03 | 1.56 | 1.50 |
| 5 | T | 301 | TQN | C62-C61 | 2.03 | 1.56 | 1.50 |
| 4 | H | 302 | TLW | O6-C6 | -2.03 | 1.40 | 1.44 |
| 5 | L | 301 | TQN | C62-C61 | 2.03 | 1.56 | 1.50 |
| 5 | W | 301 | TQN | C22-C21 | 2.03 | 1.56 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | M | 301 | TQN | C22-C21 | 2.03 | 1.56 | 1.50 |
| 5 | R | 301 | TQN | C62-C61 | 2.03 | 1.56 | 1.50 |
| 4 | S | 302 | TLW | O6-C6 | -2.03 | 1.40 | 1.44 |
| 5 | X | 301 | TQN | C22-C21 | 2.03 | 1.56 | 1.50 |
| 5 | L | 301 | TQN | C22-C21 | 2.03 | 1.56 | 1.50 |
| 5 | G | 301 | TQN | C22-C21 | 2.03 | 1.56 | 1.50 |
| 5 | W | 301 | TQN | C62-C61 | 2.03 | 1.56 | 1.50 |
| 5 | X | 301 | TQN | C62-C61 | 2.02 | 1.56 | 1.50 |
| 5 | J | 301 | TQN | C62-C61 | 2.02 | 1.56 | 1.50 |
| 5 | I | 301 | TQN | C22-C21 | 2.02 | 1.56 | 1.50 |
| 5 | V | 301 | TQN | C22-C21 | 2.02 | 1.56 | 1.50 |
| 5 | F | 301 | TQN | C22-C21 | 2.02 | 1.56 | 1.50 |
| 5 | S | 301 | TQN | C22-C21 | 2.02 | 1.56 | 1.50 |
| 5 | C | 301 | TQN | C22-C21 | 2.02 | 1.56 | 1.50 |
| 5 | Y | 301 | TQN | C62-C61 | 2.02 | 1.56 | 1.50 |
| 5 | B | 301 | TQN | C22-C21 | 2.02 | 1.56 | 1.50 |
| 5 | O | 301 | TQN | C22-C21 | 2.02 | 1.56 | 1.50 |
| 5 | I | 301 | TQN | C62-C61 | 2.02 | 1.56 | 1.50 |
| 4 | J | 302 | TLW | O6-C6 | -2.01 | 1.40 | 1.44 |
| 4 | W | 302 | TLW | O6-C6 | -2.01 | 1.40 | 1.44 |
| 5 | H | 301 | TQN | C22-C21 | 2.01 | 1.56 | 1.50 |
| 4 | D | 302 | TLW | O6-C6 | -2.01 | 1.40 | 1.44 |
| 5 | P | 301 | TQN | C22-C21 | 2.01 | 1.56 | 1.50 |
| 4 | C | 302 | TLW | O6-C6 | -2.01 | 1.40 | 1.44 |
| 4 | P | 302 | TLW | O6-C6 | -2.01 | 1.40 | 1.44 |
| 5 | A | 302 | TQN | C62-C61 | 2.01 | 1.56 | 1.50 |
| 5 | J | 301 | TQN | C22-C21 | 2.01 | 1.56 | 1.50 |
| 5 | A | 302 | TQN | C22-C21 | 2.01 | 1.56 | 1.50 |
| 5 | N | 301 | TQN | C22-C21 | 2.01 | 1.56 | 1.50 |
| 4 | X | 302 | TLW | O6-C6 | -2.00 | 1.40 | 1.44 |
| 4 | E | 302 | TLW | O6-C6 | -2.00 | 1.40 | 1.44 |
| 4 | R | 302 | TLW | O6-C6 | -2.00 | 1.40 | 1.44 |

All (433) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | B | 302 | TLW | O6-C2-C1 | 8.01 | 122.85 | 107.72 |
| 4 | H | 302 | TLW | O6-C2-C1 | 8.01 | 122.84 | 107.72 |
| 4 | G | 302 | TLW | O6-C2-C1 | 8.01 | 122.84 | 107.72 |
| 4 | P | 302 | TLW | O6-C2-C1 | 8.00 | 122.83 | 107.72 |
| 4 | A | 303 | TLW | O6-C2-C1 | 8.00 | 122.83 | 107.72 |
| 4 | V | 302 | TLW | O6-C2-C1 | 8.00 | 122.83 | 107.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | I | 302 | TLW | O6-C2-C1 | 8.00 | 122.82 | 107.72 |
| 4 | N | 302 | TLW | O6-C2-C1 | 8.00 | 122.82 | 107.72 |
| 4 | U | 302 | TLW | O6-C2-C1 | 8.00 | 122.82 | 107.72 |
| 4 | S | 302 | TLW | O6-C2-C1 | 7.99 | 122.81 | 107.72 |
| 4 | O | 302 | TLW | O6-C2-C1 | 7.99 | 122.81 | 107.72 |
| 4 | R | 302 | TLW | O6-C2-C1 | 7.99 | 122.81 | 107.72 |
| 4 | T | 302 | TLW | O6-C2-C1 | 7.99 | 122.81 | 107.72 |
| 4 | W | 302 | TLW | O6-C2-C1 | 7.99 | 122.81 | 107.72 |
| 4 | Y | 302 | TLW | O6-C2-C1 | 7.99 | 122.80 | 107.72 |
| 4 | C | 302 | TLW | O6-C2-C1 | 7.99 | 122.80 | 107.72 |
| 4 | K | 302 | TLW | O6-C2-C1 | 7.99 | 122.80 | 107.72 |
| 4 | A | 301 | TLW | O6-C2-C1 | 7.99 | 122.80 | 107.72 |
| 4 | J | 302 | TLW | O6-C2-C1 | 7.99 | 122.80 | 107.72 |
| 4 | L | 302 | TLW | O6-C2-C1 | 7.98 | 122.79 | 107.72 |
| 4 | F | 302 | TLW | O6-C2-C1 | 7.98 | 122.78 | 107.72 |
| 4 | Q | 302 | TLW | O6-C2-C1 | 7.97 | 122.77 | 107.72 |
| 4 | D | 302 | TLW | O6-C2-C1 | 7.97 | 122.77 | 107.72 |
| 4 | X | 302 | TLW | O6-C2-C1 | 7.97 | 122.76 | 107.72 |
| 4 | E | 302 | TLW | O6-C2-C1 | 7.96 | 122.74 | 107.72 |
| 4 | M | 302 | TLW | O6-C2-C1 | 7.96 | 122.74 | 107.72 |
| 5 | V | 301 | TQN | OB3-C71-C72 | 4.87 | 120.15 | 111.43 |
| 5 | S | 301 | TQN | OB3-C71-C72 | 4.86 | 120.15 | 111.43 |
| 5 | B | 301 | TQN | OB3-C71-C72 | 4.86 | 120.14 | 111.43 |
| 5 | W | 301 | TQN | OB3-C71-C72 | 4.86 | 120.14 | 111.43 |
| 5 | X | 301 | TQN | OB3-C71-C72 | 4.86 | 120.13 | 111.43 |
| 5 | R | 301 | TQN | OB3-C71-C72 | 4.85 | 120.13 | 111.43 |
| 5 | Z | 301 | TQN | OB3-C71-C72 | 4.85 | 120.13 | 111.43 |
| 5 | E | 301 | TQN | OB3-C71-C72 | 4.85 | 120.13 | 111.43 |
| 5 | O | 301 | TQN | OB3-C71-C72 | 4.85 | 120.13 | 111.43 |
| 5 | T | 301 | TQN | OB3-C71-C72 | 4.85 | 120.12 | 111.43 |
| 5 | G | 301 | TQN | OB3-C71-C72 | 4.85 | 120.12 | 111.43 |
| 5 | J | 301 | TQN | OB3-C71-C72 | 4.85 | 120.12 | 111.43 |
| 5 | D | 301 | TQN | OB3-C71-C72 | 4.85 | 120.12 | 111.43 |
| 5 | Q | 301 | TQN | OB3-C71-C72 | 4.85 | 120.12 | 111.43 |
| 5 | M | 301 | TQN | OB3-C71-C72 | 4.85 | 120.12 | 111.43 |
| 5 | N | 301 | TQN | OB3-C71-C72 | 4.85 | 120.12 | 111.43 |
| 5 | C | 301 | TQN | OB3-C71-C72 | 4.84 | 120.11 | 111.43 |
| 5 | Y | 301 | TQN | OB3-C71-C72 | 4.84 | 120.11 | 111.43 |
| 5 | H | 301 | TQN | OB3-C71-C72 | 4.84 | 120.10 | 111.43 |
| 5 | P | 301 | TQN | OB3-C71-C72 | 4.84 | 120.10 | 111.43 |
| 5 | I | 301 | TQN | OB3-C71-C72 | 4.84 | 120.10 | 111.43 |
| 5 | L | 301 | TQN | OB3-C71-C72 | 4.84 | 120.10 | 111.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | A | 302 | TQN | OB3-C71-C72 | 4.83 | 120.09 | 111.43 |
| 5 | U | 301 | TQN | OB3-C71-C72 | 4.83 | 120.08 | 111.43 |
| 5 | K | 301 | TQN | OB3-C71-C72 | 4.83 | 120.08 | 111.43 |
| 5 | F | 301 | TQN | OB3-C71-C72 | 4.82 | 120.08 | 111.43 |
| 5 | I | 301 | TQN | OA3-C31-C32 | 4.40 | 119.32 | 111.43 |
| 5 | G | 301 | TQN | OA3-C31-C32 | 4.39 | 119.29 | 111.43 |
| 5 | L | 301 | TQN | OA3-C31-C32 | 4.39 | 119.29 | 111.43 |
| 5 | V | 301 | TQN | OA3-C31-C32 | 4.38 | 119.29 | 111.43 |
| 5 | C | 301 | TQN | OA3-C31-C32 | 4.38 | 119.28 | 111.43 |
| 5 | K | 301 | TQN | OA3-C31-C32 | 4.38 | 119.28 | 111.43 |
| 5 | J | 301 | TQN | OA3-C31-C32 | 4.38 | 119.28 | 111.43 |
| 5 | A | 302 | TQN | OA3-C31-C32 | 4.38 | 119.27 | 111.43 |
| 5 | N | 301 | TQN | OA3-C31-C32 | 4.38 | 119.27 | 111.43 |
| 5 | E | 301 | TQN | OA3-C31-C32 | 4.37 | 119.27 | 111.43 |
| 5 | M | 301 | TQN | OA3-C31-C32 | 4.37 | 119.27 | 111.43 |
| 5 | P | 301 | TQN | OA3-C31-C32 | 4.37 | 119.27 | 111.43 |
| 5 | B | 301 | TQN | OA3-C31-C32 | 4.37 | 119.26 | 111.43 |
| 5 | O | 301 | TQN | OA3-C31-C32 | 4.37 | 119.26 | 111.43 |
| 5 | W | 301 | TQN | OA3-C31-C32 | 4.37 | 119.26 | 111.43 |
| 5 | Q | 301 | TQN | OA3-C31-C32 | 4.36 | 119.25 | 111.43 |
| 5 | R | 301 | TQN | OA3-C31-C32 | 4.36 | 119.25 | 111.43 |
| 5 | H | 301 | TQN | OA3-C31-C32 | 4.36 | 119.25 | 111.43 |
| 5 | U | 301 | TQN | OA3-C31-C32 | 4.36 | 119.25 | 111.43 |
| 5 | X | 301 | TQN | OA3-C31-C32 | 4.36 | 119.24 | 111.43 |
| 5 | D | 301 | TQN | OA3-C31-C32 | 4.35 | 119.23 | 111.43 |
| 5 | F | 301 | TQN | OA3-C31-C32 | 4.35 | 119.23 | 111.43 |
| 5 | S | 301 | TQN | OA3-C31-C32 | 4.35 | 119.23 | 111.43 |
| 5 | Y | 301 | TQN | OA3-C31-C32 | 4.34 | 119.21 | 111.43 |
| 5 | T | 301 | TQN | OA3-C31-C32 | 4.34 | 119.21 | 111.43 |
| 5 | Z | 301 | TQN | OA3-C31-C32 | 4.34 | 119.20 | 111.43 |
| 5 | P | 301 | TQN | O13-C21-C22 | 4.12 | 120.40 | 111.48 |
| 5 | I | 301 | TQN | O13-C21-C22 | 4.12 | 120.40 | 111.48 |
| 5 | Q | 301 | TQN | O13-C21-C22 | 4.12 | 120.40 | 111.48 |
| 5 | D | 301 | TQN | O13-C21-C22 | 4.12 | 120.39 | 111.48 |
| 5 | Z | 301 | TQN | O13-C21-C22 | 4.12 | 120.39 | 111.48 |
| 5 | B | 301 | TQN | O13-C21-C22 | 4.11 | 120.38 | 111.48 |
| 5 | L | 301 | TQN | O13-C21-C22 | 4.11 | 120.38 | 111.48 |
| 5 | E | 301 | TQN | O13-C21-C22 | 4.11 | 120.38 | 111.48 |
| 5 | Y | 301 | TQN | O13-C21-C22 | 4.11 | 120.37 | 111.48 |
| 5 | R | 301 | TQN | O13-C21-C22 | 4.11 | 120.37 | 111.48 |
| 5 | S | 301 | TQN | O13-C21-C22 | 4.11 | 120.37 | 111.48 |
| 5 | N | 301 | TQN | O13-C21-C22 | 4.11 | 120.37 | 111.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | J | 301 | TQN | O13-C21-C22 | 4.11 | 120.36 | 111.48 |
| 5 | T | 301 | TQN | O13-C21-C22 | 4.11 | 120.36 | 111.48 |
| 5 | K | 301 | TQN | O13-C21-C22 | 4.11 | 120.36 | 111.48 |
| 5 | F | 301 | TQN | O13-C21-C22 | 4.11 | 120.36 | 111.48 |
| 5 | V | 301 | TQN | O13-C21-C22 | 4.10 | 120.35 | 111.48 |
| 5 | O | 301 | TQN | O13-C21-C22 | 4.10 | 120.35 | 111.48 |
| 5 | M | 301 | TQN | O13-C21-C22 | 4.10 | 120.34 | 111.48 |
| 5 | U | 301 | TQN | O13-C21-C22 | 4.10 | 120.34 | 111.48 |
| 5 | W | 301 | TQN | O13-C21-C22 | 4.09 | 120.34 | 111.48 |
| 5 | A | 302 | TQN | O13-C21-C22 | 4.09 | 120.33 | 111.48 |
| 5 | R | 301 | TQN | O53-C61-C62 | 4.09 | 120.33 | 111.48 |
| 5 | X | 301 | TQN | O13-C21-C22 | 4.09 | 120.33 | 111.48 |
| 5 | H | 301 | TQN | O13-C21-C22 | 4.09 | 120.32 | 111.48 |
| 5 | W | 301 | TQN | O53-C61-C62 | 4.09 | 120.32 | 111.48 |
| 5 | T | 301 | TQN | O53-C61-C62 | 4.08 | 120.32 | 111.48 |
| 5 | G | 301 | TQN | O13-C21-C22 | 4.08 | 120.31 | 111.48 |
| 5 | C | 301 | TQN | O13-C21-C22 | 4.08 | 120.31 | 111.48 |
| 5 | L | 301 | TQN | O53-C61-C62 | 4.08 | 120.31 | 111.48 |
| 5 | Y | 301 | TQN | O53-C61-C62 | 4.08 | 120.31 | 111.48 |
| 5 | X | 301 | TQN | O53-C61-C62 | 4.08 | 120.31 | 111.48 |
| 5 | S | 301 | TQN | O53-C61-C62 | 4.08 | 120.31 | 111.48 |
| 5 | G | 301 | TQN | O53-C61-C62 | 4.08 | 120.30 | 111.48 |
| 5 | A | 302 | TQN | O53-C61-C62 | 4.08 | 120.30 | 111.48 |
| 5 | M | 301 | TQN | O53-C61-C62 | 4.08 | 120.30 | 111.48 |
| 5 | E | 301 | TQN | O53-C61-C62 | 4.08 | 120.30 | 111.48 |
| 5 | I | 301 | TQN | O53-C61-C62 | 4.08 | 120.30 | 111.48 |
| 5 | C | 301 | TQN | O53-C61-C62 | 4.07 | 120.29 | 111.48 |
| 5 | J | 301 | TQN | O53-C61-C62 | 4.07 | 120.29 | 111.48 |
| 5 | O | 301 | TQN | O53-C61-C62 | 4.07 | 120.28 | 111.48 |
| 5 | P | 301 | TQN | O53-C61-C62 | 4.07 | 120.28 | 111.48 |
| 5 | Z | 301 | TQN | O53-C61-C62 | 4.06 | 120.27 | 111.48 |
| 5 | N | 301 | TQN | O53-C61-C62 | 4.06 | 120.27 | 111.48 |
| 5 | V | 301 | TQN | O53-C61-C62 | 4.06 | 120.27 | 111.48 |
| 5 | F | 301 | TQN | O53-C61-C62 | 4.06 | 120.26 | 111.48 |
| 5 | B | 301 | TQN | O53-C61-C62 | 4.06 | 120.26 | 111.48 |
| 5 | U | 301 | TQN | O53-C61-C62 | 4.05 | 120.25 | 111.48 |
| 5 | H | 301 | TQN | O53-C61-C62 | 4.05 | 120.24 | 111.48 |
| 5 | D | 301 | TQN | O53-C61-C62 | 4.05 | 120.24 | 111.48 |
| 5 | Q | 301 | TQN | O53-C61-C62 | 4.05 | 120.24 | 111.48 |
| 5 | K | 301 | TQN | O53-C61-C62 | 4.05 | 120.23 | 111.48 |
| 5 | C | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.94 | 114.37 |
| 5 | G | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.94 | 114.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | A | 302 | TQN | CE1-CD9-C59 | 3.87 | 133.93 | 114.37 |
| 5 | I | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.93 | 114.37 |
| 5 | U | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.93 | 114.37 |
| 5 | N | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.92 | 114.37 |
| 5 | O | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.92 | 114.37 |
| 5 | T | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.92 | 114.37 |
| 5 | R | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.91 | 114.37 |
| 5 | P | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.91 | 114.37 |
| 5 | S | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.91 | 114.37 |
| 5 | Y | 301 | TQN | CE1-CD9-C59 | 3.87 | 133.91 | 114.37 |
| 5 | B | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.90 | 114.37 |
| 5 | E | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.90 | 114.37 |
| 5 | K | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.90 | 114.37 |
| 5 | L | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.89 | 114.37 |
| 5 | D | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.89 | 114.37 |
| 5 | H | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.89 | 114.37 |
| 5 | J | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.88 | 114.37 |
| 5 | W | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.88 | 114.37 |
| 5 | Q | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.87 | 114.37 |
| 5 | X | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.87 | 114.37 |
| 5 | V | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.86 | 114.37 |
| 5 | M | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.86 | 114.37 |
| 5 | Z | 301 | TQN | CE1-CD9-C59 | 3.86 | 133.86 | 114.37 |
| 5 | F | 301 | TQN | CE1-CD9-C59 | 3.85 | 133.85 | 114.37 |
| 5 | I | 301 | TQN | O73-C81-C82 | 3.69 | 119.46 | 111.48 |
| 5 | Y | 301 | TQN | O73-C81-C82 | 3.68 | 119.44 | 111.48 |
| 5 | Q | 301 | TQN | O73-C81-C82 | 3.68 | 119.43 | 111.48 |
| 5 | O | 301 | TQN | O73-C81-C82 | 3.67 | 119.43 | 111.48 |
| 5 | U | 301 | TQN | O73-C81-C82 | 3.67 | 119.43 | 111.48 |
| 5 | V | 301 | TQN | O73-C81-C82 | 3.67 | 119.42 | 111.48 |
| 5 | K | 301 | TQN | O73-C81-C82 | 3.67 | 119.42 | 111.48 |
| 5 | J | 301 | TQN | O73-C81-C82 | 3.67 | 119.41 | 111.48 |
| 5 | A | 302 | TQN | O73-C81-C82 | 3.66 | 119.41 | 111.48 |
| 5 | G | 301 | TQN | O73-C81-C82 | 3.66 | 119.40 | 111.48 |
| 5 | T | 301 | TQN | O73-C81-C82 | 3.66 | 119.40 | 111.48 |
| 5 | Z | 301 | TQN | O73-C81-C82 | 3.66 | 119.40 | 111.48 |
| 5 | E | 301 | TQN | O73-C81-C82 | 3.66 | 119.40 | 111.48 |
| 5 | M | 301 | TQN | O73-C81-C82 | 3.66 | 119.40 | 111.48 |
| 5 | B | 301 | TQN | O73-C81-C82 | 3.66 | 119.39 | 111.48 |
| 5 | D | 301 | TQN | O73-C81-C82 | 3.66 | 119.39 | 111.48 |
| 5 | L | 301 | TQN | O73-C81-C82 | 3.66 | 119.39 | 111.48 |
| 5 | F | 301 | TQN | O73-C81-C82 | 3.66 | 119.39 | 111.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | S | 301 | TQN | O73-C81-C82 | 3.65 | 119.39 | 111.48 |
| 5 | R | 301 | TQN | O73-C81-C82 | 3.65 | 119.38 | 111.48 |
| 5 | X | 301 | TQN | O73-C81-C82 | 3.65 | 119.38 | 111.48 |
| 5 | N | 301 | TQN | O73-C81-C82 | 3.65 | 119.38 | 111.48 |
| 5 | H | 301 | TQN | O73-C81-C82 | 3.65 | 119.38 | 111.48 |
| 5 | C | 301 | TQN | O73-C81-C82 | 3.65 | 119.38 | 111.48 |
| 5 | P | 301 | TQN | O73-C81-C82 | 3.65 | 119.37 | 111.48 |
| 5 | W | 301 | TQN | O73-C81-C82 | 3.64 | 119.36 | 111.48 |
| 5 | E | 301 | TQN | C52-C51-NB2 | 3.03 | 120.39 | 116.25 |
| 5 | T | 301 | TQN | C52-C51-NB2 | 3.02 | 120.38 | 116.25 |
| 5 | S | 301 | TQN | C52-C51-NB2 | 3.01 | 120.37 | 116.25 |
| 5 | L | 301 | TQN | C52-C51-NB2 | 3.01 | 120.37 | 116.25 |
| 5 | P | 301 | TQN | C52-C51-NB2 | 3.01 | 120.37 | 116.25 |
| 5 | Z | 301 | TQN | C52-C51-NB2 | 3.01 | 120.36 | 116.25 |
| 5 | J | 301 | TQN | C52-C51-NB2 | 3.01 | 120.36 | 116.25 |
| 5 | M | 301 | TQN | C52-C51-NB2 | 3.01 | 120.36 | 116.25 |
| 5 | Q | 301 | TQN | C52-C51-NB2 | 3.01 | 120.36 | 116.25 |
| 5 | G | 301 | TQN | C52-C51-NB2 | 3.00 | 120.36 | 116.25 |
| 5 | K | 301 | TQN | C52-C51-NB2 | 3.00 | 120.36 | 116.25 |
| 5 | W | 301 | TQN | C52-C51-NB2 | 3.00 | 120.36 | 116.25 |
| 5 | N | 301 | TQN | C52-C51-NB2 | 3.00 | 120.35 | 116.25 |
| 5 | H | 301 | TQN | C52-C51-NB2 | 3.00 | 120.35 | 116.25 |
| 5 | B | 301 | TQN | C52-C51-NB2 | 2.99 | 120.34 | 116.25 |
| 5 | X | 301 | TQN | C52-C51-NB2 | 2.99 | 120.34 | 116.25 |
| 5 | C | 301 | TQN | C52-C51-NB2 | 2.99 | 120.34 | 116.25 |
| 5 | F | 301 | TQN | C52-C51-NB2 | 2.99 | 120.34 | 116.25 |
| 5 | D | 301 | TQN | C52-C51-NB2 | 2.99 | 120.34 | 116.25 |
| 5 | R | 301 | TQN | C52-C51-NB2 | 2.99 | 120.34 | 116.25 |
| 5 | O | 301 | TQN | C52-C51-NB2 | 2.99 | 120.33 | 116.25 |
| 5 | I | 301 | TQN | C52-C51-NB2 | 2.99 | 120.33 | 116.25 |
| 5 | V | 301 | TQN | C52-C51-NB2 | 2.99 | 120.33 | 116.25 |
| 5 | Y | 301 | TQN | C52-C51-NB2 | 2.98 | 120.33 | 116.25 |
| 5 | A | 302 | TQN | C52-C51-NB2 | 2.98 | 120.32 | 116.25 |
| 5 | U | 301 | TQN | C52-C51-NB2 | 2.97 | 120.31 | 116.25 |
| 4 | X | 302 | TLW | O12-C1-C2 | 2.81 | 120.01 | 112.71 |
| 4 | Q | 302 | TLW | O12-C1-C2 | 2.80 | 120.00 | 112.71 |
| 4 | A | 303 | TLW | O12-C1-C2 | 2.80 | 119.99 | 112.71 |
| 4 | I | 302 | TLW | O12-C1-C2 | 2.80 | 119.98 | 112.71 |
| 4 | O | 302 | TLW | O12-C1-C2 | 2.80 | 119.98 | 112.71 |
| 4 | B | 302 | TLW | O12-C1-C2 | 2.80 | 119.98 | 112.71 |
| 4 | U | 302 | TLW | O12-C1-C2 | 2.80 | 119.98 | 112.71 |
| 4 | W | 302 | TLW | O12-C1-C2 | 2.79 | 119.98 | 112.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | C | 302 | TLW | O12-C1-C2 | 2.79 | 119.98 | 112.71 |
| 4 | N | 302 | TLW | O12-C1-C2 | 2.79 | 119.98 | 112.71 |
| 4 | P | 302 | TLW | O12-C1-C2 | 2.79 | 119.97 | 112.71 |
| 4 | G | 302 | TLW | O12-C1-C2 | 2.79 | 119.97 | 112.71 |
| 4 | E | 302 | TLW | O12-C1-C2 | 2.79 | 119.97 | 112.71 |
| 4 | F | 302 | TLW | O12-C1-C2 | 2.79 | 119.97 | 112.71 |
| 4 | D | 302 | TLW | O12-C1-C2 | 2.79 | 119.97 | 112.71 |
| 4 | R | 302 | TLW | O12-C1-C2 | 2.79 | 119.97 | 112.71 |
| 4 | T | 302 | TLW | O12-C1-C2 | 2.79 | 119.97 | 112.71 |
| 4 | A | 301 | TLW | O12-C1-C2 | 2.79 | 119.97 | 112.71 |
| 4 | M | 302 | TLW | O12-C1-C2 | 2.79 | 119.96 | 112.71 |
| 4 | H | 302 | TLW | O12-C1-C2 | 2.79 | 119.96 | 112.71 |
| 4 | L | 302 | TLW | O12-C1-C2 | 2.78 | 119.95 | 112.71 |
| 4 | J | 302 | TLW | O12-C1-C2 | 2.78 | 119.95 | 112.71 |
| 4 | S | 302 | TLW | O12-C1-C2 | 2.78 | 119.94 | 112.71 |
| 4 | K | 302 | TLW | O12-C1-C2 | 2.78 | 119.94 | 112.71 |
| 4 | V | 302 | TLW | O12-C1-C2 | 2.78 | 119.93 | 112.71 |
| 4 | Y | 302 | TLW | O12-C1-C2 | 2.77 | 119.93 | 112.71 |
| 5 | J | 301 | TQN | OP2-PB-OB4 | 2.27 | 114.69 | 105.85 |
| 5 | U | 301 | TQN | OP2-PB-OB4 | 2.27 | 114.69 | 105.85 |
| 5 | I | 301 | TQN | OP2-PB-OB4 | 2.27 | 114.68 | 105.85 |
| 5 | S | 301 | TQN | OP2-PB-OB4 | 2.27 | 114.68 | 105.85 |
| 5 | W | 301 | TQN | OP2-PB-OB4 | 2.27 | 114.68 | 105.85 |
| 5 | Y | 301 | TQN | OP2-PB-OB4 | 2.27 | 114.68 | 105.85 |
| 5 | R | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.67 | 105.85 |
| 5 | D | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.67 | 105.85 |
| 5 | P | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.67 | 105.85 |
| 5 | X | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.66 | 105.85 |
| 5 | L | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.66 | 105.85 |
| 5 | T | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.66 | 105.85 |
| 5 | V | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.66 | 105.85 |
| 5 | M | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.66 | 105.85 |
| 5 | Q | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.66 | 105.85 |
| 5 | F | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.65 | 105.85 |
| 5 | K | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.65 | 105.85 |
| 5 | N | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.65 | 105.85 |
| 5 | O | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.64 | 105.85 |
| 5 | A | 302 | TQN | OP2-PB-OB4 | 2.26 | 114.64 | 105.85 |
| 5 | B | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.64 | 105.85 |
| 5 | G | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.64 | 105.85 |
| 5 | Z | 301 | TQN | OP2-PB-OB4 | 2.26 | 114.64 | 105.85 |
| 5 | C | 301 | TQN | OP2-PB-OB4 | 2.25 | 114.63 | 105.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | H | 301 | TQN | OP2-PB-OB4 | 2.25 | 114.63 | 105.85 |
| 5 | E | 301 | TQN | OP2-PB-OB4 | 2.25 | 114.62 | 105.85 |
| 4 | S | 302 | TLW | O6-C6-C5 | 2.22 | 111.07 | 107.94 |
| 4 | D | 302 | TLW | O6-C6-C5 | 2.21 | 111.06 | 107.94 |
| 5 | L | 301 | TQN | C12-C11-NA2 | 2.20 | 119.26 | 116.25 |
| 5 | I | 301 | TQN | C12-C11-NA2 | 2.20 | 119.26 | 116.25 |
| 5 | H | 301 | TQN | C12-C11-NA2 | 2.20 | 119.25 | 116.25 |
| 4 | A | 301 | TLW | O6-C6-C5 | 2.19 | 111.04 | 107.94 |
| 4 | R | 302 | TLW | O6-C6-C5 | 2.19 | 111.04 | 107.94 |
| 5 | W | 301 | TQN | C12-C11-NA2 | 2.19 | 119.24 | 116.25 |
| 4 | L | 302 | TLW | O6-C6-C5 | 2.19 | 111.03 | 107.94 |
| 4 | X | 302 | TLW | O6-C6-C5 | 2.19 | 111.03 | 107.94 |
| 4 | E | 302 | TLW | O6-C6-C5 | 2.18 | 111.03 | 107.94 |
| 4 | V | 302 | TLW | O6-C6-C5 | 2.18 | 111.03 | 107.94 |
| 5 | F | 301 | TQN | C12-C11-NA2 | 2.18 | 119.23 | 116.25 |
| 4 | K | 302 | TLW | O6-C6-C5 | 2.18 | 111.02 | 107.94 |
| 5 | P | 301 | TQN | C12-C11-NA2 | 2.18 | 119.23 | 116.25 |
| 5 | S | 301 | TQN | C12-C11-NA2 | 2.18 | 119.23 | 116.25 |
| 5 | X | 301 | TQN | C12-C11-NA2 | 2.18 | 119.23 | 116.25 |
| 4 | Q | 302 | TLW | O6-C6-C5 | 2.18 | 111.02 | 107.94 |
| 5 | C | 301 | TQN | C12-C11-NA2 | 2.18 | 119.22 | 116.25 |
| 5 | O | 301 | TQN | C12-C11-NA2 | 2.18 | 119.22 | 116.25 |
| 4 | M | 302 | TLW | O6-C6-C5 | 2.18 | 111.02 | 107.94 |
| 4 | J | 302 | TLW | O6-C6-C5 | 2.17 | 111.01 | 107.94 |
| 4 | I | 302 | TLW | O6-C6-C5 | 2.17 | 111.01 | 107.94 |
| 5 | Q | 301 | TQN | C12-C11-NA2 | 2.17 | 119.22 | 116.25 |
| 5 | R | 301 | TQN | C12-C11-NA2 | 2.17 | 119.22 | 116.25 |
| 5 | M | 301 | TQN | C12-C11-NA2 | 2.17 | 119.22 | 116.25 |
| 4 | U | 302 | TLW | O6-C6-C5 | 2.17 | 111.01 | 107.94 |
| 5 | V | 301 | TQN | C12-C11-NA2 | 2.17 | 119.22 | 116.25 |
| 4 | F | 302 | TLW | O6-C6-C5 | 2.17 | 111.01 | 107.94 |
| 5 | K | 301 | TQN | C12-C11-NA2 | 2.17 | 119.22 | 116.25 |
| 4 | Y | 302 | TLW | O6-C6-C5 | 2.17 | 111.00 | 107.94 |
| 5 | B | 301 | TQN | C12-C11-NA2 | 2.17 | 119.21 | 116.25 |
| 4 | T | 302 | TLW | O6-C6-C5 | 2.17 | 111.00 | 107.94 |
| 5 | D | 301 | TQN | C12-C11-NA2 | 2.16 | 119.21 | 116.25 |
| 5 | E | 301 | TQN | C12-C11-NA2 | 2.16 | 119.21 | 116.25 |
| 4 | H | 302 | TLW | O6-C6-C5 | 2.16 | 111.00 | 107.94 |
| 4 | O | 302 | TLW | O6-C6-C5 | 2.16 | 110.99 | 107.94 |
| 5 | Y | 301 | TQN | OP7-PA-OA1 | 2.16 | 114.27 | 105.85 |
| 4 | P | 302 | TLW | O6-C6-C5 | 2.16 | 110.99 | 107.94 |
| 5 | N | 301 | TQN | C12-C11-NA2 | 2.16 | 119.20 | 116.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | U | 301 | TQN | OP7-PA-OA1 | 2.16 | 114.26 | 105.85 |
| 5 | G | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.24 | 105.85 |
| 5 | I | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.24 | 105.85 |
| 5 | H | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.24 | 105.85 |
| 5 | A | 302 | TQN | C12-C11-NA2 | 2.15 | 119.19 | 116.25 |
| 5 | O | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.24 | 105.85 |
| 5 | M | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.23 | 105.85 |
| 4 | B | 302 | TLW | O6-C6-C5 | 2.15 | 110.98 | 107.94 |
| 5 | E | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.23 | 105.85 |
| 5 | B | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.23 | 105.85 |
| 5 | V | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.23 | 105.85 |
| 5 | S | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.22 | 105.85 |
| 5 | Z | 301 | TQN | C12-C11-NA2 | 2.15 | 119.19 | 116.25 |
| 5 | Q | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.22 | 105.85 |
| 4 | N | 302 | TLW | O6-C6-C5 | 2.15 | 110.98 | 107.94 |
| 4 | A | 303 | TLW | O6-C6-C5 | 2.15 | 110.97 | 107.94 |
| 5 | L | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.22 | 105.85 |
| 5 | R | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.21 | 105.85 |
| 5 | N | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.21 | 105.85 |
| 5 | J | 301 | TQN | C12-C11-NA2 | 2.15 | 119.18 | 116.25 |
| 5 | C | 301 | TQN | OP7-PA-OA1 | 2.15 | 114.21 | 105.85 |
| 5 | F | 301 | TQN | OP7-PA-OA1 | 2.14 | 114.21 | 105.85 |
| 5 | K | 301 | TQN | OP7-PA-OA1 | 2.14 | 114.20 | 105.85 |
| 5 | Z | 301 | TQN | OP7-PA-OA1 | 2.14 | 114.20 | 105.85 |
| 4 | G | 302 | TLW | O6-C6-C5 | 2.14 | 110.97 | 107.94 |
| 4 | W | 302 | TLW | O6-C6-C5 | 2.14 | 110.97 | 107.94 |
| 5 | J | 301 | TQN | OP7-PA-OA1 | 2.14 | 114.20 | 105.85 |
| 5 | W | 301 | TQN | OP7-PA-OA1 | 2.14 | 114.20 | 105.85 |
| 5 | U | 301 | TQN | C12-C11-NA2 | 2.14 | 119.18 | 116.25 |
| 5 | X | 301 | TQN | OP7-PA-OA1 | 2.14 | 114.20 | 105.85 |
| 5 | Y | 301 | TQN | C12-C11-NA2 | 2.14 | 119.18 | 116.25 |
| 5 | T | 301 | TQN | C12-C11-NA2 | 2.14 | 119.18 | 116.25 |
| 5 | T | 301 | TQN | OP7-PA-OA1 | 2.14 | 114.19 | 105.85 |
| 5 | P | 301 | TQN | OP7-PA-OA1 | 2.14 | 114.18 | 105.85 |
| 5 | G | 301 | TQN | C12-C11-NA2 | 2.14 | 119.17 | 116.25 |
| 5 | A | 302 | TQN | OP7-PA-OA1 | 2.14 | 114.18 | 105.85 |
| 5 | D | 301 | TQN | OP7-PA-OA1 | 2.13 | 114.17 | 105.85 |
| 4 | C | 302 | TLW | O6-C6-C5 | 2.13 | 110.95 | 107.94 |
| 5 | N | 301 | TQN | OP6-PA-OA1 | 2.13 | 114.14 | 105.85 |
| 5 | B | 301 | TQN | OP6-PA-OA1 | 2.13 | 114.14 | 105.85 |
| 5 | A | 302 | TQN | OP6-PA-OA1 | 2.12 | 114.13 | 105.85 |
| 5 | M | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.13 | 105.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | L | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.13 | 105.85 |
| 5 | O | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.12 | 105.85 |
| 5 | T | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.12 | 105.85 |
| 5 | E | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.12 | 105.85 |
| 5 | W | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.12 | 105.85 |
| 5 | D | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.12 | 105.85 |
| 5 | X | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.12 | 105.85 |
| 5 | C | 301 | TQN | OP3-PB-OB4 | 2.12 | 114.12 | 105.85 |
| 5 | Y | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.12 | 105.85 |
| 5 | R | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.11 | 105.85 |
| 5 | O | 301 | TQN | OP3-PB-OB4 | 2.12 | 114.11 | 105.85 |
| 5 | Y | 301 | TQN | OP3-PB-OB4 | 2.12 | 114.11 | 105.85 |
| 5 | P | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.11 | 105.85 |
| 5 | F | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.10 | 105.85 |
| 5 | U | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.10 | 105.85 |
| 5 | C | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.10 | 105.85 |
| 5 | F | 301 | TQN | OP3-PB-OB4 | 2.12 | 114.10 | 105.85 |
| 5 | Q | 301 | TQN | OP3-PB-OB4 | 2.12 | 114.09 | 105.85 |
| 5 | H | 301 | TQN | OP6-PA-OA1 | 2.12 | 114.09 | 105.85 |
| 5 | D | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.09 | 105.85 |
| 5 | E | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.09 | 105.85 |
| 5 | P | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.09 | 105.85 |
| 5 | J | 301 | TQN | OP6-PA-OA1 | 2.11 | 114.09 | 105.85 |
| 5 | S | 301 | TQN | OP6-PA-OA1 | 2.11 | 114.08 | 105.85 |
| 5 | G | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.08 | 105.85 |
| 5 | K | 301 | TQN | OP6-PA-OA1 | 2.11 | 114.08 | 105.85 |
| 5 | V | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.08 | 105.85 |
| 5 | J | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.08 | 105.85 |
| 5 | K | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.08 | 105.85 |
| 5 | A | 302 | TQN | OP3-PB-OB4 | 2.11 | 114.07 | 105.85 |
| 5 | U | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.07 | 105.85 |
| 5 | V | 301 | TQN | OP6-PA-OA1 | 2.11 | 114.07 | 105.85 |
| 5 | Z | 301 | TQN | OP6-PA-OA1 | 2.11 | 114.07 | 105.85 |
| 5 | B | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.07 | 105.85 |
| 5 | I | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.07 | 105.85 |
| 5 | M | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.07 | 105.85 |
| 5 | N | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.07 | 105.85 |
| 5 | R | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.07 | 105.85 |
| 5 | W | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.06 | 105.85 |
| 5 | I | 301 | TQN | OP6-PA-OA1 | 2.11 | 114.06 | 105.85 |
| 5 | X | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.06 | 105.85 |
| 5 | T | 301 | TQN | OP3-PB-OB4 | 2.11 | 114.05 | 105.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | G | 301 | TQN | OP6-PA-OA1 | 2.10 | 114.05 | 105.85 |
| 5 | Q | 301 | TQN | OP6-PA-OA1 | 2.10 | 114.05 | 105.85 |
| 5 | S | 301 | TQN | OP3-PB-OB4 | 2.10 | 114.05 | 105.85 |
| 5 | E | 301 | TQN | O71-C71-C72 | -2.10 | 119.76 | 124.65 |
| 5 | L | 301 | TQN | OP3-PB-OB4 | 2.10 | 114.04 | 105.85 |
| 5 | Z | 301 | TQN | OP3-PB-OB4 | 2.10 | 114.04 | 105.85 |
| 5 | S | 301 | TQN | O71-C71-C72 | -2.10 | 119.77 | 124.65 |
| 5 | T | 301 | TQN | O71-C71-C72 | -2.10 | 119.77 | 124.65 |
| 5 | H | 301 | TQN | OP3-PB-OB4 | 2.10 | 114.03 | 105.85 |
| 5 | J | 301 | TQN | O71-C71-C72 | -2.10 | 119.77 | 124.65 |
| 5 | A | 302 | TQN | O71-C71-C72 | -2.09 | 119.79 | 124.65 |
| 5 | B | 301 | TQN | O71-C71-C72 | -2.09 | 119.79 | 124.65 |
| 5 | R | 301 | TQN | O71-C71-C72 | -2.09 | 119.79 | 124.65 |
| 5 | D | 301 | TQN | O71-C71-C72 | -2.09 | 119.79 | 124.65 |
| 5 | Q | 301 | TQN | O71-C71-C72 | -2.09 | 119.80 | 124.65 |
| 5 | V | 301 | TQN | O71-C71-C72 | -2.09 | 119.80 | 124.65 |
| 5 | O | 301 | TQN | O71-C71-C72 | -2.09 | 119.80 | 124.65 |
| 5 | G | 301 | TQN | O71-C71-C72 | -2.08 | 119.81 | 124.65 |
| 5 | Z | 301 | TQN | O71-C71-C72 | -2.08 | 119.81 | 124.65 |
| 5 | W | 301 | TQN | O71-C71-C72 | -2.08 | 119.81 | 124.65 |
| 5 | H | 301 | TQN | O71-C71-C72 | -2.08 | 119.82 | 124.65 |
| 5 | I | 301 | TQN | O71-C71-C72 | -2.08 | 119.82 | 124.65 |
| 5 | N | 301 | TQN | O71-C71-C72 | -2.08 | 119.83 | 124.65 |
| 5 | X | 301 | TQN | O71-C71-C72 | -2.08 | 119.83 | 124.65 |
| 5 | M | 301 | TQN | O71-C71-C72 | -2.07 | 119.83 | 124.65 |
| 5 | U | 301 | TQN | O71-C71-C72 | -2.07 | 119.83 | 124.65 |
| 5 | F | 301 | TQN | O71-C71-C72 | -2.07 | 119.84 | 124.65 |
| 5 | C | 301 | TQN | O71-C71-C72 | -2.07 | 119.84 | 124.65 |
| 5 | K | 301 | TQN | O71-C71-C72 | -2.07 | 119.84 | 124.65 |
| 5 | P | 301 | TQN | O71-C71-C72 | -2.07 | 119.84 | 124.65 |
| 5 | Y | 301 | TQN | O71-C71-C72 | -2.07 | 119.85 | 124.65 |
| 5 | L | 301 | TQN | O71-C71-C72 | -2.06 | 119.86 | 124.65 |
| 5 | R | 301 | TQN | O31-C31-C32 | -2.02 | 119.96 | 124.65 |
| 5 | N | 301 | TQN | O31-C31-C32 | -2.01 | 119.97 | 124.65 |
| 5 | B | 301 | TQN | O31-C31-C32 | -2.01 | 119.97 | 124.65 |
| 5 | O | 301 | TQN | O31-C31-C32 | -2.01 | 119.97 | 124.65 |
| 5 | U | 301 | TQN | O31-C31-C32 | -2.01 | 119.98 | 124.65 |
| 5 | K | 301 | TQN | O31-C31-C32 | -2.01 | 119.98 | 124.65 |
| 5 | M | 301 | TQN | O31-C31-C32 | -2.01 | 119.98 | 124.65 |
| 5 | D | 301 | TQN | O31-C31-C32 | -2.01 | 119.98 | 124.65 |
| 5 | I | 301 | TQN | O31-C31-C32 | -2.01 | 119.99 | 124.65 |
| 5 | L | 301 | TQN | O31-C31-C32 | -2.01 | 119.99 | 124.65 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | Q | 301 | TQN | O31-C31-C32 | -2.01 | 119.99 | 124.65 |
| 5 | V | 301 | TQN | O31-C31-C32 | -2.01 | 119.99 | 124.65 |
| 5 | Z | 301 | TQN | O31-C31-C32 | -2.01 | 119.99 | 124.65 |
| 5 | C | 301 | TQN | O31-C31-C32 | -2.00 | 120.00 | 124.65 |
| 5 | P | 301 | TQN | O31-C31-C32 | -2.00 | 120.00 | 124.65 |
| 5 | G | 301 | TQN | CA2-NA2-C11 | -2.00 | 119.95 | 122.90 |
| 5 | M | 301 | TQN | CA2-NA2-C11 | -2.00 | 119.95 | 122.90 |

