



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:39 PM UTC

PDB ID : 8CMO / pdb\_00008cmo  
EMDB ID : EMD-16732  
Title : Cryo-EM structure of the Photosystem I - LHCI supercomplex from Coelastrella sp.  
Authors : Fadeeva, M.; Klaiman, D.; Nelson, N.  
Deposited on : 2023-02-20  
Resolution : 2.81 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](mailto: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

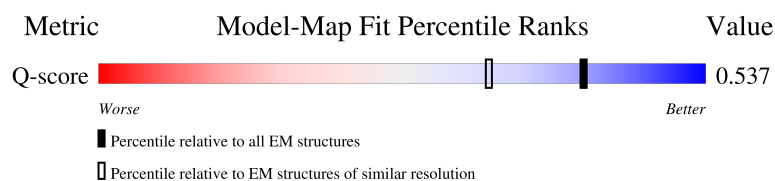
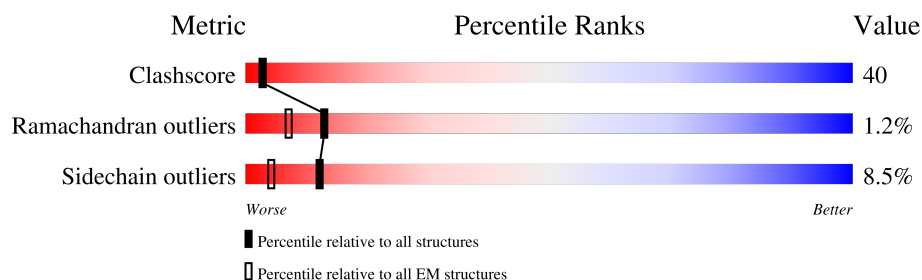
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.81 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.



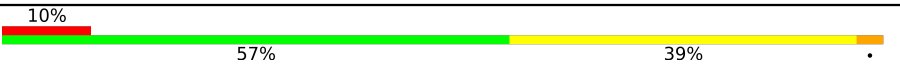
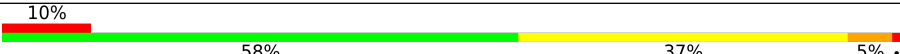
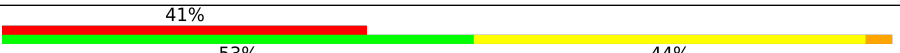
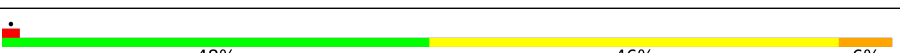
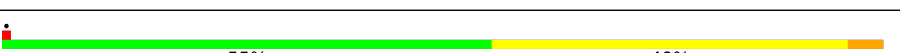
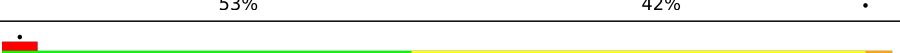
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 11740 ( 2.31 - 3.31 )                                    |

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  $\geq 3$ , 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  $\leq 5\%$ . 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     | 740    | <br>59% 39% .      |
| 2   | B     | 732    | <br>53% 44% .      |
| 3   | C     | 80     | <br>48% 51% .      |
| 4   | D     | 142    | <br>8% 55% 41% . . |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | E     | 61     |    |
| 6   | F     | 165    |    |
| 7   | G     | 93     |    |
| 8   | I     | 41     |    |
| 9   | J     | 40     |    |
| 10  | K     | 89     |    |
| 11  | L     | 123    |    |
| 12  | 1     | 194    |    |
| 12  | Z     | 194    |    |
| 13  | 3     | 218    |    |
| 14  | 7     | 220    |    |
| 15  | 8     | 214    |    |
| 16  | 4     | 207    |  |
| 17  | 5     | 226    |  |
| 18  | 6     | 226    |  |
| 19  | 9     | 184    |  |
| 20  | 2     | 70     |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21  | CL0  | A     | 801 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 304 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 305 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 306 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 307 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 308 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 309 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 310 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | 1     | 311 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 313 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 314 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 315 | X         | -        | -       | -                |
| 22  | CLA  | 1     | 316 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 301 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 302 | X         | -        | -       | -                |
| 22  | CLA  | 2     | 304 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 308 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 309 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 310 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 311 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 312 | X         | -        | X       | -                |
| 22  | CLA  | 3     | 313 | X         | -        | X       | -                |
| 22  | CLA  | 3     | 314 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 315 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 316 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 318 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 319 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 320 | X         | -        | -       | -                |
| 22  | CLA  | 3     | 322 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 805 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 806 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 807 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 808 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 809 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 810 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 811 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 812 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 815 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 817 | X         | -        | -       | -                |
| 22  | CLA  | 4     | 818 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 301 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 307 | X         | -        | X       | -                |
| 22  | CLA  | 5     | 308 | X         | -        | X       | -                |
| 22  | CLA  | 5     | 309 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 310 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 311 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 312 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 313 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 314 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 315 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | 5     | 318 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 319 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 320 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 322 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 323 | X         | -        | -       | -                |
| 22  | CLA  | 5     | 326 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 301 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 302 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 307 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 308 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 309 | X         | -        | X       | -                |
| 22  | CLA  | 6     | 310 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 311 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 312 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 313 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 314 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 317 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 319 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 321 | X         | -        | -       | -                |
| 22  | CLA  | 6     | 322 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 304 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 305 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 306 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 307 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 308 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 309 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 310 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 311 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 312 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 314 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 315 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 316 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 317 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 322 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 323 | X         | -        | -       | -                |
| 22  | CLA  | 7     | 324 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 305 | X         | -        | X       | -                |
| 22  | CLA  | 8     | 306 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 307 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 308 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 309 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 310 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | 8     | 311 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 313 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 314 | X         | -        | -       | -                |
| 22  | CLA  | 8     | 316 | X         | -        | -       | -                |
| 22  | CLA  | 9     | 303 | X         | -        | -       | -                |
| 22  | CLA  | 9     | 304 | X         | -        | -       | -                |
| 22  | CLA  | 9     | 305 | X         | -        | -       | -                |
| 22  | CLA  | 9     | 306 | X         | -        | -       | -                |
| 22  | CLA  | 9     | 307 | X         | -        | -       | -                |
| 22  | CLA  | 9     | 308 | X         | -        | -       | -                |
| 22  | CLA  | 9     | 309 | X         | -        | -       | -                |
| 22  | CLA  | 9     | 310 | X         | -        | -       | -                |
| 22  | CLA  | 9     | 311 | X         | -        | -       | -                |
| 22  | CLA  | 9     | 313 | X         | -        | -       | -                |
| 22  | CLA  | A     | 802 | X         | -        | -       | -                |
| 22  | CLA  | A     | 803 | X         | -        | -       | -                |
| 22  | CLA  | A     | 804 | X         | -        | -       | -                |
| 22  | CLA  | A     | 805 | X         | -        | -       | -                |
| 22  | CLA  | A     | 806 | X         | -        | -       | -                |
| 22  | CLA  | A     | 807 | X         | -        | -       | -                |
| 22  | CLA  | A     | 808 | X         | -        | -       | -                |
| 22  | CLA  | A     | 809 | X         | -        | -       | -                |
| 22  | CLA  | A     | 810 | X         | -        | -       | -                |
| 22  | CLA  | A     | 811 | X         | -        | -       | -                |
| 22  | CLA  | A     | 812 | X         | -        | X       | -                |
| 22  | CLA  | A     | 813 | X         | -        | -       | -                |
| 22  | CLA  | A     | 814 | X         | -        | X       | -                |
| 22  | CLA  | A     | 815 | X         | -        | -       | -                |
| 22  | CLA  | A     | 816 | X         | -        | X       | -                |
| 22  | CLA  | A     | 817 | X         | -        | -       | -                |
| 22  | CLA  | A     | 818 | X         | -        | -       | -                |
| 22  | CLA  | A     | 819 | X         | -        | -       | -                |
| 22  | CLA  | A     | 820 | X         | -        | -       | -                |
| 22  | CLA  | A     | 821 | X         | -        | X       | -                |
| 22  | CLA  | A     | 822 | X         | -        | X       | -                |
| 22  | CLA  | A     | 823 | X         | -        | X       | -                |
| 22  | CLA  | A     | 824 | X         | -        | -       | -                |
| 22  | CLA  | A     | 825 | X         | -        | -       | -                |
| 22  | CLA  | A     | 826 | X         | -        | -       | -                |
| 22  | CLA  | A     | 827 | X         | -        | -       | -                |
| 22  | CLA  | A     | 828 | X         | -        | -       | -                |
| 22  | CLA  | A     | 829 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | A     | 830 | X         | -        | -       | -                |
| 22  | CLA  | A     | 831 | X         | -        | -       | -                |
| 22  | CLA  | A     | 832 | X         | -        | -       | -                |
| 22  | CLA  | A     | 833 | X         | -        | -       | -                |
| 22  | CLA  | A     | 834 | X         | -        | -       | -                |
| 22  | CLA  | A     | 835 | X         | -        | -       | -                |
| 22  | CLA  | A     | 836 | X         | -        | -       | -                |
| 22  | CLA  | A     | 837 | X         | -        | -       | -                |
| 22  | CLA  | A     | 838 | X         | -        | -       | -                |
| 22  | CLA  | A     | 839 | X         | -        | -       | -                |
| 22  | CLA  | A     | 840 | X         | -        | -       | -                |
| 22  | CLA  | A     | 841 | X         | -        | -       | -                |
| 22  | CLA  | A     | 842 | X         | -        | -       | -                |
| 22  | CLA  | A     | 854 | X         | -        | -       | -                |
| 22  | CLA  | A     | 855 | X         | -        | -       | -                |
| 22  | CLA  | B     | 801 | X         | -        | -       | -                |
| 22  | CLA  | B     | 805 | X         | -        | -       | -                |
| 22  | CLA  | B     | 806 | X         | -        | -       | -                |
| 22  | CLA  | B     | 807 | X         | -        | -       | -                |
| 22  | CLA  | B     | 808 | X         | -        | -       | -                |
| 22  | CLA  | B     | 809 | X         | -        | -       | -                |
| 22  | CLA  | B     | 810 | X         | -        | -       | -                |
| 22  | CLA  | B     | 811 | X         | -        | X       | -                |
| 22  | CLA  | B     | 812 | X         | -        | -       | -                |
| 22  | CLA  | B     | 813 | X         | -        | -       | -                |
| 22  | CLA  | B     | 814 | X         | -        | -       | -                |
| 22  | CLA  | B     | 815 | X         | -        | X       | -                |
| 22  | CLA  | B     | 816 | X         | -        | -       | -                |
| 22  | CLA  | B     | 817 | X         | -        | -       | -                |
| 22  | CLA  | B     | 818 | X         | -        | -       | -                |
| 22  | CLA  | B     | 819 | X         | -        | -       | -                |
| 22  | CLA  | B     | 820 | X         | -        | -       | -                |
| 22  | CLA  | B     | 821 | X         | -        | -       | -                |
| 22  | CLA  | B     | 822 | X         | -        | -       | -                |
| 22  | CLA  | B     | 823 | X         | -        | -       | -                |
| 22  | CLA  | B     | 824 | X         | -        | -       | -                |
| 22  | CLA  | B     | 825 | X         | -        | X       | -                |
| 22  | CLA  | B     | 826 | X         | -        | -       | -                |
| 22  | CLA  | B     | 827 | X         | -        | X       | -                |
| 22  | CLA  | B     | 828 | X         | -        | -       | -                |
| 22  | CLA  | B     | 829 | X         | -        | -       | -                |
| 22  | CLA  | B     | 830 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22  | CLA  | B     | 831 | X         | -        | -       | -                |
| 22  | CLA  | B     | 832 | X         | -        | -       | -                |
| 22  | CLA  | B     | 833 | X         | -        | -       | -                |
| 22  | CLA  | B     | 834 | X         | -        | -       | -                |
| 22  | CLA  | B     | 835 | X         | -        | -       | -                |
| 22  | CLA  | B     | 836 | X         | -        | -       | -                |
| 22  | CLA  | B     | 837 | X         | -        | -       | -                |
| 22  | CLA  | B     | 838 | X         | -        | -       | -                |
| 22  | CLA  | B     | 839 | X         | -        | -       | -                |
| 22  | CLA  | B     | 840 | X         | -        | -       | -                |
| 22  | CLA  | B     | 841 | X         | -        | -       | -                |
| 22  | CLA  | B     | 842 | X         | -        | X       | -                |
| 22  | CLA  | F     | 301 | X         | -        | -       | -                |
| 22  | CLA  | F     | 302 | X         | -        | -       | -                |
| 22  | CLA  | F     | 304 | X         | -        | X       | -                |
| 22  | CLA  | F     | 305 | X         | -        | -       | -                |
| 22  | CLA  | G     | 201 | X         | -        | -       | -                |
| 22  | CLA  | G     | 202 | X         | -        | -       | -                |
| 22  | CLA  | J     | 103 | X         | -        | -       | -                |
| 22  | CLA  | K     | 202 | X         | -        | -       | -                |
| 22  | CLA  | K     | 203 | X         | -        | -       | -                |
| 22  | CLA  | K     | 204 | X         | -        | -       | -                |
| 22  | CLA  | K     | 205 | X         | -        | -       | -                |
| 22  | CLA  | L     | 201 | X         | -        | -       | -                |
| 22  | CLA  | L     | 202 | X         | -        | -       | -                |
| 22  | CLA  | L     | 203 | X         | -        | -       | -                |
| 22  | CLA  | Z     | 303 | X         | -        | X       | -                |
| 22  | CLA  | Z     | 304 | X         | -        | -       | -                |
| 22  | CLA  | Z     | 305 | X         | -        | -       | -                |
| 22  | CLA  | Z     | 306 | X         | -        | -       | -                |
| 22  | CLA  | Z     | 307 | X         | -        | -       | -                |
| 22  | CLA  | Z     | 308 | X         | -        | -       | -                |
| 22  | CLA  | Z     | 309 | X         | -        | X       | -                |
| 22  | CLA  | Z     | 310 | X         | -        | -       | -                |
| 22  | CLA  | Z     | 313 | X         | -        | X       | -                |
| 22  | CLA  | Z     | 314 | X         | -        | -       | -                |
| 22  | CLA  | Z     | 315 | X         | -        | -       | -                |
| 22  | CLA  | Z     | 316 | X         | -        | -       | -                |
| 24  | BCR  | 3     | 304 | -         | X        | -       | -                |
| 24  | BCR  | 3     | 307 | -         | X        | -       | -                |
| 24  | BCR  | 4     | 804 | -         | -        | X       | -                |
| 24  | BCR  | 5     | 305 | -         | X        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24  | BCR  | 6     | 306 | -         | X        | -       | -                |
| 24  | BCR  | A     | 844 | -         | -        | X       | -                |
| 24  | BCR  | A     | 856 | -         | X        | X       | -                |
| 24  | BCR  | B     | 848 | -         | X        | -       | -                |
| 29  | SF4  | B     | 802 | -         | -        | X       | -                |
| 29  | SF4  | C     | 101 | -         | -        | X       | -                |
| 29  | SF4  | C     | 102 | -         | -        | X       | -                |
| 31  | DGD  | 3     | 301 | -         | -        | X       | -                |
| 37  | DAO  | K     | 201 | -         | -        | X       | -                |
| 38  | LUT  | Z     | 301 | -         | -        | X       | -                |
| 39  | CHL  | 1     | 312 | X         | -        | -       | -                |
| 39  | CHL  | 2     | 303 | X         | -        | -       | -                |
| 39  | CHL  | 3     | 317 | X         | -        | -       | -                |
| 39  | CHL  | 4     | 813 | X         | -        | -       | -                |
| 39  | CHL  | 4     | 814 | X         | -        | -       | -                |
| 39  | CHL  | 4     | 816 | X         | -        | X       | -                |
| 39  | CHL  | 4     | 819 | X         | -        | -       | -                |
| 39  | CHL  | 5     | 316 | X         | -        | -       | -                |
| 39  | CHL  | 5     | 317 | X         | -        | -       | -                |
| 39  | CHL  | 5     | 321 | X         | -        | -       | -                |
| 39  | CHL  | 6     | 315 | X         | -        | X       | -                |
| 39  | CHL  | 6     | 316 | X         | -        | -       | -                |
| 39  | CHL  | 6     | 318 | X         | -        | -       | -                |
| 39  | CHL  | 6     | 320 | X         | -        | -       | -                |
| 39  | CHL  | 7     | 313 | X         | -        | -       | -                |
| 39  | CHL  | 8     | 301 | X         | -        | -       | -                |
| 39  | CHL  | 8     | 312 | X         | -        | -       | -                |
| 39  | CHL  | 8     | 315 | X         | -        | X       | -                |
| 39  | CHL  | 9     | 312 | X         | -        | X       | -                |
| 39  | CHL  | 9     | 314 | X         | -        | -       | -                |
| 39  | CHL  | Z     | 311 | X         | -        | -       | -                |
| 39  | CHL  | Z     | 312 | X         | -        | -       | -                |

## 2 Entry composition [i](#)

There are 44 unique types of molecules in this entry. The entry contains 50057 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1 PsaA.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 1   | A     | 740      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5819  | 3806 | 991 | 1000 | 22 |         |       |

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 PsaB.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 2   | B     | 732      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5800  | 3804 | 973 | 1005 | 18 |         |       |

- Molecule 3 is a protein called Photosystem I subunit VII PsaC.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 603   | 370 | 105 | 116 | 12 |         |       |

- Molecule 4 is a protein called Photosystem I reaction center subunit II PsaD.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 724 | 196 | 204 | 5 |         |       |

- Molecule 5 is a protein called Photosystem I reaction center subunit IV PsaE.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5   | E     | 61       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 484   | 309 | 83 | 92 |         |       |

- Molecule 6 is a protein called Photosystem I reaction center subunit III PsaF.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1265  | 813 | 219 | 230 | 3 |         |       |

- Molecule 7 is a protein called Photosystem I reaction center subunit V PsaG.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 690   | 440 | 116 | 131 | 3 |         |       |

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII PsaI.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | I     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 308   | 210 | 44 | 53 | 1 |         |       |

- Molecule 9 is a protein called Photosystem I subunit IX PsaJ.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | J     | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 319   | 217 | 47 | 54 | 1 |         |       |

- Molecule 10 is a protein called Photosystem I reaction center subunit X psaK.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | K     | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 617   | 390 | 110 | 115 | 2 |         |       |

- Molecule 11 is a protein called Photosystem I reaction centre subunit XI PsaL.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | L     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 897   | 580 | 148 | 165 | 4 |         |       |

- Molecule 12 is a protein called Light-harvesting protein of photosystem I Lhca1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | 1     | 194      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1457  | 936 | 248 | 265 | 8 |         |       |
| 12  | Z     | 194      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1457  | 936 | 248 | 265 | 8 |         |       |

- Molecule 13 is a protein called Light-harvesting protein of photosystem I Lhca3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | 3     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 1107 | 272 | 309 | 7 |         |       |

- Molecule 14 is a protein called Light-harvesting protein of photosystem I Lhca7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | 7     | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1705  | 1102 | 283 | 313 | 7 |         |       |

- Molecule 15 is a protein called Light-harvesting protein of photosystem I Lhca8.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | 8     | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1602  | 1032 | 269 | 291 | 10 |         |       |

- Molecule 16 is a protein called Light-harvesting protein of photosystem I Lhca4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | 4     | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1598  | 1036 | 272 | 284 | 6 |         |       |

- Molecule 17 is a protein called Light-harvesting protein of photosystem I Lhca5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | 5     | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1764  | 1136 | 302 | 318 | 8 |         |       |

- Molecule 18 is a protein called Light-harvesting protein of photosystem I Lhca6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | 6     | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1762  | 1162 | 289 | 303 | 8 |         |       |

- Molecule 19 is a protein called Light-harvesting protein of photosystem I Lhca9.

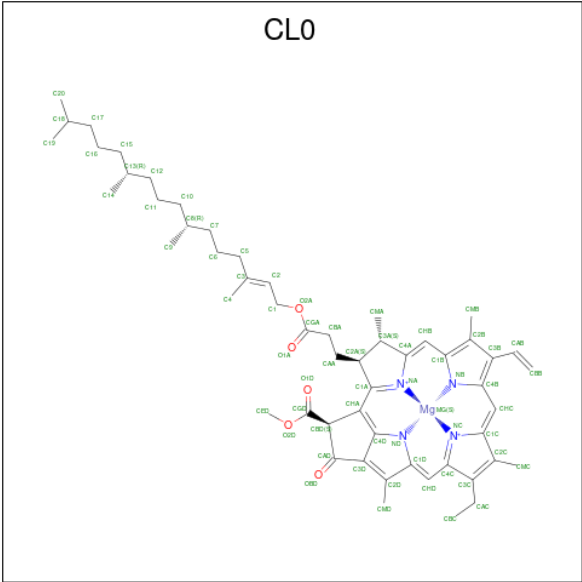
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | 9     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1416  | 914 | 239 | 254 | 9 |         |       |

- Molecule 20 is a protein called Light-harvesting protein of photosystem I Lhca2 partial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 20  | 2     | 70       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 525   | 336 | 90 | 94 | 5 |         |       |

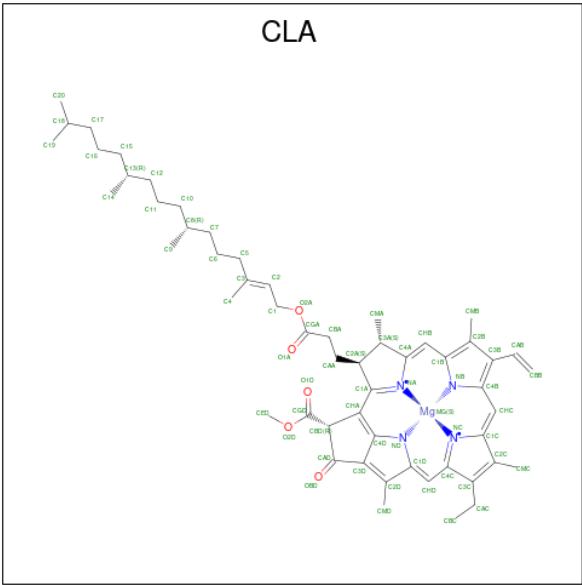
- Molecule 21 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).





| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 21  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | F     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | F     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | F     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | F     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 22  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | G     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | J     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 22  | K     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | K     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | K     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | K     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | L     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | L     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 1     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | Z     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | Z     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 3     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 22  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 22  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 22  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 22  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 22  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 22  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |

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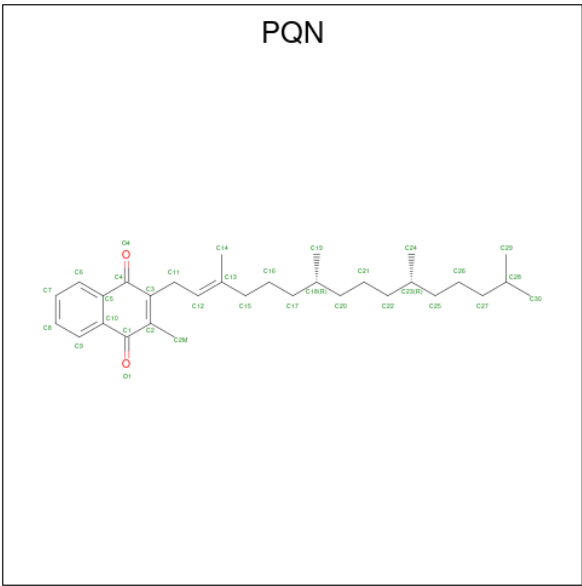
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 22  | 5     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 5     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 6     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 6     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 6     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 6     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 6     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 22  | 6     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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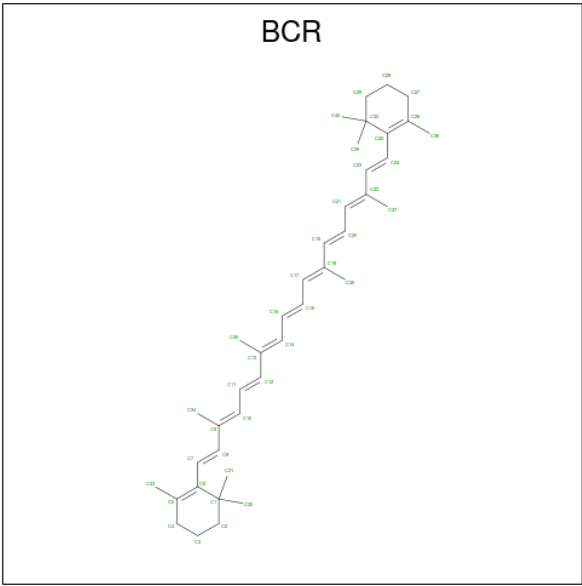
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 22  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 22  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 22  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 22  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 22  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 23  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 23  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 24  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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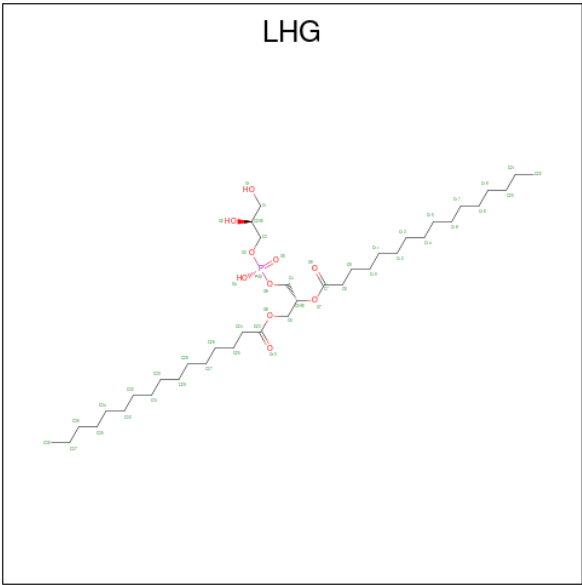
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 24  | A     | 1        | Total C<br>40 40 | 0       |
| 24  | A     | 1        | Total C<br>40 40 | 0       |
| 24  | A     | 1        | Total C<br>40 40 | 0       |
| 24  | A     | 1        | Total C<br>40 40 | 0       |
| 24  | A     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | B     | 1        | Total C<br>40 40 | 0       |
| 24  | F     | 1        | Total C<br>40 40 | 0       |
| 24  | G     | 1        | Total C<br>40 40 | 0       |
| 24  | I     | 1        | Total C<br>40 40 | 0       |
| 24  | J     | 1        | Total C<br>40 40 | 0       |
| 24  | K     | 1        | Total C<br>40 40 | 0       |
| 24  | L     | 1        | Total C<br>40 40 | 0       |
| 24  | 3     | 1        | Total C<br>40 40 | 0       |
| 24  | 3     | 1        | Total C<br>40 40 | 0       |
| 24  | 3     | 1        | Total C<br>40 40 | 0       |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 24  | 3     | 1        | Total C<br>40 40 | 0       |
| 24  | 7     | 1        | Total C<br>40 40 | 0       |
| 24  | 8     | 1        | Total C<br>40 40 | 0       |
| 24  | 4     | 1        | Total C<br>40 40 | 0       |
| 24  | 5     | 1        | Total C<br>40 40 | 0       |
| 24  | 5     | 1        | Total C<br>40 40 | 0       |
| 24  | 6     | 1        | Total C<br>40 40 | 0       |
| 24  | 6     | 1        | Total C<br>40 40 | 0       |

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



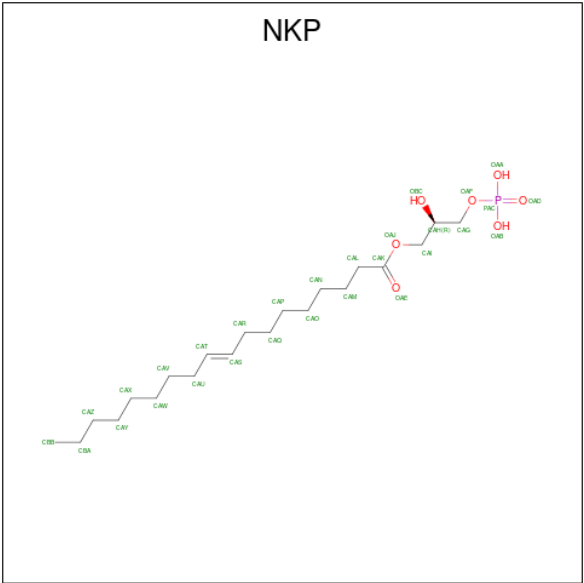
| Mol | Chain | Residues | Atoms                     | AltConf |
|-----|-------|----------|---------------------------|---------|
| 25  | A     | 1        | Total C O P<br>35 24 10 1 | 0       |
| 25  | A     | 1        | Total C O P<br>49 38 10 1 | 0       |
| 25  | B     | 1        | Total C O P<br>33 22 10 1 | 0       |

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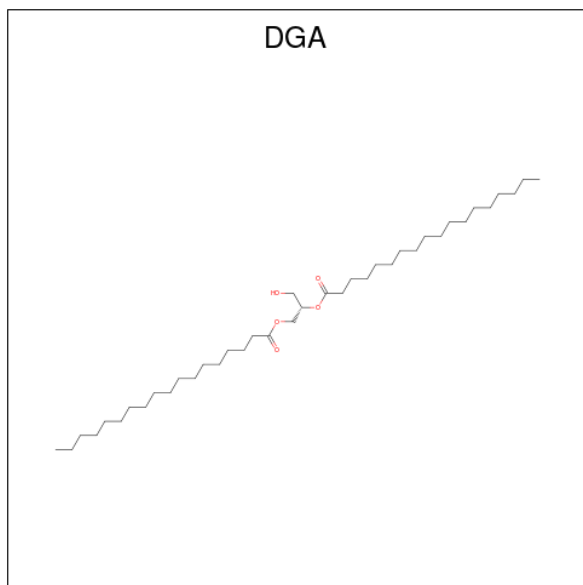
| Mol | Chain | Residues | Atoms       |    |    |   | AltConf |
|-----|-------|----------|-------------|----|----|---|---------|
|     |       |          | Total       | C  | O  | P |         |
| 25  | B     | 1        | Total<br>23 | 12 | 10 | 1 | 0       |
| 25  | B     | 1        | Total<br>20 | 9  | 10 | 1 | 0       |
| 25  | 1     | 1        | Total<br>43 | 32 | 10 | 1 | 0       |
| 25  | Z     | 1        | Total<br>43 | 32 | 10 | 1 | 0       |
| 25  | 3     | 1        | Total<br>20 | 9  | 10 | 1 | 0       |
| 25  | 7     | 1        | Total<br>37 | 26 | 10 | 1 | 0       |
| 25  | 8     | 1        | Total<br>38 | 27 | 10 | 1 | 0       |
| 25  | 4     | 1        | Total<br>49 | 38 | 10 | 1 | 0       |
| 25  | 4     | 1        | Total<br>32 | 21 | 10 | 1 | 0       |
| 25  | 5     | 1        | Total<br>37 | 26 | 10 | 1 | 0       |
| 25  | 6     | 1        | Total<br>49 | 38 | 10 | 1 | 0       |
| 25  | 9     | 1        | Total<br>33 | 22 | 10 | 1 | 0       |

- Molecule 26 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (CCD ID: NKP) (formula: C<sub>21</sub>H<sub>41</sub>O<sub>7</sub>P).



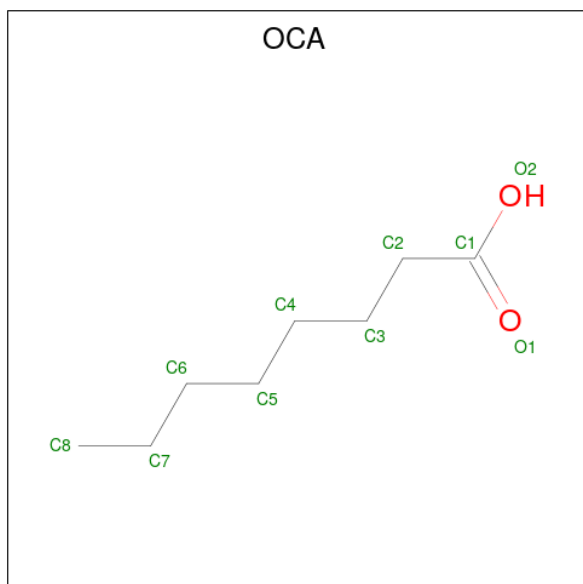
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 26  | A     | 1        | Total | C  | O | P | 0       |
|     |       |          | 23    | 15 | 7 | 1 |         |
| 26  | 8     | 1        | Total | C  | O | P | 0       |
|     |       |          | 29    | 21 | 7 | 1 |         |

- Molecule 27 is DIACYL GLYCEROL (CCD ID: DGA) (formula:  $C_{39}H_{76}O_5$ ).



| Mol | Chain | Residues | Atoms |    |   |  | AltConf |
|-----|-------|----------|-------|----|---|--|---------|
| 27  | A     | 1        | Total | C  | O |  | 0       |
|     |       |          | 40    | 35 | 5 |  |         |

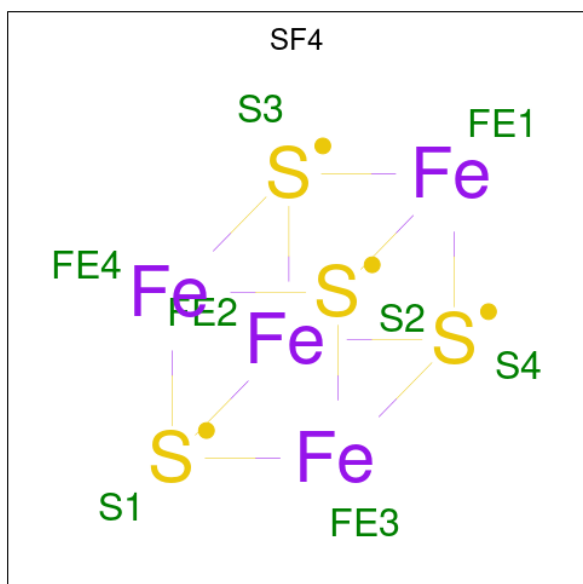
- Molecule 28 is OCTANOIC ACID (CAPRYLIC ACID) (CCD ID: OCA) (formula:  $C_8H_{16}O_2$ ).





| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 28  | A     | 1        | Total | C | O | 0       |
|     |       |          | 10    | 8 | 2 |         |

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).

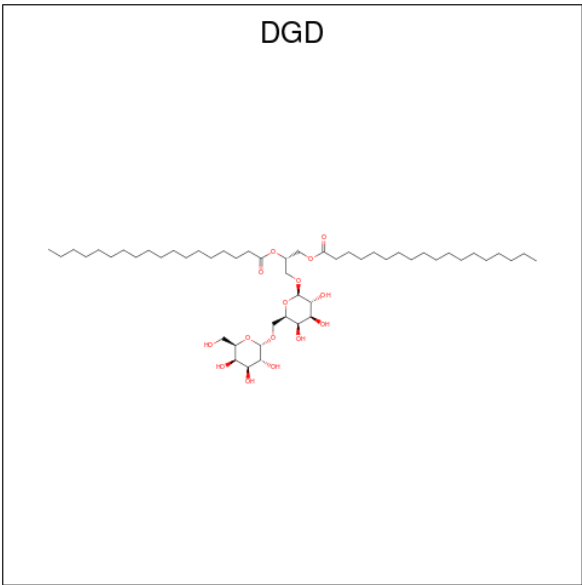


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 29  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 29  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 29  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

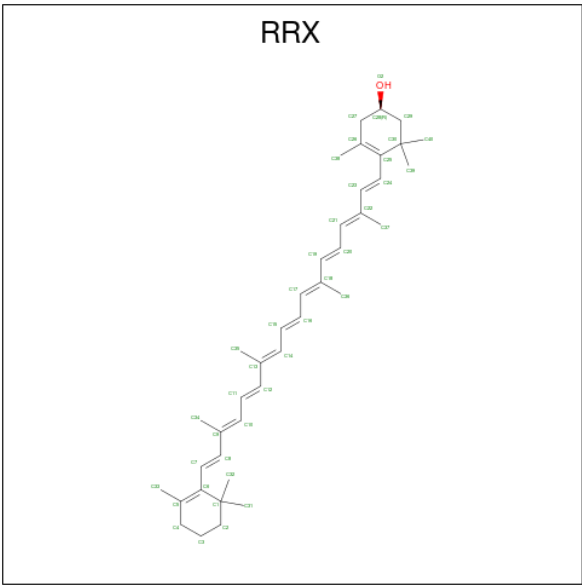
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 30  | B     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $\text{C}_{51}\text{H}_{96}\text{O}_{15}$ ).



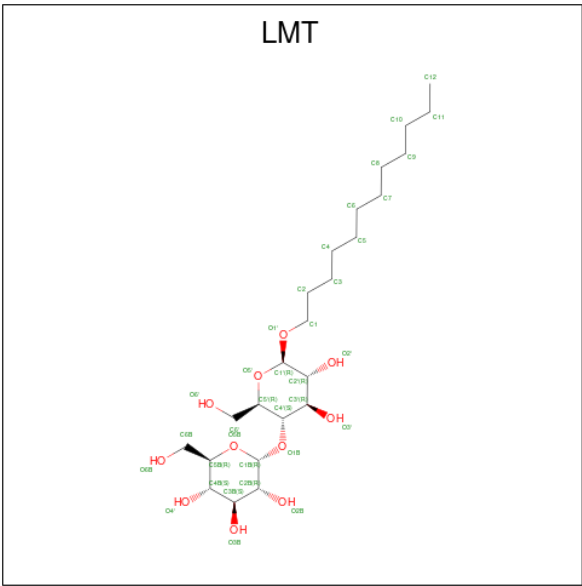
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 31  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 61    | 46 | 15 |         |
| 31  | 1     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 36 | 15 |         |
| 31  | 3     | 1        | Total | C  | O  | 0       |
|     |       |          | 51    | 36 | 15 |         |

- Molecule 32 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



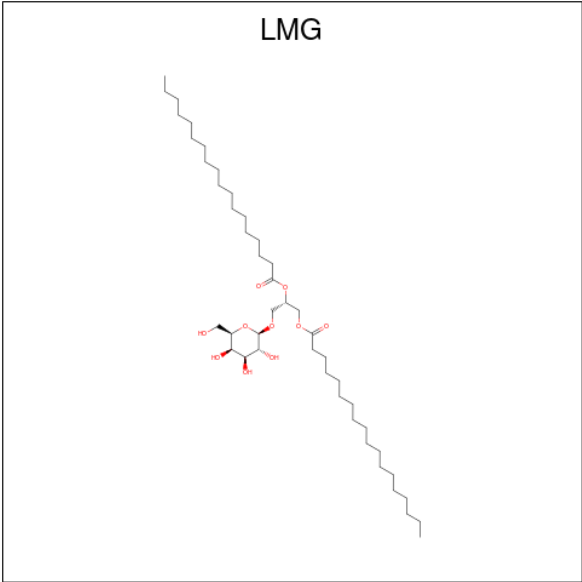
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 32  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |

- Molecule 33 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



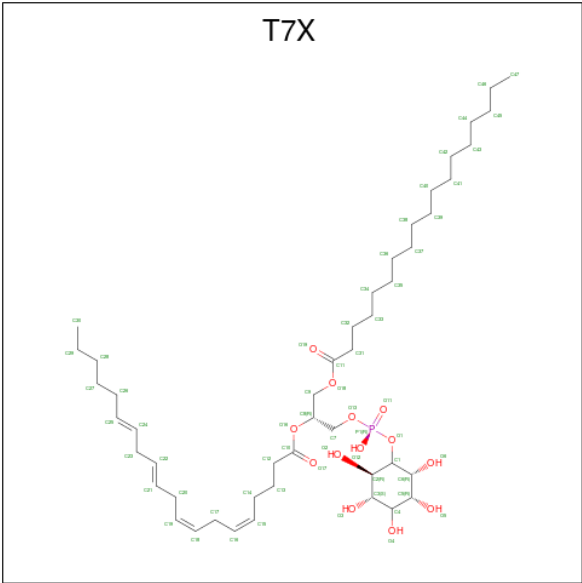
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 33  | F     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | G     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | 1     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |
| 33  | 4     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 34  | F     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 25 | 10 |         |
| 34  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 29    | 19 | 10 |         |

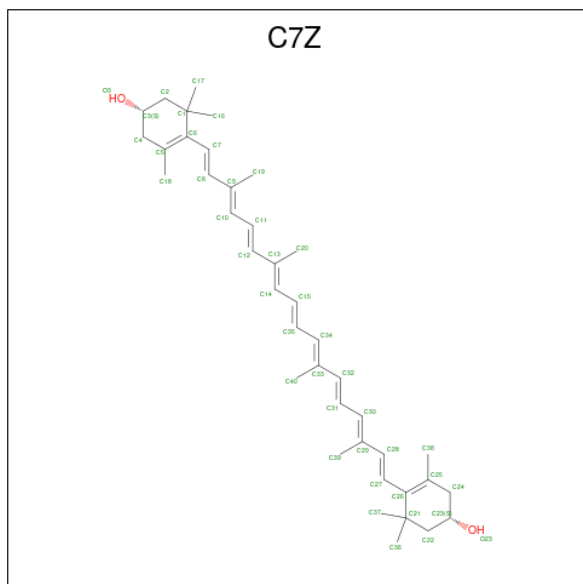
- Molecule 35 is Phosphatidylinositol (CCD ID: T7X) (formula: C<sub>47</sub>H<sub>83</sub>O<sub>13</sub>P).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 35  | J     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 35 | 13 | 1 |         |

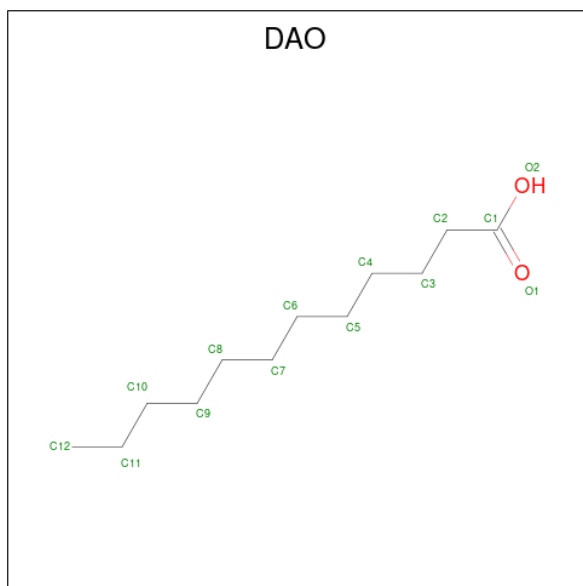
- Molecule 36 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},

15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula:  $C_{40}H_{56}O_2$ ).



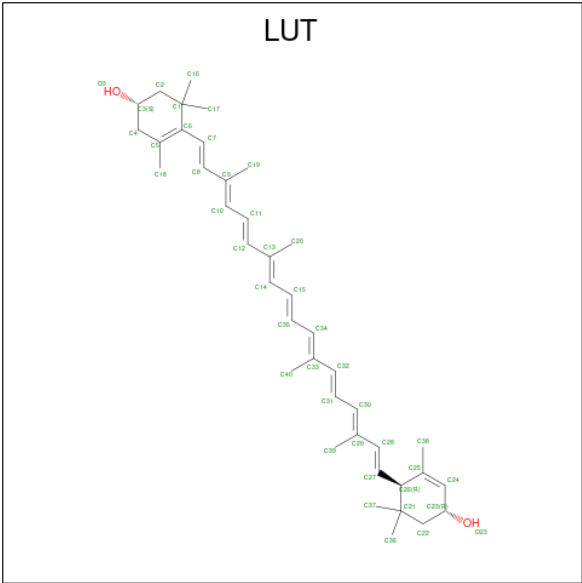
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 36  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 37 is LAURIC ACID (CCD ID: DAO) (formula:  $C_{12}H_{24}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 37  | K     | 1        | Total | C  | O | 0       |
|     |       |          | 14    | 12 | 2 |         |

- Molecule 38 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



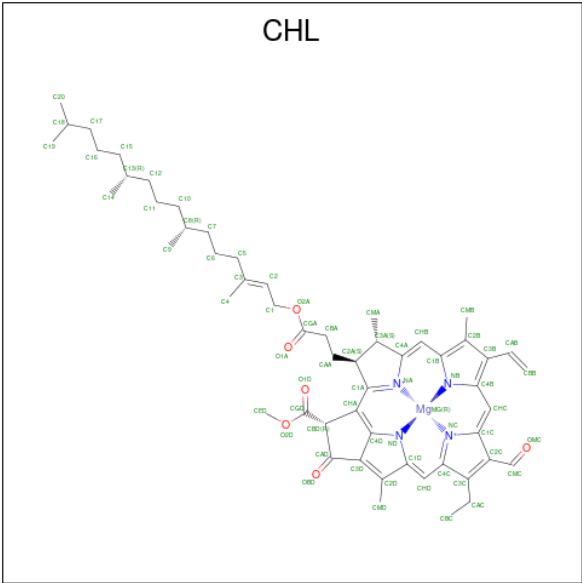
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 38  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 1     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | Z     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 38  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 38  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 39 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 39  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 39  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 39  | Z     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |

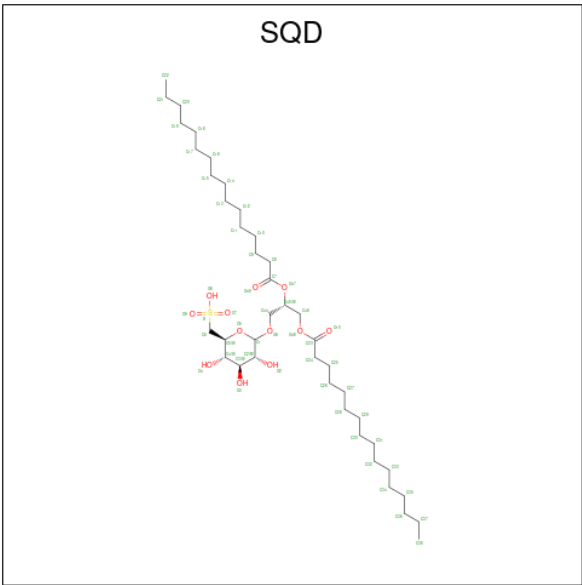
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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 39  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 39  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 43 | 1  | 4 | 6 |         |
| 39  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 47 | 1  | 4 | 6 |         |
| 39  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 39  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 39  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 39  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 39  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 39  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 39  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 39  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 39  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 39  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 39  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 39  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 39  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 39  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 39  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 33 | 1  | 4 | 4 |         |
| 39  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |

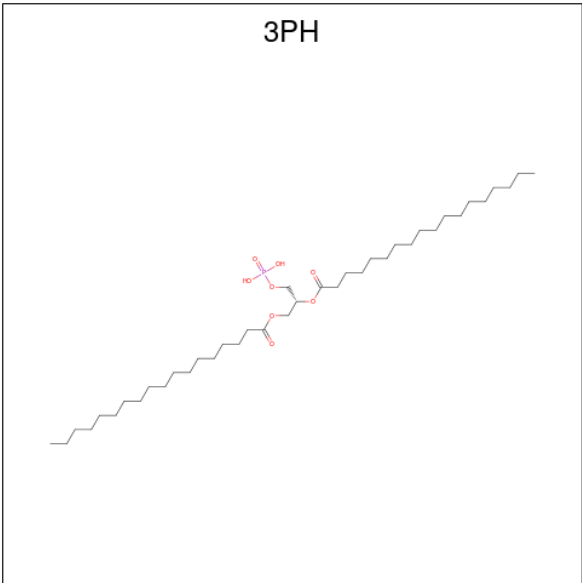
- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).





| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 40  | 1     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 48    | 35 | 12 | 1 |         |

- Molecule 41 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P).



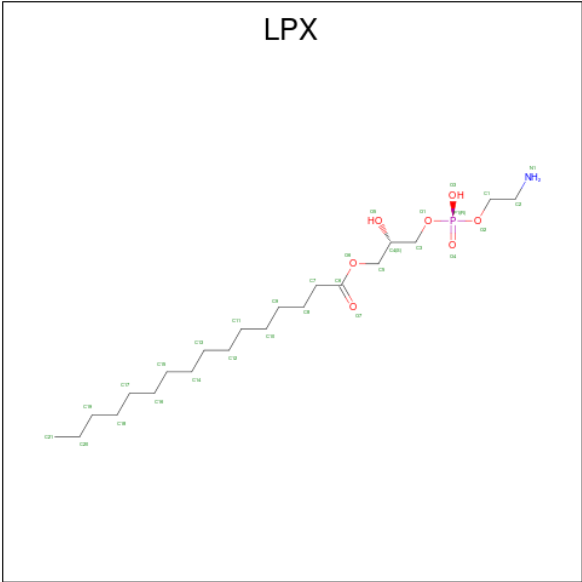
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 41  | 7     | 1        | Total | C  | O | P | 0       |
|     |       |          | 39    | 30 | 8 | 1 |         |
| 41  | 8     | 1        | Total | C  | O | P | 0       |
|     |       |          | 30    | 21 | 8 | 1 |         |

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| Mol | Chain | Residues | Atoms       |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| 41  | 5     | 1        | Total<br>23 | C<br>14 | O<br>8 | P<br>1 | 0       |
| 41  | 6     | 1        | Total<br>29 | C<br>20 | O<br>8 | P<br>1 | 0       |

- # SPH

- Molecule 43 is (2S)-3-[[ (R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C<sub>21</sub>H<sub>44</sub>NO<sub>7</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 43  | 8     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 30    | 21 | 1 | 7 | 1 |         |

- Molecule 44 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 44  | A     | 19       | Total | O  | 0       |
|     |       |          | 19    | 19 |         |
| 44  | B     | 17       | Total | O  | 0       |
|     |       |          | 17    | 17 |         |
| 44  | F     | 3        | Total | O  | 0       |
|     |       |          | 3     | 3  |         |
| 44  | I     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 44  | J     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 44  | K     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 44  | 1     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 44  | Z     | 1        | Total | O  | 0       |
|     |       |          | 1     | 1  |         |
| 44  | 3     | 2        | Total | O  | 0       |
|     |       |          | 2     | 2  |         |
| 44  | 7     | 4        | Total | O  | 0       |
|     |       |          | 4     | 4  |         |
| 44  | 8     | 4        | Total | O  | 0       |
|     |       |          | 4     | 4  |         |

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| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 44  | 4     | 5        | Total<br>5 | O<br>5 | 0       |
| 44  | 5     | 5        | Total<br>5 | O<br>5 | 0       |
| 44  | 6     | 3        | Total<br>3 | O<br>3 | 0       |
| 44  | 2     | 1        | Total<br>1 | O<br>1 | 0       |

### 3 Residue-property plots

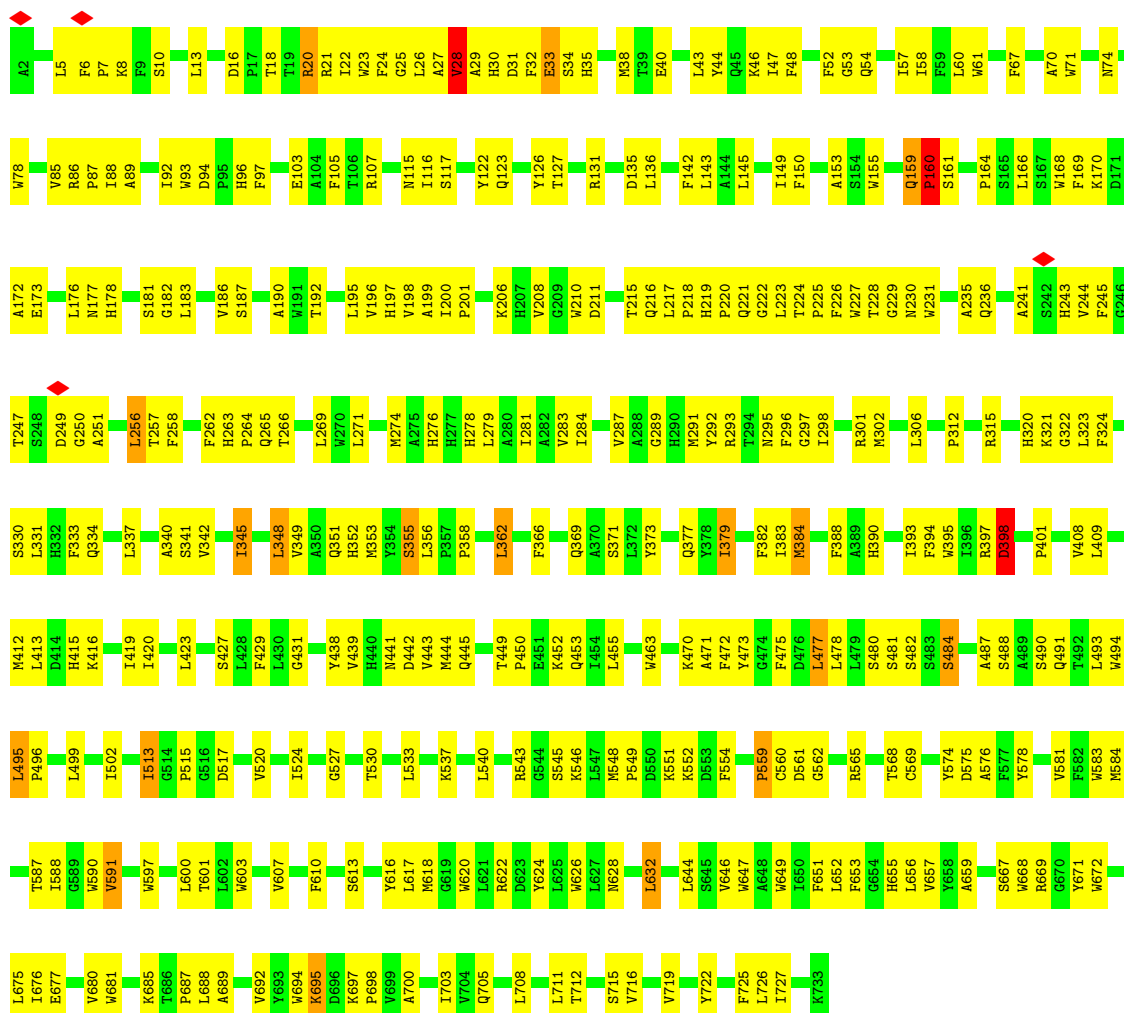
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 PsaA



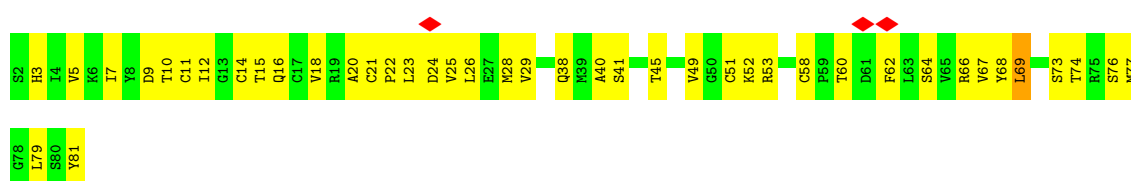
#### • Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 PsaB





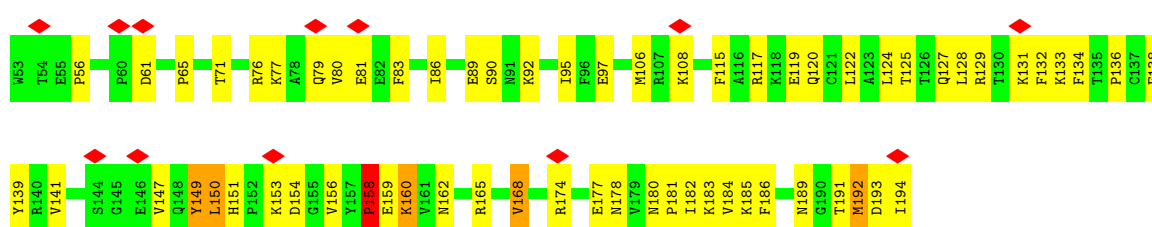
### • Molecule 3: Photosystem I subunit VII Psac

Chain C: 48% 51%

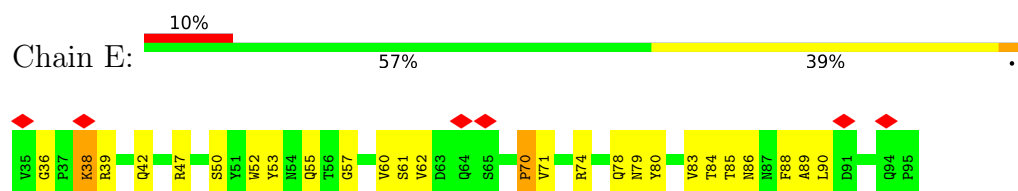


### • Molecule 4: Photosystem I reaction center subunit II Psad

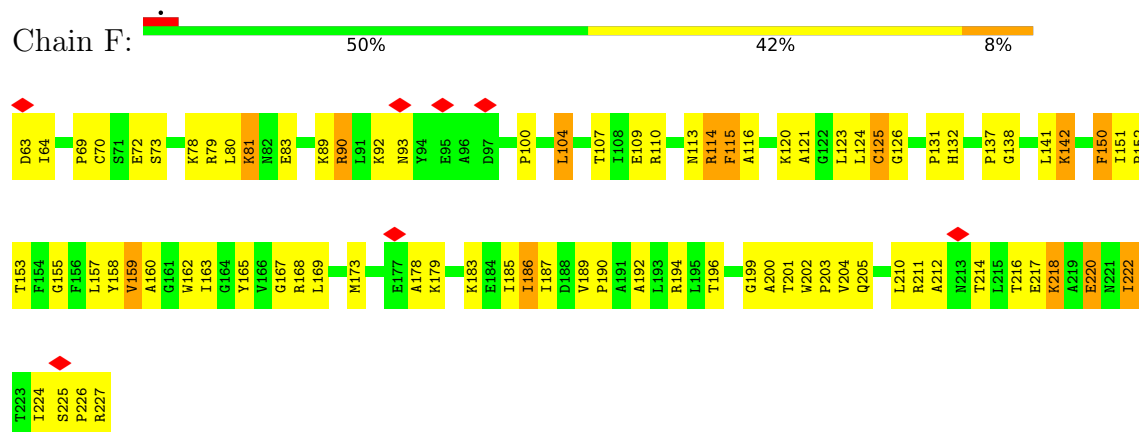
Chain D: 8% 55% 41%



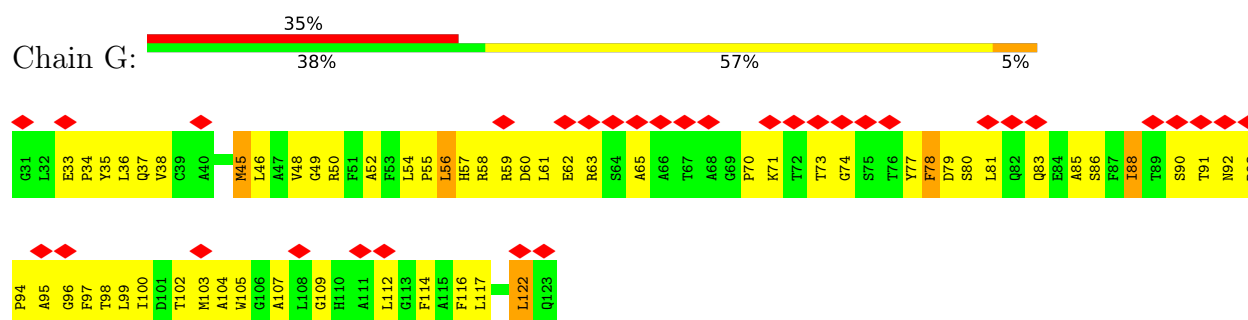
- Molecule 5: Photosystem I reaction center subunit IV PsaE



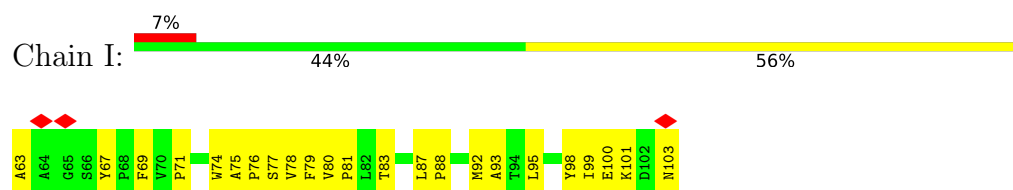
- Molecule 6: Photosystem I reaction center subunit III PsaF



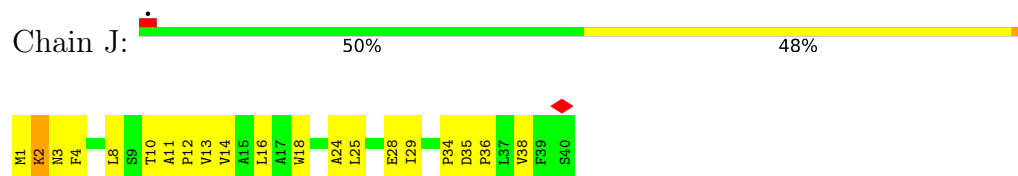
- Molecule 7: Photosystem I reaction center subunit V PsaG



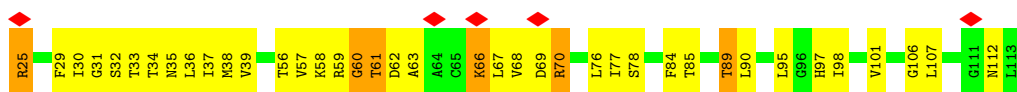
- Molecule 8: Photosystem I reaction center subunit VIII PsaI



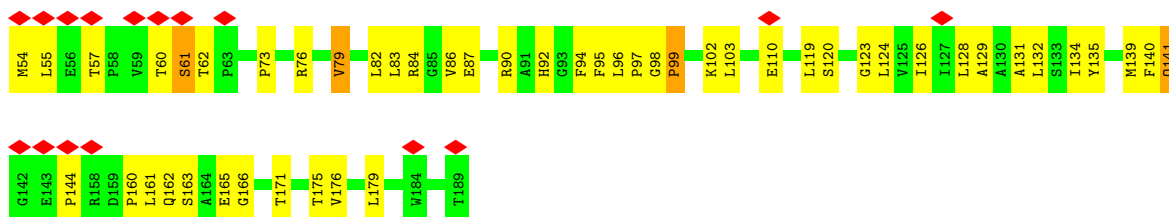
- Molecule 9: Photosystem I subunit IX PsaJ



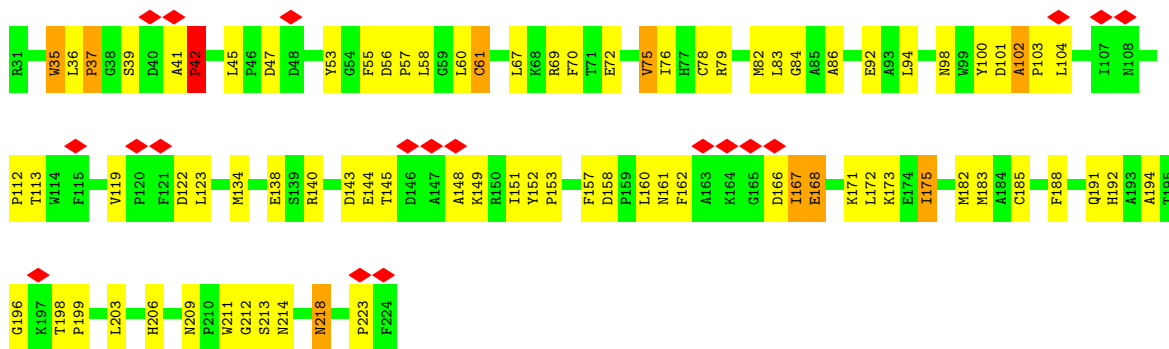
- Molecule 10: Photosystem I reaction center subunit X psaK



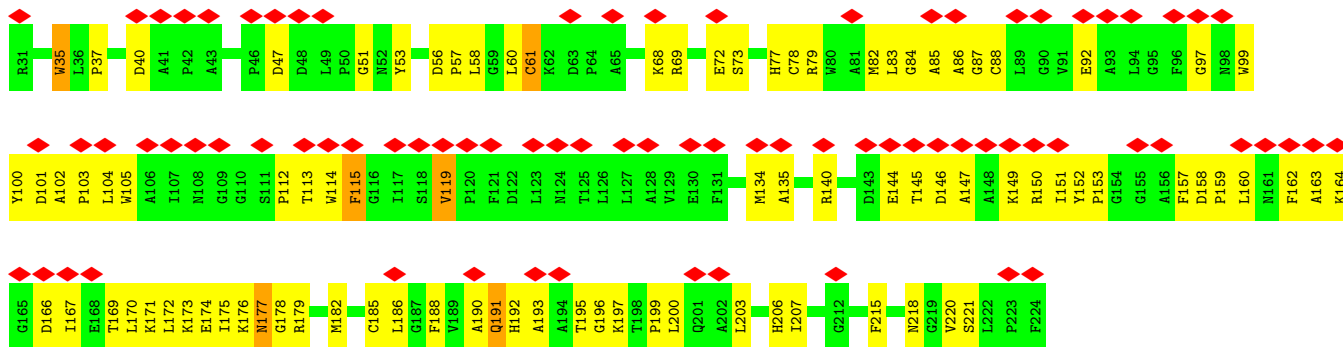
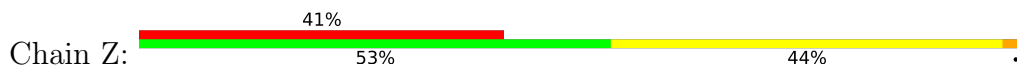
- Molecule 11: Photosystem I reaction centre subunit XI PsaL



- Molecule 12: Light-harvesting protein of photosystem I Lhca1



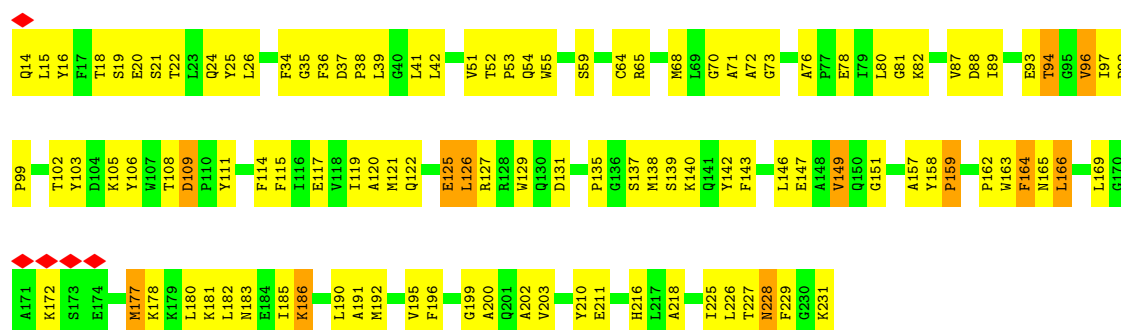
- Molecule 12: Light-harvesting protein of photosystem I Lhca1



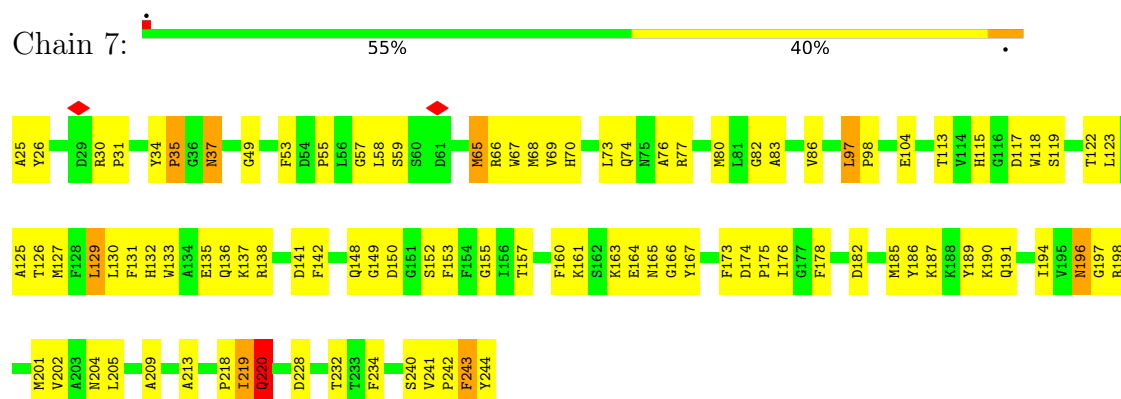
- Molecule 13: Light-harvesting protein of photosystem I Lhca3







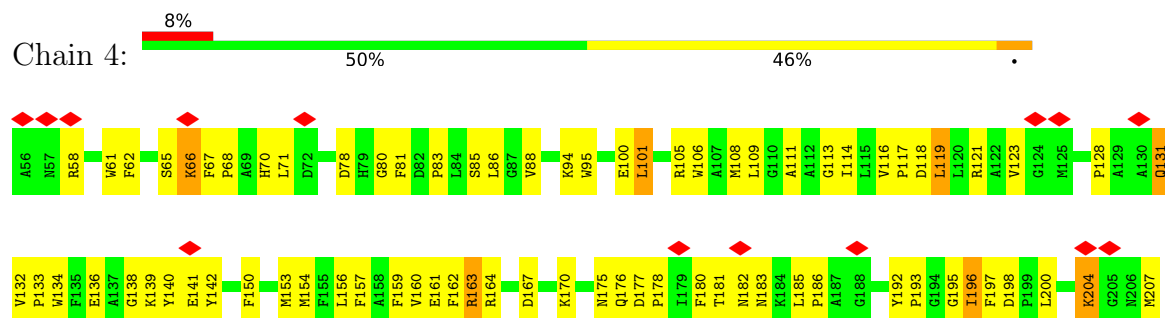
- Molecule 14: Light-harvesting protein of photosystem I Lhca7



- Molecule 15: Light-harvesting protein of photosystem I Lhca8

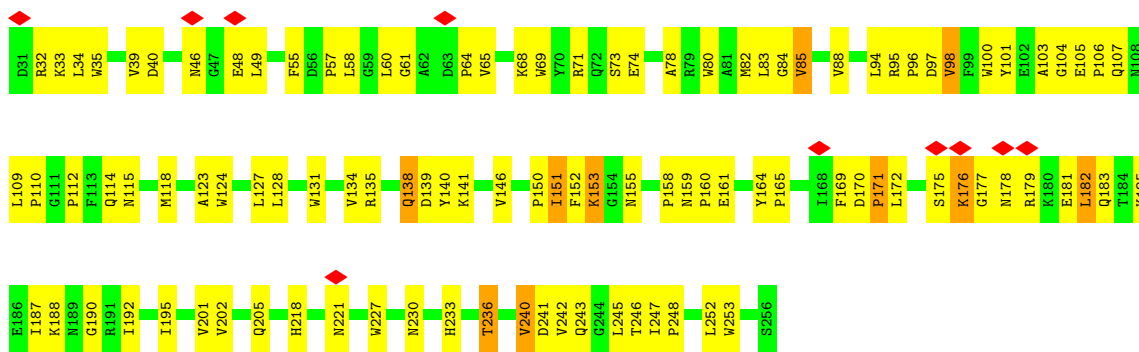


- Molecule 16: Light-harvesting protein of photosystem I Lhca4

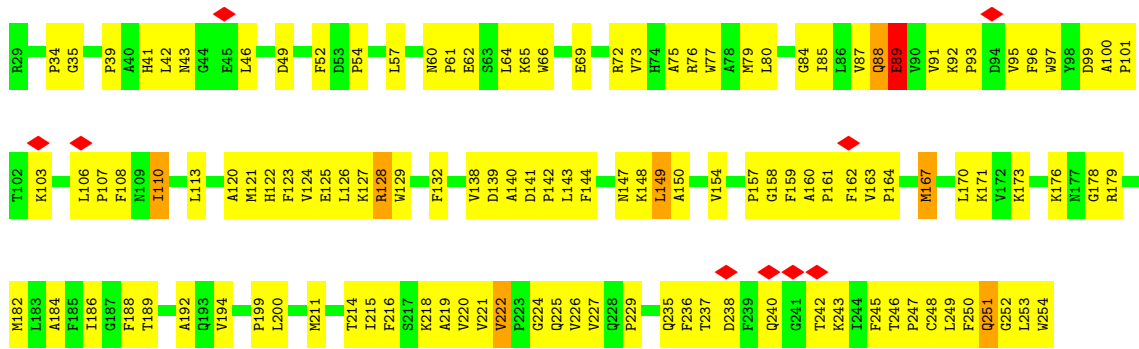




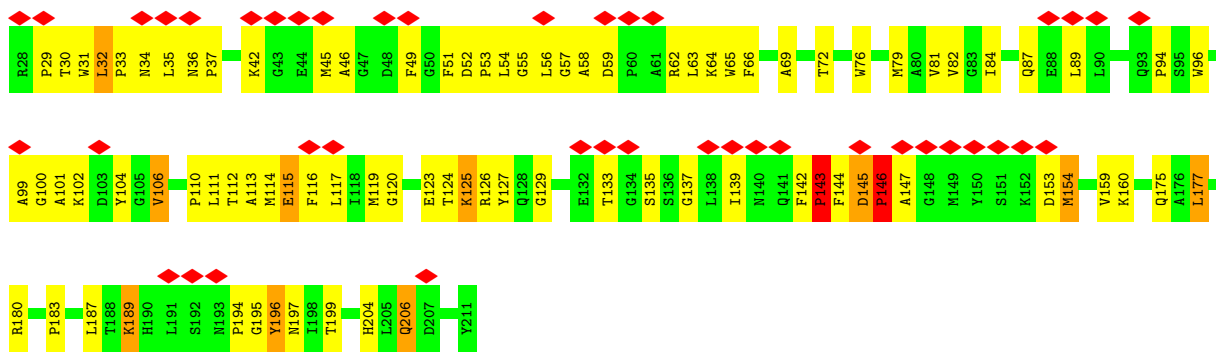
- Molecule 17: Light-harvesting protein of photosystem I Lhca5



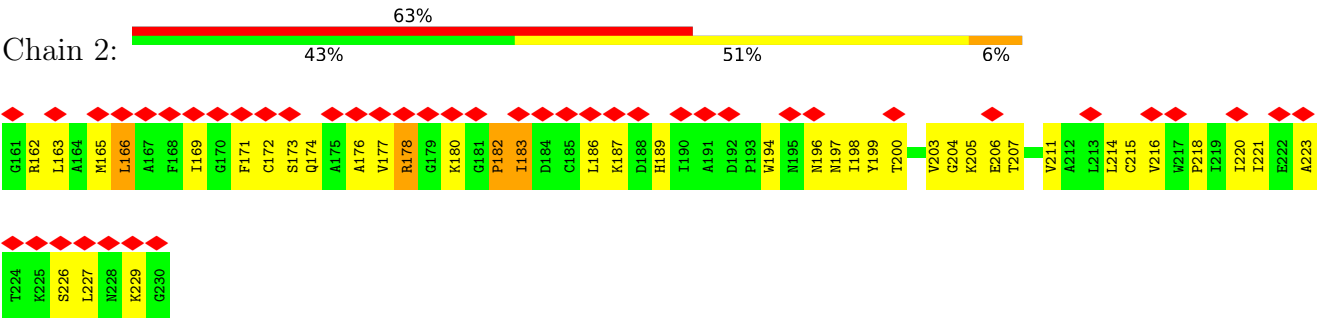
- Molecule 18: Light-harvesting protein of photosystem I Lhca6



- Molecule 19: Light-harvesting protein of photosystem I Lhca9



- Molecule 20: Light-harvesting protein of photosystem I Lhca2 partial



## 4 Experimental information

| Property                             | Value                         | Source    |
|--------------------------------------|-------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE               | Depositor |
| Imposed symmetry                     | POINT, C1                     | Depositor |
| Number of particles used             | 167160                        | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF             | Depositor |
| CTF correction method                | NONE                          | Depositor |
| Microscope                           | FEI TITAN KRIOS               | Depositor |
| Voltage (kV)                         | 300                           | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                            | Depositor |
| Minimum defocus (nm)                 | 150                           | Depositor |
| Maximum defocus (nm)                 | 1750                          | Depositor |
| Magnification                        | 130000                        | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value                    | 0.032                         | Depositor |
| Minimum map value                    | -0.012                        | Depositor |
| Average map value                    | 0.000                         | Depositor |
| Map value standard deviation         | 0.001                         | Depositor |
| Recommended contour level            | 0.007                         | Depositor |
| Map size ( $\text{\AA}$ )            | 325.5, 325.5, 325.5           | wwPDB     |
| Map dimensions                       | 500, 500, 500                 | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0              | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.651, 0.651, 0.651           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, SQD, CA, SPH, LPX, NKP, LHG, DGD, LMG, CLA, CHL, T7X, RRX, CL0, PQN, OCA, C7Z, DAO, 3PH, BCR, LUT, LMT, DGA

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     | 0.91         | 0/6016  | 1.13        | 8/8200 (0.1%)   |
| 2   | B     | 0.92         | 0/6010  | 1.13        | 3/8207 (0.0%)   |
| 3   | C     | 0.98         | 0/613   | 1.15        | 0/830           |
| 4   | D     | 0.89         | 0/1159  | 1.17        | 1/1569 (0.1%)   |
| 5   | E     | 0.98         | 0/495   | 1.09        | 0/675           |
| 6   | F     | 0.92         | 0/1292  | 1.25        | 3/1755 (0.2%)   |
| 7   | G     | 0.95         | 0/706   | 1.20        | 1/960 (0.1%)    |
| 8   | I     | 0.97         | 0/320   | 1.11        | 0/443           |
| 9   | J     | 0.96         | 0/329   | 1.20        | 0/452           |
| 10  | K     | 1.00         | 0/625   | 1.27        | 0/848           |
| 11  | L     | 0.97         | 0/919   | 1.26        | 0/1253          |
| 12  | 1     | 0.91         | 0/1501  | 1.28        | 3/2045 (0.1%)   |
| 12  | Z     | 0.78         | 0/1501  | 1.03        | 1/2045 (0.0%)   |
| 13  | 3     | 0.93         | 0/1747  | 1.21        | 2/2376 (0.1%)   |
| 14  | 7     | 0.93         | 0/1765  | 1.22        | 1/2407 (0.0%)   |
| 15  | 8     | 0.94         | 0/1643  | 1.24        | 2/2226 (0.1%)   |
| 16  | 4     | 0.92         | 0/1648  | 1.19        | 0/2240          |
| 17  | 5     | 0.92         | 0/1819  | 1.21        | 0/2480          |
| 18  | 6     | 0.92         | 0/1824  | 1.14        | 1/2488 (0.0%)   |
| 19  | 9     | 0.85         | 0/1456  | 1.30        | 5/1975 (0.3%)   |
| 20  | 2     | 0.96         | 0/535   | 1.24        | 0/726           |
| All | All   | 0.92         | 0/33923 | 1.18        | 31/46200 (0.1%) |

There are no bond length outliers.

All (31) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 19  | 9     | 143 | PRO  | CA-N-CD | -11.78 | 95.51       | 112.00   |
| 12  | 1     | 42  | PRO  | CA-N-CD | -9.96  | 98.06       | 112.00   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 19  | 9     | 189 | LYS  | N-CA-C   | -7.90 | 105.61      | 114.62   |
| 19  | 9     | 143 | PRO  | CB-CA-C  | 7.80  | 124.43      | 111.56   |
| 19  | 9     | 146 | PRO  | CA-N-CD  | -7.61 | 101.35      | 112.00   |
| 12  | 1     | 148 | ALA  | N-CA-C   | -7.60 | 105.96      | 114.62   |
| 14  | 7     | 220 | GLN  | N-CA-C   | -6.59 | 103.29      | 112.45   |
| 13  | 3     | 164 | PHE  | CB-CA-C  | 6.28  | 120.74      | 110.88   |
| 1   | A     | 44  | ASN  | N-CA-C   | -6.07 | 106.85      | 114.56   |
| 1   | A     | 274 | ASP  | N-CA-C   | -6.03 | 106.90      | 114.56   |
| 19  | 9     | 146 | PRO  | N-CA-CB  | -6.03 | 96.92       | 103.25   |
| 15  | 8     | 167 | PRO  | N-CA-C   | -5.96 | 105.24      | 113.53   |
| 1   | A     | 157 | LEU  | N-CA-C   | -5.90 | 106.21      | 113.41   |
| 12  | 1     | 42  | PRO  | CB-CA-C  | 5.85  | 121.21      | 111.56   |
| 7   | G     | 78  | PHE  | N-CA-C   | -5.58 | 107.05      | 112.97   |
| 15  | 8     | 180 | LYS  | N-CA-C   | -5.56 | 105.23      | 112.23   |
| 2   | B     | 576 | ALA  | N-CA-C   | -5.55 | 104.86      | 111.69   |
| 6   | F     | 89  | LYS  | N-CA-C   | -5.53 | 106.89      | 113.97   |
| 1   | A     | 687 | PHE  | CB-CA-C  | -5.50 | 100.87      | 110.17   |
| 4   | D     | 158 | PRO  | N-CA-CB  | -5.50 | 97.48       | 103.25   |
| 1   | A     | 426 | LEU  | N-CA-C   | -5.44 | 106.72      | 113.19   |
| 1   | A     | 469 | GLN  | N-CA-C   | -5.27 | 106.89      | 113.38   |
| 1   | A     | 433 | HIS  | CA-CB-CG | 5.24  | 119.04      | 113.80   |
| 2   | B     | 574 | TYR  | N-CA-C   | -5.22 | 105.65      | 112.23   |
| 12  | Z     | 97  | GLY  | CA-C-O   | -5.16 | 118.15      | 122.33   |
| 2   | B     | 398 | ASP  | CA-CB-CG | 5.09  | 117.69      | 112.60   |
| 13  | 3     | 186 | LYS  | N-CA-C   | -5.08 | 106.78      | 113.12   |
| 1   | A     | 593 | PHE  | CA-CB-CG | 5.07  | 118.87      | 113.80   |
| 6   | F     | 90  | ARG  | N-CA-C   | -5.07 | 107.10      | 113.28   |
| 18  | 6     | 89  | GLU  | N-CA-C   | -5.06 | 107.78      | 114.31   |
| 6   | F     | 186 | ILE  | CA-C-O   | -5.04 | 118.24      | 122.63   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5819  | 0        | 5666     | 296     | 0            |
| 2   | B     | 5800  | 0        | 5556     | 372     | 0            |
| 3   | C     | 603   | 0        | 587      | 42      | 0            |
| 4   | D     | 1129  | 0        | 1127     | 46      | 0            |
| 5   | E     | 484   | 0        | 477      | 25      | 0            |
| 6   | F     | 1265  | 0        | 1292     | 75      | 0            |
| 7   | G     | 690   | 0        | 671      | 69      | 0            |
| 8   | I     | 308   | 0        | 310      | 31      | 0            |
| 9   | J     | 319   | 0        | 327      | 23      | 0            |
| 10  | K     | 617   | 0        | 635      | 54      | 0            |
| 11  | L     | 897   | 0        | 891      | 48      | 0            |
| 12  | 1     | 1457  | 0        | 1406     | 79      | 0            |
| 12  | Z     | 1457  | 0        | 1406     | 119     | 0            |
| 13  | 3     | 1695  | 0        | 1641     | 143     | 0            |
| 14  | 7     | 1705  | 0        | 1601     | 104     | 0            |
| 15  | 8     | 1602  | 0        | 1600     | 138     | 0            |
| 16  | 4     | 1598  | 0        | 1569     | 116     | 0            |
| 17  | 5     | 1764  | 0        | 1709     | 126     | 0            |
| 18  | 6     | 1762  | 0        | 1740     | 180     | 0            |
| 19  | 9     | 1416  | 0        | 1392     | 104     | 0            |
| 20  | 2     | 525   | 0        | 539      | 46      | 0            |
| 21  | A     | 65    | 0        | 72       | 7       | 0            |
| 22  | 1     | 698   | 0        | 678      | 106     | 0            |
| 22  | 2     | 146   | 0        | 112      | 30      | 0            |
| 22  | 3     | 749   | 0        | 722      | 153     | 0            |
| 22  | 4     | 590   | 0        | 511      | 100     | 0            |
| 22  | 5     | 910   | 0        | 851      | 191     | 0            |
| 22  | 6     | 824   | 0        | 800      | 183     | 0            |
| 22  | 7     | 905   | 0        | 848      | 123     | 0            |
| 22  | 8     | 555   | 0        | 502      | 111     | 0            |
| 22  | 9     | 528   | 0        | 451      | 66      | 0            |
| 22  | A     | 2640  | 0        | 2709     | 508     | 0            |
| 22  | B     | 2340  | 0        | 2333     | 452     | 0            |
| 22  | F     | 240   | 0        | 245      | 60      | 0            |
| 22  | G     | 96    | 0        | 70       | 26      | 0            |
| 22  | J     | 42    | 0        | 30       | 1       | 0            |
| 22  | K     | 205   | 0        | 166      | 28      | 0            |
| 22  | L     | 180   | 0        | 180      | 37      | 0            |
| 22  | Z     | 679   | 0        | 631      | 147     | 0            |
| 23  | A     | 33    | 0        | 46       | 10      | 0            |
| 23  | B     | 33    | 0        | 46       | 5       | 0            |
| 24  | 3     | 160   | 0        | 224      | 59      | 0            |
| 24  | 4     | 40    | 0        | 56       | 26      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | 5     | 80    | 0        | 112      | 30      | 0            |
| 24  | 6     | 80    | 0        | 112      | 35      | 0            |
| 24  | 7     | 40    | 0        | 56       | 14      | 0            |
| 24  | 8     | 40    | 0        | 56       | 14      | 0            |
| 24  | A     | 240   | 0        | 336      | 98      | 0            |
| 24  | B     | 280   | 0        | 392      | 103     | 0            |
| 24  | F     | 40    | 0        | 56       | 14      | 0            |
| 24  | G     | 40    | 0        | 56       | 12      | 0            |
| 24  | I     | 40    | 0        | 56       | 12      | 0            |
| 24  | J     | 40    | 0        | 56       | 18      | 0            |
| 24  | K     | 40    | 0        | 55       | 12      | 0            |
| 24  | L     | 40    | 0        | 56       | 17      | 0            |
| 25  | 1     | 43    | 0        | 56       | 8       | 0            |
| 25  | 3     | 20    | 0        | 12       | 1       | 0            |
| 25  | 4     | 81    | 0        | 108      | 19      | 0            |
| 25  | 5     | 37    | 0        | 44       | 7       | 0            |
| 25  | 6     | 49    | 0        | 74       | 11      | 0            |
| 25  | 7     | 37    | 0        | 44       | 10      | 0            |
| 25  | 8     | 38    | 0        | 46       | 7       | 0            |
| 25  | 9     | 33    | 0        | 36       | 2       | 0            |
| 25  | A     | 84    | 0        | 114      | 13      | 0            |
| 25  | B     | 76    | 0        | 64       | 15      | 0            |
| 25  | Z     | 43    | 0        | 56       | 9       | 0            |
| 26  | 8     | 29    | 0        | 39       | 7       | 0            |
| 26  | A     | 23    | 0        | 24       | 3       | 0            |
| 27  | A     | 40    | 0        | 65       | 20      | 0            |
| 28  | A     | 10    | 0        | 15       | 0       | 0            |
| 29  | B     | 8     | 0        | 0        | 8       | 0            |
| 29  | C     | 16    | 0        | 0        | 8       | 0            |
| 30  | B     | 1     | 0        | 0        | 0       | 0            |
| 31  | 1     | 51    | 0        | 60       | 10      | 0            |
| 31  | 3     | 51    | 0        | 60       | 21      | 0            |
| 31  | B     | 61    | 0        | 83       | 17      | 0            |
| 32  | F     | 41    | 0        | 56       | 19      | 0            |
| 33  | 1     | 35    | 0        | 46       | 7       | 0            |
| 33  | 4     | 70    | 0        | 92       | 9       | 0            |
| 33  | F     | 35    | 0        | 46       | 5       | 0            |
| 33  | G     | 35    | 0        | 46       | 10      | 0            |
| 34  | F     | 35    | 0        | 40       | 1       | 0            |
| 34  | J     | 29    | 0        | 28       | 10      | 0            |
| 35  | J     | 49    | 0        | 0        | 2       | 0            |
| 36  | 5     | 42    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 36  | J     | 42    | 0        | 0        | 2       | 0            |
| 37  | K     | 14    | 0        | 23       | 8       | 0            |
| 38  | 1     | 84    | 0        | 112      | 26      | 0            |
| 38  | 3     | 84    | 0        | 112      | 28      | 0            |
| 38  | 4     | 84    | 0        | 112      | 34      | 0            |
| 38  | 5     | 84    | 0        | 112      | 32      | 0            |
| 38  | 6     | 84    | 0        | 112      | 24      | 0            |
| 38  | 7     | 84    | 0        | 112      | 29      | 0            |
| 38  | 8     | 84    | 0        | 112      | 28      | 0            |
| 38  | 9     | 84    | 0        | 112      | 33      | 0            |
| 38  | Z     | 84    | 0        | 112      | 36      | 0            |
| 39  | 1     | 48    | 0        | 32       | 8       | 0            |
| 39  | 2     | 51    | 0        | 36       | 8       | 0            |
| 39  | 3     | 66    | 0        | 69       | 14      | 0            |
| 39  | 4     | 192   | 0        | 130      | 42      | 0            |
| 39  | 5     | 160   | 0        | 134      | 31      | 0            |
| 39  | 6     | 206   | 0        | 156      | 51      | 0            |
| 39  | 7     | 54    | 0        | 42       | 9       | 0            |
| 39  | 8     | 180   | 0        | 165      | 44      | 0            |
| 39  | 9     | 108   | 0        | 95       | 35      | 0            |
| 39  | Z     | 99    | 0        | 68       | 23      | 0            |
| 40  | 1     | 48    | 0        | 62       | 12      | 0            |
| 41  | 5     | 23    | 0        | 19       | 3       | 0            |
| 41  | 6     | 29    | 0        | 31       | 5       | 0            |
| 41  | 7     | 39    | 0        | 51       | 14      | 0            |
| 41  | 8     | 30    | 0        | 33       | 4       | 0            |
| 42  | 7     | 42    | 0        | 74       | 12      | 0            |
| 43  | 8     | 30    | 0        | 43       | 7       | 0            |
| 44  | 1     | 1     | 0        | 0        | 0       | 0            |
| 44  | 2     | 1     | 0        | 0        | 0       | 0            |
| 44  | 3     | 2     | 0        | 0        | 1       | 0            |
| 44  | 4     | 5     | 0        | 0        | 0       | 0            |
| 44  | 5     | 5     | 0        | 0        | 0       | 0            |
| 44  | 6     | 3     | 0        | 0        | 0       | 0            |
| 44  | 7     | 4     | 0        | 0        | 0       | 0            |
| 44  | 8     | 4     | 0        | 0        | 0       | 0            |
| 44  | A     | 19    | 0        | 0        | 0       | 0            |
| 44  | B     | 17    | 0        | 0        | 0       | 0            |
| 44  | F     | 3     | 0        | 0        | 0       | 0            |
| 44  | I     | 1     | 0        | 0        | 0       | 0            |
| 44  | J     | 1     | 0        | 0        | 0       | 0            |
| 44  | K     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 44  | Z     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 50057 | 0        | 49449    | 4006    | 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 40.

All (4006) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:6:238:ASP:HA   | 18:6:243:LYS:HA    | 1.26                     | 1.13              |
| 24:3:306:BCR:H21C | 22:3:318:CLA:H91   | 1.25                     | 1.06              |
| 24:5:304:BCR:H19C | 22:5:319:CLA:HBA2  | 1.40                     | 1.04              |
| 19:9:53:PRO:HD2   | 38:9:302:LUT:H23   | 1.42                     | 1.02              |
| 38:6:304:LUT:H28  | 22:6:310:CLA:H61   | 1.39                     | 1.02              |
| 17:5:175:SER:HB3  | 22:5:307:CLA:HAA2  | 1.37                     | 1.00              |
| 12:Z:72:GLU:HG2   | 12:Z:151:ILE:HG12  | 1.45                     | 0.99              |
| 38:7:302:LUT:H32  | 22:7:307:CLA:HAB   | 1.44                     | 0.98              |
| 18:6:127:LYS:HG3  | 22:6:302:CLA:HED3  | 1.43                     | 0.98              |
| 2:B:560:CYS:HG    | 29:B:802:SF4:FE4   | 0.70                     | 0.98              |
| 22:5:309:CLA:HBD  | 22:5:309:CLA:HBA1  | 1.46                     | 0.97              |
| 22:A:817:CLA:HAB  | 24:K:206:BCR:HC32  | 1.42                     | 0.97              |
| 22:B:810:CLA:H61  | 24:I:4001:BCR:HC31 | 1.45                     | 0.97              |
| 15:8:52:PRO:HD2   | 38:8:303:LUT:H23   | 1.46                     | 0.97              |
| 22:B:811:CLA:HHC  | 22:B:811:CLA:HBB1  | 1.47                     | 0.96              |
| 16:4:198:ASP:HA   | 38:4:802:LUT:H24   | 1.47                     | 0.95              |
| 22:B:840:CLA:H161 | 24:I:4001:BCR:H19C | 1.49                     | 0.95              |
| 1:A:307:VAL:HA    | 24:A:856:BCR:H17C  | 1.45                     | 0.95              |
| 22:6:309:CLA:H71  | 25:6:323:LHG:H341  | 1.48                     | 0.95              |
| 22:B:811:CLA:HBA2 | 22:B:829:CLA:HBD   | 1.45                     | 0.95              |
| 22:3:310:CLA:HBD  | 22:3:310:CLA:HBA1  | 1.43                     | 0.94              |
| 22:7:306:CLA:H91  | 22:7:306:CLA:H142  | 1.45                     | 0.94              |
| 38:9:301:LUT:H30  | 22:9:303:CLA:H52   | 1.47                     | 0.94              |
| 17:5:58:LEU:HD13  | 38:5:303:LUT:H222  | 1.49                     | 0.93              |
| 22:7:306:CLA:HBD  | 22:7:306:CLA:HBA1  | 1.48                     | 0.93              |
| 3:C:73:SER:H      | 3:C:76:SER:HB3     | 1.32                     | 0.93              |
| 20:2:221:ILE:HG23 | 20:2:227:LEU:HD21  | 1.50                     | 0.93              |
| 22:A:808:CLA:HHC  | 22:A:808:CLA:HBB1  | 1.51                     | 0.93              |
| 22:5:311:CLA:H71  | 22:5:323:CLA:HAB   | 1.51                     | 0.92              |
| 22:B:838:CLA:H202 | 32:F:306:RRX:H34   | 1.49                     | 0.92              |
| 6:F:204:VAL:HG13  | 22:8:309:CLA:H2    | 1.49                     | 0.92              |
| 12:1:158:ASP:HA   | 38:1:302:LUT:H24   | 1.50                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:575:CYS:HG    | 29:B:802:SF4:FE3  | 0.69                     | 0.92              |
| 22:A:837:CLA:HHC  | 22:A:837:CLA:HBB1 | 1.50                     | 0.92              |
| 22:1:310:CLA:HBB1 | 22:1:310:CLA:HHC  | 1.52                     | 0.92              |
| 22:B:814:CLA:HAA1 | 7:G:81:LEU:HB3    | 1.52                     | 0.92              |
| 1:A:212:SER:HB3   | 24:A:844:BCR:H363 | 1.52                     | 0.91              |
| 22:B:823:CLA:HHC  | 22:B:823:CLA:HBB1 | 1.52                     | 0.91              |
| 2:B:348:LEU:HD11  | 22:B:828:CLA:HAA2 | 1.50                     | 0.91              |
| 22:F:302:CLA:HHC  | 22:F:302:CLA:HBB1 | 1.50                     | 0.91              |
| 22:B:814:CLA:HBA1 | 19:9:54:LEU:HB3   | 1.51                     | 0.91              |
| 22:4:809:CLA:HHC  | 22:4:809:CLA:HBB1 | 1.51                     | 0.91              |
| 22:6:314:CLA:HHC  | 22:6:314:CLA:HBB1 | 1.53                     | 0.90              |
| 22:8:306:CLA:HBB1 | 22:8:306:CLA:HHC  | 1.52                     | 0.90              |
| 2:B:210:TRP:HB2   | 25:B:851:LHG:HC5  | 1.54                     | 0.90              |
| 22:B:825:CLA:H92  | 22:B:825:CLA:H2   | 1.54                     | 0.90              |
| 22:B:805:CLA:HBB1 | 22:B:805:CLA:HHC  | 1.55                     | 0.89              |
| 5:E:78:GLN:HB3    | 5:E:84:THR:HG22   | 1.54                     | 0.89              |
| 22:A:824:CLA:H2   | 22:A:835:CLA:H171 | 1.54                     | 0.89              |
| 22:A:823:CLA:HBB1 | 22:A:823:CLA:HHC  | 1.54                     | 0.89              |
| 22:B:827:CLA:H151 | 22:B:842:CLA:H161 | 1.55                     | 0.89              |
| 2:B:382:PHE:HB3   | 22:B:809:CLA:H112 | 1.54                     | 0.89              |
| 22:A:802:CLA:H13  | 22:A:828:CLA:H143 | 1.53                     | 0.88              |
| 22:A:824:CLA:HMD3 | 22:A:825:CLA:HAB  | 1.56                     | 0.88              |
| 24:B:844:BCR:H362 | 24:G:203:BCR:H312 | 1.56                     | 0.88              |
| 22:1:305:CLA:HHC  | 22:1:305:CLA:HBB1 | 1.53                     | 0.88              |
| 13:3:195:VAL:HG11 | 38:3:303:LUT:H12  | 1.56                     | 0.88              |
| 22:B:833:CLA:H8   | 32:F:306:RRX:H27  | 1.56                     | 0.88              |
| 22:6:317:CLA:HED2 | 22:6:317:CLA:H2A  | 1.52                     | 0.88              |
| 12:Z:145:THR:HA   | 12:Z:150:ARG:HH21 | 1.39                     | 0.87              |
| 24:3:304:BCR:H281 | 22:5:301:CLA:HAB  | 1.57                     | 0.87              |
| 22:B:821:CLA:H151 | 22:B:826:CLA:H172 | 1.57                     | 0.87              |
| 24:5:305:BCR:H321 | 24:5:305:BCR:HC8  | 1.56                     | 0.87              |
| 14:7:205:LEU:HD13 | 22:7:308:CLA:HBB2 | 1.55                     | 0.87              |
| 16:4:95:TRP:HZ2   | 22:4:815:CLA:HAA2 | 1.38                     | 0.87              |
| 22:Z:316:CLA:HHC  | 22:Z:316:CLA:HBB1 | 1.55                     | 0.87              |
| 22:7:312:CLA:HHC  | 22:7:312:CLA:HBB1 | 1.57                     | 0.87              |
| 6:F:79:ARG:HG2    | 6:F:115:PHE:HZ    | 1.40                     | 0.86              |
| 38:3:302:LUT:H361 | 22:3:308:CLA:H143 | 1.57                     | 0.86              |
| 12:1:35:TRP:HH2   | 40:1:318:SQD:H2   | 1.40                     | 0.86              |
| 13:3:55:TRP:HZ2   | 22:3:318:CLA:HAA2 | 1.40                     | 0.86              |
| 18:6:247:PRO:HB2  | 22:6:301:CLA:H11  | 1.56                     | 0.86              |
| 19:9:81:VAL:HG11  | 38:9:301:LUT:H12  | 1.57                     | 0.86              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:3:203:VAL:HG22 | 31:3:301:DGD:HB62  | 1.58                     | 0.86              |
| 22:A:820:CLA:HHC  | 22:A:820:CLA:HBB1  | 1.56                     | 0.86              |
| 22:A:836:CLA:H61  | 22:K:203:CLA:HBA2  | 1.58                     | 0.86              |
| 22:B:810:CLA:HMB2 | 24:I:4001:BCR:H322 | 1.58                     | 0.85              |
| 3:C:14:CYS:SG     | 29:C:102:SF4:FE3   | 1.68                     | 0.85              |
| 12:Z:149:LYS:HB3  | 22:Z:313:CLA:HBC1  | 1.57                     | 0.85              |
| 20:2:197:ASN:HA   | 22:2:301:CLA:HBA2  | 1.58                     | 0.85              |
| 10:K:59:ARG:HA    | 10:K:69:ASP:HA     | 1.58                     | 0.85              |
| 15:8:55:LEU:HD12  | 38:8:303:LUT:H221  | 1.57                     | 0.85              |
| 22:4:807:CLA:HBD  | 22:4:807:CLA:HBA1  | 1.59                     | 0.85              |
| 22:6:309:CLA:HBD  | 22:6:309:CLA:HBA1  | 1.56                     | 0.85              |
| 22:A:835:CLA:H102 | 24:A:847:BCR:H20C  | 1.59                     | 0.85              |
| 22:B:840:CLA:H2   | 22:B:841:CLA:H121  | 1.59                     | 0.85              |
| 22:A:803:CLA:HHC  | 22:A:803:CLA:HBB1  | 1.58                     | 0.84              |
| 22:B:808:CLA:HBA1 | 22:B:815:CLA:HBA1  | 1.57                     | 0.84              |
| 15:8:169:ASP:HB2  | 22:8:305:CLA:HBD   | 1.57                     | 0.84              |
| 24:A:856:BCR:HC41 | 31:3:301:DGD:HAT1  | 1.58                     | 0.84              |
| 2:B:345:ILE:HD11  | 22:B:820:CLA:H122  | 1.59                     | 0.84              |
| 24:B:853:BCR:HC21 | 22:L:202:CLA:H62   | 1.60                     | 0.84              |
| 22:8:307:CLA:HBD  | 22:8:307:CLA:HBA1  | 1.59                     | 0.84              |
| 24:B:853:BCR:H11C | 22:L:202:CLA:HAB   | 1.58                     | 0.84              |
| 11:L:131:ALA:HB1  | 24:L:204:BCR:H19C  | 1.57                     | 0.84              |
| 22:L:201:CLA:HHC  | 22:L:201:CLA:HBB1  | 1.57                     | 0.84              |
| 17:5:227:TRP:HB3  | 22:5:309:CLA:H2    | 1.58                     | 0.84              |
| 17:5:109:LEU:HD21 | 22:5:319:CLA:HAC1  | 1.57                     | 0.84              |
| 22:G:201:CLA:HBB1 | 22:G:201:CLA:HHC   | 1.57                     | 0.83              |
| 22:B:827:CLA:H8   | 22:B:839:CLA:HMD2  | 1.58                     | 0.83              |
| 38:9:302:LUT:H28  | 22:9:306:CLA:H52   | 1.58                     | 0.83              |
| 39:9:312:CHL:HBC2 | 39:9:312:CHL:HMC   | 1.60                     | 0.83              |
| 1:A:496:GLN:HG3   | 1:A:497:LEU:HG     | 1.59                     | 0.83              |
| 6:F:204:VAL:HG22  | 22:8:309:CLA:H72   | 1.60                     | 0.83              |
| 12:Z:73:SER:HB2   | 22:Z:314:CLA:HED3  | 1.61                     | 0.83              |
| 22:A:825:CLA:H193 | 22:A:825:CLA:H13   | 1.61                     | 0.83              |
| 22:3:320:CLA:HMD1 | 41:7:319:3PH:H342  | 1.58                     | 0.83              |
| 18:6:110:ILE:HD13 | 24:6:306:BCR:HC8   | 1.59                     | 0.83              |
| 13:3:82:LYS:HZ2   | 13:3:210:TYR:HB3   | 1.42                     | 0.83              |
| 18:6:54:PRO:HD2   | 38:6:304:LUT:H23   | 1.59                     | 0.83              |
| 18:6:249:LEU:HG   | 24:6:306:BCR:H291  | 1.61                     | 0.82              |
| 17:5:170:ASP:HA   | 38:5:302:LUT:H24   | 1.59                     | 0.82              |
| 38:5:303:LUT:H28  | 22:5:310:CLA:H52   | 1.61                     | 0.82              |
| 22:6:301:CLA:H122 | 39:6:315:CHL:H43   | 1.62                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:29:TRP:HE1    | 22:A:811:CLA:CHB  | 1.93                     | 0.82              |
| 22:B:814:CLA:HHC  | 22:B:814:CLA:HBB1 | 1.59                     | 0.82              |
| 22:A:829:CLA:H2   | 24:A:845:BCR:HC7  | 1.59                     | 0.81              |
| 18:6:222:VAL:HG12 | 18:6:225:GLN:H    | 1.45                     | 0.81              |
| 1:A:338:HIS:HE1   | 25:A:849:LHG:HC12 | 1.45                     | 0.81              |
| 22:A:812:CLA:HBB1 | 22:A:812:CLA:HHC  | 1.62                     | 0.81              |
| 22:B:841:CLA:HAC2 | 24:B:849:BCR:H24C | 1.62                     | 0.81              |
| 12:Z:215:PHE:HB3  | 22:Z:305:CLA:H11  | 1.60                     | 0.81              |
| 22:1:314:CLA:H172 | 22:1:314:CLA:H91  | 1.62                     | 0.81              |
| 3:C:14:CYS:HG     | 29:C:102:SF4:FE3  | 0.96                     | 0.81              |
| 22:A:821:CLA:H101 | 24:A:847:BCR:H10C | 1.63                     | 0.81              |
| 24:A:844:BCR:H362 | 24:A:845:BCR:H21C | 1.62                     | 0.80              |
| 15:8:163:TYR:HB3  | 22:8:305:CLA:HED3 | 1.63                     | 0.80              |
| 22:3:316:CLA:HHC  | 22:3:316:CLA:HBB1 | 1.61                     | 0.80              |
| 11:L:119:LEU:O    | 22:L:201:CLA:H112 | 1.80                     | 0.80              |
| 40:1:318:SQD:H192 | 39:8:301:CHL:HMA1 | 1.64                     | 0.80              |
| 22:B:819:CLA:H92  | 22:B:828:CLA:HAB  | 1.63                     | 0.80              |
| 17:5:57:PRO:HD2   | 38:5:303:LUT:H23  | 1.63                     | 0.80              |
| 22:A:807:CLA:HMB3 | 22:A:808:CLA:HHB  | 1.64                     | 0.80              |
| 2:B:560:CYS:SG    | 29:B:802:SF4:FE4  | 1.74                     | 0.80              |
| 22:B:813:CLA:HMB3 | 22:B:813:CLA:HBB1 | 1.64                     | 0.79              |
| 22:B:830:CLA:HHC  | 22:B:830:CLA:HBB1 | 1.62                     | 0.79              |
| 15:8:127:GLY:HA3  | 39:8:301:CHL:H12  | 1.63                     | 0.79              |
| 16:4:83:PRO:HD2   | 38:4:803:LUT:H23  | 1.63                     | 0.79              |
| 19:9:56:LEU:HD11  | 38:9:302:LUT:H221 | 1.64                     | 0.79              |
| 14:7:104:GLU:HA   | 39:7:313:CHL:HED3 | 1.64                     | 0.79              |
| 22:A:840:CLA:HBC2 | 24:F:303:BCR:H21C | 1.63                     | 0.79              |
| 1:A:338:HIS:HA    | 1:A:426:LEU:HD11  | 1.62                     | 0.79              |
| 12:1:36:LEU:HD11  | 40:1:318:SQD:H172 | 1.65                     | 0.79              |
| 22:B:840:CLA:H172 | 22:B:841:CLA:H91  | 1.65                     | 0.79              |
| 12:1:86:ALA:HB1   | 22:1:304:CLA:H172 | 1.64                     | 0.78              |
| 24:3:305:BCR:H21C | 22:3:313:CLA:HAC1 | 1.63                     | 0.78              |
| 14:7:115:HIS:HB2  | 15:8:225:LEU:HD11 | 1.66                     | 0.78              |
| 22:Z:308:CLA:H61  | 22:Z:315:CLA:HAA2 | 1.65                     | 0.78              |
| 15:8:128:PHE:CE1  | 24:8:304:BCR:H10C | 2.18                     | 0.78              |
| 16:4:154:MET:HA   | 16:4:154:MET:HE2  | 1.66                     | 0.78              |
| 24:A:844:BCR:H23C | 24:3:306:BCR:H333 | 1.63                     | 0.78              |
| 24:6:306:BCR:H382 | 22:6:319:CLA:H112 | 1.65                     | 0.78              |
| 22:B:820:CLA:HBB1 | 22:B:820:CLA:HMB3 | 1.64                     | 0.78              |
| 22:A:814:CLA:H121 | 22:A:816:CLA:CAB  | 2.13                     | 0.78              |
| 19:9:142:PHE:HB3  | 19:9:143:PRO:HD2  | 1.65                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:4:802:LUT:H30  | 22:4:805:CLA:H52  | 1.65                     | 0.78              |
| 22:A:822:CLA:HMB1 | 22:A:822:CLA:HBB1 | 1.66                     | 0.78              |
| 22:A:832:CLA:H18  | 22:L:202:CLA:H18  | 1.65                     | 0.78              |
| 22:A:841:CLA:HBA2 | 25:A:850:LHG:H161 | 1.64                     | 0.78              |
| 25:1:317:LHG:H101 | 24:8:304:BCR:H313 | 1.65                     | 0.77              |
| 22:A:823:CLA:H111 | 24:A:856:BCR:H401 | 1.66                     | 0.77              |
| 22:B:828:CLA:HBB1 | 22:B:828:CLA:HHC  | 1.66                     | 0.77              |
| 7:G:94:PRO:HG2    | 22:G:202:CLA:HBC2 | 1.65                     | 0.77              |
| 22:4:810:CLA:HMA2 | 39:4:816:CHL:C3C  | 2.14                     | 0.77              |
| 22:A:814:CLA:H121 | 22:A:816:CLA:HAB  | 1.65                     | 0.77              |
| 2:B:543:ARG:HB2   | 2:B:552:LYS:HB3   | 1.65                     | 0.77              |
| 24:3:307:BCR:H311 | 22:3:315:CLA:HHB  | 1.66                     | 0.77              |
| 38:7:302:LUT:H28  | 22:7:307:CLA:H61  | 1.65                     | 0.77              |
| 6:F:142:LYS:HG3   | 33:F:307:LMT:H2'  | 1.66                     | 0.77              |
| 14:7:133:TRP:CD1  | 24:7:303:BCR:H12C | 2.18                     | 0.77              |
| 22:B:813:CLA:H11  | 22:9:307:CLA:H61  | 1.67                     | 0.77              |
| 12:Z:153:PRO:HD3  | 22:Z:313:CLA:HMD1 | 1.65                     | 0.77              |
| 12:Z:206:HIS:HB2  | 22:Z:305:CLA:HAA2 | 1.65                     | 0.77              |
| 22:7:309:CLA:H52  | 22:7:316:CLA:HBD  | 1.65                     | 0.77              |
| 12:Z:173:LYS:HD3  | 22:Z:304:CLA:HAA2 | 1.67                     | 0.77              |
| 2:B:284:ILE:HA    | 22:B:818:CLA:H172 | 1.67                     | 0.77              |
| 24:3:307:BCR:H312 | 22:3:315:CLA:HMB3 | 1.67                     | 0.77              |
| 16:4:133:PRO:HG2  | 16:4:136:GLU:HB2  | 1.66                     | 0.77              |
| 2:B:227:TRP:HH2   | 22:B:817:CLA:H71  | 1.50                     | 0.77              |
| 17:5:218:HIS:CG   | 22:5:309:CLA:HAA1 | 2.19                     | 0.77              |
| 24:6:306:BCR:H16C | 39:6:315:CHL:CHD  | 2.14                     | 0.77              |
| 22:6:307:CLA:HBB1 | 22:6:308:CLA:HAA1 | 1.65                     | 0.77              |
| 38:Z:301:LUT:H28  | 22:Z:303:CLA:H2   | 1.65                     | 0.77              |
| 24:B:844:BCR:H272 | 24:B:846:BCR:HC31 | 1.67                     | 0.76              |
| 16:4:108:MET:HE2  | 16:4:218:ALA:HB2  | 1.67                     | 0.76              |
| 22:5:322:CLA:HMB1 | 22:5:322:CLA:HBB1 | 1.66                     | 0.76              |
| 22:A:840:CLA:H111 | 22:A:840:CLA:HAB  | 1.66                     | 0.76              |
| 7:G:59:ARG:HG2    | 7:G:63:ARG:HE     | 1.48                     | 0.76              |
| 25:4:820:LHG:H191 | 22:6:321:CLA:HBA2 | 1.65                     | 0.76              |
| 38:6:303:LUT:H403 | 22:6:307:CLA:H122 | 1.66                     | 0.76              |
| 22:B:814:CLA:C4D  | 22:B:814:CLA:H2   | 2.15                     | 0.76              |
| 22:5:322:CLA:H61  | 22:6:310:CLA:H193 | 1.66                     | 0.76              |
| 39:9:312:CHL:HHC  | 39:9:312:CHL:HBB1 | 1.67                     | 0.76              |
| 22:A:854:CLA:H152 | 22:L:201:CLA:HBC1 | 1.65                     | 0.76              |
| 22:B:836:CLA:HBC2 | 31:1:319:DGD:HA32 | 1.68                     | 0.76              |
| 23:B:843:PQN:H221 | 24:B:849:BCR:H17C | 1.66                     | 0.76              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:1:35:TRP:CH2   | 40:1:318:SQD:H2    | 2.20                     | 0.76              |
| 22:3:309:CLA:HBB1 | 22:3:309:CLA:HMB3  | 1.67                     | 0.76              |
| 39:6:316:CHL:CHB  | 39:6:318:CHL:H71   | 2.16                     | 0.76              |
| 24:A:848:BCR:H372 | 2:B:439:VAL:HG21   | 1.65                     | 0.76              |
| 22:B:841:CLA:HBD  | 23:B:843:PQN:H302  | 1.68                     | 0.76              |
| 22:6:317:CLA:HBB1 | 22:6:317:CLA:HMB3  | 1.66                     | 0.76              |
| 19:9:79:MET:HG2   | 22:9:308:CLA:HAB   | 1.67                     | 0.76              |
| 8:I:83:THR:HG21   | 24:I:4001:BCR:HC42 | 1.68                     | 0.76              |
| 12:1:152:TYR:HB3  | 22:1:304:CLA:HED2  | 1.66                     | 0.76              |
| 18:6:75:ALA:HB1   | 18:6:178:GLY:HA3   | 1.67                     | 0.76              |
| 20:2:177:VAL:HG21 | 22:2:304:CLA:CMD   | 2.16                     | 0.76              |
| 22:B:834:CLA:HBA2 | 24:J:104:BCR:H272  | 1.68                     | 0.76              |
| 12:Z:203:LEU:HB2  | 38:Z:301:LUT:H22   | 1.68                     | 0.76              |
| 31:3:301:DGD:HAE2 | 24:3:306:BCR:H10C  | 1.66                     | 0.76              |
| 22:7:309:CLA:HBB1 | 22:7:309:CLA:HMB3  | 1.68                     | 0.76              |
| 6:F:204:VAL:HA    | 22:8:309:CLA:H51   | 1.68                     | 0.76              |
| 13:3:55:TRP:CZ2   | 22:3:318:CLA:HAA2  | 2.19                     | 0.76              |
| 18:6:46:LEU:H     | 18:6:46:LEU:HD12   | 1.50                     | 0.76              |
| 22:A:804:CLA:HBA2 | 22:A:811:CLA:H92   | 1.66                     | 0.75              |
| 11:L:132:LEU:HB3  | 11:L:171:THR:HG22  | 1.68                     | 0.75              |
| 15:8:80:VAL:HG11  | 38:8:302:LUT:H12   | 1.68                     | 0.75              |
| 11:L:132:LEU:HD21 | 24:L:204:BCR:H383  | 1.68                     | 0.75              |
| 16:4:136:GLU:HA   | 39:4:813:CHL:HED2  | 1.67                     | 0.75              |
| 17:5:241:ASP:HA   | 17:5:246:THR:HA    | 1.69                     | 0.75              |
| 19:9:32:LEU:HD22  | 19:9:33:PRO:HD2    | 1.69                     | 0.75              |
| 12:Z:190:ALA:HB2  | 22:Z:316:CLA:H61   | 1.68                     | 0.75              |
| 38:Z:301:LUT:H30  | 22:Z:303:CLA:H52   | 1.67                     | 0.75              |
| 22:3:313:CLA:H43  | 22:5:320:CLA:HED2  | 1.68                     | 0.75              |
| 22:B:827:CLA:H143 | 22:B:842:CLA:H18   | 1.67                     | 0.75              |
| 39:5:316:CHL:HMC  | 22:5:319:CLA:HAB   | 1.66                     | 0.75              |
| 22:A:842:CLA:HMB1 | 24:A:846:BCR:H12C  | 1.69                     | 0.75              |
| 2:B:86:ARG:NH2    | 2:B:107:ARG:HB2    | 2.02                     | 0.75              |
| 24:B:847:BCR:H323 | 33:1:301:LMT:H102  | 1.67                     | 0.75              |
| 22:F:305:CLA:HMB3 | 22:F:305:CLA:HBB1  | 1.69                     | 0.75              |
| 17:5:159:ASN:HA   | 17:5:165:PRO:HA    | 1.69                     | 0.75              |
| 2:B:351:GLN:HG3   | 22:B:827:CLA:HED2  | 1.68                     | 0.75              |
| 11:L:120:SER:HA   | 22:L:201:CLA:H71   | 1.69                     | 0.74              |
| 22:1:306:CLA:H152 | 25:1:317:LHG:HC92  | 1.69                     | 0.74              |
| 13:3:37:ASP:HA    | 38:3:303:LUT:H24   | 1.70                     | 0.74              |
| 22:B:825:CLA:HBB2 | 22:B:842:CLA:H61   | 1.70                     | 0.74              |
| 39:1:312:CHL:HAA2 | 31:1:319:DGD:HG31  | 1.67                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:820:CLA:H102 | 22:A:820:CLA:H142 | 1.69                     | 0.74              |
| 22:B:833:CLA:HBC2 | 22:B:839:CLA:HMC3 | 1.69                     | 0.74              |
| 12:Z:51:GLY:HA3   | 12:Z:175:ILE:HD13 | 1.69                     | 0.74              |
| 39:Z:311:CHL:HBC3 | 39:Z:311:CHL:HHD  | 1.68                     | 0.74              |
| 1:A:575:CYS:SG    | 29:B:802:SF4:FE3  | 1.79                     | 0.74              |
| 2:B:86:ARG:HH21   | 2:B:107:ARG:HB2   | 1.52                     | 0.74              |
| 13:3:165:ASN:HA   | 38:3:302:LUT:H24  | 1.69                     | 0.74              |
| 14:7:205:LEU:HD11 | 22:7:307:CLA:H202 | 1.69                     | 0.74              |
| 22:8:313:CLA:HMA2 | 39:8:315:CHL:H52  | 1.68                     | 0.74              |
| 22:A:854:CLA:HBB2 | 2:B:659:ALA:HB3   | 1.70                     | 0.74              |
| 22:3:310:CLA:HBA1 | 22:3:310:CLA:CBD  | 2.17                     | 0.74              |
| 22:A:802:CLA:HAB  | 2:B:583:TRP:CH2   | 2.23                     | 0.74              |
| 22:B:838:CLA:H171 | 32:F:306:RRX:H38  | 1.68                     | 0.74              |
| 12:Z:68:LYS:HD2   | 12:Z:147:ALA:HB1  | 1.69                     | 0.74              |
| 1:A:363:LEU:HD11  | 22:A:819:CLA:H111 | 1.68                     | 0.74              |
| 34:J:101:LMG:HC91 | 34:J:101:LMG:H121 | 1.70                     | 0.74              |
| 1:A:676:HIS:HB2   | 22:A:802:CLA:HBA1 | 1.70                     | 0.73              |
| 22:A:822:CLA:HBA2 | 22:A:823:CLA:H72  | 1.70                     | 0.73              |
| 22:A:836:CLA:HMB1 | 24:A:847:BCR:H281 | 1.70                     | 0.73              |
| 11:L:140:PHE:HA   | 11:L:144:PRO:HD2  | 1.70                     | 0.73              |
| 12:Z:162:PHE:HB2  | 22:Z:303:CLA:CGA  | 2.18                     | 0.73              |
| 22:A:838:CLA:HBB1 | 22:A:838:CLA:HMB3 | 1.70                     | 0.73              |
| 22:A:840:CLA:H121 | 22:F:305:CLA:HAC1 | 1.70                     | 0.73              |
| 22:Z:304:CLA:NA   | 22:Z:309:CLA:H71  | 2.03                     | 0.73              |
| 14:7:68:MET:HE1   | 22:7:308:CLA:H2   | 1.70                     | 0.73              |
| 22:5:320:CLA:HAC2 | 41:5:325:3PH:H232 | 1.70                     | 0.73              |
| 22:4:807:CLA:H102 | 25:4:820:LHG:H162 | 1.68                     | 0.73              |
| 22:6:314:CLA:H92  | 25:6:323:LHG:H152 | 1.71                     | 0.73              |
| 22:5:322:CLA:H143 | 22:6:310:CLA:H101 | 1.71                     | 0.73              |
| 22:3:320:CLA:HMA3 | 22:3:322:CLA:H112 | 1.69                     | 0.73              |
| 22:4:818:CLA:H2   | 22:4:818:CLA:HBA1 | 1.71                     | 0.73              |
| 22:B:825:CLA:HBA2 | 24:B:847:BCR:H14C | 1.71                     | 0.73              |
| 39:4:816:CHL:HMB1 | 39:4:816:CHL:HBB1 | 1.70                     | 0.73              |
| 2:B:26:LEU:HD21   | 24:L:204:BCR:H332 | 1.71                     | 0.73              |
| 10:K:59:ARG:CA    | 10:K:69:ASP:HA    | 2.19                     | 0.73              |
| 31:3:301:DGD:HB21 | 31:3:301:DGD:HG31 | 1.71                     | 0.73              |
| 14:7:174:ASP:HA   | 38:7:301:LUT:H24  | 1.70                     | 0.73              |
| 24:5:304:BCR:H353 | 39:5:317:CHL:HBB1 | 1.69                     | 0.73              |
| 39:6:320:CHL:HHC  | 39:6:320:CHL:HBB1 | 1.70                     | 0.73              |
| 19:9:100:GLY:HA2  | 39:9:314:CHL:HAC2 | 1.70                     | 0.73              |
| 22:A:840:CLA:H91  | 22:F:305:CLA:HAC2 | 1.71                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:3:305:BCR:H321 | 24:3:305:BCR:HC8  | 1.69                     | 0.72              |
| 22:7:322:CLA:H61  | 22:7:323:CLA:H72  | 1.70                     | 0.72              |
| 15:8:125:MET:HE2  | 24:8:304:BCR:H15C | 1.71                     | 0.72              |
| 24:4:804:BCR:H272 | 22:4:810:CLA:H2   | 1.69                     | 0.72              |
| 22:A:823:CLA:H191 | 10:K:98:ILE:HD12  | 1.71                     | 0.72              |
| 12:Z:182:MET:HE3  | 22:Z:306:CLA:HMC2 | 1.71                     | 0.72              |
| 2:B:569:CYS:SG    | 29:B:802:SF4:FE1  | 1.81                     | 0.72              |
| 22:B:815:CLA:HMB3 | 22:B:815:CLA:HBB1 | 1.72                     | 0.72              |
| 20:2:177:VAL:HG21 | 22:2:304:CLA:HMD2 | 1.71                     | 0.72              |
| 22:A:815:CLA:H161 | 13:3:195:VAL:HG12 | 1.70                     | 0.72              |
| 24:6:305:BCR:H16C | 39:6:316:CHL:HMB2 | 1.70                     | 0.72              |
| 22:A:818:CLA:H62  | 22:A:818:CLA:C4C  | 2.19                     | 0.72              |
| 14:7:167:TYR:HB3  | 22:7:304:CLA:HED3 | 1.70                     | 0.72              |
| 16:4:121:ARG:HH22 | 16:4:133:PRO:HA   | 1.55                     | 0.72              |
| 22:A:822:CLA:HED1 | 10:K:70:ARG:HE    | 1.54                     | 0.72              |
| 2:B:296:PHE:O     | 7:G:88:ILE:HG13   | 1.89                     | 0.72              |
| 22:B:834:CLA:H51  | 24:F:303:BCR:HC22 | 1.72                     | 0.72              |
| 22:B:827:CLA:H192 | 22:B:842:CLA:H91  | 1.70                     | 0.72              |
| 22:5:308:CLA:HMD2 | 22:5:313:CLA:H43  | 1.70                     | 0.72              |
| 1:A:615:GLN:HG2   | 1:A:630:ILE:HD12  | 1.70                     | 0.72              |
| 22:A:806:CLA:HHC  | 22:A:806:CLA:HBB1 | 1.70                     | 0.72              |
| 22:B:840:CLA:H8   | 22:B:841:CLA:H142 | 1.70                     | 0.72              |
| 13:3:70:GLY:HA2   | 38:3:303:LUT:H181 | 1.71                     | 0.72              |
| 15:8:187:LYS:HG3  | 22:8:311:CLA:HED2 | 1.69                     | 0.72              |
| 22:B:823:CLA:H71  | 22:B:824:CLA:H112 | 1.71                     | 0.71              |
| 22:8:305:CLA:H71  | 22:8:306:CLA:HMA2 | 1.72                     | 0.71              |
| 14:7:133:TRP:CZ2  | 24:7:303:BCR:HC8  | 2.24                     | 0.71              |
| 22:B:828:CLA:H112 | 24:B:847:BCR:H373 | 1.71                     | 0.71              |
| 6:F:202:TRP:CG    | 6:F:203:PRO:HD3   | 2.25                     | 0.71              |
| 22:A:827:CLA:H192 | 22:A:835:CLA:H91  | 1.70                     | 0.71              |
| 24:F:303:BCR:H321 | 24:F:303:BCR:HC8  | 1.72                     | 0.71              |
| 22:7:306:CLA:NC   | 22:7:306:CLA:H52  | 2.05                     | 0.71              |
| 39:4:819:CHL:HBB1 | 39:4:819:CHL:HHC  | 1.73                     | 0.71              |
| 22:A:822:CLA:H2   | 22:A:823:CLA:H92  | 1.73                     | 0.71              |
| 18:6:250:PHE:H    | 22:6:301:CLA:H43  | 1.55                     | 0.71              |
| 22:A:822:CLA:HMD1 | 24:A:856:BCR:H23C | 1.72                     | 0.71              |
| 7:G:38:VAL:HG11   | 22:G:201:CLA:C4D  | 2.21                     | 0.71              |
| 13:3:120:ALA:HB1  | 24:3:304:BCR:H363 | 1.72                     | 0.71              |
| 22:B:827:CLA:CAB  | 24:B:848:BCR:H19C | 2.21                     | 0.71              |
| 10:K:31:GLY:H     | 10:K:35:ASN:HD22  | 1.37                     | 0.71              |
| 6:F:202:TRP:CD1   | 6:F:203:PRO:HD3   | 2.25                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:4:813:CHL:HAB  | 39:4:816:CHL:HBB2  | 1.72                     | 0.71              |
| 18:6:126:LEU:HD12 | 22:6:302:CLA:HBA1  | 1.72                     | 0.71              |
| 22:B:815:CLA:H152 | 22:B:830:CLA:HMD3  | 1.72                     | 0.71              |
| 12:1:45:LEU:HD21  | 22:1:307:CLA:HAA2  | 1.71                     | 0.71              |
| 15:8:85:ILE:HB    | 15:8:86:PRO:HD3    | 1.72                     | 0.71              |
| 22:F:302:CLA:H193 | 32:F:306:RRX:H21   | 1.73                     | 0.71              |
| 22:1:308:CLA:HHC  | 22:1:308:CLA:HBB1  | 1.73                     | 0.71              |
| 6:F:201:THR:HA    | 22:8:309:CLA:H152  | 1.72                     | 0.70              |
| 38:1:302:LUT:H30  | 22:1:304:CLA:H52   | 1.73                     | 0.70              |
| 12:1:92:GLU:HG2   | 12:1:98:ASN:HA     | 1.72                     | 0.70              |
| 12:Z:78:CYS:HB3   | 12:Z:178:GLY:HA3   | 1.73                     | 0.70              |
| 19:9:129:GLY:HA3  | 19:9:142:PHE:CZ    | 2.26                     | 0.70              |
| 1:A:316:TRP:HD1   | 10:K:76:LEU:HD21   | 1.55                     | 0.70              |
| 22:B:824:CLA:HAB  | 24:B:847:BCR:C10   | 2.20                     | 0.70              |
| 22:7:306:CLA:HBA1 | 22:7:306:CLA:CBD   | 2.21                     | 0.70              |
| 25:4:820:LHG:HC82 | 24:6:305:BCR:HC42  | 1.73                     | 0.70              |
| 22:A:820:CLA:HBB2 | 24:A:844:BCR:H402  | 1.73                     | 0.70              |
| 2:B:549:PRO:HB3   | 6:F:226:PRO:HG2    | 1.72                     | 0.70              |
| 2:B:719:VAL:HG21  | 31:B:852:DGD:HBV1  | 1.73                     | 0.70              |
| 16:4:200:LEU:HD12 | 38:4:802:LUT:H222  | 1.74                     | 0.70              |
| 22:Z:308:CLA:H151 | 22:Z:313:CLA:HAA2  | 1.73                     | 0.70              |
| 22:A:810:CLA:HMD1 | 22:3:312:CLA:H102  | 1.74                     | 0.70              |
| 22:A:816:CLA:HBB1 | 22:A:816:CLA:HMB3  | 1.74                     | 0.70              |
| 22:A:831:CLA:HMA2 | 11:L:57:THR:HG21   | 1.72                     | 0.70              |
| 2:B:620:TRP:O     | 2:B:624:TYR:HB3    | 1.91                     | 0.70              |
| 22:Z:304:CLA:HHC  | 22:Z:304:CLA:HBB1  | 1.72                     | 0.70              |
| 38:6:303:LUT:H371 | 22:6:307:CLA:H92   | 1.73                     | 0.70              |
| 2:B:618:MET:HG3   | 2:B:622:ARG:HH12   | 1.55                     | 0.70              |
| 22:B:815:CLA:H51  | 22:B:820:CLA:HBC3  | 1.70                     | 0.70              |
| 8:I:88:PRO:HG3    | 24:I:4001:BCR:H12C | 1.72                     | 0.70              |
| 22:4:815:CLA:HED2 | 22:4:815:CLA:H2A   | 1.72                     | 0.70              |
| 17:5:106:PRO:HB2  | 17:5:115:ASN:HA    | 1.74                     | 0.70              |
| 39:5:316:CHL:H122 | 39:5:316:CHL:H91   | 1.74                     | 0.70              |
| 1:A:45:THR:HG23   | 5:E:78:GLN:HE21    | 1.55                     | 0.70              |
| 13:3:96:VAL:HG11  | 38:3:303:LUT:H172  | 1.71                     | 0.70              |
| 22:3:308:CLA:H152 | 39:3:317:CHL:H72   | 1.73                     | 0.70              |
| 22:3:312:CLA:HHC  | 22:3:312:CLA:HBB1  | 1.74                     | 0.70              |
| 22:5:311:CLA:C7   | 22:5:323:CLA:HAB   | 2.22                     | 0.70              |
| 24:B:853:BCR:H271 | 22:L:201:CLA:HED1  | 1.73                     | 0.70              |
| 18:6:247:PRO:HG3  | 22:6:301:CLA:H111  | 1.73                     | 0.70              |
| 22:6:312:CLA:HBC3 | 22:6:312:CLA:H122  | 1.74                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:B:817:CLA:HMA2 | 24:B:846:BCR:H343 | 1.74                     | 0.69              |
| 13:3:203:VAL:HG13 | 31:3:301:DGD:HG32 | 1.74                     | 0.69              |
| 1:A:205:LEU:HA    | 24:A:845:BCR:H363 | 1.74                     | 0.69              |
| 22:F:304:CLA:HBB1 | 32:F:306:RRX:H51  | 1.74                     | 0.69              |
| 24:3:304:BCR:H281 | 22:5:301:CLA:CAB  | 2.22                     | 0.69              |
| 39:3:317:CHL:HHC  | 39:3:317:CHL:HBB1 | 1.74                     | 0.69              |
| 22:6:308:CLA:HMB3 | 22:6:308:CLA:HBB1 | 1.73                     | 0.69              |
| 33:G:204:LMT:H4'  | 22:1:314:CLA:HMA2 | 1.73                     | 0.69              |
| 22:1:307:CLA:HBB1 | 22:1:307:CLA:HMB3 | 1.74                     | 0.69              |
| 38:Z:301:LUT:H403 | 22:Z:303:CLA:H141 | 1.73                     | 0.69              |
| 39:6:316:CHL:HHC  | 39:6:316:CHL:HBB1 | 1.73                     | 0.69              |
| 13:3:103:TYR:HB3  | 13:3:106:TYR:CE2  | 2.26                     | 0.69              |
| 14:7:53:PHE:HB3   | 22:7:307:CLA:CAD  | 2.23                     | 0.69              |
| 14:7:178:PHE:HE2  | 38:7:301:LUT:H221 | 1.56                     | 0.69              |
| 15:8:104:GLY:HA2  | 39:8:315:CHL:HAC2 | 1.75                     | 0.69              |
| 22:A:809:CLA:HHC  | 22:A:809:CLA:HBB1 | 1.74                     | 0.69              |
| 22:A:830:CLA:HMB3 | 22:A:830:CLA:HBB1 | 1.73                     | 0.69              |
| 12:Z:84:GLY:HA2   | 38:Z:302:LUT:H181 | 1.75                     | 0.69              |
| 22:A:813:CLA:HBA1 | 22:A:825:CLA:H41  | 1.74                     | 0.69              |
| 22:B:809:CLA:H41  | 31:B:852:DGD:HB61 | 1.75                     | 0.69              |
| 38:8:302:LUT:H11  | 22:8:306:CLA:HMC1 | 1.75                     | 0.69              |
| 18:6:123:PHE:CZ   | 39:6:320:CHL:HBB2 | 2.28                     | 0.69              |
| 39:2:303:CHL:HHC  | 39:2:303:CHL:HBB1 | 1.73                     | 0.69              |
| 22:A:822:CLA:HAA2 | 10:K:61:THR:HG21  | 1.75                     | 0.69              |
| 13:3:203:VAL:HA   | 31:3:301:DGD:HB42 | 1.73                     | 0.69              |
| 39:5:321:CHL:HBB1 | 39:5:321:CHL:HHC  | 1.74                     | 0.69              |
| 22:1:305:CLA:HBC3 | 22:1:310:CLA:H143 | 1.74                     | 0.69              |
| 17:5:185:LYS:HD3  | 22:5:308:CLA:HAA2 | 1.75                     | 0.69              |
| 22:A:823:CLA:HAA2 | 10:K:63:ALA:O     | 1.93                     | 0.68              |
| 6:F:153:THR:HA    | 22:F:302:CLA:HAC2 | 1.75                     | 0.68              |
| 19:9:115:GLU:HA   | 39:9:314:CHL:HMA3 | 1.75                     | 0.68              |
| 1:A:157:LEU:HD11  | 27:A:852:DGA:HA81 | 1.75                     | 0.68              |
| 22:A:812:CLA:HBA1 | 22:A:812:CLA:CHA  | 2.23                     | 0.68              |
| 22:A:841:CLA:H12  | 22:A:841:CLA:NA   | 2.08                     | 0.68              |
| 22:B:824:CLA:HAB  | 24:B:847:BCR:C9   | 2.24                     | 0.68              |
| 22:A:855:CLA:H122 | 22:B:841:CLA:H141 | 1.76                     | 0.68              |
| 13:3:73:GLY:HA3   | 38:3:303:LUT:H182 | 1.76                     | 0.68              |
| 18:6:142:PRO:HB2  | 22:6:302:CLA:HMD3 | 1.75                     | 0.68              |
| 1:A:59:PHE:CD2    | 22:A:805:CLA:HMC2 | 2.28                     | 0.68              |
| 2:B:283:VAL:HG13  | 24:B:844:BCR:H363 | 1.74                     | 0.68              |
| 12:Z:152:TYR:HB3  | 22:Z:303:CLA:HED3 | 1.74                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:9:314:CHL:HBB1 | 39:9:314:CHL:HHC  | 1.74                     | 0.68              |
| 22:A:808:CLA:HBB2 | 22:A:828:CLA:H171 | 1.74                     | 0.68              |
| 22:F:301:CLA:H152 | 9:J:18:TRP:HE3    | 1.58                     | 0.68              |
| 24:4:804:BCR:H373 | 39:4:816:CHL:HHB  | 1.76                     | 0.68              |
| 18:6:64:LEU:HD12  | 22:6:310:CLA:HMA2 | 1.76                     | 0.68              |
| 22:A:807:CLA:HHB  | 22:A:808:CLA:HMB3 | 1.76                     | 0.68              |
| 22:A:807:CLA:H8   | 22:A:809:CLA:H61  | 1.73                     | 0.68              |
| 22:A:823:CLA:H152 | 24:A:856:BCR:H401 | 1.73                     | 0.68              |
| 22:B:835:CLA:HMB3 | 22:B:835:CLA:HBB1 | 1.75                     | 0.68              |
| 11:L:141:GLN:HE21 | 11:L:141:GLN:H    | 1.41                     | 0.68              |
| 22:B:817:CLA:H51  | 24:B:844:BCR:H282 | 1.75                     | 0.68              |
| 22:3:313:CLA:HMB1 | 22:3:313:CLA:HBB1 | 1.75                     | 0.68              |
| 22:A:818:CLA:H8   | 22:A:836:CLA:HMA3 | 1.74                     | 0.68              |
| 2:B:687:PRO:HG2   | 22:L:202:CLA:H52  | 1.76                     | 0.68              |
| 18:6:99:ASP:HA    | 39:6:315:CHL:O1D  | 1.94                     | 0.68              |
| 2:B:499:LEU:HA    | 2:B:502:ILE:HG22  | 1.76                     | 0.67              |
| 6:F:79:ARG:HG2    | 6:F:115:PHE:CZ    | 2.26                     | 0.67              |
| 13:3:82:LYS:HZ1   | 13:3:211:GLU:HG2  | 1.59                     | 0.67              |
| 22:5:322:CLA:H152 | 22:6:319:CLA:H71  | 1.77                     | 0.67              |
| 24:A:856:BCR:H24C | 10:K:95:LEU:HD21  | 1.76                     | 0.67              |
| 2:B:197:HIS:O     | 2:B:201:PRO:HG2   | 1.95                     | 0.67              |
| 22:B:836:CLA:HMB1 | 22:B:836:CLA:HBB1 | 1.77                     | 0.67              |
| 22:G:201:CLA:CAB  | 24:G:203:BCR:H352 | 2.24                     | 0.67              |
| 10:K:39:VAL:HG22  | 22:K:202:CLA:HBA1 | 1.75                     | 0.67              |
| 12:1:168:GLU:CD   | 12:1:168:GLU:H    | 2.02                     | 0.67              |
| 22:3:309:CLA:HMD2 | 22:3:314:CLA:H43  | 1.77                     | 0.67              |
| 39:6:315:CHL:H51  | 39:6:315:CHL:H92  | 1.77                     | 0.67              |
| 22:9:306:CLA:H71  | 22:9:307:CLA:HMA3 | 1.76                     | 0.67              |
| 22:Z:313:CLA:H101 | 22:Z:313:CLA:HBA1 | 1.76                     | 0.67              |
| 22:9:306:CLA:HMB1 | 22:9:306:CLA:HBB1 | 1.76                     | 0.67              |
| 22:A:840:CLA:H111 | 22:A:840:CLA:CAB  | 2.25                     | 0.67              |
| 22:B:833:CLA:C8   | 32:F:306:RRX:H27  | 2.24                     | 0.67              |
| 13:3:89:ILE:HD13  | 13:3:94:THR:HG22  | 1.76                     | 0.67              |
| 18:6:149:LEU:HD11 | 18:6:158:GLY:HA3  | 1.75                     | 0.67              |
| 22:A:815:CLA:HBB1 | 22:A:815:CLA:HMB1 | 1.76                     | 0.67              |
| 16:4:67:PHE:HD1   | 16:4:80:GLY:HA3   | 1.60                     | 0.67              |
| 16:4:121:ARG:HG3  | 16:4:131:GLN:HA   | 1.75                     | 0.67              |
| 23:B:843:PQN:H201 | 24:B:849:BCR:H21C | 1.76                     | 0.67              |
| 22:Z:306:CLA:H71  | 22:Z:307:CLA:HMA1 | 1.76                     | 0.67              |
| 14:7:26:TYR:HE2   | 14:7:191:GLN:HB2  | 1.59                     | 0.67              |
| 22:9:313:CLA:HHC  | 22:9:313:CLA:HBB1 | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:446:ILE:HA    | 22:A:854:CLA:CGA  | 2.25                     | 0.67              |
| 22:A:815:CLA:H43  | 24:3:306:BCR:HC21 | 1.77                     | 0.67              |
| 2:B:453:GLN:HE21  | 2:B:455:LEU:HD11  | 1.58                     | 0.67              |
| 39:5:316:CHL:HHC  | 39:5:316:CHL:HBB1 | 1.76                     | 0.67              |
| 18:6:108:PHE:HD2  | 18:6:113:LEU:HD21 | 1.60                     | 0.67              |
| 22:A:804:CLA:HAB  | 22:A:806:CLA:CAD  | 2.24                     | 0.67              |
| 7:G:91:THR:HG21   | 7:G:98:THR:HA     | 1.77                     | 0.67              |
| 7:G:99:LEU:HD12   | 7:G:99:LEU:H      | 1.60                     | 0.67              |
| 13:3:146:LEU:HD22 | 24:3:305:BCR:HC32 | 1.76                     | 0.67              |
| 22:5:309:CLA:H12  | 22:5:309:CLA:NA   | 2.09                     | 0.67              |
| 22:B:827:CLA:H2   | 22:B:839:CLA:HBD  | 1.76                     | 0.67              |
| 7:G:77:TYR:HD2    | 7:G:79:ASP:HB3    | 1.59                     | 0.67              |
| 9:J:1:MET:H2      | 34:J:101:LMG:HC2  | 1.60                     | 0.67              |
| 40:1:318:SQD:C7   | 40:1:318:SQD:H121 | 2.25                     | 0.67              |
| 17:5:85:VAL:HG11  | 38:5:302:LUT:H12  | 1.77                     | 0.67              |
| 19:9:145:ASP:H    | 19:9:146:PRO:HD2  | 1.59                     | 0.67              |
| 22:B:811:CLA:CBA  | 22:B:829:CLA:HBD  | 2.24                     | 0.66              |
| 4:D:178:ASN:HB3   | 4:D:191:THR:HG22  | 1.77                     | 0.66              |
| 12:Z:79:ARG:HA    | 12:Z:82:MET:HE3   | 1.76                     | 0.66              |
| 38:3:302:LUT:C30  | 22:3:308:CLA:H72  | 2.24                     | 0.66              |
| 22:A:822:CLA:HMB2 | 22:A:823:CLA:H2   | 1.77                     | 0.66              |
| 38:1:303:LUT:H8   | 22:1:309:CLA:HBB1 | 1.78                     | 0.66              |
| 38:Z:301:LUT:H26  | 22:Z:303:CLA:H2   | 1.76                     | 0.66              |
| 14:7:209:ALA:HB2  | 22:7:317:CLA:H8   | 1.77                     | 0.66              |
| 39:8:301:CHL:HHC  | 39:8:301:CHL:HBB1 | 1.76                     | 0.66              |
| 39:6:318:CHL:HBB1 | 39:6:318:CHL:HMB3 | 1.77                     | 0.66              |
| 22:A:810:CLA:H161 | 24:A:845:BCR:H372 | 1.77                     | 0.66              |
| 22:B:808:CLA:HBB1 | 22:B:808:CLA:HMB1 | 1.76                     | 0.66              |
| 4:D:189:ASN:HD22  | 4:D:194:ILE:HD13  | 1.59                     | 0.66              |
| 38:7:302:LUT:H28  | 22:7:307:CLA:C6   | 2.25                     | 0.66              |
| 15:8:156:PHE:CE1  | 22:8:313:CLA:HAB  | 2.30                     | 0.66              |
| 24:5:304:BCR:HC8  | 22:5:326:CLA:H72  | 1.77                     | 0.66              |
| 22:B:813:CLA:HBB1 | 22:B:813:CLA:CMB  | 2.24                     | 0.66              |
| 22:B:820:CLA:HBB1 | 22:B:820:CLA:CMB  | 2.25                     | 0.66              |
| 22:3:310:CLA:H52  | 22:3:310:CLA:NC   | 2.10                     | 0.66              |
| 18:6:62:GLU:HA    | 18:6:65:LYS:HD3   | 1.76                     | 0.66              |
| 2:B:475:PHE:HB3   | 22:F:304:CLA:H191 | 1.77                     | 0.66              |
| 22:B:831:CLA:H52  | 31:B:852:DGD:HB52 | 1.77                     | 0.66              |
| 16:4:95:TRP:CZ2   | 22:4:815:CLA:HAA2 | 2.27                     | 0.66              |
| 1:A:114:SER:HB2   | 1:A:131:VAL:HG11  | 1.77                     | 0.66              |
| 22:K:202:CLA:HBB1 | 22:K:202:CLA:HMB3 | 1.75                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:5:326:CLA:H71  | 22:6:314:CLA:H72  | 1.78                     | 0.66              |
| 1:A:722:GLN:HA    | 25:A:850:LHG:HC5  | 1.78                     | 0.66              |
| 33:G:204:LMT:H51  | 22:1:314:CLA:H2   | 1.78                     | 0.66              |
| 23:A:843:PQN:H193 | 24:F:303:BCR:H23C | 1.76                     | 0.66              |
| 2:B:89:ALA:HB2    | 2:B:117:SER:HB3   | 1.77                     | 0.66              |
| 12:1:60:LEU:HD13  | 22:1:307:CLA:H42  | 1.76                     | 0.66              |
| 22:Z:303:CLA:HBB1 | 22:Z:303:CLA:HMB1 | 1.78                     | 0.66              |
| 18:6:99:ASP:HB3   | 39:6:315:CHL:HED3 | 1.77                     | 0.66              |
| 2:B:657:VAL:HG22  | 22:B:841:CLA:HMB3 | 1.77                     | 0.66              |
| 12:1:57:PRO:HD2   | 38:1:303:LUT:H23  | 1.77                     | 0.66              |
| 15:8:63:ARG:HG2   | 15:8:137:PHE:CE2  | 2.31                     | 0.66              |
| 17:5:205:GLN:HG3  | 17:5:253:TRP:HZ3  | 1.61                     | 0.66              |
| 38:9:301:LUT:H26  | 22:9:303:CLA:O1A  | 1.95                     | 0.66              |
| 22:5:309:CLA:HBA1 | 22:5:309:CLA:CBD  | 2.24                     | 0.65              |
| 1:A:680:ALA:HB3   | 22:B:801:CLA:HBB2 | 1.77                     | 0.65              |
| 22:A:824:CLA:HBB1 | 22:A:824:CLA:HHC  | 1.78                     | 0.65              |
| 13:3:89:ILE:HG12  | 22:3:313:CLA:HED2 | 1.78                     | 0.65              |
| 14:7:49:GLY:H     | 14:7:191:GLN:HE22 | 1.44                     | 0.65              |
| 17:5:230:ASN:HA   | 17:5:233:HIS:NE2  | 2.12                     | 0.65              |
| 39:9:312:CHL:HBC3 | 39:9:312:CHL:H151 | 1.77                     | 0.65              |
| 38:3:302:LUT:H383 | 39:3:317:CHL:H11  | 1.79                     | 0.65              |
| 22:3:312:CLA:O1D  | 22:3:318:CLA:H62  | 1.96                     | 0.65              |
| 22:7:304:CLA:H101 | 22:7:310:CLA:H18  | 1.78                     | 0.65              |
| 1:A:316:TRP:CD1   | 10:K:76:LEU:HD21  | 2.31                     | 0.65              |
| 22:8:311:CLA:HHC  | 22:8:311:CLA:HBB1 | 1.79                     | 0.65              |
| 19:9:117:LEU:HD21 | 39:2:303:CHL:H2   | 1.77                     | 0.65              |
| 1:A:449:GLY:HA3   | 22:A:854:CLA:O1A  | 1.95                     | 0.65              |
| 22:A:814:CLA:HBA2 | 22:A:816:CLA:HHB  | 1.78                     | 0.65              |
| 24:F:303:BCR:H12C | 22:F:305:CLA:CAB  | 2.27                     | 0.65              |
| 15:8:41:LYS:H     | 15:8:41:LYS:HD2   | 1.61                     | 0.65              |
| 6:F:160:ALA:HB1   | 22:F:302:CLA:H8   | 1.79                     | 0.65              |
| 24:3:307:BCR:H392 | 22:3:314:CLA:HAC2 | 1.78                     | 0.65              |
| 16:4:67:PHE:CD1   | 16:4:80:GLY:HA3   | 2.31                     | 0.65              |
| 1:A:80:GLN:HG2    | 22:A:805:CLA:HMA1 | 1.78                     | 0.65              |
| 22:A:822:CLA:H71  | 22:K:204:CLA:HAB  | 1.79                     | 0.65              |
| 5:E:36:GLY:HA3    | 5:E:62:VAL:HG11   | 1.78                     | 0.65              |
| 12:Z:158:ASP:HA   | 38:Z:301:LUT:H24  | 1.79                     | 0.65              |
| 13:3:82:LYS:NZ    | 13:3:211:GLU:HG2  | 2.11                     | 0.65              |
| 2:B:463:TRP:CD1   | 22:F:304:CLA:H193 | 2.32                     | 0.65              |
| 2:B:487:ALA:O     | 2:B:491:GLN:HG3   | 1.97                     | 0.65              |
| 22:B:814:CLA:H12  | 19:9:56:LEU:HD22  | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:3:146:LEU:HD11 | 22:5:315:CLA:H171 | 1.77                     | 0.65              |
| 22:3:322:CLA:HBB2 | 22:7:307:CLA:HHD  | 1.79                     | 0.65              |
| 39:7:313:CHL:HHC  | 39:7:313:CHL:HBB1 | 1.77                     | 0.65              |
| 17:5:182:LEU:HB3  | 22:5:307:CLA:CMA  | 2.26                     | 0.65              |
| 39:5:316:CHL:H162 | 22:6:322:CLA:H193 | 1.78                     | 0.65              |
| 22:B:838:CLA:H171 | 32:F:306:RRX:C35  | 2.26                     | 0.65              |
| 15:8:55:LEU:CD1   | 38:8:303:LUT:H221 | 2.25                     | 0.65              |
| 15:8:125:MET:HB3  | 24:8:304:BCR:H15C | 1.78                     | 0.65              |
| 22:5:326:CLA:HBD  | 22:5:326:CLA:HBA1 | 1.79                     | 0.65              |
| 22:A:814:CLA:H112 | 24:A:844:BCR:H353 | 1.79                     | 0.64              |
| 22:A:833:CLA:HAB  | 22:A:834:CLA:HHB  | 1.77                     | 0.64              |
| 22:A:833:CLA:NC   | 22:A:834:CLA:H101 | 2.12                     | 0.64              |
| 39:Z:311:CHL:HHC  | 39:Z:311:CHL:HBB1 | 1.78                     | 0.64              |
| 38:4:802:LUT:H383 | 39:4:814:CHL:H12  | 1.78                     | 0.64              |
| 17:5:131:TRP:CE3  | 22:6:314:CLA:HBA2 | 2.32                     | 0.64              |
| 18:6:125:GLU:HG2  | 22:6:317:CLA:C1B  | 2.26                     | 0.64              |
| 20:2:189:HIS:CG   | 22:2:301:CLA:HAA2 | 2.33                     | 0.64              |
| 24:A:856:BCR:H323 | 24:3:306:BCR:HC41 | 1.78                     | 0.64              |
| 22:B:810:CLA:H62  | 22:B:810:CLA:NC   | 2.11                     | 0.64              |
| 22:3:320:CLA:CMA  | 22:3:322:CLA:H112 | 2.28                     | 0.64              |
| 24:8:304:BCR:H292 | 22:8:310:CLA:HBA1 | 1.80                     | 0.64              |
| 22:5:326:CLA:HMD2 | 22:6:309:CLA:H2   | 1.80                     | 0.64              |
| 7:G:57:HIS:CE1    | 7:G:61:LEU:HD11   | 2.33                     | 0.64              |
| 12:Z:61:CYS:HB2   | 22:Z:306:CLA:HBA1 | 1.80                     | 0.64              |
| 12:Z:134:MET:HG3  | 22:Z:314:CLA:HMC3 | 1.79                     | 0.64              |
| 13:3:122:GLN:O    | 13:3:126:LEU:HB2  | 1.97                     | 0.64              |
| 19:9:102:LYS:HB3  | 19:9:104:TYR:CE2  | 2.32                     | 0.64              |
| 22:B:830:CLA:H151 | 24:B:845:BCR:H15C | 1.78                     | 0.64              |
| 6:F:224:ILE:HB    | 6:F:227:ARG:HH22  | 1.61                     | 0.64              |
| 7:G:35:TYR:HB3    | 22:G:201:CLA:HED2 | 1.80                     | 0.64              |
| 38:Z:301:LUT:H382 | 22:Z:303:CLA:C4D  | 2.27                     | 0.64              |
| 15:8:135:MET:HB3  | 15:8:143:GLN:NE2  | 2.13                     | 0.64              |
| 22:8:309:CLA:HED2 | 22:8:309:CLA:H2A  | 1.80                     | 0.64              |
| 38:4:802:LUT:H28  | 22:4:805:CLA:H2   | 1.78                     | 0.64              |
| 24:4:804:BCR:H19C | 39:4:816:CHL:O1A  | 1.98                     | 0.64              |
| 1:A:584:CYS:SG    | 29:B:802:SF4:FE2  | 1.90                     | 0.64              |
| 22:A:821:CLA:H72  | 24:A:846:BCR:H361 | 1.80                     | 0.64              |
| 22:B:816:CLA:H61  | 24:B:846:BCR:H362 | 1.79                     | 0.64              |
| 22:B:833:CLA:HBC2 | 22:B:839:CLA:CMC  | 2.27                     | 0.64              |
| 10:K:57:VAL:HG11  | 10:K:76:LEU:HD12  | 1.78                     | 0.64              |
| 12:1:53:TYR:HB2   | 22:1:307:CLA:HMD1 | 1.80                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:7:301:LUT:C30  | 22:7:304:CLA:H72   | 2.27                     | 0.64              |
| 22:A:855:CLA:HAB  | 2:B:692:VAL:HG11   | 1.79                     | 0.64              |
| 3:C:51:CYS:SG     | 29:C:101:SF4:FE1   | 1.89                     | 0.64              |
| 13:3:98:PRO:HD2   | 22:3:316:CLA:C1B   | 2.28                     | 0.64              |
| 39:4:813:CHL:HBB1 | 39:4:813:CHL:HMB3  | 1.78                     | 0.64              |
| 38:5:303:LUT:H28  | 22:5:310:CLA:H72   | 1.78                     | 0.64              |
| 1:A:80:GLN:HG2    | 22:A:805:CLA:CMA   | 2.28                     | 0.64              |
| 24:3:306:BCR:H19C | 22:3:312:CLA:C2C   | 2.28                     | 0.64              |
| 17:5:57:PRO:HG2   | 22:5:315:CLA:H12   | 1.78                     | 0.64              |
| 18:6:123:PHE:CD1  | 24:6:305:BCR:H10C  | 2.33                     | 0.64              |
| 18:6:247:PRO:HG2  | 24:6:306:BCR:H272  | 1.79                     | 0.64              |
| 22:A:832:CLA:H112 | 22:L:202:CLA:H171  | 1.80                     | 0.64              |
| 2:B:394:PHE:CD2   | 24:B:848:BCR:H281  | 2.32                     | 0.64              |
| 14:7:178:PHE:CE2  | 38:7:301:LUT:H221  | 2.32                     | 0.64              |
| 22:4:815:CLA:HBB1 | 22:4:815:CLA:HMB1  | 1.78                     | 0.64              |
| 38:6:304:LUT:H393 | 22:6:310:CLA:H141  | 1.80                     | 0.64              |
| 22:A:806:CLA:H43  | 25:A:850:LHG:H262  | 1.79                     | 0.63              |
| 22:A:825:CLA:H143 | 22:A:825:CLA:HMD2  | 1.79                     | 0.63              |
| 2:B:283:VAL:HG13  | 24:B:844:BCR:C36   | 2.28                     | 0.63              |
| 22:1:313:CLA:HBA1 | 22:1:313:CLA:H101  | 1.78                     | 0.63              |
| 39:6:315:CHL:HBB1 | 39:6:315:CHL:HMB1  | 1.80                     | 0.63              |
| 7:G:78:PHE:CE1    | 7:G:81:LEU:HD21    | 2.32                     | 0.63              |
| 7:G:78:PHE:CZ     | 7:G:81:LEU:HD21    | 2.33                     | 0.63              |
| 12:1:223:PRO:HG3  | 22:1:316:CLA:HAB   | 1.79                     | 0.63              |
| 13:3:22:THR:HA    | 13:3:25:TYR:CE2    | 2.34                     | 0.63              |
| 16:4:228:PHE:CD1  | 16:4:239:PRO:HB3   | 2.33                     | 0.63              |
| 38:5:302:LUT:H11  | 22:5:308:CLA:HMC1  | 1.80                     | 0.63              |
| 18:6:88:GLN:HE22  | 38:6:304:LUT:H42   | 1.62                     | 0.63              |
| 22:A:810:CLA:H71  | 22:3:312:CLA:H51   | 1.80                     | 0.63              |
| 22:A:814:CLA:HBB1 | 22:A:814:CLA:HMB3  | 1.80                     | 0.63              |
| 24:B:847:BCR:H331 | 24:B:847:BCR:HC8   | 1.80                     | 0.63              |
| 24:B:853:BCR:H403 | 24:I:4001:BCR:H372 | 1.80                     | 0.63              |
| 22:F:302:CLA:C2B  | 24:F:303:BCR:H10C  | 2.28                     | 0.63              |
| 13:3:195:VAL:HG11 | 38:3:303:LUT:C12   | 2.28                     | 0.63              |
| 24:3:307:BCR:H403 | 24:3:307:BCR:H23C  | 1.78                     | 0.63              |
| 22:7:322:CLA:HMB1 | 22:7:322:CLA:HBB1  | 1.80                     | 0.63              |
| 39:8:315:CHL:HBB1 | 39:8:315:CHL:HMB1  | 1.81                     | 0.63              |
| 22:A:838:CLA:H52  | 22:A:838:CLA:C1C   | 2.29                     | 0.63              |
| 2:B:271:LEU:HD23  | 2:B:274:MET:HE3    | 1.80                     | 0.63              |
| 10:K:57:VAL:O     | 10:K:58:LYS:HB3    | 1.97                     | 0.63              |
| 12:1:194:ALA:HB1  | 12:1:218:ASN:HD21  | 1.64                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:3:42:LEU:HB2   | 22:3:311:CLA:HBA1 | 1.78                     | 0.63              |
| 1:A:514:VAL:HG22  | 1:A:524:MET:HG3   | 1.79                     | 0.63              |
| 2:B:420:ILE:HD13  | 2:B:537:LYS:HG2   | 1.81                     | 0.63              |
| 22:B:809:CLA:H43  | 22:B:831:CLA:H2   | 1.78                     | 0.63              |
| 22:B:816:CLA:HMA2 | 24:B:846:BCR:H282 | 1.81                     | 0.63              |
| 11:L:87:GLU:HA    | 11:L:90:ARG:NH2   | 2.13                     | 0.63              |
| 1:A:690:ARG:HG3   | 1:A:717:ALA:HB3   | 1.80                     | 0.63              |
| 22:A:816:CLA:CBB  | 24:A:844:BCR:H12C | 2.28                     | 0.63              |
| 22:A:827:CLA:H193 | 22:A:827:CLA:H152 | 1.79                     | 0.63              |
| 2:B:27:ALA:HB1    | 31:B:852:DGD:HG2  | 1.79                     | 0.63              |
| 31:1:319:DGD:HG11 | 31:1:319:DGD:HB21 | 1.79                     | 0.63              |
| 18:6:88:GLN:HG2   | 22:6:312:CLA:C4D  | 2.29                     | 0.63              |
| 22:A:822:CLA:HBB1 | 37:K:201:DAO:H112 | 1.79                     | 0.63              |
| 22:B:811:CLA:HBA2 | 22:B:829:CLA:CBD  | 2.27                     | 0.63              |
| 38:1:303:LUT:H373 | 22:1:307:CLA:H91  | 1.78                     | 0.63              |
| 13:3:71:ALA:HB1   | 38:3:302:LUT:H12  | 1.81                     | 0.63              |
| 1:A:598:TRP:CH2   | 22:B:806:CLA:HAB  | 2.34                     | 0.63              |
| 22:B:827:CLA:HBA2 | 22:B:839:CLA:HAA1 | 1.81                     | 0.63              |
| 6:F:69:PRO:HG2    | 6:F:72:GLU:HB2    | 1.81                     | 0.63              |
| 14:7:70:HIS:O     | 14:7:74:GLN:HG2   | 1.99                     | 0.63              |
| 22:7:322:CLA:H2   | 22:7:323:CLA:H101 | 1.80                     | 0.63              |
| 22:A:822:CLA:H62  | 22:A:823:CLA:H92  | 1.81                     | 0.63              |
| 22:A:855:CLA:H152 | 24:B:853:BCR:H17C | 1.81                     | 0.63              |
| 2:B:258:PHE:HZ    | 22:B:819:CLA:H111 | 1.63                     | 0.63              |
| 17:5:155:ASN:HB3  | 39:5:321:CHL:C3D  | 2.27                     | 0.63              |
| 22:A:810:CLA:H43  | 22:A:812:CLA:H42  | 1.81                     | 0.62              |
| 22:A:833:CLA:HBA1 | 22:A:855:CLA:H2   | 1.81                     | 0.62              |
| 12:1:153:PRO:HB3  | 22:1:313:CLA:HBC2 | 1.80                     | 0.62              |
| 22:8:314:CLA:C4B  | 26:8:318:NKP:HAY  | 2.29                     | 0.62              |
| 16:4:66:LYS:HD3   | 25:4:821:LHG:HC31 | 1.81                     | 0.62              |
| 18:6:96:PHE:HB3   | 18:6:99:ASP:OD1   | 1.99                     | 0.62              |
| 18:6:143:LEU:HD22 | 39:6:320:CHL:HMB3 | 1.80                     | 0.62              |
| 14:7:228:ASP:HB3  | 14:7:232:THR:HG23 | 1.81                     | 0.62              |
| 18:6:238:ASP:CA   | 18:6:243:LYS:HA   | 2.17                     | 0.62              |
| 23:A:843:PQN:H212 | 22:F:301:CLA:C3B  | 2.29                     | 0.62              |
| 22:B:831:CLA:HBB1 | 22:B:831:CLA:HMB1 | 1.80                     | 0.62              |
| 4:D:115:PHE:HB3   | 4:D:120:GLN:HE21  | 1.63                     | 0.62              |
| 12:Z:203:LEU:HA   | 22:Z:305:CLA:HMA1 | 1.82                     | 0.62              |
| 14:7:133:TRP:CH2  | 24:7:303:BCR:HC8  | 2.34                     | 0.62              |
| 39:9:312:CHL:HED1 | 39:9:312:CHL:H93  | 1.80                     | 0.62              |
| 7:G:93:ASP:HB2    | 22:G:202:CLA:CHA  | 2.29                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:7:175:PRO:HD2  | 38:7:301:LUT:H23  | 1.80                     | 0.62              |
| 15:8:78:THR:HG23  | 22:8:305:CLA:CMC  | 2.30                     | 0.62              |
| 15:8:135:MET:HB3  | 15:8:143:GLN:HE22 | 1.63                     | 0.62              |
| 38:8:303:LUT:H371 | 22:8:308:CLA:H142 | 1.81                     | 0.62              |
| 39:8:312:CHL:HBB1 | 39:8:312:CHL:HMB1 | 1.81                     | 0.62              |
| 22:2:304:CLA:HBB1 | 22:2:304:CLA:HHC  | 1.82                     | 0.62              |
| 2:B:491:GLN:HA    | 2:B:495:LEU:HD12  | 1.82                     | 0.62              |
| 22:1:310:CLA:HBA1 | 22:1:310:CLA:CHA  | 2.28                     | 0.62              |
| 12:Z:103:PRO:HG2  | 39:Z:312:CHL:HED1 | 1.80                     | 0.62              |
| 16:4:86:LEU:HD23  | 33:4:801:LMT:H2'  | 1.81                     | 0.62              |
| 17:5:171:PRO:HD2  | 38:5:302:LUT:H23  | 1.82                     | 0.62              |
| 19:9:101:ALA:HB2  | 39:9:312:CHL:HBA2 | 1.81                     | 0.62              |
| 22:A:815:CLA:H41  | 24:3:306:BCR:HC8  | 1.81                     | 0.62              |
| 22:B:834:CLA:NC   | 24:J:104:BCR:H292 | 2.15                     | 0.62              |
| 1:A:59:PHE:HA     | 1:A:62:HIS:ND1    | 2.15                     | 0.62              |
| 22:A:823:CLA:HBC2 | 22:A:824:CLA:HAA1 | 1.81                     | 0.62              |
| 38:3:303:LUT:H26  | 22:3:311:CLA:H2   | 1.82                     | 0.62              |
| 11:L:135:TYR:HB2  | 24:L:204:BCR:H361 | 1.81                     | 0.62              |
| 12:Z:53:TYR:HB2   | 22:Z:306:CLA:HMD1 | 1.80                     | 0.62              |
| 13:3:26:LEU:HD13  | 13:3:35:GLY:HA2   | 1.81                     | 0.62              |
| 22:5:309:CLA:HHC  | 22:5:309:CLA:HBB1 | 1.82                     | 0.62              |
| 22:A:826:CLA:HBB1 | 22:A:826:CLA:HMB1 | 1.82                     | 0.62              |
| 22:4:811:CLA:HHC  | 22:4:811:CLA:HBB1 | 1.82                     | 0.62              |
| 22:A:818:CLA:H8   | 22:A:836:CLA:CMA  | 2.30                     | 0.62              |
| 22:B:807:CLA:HBB1 | 22:B:807:CLA:HMB1 | 1.82                     | 0.62              |
| 22:Z:309:CLA:H102 | 22:Z:309:CLA:H142 | 1.80                     | 0.62              |
| 19:9:124:THR:HG21 | 39:2:303:CHL:HED3 | 1.80                     | 0.62              |
| 1:A:153:ILE:HA    | 1:A:158:GLN:OE1   | 2.00                     | 0.61              |
| 1:A:541:PHE:HZ    | 22:B:806:CLA:HBB2 | 1.65                     | 0.61              |
| 24:A:844:BCR:H17C | 24:A:845:BCR:H382 | 1.80                     | 0.61              |
| 2:B:6:PHE:HB3     | 2:B:7:PRO:HD3     | 1.82                     | 0.61              |
| 23:B:843:PQN:H142 | 24:B:849:BCR:H281 | 1.81                     | 0.61              |
| 39:1:312:CHL:HMB3 | 39:1:312:CHL:HBB1 | 1.81                     | 0.61              |
| 13:3:82:LYS:HD2   | 13:3:210:TYR:HD2  | 1.64                     | 0.61              |
| 22:3:313:CLA:H202 | 22:5:320:CLA:HHB  | 1.82                     | 0.61              |
| 24:7:303:BCR:H332 | 25:8:317:LHG:H252 | 1.82                     | 0.61              |
| 1:A:462:MET:HE2   | 1:A:462:MET:HA    | 1.82                     | 0.61              |
| 39:Z:312:CHL:HBB1 | 39:Z:312:CHL:HMB3 | 1.80                     | 0.61              |
| 13:3:163:TRP:HH2  | 24:3:305:BCR:H10C | 1.65                     | 0.61              |
| 22:7:322:CLA:ND   | 22:7:323:CLA:H122 | 2.16                     | 0.61              |
| 15:8:170:PRO:HD2  | 38:8:302:LUT:H24  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:4:113:GLY:HA3  | 38:4:803:LUT:H182 | 1.83                     | 0.61              |
| 16:4:219:ARG:HA   | 16:4:222:MET:HE3  | 1.80                     | 0.61              |
| 19:9:56:LEU:HB2   | 22:9:306:CLA:H11  | 1.81                     | 0.61              |
| 20:2:166:LEU:HA   | 20:2:169:ILE:HG12 | 1.81                     | 0.61              |
| 22:A:814:CLA:HBD  | 22:A:816:CLA:HMA1 | 1.81                     | 0.61              |
| 2:B:597:TRP:CH2   | 2:B:613:SER:HB2   | 2.35                     | 0.61              |
| 22:B:818:CLA:HBB1 | 22:B:818:CLA:HHC  | 1.82                     | 0.61              |
| 12:1:140:ARG:HG2  | 22:1:313:CLA:HHC  | 1.81                     | 0.61              |
| 22:1:306:CLA:HBC1 | 22:1:316:CLA:H101 | 1.81                     | 0.61              |
| 24:6:306:BCR:H16C | 39:6:315:CHL:C4C  | 2.29                     | 0.61              |
| 38:9:302:LUT:H11  | 22:9:307:CLA:HAC2 | 1.82                     | 0.61              |
| 1:A:508:ALA:HB3   | 1:A:523:MET:HG3   | 1.81                     | 0.61              |
| 22:B:810:CLA:H11  | 8:I:79:PHE:HB3    | 1.81                     | 0.61              |
| 22:F:301:CLA:H121 | 9:J:14:VAL:HG13   | 1.81                     | 0.61              |
| 7:G:107:ALA:HA    | 24:G:203:BCR:H341 | 1.82                     | 0.61              |
| 12:Z:157:PHE:HA   | 22:Z:313:CLA:H72  | 1.81                     | 0.61              |
| 15:8:80:VAL:HG13  | 15:8:202:PHE:HE2  | 1.64                     | 0.61              |
| 39:4:814:CHL:HMB3 | 39:4:814:CHL:HBB1 | 1.82                     | 0.61              |
| 18:6:226:VAL:HG21 | 41:6:324:3PH:H221 | 1.80                     | 0.61              |
| 22:A:829:CLA:H11  | 24:A:845:BCR:H311 | 1.82                     | 0.61              |
| 2:B:54:GLN:HG2    | 22:B:808:CLA:CMA  | 2.30                     | 0.61              |
| 8:I:67:TYR:CE2    | 8:I:69:PHE:HB2    | 2.36                     | 0.61              |
| 22:5:307:CLA:H93  | 22:5:308:CLA:H62  | 1.81                     | 0.61              |
| 18:6:188:PHE:CE1  | 18:6:199:PRO:HB3  | 2.36                     | 0.61              |
| 22:A:829:CLA:H42  | 22:A:829:CLA:HBD  | 1.82                     | 0.61              |
| 23:A:843:PQN:H212 | 22:F:301:CLA:C4B  | 2.31                     | 0.61              |
| 12:1:98:ASN:HD21  | 12:1:101:ASP:HB2  | 1.63                     | 0.61              |
| 38:Z:301:LUT:H28  | 22:Z:303:CLA:H52  | 1.83                     | 0.61              |
| 13:3:120:ALA:HB2  | 22:3:319:CLA:H2   | 1.82                     | 0.61              |
| 16:4:243:LEU:HB2  | 38:4:802:LUT:H22  | 1.81                     | 0.61              |
| 22:6:312:CLA:H52  | 22:6:312:CLA:C3D  | 2.30                     | 0.61              |
| 19:9:120:GLY:HA2  | 22:9:313:CLA:HAB  | 1.81                     | 0.61              |
| 1:A:197:MET:HG3   | 22:A:813:CLA:HBC2 | 1.83                     | 0.61              |
| 1:A:545:VAL:HG11  | 1:A:598:TRP:CE2   | 2.35                     | 0.61              |
| 22:L:201:CLA:H162 | 22:L:201:CLA:H91  | 1.81                     | 0.61              |
| 18:6:147:ASN:HB3  | 39:6:320:CHL:C4D  | 2.30                     | 0.61              |
| 1:A:409:ALA:HB1   | 24:A:846:BCR:H271 | 1.83                     | 0.61              |
| 1:A:694:GLN:HE21  | 5:E:80:TYR:HE1    | 1.49                     | 0.61              |
| 22:A:821:CLA:H92  | 22:A:825:CLA:HMB3 | 1.83                     | 0.61              |
| 22:A:832:CLA:HMB1 | 22:A:832:CLA:HBB1 | 1.83                     | 0.61              |
| 22:A:833:CLA:HAB  | 22:A:834:CLA:CHB  | 2.30                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:B:817:CLA:HHB  | 24:B:846:BCR:HC8   | 1.83                     | 0.61              |
| 13:3:190:LEU:HB2  | 24:3:307:BCR:H393  | 1.82                     | 0.61              |
| 22:3:312:CLA:H112 | 22:3:318:CLA:H42   | 1.81                     | 0.61              |
| 22:A:836:CLA:NB   | 22:K:203:CLA:H52   | 2.15                     | 0.61              |
| 22:A:854:CLA:H142 | 24:I:4001:BCR:H271 | 1.83                     | 0.61              |
| 2:B:413:LEU:HB3   | 6:F:227:ARG:HG3    | 1.82                     | 0.61              |
| 22:B:812:CLA:H71  | 24:B:849:BCR:H343  | 1.82                     | 0.61              |
| 13:3:38:PRO:HD2   | 38:3:303:LUT:H23   | 1.82                     | 0.61              |
| 24:3:304:BCR:H382 | 24:3:305:BCR:H351  | 1.82                     | 0.61              |
| 22:3:308:CLA:H51  | 22:3:309:CLA:HMA2  | 1.81                     | 0.61              |
| 38:7:301:LUT:H383 | 22:7:314:CLA:H11   | 1.82                     | 0.61              |
| 22:9:307:CLA:H2   | 22:9:307:CLA:HED2  | 1.81                     | 0.61              |
| 2:B:694:TRP:CD1   | 2:B:698:PRO:HD3    | 2.36                     | 0.61              |
| 25:B:803:LHG:HC5  | 22:B:807:CLA:HBA2  | 1.83                     | 0.61              |
| 12:Z:188:PHE:HA   | 12:Z:191:GLN:NE2   | 2.15                     | 0.61              |
| 22:4:815:CLA:H43  | 33:4:822:LMT:H91   | 1.83                     | 0.61              |
| 17:5:131:TRP:CD1  | 24:5:304:BCR:H12C  | 2.36                     | 0.61              |
| 38:5:303:LUT:C28  | 22:5:310:CLA:H72   | 2.31                     | 0.61              |
| 24:5:304:BCR:H342 | 22:5:326:CLA:H61   | 1.83                     | 0.61              |
| 2:B:38:MET:HE3    | 2:B:38:MET:HA      | 1.82                     | 0.60              |
| 2:B:366:PHE:HB3   | 2:B:603:TRP:CZ3    | 2.36                     | 0.60              |
| 22:B:806:CLA:H171 | 22:L:201:CLA:HMC3  | 1.83                     | 0.60              |
| 16:4:159:PHE:CD2  | 24:4:804:BCR:H12C  | 2.36                     | 0.60              |
| 18:6:95:VAL:HG13  | 18:6:103:LYS:HB2   | 1.82                     | 0.60              |
| 19:9:84:ILE:HG23  | 19:9:96:TRP:CG     | 2.36                     | 0.60              |
| 19:9:110:PRO:HG3  | 20:2:199:TYR:HB2   | 1.82                     | 0.60              |
| 14:7:26:TYR:CE2   | 14:7:191:GLN:HB2   | 2.37                     | 0.60              |
| 24:8:304:BCR:H282 | 22:8:310:CLA:NB    | 2.17                     | 0.60              |
| 17:5:205:GLN:HG3  | 17:5:253:TRP:CZ3   | 2.35                     | 0.60              |
| 22:9:311:CLA:HED3 | 22:9:311:CLA:H2A   | 1.83                     | 0.60              |
| 1:A:211:LEU:HD23  | 24:A:844:BCR:H373  | 1.84                     | 0.60              |
| 1:A:363:LEU:HD21  | 22:A:819:CLA:H72   | 1.83                     | 0.60              |
| 22:B:828:CLA:H71  | 24:B:848:BCR:H16C  | 1.82                     | 0.60              |
| 14:7:49:GLY:HA3   | 14:7:194:ILE:HG21  | 1.83                     | 0.60              |
| 15:8:27:ARG:HD3   | 15:8:47:ASP:O      | 2.01                     | 0.60              |
| 16:4:86:LEU:HD11  | 38:4:803:LUT:H221  | 1.83                     | 0.60              |
| 38:4:803:LUT:H26  | 22:4:808:CLA:H52   | 1.83                     | 0.60              |
| 38:9:301:LUT:H14  | 22:9:304:CLA:HBB1  | 1.83                     | 0.60              |
| 1:A:157:LEU:HD23  | 22:A:816:CLA:HED1  | 1.82                     | 0.60              |
| 22:Z:308:CLA:H61  | 22:Z:315:CLA:CAA   | 2.30                     | 0.60              |
| 22:5:307:CLA:H72  | 22:5:308:CLA:CMA   | 2.31                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:5:317:CHL:HBB1 | 39:5:317:CHL:HMB1 | 1.84                     | 0.60              |
| 2:B:57:ILE:HG21   | 22:B:809:CLA:HMD1 | 1.82                     | 0.60              |
| 4:D:131:LYS:HE3   | 4:D:132:PHE:CE2   | 2.35                     | 0.60              |
| 22:1:305:CLA:ND   | 22:1:310:CLA:H8   | 2.17                     | 0.60              |
| 22:8:310:CLA:H121 | 43:8:319:LPX:H8A  | 1.83                     | 0.60              |
| 38:5:303:LUT:H372 | 22:5:315:CLA:H72  | 1.82                     | 0.60              |
| 24:5:304:BCR:H16C | 39:5:317:CHL:HMB3 | 1.82                     | 0.60              |
| 18:6:52:PHE:HB3   | 22:6:310:CLA:CAD  | 2.32                     | 0.60              |
| 18:6:247:PRO:HB2  | 22:6:301:CLA:C1   | 2.30                     | 0.60              |
| 22:A:828:CLA:H191 | 24:J:104:BCR:H19C | 1.83                     | 0.60              |
| 15:8:63:ARG:HG2   | 15:8:137:PHE:HE2  | 1.66                     | 0.60              |
| 15:8:102:GLU:HA   | 39:8:312:CHL:HED3 | 1.84                     | 0.60              |
| 22:5:307:CLA:H72  | 22:5:308:CLA:HMA2 | 1.82                     | 0.60              |
| 39:9:312:CHL:H2   | 39:9:312:CHL:HMA3 | 1.82                     | 0.60              |
| 22:A:823:CLA:HBA1 | 37:K:201:DAO:H51  | 1.82                     | 0.60              |
| 22:B:828:CLA:HBA2 | 24:B:848:BCR:H10C | 1.83                     | 0.60              |
| 10:K:38:MET:HG2   | 22:K:202:CLA:C3D  | 2.31                     | 0.60              |
| 10:K:97:HIS:ND1   | 24:K:206:BCR:H14C | 2.15                     | 0.60              |
| 22:1:306:CLA:C15  | 25:1:317:LHG:HC92 | 2.32                     | 0.60              |
| 22:1:306:CLA:H172 | 25:1:317:LHG:H121 | 1.82                     | 0.60              |
| 12:Z:144:GLU:HB3  | 12:Z:150:ARG:HG2  | 1.82                     | 0.60              |
| 22:Z:304:CLA:HBC3 | 22:Z:309:CLA:H143 | 1.84                     | 0.60              |
| 13:3:137:SER:HA   | 13:3:140:LYS:NZ   | 2.16                     | 0.60              |
| 22:4:815:CLA:HMB2 | 33:4:822:LMT:H51  | 1.84                     | 0.60              |
| 22:A:804:CLA:HBD  | 22:A:811:CLA:H2   | 1.83                     | 0.60              |
| 22:A:811:CLA:HBB1 | 22:A:811:CLA:HHC  | 1.83                     | 0.60              |
| 2:B:262:PHE:CE1   | 2:B:356:LEU:HA    | 2.37                     | 0.60              |
| 22:B:821:CLA:HMB1 | 22:B:826:CLA:HED1 | 1.82                     | 0.60              |
| 15:8:174:CYS:HB2  | 22:8:305:CLA:HAA2 | 1.83                     | 0.60              |
| 16:4:159:PHE:CD1  | 24:4:804:BCR:H10C | 2.37                     | 0.60              |
| 18:6:176:LYS:HD3  | 22:6:313:CLA:O1D  | 2.01                     | 0.60              |
| 1:A:680:ALA:CB    | 22:B:801:CLA:HBB2 | 2.32                     | 0.60              |
| 2:B:155:TRP:CZ2   | 2:B:159:GLN:HG2   | 2.37                     | 0.60              |
| 2:B:183:LEU:HD13  | 22:B:815:CLA:HHB  | 1.83                     | 0.60              |
| 7:G:46:LEU:HD12   | 22:G:201:CLA:H11  | 1.82                     | 0.60              |
| 7:G:49:GLY:HA3    | 7:G:105:TRP:CD2   | 2.37                     | 0.60              |
| 10:K:97:HIS:CE1   | 24:K:206:BCR:H14C | 2.37                     | 0.60              |
| 22:Z:304:CLA:C1C  | 22:Z:309:CLA:H121 | 2.31                     | 0.60              |
| 1:A:211:LEU:HD11  | 24:A:856:BCR:HC7  | 1.84                     | 0.60              |
| 22:A:817:CLA:CAB  | 24:K:206:BCR:HC32 | 2.25                     | 0.60              |
| 2:B:493:LEU:HD12  | 22:B:836:CLA:HED1 | 1.84                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:F:301:CLA:HHC  | 22:F:301:CLA:HBB1 | 1.84                     | 0.60              |
| 16:4:228:PHE:HD1  | 16:4:239:PRO:HB3  | 1.67                     | 0.60              |
| 17:5:98:VAL:HG11  | 22:5:312:CLA:HED2 | 1.84                     | 0.60              |
| 18:6:173:LYS:HD3  | 22:6:308:CLA:O1A  | 2.02                     | 0.60              |
| 1:A:136:GLN:HE22  | 6:F:104:LEU:HD11  | 1.67                     | 0.59              |
| 2:B:70:ALA:HB2    | 2:B:136:LEU:HB2   | 1.84                     | 0.59              |
| 22:B:811:CLA:HBA1 | 22:B:811:CLA:CHA  | 2.31                     | 0.59              |
| 22:G:201:CLA:HHC  | 22:G:201:CLA:CBB  | 2.31                     | 0.59              |
| 17:5:181:GLU:OE2  | 17:5:185:LYS:HE2  | 2.02                     | 0.59              |
| 22:Z:310:CLA:HBA2 | 22:Z:310:CLA:CHA  | 2.29                     | 0.59              |
| 22:7:308:CLA:HBB1 | 22:7:308:CLA:HMB3 | 1.84                     | 0.59              |
| 39:4:813:CHL:HAB  | 39:4:816:CHL:CBB  | 2.32                     | 0.59              |
| 24:5:305:BCR:H333 | 18:6:227:VAL:HG21 | 1.83                     | 0.59              |
| 19:9:115:GLU:HB2  | 39:9:312:CHL:HBB2 | 1.83                     | 0.59              |
| 22:A:805:CLA:HBD  | 22:A:825:CLA:H52  | 1.83                     | 0.59              |
| 2:B:155:TRP:CH2   | 2:B:159:GLN:HG2   | 2.37                     | 0.59              |
| 24:B:853:BCR:HC42 | 22:L:202:CLA:NC   | 2.17                     | 0.59              |
| 5:E:39:ARG:HH21   | 5:E:62:VAL:H      | 1.49                     | 0.59              |
| 22:8:308:CLA:HBC3 | 41:8:320:3PH:H3C1 | 1.83                     | 0.59              |
| 16:4:177:ASP:HB3  | 16:4:180:PHE:O    | 2.02                     | 0.59              |
| 22:4:818:CLA:HBA1 | 22:4:818:CLA:CHA  | 2.32                     | 0.59              |
| 22:6:309:CLA:HBC1 | 22:6:319:CLA:HAA1 | 1.83                     | 0.59              |
| 39:9:312:CHL:HBD  | 39:9:312:CHL:HAA2 | 1.83                     | 0.59              |
| 20:2:171:PHE:O    | 20:2:172:CYS:C    | 2.45                     | 0.59              |
| 22:A:821:CLA:C4C  | 22:A:827:CLA:H161 | 2.32                     | 0.59              |
| 2:B:195:LEU:HA    | 2:B:199:ALA:HB3   | 1.84                     | 0.59              |
| 22:B:814:CLA:HHC  | 22:B:814:CLA:CBB  | 2.32                     | 0.59              |
| 12:1:78:CYS:SG    | 12:1:182:MET:HE2  | 2.43                     | 0.59              |
| 12:Z:157:PHE:CE2  | 22:Z:313:CLA:H161 | 2.37                     | 0.59              |
| 22:Z:303:CLA:H62  | 22:Z:304:CLA:HMA2 | 1.83                     | 0.59              |
| 13:3:190:LEU:HB2  | 24:3:307:BCR:C39  | 2.33                     | 0.59              |
| 15:8:127:GLY:HA2  | 22:8:314:CLA:HMB1 | 1.83                     | 0.59              |
| 22:5:310:CLA:H101 | 22:5:315:CLA:H121 | 1.85                     | 0.59              |
| 22:5:326:CLA:HHC  | 22:5:326:CLA:HBB1 | 1.83                     | 0.59              |
| 1:A:320:HIS:HB3   | 1:A:325:ILE:HD11  | 1.83                     | 0.59              |
| 13:3:82:LYS:NZ    | 13:3:210:TYR:HB3  | 2.16                     | 0.59              |
| 24:7:303:BCR:H11C | 22:7:322:CLA:H41  | 1.84                     | 0.59              |
| 16:4:138:GLY:HA2  | 39:4:816:CHL:HAC2 | 1.83                     | 0.59              |
| 22:B:811:CLA:HBB2 | 22:B:812:CLA:HAA1 | 1.84                     | 0.59              |
| 22:B:812:CLA:HMB1 | 22:B:812:CLA:HBB1 | 1.83                     | 0.59              |
| 22:8:309:CLA:H43  | 22:8:309:CLA:HED3 | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:598:TRP:HE1   | 22:A:854:CLA:C1D  | 2.15                     | 0.59              |
| 22:A:814:CLA:H141 | 31:3:301:DGD:HA41 | 1.84                     | 0.59              |
| 2:B:349:VAL:HA    | 22:B:820:CLA:H42  | 1.85                     | 0.59              |
| 14:7:49:GLY:H     | 14:7:191:GLN:NE2  | 2.01                     | 0.59              |
| 39:8:301:CHL:HAA2 | 39:8:301:CHL:HBD  | 1.84                     | 0.59              |
| 24:5:305:BCR:H343 | 18:6:220:VAL:HG11 | 1.84                     | 0.59              |
| 20:2:207:THR:HG23 | 22:2:301:CLA:H8   | 1.82                     | 0.59              |
| 22:A:855:CLA:H102 | 22:B:840:CLA:H43  | 1.85                     | 0.59              |
| 2:B:78:TRP:HA     | 2:B:85:VAL:HB     | 1.85                     | 0.59              |
| 2:B:229:GLY:HA3   | 7:G:117:LEU:HD13  | 1.84                     | 0.59              |
| 22:B:814:CLA:O1A  | 7:G:81:LEU:HD22   | 2.02                     | 0.59              |
| 22:F:304:CLA:HMD2 | 33:F:307:LMT:H32  | 1.84                     | 0.59              |
| 15:8:133:ARG:HH12 | 22:8:314:CLA:HED3 | 1.67                     | 0.59              |
| 18:6:39:PRO:HB2   | 18:6:41:HIS:CE1   | 2.37                     | 0.59              |
| 20:2:177:VAL:C    | 20:2:178:ARG:HG3  | 2.27                     | 0.59              |
| 38:Z:302:LUT:H393 | 22:Z:306:CLA:H141 | 1.85                     | 0.59              |
| 22:8:310:CLA:HMA2 | 39:8:315:CHL:C3C  | 2.33                     | 0.59              |
| 24:5:305:BCR:C12  | 24:5:305:BCR:H341 | 2.32                     | 0.59              |
| 18:6:41:HIS:CD2   | 18:6:42:LEU:HG    | 2.38                     | 0.59              |
| 18:6:245:PHE:CZ   | 18:6:247:PRO:HB3  | 2.36                     | 0.59              |
| 22:6:314:CLA:HHC  | 22:6:314:CLA:CBB  | 2.31                     | 0.59              |
| 2:B:182:GLY:HA3   | 22:B:815:CLA:HBB1 | 1.84                     | 0.59              |
| 22:B:818:CLA:H121 | 22:B:818:CLA:HMC3 | 1.85                     | 0.59              |
| 22:B:822:CLA:HBA1 | 7:G:100:ILE:HG22  | 1.85                     | 0.59              |
| 12:Z:135:ALA:HA   | 22:Z:314:CLA:HAB  | 1.84                     | 0.59              |
| 22:Z:309:CLA:HHC  | 22:Z:309:CLA:HBB1 | 1.85                     | 0.59              |
| 22:3:322:CLA:H52  | 25:7:318:LHG:H321 | 1.84                     | 0.59              |
| 22:7:312:CLA:HHC  | 22:7:312:CLA:CBB  | 2.32                     | 0.59              |
| 22:8:309:CLA:HMD2 | 26:8:318:NKP:HAZA | 1.85                     | 0.59              |
| 38:9:301:LUT:H181 | 22:9:305:CLA:HBB1 | 1.85                     | 0.59              |
| 1:A:217:GLN:HA    | 1:A:221:SER:HB2   | 1.84                     | 0.58              |
| 22:A:814:CLA:H11  | 22:A:816:CLA:CHB  | 2.33                     | 0.58              |
| 22:B:811:CLA:HBA1 | 22:B:811:CLA:HBD  | 1.85                     | 0.58              |
| 6:F:141:LEU:HD21  | 6:F:150:PHE:CE2   | 2.37                     | 0.58              |
| 22:F:304:CLA:H12  | 22:F:304:CLA:NA   | 2.17                     | 0.58              |
| 12:Z:153:PRO:HB3  | 22:Z:313:CLA:HBC2 | 1.85                     | 0.58              |
| 15:8:40:LEU:HD11  | 15:8:51:ASP:HB2   | 1.84                     | 0.58              |
| 22:A:808:CLA:H42  | 22:A:828:CLA:HMD2 | 1.85                     | 0.58              |
| 22:B:811:CLA:HHC  | 22:B:811:CLA:CBB  | 2.28                     | 0.58              |
| 4:D:184:VAL:HG11  | 4:D:194:ILE:HG21  | 1.85                     | 0.58              |
| 15:8:39:HIS:HA    | 15:8:41:LYS:NZ    | 2.18                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:8:205:GLN:HB3  | 15:8:216:ASN:ND2  | 2.18                     | 0.58              |
| 22:B:814:CLA:O1D  | 22:B:815:CLA:HMC1 | 2.03                     | 0.58              |
| 22:B:819:CLA:HHC  | 22:B:819:CLA:HBB1 | 1.85                     | 0.58              |
| 22:B:827:CLA:H121 | 22:B:842:CLA:H202 | 1.86                     | 0.58              |
| 6:F:165:TYR:O     | 6:F:169:LEU:HG    | 2.03                     | 0.58              |
| 10:K:62:ASP:HB2   | 10:K:68:VAL:CG2   | 2.33                     | 0.58              |
| 10:K:66:LYS:HB2   | 10:K:66:LYS:NZ    | 2.18                     | 0.58              |
| 11:L:73:PRO:HB3   | 11:L:87:GLU:OE1   | 2.02                     | 0.58              |
| 16:4:116:VAL:HB   | 16:4:117:PRO:HD3  | 1.86                     | 0.58              |
| 22:4:809:CLA:OBD  | 22:4:815:CLA:HAA1 | 2.04                     | 0.58              |
| 17:5:160:PRO:HG2  | 17:5:179:ARG:NH1  | 2.18                     | 0.58              |
| 17:5:176:LYS:HD2  | 17:5:177:GLY:N    | 2.19                     | 0.58              |
| 24:A:856:BCR:C24  | 10:K:95:LEU:HD21  | 2.34                     | 0.58              |
| 2:B:10:SER:HB3    | 31:B:852:DGD:HE2  | 1.84                     | 0.58              |
| 22:B:814:CLA:H43  | 19:9:56:LEU:HD22  | 1.85                     | 0.58              |
| 22:B:842:CLA:CHC  | 22:1:308:CLA:H12  | 2.34                     | 0.58              |
| 38:1:302:LUT:H28  | 22:1:304:CLA:H2   | 1.83                     | 0.58              |
| 13:3:129:TRP:CZ3  | 41:7:319:3PH:H322 | 2.39                     | 0.58              |
| 39:7:313:CHL:CBB  | 22:7:316:CLA:HBB2 | 2.33                     | 0.58              |
| 38:5:302:LUT:H30  | 22:5:307:CLA:C5   | 2.33                     | 0.58              |
| 22:A:811:CLA:HBA1 | 22:A:811:CLA:CHA  | 2.33                     | 0.58              |
| 22:B:819:CLA:H91  | 22:B:828:CLA:HMB3 | 1.84                     | 0.58              |
| 6:F:116:ALA:HB1   | 6:F:120:LYS:HZ3   | 1.68                     | 0.58              |
| 11:L:141:GLN:H    | 11:L:141:GLN:NE2  | 2.00                     | 0.58              |
| 38:4:802:LUT:H28  | 22:4:805:CLA:C2   | 2.34                     | 0.58              |
| 25:4:821:LHG:H142 | 22:6:321:CLA:C4C  | 2.33                     | 0.58              |
| 17:5:49:LEU:HD13  | 17:5:71:ARG:HD3   | 1.84                     | 0.58              |
| 1:A:375:PRO:HG2   | 1:A:381:ALA:HB2   | 1.85                     | 0.58              |
| 22:A:855:CLA:HHC  | 22:A:855:CLA:HBB1 | 1.84                     | 0.58              |
| 2:B:628:ASN:HB2   | 2:B:725:PHE:CE1   | 2.38                     | 0.58              |
| 22:B:828:CLA:C7   | 24:B:848:BCR:H16C | 2.34                     | 0.58              |
| 22:B:841:CLA:CAC  | 24:B:849:BCR:H24C | 2.34                     | 0.58              |
| 12:Z:101:ASP:HA   | 12:Z:104:LEU:HD12 | 1.85                     | 0.58              |
| 38:Z:301:LUT:H8   | 22:Z:305:CLA:HBB1 | 1.86                     | 0.58              |
| 22:Z:307:CLA:H52  | 15:8:152:PHE:HB2  | 1.84                     | 0.58              |
| 13:3:203:VAL:HG11 | 31:3:301:DGD:HA72 | 1.86                     | 0.58              |
| 22:5:313:CLA:HBC1 | 25:5:324:LHG:H302 | 1.86                     | 0.58              |
| 18:6:182:MET:HE3  | 22:6:310:CLA:HMC3 | 1.85                     | 0.58              |
| 6:F:203:PRO:HB2   | 22:8:309:CLA:H101 | 1.86                     | 0.58              |
| 11:L:96:LEU:HD11  | 11:L:124:LEU:HD23 | 1.84                     | 0.58              |
| 12:Z:203:LEU:HA   | 22:Z:305:CLA:CMA  | 2.34                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:4:804:BCR:C19  | 39:4:816:CHL:HMA2  | 2.33                     | 0.58              |
| 17:5:164:TYR:HB3  | 22:5:307:CLA:HED3  | 1.85                     | 0.58              |
| 2:B:243:HIS:HA    | 2:B:249:ASP:O      | 2.04                     | 0.58              |
| 2:B:284:ILE:HG23  | 22:B:818:CLA:H192  | 1.86                     | 0.58              |
| 4:D:178:ASN:HB3   | 4:D:191:THR:CG2    | 2.33                     | 0.58              |
| 5:E:74:ARG:HD2    | 5:E:85:THR:HB      | 1.85                     | 0.58              |
| 24:7:303:BCR:H292 | 42:7:321:SPH:H122  | 1.85                     | 0.58              |
| 39:8:315:CHL:HAA2 | 39:8:315:CHL:HBD   | 1.86                     | 0.58              |
| 39:4:813:CHL:HAA1 | 39:4:813:CHL:HBD   | 1.85                     | 0.58              |
| 17:5:247:ILE:HG23 | 39:5:316:CHL:H42   | 1.86                     | 0.58              |
| 22:5:313:CLA:HBC2 | 25:5:324:LHG:HC91  | 1.86                     | 0.58              |
| 4:D:182:ILE:HG23  | 4:D:183:LYS:HD2    | 1.85                     | 0.58              |
| 22:F:304:CLA:C8   | 22:F:304:CLA:H2    | 2.33                     | 0.58              |
| 7:G:45:MET:HG3    | 7:G:109:GLY:HA2    | 1.85                     | 0.58              |
| 10:K:25:ARG:HA    | 10:K:29:PHE:CE1    | 2.39                     | 0.58              |
| 40:1:318:SQD:H132 | 15:8:134:TRP:CE2   | 2.39                     | 0.58              |
| 20:2:177:VAL:HG21 | 22:2:304:CLA:HMD3  | 1.86                     | 0.58              |
| 2:B:341:SER:HA    | 22:B:828:CLA:H51   | 1.84                     | 0.58              |
| 12:1:37:PRO:O     | 39:8:301:CHL:HED1  | 2.03                     | 0.58              |
| 17:5:84:GLY:HA2   | 38:5:303:LUT:H181  | 1.86                     | 0.58              |
| 18:6:108:PHE:HB2  | 18:6:113:LEU:HG    | 1.85                     | 0.58              |
| 22:2:301:CLA:HBA1 | 22:2:301:CLA:CHA   | 2.31                     | 0.58              |
| 1:A:85:PHE:CE2    | 1:A:173:MET:HE3    | 2.39                     | 0.57              |
| 22:3:313:CLA:HAA1 | 22:5:301:CLA:HMB3  | 1.86                     | 0.57              |
| 14:7:77:ARG:HA    | 14:7:80:MET:HE3    | 1.86                     | 0.57              |
| 22:A:816:CLA:HBA2 | 22:A:816:CLA:CHA   | 2.33                     | 0.57              |
| 22:A:817:CLA:H121 | 22:A:817:CLA:HMC2  | 1.85                     | 0.57              |
| 22:A:822:CLA:CMB  | 22:A:823:CLA:H2    | 2.34                     | 0.57              |
| 2:B:296:PHE:CD2   | 22:B:822:CLA:HAA2  | 2.39                     | 0.57              |
| 2:B:296:PHE:CE2   | 22:B:822:CLA:HBD   | 2.39                     | 0.57              |
| 22:B:832:CLA:C4D  | 22:B:842:CLA:H52   | 2.33                     | 0.57              |
| 22:B:832:CLA:H42  | 22:B:842:CLA:H62   | 1.86                     | 0.57              |
| 8:I:88:PRO:CG     | 24:I:4001:BCR:H12C | 2.34                     | 0.57              |
| 12:1:76:ILE:HG13  | 22:1:314:CLA:O1D   | 2.04                     | 0.57              |
| 22:4:810:CLA:CGA  | 22:4:818:CLA:HAB   | 2.34                     | 0.57              |
| 39:6:320:CHL:HAA2 | 39:6:320:CHL:HBD   | 1.87                     | 0.57              |
| 19:9:101:ALA:HB2  | 39:9:312:CHL:CBA   | 2.35                     | 0.57              |
| 1:A:362:SER:O     | 1:A:366:ILE:HG13   | 2.04                     | 0.57              |
| 1:A:670:LEU:HB3   | 22:A:802:CLA:H92   | 1.85                     | 0.57              |
| 22:A:835:CLA:ND   | 24:A:847:BCR:H282  | 2.19                     | 0.57              |
| 22:A:841:CLA:HBA1 | 22:A:841:CLA:CHA   | 2.34                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:54:GLN:HG2    | 22:B:808:CLA:HMA2 | 1.85                     | 0.57              |
| 6:F:153:THR:O     | 6:F:157:LEU:HG    | 2.04                     | 0.57              |
| 8:I:87:LEU:HB3    | 8:I:88:PRO:HD3    | 1.84                     | 0.57              |
| 12:Z:157:PHE:HZ   | 22:Z:313:CLA:NB   | 2.01                     | 0.57              |
| 14:7:153:PHE:HB3  | 14:7:160:PHE:HE2  | 1.69                     | 0.57              |
| 15:8:129:VAL:HG11 | 24:8:304:BCR:H16C | 1.86                     | 0.57              |
| 15:8:193:ARG:HA   | 15:8:196:MET:HE3  | 1.87                     | 0.57              |
| 39:9:312:CHL:HED1 | 39:9:312:CHL:C9   | 2.34                     | 0.57              |
| 22:A:807:CLA:H102 | 36:J:105:C7Z:C11  | 2.34                     | 0.57              |
| 22:A:810:CLA:HAB  | 22:A:813:CLA:H101 | 1.85                     | 0.57              |
| 2:B:646:VAL:HA    | 22:B:812:CLA:HAC1 | 1.86                     | 0.57              |
| 24:B:844:BCR:H343 | 7:G:104:ALA:HA    | 1.86                     | 0.57              |
| 24:3:304:BCR:H392 | 22:3:319:CLA:HAA1 | 1.86                     | 0.57              |
| 25:4:820:LHG:H151 | 22:6:302:CLA:H72  | 1.84                     | 0.57              |
| 18:6:157:PRO:HG3  | 39:6:316:CHL:C1D  | 2.34                     | 0.57              |
| 18:6:188:PHE:CD1  | 18:6:199:PRO:HB3  | 2.39                     | 0.57              |
| 22:A:807:CLA:HAB  | 24:J:104:BCR:C6   | 2.34                     | 0.57              |
| 22:A:832:CLA:H152 | 22:A:832:CLA:H8   | 1.87                     | 0.57              |
| 22:B:824:CLA:O1A  | 22:B:824:CLA:HBD  | 2.05                     | 0.57              |
| 22:F:304:CLA:H2   | 22:F:304:CLA:H92  | 1.86                     | 0.57              |
| 22:1:310:CLA:HHC  | 22:1:310:CLA:CBB  | 2.32                     | 0.57              |
| 24:3:304:BCR:H313 | 25:7:318:LHG:H111 | 1.86                     | 0.57              |
| 15:8:169:ASP:OD2  | 15:8:174:CYS:HB2  | 2.04                     | 0.57              |
| 18:6:120:ALA:HB1  | 24:6:305:BCR:H15C | 1.85                     | 0.57              |
| 38:9:302:LUT:H371 | 22:9:306:CLA:H112 | 1.86                     | 0.57              |
| 22:A:816:CLA:HBB2 | 24:A:844:BCR:H12C | 1.87                     | 0.57              |
| 22:A:830:CLA:H151 | 22:A:841:CLA:HMA3 | 1.86                     | 0.57              |