All (26) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 4 | A | 301 | TLW | C2 |
| 4 | A | 303 | TLW | C2 |
| 4 | B | 302 | TLW | C2 |
| 4 | C | 302 | TLW | C2 |
| 4 | D | 302 | TLW | C2 |
| 4 | E | 302 | TLW | C2 |
| 4 | F | 302 | TLW | C2 |
| 4 | G | 302 | TLW | C2 |
| 4 | H | 302 | TLW | C2 |
| 4 | I | 302 | TLW | C2 |
| 4 | J | 302 | TLW | C2 |
| 4 | K | 302 | TLW | C2 |
| 4 | L | 302 | TLW | C2 |
| 4 | M | 302 | TLW | C2 |
| 4 | N | 302 | TLW | C2 |
| 4 | O | 302 | TLW | C2 |
| 4 | P | 302 | TLW | C2 |
| 4 | Q | 302 | TLW | C2 |
| 4 | R | 302 | TLW | C2 |
| 4 | S | 302 | TLW | C2 |
| 4 | T | 302 | TLW | C2 |
| 4 | U | 302 | TLW | C2 |
| 4 | V | 302 | TLW | C2 |
| 4 | W | 302 | TLW | C2 |
| 4 | X | 302 | TLW | C2 |
| 4 | Y | 302 | TLW | C2 |