| 24:A:844:BCR:H20C | 24:A:845:BCR:H23C | 1.87                     | 0.57              |
| 2:B:210:TRP:CD1   | 25:B:851:LHG:H02  | 2.22                     | 0.57              |
| 2:B:681:TRP:O     | 2:B:685:LYS:HG2   | 2.05                     | 0.57              |
| 4:D:174:ARG:HB2   | 4:D:177:GLU:HG3   | 1.85                     | 0.57              |
| 8:I:75:ALA:HB3    | 8:I:76:PRO:HD3    | 1.87                     | 0.57              |
| 8:I:98:TYR:HD2    | 8:I:99:ILE:HD12   | 1.68                     | 0.57              |
| 22:3:314:CLA:HHC  | 22:3:314:CLA:HBB1 | 1.85                     | 0.57              |
| 22:6:307:CLA:HMB2 | 22:6:308:CLA:HBA2 | 1.87                     | 0.57              |
| 22:B:827:CLA:HAA2 | 22:B:828:CLA:OBD  | 2.05                     | 0.57              |
| 11:L:87:GLU:HA    | 11:L:90:ARG:HH21  | 1.68                     | 0.57              |
| 22:L:202:CLA:HBC1 | 24:L:204:BCR:H23C | 1.87                     | 0.57              |
| 22:1:304:CLA:HBB1 | 22:1:304:CLA:HMB1 | 1.87                     | 0.57              |
| 22:1:308:CLA:C4B  | 22:1:314:CLA:H161 | 2.34                     | 0.57              |
| 13:3:159:PRO:HD2  | 22:3:308:CLA:OBD  | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:3:312:CLA:C4B  | 22:3:318:CLA:H122 | 2.35                     | 0.57              |
| 22:7:309:CLA:CHD  | 42:7:321:SPH:H151 | 2.35                     | 0.57              |
| 15:8:115:LEU:HD21 | 39:8:312:CHL:HHD  | 1.85                     | 0.57              |
| 1:A:396:TRP:CD1   | 22:A:828:CLA:HAB  | 2.39                     | 0.57              |
| 1:A:604:SER:O     | 1:A:607:ILE:HG12  | 2.04                     | 0.57              |
| 21:A:801:CL0:H21  | 2:B:626:TRP:HD1   | 1.69                     | 0.57              |
| 22:A:819:CLA:H172 | 22:A:827:CLA:O2A  | 2.05                     | 0.57              |
| 10:K:77:ILE:HD12  | 13:3:18:THR:HG23  | 1.86                     | 0.57              |
| 38:1:303:LUT:H24  | 22:1:307:CLA:O1A  | 2.03                     | 0.57              |
| 22:Z:316:CLA:NA   | 22:Z:316:CLA:H162 | 2.19                     | 0.57              |
| 13:3:121:MET:HB2  | 22:3:318:CLA:HAB  | 1.86                     | 0.57              |
| 13:3:149:VAL:CG2  | 13:3:163:TRP:HB2  | 2.35                     | 0.57              |
| 14:7:234:PHE:CD1  | 22:7:306:CLA:H11  | 2.40                     | 0.57              |
| 38:7:301:LUT:H403 | 22:7:304:CLA:H13  | 1.86                     | 0.57              |
| 15:8:208:ALA:HA   | 15:8:234:ILE:HD13 | 1.87                     | 0.57              |
| 16:4:71:LEU:HD21  | 22:4:808:CLA:HAA2 | 1.86                     | 0.57              |
| 17:5:185:LYS:NZ   | 22:5:313:CLA:HBD  | 2.19                     | 0.57              |
| 17:5:245:LEU:HD11 | 18:6:222:VAL:HB   | 1.86                     | 0.57              |
| 1:A:160:TYR:O     | 1:A:164:ILE:HG12  | 2.03                     | 0.57              |
| 12:1:102:ALA:H    | 12:1:103:PRO:HD2  | 1.69                     | 0.57              |
| 15:8:173:MET:HB2  | 22:8:305:CLA:HBA1 | 1.86                     | 0.57              |
| 22:5:301:CLA:H51  | 22:5:301:CLA:ND   | 2.20                     | 0.57              |
| 19:9:126:ARG:HH22 | 22:9:313:CLA:CMA  | 2.17                     | 0.57              |
| 1:A:204:GLY:HA2   | 1:A:208:LEU:HD12  | 1.87                     | 0.57              |
| 22:A:808:CLA:HHC  | 22:A:808:CLA:CBB  | 2.32                     | 0.57              |
| 22:A:819:CLA:ND   | 22:A:829:CLA:H72  | 2.19                     | 0.57              |
| 22:A:823:CLA:C1C  | 37:K:201:DAO:H111 | 2.34                     | 0.57              |
| 2:B:142:PHE:HZ    | 22:B:816:CLA:H122 | 1.68                     | 0.57              |
| 22:F:302:CLA:HHC  | 22:F:302:CLA:CBB  | 2.31                     | 0.57              |
| 11:L:171:THR:O    | 11:L:175:THR:HG23 | 2.04                     | 0.57              |
| 39:1:312:CHL:HBD  | 39:1:312:CHL:HAA1 | 1.87                     | 0.57              |
| 22:3:313:CLA:HMA3 | 22:3:319:CLA:C3C  | 2.35                     | 0.57              |
| 22:3:313:CLA:H121 | 22:5:320:CLA:NC   | 2.20                     | 0.57              |
| 14:7:25:ALA:HA    | 14:7:30:ARG:HB2   | 1.87                     | 0.57              |
| 15:8:74:ARG:O     | 22:8:305:CLA:HMC1 | 2.04                     | 0.57              |
| 16:4:116:VAL:HG11 | 22:4:810:CLA:HAC2 | 1.87                     | 0.57              |
| 39:5:316:CHL:H141 | 39:5:316:CHL:H172 | 1.86                     | 0.57              |
| 22:G:202:CLA:NC   | 24:G:203:BCR:H282 | 2.20                     | 0.56              |
| 22:L:203:CLA:HBB1 | 22:L:203:CLA:HMB3 | 1.87                     | 0.56              |
| 22:Z:306:CLA:H71  | 22:Z:307:CLA:CMA  | 2.35                     | 0.56              |
| 39:4:814:CHL:HAA1 | 39:4:814:CHL:HBD  | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:9:302:LUT:H162 | 22:9:308:CLA:HHB  | 1.87                     | 0.56              |
| 20:2:178:ARG:NH1  | 20:2:203:VAL:HG22 | 2.19                     | 0.56              |
| 1:A:355:ILE:HD13  | 24:A:846:BCR:H371 | 1.86                     | 0.56              |
| 1:A:563:ILE:HD13  | 1:A:576:ASP:HB2   | 1.87                     | 0.56              |
| 22:A:821:CLA:H102 | 22:A:824:CLA:H93  | 1.87                     | 0.56              |
| 7:G:56:LEU:HD11   | 33:G:204:LMT:H3'  | 1.87                     | 0.56              |
| 22:8:307:CLA:H161 | 22:8:311:CLA:HMC3 | 1.87                     | 0.56              |
| 16:4:159:PHE:CE1  | 24:4:804:BCR:HC8  | 2.40                     | 0.56              |
| 25:4:820:LHG:H101 | 24:6:305:BCR:HC42 | 1.86                     | 0.56              |
| 22:5:315:CLA:H2A  | 25:5:324:LHG:H151 | 1.85                     | 0.56              |
| 18:6:128:ARG:HG3  | 39:6:316:CHL:C1D  | 2.35                     | 0.56              |
| 22:A:803:CLA:HHC  | 22:A:803:CLA:CBB  | 2.35                     | 0.56              |
| 22:A:824:CLA:C2   | 22:A:835:CLA:H171 | 2.30                     | 0.56              |
| 22:A:841:CLA:NC   | 22:A:841:CLA:H52  | 2.19                     | 0.56              |
| 22:B:815:CLA:H102 | 24:B:845:BCR:H381 | 1.88                     | 0.56              |
| 22:B:834:CLA:NA   | 24:J:104:BCR:H282 | 2.21                     | 0.56              |
| 10:K:95:LEU:HD13  | 22:K:204:CLA:HBB2 | 1.88                     | 0.56              |
| 14:7:163:LYS:HD3  | 14:7:164:GLU:HG3  | 1.86                     | 0.56              |
| 38:8:302:LUT:C28  | 22:8:305:CLA:H61  | 2.35                     | 0.56              |
| 22:8:307:CLA:H101 | 25:8:317:LHG:H312 | 1.86                     | 0.56              |
| 22:8:310:CLA:HBD  | 43:8:319:LPX:H3   | 1.86                     | 0.56              |
| 16:4:210:LEU:HB3  | 22:4:805:CLA:HMA2 | 1.87                     | 0.56              |
| 17:5:253:TRP:HD1  | 22:5:301:CLA:O1A  | 1.88                     | 0.56              |
| 22:5:308:CLA:C4B  | 22:5:313:CLA:H121 | 2.35                     | 0.56              |
| 38:6:304:LUT:C28  | 22:6:310:CLA:H61  | 2.26                     | 0.56              |
| 19:9:62:ARG:HA    | 19:9:62:ARG:HE    | 1.69                     | 0.56              |
| 19:9:112:THR:HG22 | 19:9:116:PHE:CZ   | 2.40                     | 0.56              |
| 39:9:312:CHL:H141 | 39:9:312:CHL:CHD  | 2.35                     | 0.56              |
| 1:A:26:PHE:HD2    | 34:J:101:LMG:HC1  | 1.69                     | 0.56              |
| 1:A:622:VAL:HA    | 1:A:627:VAL:HG22  | 1.86                     | 0.56              |
| 22:B:810:CLA:HAA2 | 8:I:80:VAL:HG22   | 1.87                     | 0.56              |
| 39:Z:312:CHL:HAB  | 22:Z:315:CLA:HBB2 | 1.86                     | 0.56              |
| 24:3:307:BCR:H352 | 22:3:315:CLA:C4D  | 2.34                     | 0.56              |
| 15:8:118:LEU:HD21 | 39:8:315:CHL:CHD  | 2.35                     | 0.56              |
| 16:4:81:PHE:HB3   | 22:4:808:CLA:C3D  | 2.35                     | 0.56              |
| 18:6:245:PHE:CE2  | 22:6:301:CLA:H112 | 2.41                     | 0.56              |
| 20:2:196:ASN:O    | 22:2:301:CLA:HAA1 | 2.06                     | 0.56              |
| 1:A:303:VAL:HG12  | 22:A:817:CLA:H142 | 1.87                     | 0.56              |
| 22:A:805:CLA:H171 | 24:A:844:BCR:H323 | 1.87                     | 0.56              |
| 2:B:224:THR:HB    | 2:B:225:PRO:HD3   | 1.88                     | 0.56              |
| 2:B:495:LEU:HB3   | 2:B:496:PRO:HD3   | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:50:ARG:HG2    | 22:G:202:CLA:CAB  | 2.35                     | 0.56              |
| 7:G:90:SER:HB2    | 19:9:34:ASN:O     | 2.05                     | 0.56              |
| 15:8:170:PRO:CD   | 38:8:302:LUT:H24  | 2.35                     | 0.56              |
| 25:8:317:LHG:H122 | 25:8:317:LHG:O7   | 2.05                     | 0.56              |
| 18:6:184:ALA:HB1  | 38:6:303:LUT:H7   | 1.86                     | 0.56              |
| 19:9:72:THR:HG21  | 22:9:313:CLA:O1D  | 2.05                     | 0.56              |
| 38:9:301:LUT:C14  | 22:9:304:CLA:HBB1 | 2.35                     | 0.56              |
| 22:2:301:CLA:C1C  | 22:2:301:CLA:H52  | 2.34                     | 0.56              |
| 22:A:803:CLA:H8   | 9:J:16:LEU:HD23   | 1.87                     | 0.56              |
| 22:A:831:CLA:HBA2 | 25:A:849:LHG:HC92 | 1.87                     | 0.56              |
| 11:L:99:PRO:HA    | 22:L:203:CLA:HMB2 | 1.87                     | 0.56              |
| 11:L:140:PHE:HD1  | 11:L:144:PRO:HD2  | 1.71                     | 0.56              |
| 12:Z:176:LYS:HD3  | 22:Z:309:CLA:O1D  | 2.05                     | 0.56              |
| 22:Z:309:CLA:H142 | 22:Z:309:CLA:H61  | 1.86                     | 0.56              |
| 22:7:308:CLA:OBD  | 22:7:315:CLA:HBA2 | 2.04                     | 0.56              |
| 22:6:309:CLA:H172 | 22:6:309:CLA:HMB3 | 1.88                     | 0.56              |
| 39:6:318:CHL:HAA2 | 39:6:318:CHL:HBD  | 1.88                     | 0.56              |
| 1:A:461:THR:HG21  | 22:B:812:CLA:HAB  | 1.87                     | 0.56              |
| 22:A:812:CLA:HBA1 | 22:A:812:CLA:HBD  | 1.87                     | 0.56              |
| 22:A:815:CLA:H121 | 24:3:306:BCR:H16C | 1.88                     | 0.56              |
| 22:A:818:CLA:HHD  | 22:A:835:CLA:H42  | 1.87                     | 0.56              |
| 22:A:820:CLA:HHC  | 22:A:820:CLA:CBB  | 2.33                     | 0.56              |
| 22:A:828:CLA:H43  | 22:A:828:CLA:HBA1 | 1.86                     | 0.56              |
| 2:B:296:PHE:HB3   | 7:G:100:ILE:HG21  | 1.86                     | 0.56              |
| 22:B:806:CLA:H13  | 24:B:849:BCR:H10C | 1.88                     | 0.56              |
| 39:Z:311:CHL:NC   | 25:Z:317:LHG:H102 | 2.21                     | 0.56              |
| 38:3:303:LUT:H28  | 22:3:311:CLA:H2   | 1.87                     | 0.56              |
| 15:8:78:THR:HG23  | 22:8:305:CLA:HMC2 | 1.87                     | 0.56              |
| 15:8:110:GLN:HB3  | 43:8:319:LPX:H2   | 1.87                     | 0.56              |
| 22:4:810:CLA:H12  | 39:4:816:CHL:C3D  | 2.35                     | 0.56              |
| 19:9:51:PHE:HB3   | 22:9:306:CLA:CAD  | 2.36                     | 0.56              |
| 1:A:201:HIS:O     | 1:A:205:LEU:HB3   | 2.05                     | 0.56              |
| 21:A:801:CL0:H12  | 22:A:802:CLA:CAD  | 2.36                     | 0.56              |
| 22:A:812:CLA:O1A  | 13:3:39:LEU:HB3   | 2.06                     | 0.56              |
| 22:A:838:CLA:H91  | 22:A:838:CLA:H143 | 1.86                     | 0.56              |
| 22:A:855:CLA:H111 | 22:B:840:CLA:H62  | 1.88                     | 0.56              |
| 2:B:481:SER:O     | 2:B:484:SER:HB2   | 2.05                     | 0.56              |
| 22:B:825:CLA:H141 | 22:B:832:CLA:HBC3 | 1.88                     | 0.56              |
| 4:D:139:TYR:CE2   | 4:D:149:TYR:HD1   | 2.23                     | 0.56              |
| 12:Z:159:PRO:HD2  | 38:Z:301:LUT:H23  | 1.88                     | 0.56              |
| 31:3:301:DGD:HA21 | 31:3:301:DGD:HA61 | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:8:312:CHL:HMC  | 26:8:318:NKP:HARA | 1.86                     | 0.56              |
| 18:6:123:PHE:CE1  | 22:6:302:CLA:HBD  | 2.41                     | 0.56              |
| 18:6:245:PHE:CE2  | 22:6:301:CLA:H91  | 2.40                     | 0.56              |
| 2:B:93:TRP:H      | 22:B:812:CLA:HED3 | 1.70                     | 0.56              |
| 2:B:190:ALA:HB1   | 22:B:816:CLA:HAB  | 1.88                     | 0.56              |
| 2:B:315:ARG:HB3   | 22:B:842:CLA:H43  | 1.88                     | 0.56              |
| 2:B:349:VAL:HA    | 22:B:820:CLA:H11  | 1.88                     | 0.56              |
| 2:B:470:LYS:HG2   | 2:B:473:TYR:CE2   | 2.41                     | 0.56              |
| 22:B:814:CLA:HAB  | 22:B:822:CLA:H72  | 1.87                     | 0.56              |
| 22:B:827:CLA:H172 | 22:B:833:CLA:HBC1 | 1.87                     | 0.56              |
| 3:C:22:PRO:HB3    | 3:C:53:ARG:NH1    | 2.21                     | 0.56              |
| 12:Z:100:TYR:O    | 12:Z:103:PRO:HD2  | 2.05                     | 0.56              |
| 22:3:320:CLA:C4D  | 41:7:319:3PH:H392 | 2.35                     | 0.56              |
| 14:7:164:GLU:HB2  | 14:7:167:TYR:HB2  | 1.87                     | 0.56              |
| 14:7:186:TYR:O    | 14:7:190:LYS:HG3  | 2.06                     | 0.56              |
| 22:7:322:CLA:HBA2 | 22:7:323:CLA:H102 | 1.88                     | 0.56              |
| 1:A:677:PHE:HB2   | 22:A:802:CLA:HAA1 | 1.89                     | 0.56              |
| 7:G:54:LEU:N      | 7:G:55:PRO:HD2    | 2.21                     | 0.56              |
| 12:Z:206:HIS:CB   | 22:Z:305:CLA:HAA2 | 2.33                     | 0.56              |
| 15:8:128:PHE:CZ   | 24:8:304:BCR:H10C | 2.41                     | 0.56              |
| 15:8:149:PHE:O    | 15:8:150:LEU:C    | 2.47                     | 0.56              |
| 38:8:302:LUT:H392 | 22:8:313:CLA:H41  | 1.89                     | 0.56              |
| 22:4:807:CLA:HBA1 | 22:4:807:CLA:CBD  | 2.33                     | 0.56              |
| 22:4:809:CLA:HHC  | 22:4:809:CLA:CBB  | 2.31                     | 0.56              |
| 19:9:51:PHE:HB3   | 22:9:306:CLA:C3D  | 2.36                     | 0.56              |
| 2:B:569:CYS:HG    | 29:B:802:SF4:FE1  | 1.22                     | 0.55              |
| 2:B:708:LEU:HD21  | 31:B:852:DGD:HA21 | 1.87                     | 0.55              |
| 22:B:805:CLA:HHC  | 22:B:805:CLA:CBB  | 2.32                     | 0.55              |
| 12:1:75:VAL:HG22  | 12:1:175:ILE:HD11 | 1.88                     | 0.55              |
| 12:Z:57:PRO:HG2   | 38:Z:302:LUT:H23  | 1.87                     | 0.55              |
| 22:Z:309:CLA:C2B  | 25:Z:317:LHG:HC2  | 2.35                     | 0.55              |
| 22:3:313:CLA:H2   | 22:3:319:CLA:CAD  | 2.36                     | 0.55              |
| 22:5:315:CLA:C1A  | 25:5:324:LHG:H142 | 2.36                     | 0.55              |
| 18:6:79:MET:HE3   | 22:6:307:CLA:HMC3 | 1.88                     | 0.55              |
| 18:6:238:ASP:HA   | 18:6:243:LYS:CA   | 2.19                     | 0.55              |
| 39:2:303:CHL:HAA1 | 39:2:303:CHL:HBD  | 1.88                     | 0.55              |
| 22:A:841:CLA:H111 | 22:B:801:CLA:H121 | 1.89                     | 0.55              |
| 27:A:852:DGA:HBW1 | 31:3:301:DGD:HA31 | 1.87                     | 0.55              |
| 2:B:427:SER:HB3   | 22:B:801:CLA:HBA1 | 1.89                     | 0.55              |
| 22:F:304:CLA:H2   | 22:F:304:CLA:H8   | 1.88                     | 0.55              |
| 38:8:303:LUT:H28  | 22:8:308:CLA:H72  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:8:304:BCR:H372 | 39:8:315:CHL:H162 | 1.87                     | 0.55              |
| 38:4:803:LUT:H193 | 39:4:816:CHL:CBB  | 2.36                     | 0.55              |
| 38:4:803:LUT:H30  | 22:4:808:CLA:H72  | 1.89                     | 0.55              |
| 22:4:810:CLA:O1A  | 22:4:818:CLA:HHC  | 2.06                     | 0.55              |
| 17:5:106:PRO:O    | 17:5:109:LEU:HB2  | 2.06                     | 0.55              |
| 17:5:127:LEU:HD13 | 22:6:314:CLA:H8   | 1.87                     | 0.55              |
| 17:5:182:LEU:HB3  | 22:5:307:CLA:HMA1 | 1.87                     | 0.55              |
| 1:A:349:TRP:CD2   | 22:A:825:CLA:H192 | 2.42                     | 0.55              |
| 1:A:535:VAL:HG22  | 1:A:539:HIS:NE2   | 2.22                     | 0.55              |
| 22:A:814:CLA:H11  | 22:A:816:CLA:HHB  | 1.88                     | 0.55              |
| 22:A:816:CLA:H43  | 22:A:816:CLA:HBA1 | 1.88                     | 0.55              |
| 2:B:6:PHE:CE2     | 2:B:25:GLY:HA3    | 2.41                     | 0.55              |
| 2:B:168:TRP:CE2   | 22:B:815:CLA:HAC2 | 2.41                     | 0.55              |
| 2:B:291:MET:HB2   | 22:B:823:CLA:HAC2 | 1.88                     | 0.55              |
| 11:L:131:ALA:HB1  | 24:L:204:BCR:C19  | 2.35                     | 0.55              |
| 12:Z:102:ALA:HB3  | 12:Z:103:PRO:HD3  | 1.88                     | 0.55              |
| 13:3:180:LEU:HB3  | 22:3:308:CLA:HMA2 | 1.87                     | 0.55              |
| 15:8:190:LYS:HD3  | 22:8:311:CLA:O1D  | 2.06                     | 0.55              |
| 17:5:202:VAL:HG22 | 17:5:252:LEU:HD12 | 1.89                     | 0.55              |
| 22:5:307:CLA:HMD2 | 39:5:317:CHL:H11  | 1.89                     | 0.55              |
| 18:6:89:GLU:HB3   | 18:6:200:LEU:HD12 | 1.88                     | 0.55              |
| 38:6:304:LUT:H28  | 22:6:310:CLA:C6   | 2.26                     | 0.55              |
| 6:F:126:GLY:H     | 6:F:132:HIS:CE1   | 2.24                     | 0.55              |
| 22:1:304:CLA:H122 | 22:1:305:CLA:CMB  | 2.36                     | 0.55              |
| 16:4:68:PRO:HG2   | 16:4:71:LEU:HD12  | 1.87                     | 0.55              |
| 1:A:438:ILE:HG13  | 1:A:556:PHE:HE2   | 1.71                     | 0.55              |
| 2:B:221:GLN:NE2   | 2:B:225:PRO:HG3   | 2.22                     | 0.55              |
| 22:B:817:CLA:H111 | 24:B:844:BCR:H383 | 1.88                     | 0.55              |
| 10:K:77:ILE:HG13  | 13:3:19:SER:HA    | 1.87                     | 0.55              |
| 12:Z:206:HIS:CG   | 22:Z:305:CLA:HAA2 | 2.42                     | 0.55              |
| 22:4:806:CLA:HMD3 | 22:4:811:CLA:C4D  | 2.37                     | 0.55              |
| 17:5:151:ILE:HD12 | 39:5:321:CHL:HMB2 | 1.87                     | 0.55              |
| 22:A:818:CLA:O1A  | 22:A:827:CLA:HBB2 | 2.05                     | 0.55              |
| 2:B:54:GLN:HE22   | 22:B:809:CLA:C1D  | 2.19                     | 0.55              |
| 2:B:87:PRO:HB3    | 2:B:122:TYR:CD1   | 2.42                     | 0.55              |
| 2:B:183:LEU:HD11  | 22:B:815:CLA:H43  | 1.87                     | 0.55              |
| 2:B:722:TYR:HB2   | 22:B:805:CLA:HED3 | 1.89                     | 0.55              |
| 8:I:80:VAL:HB     | 8:I:81:PRO:HD3    | 1.89                     | 0.55              |
| 13:3:68:MET:SD    | 22:3:308:CLA:HAB  | 2.46                     | 0.55              |
| 22:3:312:CLA:NB   | 22:3:318:CLA:H122 | 2.22                     | 0.55              |
| 22:6:308:CLA:OBD  | 22:6:313:CLA:HBD  | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:426:LEU:O     | 1:A:430:VAL:HG23  | 2.07                     | 0.55              |
| 2:B:408:VAL:O     | 2:B:412:MET:HG2   | 2.05                     | 0.55              |
| 2:B:546:LYS:HG3   | 6:F:225:SER:OG    | 2.07                     | 0.55              |
| 22:B:823:CLA:HHC  | 22:B:823:CLA:CBB  | 2.32                     | 0.55              |
| 22:B:842:CLA:HBB2 | 22:1:307:CLA:H61  | 1.88                     | 0.55              |
| 6:F:116:ALA:HB1   | 6:F:120:LYS:NZ    | 2.21                     | 0.55              |
| 6:F:201:THR:HA    | 22:8:309:CLA:C15  | 2.36                     | 0.55              |
| 8:I:63:ALA:HB2    | 20:2:206:GLU:OE2  | 2.07                     | 0.55              |
| 13:3:186:LYS:HA   | 24:3:307:BCR:H282 | 1.87                     | 0.55              |
| 22:3:320:CLA:C2D  | 41:7:319:3PH:H371 | 2.37                     | 0.55              |
| 15:8:157:LYS:HB2  | 15:8:157:LYS:NZ   | 2.22                     | 0.55              |
| 39:5:316:CHL:CBB  | 22:5:319:CLA:HBB2 | 2.37                     | 0.55              |
| 19:9:123:GLU:HB3  | 19:9:126:ARG:HH21 | 1.71                     | 0.55              |
| 20:2:211:VAL:HG13 | 39:2:303:CHL:H2   | 1.87                     | 0.55              |
| 1:A:414:VAL:HG13  | 1:A:567:ALA:HA    | 1.88                     | 0.55              |
| 1:A:575:CYS:HB3   | 1:A:584:CYS:HA    | 1.89                     | 0.55              |
| 22:A:804:CLA:C4B  | 22:A:811:CLA:H122 | 2.37                     | 0.55              |
| 22:A:806:CLA:HHC  | 22:A:806:CLA:CBB  | 2.37                     | 0.55              |
| 22:B:816:CLA:H13  | 24:B:846:BCR:H19C | 1.87                     | 0.55              |
| 4:D:128:LEU:HA    | 4:D:132:PHE:HD2   | 1.72                     | 0.55              |
| 13:3:97:ILE:HG22  | 13:3:99:PRO:HG2   | 1.89                     | 0.55              |
| 14:7:186:TYR:CE2  | 14:7:190:LYS:HD2  | 2.42                     | 0.55              |
| 22:A:824:CLA:CMD  | 22:A:825:CLA:HAB  | 2.34                     | 0.55              |
| 22:A:833:CLA:H203 | 22:B:840:CLA:HMA2 | 1.89                     | 0.55              |
| 2:B:493:LEU:O     | 2:B:496:PRO:HD2   | 2.07                     | 0.55              |
| 22:F:304:CLA:H12  | 22:F:304:CLA:C4A  | 2.36                     | 0.55              |
| 22:F:304:CLA:HBD  | 22:F:304:CLA:H151 | 1.88                     | 0.55              |
| 7:G:99:LEU:HG     | 22:G:202:CLA:CGA  | 2.37                     | 0.55              |
| 12:1:55:PHE:CD2   | 38:1:303:LUT:H383 | 2.41                     | 0.55              |
| 18:6:162:PHE:CZ   | 18:6:164:PRO:HB3  | 2.42                     | 0.55              |
| 2:B:40:GLU:O      | 2:B:44:TYR:HD1    | 1.90                     | 0.55              |
| 22:Z:304:CLA:HED2 | 22:Z:304:CLA:H2A  | 1.88                     | 0.55              |
| 22:8:305:CLA:HMB1 | 22:8:305:CLA:HBB1 | 1.88                     | 0.55              |
| 16:4:85:SER:HB2   | 16:4:88:VAL:CG2   | 2.37                     | 0.55              |
| 16:4:237:LYS:HB2  | 16:4:242:ASN:HD21 | 1.72                     | 0.55              |
| 39:4:819:CHL:HAA2 | 39:4:819:CHL:HBD  | 1.89                     | 0.55              |
| 17:5:88:VAL:HG22  | 17:5:100:TRP:CD1  | 2.42                     | 0.55              |
| 18:6:237:THR:HG21 | 39:6:315:CHL:HED2 | 1.89                     | 0.55              |
| 18:6:252:GLY:HA3  | 22:6:301:CLA:HED1 | 1.89                     | 0.55              |
| 1:A:348:SER:O     | 22:A:825:CLA:H191 | 2.07                     | 0.54              |
| 1:A:459:ASN:HB3   | 1:A:471:MET:HE3   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:822:CLA:C3D  | 24:A:856:BCR:H292 | 2.37                     | 0.54              |
| 22:B:823:CLA:H62  | 22:B:824:CLA:H72  | 1.89                     | 0.54              |
| 7:G:48:VAL:O      | 7:G:52:ALA:HB3    | 2.06                     | 0.54              |
| 22:L:201:CLA:HHC  | 22:L:201:CLA:CBB  | 2.33                     | 0.54              |
| 39:1:312:CHL:HBA1 | 31:1:319:DGD:HB31 | 1.89                     | 0.54              |
| 40:1:318:SQD:H131 | 15:8:138:LEU:HG   | 1.89                     | 0.54              |
| 13:3:121:MET:HE3  | 13:3:125:GLU:HG3  | 1.89                     | 0.54              |
| 22:8:307:CLA:HBA1 | 22:8:307:CLA:CBD  | 2.33                     | 0.54              |
| 22:5:301:CLA:H61  | 22:5:320:CLA:HED1 | 1.88                     | 0.54              |
| 19:9:206:GLN:NE2  | 19:9:206:GLN:H    | 2.05                     | 0.54              |
| 1:A:21:PRO:HD3    | 1:A:183:LYS:O     | 2.08                     | 0.54              |
| 1:A:672:PHE:CE2   | 1:A:676:HIS:HE1   | 2.26                     | 0.54              |
| 27:A:852:DGA:HA52 | 14:7:243:PHE:HB3  | 1.89                     | 0.54              |
| 22:B:810:CLA:HMB3 | 22:B:811:CLA:HHB  | 1.89                     | 0.54              |
| 22:B:833:CLA:HMB1 | 22:B:833:CLA:HBB1 | 1.90                     | 0.54              |
| 6:F:196:THR:HB    | 22:F:305:CLA:HED2 | 1.89                     | 0.54              |
| 13:3:114:PHE:CE2  | 22:3:316:CLA:H2   | 2.42                     | 0.54              |
| 13:3:226:LEU:HA   | 13:3:229:PHE:CD2  | 2.42                     | 0.54              |
| 25:7:318:LHG:H122 | 25:7:318:LHG:H322 | 1.89                     | 0.54              |
| 22:5:307:CLA:H71  | 22:5:307:CLA:H41  | 1.87                     | 0.54              |
| 1:A:13:VAL:HG12   | 22:A:812:CLA:H2A  | 1.88                     | 0.54              |
| 22:A:805:CLA:HAA2 | 22:A:825:CLA:H41  | 1.90                     | 0.54              |
| 22:A:825:CLA:HMA2 | 22:A:827:CLA:H92  | 1.90                     | 0.54              |
| 2:B:23:TRP:HB3    | 31:B:852:DGD:HA41 | 1.89                     | 0.54              |
| 12:Z:115:PHE:CD2  | 22:Z:308:CLA:HMD2 | 2.42                     | 0.54              |
| 12:Z:195:THR:CG2  | 12:Z:197:LYS:HE2  | 2.37                     | 0.54              |
| 17:5:103:ALA:HB1  | 22:5:312:CLA:HED3 | 1.89                     | 0.54              |
| 1:A:75:SER:OG     | 1:A:181:TYR:HB2   | 2.07                     | 0.54              |
| 1:A:247:ARG:NH1   | 31:3:301:DGD:HE4  | 2.22                     | 0.54              |
| 22:B:807:CLA:HBA1 | 22:B:807:CLA:CHA  | 2.38                     | 0.54              |
| 12:1:39:SER:HA    | 15:8:135:MET:HE2  | 1.89                     | 0.54              |
| 12:Z:86:ALA:HB1   | 22:Z:303:CLA:H192 | 1.89                     | 0.54              |
| 12:Z:185:CYS:HA   | 12:Z:188:PHE:CD2  | 2.42                     | 0.54              |
| 22:Z:303:CLA:HBC2 | 22:Z:313:CLA:H12  | 1.88                     | 0.54              |
| 14:7:66:ARG:HG2   | 14:7:142:PHE:CZ   | 2.43                     | 0.54              |
| 15:8:220:HIS:HA   | 15:8:227:THR:OG1  | 2.08                     | 0.54              |
| 17:5:58:LEU:HD22  | 22:5:315:CLA:H142 | 1.90                     | 0.54              |
| 18:6:123:PHE:HB2  | 22:6:302:CLA:C1   | 2.37                     | 0.54              |
| 18:6:139:ASP:O    | 18:6:148:LYS:HG3  | 2.06                     | 0.54              |
| 22:A:816:CLA:H42  | 27:A:852:DGA:HAF1 | 1.89                     | 0.54              |
| 22:A:822:CLA:HMA2 | 22:A:823:CLA:HBD  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:160:PRO:O     | 2:B:161:SER:HB3   | 2.07                     | 0.54              |
| 2:B:298:ILE:HG22  | 7:G:57:HIS:CE1    | 2.43                     | 0.54              |
| 2:B:549:PRO:HB2   | 3:C:62:PHE:CE2    | 2.42                     | 0.54              |
| 13:3:138:MET:HE1  | 14:7:35:PRO:O     | 2.08                     | 0.54              |
| 38:4:803:LUT:H28  | 22:4:808:CLA:C5   | 2.38                     | 0.54              |
| 22:6:309:CLA:C4B  | 22:6:309:CLA:H62  | 2.37                     | 0.54              |
| 2:B:92:ILE:HD11   | 2:B:115:ASN:ND2   | 2.23                     | 0.54              |
| 2:B:617:LEU:HD21  | 22:B:805:CLA:H202 | 1.90                     | 0.54              |
| 2:B:695:LYS:HD2   | 8:I:100:GLU:HB3   | 1.90                     | 0.54              |
| 2:B:697:LYS:HD3   | 3:C:81:TYR:HD2    | 1.71                     | 0.54              |
| 11:L:79:VAL:HB    | 11:L:84:ARG:HG3   | 1.90                     | 0.54              |
| 11:L:102:LYS:HG2  | 22:L:203:CLA:HMA1 | 1.88                     | 0.54              |
| 12:1:39:SER:HB2   | 40:1:318:SQD:H62  | 1.88                     | 0.54              |
| 13:3:80:LEU:HD11  | 24:3:305:BCR:H401 | 1.89                     | 0.54              |
| 13:3:216:HIS:CG   | 22:3:310:CLA:HAA1 | 2.42                     | 0.54              |
| 22:3:316:CLA:HHC  | 22:3:316:CLA:CBB  | 2.34                     | 0.54              |
| 17:5:192:ILE:HD11 | 22:5:313:CLA:HHD  | 1.89                     | 0.54              |
| 22:5:326:CLA:CMD  | 22:6:309:CLA:H2   | 2.37                     | 0.54              |
| 18:6:66:TRP:HE1   | 22:6:311:CLA:H11  | 1.72                     | 0.54              |
| 18:6:87:VAL:C     | 18:6:89:GLU:H     | 2.16                     | 0.54              |
| 18:6:254:TRP:CG   | 22:6:319:CLA:HED1 | 2.43                     | 0.54              |
| 38:6:303:LUT:C30  | 22:6:307:CLA:H8   | 2.38                     | 0.54              |
| 22:A:812:CLA:O1D  | 22:A:813:CLA:HMC1 | 2.07                     | 0.54              |
| 24:A:848:BCR:H393 | 22:B:801:CLA:H102 | 1.90                     | 0.54              |
| 2:B:263:HIS:HE1   | 2:B:265:GLN:HB3   | 1.73                     | 0.54              |
| 2:B:680:VAL:HG13  | 2:B:694:TRP:CZ2   | 2.43                     | 0.54              |
| 6:F:165:TYR:O     | 6:F:168:ARG:HG2   | 2.07                     | 0.54              |
| 7:G:56:LEU:HG     | 7:G:59:ARG:HH22   | 1.72                     | 0.54              |
| 14:7:198:ARG:HA   | 14:7:201:MET:HE2  | 1.90                     | 0.54              |
| 22:7:322:CLA:HMC2 | 15:8:221:LEU:HD21 | 1.89                     | 0.54              |
| 22:4:808:CLA:HBB2 | 22:4:809:CLA:CHB  | 2.37                     | 0.54              |
| 17:5:182:LEU:HB3  | 22:5:307:CLA:HMA2 | 1.89                     | 0.54              |
| 39:5:316:CHL:H122 | 39:5:316:CHL:C9   | 2.36                     | 0.54              |
| 18:6:238:ASP:HB2  | 18:6:243:LYS:HG2  | 1.89                     | 0.54              |
| 22:A:812:CLA:HBA1 | 22:A:812:CLA:CBD  | 2.37                     | 0.54              |
| 22:A:815:CLA:H92  | 13:3:203:VAL:HG21 | 1.90                     | 0.54              |
| 2:B:235:ALA:HA    | 2:B:257:THR:HG22  | 1.90                     | 0.54              |
| 2:B:515:PRO:HG2   | 6:F:132:HIS:CD2   | 2.42                     | 0.54              |
| 22:B:819:CLA:O1A  | 22:B:828:CLA:HBB2 | 2.07                     | 0.54              |
| 22:1:305:CLA:HHC  | 22:1:305:CLA:CBB  | 2.32                     | 0.54              |
| 12:Z:153:PRO:HD3  | 22:Z:313:CLA:CMD  | 2.35                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:7:302:LUT:C32  | 22:7:307:CLA:HAB  | 2.27                     | 0.54              |
| 15:8:39:HIS:HA    | 15:8:41:LYS:HZ3   | 1.72                     | 0.54              |
| 22:5:309:CLA:H11  | 22:5:314:CLA:HMD2 | 1.90                     | 0.54              |
| 2:B:438:TYR:CD1   | 2:B:617:LEU:HG    | 2.43                     | 0.54              |
| 39:7:313:CHL:HAA1 | 39:7:313:CHL:HBD  | 1.90                     | 0.54              |
| 22:8:310:CLA:HBA2 | 43:8:319:LPX:H3   | 1.90                     | 0.54              |
| 1:A:578:PRO:HG3   | 3:C:52:LYS:HD2    | 1.89                     | 0.54              |
| 1:A:682:SER:HB2   | 1:A:727:GLY:O     | 2.08                     | 0.54              |
| 22:A:804:CLA:C3B  | 22:A:811:CLA:H122 | 2.38                     | 0.54              |
| 22:A:814:CLA:H43  | 22:A:816:CLA:H41  | 1.90                     | 0.54              |
| 22:B:813:CLA:HMB3 | 22:B:813:CLA:CBB  | 2.35                     | 0.54              |
| 22:B:823:CLA:C1B  | 22:B:824:CLA:H8   | 2.38                     | 0.54              |
| 4:D:77:LYS:HG3    | 4:D:81:GLU:HB3    | 1.90                     | 0.54              |
| 7:G:33:GLU:HB2    | 7:G:35:TYR:CD2    | 2.43                     | 0.54              |
| 22:1:308:CLA:HHC  | 22:1:308:CLA:CBB  | 2.37                     | 0.54              |
| 12:Z:157:PHE:HA   | 22:Z:313:CLA:C7   | 2.38                     | 0.54              |
| 39:8:312:CHL:CMC  | 26:8:318:NKP:HARA | 2.38                     | 0.54              |
| 22:4:810:CLA:H43  | 39:4:816:CHL:HBD  | 1.90                     | 0.54              |
| 38:5:302:LUT:H373 | 22:5:307:CLA:H42  | 1.89                     | 0.54              |
| 22:5:308:CLA:HMB3 | 22:5:308:CLA:H151 | 1.89                     | 0.54              |
| 25:5:324:LHG:H102 | 25:5:324:LHG:H281 | 1.89                     | 0.54              |
| 18:6:251:GLN:HB2  | 22:6:301:CLA:HBA1 | 1.90                     | 0.54              |
| 19:9:137:GLY:HA2  | 19:9:144:PHE:HB2  | 1.90                     | 0.54              |
| 1:A:49:ILE:H      | 1:A:49:ILE:HD12   | 1.74                     | 0.53              |
| 1:A:646:LEU:HD12  | 1:A:650:LEU:HD12  | 1.90                     | 0.53              |
| 1:A:707:LEU:HD23  | 6:F:216:THR:HG22  | 1.90                     | 0.53              |
| 22:A:805:CLA:H101 | 24:A:845:BCR:HC8  | 1.89                     | 0.53              |
| 6:F:123:LEU:HD11  | 9:J:38:VAL:HG11   | 1.90                     | 0.53              |
| 38:4:802:LUT:C14  | 22:4:806:CLA:HAB  | 2.37                     | 0.53              |
| 17:5:128:LEU:HB3  | 24:5:304:BCR:H15C | 1.89                     | 0.53              |
| 18:6:219:ALA:HB2  | 18:6:229:PRO:HD3  | 1.90                     | 0.53              |
| 19:9:29:PRO:HB3   | 22:9:311:CLA:HED2 | 1.90                     | 0.53              |
| 1:A:80:GLN:O      | 1:A:83:VAL:HG22   | 2.08                     | 0.53              |
| 22:A:805:CLA:H143 | 24:A:844:BCR:C5   | 2.38                     | 0.53              |
| 22:A:812:CLA:H172 | 22:A:812:CLA:H143 | 1.89                     | 0.53              |
| 2:B:200:ILE:HB    | 2:B:201:PRO:HD3   | 1.90                     | 0.53              |
| 3:C:62:PHE:HE1    | 3:C:66:ARG:HH21   | 1.55                     | 0.53              |
| 6:F:190:PRO:O     | 6:F:194:ARG:HG3   | 2.08                     | 0.53              |
| 7:G:97:PHE:CD2    | 7:G:102:THR:HG22  | 2.43                     | 0.53              |
| 8:I:67:TYR:CZ     | 8:I:69:PHE:HB2    | 2.43                     | 0.53              |
| 11:L:140:PHE:HA   | 11:L:144:PRO:CD   | 2.38                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:Z:103:PRO:HB3  | 22:Z:315:CLA:HMC3 | 1.91                     | 0.53              |
| 13:3:111:TYR:CE2  | 22:3:316:CLA:HMA2 | 2.42                     | 0.53              |
| 38:7:301:LUT:H30  | 22:7:304:CLA:H72  | 1.89                     | 0.53              |
| 15:8:202:PHE:CZ   | 38:8:302:LUT:H8   | 2.42                     | 0.53              |
| 17:5:33:LYS:HB3   | 22:5:315:CLA:CBC  | 2.37                     | 0.53              |
| 22:5:301:CLA:HHC  | 22:5:301:CLA:HBB1 | 1.89                     | 0.53              |
| 22:A:812:CLA:HHC  | 22:A:812:CLA:CBB  | 2.36                     | 0.53              |
| 22:A:821:CLA:C2C  | 22:A:827:CLA:H18  | 2.38                     | 0.53              |
| 2:B:442:ASP:OD1   | 2:B:616:TYR:HB2   | 2.08                     | 0.53              |
| 12:1:94:LEU:HD12  | 22:1:309:CLA:CMD  | 2.38                     | 0.53              |
| 22:Z:308:CLA:HMA3 | 22:Z:315:CLA:C2C  | 2.38                     | 0.53              |
| 13:3:78:GLU:HB3   | 13:3:82:LYS:HE3   | 1.91                     | 0.53              |
| 24:3:305:BCR:H21C | 22:3:313:CLA:CAC  | 2.36                     | 0.53              |
| 22:3:312:CLA:HHC  | 22:3:312:CLA:CBB  | 2.38                     | 0.53              |
| 22:7:307:CLA:H92  | 22:7:308:CLA:H72  | 1.90                     | 0.53              |
| 17:5:124:TRP:NE1  | 22:5:326:CLA:HMA3 | 2.23                     | 0.53              |
| 22:A:837:CLA:HHC  | 22:A:837:CLA:CBB  | 2.31                     | 0.53              |
| 2:B:241:ALA:HA    | 2:B:264:PRO:HG3   | 1.90                     | 0.53              |
| 2:B:590:TRP:CD1   | 22:B:805:CLA:H152 | 2.42                     | 0.53              |
| 6:F:163:ILE:HG12  | 22:F:305:CLA:C4D  | 2.39                     | 0.53              |
| 8:I:78:VAL:C      | 8:I:81:PRO:HD2    | 2.33                     | 0.53              |
| 11:L:160:PRO:O    | 11:L:166:GLY:HA3  | 2.07                     | 0.53              |
| 39:Z:312:CHL:CAB  | 22:Z:315:CLA:HBB2 | 2.38                     | 0.53              |
| 15:8:136:ASP:O    | 15:8:140:PRO:HA   | 2.09                     | 0.53              |
| 16:4:106:TRP:CH2  | 24:4:804:BCR:H372 | 2.44                     | 0.53              |
| 22:4:806:CLA:C4D  | 22:4:811:CLA:H61  | 2.38                     | 0.53              |
| 18:6:221:VAL:HB   | 22:6:322:CLA:C1C  | 2.39                     | 0.53              |
| 22:A:806:CLA:CBB  | 24:A:845:BCR:HC31 | 2.39                     | 0.53              |
| 2:B:48:PHE:HB2    | 2:B:169:PHE:HE1   | 1.74                     | 0.53              |
| 2:B:355:SER:HB3   | 22:B:828:CLA:HAC2 | 1.89                     | 0.53              |
| 22:B:827:CLA:C3B  | 24:B:848:BCR:H19C | 2.38                     | 0.53              |
| 22:B:828:CLA:C11  | 24:B:847:BCR:H373 | 2.38                     | 0.53              |
| 22:3:312:CLA:C1D  | 22:3:318:CLA:H93  | 2.38                     | 0.53              |
| 22:3:313:CLA:H202 | 22:5:320:CLA:CHB  | 2.37                     | 0.53              |
| 24:7:303:BCR:H333 | 22:7:322:CLA:H8   | 1.90                     | 0.53              |
| 22:4:807:CLA:H71  | 25:4:820:LHG:H171 | 1.90                     | 0.53              |
| 22:4:807:CLA:HBB1 | 22:4:807:CLA:HMB1 | 1.90                     | 0.53              |
| 17:5:140:TYR:OH   | 22:5:323:CLA:HBA2 | 2.09                     | 0.53              |
| 24:6:305:BCR:H291 | 22:6:312:CLA:H2   | 1.91                     | 0.53              |
| 22:6:307:CLA:HMD1 | 39:6:316:CHL:CGA  | 2.38                     | 0.53              |
| 22:A:819:CLA:HHD  | 24:A:845:BCR:H352 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:244:VAL:HB    | 2:B:247:THR:OG1   | 2.09                     | 0.53              |
| 2:B:320:HIS:O     | 2:B:323:LEU:HB2   | 2.08                     | 0.53              |
| 2:B:379:ILE:O     | 2:B:383:ILE:HG13  | 2.09                     | 0.53              |
| 10:K:61:THR:HA    | 10:K:67:LEU:HA    | 1.91                     | 0.53              |
| 22:K:205:CLA:CMD  | 24:K:206:BCR:H21C | 2.39                     | 0.53              |
| 22:Z:304:CLA:HHC  | 22:Z:304:CLA:CBB  | 2.37                     | 0.53              |
| 22:Z:316:CLA:HBD  | 22:Z:316:CLA:H72  | 1.91                     | 0.53              |
| 15:8:110:GLN:HG2  | 43:8:319:LPX:H1   | 1.89                     | 0.53              |
| 17:5:131:TRP:HH2  | 24:5:304:BCR:H323 | 1.74                     | 0.53              |
| 38:5:302:LUT:H30  | 22:5:307:CLA:H51  | 1.91                     | 0.53              |
| 1:A:44:ASN:HB3    | 5:E:78:GLN:NE2    | 2.23                     | 0.53              |
| 1:A:95:GLY:HA2    | 1:A:99:SER:HB3    | 1.89                     | 0.53              |
| 2:B:312:PRO:HB2   | 25:B:850:LHG:HC32 | 1.90                     | 0.53              |
| 38:1:303:LUT:C28  | 22:1:307:CLA:H111 | 2.39                     | 0.53              |
| 22:Z:304:CLA:ND   | 22:Z:309:CLA:H62  | 2.23                     | 0.53              |
| 22:8:308:CLA:H12  | 22:8:308:CLA:CHB  | 2.39                     | 0.53              |
| 22:6:311:CLA:HBB1 | 22:6:311:CLA:HMB3 | 1.89                     | 0.53              |
| 22:2:302:CLA:HBA1 | 22:2:302:CLA:CHA  | 2.38                     | 0.53              |
| 1:A:190:TRP:CD1   | 22:A:812:CLA:HED2 | 2.43                     | 0.53              |
| 2:B:588:ILE:O     | 2:B:591:VAL:HG22  | 2.09                     | 0.53              |
| 2:B:655:HIS:HB2   | 22:B:806:CLA:HBA1 | 1.89                     | 0.53              |
| 22:B:825:CLA:H111 | 24:B:847:BCR:C15  | 2.38                     | 0.53              |
| 22:B:830:CLA:HHC  | 22:B:830:CLA:CBB  | 2.35                     | 0.53              |
| 6:F:107:THR:HA    | 6:F:110:ARG:HE    | 1.73                     | 0.53              |
| 24:G:203:BCR:H341 | 24:G:203:BCR:C12  | 2.39                     | 0.53              |
| 12:1:194:ALA:HB1  | 12:1:218:ASN:ND2  | 2.23                     | 0.53              |
| 22:Z:313:CLA:H172 | 22:Z:313:CLA:CHC  | 2.39                     | 0.53              |
| 22:3:311:CLA:HBB1 | 22:3:311:CLA:HMB1 | 1.90                     | 0.53              |
| 38:7:302:LUT:H26  | 22:7:307:CLA:H61  | 1.89                     | 0.53              |
| 22:6:302:CLA:C3D  | 24:6:305:BCR:HC41 | 2.38                     | 0.53              |
| 19:9:111:LEU:HD22 | 39:9:312:CHL:HAB  | 1.89                     | 0.53              |
| 1:A:248:GLN:CD    | 1:A:248:GLN:H     | 2.17                     | 0.53              |
| 1:A:679:TRP:CE3   | 21:A:801:CL0:H6   | 2.43                     | 0.53              |
| 22:A:809:CLA:O1A  | 22:A:809:CLA:HBD  | 2.08                     | 0.53              |
| 22:A:812:CLA:H142 | 13:3:39:LEU:HD11  | 1.89                     | 0.53              |
| 22:A:812:CLA:H92  | 22:3:311:CLA:H112 | 1.91                     | 0.53              |
| 22:A:815:CLA:H2   | 13:3:203:VAL:CG1  | 2.38                     | 0.53              |
| 24:A:856:BCR:C13  | 24:K:206:BCR:HC8  | 2.39                     | 0.53              |
| 10:K:78:SER:HB2   | 10:K:85:THR:HG22  | 1.91                     | 0.53              |
| 22:Z:316:CLA:HHC  | 22:Z:316:CLA:CBB  | 2.32                     | 0.53              |
| 13:3:180:LEU:HB3  | 22:3:308:CLA:CMA  | 2.39                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:3:303:LUT:H183 | 22:3:313:CLA:C4B  | 2.38                     | 0.53              |
| 14:7:76:ALA:HB1   | 14:7:197:GLY:HA3  | 1.91                     | 0.53              |
| 22:7:323:CLA:CAB  | 25:8:317:LHG:H151 | 2.38                     | 0.53              |
| 15:8:236:ILE:HD11 | 22:8:316:CLA:HBC3 | 1.89                     | 0.53              |
| 22:8:307:CLA:CGA  | 22:8:307:CLA:C1A  | 2.86                     | 0.53              |
| 24:5:304:BCR:H271 | 22:5:312:CLA:CHB  | 2.39                     | 0.53              |
| 22:5:311:CLA:H52  | 22:5:323:CLA:HAB  | 1.91                     | 0.53              |
| 18:6:66:TRP:CZ2   | 22:6:317:CLA:HAA2 | 2.44                     | 0.53              |
| 18:6:157:PRO:HG2  | 22:6:307:CLA:HMD2 | 1.89                     | 0.53              |
| 38:6:303:LUT:H26  | 22:6:307:CLA:O1A  | 2.08                     | 0.53              |
| 1:A:204:GLY:HA3   | 22:A:813:CLA:HBB1 | 1.90                     | 0.53              |
| 1:A:488:GLN:HA    | 1:A:510:TRP:HE3   | 1.74                     | 0.53              |
| 22:A:821:CLA:H43  | 22:A:835:CLA:H143 | 1.91                     | 0.53              |
| 12:Z:144:GLU:HB2  | 22:Z:313:CLA:HAC1 | 1.90                     | 0.53              |
| 13:3:227:THR:O    | 13:3:231:LYS:HG2  | 2.09                     | 0.53              |
| 16:4:133:PRO:HG2  | 16:4:136:GLU:CB   | 2.38                     | 0.53              |
| 17:5:185:LYS:HZ3  | 22:5:313:CLA:HBD  | 1.73                     | 0.53              |
| 17:5:227:TRP:NE1  | 22:5:314:CLA:HED2 | 2.23                     | 0.53              |
| 18:6:141:ASP:HB3  | 18:6:144:PHE:O    | 2.08                     | 0.53              |
| 19:9:81:VAL:CG1   | 38:9:301:LUT:H12  | 2.36                     | 0.53              |
| 22:9:305:CLA:HBA1 | 22:9:305:CLA:HBD  | 1.90                     | 0.53              |
| 1:A:264:PHE:HA    | 1:A:269:TRP:CD1   | 2.44                     | 0.52              |
| 1:A:681:PHE:HZ    | 22:A:841:CLA:HBC2 | 1.74                     | 0.52              |
| 22:A:802:CLA:H12  | 2:B:617:LEU:HD13  | 1.90                     | 0.52              |
| 22:A:816:CLA:NC   | 27:A:852:DGA:HB52 | 2.24                     | 0.52              |
| 22:B:810:CLA:H62  | 22:B:810:CLA:C1C  | 2.38                     | 0.52              |
| 4:D:156:VAL:HG12  | 4:D:160:LYS:HB2   | 1.90                     | 0.52              |
| 12:1:203:LEU:HB2  | 38:1:302:LUT:H22  | 1.91                     | 0.52              |
| 22:Z:304:CLA:CAD  | 22:Z:309:CLA:HBD  | 2.39                     | 0.52              |
| 22:Z:304:CLA:HMD3 | 22:Z:309:CLA:CHA  | 2.39                     | 0.52              |
| 14:7:119:SER:HB3  | 15:8:226:LYS:HG3  | 1.91                     | 0.52              |
| 16:4:185:LEU:HD11 | 16:4:197:PHE:CD2  | 2.44                     | 0.52              |
| 18:6:147:ASN:HD21 | 39:6:320:CHL:HAA1 | 1.72                     | 0.52              |
| 1:A:45:THR:HG23   | 5:E:78:GLN:NE2    | 2.21                     | 0.52              |
| 1:A:247:ARG:HB2   | 31:3:301:DGD:O3D  | 2.09                     | 0.52              |
| 22:A:855:CLA:H202 | 24:L:204:BCR:H391 | 1.91                     | 0.52              |
| 2:B:394:PHE:HA    | 2:B:398:ASP:OD1   | 2.09                     | 0.52              |
| 12:Z:88:CYS:HA    | 12:Z:99:TRP:HB3   | 1.90                     | 0.52              |
| 12:Z:144:GLU:HG3  | 22:Z:313:CLA:HBC1 | 1.91                     | 0.52              |
| 39:Z:312:CHL:HHC  | 22:Z:315:CLA:HAB  | 1.90                     | 0.52              |
| 13:3:169:LEU:HB2  | 22:3:308:CLA:O1A  | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:6:141:ASP:CB   | 18:6:147:ASN:HB2  | 2.40                     | 0.52              |
| 20:2:180:LYS:HE2  | 22:2:301:CLA:HED3 | 1.91                     | 0.52              |
| 22:1:307:CLA:H102 | 22:1:308:CLA:CMB  | 2.40                     | 0.52              |
| 39:1:312:CHL:HAA2 | 31:1:319:DGD:O2G  | 2.09                     | 0.52              |
| 22:3:322:CLA:HMB3 | 41:7:319:3PH:H2A1 | 1.89                     | 0.52              |
| 17:5:33:LYS:HB3   | 22:5:315:CLA:HBC3 | 1.91                     | 0.52              |
| 22:5:301:CLA:H62  | 22:5:301:CLA:NB   | 2.25                     | 0.52              |
| 22:9:313:CLA:HHC  | 22:9:313:CLA:CBB  | 2.40                     | 0.52              |
| 20:2:197:ASN:CA   | 22:2:301:CLA:HBA2 | 2.35                     | 0.52              |
| 1:A:366:ILE:HG22  | 1:A:370:HIS:CE1   | 2.45                     | 0.52              |
| 22:A:834:CLA:HMA1 | 11:L:103:LEU:HB3  | 1.91                     | 0.52              |
| 2:B:561:ASP:CG    | 3:C:66:ARG:HH12   | 2.17                     | 0.52              |
| 6:F:205:GLN:HG2   | 15:8:55:LEU:HD23  | 1.91                     | 0.52              |
| 7:G:38:VAL:HG11   | 22:G:201:CLA:C3D  | 2.40                     | 0.52              |
| 13:3:199:GLY:O    | 13:3:203:VAL:HG23 | 2.09                     | 0.52              |
| 24:3:304:BCR:H402 | 22:3:313:CLA:C1B  | 2.39                     | 0.52              |
| 22:4:810:CLA:HMA2 | 39:4:816:CHL:C4C  | 2.39                     | 0.52              |
| 17:5:171:PRO:HD2  | 38:5:302:LUT:C23  | 2.38                     | 0.52              |
| 1:A:32:PRO:HB2    | 1:A:48:TRP:HH2    | 1.74                     | 0.52              |
| 22:A:818:CLA:HMD2 | 22:A:827:CLA:HMB1 | 1.92                     | 0.52              |
| 22:A:826:CLA:HAA2 | 22:A:827:CLA:OBD  | 2.10                     | 0.52              |
| 26:A:851:NKP:HAGA | 26:A:851:NKP:OAE  | 2.09                     | 0.52              |
| 2:B:628:ASN:HB2   | 2:B:725:PHE:CZ    | 2.44                     | 0.52              |
| 2:B:708:LEU:HD21  | 31:B:852:DGD:HA51 | 1.91                     | 0.52              |
| 22:B:818:CLA:NC   | 22:B:818:CLA:H51  | 2.24                     | 0.52              |
| 3:C:12:ILE:HG12   | 29:C:102:SF4:S2   | 2.50                     | 0.52              |
| 8:I:92:MET:HB3    | 24:L:204:BCR:H12C | 1.91                     | 0.52              |
| 38:1:303:LUT:H28  | 22:1:307:CLA:H8   | 1.90                     | 0.52              |
| 14:7:189:TYR:HB3  | 22:7:304:CLA:CMA  | 2.40                     | 0.52              |
| 39:9:312:CHL:H2A  | 39:9:312:CHL:O2A  | 2.09                     | 0.52              |
| 1:A:278:PHE:HZ    | 22:A:818:CLA:H43  | 1.75                     | 0.52              |
| 22:A:823:CLA:NB   | 37:K:201:DAO:H91  | 2.24                     | 0.52              |
| 22:B:828:CLA:HHC  | 22:B:828:CLA:CBB  | 2.38                     | 0.52              |
| 10:K:107:LEU:HD21 | 22:K:203:CLA:HBB1 | 1.91                     | 0.52              |
| 24:3:307:BCR:H402 | 25:3:321:LHG:O6   | 2.09                     | 0.52              |
| 22:8:311:CLA:HMA2 | 33:4:801:LMT:H5'  | 1.92                     | 0.52              |
| 18:6:107:PRO:HD2  | 39:6:318:CHL:CMD  | 2.40                     | 0.52              |
| 18:6:186:ILE:HD11 | 22:6:311:CLA:HAB  | 1.91                     | 0.52              |
| 22:A:804:CLA:HED1 | 22:A:811:CLA:HBD  | 1.90                     | 0.52              |
| 2:B:390:HIS:HA    | 2:B:393:ILE:HD12  | 1.91                     | 0.52              |
| 22:Z:304:CLA:OBD  | 22:Z:309:CLA:HBD  | 2.08                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:3:38:PRO:HD2   | 38:3:303:LUT:C23  | 2.40                     | 0.52              |
| 24:3:305:BCR:H24C | 22:3:313:CLA:CAC  | 2.39                     | 0.52              |
| 24:3:305:BCR:H342 | 39:3:317:CHL:HHB  | 1.92                     | 0.52              |
| 24:3:307:BCR:H311 | 22:3:315:CLA:HMA1 | 1.90                     | 0.52              |
| 16:4:210:LEU:HB3  | 22:4:805:CLA:CMA  | 2.39                     | 0.52              |
| 38:4:802:LUT:H382 | 22:4:805:CLA:C4D  | 2.39                     | 0.52              |
| 17:5:95:ARG:NH1   | 17:5:110:PRO:HB3  | 2.25                     | 0.52              |
| 17:5:138:GLN:NE2  | 18:6:35:GLY:HA3   | 2.25                     | 0.52              |
| 22:5:311:CLA:OBD  | 22:5:318:CLA:HAA1 | 2.09                     | 0.52              |
| 18:6:34:PRO:HD2   | 22:6:314:CLA:O1D  | 2.09                     | 0.52              |
| 18:6:108:PHE:CD2  | 18:6:113:LEU:HD21 | 2.44                     | 0.52              |
| 22:6:319:CLA:HHC  | 22:6:319:CLA:HBB1 | 1.91                     | 0.52              |
| 1:A:197:MET:CG    | 22:A:813:CLA:HBC2 | 2.38                     | 0.52              |
| 2:B:477:LEU:H     | 2:B:480:SER:HB2   | 1.75                     | 0.52              |
| 2:B:688:LEU:HB2   | 24:B:853:BCR:HC31 | 1.92                     | 0.52              |
| 22:B:827:CLA:HMB1 | 22:B:827:CLA:HBB1 | 1.92                     | 0.52              |
| 12:Z:87:GLY:HA3   | 38:Z:302:LUT:H182 | 1.91                     | 0.52              |
| 12:Z:203:LEU:HD22 | 38:Z:301:LUT:H172 | 1.92                     | 0.52              |
| 14:7:55:PRO:HD2   | 38:7:302:LUT:H23  | 1.90                     | 0.52              |
| 24:7:303:BCR:H292 | 22:7:309:CLA:H71  | 1.90                     | 0.52              |
| 38:8:302:LUT:H373 | 22:8:305:CLA:H42  | 1.91                     | 0.52              |
| 17:5:106:PRO:HG3  | 17:5:243:GLN:HG3  | 1.91                     | 0.52              |
| 22:A:829:CLA:C1C  | 24:A:845:BCR:HC42 | 2.40                     | 0.52              |
| 22:A:832:CLA:H121 | 22:A:834:CLA:H201 | 1.91                     | 0.52              |
| 22:A:833:CLA:H202 | 24:L:204:BCR:C10  | 2.40                     | 0.52              |
| 2:B:552:LYS:HD2   | 4:D:181:PRO:HD3   | 1.91                     | 0.52              |
| 22:B:814:CLA:H3A  | 19:9:54:LEU:HD22  | 1.92                     | 0.52              |
| 22:B:827:CLA:H2   | 22:B:839:CLA:HBA2 | 1.91                     | 0.52              |
| 22:B:828:CLA:HBA2 | 24:B:848:BCR:C10  | 2.40                     | 0.52              |
| 22:B:833:CLA:H112 | 22:F:302:CLA:H151 | 1.92                     | 0.52              |
| 11:L:92:HIS:HA    | 11:L:95:PHE:HE2   | 1.75                     | 0.52              |
| 12:1:60:LEU:CD1   | 22:1:307:CLA:H42  | 2.40                     | 0.52              |
| 12:Z:105:TRP:CH2  | 12:Z:112:PRO:HG3  | 2.45                     | 0.52              |
| 24:3:307:BCR:HC7  | 22:3:315:CLA:H3A  | 1.90                     | 0.52              |
| 14:7:82:GLY:O     | 14:7:86:VAL:HG23  | 2.10                     | 0.52              |
| 16:4:86:LEU:CD1   | 38:4:803:LUT:H221 | 2.40                     | 0.52              |
| 16:4:139:LYS:HG3  | 39:4:813:CHL:O2D  | 2.10                     | 0.52              |
| 17:5:131:TRP:CH2  | 24:5:304:BCR:H323 | 2.44                     | 0.52              |
| 17:5:243:GLN:HB3  | 24:5:305:BCR:H312 | 1.91                     | 0.52              |
| 18:6:76:ARG:HA    | 18:6:79:MET:HE3   | 1.92                     | 0.52              |
| 18:6:88:GLN:NE2   | 38:6:304:LUT:H42  | 2.24                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:9:82:VAL:HG12  | 22:9:308:CLA:HBC2 | 1.91                     | 0.52              |
| 19:9:101:ALA:N    | 39:9:312:CHL:HAA1 | 2.25                     | 0.52              |
| 2:B:127:THR:HA    | 2:B:245:PHE:CZ    | 2.45                     | 0.52              |
| 2:B:394:PHE:HZ    | 2:B:409:LEU:HD21  | 1.75                     | 0.52              |
| 12:1:194:ALA:HB2  | 22:1:316:CLA:HED3 | 1.91                     | 0.52              |
| 12:Z:53:TYR:CE1   | 39:Z:311:CHL:HAC2 | 2.45                     | 0.52              |
| 14:7:175:PRO:HD2  | 38:7:301:LUT:C23  | 2.40                     | 0.52              |
| 39:5:317:CHL:HAA1 | 39:5:317:CHL:HBD  | 1.90                     | 0.52              |
| 22:6:312:CLA:H193 | 22:6:312:CLA:H152 | 1.92                     | 0.52              |
| 22:A:824:CLA:HHC  | 22:A:824:CLA:CBB  | 2.41                     | 0.51              |
| 2:B:394:PHE:CZ    | 2:B:409:LEU:HD21  | 2.45                     | 0.51              |
| 22:B:824:CLA:C1C  | 33:1:301:LMT:H101 | 2.39                     | 0.51              |
| 12:1:94:LEU:HD12  | 22:1:309:CLA:HMD1 | 1.92                     | 0.51              |
| 22:1:313:CLA:CHC  | 22:1:313:CLA:H172 | 2.41                     | 0.51              |
| 39:Z:311:CHL:CMA  | 25:Z:317:LHG:H192 | 2.40                     | 0.51              |
| 14:7:149:GLY:HA3  | 14:7:161:LYS:HE3  | 1.93                     | 0.51              |
| 22:4:806:CLA:HMD2 | 22:4:811:CLA:H2   | 1.91                     | 0.51              |
| 1:A:360:PHE:HD1   | 22:A:829:CLA:H192 | 1.76                     | 0.51              |
| 2:B:362:LEU:HD22  | 2:B:369:GLN:HE21  | 1.75                     | 0.51              |
| 12:1:140:ARG:HG3  | 22:1:313:CLA:HMC2 | 1.92                     | 0.51              |
| 12:Z:56:ASP:HA    | 38:Z:302:LUT:H24  | 1.91                     | 0.51              |
| 13:3:42:LEU:HD13  | 22:3:311:CLA:HMA2 | 1.92                     | 0.51              |
| 13:3:129:TRP:HZ3  | 41:7:319:3PH:H322 | 1.74                     | 0.51              |
| 24:7:303:BCR:H383 | 22:7:316:CLA:NA   | 2.25                     | 0.51              |
| 22:7:304:CLA:HMB2 | 22:7:305:CLA:HBA2 | 1.92                     | 0.51              |
| 22:7:312:CLA:H72  | 22:7:312:CLA:C4B  | 2.40                     | 0.51              |
| 22:7:323:CLA:H92  | 25:8:317:LHG:H321 | 1.93                     | 0.51              |
| 15:8:143:GLN:HG3  | 22:8:313:CLA:HMC2 | 1.92                     | 0.51              |
| 16:4:108:MET:SD   | 22:4:805:CLA:HAB  | 2.50                     | 0.51              |
| 16:4:254:THR:HA   | 22:4:807:CLA:HBA2 | 1.91                     | 0.51              |
| 22:6:319:CLA:C3D  | 25:6:323:LHG:H372 | 2.40                     | 0.51              |
| 19:9:65:TRP:CZ2   | 22:9:313:CLA:HAA1 | 2.45                     | 0.51              |
| 1:A:460:ASP:OD1   | 1:A:641:THR:HB    | 2.10                     | 0.51              |
| 22:A:810:CLA:HBA2 | 22:A:810:CLA:H42  | 1.92                     | 0.51              |
| 2:B:463:TRP:NE1   | 2:B:477:LEU:HG    | 2.24                     | 0.51              |
| 22:B:810:CLA:H2   | 22:B:810:CLA:C4D  | 2.41                     | 0.51              |
| 22:B:824:CLA:HBC2 | 22:B:825:CLA:HBA1 | 1.91                     | 0.51              |
| 22:G:202:CLA:C4C  | 24:G:203:BCR:H282 | 2.41                     | 0.51              |
| 22:1:310:CLA:C1C  | 25:1:317:LHG:HC41 | 2.41                     | 0.51              |
| 13:3:139:SER:HB3  | 13:3:151:GLY:HA2  | 1.92                     | 0.51              |
| 16:4:163:ARG:NH2  | 16:4:178:PRO:HG3  | 2.26                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:6:132:PHE:HD1  | 18:6:154:VAL:HG11 | 1.75                     | 0.51              |
| 18:6:147:ASN:HB3  | 39:6:320:CHL:C3D  | 2.40                     | 0.51              |
| 20:2:218:PRO:HD3  | 39:2:303:CHL:HMA3 | 1.93                     | 0.51              |
| 1:A:267:LEU:HD12  | 10:K:34:THR:HG23  | 1.92                     | 0.51              |
| 1:A:407:ALA:O     | 1:A:411:ILE:HG13  | 2.10                     | 0.51              |
| 22:A:842:CLA:H42  | 22:A:842:CLA:HED2 | 1.92                     | 0.51              |
| 2:B:530:THR:HG21  | 2:B:583:TRP:CE2   | 2.46                     | 0.51              |
| 2:B:694:TRP:HA    | 22:B:840:CLA:O1D  | 2.10                     | 0.51              |
| 22:B:811:CLA:HBA1 | 22:B:811:CLA:CBD  | 2.40                     | 0.51              |
| 22:B:814:CLA:H112 | 22:B:814:CLA:C3B  | 2.41                     | 0.51              |
| 22:B:840:CLA:H111 | 22:B:841:CLA:H142 | 1.92                     | 0.51              |
| 10:K:59:ARG:N     | 10:K:69:ASP:HA    | 2.25                     | 0.51              |
| 38:1:303:LUT:C28  | 22:1:307:CLA:H8   | 2.40                     | 0.51              |
| 15:8:118:LEU:HD21 | 39:8:315:CHL:C1D  | 2.40                     | 0.51              |
| 22:8:311:CLA:HHC  | 22:8:311:CLA:CBB  | 2.40                     | 0.51              |
| 17:5:227:TRP:HH2  | 22:5:301:CLA:HBC2 | 1.75                     | 0.51              |
| 22:5:326:CLA:H51  | 22:6:314:CLA:H61  | 1.93                     | 0.51              |
| 18:6:79:MET:SD    | 22:6:307:CLA:HAB  | 2.50                     | 0.51              |
| 1:A:413:MET:HG3   | 1:A:558:ARG:HG3   | 1.93                     | 0.51              |
| 22:A:820:CLA:H143 | 10:K:90:LEU:HD21  | 1.91                     | 0.51              |
| 2:B:687:PRO:C     | 2:B:689:ALA:H     | 2.19                     | 0.51              |
| 10:K:32:SER:O     | 10:K:36:LEU:HG    | 2.10                     | 0.51              |
| 17:5:82:MET:SD    | 22:5:307:CLA:HAB  | 2.51                     | 0.51              |
| 18:6:235:GLN:HG2  | 18:6:245:PHE:HE1  | 1.76                     | 0.51              |
| 1:A:75:SER:HA     | 1:A:78:PHE:HD2    | 1.76                     | 0.51              |
| 1:A:104:TRP:CH2   | 1:A:149:ARG:HD2   | 2.45                     | 0.51              |
| 22:A:816:CLA:CMB  | 24:A:844:BCR:H341 | 2.40                     | 0.51              |
| 22:A:824:CLA:H11  | 24:A:846:BCR:H363 | 1.92                     | 0.51              |
| 2:B:355:SER:CB    | 22:B:828:CLA:HAC2 | 2.41                     | 0.51              |
| 22:B:842:CLA:HAB  | 12:1:70:PHE:CZ    | 2.45                     | 0.51              |
| 3:C:29:VAL:HG12   | 4:D:165:ARG:HB3   | 1.92                     | 0.51              |
| 6:F:162:TRP:CD1   | 22:F:305:CLA:HBD  | 2.46                     | 0.51              |
| 11:L:123:GLY:HA2  | 22:L:201:CLA:H161 | 1.91                     | 0.51              |
| 12:Z:100:TYR:O    | 39:Z:312:CHL:HED1 | 2.10                     | 0.51              |
| 14:7:196:ASN:HD22 | 14:7:196:ASN:N    | 2.08                     | 0.51              |
| 22:7:306:CLA:CMB  | 22:7:306:CLA:HBB1 | 2.41                     | 0.51              |
| 22:7:310:CLA:HBA2 | 22:7:310:CLA:CHA  | 2.40                     | 0.51              |
| 38:8:303:LUT:H163 | 39:8:315:CHL:HMC  | 1.92                     | 0.51              |
| 39:8:312:CHL:HBD  | 39:8:312:CHL:HAA1 | 1.93                     | 0.51              |
| 22:4:811:CLA:HHC  | 22:4:811:CLA:CBB  | 2.40                     | 0.51              |
| 25:4:820:LHG:H312 | 22:6:321:CLA:HED1 | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:6:120:ALA:HB1  | 24:6:305:BCR:C15  | 2.40                     | 0.51              |
| 24:6:306:BCR:H352 | 39:6:315:CHL:HAC2 | 1.91                     | 0.51              |
| 1:A:349:TRP:HZ3   | 22:A:825:CLA:H91  | 1.76                     | 0.51              |
| 22:A:803:CLA:HMA1 | 22:A:808:CLA:H201 | 1.92                     | 0.51              |
| 22:A:815:CLA:C4   | 24:3:306:BCR:HC8  | 2.40                     | 0.51              |
| 2:B:93:TRP:CZ2    | 8:I:77:SER:HA     | 2.46                     | 0.51              |
| 2:B:463:TRP:HD1   | 22:F:304:CLA:H193 | 1.75                     | 0.51              |
| 22:B:842:CLA:HBB2 | 22:1:307:CLA:H41  | 1.93                     | 0.51              |
| 6:F:78:LYS:HZ1    | 6:F:81:LYS:HD3    | 1.76                     | 0.51              |
| 22:F:302:CLA:C1B  | 24:F:303:BCR:H10C | 2.41                     | 0.51              |
| 22:8:306:CLA:HHC  | 22:8:306:CLA:CBB  | 2.32                     | 0.51              |
| 16:4:234:THR:HG22 | 22:4:817:CLA:O1D  | 2.10                     | 0.51              |
| 17:5:165:PRO:HD2  | 22:5:307:CLA:OBD  | 2.10                     | 0.51              |
| 18:6:106:LEU:CD1  | 18:6:110:ILE:HG23 | 2.41                     | 0.51              |
| 1:A:396:TRP:HA    | 1:A:603:LEU:HD23  | 1.93                     | 0.51              |
| 22:A:822:CLA:HBC3 | 22:A:823:CLA:H171 | 1.93                     | 0.51              |
| 2:B:145:LEU:O     | 2:B:149:ILE:HG13  | 2.11                     | 0.51              |
| 22:B:822:CLA:C1B  | 24:B:844:BCR:H351 | 2.40                     | 0.51              |
| 22:B:823:CLA:HMD1 | 24:B:844:BCR:HC7  | 1.92                     | 0.51              |
| 33:G:204:LMT:H62  | 22:1:308:CLA:HMD2 | 1.93                     | 0.51              |
| 10:K:62:ASP:HB2   | 10:K:68:VAL:HG23  | 1.92                     | 0.51              |
| 13:3:14:GLN:N     | 13:3:16:TYR:HH    | 2.09                     | 0.51              |
| 16:4:157:PHE:CZ   | 22:4:815:CLA:HBC2 | 2.46                     | 0.51              |
| 22:5:313:CLA:HHC  | 22:5:313:CLA:HBB1 | 1.93                     | 0.51              |
| 22:5:326:CLA:HHC  | 22:5:326:CLA:CBB  | 2.41                     | 0.51              |
| 22:A:810:CLA:C4C  | 22:A:813:CLA:H203 | 2.40                     | 0.51              |
| 22:A:818:CLA:H41  | 22:A:836:CLA:HMA1 | 1.93                     | 0.51              |
| 22:A:833:CLA:H43  | 22:A:855:CLA:H43  | 1.92                     | 0.51              |
| 23:A:843:PQN:C19  | 24:F:303:BCR:H23C | 2.41                     | 0.51              |
| 22:F:304:CLA:H2   | 22:F:304:CLA:C9   | 2.41                     | 0.51              |
| 9:J:1:MET:H2      | 34:J:101:LMG:C2   | 2.22                     | 0.51              |
| 13:3:64:CYS:SG    | 13:3:192:MET:HE2  | 2.51                     | 0.51              |
| 18:6:142:PRO:HD2  | 39:6:320:CHL:CHC  | 2.41                     | 0.51              |
| 25:6:323:LHG:C12  | 25:6:323:LHG:H292 | 2.40                     | 0.51              |
| 19:9:114:MET:SD   | 22:2:302:CLA:HAA1 | 2.51                     | 0.51              |
| 19:9:204:HIS:HA   | 19:9:206:GLN:OE1  | 2.11                     | 0.51              |
| 20:2:197:ASN:HA   | 22:2:301:CLA:CBA  | 2.34                     | 0.51              |
| 1:A:453:PHE:HE1   | 22:B:806:CLA:HMA1 | 1.73                     | 0.51              |
| 1:A:493:LEU:O     | 1:A:496:GLN:HG2   | 2.09                     | 0.51              |
| 22:A:833:CLA:CAD  | 24:B:853:BCR:H10C | 2.41                     | 0.51              |
| 2:B:46:LYS:HG2    | 25:B:803:LHG:HC12 | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:B:841:CLA:HBA2 | 23:B:843:PQN:H241 | 1.92                     | 0.51              |
| 6:F:186:ILE:HG12  | 9:J:10:THR:HG22   | 1.92                     | 0.51              |
| 11:L:94:PHE:O     | 11:L:97:PRO:HD2   | 2.11                     | 0.51              |
| 12:1:58:LEU:HD12  | 38:1:303:LUT:H222 | 1.92                     | 0.51              |
| 12:1:173:LYS:HD3  | 22:1:305:CLA:HAA2 | 1.92                     | 0.51              |
| 15:8:164:PRO:HB3  | 22:8:313:CLA:HBC2 | 1.94                     | 0.51              |
| 16:4:71:LEU:HB3   | 16:4:78:ASP:OD1   | 2.11                     | 0.51              |
| 24:4:804:BCR:H282 | 22:4:818:CLA:HMC2 | 1.92                     | 0.51              |
| 25:4:820:LHG:H131 | 22:6:302:CLA:H2   | 1.92                     | 0.51              |
| 18:6:245:PHE:HE2  | 22:6:301:CLA:H91  | 1.76                     | 0.51              |
| 22:2:304:CLA:HHC  | 22:2:304:CLA:CBB  | 2.41                     | 0.51              |
| 1:A:526:ILE:HG23  | 1:A:613:LYS:HE3   | 1.93                     | 0.50              |
| 22:A:829:CLA:HHC  | 22:A:829:CLA:HBB1 | 1.92                     | 0.50              |
| 22:A:855:CLA:HHC  | 22:A:855:CLA:CBB  | 2.41                     | 0.50              |
| 2:B:263:HIS:HB3   | 2:B:266:THR:OG1   | 2.11                     | 0.50              |
| 2:B:276:HIS:ND1   | 22:B:819:CLA:HAB  | 2.26                     | 0.50              |
| 22:B:825:CLA:HMB3 | 22:B:825:CLA:HBB1 | 1.91                     | 0.50              |
| 22:F:304:CLA:C2D  | 22:F:304:CLA:H72  | 2.40                     | 0.50              |
| 10:K:58:LYS:O     | 10:K:59:ARG:HB2   | 2.09                     | 0.50              |
| 12:1:84:GLY:HA2   | 38:1:303:LUT:H181 | 1.93                     | 0.50              |
| 24:3:305:BCR:H16C | 39:3:317:CHL:H112 | 1.94                     | 0.50              |
| 15:8:125:MET:HB3  | 24:8:304:BCR:C15  | 2.41                     | 0.50              |
| 36:5:306:C7Z:C36  | 22:5:322:CLA:HAC1 | 2.42                     | 0.50              |
| 22:A:809:CLA:H11  | 24:J:104:BCR:C12  | 2.41                     | 0.50              |
| 22:A:840:CLA:H92  | 24:F:303:BCR:H17C | 1.93                     | 0.50              |
| 2:B:463:TRP:HE1   | 2:B:477:LEU:HG    | 1.75                     | 0.50              |
| 2:B:597:TRP:HH2   | 2:B:613:SER:HB2   | 1.77                     | 0.50              |
| 14:7:234:PHE:HD1  | 22:7:306:CLA:H11  | 1.75                     | 0.50              |
| 22:7:310:CLA:H171 | 22:7:310:CLA:H122 | 1.94                     | 0.50              |
| 38:5:303:LUT:H373 | 22:5:310:CLA:H8   | 1.94                     | 0.50              |
| 22:6:309:CLA:HBA1 | 22:6:309:CLA:CBD  | 2.34                     | 0.50              |
| 1:A:49:ILE:O      | 1:A:52:LEU:HD23   | 2.11                     | 0.50              |
| 1:A:204:GLY:O     | 1:A:208:LEU:HB2   | 2.12                     | 0.50              |
| 1:A:552:LYS:HD3   | 2:B:671:TYR:CE1   | 2.46                     | 0.50              |
| 22:A:809:CLA:HHC  | 22:A:809:CLA:CBB  | 2.39                     | 0.50              |
| 24:A:844:BCR:C40  | 24:A:856:BCR:H12C | 2.42                     | 0.50              |
| 2:B:488:SER:HA    | 2:B:491:GLN:CD    | 2.35                     | 0.50              |
| 25:B:803:LHG:HC32 | 25:B:803:LHG:H242 | 1.91                     | 0.50              |
| 12:Z:163:ALA:HB2  | 22:Z:303:CLA:HAA2 | 1.92                     | 0.50              |
| 14:7:97:LEU:HD12  | 22:6:301:CLA:HMA1 | 1.94                     | 0.50              |
| 22:7:311:CLA:HBA2 | 22:7:311:CLA:CHA  | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:8:52:PRO:HD2   | 38:8:303:LUT:C23  | 2.31                     | 0.50              |
| 15:8:152:PHE:HB3  | 15:8:156:PHE:CE2  | 2.47                     | 0.50              |
| 15:8:169:ASP:HA   | 38:8:302:LUT:C24  | 2.42                     | 0.50              |
| 17:5:127:LEU:HD12 | 22:5:326:CLA:CBA  | 2.42                     | 0.50              |
| 1:A:75:SER:O      | 1:A:78:PHE:HB2    | 2.11                     | 0.50              |
| 1:A:190:TRP:CZ2   | 22:A:810:CLA:HMA1 | 2.45                     | 0.50              |
| 22:A:833:CLA:CHA  | 24:B:853:BCR:H12C | 2.41                     | 0.50              |
| 2:B:340:ALA:HA    | 2:B:384:MET:HE3   | 1.93                     | 0.50              |
| 3:C:22:PRO:HG2    | 3:C:23:LEU:HD12   | 1.94                     | 0.50              |
| 6:F:155:GLY:O     | 6:F:159:VAL:HG12  | 2.11                     | 0.50              |
| 22:F:302:CLA:H162 | 32:F:306:RRX:C40  | 2.42                     | 0.50              |
| 11:L:92:HIS:HA    | 11:L:95:PHE:CE2   | 2.47                     | 0.50              |
| 24:3:307:BCR:C31  | 22:3:315:CLA:HHB  | 2.38                     | 0.50              |
| 18:6:214:THR:HA   | 22:6:309:CLA:CBA  | 2.40                     | 0.50              |
| 25:6:323:LHG:HC92 | 25:6:323:LHG:H272 | 1.93                     | 0.50              |
| 1:A:28:LYS:HE2    | 1:A:34:HIS:CG     | 2.47                     | 0.50              |
| 22:A:806:CLA:C4   | 25:A:850:LHG:H262 | 2.42                     | 0.50              |
| 2:B:444:MET:HB3   | 2:B:449:THR:O     | 2.11                     | 0.50              |
| 24:B:847:BCR:H311 | 22:1:308:CLA:H72  | 1.93                     | 0.50              |
| 6:F:114:ARG:C     | 6:F:116:ALA:H     | 2.20                     | 0.50              |
| 15:8:169:ASP:N    | 15:8:170:PRO:HD3  | 2.27                     | 0.50              |
| 38:5:302:LUT:C11  | 22:5:308:CLA:HMC1 | 2.41                     | 0.50              |
| 22:A:839:CLA:H11  | 24:A:847:BCR:C15  | 2.41                     | 0.50              |
| 24:A:844:BCR:H23C | 24:3:306:BCR:C33  | 2.40                     | 0.50              |
| 22:B:806:CLA:H171 | 22:L:201:CLA:CMC  | 2.41                     | 0.50              |
| 22:B:811:CLA:CBB  | 22:B:812:CLA:HAA1 | 2.42                     | 0.50              |
| 22:B:820:CLA:HMB3 | 22:B:820:CLA:CBB  | 2.37                     | 0.50              |
| 22:B:825:CLA:NA   | 24:B:847:BCR:H362 | 2.27                     | 0.50              |
| 11:L:99:PRO:HG3   | 22:L:203:CLA:CAB  | 2.41                     | 0.50              |
| 12:1:160:LEU:H    | 12:1:160:LEU:HD12 | 1.77                     | 0.50              |
| 38:Z:301:LUT:H30  | 22:Z:303:CLA:C5   | 2.39                     | 0.50              |
| 14:7:129:LEU:HD21 | 25:8:317:LHG:H322 | 1.94                     | 0.50              |
| 15:8:202:PHE:CD1  | 38:8:302:LUT:H41  | 2.47                     | 0.50              |
| 16:4:183:ASN:HB3  | 39:4:819:CHL:C3D  | 2.41                     | 0.50              |
| 38:4:803:LUT:H32  | 22:4:808:CLA:CAB  | 2.41                     | 0.50              |
| 18:6:127:LYS:HB3  | 39:6:316:CHL:CMC  | 2.40                     | 0.50              |
| 1:A:305:PHE:HE1   | 22:A:821:CLA:HAB  | 1.76                     | 0.50              |
| 1:A:359:LEU:HD21  | 22:A:821:CLA:H93  | 1.94                     | 0.50              |
| 22:A:814:CLA:H143 | 27:A:852:DGA:HBT1 | 1.94                     | 0.50              |
| 2:B:16:ASP:OD2    | 2:B:20:ARG:HG3    | 2.12                     | 0.50              |
| 22:B:811:CLA:CGA  | 22:B:811:CLA:C1A  | 2.89                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:B:817:CLA:H112 | 24:B:844:BCR:H21C | 1.93                     | 0.50              |
| 22:B:818:CLA:HHC  | 22:B:818:CLA:CBB  | 2.42                     | 0.50              |
| 4:D:125:THR:HG22  | 4:D:129:ARG:HD2   | 1.93                     | 0.50              |
| 9:J:35:ASP:N      | 9:J:36:PRO:HD3    | 2.27                     | 0.50              |
| 22:1:305:CLA:C4D  | 22:1:310:CLA:H8   | 2.42                     | 0.50              |
| 12:Z:221:SER:HA   | 22:Z:316:CLA:C4D  | 2.41                     | 0.50              |
| 22:Z:306:CLA:H72  | 22:Z:307:CLA:HHB  | 1.92                     | 0.50              |
| 38:9:301:LUT:H403 | 22:9:303:CLA:H13  | 1.93                     | 0.50              |
| 38:9:302:LUT:H162 | 22:9:308:CLA:HMA1 | 1.94                     | 0.50              |
| 38:9:302:LUT:C32  | 22:9:306:CLA:HAB  | 2.42                     | 0.50              |
| 1:A:536:HIS:HA    | 1:A:539:HIS:HD2   | 1.76                     | 0.50              |
| 1:A:572:ARG:HH21  | 25:A:850:LHG:C3   | 2.24                     | 0.50              |
| 22:A:813:CLA:H201 | 22:3:312:CLA:H72  | 1.93                     | 0.50              |
| 22:A:829:CLA:CHA  | 22:A:829:CLA:H12  | 2.42                     | 0.50              |
| 2:B:5:LEU:HD12    | 8:I:101:LYS:HG3   | 1.94                     | 0.50              |
| 2:B:222:GLY:O     | 2:B:225:PRO:HD2   | 2.12                     | 0.50              |
| 22:B:830:CLA:H8   | 24:B:845:BCR:H19C | 1.94                     | 0.50              |
| 22:B:836:CLA:NC   | 31:1:319:DGD:HA82 | 2.26                     | 0.50              |
| 11:L:86:VAL:HG22  | 11:L:90:ARG:HD3   | 1.93                     | 0.50              |
| 11:L:120:SER:OG   | 22:L:201:CLA:H2   | 2.12                     | 0.50              |
| 12:Z:58:LEU:HD21  | 15:8:170:PRO:HB3  | 1.93                     | 0.50              |
| 22:Z:303:CLA:H102 | 22:Z:304:CLA:CMB  | 2.41                     | 0.50              |
| 14:7:130:LEU:HB3  | 24:7:303:BCR:C15  | 2.42                     | 0.50              |
| 25:4:820:LHG:H381 | 22:6:321:CLA:HBD  | 1.94                     | 0.50              |
| 17:5:64:PRO:O     | 17:5:68:LYS:HG3   | 2.11                     | 0.50              |
| 18:6:147:ASN:ND2  | 39:6:320:CHL:HAA1 | 2.27                     | 0.50              |
| 18:6:157:PRO:HG3  | 39:6:316:CHL:C2D  | 2.42                     | 0.50              |
| 22:6:309:CLA:HMB3 | 22:6:309:CLA:HBB1 | 1.94                     | 0.50              |
| 22:9:307:CLA:HED2 | 22:9:307:CLA:H2A  | 1.94                     | 0.50              |
| 20:2:166:LEU:HA   | 20:2:169:ILE:CG1  | 2.41                     | 0.50              |
| 1:A:71:ARG:HH21   | 1:A:187:LYS:HA    | 1.77                     | 0.50              |
| 1:A:245:LEU:HD23  | 31:3:301:DGD:HG12 | 1.93                     | 0.50              |
| 1:A:697:ILE:O     | 1:A:701:ILE:HG13  | 2.12                     | 0.50              |
| 22:A:815:CLA:H51  | 13:3:200:ALA:HA   | 1.93                     | 0.50              |
| 2:B:13:LEU:HD21   | 2:B:20:ARG:HH11   | 1.76                     | 0.50              |
| 12:1:211:TRP:CZ3  | 15:8:118:LEU:HA   | 2.47                     | 0.50              |
| 12:Z:82:MET:HE3   | 22:Z:303:CLA:HMC3 | 1.93                     | 0.50              |
| 12:Z:103:PRO:HG2  | 39:Z:312:CHL:CED  | 2.41                     | 0.50              |
| 12:Z:140:ARG:HG2  | 22:Z:313:CLA:CAB  | 2.42                     | 0.50              |
| 22:Z:309:CLA:CBB  | 24:4:804:BCR:H323 | 2.42                     | 0.50              |
| 16:4:185:LEU:HD11 | 16:4:197:PHE:CE2  | 2.47                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:4:804:BCR:H402 | 22:4:810:CLA:C5   | 2.42                     | 0.50              |
| 1:A:60:ASP:HA     | 1:A:69:ILE:HD13   | 1.93                     | 0.49              |
| 22:A:854:CLA:HMA3 | 22:A:854:CLA:C2   | 2.42                     | 0.49              |
| 2:B:143:LEU:HD21  | 24:B:846:BCR:H24C | 1.94                     | 0.49              |
| 2:B:178:HIS:HB3   | 22:B:815:CLA:CAB  | 2.42                     | 0.49              |
| 2:B:478:LEU:HD13  | 22:B:835:CLA:HHD  | 1.94                     | 0.49              |
| 22:B:838:CLA:H152 | 32:F:306:RRX:C35  | 2.42                     | 0.49              |
| 7:G:78:PHE:CG     | 7:G:78:PHE:O      | 2.65                     | 0.49              |
| 7:G:114:PHE:CE2   | 22:G:201:CLA:HBC2 | 2.47                     | 0.49              |
| 22:K:205:CLA:HMD3 | 24:K:206:BCR:H21C | 1.94                     | 0.49              |
| 22:1:307:CLA:HHD  | 39:8:301:CHL:HBB2 | 1.93                     | 0.49              |
| 38:Z:302:LUT:H28  | 22:Z:306:CLA:H61  | 1.94                     | 0.49              |
| 39:Z:311:CHL:HAA1 | 39:Z:311:CHL:HBD  | 1.93                     | 0.49              |
| 22:7:315:CLA:HBB1 | 22:7:315:CLA:HMB3 | 1.93                     | 0.49              |
| 38:8:302:LUT:C30  | 22:8:305:CLA:H61  | 2.41                     | 0.49              |
| 17:5:188:LYS:HE3  | 25:5:324:LHG:HC61 | 1.94                     | 0.49              |
| 19:9:115:GLU:CB   | 39:9:312:CHL:HBB2 | 2.41                     | 0.49              |
| 1:A:197:MET:HE1   | 22:A:825:CLA:H71  | 1.93                     | 0.49              |
| 22:A:823:CLA:HHC  | 22:A:823:CLA:CBB  | 2.33                     | 0.49              |
| 24:A:856:BCR:H321 | 24:A:856:BCR:HC8  | 1.94                     | 0.49              |
| 2:B:393:ILE:CG2   | 2:B:397:ARG:HD2   | 2.42                     | 0.49              |
| 2:B:646:VAL:HG21  | 22:B:811:CLA:HAC1 | 1.93                     | 0.49              |
| 22:B:815:CLA:H141 | 22:B:820:CLA:NB   | 2.27                     | 0.49              |
| 6:F:138:GLY:HA3   | 22:F:304:CLA:C2D  | 2.41                     | 0.49              |
| 12:1:160:LEU:HD12 | 12:1:160:LEU:N    | 2.28                     | 0.49              |
| 12:Z:144:GLU:HG3  | 22:Z:313:CLA:HAC1 | 1.93                     | 0.49              |
| 17:5:128:LEU:HB3  | 24:5:304:BCR:C15  | 2.42                     | 0.49              |
| 38:9:301:LUT:H34  | 22:9:303:CLA:HBB2 | 1.94                     | 0.49              |
| 38:9:301:LUT:H28  | 22:9:303:CLA:H2   | 1.92                     | 0.49              |
| 22:A:816:CLA:HBB1 | 22:A:816:CLA:CMB  | 2.41                     | 0.49              |
| 22:A:826:CLA:HHB  | 22:A:839:CLA:O2A  | 2.12                     | 0.49              |
| 2:B:71:TRP:CD1    | 8:I:71:PRO:HD2    | 2.47                     | 0.49              |
| 2:B:278:HIS:HA    | 2:B:281:ILE:HG12  | 1.94                     | 0.49              |
| 2:B:349:VAL:O     | 2:B:353:MET:HB2   | 2.13                     | 0.49              |
| 2:B:689:ALA:HB2   | 24:B:853:BCR:HC22 | 1.94                     | 0.49              |
| 2:B:705:GLN:O     | 2:B:708:LEU:HG    | 2.11                     | 0.49              |
| 3:C:18:VAL:C      | 3:C:20:ALA:H      | 2.19                     | 0.49              |
| 22:F:301:CLA:HHC  | 22:F:301:CLA:CBB  | 2.42                     | 0.49              |
| 12:Z:144:GLU:HG3  | 22:Z:313:CLA:CAC  | 2.43                     | 0.49              |
| 22:3:311:CLA:H62  | 22:3:312:CLA:HHB  | 1.95                     | 0.49              |
| 22:8:306:CLA:HMD3 | 22:8:311:CLA:C4D  | 2.43                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:4:812:CLA:C4D  | 22:6:302:CLA:H111 | 2.42                     | 0.49              |
| 17:5:106:PRO:C    | 17:5:115:ASN:H    | 2.21                     | 0.49              |
| 22:5:309:CLA:HHC  | 22:5:309:CLA:CBB  | 2.41                     | 0.49              |
| 18:6:140:ALA:HA   | 18:6:148:LYS:HA   | 1.93                     | 0.49              |
| 19:9:84:ILE:HG22  | 19:9:183:PRO:HG2  | 1.94                     | 0.49              |
| 19:9:126:ARG:HH22 | 22:9:313:CLA:HMA3 | 1.77                     | 0.49              |
| 2:B:6:PHE:CE2     | 2:B:22:ILE:HA     | 2.47                     | 0.49              |
| 2:B:478:LEU:CD1   | 22:B:835:CLA:HHD  | 2.42                     | 0.49              |
| 4:D:184:VAL:CG1   | 4:D:194:ILE:HG21  | 2.42                     | 0.49              |
| 22:1:304:CLA:H122 | 22:1:305:CLA:HMB2 | 1.95                     | 0.49              |
| 22:1:305:CLA:HED2 | 22:1:305:CLA:H2A  | 1.93                     | 0.49              |
| 22:1:316:CLA:HED1 | 22:1:316:CLA:H2   | 1.95                     | 0.49              |
| 24:3:305:BCR:H312 | 39:3:317:CHL:HMB3 | 1.95                     | 0.49              |
| 22:3:314:CLA:HHC  | 22:3:314:CLA:CBB  | 2.42                     | 0.49              |
| 16:4:118:ASP:HA   | 16:4:121:ARG:HE   | 1.78                     | 0.49              |
| 17:5:74:GLU:CD    | 17:5:187:ILE:HD11 | 2.38                     | 0.49              |
| 17:5:106:PRO:HA   | 17:5:109:LEU:HD12 | 1.93                     | 0.49              |
| 1:A:272:TYR:HB3   | 1:A:275:PHE:CZ    | 2.48                     | 0.49              |
| 22:A:805:CLA:HAA2 | 22:A:825:CLA:C4   | 2.41                     | 0.49              |
| 22:A:806:CLA:H8   | 22:A:830:CLA:HBC3 | 1.94                     | 0.49              |
| 2:B:18:THR:HG22   | 3:C:79:LEU:HD11   | 1.94                     | 0.49              |
| 2:B:107:ARG:HH22  | 2:B:115:ASN:HD22  | 1.60                     | 0.49              |
| 25:Z:317:LHG:HC92 | 24:4:804:BCR:HC22 | 1.94                     | 0.49              |
| 13:3:103:TYR:HE2  | 13:3:105:LYS:O    | 1.95                     | 0.49              |
| 14:7:58:LEU:HD11  | 38:7:302:LUT:H221 | 1.94                     | 0.49              |
| 17:5:127:LEU:HD12 | 22:5:326:CLA:HBA1 | 1.93                     | 0.49              |
| 18:6:235:GLN:HE21 | 22:6:301:CLA:HHB  | 1.78                     | 0.49              |
| 19:9:62:ARG:HB3   | 19:9:66:PHE:CE2   | 2.47                     | 0.49              |
| 22:A:810:CLA:HMB3 | 22:A:810:CLA:HBB1 | 1.95                     | 0.49              |
| 22:A:815:CLA:H122 | 13:3:196:PHE:CD2  | 2.47                     | 0.49              |
| 22:A:841:CLA:H51  | 22:B:801:CLA:H203 | 1.94                     | 0.49              |
| 22:A:855:CLA:H193 | 24:B:853:BCR:C35  | 2.43                     | 0.49              |
| 2:B:548:MET:HE3   | 2:B:551:LYS:HA    | 1.93                     | 0.49              |
| 2:B:651:PHE:CE2   | 2:B:655:HIS:HE1   | 2.31                     | 0.49              |
| 2:B:715:SER:HB2   | 31:B:852:DGD:HBH2 | 1.95                     | 0.49              |
| 39:1:312:CHL:HAB  | 22:1:315:CLA:HBB2 | 1.93                     | 0.49              |
| 13:3:225:ILE:HG13 | 22:3:310:CLA:HMD3 | 1.95                     | 0.49              |
| 14:7:202:VAL:HG21 | 25:7:318:LHG:H271 | 1.93                     | 0.49              |
| 22:5:307:CLA:H101 | 22:5:308:CLA:H122 | 1.94                     | 0.49              |
| 22:A:824:CLA:H141 | 25:A:849:LHG:H171 | 1.94                     | 0.49              |
| 22:A:837:CLA:C3A  | 22:A:838:CLA:HAA2 | 2.42                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:A:841:CLA:HHC  | 22:A:841:CLA:HBB1  | 1.94                     | 0.49              |
| 2:B:164:PRO:HB2   | 2:B:169:PHE:CE2    | 2.48                     | 0.49              |
| 2:B:227:TRP:CZ2   | 22:B:817:CLA:H52   | 2.48                     | 0.49              |
| 22:B:838:CLA:CGA  | 22:B:838:CLA:C1A   | 2.90                     | 0.49              |
| 22:B:838:CLA:NC   | 22:B:838:CLA:H42   | 2.28                     | 0.49              |
| 4:D:76:ARG:O      | 4:D:80:VAL:HG12    | 2.12                     | 0.49              |
| 24:L:204:BCR:C12  | 24:L:204:BCR:H341  | 2.43                     | 0.49              |
| 22:1:310:CLA:HBC3 | 25:1:317:LHG:O8    | 2.13                     | 0.49              |
| 12:Z:191:GLN:HE22 | 12:Z:199:PRO:HG3   | 1.77                     | 0.49              |
| 22:Z:307:CLA:H12  | 15:8:151:GLY:O     | 2.13                     | 0.49              |
| 22:3:314:CLA:H41  | 22:3:314:CLA:H101  | 1.93                     | 0.49              |
| 14:7:58:LEU:HB2   | 22:7:307:CLA:H11   | 1.94                     | 0.49              |
| 14:7:83:ALA:HB1   | 38:7:301:LUT:H12   | 1.93                     | 0.49              |
| 25:4:820:LHG:H122 | 24:6:305:BCR:H333  | 1.94                     | 0.49              |
| 17:5:35:TRP:CZ3   | 22:5:315:CLA:HAA1  | 2.48                     | 0.49              |
| 17:5:80:TRP:CE2   | 22:5:318:CLA:HBC3  | 2.47                     | 0.49              |
| 18:6:73:VAL:HG21  | 18:6:128:ARG:CZ    | 2.41                     | 0.49              |
| 22:6:310:CLA:H151 | 22:6:311:CLA:HBB1  | 1.94                     | 0.49              |
| 22:A:807:CLA:HHC  | 22:A:807:CLA:HBB1  | 1.94                     | 0.49              |
| 2:B:306:LEU:HD23  | 22:B:825:CLA:O1D   | 2.12                     | 0.49              |
| 22:B:810:CLA:C1B  | 24:I:4001:BCR:HC22 | 2.42                     | 0.49              |
| 13:3:121:MET:CB   | 22:3:318:CLA:HAB   | 2.42                     | 0.49              |
| 38:8:303:LUT:H163 | 39:8:315:CHL:CMC   | 2.43                     | 0.49              |
| 16:4:259:ASP:HB3  | 22:4:817:CLA:CHB   | 2.42                     | 0.49              |
| 22:5:322:CLA:C14  | 22:6:310:CLA:H101  | 2.42                     | 0.49              |
| 18:6:170:LEU:HB3  | 22:6:307:CLA:HMA1  | 1.95                     | 0.49              |
| 1:A:21:PRO:HG2    | 1:A:185:ALA:HB3    | 1.95                     | 0.49              |
| 1:A:53:HIS:HD2    | 22:A:804:CLA:HAC1  | 1.77                     | 0.49              |
| 1:A:545:VAL:HG11  | 1:A:598:TRP:CZ2    | 2.48                     | 0.49              |
| 22:A:815:CLA:HBC1 | 22:A:817:CLA:HMB2  | 1.95                     | 0.49              |
| 2:B:71:TRP:CZ2    | 8:I:71:PRO:HB2     | 2.47                     | 0.49              |
| 2:B:117:SER:HA    | 22:B:811:CLA:HMD1  | 1.94                     | 0.49              |
| 22:B:809:CLA:H62  | 22:B:809:CLA:HMA3  | 1.95                     | 0.49              |
| 6:F:138:GLY:O     | 6:F:142:LYS:HB2    | 2.13                     | 0.49              |
| 7:G:71:LYS:HA     | 7:G:71:LYS:HE2     | 1.94                     | 0.49              |
| 10:K:30:ILE:HA    | 10:K:35:ASN:ND2    | 2.28                     | 0.49              |
| 22:1:306:CLA:H171 | 24:8:304:BCR:H321  | 1.93                     | 0.49              |
| 22:Z:308:CLA:HBA2 | 22:Z:308:CLA:CHA   | 2.43                     | 0.49              |
| 13:3:114:PHE:HB2  | 22:3:316:CLA:HAA1  | 1.95                     | 0.49              |
| 38:9:301:LUT:H34  | 22:9:303:CLA:CBB   | 2.42                     | 0.49              |
| 22:A:810:CLA:H142 | 22:A:813:CLA:H151  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:835:CLA:H201 | 22:A:842:CLA:HBB2 | 1.95                     | 0.49              |
| 8:I:74:TRP:HZ2    | 22:2:304:CLA:HHB  | 1.78                     | 0.49              |
| 10:K:38:MET:HE1   | 10:K:101:VAL:HG23 | 1.95                     | 0.49              |
| 10:K:107:LEU:HD22 | 10:K:112:ASN:HD22 | 1.78                     | 0.49              |
| 22:K:205:CLA:CHA  | 24:K:206:BCR:H393 | 2.43                     | 0.49              |
| 22:Z:316:CLA:HMB2 | 22:8:310:CLA:H143 | 1.94                     | 0.49              |
| 13:3:117:GLU:O    | 13:3:121:MET:HG2  | 2.13                     | 0.49              |
| 13:3:203:VAL:O    | 31:3:301:DGD:HG31 | 2.12                     | 0.49              |
| 39:7:313:CHL:C1C  | 39:7:313:CHL:H71  | 2.43                     | 0.49              |
| 15:8:187:LYS:HD3  | 22:8:306:CLA:HBA1 | 1.94                     | 0.49              |
| 16:4:180:PHE:HB3  | 16:4:182:ASN:OD1  | 2.12                     | 0.49              |
| 39:4:816:CHL:HBA2 | 39:4:816:CHL:O2D  | 2.12                     | 0.49              |
| 22:6:322:CLA:H112 | 22:6:322:CLA:H72  | 1.60                     | 0.49              |
| 22:9:307:CLA:C3D  | 22:9:313:CLA:H43  | 2.43                     | 0.49              |
| 20:2:178:ARG:HB3  | 22:2:304:CLA:HED2 | 1.94                     | 0.49              |
| 1:A:202:LEU:O     | 1:A:305:PHE:HB3   | 2.12                     | 0.48              |
| 1:A:203:ALA:HB2   | 1:A:309:GLY:HA3   | 1.93                     | 0.48              |
| 1:A:668:TYR:CE1   | 22:A:808:CLA:HAC1 | 2.48                     | 0.48              |
| 22:A:804:CLA:HBB1 | 22:A:804:CLA:HMB1 | 1.94                     | 0.48              |
| 2:B:142:PHE:CZ    | 22:B:816:CLA:H122 | 2.48                     | 0.48              |
| 3:C:5:VAL:HG11    | 3:C:26:LEU:HD21   | 1.95                     | 0.48              |
| 6:F:107:THR:HA    | 6:F:110:ARG:NE    | 2.27                     | 0.48              |
| 22:F:301:CLA:H122 | 22:F:301:CLA:H8   | 1.61                     | 0.48              |
| 10:K:59:ARG:H     | 10:K:69:ASP:HA    | 1.78                     | 0.48              |
| 12:Z:192:HIS:O    | 12:Z:196:GLY:HA2  | 2.12                     | 0.48              |
| 15:8:77:MET:HE3   | 22:8:305:CLA:HMC3 | 1.94                     | 0.48              |
| 15:8:153:GLU:HA   | 15:8:156:PHE:HD2  | 1.78                     | 0.48              |
| 22:4:808:CLA:HBC1 | 25:4:820:LHG:H282 | 1.95                     | 0.48              |
| 17:5:109:LEU:HD23 | 22:5:312:CLA:HAA2 | 1.95                     | 0.48              |
| 18:6:110:ILE:CD1  | 24:6:306:BCR:HC8  | 2.38                     | 0.48              |
| 18:6:141:ASP:HB2  | 18:6:147:ASN:HB2  | 1.95                     | 0.48              |
| 22:6:309:CLA:NC   | 22:6:309:CLA:H51  | 2.28                     | 0.48              |
| 19:9:127:TYR:HB2  | 22:9:313:CLA:HMA3 | 1.93                     | 0.48              |
| 39:9:312:CHL:CHB  | 39:9:314:CHL:HBC2 | 2.43                     | 0.48              |
| 1:A:396:TRP:CZ3   | 1:A:600:TYR:HA    | 2.48                     | 0.48              |
| 2:B:223:LEU:HB3   | 2:B:227:TRP:NE1   | 2.28                     | 0.48              |
| 2:B:412:MET:HA    | 2:B:415:HIS:CE1   | 2.48                     | 0.48              |
| 12:Z:69:ARG:NH2   | 15:8:150:LEU:HD23 | 2.27                     | 0.48              |
| 22:Z:309:CLA:HHC  | 22:Z:309:CLA:CBB  | 2.43                     | 0.48              |
| 13:3:143:PHE:CE2  | 39:3:317:CHL:HBB2 | 2.48                     | 0.48              |
| 13:3:159:PRO:HG3  | 39:3:317:CHL:HMD1 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:7:309:CLA:HMA2 | 22:7:316:CLA:C3C  | 2.43                     | 0.48              |
| 16:4:258:ASN:O    | 16:4:262:ARG:HG3  | 2.13                     | 0.48              |
| 17:5:105:GLU:HB3  | 17:5:107:GLN:NE2  | 2.27                     | 0.48              |
| 24:5:305:BCR:H21C | 24:5:305:BCR:H361 | 1.94                     | 0.48              |
| 19:9:31:TRP:CD1   | 19:9:51:PHE:HA    | 2.48                     | 0.48              |
| 1:A:501:THR:HG21  | 22:K:203:CLA:HED1 | 1.94                     | 0.48              |
| 2:B:54:GLN:O      | 2:B:58:ILE:HG13   | 2.14                     | 0.48              |
| 2:B:584:MET:O     | 2:B:588:ILE:HG12  | 2.13                     | 0.48              |
| 22:B:814:CLA:HBB2 | 22:B:822:CLA:H93  | 1.95                     | 0.48              |
| 13:3:149:VAL:HG22 | 13:3:163:TRP:HB2  | 1.93                     | 0.48              |
| 14:7:82:GLY:HA2   | 38:7:302:LUT:H181 | 1.95                     | 0.48              |
| 14:7:125:ALA:HB2  | 15:8:230:VAL:HG21 | 1.94                     | 0.48              |
| 22:8:309:CLA:HAC1 | 39:8:312:CHL:HBB2 | 1.95                     | 0.48              |
| 16:4:161:GLU:HG3  | 22:4:815:CLA:C4B  | 2.43                     | 0.48              |
| 22:5:301:CLA:HHC  | 22:5:301:CLA:CBB  | 2.43                     | 0.48              |
| 19:9:76:TRP:CD2   | 22:9:313:CLA:HAC2 | 2.47                     | 0.48              |
| 1:A:678:VAL:HG21  | 24:A:848:BCR:H353 | 1.95                     | 0.48              |
| 22:A:822:CLA:C4D  | 24:A:856:BCR:H292 | 2.44                     | 0.48              |
| 23:A:843:PQN:H201 | 24:F:303:BCR:H382 | 1.95                     | 0.48              |
| 24:A:848:BCR:H24C | 22:B:801:CLA:H101 | 1.95                     | 0.48              |
| 2:B:23:TRP:HB3    | 31:B:852:DGD:C4A  | 2.44                     | 0.48              |
| 2:B:32:PHE:HB2    | 2:B:43:LEU:HD13   | 1.95                     | 0.48              |
| 2:B:177:ASN:OD1   | 2:B:292:TYR:HD2   | 1.97                     | 0.48              |
| 22:B:824:CLA:H11  | 33:G:204:LMT:C6'  | 2.43                     | 0.48              |
| 22:B:841:CLA:H203 | 24:L:204:BCR:H15C | 1.95                     | 0.48              |
| 24:B:844:BCR:H272 | 24:B:846:BCR:H323 | 1.96                     | 0.48              |
| 3:C:3:HIS:ND1     | 3:C:69:LEU:HA     | 2.28                     | 0.48              |
| 6:F:121:ALA:HB3   | 6:F:123:LEU:HD13  | 1.95                     | 0.48              |
| 22:F:304:CLA:C1D  | 22:F:304:CLA:H52  | 2.44                     | 0.48              |
| 7:G:33:GLU:HB3    | 7:G:34:PRO:HD2    | 1.95                     | 0.48              |
| 7:G:54:LEU:O      | 7:G:58:ARG:HG2    | 2.13                     | 0.48              |
| 9:J:34:PRO:HD2    | 35:J:102:T7X:C5   | 2.43                     | 0.48              |
| 12:1:79:ARG:HA    | 12:1:82:MET:HE3   | 1.95                     | 0.48              |
| 12:1:191:GLN:HG3  | 12:1:192:HIS:N    | 2.27                     | 0.48              |
| 22:7:310:CLA:H2   | 22:7:310:CLA:H61  | 1.64                     | 0.48              |
| 22:8:306:CLA:HMD2 | 33:4:801:LMT:H61  | 1.95                     | 0.48              |
| 39:8:312:CHL:CHD  | 39:8:315:CHL:HBC2 | 2.43                     | 0.48              |
| 16:4:114:ILE:HG23 | 16:4:134:TRP:CD1  | 2.48                     | 0.48              |
| 16:4:177:ASP:CB   | 16:4:183:ASN:HB2  | 2.42                     | 0.48              |
| 18:6:159:PHE:O    | 38:6:303:LUT:H24  | 2.12                     | 0.48              |
| 1:A:69:ILE:O      | 1:A:73:VAL:HG23   | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:296:HIS:HB3   | 22:A:818:CLA:HMB1 | 1.95                     | 0.48              |
| 1:A:382:THR:HG21  | 1:A:517:VAL:HB    | 1.94                     | 0.48              |
| 1:A:487:ILE:HD11  | 22:A:837:CLA:H43  | 1.95                     | 0.48              |
| 1:A:563:ILE:HD11  | 1:A:583:THR:HB    | 1.95                     | 0.48              |
| 22:A:810:CLA:O1A  | 22:A:813:CLA:H193 | 2.13                     | 0.48              |
| 22:A:813:CLA:H191 | 22:3:312:CLA:H41  | 1.95                     | 0.48              |
| 22:A:835:CLA:NB   | 24:A:847:BCR:H292 | 2.28                     | 0.48              |
| 22:A:836:CLA:C4D  | 22:K:203:CLA:H12  | 2.44                     | 0.48              |
| 22:A:841:CLA:H62  | 22:A:841:CLA:H102 | 1.48                     | 0.48              |
| 22:B:819:CLA:HHC  | 22:B:819:CLA:CBB  | 2.43                     | 0.48              |
| 22:B:821:CLA:H42  | 22:B:825:CLA:O1A  | 2.14                     | 0.48              |
| 22:B:842:CLA:HBA1 | 25:B:850:LHG:HC42 | 1.95                     | 0.48              |
| 33:1:301:LMT:H31  | 22:1:308:CLA:H42  | 1.95                     | 0.48              |
| 13:3:163:TRP:O    | 13:3:166:LEU:HB3  | 2.14                     | 0.48              |
| 38:3:302:LUT:H382 | 22:3:308:CLA:C4D  | 2.43                     | 0.48              |
| 22:8:306:CLA:HMD3 | 22:8:311:CLA:CHA  | 2.43                     | 0.48              |
| 25:4:820:LHG:HC91 | 25:4:820:LHG:H292 | 1.94                     | 0.48              |
| 25:6:323:LHG:H292 | 25:6:323:LHG:H122 | 1.96                     | 0.48              |
| 38:9:302:LUT:H161 | 39:9:314:CHL:HBB1 | 1.96                     | 0.48              |
| 39:9:312:CHL:HBC2 | 39:9:312:CHL:CMC  | 2.39                     | 0.48              |
| 1:A:25:SER:O      | 22:A:811:CLA:HHB  | 2.13                     | 0.48              |
| 1:A:427:LEU:O     | 1:A:431:ILE:HG13  | 2.14                     | 0.48              |
| 1:A:441:LEU:O     | 1:A:444:VAL:HG12  | 2.13                     | 0.48              |
| 1:A:541:PHE:CZ    | 22:B:806:CLA:HBB2 | 2.46                     | 0.48              |
| 22:A:811:CLA:HHC  | 22:A:811:CLA:CBB  | 2.42                     | 0.48              |
| 22:A:823:CLA:NC   | 37:K:201:DAO:H111 | 2.29                     | 0.48              |
| 2:B:490:SER:CB    | 2:B:495:LEU:HB2   | 2.44                     | 0.48              |
| 22:B:832:CLA:H2   | 22:B:842:CLA:C3   | 2.43                     | 0.48              |
| 22:Z:305:CLA:H43  | 22:Z:310:CLA:OBD  | 2.14                     | 0.48              |
| 13:3:202:ALA:O    | 31:3:301:DGD:HB31 | 2.13                     | 0.48              |
| 24:3:306:BCR:C12  | 24:3:306:BCR:H341 | 2.42                     | 0.48              |
| 22:3:320:CLA:CMD  | 41:7:319:3PH:H342 | 2.36                     | 0.48              |
| 15:8:208:ALA:HA   | 15:8:234:ILE:HG21 | 1.95                     | 0.48              |
| 22:4:807:CLA:C1A  | 22:4:807:CLA:CGA  | 2.91                     | 0.48              |
| 18:6:142:PRO:HB2  | 22:6:302:CLA:CMD  | 2.44                     | 0.48              |
| 20:2:199:TYR:O    | 20:2:204:GLY:HA3  | 2.14                     | 0.48              |
| 1:A:82:GLY:O      | 1:A:86:ILE:HG13   | 2.13                     | 0.48              |
| 1:A:495:PRO:O     | 1:A:500:PRO:HA    | 2.13                     | 0.48              |
| 1:A:673:LEU:HB3   | 22:A:802:CLA:O2A  | 2.13                     | 0.48              |
| 1:A:684:MET:HE3   | 23:A:843:PQN:H2M1 | 1.94                     | 0.48              |
| 22:A:814:CLA:HBA1 | 24:A:844:BCR:C34  | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:814:CLA:HMC2 | 24:A:844:BCR:H352 | 1.94                     | 0.48              |
| 22:A:821:CLA:H2   | 22:A:821:CLA:H61  | 1.56                     | 0.48              |
| 22:A:821:CLA:C10  | 24:A:847:BCR:H10C | 2.41                     | 0.48              |
| 24:A:848:BCR:H292 | 22:F:302:CLA:HMA1 | 1.96                     | 0.48              |
| 2:B:295:ASN:HB2   | 7:G:83:GLN:O      | 2.13                     | 0.48              |
| 6:F:123:LEU:HB3   | 6:F:131:PRO:HB3   | 1.96                     | 0.48              |
| 9:J:16:LEU:HD21   | 36:J:105:C7Z:C12  | 2.44                     | 0.48              |
| 22:Z:303:CLA:H41  | 22:Z:304:CLA:HBA1 | 1.95                     | 0.48              |
| 22:Z:304:CLA:HMD3 | 22:Z:309:CLA:HBA2 | 1.95                     | 0.48              |
| 22:Z:305:CLA:HBC1 | 22:Z:316:CLA:C10  | 2.42                     | 0.48              |
| 13:3:138:MET:HE2  | 13:3:138:MET:HA   | 1.96                     | 0.48              |
| 14:7:243:PHE:HE2  | 22:7:317:CLA:CAB  | 2.26                     | 0.48              |
| 16:4:183:ASN:OD1  | 39:4:819:CHL:HAA1 | 2.14                     | 0.48              |
| 17:5:160:PRO:HG2  | 17:5:179:ARG:HH12 | 1.77                     | 0.48              |
| 39:5:316:CHL:HAA1 | 39:5:316:CHL:HBD  | 1.95                     | 0.48              |
| 18:6:237:THR:HG23 | 18:6:246:THR:OG1  | 2.13                     | 0.48              |
| 22:6:311:CLA:CBB  | 22:6:319:CLA:H42  | 2.44                     | 0.48              |
| 19:9:100:GLY:O    | 39:9:314:CHL:HBC1 | 2.14                     | 0.48              |
| 39:9:312:CHL:HBC1 | 22:9:313:CLA:HBC3 | 1.94                     | 0.48              |
| 22:A:822:CLA:H8   | 22:A:823:CLA:C9   | 2.44                     | 0.48              |
| 2:B:613:SER:HA    | 2:B:616:TYR:CE1   | 2.49                     | 0.48              |
| 22:B:834:CLA:O2A  | 9:J:36:PRO:HG2    | 2.14                     | 0.48              |
| 22:B:836:CLA:HBB1 | 22:B:836:CLA:CMB  | 2.43                     | 0.48              |
| 11:L:126:ILE:HD12 | 22:L:201:CLA:H152 | 1.96                     | 0.48              |
| 14:7:137:LYS:HB3  | 22:7:314:CLA:HMC2 | 1.95                     | 0.48              |
| 15:8:107:SER:OG   | 39:8:315:CHL:HAC1 | 2.14                     | 0.48              |
| 22:5:312:CLA:HBA1 | 22:5:312:CLA:H3A  | 1.72                     | 0.48              |
| 22:5:318:CLA:H92  | 22:6:322:CLA:H62  | 1.95                     | 0.48              |
| 18:6:122:HIS:CE1  | 18:6:126:LEU:HD11 | 2.48                     | 0.48              |
| 20:2:199:TYR:OH   | 20:2:211:VAL:HG21 | 2.13                     | 0.48              |
| 1:A:26:PHE:CD2    | 34:J:101:LMG:HC1  | 2.49                     | 0.48              |
| 22:A:805:CLA:C17  | 24:A:844:BCR:H323 | 2.44                     | 0.48              |
| 22:A:822:CLA:O1A  | 22:K:204:CLA:HMB3 | 2.14                     | 0.48              |
| 2:B:217:LEU:HD23  | 22:B:817:CLA:O1D  | 2.14                     | 0.48              |
| 2:B:688:LEU:CB    | 24:B:853:BCR:HC31 | 2.43                     | 0.48              |
| 22:B:815:CLA:H71  | 22:B:815:CLA:H111 | 1.56                     | 0.48              |
| 22:B:815:CLA:H172 | 22:B:830:CLA:CAD  | 2.44                     | 0.48              |
| 22:G:202:CLA:HED2 | 22:G:202:CLA:H2A  | 1.95                     | 0.48              |
| 9:J:3:ASN:HB2     | 34:J:101:LMG:HC3  | 1.95                     | 0.48              |
| 11:L:135:TYR:CZ   | 11:L:139:MET:HG3  | 2.49                     | 0.48              |
| 39:Z:312:CHL:HAA1 | 39:Z:312:CHL:HBD  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:3:322:CLA:H141 | 22:7:317:CLA:HBC2  | 1.96                     | 0.48              |
| 39:8:312:CHL:C1C  | 26:8:318:NKP:HAPA  | 2.44                     | 0.48              |
| 16:4:100:GLU:CD   | 16:4:215:ILE:HD11  | 2.38                     | 0.48              |
| 16:4:237:LYS:HB2  | 16:4:242:ASN:ND2   | 2.28                     | 0.48              |
| 22:5:322:CLA:H2A  | 22:5:322:CLA:HED3  | 1.95                     | 0.48              |
| 18:6:52:PHE:HB3   | 22:6:310:CLA:C3D   | 2.43                     | 0.48              |
| 19:9:69:ALA:HA    | 19:9:72:THR:HG22   | 1.96                     | 0.48              |
| 22:A:810:CLA:H51  | 22:3:312:CLA:H51   | 1.95                     | 0.48              |
| 2:B:32:PHE:HB2    | 2:B:43:LEU:CD1     | 2.43                     | 0.48              |
| 2:B:312:PRO:HD2   | 25:B:850:LHG:P     | 2.54                     | 0.48              |
| 2:B:655:HIS:HB3   | 22:B:806:CLA:HBD   | 1.96                     | 0.48              |
| 22:B:827:CLA:C3B  | 22:B:839:CLA:HMA3  | 2.44                     | 0.48              |
| 5:E:47:ARG:HB3    | 5:E:50:SER:OG      | 2.13                     | 0.48              |
| 11:L:96:LEU:HB3   | 11:L:97:PRO:HD3    | 1.95                     | 0.48              |
| 12:Z:60:LEU:CD1   | 38:Z:302:LUT:H221  | 2.43                     | 0.48              |
| 13:3:20:GLU:O     | 13:3:24:GLN:HG3    | 2.14                     | 0.48              |
| 38:7:301:LUT:H26  | 22:7:304:CLA:O1A   | 2.14                     | 0.48              |
| 22:4:812:CLA:H72  | 22:6:302:CLA:H121  | 1.96                     | 0.48              |
| 22:6:309:CLA:HBD  | 22:6:309:CLA:CBA   | 2.38                     | 0.48              |
| 1:A:307:VAL:CA    | 24:A:856:BCR:H17C  | 2.31                     | 0.47              |
| 22:A:823:CLA:H12  | 37:K:201:DAO:H82   | 1.95                     | 0.47              |
| 22:A:830:CLA:H112 | 25:A:850:LHG:H202  | 1.95                     | 0.47              |
| 22:A:833:CLA:CBD  | 24:B:853:BCR:H12C  | 2.43                     | 0.47              |
| 22:A:855:CLA:H141 | 24:B:853:BCR:C17   | 2.44                     | 0.47              |
| 22:B:811:CLA:H111 | 22:B:811:CLA:H2    | 1.95                     | 0.47              |
| 22:Z:303:CLA:HBB1 | 22:Z:303:CLA:CMB   | 2.44                     | 0.47              |
| 14:7:58:LEU:CD1   | 38:7:302:LUT:H221  | 2.44                     | 0.47              |
| 22:8:313:CLA:CHA  | 22:8:313:CLA:HBA2  | 2.44                     | 0.47              |
| 22:8:313:CLA:CMA  | 39:8:315:CHL:H52   | 2.40                     | 0.47              |
| 16:4:192:TYR:HB3  | 22:4:805:CLA:O1D   | 2.14                     | 0.47              |
| 18:6:179:ARG:HA   | 18:6:182:MET:HE2   | 1.96                     | 0.47              |
| 39:9:312:CHL:HHC  | 39:9:312:CHL:CBB   | 2.41                     | 0.47              |
| 1:A:409:ALA:CB    | 24:A:846:BCR:H271  | 2.43                     | 0.47              |
| 22:A:821:CLA:HMB1 | 22:A:821:CLA:HBB1  | 1.96                     | 0.47              |
| 22:A:822:CLA:C1D  | 24:A:856:BCR:H402  | 2.43                     | 0.47              |
| 22:A:833:CLA:H42  | 22:B:840:CLA:H41   | 1.96                     | 0.47              |
| 22:A:835:CLA:O1A  | 22:A:836:CLA:HHB   | 2.13                     | 0.47              |
| 22:A:842:CLA:CBB  | 24:A:846:BCR:H12C  | 2.44                     | 0.47              |
| 22:B:810:CLA:C2B  | 24:I:4001:BCR:HC22 | 2.45                     | 0.47              |
| 22:B:818:CLA:H143 | 22:B:818:CLA:H111  | 1.64                     | 0.47              |
| 6:F:153:THR:HG21  | 32:F:306:RRX:H57   | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:35:TYR:HA     | 22:G:201:CLA:OBD  | 2.15                     | 0.47              |
| 33:1:301:LMT:H52  | 22:1:314:CLA:H42  | 1.95                     | 0.47              |
| 12:Z:203:LEU:O    | 12:Z:207:ILE:HG13 | 2.14                     | 0.47              |
| 22:Z:306:CLA:H72  | 22:Z:307:CLA:HMB1 | 1.96                     | 0.47              |
| 13:3:59:SER:OG    | 22:3:312:CLA:HAA1 | 2.14                     | 0.47              |
| 13:3:70:GLY:HA2   | 38:3:303:LUT:C18  | 2.40                     | 0.47              |
| 15:8:30:TRP:CH2   | 41:8:320:3PH:H332 | 2.49                     | 0.47              |
| 16:4:183:ASN:HB3  | 39:4:819:CHL:C4D  | 2.43                     | 0.47              |
| 17:5:134:VAL:HG12 | 22:6:314:CLA:HED1 | 1.95                     | 0.47              |
| 22:5:307:CLA:H52  | 22:5:307:CLA:H8   | 1.66                     | 0.47              |
| 19:9:195:GLY:O    | 19:9:196:TYR:C    | 2.57                     | 0.47              |
| 22:A:805:CLA:OBD  | 22:A:825:CLA:H101 | 2.14                     | 0.47              |
| 22:A:838:CLA:H72  | 22:A:839:CLA:HMD3 | 1.97                     | 0.47              |
| 22:B:825:CLA:HHC  | 22:B:832:CLA:HMD1 | 1.95                     | 0.47              |
| 3:C:66:ARG:HB3    | 3:C:68:TYR:CE1    | 2.48                     | 0.47              |
| 5:E:50:SER:OG     | 5:E:88:PHE:HE1    | 1.97                     | 0.47              |
| 7:G:112:LEU:O     | 7:G:116:PHE:HD1   | 1.97                     | 0.47              |
| 12:Z:170:LEU:HA   | 12:Z:173:LYS:HD2  | 1.95                     | 0.47              |
| 13:3:82:LYS:HD2   | 13:3:210:TYR:CD2  | 2.47                     | 0.47              |
| 24:3:306:BCR:C21  | 22:3:318:CLA:H91  | 2.19                     | 0.47              |
| 22:8:307:CLA:H62  | 22:8:307:CLA:CHC  | 2.44                     | 0.47              |
| 17:5:107:GLN:H    | 17:5:107:GLN:CD   | 2.21                     | 0.47              |
| 18:6:216:PHE:CD1  | 22:6:322:CLA:HBB1 | 2.48                     | 0.47              |
| 19:9:123:GLU:HG3  | 22:9:313:CLA:C4B  | 2.43                     | 0.47              |
| 22:A:805:CLA:H151 | 24:A:844:BCR:HC31 | 1.96                     | 0.47              |
| 2:B:31:ASP:HB2    | 22:B:831:CLA:CAA  | 2.45                     | 0.47              |
| 2:B:153:ALA:HB2   | 22:B:813:CLA:HBC2 | 1.95                     | 0.47              |
| 2:B:680:VAL:HG13  | 2:B:694:TRP:HZ2   | 1.79                     | 0.47              |
| 2:B:705:GLN:HG3   | 31:B:852:DGD:HA52 | 1.95                     | 0.47              |
| 22:B:806:CLA:H72  | 22:B:806:CLA:H112 | 1.77                     | 0.47              |
| 24:B:853:BCR:H272 | 22:L:201:CLA:H92  | 1.95                     | 0.47              |
| 7:G:102:THR:HG21  | 22:G:202:CLA:HBA1 | 1.96                     | 0.47              |
| 9:J:8:LEU:HA      | 9:J:13:VAL:HG11   | 1.96                     | 0.47              |
| 12:Z:112:PRO:HB2  | 12:Z:119:VAL:HG23 | 1.97                     | 0.47              |
| 22:Z:304:CLA:HMD2 | 22:Z:309:CLA:H12  | 1.96                     | 0.47              |
| 13:3:127:ARG:HG3  | 22:3:322:CLA:O1D  | 2.14                     | 0.47              |
| 16:4:176:GLN:NE2  | 16:4:181:THR:HA   | 2.29                     | 0.47              |
| 17:5:55:PHE:CE1   | 22:5:315:CLA:HAA2 | 2.49                     | 0.47              |
| 22:5:310:CLA:H172 | 22:5:311:CLA:HBB2 | 1.96                     | 0.47              |
| 18:6:123:PHE:HZ   | 39:6:320:CHL:HBB2 | 1.76                     | 0.47              |
| 22:A:821:CLA:H18  | 24:A:846:BCR:H272 | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:330:SER:O     | 2:B:334:GLN:HG3   | 2.13                     | 0.47              |
| 22:B:808:CLA:CBA  | 22:B:815:CLA:HBA1 | 2.38                     | 0.47              |
| 22:B:840:CLA:HBB1 | 22:B:840:CLA:HMB3 | 1.95                     | 0.47              |
| 4:D:192:MET:SD    | 4:D:192:MET:N     | 2.83                     | 0.47              |
| 12:1:185:CYS:HA   | 12:1:188:PHE:CD2  | 2.49                     | 0.47              |
| 38:Z:301:LUT:C28  | 22:Z:303:CLA:H52  | 2.45                     | 0.47              |
| 13:3:131:ASP:O    | 13:3:135:PRO:HA   | 2.15                     | 0.47              |
| 24:3:304:BCR:HC31 | 22:7:310:CLA:HAB  | 1.96                     | 0.47              |
| 22:3:322:CLA:C4B  | 25:7:318:LHG:H101 | 2.44                     | 0.47              |
| 22:7:306:CLA:H8   | 22:7:306:CLA:H51  | 1.48                     | 0.47              |
| 25:4:820:LHG:H121 | 25:4:820:LHG:HC92 | 1.60                     | 0.47              |
| 17:5:123:ALA:HB1  | 22:5:326:CLA:HAA1 | 1.95                     | 0.47              |
| 22:5:315:CLA:H152 | 22:5:315:CLA:H18  | 1.76                     | 0.47              |
| 18:6:73:VAL:HG21  | 18:6:128:ARG:NH1  | 2.30                     | 0.47              |
| 18:6:123:PHE:HE1  | 24:6:305:BCR:H332 | 1.80                     | 0.47              |
| 18:6:161:PRO:HD2  | 38:6:303:LUT:C23  | 2.44                     | 0.47              |
| 18:6:251:GLN:HG2  | 18:6:254:TRP:CZ3  | 2.50                     | 0.47              |
| 22:6:308:CLA:C1D  | 22:6:313:CLA:H72  | 2.44                     | 0.47              |
| 19:9:111:LEU:HD11 | 39:9:314:CHL:C2D  | 2.45                     | 0.47              |
| 22:2:302:CLA:HED2 | 22:2:302:CLA:H2A  | 1.95                     | 0.47              |
| 1:A:87:TRP:O      | 1:A:91:MET:HG2    | 2.15                     | 0.47              |
| 1:A:264:PHE:HA    | 1:A:269:TRP:HD1   | 1.80                     | 0.47              |
| 1:A:437:ILE:HG23  | 22:A:839:CLA:HBB2 | 1.95                     | 0.47              |
| 21:A:801:CL0:H34  | 21:A:801:CL0:H41  | 1.52                     | 0.47              |
| 22:A:807:CLA:CHC  | 26:A:851:NKP:HAUA | 2.44                     | 0.47              |
| 22:A:831:CLA:CMA  | 11:L:57:THR:HG21  | 2.43                     | 0.47              |
| 2:B:18:THR:HG21   | 3:C:77:MET:HG3    | 1.96                     | 0.47              |
| 2:B:30:HIS:CD2    | 22:B:808:CLA:HBB2 | 2.50                     | 0.47              |
| 2:B:269:LEU:HD21  | 2:B:356:LEU:HB3   | 1.95                     | 0.47              |
| 22:B:823:CLA:HBD  | 7:G:57:HIS:HD2    | 1.79                     | 0.47              |
| 22:B:842:CLA:HAB  | 12:1:70:PHE:HZ    | 1.79                     | 0.47              |
| 6:F:157:LEU:HB3   | 22:F:302:CLA:H142 | 1.97                     | 0.47              |
| 7:G:59:ARG:HG2    | 7:G:63:ARG:NE     | 2.24                     | 0.47              |
| 9:J:11:ALA:N      | 9:J:12:PRO:HD2    | 2.29                     | 0.47              |
| 22:L:202:CLA:H2   | 22:L:202:CLA:H92  | 1.97                     | 0.47              |
| 12:Z:144:GLU:HG3  | 22:Z:313:CLA:CBC  | 2.45                     | 0.47              |
| 13:3:203:VAL:CG1  | 31:3:301:DGD:HG32 | 2.42                     | 0.47              |
| 15:8:37:PRO:HG2   | 15:8:40:LEU:HD12  | 1.96                     | 0.47              |
| 15:8:51:ASP:HA    | 38:8:303:LUT:H24  | 1.96                     | 0.47              |
| 15:8:62:LEU:HD12  | 22:8:308:CLA:HMA2 | 1.97                     | 0.47              |
| 15:8:105:LYS:HB2  | 39:8:312:CHL:OBD  | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:8:307:CLA:HBB1 | 22:8:307:CLA:HMB3 | 1.96                     | 0.47              |
| 16:4:85:SER:HB2   | 16:4:88:VAL:HG23  | 1.95                     | 0.47              |
| 16:4:192:TYR:HD1  | 22:4:805:CLA:O1D  | 1.98                     | 0.47              |
| 22:5:311:CLA:O2D  | 22:5:311:CLA:HBA2 | 2.15                     | 0.47              |
| 1:A:200:HIS:HB3   | 22:A:813:CLA:CAB  | 2.44                     | 0.47              |
| 1:A:204:GLY:HA3   | 22:A:813:CLA:CBB  | 2.45                     | 0.47              |
| 22:A:809:CLA:HAB  | 24:J:104:BCR:H383 | 1.97                     | 0.47              |
| 22:A:829:CLA:HHC  | 22:A:829:CLA:CBB  | 2.45                     | 0.47              |
| 2:B:27:ALA:C      | 2:B:29:ALA:H      | 2.22                     | 0.47              |
| 2:B:31:ASP:HB2    | 22:B:831:CLA:HAA1 | 1.97                     | 0.47              |
| 2:B:92:ILE:HG23   | 22:B:812:CLA:CAD  | 2.45                     | 0.47              |
| 2:B:218:PRO:HD2   | 22:B:817:CLA:CAD  | 2.45                     | 0.47              |
| 2:B:262:PHE:HZ    | 2:B:356:LEU:HD23  | 1.79                     | 0.47              |
| 2:B:384:MET:HE1   | 24:B:848:BCR:H361 | 1.95                     | 0.47              |
| 2:B:429:PHE:HA    | 22:F:302:CLA:O1D  | 2.15                     | 0.47              |
| 22:B:808:CLA:HBB1 | 22:B:808:CLA:CMB  | 2.44                     | 0.47              |
| 22:B:809:CLA:HMA2 | 22:B:831:CLA:C3B  | 2.44                     | 0.47              |
| 22:B:811:CLA:H11  | 22:B:829:CLA:O1A  | 2.13                     | 0.47              |
| 22:B:813:CLA:HBA1 | 22:B:814:CLA:H11  | 1.97                     | 0.47              |
| 22:B:841:CLA:H91  | 22:B:841:CLA:H111 | 1.68                     | 0.47              |
| 3:C:14:CYS:HB2    | 3:C:16:GLN:HG2    | 1.97                     | 0.47              |
| 5:E:71:VAL:CG2    | 5:E:90:LEU:HD23   | 2.44                     | 0.47              |
| 6:F:79:ARG:O      | 6:F:83:GLU:HB2    | 2.14                     | 0.47              |
| 7:G:78:PHE:CD1    | 19:9:58:ALA:HB3   | 2.49                     | 0.47              |
| 33:G:204:LMT:H91  | 22:1:308:CLA:HMD2 | 1.97                     | 0.47              |
| 8:I:75:ALA:O      | 8:I:79:PHE:HD1    | 1.98                     | 0.47              |
| 11:L:86:VAL:O     | 11:L:90:ARG:HG3   | 2.14                     | 0.47              |
| 12:Z:83:LEU:HD11  | 22:Z:303:CLA:HAC1 | 1.94                     | 0.47              |
| 12:Z:166:ASP:O    | 12:Z:170:LEU:HD13 | 2.14                     | 0.47              |
| 39:7:313:CHL:HMC  | 22:7:316:CLA:HAB  | 1.95                     | 0.47              |
| 22:7:323:CLA:H18  | 22:7:324:CLA:HMC2 | 1.95                     | 0.47              |
| 15:8:72:HIS:HB3   | 15:8:196:MET:SD   | 2.55                     | 0.47              |
| 16:4:210:LEU:C    | 22:4:805:CLA:HMA1 | 2.39                     | 0.47              |
| 22:4:815:CLA:HBB1 | 22:4:815:CLA:CMB  | 2.44                     | 0.47              |
| 22:5:311:CLA:C1B  | 22:5:318:CLA:H191 | 2.45                     | 0.47              |
| 39:5:317:CHL:CHB  | 22:5:319:CLA:H71  | 2.44                     | 0.47              |
| 18:6:125:GLU:HG2  | 22:6:317:CLA:CHB  | 2.45                     | 0.47              |
| 22:9:311:CLA:NC   | 25:9:315:LHG:H271 | 2.30                     | 0.47              |
| 22:A:809:CLA:CAB  | 24:J:104:BCR:H24C | 2.45                     | 0.47              |
| 22:A:827:CLA:C3B  | 22:A:835:CLA:HMA3 | 2.45                     | 0.47              |
| 22:A:830:CLA:HMD1 | 25:A:850:LHG:H291 | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:301:ARG:HG3   | 7:G:65:ALA:HA     | 1.97                     | 0.47              |
| 2:B:395:TRP:NE1   | 24:B:848:BCR:H272 | 2.29                     | 0.47              |
| 7:G:58:ARG:NH2    | 7:G:96:GLY:O      | 2.46                     | 0.47              |
| 13:3:186:LYS:HD3  | 22:3:314:CLA:O1D  | 2.15                     | 0.47              |
| 14:7:131:PHE:HB3  | 22:7:315:CLA:HAB  | 1.96                     | 0.47              |
| 14:7:132:HIS:CD2  | 22:7:315:CLA:HMB3 | 2.50                     | 0.47              |
| 15:8:80:VAL:HG13  | 15:8:202:PHE:CE2  | 2.46                     | 0.47              |
| 38:8:303:LUT:C28  | 22:8:308:CLA:H72  | 2.45                     | 0.47              |
| 22:8:305:CLA:H71  | 22:8:306:CLA:CMA  | 2.44                     | 0.47              |
| 16:4:81:PHE:HB3   | 22:4:808:CLA:CAD  | 2.44                     | 0.47              |
| 16:4:140:TYR:CD2  | 22:4:810:CLA:HED1 | 2.49                     | 0.47              |
| 22:5:301:CLA:H61  | 22:5:301:CLA:H2   | 1.68                     | 0.47              |
| 38:5:302:LUT:H183 | 22:5:309:CLA:C3B  | 2.45                     | 0.47              |
| 24:5:304:BCR:H17C | 22:5:319:CLA:H2   | 1.97                     | 0.47              |
| 18:6:61:PRO:O     | 18:6:65:LYS:HG3   | 2.15                     | 0.47              |
| 18:6:84:GLY:O     | 18:6:88:GLN:HG3   | 2.15                     | 0.47              |
| 18:6:160:ALA:HA   | 22:6:307:CLA:HBA2 | 1.97                     | 0.47              |
| 1:A:262:ALA:HB3   | 1:A:263:PRO:HD3   | 1.97                     | 0.47              |
| 22:A:804:CLA:HAA1 | 22:A:811:CLA:H2   | 1.97                     | 0.47              |
| 22:A:821:CLA:H72  | 24:A:846:BCR:C36  | 2.44                     | 0.47              |
| 22:A:833:CLA:C1D  | 22:A:834:CLA:H121 | 2.45                     | 0.47              |
| 2:B:54:GLN:HG2    | 22:B:808:CLA:HMA1 | 1.97                     | 0.47              |
| 2:B:219:HIS:CG    | 2:B:220:PRO:HD2   | 2.50                     | 0.47              |
| 2:B:705:GLN:HG3   | 31:B:852:DGD:C5A  | 2.45                     | 0.47              |
| 22:B:813:CLA:H42  | 22:9:307:CLA:H72  | 1.96                     | 0.47              |
| 22:B:823:CLA:HED2 | 22:B:823:CLA:H2A  | 1.97                     | 0.47              |
| 22:B:828:CLA:H143 | 22:B:828:CLA:H111 | 1.75                     | 0.47              |
| 3:C:5:VAL:HG22    | 3:C:67:VAL:HG22   | 1.96                     | 0.47              |
| 22:F:302:CLA:H162 | 32:F:306:RRX:H6   | 1.95                     | 0.47              |
| 22:G:201:CLA:HHB  | 24:G:203:BCR:H363 | 1.96                     | 0.47              |
| 15:8:97:VAL:HG13  | 22:8:310:CLA:O1D  | 2.14                     | 0.47              |
| 38:4:803:LUT:H24  | 22:4:808:CLA:O1A  | 2.15                     | 0.47              |
| 22:5:318:CLA:HBB1 | 22:5:318:CLA:HMB1 | 1.96                     | 0.47              |
| 18:6:69:GLU:HG3   | 18:6:132:PHE:CD1  | 2.50                     | 0.47              |
| 18:6:248:CYS:O    | 18:6:249:LEU:C    | 2.57                     | 0.47              |
| 22:6:301:CLA:C1   | 22:6:301:CLA:H92  | 2.45                     | 0.47              |
| 22:6:309:CLA:H121 | 25:6:323:LHG:H122 | 1.97                     | 0.47              |
| 19:9:49:PHE:HZ    | 19:9:160:LYS:HE2  | 1.80                     | 0.47              |
| 19:9:87:GLN:HG2   | 22:9:308:CLA:C1D  | 2.45                     | 0.47              |
| 22:9:306:CLA:HBB1 | 22:9:306:CLA:CMB  | 2.44                     | 0.47              |
| 1:A:410:ALA:O     | 1:A:414:VAL:HG23  | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:817:CLA:H62  | 22:A:817:CLA:H41  | 1.51                     | 0.47              |
| 2:B:208:VAL:HG22  | 2:B:216:GLN:HG2   | 1.97                     | 0.47              |
| 22:B:830:CLA:H72  | 24:B:846:BCR:H372 | 1.96                     | 0.47              |
| 12:1:157:PHE:HZ   | 22:1:313:CLA:NB   | 2.13                     | 0.47              |
| 12:Z:195:THR:HG22 | 12:Z:197:LYS:H    | 1.80                     | 0.47              |
| 38:Z:301:LUT:H26  | 22:Z:303:CLA:C2   | 2.44                     | 0.47              |
| 22:3:311:CLA:C6   | 22:3:312:CLA:HMA3 | 2.45                     | 0.47              |
| 14:7:55:PRO:HG2   | 38:7:302:LUT:H23  | 1.97                     | 0.47              |
| 42:7:321:SPH:H4   | 42:7:321:SPH:H71  | 1.72                     | 0.47              |
| 15:8:50:PHE:HB3   | 22:8:308:CLA:CAD  | 2.45                     | 0.47              |
| 15:8:124:PHE:CD1  | 39:8:301:CHL:H51  | 2.50                     | 0.47              |
| 22:8:309:CLA:HBD  | 22:8:314:CLA:HBD  | 1.97                     | 0.47              |
| 17:5:188:LYS:HD3  | 22:5:313:CLA:O1D  | 2.15                     | 0.47              |
| 39:6:315:CHL:HAB  | 39:6:318:CHL:HBB2 | 1.96                     | 0.47              |
| 19:9:62:ARG:HB3   | 19:9:66:PHE:CZ    | 2.50                     | 0.47              |
| 19:9:117:LEU:HD23 | 20:2:215:CYS:SG   | 2.55                     | 0.47              |
| 20:2:214:LEU:HB3  | 39:2:303:CHL:HBA1 | 1.97                     | 0.47              |
| 22:2:302:CLA:HHC  | 22:2:302:CLA:HBB1 | 1.96                     | 0.47              |
| 1:A:301:ILE:HD12  | 1:A:305:PHE:CE2   | 2.50                     | 0.46              |
| 22:A:814:CLA:HBA1 | 24:A:844:BCR:H341 | 1.97                     | 0.46              |
| 2:B:187:SER:O     | 22:B:816:CLA:HBB2 | 2.15                     | 0.46              |
| 2:B:495:LEU:O     | 2:B:495:LEU:HD22  | 2.15                     | 0.46              |
| 22:B:812:CLA:HBB1 | 22:B:812:CLA:CMB  | 2.45                     | 0.46              |
| 22:B:823:CLA:CMB  | 33:1:301:LMT:H71  | 2.45                     | 0.46              |
| 7:G:86:SER:HB3    | 19:9:36:ASN:HB2   | 1.97                     | 0.46              |
| 10:K:35:ASN:HA    | 22:K:202:CLA:OBD  | 2.15                     | 0.46              |
| 22:Z:307:CLA:CBC  | 22:Z:314:CLA:HAC1 | 2.45                     | 0.46              |
| 13:3:146:LEU:HD11 | 22:5:315:CLA:C17  | 2.42                     | 0.46              |
| 13:3:149:VAL:HG21 | 17:5:57:PRO:O     | 2.15                     | 0.46              |
| 13:3:149:VAL:HG23 | 13:3:162:PRO:HD2  | 1.96                     | 0.46              |
| 24:3:304:BCR:H312 | 22:3:322:CLA:C1D  | 2.44                     | 0.46              |
| 22:3:316:CLA:CHA  | 22:3:316:CLA:HBA1 | 2.45                     | 0.46              |
| 42:7:321:SPH:H5   | 42:7:321:SPH:H2   | 1.58                     | 0.46              |
| 15:8:184:LEU:C    | 22:8:305:CLA:HMA1 | 2.40                     | 0.46              |
| 16:4:198:ASP:HA   | 38:4:802:LUT:C24  | 2.31                     | 0.46              |
| 38:4:802:LUT:H181 | 38:4:802:LUT:H8   | 1.97                     | 0.46              |
| 24:4:804:BCR:H271 | 22:4:810:CLA:C4A  | 2.45                     | 0.46              |
| 24:4:804:BCR:H271 | 22:4:810:CLA:NA   | 2.30                     | 0.46              |
| 22:4:818:CLA:C2D  | 22:4:818:CLA:H42  | 2.45                     | 0.46              |
| 18:6:164:PRO:O    | 18:6:170:LEU:HD21 | 2.15                     | 0.46              |
| 22:6:307:CLA:H71  | 22:6:308:CLA:HMA2 | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:6:314:CLA:NC   | 25:6:323:LHG:HC91 | 2.29                     | 0.46              |
| 1:A:114:SER:CB    | 1:A:131:VAL:HG21  | 2.46                     | 0.46              |
| 1:A:310:HIS:HB2   | 24:A:856:BCR:H19C | 1.96                     | 0.46              |
| 1:A:316:TRP:HH2   | 22:A:812:CLA:HHB  | 1.80                     | 0.46              |
| 1:A:528:LEU:HD11  | 22:A:837:CLA:CAD  | 2.46                     | 0.46              |
| 22:A:807:CLA:HHC  | 22:A:807:CLA:CBB  | 2.46                     | 0.46              |
| 3:C:7:ILE:HG13    | 3:C:40:ALA:O      | 2.15                     | 0.46              |
| 3:C:25:VAL:HG13   | 3:C:45:THR:HA     | 1.97                     | 0.46              |
| 11:L:129:ALA:CB   | 11:L:175:THR:HG22 | 2.45                     | 0.46              |
| 12:Z:85:ALA:HB1   | 38:Z:301:LUT:H12  | 1.96                     | 0.46              |
| 12:Z:195:THR:HG22 | 12:Z:197:LYS:HE2  | 1.96                     | 0.46              |
| 13:3:228:ASN:HA   | 13:3:231:LYS:HG2  | 1.96                     | 0.46              |
| 14:7:117:ASP:HB3  | 15:8:226:LYS:HD2  | 1.97                     | 0.46              |
| 24:7:303:BCR:H271 | 22:7:309:CLA:C4A  | 2.44                     | 0.46              |
| 22:8:307:CLA:H111 | 22:8:307:CLA:H152 | 1.66                     | 0.46              |
| 22:5:313:CLA:HHC  | 22:5:313:CLA:CBB  | 2.46                     | 0.46              |
| 18:6:167:MET:SD   | 18:6:171:LYS:HE3  | 2.55                     | 0.46              |
| 1:A:366:ILE:HA    | 22:A:826:CLA:HED2 | 1.96                     | 0.46              |
| 1:A:498:THR:HG21  | 22:A:835:CLA:HMD2 | 1.97                     | 0.46              |
| 22:A:808:CLA:HAB  | 24:J:104:BCR:H352 | 1.98                     | 0.46              |
| 2:B:196:VAL:HA    | 2:B:200:ILE:HD12  | 1.98                     | 0.46              |
| 2:B:632:LEU:HD11  | 2:B:651:PHE:HB2   | 1.97                     | 0.46              |
| 3:C:58:CYS:HA     | 29:C:102:SF4:S4   | 2.56                     | 0.46              |
| 4:D:150:LEU:O     | 4:D:153:LYS:HE3   | 2.15                     | 0.46              |
| 22:F:302:CLA:H61  | 32:F:306:RRX:H7   | 1.96                     | 0.46              |
| 22:F:304:CLA:H72  | 22:F:304:CLA:C3D  | 2.44                     | 0.46              |
| 10:K:38:MET:HB3   | 22:K:202:CLA:CAD  | 2.46                     | 0.46              |
| 12:1:98:ASN:ND2   | 12:1:101:ASP:HB2  | 2.29                     | 0.46              |
| 22:1:304:CLA:HMB2 | 22:1:305:CLA:HBA2 | 1.97                     | 0.46              |
| 22:1:315:CLA:HBB1 | 22:1:315:CLA:HMB1 | 1.96                     | 0.46              |
| 13:3:137:SER:HA   | 13:3:140:LYS:HZ1  | 1.78                     | 0.46              |
| 13:3:177:MET:HE1  | 22:3:308:CLA:HAA2 | 1.96                     | 0.46              |
| 38:7:301:LUT:H382 | 22:7:304:CLA:C4D  | 2.44                     | 0.46              |
| 25:7:318:LHG:H111 | 25:7:318:LHG:HC81 | 1.41                     | 0.46              |
| 22:7:322:CLA:C2   | 22:7:323:CLA:H101 | 2.45                     | 0.46              |
| 15:8:157:LYS:HB2  | 15:8:157:LYS:HZ3  | 1.80                     | 0.46              |
| 15:8:196:MET:HE3  | 22:8:308:CLA:HMC3 | 1.97                     | 0.46              |
| 38:8:303:LUT:H162 | 22:8:310:CLA:HHB  | 1.96                     | 0.46              |
| 16:4:237:LYS:HB3  | 16:4:241:GLN:OE1  | 2.15                     | 0.46              |
| 17:5:131:TRP:HZ2  | 17:5:150:PRO:HG3  | 1.80                     | 0.46              |
| 17:5:171:PRO:HD2  | 38:5:302:LUT:C24  | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:5:248:PRO:O    | 39:5:316:CHL:H2   | 2.14                     | 0.46              |
| 22:5:310:CLA:H92  | 22:5:310:CLA:H61  | 1.64                     | 0.46              |
| 18:6:149:LEU:HD13 | 18:6:150:ALA:N    | 2.31                     | 0.46              |
| 18:6:215:ILE:HG13 | 22:6:322:CLA:HBB2 | 1.97                     | 0.46              |
| 39:9:312:CHL:HAA2 | 39:9:312:CHL:CBD  | 2.46                     | 0.46              |
| 22:2:301:CLA:HHC  | 22:2:301:CLA:HBB1 | 1.97                     | 0.46              |
| 1:A:80:GLN:O      | 1:A:84:ILE:HG13   | 2.16                     | 0.46              |
| 1:A:91:MET:HE1    | 22:A:808:CLA:HMA2 | 1.97                     | 0.46              |
| 1:A:175:PHE:CD2   | 22:A:810:CLA:HAC2 | 2.50                     | 0.46              |
| 1:A:289:LEU:HD21  | 1:A:374:MET:HB3   | 1.97                     | 0.46              |
| 22:A:827:CLA:C4B  | 22:A:835:CLA:HMA3 | 2.45                     | 0.46              |
| 2:B:450:PRO:O     | 2:B:453:GLN:HG2   | 2.16                     | 0.46              |
| 2:B:543:ARG:CB    | 2:B:552:LYS:HB3   | 2.39                     | 0.46              |
| 2:B:601:THR:HG21  | 2:B:610:PHE:HB2   | 1.97                     | 0.46              |
| 22:B:824:CLA:HHC  | 24:B:847:BCR:C10  | 2.45                     | 0.46              |
| 22:B:842:CLA:HED2 | 24:B:847:BCR:H11C | 1.97                     | 0.46              |
| 7:G:98:THR:OG1    | 7:G:100:ILE:HG12  | 2.15                     | 0.46              |
| 12:1:79:ARG:O     | 12:1:83:LEU:HG    | 2.15                     | 0.46              |
| 12:Z:220:VAL:HG12 | 22:Z:316:CLA:H2A  | 1.97                     | 0.46              |
| 13:3:65:ARG:HA    | 13:3:68:MET:HE3   | 1.96                     | 0.46              |
| 22:3:313:CLA:H121 | 22:5:320:CLA:C1C  | 2.45                     | 0.46              |
| 24:7:303:BCR:H291 | 42:7:321:SPH:H142 | 1.98                     | 0.46              |
| 39:8:312:CHL:HHD  | 39:8:315:CHL:HBC2 | 1.96                     | 0.46              |
| 18:6:141:ASP:HA   | 39:6:320:CHL:C1C  | 2.46                     | 0.46              |
| 19:9:106:VAL:HG13 | 19:9:111:LEU:HD12 | 1.98                     | 0.46              |
| 22:9:307:CLA:HMD3 | 22:9:313:CLA:C1D  | 2.46                     | 0.46              |
| 1:A:150:ALA:HB2   | 1:A:378:PRO:CD    | 2.46                     | 0.46              |
| 1:A:450:PHE:CD2   | 22:A:854:CLA:H12  | 2.51                     | 0.46              |
| 1:A:493:LEU:HB3   | 1:A:496:GLN:NE2   | 2.30                     | 0.46              |
| 22:A:803:CLA:H193 | 24:J:104:BCR:H17C | 1.98                     | 0.46              |
| 22:A:826:CLA:HBB1 | 22:A:826:CLA:CMB  | 2.44                     | 0.46              |
| 22:A:830:CLA:HBB1 | 22:A:830:CLA:CMB  | 2.42                     | 0.46              |
| 22:A:832:CLA:HBB1 | 22:A:832:CLA:CMB  | 2.45                     | 0.46              |
| 2:B:256:LEU:HD11  | 22:B:817:CLA:HBC1 | 1.98                     | 0.46              |
| 2:B:337:LEU:HD13  | 22:B:826:CLA:C3B  | 2.46                     | 0.46              |
| 24:B:844:BCR:C36  | 24:G:203:BCR:H312 | 2.36                     | 0.46              |
| 4:D:125:THR:HA    | 4:D:136:PRO:HG2   | 1.97                     | 0.46              |
| 7:G:49:GLY:HA3    | 7:G:105:TRP:CE2   | 2.50                     | 0.46              |
| 7:G:98:THR:O      | 7:G:102:THR:HG23  | 2.15                     | 0.46              |
| 22:Z:307:CLA:OBD  | 22:Z:314:CLA:HAA1 | 2.15                     | 0.46              |
| 39:Z:312:CHL:HMC  | 22:Z:315:CLA:HAB  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:3:308:CLA:CMD  | 39:3:317:CHL:HBA2 | 2.45                     | 0.46              |
| 22:8:307:CLA:H18  | 22:8:311:CLA:HAC2 | 1.98                     | 0.46              |
| 39:8:312:CHL:ND   | 26:8:318:NKP:HAL  | 2.30                     | 0.46              |
| 16:4:230:ALA:CB   | 22:4:807:CLA:HAC2 | 2.46                     | 0.46              |
| 22:5:307:CLA:CHB  | 22:5:307:CLA:H2   | 2.46                     | 0.46              |
| 22:6:301:CLA:H41  | 22:6:301:CLA:H61  | 1.75                     | 0.46              |
| 38:6:303:LUT:H35  | 38:6:303:LUT:H401 | 1.73                     | 0.46              |
| 38:6:303:LUT:H30  | 22:6:307:CLA:H52  | 1.96                     | 0.46              |
| 39:6:315:CHL:HBC3 | 39:6:318:CHL:CBC  | 2.45                     | 0.46              |
| 22:6:322:CLA:HBC2 | 41:6:324:3PH:H281 | 1.98                     | 0.46              |
| 22:2:301:CLA:HHC  | 22:2:301:CLA:CBB  | 2.46                     | 0.46              |
| 1:A:119:TRP:HE3   | 22:A:809:CLA:H2A  | 1.81                     | 0.46              |
| 1:A:526:ILE:CG2   | 1:A:613:LYS:HE3   | 2.46                     | 0.46              |
| 1:A:694:GLN:O     | 1:A:698:GLU:HG3   | 2.14                     | 0.46              |
| 22:A:812:CLA:H142 | 22:A:812:CLA:HMB2 | 1.97                     | 0.46              |
| 22:A:826:CLA:HMA1 | 24:A:847:BCR:H15C | 1.98                     | 0.46              |
| 2:B:263:HIS:CE1   | 2:B:265:GLN:HB3   | 2.48                     | 0.46              |
| 2:B:692:VAL:HG13  | 11:L:135:TYR:CE1  | 2.50                     | 0.46              |
| 22:B:841:CLA:H161 | 24:L:204:BCR:H15C | 1.97                     | 0.46              |
| 4:D:125:THR:O     | 4:D:129:ARG:HG3   | 2.16                     | 0.46              |
| 10:K:66:LYS:O     | 10:K:68:VAL:HG23  | 2.16                     | 0.46              |
| 12:1:153:PRO:HD2  | 22:1:304:CLA:OBD  | 2.16                     | 0.46              |
| 12:Z:182:MET:HE3  | 22:Z:306:CLA:CMC  | 2.45                     | 0.46              |
| 38:3:303:LUT:H42  | 44:3:402:HOH:O    | 2.16                     | 0.46              |
| 15:8:151:GLY:O    | 15:8:152:PHE:HB2  | 2.16                     | 0.46              |
| 16:4:231:GLN:HB3  | 16:4:242:ASN:OD1  | 2.16                     | 0.46              |
| 22:4:806:CLA:H12  | 22:4:806:CLA:H52  | 1.66                     | 0.46              |
| 17:5:61:GLY:HA3   | 22:5:310:CLA:HBA1 | 1.96                     | 0.46              |
| 17:5:164:TYR:CE1  | 17:5:183:GLN:HG2  | 2.50                     | 0.46              |
| 22:5:315:CLA:H2   | 22:5:315:CLA:H61  | 1.55                     | 0.46              |
| 18:6:66:TRP:NE1   | 22:6:311:CLA:H11  | 2.30                     | 0.46              |
| 18:6:164:PRO:CG   | 22:6:308:CLA:H12  | 2.45                     | 0.46              |
| 22:6:308:CLA:ND   | 22:6:313:CLA:H72  | 2.30                     | 0.46              |
| 22:A:806:CLA:HBB2 | 24:A:845:BCR:HC31 | 1.96                     | 0.46              |
| 22:A:821:CLA:H43  | 22:A:824:CLA:H12  | 1.98                     | 0.46              |
| 22:A:825:CLA:H122 | 22:A:825:CLA:H8   | 1.65                     | 0.46              |
| 22:A:828:CLA:H191 | 24:J:104:BCR:C19  | 2.45                     | 0.46              |
| 2:B:190:ALA:CB    | 22:B:816:CLA:HAB  | 2.44                     | 0.46              |
| 22:B:822:CLA:HBA2 | 22:B:822:CLA:H12  | 1.73                     | 0.46              |
| 9:J:4:PHE:O       | 9:J:8:LEU:HG      | 2.16                     | 0.46              |
| 14:7:53:PHE:HB3   | 22:7:307:CLA:C3D  | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:7:218:PRO:C    | 14:7:220:GLN:H    | 2.24                     | 0.46              |
| 39:7:313:CHL:HMC  | 22:7:316:CLA:CAB  | 2.46                     | 0.46              |
| 39:4:813:CHL:HHC  | 39:4:816:CHL:HAB  | 1.98                     | 0.46              |
| 22:4:815:CLA:H2A  | 22:4:815:CLA:CED  | 2.43                     | 0.46              |
| 18:6:173:LYS:HG3  | 22:6:313:CLA:HED2 | 1.97                     | 0.46              |
| 22:6:314:CLA:H11  | 22:6:314:CLA:H51  | 1.75                     | 0.46              |
| 22:2:302:CLA:HHC  | 22:2:302:CLA:CBB  | 2.46                     | 0.46              |
| 1:A:87:TRP:HA     | 22:A:807:CLA:HBB2 | 1.97                     | 0.46              |
| 1:A:178:TRP:HB2   | 22:A:811:CLA:HMC2 | 1.97                     | 0.46              |
| 1:A:687:PHE:HB2   | 22:B:801:CLA:HBC2 | 1.97                     | 0.46              |
| 22:A:805:CLA:H202 | 22:A:805:CLA:H161 | 1.71                     | 0.46              |
| 22:A:839:CLA:H11  | 24:A:847:BCR:H15C | 1.98                     | 0.46              |
| 27:A:852:DGA:HAW1 | 27:A:852:DGA:HAN2 | 1.57                     | 0.46              |
| 2:B:87:PRO:HB3    | 2:B:122:TYR:CG    | 2.51                     | 0.46              |
| 2:B:296:PHE:HE2   | 22:B:822:CLA:HBD  | 1.79                     | 0.46              |
| 2:B:358:PRO:HG3   | 22:B:820:CLA:HBA1 | 1.98                     | 0.46              |
| 2:B:401:PRO:HD2   | 4:D:180:ASN:ND2   | 2.30                     | 0.46              |
| 2:B:540:LEU:HD21  | 24:B:847:BCR:H282 | 1.97                     | 0.46              |
| 22:B:812:CLA:H8   | 22:B:812:CLA:H51  | 1.27                     | 0.46              |
| 4:D:131:LYS:HE3   | 4:D:132:PHE:CZ    | 2.51                     | 0.46              |
| 22:F:304:CLA:HMC1 | 33:F:307:LMT:H121 | 1.98                     | 0.46              |
| 7:G:33:GLU:CD     | 7:G:33:GLU:H      | 2.23                     | 0.46              |
| 7:G:99:LEU:HD21   | 19:9:32:LEU:HD21  | 1.98                     | 0.46              |
| 10:K:107:LEU:CD2  | 22:K:203:CLA:HBB1 | 2.45                     | 0.46              |
| 22:Z:304:CLA:C4D  | 22:Z:309:CLA:H62  | 2.45                     | 0.46              |
| 31:3:301:DGD:O2G  | 31:3:301:DGD:HD1  | 2.16                     | 0.46              |
| 17:5:73:SER:OG    | 22:5:311:CLA:HAA2 | 2.15                     | 0.46              |
| 17:5:105:GLU:OE1  | 17:5:240:VAL:HG21 | 2.16                     | 0.46              |
| 17:5:153:LYS:HA   | 17:5:153:LYS:HD3  | 1.69                     | 0.46              |
| 18:6:250:PHE:H    | 22:6:301:CLA:C4   | 2.27                     | 0.46              |
| 18:6:250:PHE:N    | 22:6:301:CLA:H43  | 2.28                     | 0.46              |
| 1:A:200:HIS:CD2   | 22:A:813:CLA:HAB  | 2.50                     | 0.46              |
| 1:A:263:PRO:HB2   | 1:A:272:TYR:CZ    | 2.50                     | 0.46              |
| 1:A:695:GLU:HA    | 1:A:698:GLU:CD    | 2.41                     | 0.46              |
| 24:A:844:BCR:H15C | 24:A:844:BCR:H351 | 1.39                     | 0.46              |
| 22:B:808:CLA:H43  | 24:B:845:BCR:H24C | 1.97                     | 0.46              |
| 22:B:810:CLA:CAA  | 8:I:80:VAL:HG22   | 2.46                     | 0.46              |
| 22:B:816:CLA:C6   | 24:B:846:BCR:H362 | 2.46                     | 0.46              |
| 22:B:817:CLA:C4B  | 24:B:844:BCR:H271 | 2.46                     | 0.46              |
| 24:B:847:BCR:H15C | 24:B:847:BCR:H351 | 1.75                     | 0.46              |
| 6:F:218:LYS:HE2   | 6:F:218:LYS:HB2   | 1.63                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:G:92:ASN:HB3    | 22:G:202:CLA:OBD   | 2.16                     | 0.46              |
| 12:1:61:CYS:SG    | 12:1:67:LEU:HA     | 2.56                     | 0.46              |
| 12:1:82:MET:HE3   | 22:1:304:CLA:HMC3  | 1.97                     | 0.46              |
| 22:1:308:CLA:CMD  | 22:1:314:CLA:ND    | 2.79                     | 0.46              |
| 25:Z:317:LHG:H121 | 25:Z:317:LHG:HC91  | 1.78                     | 0.46              |
| 22:3:313:CLA:HBB1 | 22:3:313:CLA:CMB   | 2.44                     | 0.46              |
| 22:7:308:CLA:HBB1 | 22:7:308:CLA:CMB   | 2.45                     | 0.46              |
| 42:7:320:SPH:H11  | 42:7:320:SPH:H4    | 1.55                     | 0.46              |
| 16:4:128:PRO:HD2  | 22:4:818:CLA:HMA1  | 1.98                     | 0.46              |
| 16:4:163:ARG:NE   | 39:4:819:CHL:OMC   | 2.49                     | 0.46              |
| 17:5:57:PRO:HB2   | 17:5:58:LEU:HD12   | 1.97                     | 0.46              |
| 22:5:326:CLA:HBA1 | 22:5:326:CLA:CBD   | 2.45                     | 0.46              |
| 24:6:306:BCR:H19C | 39:6:315:CHL:H2    | 1.98                     | 0.46              |
| 22:6:311:CLA:HED3 | 22:6:317:CLA:CGA   | 2.46                     | 0.46              |
| 19:9:51:PHE:HE1   | 22:9:311:CLA:HBC3  | 1.80                     | 0.46              |
| 38:9:302:LUT:C16  | 22:9:308:CLA:HMA1  | 2.46                     | 0.46              |
| 20:2:163:LEU:C    | 20:2:165:MET:H     | 2.24                     | 0.46              |
| 1:A:12:LYS:HE3    | 1:A:12:LYS:HB3     | 1.70                     | 0.46              |
| 22:A:814:CLA:H121 | 22:A:816:CLA:CBB   | 2.44                     | 0.46              |
| 22:A:823:CLA:H172 | 24:A:856:BCR:H403  | 1.98                     | 0.46              |
| 2:B:172:ALA:O     | 2:B:173:GLU:C      | 2.59                     | 0.46              |
| 2:B:653:PHE:HD1   | 22:B:806:CLA:H71   | 1.81                     | 0.46              |
| 22:B:809:CLA:H71  | 22:B:809:CLA:H111  | 1.52                     | 0.46              |
| 24:B:853:BCR:H372 | 24:I:4001:BCR:H403 | 1.98                     | 0.46              |
| 10:K:98:ILE:HG12  | 24:K:206:BCR:H311  | 1.98                     | 0.46              |
| 22:K:202:CLA:HBB1 | 22:K:202:CLA:CMB   | 2.45                     | 0.46              |
| 22:1:306:CLA:C4B  | 22:1:306:CLA:H72   | 2.46                     | 0.46              |
| 22:Z:307:CLA:HBC1 | 22:Z:314:CLA:HAC1  | 1.98                     | 0.46              |
| 22:Z:308:CLA:HMA3 | 22:Z:315:CLA:C1C   | 2.45                     | 0.46              |
| 39:Z:311:CHL:C1C  | 25:Z:317:LHG:H102  | 2.46                     | 0.46              |
| 13:3:182:LEU:HA   | 13:3:185:ILE:HG22  | 1.98                     | 0.46              |
| 24:3:307:BCR:C19  | 22:3:310:CLA:H91   | 2.46                     | 0.46              |
| 16:4:119:LEU:O    | 16:4:123:VAL:HG23  | 2.16                     | 0.46              |
| 24:5:305:BCR:H343 | 18:6:220:VAL:HG21  | 1.97                     | 0.46              |
| 22:5:315:CLA:HHC  | 22:5:315:CLA:HBB1  | 1.97                     | 0.46              |
| 39:5:316:CHL:H152 | 22:6:322:CLA:HAA1  | 1.97                     | 0.46              |
| 18:6:96:PHE:HZ    | 18:6:192:ALA:HB1   | 1.81                     | 0.46              |
| 18:6:249:LEU:O    | 18:6:250:PHE:C     | 2.58                     | 0.46              |
| 22:6:309:CLA:HBC2 | 22:6:319:CLA:HBD   | 1.98                     | 0.46              |
| 22:6:311:CLA:HBB1 | 22:6:311:CLA:CMB   | 2.46                     | 0.46              |
| 39:6:315:CHL:HBC3 | 39:6:318:CHL:HBC3  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:9:142:PHE:HB3  | 19:9:143:PRO:CD   | 2.40                     | 0.46              |
| 1:A:572:ARG:HH21  | 25:A:850:LHG:HC31 | 1.82                     | 0.45              |
| 1:A:676:HIS:HB3   | 22:A:802:CLA:HBD  | 1.98                     | 0.45              |
| 22:A:802:CLA:H202 | 22:A:830:CLA:H192 | 1.97                     | 0.45              |
| 22:A:817:CLA:H122 | 22:A:817:CLA:H8   | 1.64                     | 0.45              |
| 2:B:470:LYS:HG2   | 2:B:473:TYR:HE2   | 1.80                     | 0.45              |
| 25:B:803:LHG:HC32 | 25:B:803:LHG:H262 | 1.98                     | 0.45              |
| 22:B:821:CLA:H93  | 22:B:821:CLA:H111 | 1.63                     | 0.45              |
| 5:E:53:TYR:C      | 5:E:55:GLN:H      | 2.25                     | 0.45              |
| 6:F:199:GLY:O     | 6:F:202:TRP:HD1   | 1.99                     | 0.45              |
| 22:F:304:CLA:H172 | 22:F:304:CLA:HAA1 | 1.98                     | 0.45              |
| 8:I:95:LEU:CD1    | 24:L:204:BCR:HC8  | 2.46                     | 0.45              |
| 12:Z:190:ALA:CB   | 22:Z:316:CLA:H61  | 2.41                     | 0.45              |
| 22:3:308:CLA:HMD3 | 39:3:317:CHL:HBA2 | 1.98                     | 0.45              |
| 22:7:324:CLA:H102 | 22:4:817:CLA:C4B  | 2.45                     | 0.45              |
| 15:8:202:PHE:HD1  | 38:8:302:LUT:H41  | 1.81                     | 0.45              |
| 16:4:66:LYS:CD    | 25:4:821:LHG:HC31 | 2.44                     | 0.45              |
| 17:5:151:ILE:HD12 | 39:5:321:CHL:CMB  | 2.46                     | 0.45              |
| 24:5:305:BCR:H351 | 39:5:316:CHL:HAC1 | 1.97                     | 0.45              |
| 22:6:319:CLA:HHC  | 22:6:319:CLA:CBB  | 2.45                     | 0.45              |
| 19:9:59:ASP:OD1   | 19:9:62:ARG:HB2   | 2.16                     | 0.45              |
| 19:9:119:MET:HE3  | 39:9:314:CHL:HHB  | 1.98                     | 0.45              |
| 20:2:163:LEU:HB3  | 20:2:165:MET:HG2  | 1.99                     | 0.45              |
| 1:A:578:PRO:HD3   | 2:B:562:GLY:HA2   | 1.97                     | 0.45              |
| 22:A:842:CLA:HMB1 | 24:A:846:BCR:C12  | 2.44                     | 0.45              |
| 27:A:852:DGA:HA61 | 14:7:242:PRO:HB2  | 1.97                     | 0.45              |
| 2:B:423:LEU:HD11  | 22:B:839:CLA:HMB1 | 1.98                     | 0.45              |
| 22:B:808:CLA:H18  | 22:B:815:CLA:HMD3 | 1.97                     | 0.45              |
| 22:B:824:CLA:HMB2 | 22:B:842:CLA:ND   | 2.31                     | 0.45              |
| 22:B:829:CLA:ND   | 22:B:829:CLA:H8   | 2.31                     | 0.45              |
| 22:B:836:CLA:O2A  | 31:1:319:DGD:HA72 | 2.16                     | 0.45              |
| 22:B:842:CLA:HHC  | 12:1:70:PHE:HZ    | 1.81                     | 0.45              |
| 9:J:2:LYS:HE3     | 9:J:2:LYS:HB3     | 1.59                     | 0.45              |
| 12:1:37:PRO:HG2   | 39:8:301:CHL:CMD  | 2.46                     | 0.45              |
| 24:3:307:BCR:H11C | 24:3:307:BCR:H341 | 1.67                     | 0.45              |
| 22:3:322:CLA:H92  | 22:7:306:CLA:H72  | 1.99                     | 0.45              |
| 15:8:201:GLY:O    | 15:8:205:GLN:HG2  | 2.16                     | 0.45              |
| 18:6:126:LEU:CD1  | 22:6:302:CLA:HBA1 | 2.42                     | 0.45              |
| 18:6:219:ALA:CB   | 18:6:229:PRO:HD3  | 2.47                     | 0.45              |
| 20:2:223:ALA:HB3  | 20:2:226:SER:OG   | 2.16                     | 0.45              |
| 1:A:516:ALA:HB2   | 1:A:622:VAL:HG21  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:812:CLA:C1C  | 22:A:812:CLA:H51  | 2.46                     | 0.45              |
| 22:A:815:CLA:HBB1 | 22:A:815:CLA:CMB  | 2.45                     | 0.45              |
| 2:B:226:PHE:HA    | 2:B:231:TRP:CD1   | 2.51                     | 0.45              |
| 2:B:348:LEU:HG    | 2:B:352:HIS:CE1   | 2.52                     | 0.45              |
| 4:D:127:GLN:HG3   | 4:D:131:LYS:HE2   | 1.98                     | 0.45              |
| 4:D:129:ARG:O     | 4:D:133:LYS:HA    | 2.16                     | 0.45              |
| 4:D:141:VAL:HG22  | 4:D:147:VAL:HG22  | 1.98                     | 0.45              |
| 22:G:202:CLA:HBB1 | 22:G:202:CLA:HMB3 | 1.98                     | 0.45              |
| 13:3:192:MET:SD   | 22:3:311:CLA:HAB  | 2.57                     | 0.45              |
| 24:3:307:BCR:H401 | 22:3:314:CLA:CHD  | 2.47                     | 0.45              |
| 22:7:322:CLA:HBB1 | 22:7:322:CLA:CMB  | 2.44                     | 0.45              |
| 22:8:310:CLA:H62  | 22:8:310:CLA:H2   | 1.72                     | 0.45              |
| 17:5:118:MET:HB3  | 24:5:305:BCR:H12C | 1.98                     | 0.45              |
| 17:5:131:TRP:HZ3  | 24:5:304:BCR:HC41 | 1.81                     | 0.45              |
| 39:5:316:CHL:H13  | 22:6:322:CLA:HBD  | 1.98                     | 0.45              |
| 39:6:315:CHL:HBD  | 39:6:315:CHL:HAA1 | 1.97                     | 0.45              |
| 22:9:311:CLA:CGA  | 25:9:315:LHG:HC62 | 2.47                     | 0.45              |
| 1:A:265:PHE:HA    | 22:K:202:CLA:HAC2 | 1.99                     | 0.45              |
| 1:A:700:ILE:HG23  | 22:A:840:CLA:O1D  | 2.16                     | 0.45              |
| 22:A:802:CLA:H51  | 2:B:439:VAL:HG13  | 1.98                     | 0.45              |
| 22:A:833:CLA:H13  | 22:B:840:CLA:HBA1 | 1.98                     | 0.45              |
| 22:A:834:CLA:HBC3 | 22:A:854:CLA:H13  | 1.97                     | 0.45              |
| 2:B:293:ARG:HD2   | 2:B:301:ARG:HD3   | 1.98                     | 0.45              |
| 2:B:321:LYS:HD2   | 2:B:322:GLY:N     | 2.31                     | 0.45              |
| 25:B:803:LHG:H111 | 22:B:807:CLA:C1D  | 2.46                     | 0.45              |
| 22:B:816:CLA:H61  | 22:B:816:CLA:H2   | 1.52                     | 0.45              |
| 22:B:825:CLA:H13  | 24:B:847:BCR:H17C | 1.99                     | 0.45              |
| 22:B:827:CLA:CHB  | 22:B:839:CLA:HAA2 | 2.47                     | 0.45              |
| 22:B:834:CLA:HBA2 | 22:B:834:CLA:CHA  | 2.43                     | 0.45              |
| 3:C:10:THR:O      | 3:C:60:THR:HG21   | 2.17                     | 0.45              |
| 6:F:125:CYS:HB3   | 6:F:131:PRO:HA    | 1.99                     | 0.45              |
| 10:K:60:GLY:O     | 10:K:67:LEU:HG    | 2.16                     | 0.45              |
| 22:Z:306:CLA:HBC1 | 25:Z:317:LHG:H292 | 1.98                     | 0.45              |
| 22:7:322:CLA:H72  | 22:7:323:CLA:H171 | 1.99                     | 0.45              |
| 22:8:305:CLA:HBB1 | 22:8:306:CLA:HAA1 | 1.98                     | 0.45              |
| 22:8:311:CLA:C2B  | 25:8:317:LHG:HC2  | 2.46                     | 0.45              |
| 1:A:101:TYR:O     | 1:A:105:LEU:HG    | 2.16                     | 0.45              |
| 1:A:113:PRO:O     | 1:A:139:GLN:HA    | 2.17                     | 0.45              |
| 1:A:248:GLN:H     | 1:A:248:GLN:NE2   | 2.14                     | 0.45              |
| 1:A:442:ASN:HD22  | 2:B:675:LEU:HD11  | 1.82                     | 0.45              |
| 22:A:810:CLA:H121 | 22:A:812:CLA:HBC1 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:814:CLA:H92  | 27:A:852:DGA:HB81 | 1.99                     | 0.45              |
| 22:A:815:CLA:C1B  | 24:A:856:BCR:HC42 | 2.47                     | 0.45              |
| 22:A:829:CLA:H11  | 24:A:845:BCR:H321 | 1.98                     | 0.45              |
| 2:B:228:THR:O     | 7:G:34:PRO:HG3    | 2.17                     | 0.45              |
| 2:B:616:TYR:HD2   | 2:B:618:MET:HB3   | 1.81                     | 0.45              |
| 22:B:806:CLA:C19  | 22:B:812:CLA:H52  | 2.46                     | 0.45              |
| 6:F:151:ILE:HB    | 6:F:152:PRO:HD3   | 1.97                     | 0.45              |
| 7:G:46:LEU:HB3    | 22:G:202:CLA:HMB3 | 1.98                     | 0.45              |
| 11:L:134:ILE:HG13 | 24:L:204:BCR:H363 | 1.97                     | 0.45              |
| 12:1:72:GLU:O     | 12:1:76:ILE:HG12  | 2.17                     | 0.45              |
| 12:1:112:PRO:HB3  | 22:1:315:CLA:HMD1 | 1.97                     | 0.45              |
| 12:1:138:GLU:HG3  | 22:1:314:CLA:C4B  | 2.47                     | 0.45              |
| 38:Z:302:LUT:C28  | 22:Z:306:CLA:H61  | 2.47                     | 0.45              |
| 13:3:191:ALA:O    | 13:3:195:VAL:HG23 | 2.17                     | 0.45              |
| 24:4:804:BCR:H393 | 22:4:810:CLA:CHC  | 2.47                     | 0.45              |
| 25:4:820:LHG:HC61 | 22:6:302:CLA:HAC2 | 1.99                     | 0.45              |
| 18:6:66:TRP:HZ2   | 22:6:317:CLA:HAA2 | 1.80                     | 0.45              |
| 18:6:101:PRO:HG3  | 39:6:318:CHL:OMC  | 2.16                     | 0.45              |
| 19:9:57:GLY:HA3   | 19:9:63:LEU:HD13  | 1.98                     | 0.45              |
| 38:9:302:LUT:C37  | 22:9:306:CLA:H112 | 2.47                     | 0.45              |
| 20:2:197:ASN:CB   | 22:2:301:CLA:HBA2 | 2.47                     | 0.45              |
| 20:2:216:VAL:O    | 20:2:220:ILE:HG13 | 2.16                     | 0.45              |
| 1:A:49:ILE:HD12   | 1:A:49:ILE:N      | 2.32                     | 0.45              |
| 1:A:403:VAL:HG11  | 1:A:596:LEU:CD2   | 2.46                     | 0.45              |
| 22:A:822:CLA:H71  | 22:K:204:CLA:CAB  | 2.45                     | 0.45              |
| 23:A:843:PQN:H262 | 23:A:843:PQN:H302 | 1.63                     | 0.45              |
| 2:B:647:TRP:CZ2   | 2:B:727:ILE:HG21  | 2.52                     | 0.45              |
| 22:B:818:CLA:H112 | 22:B:818:CLA:H93  | 1.69                     | 0.45              |
| 4:D:117:ARG:HB3   | 4:D:120:GLN:HG3   | 1.99                     | 0.45              |
| 6:F:163:ILE:HG23  | 22:F:305:CLA:C1D  | 2.47                     | 0.45              |
| 7:G:78:PHE:CE1    | 19:9:58:ALA:HB3   | 2.52                     | 0.45              |
| 11:L:129:ALA:HB2  | 11:L:175:THR:HG22 | 1.97                     | 0.45              |
| 12:Z:147:ALA:HA   | 12:Z:150:ARG:CD   | 2.47                     | 0.45              |
| 22:3:313:CLA:H111 | 22:3:313:CLA:H152 | 1.68                     | 0.45              |
| 14:7:118:TRP:CZ3  | 14:7:123:LEU:HA   | 2.52                     | 0.45              |
| 15:8:78:THR:HG23  | 22:8:305:CLA:HMC1 | 1.97                     | 0.45              |
| 22:8:307:CLA:NC   | 22:8:307:CLA:H51  | 2.32                     | 0.45              |
| 17:5:60:LEU:HD12  | 38:5:303:LUT:H221 | 1.99                     | 0.45              |
| 17:5:104:GLY:HA2  | 22:5:319:CLA:HAC2 | 1.98                     | 0.45              |
| 18:6:127:LYS:O    | 18:6:138:VAL:HG21 | 2.16                     | 0.45              |
| 22:6:302:CLA:C4D  | 24:6:305:BCR:HC41 | 2.47                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:9:94:PRO:HB2   | 19:9:99:ALA:HA    | 1.98                     | 0.45              |
| 1:A:175:PHE:CE2   | 22:A:810:CLA:HAC2 | 2.52                     | 0.45              |
| 21:A:801:CL0:H72  | 21:A:801:CL0:H10  | 1.57                     | 0.45              |
| 2:B:107:ARG:NH2   | 2:B:115:ASN:HA    | 2.32                     | 0.45              |
| 2:B:227:TRP:CH2   | 22:B:817:CLA:H52  | 2.50                     | 0.45              |
| 2:B:243:HIS:CD2   | 2:B:251:ALA:HA    | 2.52                     | 0.45              |
| 2:B:423:LEU:HD13  | 2:B:533:LEU:HA    | 1.97                     | 0.45              |
| 22:B:810:CLA:C1D  | 22:B:810:CLA:H51  | 2.46                     | 0.45              |
| 22:B:824:CLA:NC   | 33:1:301:LMT:H101 | 2.32                     | 0.45              |
| 22:B:825:CLA:H2   | 22:B:825:CLA:H61  | 1.76                     | 0.45              |
| 22:B:825:CLA:O1A  | 24:B:847:BCR:H16C | 2.16                     | 0.45              |
| 22:B:835:CLA:CMB  | 24:B:848:BCR:H332 | 2.47                     | 0.45              |
| 22:F:301:CLA:H152 | 9:J:18:TRP:CE3    | 2.46                     | 0.45              |
| 13:3:164:PHE:HB3  | 22:3:308:CLA:OBD  | 2.16                     | 0.45              |
| 41:7:319:3PH:H362 | 41:7:319:3PH:H231 | 1.98                     | 0.45              |
| 15:8:101:TYR:CD1  | 15:8:102:GLU:HG3  | 2.52                     | 0.45              |
| 16:4:156:LEU:O    | 24:4:804:BCR:H14C | 2.17                     | 0.45              |
| 22:4:805:CLA:H61  | 22:4:805:CLA:H92  | 1.74                     | 0.45              |
| 17:5:60:LEU:HD11  | 22:5:315:CLA:C14  | 2.47                     | 0.45              |
| 22:5:301:CLA:HBA1 | 22:5:320:CLA:HED3 | 1.97                     | 0.45              |
| 38:5:303:LUT:H183 | 22:5:312:CLA:C3B  | 2.47                     | 0.45              |
| 22:5:310:CLA:HMB2 | 22:5:310:CLA:H51  | 1.99                     | 0.45              |
| 18:6:97:TRP:HH2   | 18:6:189:THR:HG22 | 1.80                     | 0.45              |
| 24:6:305:BCR:C27  | 22:6:312:CLA:H101 | 2.46                     | 0.45              |
| 24:6:306:BCR:H11C | 24:6:306:BCR:H341 | 1.80                     | 0.45              |
| 19:9:65:TRP:HZ2   | 22:9:313:CLA:HAA1 | 1.81                     | 0.45              |
| 19:9:106:VAL:HG22 | 19:9:111:LEU:HB2  | 1.98                     | 0.45              |
| 19:9:120:GLY:CA   | 22:9:313:CLA:HAB  | 2.44                     | 0.45              |
| 1:A:114:SER:HB3   | 1:A:131:VAL:HG21  | 1.99                     | 0.45              |
| 1:A:222:LEU:N     | 1:A:223:PRO:HD2   | 2.32                     | 0.45              |
| 1:A:571:PHE:HD2   | 22:A:830:CLA:HED1 | 1.82                     | 0.45              |
| 22:A:829:CLA:H61  | 24:A:845:BCR:H342 | 1.97                     | 0.45              |
| 22:A:841:CLA:HHC  | 22:A:841:CLA:CBB  | 2.47                     | 0.45              |
| 2:B:192:THR:HG21  | 2:B:279:LEU:HB2   | 1.99                     | 0.45              |
| 2:B:262:PHE:HE1   | 2:B:356:LEU:HA    | 1.82                     | 0.45              |
| 22:B:821:CLA:H172 | 22:B:826:CLA:H203 | 1.99                     | 0.45              |
| 22:B:825:CLA:H141 | 22:B:832:CLA:CBC  | 2.47                     | 0.45              |
| 22:B:829:CLA:O1D  | 22:B:830:CLA:HHB  | 2.16                     | 0.45              |
| 3:C:74:THR:HG23   | 3:C:79:LEU:HB2    | 1.98                     | 0.45              |
| 5:E:39:ARG:HE     | 5:E:62:VAL:N      | 2.15                     | 0.45              |
| 6:F:158:TYR:HA    | 6:F:202:TRP:HZ2   | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:24:ALA:O      | 9:J:28:GLU:HG2    | 2.17                     | 0.45              |
| 12:1:134:MET:HE2  | 22:1:314:CLA:HMC2 | 1.98                     | 0.45              |
| 22:Z:306:CLA:H3A  | 22:Z:306:CLA:HBA2 | 1.15                     | 0.45              |
| 13:3:157:ALA:O    | 13:3:159:PRO:HD3  | 2.17                     | 0.45              |
| 14:7:122:THR:O    | 14:7:126:THR:HG23 | 2.17                     | 0.45              |
| 15:8:50:PHE:CZ    | 41:8:320:3PH:H391 | 2.52                     | 0.45              |
| 15:8:83:ILE:HG23  | 15:8:100:TRP:HB3  | 1.99                     | 0.45              |
| 16:4:204:LYS:H    | 16:4:204:LYS:HG2  | 1.66                     | 0.45              |
| 17:5:46:ASN:HB2   | 17:5:48:GLU:OE1   | 2.17                     | 0.45              |
| 17:5:83:LEU:HG    | 22:5:307:CLA:HMC3 | 1.97                     | 0.45              |
| 22:5:307:CLA:H3A  | 22:5:307:CLA:HBA2 | 1.35                     | 0.45              |
| 22:5:311:CLA:OBD  | 22:5:318:CLA:H12  | 2.17                     | 0.45              |
| 22:9:313:CLA:CHA  | 22:9:313:CLA:HBA2 | 2.45                     | 0.45              |
| 22:2:301:CLA:HBC1 | 22:2:304:CLA:HMD1 | 1.99                     | 0.45              |
| 1:A:80:GLN:HE21   | 1:A:84:ILE:HG13   | 1.82                     | 0.45              |
| 22:A:821:CLA:H101 | 24:A:847:BCR:C10  | 2.40                     | 0.45              |
| 2:B:475:PHE:HB3   | 22:F:304:CLA:C19  | 2.44                     | 0.45              |
| 2:B:548:MET:HG2   | 2:B:565:ARG:NH2   | 2.32                     | 0.45              |
| 2:B:561:ASP:HB3   | 2:B:568:THR:HG21  | 1.99                     | 0.45              |
| 2:B:681:TRP:CZ2   | 4:D:71:THR:HB     | 2.52                     | 0.45              |
| 5:E:42:GLN:HA     | 5:E:57:GLY:O      | 2.16                     | 0.45              |
| 14:7:53:PHE:HZ    | 41:7:319:3PH:H282 | 1.82                     | 0.45              |
| 15:8:115:LEU:HD21 | 39:8:312:CHL:CHD  | 2.47                     | 0.45              |
| 15:8:139:LYS:HB3  | 15:8:139:LYS:HE2  | 1.71                     | 0.45              |
| 17:5:169:PHE:HD1  | 39:5:317:CHL:O1A  | 1.98                     | 0.45              |
| 22:5:308:CLA:C1C  | 22:5:313:CLA:H143 | 2.47                     | 0.45              |
| 22:6:322:CLA:H2   | 22:6:322:CLA:H121 | 1.99                     | 0.45              |
| 1:A:85:PHE:HE1    | 24:A:844:BCR:HC21 | 1.82                     | 0.45              |
| 2:B:293:ARG:HH22  | 7:G:61:LEU:HB3    | 1.81                     | 0.45              |
| 22:B:838:CLA:H152 | 32:F:306:RRX:H37  | 1.98                     | 0.45              |
| 6:F:162:TRP:CD1   | 6:F:162:TRP:C     | 2.94                     | 0.45              |
| 7:G:80:SER:O      | 7:G:83:GLN:HB3    | 2.17                     | 0.45              |
| 22:G:201:CLA:HAB  | 24:G:203:BCR:H352 | 1.98                     | 0.45              |
| 8:I:87:LEU:C      | 8:I:87:LEU:HD13   | 2.42                     | 0.45              |
| 10:K:68:VAL:O     | 10:K:68:VAL:HG12  | 2.16                     | 0.45              |
| 12:Z:147:ALA:HA   | 12:Z:150:ARG:HD2  | 1.99                     | 0.45              |
| 38:Z:301:LUT:H15  | 38:Z:301:LUT:H201 | 1.79                     | 0.45              |
| 24:3:304:BCR:H341 | 24:3:304:BCR:H11C | 1.34                     | 0.45              |
| 14:7:58:LEU:HD11  | 22:7:308:CLA:H92  | 1.99                     | 0.45              |
| 15:8:113:ILE:HG22 | 15:8:118:LEU:HB2  | 1.99                     | 0.45              |
| 16:4:140:TYR:HD2  | 16:4:142:TYR:CE1  | 2.35                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:4:804:BCR:C37  | 39:4:816:CHL:HHB  | 2.44                     | 0.45              |
| 17:5:69:TRP:CG    | 22:5:323:CLA:HAA1 | 2.52                     | 0.45              |
| 22:5:311:CLA:CMD  | 22:6:322:CLA:H92  | 2.47                     | 0.45              |
| 22:5:326:CLA:C1   | 22:6:314:CLA:H152 | 2.46                     | 0.45              |
| 19:9:133:THR:C    | 19:9:135:SER:H    | 2.25                     | 0.45              |
| 39:9:312:CHL:H2A  | 39:9:312:CHL:C2   | 2.47                     | 0.45              |
| 1:A:172:ALA:HA    | 22:3:312:CLA:H18  | 1.99                     | 0.44              |
| 1:A:442:ASN:ND2   | 2:B:675:LEU:HD11  | 2.33                     | 0.44              |
| 1:A:481:PRO:HG3   | 1:A:533:PHE:HB2   | 1.99                     | 0.44              |
| 1:A:536:HIS:HA    | 1:A:539:HIS:CD2   | 2.52                     | 0.44              |
| 22:A:807:CLA:HAB  | 24:J:104:BCR:C7   | 2.47                     | 0.44              |
| 22:A:820:CLA:H62  | 22:A:820:CLA:H2   | 1.41                     | 0.44              |
| 22:A:840:CLA:HBB2 | 6:F:167:GLY:HA3   | 1.99                     | 0.44              |
| 27:A:852:DGA:HA22 | 27:A:852:DGA:HA51 | 1.65                     | 0.44              |
| 2:B:181:SER:HB3   | 2:B:289:GLY:HA3   | 2.00                     | 0.44              |
| 22:B:801:CLA:H122 | 22:B:801:CLA:H161 | 1.67                     | 0.44              |
| 22:B:811:CLA:C3D  | 22:B:829:CLA:HBA1 | 2.47                     | 0.44              |
| 22:B:842:CLA:C4B  | 22:1:308:CLA:H51  | 2.47                     | 0.44              |
| 22:B:842:CLA:HBC1 | 33:1:301:LMT:O6'  | 2.16                     | 0.44              |
| 6:F:224:ILE:HB    | 6:F:227:ARG:NH2   | 2.30                     | 0.44              |
| 7:G:94:PRO:O      | 7:G:95:ALA:HB3    | 2.17                     | 0.44              |
| 11:L:128:LEU:HB3  | 24:L:204:BCR:H401 | 1.99                     | 0.44              |
| 12:1:144:GLU:CB   | 22:1:313:CLA:HAC1 | 2.47                     | 0.44              |
| 12:Z:145:THR:CA   | 12:Z:150:ARG:HH21 | 2.22                     | 0.44              |
| 38:3:303:LUT:H32  | 22:3:311:CLA:CAB  | 2.47                     | 0.44              |
| 22:7:308:CLA:HMD3 | 22:7:315:CLA:ND   | 2.32                     | 0.44              |
| 38:4:803:LUT:H32  | 22:4:808:CLA:HAB  | 1.99                     | 0.44              |
| 22:4:805:CLA:HMD1 | 39:4:814:CHL:O1A  | 2.16                     | 0.44              |
| 17:5:131:TRP:CZ3  | 22:6:314:CLA:HBA2 | 2.52                     | 0.44              |
| 41:5:325:3PH:H221 | 41:5:325:3PH:H2   | 1.51                     | 0.44              |
| 19:9:64:LYS:HD2   | 19:9:64:LYS:C     | 2.42                     | 0.44              |
| 19:9:145:ASP:N    | 19:9:146:PRO:HD2  | 2.27                     | 0.44              |
| 19:9:187:LEU:HD13 | 38:9:301:LUT:H163 | 1.99                     | 0.44              |
| 1:A:53:HIS:CD2    | 22:A:804:CLA:HAC1 | 2.52                     | 0.44              |
| 1:A:658:ILE:HD12  | 2:B:622:ARG:HG3   | 2.00                     | 0.44              |
| 22:A:804:CLA:C4A  | 22:A:811:CLA:H71  | 2.48                     | 0.44              |
| 22:A:816:CLA:O1A  | 27:A:852:DGA:HG12 | 2.16                     | 0.44              |
| 22:A:817:CLA:C4D  | 22:A:817:CLA:H12  | 2.47                     | 0.44              |
| 22:A:830:CLA:H151 | 22:A:841:CLA:CMA  | 2.48                     | 0.44              |
| 22:A:832:CLA:H101 | 22:L:202:CLA:H11  | 2.00                     | 0.44              |
| 22:A:836:CLA:H61  | 22:K:203:CLA:CBA  | 2.39                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:32:PHE:HA     | 2:B:35:HIS:CG     | 2.52                     | 0.44              |
| 2:B:548:MET:HE1   | 2:B:554:PHE:CD1   | 2.52                     | 0.44              |
| 2:B:622:ARG:HA    | 2:B:626:TRP:HB3   | 1.98                     | 0.44              |
| 22:B:811:CLA:H202 | 22:B:811:CLA:H162 | 1.64                     | 0.44              |
| 22:B:819:CLA:H111 | 22:B:819:CLA:H71  | 1.25                     | 0.44              |
| 22:B:824:CLA:H91  | 22:B:824:CLA:H111 | 1.75                     | 0.44              |
| 22:B:826:CLA:HMA1 | 22:B:826:CLA:H92  | 1.99                     | 0.44              |
| 22:B:827:CLA:HBB1 | 22:B:827:CLA:CMB  | 2.47                     | 0.44              |
| 6:F:186:ILE:HA    | 9:J:10:THR:HA     | 1.97                     | 0.44              |
| 12:1:57:PRO:CD    | 38:1:303:LUT:H23  | 2.45                     | 0.44              |
| 12:1:211:TRP:HZ3  | 15:8:118:LEU:HA   | 1.81                     | 0.44              |
| 12:Z:68:LYS:HD2   | 12:Z:147:ALA:CB   | 2.44                     | 0.44              |
| 13:3:36:PHE:HB3   | 22:3:311:CLA:HMD3 | 1.98                     | 0.44              |
| 22:3:309:CLA:HMC2 | 22:3:314:CLA:H143 | 1.98                     | 0.44              |
| 22:3:312:CLA:HBD  | 22:3:318:CLA:HBD  | 1.99                     | 0.44              |
| 14:7:157:THR:O    | 14:7:161:LYS:HD3  | 2.17                     | 0.44              |
| 14:7:198:ARG:HA   | 14:7:201:MET:CE   | 2.47                     | 0.44              |
| 22:7:306:CLA:HBB1 | 22:7:306:CLA:HMB3 | 1.98                     | 0.44              |
| 22:7:310:CLA:H122 | 22:7:310:CLA:C17  | 2.46                     | 0.44              |
| 15:8:50:PHE:HB3   | 22:8:308:CLA:C3D  | 2.48                     | 0.44              |
| 15:8:205:GLN:HG3  | 38:8:302:LUT:H42  | 1.99                     | 0.44              |
| 22:4:809:CLA:HBA1 | 22:4:809:CLA:H11  | 1.62                     | 0.44              |
| 25:4:821:LHG:H142 | 22:6:321:CLA:CHD  | 2.47                     | 0.44              |
| 25:5:324:LHG:H111 | 25:5:324:LHG:HC82 | 1.50                     | 0.44              |
| 22:A:809:CLA:HBA1 | 24:J:104:BCR:H363 | 1.99                     | 0.44              |
| 22:A:833:CLA:H41  | 22:A:855:CLA:HBC2 | 1.99                     | 0.44              |
| 24:A:844:BCR:C20  | 24:A:845:BCR:H23C | 2.47                     | 0.44              |
| 24:A:844:BCR:H21C | 24:A:845:BCR:H271 | 1.99                     | 0.44              |
| 27:A:852:DGA:HG11 | 14:7:243:PHE:HB3  | 1.99                     | 0.44              |
| 2:B:135:ASP:HB3   | 22:B:816:CLA:HED1 | 1.99                     | 0.44              |
| 2:B:292:TYR:CD1   | 2:B:302:MET:HG2   | 2.52                     | 0.44              |
| 2:B:649:TRP:CZ2   | 22:B:806:CLA:H72  | 2.52                     | 0.44              |
| 22:B:823:CLA:NA   | 22:B:824:CLA:H92  | 2.32                     | 0.44              |
| 22:B:839:CLA:H61  | 22:B:839:CLA:H2   | 1.67                     | 0.44              |
| 33:G:204:LMT:H62  | 33:G:204:LMT:H91  | 1.79                     | 0.44              |
| 12:Z:193:ALA:HB3  | 22:Z:316:CLA:HED1 | 1.99                     | 0.44              |
| 22:Z:303:CLA:H62  | 22:Z:304:CLA:CMA  | 2.47                     | 0.44              |
| 22:Z:309:CLA:HBB2 | 24:4:804:BCR:H323 | 1.99                     | 0.44              |
| 13:3:71:ALA:CB    | 38:3:302:LUT:H12  | 2.47                     | 0.44              |
| 13:3:146:LEU:O    | 13:3:149:VAL:N    | 2.46                     | 0.44              |
| 24:3:307:BCR:H342 | 22:3:315:CLA:HAA1 | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:3:317:CHL:H61  | 39:3:317:CHL:H101 | 1.65                     | 0.44              |
| 14:7:141:ASP:HB2  | 14:7:148:GLN:HG2  | 1.98                     | 0.44              |
| 22:7:310:CLA:HBC1 | 25:7:318:LHG:H281 | 1.99                     | 0.44              |
| 15:8:51:ASP:OD2   | 22:8:308:CLA:HBA1 | 2.18                     | 0.44              |
| 22:8:310:CLA:H72  | 22:8:310:CLA:H112 | 1.31                     | 0.44              |
| 16:4:83:PRO:HD2   | 38:4:803:LUT:C23  | 2.42                     | 0.44              |
| 16:4:193:PRO:HB2  | 16:4:197:PHE:HB2  | 2.00                     | 0.44              |
| 22:4:805:CLA:HBA2 | 22:4:805:CLA:H3A  | 1.29                     | 0.44              |
| 39:4:813:CHL:CAB  | 39:4:816:CHL:HBB2 | 2.41                     | 0.44              |
| 17:5:230:ASN:HA   | 17:5:233:HIS:HE2  | 1.82                     | 0.44              |
| 38:5:303:LUT:H15  | 38:5:303:LUT:H201 | 1.85                     | 0.44              |
| 19:9:31:TRP:NE1   | 19:9:51:PHE:HA    | 2.32                     | 0.44              |
| 1:A:212:SER:HA    | 22:A:815:CLA:HBB2 | 1.98                     | 0.44              |
| 1:A:269:TRP:HB3   | 22:A:817:CLA:HHB  | 1.98                     | 0.44              |
| 1:A:369:HIS:HA    | 1:A:372:TYR:CD2   | 2.53                     | 0.44              |
| 1:A:412:PHE:CD1   | 1:A:416:ASP:HB2   | 2.53                     | 0.44              |
| 22:A:821:CLA:NC   | 22:A:827:CLA:H161 | 2.32                     | 0.44              |
| 2:B:52:PHE:HD1    | 2:B:150:PHE:HD1   | 1.64                     | 0.44              |
| 2:B:287:VAL:HB    | 22:B:818:CLA:H202 | 1.98                     | 0.44              |
| 25:B:803:LHG:H262 | 22:B:807:CLA:HAA2 | 2.00                     | 0.44              |
| 22:B:831:CLA:HBB1 | 22:B:831:CLA:CMB  | 2.45                     | 0.44              |
| 22:B:835:CLA:HBA2 | 22:B:835:CLA:H3A  | 1.25                     | 0.44              |
| 24:B:848:BCR:C8   | 24:B:848:BCR:H321 | 2.47                     | 0.44              |
| 5:E:70:PRO:HD2    | 5:E:89:ALA:HA     | 1.97                     | 0.44              |
| 10:K:62:ASP:HB2   | 10:K:68:VAL:HG21  | 1.99                     | 0.44              |
| 12:Z:160:LEU:HB2  | 38:Z:301:LUT:H222 | 1.99                     | 0.44              |
| 13:3:127:ARG:HD3  | 39:3:317:CHL:CBB  | 2.47                     | 0.44              |
| 15:8:105:LYS:NZ   | 15:8:105:LYS:HB3  | 2.32                     | 0.44              |
| 15:8:152:PHE:O    | 15:8:153:GLU:C    | 2.60                     | 0.44              |
| 22:4:818:CLA:HBA1 | 22:4:818:CLA:C2   | 2.45                     | 0.44              |
| 17:5:100:TRP:HD1  | 38:5:303:LUT:H41  | 1.82                     | 0.44              |
| 17:5:245:LEU:HD22 | 18:6:220:VAL:HG11 | 1.99                     | 0.44              |
| 22:5:307:CLA:H43  | 22:5:308:CLA:H2   | 1.99                     | 0.44              |
| 18:6:57:LEU:CD1   | 38:6:304:LUT:H221 | 2.47                     | 0.44              |
| 1:A:367:VAL:HG12  | 1:A:371:MET:HE2   | 1.98                     | 0.44              |
| 1:A:454:GLY:C     | 1:A:456:TYR:H     | 2.25                     | 0.44              |
| 22:A:815:CLA:H143 | 13:3:196:PHE:HA   | 1.98                     | 0.44              |
| 27:A:852:DGA:HA22 | 27:A:852:DGA:HG12 | 1.72                     | 0.44              |
| 2:B:373:TYR:CE2   | 2:B:377:GLN:HG3   | 2.52                     | 0.44              |
| 2:B:667:SER:C     | 2:B:668:TRP:HD1   | 2.26                     | 0.44              |
| 22:L:203:CLA:HBB1 | 22:L:203:CLA:CMB  | 2.47                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:1:308:CLA:C1C  | 22:1:314:CLA:H18  | 2.48                     | 0.44              |
| 39:1:312:CHL:CAA  | 31:1:319:DGD:HG31 | 2.42                     | 0.44              |
| 25:1:317:LHG:C10  | 24:8:304:BCR:H313 | 2.43                     | 0.44              |
| 12:Z:79:ARG:O     | 12:Z:83:LEU:HG    | 2.17                     | 0.44              |
| 12:Z:190:ALA:CB   | 22:Z:305:CLA:HAC2 | 2.47                     | 0.44              |
| 15:8:114:ALA:HB3  | 15:8:117:PRO:HD2  | 2.00                     | 0.44              |
| 15:8:126:CYS:HB2  | 22:8:314:CLA:HAB  | 1.99                     | 0.44              |
| 22:8:306:CLA:CMD  | 22:8:311:CLA:C4D  | 2.96                     | 0.44              |
| 38:5:302:LUT:H401 | 38:5:302:LUT:H35  | 1.77                     | 0.44              |
| 18:6:253:LEU:HA   | 41:6:324:3PH:H292 | 1.98                     | 0.44              |
| 38:9:302:LUT:H28  | 22:9:306:CLA:C5   | 2.40                     | 0.44              |
| 22:9:306:CLA:H111 | 22:9:306:CLA:H72  | 1.27                     | 0.44              |
| 20:2:182:PRO:HG2  | 20:2:183:ILE:H    | 1.81                     | 0.44              |
| 1:A:71:ARG:HD3    | 1:A:185:ALA:HB1   | 1.99                     | 0.44              |
| 22:A:812:CLA:H91  | 22:A:812:CLA:H111 | 1.71                     | 0.44              |
| 22:A:814:CLA:H41  | 22:A:814:CLA:H61  | 1.65                     | 0.44              |
| 22:A:832:CLA:H13  | 22:A:832:CLA:H91  | 2.00                     | 0.44              |
| 24:A:844:BCR:C21  | 24:A:845:BCR:H291 | 2.47                     | 0.44              |
| 2:B:423:LEU:HB3   | 2:B:533:LEU:HD13  | 1.98                     | 0.44              |
| 2:B:429:PHE:CE2   | 22:B:838:CLA:HAB  | 2.52                     | 0.44              |
| 2:B:473:TYR:HB3   | 2:B:475:PHE:CE2   | 2.53                     | 0.44              |
| 22:B:818:CLA:H72  | 22:B:818:CLA:H122 | 1.99                     | 0.44              |
| 22:B:818:CLA:HBA2 | 22:B:818:CLA:H3A  | 1.53                     | 0.44              |
| 3:C:49:VAL:HG11   | 4:D:117:ARG:HH21  | 1.82                     | 0.44              |
| 4:D:115:PHE:HB3   | 4:D:120:GLN:NE2   | 2.29                     | 0.44              |
| 22:F:304:CLA:H92  | 22:F:304:CLA:H61  | 1.57                     | 0.44              |
| 22:G:201:CLA:C1C  | 24:G:203:BCR:H10C | 2.48                     | 0.44              |
| 10:K:107:LEU:HD22 | 10:K:112:ASN:CB   | 2.47                     | 0.44              |
| 22:Z:307:CLA:H12  | 22:Z:307:CLA:H51  | 1.70                     | 0.44              |
| 24:3:307:BCR:C39  | 22:3:314:CLA:HAC2 | 2.46                     | 0.44              |
| 22:7:309:CLA:C2   | 22:7:309:CLA:H72  | 2.44                     | 0.44              |
| 22:7:310:CLA:CBC  | 25:7:318:LHG:H281 | 2.48                     | 0.44              |
| 22:8:311:CLA:C4A  | 33:4:801:LMT:H62  | 2.47                     | 0.44              |
| 16:4:113:GLY:O    | 38:4:803:LUT:H42  | 2.17                     | 0.44              |
| 16:4:121:ARG:NH2  | 16:4:133:PRO:HA   | 2.28                     | 0.44              |
| 16:4:164:ARG:HH12 | 22:4:815:CLA:CED  | 2.31                     | 0.44              |
| 22:5:307:CLA:HMB2 | 22:5:308:CLA:HBA2 | 2.00                     | 0.44              |
| 22:5:310:CLA:H51  | 22:5:310:CLA:C2B  | 2.48                     | 0.44              |
| 22:6:309:CLA:HBC1 | 22:6:319:CLA:CAA  | 2.46                     | 0.44              |
| 22:6:312:CLA:H52  | 22:6:312:CLA:C2D  | 2.48                     | 0.44              |
| 19:9:102:LYS:HD2  | 22:9:308:CLA:HED1 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:511:GLY:HA2   | 1:A:525:PRO:HB3   | 1.99                     | 0.44              |
| 1:A:606:ALA:HB2   | 22:A:837:CLA:HBB2 | 1.99                     | 0.44              |
| 21:A:801:CL0:CAC  | 2:B:626:TRP:HD1   | 2.31                     | 0.44              |
| 22:A:812:CLA:C4   | 13:3:41:LEU:HD21  | 2.48                     | 0.44              |
| 22:B:840:CLA:C2   | 22:B:841:CLA:H143 | 2.47                     | 0.44              |
| 24:B:844:BCR:H341 | 24:B:844:BCR:H11C | 1.52                     | 0.44              |
| 3:C:28:MET:CE     | 3:C:38:GLN:HB3    | 2.48                     | 0.44              |
| 22:F:302:CLA:H62  | 22:F:302:CLA:H2   | 1.48                     | 0.44              |
| 22:F:304:CLA:H111 | 22:F:304:CLA:H152 | 1.71                     | 0.44              |
| 13:3:203:VAL:HG11 | 31:3:301:DGD:C7A  | 2.48                     | 0.44              |
| 14:7:187:LYS:HD3  | 14:7:190:LYS:HD3  | 1.98                     | 0.44              |
| 22:7:309:CLA:C3C  | 42:7:321:SPH:H162 | 2.48                     | 0.44              |
| 41:7:319:3PH:H372 | 41:7:319:3PH:H3A1 | 1.41                     | 0.44              |
| 22:8:309:CLA:H93  | 22:8:309:CLA:H111 | 1.71                     | 0.44              |
| 18:6:235:GLN:NE2  | 22:6:301:CLA:HHB  | 2.32                     | 0.44              |
| 41:6:324:3PH:H221 | 41:6:324:3PH:H251 | 1.52                     | 0.44              |
| 1:A:399:GLY:HA3   | 1:A:603:LEU:HD21  | 2.00                     | 0.44              |
| 22:A:807:CLA:H2   | 22:A:807:CLA:H61  | 1.62                     | 0.44              |
| 2:B:178:HIS:CE1   | 22:B:822:CLA:HMD3 | 2.53                     | 0.44              |
| 2:B:183:LEU:CD1   | 22:B:815:CLA:H43  | 2.47                     | 0.44              |
| 2:B:695:LYS:HE2   | 11:L:141:GLN:NE2  | 2.32                     | 0.44              |
| 22:B:821:CLA:O1A  | 22:B:826:CLA:H142 | 2.17                     | 0.44              |
| 22:B:830:CLA:H193 | 24:B:846:BCR:H17C | 1.99                     | 0.44              |
| 22:L:201:CLA:HBA2 | 22:L:201:CLA:HBD  | 1.99                     | 0.44              |
| 22:L:202:CLA:CBC  | 24:L:204:BCR:H23C | 2.48                     | 0.44              |
| 12:1:209:ASN:ND2  | 12:1:212:GLY:HA3  | 2.33                     | 0.44              |
| 38:1:303:LUT:H11  | 38:1:303:LUT:H191 | 1.88                     | 0.44              |
| 38:1:303:LUT:H382 | 22:1:307:CLA:O2A  | 2.17                     | 0.44              |
| 12:Z:149:LYS:CB   | 22:Z:313:CLA:HBC1 | 2.40                     | 0.44              |
| 12:Z:177:ASN:HD22 | 12:Z:177:ASN:H    | 1.65                     | 0.44              |
| 13:3:149:VAL:HG21 | 13:3:163:TRP:HB2  | 2.00                     | 0.44              |
| 14:7:135:GLU:HG3  | 22:7:315:CLA:C4B  | 2.48                     | 0.44              |
| 38:7:301:LUT:C14  | 22:7:305:CLA:HAB  | 2.48                     | 0.44              |
| 15:8:115:LEU:HD22 | 15:8:115:LEU:HA   | 1.74                     | 0.44              |
| 15:8:141:GLY:HA2  | 15:8:157:LYS:O    | 2.18                     | 0.44              |
| 39:8:315:CHL:H61  | 39:8:315:CHL:H111 | 1.98                     | 0.44              |
| 38:4:803:LUT:H28  | 22:4:808:CLA:H72  | 2.00                     | 0.44              |
| 22:4:807:CLA:H152 | 22:4:807:CLA:H111 | 1.67                     | 0.44              |
| 17:5:155:ASN:HB3  | 39:5:321:CHL:C2D  | 2.47                     | 0.44              |
| 17:5:179:ARG:O    | 17:5:183:GLN:HG3  | 2.17                     | 0.44              |
| 39:6:320:CHL:HHC  | 39:6:320:CHL:CBB  | 2.46                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:453:PHE:CE1   | 22:B:806:CLA:HMA1 | 2.52                     | 0.44              |
| 2:B:258:PHE:CD1   | 2:B:494:TRP:HB3   | 2.53                     | 0.44              |
| 22:B:808:CLA:H122 | 22:B:808:CLA:HBD  | 1.99                     | 0.44              |
| 22:B:817:CLA:H3A  | 22:B:817:CLA:HBA2 | 1.21                     | 0.44              |
| 6:F:222:ILE:O     | 6:F:222:ILE:HD12  | 2.18                     | 0.44              |
| 38:1:302:LUT:C30  | 22:1:304:CLA:H8   | 2.47                     | 0.44              |
| 12:Z:114:TRP:HB2  | 22:Z:308:CLA:CGA  | 2.47                     | 0.44              |
| 38:Z:302:LUT:H8   | 22:Z:308:CLA:HBB1 | 2.00                     | 0.44              |
| 13:3:42:LEU:HD12  | 13:3:53:PRO:HA    | 2.00                     | 0.44              |
| 13:3:81:GLY:HA3   | 13:3:88:ASP:HA    | 2.00                     | 0.44              |
| 13:3:146:LEU:O    | 13:3:147:GLU:C    | 2.61                     | 0.44              |
| 22:3:313:CLA:H112 | 22:5:320:CLA:ND   | 2.33                     | 0.44              |
| 22:7:305:CLA:HAC2 | 22:7:306:CLA:H191 | 2.00                     | 0.44              |
| 39:4:816:CHL:HAC2 | 39:4:816:CHL:OMC  | 2.18                     | 0.44              |
| 17:5:179:ARG:HG2  | 17:5:183:GLN:HG3  | 2.00                     | 0.44              |
| 24:5:304:BCR:HC32 | 22:6:314:CLA:C1D  | 2.48                     | 0.44              |
| 19:9:57:GLY:N     | 22:9:306:CLA:O1A  | 2.51                     | 0.44              |
| 20:2:173:SER:HB2  | 20:2:176:ALA:C    | 2.43                     | 0.44              |
| 1:A:316:TRP:CZ3   | 22:A:820:CLA:HBD  | 2.52                     | 0.43              |
| 1:A:693:TRP:HZ3   | 22:B:801:CLA:O1D  | 2.01                     | 0.43              |
| 22:A:818:CLA:H62  | 22:A:818:CLA:NC   | 2.32                     | 0.43              |
| 22:A:823:CLA:HBA2 | 37:K:201:DAO:H81  | 2.00                     | 0.43              |
| 2:B:231:TRP:HB2   | 22:B:818:CLA:O1A  | 2.18                     | 0.43              |
| 2:B:320:HIS:HA    | 2:B:323:LEU:HD12  | 2.00                     | 0.43              |
| 2:B:351:GLN:HG3   | 22:B:827:CLA:CED  | 2.44                     | 0.43              |
| 2:B:388:PHE:CZ    | 24:B:848:BCR:H20C | 2.53                     | 0.43              |
| 2:B:449:THR:HB    | 2:B:452:LYS:HG3   | 1.99                     | 0.43              |
| 2:B:471:ALA:O     | 2:B:472:PHE:C     | 2.60                     | 0.43              |
| 2:B:616:TYR:CD2   | 2:B:618:MET:HB3   | 2.52                     | 0.43              |
| 22:B:817:CLA:NC   | 24:B:844:BCR:H291 | 2.33                     | 0.43              |
| 22:B:825:CLA:HBB1 | 22:B:825:CLA:CMB  | 2.48                     | 0.43              |
| 22:B:827:CLA:C2B  | 22:B:839:CLA:HMA3 | 2.48                     | 0.43              |
| 22:B:829:CLA:H92  | 22:B:829:CLA:H62  | 1.55                     | 0.43              |
| 22:B:833:CLA:HBB1 | 22:B:833:CLA:CMB  | 2.48                     | 0.43              |
| 22:B:834:CLA:C2   | 24:F:303:BCR:HC42 | 2.47                     | 0.43              |
| 7:G:50:ARG:HG2    | 22:G:202:CLA:C3B  | 2.48                     | 0.43              |