All (1508) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | A | 301 | TLW | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | A | 301 | TLW | C5-C6-C7-O7 |
| 4 | A | 301 | TLW | O6-C6-C7-C8 |
| 4 | A | 301 | TLW | O6-C6-C7-O7 |
| 4 | A | 303 | TLW | C5-C6-C7-C8 |
| 4 | A | 303 | TLW | C5-C6-C7-O7 |
| 4 | A | 303 | TLW | O6-C6-C7-C8 |
| 4 | A | 303 | TLW | O6-C6-C7-O7 |
| 4 | B | 302 | TLW | C5-C6-C7-C8 |
| 4 | B | 302 | TLW | C5-C6-C7-O7 |
| 4 | B | 302 | TLW | O6-C6-C7-C8 |
| 4 | B | 302 | TLW | O6-C6-C7-O7 |
| 4 | C | 302 | TLW | C5-C6-C7-C8 |
| 4 | C | 302 | TLW | C5-C6-C7-O7 |
| 4 | C | 302 | TLW | O6-C6-C7-C8 |
| 4 | C | 302 | TLW | O6-C6-C7-O7 |
| 4 | D | 302 | TLW | C5-C6-C7-C8 |
| 4 | D | 302 | TLW | C5-C6-C7-O7 |
| 4 | D | 302 | TLW | O6-C6-C7-C8 |
| 4 | D | 302 | TLW | O6-C6-C7-O7 |
| 4 | E | 302 | TLW | C5-C6-C7-C8 |
| 4 | E | 302 | TLW | C5-C6-C7-O7 |
| 4 | E | 302 | TLW | O6-C6-C7-C8 |
| 4 | E | 302 | TLW | O6-C6-C7-O7 |
| 4 | F | 302 | TLW | C5-C6-C7-C8 |
| 4 | F | 302 | TLW | C5-C6-C7-O7 |
| 4 | F | 302 | TLW | O6-C6-C7-C8 |
| 4 | F | 302 | TLW | O6-C6-C7-O7 |
| 4 | G | 302 | TLW | C5-C6-C7-C8 |
| 4 | G | 302 | TLW | C5-C6-C7-O7 |
| 4 | G | 302 | TLW | O6-C6-C7-C8 |
| 4 | G | 302 | TLW | O6-C6-C7-O7 |
| 4 | H | 302 | TLW | C5-C6-C7-C8 |
| 4 | H | 302 | TLW | C5-C6-C7-O7 |
| 4 | H | 302 | TLW | O6-C6-C7-C8 |
| 4 | H | 302 | TLW | O6-C6-C7-O7 |
| 4 | I | 302 | TLW | C5-C6-C7-C8 |
| 4 | I | 302 | TLW | C5-C6-C7-O7 |
| 4 | I | 302 | TLW | O6-C6-C7-C8 |
| 4 | I | 302 | TLW | O6-C6-C7-O7 |
| 4 | J | 302 | TLW | C5-C6-C7-C8 |
| 4 | J | 302 | TLW | C5-C6-C7-O7 |
| 4 | J | 302 | TLW | O6-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | J | 302 | TLW | O6-C6-C7-O7 |
| 4 | K | 302 | TLW | C5-C6-C7-C8 |
| 4 | K | 302 | TLW | C5-C6-C7-O7 |
| 4 | K | 302 | TLW | O6-C6-C7-C8 |
| 4 | K | 302 | TLW | O6-C6-C7-O7 |
| 4 | L | 302 | TLW | C5-C6-C7-C8 |
| 4 | L | 302 | TLW | C5-C6-C7-O7 |
| 4 | L | 302 | TLW | O6-C6-C7-C8 |
| 4 | L | 302 | TLW | O6-C6-C7-O7 |
| 4 | M | 302 | TLW | C5-C6-C7-C8 |
| 4 | M | 302 | TLW | C5-C6-C7-O7 |
| 4 | M | 302 | TLW | O6-C6-C7-C8 |
| 4 | M | 302 | TLW | O6-C6-C7-O7 |
| 4 | N | 302 | TLW | C5-C6-C7-C8 |
| 4 | N | 302 | TLW | C5-C6-C7-O7 |
| 4 | N | 302 | TLW | O6-C6-C7-C8 |
| 4 | N | 302 | TLW | O6-C6-C7-O7 |
| 4 | O | 302 | TLW | C5-C6-C7-C8 |
| 4 | O | 302 | TLW | C5-C6-C7-O7 |
| 4 | O | 302 | TLW | O6-C6-C7-C8 |
| 4 | O | 302 | TLW | O6-C6-C7-O7 |
| 4 | P | 302 | TLW | C5-C6-C7-C8 |
| 4 | P | 302 | TLW | C5-C6-C7-O7 |
| 4 | P | 302 | TLW | O6-C6-C7-C8 |
| 4 | P | 302 | TLW | O6-C6-C7-O7 |
| 4 | Q | 302 | TLW | C5-C6-C7-C8 |
| 4 | Q | 302 | TLW | C5-C6-C7-O7 |
| 4 | Q | 302 | TLW | O6-C6-C7-C8 |
| 4 | Q | 302 | TLW | O6-C6-C7-O7 |
| 4 | R | 302 | TLW | C5-C6-C7-C8 |
| 4 | R | 302 | TLW | C5-C6-C7-O7 |
| 4 | R | 302 | TLW | O6-C6-C7-C8 |
| 4 | R | 302 | TLW | O6-C6-C7-O7 |
| 4 | S | 302 | TLW | C5-C6-C7-C8 |
| 4 | S | 302 | TLW | C5-C6-C7-O7 |
| 4 | S | 302 | TLW | O6-C6-C7-C8 |
| 4 | S | 302 | TLW | O6-C6-C7-O7 |
| 4 | T | 302 | TLW | C5-C6-C7-C8 |
| 4 | T | 302 | TLW | C5-C6-C7-O7 |
| 4 | T | 302 | TLW | O6-C6-C7-C8 |
| 4 | T | 302 | TLW | O6-C6-C7-O7 |
| 4 | U | 302 | TLW | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | U | 302 | TLW | C5-C6-C7-O7 |
| 4 | U | 302 | TLW | O6-C6-C7-C8 |
| 4 | U | 302 | TLW | O6-C6-C7-O7 |
| 4 | V | 302 | TLW | C5-C6-C7-C8 |
| 4 | V | 302 | TLW | C5-C6-C7-O7 |
| 4 | V | 302 | TLW | O6-C6-C7-C8 |
| 4 | V | 302 | TLW | O6-C6-C7-O7 |
| 4 | W | 302 | TLW | C5-C6-C7-C8 |
| 4 | W | 302 | TLW | C5-C6-C7-O7 |
| 4 | W | 302 | TLW | O6-C6-C7-C8 |
| 4 | W | 302 | TLW | O6-C6-C7-O7 |
| 4 | X | 302 | TLW | C5-C6-C7-C8 |
| 4 | X | 302 | TLW | C5-C6-C7-O7 |
| 4 | X | 302 | TLW | O6-C6-C7-C8 |
| 4 | X | 302 | TLW | O6-C6-C7-O7 |
| 4 | Y | 302 | TLW | C5-C6-C7-C8 |
| 4 | Y | 302 | TLW | C5-C6-C7-O7 |
| 4 | Y | 302 | TLW | O6-C6-C7-C8 |
| 4 | Y | 302 | TLW | O6-C6-C7-O7 |
| 5 | A | 302 | TQN | C11-C12-C13-C14 |
| 5 | A | 302 | TQN | C11-C12-C13-O13 |
| 5 | A | 302 | TQN | C22-C21-O13-C13 |
| 5 | A | 302 | TQN | O21-C21-O13-C13 |
| 5 | A | 302 | TQN | C51-C52-C53-C54 |
| 5 | A | 302 | TQN | C51-C52-C53-O53 |
| 5 | A | 302 | TQN | C62-C61-O53-C53 |
| 5 | A | 302 | TQN | O61-C61-O53-C53 |
| 5 | A | 302 | TQN | C71-C72-C73-O73 |
| 5 | A | 302 | TQN | C72-C73-O73-C81 |
| 5 | A | 302 | TQN | C82-C81-O73-C73 |
| 5 | A | 302 | TQN | O81-C81-O73-C73 |
| 5 | B | 301 | TQN | C11-C12-C13-C14 |
| 5 | B | 301 | TQN | C11-C12-C13-O13 |
| 5 | B | 301 | TQN | C22-C21-O13-C13 |
| 5 | B | 301 | TQN | O21-C21-O13-C13 |
| 5 | B | 301 | TQN | C51-C52-C53-C54 |
| 5 | B | 301 | TQN | C51-C52-C53-O53 |
| 5 | B | 301 | TQN | C62-C61-O53-C53 |
| 5 | B | 301 | TQN | O61-C61-O53-C53 |
| 5 | B | 301 | TQN | C71-C72-C73-O73 |
| 5 | B | 301 | TQN | C72-C73-O73-C81 |
| 5 | B | 301 | TQN | C82-C81-O73-C73 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | B | 301 | TQN | O81-C81-O73-C73 |
| 5 | C | 301 | TQN | C11-C12-C13-C14 |
| 5 | C | 301 | TQN | C11-C12-C13-O13 |
| 5 | C | 301 | TQN | C22-C21-O13-C13 |
| 5 | C | 301 | TQN | O21-C21-O13-C13 |
| 5 | C | 301 | TQN | C51-C52-C53-C54 |
| 5 | C | 301 | TQN | C51-C52-C53-O53 |
| 5 | C | 301 | TQN | C62-C61-O53-C53 |
| 5 | C | 301 | TQN | O61-C61-O53-C53 |
| 5 | C | 301 | TQN | C71-C72-C73-O73 |
| 5 | C | 301 | TQN | C72-C73-O73-C81 |
| 5 | C | 301 | TQN | C82-C81-O73-C73 |
| 5 | C | 301 | TQN | O81-C81-O73-C73 |
| 5 | D | 301 | TQN | C11-C12-C13-C14 |
| 5 | D | 301 | TQN | C11-C12-C13-O13 |
| 5 | D | 301 | TQN | C22-C21-O13-C13 |
| 5 | D | 301 | TQN | O21-C21-O13-C13 |
| 5 | D | 301 | TQN | C51-C52-C53-C54 |
| 5 | D | 301 | TQN | C51-C52-C53-O53 |
| 5 | D | 301 | TQN | C62-C61-O53-C53 |
| 5 | D | 301 | TQN | O61-C61-O53-C53 |
| 5 | D | 301 | TQN | C71-C72-C73-O73 |
| 5 | D | 301 | TQN | C72-C73-O73-C81 |
| 5 | D | 301 | TQN | C82-C81-O73-C73 |
| 5 | D | 301 | TQN | O81-C81-O73-C73 |
| 5 | E | 301 | TQN | C11-C12-C13-C14 |
| 5 | E | 301 | TQN | C11-C12-C13-O13 |
| 5 | E | 301 | TQN | C22-C21-O13-C13 |
| 5 | E | 301 | TQN | O21-C21-O13-C13 |
| 5 | E | 301 | TQN | C51-C52-C53-C54 |
| 5 | E | 301 | TQN | C51-C52-C53-O53 |
| 5 | E | 301 | TQN | C62-C61-O53-C53 |
| 5 | E | 301 | TQN | O61-C61-O53-C53 |
| 5 | E | 301 | TQN | C71-C72-C73-O73 |
| 5 | E | 301 | TQN | C72-C73-O73-C81 |
| 5 | E | 301 | TQN | C82-C81-O73-C73 |
| 5 | E | 301 | TQN | O81-C81-O73-C73 |
| 5 | F | 301 | TQN | C11-C12-C13-C14 |
| 5 | F | 301 | TQN | C11-C12-C13-O13 |
| 5 | F | 301 | TQN | C22-C21-O13-C13 |
| 5 | F | 301 | TQN | O21-C21-O13-C13 |
| 5 | F | 301 | TQN | C51-C52-C53-C54 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | F | 301 | TQN | C51-C52-C53-O53 |
| 5 | F | 301 | TQN | C62-C61-O53-C53 |
| 5 | F | 301 | TQN | O61-C61-O53-C53 |
| 5 | F | 301 | TQN | C71-C72-C73-O73 |
| 5 | F | 301 | TQN | C72-C73-O73-C81 |
| 5 | F | 301 | TQN | C82-C81-O73-C73 |
| 5 | F | 301 | TQN | O81-C81-O73-C73 |
| 5 | G | 301 | TQN | C11-C12-C13-C14 |
| 5 | G | 301 | TQN | C11-C12-C13-O13 |
| 5 | G | 301 | TQN | C22-C21-O13-C13 |
| 5 | G | 301 | TQN | O21-C21-O13-C13 |
| 5 | G | 301 | TQN | C51-C52-C53-C54 |
| 5 | G | 301 | TQN | C51-C52-C53-O53 |
| 5 | G | 301 | TQN | C62-C61-O53-C53 |
| 5 | G | 301 | TQN | O61-C61-O53-C53 |
| 5 | G | 301 | TQN | C71-C72-C73-O73 |
| 5 | G | 301 | TQN | C72-C73-O73-C81 |
| 5 | G | 301 | TQN | C82-C81-O73-C73 |
| 5 | G | 301 | TQN | O81-C81-O73-C73 |
| 5 | H | 301 | TQN | C11-C12-C13-C14 |
| 5 | H | 301 | TQN | C11-C12-C13-O13 |
| 5 | H | 301 | TQN | C22-C21-O13-C13 |
| 5 | H | 301 | TQN | O21-C21-O13-C13 |
| 5 | H | 301 | TQN | C51-C52-C53-C54 |
| 5 | H | 301 | TQN | C51-C52-C53-O53 |
| 5 | H | 301 | TQN | C62-C61-O53-C53 |
| 5 | H | 301 | TQN | O61-C61-O53-C53 |
| 5 | H | 301 | TQN | C71-C72-C73-O73 |
| 5 | H | 301 | TQN | C72-C73-O73-C81 |
| 5 | H | 301 | TQN | C82-C81-O73-C73 |
| 5 | H | 301 | TQN | O81-C81-O73-C73 |
| 5 | I | 301 | TQN | C11-C12-C13-C14 |
| 5 | I | 301 | TQN | C11-C12-C13-O13 |
| 5 | I | 301 | TQN | C22-C21-O13-C13 |
| 5 | I | 301 | TQN | O21-C21-O13-C13 |
| 5 | I | 301 | TQN | C51-C52-C53-C54 |
| 5 | I | 301 | TQN | C51-C52-C53-O53 |
| 5 | I | 301 | TQN | C62-C61-O53-C53 |
| 5 | I | 301 | TQN | O61-C61-O53-C53 |
| 5 | I | 301 | TQN | C71-C72-C73-O73 |
| 5 | I | 301 | TQN | C72-C73-O73-C81 |
| 5 | I | 301 | TQN | C82-C81-O73-C73 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | I | 301 | TQN | O81-C81-O73-C73 |
| 5 | J | 301 | TQN | C11-C12-C13-C14 |
| 5 | J | 301 | TQN | C11-C12-C13-O13 |
| 5 | J | 301 | TQN | C22-C21-O13-C13 |
| 5 | J | 301 | TQN | O21-C21-O13-C13 |
| 5 | J | 301 | TQN | C51-C52-C53-C54 |
| 5 | J | 301 | TQN | C51-C52-C53-O53 |
| 5 | J | 301 | TQN | C62-C61-O53-C53 |
| 5 | J | 301 | TQN | O61-C61-O53-C53 |
| 5 | J | 301 | TQN | C71-C72-C73-O73 |
| 5 | J | 301 | TQN | C72-C73-O73-C81 |
| 5 | J | 301 | TQN | C82-C81-O73-C73 |
| 5 | J | 301 | TQN | O81-C81-O73-C73 |
| 5 | K | 301 | TQN | C11-C12-C13-C14 |
| 5 | K | 301 | TQN | C11-C12-C13-O13 |
| 5 | K | 301 | TQN | C22-C21-O13-C13 |
| 5 | K | 301 | TQN | O21-C21-O13-C13 |
| 5 | K | 301 | TQN | C51-C52-C53-C54 |
| 5 | K | 301 | TQN | C51-C52-C53-O53 |
| 5 | K | 301 | TQN | C62-C61-O53-C53 |
| 5 | K | 301 | TQN | O61-C61-O53-C53 |
| 5 | K | 301 | TQN | C71-C72-C73-O73 |
| 5 | K | 301 | TQN | C72-C73-O73-C81 |
| 5 | K | 301 | TQN | C82-C81-O73-C73 |
| 5 | K | 301 | TQN | O81-C81-O73-C73 |
| 5 | L | 301 | TQN | C11-C12-C13-C14 |
| 5 | L | 301 | TQN | C11-C12-C13-O13 |
| 5 | L | 301 | TQN | C22-C21-O13-C13 |
| 5 | L | 301 | TQN | O21-C21-O13-C13 |
| 5 | L | 301 | TQN | C51-C52-C53-C54 |
| 5 | L | 301 | TQN | C51-C52-C53-O53 |
| 5 | L | 301 | TQN | C62-C61-O53-C53 |
| 5 | L | 301 | TQN | O61-C61-O53-C53 |
| 5 | L | 301 | TQN | C71-C72-C73-O73 |
| 5 | L | 301 | TQN | C72-C73-O73-C81 |
| 5 | L | 301 | TQN | C82-C81-O73-C73 |
| 5 | L | 301 | TQN | O81-C81-O73-C73 |
| 5 | M | 301 | TQN | C11-C12-C13-C14 |
| 5 | M | 301 | TQN | C11-C12-C13-O13 |
| 5 | M | 301 | TQN | C22-C21-O13-C13 |
| 5 | M | 301 | TQN | O21-C21-O13-C13 |
| 5 | M | 301 | TQN | C51-C52-C53-C54 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | M | 301 | TQN | C51-C52-C53-O53 |
| 5 | M | 301 | TQN | C62-C61-O53-C53 |
| 5 | M | 301 | TQN | O61-C61-O53-C53 |
| 5 | M | 301 | TQN | C71-C72-C73-O73 |
| 5 | M | 301 | TQN | C72-C73-O73-C81 |
| 5 | M | 301 | TQN | C82-C81-O73-C73 |
| 5 | M | 301 | TQN | O81-C81-O73-C73 |
| 5 | N | 301 | TQN | C11-C12-C13-C14 |
| 5 | N | 301 | TQN | C11-C12-C13-O13 |
| 5 | N | 301 | TQN | C22-C21-O13-C13 |
| 5 | N | 301 | TQN | O21-C21-O13-C13 |
| 5 | N | 301 | TQN | C51-C52-C53-C54 |
| 5 | N | 301 | TQN | C51-C52-C53-O53 |
| 5 | N | 301 | TQN | C62-C61-O53-C53 |
| 5 | N | 301 | TQN | O61-C61-O53-C53 |
| 5 | N | 301 | TQN | C71-C72-C73-O73 |
| 5 | N | 301 | TQN | C72-C73-O73-C81 |
| 5 | N | 301 | TQN | C82-C81-O73-C73 |
| 5 | N | 301 | TQN | O81-C81-O73-C73 |
| 5 | O | 301 | TQN | C11-C12-C13-C14 |
| 5 | O | 301 | TQN | C11-C12-C13-O13 |
| 5 | O | 301 | TQN | C22-C21-O13-C13 |
| 5 | O | 301 | TQN | O21-C21-O13-C13 |
| 5 | O | 301 | TQN | C51-C52-C53-C54 |
| 5 | O | 301 | TQN | C51-C52-C53-O53 |
| 5 | O | 301 | TQN | C62-C61-O53-C53 |
| 5 | O | 301 | TQN | O61-C61-O53-C53 |
| 5 | O | 301 | TQN | C71-C72-C73-O73 |
| 5 | O | 301 | TQN | C72-C73-O73-C81 |
| 5 | O | 301 | TQN | C82-C81-O73-C73 |
| 5 | O | 301 | TQN | O81-C81-O73-C73 |
| 5 | P | 301 | TQN | C11-C12-C13-C14 |
| 5 | P | 301 | TQN | C11-C12-C13-O13 |
| 5 | P | 301 | TQN | C22-C21-O13-C13 |
| 5 | P | 301 | TQN | O21-C21-O13-C13 |
| 5 | P | 301 | TQN | C51-C52-C53-C54 |
| 5 | P | 301 | TQN | C51-C52-C53-O53 |
| 5 | P | 301 | TQN | C62-C61-O53-C53 |
| 5 | P | 301 | TQN | O61-C61-O53-C53 |
| 5 | P | 301 | TQN | C71-C72-C73-O73 |
| 5 | P | 301 | TQN | C72-C73-O73-C81 |
| 5 | P | 301 | TQN | C82-C81-O73-C73 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | P | 301 | TQN | O81-C81-O73-C73 |
| 5 | Q | 301 | TQN | C11-C12-C13-C14 |
| 5 | Q | 301 | TQN | C11-C12-C13-O13 |
| 5 | Q | 301 | TQN | C22-C21-O13-C13 |
| 5 | Q | 301 | TQN | O21-C21-O13-C13 |
| 5 | Q | 301 | TQN | C51-C52-C53-C54 |
| 5 | Q | 301 | TQN | C51-C52-C53-O53 |
| 5 | Q | 301 | TQN | C62-C61-O53-C53 |
| 5 | Q | 301 | TQN | O61-C61-O53-C53 |
| 5 | Q | 301 | TQN | C71-C72-C73-O73 |
| 5 | Q | 301 | TQN | C72-C73-O73-C81 |
| 5 | Q | 301 | TQN | C82-C81-O73-C73 |
| 5 | Q | 301 | TQN | O81-C81-O73-C73 |
| 5 | R | 301 | TQN | C11-C12-C13-C14 |
| 5 | R | 301 | TQN | C11-C12-C13-O13 |
| 5 | R | 301 | TQN | C22-C21-O13-C13 |
| 5 | R | 301 | TQN | O21-C21-O13-C13 |
| 5 | R | 301 | TQN | C51-C52-C53-C54 |
| 5 | R | 301 | TQN | C51-C52-C53-O53 |
| 5 | R | 301 | TQN | C62-C61-O53-C53 |
| 5 | R | 301 | TQN | O61-C61-O53-C53 |
| 5 | R | 301 | TQN | C71-C72-C73-O73 |
| 5 | R | 301 | TQN | C72-C73-O73-C81 |
| 5 | R | 301 | TQN | O81-C81-O73-C73 |
| 5 | S | 301 | TQN | C11-C12-C13-C14 |
| 5 | S | 301 | TQN | C11-C12-C13-O13 |
| 5 | S | 301 | TQN | C22-C21-O13-C13 |
| 5 | S | 301 | TQN | O21-C21-O13-C13 |
| 5 | S | 301 | TQN | C51-C52-C53-C54 |
| 5 | S | 301 | TQN | C51-C52-C53-O53 |
| 5 | S | 301 | TQN | C62-C61-O53-C53 |
| 5 | S | 301 | TQN | O61-C61-O53-C53 |
| 5 | S | 301 | TQN | C71-C72-C73-O73 |
| 5 | S | 301 | TQN | C72-C73-O73-C81 |
| 5 | S | 301 | TQN | C82-C81-O73-C73 |
| 5 | S | 301 | TQN | O81-C81-O73-C73 |
| 5 | T | 301 | TQN | C11-C12-C13-C14 |
| 5 | T | 301 | TQN | C11-C12-C13-O13 |
| 5 | T | 301 | TQN | C22-C21-O13-C13 |
| 5 | T | 301 | TQN | O21-C21-O13-C13 |
| 5 | T | 301 | TQN | C51-C52-C53-C54 |
| 5 | T | 301 | TQN | C51-C52-C53-O53 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | T | 301 | TQN | C62-C61-O53-C53 |
| 5 | T | 301 | TQN | O61-C61-O53-C53 |
| 5 | T | 301 | TQN | C71-C72-C73-O73 |
| 5 | T | 301 | TQN | C72-C73-O73-C81 |
| 5 | T | 301 | TQN | C82-C81-O73-C73 |
| 5 | T | 301 | TQN | O81-C81-O73-C73 |
| 5 | U | 301 | TQN | C11-C12-C13-C14 |
| 5 | U | 301 | TQN | C11-C12-C13-O13 |
| 5 | U | 301 | TQN | C22-C21-O13-C13 |
| 5 | U | 301 | TQN | O21-C21-O13-C13 |
| 5 | U | 301 | TQN | C51-C52-C53-C54 |
| 5 | U | 301 | TQN | C51-C52-C53-O53 |
| 5 | U | 301 | TQN | C62-C61-O53-C53 |
| 5 | U | 301 | TQN | O61-C61-O53-C53 |
| 5 | U | 301 | TQN | C71-C72-C73-O73 |
| 5 | U | 301 | TQN | C72-C73-O73-C81 |
| 5 | U | 301 | TQN | C82-C81-O73-C73 |
| 5 | U | 301 | TQN | O81-C81-O73-C73 |
| 5 | V | 301 | TQN | C11-C12-C13-C14 |
| 5 | V | 301 | TQN | C11-C12-C13-O13 |
| 5 | V | 301 | TQN | C22-C21-O13-C13 |
| 5 | V | 301 | TQN | O21-C21-O13-C13 |
| 5 | V | 301 | TQN | C51-C52-C53-C54 |
| 5 | V | 301 | TQN | C51-C52-C53-O53 |
| 5 | V | 301 | TQN | C62-C61-O53-C53 |
| 5 | V | 301 | TQN | O61-C61-O53-C53 |
| 5 | V | 301 | TQN | C71-C72-C73-O73 |
| 5 | V | 301 | TQN | C72-C73-O73-C81 |
| 5 | V | 301 | TQN | C82-C81-O73-C73 |
| 5 | V | 301 | TQN | O81-C81-O73-C73 |
| 5 | W | 301 | TQN | C11-C12-C13-C14 |
| 5 | W | 301 | TQN | C11-C12-C13-O13 |
| 5 | W | 301 | TQN | C22-C21-O13-C13 |
| 5 | W | 301 | TQN | O21-C21-O13-C13 |
| 5 | W | 301 | TQN | C51-C52-C53-C54 |
| 5 | W | 301 | TQN | C51-C52-C53-O53 |
| 5 | W | 301 | TQN | C62-C61-O53-C53 |
| 5 | W | 301 | TQN | O61-C61-O53-C53 |
| 5 | W | 301 | TQN | C71-C72-C73-O73 |
| 5 | W | 301 | TQN | C72-C73-O73-C81 |
| 5 | W | 301 | TQN | C82-C81-O73-C73 |
| 5 | W | 301 | TQN | O81-C81-O73-C73 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | X | 301 | TQN | C11-C12-C13-C14 |
| 5 | X | 301 | TQN | C11-C12-C13-O13 |
| 5 | X | 301 | TQN | C22-C21-O13-C13 |
| 5 | X | 301 | TQN | O21-C21-O13-C13 |
| 5 | X | 301 | TQN | C51-C52-C53-C54 |
| 5 | X | 301 | TQN | C51-C52-C53-O53 |
| 5 | X | 301 | TQN | C62-C61-O53-C53 |
| 5 | X | 301 | TQN | O61-C61-O53-C53 |
| 5 | X | 301 | TQN | C71-C72-C73-O73 |
| 5 | X | 301 | TQN | C72-C73-O73-C81 |
| 5 | X | 301 | TQN | C82-C81-O73-C73 |
| 5 | X | 301 | TQN | O81-C81-O73-C73 |
| 5 | Y | 301 | TQN | C11-C12-C13-C14 |
| 5 | Y | 301 | TQN | C11-C12-C13-O13 |
| 5 | Y | 301 | TQN | C22-C21-O13-C13 |
| 5 | Y | 301 | TQN | O21-C21-O13-C13 |
| 5 | Y | 301 | TQN | C51-C52-C53-C54 |
| 5 | Y | 301 | TQN | C51-C52-C53-O53 |
| 5 | Y | 301 | TQN | C62-C61-O53-C53 |
| 5 | Y | 301 | TQN | O61-C61-O53-C53 |
| 5 | Y | 301 | TQN | C71-C72-C73-O73 |
| 5 | Y | 301 | TQN | C72-C73-O73-C81 |
| 5 | Y | 301 | TQN | C82-C81-O73-C73 |
| 5 | Y | 301 | TQN | O81-C81-O73-C73 |
| 5 | Z | 301 | TQN | C11-C12-C13-C14 |
| 5 | Z | 301 | TQN | C11-C12-C13-O13 |
| 5 | Z | 301 | TQN | C22-C21-O13-C13 |
| 5 | Z | 301 | TQN | O21-C21-O13-C13 |
| 5 | Z | 301 | TQN | C51-C52-C53-C54 |
| 5 | Z | 301 | TQN | C51-C52-C53-O53 |
| 5 | Z | 301 | TQN | C62-C61-O53-C53 |
| 5 | Z | 301 | TQN | O61-C61-O53-C53 |
| 5 | Z | 301 | TQN | C71-C72-C73-O73 |
| 5 | Z | 301 | TQN | C72-C73-O73-C81 |
| 5 | Z | 301 | TQN | C82-C81-O73-C73 |
| 5 | Z | 301 | TQN | O81-C81-O73-C73 |
| 5 | R | 301 | TQN | C82-C81-O73-C73 |
| 5 | A | 302 | TQN | C59-CD9-CE1-CE2 |
| 5 | B | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | C | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | D | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | F | 301 | TQN | C59-CD9-CE1-CE2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | G | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | I | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | L | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | M | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | Q | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | R | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | S | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | T | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | U | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | V | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | W | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | Y | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | Z | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | H | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | K | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | N | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | O | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | P | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | X | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | E | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | J | 301 | TQN | C59-CD9-CE1-CE2 |
| 5 | A | 302 | TQN | C74-C73-O73-C81 |
| 5 | B | 301 | TQN | C74-C73-O73-C81 |
| 5 | C | 301 | TQN | C74-C73-O73-C81 |
| 5 | D | 301 | TQN | C74-C73-O73-C81 |
| 5 | E | 301 | TQN | C74-C73-O73-C81 |
| 5 | F | 301 | TQN | C74-C73-O73-C81 |
| 5 | G | 301 | TQN | C74-C73-O73-C81 |
| 5 | H | 301 | TQN | C74-C73-O73-C81 |
| 5 | I | 301 | TQN | C74-C73-O73-C81 |
| 5 | J | 301 | TQN | C74-C73-O73-C81 |
| 5 | K | 301 | TQN | C74-C73-O73-C81 |
| 5 | L | 301 | TQN | C74-C73-O73-C81 |
| 5 | M | 301 | TQN | C74-C73-O73-C81 |
| 5 | N | 301 | TQN | C74-C73-O73-C81 |
| 5 | O | 301 | TQN | C74-C73-O73-C81 |
| 5 | P | 301 | TQN | C74-C73-O73-C81 |
| 5 | Q | 301 | TQN | C74-C73-O73-C81 |
| 5 | R | 301 | TQN | C74-C73-O73-C81 |
| 5 | S | 301 | TQN | C74-C73-O73-C81 |
| 5 | T | 301 | TQN | C74-C73-O73-C81 |
| 5 | U | 301 | TQN | C74-C73-O73-C81 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | V | 301 | TQN | C74-C73-O73-C81 |
| 5 | W | 301 | TQN | C74-C73-O73-C81 |
| 5 | X | 301 | TQN | C74-C73-O73-C81 |
| 5 | Y | 301 | TQN | C74-C73-O73-C81 |
| 5 | Z | 301 | TQN | C74-C73-O73-C81 |
| 5 | A | 302 | TQN | C72-C71-OB3-CB3 |
| 5 | B | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | C | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | D | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | E | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | F | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | G | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | H | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | I | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | J | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | K | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | L | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | M | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | N | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | O | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | P | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | Q | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | R | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | S | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | T | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | U | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | V | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | W | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | X | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | Y | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | Z | 301 | TQN | C72-C71-OB3-CB3 |
| 5 | A | 302 | TQN | O71-C71-OB3-CB3 |
| 5 | B | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | C | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | D | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | E | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | F | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | G | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | H | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | I | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | J | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | K | 301 | TQN | O71-C71-OB3-CB3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | L | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | M | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | N | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | O | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | P | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | Q | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | R | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | S | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | T | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | U | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | V | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | W | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | X | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | Y | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | Z | 301 | TQN | O71-C71-OB3-CB3 |
| 5 | G | 301 | TQN | C85-C86-C87-C88 |
| 5 | H | 301 | TQN | C85-C86-C87-C88 |
| 5 | Q | 301 | TQN | C85-C86-C87-C88 |
| 5 | S | 301 | TQN | C85-C86-C87-C88 |
| 5 | Z | 301 | TQN | C85-C86-C87-C88 |
| 5 | A | 302 | TQN | C85-C86-C87-C88 |
| 5 | B | 301 | TQN | C85-C86-C87-C88 |
| 5 | C | 301 | TQN | C85-C86-C87-C88 |
| 5 | D | 301 | TQN | C85-C86-C87-C88 |
| 5 | E | 301 | TQN | C85-C86-C87-C88 |
| 5 | F | 301 | TQN | C85-C86-C87-C88 |
| 5 | I | 301 | TQN | C85-C86-C87-C88 |
| 5 | J | 301 | TQN | C85-C86-C87-C88 |
| 5 | K | 301 | TQN | C85-C86-C87-C88 |
| 5 | L | 301 | TQN | C85-C86-C87-C88 |
| 5 | M | 301 | TQN | C85-C86-C87-C88 |
| 5 | N | 301 | TQN | C85-C86-C87-C88 |
| 5 | O | 301 | TQN | C85-C86-C87-C88 |
| 5 | P | 301 | TQN | C85-C86-C87-C88 |
| 5 | R | 301 | TQN | C85-C86-C87-C88 |
| 5 | T | 301 | TQN | C85-C86-C87-C88 |
| 5 | U | 301 | TQN | C85-C86-C87-C88 |
| 5 | V | 301 | TQN | C85-C86-C87-C88 |
| 5 | W | 301 | TQN | C85-C86-C87-C88 |
| 5 | X | 301 | TQN | C85-C86-C87-C88 |
| 5 | Y | 301 | TQN | C85-C86-C87-C88 |
| 5 | E | 301 | TQN | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | C | 301 | TQN | C55-C56-C57-C58 |
| 5 | D | 301 | TQN | C55-C56-C57-C58 |
| 5 | E | 301 | TQN | C55-C56-C57-C58 |
| 5 | H | 301 | TQN | C55-C56-C57-C58 |
| 5 | I | 301 | TQN | C55-C56-C57-C58 |
| 5 | J | 301 | TQN | C55-C56-C57-C58 |
| 5 | M | 301 | TQN | C55-C56-C57-C58 |
| 5 | N | 301 | TQN | C55-C56-C57-C58 |
| 5 | O | 301 | TQN | C24-C25-C26-C27 |
| 5 | P | 301 | TQN | C55-C56-C57-C58 |
| 5 | Q | 301 | TQN | C55-C56-C57-C58 |
| 5 | R | 301 | TQN | C24-C25-C26-C27 |
| 5 | R | 301 | TQN | C55-C56-C57-C58 |
| 5 | S | 301 | TQN | C55-C56-C57-C58 |
| 5 | U | 301 | TQN | C55-C56-C57-C58 |
| 5 | W | 301 | TQN | C55-C56-C57-C58 |
| 5 | X | 301 | TQN | C55-C56-C57-C58 |
| 5 | Y | 301 | TQN | C55-C56-C57-C58 |
| 5 | Z | 301 | TQN | C55-C56-C57-C58 |
| 5 | A | 302 | TQN | C24-C25-C26-C27 |
| 5 | A | 302 | TQN | C55-C56-C57-C58 |
| 5 | B | 301 | TQN | C24-C25-C26-C27 |
| 5 | B | 301 | TQN | C55-C56-C57-C58 |
| 5 | C | 301 | TQN | C24-C25-C26-C27 |
| 5 | D | 301 | TQN | C24-C25-C26-C27 |
| 5 | F | 301 | TQN | C24-C25-C26-C27 |
| 5 | F | 301 | TQN | C55-C56-C57-C58 |
| 5 | G | 301 | TQN | C24-C25-C26-C27 |
| 5 | G | 301 | TQN | C55-C56-C57-C58 |
| 5 | H | 301 | TQN | C24-C25-C26-C27 |
| 5 | I | 301 | TQN | C24-C25-C26-C27 |
| 5 | J | 301 | TQN | C24-C25-C26-C27 |
| 5 | K | 301 | TQN | C24-C25-C26-C27 |
| 5 | K | 301 | TQN | C55-C56-C57-C58 |
| 5 | L | 301 | TQN | C24-C25-C26-C27 |
| 5 | L | 301 | TQN | C55-C56-C57-C58 |
| 5 | M | 301 | TQN | C24-C25-C26-C27 |
| 5 | N | 301 | TQN | C24-C25-C26-C27 |
| 5 | O | 301 | TQN | C55-C56-C57-C58 |
| 5 | P | 301 | TQN | C24-C25-C26-C27 |
| 5 | Q | 301 | TQN | C24-C25-C26-C27 |
| 5 | S | 301 | TQN | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | T | 301 | TQN | C24-C25-C26-C27 |
| 5 | T | 301 | TQN | C55-C56-C57-C58 |
| 5 | U | 301 | TQN | C24-C25-C26-C27 |
| 5 | V | 301 | TQN | C24-C25-C26-C27 |
| 5 | V | 301 | TQN | C55-C56-C57-C58 |
| 5 | W | 301 | TQN | C24-C25-C26-C27 |
| 5 | X | 301 | TQN | C24-C25-C26-C27 |
| 5 | Y | 301 | TQN | C24-C25-C26-C27 |
| 5 | Z | 301 | TQN | C24-C25-C26-C27 |
| 5 | B | 301 | TQN | C23-C24-C25-C26 |
| 5 | H | 301 | TQN | C23-C24-C25-C26 |
| 5 | J | 301 | TQN | C23-C24-C25-C26 |
| 5 | K | 301 | TQN | C23-C24-C25-C26 |
| 5 | N | 301 | TQN | C23-C24-C25-C26 |
| 5 | O | 301 | TQN | C23-C24-C25-C26 |
| 5 | R | 301 | TQN | C23-C24-C25-C26 |
| 5 | V | 301 | TQN | C23-C24-C25-C26 |
| 5 | Y | 301 | TQN | C23-C24-C25-C26 |
| 5 | A | 302 | TQN | C23-C24-C25-C26 |
| 5 | C | 301 | TQN | C23-C24-C25-C26 |
| 5 | D | 301 | TQN | C23-C24-C25-C26 |
| 5 | E | 301 | TQN | C23-C24-C25-C26 |
| 5 | F | 301 | TQN | C23-C24-C25-C26 |
| 5 | G | 301 | TQN | C23-C24-C25-C26 |
| 5 | I | 301 | TQN | C23-C24-C25-C26 |
| 5 | L | 301 | TQN | C23-C24-C25-C26 |
| 5 | M | 301 | TQN | C23-C24-C25-C26 |
| 5 | P | 301 | TQN | C23-C24-C25-C26 |
| 5 | Q | 301 | TQN | C23-C24-C25-C26 |
| 5 | S | 301 | TQN | C23-C24-C25-C26 |
| 5 | T | 301 | TQN | C23-C24-C25-C26 |
| 5 | U | 301 | TQN | C23-C24-C25-C26 |
| 5 | W | 301 | TQN | C23-C24-C25-C26 |
| 5 | X | 301 | TQN | C23-C24-C25-C26 |
| 5 | Z | 301 | TQN | C23-C24-C25-C26 |
| 5 | A | 302 | TQN | C37-C38-C39-CD4 |
| 5 | B | 301 | TQN | C37-C38-C39-CD4 |
| 5 | C | 301 | TQN | C37-C38-C39-CD4 |
| 5 | D | 301 | TQN | C37-C38-C39-CD4 |
| 5 | E | 301 | TQN | C37-C38-C39-CD4 |
| 5 | G | 301 | TQN | C37-C38-C39-CD4 |
| 5 | I | 301 | TQN | C37-C38-C39-CD4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | J | 301 | TQN | C37-C38-C39-CD4 |
| 5 | K | 301 | TQN | C37-C38-C39-CD4 |
| 5 | M | 301 | TQN | C37-C38-C39-CD4 |
| 5 | O | 301 | TQN | C37-C38-C39-CD4 |
| 5 | P | 301 | TQN | C37-C38-C39-CD4 |
| 5 | S | 301 | TQN | C37-C38-C39-CD4 |
| 5 | U | 301 | TQN | C37-C38-C39-CD4 |
| 5 | V | 301 | TQN | C37-C38-C39-CD4 |
| 5 | W | 301 | TQN | C37-C38-C39-CD4 |
| 5 | Y | 301 | TQN | C37-C38-C39-CD4 |
| 5 | F | 301 | TQN | C37-C38-C39-CD4 |
| 5 | H | 301 | TQN | C37-C38-C39-CD4 |
| 5 | T | 301 | TQN | C37-C38-C39-CD4 |
| 5 | X | 301 | TQN | C37-C38-C39-CD4 |
| 5 | L | 301 | TQN | C37-C38-C39-CD4 |
| 5 | N | 301 | TQN | C37-C38-C39-CD4 |
| 5 | Q | 301 | TQN | C37-C38-C39-CD4 |
| 5 | R | 301 | TQN | C37-C38-C39-CD4 |
| 5 | Z | 301 | TQN | C37-C38-C39-CD4 |
| 5 | V | 301 | TQN | C54-C55-C56-C57 |
| 5 | A | 302 | TQN | C54-C55-C56-C57 |
| 5 | B | 301 | TQN | C54-C55-C56-C57 |
| 5 | C | 301 | TQN | C54-C55-C56-C57 |
| 5 | D | 301 | TQN | C54-C55-C56-C57 |
| 5 | E | 301 | TQN | C54-C55-C56-C57 |
| 5 | F | 301 | TQN | C54-C55-C56-C57 |
| 5 | H | 301 | TQN | C54-C55-C56-C57 |
| 5 | I | 301 | TQN | C54-C55-C56-C57 |
| 5 | J | 301 | TQN | C54-C55-C56-C57 |
| 5 | K | 301 | TQN | C54-C55-C56-C57 |
| 5 | L | 301 | TQN | C54-C55-C56-C57 |
| 5 | M | 301 | TQN | C54-C55-C56-C57 |
| 5 | N | 301 | TQN | C54-C55-C56-C57 |
| 5 | O | 301 | TQN | C54-C55-C56-C57 |
| 5 | P | 301 | TQN | C54-C55-C56-C57 |
| 5 | Q | 301 | TQN | C54-C55-C56-C57 |
| 5 | R | 301 | TQN | C54-C55-C56-C57 |
| 5 | S | 301 | TQN | C54-C55-C56-C57 |
| 5 | T | 301 | TQN | C54-C55-C56-C57 |
| 5 | U | 301 | TQN | C54-C55-C56-C57 |
| 5 | W | 301 | TQN | C54-C55-C56-C57 |
| 5 | X | 301 | TQN | C54-C55-C56-C57 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | Y | 301 | TQN | C54-C55-C56-C57 |
| 5 | Z | 301 | TQN | C54-C55-C56-C57 |
| 5 | G | 301 | TQN | C54-C55-C56-C57 |
| 5 | A | 302 | TQN | O73-C73-C74-C75 |
| 5 | B | 301 | TQN | O73-C73-C74-C75 |
| 5 | C | 301 | TQN | O73-C73-C74-C75 |
| 5 | D | 301 | TQN | O73-C73-C74-C75 |
| 5 | E | 301 | TQN | O73-C73-C74-C75 |
| 5 | F | 301 | TQN | O73-C73-C74-C75 |
| 5 | G | 301 | TQN | O73-C73-C74-C75 |
| 5 | H | 301 | TQN | O73-C73-C74-C75 |
| 5 | I | 301 | TQN | O73-C73-C74-C75 |
| 5 | J | 301 | TQN | O73-C73-C74-C75 |
| 5 | K | 301 | TQN | O73-C73-C74-C75 |
| 5 | L | 301 | TQN | O73-C73-C74-C75 |
| 5 | M | 301 | TQN | O73-C73-C74-C75 |
| 5 | N | 301 | TQN | O73-C73-C74-C75 |
| 5 | O | 301 | TQN | O73-C73-C74-C75 |
| 5 | P | 301 | TQN | O73-C73-C74-C75 |
| 5 | Q | 301 | TQN | O73-C73-C74-C75 |
| 5 | R | 301 | TQN | O73-C73-C74-C75 |
| 5 | S | 301 | TQN | O73-C73-C74-C75 |
| 5 | T | 301 | TQN | O73-C73-C74-C75 |
| 5 | U | 301 | TQN | O73-C73-C74-C75 |
| 5 | V | 301 | TQN | O73-C73-C74-C75 |
| 5 | W | 301 | TQN | O73-C73-C74-C75 |
| 5 | X | 301 | TQN | O73-C73-C74-C75 |
| 5 | Y | 301 | TQN | O73-C73-C74-C75 |
| 5 | Z | 301 | TQN | O73-C73-C74-C75 |
| 5 | P | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | Y | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | C | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | D | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | F | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | G | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | H | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | I | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | L | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | M | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | N | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | O | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | S | 301 | TQN | C68-C69-CE5-CE6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | T | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | U | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | V | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | W | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | Z | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | A | 302 | TQN | C68-C69-CE5-CE6 |
| 5 | B | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | E | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | J | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | K | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | Q | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | R | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | X | 301 | TQN | C68-C69-CE5-CE6 |
| 5 | C | 301 | TQN | C87-C88-C89-CF4 |
| 5 | D | 301 | TQN | C87-C88-C89-CF4 |
| 5 | H | 301 | TQN | C87-C88-C89-CF4 |
| 5 | L | 301 | TQN | C87-C88-C89-CF4 |
| 5 | N | 301 | TQN | C87-C88-C89-CF4 |
| 5 | O | 301 | TQN | C87-C88-C89-CF4 |
| 5 | Q | 301 | TQN | C87-C88-C89-CF4 |
| 5 | R | 301 | TQN | C87-C88-C89-CF4 |
| 5 | S | 301 | TQN | C87-C88-C89-CF4 |
| 5 | T | 301 | TQN | C87-C88-C89-CF4 |
| 5 | X | 301 | TQN | C87-C88-C89-CF4 |
| 5 | Y | 301 | TQN | C87-C88-C89-CF4 |
| 5 | A | 302 | TQN | C87-C88-C89-CF4 |
| 5 | B | 301 | TQN | C87-C88-C89-CF4 |
| 5 | E | 301 | TQN | C87-C88-C89-CF4 |
| 5 | F | 301 | TQN | C87-C88-C89-CF4 |
| 5 | G | 301 | TQN | C87-C88-C89-CF4 |
| 5 | I | 301 | TQN | C87-C88-C89-CF4 |
| 5 | J | 301 | TQN | C87-C88-C89-CF4 |
| 5 | K | 301 | TQN | C87-C88-C89-CF4 |
| 5 | M | 301 | TQN | C87-C88-C89-CF4 |
| 5 | P | 301 | TQN | C87-C88-C89-CF4 |
| 5 | U | 301 | TQN | C87-C88-C89-CF4 |
| 5 | V | 301 | TQN | C87-C88-C89-CF4 |
| 5 | W | 301 | TQN | C87-C88-C89-CF4 |
| 5 | Z | 301 | TQN | C87-C88-C89-CF4 |
| 4 | A | 301 | TLW | O11-C1-C2-O6 |
| 4 | A | 303 | TLW | O11-C1-C2-O6 |
| 4 | B | 302 | TLW | O11-C1-C2-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | C | 302 | TLW | O11-C1-C2-O6 |
| 4 | D | 302 | TLW | O11-C1-C2-O6 |
| 4 | E | 302 | TLW | O11-C1-C2-O6 |
| 4 | F | 302 | TLW | O11-C1-C2-O6 |
| 4 | G | 302 | TLW | O11-C1-C2-O6 |
| 4 | H | 302 | TLW | O11-C1-C2-O6 |
| 4 | I | 302 | TLW | O11-C1-C2-O6 |
| 4 | J | 302 | TLW | O11-C1-C2-O6 |
| 4 | K | 302 | TLW | O11-C1-C2-O6 |
| 4 | L | 302 | TLW | O11-C1-C2-O6 |
| 4 | M | 302 | TLW | O11-C1-C2-O6 |
| 4 | N | 302 | TLW | O11-C1-C2-O6 |
| 4 | O | 302 | TLW | O11-C1-C2-O6 |
| 4 | P | 302 | TLW | O11-C1-C2-O6 |
| 4 | Q | 302 | TLW | O11-C1-C2-O6 |
| 4 | R | 302 | TLW | O11-C1-C2-O6 |
| 4 | S | 302 | TLW | O11-C1-C2-O6 |
| 4 | T | 302 | TLW | O11-C1-C2-O6 |
| 4 | U | 302 | TLW | O11-C1-C2-O6 |
| 4 | V | 302 | TLW | O11-C1-C2-O6 |
| 4 | W | 302 | TLW | O11-C1-C2-O6 |
| 4 | X | 302 | TLW | O11-C1-C2-O6 |
| 4 | Y | 302 | TLW | O11-C1-C2-O6 |
| 5 | Q | 301 | TQN | C74-C75-C76-C77 |
| 5 | A | 302 | TQN | C74-C75-C76-C77 |
| 5 | B | 301 | TQN | C74-C75-C76-C77 |
| 5 | F | 301 | TQN | C74-C75-C76-C77 |
| 5 | H | 301 | TQN | C74-C75-C76-C77 |
| 5 | J | 301 | TQN | C74-C75-C76-C77 |
| 5 | L | 301 | TQN | C74-C75-C76-C77 |
| 5 | M | 301 | TQN | C74-C75-C76-C77 |
| 5 | O | 301 | TQN | C74-C75-C76-C77 |
| 5 | P | 301 | TQN | C74-C75-C76-C77 |
| 5 | T | 301 | TQN | C74-C75-C76-C77 |
| 5 | U | 301 | TQN | C74-C75-C76-C77 |
| 5 | V | 301 | TQN | C74-C75-C76-C77 |
| 5 | X | 301 | TQN | C74-C75-C76-C77 |
| 5 | Y | 301 | TQN | C74-C75-C76-C77 |
| 5 | Z | 301 | TQN | C74-C75-C76-C77 |
| 5 | C | 301 | TQN | C74-C75-C76-C77 |
| 5 | D | 301 | TQN | C74-C75-C76-C77 |
| 5 | E | 301 | TQN | C74-C75-C76-C77 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | G | 301 | TQN | C74-C75-C76-C77 |
| 5 | I | 301 | TQN | C74-C75-C76-C77 |
| 5 | K | 301 | TQN | C74-C75-C76-C77 |
| 5 | N | 301 | TQN | C74-C75-C76-C77 |
| 5 | R | 301 | TQN | C74-C75-C76-C77 |
| 5 | S | 301 | TQN | C74-C75-C76-C77 |
| 5 | W | 301 | TQN | C74-C75-C76-C77 |
| 5 | P | 301 | TQN | C15-C16-C17-C18 |
| 5 | U | 301 | TQN | C15-C16-C17-C18 |
| 5 | H | 301 | TQN | C15-C16-C17-C18 |
| 5 | M | 301 | TQN | C15-C16-C17-C18 |
| 5 | O | 301 | TQN | C15-C16-C17-C18 |
| 5 | W | 301 | TQN | C15-C16-C17-C18 |
| 5 | A | 302 | TQN | C15-C16-C17-C18 |
| 5 | B | 301 | TQN | C15-C16-C17-C18 |
| 5 | C | 301 | TQN | C15-C16-C17-C18 |
| 5 | D | 301 | TQN | C15-C16-C17-C18 |
| 5 | E | 301 | TQN | C15-C16-C17-C18 |
| 5 | F | 301 | TQN | C15-C16-C17-C18 |
| 5 | G | 301 | TQN | C15-C16-C17-C18 |
| 5 | I | 301 | TQN | C15-C16-C17-C18 |
| 5 | J | 301 | TQN | C15-C16-C17-C18 |
| 5 | K | 301 | TQN | C15-C16-C17-C18 |
| 5 | L | 301 | TQN | C15-C16-C17-C18 |
| 5 | N | 301 | TQN | C15-C16-C17-C18 |
| 5 | Q | 301 | TQN | C15-C16-C17-C18 |
| 5 | R | 301 | TQN | C15-C16-C17-C18 |
| 5 | S | 301 | TQN | C15-C16-C17-C18 |
| 5 | T | 301 | TQN | C15-C16-C17-C18 |
| 5 | V | 301 | TQN | C15-C16-C17-C18 |
| 5 | X | 301 | TQN | C15-C16-C17-C18 |
| 5 | Y | 301 | TQN | C15-C16-C17-C18 |
| 5 | Z | 301 | TQN | C15-C16-C17-C18 |
| 5 | A | 302 | TQN | C72-C73-C74-C75 |
| 5 | B | 301 | TQN | C72-C73-C74-C75 |
| 5 | C | 301 | TQN | C72-C73-C74-C75 |
| 5 | D | 301 | TQN | C72-C73-C74-C75 |
| 5 | E | 301 | TQN | C72-C73-C74-C75 |
| 5 | F | 301 | TQN | C72-C73-C74-C75 |
| 5 | G | 301 | TQN | C72-C73-C74-C75 |
| 5 | H | 301 | TQN | C72-C73-C74-C75 |
| 5 | I | 301 | TQN | C72-C73-C74-C75 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | J | 301 | TQN | C72-C73-C74-C75 |
| 5 | K | 301 | TQN | C72-C73-C74-C75 |
| 5 | L | 301 | TQN | C72-C73-C74-C75 |
| 5 | M | 301 | TQN | C72-C73-C74-C75 |
| 5 | N | 301 | TQN | C72-C73-C74-C75 |
| 5 | O | 301 | TQN | C72-C73-C74-C75 |
| 5 | P | 301 | TQN | C72-C73-C74-C75 |
| 5 | Q | 301 | TQN | C72-C73-C74-C75 |
| 5 | R | 301 | TQN | C72-C73-C74-C75 |
| 5 | S | 301 | TQN | C72-C73-C74-C75 |
| 5 | T | 301 | TQN | C72-C73-C74-C75 |
| 5 | U | 301 | TQN | C72-C73-C74-C75 |
| 5 | V | 301 | TQN | C72-C73-C74-C75 |
| 5 | W | 301 | TQN | C72-C73-C74-C75 |
| 5 | X | 301 | TQN | C72-C73-C74-C75 |
| 5 | Y | 301 | TQN | C72-C73-C74-C75 |
| 5 | Z | 301 | TQN | C72-C73-C74-C75 |
| 5 | A | 302 | TQN | C18-C19-CC1-CC2 |
| 5 | B | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | C | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | D | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | E | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | F | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | G | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | H | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | I | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | J | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | K | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | L | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | M | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | N | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | O | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | P | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | Q | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | R | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | S | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | T | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | U | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | V | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | W | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | X | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | Y | 301 | TQN | C18-C19-CC1-CC2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | Z | 301 | TQN | C18-C19-CC1-CC2 |
| 5 | A | 302 | TQN | C14-C13-O13-C21 |
| 5 | B | 301 | TQN | C14-C13-O13-C21 |
| 5 | C | 301 | TQN | C14-C13-O13-C21 |
| 5 | D | 301 | TQN | C14-C13-O13-C21 |
| 5 | E | 301 | TQN | C14-C13-O13-C21 |
| 5 | F | 301 | TQN | C14-C13-O13-C21 |
| 5 | G | 301 | TQN | C14-C13-O13-C21 |
| 5 | H | 301 | TQN | C14-C13-O13-C21 |
| 5 | J | 301 | TQN | C14-C13-O13-C21 |
| 5 | K | 301 | TQN | C14-C13-O13-C21 |
| 5 | M | 301 | TQN | C14-C13-O13-C21 |
| 5 | N | 301 | TQN | C14-C13-O13-C21 |
| 5 | O | 301 | TQN | C14-C13-O13-C21 |
| 5 | P | 301 | TQN | C14-C13-O13-C21 |
| 5 | R | 301 | TQN | C14-C13-O13-C21 |
| 5 | U | 301 | TQN | C14-C13-O13-C21 |
| 5 | V | 301 | TQN | C14-C13-O13-C21 |
| 5 | W | 301 | TQN | C14-C13-O13-C21 |
| 5 | X | 301 | TQN | C14-C13-O13-C21 |
| 5 | N | 301 | TQN | C36-C37-C38-C39 |
| 5 | O | 301 | TQN | C36-C37-C38-C39 |
| 5 | S | 301 | TQN | C36-C37-C38-C39 |
| 5 | T | 301 | TQN | C36-C37-C38-C39 |
| 5 | F | 301 | TQN | C36-C37-C38-C39 |
| 5 | G | 301 | TQN | C36-C37-C38-C39 |
| 5 | H | 301 | TQN | C36-C37-C38-C39 |
| 5 | Q | 301 | TQN | C36-C37-C38-C39 |
| 5 | R | 301 | TQN | C36-C37-C38-C39 |
| 5 | X | 301 | TQN | C36-C37-C38-C39 |
| 5 | B | 301 | TQN | C36-C37-C38-C39 |
| 5 | C | 301 | TQN | C36-C37-C38-C39 |
| 5 | E | 301 | TQN | C36-C37-C38-C39 |
| 5 | I | 301 | TQN | C36-C37-C38-C39 |
| 5 | Z | 301 | TQN | C36-C37-C38-C39 |
| 5 | A | 302 | TQN | C36-C37-C38-C39 |
| 5 | D | 301 | TQN | C36-C37-C38-C39 |
| 5 | J | 301 | TQN | C36-C37-C38-C39 |
| 5 | K | 301 | TQN | C36-C37-C38-C39 |
| 5 | L | 301 | TQN | C36-C37-C38-C39 |
| 5 | M | 301 | TQN | C36-C37-C38-C39 |
| 5 | P | 301 | TQN | C36-C37-C38-C39 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | U | 301 | TQN | C36-C37-C38-C39 |
| 5 | V | 301 | TQN | C36-C37-C38-C39 |
| 5 | W | 301 | TQN | C36-C37-C38-C39 |
| 5 | Y | 301 | TQN | C36-C37-C38-C39 |
| 5 | C | 301 | TQN | C81-C82-C83-C84 |
| 5 | G | 301 | TQN | C81-C82-C83-C84 |
| 5 | L | 301 | TQN | C81-C82-C83-C84 |
| 5 | R | 301 | TQN | C81-C82-C83-C84 |
| 5 | X | 301 | TQN | C81-C82-C83-C84 |
| 5 | B | 301 | TQN | C81-C82-C83-C84 |
| 5 | E | 301 | TQN | C81-C82-C83-C84 |
| 5 | H | 301 | TQN | C81-C82-C83-C84 |
| 5 | M | 301 | TQN | C81-C82-C83-C84 |
| 5 | N | 301 | TQN | C81-C82-C83-C84 |
| 5 | O | 301 | TQN | C81-C82-C83-C84 |
| 5 | Q | 301 | TQN | C81-C82-C83-C84 |
| 5 | T | 301 | TQN | C81-C82-C83-C84 |
| 5 | U | 301 | TQN | C81-C82-C83-C84 |
| 5 | V | 301 | TQN | C81-C82-C83-C84 |
| 5 | W | 301 | TQN | C81-C82-C83-C84 |
| 5 | Y | 301 | TQN | C81-C82-C83-C84 |
| 5 | A | 302 | TQN | C81-C82-C83-C84 |
| 5 | D | 301 | TQN | C81-C82-C83-C84 |
| 5 | F | 301 | TQN | C81-C82-C83-C84 |
| 5 | I | 301 | TQN | C81-C82-C83-C84 |
| 5 | J | 301 | TQN | C81-C82-C83-C84 |
| 5 | K | 301 | TQN | C81-C82-C83-C84 |
| 5 | P | 301 | TQN | C81-C82-C83-C84 |
| 5 | S | 301 | TQN | C81-C82-C83-C84 |
| 5 | Z | 301 | TQN | C81-C82-C83-C84 |
| 5 | I | 301 | TQN | C14-C13-O13-C21 |
| 5 | L | 301 | TQN | C14-C13-O13-C21 |
| 5 | Q | 301 | TQN | C14-C13-O13-C21 |
| 5 | S | 301 | TQN | C14-C13-O13-C21 |
| 5 | T | 301 | TQN | C14-C13-O13-C21 |
| 5 | Y | 301 | TQN | C14-C13-O13-C21 |
| 5 | Z | 301 | TQN | C14-C13-O13-C21 |
| 5 | F | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | K | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | U | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | V | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | Z | 301 | TQN | CC8-CC9-CD1-CD2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | B | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | C | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | D | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | E | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | G | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | H | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | I | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | J | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | L | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | M | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | N | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | O | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | P | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | Q | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | S | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | T | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | W | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | X | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | Y | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | A | 302 | TQN | CC8-CC9-CD1-CD2 |
| 5 | R | 301 | TQN | CC8-CC9-CD1-CD2 |
| 5 | A | 302 | TQN | CE8-CE9-CF1-CF2 |
| 5 | B | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | E | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | D | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | F | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | I | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | J | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | K | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | L | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | M | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | N | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | O | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | R | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | S | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | T | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | U | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | V | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | Z | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | C | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | G | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | P | 301 | TQN | CE8-CE9-CF1-CF2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | Q | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | W | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | X | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | Y | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | H | 301 | TQN | CE8-CE9-CF1-CF2 |
| 5 | A | 302 | TQN | C71-C72-C73-C74 |
| 5 | B | 301 | TQN | C71-C72-C73-C74 |
| 5 | C | 301 | TQN | C71-C72-C73-C74 |
| 5 | D | 301 | TQN | C71-C72-C73-C74 |
| 5 | E | 301 | TQN | C71-C72-C73-C74 |
| 5 | F | 301 | TQN | C71-C72-C73-C74 |
| 5 | G | 301 | TQN | C71-C72-C73-C74 |
| 5 | H | 301 | TQN | C71-C72-C73-C74 |
| 5 | I | 301 | TQN | C71-C72-C73-C74 |
| 5 | J | 301 | TQN | C71-C72-C73-C74 |
| 5 | K | 301 | TQN | C71-C72-C73-C74 |
| 5 | L | 301 | TQN | C71-C72-C73-C74 |
| 5 | M | 301 | TQN | C71-C72-C73-C74 |
| 5 | N | 301 | TQN | C71-C72-C73-C74 |
| 5 | O | 301 | TQN | C71-C72-C73-C74 |
| 5 | P | 301 | TQN | C71-C72-C73-C74 |
| 5 | Q | 301 | TQN | C71-C72-C73-C74 |
| 5 | R | 301 | TQN | C71-C72-C73-C74 |
| 5 | S | 301 | TQN | C71-C72-C73-C74 |
| 5 | T | 301 | TQN | C71-C72-C73-C74 |
| 5 | U | 301 | TQN | C71-C72-C73-C74 |
| 5 | V | 301 | TQN | C71-C72-C73-C74 |
| 5 | W | 301 | TQN | C71-C72-C73-C74 |
| 5 | X | 301 | TQN | C71-C72-C73-C74 |
| 5 | Y | 301 | TQN | C71-C72-C73-C74 |
| 5 | Z | 301 | TQN | C71-C72-C73-C74 |
| 5 | Q | 301 | TQN | C16-C17-C18-C19 |
| 5 | J | 301 | TQN | C16-C17-C18-C19 |
| 5 | S | 301 | TQN | C16-C17-C18-C19 |
| 5 | B | 301 | TQN | C16-C17-C18-C19 |
| 5 | D | 301 | TQN | C16-C17-C18-C19 |
| 5 | F | 301 | TQN | C16-C17-C18-C19 |
| 5 | G | 301 | TQN | C16-C17-C18-C19 |
| 5 | H | 301 | TQN | C16-C17-C18-C19 |
| 5 | I | 301 | TQN | C16-C17-C18-C19 |
| 5 | K | 301 | TQN | C16-C17-C18-C19 |
| 5 | L | 301 | TQN | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | N | 301 | TQN | C16-C17-C18-C19 |
| 5 | O | 301 | TQN | C16-C17-C18-C19 |
| 5 | P | 301 | TQN | C16-C17-C18-C19 |
| 5 | R | 301 | TQN | C16-C17-C18-C19 |
| 5 | V | 301 | TQN | C16-C17-C18-C19 |
| 5 | X | 301 | TQN | C16-C17-C18-C19 |
| 5 | A | 302 | TQN | C16-C17-C18-C19 |
| 5 | C | 301 | TQN | C16-C17-C18-C19 |
| 5 | E | 301 | TQN | C16-C17-C18-C19 |
| 5 | M | 301 | TQN | C16-C17-C18-C19 |
| 5 | T | 301 | TQN | C16-C17-C18-C19 |
| 5 | U | 301 | TQN | C16-C17-C18-C19 |
| 5 | W | 301 | TQN | C16-C17-C18-C19 |
| 5 | Y | 301 | TQN | C16-C17-C18-C19 |
| 5 | Z | 301 | TQN | C16-C17-C18-C19 |
| 5 | A | 302 | TQN | CB4-OB4-PB-OP4 |
| 5 | B | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | C | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | D | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | E | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | F | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | G | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | H | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | I | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | J | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | K | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | L | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | M | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | N | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | O | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | P | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | Q | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | R | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | S | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | T | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | U | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | V | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | W | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | X | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | Y | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | Z | 301 | TQN | CB4-OB4-PB-OP4 |
| 5 | Z | 301 | TQN | C19-CC1-CC2-CC3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | A | 302 | TQN | C19-CC1-CC2-CC3 |
| 5 | C | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | I | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | S | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | T | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | B | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | H | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | K | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | M | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | O | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | Q | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | R | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | U | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | W | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | X | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | D | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | E | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | F | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | J | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | L | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | N | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | Y | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | G | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | P | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | V | 301 | TQN | C19-CC1-CC2-CC3 |
| 5 | I | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | A | 302 | TQN | CF4-CF5-CF6-CF7 |
| 5 | B | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | C | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | E | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | F | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | H | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | K | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | L | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | M | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | N | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | O | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | P | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | Q | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | R | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | S | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | T | 301 | TQN | CF4-CF5-CF6-CF7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | U | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | W | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | Y | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | Z | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | D | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | J | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | V | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | X | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | G | 301 | TQN | CF4-CF5-CF6-CF7 |
| 5 | K | 301 | TQN | C75-C76-C77-C78 |
| 5 | O | 301 | TQN | C75-C76-C77-C78 |
| 5 | R | 301 | TQN | C75-C76-C77-C78 |
| 5 | S | 301 | TQN | C75-C76-C77-C78 |
| 5 | B | 301 | TQN | C75-C76-C77-C78 |
| 5 | C | 301 | TQN | C75-C76-C77-C78 |
| 5 | D | 301 | TQN | C75-C76-C77-C78 |
| 5 | F | 301 | TQN | C75-C76-C77-C78 |
| 5 | G | 301 | TQN | C75-C76-C77-C78 |
| 5 | H | 301 | TQN | C75-C76-C77-C78 |
| 5 | I | 301 | TQN | C75-C76-C77-C78 |
| 5 | J | 301 | TQN | C75-C76-C77-C78 |
| 5 | M | 301 | TQN | C75-C76-C77-C78 |
| 5 | P | 301 | TQN | C75-C76-C77-C78 |
| 5 | Q | 301 | TQN | C75-C76-C77-C78 |
| 5 | T | 301 | TQN | C75-C76-C77-C78 |
| 5 | V | 301 | TQN | C75-C76-C77-C78 |
| 5 | W | 301 | TQN | C75-C76-C77-C78 |
| 5 | X | 301 | TQN | C75-C76-C77-C78 |
| 5 | Y | 301 | TQN | C75-C76-C77-C78 |
| 5 | Z | 301 | TQN | C75-C76-C77-C78 |
| 5 | A | 302 | TQN | C75-C76-C77-C78 |
| 5 | L | 301 | TQN | C75-C76-C77-C78 |
| 5 | N | 301 | TQN | C75-C76-C77-C78 |
| 5 | U | 301 | TQN | C75-C76-C77-C78 |
| 5 | E | 301 | TQN | C75-C76-C77-C78 |
| 5 | U | 301 | TQN | C35-C36-C37-C38 |
| 5 | B | 301 | TQN | C35-C36-C37-C38 |
| 5 | D | 301 | TQN | C35-C36-C37-C38 |
| 5 | E | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | K | 301 | TQN | C35-C36-C37-C38 |
| 5 | L | 301 | TQN | C35-C36-C37-C38 |
| 5 | M | 301 | TQN | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | S | 301 | TQN | C35-C36-C37-C38 |
| 5 | S | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | U | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | V | 301 | TQN | C35-C36-C37-C38 |
| 5 | X | 301 | TQN | C35-C36-C37-C38 |
| 5 | Y | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | Z | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | A | 302 | TQN | C35-C36-C37-C38 |
| 5 | A | 302 | TQN | CC6-CC7-CC8-CC9 |
| 5 | B | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | C | 301 | TQN | C35-C36-C37-C38 |
| 5 | C | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | D | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | E | 301 | TQN | C35-C36-C37-C38 |
| 5 | F | 301 | TQN | C35-C36-C37-C38 |
| 5 | F | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | G | 301 | TQN | C35-C36-C37-C38 |
| 5 | G | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | H | 301 | TQN | C35-C36-C37-C38 |
| 5 | H | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | I | 301 | TQN | C35-C36-C37-C38 |
| 5 | I | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | J | 301 | TQN | C35-C36-C37-C38 |
| 5 | J | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | K | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | L | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | M | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | N | 301 | TQN | C35-C36-C37-C38 |
| 5 | N | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | O | 301 | TQN | C35-C36-C37-C38 |
| 5 | O | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | P | 301 | TQN | C35-C36-C37-C38 |
| 5 | P | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | Q | 301 | TQN | C35-C36-C37-C38 |
| 5 | Q | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | R | 301 | TQN | C35-C36-C37-C38 |
| 5 | R | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | T | 301 | TQN | C35-C36-C37-C38 |
| 5 | T | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | V | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | W | 301 | TQN | C35-C36-C37-C38 |
| 5 | W | 301 | TQN | CC6-CC7-CC8-CC9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | X | 301 | TQN | CC6-CC7-CC8-CC9 |
| 5 | Y | 301 | TQN | C35-C36-C37-C38 |
| 5 | Z | 301 | TQN | C35-C36-C37-C38 |
| 5 | A | 302 | TQN | C12-C13-O13-C21 |
| 5 | B | 301 | TQN | C12-C13-O13-C21 |
| 5 | C | 301 | TQN | C12-C13-O13-C21 |
| 5 | D | 301 | TQN | C12-C13-O13-C21 |
| 5 | E | 301 | TQN | C12-C13-O13-C21 |
| 5 | F | 301 | TQN | C12-C13-O13-C21 |
| 5 | G | 301 | TQN | C12-C13-O13-C21 |
| 5 | H | 301 | TQN | C12-C13-O13-C21 |
| 5 | I | 301 | TQN | C12-C13-O13-C21 |
| 5 | J | 301 | TQN | C12-C13-O13-C21 |
| 5 | K | 301 | TQN | C12-C13-O13-C21 |
| 5 | L | 301 | TQN | C12-C13-O13-C21 |
| 5 | M | 301 | TQN | C12-C13-O13-C21 |
| 5 | N | 301 | TQN | C12-C13-O13-C21 |
| 5 | O | 301 | TQN | C12-C13-O13-C21 |
| 5 | P | 301 | TQN | C12-C13-O13-C21 |
| 5 | Q | 301 | TQN | C12-C13-O13-C21 |
| 5 | R | 301 | TQN | C12-C13-O13-C21 |
| 5 | S | 301 | TQN | C12-C13-O13-C21 |
| 5 | T | 301 | TQN | C12-C13-O13-C21 |
| 5 | U | 301 | TQN | C12-C13-O13-C21 |
| 5 | V | 301 | TQN | C12-C13-O13-C21 |
| 5 | W | 301 | TQN | C12-C13-O13-C21 |
| 5 | X | 301 | TQN | C12-C13-O13-C21 |
| 5 | Y | 301 | TQN | C12-C13-O13-C21 |
| 5 | Z | 301 | TQN | C12-C13-O13-C21 |
| 5 | R | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | B | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | F | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | G | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | H | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | J | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | L | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | N | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | O | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | P | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | T | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | U | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | W | 301 | TQN | C28-C29-CC6-CC7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | Z | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | A | 302 | TQN | C28-C29-CC6-CC7 |
| 5 | E | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | Q | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | V | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | M | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | I | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | K | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | S | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | Y | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | C | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | D | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | X | 301 | TQN | C28-C29-CC6-CC7 |
| 5 | A | 302 | TQN | CD5-CD6-CD7-CD8 |
| 5 | B | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | C | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | E | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | F | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | I | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | L | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | Q | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | U | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | V | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | X | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | O | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | Z | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | D | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | G | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | H | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | J | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | K | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | M | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | N | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | P | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | R | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | S | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | T | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | W | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | Y | 301 | TQN | CD5-CD6-CD7-CD8 |
| 5 | Q | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | A | 302 | TQN | C39-CD4-CD5-CD6 |
| 5 | B | 301 | TQN | C39-CD4-CD5-CD6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | C | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | E | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | F | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | G | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | I | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | L | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | M | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | U | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | W | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | Y | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | Z | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | D | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | H | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | J | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | K | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | N | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | O | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | P | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | R | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | S | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | T | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | V | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | X | 301 | TQN | C39-CD4-CD5-CD6 |
| 5 | B | 301 | TQN | C14-C15-C16-C17 |
| 5 | E | 301 | TQN | C14-C15-C16-C17 |
| 5 | F | 301 | TQN | C14-C15-C16-C17 |
| 5 | H | 301 | TQN | C14-C15-C16-C17 |
| 5 | L | 301 | TQN | C14-C15-C16-C17 |
| 5 | M | 301 | TQN | C14-C15-C16-C17 |
| 5 | N | 301 | TQN | C14-C15-C16-C17 |
| 5 | P | 301 | TQN | C14-C15-C16-C17 |
| 5 | Q | 301 | TQN | C14-C15-C16-C17 |
| 5 | R | 301 | TQN | C14-C15-C16-C17 |
| 5 | S | 301 | TQN | C14-C15-C16-C17 |
| 5 | T | 301 | TQN | C14-C15-C16-C17 |
| 5 | U | 301 | TQN | C14-C15-C16-C17 |
| 5 | V | 301 | TQN | C14-C15-C16-C17 |
| 5 | W | 301 | TQN | C14-C15-C16-C17 |
| 5 | X | 301 | TQN | C14-C15-C16-C17 |
| 5 | Z | 301 | TQN | C14-C15-C16-C17 |
| 5 | C | 301 | TQN | C14-C15-C16-C17 |
| 5 | K | 301 | TQN | C14-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | Y | 301 | TQN | C14-C15-C16-C17 |
| 5 | A | 302 | TQN | C14-C15-C16-C17 |
| 5 | D | 301 | TQN | C14-C15-C16-C17 |
| 5 | G | 301 | TQN | C14-C15-C16-C17 |
| 5 | I | 301 | TQN | C14-C15-C16-C17 |
| 5 | J | 301 | TQN | C14-C15-C16-C17 |
| 5 | O | 301 | TQN | C14-C15-C16-C17 |
| 5 | L | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | V | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | C | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | F | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | T | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | U | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | X | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | Q | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | S | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | D | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | E | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | G | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | M | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | O | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | Z | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | H | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | I | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | N | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | P | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | R | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | W | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | Y | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | A | 302 | TQN | CD4-CD5-CD6-CD7 |
| 5 | B | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | J | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | K | 301 | TQN | CD4-CD5-CD6-CD7 |
| 5 | A | 302 | TQN | O33-C33-C34-C35 |
| 5 | B | 301 | TQN | O33-C33-C34-C35 |
| 5 | C | 301 | TQN | O33-C33-C34-C35 |
| 5 | D | 301 | TQN | O33-C33-C34-C35 |
| 5 | E | 301 | TQN | O33-C33-C34-C35 |
| 5 | F | 301 | TQN | O33-C33-C34-C35 |
| 5 | G | 301 | TQN | O33-C33-C34-C35 |
| 5 | H | 301 | TQN | O33-C33-C34-C35 |
| 5 | I | 301 | TQN | O33-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | J | 301 | TQN | O33-C33-C34-C35 |
| 5 | K | 301 | TQN | O33-C33-C34-C35 |
| 5 | L | 301 | TQN | O33-C33-C34-C35 |
| 5 | M | 301 | TQN | O33-C33-C34-C35 |
| 5 | N | 301 | TQN | O33-C33-C34-C35 |
| 5 | O | 301 | TQN | O33-C33-C34-C35 |
| 5 | P | 301 | TQN | O33-C33-C34-C35 |
| 5 | Q | 301 | TQN | O33-C33-C34-C35 |
| 5 | R | 301 | TQN | O33-C33-C34-C35 |
| 5 | S | 301 | TQN | O33-C33-C34-C35 |
| 5 | T | 301 | TQN | O33-C33-C34-C35 |
| 5 | U | 301 | TQN | O33-C33-C34-C35 |
| 5 | V | 301 | TQN | O33-C33-C34-C35 |
| 5 | W | 301 | TQN | O33-C33-C34-C35 |
| 5 | X | 301 | TQN | O33-C33-C34-C35 |
| 5 | Y | 301 | TQN | O33-C33-C34-C35 |
| 5 | Z | 301 | TQN | O33-C33-C34-C35 |
| 5 | A | 302 | TQN | C13-C14-C15-C16 |
| 5 | B | 301 | TQN | C13-C14-C15-C16 |
| 5 | C | 301 | TQN | C13-C14-C15-C16 |
| 5 | D | 301 | TQN | C13-C14-C15-C16 |
| 5 | E | 301 | TQN | C13-C14-C15-C16 |
| 5 | F | 301 | TQN | C13-C14-C15-C16 |
| 5 | G | 301 | TQN | C13-C14-C15-C16 |
| 5 | H | 301 | TQN | C13-C14-C15-C16 |
| 5 | I | 301 | TQN | C13-C14-C15-C16 |
| 5 | J | 301 | TQN | C13-C14-C15-C16 |
| 5 | K | 301 | TQN | C13-C14-C15-C16 |
| 5 | L | 301 | TQN | C13-C14-C15-C16 |
| 5 | M | 301 | TQN | C13-C14-C15-C16 |
| 5 | N | 301 | TQN | C13-C14-C15-C16 |
| 5 | O | 301 | TQN | C13-C14-C15-C16 |
| 5 | P | 301 | TQN | C13-C14-C15-C16 |
| 5 | Q | 301 | TQN | C13-C14-C15-C16 |
| 5 | R | 301 | TQN | C13-C14-C15-C16 |
| 5 | S | 301 | TQN | C13-C14-C15-C16 |
| 5 | T | 301 | TQN | C13-C14-C15-C16 |
| 5 | U | 301 | TQN | C13-C14-C15-C16 |
| 5 | V | 301 | TQN | C13-C14-C15-C16 |
| 5 | W | 301 | TQN | C13-C14-C15-C16 |
| 5 | X | 301 | TQN | C13-C14-C15-C16 |
| 5 | Y | 301 | TQN | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | Z | 301 | TQN | C13-C14-C15-C16 |
| 5 | L | 301 | TQN | C82-C83-C84-C85 |
| 5 | N | 301 | TQN | C82-C83-C84-C85 |
| 5 | S | 301 | TQN | C82-C83-C84-C85 |
| 5 | W | 301 | TQN | C82-C83-C84-C85 |
| 5 | B | 301 | TQN | C82-C83-C84-C85 |
| 5 | D | 301 | TQN | C82-C83-C84-C85 |
| 5 | G | 301 | TQN | C82-C83-C84-C85 |
| 5 | O | 301 | TQN | C82-C83-C84-C85 |
| 5 | R | 301 | TQN | C82-C83-C84-C85 |
| 5 | A | 302 | TQN | C82-C83-C84-C85 |
| 5 | V | 301 | TQN | C82-C83-C84-C85 |
| 5 | X | 301 | TQN | C82-C83-C84-C85 |
| 5 | Y | 301 | TQN | C82-C83-C84-C85 |
| 5 | C | 301 | TQN | C82-C83-C84-C85 |
| 5 | H | 301 | TQN | C82-C83-C84-C85 |
| 5 | K | 301 | TQN | C82-C83-C84-C85 |
| 5 | T | 301 | TQN | C82-C83-C84-C85 |
| 5 | U | 301 | TQN | C82-C83-C84-C85 |
| 5 | F | 301 | TQN | C82-C83-C84-C85 |
| 5 | I | 301 | TQN | C82-C83-C84-C85 |
| 5 | Q | 301 | TQN | C82-C83-C84-C85 |
| 5 | Z | 301 | TQN | C82-C83-C84-C85 |
| 5 | M | 301 | TQN | C82-C83-C84-C85 |
| 5 | P | 301 | TQN | C82-C83-C84-C85 |
| 5 | J | 301 | TQN | C82-C83-C84-C85 |
| 5 | E | 301 | TQN | C82-C83-C84-C85 |
| 5 | A | 302 | TQN | C52-C53-C54-C55 |
| 5 | B | 301 | TQN | C52-C53-C54-C55 |
| 5 | C | 301 | TQN | C52-C53-C54-C55 |
| 5 | D | 301 | TQN | C52-C53-C54-C55 |
| 5 | E | 301 | TQN | C52-C53-C54-C55 |
| 5 | F | 301 | TQN | C52-C53-C54-C55 |
| 5 | G | 301 | TQN | C52-C53-C54-C55 |
| 5 | H | 301 | TQN | C52-C53-C54-C55 |
| 5 | I | 301 | TQN | C52-C53-C54-C55 |
| 5 | J | 301 | TQN | C52-C53-C54-C55 |
| 5 | K | 301 | TQN | C52-C53-C54-C55 |
| 5 | L | 301 | TQN | C52-C53-C54-C55 |
| 5 | M | 301 | TQN | C52-C53-C54-C55 |
| 5 | N | 301 | TQN | C52-C53-C54-C55 |
| 5 | O | 301 | TQN | C52-C53-C54-C55 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | P | 301 | TQN | C52-C53-C54-C55 |
| 5 | Q | 301 | TQN | C52-C53-C54-C55 |
| 5 | R | 301 | TQN | C52-C53-C54-C55 |
| 5 | S | 301 | TQN | C52-C53-C54-C55 |
| 5 | T | 301 | TQN | C52-C53-C54-C55 |
| 5 | U | 301 | TQN | C52-C53-C54-C55 |
| 5 | V | 301 | TQN | C52-C53-C54-C55 |
| 5 | W | 301 | TQN | C52-C53-C54-C55 |
| 5 | X | 301 | TQN | C52-C53-C54-C55 |
| 5 | Y | 301 | TQN | C52-C53-C54-C55 |
| 5 | Z | 301 | TQN | C52-C53-C54-C55 |
| 5 | A | 302 | TQN | CA5-CA6-OA6-CB1 |
| 5 | B | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | C | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | D | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | E | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | F | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | G | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | H | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | I | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | J | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | K | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | L | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | M | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | N | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | O | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | P | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | Q | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | R | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | S | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | T | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | U | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | V | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | W | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | X | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | Y | 301 | TQN | CA5-CA6-OA6-CB1 |
| 5 | Z | 301 | TQN | CA5-CA6-OA6-CB1 |

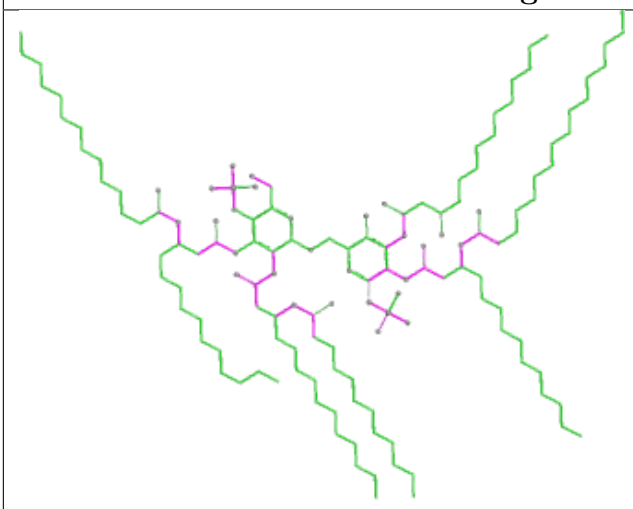
There are no ring outliers.

26 monomers are involved in 52 short contacts:

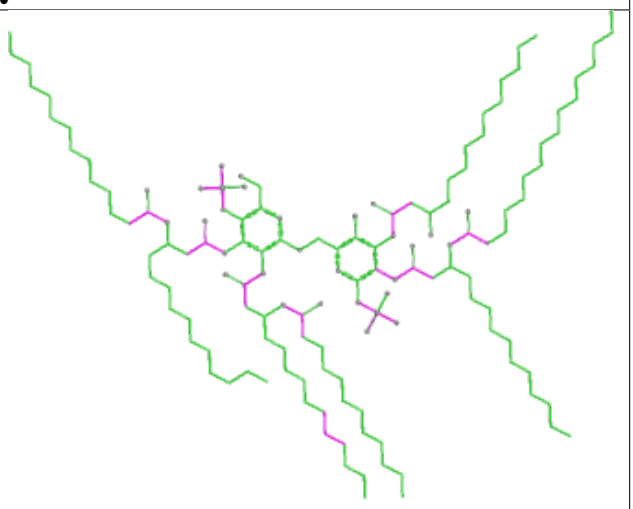
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | G | 301 | TQN | 2 | 0 |
| 5 | U | 301 | TQN | 2 | 0 |
| 5 | H | 301 | TQN | 2 | 0 |
| 5 | W | 301 | TQN | 2 | 0 |
| 5 | O | 301 | TQN | 2 | 0 |
| 5 | L | 301 | TQN | 2 | 0 |
| 5 | D | 301 | TQN | 2 | 0 |
| 5 | F | 301 | TQN | 2 | 0 |
| 5 | I | 301 | TQN | 2 | 0 |
| 5 | M | 301 | TQN | 2 | 0 |
| 5 | Q | 301 | TQN | 2 | 0 |
| 5 | N | 301 | TQN | 2 | 0 |
| 5 | Y | 301 | TQN | 2 | 0 |
| 5 | Z | 301 | TQN | 2 | 0 |
| 5 | E | 301 | TQN | 2 | 0 |
| 5 | S | 301 | TQN | 2 | 0 |
| 5 | A | 302 | TQN | 2 | 0 |
| 5 | K | 301 | TQN | 2 | 0 |
| 5 | T | 301 | TQN | 2 | 0 |
| 5 | B | 301 | TQN | 2 | 0 |
| 5 | V | 301 | TQN | 2 | 0 |
| 5 | R | 301 | TQN | 2 | 0 |
| 5 | C | 301 | TQN | 2 | 0 |
| 5 | X | 301 | TQN | 2 | 0 |
| 5 | J | 301 | TQN | 2 | 0 |
| 5 | P | 301 | TQN | 2 | 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.