| 11:L:96:LEU:O     | 11:L:99:PRO:HD2   | 2.18                     | 0.43              |
| 12:Z:179:ARG:HA   | 12:Z:182:MET:CE   | 2.48                     | 0.43              |
| 39:Z:311:CHL:HBC3 | 39:Z:311:CHL:CHD  | 2.44                     | 0.43              |
| 13:3:21:SER:HA    | 13:3:24:GLN:CD    | 2.43                     | 0.43              |
| 13:3:115:PHE:O    | 13:3:119:ILE:HG12 | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:3:311:CLA:HBB1 | 22:3:311:CLA:CMB  | 2.47                     | 0.43              |
| 16:4:259:ASP:HA   | 16:4:262:ARG:HD3  | 1.99                     | 0.43              |
| 22:5:315:CLA:HHC  | 22:5:315:CLA:CBB  | 2.48                     | 0.43              |
| 22:6:302:CLA:HHC  | 22:6:302:CLA:CBB  | 2.48                     | 0.43              |
| 1:A:32:PRO:HB2    | 1:A:48:TRP:CH2    | 2.53                     | 0.43              |
| 1:A:127:LEU:HD22  | 1:A:667:ALA:HB2   | 2.00                     | 0.43              |
| 1:A:227:LEU:HD12  | 1:A:237:ILE:HG23  | 2.00                     | 0.43              |
| 1:A:338:HIS:CE1   | 25:A:849:LHG:HC12 | 2.36                     | 0.43              |
| 1:A:392:THR:HG23  | 1:A:607:ILE:HG21  | 2.00                     | 0.43              |
| 22:A:817:CLA:H61  | 22:A:817:CLA:C4C  | 2.48                     | 0.43              |
| 22:A:821:CLA:H11  | 22:A:827:CLA:H122 | 2.00                     | 0.43              |
| 23:A:843:PQN:H142 | 24:F:303:BCR:H291 | 2.00                     | 0.43              |
| 2:B:5:LEU:HB3     | 2:B:8:LYS:HE3     | 2.00                     | 0.43              |
| 2:B:520:VAL:O     | 2:B:524:ILE:HG13  | 2.18                     | 0.43              |
| 22:B:821:CLA:HMB2 | 22:B:826:CLA:HMA3 | 1.99                     | 0.43              |
| 22:B:831:CLA:HMD2 | 31:B:852:DGD:HB62 | 2.00                     | 0.43              |
| 22:B:833:CLA:H18  | 22:B:833:CLA:H152 | 1.74                     | 0.43              |
| 9:J:1:MET:N       | 34:J:101:LMG:HC71 | 2.32                     | 0.43              |
| 12:1:57:PRO:HD2   | 38:1:303:LUT:C23  | 2.46                     | 0.43              |
| 22:Z:316:CLA:C2   | 22:Z:316:CLA:H71  | 2.42                     | 0.43              |
| 13:3:103:TYR:CE2  | 13:3:105:LYS:HB2  | 2.53                     | 0.43              |
| 14:7:70:HIS:CE1   | 14:7:138:ARG:HH11 | 2.35                     | 0.43              |
| 22:7:308:CLA:HMA3 | 22:7:308:CLA:H43  | 2.00                     | 0.43              |
| 38:4:803:LUT:H28  | 22:4:808:CLA:H52  | 2.00                     | 0.43              |
| 24:5:304:BCR:HC42 | 25:6:323:LHG:HC81 | 2.00                     | 0.43              |
| 22:5:318:CLA:H12  | 22:5:318:CLA:H51  | 1.80                     | 0.43              |
| 22:5:322:CLA:HED1 | 25:6:323:LHG:H301 | 2.00                     | 0.43              |
| 22:6:312:CLA:HMA3 | 39:6:318:CHL:HAC2 | 1.99                     | 0.43              |
| 39:6:316:CHL:HBD  | 39:6:316:CHL:HAA1 | 2.00                     | 0.43              |
| 19:9:35:LEU:HG    | 19:9:36:ASN:N     | 2.32                     | 0.43              |
| 19:9:129:GLY:HA3  | 19:9:142:PHE:CE1  | 2.53                     | 0.43              |
| 20:2:186:LEU:HD23 | 20:2:186:LEU:C    | 2.42                     | 0.43              |
| 1:A:521:VAL:HG21  | 1:A:627:VAL:HG11  | 1.99                     | 0.43              |
| 1:A:550:LEU:CB    | 24:A:847:BCR:H322 | 2.48                     | 0.43              |
| 22:A:835:CLA:H51  | 22:A:835:CLA:H12  | 1.76                     | 0.43              |
| 2:B:16:ASP:HB3    | 2:B:21:ARG:HB3    | 1.98                     | 0.43              |
| 22:B:812:CLA:NB   | 24:B:849:BCR:H322 | 2.34                     | 0.43              |
| 22:B:817:CLA:H51  | 22:B:817:CLA:H11  | 1.76                     | 0.43              |
| 22:B:821:CLA:HAA2 | 22:B:825:CLA:OBD  | 2.17                     | 0.43              |
| 22:B:825:CLA:H111 | 24:B:847:BCR:C16  | 2.49                     | 0.43              |
| 22:B:838:CLA:HHC  | 22:B:838:CLA:H102 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:66:ARG:HD3    | 3:C:66:ARG:HA     | 1.84                     | 0.43              |
| 12:1:55:PHE:HZ    | 40:1:318:SQD:H271 | 1.83                     | 0.43              |
| 12:1:69:ARG:NH2   | 22:1:308:CLA:O1D  | 2.51                     | 0.43              |
| 12:Z:82:MET:SD    | 22:Z:303:CLA:HAB  | 2.58                     | 0.43              |
| 38:Z:301:LUT:H362 | 22:Z:313:CLA:H42  | 1.99                     | 0.43              |
| 22:7:324:CLA:H143 | 22:4:817:CLA:ND   | 2.32                     | 0.43              |
| 15:8:74:ARG:HA    | 15:8:77:MET:HE3   | 1.99                     | 0.43              |
| 15:8:121:VAL:O    | 15:8:125:MET:HG3  | 2.18                     | 0.43              |
| 24:8:304:BCR:H19C | 39:8:315:CHL:CGA  | 2.49                     | 0.43              |
| 22:8:316:CLA:CBB  | 22:8:316:CLA:HHC  | 2.48                     | 0.43              |
| 22:8:316:CLA:HHC  | 22:8:316:CLA:HBB1 | 2.00                     | 0.43              |
| 17:5:230:ASN:HA   | 17:5:233:HIS:CE1  | 2.53                     | 0.43              |
| 22:5:308:CLA:H151 | 22:5:308:CLA:CMB  | 2.48                     | 0.43              |
| 22:5:318:CLA:HBC2 | 22:5:319:CLA:HMB1 | 2.00                     | 0.43              |
| 18:6:215:ILE:O    | 18:6:218:LYS:HG2  | 2.18                     | 0.43              |
| 18:6:240:GLN:HB2  | 24:6:306:BCR:H313 | 1.99                     | 0.43              |
| 24:6:305:BCR:H20C | 22:6:312:CLA:H203 | 1.99                     | 0.43              |
| 19:9:30:THR:HB    | 19:9:35:LEU:HB3   | 2.00                     | 0.43              |
| 1:A:412:PHE:HD1   | 1:A:416:ASP:HB2   | 1.83                     | 0.43              |
| 1:A:675:ALA:HB1   | 1:A:734:GLY:O     | 2.18                     | 0.43              |
| 22:A:823:CLA:H191 | 10:K:98:ILE:CD1   | 2.46                     | 0.43              |
| 22:A:828:CLA:C9   | 24:J:104:BCR:H341 | 2.48                     | 0.43              |
| 22:B:820:CLA:CMB  | 22:B:820:CLA:CBB  | 2.96                     | 0.43              |
| 22:B:823:CLA:NB   | 22:B:824:CLA:H8   | 2.33                     | 0.43              |
| 3:C:14:CYS:SG     | 29:C:102:SF4:S4   | 3.17                     | 0.43              |
| 4:D:160:LYS:HB3   | 4:D:160:LYS:HE2   | 1.78                     | 0.43              |
| 5:E:78:GLN:CB     | 5:E:84:THR:HG22   | 2.38                     | 0.43              |
| 6:F:137:PRO:HG2   | 22:F:304:CLA:C2C  | 2.49                     | 0.43              |
| 33:G:204:LMT:H111 | 22:1:314:CLA:HMC3 | 2.00                     | 0.43              |
| 12:1:143:ASP:O    | 12:1:145:THR:HG23 | 2.18                     | 0.43              |
| 38:1:302:LUT:H35  | 38:1:302:LUT:H401 | 1.84                     | 0.43              |
| 13:3:142:TYR:HA   | 13:3:147:GLU:CD   | 2.44                     | 0.43              |
| 39:3:317:CHL:HAA1 | 39:3:317:CHL:HBD  | 1.99                     | 0.43              |
| 38:7:301:LUT:H35  | 38:7:301:LUT:H401 | 1.83                     | 0.43              |
| 15:8:228:THR:HA   | 22:8:307:CLA:CBA  | 2.48                     | 0.43              |
| 22:8:308:CLA:C17  | 22:8:308:CLA:H122 | 2.48                     | 0.43              |
| 16:4:101:LEU:HD12 | 16:4:101:LEU:HA   | 1.82                     | 0.43              |
| 17:5:135:ARG:HB3  | 39:5:317:CHL:CMC  | 2.48                     | 0.43              |
| 17:5:178:ASN:ND2  | 17:5:181:GLU:HB2  | 2.32                     | 0.43              |
| 38:5:303:LUT:H31  | 38:5:303:LUT:H391 | 1.91                     | 0.43              |
| 22:5:318:CLA:H2   | 22:5:323:CLA:HAC1 | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:6:235:GLN:HG2  | 18:6:245:PHE:CE1  | 2.53                     | 0.43              |
| 24:6:305:BCR:H16C | 39:6:316:CHL:CMB  | 2.42                     | 0.43              |
| 22:6:309:CLA:H203 | 22:6:309:CLA:H152 | 2.01                     | 0.43              |
| 22:9:305:CLA:H92  | 22:9:305:CLA:H61  | 1.68                     | 0.43              |
| 1:A:26:PHE:H      | 34:J:101:LMG:HC5  | 1.83                     | 0.43              |
| 22:A:804:CLA:HED1 | 22:A:811:CLA:HED2 | 2.00                     | 0.43              |
| 22:A:807:CLA:ND   | 26:A:851:NKP:HARA | 2.33                     | 0.43              |
| 22:A:810:CLA:HAA1 | 13:3:51:VAL:HG21  | 2.01                     | 0.43              |
| 22:A:814:CLA:HBB1 | 22:A:814:CLA:CMB  | 2.46                     | 0.43              |
| 22:A:814:CLA:H61  | 27:A:852:DGA:HB62 | 1.99                     | 0.43              |
| 22:A:841:CLA:CAB  | 22:B:801:CLA:H162 | 2.48                     | 0.43              |
| 22:A:842:CLA:H62  | 22:A:842:CLA:H2   | 1.65                     | 0.43              |
| 2:B:32:PHE:C      | 2:B:34:SER:N      | 2.76                     | 0.43              |
| 2:B:258:PHE:HE1   | 22:B:819:CLA:H52  | 1.83                     | 0.43              |
| 25:B:803:LHG:H122 | 22:B:807:CLA:ND   | 2.32                     | 0.43              |
| 22:B:807:CLA:HAB  | 22:B:809:CLA:CAD  | 2.48                     | 0.43              |
| 22:B:817:CLA:H111 | 24:B:844:BCR:H23C | 2.01                     | 0.43              |
| 22:B:835:CLA:HMB3 | 24:B:848:BCR:H332 | 1.99                     | 0.43              |
| 4:D:191:THR:O     | 4:D:194:ILE:HG22  | 2.19                     | 0.43              |
| 12:Z:164:LYS:HB2  | 12:Z:164:LYS:NZ   | 2.34                     | 0.43              |
| 14:7:80:MET:SD    | 22:7:304:CLA:HAB  | 2.58                     | 0.43              |
| 15:8:82:GLY:O     | 15:8:86:PRO:HG2   | 2.19                     | 0.43              |
| 16:4:193:PRO:HD2  | 22:4:805:CLA:OBD  | 2.18                     | 0.43              |
| 17:5:131:TRP:HB2  | 22:6:314:CLA:H2   | 2.00                     | 0.43              |
| 22:5:309:CLA:H12  | 22:5:309:CLA:C1A  | 2.49                     | 0.43              |
| 22:6:312:CLA:C4D  | 22:6:312:CLA:H52  | 2.48                     | 0.43              |
| 39:6:315:CHL:HBB2 | 39:6:318:CHL:HBB2 | 2.00                     | 0.43              |
| 39:6:315:CHL:HBB2 | 22:6:317:CLA:HBC1 | 2.00                     | 0.43              |
| 19:9:194:PRO:HB3  | 22:9:310:CLA:HMB2 | 2.00                     | 0.43              |
| 1:A:161:THR:HG21  | 22:A:816:CLA:HAA2 | 2.00                     | 0.43              |
| 1:A:343:GLU:H     | 1:A:343:GLU:CD    | 2.26                     | 0.43              |
| 1:A:487:ILE:HG21  | 22:A:837:CLA:HED1 | 2.01                     | 0.43              |
| 1:A:674:GLY:HA2   | 24:A:848:BCR:H17C | 2.00                     | 0.43              |
| 22:A:833:CLA:H102 | 22:B:840:CLA:C5   | 2.48                     | 0.43              |
| 2:B:48:PHE:HB2    | 2:B:169:PHE:CE1   | 2.54                     | 0.43              |
| 2:B:262:PHE:CZ    | 2:B:356:LEU:HA    | 2.54                     | 0.43              |
| 2:B:687:PRO:HG2   | 22:L:202:CLA:C5   | 2.45                     | 0.43              |
| 22:B:831:CLA:CHA  | 22:B:831:CLA:HBA1 | 2.42                     | 0.43              |
| 22:B:832:CLA:HAA1 | 22:B:842:CLA:H41  | 2.00                     | 0.43              |
| 22:B:838:CLA:H122 | 32:F:306:RRX:H38  | 2.00                     | 0.43              |
| 4:D:56:PRO:HD2    | 4:D:149:TYR:CZ    | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:39:ARG:HG3    | 5:E:61:SER:HA     | 1.98                     | 0.43              |
| 5:E:86:ASN:HB3    | 5:E:88:PHE:CE2    | 2.53                     | 0.43              |
| 22:F:304:CLA:OBD  | 22:F:304:CLA:H122 | 2.19                     | 0.43              |
| 34:J:101:LMG:HC8  | 14:7:57:GLY:HA3   | 2.00                     | 0.43              |
| 12:1:100:TYR:O    | 12:1:103:PRO:HD2  | 2.17                     | 0.43              |
| 22:1:307:CLA:C1B  | 22:1:307:CLA:H2   | 2.49                     | 0.43              |
| 14:7:205:LEU:HD21 | 22:7:307:CLA:H171 | 2.00                     | 0.43              |
| 22:7:323:CLA:HED2 | 15:8:31:MET:HG2   | 2.00                     | 0.43              |
| 41:8:320:3PH:H3A1 | 41:8:320:3PH:H3D1 | 1.45                     | 0.43              |
| 16:4:196:ILE:HD12 | 16:4:196:ILE:HA   | 1.80                     | 0.43              |
| 24:4:804:BCR:H281 | 22:4:810:CLA:NB   | 2.33                     | 0.43              |
| 17:5:242:VAL:HG21 | 39:5:316:CHL:HMD3 | 1.99                     | 0.43              |
| 22:5:308:CLA:H72  | 22:5:308:CLA:H112 | 1.68                     | 0.43              |
| 22:5:323:CLA:O1A  | 22:5:323:CLA:H2A  | 2.19                     | 0.43              |
| 18:6:88:GLN:HG2   | 22:6:312:CLA:C3D  | 2.48                     | 0.43              |
| 1:A:119:TRP:CE3   | 22:A:809:CLA:H2A  | 2.53                     | 0.43              |
| 1:A:651:TRP:HD1   | 22:B:805:CLA:CAC  | 2.31                     | 0.43              |
| 1:A:673:LEU:HD12  | 22:A:802:CLA:H42  | 1.99                     | 0.43              |
| 22:A:834:CLA:H92  | 22:A:834:CLA:H61  | 1.71                     | 0.43              |
| 2:B:38:MET:O      | 4:D:186:PHE:HD1   | 2.02                     | 0.43              |
| 2:B:590:TRP:CG    | 22:B:805:CLA:H152 | 2.53                     | 0.43              |
| 22:B:833:CLA:C1B  | 32:F:306:RRX:H26  | 2.48                     | 0.43              |
| 22:B:838:CLA:HMA2 | 22:B:839:CLA:HED2 | 2.01                     | 0.43              |
| 33:G:204:LMT:H111 | 22:1:314:CLA:CMC  | 2.47                     | 0.43              |
| 9:J:1:MET:N       | 34:J:101:LMG:HC2  | 2.29                     | 0.43              |
| 12:1:173:LYS:HG3  | 22:1:310:CLA:HED2 | 2.00                     | 0.43              |
| 22:1:304:CLA:HBB1 | 22:1:304:CLA:CMB  | 2.47                     | 0.43              |
| 22:1:308:CLA:HMD3 | 22:1:314:CLA:ND   | 2.34                     | 0.43              |
| 12:Z:144:GLU:CG   | 22:Z:313:CLA:HAC1 | 2.49                     | 0.43              |
| 12:Z:144:GLU:CD   | 12:Z:146:ASP:H    | 2.27                     | 0.43              |
| 12:Z:195:THR:HG23 | 12:Z:197:LYS:HE2  | 2.01                     | 0.43              |
| 38:Z:301:LUT:H35  | 38:Z:301:LUT:H401 | 1.81                     | 0.43              |
| 22:Z:306:CLA:C1B  | 22:Z:306:CLA:H2   | 2.49                     | 0.43              |
| 13:3:52:THR:HG23  | 13:3:55:TRP:H     | 1.84                     | 0.43              |
| 14:7:204:ASN:CG   | 38:7:302:LUT:H12  | 2.44                     | 0.43              |
| 38:7:302:LUT:C28  | 22:7:307:CLA:H61  | 2.44                     | 0.43              |
| 24:4:804:BCR:H343 | 39:4:819:CHL:HAB  | 2.01                     | 0.43              |
| 22:4:805:CLA:H71  | 22:4:806:CLA:CMA  | 2.49                     | 0.43              |
| 24:5:304:BCR:HC7  | 39:5:321:CHL:HBB2 | 2.01                     | 0.43              |
| 22:5:318:CLA:H2   | 22:5:323:CLA:CAC  | 2.49                     | 0.43              |
| 38:9:302:LUT:H35  | 38:9:302:LUT:H401 | 1.81                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:A:801:CL0:H22  | 2:B:626:TRP:CD1   | 2.54                     | 0.43              |
| 22:A:816:CLA:H92  | 27:A:852:DGA:HB61 | 2.01                     | 0.43              |
| 22:A:821:CLA:H111 | 22:A:821:CLA:H152 | 1.75                     | 0.43              |
| 22:A:826:CLA:O1A  | 22:A:839:CLA:HAA2 | 2.19                     | 0.43              |
| 22:A:832:CLA:C11  | 22:L:202:CLA:H171 | 2.47                     | 0.43              |
| 2:B:126:TYR:O     | 2:B:131:ARG:NH1   | 2.51                     | 0.43              |
| 2:B:431:GLY:HA3   | 22:B:801:CLA:H11  | 2.00                     | 0.43              |
| 22:B:815:CLA:H142 | 22:B:815:CLA:H112 | 1.80                     | 0.43              |
| 22:B:815:CLA:H151 | 22:B:820:CLA:C4D  | 2.48                     | 0.43              |
| 22:B:824:CLA:HBC2 | 22:B:825:CLA:CBA  | 2.48                     | 0.43              |
| 22:F:304:CLA:CBB  | 32:F:306:RRX:H51  | 2.45                     | 0.43              |
| 7:G:45:MET:HG3    | 7:G:109:GLY:CA    | 2.47                     | 0.43              |
| 12:Z:35:TRP:HD1   | 39:Z:311:CHL:C1B  | 2.32                     | 0.43              |
| 12:Z:160:LEU:HB3  | 12:Z:162:PHE:CZ   | 2.54                     | 0.43              |
| 12:Z:166:ASP:OD1  | 12:Z:169:THR:OG1  | 2.28                     | 0.43              |
| 31:3:301:DGD:HE5  | 31:3:301:DGD:O4D  | 2.18                     | 0.43              |
| 24:3:304:BCR:H23C | 24:3:305:BCR:H353 | 2.01                     | 0.43              |
| 24:3:305:BCR:C16  | 39:3:317:CHL:H112 | 2.48                     | 0.43              |
| 14:7:59:SER:HB2   | 14:7:65:MET:HG2   | 2.01                     | 0.43              |
| 14:7:135:GLU:HG3  | 22:7:315:CLA:C1B  | 2.48                     | 0.43              |
| 22:7:308:CLA:H92  | 22:7:308:CLA:H62  | 1.71                     | 0.43              |
| 15:8:37:PRO:O     | 15:8:38:ALA:HB2   | 2.19                     | 0.43              |
| 22:8:307:CLA:O1D  | 22:8:307:CLA:H2A  | 2.19                     | 0.43              |
| 16:4:70:HIS:CD2   | 16:4:71:LEU:HG    | 2.54                     | 0.43              |
| 16:4:105:ARG:HB3  | 39:4:814:CHL:HED2 | 2.00                     | 0.43              |
| 17:5:78:ALA:HB1   | 17:5:190:GLY:HA3  | 2.01                     | 0.43              |
| 24:5:304:BCR:H381 | 22:5:319:CLA:NC   | 2.34                     | 0.43              |
| 22:5:310:CLA:H152 | 22:5:311:CLA:HBB1 | 2.00                     | 0.43              |
| 18:6:167:MET:O    | 18:6:171:LYS:HG3  | 2.19                     | 0.43              |
| 18:6:173:LYS:NZ   | 22:6:308:CLA:H43  | 2.34                     | 0.43              |
| 19:9:32:LEU:O     | 19:9:35:LEU:HB2   | 2.18                     | 0.43              |
| 20:2:177:VAL:O    | 20:2:178:ARG:HG3  | 2.19                     | 0.43              |
| 1:A:521:VAL:HG11  | 1:A:524:MET:HB2   | 2.00                     | 0.43              |
| 22:A:819:CLA:H151 | 22:A:819:CLA:H18  | 1.74                     | 0.43              |
| 22:A:821:CLA:O2A  | 22:A:824:CLA:HBA2 | 2.19                     | 0.43              |
| 2:B:669:ARG:NE    | 2:B:700:ALA:HB3   | 2.34                     | 0.43              |
| 22:B:805:CLA:H51  | 22:B:805:CLA:H8   | 1.64                     | 0.43              |
| 22:B:814:CLA:H2   | 22:B:814:CLA:ND   | 2.33                     | 0.43              |
| 22:B:827:CLA:HBA1 | 22:B:827:CLA:H12  | 1.73                     | 0.43              |
| 5:E:53:TYR:C      | 5:E:55:GLN:N      | 2.77                     | 0.43              |
| 6:F:201:THR:O     | 6:F:205:GLN:HG3   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:1:56:ASP:HA    | 38:1:303:LUT:H24  | 2.00                     | 0.43              |
| 22:1:316:CLA:H141 | 39:8:301:CHL:H111 | 2.00                     | 0.43              |
| 38:3:303:LUT:H15  | 38:3:303:LUT:H201 | 1.86                     | 0.43              |
| 22:4:808:CLA:H62  | 22:4:808:CLA:H41  | 1.58                     | 0.43              |
| 17:5:58:LEU:HD12  | 17:5:58:LEU:N     | 2.34                     | 0.43              |
| 22:5:309:CLA:C1   | 22:5:314:CLA:HMD2 | 2.49                     | 0.43              |
| 38:6:303:LUT:C28  | 22:6:307:CLA:H52  | 2.49                     | 0.43              |
| 19:9:119:MET:HE3  | 39:9:314:CHL:HMB3 | 2.01                     | 0.43              |
| 22:2:301:CLA:HBA1 | 22:2:301:CLA:H11  | 1.61                     | 0.43              |
| 1:A:494:ALA:HB1   | 1:A:498:THR:OG1   | 2.18                     | 0.43              |
| 1:A:726:VAL:HG22  | 22:A:841:CLA:O1D  | 2.19                     | 0.43              |
| 22:A:822:CLA:HAA2 | 10:K:61:THR:CG2   | 2.47                     | 0.43              |
| 22:A:832:CLA:H112 | 22:L:202:CLA:H152 | 2.00                     | 0.43              |
| 2:B:482:SER:C     | 2:B:484:SER:H     | 2.27                     | 0.43              |
| 2:B:652:LEU:O     | 22:B:806:CLA:HBA1 | 2.19                     | 0.43              |
| 22:B:809:CLA:CBC  | 22:B:811:CLA:H193 | 2.49                     | 0.43              |
| 22:B:819:CLA:H93  | 22:B:835:CLA:HBA1 | 2.00                     | 0.43              |
| 24:B:848:BCR:H321 | 24:B:848:BCR:HC8  | 2.00                     | 0.43              |
| 3:C:79:LEU:HD22   | 3:C:81:TYR:CE2    | 2.54                     | 0.43              |
| 6:F:70:CYS:HA     | 6:F:73:SER:HB3    | 2.01                     | 0.43              |
| 22:G:202:CLA:CHC  | 24:G:203:BCR:H402 | 2.49                     | 0.43              |
| 8:I:74:TRP:CZ2    | 22:2:304:CLA:HHB  | 2.54                     | 0.43              |
| 38:Z:301:LUT:H371 | 22:Z:303:CLA:H92  | 2.01                     | 0.43              |
| 13:3:109:ASP:OD1  | 13:3:109:ASP:N    | 2.52                     | 0.43              |
| 38:3:302:LUT:H30  | 22:3:308:CLA:H72  | 1.98                     | 0.43              |
| 22:3:308:CLA:H3A  | 22:3:308:CLA:HBA2 | 1.17                     | 0.43              |
| 22:3:312:CLA:H61  | 22:3:312:CLA:H2   | 1.73                     | 0.43              |
| 22:3:312:CLA:H61  | 22:3:312:CLA:H92  | 1.76                     | 0.43              |
| 22:3:322:CLA:HHC  | 22:3:322:CLA:HBB1 | 2.01                     | 0.43              |
| 42:7:320:SPH:H91  | 42:7:320:SPH:H61  | 1.63                     | 0.43              |
| 15:8:105:LYS:O    | 15:8:109:GLU:HG2  | 2.19                     | 0.43              |
| 16:4:225:PHE:HA   | 16:4:228:PHE:HD2  | 1.83                     | 0.43              |
| 22:4:805:CLA:H71  | 22:4:806:CLA:HMA2 | 2.00                     | 0.43              |
| 22:4:806:CLA:HBA1 | 22:4:806:CLA:H61  | 2.01                     | 0.43              |
| 17:5:94:LEU:O     | 17:5:96:PRO:HD3   | 2.18                     | 0.43              |
| 17:5:227:TRP:N    | 22:5:309:CLA:O1A  | 2.52                     | 0.43              |
| 18:6:121:MET:HE2  | 22:6:317:CLA:C2C  | 2.49                     | 0.43              |
| 18:6:222:VAL:CG1  | 18:6:224:GLY:H    | 2.32                     | 0.43              |
| 24:6:306:BCR:H19C | 39:6:315:CHL:C2   | 2.49                     | 0.43              |
| 24:6:306:BCR:C8   | 24:6:306:BCR:H311 | 2.48                     | 0.43              |
| 1:A:694:GLN:NE2   | 5:E:80:TYR:HE1    | 2.16                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:819:CLA:H203 | 22:A:827:CLA:HAA1 | 2.00                     | 0.42              |
| 22:A:840:CLA:H11  | 22:A:840:CLA:C1A  | 2.49                     | 0.42              |
| 2:B:600:LEU:HD23  | 2:B:600:LEU:HA    | 1.94                     | 0.42              |
| 22:B:809:CLA:HBA1 | 22:B:809:CLA:H3A  | 1.55                     | 0.42              |
| 24:B:844:BCR:C22  | 24:G:203:BCR:HC42 | 2.49                     | 0.42              |
| 3:C:74:THR:HG21   | 4:D:81:GLU:OE1    | 2.18                     | 0.42              |
| 5:E:47:ARG:HD2    | 5:E:50:SER:OG     | 2.18                     | 0.42              |
| 12:Z:149:LYS:HB3  | 22:Z:313:CLA:CBC  | 2.40                     | 0.42              |
| 14:7:113:THR:HG22 | 14:7:115:HIS:H    | 1.84                     | 0.42              |
| 24:8:304:BCR:H19C | 39:8:315:CHL:CMA  | 2.49                     | 0.42              |
| 16:4:106:TRP:CZ3  | 24:4:804:BCR:H372 | 2.54                     | 0.42              |
| 16:4:216:LYS:HD2  | 22:4:811:CLA:O1D  | 2.19                     | 0.42              |
| 17:5:69:TRP:CZ2   | 22:5:318:CLA:HAA2 | 2.54                     | 0.42              |
| 22:5:309:CLA:H11  | 22:5:314:CLA:CMD  | 2.49                     | 0.42              |
| 18:6:87:VAL:C     | 18:6:89:GLU:N     | 2.76                     | 0.42              |
| 18:6:242:THR:HG23 | 24:6:306:BCR:H312 | 2.01                     | 0.42              |
| 38:6:304:LUT:H15  | 38:6:304:LUT:H201 | 1.84                     | 0.42              |
| 20:2:198:ILE:HD12 | 22:2:301:CLA:CHD  | 2.48                     | 0.42              |
| 1:A:365:ILE:CD1   | 1:A:398:GLY:HA3   | 2.49                     | 0.42              |
| 22:A:806:CLA:H12  | 22:A:806:CLA:HBA2 | 1.53                     | 0.42              |
| 22:A:821:CLA:H93  | 22:A:821:CLA:H62  | 1.85                     | 0.42              |
| 22:A:831:CLA:HAB  | 22:A:839:CLA:CBB  | 2.49                     | 0.42              |
| 2:B:107:ARG:HE    | 2:B:116:ILE:HG12  | 1.84                     | 0.42              |
| 2:B:371:SER:HA    | 2:B:726:LEU:HD21  | 2.00                     | 0.42              |
| 2:B:513:ILE:HG22  | 2:B:517:ASP:OD2   | 2.19                     | 0.42              |
| 22:B:833:CLA:HMC2 | 22:B:839:CLA:HAC1 | 2.00                     | 0.42              |
| 24:B:847:BCR:HC31 | 22:1:314:CLA:H41  | 2.00                     | 0.42              |
| 5:E:38:LYS:HB3    | 5:E:38:LYS:HE3    | 1.65                     | 0.42              |
| 11:L:165:GLU:H    | 11:L:165:GLU:CD   | 2.26                     | 0.42              |
| 12:1:134:MET:HE2  | 22:1:314:CLA:C2C  | 2.48                     | 0.42              |
| 22:1:308:CLA:C1D  | 22:1:314:CLA:H93  | 2.49                     | 0.42              |
| 12:Z:115:PHE:H    | 22:Z:308:CLA:CAD  | 2.32                     | 0.42              |
| 22:Z:309:CLA:HMC2 | 24:4:804:BCR:HC21 | 2.01                     | 0.42              |
| 39:Z:312:CHL:HAB  | 22:Z:315:CLA:CBB  | 2.49                     | 0.42              |
| 14:7:65:MET:O     | 14:7:69:VAL:HG23  | 2.20                     | 0.42              |
| 24:7:303:BCR:H373 | 22:7:316:CLA:HHB  | 2.00                     | 0.42              |
| 22:7:310:CLA:H93  | 22:7:310:CLA:H62  | 1.80                     | 0.42              |
| 15:8:135:MET:HE3  | 15:8:139:LYS:HB2  | 2.01                     | 0.42              |
| 15:8:164:PRO:HD3  | 22:8:313:CLA:HMD1 | 2.01                     | 0.42              |
| 16:4:85:SER:HB2   | 16:4:88:VAL:HG21  | 2.00                     | 0.42              |
| 17:5:227:TRP:HE1  | 22:5:314:CLA:HED2 | 1.83                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:5:314:CLA:CBB  | 22:5:314:CLA:HHC  | 2.49                     | 0.42              |
| 19:9:59:ASP:OD2   | 19:9:62:ARG:HG3   | 2.19                     | 0.42              |
| 38:9:301:LUT:H162 | 22:9:305:CLA:HBB  | 2.01                     | 0.42              |
| 1:A:365:ILE:HG13  | 1:A:395:ASN:HA    | 2.01                     | 0.42              |
| 1:A:366:ILE:HD12  | 22:A:827:CLA:H42  | 2.01                     | 0.42              |
| 22:A:810:CLA:CAB  | 22:A:813:CLA:H121 | 2.48                     | 0.42              |
| 22:A:814:CLA:C2C  | 24:A:844:BCR:H352 | 2.49                     | 0.42              |
| 2:B:5:LEU:HG      | 8:I:103:ASN:HB2   | 2.01                     | 0.42              |
| 2:B:176:LEU:HD12  | 2:B:176:LEU:HA    | 1.87                     | 0.42              |
| 2:B:211:ASP:HB3   | 25:B:851:LHG:HC42 | 2.01                     | 0.42              |
| 2:B:527:GLY:HA2   | 2:B:583:TRP:CZ3   | 2.53                     | 0.42              |
| 22:B:835:CLA:HBB1 | 22:B:835:CLA:CMB  | 2.44                     | 0.42              |
| 24:B:853:BCR:HC32 | 22:L:202:CLA:C4C  | 2.49                     | 0.42              |
| 22:F:304:CLA:C2   | 22:F:304:CLA:HBA1 | 2.49                     | 0.42              |
| 22:G:202:CLA:HBB1 | 22:G:202:CLA:CMB  | 2.50                     | 0.42              |
| 8:I:98:TYR:CD2    | 8:I:99:ILE:HD12   | 2.51                     | 0.42              |
| 10:K:33:THR:O     | 10:K:37:ILE:HG13  | 2.19                     | 0.42              |
| 38:Z:301:LUT:C30  | 22:Z:303:CLA:H8   | 2.49                     | 0.42              |
| 22:3:309:CLA:O1D  | 22:3:314:CLA:H51  | 2.19                     | 0.42              |
| 22:7:307:CLA:H18  | 22:7:307:CLA:H151 | 1.80                     | 0.42              |
| 38:8:302:LUT:H30  | 22:8:305:CLA:H61  | 2.00                     | 0.42              |
| 22:4:807:CLA:HBB1 | 22:4:807:CLA:CMB  | 2.49                     | 0.42              |
| 18:6:46:LEU:H     | 18:6:46:LEU:CD1   | 2.27                     | 0.42              |
| 18:6:170:LEU:HB3  | 22:6:307:CLA:CMA  | 2.49                     | 0.42              |
| 18:6:216:PHE:HA   | 22:6:322:CLA:HMB1 | 2.01                     | 0.42              |
| 24:6:305:BCR:H402 | 22:6:312:CLA:C1B  | 2.50                     | 0.42              |
| 1:A:483:PHE:HB3   | 22:A:837:CLA:C3   | 2.48                     | 0.42              |
| 22:A:812:CLA:C9   | 38:3:303:LUT:H372 | 2.49                     | 0.42              |
| 22:A:824:CLA:H52  | 24:A:847:BCR:H363 | 2.01                     | 0.42              |
| 22:A:832:CLA:H18  | 22:A:832:CLA:H151 | 1.69                     | 0.42              |
| 22:A:835:CLA:H11  | 22:A:835:CLA:HBA1 | 1.72                     | 0.42              |
| 2:B:43:LEU:O      | 2:B:47:ILE:HG13   | 2.20                     | 0.42              |
| 2:B:159:GLN:O     | 2:B:160:PRO:C     | 2.62                     | 0.42              |
| 2:B:243:HIS:HD2   | 2:B:251:ALA:HA    | 1.84                     | 0.42              |
| 22:B:815:CLA:H192 | 22:B:830:CLA:H93  | 2.01                     | 0.42              |
| 22:B:817:CLA:HBA1 | 19:9:177:LEU:HD22 | 2.00                     | 0.42              |
| 22:B:834:CLA:HMA3 | 35:J:102:T7X:C15  | 2.48                     | 0.42              |
| 3:C:15:THR:HG22   | 3:C:28:MET:HE2    | 2.00                     | 0.42              |
| 4:D:138:PHE:CZ    | 4:D:151:HIS:HB2   | 2.54                     | 0.42              |
| 6:F:162:TRP:CZ3   | 6:F:200:ALA:HA    | 2.54                     | 0.42              |
| 7:G:77:TYR:CG     | 7:G:78:PHE:N      | 2.87                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:1:158:ASP:O    | 12:1:161:ASN:ND2  | 2.50                     | 0.42              |
| 38:Z:302:LUT:H35  | 38:Z:302:LUT:H401 | 1.83                     | 0.42              |
| 13:3:182:LEU:HD23 | 22:3:314:CLA:HED2 | 2.01                     | 0.42              |
| 13:3:231:LYS:C    | 31:3:301:DGD:HE2  | 2.44                     | 0.42              |
| 22:3:318:CLA:H62  | 22:3:318:CLA:H2   | 1.64                     | 0.42              |
| 38:7:302:LUT:H35  | 38:7:302:LUT:H401 | 1.87                     | 0.42              |
| 42:7:320:SPH:H121 | 42:7:320:SPH:H152 | 1.45                     | 0.42              |
| 15:8:155:SER:HB3  | 15:8:167:PRO:HD3  | 2.02                     | 0.42              |
| 22:8:310:CLA:H62  | 43:8:319:LPX:H5A  | 2.01                     | 0.42              |
| 39:8:312:CHL:C1D  | 26:8:318:NKP:HAL  | 2.50                     | 0.42              |
| 16:4:62:PHE:HD2   | 16:4:65:SER:HB3   | 1.85                     | 0.42              |
| 18:6:72:ARG:O     | 18:6:76:ARG:HG3   | 2.20                     | 0.42              |
| 18:6:91:VAL:O     | 18:6:93:PRO:HD3   | 2.20                     | 0.42              |
| 18:6:95:VAL:HA    | 18:6:103:LYS:HE2  | 2.02                     | 0.42              |
| 18:6:123:PHE:CD2  | 24:6:305:BCR:H12C | 2.54                     | 0.42              |
| 22:6:302:CLA:HHC  | 22:6:302:CLA:HBB1 | 2.01                     | 0.42              |
| 22:6:310:CLA:H13  | 22:6:310:CLA:H102 | 1.82                     | 0.42              |
| 19:9:110:PRO:HB2  | 20:2:194:TRP:CZ3  | 2.54                     | 0.42              |
| 19:9:125:LYS:NZ   | 19:9:125:LYS:HB3  | 2.35                     | 0.42              |
| 20:2:189:HIS:ND1  | 22:2:301:CLA:HAA2 | 2.34                     | 0.42              |
| 1:A:101:TYR:CZ    | 1:A:105:LEU:HD21  | 2.54                     | 0.42              |
| 1:A:150:ALA:HB2   | 1:A:378:PRO:HD2   | 2.02                     | 0.42              |
| 1:A:650:LEU:HD13  | 22:B:805:CLA:CBB  | 2.50                     | 0.42              |
| 1:A:686:LEU:HG    | 1:A:727:GLY:HA3   | 2.00                     | 0.42              |
| 22:A:808:CLA:H93  | 22:A:808:CLA:H62  | 1.87                     | 0.42              |
| 22:A:810:CLA:HBD  | 13:3:51:VAL:HG23  | 2.00                     | 0.42              |
| 22:A:829:CLA:H2   | 22:A:829:CLA:H62  | 1.73                     | 0.42              |
| 22:A:838:CLA:HHB  | 22:A:839:CLA:O1D  | 2.19                     | 0.42              |
| 24:A:846:BCR:H15C | 24:A:846:BCR:H351 | 1.66                     | 0.42              |
| 2:B:231:TRP:CH2   | 22:B:818:CLA:H92  | 2.54                     | 0.42              |
| 22:B:840:CLA:HBB1 | 22:B:840:CLA:CMB  | 2.49                     | 0.42              |
| 22:B:841:CLA:NB   | 24:B:849:BCR:H15C | 2.35                     | 0.42              |
| 24:B:844:BCR:H20C | 24:B:844:BCR:H361 | 1.42                     | 0.42              |
| 25:B:850:LHG:HC81 | 25:B:850:LHG:HC5  | 1.83                     | 0.42              |
| 4:D:86:ILE:HG21   | 4:D:124:LEU:HD23  | 2.01                     | 0.42              |
| 8:I:95:LEU:HD13   | 24:L:204:BCR:HC8  | 2.00                     | 0.42              |
| 12:Z:160:LEU:N    | 12:Z:160:LEU:HD22 | 2.34                     | 0.42              |
| 12:Z:188:PHE:HA   | 12:Z:191:GLN:HE22 | 1.82                     | 0.42              |
| 38:Z:302:LUT:H15  | 38:Z:302:LUT:H201 | 1.83                     | 0.42              |
| 39:Z:312:CHL:HED2 | 39:Z:312:CHL:H2A  | 2.00                     | 0.42              |
| 13:3:41:LEU:HD12  | 13:3:41:LEU:N     | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:3:307:BCR:H351 | 24:3:307:BCR:H15C | 1.46                     | 0.42              |
| 14:7:149:GLY:HA3  | 14:7:161:LYS:HD2  | 2.02                     | 0.42              |
| 14:7:167:TYR:CZ   | 14:7:190:LYS:HE3  | 2.54                     | 0.42              |
| 38:7:302:LUT:H15  | 38:7:302:LUT:H201 | 1.83                     | 0.42              |
| 22:8:307:CLA:HBB1 | 22:8:307:CLA:CMB  | 2.50                     | 0.42              |
| 16:4:118:ASP:HB2  | 16:4:240:LEU:HD23 | 2.01                     | 0.42              |
| 22:4:812:CLA:H61  | 22:4:812:CLA:H2   | 1.60                     | 0.42              |
| 22:5:318:CLA:H11  | 22:6:322:CLA:H91  | 2.00                     | 0.42              |
| 18:6:80:LEU:HD11  | 22:6:307:CLA:CBC  | 2.49                     | 0.42              |
| 22:6:311:CLA:OBD  | 22:6:317:CLA:HAA1 | 2.19                     | 0.42              |
| 1:A:278:PHE:HB2   | 22:A:817:CLA:O1D  | 2.20                     | 0.42              |
| 1:A:490:THR:O     | 1:A:494:ALA:HB2   | 2.20                     | 0.42              |
| 22:A:805:CLA:H93  | 22:A:805:CLA:H111 | 1.71                     | 0.42              |
| 22:A:812:CLA:H2   | 22:A:812:CLA:ND   | 2.35                     | 0.42              |
| 22:A:812:CLA:H71  | 22:A:812:CLA:CHC  | 2.48                     | 0.42              |
| 22:A:841:CLA:HBC1 | 24:F:303:BCR:H392 | 2.00                     | 0.42              |
| 2:B:166:LEU:HD11  | 2:B:170:LYS:HE3   | 2.01                     | 0.42              |
| 2:B:517:ASP:HA    | 2:B:520:VAL:HG12  | 2.01                     | 0.42              |
| 2:B:712:THR:O     | 2:B:716:VAL:HG23  | 2.19                     | 0.42              |
| 22:B:821:CLA:O1A  | 22:B:826:CLA:H112 | 2.20                     | 0.42              |
| 6:F:192:ALA:O     | 6:F:196:THR:HG23  | 2.18                     | 0.42              |
| 7:G:122:LEU:HD22  | 7:G:122:LEU:HA    | 1.83                     | 0.42              |
| 12:1:192:HIS:O    | 12:1:196:GLY:HA2  | 2.19                     | 0.42              |
| 12:Z:218:ASN:ND2  | 22:Z:305:CLA:HMD2 | 2.35                     | 0.42              |
| 13:3:15:LEU:HA    | 13:3:34:PHE:O     | 2.19                     | 0.42              |
| 22:7:324:CLA:H11  | 22:7:324:CLA:H51  | 1.83                     | 0.42              |
| 15:8:186:LEU:HD23 | 22:8:311:CLA:HED3 | 2.00                     | 0.42              |
| 16:4:225:PHE:CD2  | 38:4:803:LUT:H14  | 2.54                     | 0.42              |
| 38:4:802:LUT:H31  | 38:4:802:LUT:H391 | 1.90                     | 0.42              |
| 22:4:812:CLA:H93  | 24:6:305:BCR:H311 | 2.01                     | 0.42              |
| 17:5:55:PHE:HB3   | 22:5:310:CLA:C3D  | 2.50                     | 0.42              |
| 22:6:322:CLA:HBB1 | 22:6:322:CLA:HMB1 | 2.02                     | 0.42              |
| 19:9:76:TRP:CE3   | 22:9:313:CLA:HAC2 | 2.55                     | 0.42              |
| 1:A:161:THR:HA    | 27:A:852:DGA:HAW1 | 2.01                     | 0.42              |
| 22:A:810:CLA:HBB1 | 22:A:810:CLA:CMB  | 2.49                     | 0.42              |
| 22:A:817:CLA:H61  | 22:A:817:CLA:C3C  | 2.50                     | 0.42              |
| 22:A:829:CLA:C2   | 24:A:845:BCR:HC7  | 2.41                     | 0.42              |
| 23:A:843:PQN:H18  | 23:A:843:PQN:H222 | 1.42                     | 0.42              |
| 2:B:33:GLU:H      | 2:B:33:GLU:HG3    | 1.48                     | 0.42              |
| 2:B:61:TRP:CG     | 22:B:809:CLA:HBC1 | 2.54                     | 0.42              |
| 2:B:443:VAL:HG21  | 22:B:834:CLA:HAC2 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:453:GLN:NE2   | 2:B:455:LEU:HD11  | 2.32                     | 0.42              |
| 22:B:822:CLA:NB   | 24:B:844:BCR:H351 | 2.35                     | 0.42              |
| 22:B:823:CLA:CMD  | 24:B:844:BCR:HC7  | 2.50                     | 0.42              |
| 22:B:829:CLA:H111 | 22:B:829:CLA:C2D  | 2.50                     | 0.42              |
| 6:F:202:TRP:N     | 6:F:203:PRO:CD    | 2.83                     | 0.42              |
| 22:L:201:CLA:H62  | 22:L:201:CLA:H102 | 1.30                     | 0.42              |
| 12:1:122:ASP:O    | 12:1:123:LEU:C    | 2.62                     | 0.42              |
| 38:Z:302:LUT:H8   | 22:Z:308:CLA:HMB2 | 2.01                     | 0.42              |
| 13:3:72:ALA:HB1   | 24:3:305:BCR:H383 | 2.01                     | 0.42              |
| 22:3:320:CLA:NA   | 41:7:319:3PH:H3D2 | 2.34                     | 0.42              |
| 22:3:322:CLA:CMB  | 41:7:319:3PH:H2A1 | 2.49                     | 0.42              |
| 14:7:34:TYR:O     | 14:7:35:PRO:C     | 2.62                     | 0.42              |
| 22:7:307:CLA:HBB1 | 22:7:307:CLA:HMB3 | 2.01                     | 0.42              |
| 16:4:111:ALA:HB1  | 38:4:802:LUT:H12  | 2.00                     | 0.42              |
| 16:4:185:LEU:HD23 | 39:4:819:CHL:HMD2 | 2.02                     | 0.42              |
| 17:5:252:LEU:HD23 | 41:5:325:3PH:H342 | 2.00                     | 0.42              |
| 22:6:301:CLA:H11  | 22:6:301:CLA:H52  | 1.71                     | 0.42              |
| 22:6:314:CLA:H93  | 22:6:314:CLA:H112 | 1.63                     | 0.42              |
| 19:9:113:ALA:HA   | 19:9:116:PHE:HD2  | 1.84                     | 0.42              |
| 20:2:165:MET:O    | 20:2:169:ILE:HG12 | 2.20                     | 0.42              |
| 1:A:478:GLN:HB3   | 1:A:480:GLN:HE21  | 1.83                     | 0.42              |
| 22:A:804:CLA:HBB1 | 22:A:804:CLA:CMB  | 2.49                     | 0.42              |
| 22:A:805:CLA:H62  | 22:A:805:CLA:H2   | 1.55                     | 0.42              |
| 22:A:822:CLA:CBB  | 37:K:201:DAO:H112 | 2.46                     | 0.42              |
| 22:A:833:CLA:HBB1 | 22:L:203:CLA:HBB2 | 2.02                     | 0.42              |
| 2:B:67:PHE:HZ     | 8:I:71:PRO:HG2    | 1.85                     | 0.42              |
| 2:B:89:ALA:HB1    | 22:B:811:CLA:O2D  | 2.19                     | 0.42              |
| 25:B:803:LHG:HC91 | 22:B:807:CLA:C3D  | 2.50                     | 0.42              |
| 22:B:829:CLA:H62  | 22:B:829:CLA:H2   | 1.63                     | 0.42              |
| 5:E:79:ASN:OD1    | 5:E:83:VAL:N      | 2.53                     | 0.42              |
| 6:F:220:GLU:H     | 6:F:220:GLU:HG3   | 1.50                     | 0.42              |
| 7:G:36:LEU:HD13   | 7:G:36:LEU:C      | 2.43                     | 0.42              |
| 22:Z:316:CLA:H111 | 22:Z:316:CLA:H152 | 1.49                     | 0.42              |
| 22:3:311:CLA:H62  | 22:3:311:CLA:H93  | 1.80                     | 0.42              |
| 22:3:322:CLA:HHC  | 22:3:322:CLA:CBB  | 2.48                     | 0.42              |
| 14:7:67:TRP:CH2   | 22:7:315:CLA:HAA1 | 2.54                     | 0.42              |
| 14:7:135:GLU:HG3  | 22:7:315:CLA:NB   | 2.35                     | 0.42              |
| 22:7:323:CLA:H93  | 22:7:323:CLA:H111 | 1.68                     | 0.42              |
| 15:8:205:GLN:NE2  | 38:8:302:LUT:H42  | 2.35                     | 0.42              |
| 22:8:305:CLA:HBB1 | 22:8:305:CLA:CMB  | 2.48                     | 0.42              |
| 22:8:307:CLA:H51  | 22:8:307:CLA:C4C  | 2.50                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:8:315:CHL:HAA2 | 39:8:315:CHL:CBD  | 2.50                     | 0.42              |
| 24:4:804:BCR:H24C | 39:4:816:CHL:HAA1 | 2.01                     | 0.42              |
| 17:5:100:TRP:CH2  | 17:5:201:VAL:HA   | 2.55                     | 0.42              |
| 17:5:123:ALA:CB   | 22:5:326:CLA:HAA1 | 2.50                     | 0.42              |
| 39:5:316:CHL:HMC  | 22:5:319:CLA:CAB  | 2.45                     | 0.42              |
| 18:6:214:THR:HA   | 22:6:309:CLA:HBA2 | 2.01                     | 0.42              |
| 18:6:248:CYS:HB3  | 18:6:254:TRP:CH2  | 2.55                     | 0.42              |
| 39:9:312:CHL:H162 | 39:9:312:CHL:H121 | 1.85                     | 0.42              |
| 20:2:214:LEU:C    | 39:2:303:CHL:HAA2 | 2.44                     | 0.42              |
| 1:A:341:LEU:HD11  | 1:A:426:LEU:CD1   | 2.50                     | 0.42              |
| 1:A:426:LEU:HB2   | 22:A:824:CLA:HMC2 | 2.01                     | 0.42              |
| 1:A:461:THR:CG2   | 22:B:812:CLA:HAB  | 2.48                     | 0.42              |
| 22:A:815:CLA:C1C  | 24:A:856:BCR:H312 | 2.49                     | 0.42              |
| 2:B:13:LEU:HD11   | 31:B:852:DGD:HE1  | 2.02                     | 0.42              |
| 2:B:297:GLY:O     | 2:B:298:ILE:C     | 2.63                     | 0.42              |
| 2:B:653:PHE:CD1   | 22:B:806:CLA:H71  | 2.54                     | 0.42              |
| 22:B:801:CLA:H152 | 22:B:801:CLA:H18  | 1.83                     | 0.42              |
| 22:B:819:CLA:H43  | 22:B:835:CLA:HED1 | 2.02                     | 0.42              |
| 6:F:114:ARG:HB2   | 9:J:35:ASP:OD2    | 2.20                     | 0.42              |
| 13:3:216:HIS:CD2  | 22:3:310:CLA:HAA1 | 2.54                     | 0.42              |
| 14:7:127:MET:HE3  | 14:7:127:MET:HB3  | 1.94                     | 0.42              |
| 14:7:209:ALA:CB   | 22:7:317:CLA:H8   | 2.48                     | 0.42              |
| 22:7:305:CLA:C4B  | 22:7:310:CLA:H121 | 2.50                     | 0.42              |
| 15:8:187:LYS:HG2  | 22:8:306:CLA:HBD  | 2.01                     | 0.42              |
| 17:5:158:PRO:HB2  | 17:5:160:PRO:HD3  | 2.02                     | 0.42              |
| 24:5:304:BCR:H19C | 22:5:319:CLA:CBA  | 2.28                     | 0.42              |
| 19:9:52:ASP:CG    | 19:9:55:GLY:HA2   | 2.44                     | 0.42              |
| 39:9:312:CHL:H18  | 39:9:312:CHL:C1C  | 2.50                     | 0.42              |
| 39:9:314:CHL:HED2 | 20:2:194:TRP:CH2  | 2.54                     | 0.42              |
| 1:A:129:GLY:O     | 1:A:136:GLN:HA    | 2.20                     | 0.42              |
| 1:A:205:LEU:HD12  | 24:A:845:BCR:H363 | 2.02                     | 0.42              |
| 1:A:278:PHE:CZ    | 22:A:818:CLA:H43  | 2.54                     | 0.42              |
| 1:A:369:HIS:HA    | 1:A:372:TYR:CE2   | 2.55                     | 0.42              |
| 1:A:651:TRP:CD1   | 22:B:805:CLA:HBC1 | 2.55                     | 0.42              |
| 22:A:806:CLA:H62  | 22:A:806:CLA:H2   | 1.64                     | 0.42              |
| 22:A:815:CLA:O1A  | 13:3:203:VAL:HG12 | 2.20                     | 0.42              |
| 22:A:840:CLA:HHB  | 24:F:303:BCR:H383 | 2.01                     | 0.42              |
| 2:B:229:GLY:O     | 2:B:231:TRP:N     | 2.50                     | 0.42              |
| 2:B:419:ILE:HG23  | 22:B:839:CLA:HBB2 | 2.02                     | 0.42              |
| 2:B:490:SER:HB3   | 2:B:495:LEU:HB2   | 2.01                     | 0.42              |
| 2:B:712:THR:HG22  | 31:B:852:DGD:HBW1 | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:23:LEU:O      | 3:C:24:ASP:C      | 2.62                     | 0.42              |
| 8:I:93:ALA:HB1    | 11:L:134:ILE:HG21 | 2.00                     | 0.42              |
| 11:L:140:PHE:CD1  | 11:L:144:PRO:HD2  | 2.53                     | 0.42              |
| 12:1:206:HIS:HA   | 12:1:213:SER:OG   | 2.20                     | 0.42              |
| 22:1:315:CLA:HBB1 | 22:1:315:CLA:CMB  | 2.50                     | 0.42              |
| 12:Z:186:LEU:HG   | 22:Z:305:CLA:HAC1 | 2.02                     | 0.42              |
| 22:Z:309:CLA:HHD  | 25:Z:317:LHG:H242 | 2.02                     | 0.42              |
| 39:Z:311:CHL:HMA1 | 25:Z:317:LHG:H192 | 2.01                     | 0.42              |
| 22:3:320:CLA:C4A  | 41:7:319:3PH:H3D2 | 2.50                     | 0.42              |
| 22:7:307:CLA:H93  | 22:7:307:CLA:H111 | 1.77                     | 0.42              |
| 22:8:309:CLA:HMD1 | 22:8:314:CLA:C4C  | 2.50                     | 0.42              |
| 16:4:193:PRO:HD2  | 22:4:805:CLA:CAD  | 2.50                     | 0.42              |
| 25:4:820:LHG:H352 | 22:6:321:CLA:C1   | 2.50                     | 0.42              |
| 18:6:85:ILE:HG12  | 38:6:304:LUT:H41  | 2.01                     | 0.42              |
| 18:6:100:ALA:HB3  | 18:6:101:PRO:HD3  | 2.02                     | 0.42              |
| 39:6:315:CHL:H61  | 39:6:315:CHL:H41  | 1.88                     | 0.42              |
| 39:6:318:CHL:H62  | 39:6:318:CHL:H41  | 1.74                     | 0.42              |
| 19:9:102:LYS:CD   | 22:9:308:CLA:HED1 | 2.50                     | 0.42              |
| 19:9:175:GLN:OE1  | 38:9:301:LUT:H42  | 2.19                     | 0.42              |
| 22:9:305:CLA:H142 | 22:9:305:CLA:H112 | 1.89                     | 0.42              |
| 20:2:171:PHE:C    | 20:2:174:GLN:H    | 2.27                     | 0.42              |
| 1:A:634:ASN:O     | 1:A:638:SER:HB2   | 2.19                     | 0.41              |
| 22:A:820:CLA:H71  | 22:A:820:CLA:H111 | 1.20                     | 0.41              |
| 22:A:832:CLA:H112 | 22:A:832:CLA:H152 | 1.66                     | 0.41              |
| 22:A:855:CLA:H161 | 24:B:853:BCR:H351 | 2.01                     | 0.41              |
| 2:B:198:VAL:C     | 2:B:201:PRO:HD2   | 2.45                     | 0.41              |
| 2:B:687:PRO:O     | 2:B:688:LEU:HB2   | 2.20                     | 0.41              |
| 22:B:821:CLA:HMB1 | 22:B:826:CLA:H2   | 2.02                     | 0.41              |
| 22:B:824:CLA:HMB3 | 22:B:824:CLA:HBB1 | 2.02                     | 0.41              |
| 22:B:826:CLA:H92  | 22:B:826:CLA:H61  | 1.65                     | 0.41              |
| 3:C:15:THR:HG22   | 3:C:28:MET:HG3    | 2.02                     | 0.41              |
| 11:L:61:SER:O     | 11:L:62:THR:C     | 2.63                     | 0.41              |
| 38:Z:301:LUT:H403 | 22:Z:303:CLA:C14  | 2.47                     | 0.41              |
| 22:3:314:CLA:H41  | 22:3:314:CLA:H62  | 1.32                     | 0.41              |
| 14:7:241:VAL:CG1  | 14:7:244:TYR:HB3  | 2.50                     | 0.41              |
| 22:7:312:CLA:HED2 | 22:7:312:CLA:HBD  | 1.85                     | 0.41              |
| 39:7:313:CHL:CMC  | 22:7:316:CLA:HAB  | 2.50                     | 0.41              |
| 38:8:302:LUT:H35  | 38:8:302:LUT:H401 | 1.79                     | 0.41              |
| 38:5:302:LUT:C33  | 22:5:308:CLA:HMB2 | 2.50                     | 0.41              |
| 38:5:303:LUT:H35  | 38:5:303:LUT:H401 | 1.85                     | 0.41              |
| 22:6:307:CLA:H41  | 22:6:308:CLA:HBA1 | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:6:308:CLA:H51  | 22:6:308:CLA:H11  | 1.63                     | 0.41              |
| 39:6:320:CHL:OMC  | 39:6:320:CHL:HAC2 | 2.20                     | 0.41              |
| 22:6:322:CLA:HMC3 | 41:6:324:3PH:H2A1 | 2.02                     | 0.41              |
| 19:9:111:LEU:HD23 | 19:9:111:LEU:C    | 2.44                     | 0.41              |
| 1:A:179:PHE:O     | 1:A:183:LYS:HB2   | 2.20                     | 0.41              |
| 1:A:483:PHE:HB3   | 22:A:837:CLA:H42  | 2.01                     | 0.41              |
| 22:A:823:CLA:H111 | 22:A:823:CLA:H152 | 1.46                     | 0.41              |
| 24:A:844:BCR:H393 | 24:3:306:BCR:HC42 | 2.02                     | 0.41              |
| 2:B:105:PHE:HD2   | 2:B:107:ARG:HH12  | 1.67                     | 0.41              |
| 2:B:388:PHE:HZ    | 22:B:827:CLA:HAB  | 1.85                     | 0.41              |
| 2:B:495:LEU:HD22  | 2:B:495:LEU:C     | 2.46                     | 0.41              |
| 2:B:587:THR:O     | 2:B:591:VAL:HG13  | 2.21                     | 0.41              |
| 2:B:656:LEU:HA    | 22:B:806:CLA:HAA1 | 2.01                     | 0.41              |
| 2:B:727:ILE:CD1   | 22:B:829:CLA:H12  | 2.50                     | 0.41              |
| 22:B:806:CLA:H92  | 22:B:806:CLA:H62  | 1.71                     | 0.41              |
| 22:B:810:CLA:C1   | 8:I:79:PHE:HB3    | 2.50                     | 0.41              |
| 22:B:822:CLA:HMA2 | 7:G:103:MET:HE3   | 2.00                     | 0.41              |
| 22:B:825:CLA:HAB  | 22:B:832:CLA:HMD1 | 2.01                     | 0.41              |
| 22:B:830:CLA:H52  | 24:B:845:BCR:C23  | 2.50                     | 0.41              |
| 6:F:222:ILE:H     | 6:F:222:ILE:HG13  | 1.79                     | 0.41              |
| 33:G:204:LMT:H41  | 33:G:204:LMT:H12  | 1.79                     | 0.41              |
| 12:Z:167:ILE:O    | 12:Z:171:LYS:HG3  | 2.20                     | 0.41              |
| 13:3:183:ASN:HB3  | 22:3:309:CLA:CAA  | 2.51                     | 0.41              |
| 14:7:155:GLY:N    | 42:7:320:SPH:H62  | 2.35                     | 0.41              |
| 38:7:302:LUT:H24  | 22:7:307:CLA:O1A  | 2.20                     | 0.41              |
| 15:8:111:THR:HG21 | 39:8:315:CHL:CMD  | 2.50                     | 0.41              |
| 38:8:303:LUT:H15  | 38:8:303:LUT:H201 | 1.95                     | 0.41              |
| 16:4:156:LEU:HD22 | 24:4:804:BCR:H15C | 2.02                     | 0.41              |
| 22:4:810:CLA:HMA2 | 39:4:816:CHL:C2C  | 2.49                     | 0.41              |
| 17:5:172:LEU:HD12 | 38:5:302:LUT:H222 | 2.01                     | 0.41              |
| 22:5:311:CLA:CHB  | 22:5:318:CLA:H191 | 2.51                     | 0.41              |
| 22:5:318:CLA:C9   | 22:6:322:CLA:H62  | 2.49                     | 0.41              |
| 19:9:31:TRP:CZ3   | 19:9:32:LEU:HD23  | 2.55                     | 0.41              |
| 1:A:46:THR:CG2    | 1:A:715:PRO:HA    | 2.51                     | 0.41              |
| 1:A:376:PRO:HG3   | 22:A:819:CLA:HBA1 | 2.03                     | 0.41              |
| 22:A:828:CLA:H72  | 22:A:828:CLA:H111 | 1.19                     | 0.41              |
| 22:A:828:CLA:H93  | 24:J:104:BCR:H353 | 2.01                     | 0.41              |
| 22:A:841:CLA:H141 | 22:A:841:CLA:H162 | 1.94                     | 0.41              |
| 2:B:495:LEU:HD22  | 2:B:499:LEU:HG    | 2.02                     | 0.41              |
| 22:B:811:CLA:H51  | 22:B:811:CLA:H8   | 1.22                     | 0.41              |
| 22:B:816:CLA:HMB3 | 22:B:830:CLA:H13  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:B:821:CLA:H41  | 22:B:825:CLA:H91  | 2.02                     | 0.41              |
| 22:B:823:CLA:HAA2 | 7:G:60:ASP:OD2    | 2.21                     | 0.41              |
| 22:B:830:CLA:C1D  | 24:B:845:BCR:H272 | 2.50                     | 0.41              |
| 6:F:204:VAL:CG2   | 22:8:309:CLA:H72  | 2.42                     | 0.41              |
| 22:1:308:CLA:HBC1 | 22:1:314:CLA:HAC1 | 2.02                     | 0.41              |
| 22:1:313:CLA:H102 | 22:1:313:CLA:H13  | 1.88                     | 0.41              |
| 12:Z:83:LEU:HB2   | 22:Z:308:CLA:HBB2 | 2.02                     | 0.41              |
| 13:3:114:PHE:CD1  | 22:3:316:CLA:HBD  | 2.55                     | 0.41              |
| 13:3:122:GLN:HE21 | 13:3:122:GLN:HB3  | 1.73                     | 0.41              |
| 13:3:158:TYR:CE1  | 13:3:181:LYS:HG2  | 2.55                     | 0.41              |
| 22:3:311:CLA:H61  | 22:3:312:CLA:HMA3 | 2.01                     | 0.41              |
| 14:7:150:ASP:OD1  | 14:7:150:ASP:N    | 2.53                     | 0.41              |
| 39:4:813:CHL:HAB  | 39:4:816:CHL:CAB  | 2.50                     | 0.41              |
| 38:5:303:LUT:H162 | 22:5:312:CLA:HMB3 | 2.00                     | 0.41              |
| 24:5:305:BCR:H363 | 39:5:316:CHL:ND   | 2.34                     | 0.41              |
| 22:5:308:CLA:CMA  | 22:5:308:CLA:HBA1 | 2.49                     | 0.41              |
| 22:5:314:CLA:HHC  | 22:5:314:CLA:HBB1 | 2.02                     | 0.41              |
| 18:6:194:VAL:HG21 | 22:6:309:CLA:HMD1 | 2.02                     | 0.41              |
| 22:6:309:CLA:H62  | 22:6:309:CLA:CHC  | 2.51                     | 0.41              |
| 1:A:346:THR:HG23  | 22:A:825:CLA:HBC1 | 2.00                     | 0.41              |
| 1:A:690:ARG:HG3   | 1:A:717:ALA:CB    | 2.48                     | 0.41              |
| 1:A:740:TRP:CG    | 24:A:848:BCR:HC41 | 2.55                     | 0.41              |
| 22:A:808:CLA:CAD  | 22:A:828:CLA:HAA2 | 2.51                     | 0.41              |
| 22:A:823:CLA:C11  | 24:A:856:BCR:H401 | 2.41                     | 0.41              |
| 22:A:840:CLA:CBB  | 6:F:167:GLY:HA3   | 2.51                     | 0.41              |
| 27:A:852:DGA:HB91 | 22:3:316:CLA:HMC1 | 2.03                     | 0.41              |
| 2:B:356:LEU:HD13  | 22:B:819:CLA:HAA2 | 2.03                     | 0.41              |
| 2:B:439:VAL:HG12  | 22:B:834:CLA:HAC1 | 2.03                     | 0.41              |
| 2:B:513:ILE:HG23  | 22:B:837:CLA:HMD3 | 2.02                     | 0.41              |
| 22:B:824:CLA:HBB1 | 22:B:824:CLA:CMB  | 2.50                     | 0.41              |
| 22:B:827:CLA:C2   | 22:B:839:CLA:HBD  | 2.46                     | 0.41              |
| 3:C:5:VAL:HA      | 3:C:66:ARG:O      | 2.21                     | 0.41              |
| 22:F:304:CLA:NB   | 22:F:304:CLA:H43  | 2.36                     | 0.41              |
| 32:F:306:RRX:H40  | 32:F:306:RRX:H36  | 1.34                     | 0.41              |
| 22:L:202:CLA:H2   | 22:L:202:CLA:H61  | 1.61                     | 0.41              |
| 12:1:140:ARG:HG2  | 22:1:313:CLA:CHC  | 2.50                     | 0.41              |
| 38:1:302:LUT:H15  | 38:1:302:LUT:H201 | 1.86                     | 0.41              |
| 22:1:313:CLA:O1A  | 22:1:313:CLA:H93  | 2.21                     | 0.41              |
| 12:Z:85:ALA:CB    | 38:Z:301:LUT:H12  | 2.51                     | 0.41              |
| 39:Z:311:CHL:HAA2 | 16:4:162:PHE:HB2  | 2.01                     | 0.41              |
| 13:3:38:PRO:HD2   | 38:3:303:LUT:C24  | 2.50                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:3:111:TYR:CE2  | 14:7:244:TYR:HB2   | 2.55                     | 0.41              |
| 38:3:303:LUT:H31  | 38:3:303:LUT:H391  | 1.92                     | 0.41              |
| 24:3:306:BCR:H393 | 22:3:318:CLA:H92   | 2.02                     | 0.41              |
| 22:3:322:CLA:C2C  | 25:7:318:LHG:HC82  | 2.51                     | 0.41              |
| 22:7:305:CLA:O1D  | 22:7:310:CLA:H92   | 2.19                     | 0.41              |
| 16:4:85:SER:OG    | 33:4:801:LMT:H1B   | 2.20                     | 0.41              |
| 17:5:240:VAL:HG13 | 17:5:247:ILE:HB    | 2.03                     | 0.41              |
| 38:5:302:LUT:H11  | 22:5:308:CLA:CMC   | 2.47                     | 0.41              |
| 24:5:304:BCR:H382 | 22:5:319:CLA:NB    | 2.36                     | 0.41              |
| 22:5:315:CLA:H93  | 22:5:315:CLA:H62   | 1.75                     | 0.41              |
| 22:5:318:CLA:H42  | 22:5:323:CLA:HAC2  | 2.02                     | 0.41              |
| 18:6:95:VAL:HA    | 18:6:103:LYS:HZ3   | 1.85                     | 0.41              |
| 18:6:245:PHE:HE2  | 22:6:301:CLA:H112  | 1.85                     | 0.41              |
| 22:6:308:CLA:HBB1 | 22:6:308:CLA:CMB   | 2.45                     | 0.41              |
| 22:6:309:CLA:HBB1 | 22:6:309:CLA:CMB   | 2.49                     | 0.41              |
| 39:6:316:CHL:H12  | 39:6:316:CHL:HBA1  | 1.52                     | 0.41              |
| 38:9:302:LUT:H31  | 38:9:302:LUT:H391  | 1.90                     | 0.41              |
| 1:A:495:PRO:HA    | 1:A:499:ALA:O      | 2.20                     | 0.41              |
| 22:A:814:CLA:C9   | 27:A:852:DGA:HB81  | 2.50                     | 0.41              |
| 22:A:817:CLA:C1A  | 22:A:817:CLA:CGA   | 2.98                     | 0.41              |
| 22:A:822:CLA:CBC  | 22:A:823:CLA:H171  | 2.50                     | 0.41              |
| 22:A:834:CLA:CHC  | 24:I:4001:BCR:H291 | 2.51                     | 0.41              |
| 2:B:298:ILE:HG22  | 7:G:57:HIS:NE2     | 2.35                     | 0.41              |
| 2:B:398:ASP:OD2   | 4:D:185:LYS:HE3    | 2.21                     | 0.41              |
| 2:B:559:PRO:HB3   | 2:B:703:ILE:HB     | 2.02                     | 0.41              |
| 22:B:815:CLA:H102 | 24:B:845:BCR:C38   | 2.50                     | 0.41              |
| 22:B:829:CLA:HBC3 | 31:B:852:DGD:HBG3  | 2.02                     | 0.41              |
| 22:B:838:CLA:HAC2 | 32:F:306:RRX:H2    | 2.02                     | 0.41              |
| 22:B:838:CLA:C19  | 22:F:302:CLA:H101  | 2.51                     | 0.41              |
| 22:B:842:CLA:CED  | 24:B:847:BCR:H11C  | 2.51                     | 0.41              |
| 3:C:22:PRO:O      | 4:D:122:LEU:HD23   | 2.20                     | 0.41              |
| 12:1:162:PHE:HB2  | 22:1:304:CLA:O2A   | 2.20                     | 0.41              |
| 22:1:310:CLA:H91  | 22:1:310:CLA:H111  | 1.77                     | 0.41              |
| 12:Z:140:ARG:HG3  | 22:Z:313:CLA:CMC   | 2.50                     | 0.41              |
| 12:Z:174:GLU:HG3  | 22:Z:303:CLA:C4B   | 2.50                     | 0.41              |
| 14:7:136:GLN:HG3  | 22:7:323:CLA:HBA1  | 2.02                     | 0.41              |
| 14:7:241:VAL:HG12 | 14:7:244:TYR:H     | 1.85                     | 0.41              |
| 22:7:309:CLA:C4C  | 42:7:321:SPH:H151  | 2.49                     | 0.41              |
| 15:8:61:ALA:HB1   | 15:8:65:TYR:CE2    | 2.56                     | 0.41              |
| 15:8:106:VAL:O    | 15:8:110:GLN:HB2   | 2.21                     | 0.41              |
| 39:8:315:CHL:H111 | 39:8:315:CHL:C6    | 2.46                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:4:816:CHL:HBB1 | 39:4:816:CHL:CMB  | 2.45                     | 0.41              |
| 17:5:112:PRO:C    | 17:5:114:GLN:N    | 2.78                     | 0.41              |
| 22:5:307:CLA:HBB1 | 22:5:307:CLA:HMB1 | 2.02                     | 0.41              |
| 22:5:322:CLA:H152 | 22:6:319:CLA:H52  | 2.03                     | 0.41              |
| 18:6:77:TRP:HZ2   | 18:6:121:MET:HE1  | 1.85                     | 0.41              |
| 38:6:304:LUT:H35  | 38:6:304:LUT:H401 | 1.86                     | 0.41              |
| 24:6:305:BCR:H271 | 22:6:312:CLA:H101 | 2.03                     | 0.41              |
| 24:6:306:BCR:H363 | 39:6:315:CHL:C4D  | 2.50                     | 0.41              |
| 22:6:322:CLA:H2A  | 22:6:322:CLA:CED  | 2.49                     | 0.41              |
| 19:9:110:PRO:HG2  | 20:2:200:THR:HG23 | 2.02                     | 0.41              |
| 20:2:177:VAL:O    | 20:2:178:ARG:C    | 2.63                     | 0.41              |
| 1:A:14:LYS:HA     | 22:A:812:CLA:HAA1 | 2.03                     | 0.41              |
| 1:A:15:ILE:HG12   | 22:A:812:CLA:OBD  | 2.21                     | 0.41              |
| 1:A:211:LEU:CD2   | 24:A:844:BCR:H373 | 2.50                     | 0.41              |
| 1:A:584:CYS:HB3   | 2:B:668:TRP:HE3   | 1.86                     | 0.41              |
| 22:A:809:CLA:NC   | 22:A:828:CLA:H172 | 2.35                     | 0.41              |
| 22:A:813:CLA:H42  | 22:A:813:CLA:HMA2 | 2.02                     | 0.41              |
| 22:A:814:CLA:H43  | 22:A:816:CLA:C4   | 2.50                     | 0.41              |
| 2:B:78:TRP:HH2    | 2:B:123:GLN:HA    | 1.85                     | 0.41              |
| 22:B:808:CLA:H2   | 22:B:808:CLA:H61  | 1.61                     | 0.41              |
| 22:B:808:CLA:H143 | 22:B:815:CLA:C3D  | 2.50                     | 0.41              |
| 22:B:830:CLA:H52  | 24:B:845:BCR:H23C | 2.02                     | 0.41              |
| 12:1:206:HIS:CG   | 22:1:306:CLA:HAA2 | 2.56                     | 0.41              |
| 22:Z:316:CLA:ND   | 22:Z:316:CLA:H13  | 2.35                     | 0.41              |
| 22:Z:316:CLA:H141 | 22:Z:316:CLA:H172 | 2.01                     | 0.41              |
| 22:3:313:CLA:H13  | 22:5:320:CLA:NB   | 2.35                     | 0.41              |
| 22:3:313:CLA:H3A  | 22:3:313:CLA:HBA2 | 1.46                     | 0.41              |
| 22:3:322:CLA:HBC1 | 14:7:31:PRO:HB2   | 2.03                     | 0.41              |
| 22:7:322:CLA:H61  | 22:7:322:CLA:H2   | 1.66                     | 0.41              |
| 22:7:322:CLA:C3   | 22:7:323:CLA:H193 | 2.50                     | 0.41              |
| 22:7:323:CLA:H161 | 22:7:323:CLA:H121 | 1.79                     | 0.41              |
| 22:5:308:CLA:HMA2 | 22:5:308:CLA:HBA1 | 2.02                     | 0.41              |
| 19:9:56:LEU:CD1   | 38:9:302:LUT:H221 | 2.45                     | 0.41              |
| 19:9:113:ALA:HA   | 19:9:116:PHE:CD2  | 2.56                     | 0.41              |
| 1:A:368:ALA:HB2   | 1:A:394:HIS:HB2   | 2.03                     | 0.41              |
| 1:A:377:TYR:CE2   | 22:A:829:CLA:HED2 | 2.56                     | 0.41              |
| 1:A:396:TRP:HZ3   | 1:A:600:TYR:HA    | 1.85                     | 0.41              |
| 1:A:406:GLY:CA    | 24:A:847:BCR:H323 | 2.51                     | 0.41              |
| 1:A:499:ALA:HB1   | 22:A:836:CLA:HED3 | 2.02                     | 0.41              |
| 22:A:803:CLA:HBA2 | 22:A:803:CLA:H12  | 1.72                     | 0.41              |
| 22:A:807:CLA:O2D  | 22:A:809:CLA:HED1 | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:822:CLA:CHD  | 24:A:856:BCR:H402 | 2.50                     | 0.41              |
| 22:A:823:CLA:C9   | 22:K:204:CLA:HMB2 | 2.50                     | 0.41              |
| 22:A:832:CLA:HMA2 | 2:B:685:LYS:HB2   | 2.03                     | 0.41              |
| 22:A:836:CLA:HBA2 | 22:A:836:CLA:CHA  | 2.49                     | 0.41              |
| 22:A:840:CLA:HMC2 | 23:A:843:PQN:H272 | 2.01                     | 0.41              |
| 2:B:24:PHE:O      | 2:B:28:VAL:HG23   | 2.21                     | 0.41              |
| 2:B:413:LEU:HA    | 2:B:416:LYS:HB3   | 2.03                     | 0.41              |
| 22:B:819:CLA:C9   | 22:B:828:CLA:HAB  | 2.41                     | 0.41              |
| 22:B:832:CLA:CHA  | 22:B:842:CLA:H52  | 2.51                     | 0.41              |
| 3:C:9:ASP:C       | 3:C:11:CYS:H      | 2.29                     | 0.41              |
| 4:D:106:MET:SD    | 4:D:134:PHE:HE2   | 2.43                     | 0.41              |
| 6:F:142:LYS:HA    | 33:F:307:LMT:H2'  | 2.03                     | 0.41              |
| 12:1:157:PHE:CE2  | 22:1:313:CLA:H161 | 2.55                     | 0.41              |
| 22:1:308:CLA:HMD1 | 22:1:314:CLA:C4C  | 2.50                     | 0.41              |
| 12:Z:215:PHE:CG   | 22:Z:305:CLA:H42  | 2.55                     | 0.41              |
| 22:3:312:CLA:ND   | 22:3:318:CLA:H101 | 2.35                     | 0.41              |
| 15:8:124:PHE:HD1  | 39:8:301:CHL:H51  | 1.85                     | 0.41              |
| 22:8:305:CLA:HBB1 | 22:8:306:CLA:CAA  | 2.51                     | 0.41              |
| 16:4:78:ASP:HA    | 22:4:808:CLA:O1D  | 2.21                     | 0.41              |
| 16:4:83:PRO:CD    | 38:4:803:LUT:H23  | 2.42                     | 0.41              |
| 16:4:150:PHE:HB2  | 39:4:813:CHL:HAC2 | 2.01                     | 0.41              |
| 16:4:238:THR:HB   | 16:4:239:PRO:HD2  | 2.03                     | 0.41              |
| 17:5:161:GLU:HG3  | 17:5:179:ARG:HH22 | 1.86                     | 0.41              |
| 22:5:322:CLA:H121 | 22:6:311:CLA:HMB2 | 2.03                     | 0.41              |
| 18:6:95:VAL:CG1   | 18:6:100:ALA:HA   | 2.50                     | 0.41              |
| 39:9:312:CHL:C3C  | 39:9:314:CHL:CBB  | 2.98                     | 0.41              |
| 1:A:575:CYS:SG    | 29:B:802:SF4:S1   | 3.19                     | 0.41              |
| 1:A:661:TYR:OH    | 1:A:670:LEU:HD23  | 2.21                     | 0.41              |
| 22:A:817:CLA:H12  | 22:A:817:CLA:ND   | 2.35                     | 0.41              |
| 2:B:32:PHE:HD1    | 2:B:35:HIS:CE1    | 2.38                     | 0.41              |
| 2:B:143:LEU:HD21  | 24:B:846:BCR:C24  | 2.50                     | 0.41              |
| 2:B:243:HIS:HB2   | 2:B:250:GLY:O     | 2.21                     | 0.41              |
| 2:B:315:ARG:HB2   | 22:B:842:CLA:O1A  | 2.21                     | 0.41              |
| 2:B:331:LEU:HD23  | 2:B:331:LEU:HA    | 1.90                     | 0.41              |
| 22:B:830:CLA:ND   | 24:B:845:BCR:H282 | 2.35                     | 0.41              |
| 22:B:838:CLA:H2   | 22:B:839:CLA:CMD  | 2.51                     | 0.41              |
| 6:F:153:THR:HG21  | 32:F:306:RRX:C4   | 2.51                     | 0.41              |
| 22:F:305:CLA:HMB3 | 22:F:305:CLA:CBB  | 2.46                     | 0.41              |
| 38:1:303:LUT:H161 | 22:1:309:CLA:HMB2 | 2.02                     | 0.41              |
| 12:Z:176:LYS:HE2  | 22:Z:309:CLA:C2D  | 2.50                     | 0.41              |
| 38:Z:302:LUT:H371 | 22:Z:306:CLA:H142 | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:3:312:CLA:H162 | 22:3:312:CLA:H141 | 1.85                     | 0.41              |
| 14:7:73:LEU:HD13  | 14:7:166:GLY:HA3  | 2.03                     | 0.41              |
| 14:7:129:LEU:O    | 22:7:323:CLA:H11  | 2.21                     | 0.41              |
| 14:7:173:PHE:HZ   | 22:7:314:CLA:CHC  | 2.34                     | 0.41              |
| 22:7:322:CLA:C3D  | 22:7:323:CLA:H91  | 2.51                     | 0.41              |
| 15:8:184:LEU:HB3  | 22:8:305:CLA:CMA  | 2.50                     | 0.41              |
| 16:4:109:LEU:HB3  | 22:4:810:CLA:HAB  | 2.03                     | 0.41              |
| 18:6:164:PRO:HG2  | 22:6:308:CLA:H12  | 2.03                     | 0.41              |
| 19:9:82:VAL:HG21  | 38:9:301:LUT:H401 | 2.03                     | 0.41              |
| 19:9:111:LEU:HD21 | 39:9:314:CHL:ND   | 2.35                     | 0.41              |
| 1:A:59:PHE:HB2    | 1:A:69:ILE:HG23   | 2.03                     | 0.41              |
| 1:A:205:LEU:HD13  | 22:A:813:CLA:HHB  | 2.03                     | 0.41              |
| 22:A:807:CLA:H91  | 22:A:807:CLA:H111 | 1.69                     | 0.41              |
| 22:A:808:CLA:CHC  | 22:A:809:CLA:HMD2 | 2.51                     | 0.41              |
| 22:A:816:CLA:HBC2 | 22:3:316:CLA:CBB  | 2.51                     | 0.41              |
| 22:A:821:CLA:O1A  | 22:A:824:CLA:HBD  | 2.21                     | 0.41              |
| 22:A:828:CLA:H91  | 24:J:104:BCR:H11C | 2.02                     | 0.41              |
| 22:A:829:CLA:NC   | 24:A:845:BCR:HC42 | 2.35                     | 0.41              |
| 22:A:838:CLA:H52  | 22:A:838:CLA:NC   | 2.36                     | 0.41              |
| 24:A:847:BCR:H311 | 24:A:847:BCR:HC7  | 1.81                     | 0.41              |
| 2:B:74:ASN:ND2    | 2:B:88:ILE:HG13   | 2.35                     | 0.41              |
| 2:B:94:ASP:C      | 2:B:96:HIS:H      | 2.28                     | 0.41              |
| 2:B:127:THR:HA    | 2:B:245:PHE:HZ    | 1.84                     | 0.41              |
| 2:B:168:TRP:NE1   | 22:B:815:CLA:HAC2 | 2.36                     | 0.41              |
| 2:B:302:MET:HB2   | 2:B:324:PHE:CE2   | 2.55                     | 0.41              |
| 2:B:362:LEU:HD22  | 2:B:369:GLN:NE2   | 2.35                     | 0.41              |
| 2:B:478:LEU:HD13  | 22:B:835:CLA:CMD  | 2.51                     | 0.41              |
| 2:B:575:ASP:HA    | 2:B:578:TYR:HB3   | 2.02                     | 0.41              |
| 22:B:812:CLA:H41  | 22:B:812:CLA:H62  | 1.88                     | 0.41              |
| 22:B:821:CLA:H51  | 22:B:828:CLA:H101 | 2.03                     | 0.41              |
| 22:B:826:CLA:H161 | 22:B:826:CLA:H122 | 1.67                     | 0.41              |
| 22:B:827:CLA:HBA1 | 22:B:828:CLA:HED2 | 2.03                     | 0.41              |
| 24:B:853:BCR:H312 | 22:L:202:CLA:C2C  | 2.50                     | 0.41              |
| 34:F:308:LMG:H161 | 34:F:308:LMG:H132 | 1.83                     | 0.41              |
| 22:J:103:CLA:HED1 | 15:8:240:LEU:HB2  | 2.03                     | 0.41              |
| 22:K:202:CLA:HMB3 | 24:K:206:BCR:H352 | 2.03                     | 0.41              |
| 22:K:205:CLA:NA   | 24:K:206:BCR:H281 | 2.36                     | 0.41              |
| 38:1:303:LUT:H35  | 38:1:303:LUT:H401 | 1.84                     | 0.41              |
| 39:1:312:CHL:H11  | 31:1:319:DGD:HD3  | 2.02                     | 0.41              |
| 12:Z:92:GLU:OE1   | 12:Z:199:PRO:HD2  | 2.20                     | 0.41              |
| 12:Z:92:GLU:OE1   | 12:Z:200:LEU:HD23 | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:Z:103:PRO:HB2  | 39:Z:312:CHL:C1D  | 2.51                     | 0.41              |
| 13:3:54:GLN:H     | 13:3:54:GLN:CD    | 2.29                     | 0.41              |
| 13:3:98:PRO:N     | 13:3:99:PRO:HD2   | 2.36                     | 0.41              |
| 13:3:111:TYR:CZ   | 22:3:316:CLA:HMA2 | 2.55                     | 0.41              |
| 13:3:158:TYR:HB3  | 22:3:308:CLA:HED3 | 2.03                     | 0.41              |
| 24:3:304:BCR:H383 | 22:3:313:CLA:CAB  | 2.51                     | 0.41              |
| 22:3:313:CLA:H13  | 22:5:320:CLA:C4B  | 2.51                     | 0.41              |
| 14:7:58:LEU:CD1   | 22:7:308:CLA:H92  | 2.51                     | 0.41              |
| 24:7:303:BCR:C29  | 42:7:321:SPH:H122 | 2.50                     | 0.41              |
| 22:7:308:CLA:CMD  | 22:7:315:CLA:C1D  | 2.99                     | 0.41              |
| 15:8:77:MET:SD    | 22:8:305:CLA:HAB  | 2.61                     | 0.41              |
| 15:8:113:ILE:CG2  | 15:8:118:LEU:HB2  | 2.51                     | 0.41              |
| 15:8:144:SER:OG   | 15:8:157:LYS:HD3  | 2.21                     | 0.41              |
| 15:8:189:ILE:HD12 | 15:8:189:ILE:HA   | 1.62                     | 0.41              |
| 22:8:305:CLA:H111 | 43:8:319:LPX:H19A | 2.03                     | 0.41              |
| 16:4:132:VAL:HG21 | 16:4:140:TYR:CD1  | 2.56                     | 0.41              |
| 16:4:231:GLN:NE2  | 38:4:802:LUT:H42  | 2.35                     | 0.41              |
| 16:4:251:TRP:HB3  | 18:6:108:PHE:HB3  | 2.02                     | 0.41              |
| 38:4:803:LUT:H31  | 38:4:803:LUT:H391 | 1.91                     | 0.41              |
| 22:4:807:CLA:HBB1 | 22:4:807:CLA:H171 | 2.02                     | 0.41              |
| 22:5:318:CLA:HBB1 | 22:5:318:CLA:CMB  | 2.50                     | 0.41              |
| 18:6:61:PRO:HG2   | 18:6:62:GLU:OE1   | 2.21                     | 0.41              |
| 18:6:215:ILE:HA   | 18:6:218:LYS:HG2  | 2.01                     | 0.41              |
| 22:6:310:CLA:HBC1 | 25:6:323:LHG:H282 | 2.03                     | 0.41              |
| 39:6:315:CHL:CBB  | 39:6:318:CHL:HBB2 | 2.51                     | 0.41              |
| 19:9:36:ASN:O     | 19:9:37:PRO:C     | 2.64                     | 0.41              |
| 38:9:302:LUT:H32  | 22:9:306:CLA:CAB  | 2.50                     | 0.41              |
| 22:9:308:CLA:HMB3 | 22:9:308:CLA:HBB1 | 2.03                     | 0.41              |
| 20:2:178:ARG:O    | 20:2:178:ARG:NE   | 2.52                     | 0.41              |
| 20:2:194:TRP:O    | 20:2:200:THR:HG21 | 2.21                     | 0.41              |
| 1:A:562:LEU:HB2   | 2:B:677:GLU:OE2   | 2.21                     | 0.41              |
| 22:A:803:CLA:HMA2 | 22:A:808:CLA:H191 | 2.03                     | 0.41              |
| 22:A:836:CLA:H42  | 22:K:203:CLA:C2D  | 2.51                     | 0.41              |
| 22:A:840:CLA:H61  | 22:A:840:CLA:H2   | 1.75                     | 0.41              |
| 2:B:53:GLY:O      | 2:B:57:ILE:HG13   | 2.21                     | 0.41              |
| 22:B:809:CLA:HMA2 | 22:B:831:CLA:C4B  | 2.51                     | 0.41              |
| 24:B:847:BCR:C8   | 22:1:308:CLA:H92  | 2.51                     | 0.41              |
| 3:C:21:CYS:HA     | 29:C:101:SF4:S4   | 2.61                     | 0.41              |
| 6:F:79:ARG:HB2    | 6:F:79:ARG:NH1    | 2.36                     | 0.41              |
| 10:K:59:ARG:NH2   | 10:K:67:LEU:HD22  | 2.36                     | 0.41              |
| 24:K:206:BCR:H15C | 24:K:206:BCR:H351 | 1.96                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:1:36:LEU:HD21  | 40:1:318:SQD:H161 | 2.03                     | 0.41              |
| 12:1:167:ILE:O    | 12:1:171:LYS:HG3  | 2.20                     | 0.41              |
| 22:1:306:CLA:H112 | 25:1:317:LHG:H312 | 2.02                     | 0.41              |
| 22:1:307:CLA:H61  | 22:1:307:CLA:H92  | 1.76                     | 0.41              |
| 12:Z:60:LEU:CD1   | 22:Z:306:CLA:H42  | 2.51                     | 0.41              |
| 12:Z:77:HIS:HB3   | 12:Z:182:MET:SD   | 2.61                     | 0.41              |
| 38:3:302:LUT:H31  | 38:3:302:LUT:H391 | 1.88                     | 0.41              |
| 24:3:307:BCR:H10C | 22:3:315:CLA:C1B  | 2.50                     | 0.41              |
| 22:3:309:CLA:HBB1 | 22:3:309:CLA:CMB  | 2.46                     | 0.41              |
| 39:7:313:CHL:OMC  | 39:7:313:CHL:HAC1 | 2.20                     | 0.41              |
| 22:8:306:CLA:CMD  | 33:4:801:LMT:H61  | 2.51                     | 0.41              |
| 39:8:315:CHL:HAC2 | 39:8:315:CHL:OMC  | 2.20                     | 0.41              |
| 16:4:225:PHE:CE1  | 38:4:803:LUT:H10  | 2.56                     | 0.41              |
| 18:6:99:ASP:CB    | 39:6:315:CHL:HED3 | 2.48                     | 0.41              |
| 18:6:123:PHE:CG   | 24:6:305:BCR:H10C | 2.55                     | 0.41              |
| 18:6:157:PRO:HG2  | 22:6:307:CLA:CMD  | 2.51                     | 0.41              |
| 18:6:199:PRO:HB2  | 38:6:303:LUT:H183 | 2.03                     | 0.41              |
| 22:6:317:CLA:HBA2 | 22:6:317:CLA:H12  | 1.69                     | 0.41              |
| 39:9:314:CHL:HHC  | 39:9:314:CHL:CBB  | 2.48                     | 0.41              |
| 20:2:177:VAL:HG22 | 22:2:301:CLA:HHD  | 2.03                     | 0.41              |
| 1:A:578:PRO:HB3   | 2:B:560:CYS:SG    | 2.60                     | 0.40              |
| 22:A:807:CLA:HAA2 | 22:A:809:CLA:O2D  | 2.22                     | 0.40              |
| 22:A:821:CLA:HBB1 | 22:A:821:CLA:CMB  | 2.50                     | 0.40              |
| 22:A:834:CLA:HED2 | 22:A:834:CLA:H2A  | 2.02                     | 0.40              |
| 31:B:852:DGD:HE5  | 31:B:852:DGD:HD4  | 2.03                     | 0.40              |
| 4:D:117:ARG:HD2   | 4:D:119:GLU:HB3   | 2.03                     | 0.40              |
| 4:D:192:MET:HG2   | 4:D:193:ASP:N     | 2.36                     | 0.40              |
| 5:E:52:TRP:O      | 5:E:55:GLN:HB2    | 2.21                     | 0.40              |
| 10:K:106:GLY:HA3  | 22:K:203:CLA:C1B  | 2.52                     | 0.40              |
| 13:3:126:LEU:HD13 | 22:3:318:CLA:HMB3 | 2.02                     | 0.40              |
| 22:7:310:CLA:HBC3 | 25:7:318:LHG:O8   | 2.21                     | 0.40              |
| 22:8:311:CLA:CMA  | 33:4:801:LMT:H5'  | 2.51                     | 0.40              |
| 16:4:150:PHE:O    | 16:4:153:MET:HG2  | 2.22                     | 0.40              |
| 16:4:258:ASN:HD22 | 16:4:258:ASN:H    | 1.69                     | 0.40              |
| 17:5:101:TYR:HD1  | 39:5:316:CHL:HED3 | 1.86                     | 0.40              |
| 22:5:308:CLA:HBB1 | 22:5:308:CLA:HMB1 | 2.03                     | 0.40              |
| 18:6:57:LEU:HD11  | 38:6:304:LUT:H221 | 2.01                     | 0.40              |
| 18:6:60:ASN:OD1   | 18:6:61:PRO:HD2   | 2.21                     | 0.40              |
| 18:6:163:VAL:HG22 | 22:6:307:CLA:HAA2 | 2.02                     | 0.40              |
| 1:A:323:LYS:O     | 1:A:327:GLU:HG3   | 2.21                     | 0.40              |
| 1:A:360:PHE:CE2   | 22:A:829:CLA:HMC3 | 2.57                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:814:CLA:CMC  | 24:A:844:BCR:H352 | 2.51                     | 0.40              |
| 22:A:821:CLA:H71  | 22:A:824:CLA:H71  | 2.01                     | 0.40              |
| 22:A:827:CLA:H2   | 22:A:827:CLA:H61  | 1.69                     | 0.40              |
| 22:A:828:CLA:H91  | 24:J:104:BCR:H341 | 2.03                     | 0.40              |
| 22:A:833:CLA:H192 | 22:B:840:CLA:HHB  | 2.04                     | 0.40              |
| 2:B:439:VAL:HB    | 22:B:834:CLA:HMC2 | 2.02                     | 0.40              |
| 2:B:672:TRP:O     | 2:B:676:ILE:HG13  | 2.20                     | 0.40              |
| 22:B:821:CLA:H193 | 22:B:826:CLA:H203 | 2.03                     | 0.40              |
| 22:B:836:CLA:C1B  | 31:1:319:DGD:HAT2 | 2.51                     | 0.40              |
| 5:E:39:ARG:NH2    | 5:E:62:VAL:H      | 2.17                     | 0.40              |
| 6:F:69:PRO:HA     | 6:F:124:LEU:HD23  | 2.03                     | 0.40              |
| 22:F:304:CLA:HAC1 | 33:F:307:LMT:H121 | 2.02                     | 0.40              |
| 7:G:73:THR:O      | 7:G:74:GLY:C      | 2.64                     | 0.40              |
| 22:Z:303:CLA:H12  | 22:Z:303:CLA:HBA2 | 1.59                     | 0.40              |
| 22:3:312:CLA:H111 | 22:3:312:CLA:H93  | 1.62                     | 0.40              |
| 14:7:150:ASP:C    | 14:7:152:SER:H    | 2.28                     | 0.40              |
| 15:8:77:MET:HB2   | 22:8:305:CLA:HMC3 | 2.02                     | 0.40              |
| 16:4:178:PRO:HD2  | 39:4:819:CHL:CHC  | 2.51                     | 0.40              |
| 22:6:301:CLA:HHC  | 22:6:301:CLA:CBB  | 2.52                     | 0.40              |
| 1:A:104:TRP:CD1   | 1:A:108:PRO:HA    | 2.56                     | 0.40              |
| 1:A:651:TRP:HB2   | 22:B:805:CLA:CBC  | 2.51                     | 0.40              |
| 22:A:815:CLA:H42  | 31:3:301:DGD:HAT2 | 2.03                     | 0.40              |
| 22:A:831:CLA:NA   | 25:A:849:LHG:H111 | 2.37                     | 0.40              |
| 24:A:844:BCR:H403 | 24:A:856:BCR:H10C | 2.02                     | 0.40              |
| 24:A:856:BCR:H392 | 10:K:95:LEU:CD2   | 2.52                     | 0.40              |
| 2:B:258:PHE:CE1   | 22:B:819:CLA:H52  | 2.57                     | 0.40              |
| 22:B:814:CLA:H111 | 19:9:54:LEU:HD11  | 2.04                     | 0.40              |
| 22:B:833:CLA:H2   | 22:B:833:CLA:H61  | 1.77                     | 0.40              |
| 10:K:38:MET:HG2   | 22:K:202:CLA:C2D  | 2.52                     | 0.40              |
| 10:K:107:LEU:CD2  | 10:K:112:ASN:HD22 | 2.34                     | 0.40              |
| 11:L:144:PRO:O    | 11:L:163:SER:HA   | 2.21                     | 0.40              |
| 12:1:191:GLN:OE1  | 12:1:199:PRO:HA   | 2.20                     | 0.40              |
| 40:1:318:SQD:H291 | 39:8:301:CHL:HMB2 | 2.03                     | 0.40              |
| 12:Z:146:ASP:O    | 12:Z:147:ALA:HB3  | 2.20                     | 0.40              |
| 22:3:308:CLA:HMB1 | 22:3:308:CLA:HBB1 | 2.02                     | 0.40              |
| 14:7:129:LEU:HD13 | 22:7:322:CLA:O1A  | 2.22                     | 0.40              |
| 14:7:173:PHE:C    | 14:7:175:PRO:HD3  | 2.46                     | 0.40              |
| 15:8:228:THR:HA   | 22:8:307:CLA:HBA2 | 2.02                     | 0.40              |
| 16:4:108:MET:HE2  | 16:4:218:ALA:CB   | 2.45                     | 0.40              |
| 22:5:308:CLA:H101 | 22:5:308:CLA:H13  | 1.80                     | 0.40              |
| 22:5:311:CLA:CHD  | 22:5:318:CLA:H101 | 2.50                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:6:110:ILE:HD13 | 24:6:306:BCR:C8   | 2.41                     | 0.40              |
| 22:6:308:CLA:HMD3 | 22:6:313:CLA:CHA  | 2.52                     | 0.40              |
| 19:9:154:MET:HE2  | 19:9:154:MET:HB2  | 1.72                     | 0.40              |
| 1:A:121:VAL:HG13  | 1:A:122:VAL:HG22  | 2.03                     | 0.40              |
| 1:A:310:HIS:O     | 22:A:822:CLA:HAC2 | 2.22                     | 0.40              |
| 1:A:370:HIS:NE2   | 22:A:827:CLA:NB   | 2.70                     | 0.40              |
| 1:A:571:PHE:O     | 1:A:587:SER:HB2   | 2.22                     | 0.40              |
| 22:A:810:CLA:H62  | 22:A:810:CLA:H2   | 1.77                     | 0.40              |
| 22:A:833:CLA:HBD  | 24:B:853:BCR:H12C | 2.03                     | 0.40              |
| 22:A:854:CLA:HMA3 | 22:A:854:CLA:C3   | 2.51                     | 0.40              |
| 2:B:441:ASN:O     | 2:B:445:GLN:HG2   | 2.21                     | 0.40              |
| 3:C:22:PRO:HD2    | 29:C:101:SF4:S3   | 2.61                     | 0.40              |
| 3:C:41:SER:HB2    | 4:D:168:VAL:H     | 1.87                     | 0.40              |
| 4:D:83:PHE:CZ     | 4:D:141:VAL:HB    | 2.56                     | 0.40              |
| 6:F:107:THR:O     | 6:F:110:ARG:HG2   | 2.21                     | 0.40              |
| 6:F:185:ILE:HG13  | 6:F:186:ILE:H     | 1.87                     | 0.40              |
| 9:J:25:LEU:O      | 9:J:29:ILE:HG13   | 2.22                     | 0.40              |
| 12:1:144:GLU:HB2  | 22:1:313:CLA:HAC1 | 2.03                     | 0.40              |
| 38:1:302:LUT:H371 | 22:1:304:CLA:H92  | 2.04                     | 0.40              |
| 38:1:303:LUT:H15  | 38:1:303:LUT:H201 | 1.86                     | 0.40              |
| 22:1:308:CLA:ND   | 22:1:314:CLA:H93  | 2.37                     | 0.40              |
| 22:Z:305:CLA:CGA  | 22:Z:305:CLA:C1A  | 2.99                     | 0.40              |
| 22:3:318:CLA:HMB2 | 22:3:320:CLA:C1C  | 2.52                     | 0.40              |
| 22:3:320:CLA:HBA1 | 41:7:319:3PH:C3D  | 2.51                     | 0.40              |
| 14:7:37:ASN:HD22  | 14:7:37:ASN:HA    | 1.57                     | 0.40              |
| 16:4:138:GLY:HA3  | 39:4:813:CHL:C3D  | 2.51                     | 0.40              |
| 16:4:186:PRO:HD2  | 16:4:195:GLY:HA3  | 2.04                     | 0.40              |
| 38:4:802:LUT:H7   | 38:4:802:LUT:H171 | 1.85                     | 0.40              |
| 24:4:804:BCR:C27  | 22:4:810:CLA:H2   | 2.44                     | 0.40              |
| 22:4:807:CLA:H93  | 22:4:807:CLA:H61  | 1.90                     | 0.40              |
| 17:5:69:TRP:HZ2   | 22:5:318:CLA:HAA2 | 1.86                     | 0.40              |
| 38:5:303:LUT:H193 | 22:5:319:CLA:HBB2 | 2.03                     | 0.40              |
| 24:5:304:BCR:H271 | 22:5:312:CLA:C1B  | 2.51                     | 0.40              |
| 22:5:308:CLA:HMA1 | 22:5:308:CLA:H121 | 2.03                     | 0.40              |
| 22:5:326:CLA:C1D  | 22:6:314:CLA:H13  | 2.52                     | 0.40              |
| 18:6:49:ASP:HA    | 22:6:310:CLA:O1D  | 2.21                     | 0.40              |
| 18:6:54:PRO:HD2   | 38:6:304:LUT:C23  | 2.40                     | 0.40              |
| 38:9:301:LUT:H162 | 22:9:305:CLA:CHB  | 2.51                     | 0.40              |
| 38:9:302:LUT:H371 | 22:9:306:CLA:H142 | 2.03                     | 0.40              |
| 1:A:161:THR:HG23  | 27:A:852:DGA:HAW2 | 2.03                     | 0.40              |
| 1:A:223:PRO:HD3   | 1:A:250:MET:HE1   | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:247:ARG:HD3   | 1:A:257:PHE:O     | 2.21                     | 0.40              |
| 1:A:457:ILE:HG21  | 22:B:806:CLA:H92  | 2.03                     | 0.40              |
| 1:A:494:ALA:N     | 1:A:495:PRO:CD    | 2.84                     | 0.40              |
| 1:A:645:TRP:O     | 1:A:649:PHE:HB3   | 2.22                     | 0.40              |
| 22:A:804:CLA:HBA1 | 22:A:811:CLA:C1D  | 2.52                     | 0.40              |
| 22:A:809:CLA:H42  | 24:J:104:BCR:C10  | 2.52                     | 0.40              |
| 22:A:813:CLA:HBA1 | 22:A:825:CLA:C4   | 2.49                     | 0.40              |
| 22:A:822:CLA:H8   | 22:A:823:CLA:H93  | 2.02                     | 0.40              |
| 22:A:822:CLA:C9   | 22:K:204:CLA:HAB  | 2.52                     | 0.40              |
| 22:A:836:CLA:HED3 | 22:A:836:CLA:H2A  | 2.03                     | 0.40              |
| 27:A:852:DGA:HG32 | 22:3:316:CLA:HMB1 | 2.03                     | 0.40              |
| 2:B:263:HIS:CG    | 2:B:264:PRO:HD2   | 2.56                     | 0.40              |
| 2:B:333:PHE:CD2   | 24:B:848:BCR:H292 | 2.56                     | 0.40              |
| 2:B:581:VAL:HG21  | 2:B:711:LEU:HD21  | 2.03                     | 0.40              |
| 2:B:695:LYS:HE2   | 11:L:141:GLN:HE22 | 1.86                     | 0.40              |
| 22:B:819:CLA:ND   | 22:B:819:CLA:H8   | 2.36                     | 0.40              |
| 3:C:10:THR:O      | 3:C:64:SER:HB2    | 2.21                     | 0.40              |
| 4:D:76:ARG:HA     | 4:D:79:GLN:OE1    | 2.21                     | 0.40              |
| 4:D:128:LEU:HB3   | 4:D:134:PHE:HB2   | 2.03                     | 0.40              |
| 10:K:84:PHE:CD2   | 10:K:89:THR:HG22  | 2.57                     | 0.40              |
| 40:1:318:SQD:H171 | 40:1:318:SQD:H141 | 1.92                     | 0.40              |
| 22:Z:303:CLA:H41  | 22:Z:304:CLA:HMA2 | 2.03                     | 0.40              |
| 13:3:22:THR:HA    | 13:3:25:TYR:CZ    | 2.56                     | 0.40              |
| 13:3:76:ALA:CB    | 24:3:305:BCR:H292 | 2.52                     | 0.40              |
| 13:3:169:LEU:HD12 | 38:3:302:LUT:H221 | 2.03                     | 0.40              |
| 24:3:304:BCR:H19C | 22:3:319:CLA:HBA1 | 2.03                     | 0.40              |
| 22:3:318:CLA:H13  | 22:3:318:CLA:H102 | 1.89                     | 0.40              |
| 14:7:155:GLY:O    | 14:7:157:THR:HG23 | 2.22                     | 0.40              |
| 22:7:305:CLA:ND   | 22:7:310:CLA:H8   | 2.36                     | 0.40              |
| 22:7:307:CLA:HBB1 | 22:7:307:CLA:CMB  | 2.52                     | 0.40              |
| 15:8:164:PRO:HG3  | 22:8:313:CLA:C1D  | 2.52                     | 0.40              |
| 24:4:804:BCR:H282 | 22:4:818:CLA:CMC  | 2.51                     | 0.40              |
| 39:4:813:CHL:HMB3 | 39:4:813:CHL:CBB  | 2.50                     | 0.40              |
| 38:5:302:LUT:H30  | 22:5:307:CLA:H52  | 2.01                     | 0.40              |
| 22:5:308:CLA:OBD  | 22:5:313:CLA:H12  | 2.22                     | 0.40              |
| 22:5:310:CLA:HMD1 | 22:5:315:CLA:OBD  | 2.22                     | 0.40              |
| 18:6:236:PHE:CE2  | 18:6:245:PHE:HB2  | 2.56                     | 0.40              |
| 22:6:309:CLA:H51  | 22:6:309:CLA:C1C  | 2.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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     | 738/740 (100%)  | 685 (93%)  | 51 (7%)  | 2 (0%)   | 36          | 64  |
| 2   | B     | 730/732 (100%)  | 683 (94%)  | 42 (6%)  | 5 (1%)   | 18          | 45  |
| 3   | C     | 78/80 (98%)     | 72 (92%)   | 6 (8%)   | 0        | 100         | 100 |
| 4   | D     | 140/142 (99%)   | 124 (89%)  | 13 (9%)  | 3 (2%)   | 5           | 18  |
| 5   | E     | 59/61 (97%)     | 50 (85%)   | 8 (14%)  | 1 (2%)   | 7           | 23  |
| 6   | F     | 163/165 (99%)   | 145 (89%)  | 14 (9%)  | 4 (2%)   | 4           | 15  |
| 7   | G     | 91/93 (98%)     | 73 (80%)   | 16 (18%) | 2 (2%)   | 5           | 17  |
| 8   | I     | 39/41 (95%)     | 34 (87%)   | 5 (13%)  | 0        | 100         | 100 |
| 9   | J     | 38/40 (95%)     | 38 (100%)  | 0        | 0        | 100         | 100 |
| 10  | K     | 87/89 (98%)     | 78 (90%)   | 8 (9%)   | 1 (1%)   | 11          | 34  |
| 11  | L     | 119/123 (97%)   | 106 (89%)  | 11 (9%)  | 2 (2%)   | 7           | 23  |
| 12  | 1     | 192/194 (99%)   | 165 (86%)  | 23 (12%) | 4 (2%)   | 5           | 18  |
| 12  | Z     | 192/194 (99%)   | 181 (94%)  | 10 (5%)  | 1 (0%)   | 24          | 53  |
| 13  | 3     | 216/218 (99%)   | 195 (90%)  | 18 (8%)  | 3 (1%)   | 9           | 27  |
| 14  | 7     | 218/220 (99%)   | 202 (93%)  | 12 (6%)  | 4 (2%)   | 6           | 22  |
| 15  | 8     | 212/214 (99%)   | 181 (85%)  | 24 (11%) | 7 (3%)   | 3           | 10  |
| 16  | 4     | 205/207 (99%)   | 190 (93%)  | 15 (7%)  | 0        | 100         | 100 |
| 17  | 5     | 224/226 (99%)   | 207 (92%)  | 13 (6%)  | 4 (2%)   | 6           | 22  |
| 18  | 6     | 224/226 (99%)   | 212 (95%)  | 11 (5%)  | 1 (0%)   | 30          | 58  |
| 19  | 9     | 182/184 (99%)   | 152 (84%)  | 23 (13%) | 7 (4%)   | 2           | 8   |
| 20  | 2     | 68/70 (97%)     | 53 (78%)   | 14 (21%) | 1 (2%)   | 8           | 26  |
| All | All   | 4215/4259 (99%) | 3826 (91%) | 337 (8%) | 52 (1%)  | 13          | 31  |