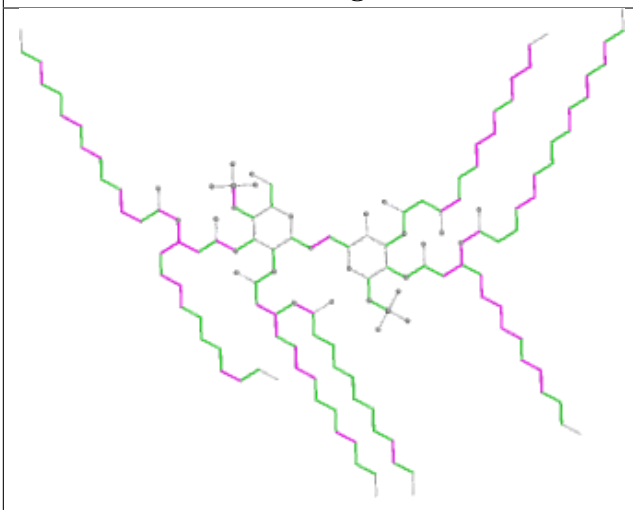
**Ligand TQN G 301**



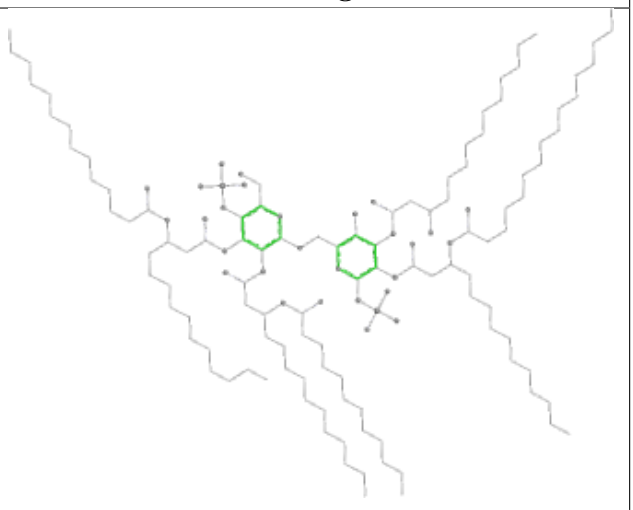
**Bond lengths**



**Bond angles**

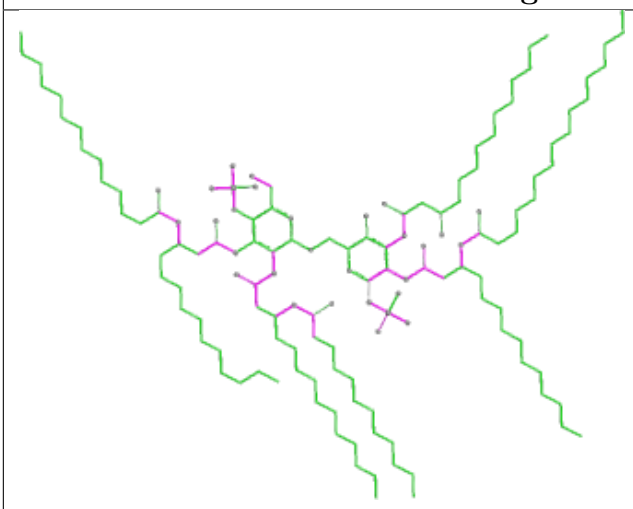


**Torsions**

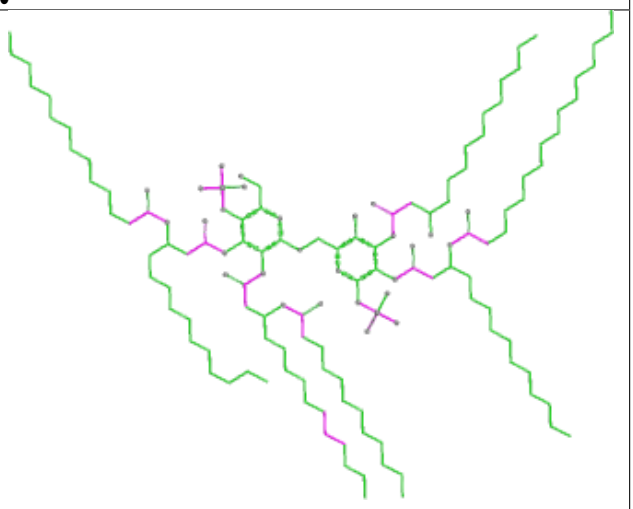


**Rings**

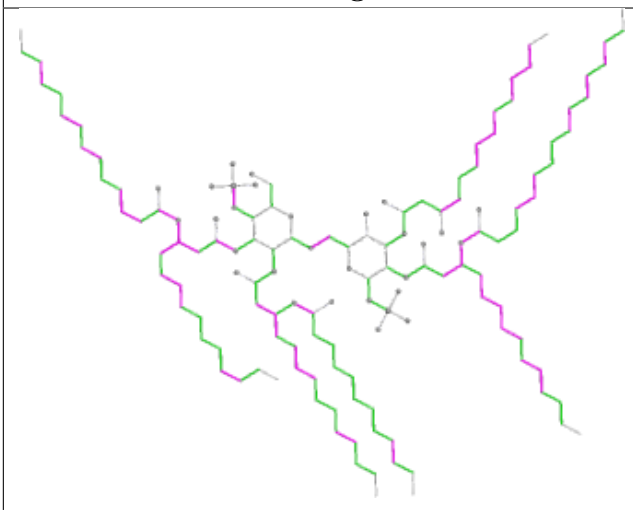
**Ligand TQN U 301**



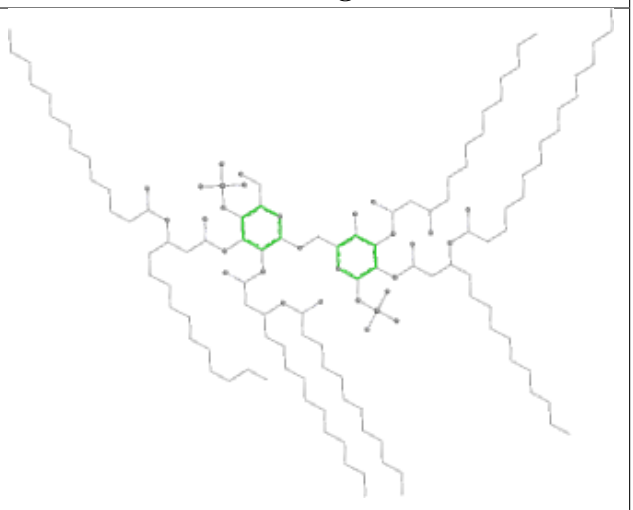
**Bond lengths**



**Bond angles**

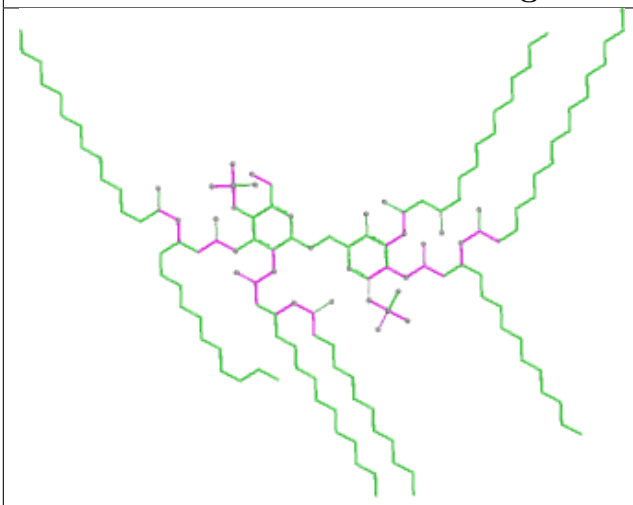


**Torsions**

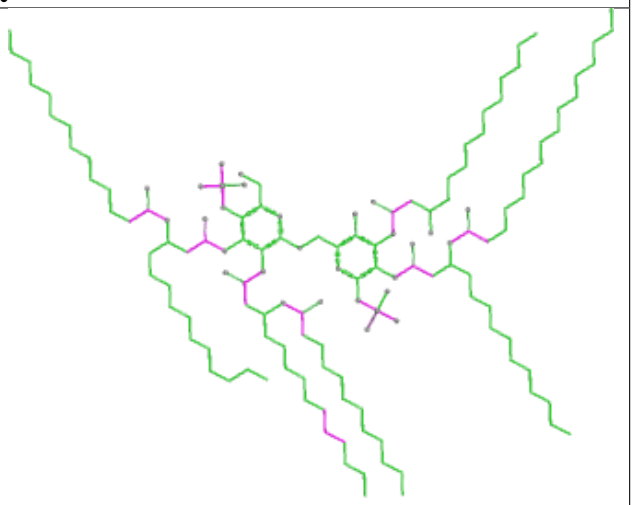


**Rings**

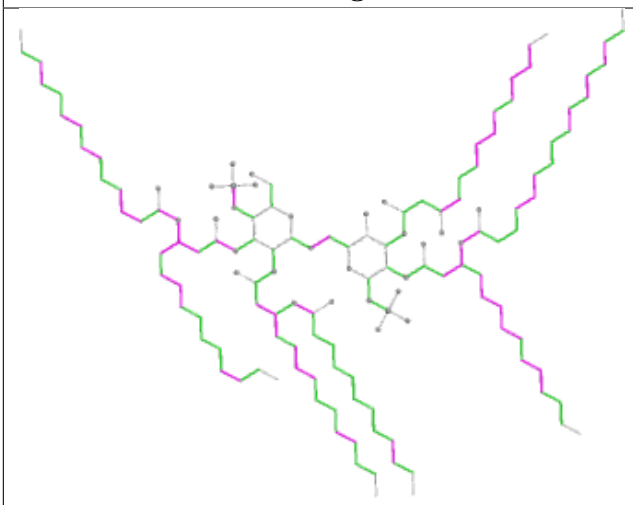
**Ligand TQN H 301**



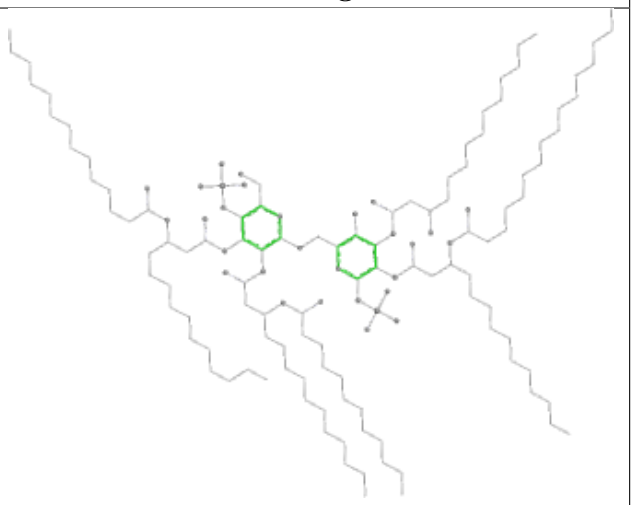
**Bond lengths**



**Bond angles**

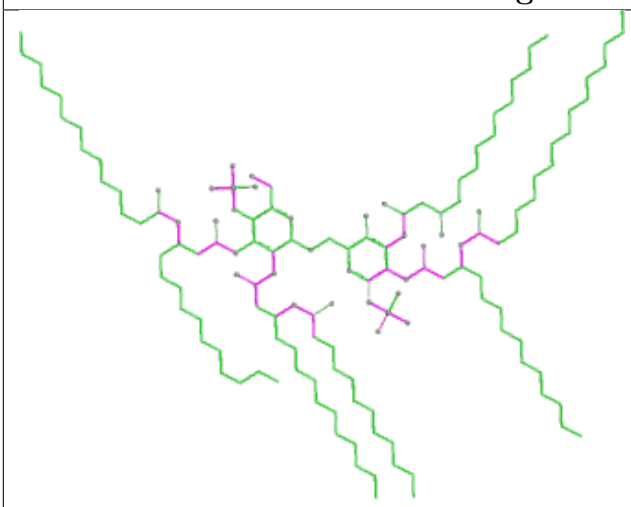


**Torsions**

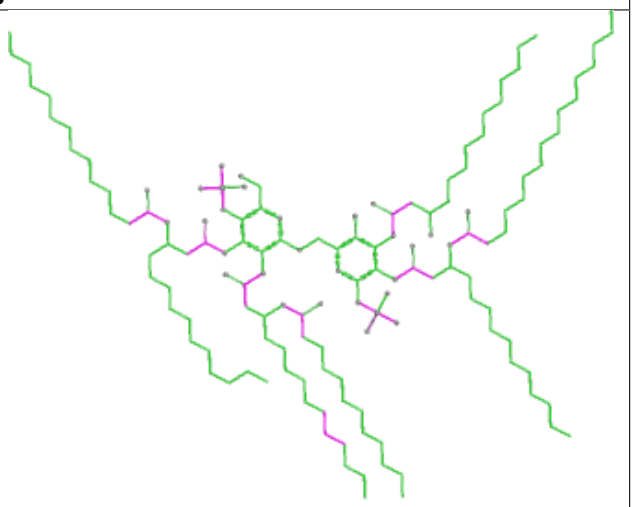


**Rings**

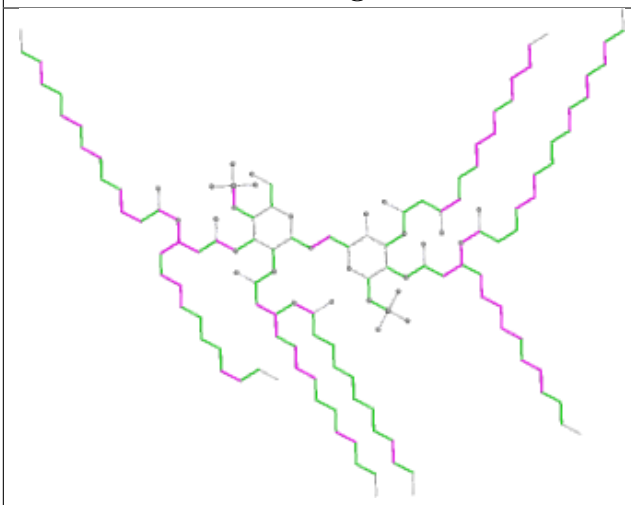
**Ligand TQN W 301**



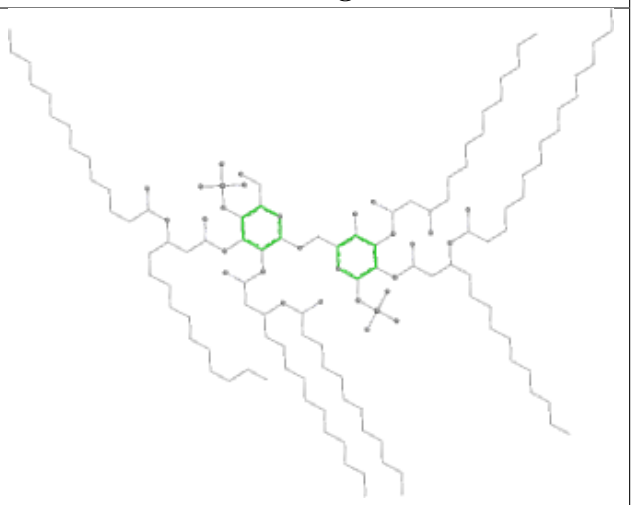
**Bond lengths**



**Bond angles**

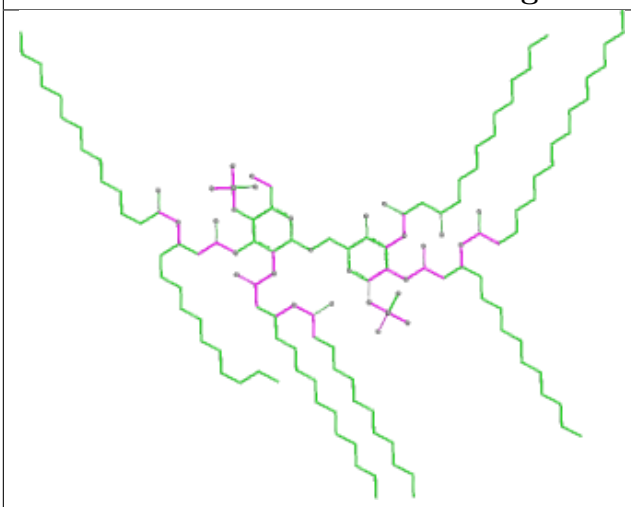


**Torsions**

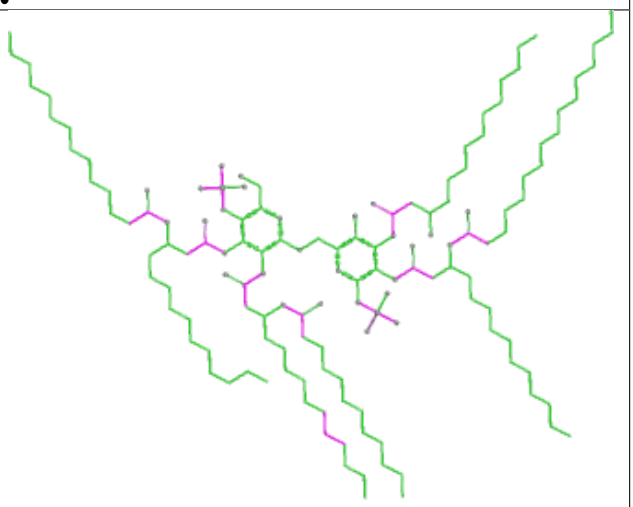


**Rings**

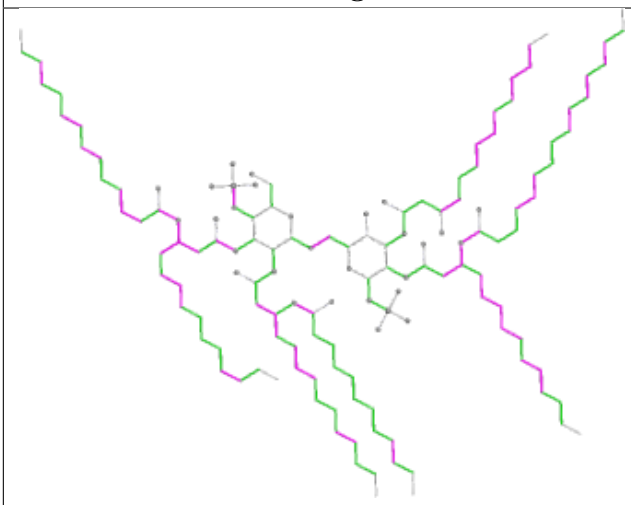
**Ligand TQN O 301**



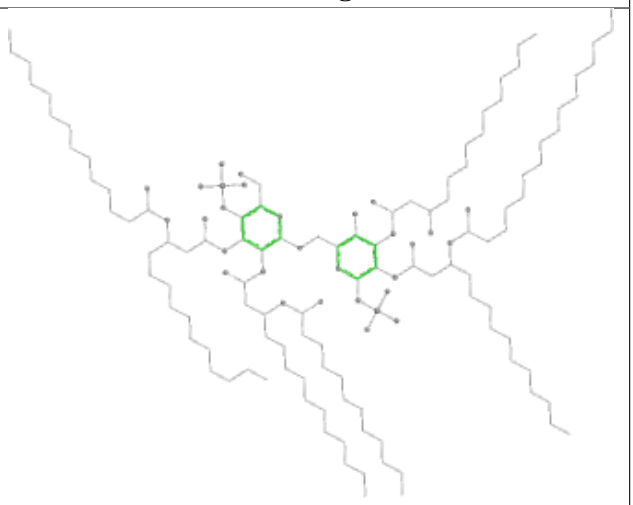
**Bond lengths**



**Bond angles**

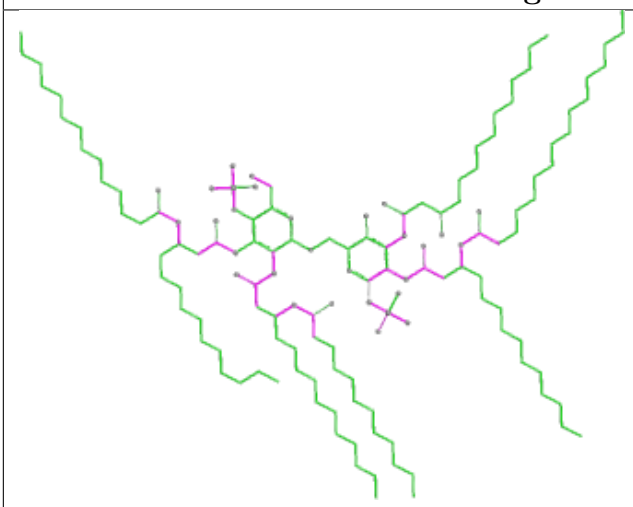


**Torsions**

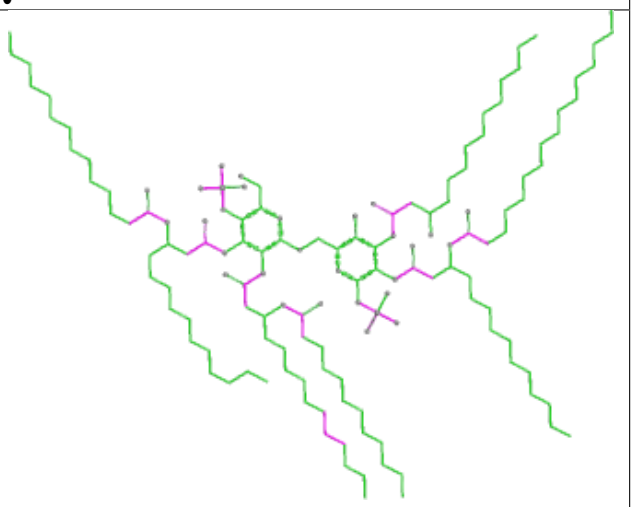


**Rings**

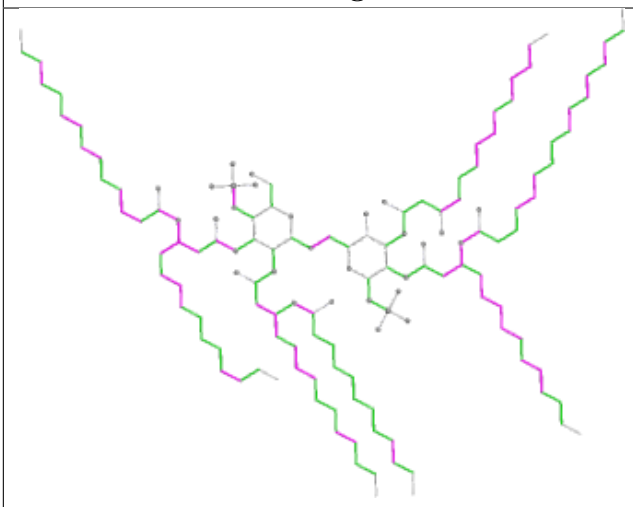
**Ligand TQN L 301**



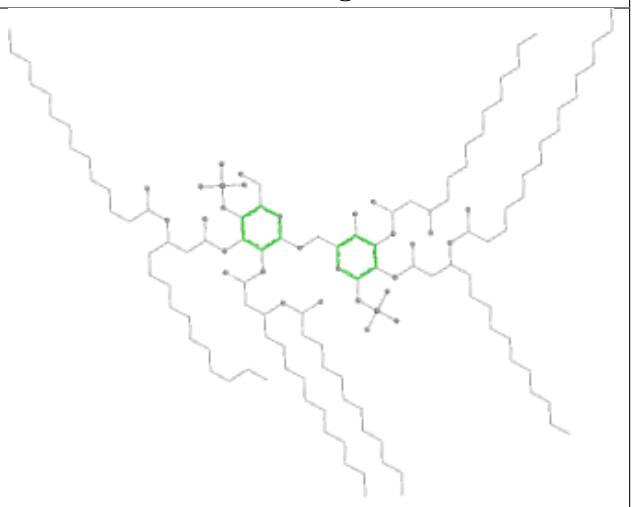
**Bond lengths**



**Bond angles**

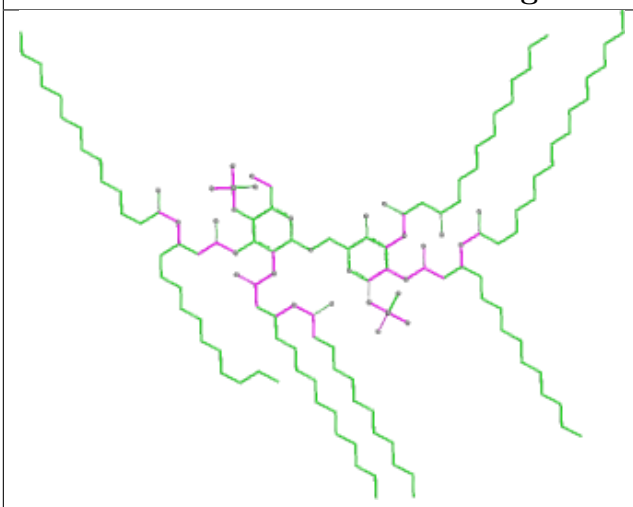


**Torsions**

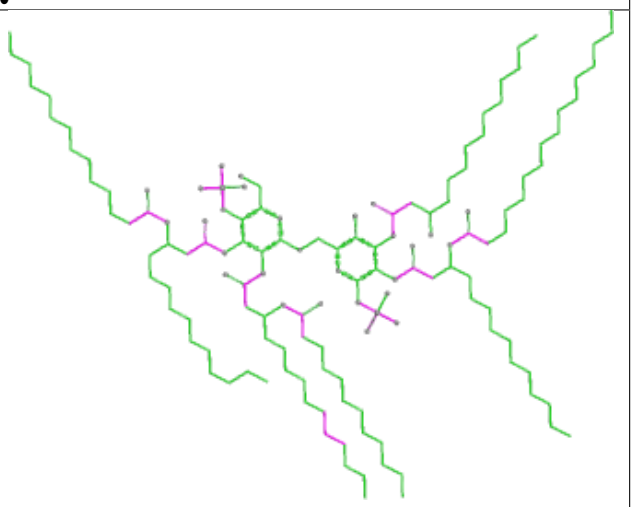


**Rings**

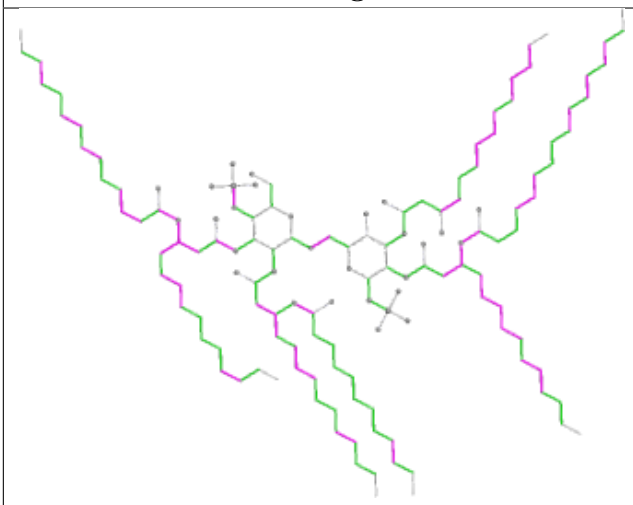
**Ligand TQN D 301**



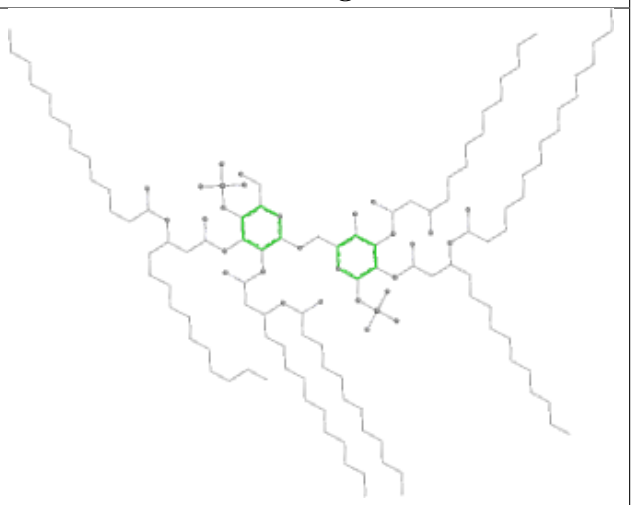
**Bond lengths**



**Bond angles**

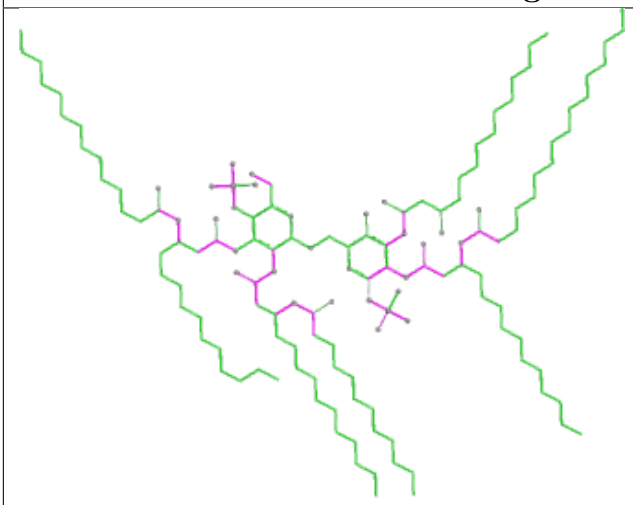


**Torsions**



**Rings**

**Ligand TQN F 301**



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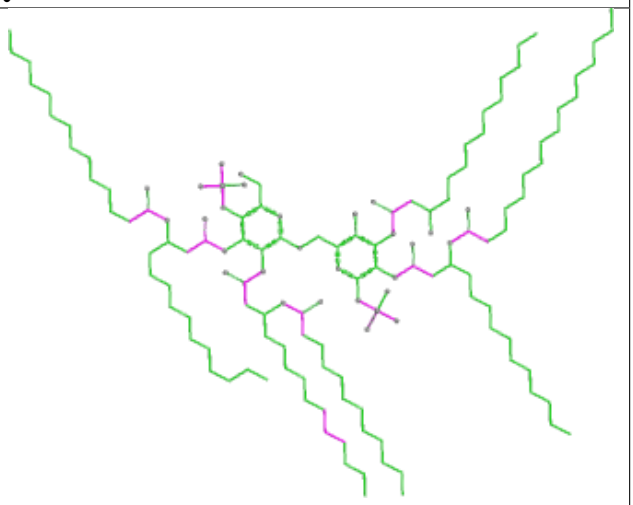

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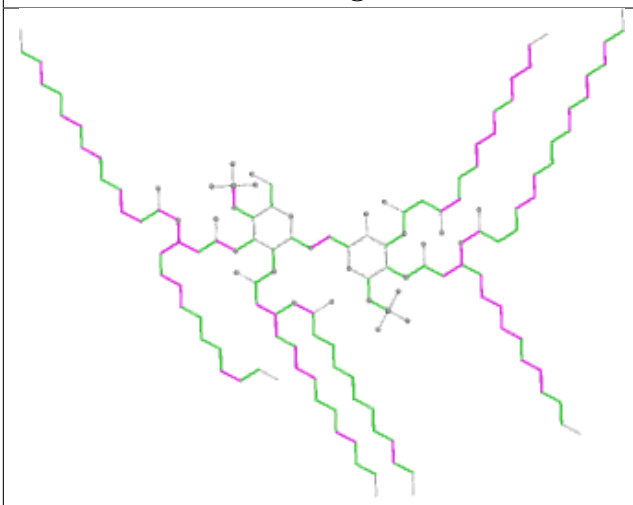

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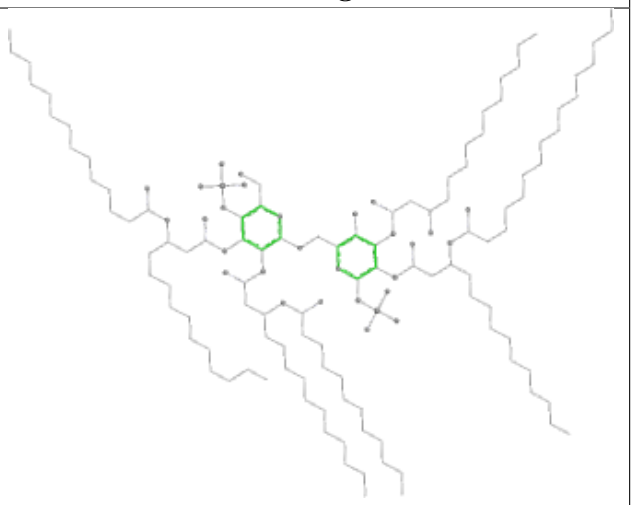
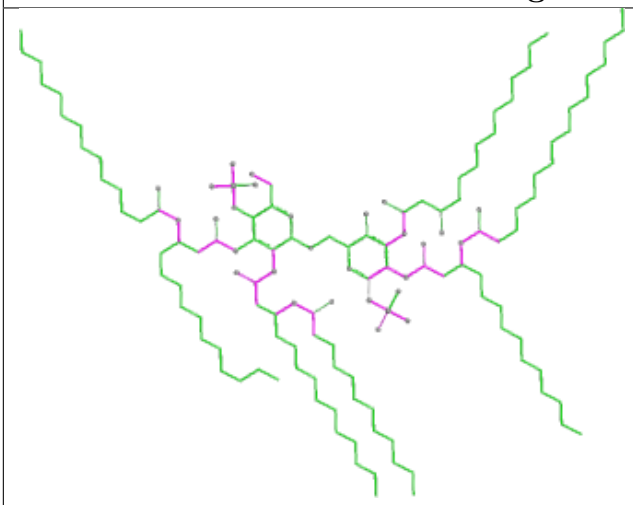


**Rings**

**Ligand TQN I 301**



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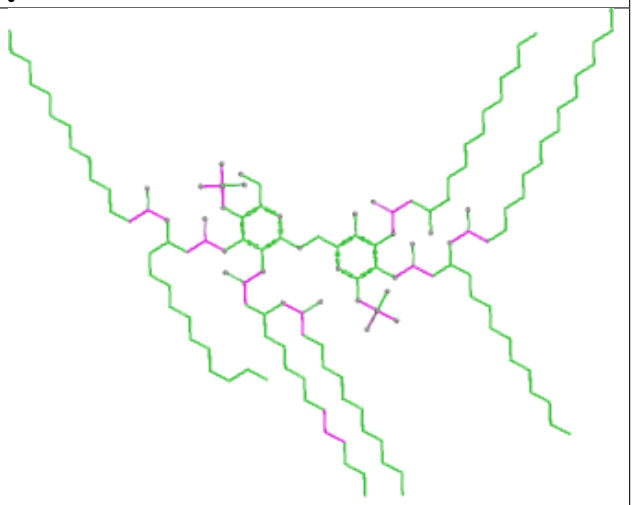

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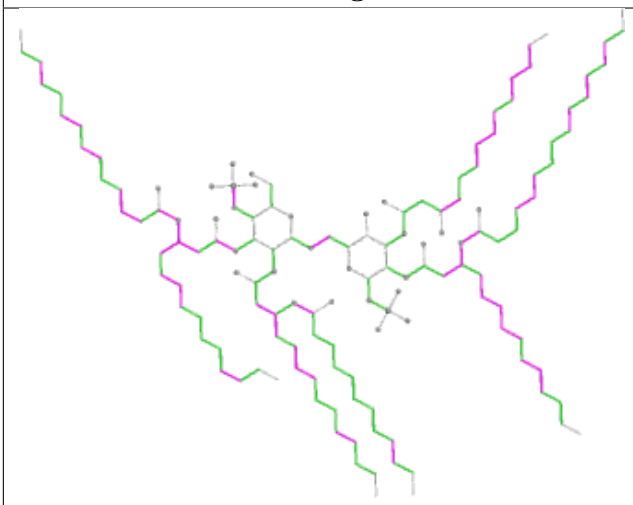
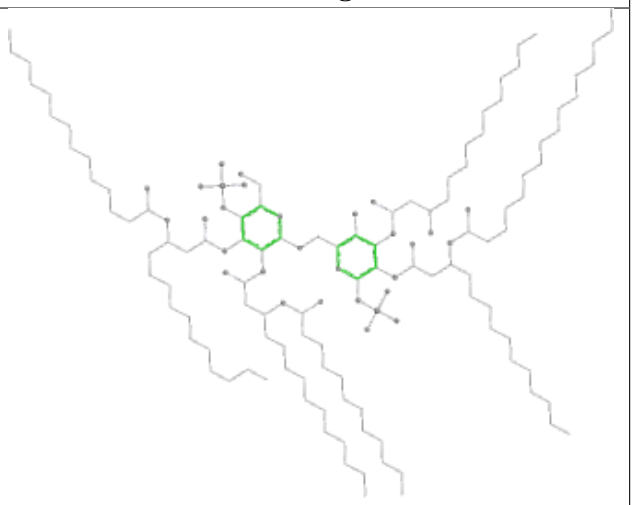


**Torsions**



**Rings**

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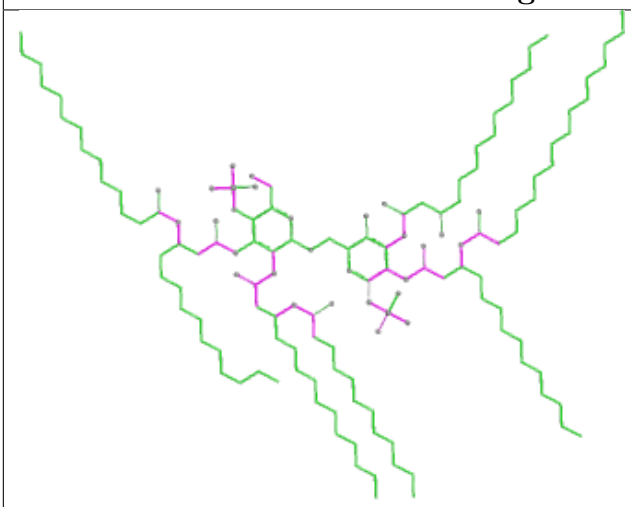

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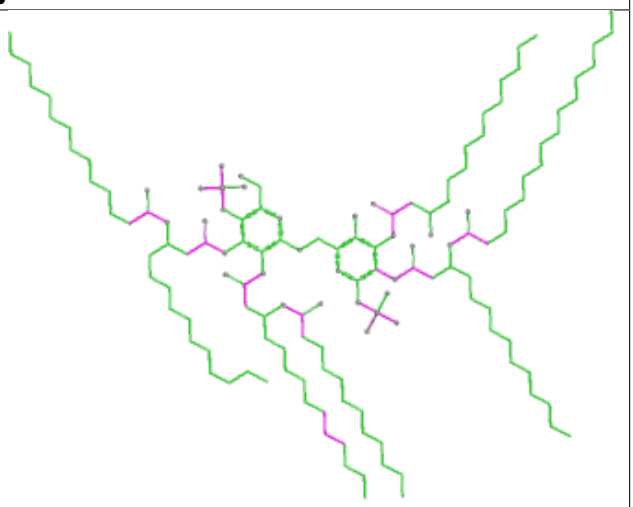

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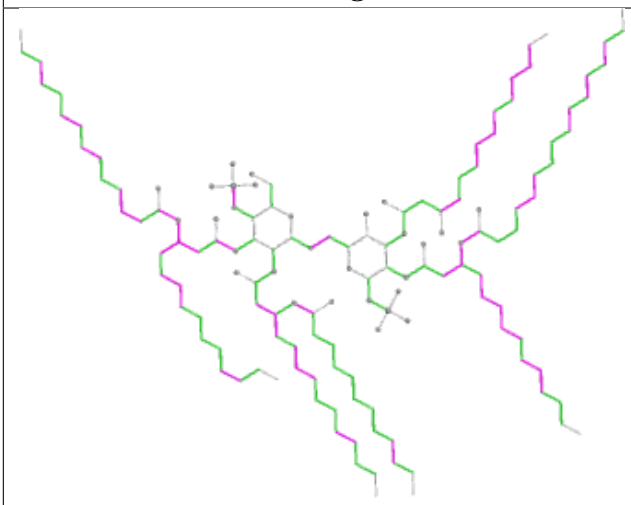

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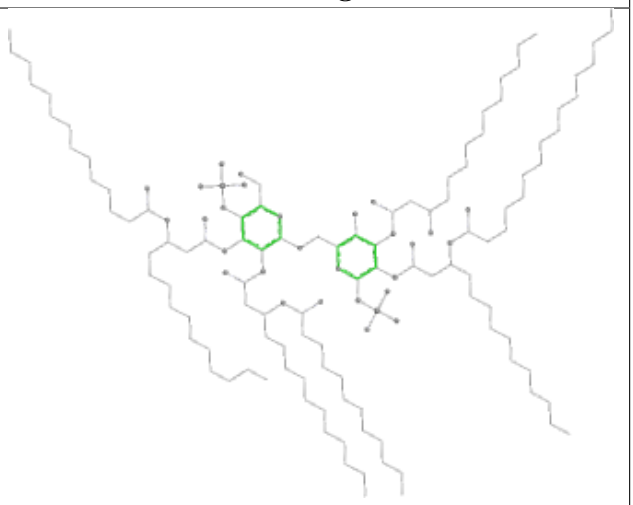
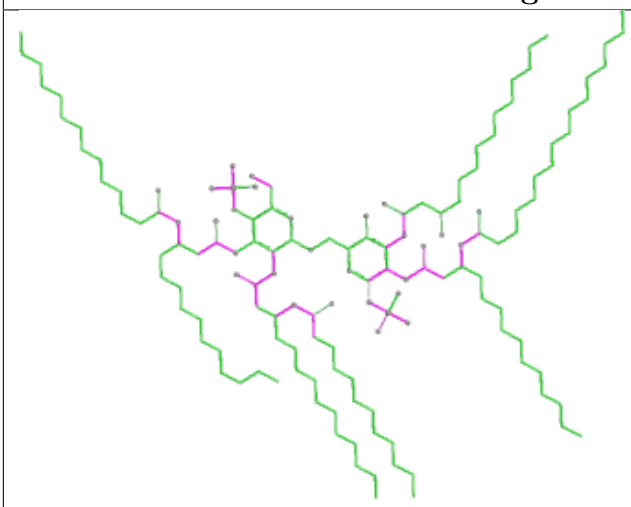


**Rings**

**Ligand TQN Q 301**



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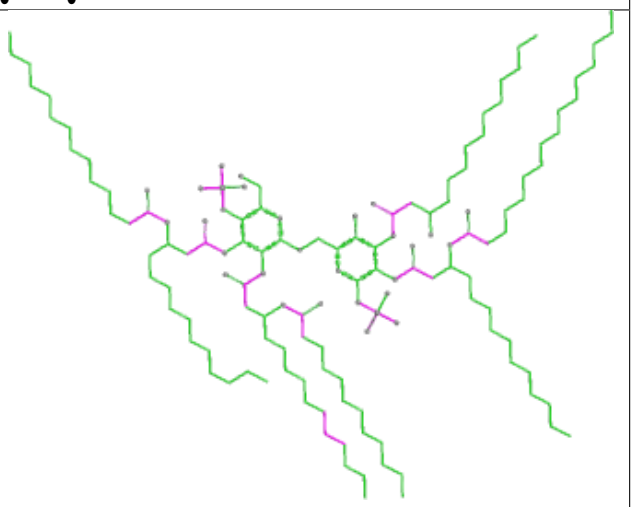

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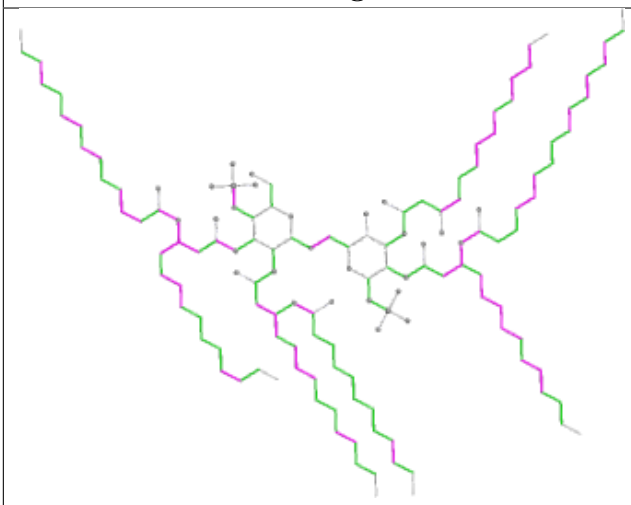

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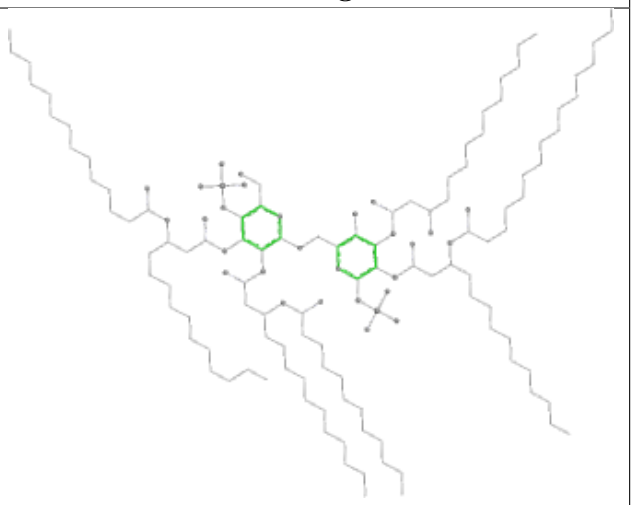

**Rings**

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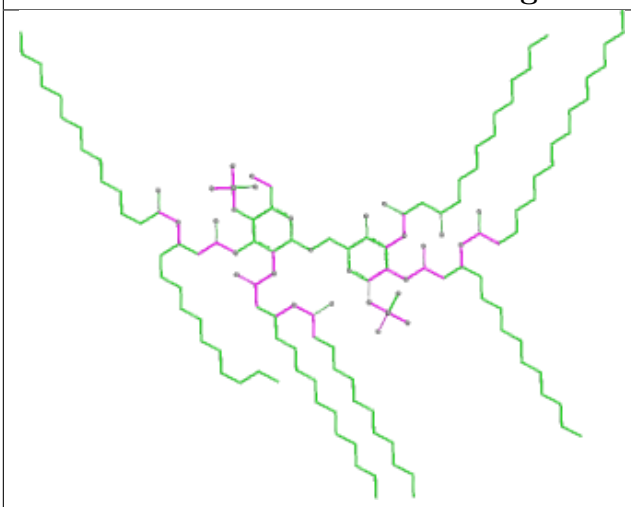

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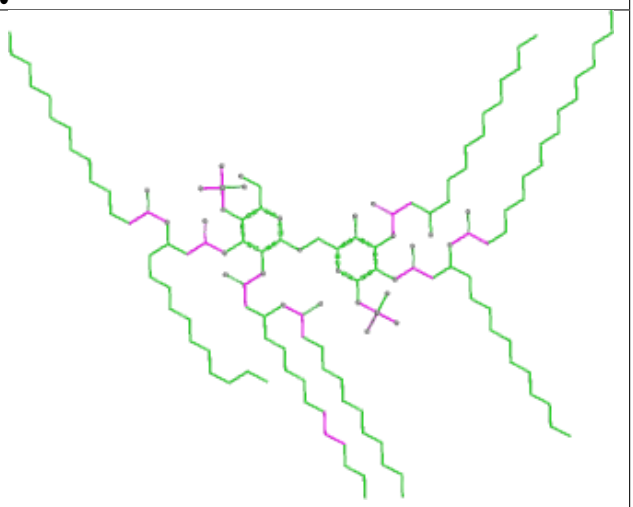

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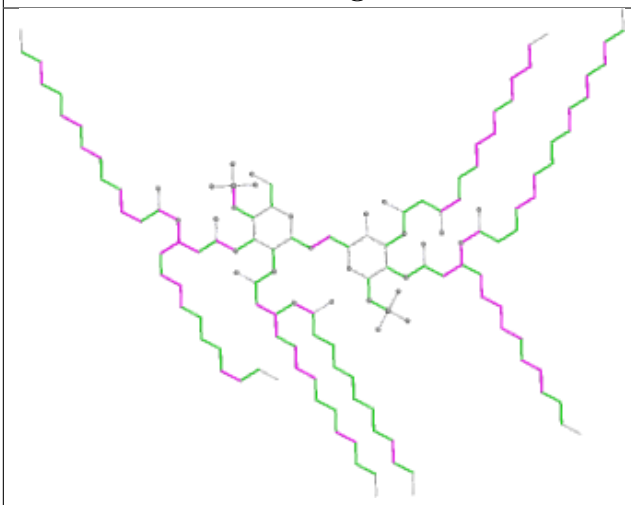

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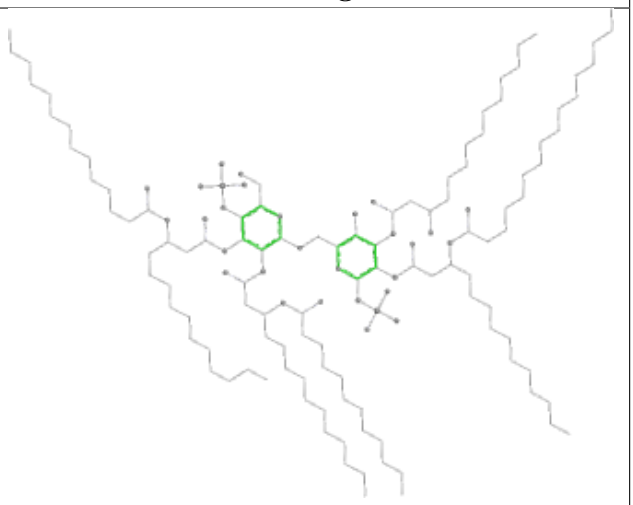

**Rings**

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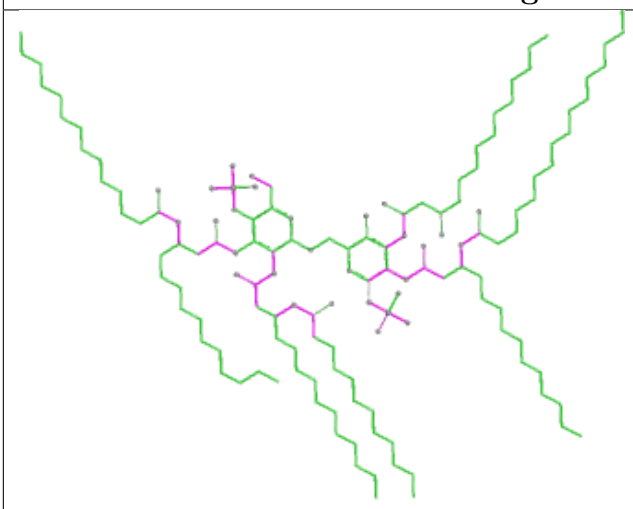

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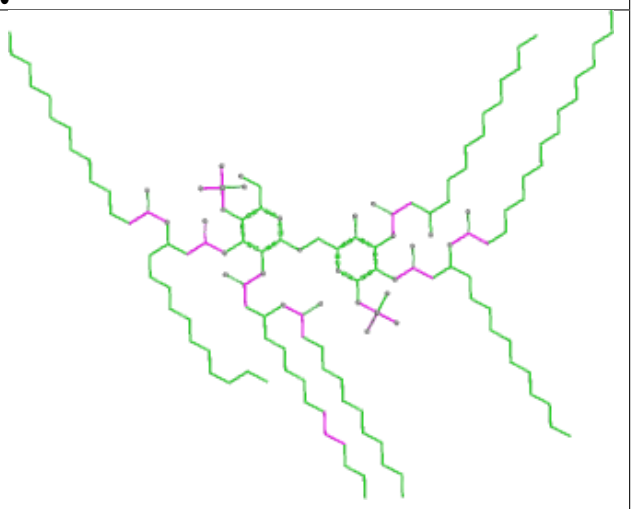

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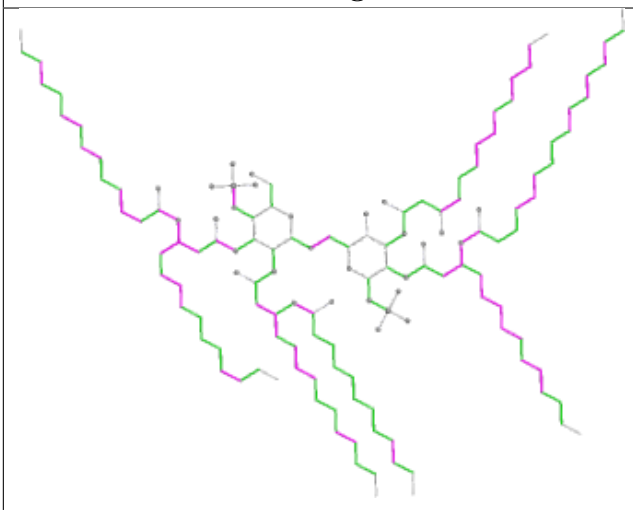

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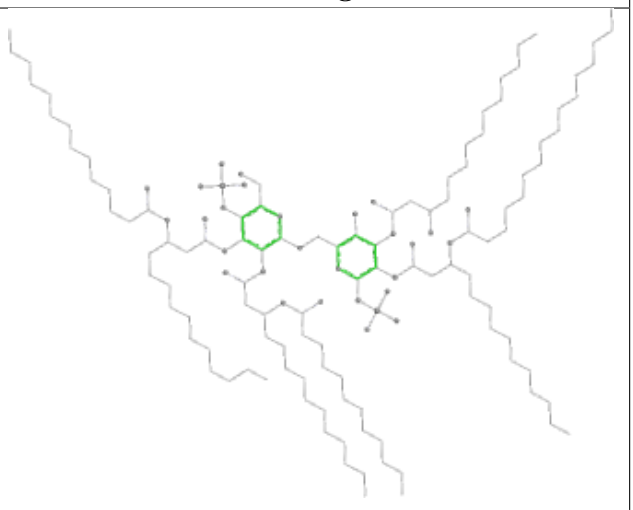

**Rings**

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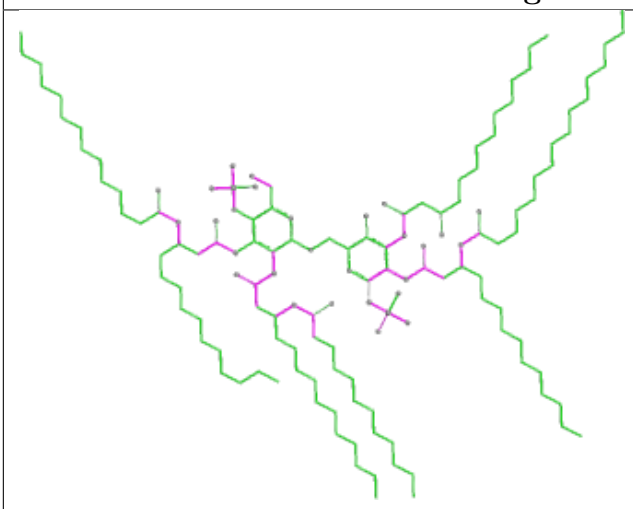

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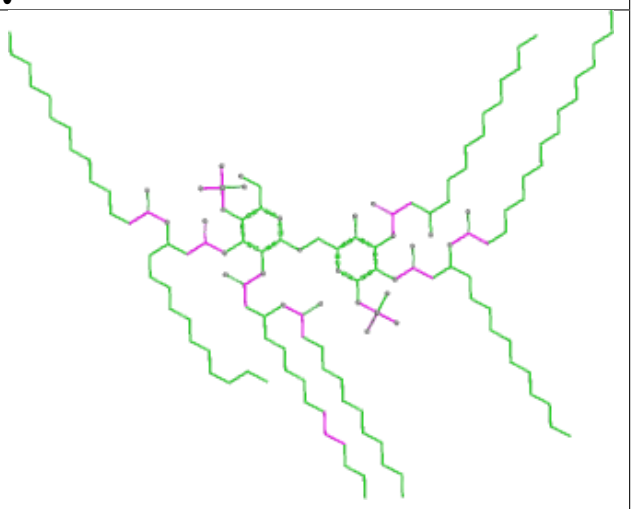

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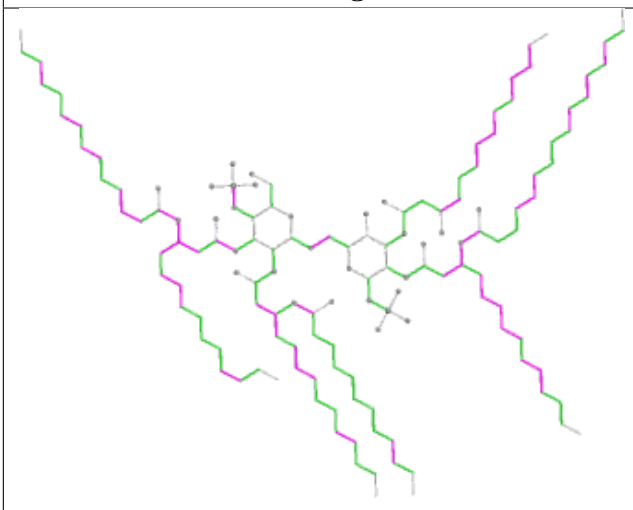
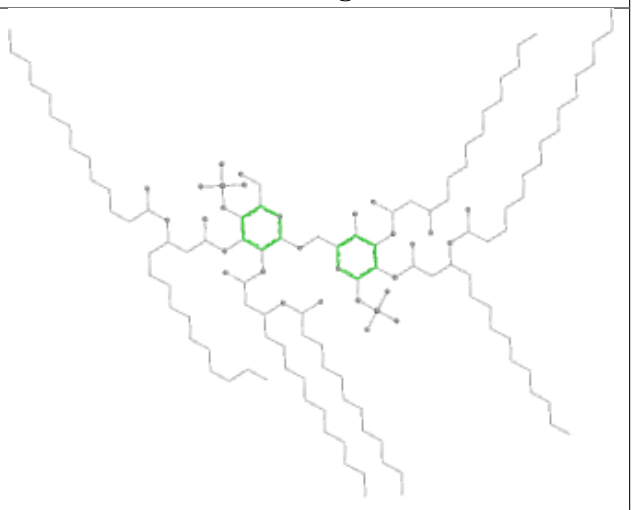


**Torsions**



**Rings**

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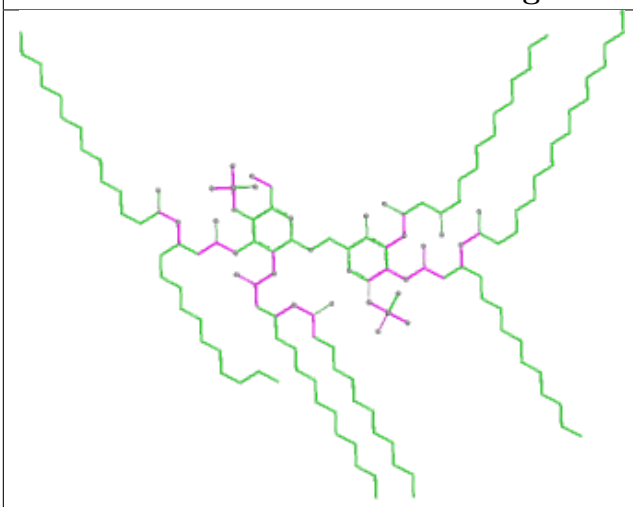

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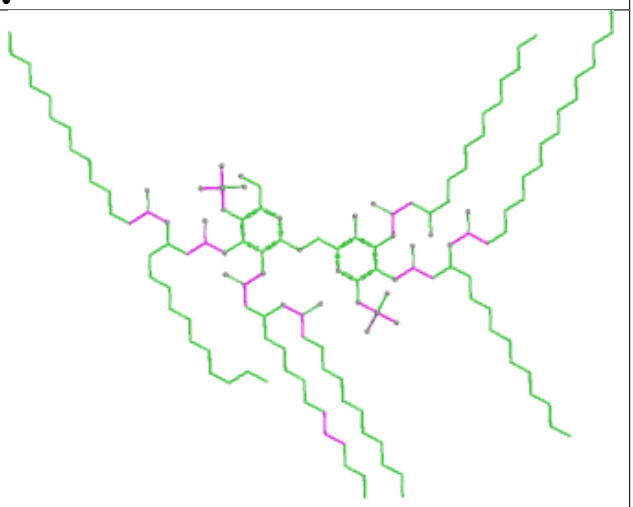

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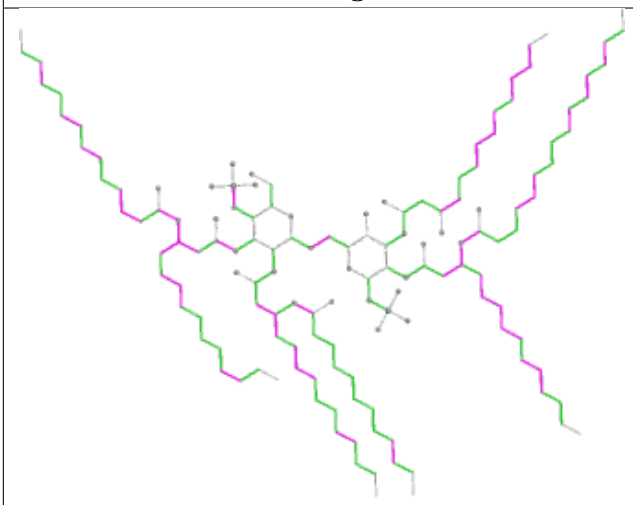

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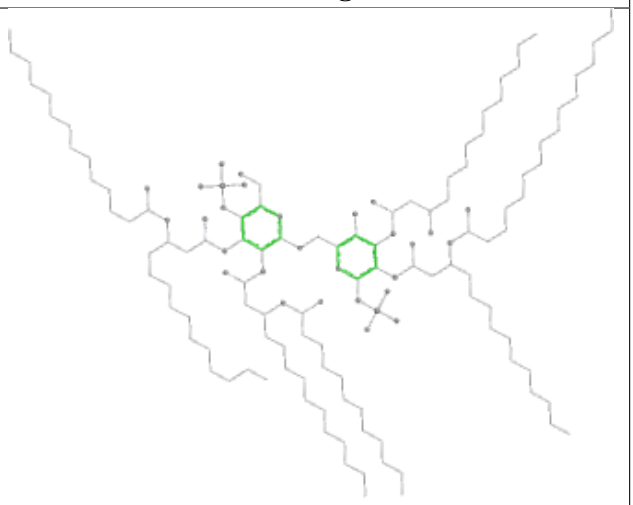

**Rings**

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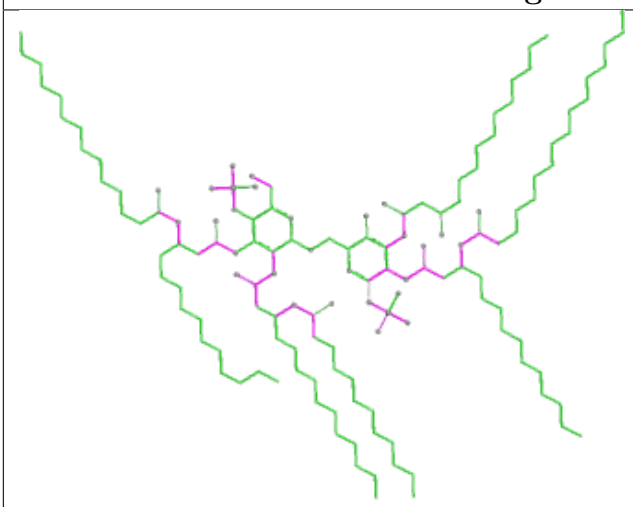

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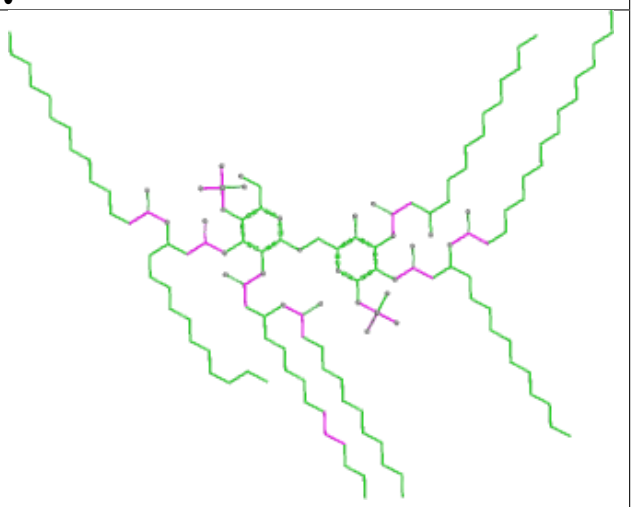

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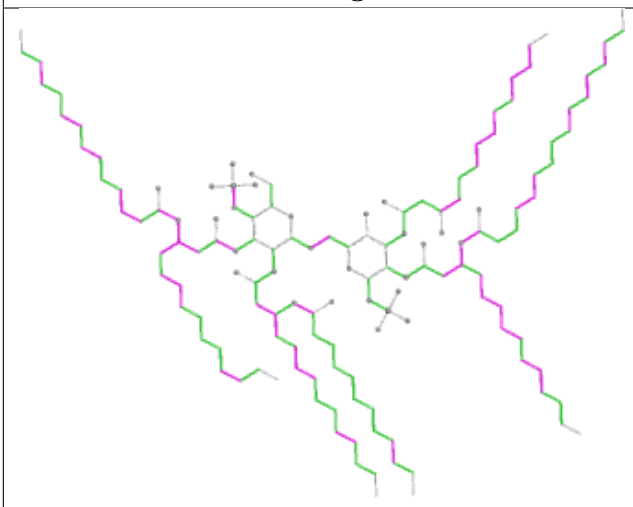

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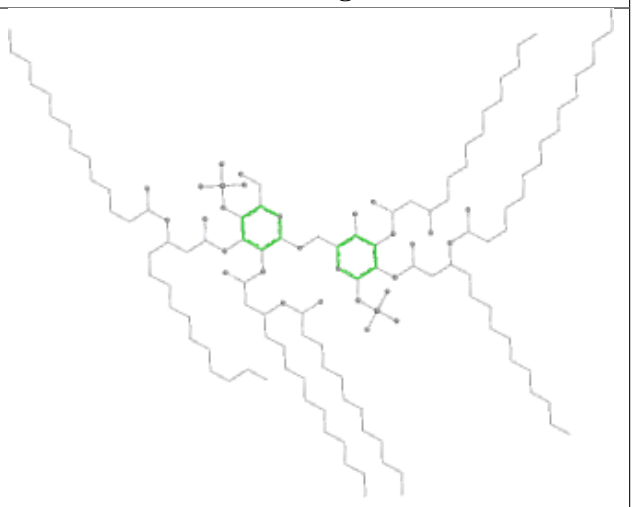

**Rings**

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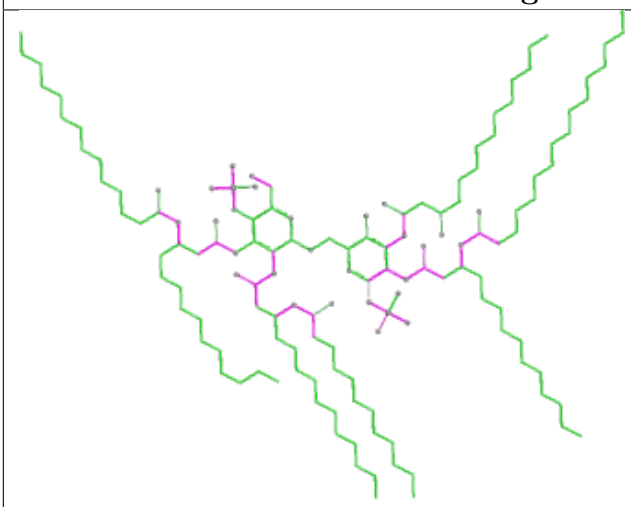

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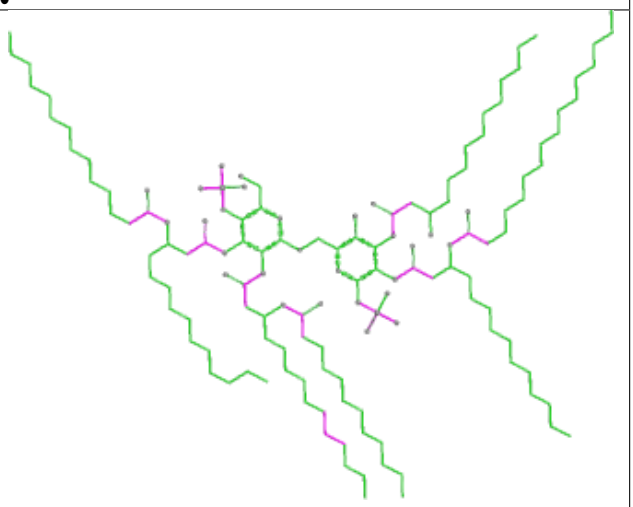
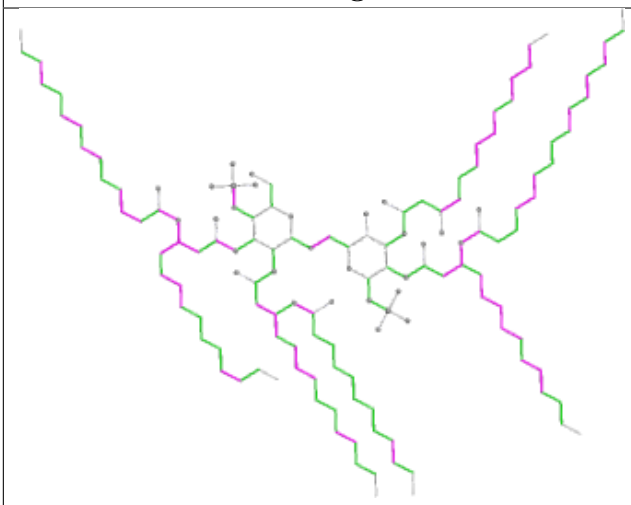


**Bond angles**



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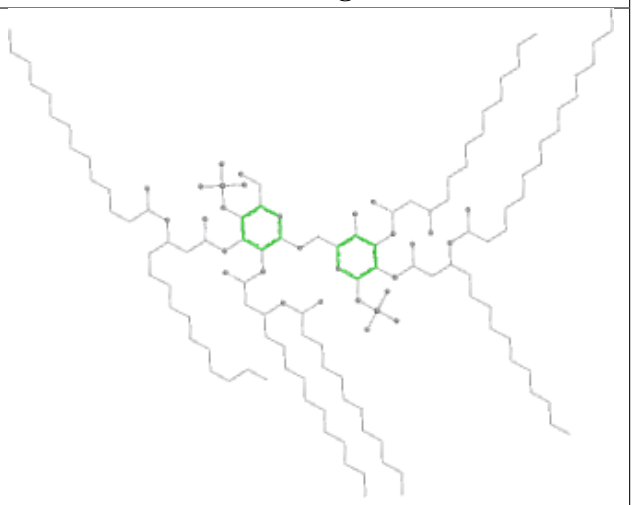

**Rings**

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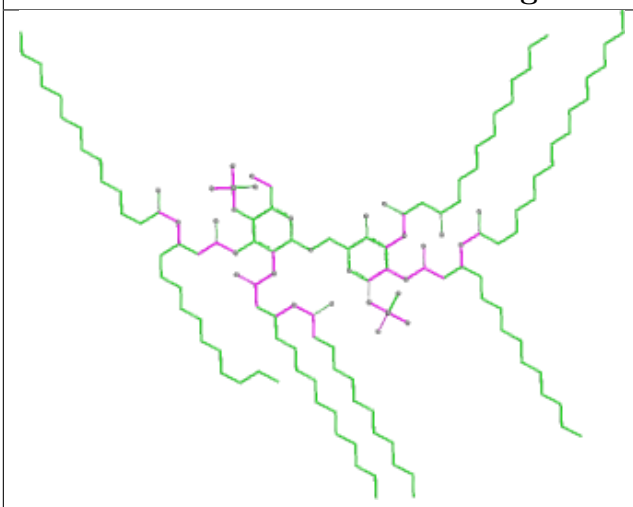

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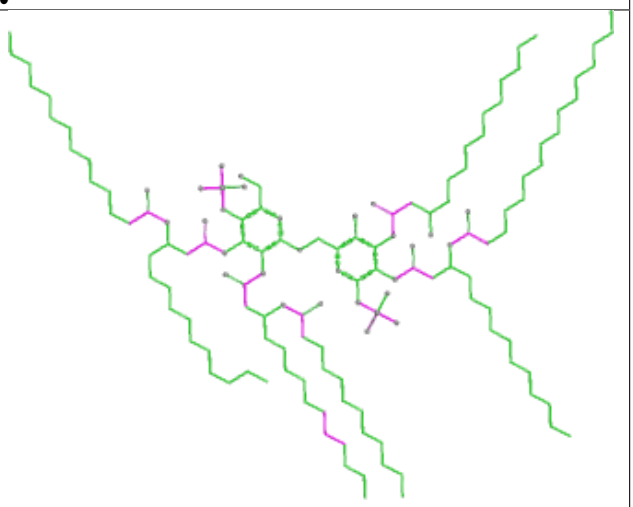
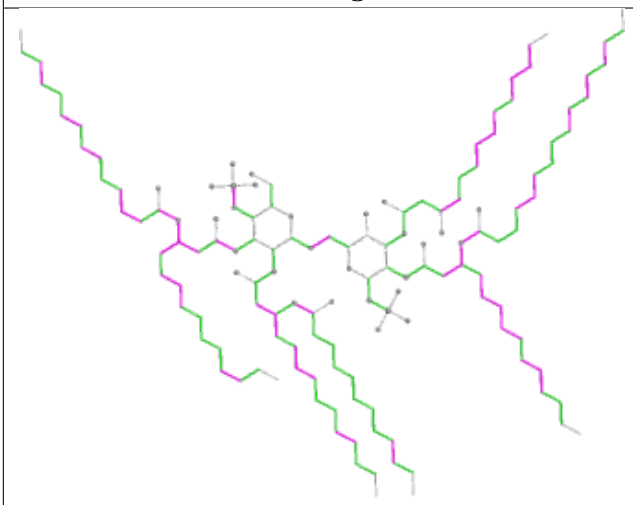
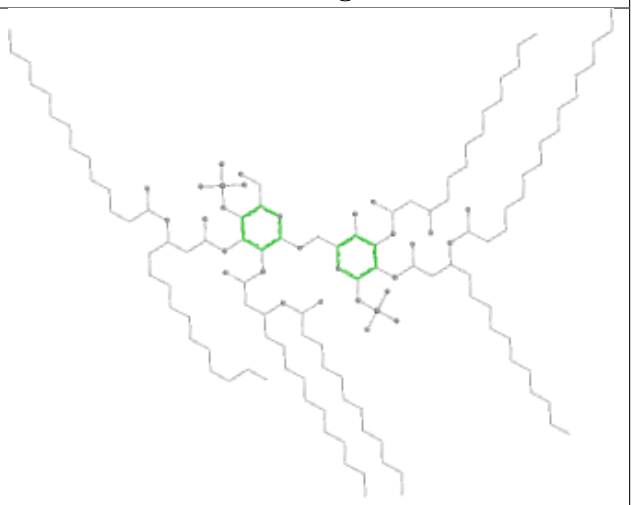


**Bond angles**



**Torsions**



**Rings**

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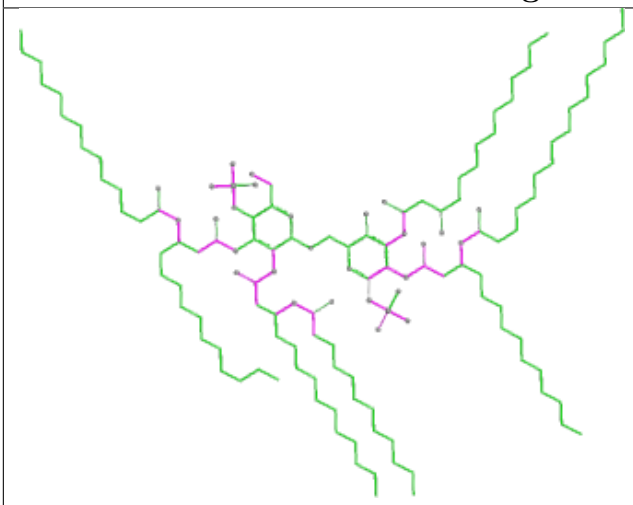

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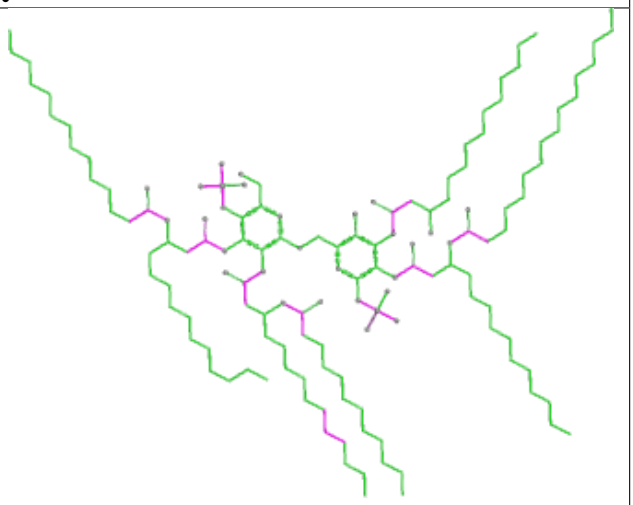
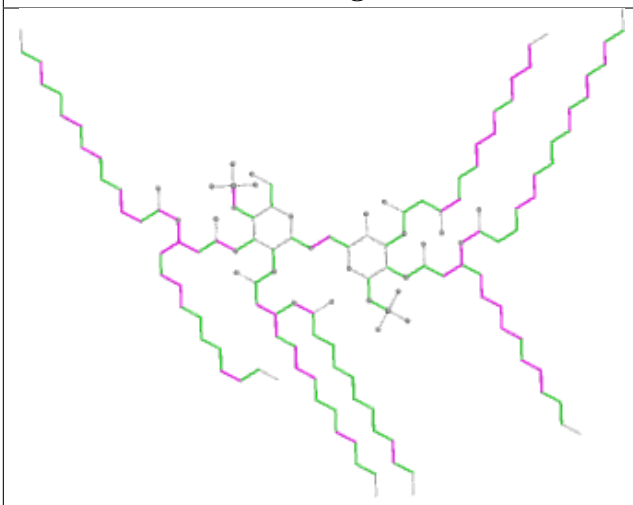
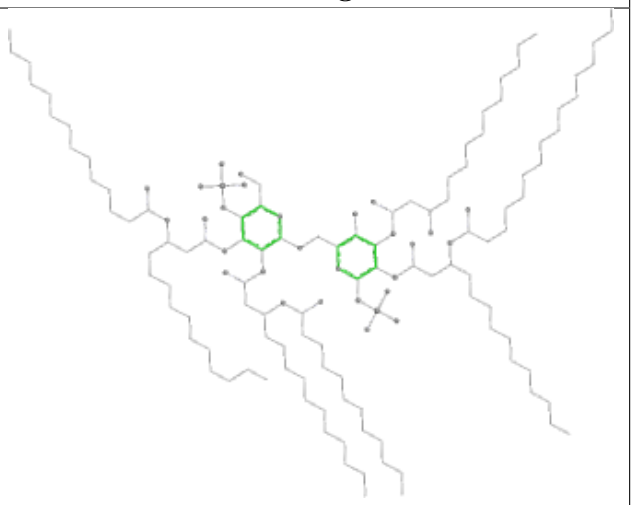


**Bond angles**



**Torsions**



**Rings**

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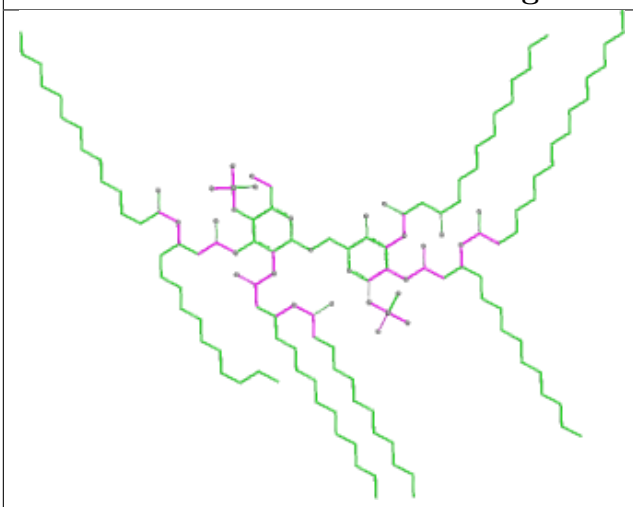