All (52) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 154 | ASP  |
| 12  | 1     | 41  | ALA  |
| 12  | 1     | 42  | PRO  |
| 14  | 7     | 219 | ILE  |
| 15  | 8     | 38  | ALA  |
| 15  | 8     | 148 | SER  |
| 15  | 8     | 152 | PHE  |
| 15  | 8     | 161 | ASN  |
| 19  | 9     | 46  | ALA  |
| 19  | 9     | 143 | PRO  |
| 19  | 9     | 146 | PRO  |
| 19  | 9     | 147 | ALA  |
| 20  | 2     | 182 | PRO  |
| 1   | A     | 21  | PRO  |
| 2   | B     | 28  | VAL  |
| 6   | F     | 64  | ILE  |
| 6   | F     | 150 | PHE  |
| 12  | 1     | 166 | ASP  |
| 15  | 8     | 42  | GLY  |
| 19  | 9     | 139 | ILE  |
| 6   | F     | 178 | ALA  |
| 6   | F     | 212 | ALA  |
| 11  | L     | 61  | SER  |
| 13  | 3     | 87  | VAL  |
| 13  | 3     | 159 | PRO  |
| 14  | 7     | 213 | ALA  |
| 15  | 8     | 37  | PRO  |
| 19  | 9     | 196 | TYR  |
| 2   | B     | 230 | ASN  |
| 7   | G     | 70  | PRO  |
| 7   | G     | 85  | ALA  |
| 12  | 1     | 102 | ALA  |
| 12  | Z     | 40  | ASP  |
| 14  | 7     | 98  | PRO  |
| 14  | 7     | 240 | SER  |
| 15  | 8     | 150 | LEU  |
| 18  | 6     | 88  | GLN  |
| 19  | 9     | 145 | ASP  |
| 1   | A     | 574 | PRO  |
| 4   | D     | 149 | TYR  |
| 13  | 3     | 218 | ALA  |
| 17  | 5     | 152 | PHE  |
| 2   | B     | 160 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 545 | SER  |
| 2   | B     | 559 | PRO  |
| 17  | 5     | 236 | THR  |
| 4   | D     | 158 | PRO  |
| 5   | E     | 70  | PRO  |
| 11  | L     | 98  | GLY  |
| 17  | 5     | 171 | PRO  |
| 10  | K     | 60  | GLY  |
| 17  | 5     | 151 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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     | 602/602 (100%) | 574 (95%) | 28 (5%)  | 23          | 55  |
| 2   | B     | 596/596 (100%) | 566 (95%) | 30 (5%)  | 22          | 53  |
| 3   | C     | 70/70 (100%)   | 69 (99%)  | 1 (1%)   | 59          | 84  |
| 4   | D     | 122/122 (100%) | 107 (88%) | 15 (12%) | 4           | 15  |
| 5   | E     | 54/54 (100%)   | 52 (96%)  | 2 (4%)   | 30          | 63  |
| 6   | F     | 128/128 (100%) | 101 (79%) | 27 (21%) | 1           | 3   |
| 7   | G     | 69/69 (100%)   | 63 (91%)  | 6 (9%)   | 9           | 29  |
| 8   | I     | 33/33 (100%)   | 33 (100%) | 0        | 100         | 100 |
| 9   | J     | 35/35 (100%)   | 34 (97%)  | 1 (3%)   | 37          | 71  |
| 10  | K     | 60/60 (100%)   | 54 (90%)  | 6 (10%)  | 7           | 23  |
| 11  | L     | 90/90 (100%)   | 76 (84%)  | 14 (16%) | 2           | 8   |
| 12  | 1     | 144/144 (100%) | 125 (87%) | 19 (13%) | 4           | 13  |
| 12  | Z     | 144/144 (100%) | 134 (93%) | 10 (7%)  | 14          | 39  |
| 13  | 3     | 173/173 (100%) | 159 (92%) | 14 (8%)  | 11          | 32  |
| 14  | 7     | 169/169 (100%) | 156 (92%) | 13 (8%)  | 12          | 34  |
| 15  | 8     | 162/162 (100%) | 137 (85%) | 25 (15%) | 2           | 9   |
| 16  | 4     | 162/162 (100%) | 141 (87%) | 21 (13%) | 4           | 13  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 17  | 5     | 185/185 (100%)   | 166 (90%)  | 19 (10%) | 7           | 22 |
| 18  | 6     | 184/184 (100%)   | 172 (94%)  | 12 (6%)  | 15          | 42 |
| 19  | 9     | 143/143 (100%)   | 125 (87%)  | 18 (13%) | 4           | 14 |
| 20  | 2     | 57/57 (100%)     | 50 (88%)   | 7 (12%)  | 4           | 15 |
| All | All   | 3382/3382 (100%) | 3094 (92%) | 288 (8%) | 12          | 30 |