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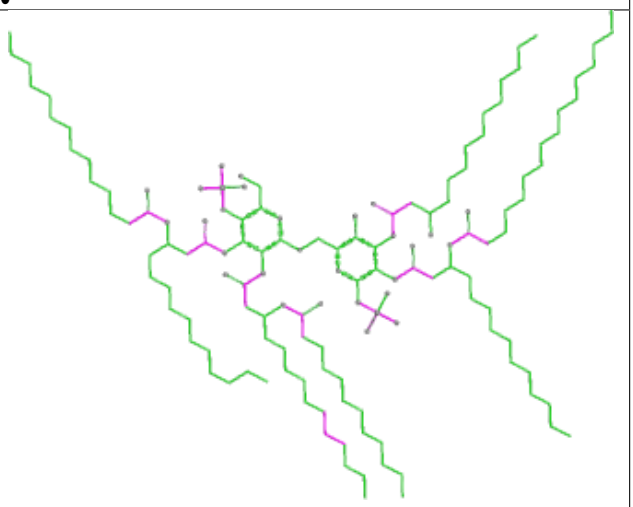
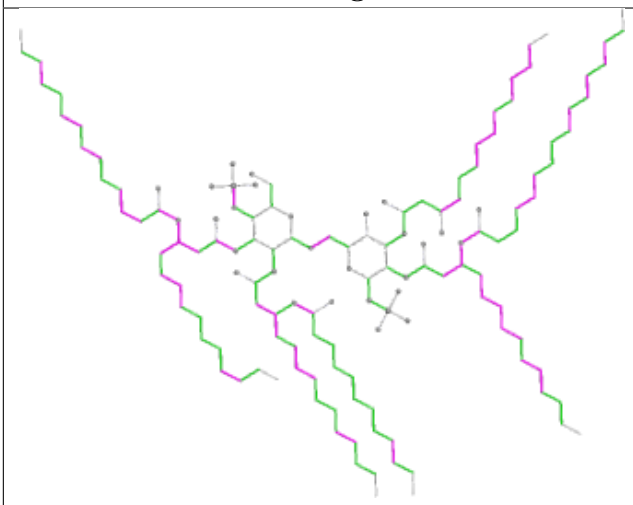
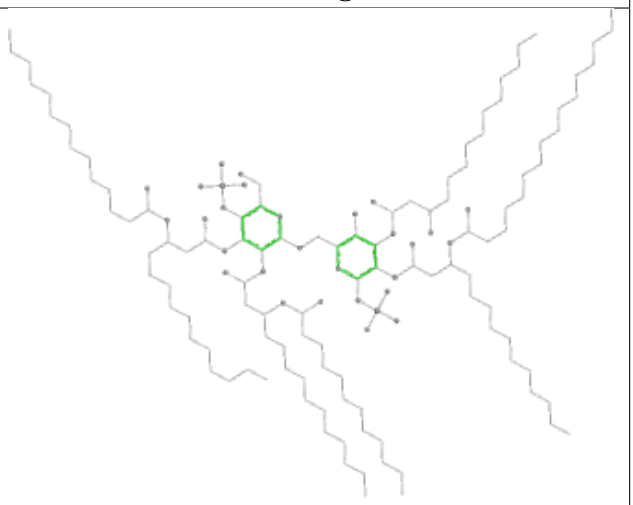


**Bond angles**

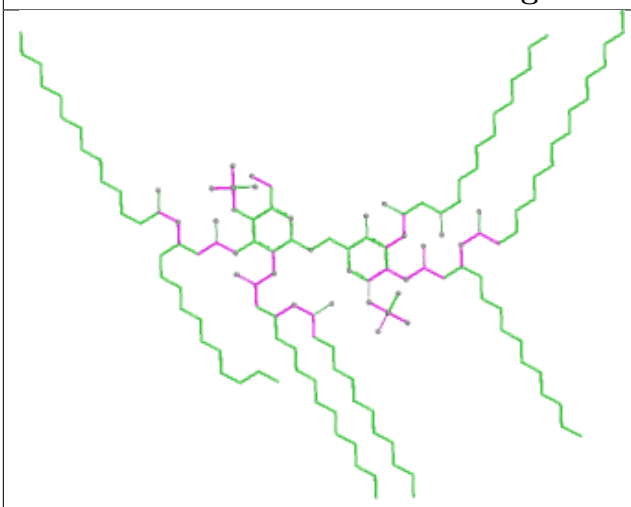


**Torsions**

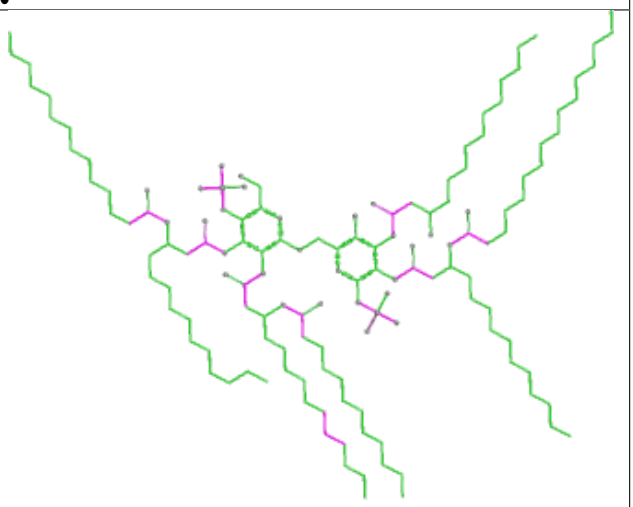


**Rings**

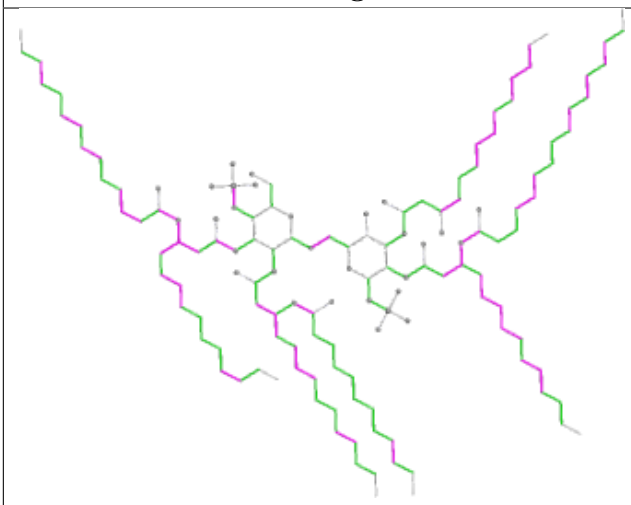
**Ligand TQN V 301**



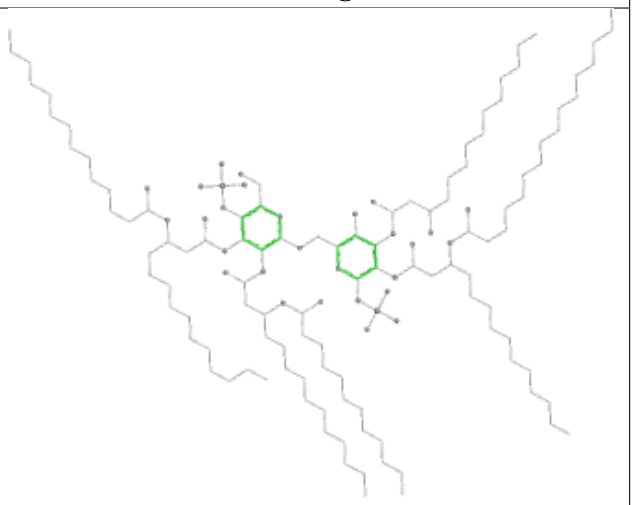
**Bond lengths**



**Bond angles**

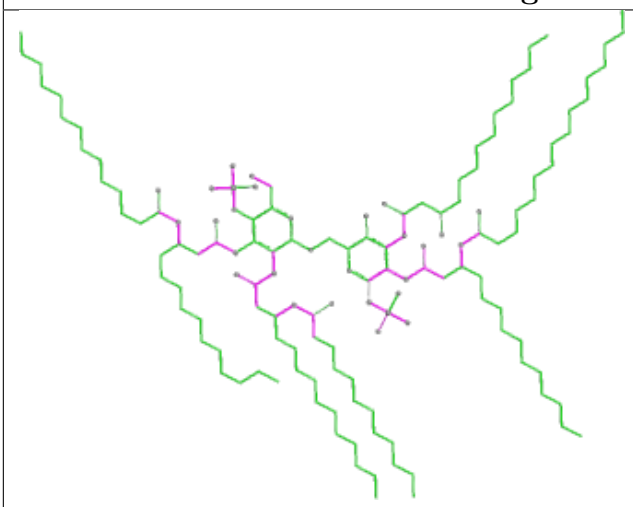


**Torsions**

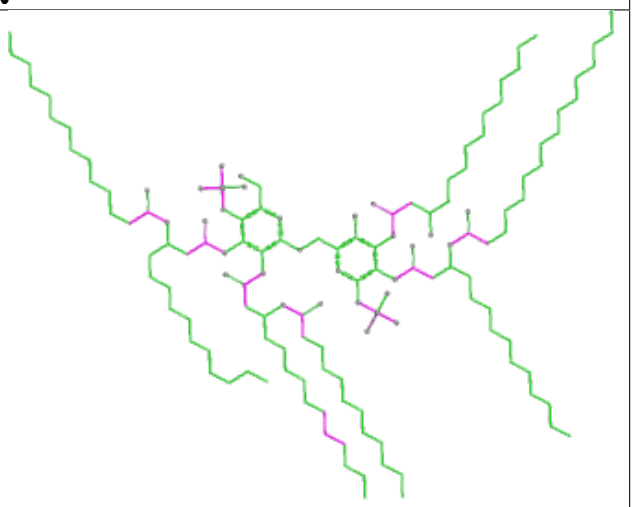


**Rings**

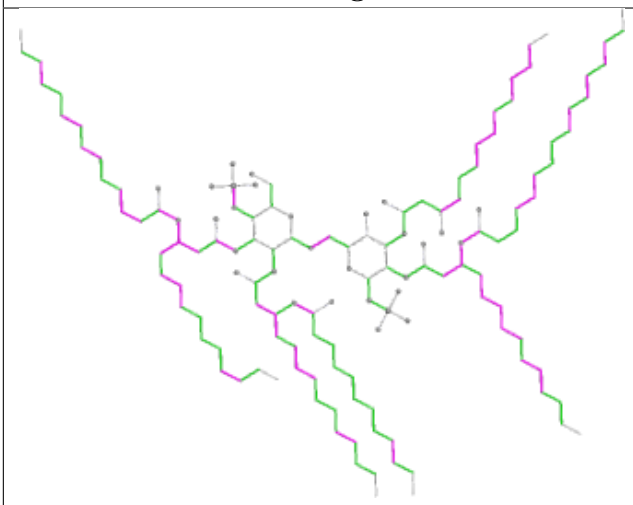
**Ligand TQN R 301**



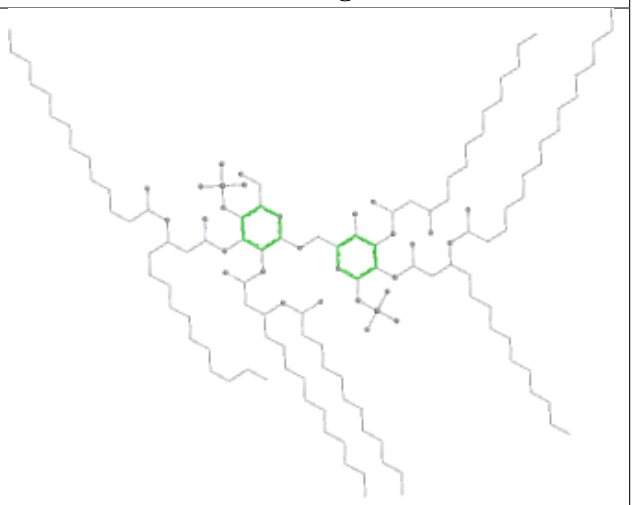
**Bond lengths**



**Bond angles**

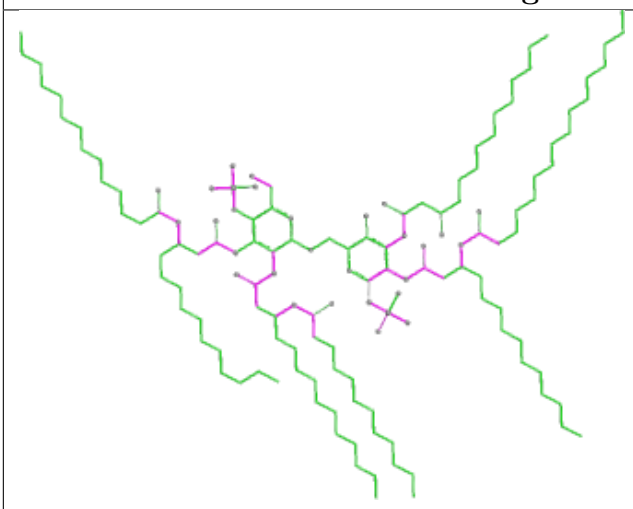


**Torsions**

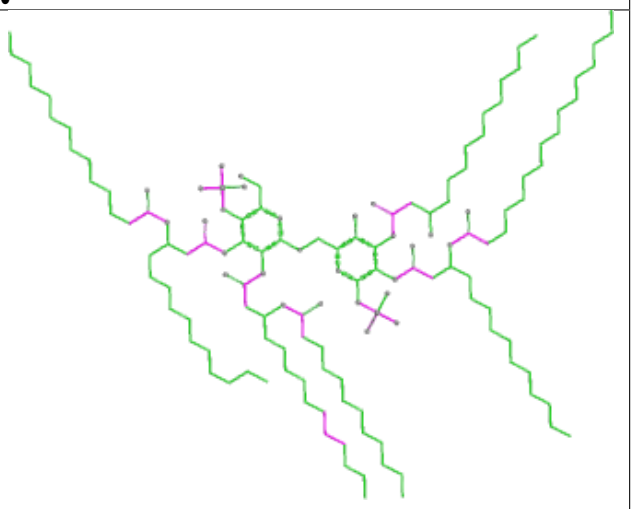


**Rings**

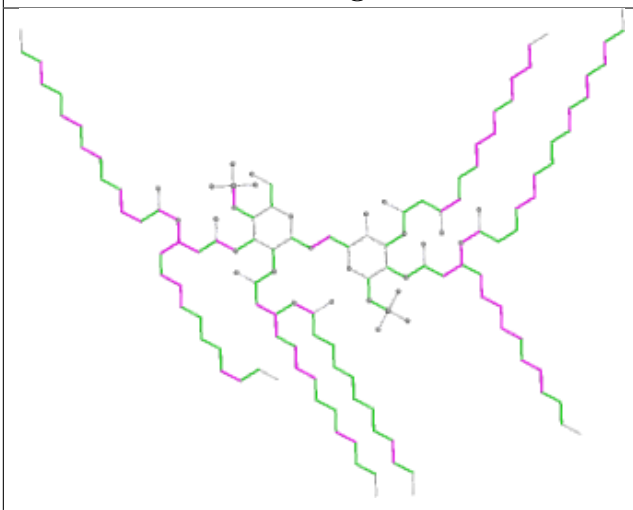
**Ligand TQN C 301**



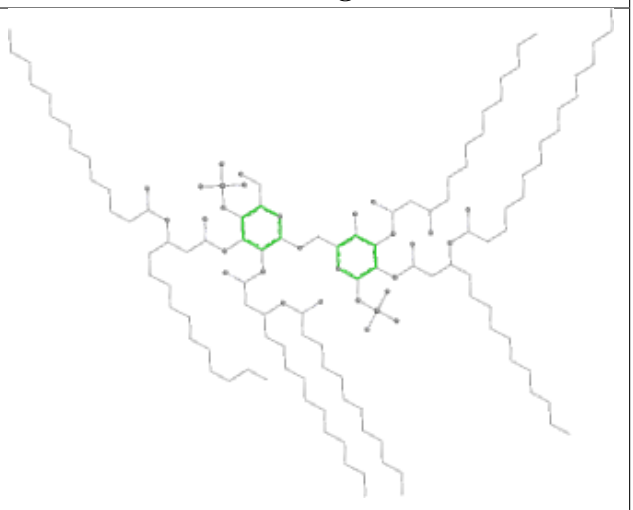
**Bond lengths**



**Bond angles**

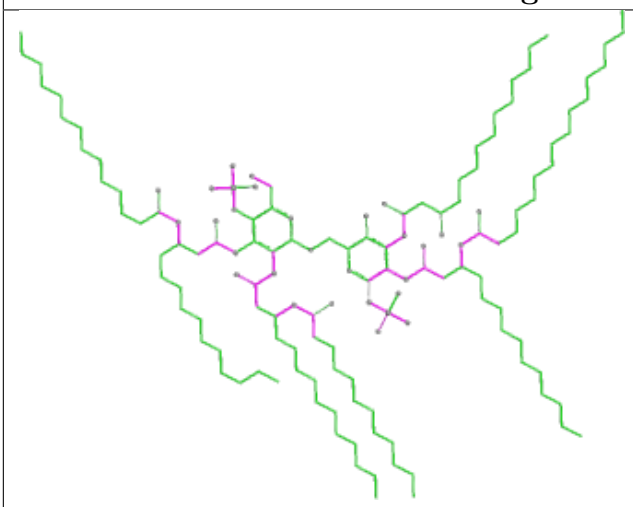


**Torsions**

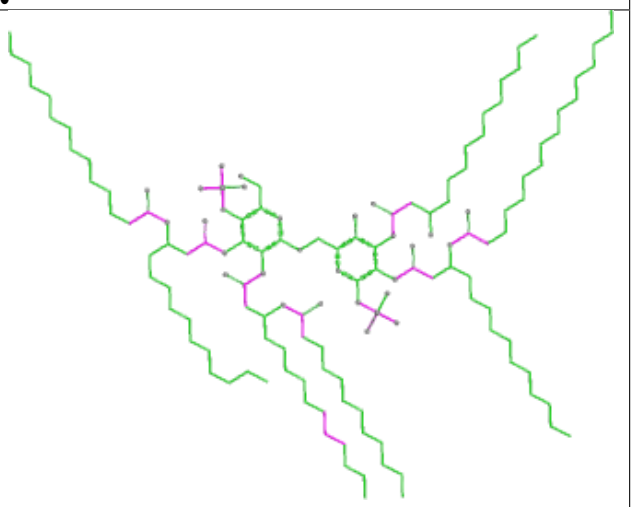


**Rings**

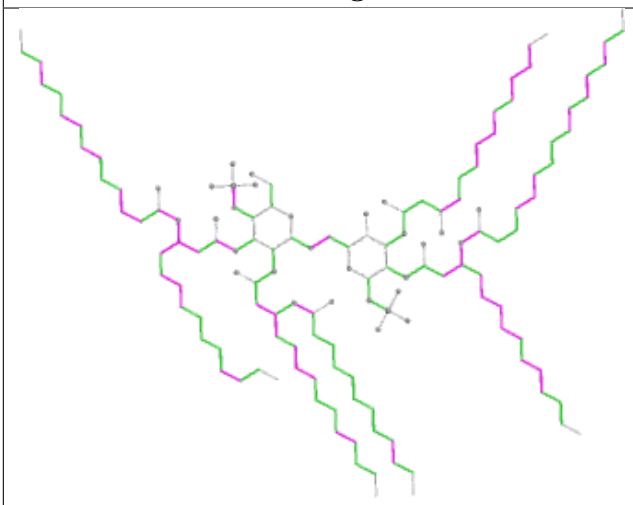
**Ligand TQN X 301**



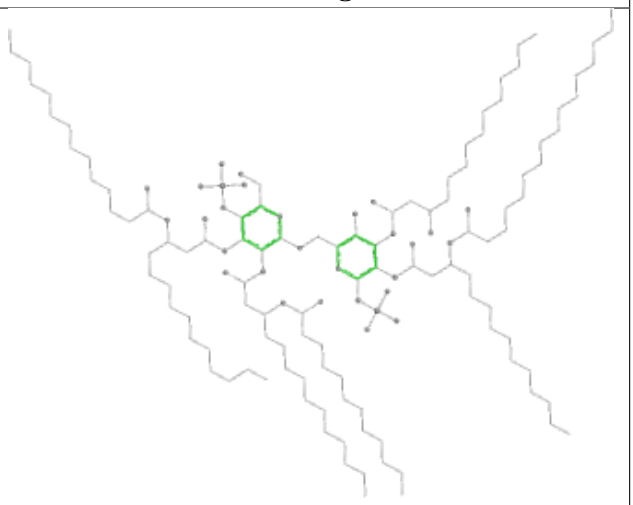
**Bond lengths**



**Bond angles**

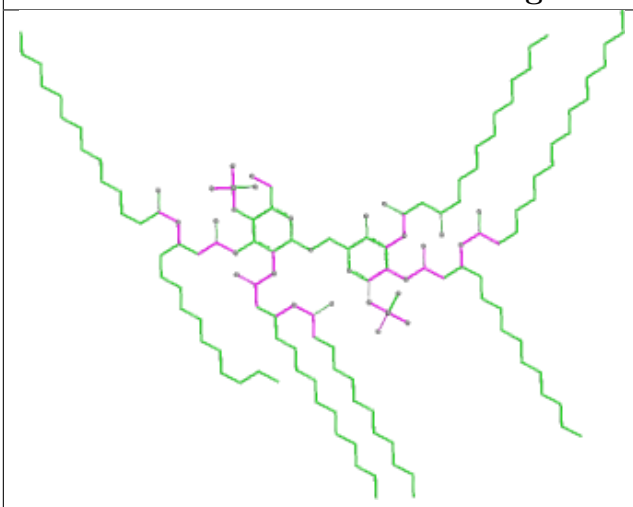


**Torsions**

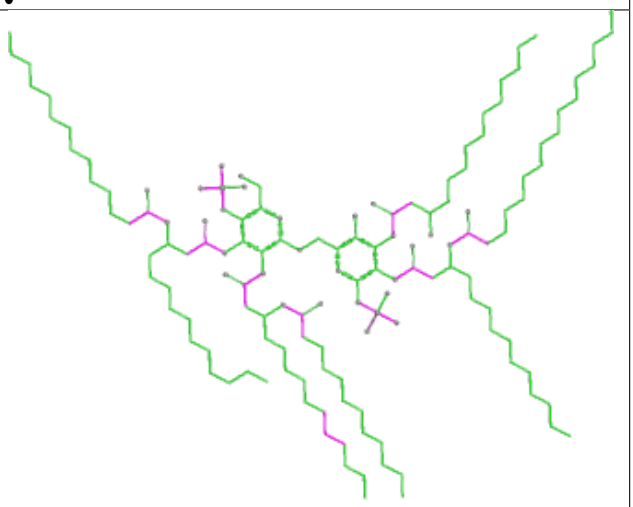


**Rings**

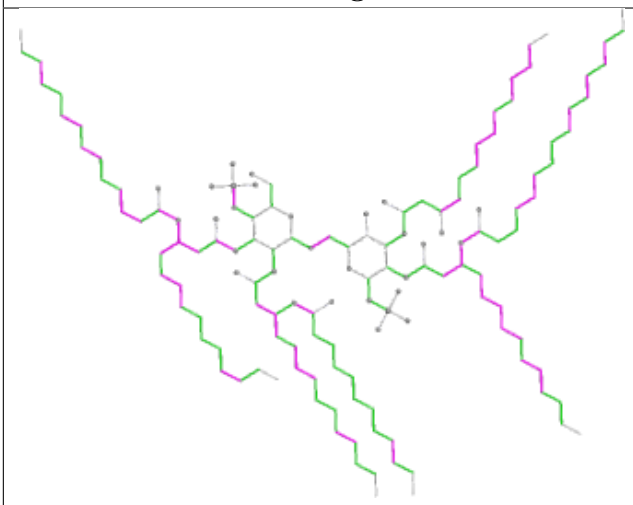
**Ligand TQN J 301**



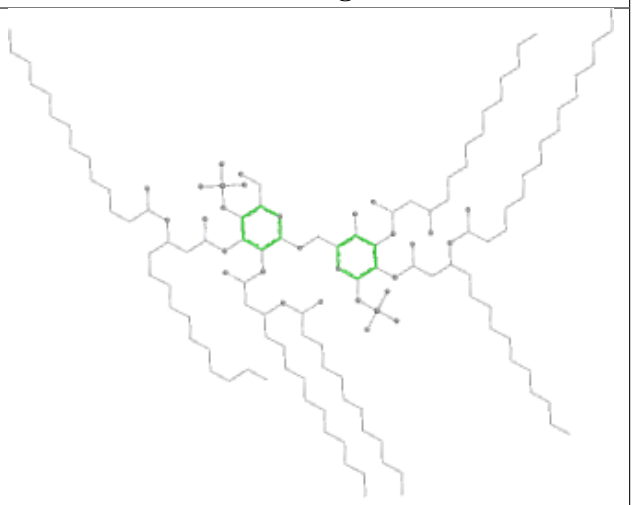
**Bond lengths**



**Bond angles**

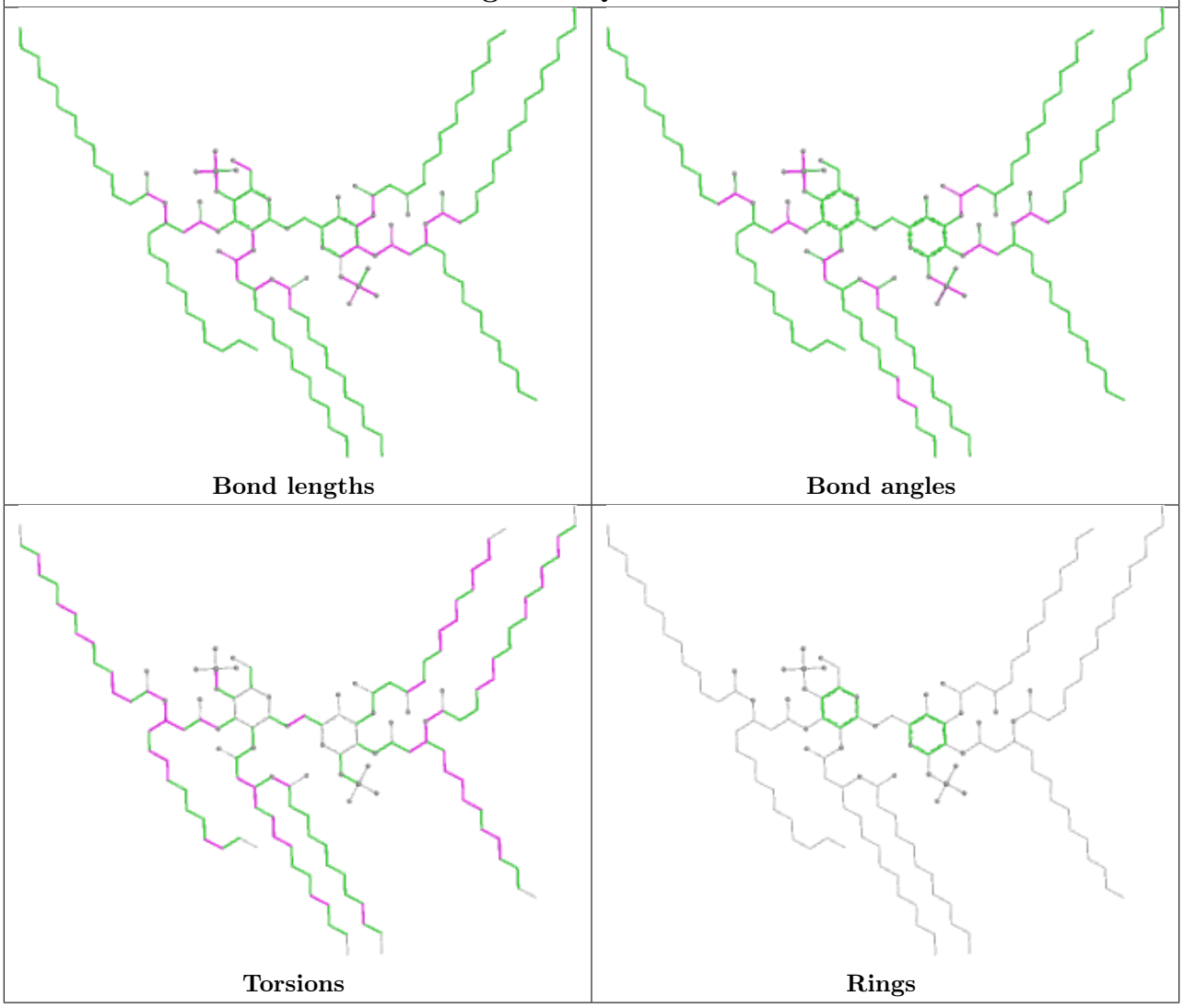


**Torsions**



**Rings**

**Ligand TQN P 301**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

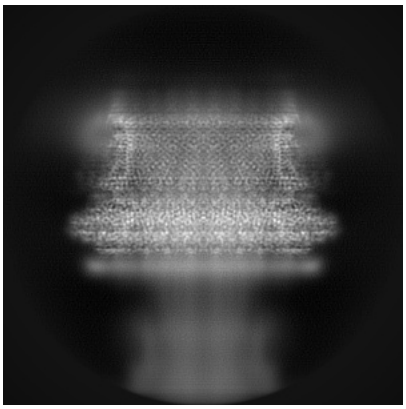
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12183. These allow visual inspection of the internal detail of the map and identification of artifacts.

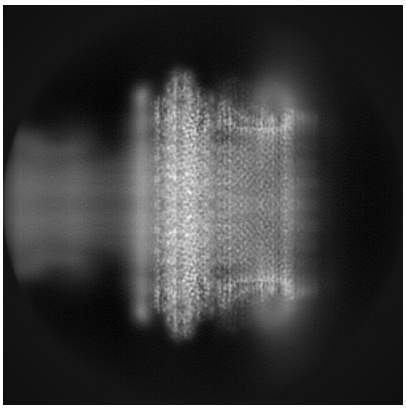
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

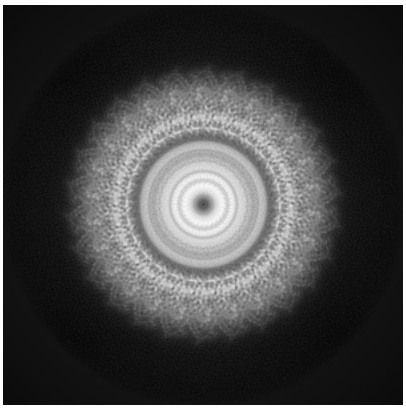
### 6.1.1 Primary map



X

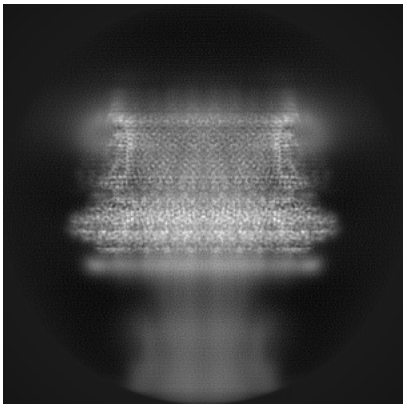


Y

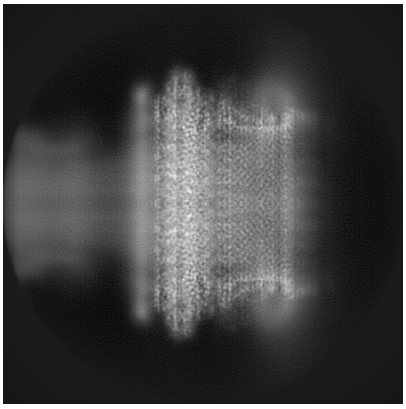


Z

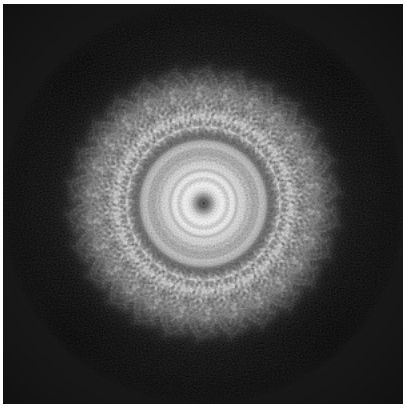
### 6.1.2 Raw map



X



Y

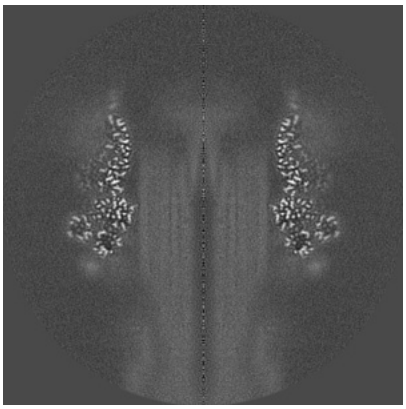


Z

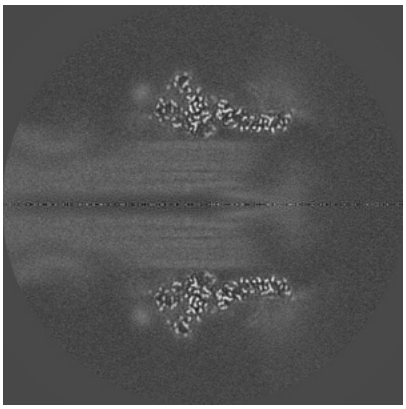
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

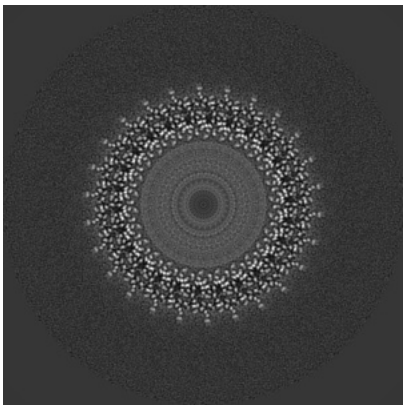
### 6.2.1 Primary map



X Index: 216

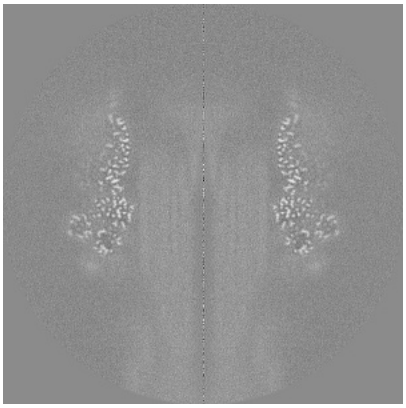


Y Index: 216



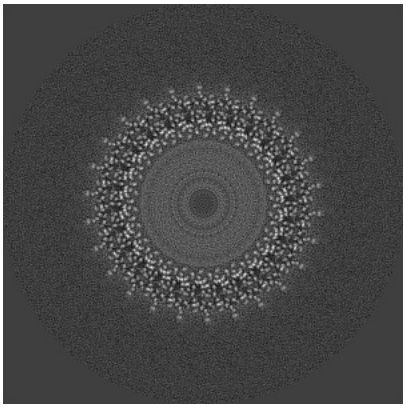
Z Index: 216

### 6.2.2 Raw map



X Index: 216

Y Index: 216

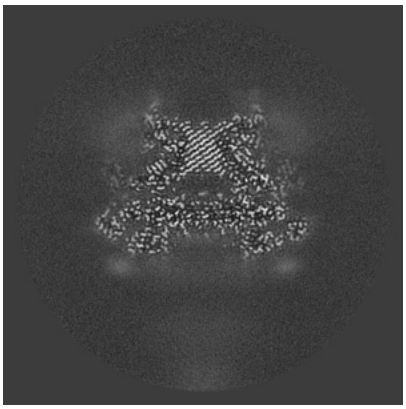


Z Index: 216

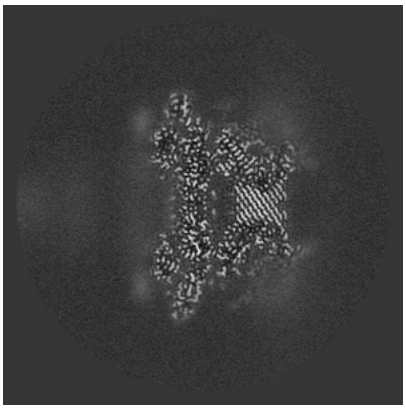
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

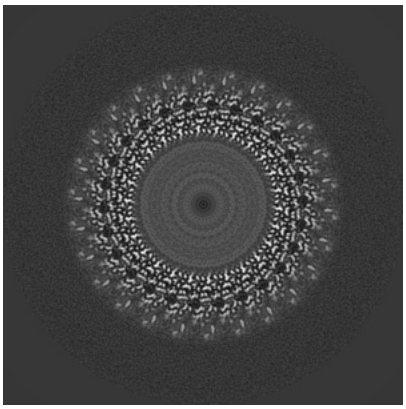
### 6.3.1 Primary map



X Index: 134

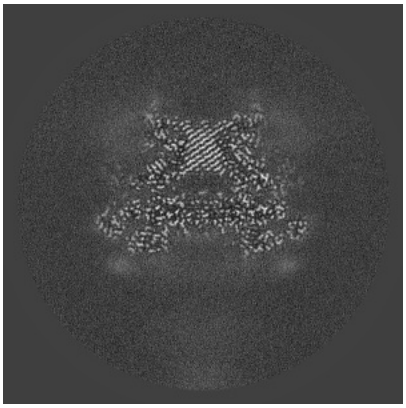


Y Index: 134

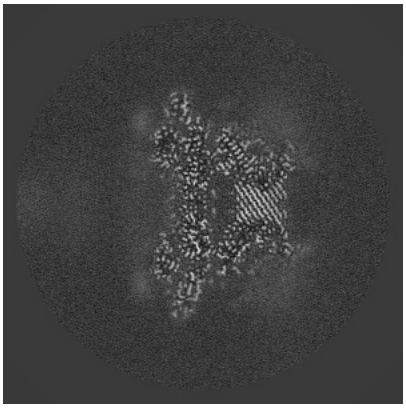


Z Index: 204

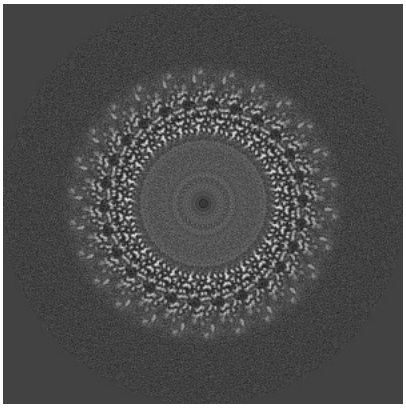
### 6.3.2 Raw map



X Index: 134



Y Index: 134

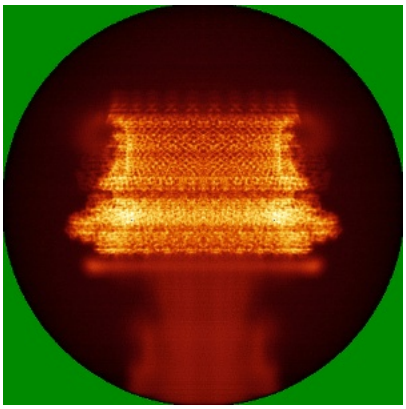


Z Index: 204

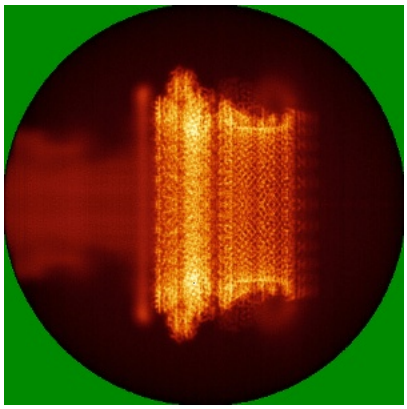
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

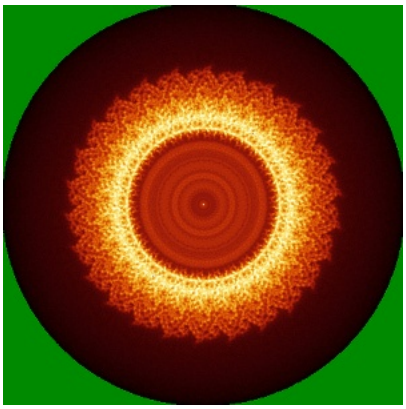
### 6.4.1 Primary map



X

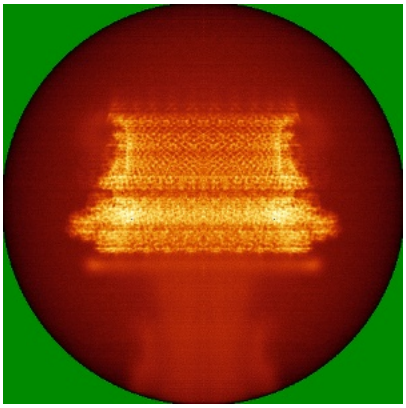


Y

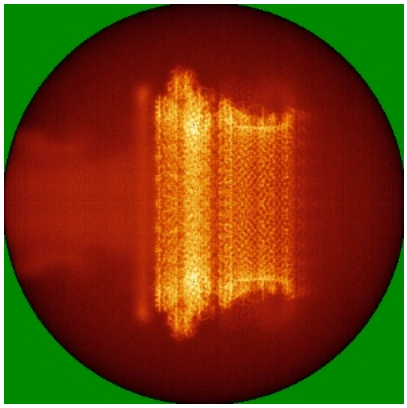


Z

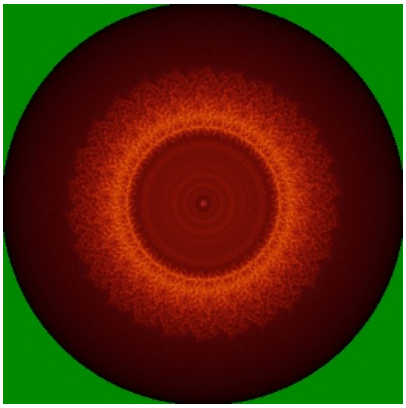
### 6.4.2 Raw map



X



Y

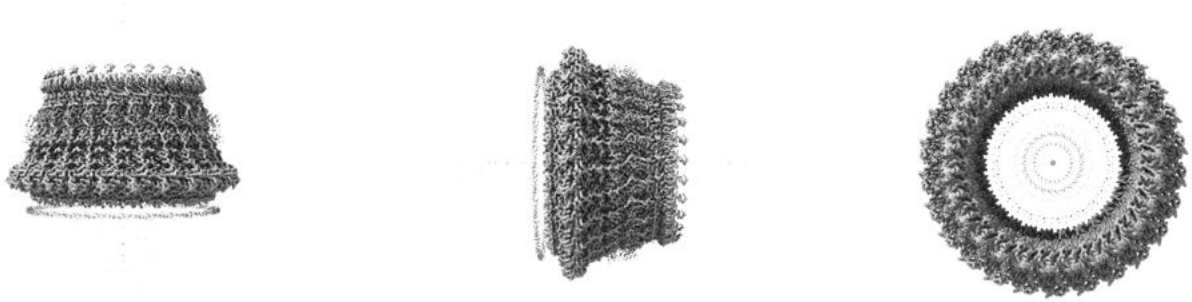


Z

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)

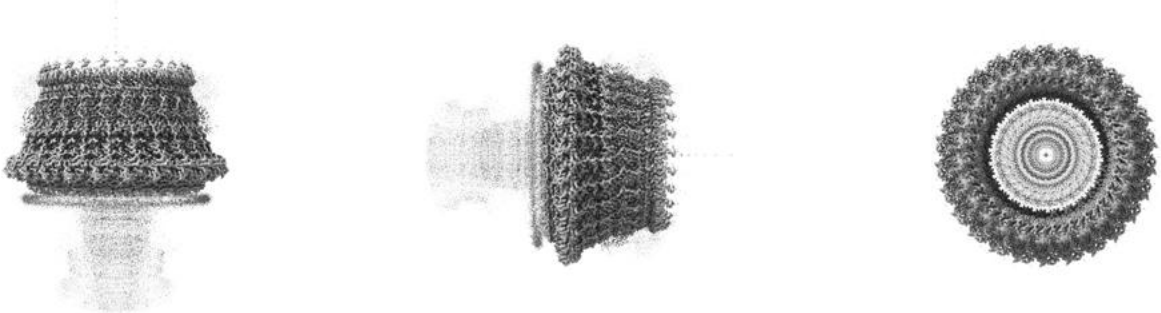
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

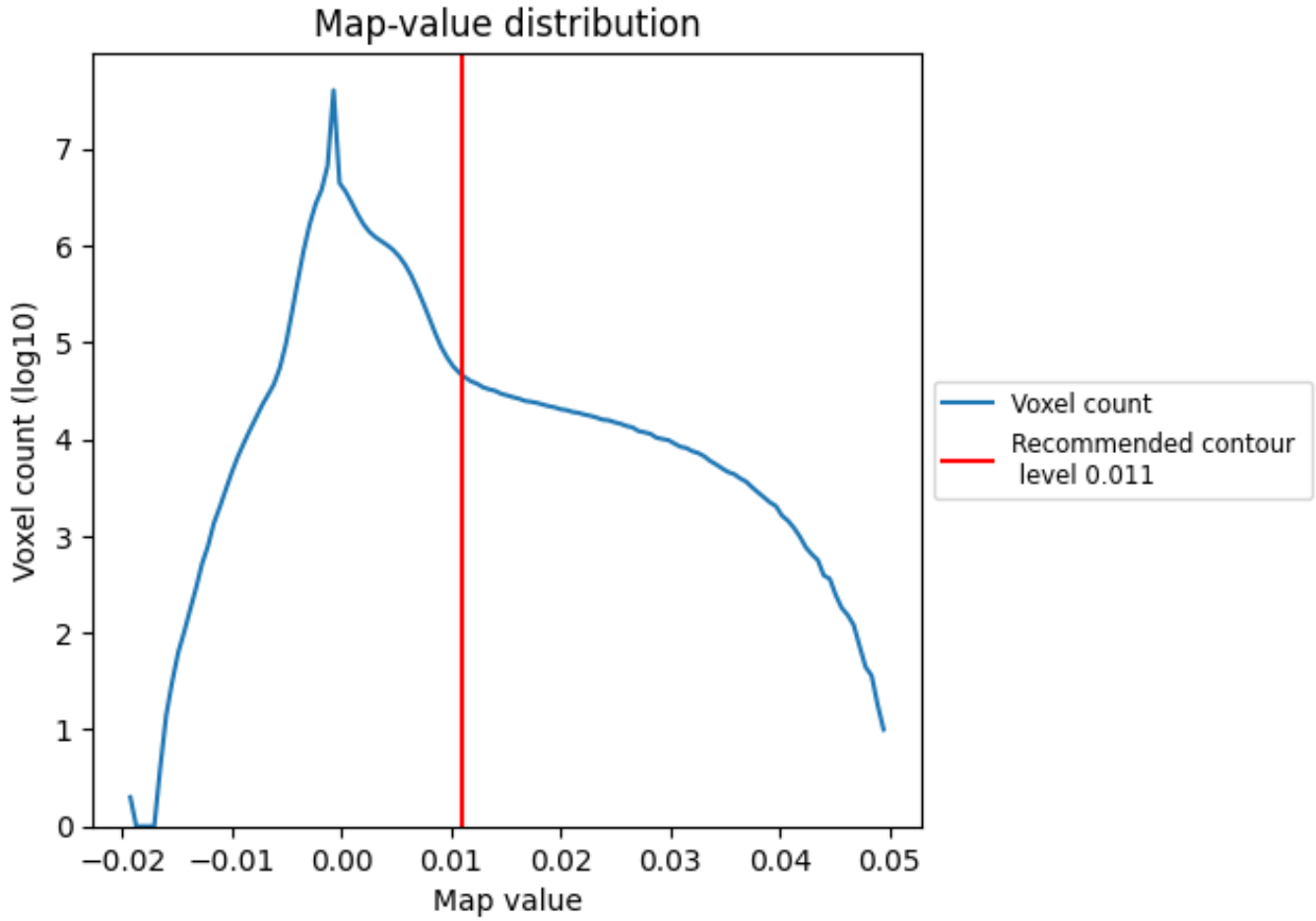
## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

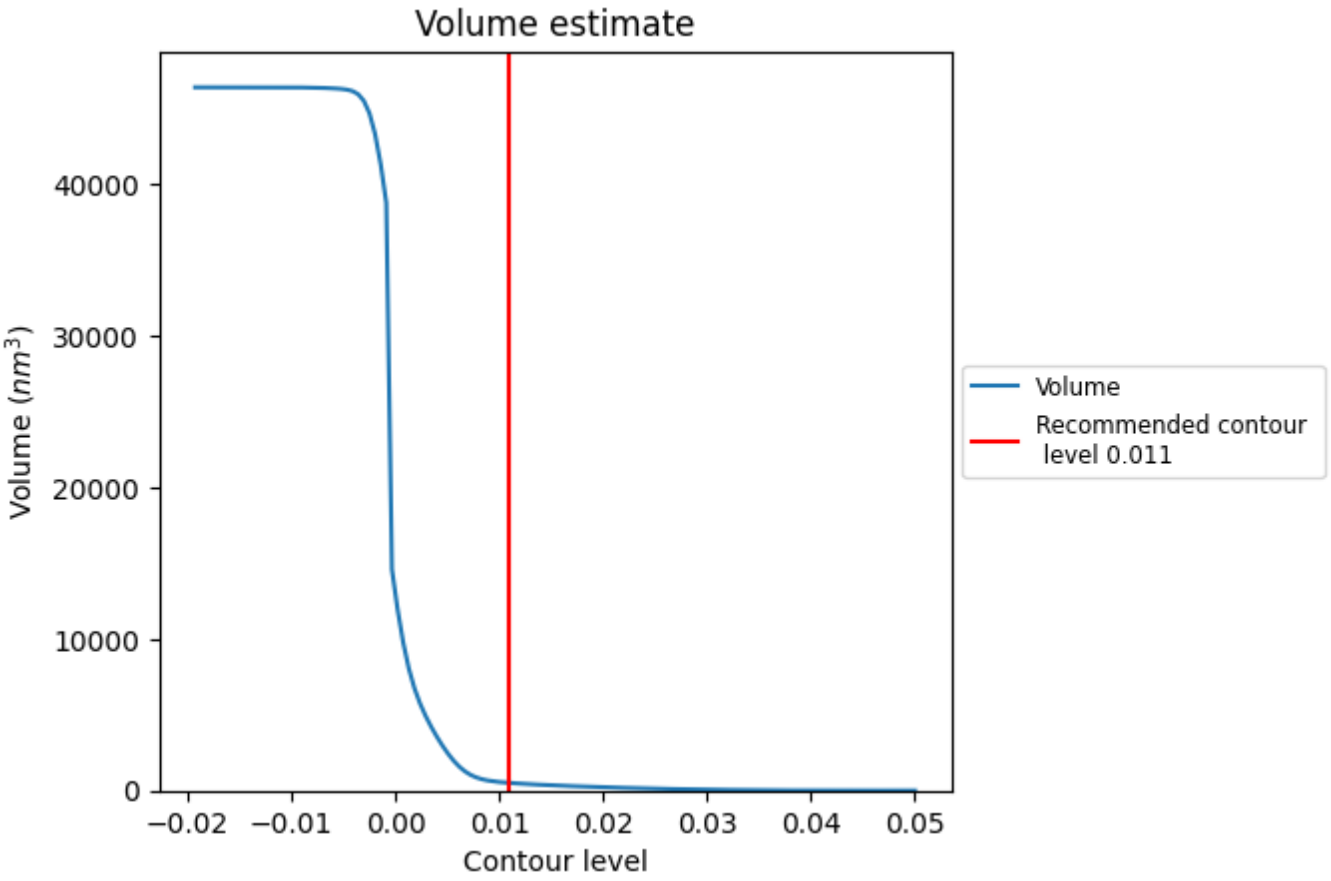
This section contains the results of statistical analysis of the map.

## 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.

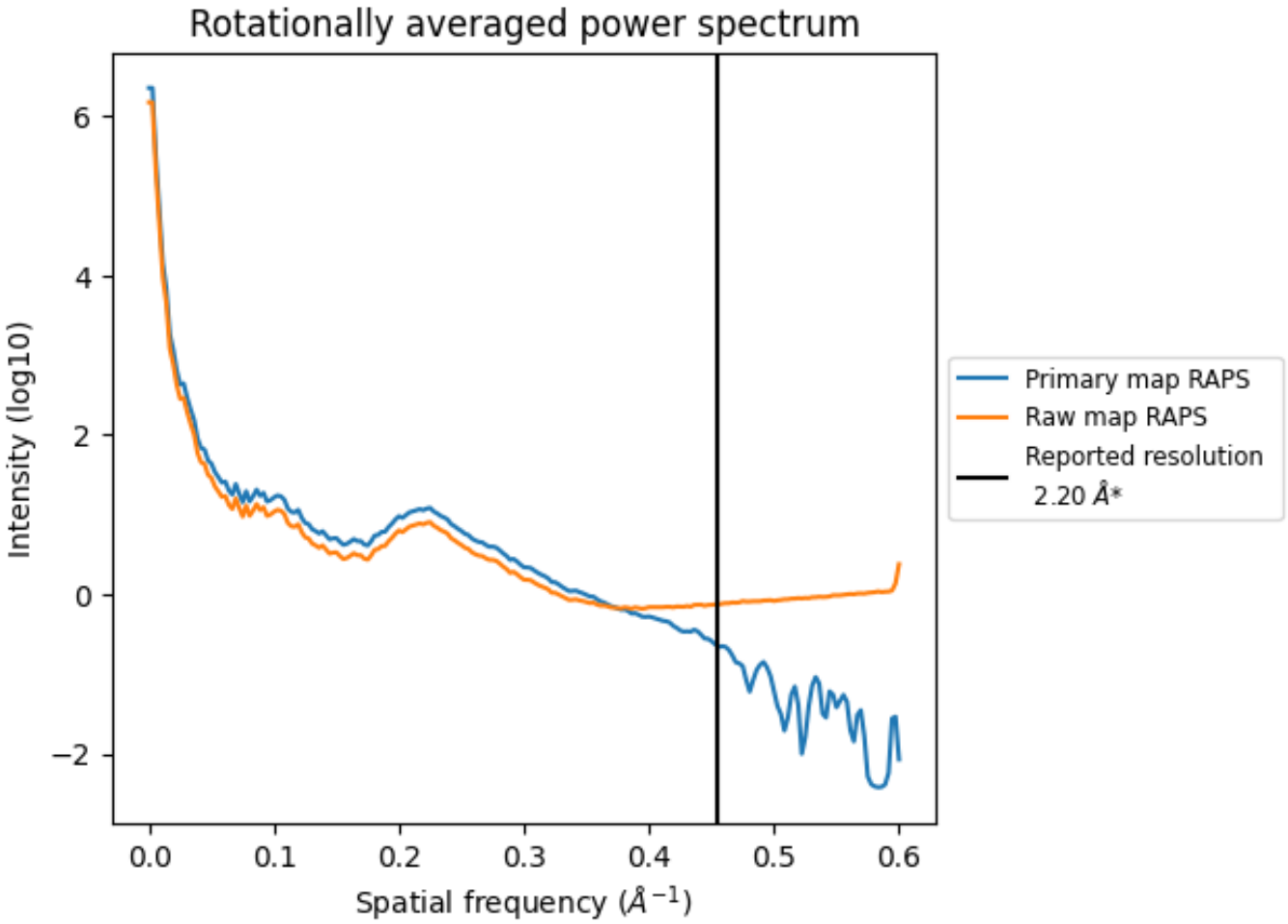
## 7.2 Volume estimate




The volume at the recommended contour level is 505 $nm^3$; this corresponds to an approximate mass of 456 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)

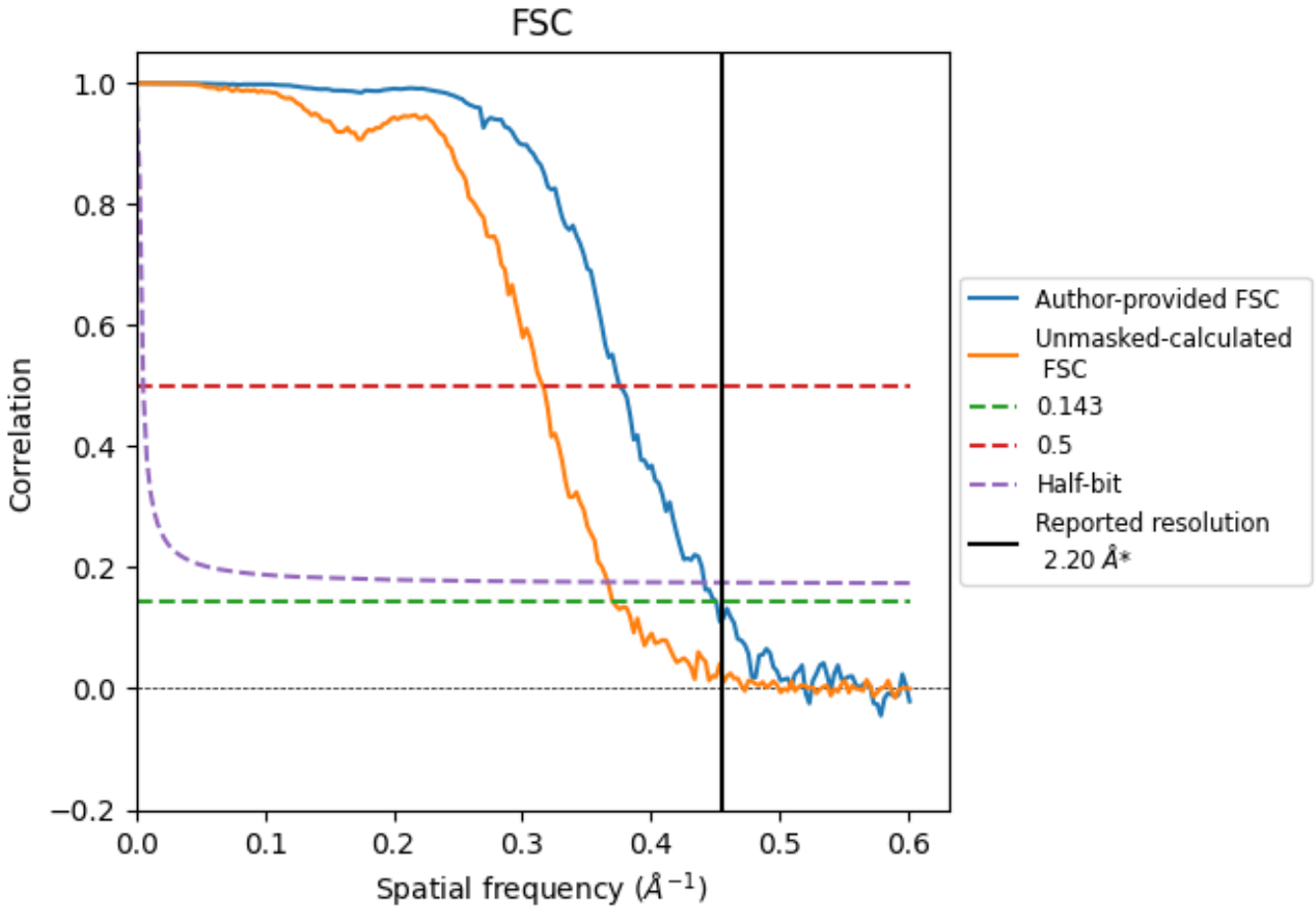



*Reported resolution corresponds to spatial frequency of 0.455 Å$^{-1}$

# 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 0.455 Å$^{-1}$

## 8.2 Resolution estimates (i)

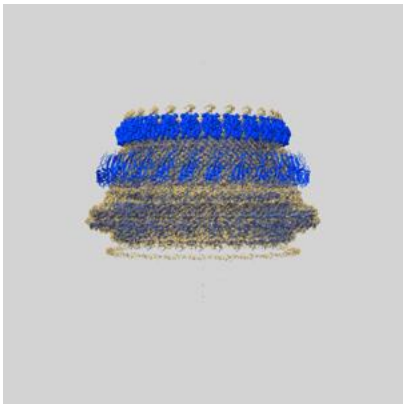
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.20 | - | - |
| Author-provided FSC curve | 2.22 | 2.66 | 2.27 |
| Unmasked-calculated* | 2.70 | 3.16 | 2.73 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.70 differs from the reported value 2.2 by more than 10 %

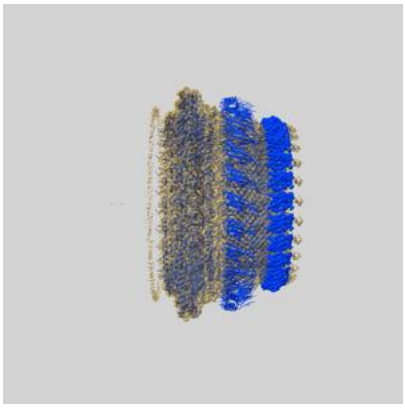
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12183 and PDB model 7BGL. Per-residue inclusion information can be found in section 3 on page 15.

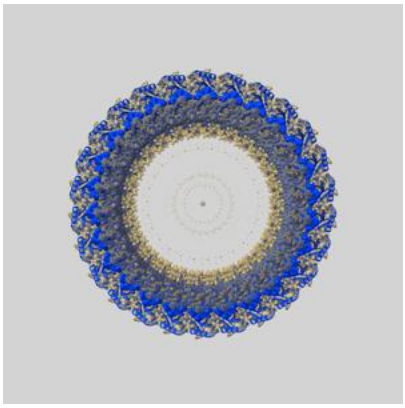
## 9.1 Map-model overlay



X



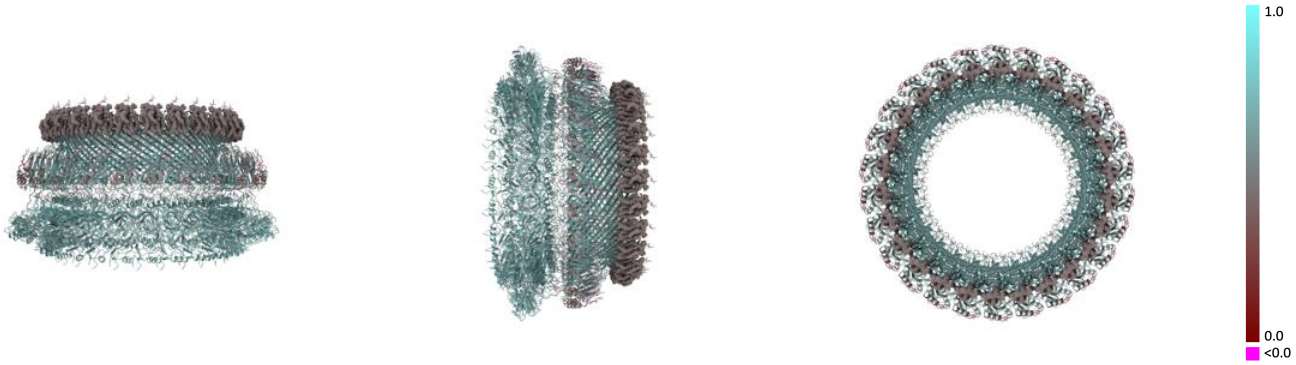
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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 (i)



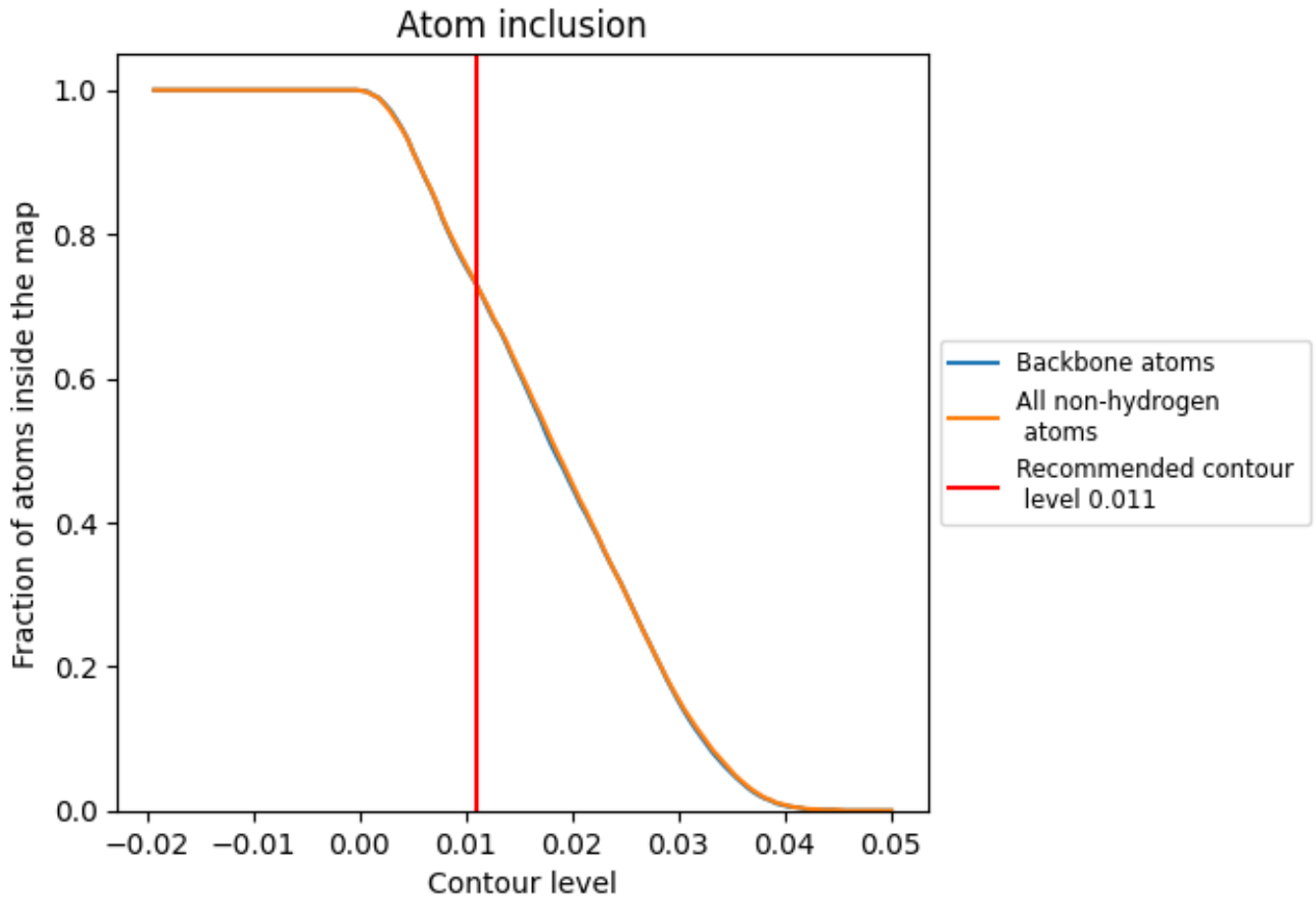

X Y Z

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 (i)

This section was not generated.

## 9.4 Atom inclusion (i)




At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.011) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7300 | 0.6030 |
| 1 | 0.0440 | 0.4570 |
| 10 | 0.0460 | 0.4580 |
| 11 | 0.0480 | 0.4580 |
| 12 | 0.0460 | 0.4610 |
| 13 | 0.0460 | 0.4630 |
| 14 | 0.0440 | 0.4600 |
| 15 | 0.0460 | 0.4590 |
| 16 | 0.0490 | 0.4600 |
| 17 | 0.0460 | 0.4600 |
| 18 | 0.0460 | 0.4580 |
| 19 | 0.0460 | 0.4580 |
| 2 | 0.0460 | 0.4580 |
| 20 | 0.0520 | 0.4590 |
| 21 | 0.0490 | 0.4590 |
| 22 | 0.0480 | 0.4610 |
| 23 | 0.0460 | 0.4590 |
| 24 | 0.0480 | 0.4550 |
| 25 | 0.0460 | 0.4580 |
| 26 | 0.0480 | 0.4570 |
| 3 | 0.0490 | 0.4570 |
| 4 | 0.0460 | 0.4570 |
| 5 | 0.0460 | 0.4570 |
| 6 | 0.0460 | 0.4590 |
| 7 | 0.0520 | 0.4610 |
| 8 | 0.0490 | 0.4620 |
| 9 | 0.0480 | 0.4610 |
| A | 0.8390 | 0.6140 |
| B | 0.8460 | 0.6150 |
| C | 0.8410 | 0.6140 |
| D | 0.8370 | 0.6140 |
| E | 0.8410 | 0.6140 |
| F | 0.8400 | 0.6140 |
| G | 0.8420 | 0.6140 |
| H | 0.8410 | 0.6140 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| I | 0.8400 | 0.6140 |
| J | 0.8410 | 0.6150 |
| K | 0.8430 | 0.6160 |
| L | 0.8400 | 0.6160 |
| M | 0.8430 | 0.6150 |
| N | 0.8380 | 0.6160 |
| O | 0.8440 | 0.6160 |
| P | 0.8390 | 0.6160 |
| Q | 0.8390 | 0.6160 |
| R | 0.8400 | 0.6160 |
| S | 0.8400 | 0.6160 |
| T | 0.8400 | 0.6170 |
| U | 0.8390 | 0.6160 |
| V | 0.8400 | 0.6160 |
| W | 0.8390 | 0.6150 |
| X | 0.8430 | 0.6150 |
| Y | 0.8400 | 0.6160 |
| Z | 0.8440 | 0.6170 |
| a | 0.8610 | 0.6350 |
| b | 0.8630 | 0.6350 |
| c | 0.8580 | 0.6340 |
| d | 0.8620 | 0.6330 |
| e | 0.8600 | 0.6340 |
| f | 0.8590 | 0.6350 |
| g | 0.8580 | 0.6350 |
| h | 0.8580 | 0.6340 |
| i | 0.8600 | 0.6330 |
| j | 0.8600 | 0.6340 |
| k | 0.8590 | 0.6350 |
| l | 0.8570 | 0.6350 |
| m | 0.8610 | 0.6350 |
| n | 0.8620 | 0.6350 |
| o | 0.8630 | 0.6340 |
| p | 0.8600 | 0.6340 |
| q | 0.8630 | 0.6340 |
| r | 0.8590 | 0.6340 |
| s | 0.8580 | 0.6340 |
| t | 0.8580 | 0.6330 |
| u | 0.8590 | 0.6330 |
| v | 0.8600 | 0.6340 |
| w | 0.8590 | 0.6330 |
| x | 0.8600 | 0.6340 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| y | 0.8590 | 0.6330 |
| z | 0.8600 | 0.6330 |