All (288) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | LYS  |
| 1   | A     | 14  | LYS  |
| 1   | A     | 17  | VAL  |
| 1   | A     | 36  | SER  |
| 1   | A     | 37  | ARG  |
| 1   | A     | 52  | LEU  |
| 1   | A     | 55  | ASP  |
| 1   | A     | 68  | GLU  |
| 1   | A     | 83  | VAL  |
| 1   | A     | 116 | GLN  |
| 1   | A     | 144 | PHE  |
| 1   | A     | 154 | THR  |
| 1   | A     | 187 | LYS  |
| 1   | A     | 189 | GLU  |
| 1   | A     | 225 | ASN  |
| 1   | A     | 244 | LEU  |
| 1   | A     | 248 | GLN  |
| 1   | A     | 291 | LEU  |
| 1   | A     | 299 | LEU  |
| 1   | A     | 301 | ILE  |
| 1   | A     | 339 | VAL  |
| 1   | A     | 363 | LEU  |
| 1   | A     | 426 | LEU  |
| 1   | A     | 455 | LEU  |
| 1   | A     | 489 | LYS  |
| 1   | A     | 490 | THR  |
| 1   | A     | 503 | LEU  |
| 1   | A     | 642 | ILE  |
| 2   | B     | 20  | ARG  |
| 2   | B     | 28  | VAL  |
| 2   | B     | 33  | GLU  |
| 2   | B     | 60  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 97  | PHE  |
| 2   | B     | 103 | GLU  |
| 2   | B     | 159 | GLN  |
| 2   | B     | 160 | PRO  |
| 2   | B     | 186 | VAL  |
| 2   | B     | 206 | LYS  |
| 2   | B     | 215 | THR  |
| 2   | B     | 236 | GLN  |
| 2   | B     | 256 | LEU  |
| 2   | B     | 342 | VAL  |
| 2   | B     | 345 | ILE  |
| 2   | B     | 348 | LEU  |
| 2   | B     | 355 | SER  |
| 2   | B     | 362 | LEU  |
| 2   | B     | 379 | ILE  |
| 2   | B     | 384 | MET  |
| 2   | B     | 398 | ASP  |
| 2   | B     | 477 | LEU  |
| 2   | B     | 484 | SER  |
| 2   | B     | 495 | LEU  |
| 2   | B     | 513 | ILE  |
| 2   | B     | 591 | VAL  |
| 2   | B     | 607 | VAL  |
| 2   | B     | 632 | LEU  |
| 2   | B     | 644 | LEU  |
| 2   | B     | 695 | LYS  |
| 3   | C     | 69  | LEU  |
| 4   | D     | 61  | ASP  |
| 4   | D     | 65  | PRO  |
| 4   | D     | 89  | GLU  |
| 4   | D     | 90  | SER  |
| 4   | D     | 92  | LYS  |
| 4   | D     | 95  | ILE  |
| 4   | D     | 97  | GLU  |
| 4   | D     | 108 | LYS  |
| 4   | D     | 150 | LEU  |
| 4   | D     | 158 | PRO  |
| 4   | D     | 159 | GLU  |
| 4   | D     | 160 | LYS  |
| 4   | D     | 162 | ASN  |
| 4   | D     | 168 | VAL  |
| 4   | D     | 192 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 38  | LYS  |
| 5   | E     | 60  | VAL  |
| 6   | F     | 63  | ASP  |
| 6   | F     | 80  | LEU  |
| 6   | F     | 81  | LYS  |
| 6   | F     | 90  | ARG  |
| 6   | F     | 92  | LYS  |
| 6   | F     | 93  | ASN  |
| 6   | F     | 100 | PRO  |
| 6   | F     | 104 | LEU  |
| 6   | F     | 109 | GLU  |
| 6   | F     | 113 | ASN  |
| 6   | F     | 114 | ARG  |
| 6   | F     | 115 | PHE  |
| 6   | F     | 125 | CYS  |
| 6   | F     | 142 | LYS  |
| 6   | F     | 159 | VAL  |
| 6   | F     | 173 | MET  |
| 6   | F     | 179 | LYS  |
| 6   | F     | 183 | LYS  |
| 6   | F     | 187 | ILE  |
| 6   | F     | 189 | VAL  |
| 6   | F     | 210 | LEU  |
| 6   | F     | 211 | ARG  |
| 6   | F     | 214 | THR  |
| 6   | F     | 217 | GLU  |
| 6   | F     | 218 | LYS  |
| 6   | F     | 220 | GLU  |
| 6   | F     | 222 | ILE  |
| 7   | G     | 37  | GLN  |
| 7   | G     | 45  | MET  |
| 7   | G     | 56  | LEU  |
| 7   | G     | 62  | GLU  |
| 7   | G     | 88  | ILE  |
| 7   | G     | 122 | LEU  |
| 9   | J     | 2   | LYS  |
| 10  | K     | 25  | ARG  |
| 10  | K     | 56  | THR  |
| 10  | K     | 61  | THR  |
| 10  | K     | 66  | LYS  |
| 10  | K     | 70  | ARG  |
| 10  | K     | 89  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | L     | 54  | MET  |
| 11  | L     | 55  | LEU  |
| 11  | L     | 60  | THR  |
| 11  | L     | 76  | ARG  |
| 11  | L     | 79  | VAL  |
| 11  | L     | 82  | LEU  |
| 11  | L     | 83  | LEU  |
| 11  | L     | 99  | PRO  |
| 11  | L     | 110 | GLU  |
| 11  | L     | 141 | GLN  |
| 11  | L     | 161 | LEU  |
| 11  | L     | 162 | GLN  |
| 11  | L     | 176 | VAL  |
| 11  | L     | 179 | LEU  |
| 12  | 1     | 35  | TRP  |
| 12  | 1     | 37  | PRO  |
| 12  | 1     | 42  | PRO  |
| 12  | 1     | 47  | ASP  |
| 12  | 1     | 61  | CYS  |
| 12  | 1     | 75  | VAL  |
| 12  | 1     | 104 | LEU  |
| 12  | 1     | 113 | THR  |
| 12  | 1     | 119 | VAL  |
| 12  | 1     | 149 | LYS  |
| 12  | 1     | 151 | ILE  |
| 12  | 1     | 167 | ILE  |
| 12  | 1     | 168 | GLU  |
| 12  | 1     | 172 | LEU  |
| 12  | 1     | 175 | ILE  |
| 12  | 1     | 183 | MET  |
| 12  | 1     | 198 | THR  |
| 12  | 1     | 214 | ASN  |
| 12  | 1     | 218 | ASN  |
| 12  | Z     | 35  | TRP  |
| 12  | Z     | 37  | PRO  |
| 12  | Z     | 47  | ASP  |
| 12  | Z     | 61  | CYS  |
| 12  | Z     | 113 | THR  |
| 12  | Z     | 115 | PHE  |
| 12  | Z     | 119 | VAL  |
| 12  | Z     | 172 | LEU  |
| 12  | Z     | 177 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | Z     | 191 | GLN  |
| 13  | 3     | 93  | GLU  |
| 13  | 3     | 94  | THR  |
| 13  | 3     | 96  | VAL  |
| 13  | 3     | 102 | THR  |
| 13  | 3     | 108 | THR  |
| 13  | 3     | 109 | ASP  |
| 13  | 3     | 125 | GLU  |
| 13  | 3     | 126 | LEU  |
| 13  | 3     | 149 | VAL  |
| 13  | 3     | 166 | LEU  |
| 13  | 3     | 172 | LYS  |
| 13  | 3     | 177 | MET  |
| 13  | 3     | 178 | LYS  |
| 13  | 3     | 228 | ASN  |
| 14  | 7     | 35  | PRO  |
| 14  | 7     | 37  | ASN  |
| 14  | 7     | 65  | MET  |
| 14  | 7     | 97  | LEU  |
| 14  | 7     | 129 | LEU  |
| 14  | 7     | 165 | ASN  |
| 14  | 7     | 176 | ILE  |
| 14  | 7     | 182 | ASP  |
| 14  | 7     | 185 | MET  |
| 14  | 7     | 196 | ASN  |
| 14  | 7     | 219 | ILE  |
| 14  | 7     | 220 | GLN  |
| 14  | 7     | 243 | PHE  |
| 15  | 8     | 31  | MET  |
| 15  | 8     | 41  | LYS  |
| 15  | 8     | 91  | LYS  |
| 15  | 8     | 95  | LEU  |
| 15  | 8     | 105 | LYS  |
| 15  | 8     | 110 | GLN  |
| 15  | 8     | 115 | LEU  |
| 15  | 8     | 138 | LEU  |
| 15  | 8     | 149 | PHE  |
| 15  | 8     | 152 | PHE  |
| 15  | 8     | 153 | GLU  |
| 15  | 8     | 157 | LYS  |
| 15  | 8     | 173 | MET  |
| 15  | 8     | 174 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | 8     | 178 | GLU  |
| 15  | 8     | 180 | LYS  |
| 15  | 8     | 183 | ASP  |
| 15  | 8     | 185 | LYS  |
| 15  | 8     | 189 | ILE  |
| 15  | 8     | 215 | ASP  |
| 15  | 8     | 225 | LEU  |
| 15  | 8     | 231 | ASP  |
| 15  | 8     | 234 | ILE  |
| 15  | 8     | 238 | ILE  |
| 15  | 8     | 240 | LEU  |
| 16  | 4     | 58  | ARG  |
| 16  | 4     | 61  | TRP  |
| 16  | 4     | 66  | LYS  |
| 16  | 4     | 94  | LYS  |
| 16  | 4     | 101 | LEU  |
| 16  | 4     | 119 | LEU  |
| 16  | 4     | 131 | GLN  |
| 16  | 4     | 141 | GLU  |
| 16  | 4     | 160 | VAL  |
| 16  | 4     | 163 | ARG  |
| 16  | 4     | 167 | ASP  |
| 16  | 4     | 170 | LYS  |
| 16  | 4     | 175 | ASN  |
| 16  | 4     | 196 | ILE  |
| 16  | 4     | 204 | LYS  |
| 16  | 4     | 207 | MET  |
| 16  | 4     | 208 | GLU  |
| 16  | 4     | 210 | LEU  |
| 16  | 4     | 212 | LEU  |
| 16  | 4     | 213 | LYS  |
| 16  | 4     | 257 | SER  |
| 17  | 5     | 32  | ARG  |
| 17  | 5     | 34  | LEU  |
| 17  | 5     | 39  | VAL  |
| 17  | 5     | 40  | ASP  |
| 17  | 5     | 65  | VAL  |
| 17  | 5     | 85  | VAL  |
| 17  | 5     | 97  | ASP  |
| 17  | 5     | 98  | VAL  |
| 17  | 5     | 138 | GLN  |
| 17  | 5     | 139 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | 5     | 141 | LYS  |
| 17  | 5     | 146 | VAL  |
| 17  | 5     | 153 | LYS  |
| 17  | 5     | 176 | LYS  |
| 17  | 5     | 182 | LEU  |
| 17  | 5     | 195 | ILE  |
| 17  | 5     | 221 | ASN  |
| 17  | 5     | 236 | THR  |
| 17  | 5     | 240 | VAL  |
| 18  | 6     | 43  | ASN  |
| 18  | 6     | 89  | GLU  |
| 18  | 6     | 92  | LYS  |
| 18  | 6     | 110 | ILE  |
| 18  | 6     | 124 | VAL  |
| 18  | 6     | 128 | ARG  |
| 18  | 6     | 129 | TRP  |
| 18  | 6     | 149 | LEU  |
| 18  | 6     | 167 | MET  |
| 18  | 6     | 211 | MET  |
| 18  | 6     | 222 | VAL  |
| 18  | 6     | 251 | GLN  |
| 19  | 9     | 32  | LEU  |
| 19  | 9     | 42  | LYS  |
| 19  | 9     | 45  | MET  |
| 19  | 9     | 89  | LEU  |
| 19  | 9     | 106 | VAL  |
| 19  | 9     | 115 | GLU  |
| 19  | 9     | 125 | LYS  |
| 19  | 9     | 143 | PRO  |
| 19  | 9     | 146 | PRO  |
| 19  | 9     | 153 | ASP  |
| 19  | 9     | 154 | MET  |
| 19  | 9     | 159 | VAL  |
| 19  | 9     | 177 | LEU  |
| 19  | 9     | 180 | ARG  |
| 19  | 9     | 189 | LYS  |
| 19  | 9     | 197 | ASN  |
| 19  | 9     | 199 | THR  |
| 19  | 9     | 206 | GLN  |
| 20  | 2     | 162 | ARG  |
| 20  | 2     | 166 | LEU  |
| 20  | 2     | 178 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | 2     | 183 | ILE  |
| 20  | 2     | 187 | LYS  |
| 20  | 2     | 205 | LYS  |
| 20  | 2     | 229 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 80  | GLN  |
| 1   | A     | 116 | GLN  |
| 1   | A     | 136 | GLN  |
| 1   | A     | 248 | GLN  |
| 1   | A     | 279 | ASN  |
| 1   | A     | 338 | HIS  |
| 1   | A     | 442 | ASN  |
| 1   | A     | 485 | GLN  |
| 1   | A     | 539 | HIS  |
| 1   | A     | 637 | GLN  |
| 1   | A     | 659 | GLN  |
| 1   | A     | 676 | HIS  |
| 1   | A     | 722 | GLN  |
| 2   | B     | 11  | GLN  |
| 2   | B     | 30  | HIS  |
| 2   | B     | 35  | HIS  |
| 2   | B     | 42  | ASN  |
| 2   | B     | 72  | GLN  |
| 2   | B     | 90  | HIS  |
| 2   | B     | 115 | ASN  |
| 2   | B     | 216 | GLN  |
| 2   | B     | 221 | GLN  |
| 2   | B     | 267 | GLN  |
| 2   | B     | 300 | HIS  |
| 2   | B     | 364 | ASN  |
| 2   | B     | 369 | GLN  |
| 2   | B     | 376 | HIS  |
| 2   | B     | 453 | GLN  |
| 2   | B     | 491 | GLN  |
| 2   | B     | 503 | ASN  |
| 2   | B     | 521 | HIS  |
| 2   | B     | 599 | HIS  |
| 2   | B     | 604 | GLN  |
| 2   | B     | 655 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 37  | ASN  |
| 4   | D     | 91  | ASN  |
| 4   | D     | 120 | GLN  |
| 4   | D     | 180 | ASN  |
| 4   | D     | 189 | ASN  |
| 5   | E     | 78  | GLN  |
| 5   | E     | 94  | GLN  |
| 6   | F     | 82  | ASN  |
| 6   | F     | 132 | HIS  |
| 6   | F     | 145 | HIS  |
| 6   | F     | 205 | GLN  |
| 7   | G     | 37  | GLN  |
| 7   | G     | 57  | HIS  |
| 7   | G     | 92  | ASN  |
| 8   | I     | 103 | ASN  |
| 10  | K     | 35  | ASN  |
| 10  | K     | 112 | ASN  |
| 11  | L     | 141 | GLN  |
| 12  | 1     | 124 | ASN  |
| 12  | 1     | 161 | ASN  |
| 12  | 1     | 192 | HIS  |
| 12  | Z     | 191 | GLN  |
| 13  | 3     | 130 | GLN  |
| 13  | 3     | 141 | GLN  |
| 13  | 3     | 212 | ASN  |
| 13  | 3     | 222 | ASN  |
| 13  | 3     | 223 | ASN  |
| 14  | 7     | 37  | ASN  |
| 14  | 7     | 74  | GLN  |
| 14  | 7     | 75  | ASN  |
| 14  | 7     | 132 | HIS  |
| 14  | 7     | 191 | GLN  |
| 14  | 7     | 196 | ASN  |
| 15  | 8     | 110 | GLN  |
| 15  | 8     | 191 | ASN  |
| 15  | 8     | 205 | GLN  |
| 16  | 4     | 79  | HIS  |
| 16  | 4     | 98  | GLN  |
| 16  | 4     | 176 | GLN  |
| 16  | 4     | 231 | GLN  |
| 16  | 4     | 233 | GLN  |
| 16  | 4     | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | 4     | 258 | ASN  |
| 17  | 5     | 72  | GLN  |
| 17  | 5     | 108 | ASN  |
| 17  | 5     | 114 | GLN  |
| 17  | 5     | 130 | HIS  |
| 17  | 5     | 230 | ASN  |
| 18  | 6     | 122 | HIS  |
| 18  | 6     | 134 | ASN  |
| 18  | 6     | 147 | ASN  |
| 18  | 6     | 193 | GLN  |
| 18  | 6     | 228 | GLN  |
| 18  | 6     | 235 | GLN  |
| 19  | 9     | 40  | HIS  |
| 19  | 9     | 128 | GLN  |
| 19  | 9     | 193 | ASN  |
| 19  | 9     | 201 | ASN  |
| 19  | 9     | 206 | GLN  |
| 20  | 2     | 228 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 332 ligands modelled in this entry, 1 is monoatomic - leaving 331 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 24  | BCR  | 7     | 303 | -    | 41,41,41     | 4.92 | 27 (65%)    | 56,56,56    | 2.42 | 20 (35%)    |
| 24  | BCR  | A     | 846 | -    | 41,41,41     | 4.94 | 27 (65%)    | 56,56,56    | 2.50 | 20 (35%)    |
| 22  | CLA  | 1     | 314 | 12   | 69,73,73     | 1.34 | 5 (7%)      | 82,113,113  | 1.86 | 19 (23%)    |
| 39  | CHL  | 8     | 312 | -    | 50,64,74     | 1.47 | 9 (18%)     | 46,102,114  | 1.83 | 12 (26%)    |
| 25  | LHG  | 3     | 321 | 22   | 19,19,48     | 0.95 | 1 (5%)      | 20,24,54    | 1.55 | 1 (5%)      |
| 25  | LHG  | B     | 803 | -    | 32,32,48     | 0.47 | 0           | 35,38,54    | 1.20 | 3 (8%)      |
| 24  | BCR  | B     | 848 | -    | 41,41,41     | 4.93 | 27 (65%)    | 56,56,56    | 6.50 | 24 (42%)    |
| 22  | CLA  | A     | 815 | -    | 69,73,73     | 1.34 | 7 (10%)     | 82,113,113  | 1.90 | 19 (23%)    |
| 22  | CLA  | A     | 803 | -    | 69,73,73     | 1.34 | 7 (10%)     | 82,113,113  | 1.91 | 19 (23%)    |
| 22  | CLA  | 3     | 314 | 25   | 64,68,73     | 1.40 | 6 (9%)      | 76,107,113  | 1.94 | 18 (23%)    |
| 22  | CLA  | Z     | 307 | -    | 59,63,73     | 1.47 | 7 (11%)     | 70,101,113  | 2.08 | 19 (27%)    |
| 22  | CLA  | B     | 830 | -    | 69,73,73     | 1.34 | 6 (8%)      | 82,113,113  | 1.87 | 18 (21%)    |
| 38  | LUT  | 5     | 302 | -    | 42,43,43     | 6.39 | 26 (61%)    | 51,60,60    | 2.10 | 14 (27%)    |
| 22  | CLA  | 3     | 315 | -    | 49,53,73     | 1.67 | 6 (12%)     | 58,89,113   | 2.10 | 14 (24%)    |
| 22  | CLA  | 1     | 305 | 12   | 49,53,73     | 1.60 | 6 (12%)     | 58,89,113   | 2.06 | 18 (31%)    |
| 22  | CLA  | 7     | 314 | 44   | 54,58,73     | 1.51 | 5 (9%)      | 64,95,113   | 2.12 | 19 (29%)    |
| 38  | LUT  | Z     | 302 | -    | 42,43,43     | 6.40 | 26 (61%)    | 51,60,60    | 2.15 | 13 (25%)    |
| 38  | LUT  | 1     | 302 | -    | 42,43,43     | 6.42 | 27 (64%)    | 51,60,60    | 2.16 | 15 (29%)    |
| 22  | CLA  | 5     | 320 | -    | 54,58,73     | 1.59 | 7 (12%)     | 64,95,113   | 2.08 | 17 (26%)    |
| 22  | CLA  | A     | 807 | -    | 64,68,73     | 1.39 | 6 (9%)      | 76,107,113  | 1.97 | 19 (25%)    |
| 24  | BCR  | B     | 846 | -    | 41,41,41     | 4.94 | 27 (65%)    | 56,56,56    | 2.41 | 20 (35%)    |
| 22  | CLA  | 7     | 324 | -    | 64,68,73     | 1.41 | 6 (9%)      | 76,107,113  | 1.96 | 20 (26%)    |
| 22  | CLA  | 4     | 805 | 16   | 64,68,73     | 1.44 | 8 (12%)     | 76,107,113  | 1.85 | 17 (22%)    |
| 22  | CLA  | 8     | 309 | -    | 69,73,73     | 1.36 | 7 (10%)     | 82,113,113  | 1.88 | 19 (23%)    |
| 22  | CLA  | B     | 810 | -    | 60,64,73     | 1.44 | 5 (8%)      | 71,102,113  | 2.08 | 22 (30%)    |
| 22  | CLA  | B     | 812 | 2    | 63,67,73     | 1.41 | 5 (7%)      | 74,105,113  | 1.90 | 18 (24%)    |
| 22  | CLA  | 1     | 308 | -    | 59,63,73     | 1.46 | 7 (11%)     | 70,101,113  | 2.11 | 18 (25%)    |
| 26  | NKP  | A     | 851 | -    | 22,22,28     | 0.37 | 0           | 24,26,32    | 0.38 | 0           |
| 24  | BCR  | B     | 853 | -    | 41,41,41     | 4.98 | 27 (65%)    | 56,56,56    | 2.40 | 20 (35%)    |
| 22  | CLA  | 6     | 307 | 18   | 64,68,73     | 1.40 | 8 (12%)     | 76,107,113  | 1.96 | 18 (23%)    |
| 22  | CLA  | B     | 832 | -    | 54,58,73     | 1.52 | 6 (11%)     | 64,95,113   | 2.09 | 19 (29%)    |
| 24  | BCR  | 3     | 305 | -    | 41,41,41     | 4.93 | 27 (65%)    | 56,56,56    | 2.23 | 19 (33%)    |
| 42  | SPH  | 7     | 320 | -    | 19,20,20     | 0.65 | 0           | 18,21,21    | 1.10 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | K     | 203 | 44   | 59,63,73     | 1.46 | 6 (10%)  | 70,101,113  | 2.04 | 20 (28%) |
| 25  | LHG  | 5     | 324 | 22   | 36,36,48     | 0.44 | 0        | 39,42,54    | 1.14 | 3 (7%)   |
| 22  | CLA  | Z     | 314 | 12   | 55,59,73     | 1.50 | 6 (10%)  | 64,96,113   | 2.07 | 18 (28%) |
| 39  | CHL  | 7     | 313 | 44   | 48,62,74     | 1.44 | 9 (18%)  | 43,99,114   | 1.88 | 11 (25%) |
| 22  | CLA  | K     | 205 | 10   | 59,63,73     | 1.56 | 7 (11%)  | 70,101,113  | 2.12 | 17 (24%) |
| 22  | CLA  | 3     | 309 | 13   | 50,54,73     | 1.59 | 6 (12%)  | 59,90,113   | 2.02 | 16 (27%) |
| 22  | CLA  | 5     | 315 | 17   | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.90 | 20 (24%) |
| 24  | BCR  | A     | 845 | -    | 41,41,41     | 4.91 | 27 (65%) | 56,56,56    | 2.53 | 22 (39%) |
| 38  | LUT  | 8     | 302 | -    | 42,43,43     | 6.34 | 26 (61%) | 51,60,60    | 2.07 | 16 (31%) |
| 22  | CLA  | B     | 833 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.88 | 20 (24%) |
| 22  | CLA  | Z     | 315 | -    | 50,54,73     | 1.58 | 6 (12%)  | 59,90,113   | 2.08 | 15 (25%) |
| 39  | CHL  | 4     | 814 | 44   | 45,59,74     | 1.39 | 8 (17%)  | 40,96,114   | 2.01 | 11 (27%) |
| 22  | CLA  | 7     | 304 | 14   | 64,68,73     | 1.39 | 6 (9%)   | 76,107,113  | 2.01 | 21 (27%) |
| 22  | CLA  | A     | 826 | 44   | 54,58,73     | 1.52 | 6 (11%)  | 64,95,113   | 2.11 | 18 (28%) |
| 22  | CLA  | G     | 201 | -    | 54,58,73     | 1.54 | 6 (11%)  | 64,95,113   | 2.12 | 21 (32%) |
| 22  | CLA  | 6     | 312 | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.91 | 21 (25%) |
| 22  | CLA  | A     | 827 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.91 | 21 (25%) |
| 22  | CLA  | 4     | 810 | 44   | 54,58,73     | 1.52 | 5 (9%)   | 64,95,113   | 2.11 | 20 (31%) |
| 22  | CLA  | 8     | 316 | 15   | 50,54,73     | 1.57 | 7 (14%)  | 59,90,113   | 2.04 | 15 (25%) |
| 22  | CLA  | 3     | 310 | 13   | 69,73,73     | 1.36 | 7 (10%)  | 82,113,113  | 1.97 | 21 (25%) |
| 22  | CLA  | 5     | 318 | 17   | 69,73,73     | 1.34 | 5 (7%)   | 82,113,113  | 1.86 | 18 (21%) |
| 22  | CLA  | A     | 828 | -    | 69,73,73     | 1.34 | 5 (7%)   | 82,113,113  | 1.91 | 17 (20%) |
| 22  | CLA  | A     | 802 | 44   | 69,73,73     | 1.35 | 5 (7%)   | 82,113,113  | 1.93 | 20 (24%) |
| 22  | CLA  | A     | 834 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.87 | 20 (24%) |
| 22  | CLA  | 8     | 313 | 44   | 54,58,73     | 1.52 | 6 (11%)  | 64,95,113   | 2.09 | 18 (28%) |
| 22  | CLA  | 3     | 312 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.88 | 19 (23%) |
| 22  | CLA  | 2     | 304 | 44   | 50,54,73     | 1.57 | 6 (12%)  | 59,90,113   | 2.05 | 16 (27%) |
| 39  | CHL  | 5     | 321 | 17   | 37,51,74     | 1.59 | 7 (18%)  | 30,86,114   | 2.19 | 9 (30%)  |
| 22  | CLA  | 7     | 312 | -    | 64,68,73     | 1.40 | 5 (7%)   | 76,107,113  | 1.95 | 19 (25%) |
| 22  | CLA  | 5     | 308 | 17   | 65,69,73     | 1.39 | 6 (9%)   | 77,108,113  | 1.94 | 20 (25%) |
| 39  | CHL  | 4     | 819 | 16   | 37,51,74     | 1.64 | 8 (21%)  | 30,86,114   | 2.15 | 9 (30%)  |
| 22  | CLA  | B     | 808 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.88 | 20 (24%) |
| 22  | CLA  | B     | 828 | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.89 | 20 (24%) |
| 22  | CLA  | 7     | 306 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.97 | 19 (23%) |
| 38  | LUT  | 7     | 302 | -    | 42,43,43     | 6.40 | 26 (61%) | 51,60,60    | 2.18 | 15 (29%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | 1     | 310 | 25   | 64,68,73     | 1.39 | 6 (9%)   | 76,107,113  | 1.95 | 18 (23%) |
| 22  | CLA  | A     | 840 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.90 | 18 (21%) |
| 22  | CLA  | 6     | 311 | -    | 59,63,73     | 1.46 | 6 (10%)  | 70,101,113  | 1.96 | 18 (25%) |
| 38  | LUT  | 4     | 802 | -    | 42,43,43     | 6.39 | 26 (61%) | 51,60,60    | 2.14 | 14 (27%) |
| 22  | CLA  | 6     | 321 | -    | 50,54,73     | 1.58 | 6 (12%)  | 59,90,113   | 2.06 | 16 (27%) |
| 22  | CLA  | 7     | 308 | 14   | 65,69,73     | 1.41 | 7 (10%)  | 77,108,113  | 1.93 | 19 (24%) |
| 24  | BCR  | 5     | 305 | -    | 41,41,41     | 4.95 | 27 (65%) | 56,56,56    | 2.69 | 25 (44%) |
| 22  | CLA  | B     | 809 | 2    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.88 | 19 (23%) |
| 25  | LHG  | Z     | 317 | 22   | 42,42,48     | 0.41 | 0        | 45,48,54    | 1.10 | 3 (6%)   |
| 35  | T7X  | J     | 102 | -    | 49,49,61     | 0.93 | 4 (8%)   | 58,61,73    | 0.94 | 3 (5%)   |
| 22  | CLA  | 6     | 302 | 16   | 64,68,73     | 1.40 | 5 (7%)   | 76,107,113  | 1.92 | 19 (25%) |
| 24  | BCR  | A     | 856 | -    | 41,41,41     | 4.91 | 27 (65%) | 56,56,56    | 2.54 | 22 (39%) |
| 22  | CLA  | A     | 813 | -    | 69,73,73     | 1.36 | 5 (7%)   | 82,113,113  | 1.92 | 20 (24%) |
| 39  | CHL  | 6     | 318 | -    | 50,64,74     | 1.55 | 9 (18%)  | 46,102,114  | 1.85 | 13 (28%) |
| 22  | CLA  | 5     | 311 | -    | 59,63,73     | 1.47 | 8 (13%)  | 70,101,113  | 2.01 | 20 (28%) |
| 38  | LUT  | 3     | 303 | -    | 42,43,43     | 6.37 | 26 (61%) | 51,60,60    | 2.10 | 16 (31%) |
| 22  | CLA  | 8     | 306 | 15   | 55,59,73     | 1.52 | 7 (12%)  | 64,96,113   | 2.06 | 18 (28%) |
| 22  | CLA  | Z     | 316 | 12   | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.88 | 18 (21%) |
| 25  | LHG  | 7     | 318 | 22   | 36,36,48     | 0.43 | 0        | 39,42,54    | 1.15 | 3 (7%)   |
| 25  | LHG  | 4     | 820 | 22   | 48,48,48     | 0.42 | 0        | 51,54,54    | 1.06 | 4 (7%)   |
| 22  | CLA  | 6     | 313 | 25   | 59,63,73     | 1.47 | 6 (10%)  | 70,101,113  | 2.00 | 18 (25%) |
| 22  | CLA  | 4     | 808 | 16   | 64,68,73     | 1.40 | 7 (10%)  | 76,107,113  | 1.95 | 20 (26%) |
| 22  | CLA  | 5     | 319 | 44   | 59,63,73     | 1.45 | 6 (10%)  | 70,101,113  | 2.04 | 20 (28%) |
| 22  | CLA  | 7     | 315 | 14   | 54,58,73     | 1.52 | 7 (12%)  | 64,95,113   | 2.13 | 19 (29%) |
| 22  | CLA  | B     | 826 | 44   | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.91 | 20 (24%) |
| 22  | CLA  | 9     | 309 | 25   | 59,63,73     | 1.47 | 6 (10%)  | 70,101,113  | 2.07 | 16 (22%) |
| 33  | LMT  | 4     | 801 | -    | 36,36,36     | 0.36 | 0        | 47,47,47    | 0.73 | 1 (2%)   |
| 38  | LUT  | 1     | 303 | -    | 42,43,43     | 6.40 | 26 (61%) | 51,60,60    | 2.17 | 14 (27%) |
| 22  | CLA  | B     | 834 | -    | 62,66,73     | 1.43 | 5 (8%)   | 73,104,113  | 2.00 | 20 (27%) |
| 22  | CLA  | B     | 839 | -    | 56,60,73     | 1.50 | 6 (10%)  | 65,97,113   | 2.09 | 19 (29%) |
| 22  | CLA  | B     | 824 | -    | 63,67,73     | 1.42 | 6 (9%)   | 74,105,113  | 2.02 | 20 (27%) |
| 22  | CLA  | 3     | 313 | 44   | 69,73,73     | 1.33 | 6 (8%)   | 82,113,113  | 1.90 | 20 (24%) |
| 39  | CHL  | 6     | 316 | -    | 45,59,74     | 1.60 | 9 (20%)  | 40,96,114   | 1.97 | 12 (30%) |
| 42  | SPH  | 7     | 321 | -    | 19,20,20     | 0.66 | 1 (5%)   | 18,21,21    | 1.15 | 1 (5%)   |
| 22  | CLA  | A     | 842 | 25   | 56,60,73     | 1.50 | 6 (10%)  | 65,97,113   | 2.07 | 18 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | 8     | 311 | 25   | 54,58,73     | 1.52 | 6 (11%)  | 64,95,113   | 2.07 | 17 (26%) |
| 38  | LUT  | 7     | 301 | -    | 42,43,43     | 6.37 | 26 (61%) | 51,60,60    | 2.07 | 15 (29%) |
| 22  | CLA  | A     | 838 | -    | 69,73,73     | 1.34 | 5 (7%)   | 82,113,113  | 1.92 | 19 (23%) |
| 22  | CLA  | 4     | 806 | 16   | 56,60,73     | 1.51 | 7 (12%)  | 65,97,113   | 2.11 | 19 (29%) |
| 22  | CLA  | G     | 202 | 7    | 50,54,73     | 1.58 | 7 (14%)  | 59,90,113   | 2.05 | 17 (28%) |
| 22  | CLA  | B     | 814 | -    | 64,68,73     | 1.39 | 6 (9%)   | 76,107,113  | 1.96 | 18 (23%) |
| 22  | CLA  | A     | 819 | -    | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.86 | 19 (23%) |
| 22  | CLA  | 1     | 307 | 12   | 64,68,73     | 1.41 | 7 (10%)  | 76,107,113  | 1.99 | 18 (23%) |
| 33  | LMT  | F     | 307 | -    | 36,36,36     | 0.38 | 0        | 47,47,47    | 0.64 | 0        |
| 37  | DAO  | K     | 201 | -    | 13,13,13     | 0.61 | 0        | 13,13,13    | 0.57 | 0        |
| 22  | CLA  | 4     | 817 | 16   | 45,49,73     | 1.66 | 6 (13%)  | 54,84,113   | 2.14 | 17 (31%) |
| 22  | CLA  | B     | 831 | -    | 62,66,73     | 1.43 | 7 (11%)  | 73,104,113  | 2.01 | 18 (24%) |
| 22  | CLA  | 1     | 304 | -    | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.89 | 19 (23%) |
| 38  | LUT  | 9     | 302 | -    | 42,43,43     | 6.39 | 27 (64%) | 51,60,60    | 1.98 | 14 (27%) |
| 22  | CLA  | 5     | 314 | -    | 49,53,73     | 1.59 | 6 (12%)  | 58,89,113   | 2.05 | 15 (25%) |
| 22  | CLA  | B     | 825 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.88 | 20 (24%) |
| 22  | CLA  | 9     | 313 | 19   | 54,58,73     | 1.52 | 5 (9%)   | 64,95,113   | 2.11 | 20 (31%) |
| 22  | CLA  | 9     | 308 | -    | 54,58,73     | 1.53 | 5 (9%)   | 64,95,113   | 2.08 | 20 (31%) |
| 22  | CLA  | B     | 820 | -    | 64,68,73     | 1.41 | 6 (9%)   | 76,107,113  | 1.92 | 19 (25%) |
| 21  | CL0  | A     | 801 | -    | 58,73,73     | 3.23 | 16 (27%) | 60,113,113  | 2.88 | 17 (28%) |
| 22  | CLA  | Z     | 313 | 44   | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.90 | 19 (23%) |
| 22  | CLA  | A     | 804 | 22   | 49,53,73     | 1.59 | 5 (10%)  | 58,89,113   | 2.06 | 16 (27%) |
| 22  | CLA  | A     | 817 | -    | 64,68,73     | 1.40 | 6 (9%)   | 76,107,113  | 1.99 | 17 (22%) |
| 22  | CLA  | A     | 812 | -    | 69,73,73     | 1.34 | 7 (10%)  | 82,113,113  | 1.90 | 19 (23%) |
| 22  | CLA  | K     | 204 | 10   | 53,57,73     | 1.54 | 6 (11%)  | 61,93,113   | 2.17 | 19 (31%) |
| 22  | CLA  | L     | 202 | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.88 | 19 (23%) |
| 22  | CLA  | B     | 806 | 44   | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.90 | 20 (24%) |
| 29  | SF4  | C     | 101 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 24  | BCR  | F     | 303 | -    | 41,41,41     | 4.95 | 27 (65%) | 56,56,56    | 2.23 | 17 (30%) |
| 41  | 3PH  | 5     | 325 | -    | 22,22,47     | 1.24 | 4 (18%)  | 25,27,52    | 1.32 | 2 (8%)   |
| 22  | CLA  | B     | 842 | 25   | 69,73,73     | 1.35 | 5 (7%)   | 82,113,113  | 1.90 | 19 (23%) |
| 29  | SF4  | B     | 802 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 40  | SQD  | 1     | 318 | -    | 46,48,54     | 0.82 | 1 (2%)   | 56,59,65    | 0.89 | 2 (3%)   |
| 22  | CLA  | 5     | 310 | 17   | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.91 | 19 (23%) |
| 22  | CLA  | 7     | 309 | -    | 60,64,73     | 1.45 | 6 (10%)  | 71,102,113  | 2.05 | 21 (29%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 39  | CHL  | 5     | 316 | 44   | 60,74,74     | 1.35 | 9 (15%)  | 58,114,114  | 1.61 | 13 (22%) |
| 22  | CLA  | 7     | 307 | 14   | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.92 | 18 (21%) |
| 34  | LMG  | F     | 308 | -    | 35,35,55     | 0.47 | 0        | 43,43,63    | 1.40 | 5 (11%)  |
| 38  | LUT  | 9     | 301 | -    | 42,43,43     | 6.39 | 26 (61%) | 51,60,60    | 2.05 | 14 (27%) |
| 22  | CLA  | 3     | 308 | 13   | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.93 | 19 (23%) |
| 22  | CLA  | B     | 841 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.95 | 20 (24%) |
| 22  | CLA  | B     | 829 | -    | 61,65,73     | 1.43 | 6 (9%)   | 72,103,113  | 2.00 | 21 (29%) |
| 25  | LHG  | B     | 850 | 22   | 22,22,48     | 0.57 | 0        | 25,28,54    | 1.28 | 2 (8%)   |
| 24  | BCR  | 3     | 306 | -    | 41,41,41     | 4.94 | 27 (65%) | 56,56,56    | 2.31 | 18 (32%) |
| 28  | OCA  | A     | 853 | -    | 9,9,9        | 0.72 | 0        | 9,9,9       | 0.71 | 0        |
| 22  | CLA  | A     | 820 | -    | 64,68,73     | 1.40 | 7 (10%)  | 76,107,113  | 1.92 | 19 (25%) |
| 22  | CLA  | A     | 818 | -    | 64,68,73     | 1.40 | 7 (10%)  | 76,107,113  | 2.01 | 21 (27%) |
| 22  | CLA  | 1     | 306 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.92 | 19 (23%) |
| 22  | CLA  | A     | 835 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.86 | 19 (23%) |
| 24  | BCR  | A     | 847 | -    | 41,41,41     | 4.94 | 27 (65%) | 56,56,56    | 2.41 | 19 (33%) |
| 25  | LHG  | A     | 850 | -    | 48,48,48     | 0.39 | 0        | 51,54,54    | 1.05 | 3 (5%)   |
| 22  | CLA  | A     | 816 | 44   | 60,64,73     | 1.45 | 6 (10%)  | 71,102,113  | 2.08 | 21 (29%) |
| 24  | BCR  | 5     | 304 | -    | 41,41,41     | 4.93 | 26 (63%) | 56,56,56    | 2.57 | 21 (37%) |
| 22  | CLA  | Z     | 308 | -    | 65,69,73     | 1.38 | 6 (9%)   | 77,108,113  | 1.95 | 20 (25%) |
| 22  | CLA  | B     | 836 | -    | 49,53,73     | 1.59 | 6 (12%)  | 58,89,113   | 2.04 | 17 (29%) |
| 22  | CLA  | B     | 835 | -    | 54,58,73     | 1.52 | 7 (12%)  | 64,95,113   | 2.16 | 19 (29%) |
| 39  | CHL  | 1     | 312 | -    | 42,56,74     | 1.64 | 9 (21%)  | 36,92,114   | 1.96 | 11 (30%) |
| 22  | CLA  | 8     | 305 | 15   | 64,68,73     | 1.40 | 6 (9%)   | 76,107,113  | 1.98 | 19 (25%) |
| 22  | CLA  | 3     | 318 | 13   | 64,68,73     | 1.39 | 6 (9%)   | 76,107,113  | 1.96 | 22 (28%) |
| 22  | CLA  | B     | 840 | 44   | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.88 | 18 (21%) |
| 22  | CLA  | 6     | 309 | 44   | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.97 | 20 (24%) |
| 27  | DGA  | A     | 852 | -    | 39,39,43     | 1.17 | 3 (7%)   | 41,41,45    | 1.34 | 3 (7%)   |
| 22  | CLA  | 1     | 315 | -    | 50,54,73     | 1.58 | 7 (14%)  | 59,90,113   | 2.06 | 15 (25%) |
| 24  | BCR  | B     | 845 | -    | 41,41,41     | 4.93 | 27 (65%) | 56,56,56    | 2.43 | 20 (35%) |
| 22  | CLA  | B     | 821 | 44   | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.89 | 18 (21%) |
| 22  | CLA  | 4     | 811 | 25   | 59,63,73     | 1.45 | 7 (11%)  | 70,101,113  | 2.05 | 19 (27%) |
| 22  | CLA  | B     | 827 | 44   | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.92 | 20 (24%) |
| 22  | CLA  | 6     | 308 | 18   | 56,60,73     | 1.49 | 5 (8%)   | 65,97,113   | 2.11 | 21 (32%) |
| 25  | LHG  | A     | 849 | 22   | 34,34,48     | 0.44 | 0        | 37,40,54    | 1.16 | 3 (8%)   |
| 22  | CLA  | A     | 821 | 44   | 69,73,73     | 1.35 | 5 (7%)   | 82,113,113  | 1.87 | 18 (21%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | PQN  | B     | 843 | -    | 34,34,34     | 0.39 | 0        | 43,45,45    | 1.18 | 4 (9%)   |
| 25  | LHG  | 1     | 317 | 22   | 42,42,48     | 0.46 | 1 (2%)   | 45,48,54    | 1.19 | 3 (6%)   |
| 38  | LUT  | 8     | 303 | -    | 42,43,43     | 6.39 | 26 (61%) | 51,60,60    | 2.08 | 16 (31%) |
| 22  | CLA  | A     | 837 | -    | 55,59,73     | 1.51 | 5 (9%)   | 64,96,113   | 2.09 | 19 (29%) |
| 29  | SF4  | C     | 102 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 22  | CLA  | 2     | 301 | -    | 59,63,73     | 1.45 | 6 (10%)  | 70,101,113  | 2.05 | 18 (25%) |
| 22  | CLA  | 9     | 305 | 19   | 64,68,73     | 1.46 | 8 (12%)  | 76,107,113  | 2.33 | 23 (30%) |
| 22  | CLA  | Z     | 310 | -    | 54,58,73     | 1.52 | 6 (11%)  | 64,95,113   | 2.06 | 20 (31%) |
| 38  | LUT  | 6     | 303 | -    | 42,43,43     | 6.43 | 25 (59%) | 51,60,60    | 2.03 | 17 (33%) |
| 22  | CLA  | 3     | 322 | 14   | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.87 | 19 (23%) |
| 22  | CLA  | 3     | 319 | -    | 59,63,73     | 1.46 | 6 (10%)  | 70,101,113  | 2.01 | 19 (27%) |
| 41  | 3PH  | 6     | 324 | -    | 28,28,47     | 1.11 | 4 (14%)  | 31,33,52    | 1.24 | 2 (6%)   |
| 22  | CLA  | A     | 831 | -    | 54,58,73     | 1.52 | 6 (11%)  | 64,95,113   | 2.10 | 19 (29%) |
| 22  | CLA  | 7     | 305 | -    | 54,58,73     | 1.53 | 7 (12%)  | 64,95,113   | 2.12 | 19 (29%) |
| 22  | CLA  | 4     | 812 | -    | 59,63,73     | 1.46 | 5 (8%)   | 70,101,113  | 2.04 | 20 (28%) |
| 39  | CHL  | 3     | 317 | -    | 60,74,74     | 1.28 | 8 (13%)  | 58,114,114  | 1.65 | 11 (18%) |
| 22  | CLA  | 4     | 815 | 16   | 54,58,73     | 1.52 | 6 (11%)  | 64,95,113   | 2.10 | 18 (28%) |
| 22  | CLA  | B     | 813 | -    | 60,64,73     | 1.44 | 7 (11%)  | 71,102,113  | 2.07 | 20 (28%) |
| 22  | CLA  | 5     | 322 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.87 | 19 (23%) |
| 22  | CLA  | 8     | 314 | 15   | 50,54,73     | 1.58 | 7 (14%)  | 59,90,113   | 2.01 | 16 (27%) |
| 22  | CLA  | 5     | 313 | 25   | 65,69,73     | 1.39 | 7 (10%)  | 77,108,113  | 1.97 | 19 (24%) |
| 22  | CLA  | 5     | 323 | 44   | 50,54,73     | 1.56 | 5 (10%)  | 59,90,113   | 2.12 | 16 (27%) |
| 24  | BCR  | 6     | 306 | -    | 41,41,41     | 4.91 | 27 (65%) | 56,56,56    | 2.83 | 22 (39%) |
| 22  | CLA  | Z     | 304 | 12   | 49,53,73     | 1.60 | 6 (12%)  | 58,89,113   | 2.00 | 14 (24%) |
| 22  | CLA  | 1     | 313 | 44   | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.93 | 21 (25%) |
| 38  | LUT  | 3     | 302 | -    | 42,43,43     | 6.38 | 26 (61%) | 51,60,60    | 2.12 | 15 (29%) |
| 22  | CLA  | 8     | 310 | 44   | 64,68,73     | 1.40 | 6 (9%)   | 76,107,113  | 1.98 | 19 (25%) |
| 22  | CLA  | 4     | 807 | 16   | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.94 | 20 (24%) |
| 22  | CLA  | 7     | 316 | 44   | 46,50,73     | 1.64 | 6 (13%)  | 53,85,113   | 2.13 | 16 (30%) |
| 24  | BCR  | B     | 849 | -    | 41,41,41     | 4.96 | 28 (68%) | 56,56,56    | 2.37 | 19 (33%) |
| 22  | CLA  | A     | 805 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.89 | 20 (24%) |
| 22  | CLA  | 4     | 809 | 16   | 55,59,73     | 1.52 | 6 (10%)  | 64,96,113   | 2.06 | 20 (31%) |
| 39  | CHL  | 2     | 303 | -    | 45,59,74     | 1.51 | 7 (15%)  | 40,96,114   | 1.96 | 11 (27%) |
| 22  | CLA  | 3     | 316 | 13   | 56,60,73     | 1.49 | 6 (10%)  | 65,97,113   | 2.04 | 19 (29%) |
| 22  | CLA  | A     | 811 | 22   | 69,73,73     | 1.34 | 7 (10%)  | 82,113,113  | 1.86 | 19 (23%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | 7     | 323  | 15   | 69,73,73     | 1.35 | 5 (7%)   | 82,113,113  | 1.91 | 21 (25%) |
| 22  | CLA  | L     | 201  | -    | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.92 | 19 (23%) |
| 22  | CLA  | 5     | 312  | 44   | 54,58,73     | 1.53 | 5 (9%)   | 64,95,113   | 2.06 | 19 (29%) |
| 39  | CHL  | Z     | 311  | 12   | 45,59,74     | 1.65 | 9 (20%)  | 40,96,114   | 2.00 | 13 (32%) |
| 22  | CLA  | B     | 811  | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.93 | 20 (24%) |
| 22  | CLA  | 6     | 317  | 18   | 54,58,73     | 1.53 | 6 (11%)  | 64,95,113   | 2.10 | 19 (29%) |
| 24  | BCR  | I     | 4001 | -    | 41,41,41     | 4.92 | 27 (65%) | 56,56,56    | 2.61 | 20 (35%) |
| 22  | CLA  | 5     | 301  | 44   | 60,64,73     | 1.44 | 5 (8%)   | 71,102,113  | 2.00 | 20 (28%) |
| 22  | CLA  | B     | 838  | -    | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.84 | 18 (21%) |
| 39  | CHL  | 8     | 315  | 44   | 60,74,74     | 1.20 | 7 (11%)  | 58,114,114  | 1.62 | 10 (17%) |
| 24  | BCR  | 3     | 307  | -    | 41,41,41     | 4.92 | 27 (65%) | 56,56,56    | 3.29 | 28 (50%) |
| 31  | DGD  | 3     | 301  | -    | 52,52,67     | 0.92 | 2 (3%)   | 66,66,81    | 1.07 | 4 (6%)   |
| 22  | CLA  | B     | 819  | -    | 63,67,73     | 1.41 | 6 (9%)   | 74,105,113  | 1.99 | 21 (28%) |
| 22  | CLA  | A     | 810  | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.88 | 18 (21%) |
| 24  | BCR  | 8     | 304  | -    | 41,41,41     | 4.94 | 27 (65%) | 56,56,56    | 2.46 | 21 (37%) |
| 22  | CLA  | 2     | 302  | -    | 49,53,73     | 1.59 | 5 (10%)  | 58,89,113   | 2.11 | 17 (29%) |
| 22  | CLA  | 9     | 306  | 19   | 66,70,73     | 1.38 | 6 (9%)   | 78,109,113  | 1.99 | 21 (26%) |
| 24  | BCR  | J     | 104  | -    | 41,41,41     | 4.91 | 27 (65%) | 56,56,56    | 2.43 | 20 (35%) |
| 24  | BCR  | B     | 844  | -    | 41,41,41     | 4.94 | 27 (65%) | 56,56,56    | 2.77 | 24 (42%) |
| 39  | CHL  | 5     | 317  | 44   | 45,59,74     | 1.33 | 7 (15%)  | 40,96,114   | 1.98 | 11 (27%) |
| 25  | LHG  | 6     | 323  | 22   | 48,48,48     | 0.38 | 0        | 51,54,54    | 1.10 | 4 (7%)   |
| 33  | LMT  | 1     | 301  | -    | 36,36,36     | 0.38 | 0        | 47,47,47    | 0.85 | 0        |
| 22  | CLA  | 7     | 322  | -    | 59,63,73     | 1.45 | 6 (10%)  | 70,101,113  | 2.00 | 20 (28%) |
| 22  | CLA  | L     | 203  | -    | 54,58,73     | 1.53 | 6 (11%)  | 64,95,113   | 2.09 | 18 (28%) |
| 43  | LPX  | 8     | 319  | -    | 29,29,29     | 0.30 | 0        | 31,33,33    | 0.35 | 0        |
| 38  | LUT  | 4     | 803  | -    | 42,43,43     | 6.38 | 26 (61%) | 51,60,60    | 2.28 | 14 (27%) |
| 22  | CLA  | B     | 817  | -    | 61,65,73     | 1.43 | 6 (9%)   | 72,103,113  | 1.99 | 18 (25%) |
| 41  | 3PH  | 7     | 319  | -    | 38,38,47     | 0.95 | 4 (10%)  | 41,43,52    | 1.15 | 2 (4%)   |
| 22  | CLA  | A     | 832  | -    | 69,73,73     | 1.34 | 5 (7%)   | 82,113,113  | 1.87 | 21 (25%) |
| 39  | CHL  | 4     | 813  | 44   | 45,59,74     | 1.59 | 8 (17%)  | 40,96,114   | 1.97 | 13 (32%) |
| 22  | CLA  | 1     | 311  | -    | 50,54,73     | 1.58 | 7 (14%)  | 59,90,113   | 2.14 | 13 (22%) |
| 22  | CLA  | A     | 814  | -    | 64,68,73     | 1.40 | 6 (9%)   | 76,107,113  | 1.98 | 20 (26%) |
| 22  | CLA  | B     | 823  | -    | 59,63,73     | 1.46 | 7 (11%)  | 70,101,113  | 2.01 | 21 (30%) |
| 22  | CLA  | 9     | 303  | 19   | 64,68,73     | 1.45 | 6 (9%)   | 76,107,113  | 2.03 | 20 (26%) |
| 22  | CLA  | 9     | 310  | -    | 49,53,73     | 1.60 | 7 (14%)  | 58,89,113   | 2.14 | 15 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | BCR  | 6     | 305 | -    | 41,41,41     | 4.93 | 27 (65%) | 56,56,56    | 2.52 | 20 (35%) |
| 22  | CLA  | A     | 808 | 1    | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.93 | 19 (23%) |
| 22  | CLA  | F     | 301 | 44   | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.93 | 21 (25%) |
| 25  | LHG  | 4     | 821 | -    | 31,31,48     | 0.48 | 0        | 34,37,54    | 1.21 | 3 (8%)   |
| 22  | CLA  | 5     | 309 | -    | 60,64,73     | 1.45 | 7 (11%)  | 71,102,113  | 2.12 | 22 (30%) |
| 39  | CHL  | 4     | 816 | 44   | 41,55,74     | 1.68 | 7 (17%)  | 35,91,114   | 2.06 | 10 (28%) |
| 22  | CLA  | F     | 305 | -    | 49,53,73     | 1.60 | 7 (14%)  | 58,89,113   | 2.02 | 16 (27%) |
| 22  | CLA  | 9     | 304 | -    | 49,53,73     | 1.61 | 6 (12%)  | 58,89,113   | 2.05 | 14 (24%) |
| 22  | CLA  | K     | 202 | -    | 50,54,73     | 1.59 | 6 (12%)  | 59,90,113   | 2.09 | 17 (28%) |
| 22  | CLA  | A     | 806 | 1    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.89 | 19 (23%) |
| 22  | CLA  | A     | 833 | -    | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.91 | 21 (25%) |
| 22  | CLA  | J     | 103 | 9    | 46,50,73     | 1.65 | 6 (13%)  | 53,85,113   | 2.11 | 16 (30%) |
| 22  | CLA  | B     | 818 | -    | 69,73,73     | 1.34 | 7 (10%)  | 82,113,113  | 1.88 | 19 (23%) |
| 24  | BCR  | B     | 847 | -    | 41,41,41     | 4.93 | 27 (65%) | 56,56,56    | 2.49 | 22 (39%) |
| 22  | CLA  | B     | 815 | -    | 69,73,73     | 1.36 | 5 (7%)   | 82,113,113  | 1.95 | 20 (24%) |
| 22  | CLA  | 6     | 314 | 18   | 69,73,73     | 1.34 | 5 (7%)   | 82,113,113  | 1.88 | 18 (21%) |
| 22  | CLA  | B     | 807 | -    | 49,53,73     | 1.59 | 7 (14%)  | 58,89,113   | 2.04 | 17 (29%) |
| 22  | CLA  | A     | 809 | 1    | 59,63,73     | 1.46 | 7 (11%)  | 70,101,113  | 2.04 | 21 (30%) |
| 22  | CLA  | Z     | 306 | 12   | 64,68,73     | 1.41 | 7 (10%)  | 76,107,113  | 1.96 | 19 (25%) |
| 24  | BCR  | 4     | 804 | -    | 41,41,41     | 4.96 | 27 (65%) | 56,56,56    | 2.27 | 21 (37%) |
| 23  | PQN  | A     | 843 | -    | 34,34,34     | 0.39 | 0        | 43,45,45    | 1.24 | 6 (13%)  |
| 22  | CLA  | A     | 822 | -    | 59,63,73     | 1.47 | 7 (11%)  | 70,101,113  | 2.08 | 19 (27%) |
| 22  | CLA  | 1     | 309 | -    | 65,69,73     | 1.38 | 7 (10%)  | 77,108,113  | 1.98 | 18 (23%) |
| 22  | CLA  | A     | 839 | -    | 55,59,73     | 1.52 | 7 (12%)  | 64,96,113   | 2.12 | 20 (31%) |
| 22  | CLA  | A     | 824 | -    | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.87 | 19 (23%) |
| 22  | CLA  | B     | 805 | -    | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.89 | 21 (25%) |
| 22  | CLA  | 8     | 308 | 15   | 66,70,73     | 1.37 | 6 (9%)   | 78,109,113  | 1.93 | 20 (25%) |
| 32  | RRX  | F     | 306 | -    | 42,42,42     | 5.17 | 24 (57%) | 56,58,58    | 2.61 | 20 (35%) |
| 38  | LUT  | 6     | 304 | -    | 42,43,43     | 6.39 | 26 (61%) | 51,60,60    | 2.16 | 15 (29%) |
| 38  | LUT  | 5     | 303 | -    | 42,43,43     | 6.43 | 27 (64%) | 51,60,60    | 2.11 | 14 (27%) |
| 22  | CLA  | 9     | 307 | 19   | 59,63,73     | 1.47 | 7 (11%)  | 70,101,113  | 1.96 | 18 (25%) |
| 22  | CLA  | B     | 822 | -    | 60,64,73     | 1.45 | 6 (10%)  | 71,102,113  | 1.96 | 19 (26%) |
| 24  | BCR  | G     | 203 | -    | 41,41,41     | 4.93 | 27 (65%) | 56,56,56    | 2.44 | 20 (35%) |
| 22  | CLA  | 7     | 311 | -    | 47,51,73     | 1.62 | 6 (12%)  | 55,86,113   | 2.11 | 16 (29%) |
| 22  | CLA  | F     | 302 | -    | 69,73,73     | 1.34 | 7 (10%)  | 82,113,113  | 1.90 | 22 (26%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 39  | CHL  | 6     | 315 | 44   | 50,64,74     | 1.36 | 8 (16%)  | 46,102,114  | 1.83 | 10 (21%) |
| 24  | BCR  | 3     | 304 | -    | 41,41,41     | 4.96 | 27 (65%) | 56,56,56    | 3.11 | 28 (50%) |
| 24  | BCR  | A     | 848 | -    | 41,41,41     | 4.92 | 27 (65%) | 56,56,56    | 2.43 | 20 (35%) |
| 25  | LHG  | B     | 851 | -    | 19,19,48     | 0.78 | 1 (5%)   | 20,24,54    | 1.38 | 1 (5%)   |
| 22  | CLA  | 1     | 316 | 12   | 69,73,73     | 1.41 | 7 (10%)  | 82,113,113  | 1.86 | 17 (20%) |
| 31  | DGD  | 1     | 319 | -    | 52,52,67     | 0.93 | 2 (3%)   | 66,66,81    | 0.98 | 4 (6%)   |
| 41  | 3PH  | 8     | 320 | -    | 29,29,47     | 1.08 | 4 (13%)  | 32,34,52    | 1.13 | 2 (6%)   |
| 24  | BCR  | A     | 844 | -    | 41,41,41     | 4.92 | 27 (65%) | 56,56,56    | 3.14 | 24 (42%) |
| 31  | DGD  | B     | 852 | -    | 62,62,67     | 1.22 | 6 (9%)   | 76,76,81    | 0.97 | 3 (3%)   |
| 22  | CLA  | 7     | 317 | -    | 62,66,73     | 1.42 | 7 (11%)  | 73,104,113  | 1.98 | 20 (27%) |
| 33  | LMT  | G     | 204 | -    | 36,36,36     | 0.39 | 0        | 47,47,47    | 0.75 | 2 (4%)   |
| 24  | BCR  | L     | 204 | -    | 41,41,41     | 4.92 | 27 (65%) | 56,56,56    | 2.38 | 19 (33%) |
| 38  | LUT  | Z     | 301 | -    | 42,43,43     | 6.39 | 27 (64%) | 51,60,60    | 2.07 | 14 (27%) |
| 26  | NKP  | 8     | 318 | -    | 28,28,28     | 0.33 | 0        | 30,32,32    | 0.34 | 0        |
| 39  | CHL  | 6     | 320 | 18   | 37,51,74     | 1.66 | 8 (21%)  | 30,86,114   | 2.14 | 9 (30%)  |
| 22  | CLA  | 4     | 818 | 44   | 55,59,73     | 1.51 | 5 (9%)   | 64,96,113   | 2.16 | 21 (32%) |
| 25  | LHG  | 9     | 315 | 22   | 32,32,48     | 0.49 | 0        | 35,38,54    | 1.06 | 3 (8%)   |
| 22  | CLA  | A     | 854 | -    | 69,73,73     | 1.34 | 5 (7%)   | 82,113,113  | 1.86 | 18 (21%) |
| 22  | CLA  | Z     | 303 | 12   | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.93 | 20 (24%) |
| 22  | CLA  | B     | 816 | -    | 64,68,73     | 1.40 | 6 (9%)   | 76,107,113  | 1.94 | 19 (25%) |
| 39  | CHL  | 9     | 314 | -    | 36,50,74     | 1.63 | 9 (25%)  | 29,85,114   | 2.17 | 9 (31%)  |
| 25  | LHG  | 8     | 317 | 22   | 37,37,48     | 0.43 | 0        | 40,43,54    | 1.05 | 2 (5%)   |
| 22  | CLA  | 7     | 310 | 25   | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.89 | 18 (21%) |
| 22  | CLA  | B     | 801 | -    | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.82 | 18 (21%) |
| 34  | LMG  | J     | 101 | -    | 29,29,55     | 0.54 | 0        | 37,37,63    | 1.14 | 3 (8%)   |
| 39  | CHL  | 8     | 301 | 12   | 52,66,74     | 1.48 | 9 (17%)  | 48,104,114  | 1.83 | 12 (25%) |
| 22  | CLA  | A     | 825 | 44   | 69,73,73     | 1.36 | 6 (8%)   | 82,113,113  | 1.92 | 20 (24%) |
| 22  | CLA  | B     | 837 | -    | 55,59,73     | 1.51 | 6 (10%)  | 64,96,113   | 2.14 | 19 (29%) |
| 22  | CLA  | 6     | 310 | 18   | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.88 | 20 (24%) |
| 22  | CLA  | A     | 823 | -    | 69,73,73     | 1.34 | 7 (10%)  | 82,113,113  | 1.92 | 19 (23%) |
| 22  | CLA  | 3     | 320 | 13   | 50,54,73     | 1.61 | 6 (12%)  | 59,90,113   | 2.12 | 15 (25%) |
| 22  | CLA  | A     | 830 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.89 | 18 (21%) |
| 22  | CLA  | 5     | 307 | 17   | 64,68,73     | 1.40 | 6 (9%)   | 76,107,113  | 1.97 | 18 (23%) |
| 22  | CLA  | 6     | 301 | 44   | 64,68,73     | 1.40 | 6 (9%)   | 76,107,113  | 1.99 | 20 (26%) |
| 24  | BCR  | K     | 206 | -    | 41,41,41     | 4.93 | 27 (65%) | 56,56,56    | 2.52 | 20 (35%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | CLA  | A     | 841 | -    | 69,73,73     | 1.34 | 6 (8%)   | 82,113,113  | 1.92 | 20 (24%) |
| 22  | CLA  | A     | 829 | -    | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.84 | 18 (21%) |
| 36  | C7Z  | 5     | 306 | -    | 43,43,43     | 5.42 | 27 (62%) | 56,60,60    | 2.41 | 18 (32%) |
| 22  | CLA  | F     | 304 | 6    | 69,73,73     | 1.34 | 5 (7%)   | 82,113,113  | 1.92 | 19 (23%) |
| 39  | CHL  | Z     | 312 | -    | 42,56,74     | 1.60 | 8 (19%)  | 36,92,114   | 1.96 | 10 (27%) |
| 33  | LMT  | 4     | 822 | -    | 36,36,36     | 0.45 | 0        | 47,47,47    | 1.19 | 4 (8%)   |
| 39  | CHL  | 9     | 312 | -    | 60,74,74     | 1.19 | 8 (13%)  | 58,114,114  | 1.73 | 12 (20%) |
| 22  | CLA  | 6     | 322 | 18   | 69,73,73     | 1.35 | 6 (8%)   | 82,113,113  | 1.92 | 19 (23%) |
| 22  | CLA  | A     | 836 | -    | 59,63,73     | 1.45 | 7 (11%)  | 70,101,113  | 2.00 | 21 (30%) |
| 22  | CLA  | A     | 855 | 44   | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.88 | 19 (23%) |
| 36  | C7Z  | J     | 105 | -    | 43,43,43     | 5.44 | 27 (62%) | 56,60,60    | 2.25 | 18 (32%) |
| 22  | CLA  | 9     | 311 | 19   | 50,54,73     | 1.58 | 6 (12%)  | 59,90,113   | 2.05 | 17 (28%) |
| 22  | CLA  | Z     | 305 | -    | 60,64,73     | 1.44 | 5 (8%)   | 71,102,113  | 1.99 | 17 (23%) |
| 22  | CLA  | 5     | 326 | -    | 59,63,73     | 1.45 | 6 (10%)  | 70,101,113  | 2.03 | 20 (28%) |
| 22  | CLA  | 8     | 307 | -    | 69,73,73     | 1.35 | 7 (10%)  | 82,113,113  | 1.96 | 18 (21%) |
| 22  | CLA  | 3     | 311 | 13   | 64,68,73     | 1.40 | 6 (9%)   | 76,107,113  | 1.95 | 21 (27%) |
| 22  | CLA  | Z     | 309 | 25   | 64,68,73     | 1.39 | 6 (9%)   | 76,107,113  | 1.95 | 18 (23%) |
| 22  | CLA  | 6     | 319 | 44   | 65,69,73     | 1.39 | 6 (9%)   | 77,108,113  | 1.97 | 19 (24%) |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24  | BCR  | 7     | 303 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 24  | BCR  | A     | 846 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | 1     | 314 | 12   | 1/1/15/20 | 12/39/115/115 | -       |
| 39  | CHL  | 8     | 312 | -    | 3/3/18/26 | 6/27/125/137  | -       |
| 25  | LHG  | 3     | 321 | 22   | -         | 9/22/22/53    | -       |
| 25  | LHG  | B     | 803 | -    | -         | 21/37/37/53   | -       |
| 24  | BCR  | B     | 848 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 22  | CLA  | A     | 815 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | A     | 803 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | 3     | 314 | 25   | 1/1/14/20 | 19/33/109/115 | -       |
| 22  | CLA  | Z     | 307 | -    | 1/1/13/20 | 10/27/103/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | B     | 830 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 38  | LUT  | 5     | 302 | -    | -         | 9/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 3     | 315 | -    | 1/1/11/20 | 7/15/91/115   | -       |
| 22  | CLA  | 1     | 305 | 12   | 1/1/11/20 | 6/15/91/115   | -       |
| 22  | CLA  | 7     | 314 | 44   | 1/1/12/20 | 5/21/97/115   | -       |
| 38  | LUT  | Z     | 302 | -    | -         | 7/29/67/67    | 0/2/2/2 |
| 38  | LUT  | 1     | 302 | -    | -         | 9/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 5     | 320 | -    | 1/1/12/20 | 7/21/97/115   | -       |
| 22  | CLA  | A     | 807 | -    | 1/1/14/20 | 16/33/109/115 | -       |
| 24  | BCR  | B     | 846 | -    | -         | 17/29/63/63   | 0/2/2/2 |
| 22  | CLA  | 7     | 324 | -    | 1/1/14/20 | 21/33/109/115 | -       |
| 22  | CLA  | 4     | 805 | 16   | 1/1/14/20 | 15/33/109/115 | -       |
| 22  | CLA  | 8     | 309 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | B     | 810 | -    | 1/1/13/20 | 9/29/105/115  | -       |
| 22  | CLA  | B     | 812 | 2    | 2/2/14/20 | 14/29/105/115 | -       |
| 22  | CLA  | 1     | 308 | -    | 1/1/13/20 | 13/27/103/115 | -       |
| 26  | NKP  | A     | 851 | -    | -         | 9/22/22/28    | -       |
| 24  | BCR  | B     | 853 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 22  | CLA  | 6     | 307 | 18   | 1/1/14/20 | 12/33/109/115 | -       |
| 22  | CLA  | B     | 832 | -    | 1/1/12/20 | 4/21/97/115   | -       |
| 24  | BCR  | 3     | 305 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 42  | SPH  | 7     | 320 | -    | -         | 11/21/21/21   | -       |
| 22  | CLA  | K     | 203 | 44   | 1/1/13/20 | 7/27/103/115  | -       |
| 25  | LHG  | 5     | 324 | 22   | -         | 23/41/41/53   | -       |
| 22  | CLA  | Z     | 314 | 12   | 1/1/12/20 | 6/23/99/115   | -       |
| 39  | CHL  | 7     | 313 | 44   | 3/3/17/26 | 5/25/123/137  | -       |
| 22  | CLA  | K     | 205 | 10   | 1/1/13/20 | 17/27/103/115 | -       |
| 22  | CLA  | 3     | 309 | 13   | 1/1/11/20 | 4/17/93/115   | -       |
| 22  | CLA  | 5     | 315 | 17   | 1/1/15/20 | 12/39/115/115 | -       |
| 24  | BCR  | A     | 845 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 38  | LUT  | 8     | 302 | -    | -         | 8/29/67/67    | 0/2/2/2 |
| 22  | CLA  | B     | 833 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | Z     | 315 | -    | 1/1/11/20 | 9/17/93/115   | -       |
| 39  | CHL  | 4     | 814 | 44   | 3/3/17/26 | 6/21/119/137  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | 7     | 304 | 14   | 1/1/14/20 | 11/33/109/115 | -       |
| 22  | CLA  | A     | 826 | 44   | 1/1/12/20 | 7/21/97/115   | -       |
| 22  | CLA  | G     | 201 | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 22  | CLA  | 6     | 312 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | A     | 827 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | 4     | 810 | 44   | 1/1/12/20 | 6/21/97/115   | -       |
| 22  | CLA  | 8     | 316 | 15   | 1/1/11/20 | 9/17/93/115   | -       |
| 22  | CLA  | 3     | 310 | 13   | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | 5     | 318 | 17   | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | A     | 828 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | A     | 802 | 44   | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | A     | 834 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | 8     | 313 | 44   | 1/1/12/20 | 5/21/97/115   | -       |
| 22  | CLA  | 3     | 312 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | 2     | 304 | 44   | 1/1/11/20 | 7/17/93/115   | -       |
| 39  | CHL  | 5     | 321 | 17   | 3/3/15/26 | 5/12/110/137  | -       |
| 22  | CLA  | 7     | 312 | -    | 1/1/14/20 | 16/33/109/115 | -       |
| 22  | CLA  | 5     | 308 | 17   | 1/1/14/20 | 16/35/111/115 | -       |
| 39  | CHL  | 4     | 819 | 16   | 3/3/15/26 | 2/12/110/137  | -       |
| 22  | CLA  | B     | 808 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | B     | 828 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | 7     | 306 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 38  | LUT  | 7     | 302 | -    | -         | 5/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 1     | 310 | 25   | 1/1/14/20 | 15/33/109/115 | -       |
| 22  | CLA  | A     | 840 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | 6     | 311 | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 38  | LUT  | 4     | 802 | -    | -         | 9/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 6     | 321 | -    | 1/1/11/20 | 4/17/93/115   | -       |
| 22  | CLA  | 7     | 308 | 14   | 1/1/14/20 | 14/35/111/115 | -       |
| 24  | BCR  | 5     | 305 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | B     | 809 | 2    | 1/1/15/20 | 16/39/115/115 | -       |
| 25  | LHG  | Z     | 317 | 22   | -         | 26/47/47/53   | -       |
| 35  | T7X  | J     | 102 | -    | -         | 15/44/68/80   | 0/1/1/1 |
| 22  | CLA  | 6     | 302 | 16   | 1/1/14/20 | 15/33/109/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 24  | BCR  | A     | 856 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 22  | CLA  | A     | 813 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 39  | CHL  | 6     | 318 | -    | 3/3/18/26 | 7/27/125/137  | -       |
| 22  | CLA  | 5     | 311 | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 38  | LUT  | 3     | 303 | -    | -         | 8/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 8     | 306 | 15   | 1/1/12/20 | 7/23/99/115   | -       |
| 22  | CLA  | Z     | 316 | 12   | 1/1/15/20 | 18/39/115/115 | -       |
| 25  | LHG  | 7     | 318 | 22   | -         | 24/41/41/53   | -       |
| 25  | LHG  | 4     | 820 | 22   | -         | 29/53/53/53   | -       |
| 22  | CLA  | 6     | 313 | 25   | 1/1/13/20 | 7/27/103/115  | -       |
| 22  | CLA  | 4     | 808 | 16   | 1/1/14/20 | 17/33/109/115 | -       |
| 22  | CLA  | 5     | 319 | 44   | 1/1/13/20 | 11/27/103/115 | -       |
| 22  | CLA  | 7     | 315 | 14   | 1/1/12/20 | 8/21/97/115   | -       |
| 22  | CLA  | B     | 826 | 44   | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | 9     | 309 | 25   | 1/1/13/20 | 6/27/103/115  | -       |
| 33  | LMT  | 4     | 801 | -    | -         | 1/21/61/61    | 0/2/2/2 |
| 38  | LUT  | 1     | 303 | -    | -         | 6/29/67/67    | 0/2/2/2 |
| 22  | CLA  | B     | 834 | -    | 1/1/13/20 | 15/31/107/115 | -       |
| 22  | CLA  | B     | 839 | -    | 1/1/12/20 | 8/24/100/115  | -       |
| 22  | CLA  | B     | 824 | -    | 1/1/13/20 | 17/32/108/115 | -       |
| 22  | CLA  | 3     | 313 | 44   | 1/1/15/20 | 14/39/115/115 | -       |
| 39  | CHL  | 6     | 316 | -    | 3/3/17/26 | 9/21/119/137  | -       |
| 42  | SPH  | 7     | 321 | -    | -         | 12/21/21/21   | -       |
| 22  | CLA  | A     | 842 | 25   | 1/1/12/20 | 10/24/100/115 | -       |
| 22  | CLA  | 8     | 311 | 25   | 1/1/12/20 | 8/21/97/115   | -       |
| 38  | LUT  | 7     | 301 | -    | -         | 9/29/67/67    | 0/2/2/2 |
| 22  | CLA  | A     | 838 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | 4     | 806 | 16   | 1/1/12/20 | 13/24/100/115 | -       |
| 22  | CLA  | G     | 202 | 7    | 1/1/11/20 | 8/17/93/115   | -       |
| 22  | CLA  | B     | 814 | -    | 1/1/14/20 | 17/33/109/115 | -       |
| 22  | CLA  | A     | 819 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | 1     | 307 | 12   | 1/1/14/20 | 17/33/109/115 | -       |
| 33  | LMT  | F     | 307 | -    | -         | 9/21/61/61    | 0/2/2/2 |
| 37  | DAO  | K     | 201 | -    | -         | 1/11/11/11    | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | 4     | 817 | 16   | 1/1/10/20 | 2/10/86/115   | -       |
| 22  | CLA  | B     | 831 | -    | 1/1/13/20 | 16/31/107/115 | -       |
| 22  | CLA  | 1     | 304 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 38  | LUT  | 9     | 302 | -    | -         | 4/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 5     | 314 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 22  | CLA  | B     | 825 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | 9     | 313 | 19   | 1/1/12/20 | 6/21/97/115   | -       |
| 22  | CLA  | 9     | 308 | -    | 1/1/12/20 | 8/21/97/115   | -       |
| 22  | CLA  | B     | 820 | -    | 1/1/14/20 | 16/33/109/115 | -       |
| 21  | CL0  | A     | 801 | -    | 3/3/20/25 | 15/37/135/135 | -       |
| 22  | CLA  | Z     | 313 | 44   | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | A     | 804 | 22   | 1/1/11/20 | 6/15/91/115   | -       |
| 22  | CLA  | A     | 817 | -    | 1/1/14/20 | 11/33/109/115 | -       |
| 22  | CLA  | A     | 812 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | K     | 204 | 10   | 1/1/11/20 | 10/20/96/115  | -       |
| 22  | CLA  | L     | 202 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | B     | 806 | 44   | 1/1/15/20 | 11/39/115/115 | -       |
| 29  | SF4  | C     | 101 | 3    | -         | -             | 0/6/5/5 |
| 24  | BCR  | F     | 303 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 41  | 3PH  | 5     | 325 | -    | -         | 5/24/24/49    | -       |
| 22  | CLA  | B     | 842 | 25   | 1/1/15/20 | 15/39/115/115 | -       |
| 40  | SQD  | 1     | 318 | -    | -         | 13/43/63/69   | 0/1/1/1 |
| 29  | SF4  | B     | 802 | -    | -         | -             | 0/6/5/5 |
| 22  | CLA  | 5     | 310 | 17   | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | 7     | 309 | -    | 1/1/13/20 | 12/29/105/115 | -       |
| 39  | CHL  | 5     | 316 | 44   | 3/3/20/26 | 13/39/137/137 | -       |
| 22  | CLA  | 7     | 307 | 14   | 1/1/15/20 | 12/39/115/115 | -       |
| 34  | LMG  | F     | 308 | -    | -         | 16/30/50/70   | 0/1/1/1 |
| 38  | LUT  | 9     | 301 | -    | -         | 4/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 3     | 308 | 13   | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | B     | 841 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | B     | 829 | -    | 1/1/13/20 | 13/30/106/115 | -       |
| 25  | LHG  | B     | 850 | 22   | -         | 16/26/26/53   | -       |
| 24  | BCR  | 3     | 306 | -    | -         | 13/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 28  | OCA  | A     | 853 | -    | -         | 3/7/7/7       | -       |
| 22  | CLA  | A     | 820 | -    | 1/1/14/20 | 19/33/109/115 | -       |
| 22  | CLA  | A     | 818 | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 22  | CLA  | 1     | 306 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | A     | 835 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 24  | BCR  | A     | 847 | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 25  | LHG  | A     | 850 | -    | -         | 28/53/53/53   | -       |
| 22  | CLA  | A     | 816 | 44   | 1/1/13/20 | 14/29/105/115 | -       |
| 24  | BCR  | 5     | 304 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 22  | CLA  | Z     | 308 | -    | 1/1/14/20 | 12/35/111/115 | -       |
| 22  | CLA  | B     | 836 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 22  | CLA  | B     | 835 | -    | 1/1/12/20 | 8/21/97/115   | -       |
| 39  | CHL  | 1     | 312 | -    | 3/3/16/26 | 2/18/116/137  | -       |
| 22  | CLA  | 8     | 305 | 15   | 1/1/14/20 | 12/33/109/115 | -       |
| 22  | CLA  | 3     | 318 | 13   | 1/1/14/20 | 10/33/109/115 | -       |
| 22  | CLA  | B     | 840 | 44   | 1/1/15/20 | 10/39/115/115 | -       |
| 22  | CLA  | 6     | 309 | 44   | 1/1/15/20 | 15/39/115/115 | -       |
| 27  | DGA  | A     | 852 | -    | -         | 23/41/41/45   | -       |
| 22  | CLA  | 1     | 315 | -    | 1/1/11/20 | 7/17/93/115   | -       |
| 24  | BCR  | B     | 845 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 22  | CLA  | B     | 821 | 44   | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | 4     | 811 | 25   | 1/1/13/20 | 8/27/103/115  | -       |
| 22  | CLA  | B     | 827 | 44   | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | 6     | 308 | 18   | 1/1/12/20 | 7/24/100/115  | -       |
| 25  | LHG  | A     | 849 | 22   | -         | 25/39/39/53   | -       |
| 22  | CLA  | A     | 821 | 44   | 1/1/15/20 | 10/39/115/115 | -       |
| 23  | PQN  | B     | 843 | -    | -         | 9/23/43/43    | 0/2/2/2 |
| 25  | LHG  | 1     | 317 | 22   | -         | 22/47/47/53   | -       |
| 22  | CLA  | A     | 837 | -    | 1/1/12/20 | 8/23/99/115   | -       |
| 38  | LUT  | 8     | 303 | -    | -         | 3/29/67/67    | 0/2/2/2 |
| 29  | SF4  | C     | 102 | 3    | -         | -             | 0/6/5/5 |
| 22  | CLA  | 2     | 301 | -    | 1/1/13/20 | 9/27/103/115  | -       |
| 22  | CLA  | 9     | 305 | 19   | 1/1/14/20 | 19/33/109/115 | -       |
| 22  | CLA  | Z     | 310 | -    | 1/1/12/20 | 8/21/97/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 38  | LUT  | 6     | 303  | -    | -         | 9/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 3     | 322  | 14   | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | 3     | 319  | -    | 1/1/13/20 | 7/27/103/115  | -       |
| 41  | 3PH  | 6     | 324  | -    | -         | 11/30/30/49   | -       |
| 22  | CLA  | A     | 831  | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 22  | CLA  | 7     | 305  | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 22  | CLA  | 4     | 812  | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 39  | CHL  | 3     | 317  | -    | 3/3/20/26 | 13/39/137/137 | -       |
| 22  | CLA  | 4     | 815  | 16   | 1/1/12/20 | 8/21/97/115   | -       |
| 22  | CLA  | B     | 813  | -    | 1/1/13/20 | 14/29/105/115 | -       |
| 22  | CLA  | 5     | 322  | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 22  | CLA  | 8     | 314  | 15   | 1/1/11/20 | 8/17/93/115   | -       |
| 22  | CLA  | 5     | 313  | 25   | 1/1/14/20 | 10/35/111/115 | -       |
| 22  | CLA  | 5     | 323  | 44   | 1/1/11/20 | 8/17/93/115   | -       |
| 24  | BCR  | 6     | 306  | -    | -         | 16/29/63/63   | 0/2/2/2 |
| 22  | CLA  | Z     | 304  | 12   | 1/1/11/20 | 6/15/91/115   | -       |
| 22  | CLA  | 1     | 313  | 44   | 1/1/15/20 | 12/39/115/115 | -       |
| 38  | LUT  | 3     | 302  | -    | -         | 4/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 8     | 310  | 44   | 1/1/14/20 | 13/33/109/115 | -       |
| 22  | CLA  | 4     | 807  | 16   | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | 7     | 316  | 44   | 1/1/10/20 | 4/12/88/115   | -       |
| 24  | BCR  | B     | 849  | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | A     | 805  | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | 4     | 809  | 16   | 1/1/12/20 | 4/23/99/115   | -       |
| 39  | CHL  | 2     | 303  | -    | 3/3/17/26 | 9/21/119/137  | -       |
| 22  | CLA  | 3     | 316  | 13   | 1/1/12/20 | 9/24/100/115  | -       |
| 22  | CLA  | A     | 811  | 22   | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | 7     | 323  | 15   | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | L     | 201  | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | 5     | 312  | 44   | 1/1/12/20 | 3/21/97/115   | -       |
| 39  | CHL  | Z     | 311  | 12   | 3/3/17/26 | 8/21/119/137  | -       |
| 22  | CLA  | B     | 811  | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | 6     | 317  | 18   | 1/1/12/20 | 10/21/97/115  | -       |
| 24  | BCR  | I     | 4001 | -    | -         | 13/29/63/63   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | 5     | 301 | 44   | 1/1/13/20 | 11/29/105/115 | -       |
| 22  | CLA  | B     | 838 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 39  | CHL  | 8     | 315 | 44   | 3/3/20/26 | 12/39/137/137 | -       |
| 24  | BCR  | 3     | 307 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 31  | DGD  | 3     | 301 | -    | -         | 12/40/80/95   | 0/2/2/2 |
| 22  | CLA  | B     | 819 | -    | 1/1/13/20 | 12/32/108/115 | -       |
| 22  | CLA  | A     | 810 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 24  | BCR  | 8     | 304 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 22  | CLA  | 2     | 302 | -    | 1/1/11/20 | 8/15/91/115   | -       |
| 22  | CLA  | 9     | 306 | 19   | 1/1/14/20 | 12/36/112/115 | -       |
| 24  | BCR  | J     | 104 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 24  | BCR  | B     | 844 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 39  | CHL  | 5     | 317 | 44   | 3/3/17/26 | 5/21/119/137  | -       |
| 25  | LHG  | 6     | 323 | 22   | -         | 38/53/53/53   | -       |
| 33  | LMT  | 1     | 301 | -    | -         | 4/21/61/61    | 0/2/2/2 |
| 22  | CLA  | 7     | 322 | -    | 1/1/13/20 | 7/27/103/115  | -       |
| 22  | CLA  | L     | 203 | -    | 1/1/12/20 | 7/21/97/115   | -       |
| 43  | LPX  | 8     | 319 | -    | -         | 4/31/31/31    | -       |
| 38  | LUT  | 4     | 803 | -    | -         | 8/29/67/67    | 0/2/2/2 |
| 22  | CLA  | B     | 817 | -    | 1/1/13/20 | 18/30/106/115 | -       |
| 41  | 3PH  | 7     | 319 | -    | -         | 18/40/40/49   | -       |
| 22  | CLA  | A     | 832 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 39  | CHL  | 4     | 813 | 44   | 3/3/17/26 | 4/21/119/137  | -       |
| 22  | CLA  | 1     | 311 | -    | 1/1/11/20 | 8/17/93/115   | -       |
| 22  | CLA  | A     | 814 | -    | 1/1/14/20 | 19/33/109/115 | -       |
| 22  | CLA  | B     | 823 | -    | 1/1/13/20 | 12/27/103/115 | -       |
| 22  | CLA  | 9     | 303 | 19   | 1/1/14/20 | 13/33/109/115 | -       |
| 22  | CLA  | 9     | 310 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 24  | BCR  | 6     | 305 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | A     | 808 | 1    | 1/1/15/20 | 19/39/115/115 | -       |
| 22  | CLA  | F     | 301 | 44   | 1/1/15/20 | 11/39/115/115 | -       |
| 25  | LHG  | 4     | 821 | -    | -         | 15/36/36/53   | -       |
| 22  | CLA  | 5     | 309 | -    | 1/1/13/20 | 15/29/105/115 | -       |
| 39  | CHL  | 4     | 816 | 44   | 3/3/16/26 | 4/17/115/137  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22  | CLA  | F     | 305 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 22  | CLA  | 9     | 304 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 22  | CLA  | K     | 202 | -    | 1/1/11/20 | 7/17/93/115   | -       |
| 22  | CLA  | A     | 806 | 1    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | A     | 833 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | J     | 103 | 9    | 1/1/10/20 | 3/12/88/115   | -       |
| 22  | CLA  | B     | 818 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 24  | BCR  | B     | 847 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 22  | CLA  | B     | 815 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 22  | CLA  | 6     | 314 | 18   | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | B     | 807 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 22  | CLA  | A     | 809 | 1    | 1/1/13/20 | 7/27/103/115  | -       |
| 22  | CLA  | Z     | 306 | 12   | 1/1/14/20 | 19/33/109/115 | -       |
| 24  | BCR  | 4     | 804 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 23  | PQN  | A     | 843 | -    | -         | 7/23/43/43    | 0/2/2/2 |
| 22  | CLA  | A     | 822 | -    | 1/1/13/20 | 12/27/103/115 | -       |
| 22  | CLA  | 1     | 309 | -    | 1/1/14/20 | 13/35/111/115 | -       |
| 22  | CLA  | A     | 839 | -    | 1/1/12/20 | 8/23/99/115   | -       |
| 22  | CLA  | A     | 824 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | B     | 805 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | 8     | 308 | 15   | 1/1/14/20 | 14/36/112/115 | -       |
| 32  | RRX  | F     | 306 | -    | -         | 15/29/65/65   | 0/2/2/2 |
| 38  | LUT  | 6     | 304 | -    | -         | 6/29/67/67    | 0/2/2/2 |
| 38  | LUT  | 5     | 303 | -    | -         | 6/29/67/67    | 0/2/2/2 |
| 22  | CLA  | 9     | 307 | 19   | 1/1/13/20 | 10/27/103/115 | -       |
| 22  | CLA  | B     | 822 | -    | 1/1/13/20 | 14/29/105/115 | -       |
| 24  | BCR  | G     | 203 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 22  | CLA  | 7     | 311 | -    | 1/1/10/20 | 5/13/89/115   | -       |
| 22  | CLA  | F     | 302 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 39  | CHL  | 6     | 315 | 44   | 3/3/18/26 | 10/27/125/137 | -       |
| 24  | BCR  | 3     | 304 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 24  | BCR  | A     | 848 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 25  | LHG  | B     | 851 | -    | -         | 14/22/22/53   | -       |
| 22  | CLA  | 1     | 316 | 12   | 1/1/15/20 | 19/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | DGD  | 1     | 319 | -    | -         | 13/40/80/95   | 0/2/2/2 |
| 41  | 3PH  | 8     | 320 | -    | -         | 13/31/31/49   | -       |
| 24  | BCR  | A     | 844 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 31  | DGD  | B     | 852 | -    | -         | 11/50/90/95   | 0/2/2/2 |
| 22  | CLA  | 7     | 317 | -    | 1/1/13/20 | 13/31/107/115 | -       |
| 33  | LMT  | G     | 204 | -    | -         | 8/21/61/61    | 0/2/2/2 |
| 24  | BCR  | L     | 204 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 38  | LUT  | Z     | 301 | -    | -         | 7/29/67/67    | 0/2/2/2 |
| 26  | NKP  | 8     | 318 | -    | -         | 7/28/28/28    | -       |
| 39  | CHL  | 6     | 320 | 18   | 3/3/15/26 | 2/12/110/137  | -       |
| 22  | CLA  | 4     | 818 | 44   | 1/1/12/20 | 11/23/99/115  | -       |
| 25  | LHG  | 9     | 315 | 22   | -         | 20/37/37/53   | -       |
| 22  | CLA  | A     | 854 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 22  | CLA  | Z     | 303 | 12   | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | B     | 816 | -    | 1/1/14/20 | 11/33/109/115 | -       |
| 39  | CHL  | 9     | 314 | -    | 3/3/15/26 | 2/10/108/137  | -       |
| 25  | LHG  | 8     | 317 | 22   | -         | 26/42/42/53   | -       |
| 22  | CLA  | 7     | 310 | 25   | 1/1/15/20 | 17/39/115/115 | -       |
| 22  | CLA  | B     | 801 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 34  | LMG  | J     | 101 | -    | -         | 7/24/44/70    | 0/1/1/1 |
| 39  | CHL  | 8     | 301 | 12   | 3/3/18/26 | 4/30/128/137  | -       |
| 22  | CLA  | A     | 825 | 44   | 1/1/15/20 | 14/39/115/115 | -       |
| 22  | CLA  | B     | 837 | -    | 1/1/12/20 | 8/23/99/115   | -       |
| 22  | CLA  | 6     | 310 | 18   | 1/1/15/20 | 16/39/115/115 | -       |
| 22  | CLA  | A     | 823 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 22  | CLA  | 3     | 320 | 13   | 1/1/11/20 | 7/17/93/115   | -       |
| 22  | CLA  | A     | 830 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | 5     | 307 | 17   | 1/1/14/20 | 14/33/109/115 | -       |
| 22  | CLA  | 6     | 301 | 44   | 1/1/14/20 | 16/33/109/115 | -       |
| 24  | BCR  | K     | 206 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 22  | CLA  | A     | 841 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 22  | CLA  | A     | 829 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 36  | C7Z  | 5     | 306 | -    | -         | 13/29/67/67   | 0/2/2/2 |
| 22  | CLA  | F     | 304 | 6    | 1/1/15/20 | 22/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 39  | CHL  | Z     | 312 | -    | 3/3/16/26 | 7/18/116/137  | -       |
| 33  | LMT  | 4     | 822 | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 39  | CHL  | 9     | 312 | -    | 3/3/20/26 | 14/39/137/137 | -       |
| 22  | CLA  | 6     | 322 | 18   | 1/1/15/20 | 15/39/115/115 | -       |
| 22  | CLA  | A     | 836 | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 22  | CLA  | A     | 855 | 44   | 1/1/15/20 | 16/39/115/115 | -       |
| 36  | C7Z  | J     | 105 | -    | -         | 12/29/67/67   | 0/2/2/2 |
| 22  | CLA  | 9     | 311 | 19   | 1/1/11/20 | 5/17/93/115   | -       |
| 22  | CLA  | Z     | 305 | -    | 1/1/13/20 | 10/29/105/115 | -       |
| 22  | CLA  | 5     | 326 | -    | 1/1/13/20 | 8/27/103/115  | -       |
| 22  | CLA  | 8     | 307 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 22  | CLA  | 3     | 311 | 13   | 1/1/14/20 | 11/33/109/115 | -       |
| 22  | CLA  | Z     | 309 | 25   | 1/1/14/20 | 16/33/109/115 | -       |
| 22  | CLA  | 6     | 319 | 44   | 1/1/14/20 | 16/35/111/115 | -       |

All (2908) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 38  | 6     | 303 | LUT  | C24-C25 | 24.55 | 1.62        | 1.33     |
| 38  | 5     | 303 | LUT  | C24-C25 | 24.53 | 1.62        | 1.33     |
| 38  | 1     | 302 | LUT  | C24-C25 | 24.50 | 1.62        | 1.33     |
| 38  | 7     | 302 | LUT  | C24-C25 | 24.42 | 1.62        | 1.33     |
| 38  | Z     | 302 | LUT  | C24-C25 | 24.41 | 1.62        | 1.33     |
| 38  | 6     | 304 | LUT  | C24-C25 | 24.37 | 1.62        | 1.33     |
| 38  | 5     | 302 | LUT  | C24-C25 | 24.35 | 1.62        | 1.33     |
| 38  | 4     | 803 | LUT  | C24-C25 | 24.34 | 1.62        | 1.33     |
| 38  | 1     | 303 | LUT  | C24-C25 | 24.32 | 1.62        | 1.33     |
| 38  | 9     | 302 | LUT  | C24-C25 | 24.32 | 1.62        | 1.33     |
| 38  | 9     | 301 | LUT  | C24-C25 | 24.31 | 1.62        | 1.33     |
| 38  | 8     | 303 | LUT  | C24-C25 | 24.26 | 1.62        | 1.33     |
| 38  | 3     | 303 | LUT  | C24-C25 | 24.25 | 1.61        | 1.33     |
| 38  | 4     | 802 | LUT  | C24-C25 | 24.23 | 1.61        | 1.33     |
| 38  | 3     | 302 | LUT  | C24-C25 | 24.22 | 1.61        | 1.33     |
| 38  | Z     | 301 | LUT  | C24-C25 | 24.18 | 1.61        | 1.33     |
| 38  | 7     | 301 | LUT  | C24-C25 | 24.04 | 1.61        | 1.33     |
| 38  | 8     | 302 | LUT  | C24-C25 | 23.86 | 1.61        | 1.33     |
| 36  | J     | 105 | C7Z  | C25-C26 | 16.33 | 1.61        | 1.34     |
| 32  | F     | 306 | RRX  | C26-C25 | 16.29 | 1.61        | 1.34     |
| 36  | 5     | 306 | C7Z  | C25-C26 | 16.24 | 1.61        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | 5     | 305  | BCR  | C26-C25 | 16.08 | 1.61        | 1.34     |
| 24  | B     | 848  | BCR  | C26-C25 | 16.05 | 1.61        | 1.34     |
| 24  | 6     | 306  | BCR  | C26-C25 | 16.02 | 1.61        | 1.34     |
| 24  | F     | 303  | BCR  | C26-C25 | 15.99 | 1.61        | 1.34     |
| 24  | 7     | 303  | BCR  | C26-C25 | 15.96 | 1.61        | 1.34     |
| 24  | A     | 846  | BCR  | C26-C25 | 15.93 | 1.61        | 1.34     |
| 24  | 3     | 304  | BCR  | C26-C25 | 15.92 | 1.61        | 1.34     |
| 24  | 4     | 804  | BCR  | C26-C25 | 15.92 | 1.61        | 1.34     |
| 24  | 6     | 305  | BCR  | C26-C25 | 15.90 | 1.61        | 1.34     |
| 24  | 8     | 304  | BCR  | C26-C25 | 15.89 | 1.61        | 1.34     |
| 24  | B     | 844  | BCR  | C26-C25 | 15.88 | 1.61        | 1.34     |
| 24  | B     | 846  | BCR  | C26-C25 | 15.87 | 1.61        | 1.34     |
| 24  | A     | 847  | BCR  | C26-C25 | 15.86 | 1.61        | 1.34     |
| 24  | G     | 203  | BCR  | C26-C25 | 15.83 | 1.61        | 1.34     |
| 24  | B     | 853  | BCR  | C26-C25 | 15.82 | 1.61        | 1.34     |
| 24  | A     | 848  | BCR  | C26-C25 | 15.78 | 1.61        | 1.34     |
| 24  | 3     | 307  | BCR  | C26-C25 | 15.78 | 1.61        | 1.34     |
| 24  | A     | 845  | BCR  | C26-C25 | 15.76 | 1.60        | 1.34     |
| 38  | 4     | 802  | LUT  | C5-C6   | 15.76 | 1.60        | 1.34     |
| 24  | L     | 204  | BCR  | C26-C25 | 15.75 | 1.60        | 1.34     |
| 38  | 6     | 303  | LUT  | C5-C6   | 15.75 | 1.60        | 1.34     |
| 24  | B     | 849  | BCR  | C26-C25 | 15.73 | 1.60        | 1.34     |
| 38  | 5     | 303  | LUT  | C5-C6   | 15.72 | 1.60        | 1.34     |
| 24  | 3     | 306  | BCR  | C26-C25 | 15.72 | 1.60        | 1.34     |
| 38  | 1     | 302  | LUT  | C5-C6   | 15.69 | 1.60        | 1.34     |
| 38  | 9     | 302  | LUT  | C5-C6   | 15.67 | 1.60        | 1.34     |
| 38  | 7     | 301  | LUT  | C5-C6   | 15.66 | 1.60        | 1.34     |
| 38  | Z     | 301  | LUT  | C5-C6   | 15.65 | 1.60        | 1.34     |
| 38  | 9     | 301  | LUT  | C5-C6   | 15.63 | 1.60        | 1.34     |
| 24  | K     | 206  | BCR  | C26-C25 | 15.63 | 1.60        | 1.34     |
| 24  | 3     | 305  | BCR  | C26-C25 | 15.62 | 1.60        | 1.34     |
| 38  | 7     | 302  | LUT  | C5-C6   | 15.61 | 1.60        | 1.34     |
| 38  | 8     | 302  | LUT  | C5-C6   | 15.60 | 1.60        | 1.34     |
| 24  | B     | 847  | BCR  | C26-C25 | 15.59 | 1.60        | 1.34     |
| 38  | 6     | 304  | LUT  | C5-C6   | 15.57 | 1.60        | 1.34     |
| 38  | Z     | 302  | LUT  | C5-C6   | 15.56 | 1.60        | 1.34     |
| 24  | I     | 4001 | BCR  | C26-C25 | 15.56 | 1.60        | 1.34     |
| 24  | B     | 845  | BCR  | C26-C25 | 15.55 | 1.60        | 1.34     |
| 38  | 8     | 303  | LUT  | C5-C6   | 15.55 | 1.60        | 1.34     |
| 24  | A     | 844  | BCR  | C26-C25 | 15.55 | 1.60        | 1.34     |
| 36  | J     | 105  | C7Z  | C5-C6   | 15.54 | 1.60        | 1.34     |
| 24  | 5     | 304  | BCR  | C26-C25 | 15.54 | 1.60        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 38  | 5     | 302  | LUT  | C5-C6   | 15.53  | 1.60        | 1.34     |
| 38  | 3     | 302  | LUT  | C5-C6   | 15.53  | 1.60        | 1.34     |
| 38  | 3     | 303  | LUT  | C5-C6   | 15.51  | 1.60        | 1.34     |
| 38  | 1     | 303  | LUT  | C5-C6   | 15.51  | 1.60        | 1.34     |
| 38  | 4     | 803  | LUT  | C5-C6   | 15.47  | 1.60        | 1.34     |
| 24  | A     | 856  | BCR  | C26-C25 | 15.46  | 1.60        | 1.34     |
| 24  | J     | 104  | BCR  | C26-C25 | 15.45  | 1.60        | 1.34     |
| 36  | 5     | 306  | C7Z  | C5-C6   | 15.36  | 1.60        | 1.34     |
| 32  | F     | 306  | RRX  | C5-C6   | 14.82  | 1.59        | 1.34     |
| 24  | 3     | 304  | BCR  | C5-C6   | 14.64  | 1.59        | 1.34     |
| 24  | B     | 849  | BCR  | C5-C6   | 14.63  | 1.59        | 1.34     |
| 24  | 4     | 804  | BCR  | C5-C6   | 14.63  | 1.59        | 1.34     |
| 24  | F     | 303  | BCR  | C5-C6   | 14.53  | 1.58        | 1.34     |
| 24  | A     | 844  | BCR  | C5-C6   | 14.51  | 1.58        | 1.34     |
| 24  | B     | 853  | BCR  | C5-C6   | 14.50  | 1.58        | 1.34     |
| 24  | A     | 847  | BCR  | C5-C6   | 14.50  | 1.58        | 1.34     |
| 24  | B     | 847  | BCR  | C5-C6   | 14.48  | 1.58        | 1.34     |
| 24  | 3     | 305  | BCR  | C5-C6   | 14.46  | 1.58        | 1.34     |
| 24  | A     | 846  | BCR  | C5-C6   | 14.45  | 1.58        | 1.34     |
| 24  | B     | 844  | BCR  | C5-C6   | 14.44  | 1.58        | 1.34     |
| 24  | G     | 203  | BCR  | C5-C6   | 14.42  | 1.58        | 1.34     |
| 24  | K     | 206  | BCR  | C5-C6   | 14.41  | 1.58        | 1.34     |
| 24  | B     | 846  | BCR  | C5-C6   | 14.41  | 1.58        | 1.34     |
| 24  | 5     | 304  | BCR  | C5-C6   | 14.39  | 1.58        | 1.34     |
| 24  | 6     | 305  | BCR  | C5-C6   | 14.38  | 1.58        | 1.34     |
| 24  | 5     | 305  | BCR  | C5-C6   | 14.36  | 1.58        | 1.34     |
| 24  | A     | 856  | BCR  | C5-C6   | 14.35  | 1.58        | 1.34     |
| 24  | 6     | 306  | BCR  | C5-C6   | 14.33  | 1.58        | 1.34     |
| 24  | B     | 845  | BCR  | C5-C6   | 14.30  | 1.58        | 1.34     |
| 24  | B     | 848  | BCR  | C5-C6   | 14.29  | 1.58        | 1.34     |
| 24  | J     | 104  | BCR  | C5-C6   | 14.24  | 1.58        | 1.34     |
| 24  | I     | 4001 | BCR  | C5-C6   | 14.22  | 1.58        | 1.34     |
| 24  | 3     | 306  | BCR  | C5-C6   | 14.22  | 1.58        | 1.34     |
| 24  | A     | 845  | BCR  | C5-C6   | 14.21  | 1.58        | 1.34     |
| 24  | 8     | 304  | BCR  | C5-C6   | 14.14  | 1.58        | 1.34     |
| 24  | L     | 204  | BCR  | C5-C6   | 14.13  | 1.58        | 1.34     |
| 24  | A     | 848  | BCR  | C5-C6   | 14.09  | 1.58        | 1.34     |
| 24  | 3     | 307  | BCR  | C5-C6   | 14.08  | 1.58        | 1.34     |
| 24  | 7     | 303  | BCR  | C5-C6   | 14.05  | 1.58        | 1.34     |
| 38  | 4     | 802  | LUT  | C22-C21 | -13.44 | 1.38        | 1.54     |
| 38  | 5     | 302  | LUT  | C22-C21 | -13.42 | 1.38        | 1.54     |
| 38  | 5     | 303  | LUT  | C22-C21 | -13.41 | 1.38        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 38  | 6     | 303 | LUT  | C22-C21 | -13.39 | 1.38        | 1.54     |
| 38  | 4     | 803 | LUT  | C22-C21 | -13.33 | 1.38        | 1.54     |
| 38  | 8     | 303 | LUT  | C22-C21 | -13.33 | 1.38        | 1.54     |
| 38  | 6     | 304 | LUT  | C22-C21 | -13.28 | 1.38        | 1.54     |
| 38  | Z     | 302 | LUT  | C22-C21 | -13.27 | 1.38        | 1.54     |
| 38  | 7     | 301 | LUT  | C22-C21 | -13.22 | 1.38        | 1.54     |
| 38  | 9     | 302 | LUT  | C22-C21 | -13.20 | 1.38        | 1.54     |
| 38  | 7     | 302 | LUT  | C22-C21 | -13.19 | 1.38        | 1.54     |
| 38  | 1     | 303 | LUT  | C22-C21 | -13.18 | 1.38        | 1.54     |
| 38  | 9     | 301 | LUT  | C22-C21 | -13.17 | 1.38        | 1.54     |
| 38  | 3     | 303 | LUT  | C22-C21 | -13.17 | 1.38        | 1.54     |
| 38  | 1     | 302 | LUT  | C22-C21 | -13.14 | 1.38        | 1.54     |
| 38  | 3     | 302 | LUT  | C22-C21 | -13.06 | 1.38        | 1.54     |
| 38  | Z     | 301 | LUT  | C22-C21 | -12.99 | 1.38        | 1.54     |
| 38  | 8     | 302 | LUT  | C22-C21 | -12.86 | 1.39        | 1.54     |
| 38  | 1     | 303 | LUT  | C22-C23 | 12.35  | 1.66        | 1.52     |
| 38  | 3     | 302 | LUT  | C22-C23 | 12.24  | 1.66        | 1.52     |
| 38  | 6     | 303 | LUT  | C22-C23 | 12.13  | 1.66        | 1.52     |
| 38  | 8     | 302 | LUT  | C22-C23 | 12.12  | 1.66        | 1.52     |
| 38  | Z     | 301 | LUT  | C22-C23 | 12.08  | 1.66        | 1.52     |
| 38  | 7     | 301 | LUT  | C22-C23 | 12.05  | 1.66        | 1.52     |
| 38  | 9     | 302 | LUT  | C22-C23 | 12.04  | 1.66        | 1.52     |
| 38  | 5     | 303 | LUT  | C22-C23 | 12.02  | 1.66        | 1.52     |
| 38  | 8     | 303 | LUT  | C22-C23 | 11.99  | 1.66        | 1.52     |
| 38  | 7     | 302 | LUT  | C22-C23 | 11.99  | 1.66        | 1.52     |
| 38  | 4     | 803 | LUT  | C22-C23 | 11.98  | 1.66        | 1.52     |
| 38  | Z     | 302 | LUT  | C22-C23 | 11.94  | 1.66        | 1.52     |
| 38  | 6     | 304 | LUT  | C22-C23 | 11.93  | 1.66        | 1.52     |
| 38  | 1     | 302 | LUT  | C22-C23 | 11.86  | 1.66        | 1.52     |
| 38  | 5     | 302 | LUT  | C22-C23 | 11.85  | 1.66        | 1.52     |
| 38  | 9     | 301 | LUT  | C22-C23 | 11.83  | 1.66        | 1.52     |
| 38  | 3     | 303 | LUT  | C22-C23 | 11.82  | 1.66        | 1.52     |
| 38  | 4     | 802 | LUT  | C22-C23 | 11.81  | 1.66        | 1.52     |
| 36  | J     | 105 | C7Z  | C24-C23 | 11.57  | 1.72        | 1.52     |
| 36  | 5     | 306 | C7Z  | C24-C23 | 11.53  | 1.72        | 1.52     |
| 38  | 4     | 802 | LUT  | C2-C3   | -11.43 | 1.36        | 1.52     |
| 38  | 7     | 301 | LUT  | C2-C3   | -11.26 | 1.36        | 1.52     |
| 38  | 9     | 301 | LUT  | C2-C3   | -11.23 | 1.36        | 1.52     |
| 38  | 5     | 302 | LUT  | C2-C3   | -11.21 | 1.36        | 1.52     |
| 38  | 9     | 302 | LUT  | C2-C3   | -11.20 | 1.36        | 1.52     |
| 38  | 3     | 302 | LUT  | C2-C3   | -11.20 | 1.36        | 1.52     |
| 38  | 8     | 302 | LUT  | C2-C3   | -11.19 | 1.36        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 36  | J     | 105 | C7Z  | C22-C23 | -11.18 | 1.36        | 1.52     |
| 38  | 5     | 303 | LUT  | C2-C3   | -11.18 | 1.36        | 1.52     |
| 38  | 3     | 303 | LUT  | C2-C3   | -11.14 | 1.36        | 1.52     |
| 36  | 5     | 306 | C7Z  | C22-C23 | -11.12 | 1.36        | 1.52     |
| 38  | 1     | 302 | LUT  | C2-C3   | -11.11 | 1.36        | 1.52     |
| 38  | 7     | 302 | LUT  | C2-C3   | -11.09 | 1.36        | 1.52     |
| 38  | 4     | 803 | LUT  | C2-C3   | -11.05 | 1.36        | 1.52     |
| 38  | 6     | 304 | LUT  | C2-C3   | -11.03 | 1.36        | 1.52     |
| 38  | 1     | 303 | LUT  | C2-C3   | -11.01 | 1.36        | 1.52     |
| 38  | Z     | 302 | LUT  | C2-C3   | -11.01 | 1.36        | 1.52     |
| 38  | 8     | 303 | LUT  | C2-C3   | -11.01 | 1.36        | 1.52     |
| 38  | Z     | 301 | LUT  | C2-C3   | -10.98 | 1.36        | 1.52     |
| 38  | 6     | 303 | LUT  | C2-C3   | -10.95 | 1.36        | 1.52     |
| 32  | F     | 306 | RRX  | C29-C28 | -10.80 | 1.37        | 1.52     |
| 36  | J     | 105 | C7Z  | C2-C3   | -10.00 | 1.38        | 1.52     |
| 36  | 5     | 306 | C7Z  | C2-C3   | -9.98  | 1.38        | 1.52     |
| 21  | A     | 801 | CL0  | C1A-CHA | 9.44   | 1.50        | 1.40     |
| 21  | A     | 801 | CL0  | C1D-C2D | 9.36   | 1.50        | 1.39     |
| 21  | A     | 801 | CL0  | C1B-C2B | 9.25   | 1.50        | 1.39     |
| 36  | 5     | 306 | C7Z  | C4-C3   | 8.47   | 1.67        | 1.52     |
| 36  | J     | 105 | C7Z  | C4-C3   | 8.40   | 1.67        | 1.52     |
| 32  | F     | 306 | RRX  | C27-C28 | 7.98   | 1.66        | 1.52     |
| 38  | 3     | 302 | LUT  | C4-C3   | 7.95   | 1.66        | 1.52     |
| 38  | 1     | 302 | LUT  | C4-C3   | 7.95   | 1.66        | 1.52     |
| 38  | Z     | 301 | LUT  | C4-C3   | 7.89   | 1.66        | 1.52     |
| 38  | 1     | 303 | LUT  | C4-C3   | 7.89   | 1.66        | 1.52     |
| 38  | 6     | 303 | LUT  | C4-C3   | 7.85   | 1.66        | 1.52     |
| 38  | Z     | 302 | LUT  | C4-C3   | 7.83   | 1.66        | 1.52     |
| 38  | 8     | 302 | LUT  | C4-C3   | 7.81   | 1.65        | 1.52     |
| 38  | 5     | 303 | LUT  | C4-C3   | 7.80   | 1.65        | 1.52     |
| 38  | 5     | 302 | LUT  | C4-C3   | 7.80   | 1.65        | 1.52     |
| 38  | 9     | 301 | LUT  | C4-C3   | 7.79   | 1.65        | 1.52     |
| 38  | 6     | 304 | LUT  | C4-C3   | 7.78   | 1.65        | 1.52     |
| 38  | 3     | 303 | LUT  | C4-C3   | 7.76   | 1.65        | 1.52     |
| 38  | 8     | 303 | LUT  | C4-C3   | 7.75   | 1.65        | 1.52     |
| 38  | 7     | 301 | LUT  | C4-C3   | 7.74   | 1.65        | 1.52     |
| 38  | 7     | 302 | LUT  | C4-C3   | 7.72   | 1.65        | 1.52     |
| 38  | 4     | 803 | LUT  | C4-C3   | 7.71   | 1.65        | 1.52     |
| 38  | 4     | 802 | LUT  | C4-C3   | 7.66   | 1.65        | 1.52     |
| 24  | 3     | 306 | BCR  | C30-C25 | -7.64  | 1.44        | 1.53     |
| 38  | Z     | 301 | LUT  | C32-C33 | 7.64   | 1.62        | 1.46     |
| 24  | 5     | 304 | BCR  | C30-C25 | -7.63  | 1.44        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | B     | 845  | BCR  | C30-C25 | -7.56 | 1.44        | 1.53     |
| 24  | L     | 204  | BCR  | C30-C25 | -7.56 | 1.44        | 1.53     |
| 38  | 9     | 302  | LUT  | C4-C3   | 7.55  | 1.65        | 1.52     |
| 24  | B     | 847  | BCR  | C30-C25 | -7.54 | 1.44        | 1.53     |
| 24  | A     | 844  | BCR  | C30-C25 | -7.54 | 1.44        | 1.53     |
| 24  | I     | 4001 | BCR  | C30-C25 | -7.54 | 1.44        | 1.53     |
| 38  | 7     | 302  | LUT  | C32-C33 | 7.52  | 1.62        | 1.46     |
| 38  | 1     | 303  | LUT  | C32-C33 | 7.51  | 1.62        | 1.46     |
| 38  | 1     | 302  | LUT  | C32-C33 | 7.51  | 1.62        | 1.46     |
| 24  | A     | 847  | BCR  | C30-C25 | -7.51 | 1.44        | 1.53     |
| 38  | 5     | 303  | LUT  | C32-C33 | 7.49  | 1.62        | 1.46     |
| 38  | Z     | 302  | LUT  | C32-C33 | 7.49  | 1.62        | 1.46     |
| 24  | K     | 206  | BCR  | C30-C25 | -7.47 | 1.44        | 1.53     |
| 38  | 7     | 301  | LUT  | C32-C33 | 7.45  | 1.61        | 1.46     |
| 38  | 6     | 304  | LUT  | C32-C33 | 7.44  | 1.61        | 1.46     |
| 38  | 3     | 303  | LUT  | C32-C33 | 7.44  | 1.61        | 1.46     |
| 38  | 6     | 303  | LUT  | C32-C33 | 7.42  | 1.61        | 1.46     |
| 38  | 3     | 302  | LUT  | C32-C33 | 7.42  | 1.61        | 1.46     |
| 38  | 9     | 301  | LUT  | C32-C33 | 7.41  | 1.61        | 1.46     |
| 24  | 8     | 304  | BCR  | C1-C6   | -7.41 | 1.44        | 1.53     |
| 24  | 3     | 305  | BCR  | C30-C25 | -7.40 | 1.44        | 1.53     |
| 24  | I     | 4001 | BCR  | C1-C6   | -7.40 | 1.44        | 1.53     |
| 38  | 4     | 802  | LUT  | C32-C33 | 7.39  | 1.61        | 1.46     |
| 38  | 8     | 303  | LUT  | C32-C33 | 7.38  | 1.61        | 1.46     |
| 38  | 9     | 302  | LUT  | C32-C33 | 7.38  | 1.61        | 1.46     |
| 24  | B     | 853  | BCR  | C30-C25 | -7.37 | 1.44        | 1.53     |
| 38  | 4     | 803  | LUT  | C32-C33 | 7.37  | 1.61        | 1.46     |
| 24  | B     | 849  | BCR  | C30-C25 | -7.37 | 1.44        | 1.53     |
| 24  | A     | 856  | BCR  | C30-C25 | -7.36 | 1.44        | 1.53     |
| 24  | J     | 104  | BCR  | C30-C25 | -7.35 | 1.44        | 1.53     |
| 38  | 5     | 302  | LUT  | C32-C33 | 7.34  | 1.61        | 1.46     |
| 24  | B     | 848  | BCR  | C30-C25 | -7.31 | 1.44        | 1.53     |
| 38  | 8     | 302  | LUT  | C32-C33 | 7.30  | 1.61        | 1.46     |
| 24  | A     | 848  | BCR  | C30-C25 | -7.30 | 1.44        | 1.53     |
| 24  | 3     | 307  | BCR  | C30-C25 | -7.30 | 1.44        | 1.53     |
| 24  | 4     | 804  | BCR  | C30-C25 | -7.30 | 1.44        | 1.53     |
| 24  | B     | 844  | BCR  | C30-C25 | -7.29 | 1.44        | 1.53     |
| 24  | A     | 845  | BCR  | C30-C25 | -7.28 | 1.44        | 1.53     |
| 24  | A     | 846  | BCR  | C30-C25 | -7.27 | 1.44        | 1.53     |
| 24  | 5     | 305  | BCR  | C30-C25 | -7.27 | 1.44        | 1.53     |
| 24  | 6     | 305  | BCR  | C30-C25 | -7.24 | 1.44        | 1.53     |
| 24  | 6     | 306  | BCR  | C30-C25 | -7.24 | 1.44        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | 7     | 303 | BCR  | C30-C25 | -7.22 | 1.44        | 1.53     |
| 24  | 3     | 304 | BCR  | C30-C25 | -7.21 | 1.44        | 1.53     |
| 24  | B     | 847 | BCR  | C1-C6   | -7.20 | 1.44        | 1.53     |
| 24  | L     | 204 | BCR  | C1-C6   | -7.20 | 1.44        | 1.53     |
| 24  | F     | 303 | BCR  | C30-C25 | -7.19 | 1.44        | 1.53     |
| 24  | 8     | 304 | BCR  | C30-C25 | -7.19 | 1.44        | 1.53     |
| 24  | B     | 845 | BCR  | C1-C6   | -7.18 | 1.44        | 1.53     |
| 21  | A     | 801 | CL0  | C3B-C4B | 7.16  | 1.48        | 1.41     |
| 24  | 3     | 307 | BCR  | C1-C6   | -7.16 | 1.44        | 1.53     |
| 24  | 5     | 304 | BCR  | C1-C6   | -7.12 | 1.44        | 1.53     |
| 24  | B     | 846 | BCR  | C30-C25 | -7.11 | 1.44        | 1.53     |
| 24  | K     | 206 | BCR  | C1-C6   | -7.11 | 1.44        | 1.53     |
| 24  | A     | 848 | BCR  | C1-C6   | -7.08 | 1.44        | 1.53     |
| 24  | 3     | 304 | BCR  | C2-C3   | -7.08 | 1.35        | 1.52     |
| 24  | G     | 203 | BCR  | C30-C25 | -7.05 | 1.44        | 1.53     |
| 24  | A     | 847 | BCR  | C1-C6   | -7.03 | 1.44        | 1.53     |
| 24  | 6     | 306 | BCR  | C1-C6   | -7.00 | 1.44        | 1.53     |
| 24  | B     | 846 | BCR  | C1-C6   | -6.98 | 1.44        | 1.53     |
| 24  | G     | 203 | BCR  | C2-C3   | -6.98 | 1.36        | 1.52     |
| 24  | 6     | 305 | BCR  | C2-C3   | -6.97 | 1.36        | 1.52     |
| 24  | G     | 203 | BCR  | C1-C6   | -6.97 | 1.44        | 1.53     |
| 32  | F     | 306 | RRX  | C30-C25 | -6.96 | 1.44        | 1.53     |
| 24  | 3     | 305 | BCR  | C1-C6   | -6.96 | 1.44        | 1.53     |
| 24  | A     | 844 | BCR  | C2-C3   | -6.96 | 1.36        | 1.52     |
| 24  | 5     | 304 | BCR  | C2-C3   | -6.96 | 1.36        | 1.52     |
| 24  | B     | 844 | BCR  | C2-C3   | -6.96 | 1.36        | 1.52     |
| 24  | J     | 104 | BCR  | C1-C6   | -6.95 | 1.44        | 1.53     |
| 24  | K     | 206 | BCR  | C2-C3   | -6.95 | 1.36        | 1.52     |
| 24  | 3     | 305 | BCR  | C2-C3   | -6.95 | 1.36        | 1.52     |
| 24  | B     | 849 | BCR  | C2-C3   | -6.95 | 1.36        | 1.52     |
| 24  | B     | 848 | BCR  | C2-C3   | -6.94 | 1.36        | 1.52     |
| 24  | 4     | 804 | BCR  | C2-C3   | -6.94 | 1.36        | 1.52     |
| 24  | A     | 846 | BCR  | C1-C6   | -6.94 | 1.44        | 1.53     |
| 24  | F     | 303 | BCR  | C2-C3   | -6.93 | 1.36        | 1.52     |
| 24  | A     | 856 | BCR  | C1-C6   | -6.93 | 1.44        | 1.53     |
| 24  | B     | 846 | BCR  | C2-C3   | -6.93 | 1.36        | 1.52     |
| 24  | A     | 846 | BCR  | C2-C3   | -6.91 | 1.36        | 1.52     |
| 24  | 5     | 305 | BCR  | C2-C3   | -6.90 | 1.36        | 1.52     |
| 24  | A     | 847 | BCR  | C2-C3   | -6.90 | 1.36        | 1.52     |
| 24  | B     | 847 | BCR  | C2-C3   | -6.89 | 1.36        | 1.52     |
| 24  | B     | 844 | BCR  | C1-C6   | -6.88 | 1.45        | 1.53     |
| 24  | B     | 849 | BCR  | C1-C6   | -6.88 | 1.45        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | A     | 845  | BCR  | C1-C6   | -6.88 | 1.45        | 1.53     |
| 24  | A     | 856  | BCR  | C2-C3   | -6.86 | 1.36        | 1.52     |
| 38  | 6     | 303  | LUT  | C1-C6   | -6.86 | 1.45        | 1.53     |
| 24  | B     | 853  | BCR  | C2-C3   | -6.85 | 1.36        | 1.52     |
| 24  | 3     | 306  | BCR  | C2-C3   | -6.83 | 1.36        | 1.52     |
| 24  | B     | 853  | BCR  | C1-C6   | -6.81 | 1.45        | 1.53     |
| 24  | 6     | 306  | BCR  | C2-C3   | -6.81 | 1.36        | 1.52     |
| 24  | I     | 4001 | BCR  | C2-C3   | -6.81 | 1.36        | 1.52     |
| 24  | 7     | 303  | BCR  | C1-C6   | -6.81 | 1.45        | 1.53     |
| 32  | F     | 306  | RRX  | C2-C3   | -6.80 | 1.36        | 1.52     |
| 24  | 4     | 804  | BCR  | C1-C6   | -6.79 | 1.45        | 1.53     |
| 24  | A     | 845  | BCR  | C2-C3   | -6.78 | 1.36        | 1.52     |
| 24  | F     | 303  | BCR  | C1-C6   | -6.75 | 1.45        | 1.53     |
| 24  | B     | 845  | BCR  | C2-C3   | -6.74 | 1.36        | 1.52     |
| 24  | J     | 104  | BCR  | C2-C3   | -6.74 | 1.36        | 1.52     |
| 24  | L     | 204  | BCR  | C2-C3   | -6.73 | 1.36        | 1.52     |
| 38  | 8     | 303  | LUT  | C1-C6   | -6.73 | 1.45        | 1.53     |
| 38  | Z     | 301  | LUT  | C1-C6   | -6.72 | 1.45        | 1.53     |
| 24  | 8     | 304  | BCR  | C2-C3   | -6.72 | 1.36        | 1.52     |
| 38  | 4     | 803  | LUT  | C1-C6   | -6.72 | 1.45        | 1.53     |
| 24  | A     | 848  | BCR  | C2-C3   | -6.71 | 1.36        | 1.52     |
| 38  | 1     | 303  | LUT  | C1-C6   | -6.70 | 1.45        | 1.53     |
| 24  | 5     | 305  | BCR  | C29-C28 | -6.70 | 1.36        | 1.52     |
| 38  | 3     | 302  | LUT  | C1-C6   | -6.69 | 1.45        | 1.53     |
| 24  | 3     | 307  | BCR  | C2-C3   | -6.69 | 1.36        | 1.52     |
| 24  | 6     | 305  | BCR  | C29-C28 | -6.69 | 1.36        | 1.52     |
| 24  | A     | 847  | BCR  | C29-C28 | -6.69 | 1.36        | 1.52     |
| 24  | A     | 844  | BCR  | C1-C6   | -6.68 | 1.45        | 1.53     |
| 24  | 7     | 303  | BCR  | C29-C28 | -6.68 | 1.36        | 1.52     |
| 24  | B     | 848  | BCR  | C1-C6   | -6.67 | 1.45        | 1.53     |
| 24  | 5     | 305  | BCR  | C1-C6   | -6.67 | 1.45        | 1.53     |
| 24  | B     | 848  | BCR  | C29-C28 | -6.67 | 1.36        | 1.52     |
| 24  | 4     | 804  | BCR  | C29-C28 | -6.66 | 1.36        | 1.52     |
| 24  | F     | 303  | BCR  | C29-C28 | -6.66 | 1.36        | 1.52     |
| 24  | 3     | 306  | BCR  | C1-C6   | -6.65 | 1.45        | 1.53     |
| 38  | 8     | 302  | LUT  | C1-C6   | -6.65 | 1.45        | 1.53     |
| 24  | 8     | 304  | BCR  | C29-C28 | -6.65 | 1.36        | 1.52     |
| 38  | 1     | 302  | LUT  | C1-C6   | -6.64 | 1.45        | 1.53     |
| 24  | 7     | 303  | BCR  | C2-C3   | -6.64 | 1.36        | 1.52     |
| 38  | Z     | 302  | LUT  | C1-C6   | -6.64 | 1.45        | 1.53     |
| 24  | 6     | 306  | BCR  | C29-C28 | -6.64 | 1.36        | 1.52     |
| 38  | 3     | 303  | LUT  | C1-C6   | -6.62 | 1.45        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | 6     | 305  | BCR  | C1-C6   | -6.62 | 1.45        | 1.53     |
| 38  | 5     | 302  | LUT  | C1-C6   | -6.62 | 1.45        | 1.53     |
| 38  | 6     | 304  | LUT  | C1-C6   | -6.61 | 1.45        | 1.53     |
| 24  | 3     | 304  | BCR  | C29-C28 | -6.60 | 1.36        | 1.52     |
| 24  | B     | 844  | BCR  | C29-C28 | -6.60 | 1.37        | 1.52     |
| 24  | B     | 846  | BCR  | C29-C28 | -6.60 | 1.37        | 1.52     |
| 24  | A     | 846  | BCR  | C29-C28 | -6.59 | 1.37        | 1.52     |
| 24  | G     | 203  | BCR  | C29-C28 | -6.58 | 1.37        | 1.52     |
| 24  | 3     | 304  | BCR  | C1-C6   | -6.57 | 1.45        | 1.53     |
| 24  | 3     | 306  | BCR  | C29-C28 | -6.55 | 1.37        | 1.52     |
| 38  | 7     | 302  | LUT  | C1-C6   | -6.54 | 1.45        | 1.53     |
| 24  | 3     | 307  | BCR  | C29-C28 | -6.53 | 1.37        | 1.52     |
| 24  | K     | 206  | BCR  | C29-C28 | -6.52 | 1.37        | 1.52     |
| 24  | A     | 845  | BCR  | C29-C28 | -6.52 | 1.37        | 1.52     |
| 38  | 9     | 301  | LUT  | C1-C6   | -6.50 | 1.45        | 1.53     |
| 24  | A     | 848  | BCR  | C29-C28 | -6.50 | 1.37        | 1.52     |
| 22  | 4     | 805  | CLA  | MG-NA   | 6.49  | 2.21        | 2.06     |
| 38  | 5     | 303  | LUT  | C1-C6   | -6.49 | 1.45        | 1.53     |
| 38  | 9     | 302  | LUT  | C1-C6   | -6.47 | 1.45        | 1.53     |
| 24  | B     | 849  | BCR  | C29-C28 | -6.47 | 1.37        | 1.52     |
| 38  | 7     | 301  | LUT  | C1-C6   | -6.46 | 1.45        | 1.53     |
| 24  | 3     | 305  | BCR  | C29-C28 | -6.44 | 1.37        | 1.52     |
| 24  | 5     | 304  | BCR  | C29-C28 | -6.44 | 1.37        | 1.52     |
| 24  | B     | 847  | BCR  | C29-C28 | -6.44 | 1.37        | 1.52     |
| 24  | B     | 845  | BCR  | C29-C28 | -6.42 | 1.37        | 1.52     |
| 22  | 8     | 307  | CLA  | MG-NA   | 6.42  | 2.21        | 2.06     |
| 24  | A     | 844  | BCR  | C29-C28 | -6.42 | 1.37        | 1.52     |
| 24  | L     | 204  | BCR  | C29-C28 | -6.40 | 1.37        | 1.52     |
| 22  | 4     | 807  | CLA  | MG-NA   | 6.40  | 2.21        | 2.06     |
| 22  | 4     | 806  | CLA  | MG-NA   | 6.38  | 2.21        | 2.06     |
| 22  | 7     | 308  | CLA  | MG-NA   | 6.38  | 2.21        | 2.06     |
| 22  | 4     | 809  | CLA  | MG-NA   | 6.38  | 2.21        | 2.06     |
| 22  | 6     | 309  | CLA  | MG-NA   | 6.38  | 2.21        | 2.06     |
| 24  | I     | 4001 | BCR  | C29-C28 | -6.38 | 1.37        | 1.52     |
| 22  | A     | 816  | CLA  | MG-NA   | 6.37  | 2.21        | 2.06     |
| 22  | 5     | 311  | CLA  | MG-NA   | 6.37  | 2.21        | 2.06     |
| 24  | B     | 853  | BCR  | C29-C28 | -6.37 | 1.37        | 1.52     |
| 22  | B     | 820  | CLA  | MG-NA   | 6.37  | 2.21        | 2.06     |
| 22  | 7     | 306  | CLA  | MG-NA   | 6.36  | 2.21        | 2.06     |
| 22  | 3     | 310  | CLA  | MG-NA   | 6.36  | 2.21        | 2.06     |
| 22  | A     | 817  | CLA  | MG-NA   | 6.36  | 2.21        | 2.06     |
| 22  | 3     | 312  | CLA  | MG-NA   | 6.36  | 2.21        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | J     | 104 | BCR  | C29-C28 | -6.36 | 1.37        | 1.52     |
| 22  | A     | 825 | CLA  | MG-NA   | 6.36  | 2.21        | 2.06     |
| 22  | 5     | 315 | CLA  | MG-NA   | 6.35  | 2.21        | 2.06     |
| 22  | B     | 828 | CLA  | MG-NA   | 6.35  | 2.21        | 2.06     |
| 22  | Z     | 313 | CLA  | MG-NA   | 6.34  | 2.21        | 2.06     |
| 22  | 7     | 324 | CLA  | MG-NA   | 6.34  | 2.21        | 2.06     |
| 22  | 6     | 301 | CLA  | MG-NA   | 6.34  | 2.21        | 2.06     |
| 22  | A     | 837 | CLA  | MG-NA   | 6.34  | 2.21        | 2.06     |
| 22  | 1     | 315 | CLA  | MG-NA   | 6.33  | 2.21        | 2.06     |
| 22  | 5     | 313 | CLA  | MG-NA   | 6.33  | 2.21        | 2.06     |
| 22  | G     | 201 | CLA  | MG-NA   | 6.33  | 2.21        | 2.06     |
| 22  | B     | 826 | CLA  | MG-NA   | 6.33  | 2.21        | 2.06     |
| 22  | A     | 820 | CLA  | MG-NA   | 6.32  | 2.21        | 2.06     |
| 22  | A     | 822 | CLA  | MG-NA   | 6.32  | 2.21        | 2.06     |
| 22  | 5     | 322 | CLA  | MG-NA   | 6.32  | 2.21        | 2.06     |
| 22  | A     | 813 | CLA  | MG-NA   | 6.32  | 2.21        | 2.06     |
| 22  | A     | 829 | CLA  | MG-NA   | 6.32  | 2.21        | 2.06     |
| 22  | F     | 301 | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 22  | K     | 203 | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 22  | 9     | 308 | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 22  | 1     | 310 | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 22  | 8     | 306 | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 22  | 5     | 326 | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 22  | 3     | 322 | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 22  | 5     | 309 | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 38  | 4     | 802 | LUT  | C1-C6   | -6.31 | 1.45        | 1.53     |
| 22  | B     | 810 | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 22  | L     | 203 | CLA  | MG-NA   | 6.31  | 2.21        | 2.06     |
| 22  | B     | 824 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | B     | 840 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | 7     | 323 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | A     | 840 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | L     | 202 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | 4     | 811 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | 1     | 305 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | A     | 834 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | J     | 103 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | B     | 829 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | Z     | 315 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | 8     | 309 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | 9     | 307 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | 6     | 319 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 834 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | B     | 806 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | 1     | 304 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | A     | 807 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | 7     | 310 | CLA  | MG-NA   | 6.30  | 2.21        | 2.06     |
| 22  | A     | 839 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | A     | 855 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | Z     | 304 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | K     | 202 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | 2     | 302 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | F     | 302 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | Z     | 310 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | 7     | 305 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | 2     | 304 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | A     | 814 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | 7     | 312 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | A     | 824 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | B     | 823 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | B     | 822 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | 7     | 317 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | 6     | 311 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | B     | 842 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | A     | 812 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 24  | A     | 856 | BCR  | C29-C28 | -6.29 | 1.37        | 1.52     |
| 22  | F     | 305 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | A     | 841 | CLA  | MG-NA   | 6.29  | 2.21        | 2.06     |
| 22  | A     | 808 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | A     | 809 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | B     | 833 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | B     | 815 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | 6     | 322 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | 4     | 812 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | B     | 837 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | 9     | 313 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | K     | 204 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | A     | 826 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | 4     | 808 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | A     | 827 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | Z     | 307 | CLA  | MG-NA   | 6.28  | 2.21        | 2.06     |
| 22  | 7     | 315 | CLA  | MG-NA   | 6.27  | 2.21        | 2.06     |
| 22  | B     | 805 | CLA  | MG-NA   | 6.27  | 2.21        | 2.06     |
| 22  | 6     | 314 | CLA  | MG-NA   | 6.27  | 2.21        | 2.06     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 22  | 7     | 314 | CLA  | MG-NA | 6.27 | 2.21        | 2.06     |
| 22  | A     | 810 | CLA  | MG-NA | 6.27 | 2.21        | 2.06     |
| 22  | A     | 842 | CLA  | MG-NA | 6.27 | 2.21        | 2.06     |
| 22  | L     | 201 | CLA  | MG-NA | 6.27 | 2.21        | 2.06     |
| 22  | 3     | 319 | CLA  | MG-NA | 6.27 | 2.21        | 2.06     |
| 22  | B     | 827 | CLA  | MG-NA | 6.27 | 2.21        | 2.06     |
| 22  | 3     | 309 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | 3     | 316 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | 6     | 313 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | B     | 839 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | 7     | 311 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | 6     | 321 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | B     | 821 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | 9     | 311 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | B     | 819 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | 1     | 307 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | 1     | 306 | CLA  | MG-NA | 6.26 | 2.21        | 2.06     |
| 22  | B     | 811 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | 6     | 312 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | Z     | 314 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | Z     | 316 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | A     | 830 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | A     | 802 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | 7     | 316 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | 4     | 818 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | 6     | 302 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | A     | 803 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | A     | 806 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | 7     | 309 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | A     | 833 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | B     | 831 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | 1     | 314 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | 8     | 314 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | A     | 815 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | 5     | 310 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | 6     | 310 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | A     | 832 | CLA  | MG-NA | 6.25 | 2.21        | 2.06     |
| 22  | B     | 816 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | B     | 825 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | F     | 304 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | B     | 841 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | 8     | 316 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 22  | B     | 809 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | B     | 813 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | 1     | 313 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | A     | 854 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | 4     | 817 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | 6     | 317 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | 3     | 314 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | 5     | 308 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | 5     | 319 | CLA  | MG-NA | 6.24 | 2.21        | 2.06     |
| 22  | 5     | 314 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | A     | 811 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | Z     | 309 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | A     | 818 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | B     | 807 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | B     | 808 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | Z     | 308 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | 8     | 311 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | 5     | 307 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | 8     | 310 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | A     | 831 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | B     | 812 | CLA  | MG-NA | 6.23 | 2.21        | 2.06     |
| 22  | B     | 830 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | 4     | 815 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | G     | 202 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | 5     | 312 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | B     | 836 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | A     | 804 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | A     | 819 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | 4     | 810 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | A     | 821 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | 5     | 301 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | B     | 801 | CLA  | MG-NA | 6.22 | 2.21        | 2.06     |
| 22  | A     | 838 | CLA  | MG-NA | 6.21 | 2.21        | 2.06     |
| 22  | 6     | 308 | CLA  | MG-NA | 6.21 | 2.21        | 2.06     |
| 22  | 9     | 306 | CLA  | MG-NA | 6.21 | 2.21        | 2.06     |
| 22  | B     | 835 | CLA  | MG-NA | 6.21 | 2.21        | 2.06     |
| 22  | 3     | 308 | CLA  | MG-NA | 6.21 | 2.21        | 2.06     |
| 22  | 8     | 313 | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | 3     | 311 | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | 8     | 308 | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | A     | 805 | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |
| 22  | B     | 832 | CLA  | MG-NA | 6.20 | 2.21        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 6     | 307 | CLA  | MG-NA   | 6.20  | 2.21        | 2.06     |
| 22  | 5     | 318 | CLA  | MG-NA   | 6.20  | 2.21        | 2.06     |
| 22  | 7     | 322 | CLA  | MG-NA   | 6.20  | 2.21        | 2.06     |
| 22  | B     | 817 | CLA  | MG-NA   | 6.19  | 2.21        | 2.06     |
| 22  | B     | 838 | CLA  | MG-NA   | 6.19  | 2.21        | 2.06     |
| 22  | 2     | 301 | CLA  | MG-NA   | 6.19  | 2.21        | 2.06     |
| 22  | A     | 823 | CLA  | MG-NA   | 6.19  | 2.21        | 2.06     |
| 22  | 7     | 307 | CLA  | MG-NA   | 6.19  | 2.21        | 2.06     |
| 22  | A     | 828 | CLA  | MG-NA   | 6.18  | 2.21        | 2.06     |
| 22  | Z     | 306 | CLA  | MG-NA   | 6.18  | 2.21        | 2.06     |
| 22  | 1     | 308 | CLA  | MG-NA   | 6.18  | 2.21        | 2.06     |
| 22  | 3     | 318 | CLA  | MG-NA   | 6.18  | 2.20        | 2.06     |
| 22  | 5     | 323 | CLA  | MG-NA   | 6.15  | 2.20        | 2.06     |
| 22  | Z     | 303 | CLA  | MG-NA   | 6.15  | 2.20        | 2.06     |
| 22  | B     | 818 | CLA  | MG-NA   | 6.15  | 2.20        | 2.06     |
| 22  | Z     | 305 | CLA  | MG-NA   | 6.15  | 2.20        | 2.06     |
| 22  | A     | 835 | CLA  | MG-NA   | 6.15  | 2.20        | 2.06     |
| 22  | 1     | 309 | CLA  | MG-NA   | 6.14  | 2.20        | 2.06     |
| 32  | F     | 306 | RRX  | C19-C18 | 6.14  | 1.59        | 1.46     |
| 22  | A     | 836 | CLA  | MG-NA   | 6.14  | 2.20        | 2.06     |
| 22  | B     | 814 | CLA  | MG-NA   | 6.14  | 2.20        | 2.06     |
| 22  | 3     | 313 | CLA  | MG-NA   | 6.12  | 2.20        | 2.06     |
| 22  | 7     | 304 | CLA  | MG-NA   | 6.10  | 2.20        | 2.06     |
| 22  | 8     | 305 | CLA  | MG-NA   | 6.10  | 2.20        | 2.06     |
| 22  | 1     | 316 | CLA  | MG-NA   | 6.09  | 2.20        | 2.06     |
| 22  | 9     | 304 | CLA  | MG-NA   | 6.09  | 2.20        | 2.06     |
| 39  | Z     | 311 | CHL  | C3A-C2A | -6.05 | 1.49        | 1.54     |
| 22  | 9     | 310 | CLA  | MG-NA   | 6.05  | 2.20        | 2.06     |
| 36  | J     | 105 | C7Z  | C12-C13 | 6.04  | 1.58        | 1.46     |
| 24  | B     | 853 | BCR  | C12-C13 | 6.02  | 1.58        | 1.46     |
| 22  | K     | 205 | CLA  | MG-NA   | 5.99  | 2.20        | 2.06     |
| 22  | 9     | 309 | CLA  | MG-NA   | 5.96  | 2.20        | 2.06     |
| 22  | 3     | 315 | CLA  | MG-NA   | 5.95  | 2.20        | 2.06     |
| 36  | 5     | 306 | C7Z  | C12-C13 | 5.94  | 1.58        | 1.46     |
| 22  | 5     | 320 | CLA  | MG-NA   | 5.93  | 2.20        | 2.06     |
| 22  | 3     | 320 | CLA  | MG-NA   | 5.92  | 2.20        | 2.06     |
| 22  | 1     | 311 | CLA  | MG-NA   | 5.91  | 2.20        | 2.06     |
| 24  | 3     | 306 | BCR  | C12-C13 | 5.91  | 1.58        | 1.46     |
| 22  | 9     | 305 | CLA  | MG-NA   | 5.89  | 2.20        | 2.06     |
| 24  | 3     | 304 | BCR  | C12-C13 | 5.87  | 1.58        | 1.46     |
| 24  | A     | 844 | BCR  | C12-C13 | 5.84  | 1.58        | 1.46     |
| 32  | F     | 306 | RRX  | C1-C6   | -5.82 | 1.46        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | J     | 104  | BCR  | C12-C13 | 5.82  | 1.58        | 1.46     |
| 36  | 5     | 306  | C7Z  | C1-C6   | -5.82 | 1.46        | 1.53     |
| 24  | A     | 848  | BCR  | C12-C13 | 5.81  | 1.58        | 1.46     |
| 24  | B     | 846  | BCR  | C12-C13 | 5.77  | 1.58        | 1.46     |
| 24  | A     | 856  | BCR  | C12-C13 | 5.76  | 1.58        | 1.46     |
| 39  | 6     | 318  | CHL  | C3A-C2A | -5.75 | 1.49        | 1.54     |
| 39  | 1     | 312  | CHL  | C3A-C2A | -5.75 | 1.49        | 1.54     |
| 24  | A     | 845  | BCR  | C12-C13 | 5.74  | 1.58        | 1.46     |
| 24  | B     | 849  | BCR  | C12-C13 | 5.74  | 1.58        | 1.46     |
| 24  | B     | 845  | BCR  | C12-C13 | 5.74  | 1.58        | 1.46     |
| 24  | B     | 844  | BCR  | C12-C13 | 5.74  | 1.58        | 1.46     |
| 24  | G     | 203  | BCR  | C12-C13 | 5.73  | 1.58        | 1.46     |
| 24  | 3     | 307  | BCR  | C12-C13 | 5.73  | 1.58        | 1.46     |
| 22  | 9     | 303  | CLA  | MG-NA   | 5.73  | 2.19        | 2.06     |
| 24  | I     | 4001 | BCR  | C12-C13 | 5.73  | 1.58        | 1.46     |
| 24  | F     | 303  | BCR  | C12-C13 | 5.73  | 1.58        | 1.46     |
| 24  | 7     | 303  | BCR  | C12-C13 | 5.73  | 1.58        | 1.46     |
| 24  | 3     | 305  | BCR  | C12-C13 | 5.70  | 1.58        | 1.46     |
| 24  | 6     | 305  | BCR  | C12-C13 | 5.70  | 1.58        | 1.46     |
| 24  | 4     | 804  | BCR  | C12-C13 | 5.70  | 1.58        | 1.46     |
| 24  | 8     | 304  | BCR  | C12-C13 | 5.70  | 1.58        | 1.46     |
| 24  | B     | 853  | BCR  | C8-C9   | 5.69  | 1.58        | 1.46     |
| 24  | 5     | 304  | BCR  | C12-C13 | 5.69  | 1.58        | 1.46     |
| 24  | B     | 847  | BCR  | C12-C13 | 5.66  | 1.58        | 1.46     |
| 39  | 6     | 316  | CHL  | C3A-C2A | -5.66 | 1.49        | 1.54     |
| 24  | 5     | 305  | BCR  | C12-C13 | 5.66  | 1.58        | 1.46     |
| 24  | L     | 204  | BCR  | C12-C13 | 5.64  | 1.58        | 1.46     |
| 36  | J     | 105  | C7Z  | C1-C6   | -5.64 | 1.46        | 1.53     |
| 24  | A     | 846  | BCR  | C12-C13 | 5.64  | 1.58        | 1.46     |
| 24  | K     | 206  | BCR  | C12-C13 | 5.63  | 1.58        | 1.46     |
| 24  | A     | 847  | BCR  | C12-C13 | 5.62  | 1.58        | 1.46     |
| 24  | B     | 848  | BCR  | C12-C13 | 5.62  | 1.58        | 1.46     |
| 24  | 6     | 306  | BCR  | C12-C13 | 5.61  | 1.58        | 1.46     |
| 24  | B     | 844  | BCR  | C8-C9   | 5.58  | 1.57        | 1.46     |
| 24  | 4     | 804  | BCR  | C8-C9   | 5.54  | 1.57        | 1.46     |
| 24  | I     | 4001 | BCR  | C8-C9   | 5.52  | 1.57        | 1.46     |
| 24  | A     | 856  | BCR  | C8-C9   | 5.51  | 1.57        | 1.46     |
| 39  | 8     | 312  | CHL  | C3A-C2A | -5.50 | 1.50        | 1.54     |
| 24  | 3     | 307  | BCR  | C8-C9   | 5.49  | 1.57        | 1.46     |
| 24  | B     | 845  | BCR  | C8-C9   | 5.47  | 1.57        | 1.46     |
| 21  | A     | 801  | CL0  | CHB-C1B | 5.46  | 1.48        | 1.39     |
| 24  | F     | 303  | BCR  | C8-C9   | 5.46  | 1.57        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | 3     | 305  | BCR  | C8-C9   | 5.46  | 1.57        | 1.46     |
| 24  | B     | 849  | BCR  | C8-C9   | 5.45  | 1.57        | 1.46     |
| 24  | J     | 104  | BCR  | C8-C9   | 5.45  | 1.57        | 1.46     |
| 24  | A     | 845  | BCR  | C8-C9   | 5.45  | 1.57        | 1.46     |
| 24  | B     | 846  | BCR  | C8-C9   | 5.44  | 1.57        | 1.46     |
| 24  | A     | 848  | BCR  | C8-C9   | 5.44  | 1.57        | 1.46     |
| 24  | L     | 204  | BCR  | C8-C9   | 5.42  | 1.57        | 1.46     |
| 24  | 3     | 306  | BCR  | C8-C9   | 5.42  | 1.57        | 1.46     |
| 24  | 5     | 305  | BCR  | C8-C9   | 5.42  | 1.57        | 1.46     |
| 24  | B     | 853  | BCR  | C23-C22 | 5.42  | 1.57        | 1.46     |
| 24  | B     | 848  | BCR  | C8-C9   | 5.41  | 1.57        | 1.46     |
| 24  | 7     | 303  | BCR  | C8-C9   | 5.41  | 1.57        | 1.46     |
| 24  | 6     | 305  | BCR  | C8-C9   | 5.41  | 1.57        | 1.46     |
| 24  | 8     | 304  | BCR  | C29-C30 | 5.40  | 1.66        | 1.54     |
| 24  | 8     | 304  | BCR  | C8-C9   | 5.40  | 1.57        | 1.46     |
| 24  | A     | 846  | BCR  | C8-C9   | 5.39  | 1.57        | 1.46     |
| 24  | A     | 856  | BCR  | C23-C22 | 5.39  | 1.57        | 1.46     |
| 24  | A     | 856  | BCR  | C29-C30 | 5.38  | 1.66        | 1.54     |
| 24  | 5     | 304  | BCR  | C29-C30 | 5.37  | 1.66        | 1.54     |
| 21  | A     | 801  | CL0  | CHC-C4B | 5.37  | 1.48        | 1.39     |
| 24  | B     | 846  | BCR  | C29-C30 | 5.37  | 1.66        | 1.54     |
| 39  | 8     | 301  | CHL  | C3A-C2A | -5.37 | 1.50        | 1.54     |
| 24  | G     | 203  | BCR  | C29-C30 | 5.37  | 1.66        | 1.54     |
| 39  | 4     | 816  | CHL  | C3A-C2A | -5.36 | 1.50        | 1.54     |
| 24  | 3     | 304  | BCR  | C8-C9   | 5.36  | 1.57        | 1.46     |
| 24  | 3     | 305  | BCR  | C23-C22 | 5.36  | 1.57        | 1.46     |
| 24  | 5     | 304  | BCR  | C8-C9   | 5.36  | 1.57        | 1.46     |
| 24  | B     | 849  | BCR  | C29-C30 | 5.35  | 1.66        | 1.54     |
| 24  | J     | 104  | BCR  | C29-C30 | 5.35  | 1.66        | 1.54     |
| 24  | A     | 847  | BCR  | C8-C9   | 5.35  | 1.57        | 1.46     |
| 24  | K     | 206  | BCR  | C8-C9   | 5.35  | 1.57        | 1.46     |
| 21  | A     | 801  | CL0  | O2A-C1  | 5.34  | 1.60        | 1.46     |
| 24  | B     | 847  | BCR  | C8-C9   | 5.34  | 1.57        | 1.46     |
| 24  | G     | 203  | BCR  | C8-C9   | 5.33  | 1.57        | 1.46     |
| 24  | 3     | 304  | BCR  | C29-C30 | 5.33  | 1.66        | 1.54     |
| 24  | 8     | 304  | BCR  | C23-C22 | 5.33  | 1.57        | 1.46     |
| 24  | 3     | 305  | BCR  | C29-C30 | 5.33  | 1.66        | 1.54     |
| 24  | I     | 4001 | BCR  | C29-C30 | 5.32  | 1.66        | 1.54     |
| 24  | F     | 303  | BCR  | C23-C22 | 5.32  | 1.57        | 1.46     |
| 24  | A     | 846  | BCR  | C29-C30 | 5.32  | 1.66        | 1.54     |
| 24  | A     | 844  | BCR  | C29-C30 | 5.32  | 1.66        | 1.54     |
| 24  | A     | 848  | BCR  | C23-C22 | 5.31  | 1.57        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 24  | K     | 206  | BCR  | C29-C30 | 5.31 | 1.66        | 1.54     |
| 24  | B     | 849  | BCR  | C23-C22 | 5.30 | 1.57        | 1.46     |
| 24  | A     | 845  | BCR  | C29-C30 | 5.30 | 1.66        | 1.54     |
| 24  | A     | 844  | BCR  | C8-C9   | 5.30 | 1.57        | 1.46     |
| 24  | 6     | 306  | BCR  | C8-C9   | 5.30 | 1.57        | 1.46     |
| 24  | B     | 847  | BCR  | C29-C30 | 5.30 | 1.66        | 1.54     |
| 24  | K     | 206  | BCR  | C23-C22 | 5.30 | 1.57        | 1.46     |
| 32  | F     | 306  | RRX  | C8-C9   | 5.29 | 1.57        | 1.46     |
| 24  | 6     | 305  | BCR  | C29-C30 | 5.29 | 1.66        | 1.54     |
| 24  | A     | 845  | BCR  | C23-C22 | 5.29 | 1.57        | 1.46     |
| 24  | 7     | 303  | BCR  | C23-C22 | 5.29 | 1.57        | 1.46     |
| 24  | 5     | 304  | BCR  | C23-C22 | 5.29 | 1.57        | 1.46     |
| 24  | B     | 844  | BCR  | C23-C22 | 5.29 | 1.57        | 1.46     |
| 24  | 3     | 306  | BCR  | C23-C22 | 5.28 | 1.57        | 1.46     |
| 24  | A     | 848  | BCR  | C29-C30 | 5.27 | 1.66        | 1.54     |
| 24  | L     | 204  | BCR  | C29-C30 | 5.27 | 1.66        | 1.54     |
| 24  | 3     | 304  | BCR  | C23-C22 | 5.27 | 1.57        | 1.46     |
| 24  | J     | 104  | BCR  | C23-C22 | 5.27 | 1.57        | 1.46     |
| 24  | 3     | 306  | BCR  | C29-C30 | 5.26 | 1.66        | 1.54     |
| 24  | B     | 845  | BCR  | C23-C22 | 5.26 | 1.57        | 1.46     |
| 24  | 4     | 804  | BCR  | C23-C22 | 5.26 | 1.57        | 1.46     |
| 24  | B     | 845  | BCR  | C29-C30 | 5.26 | 1.66        | 1.54     |
| 24  | 3     | 307  | BCR  | C29-C30 | 5.25 | 1.66        | 1.54     |
| 24  | B     | 844  | BCR  | C29-C30 | 5.24 | 1.66        | 1.54     |
| 24  | B     | 846  | BCR  | C23-C22 | 5.24 | 1.57        | 1.46     |
| 24  | F     | 303  | BCR  | C29-C30 | 5.23 | 1.66        | 1.54     |
| 24  | G     | 203  | BCR  | C23-C22 | 5.22 | 1.57        | 1.46     |
| 24  | 6     | 306  | BCR  | C29-C30 | 5.21 | 1.66        | 1.54     |
| 24  | 6     | 305  | BCR  | C23-C22 | 5.21 | 1.57        | 1.46     |
| 24  | A     | 847  | BCR  | C23-C22 | 5.21 | 1.57        | 1.46     |
| 24  | B     | 847  | BCR  | C23-C22 | 5.20 | 1.57        | 1.46     |
| 24  | L     | 204  | BCR  | C23-C22 | 5.20 | 1.57        | 1.46     |
| 24  | A     | 846  | BCR  | C23-C22 | 5.20 | 1.57        | 1.46     |
| 24  | A     | 844  | BCR  | C23-C22 | 5.20 | 1.57        | 1.46     |
| 24  | 4     | 804  | BCR  | C29-C30 | 5.19 | 1.66        | 1.54     |
| 24  | 3     | 307  | BCR  | C23-C22 | 5.19 | 1.57        | 1.46     |
| 24  | B     | 848  | BCR  | C23-C22 | 5.18 | 1.57        | 1.46     |
| 24  | 5     | 305  | BCR  | C23-C22 | 5.18 | 1.57        | 1.46     |
| 24  | I     | 4001 | BCR  | C23-C22 | 5.17 | 1.57        | 1.46     |
| 24  | 7     | 303  | BCR  | C29-C30 | 5.17 | 1.65        | 1.54     |
| 24  | B     | 848  | BCR  | C29-C30 | 5.15 | 1.65        | 1.54     |
| 24  | 5     | 305  | BCR  | C29-C30 | 5.15 | 1.65        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 39  | 4     | 813  | CHL  | C3A-C2A | -5.11 | 1.50        | 1.54     |
| 21  | A     | 801  | CL0  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 24  | B     | 853  | BCR  | C15-C14 | 5.09  | 1.59        | 1.43     |
| 38  | 1     | 302  | LUT  | C8-C9   | 5.08  | 1.56        | 1.46     |
| 32  | F     | 306  | RRX  | C2-C1   | 5.07  | 1.65        | 1.54     |
| 38  | Z     | 301  | LUT  | C8-C9   | 5.04  | 1.56        | 1.46     |
| 39  | Z     | 312  | CHL  | C3A-C2A | -5.04 | 1.50        | 1.54     |
| 38  | 6     | 303  | LUT  | C8-C9   | 5.04  | 1.56        | 1.46     |
| 21  | A     | 801  | CL0  | OBD-CAD | 5.02  | 1.28        | 1.22     |
| 38  | 7     | 302  | LUT  | C8-C9   | 5.01  | 1.56        | 1.46     |
| 38  | Z     | 302  | LUT  | C8-C9   | 5.01  | 1.56        | 1.46     |
| 24  | A     | 847  | BCR  | C29-C30 | 5.01  | 1.65        | 1.54     |
| 38  | 8     | 303  | LUT  | C8-C9   | 5.00  | 1.56        | 1.46     |
| 24  | 3     | 306  | BCR  | C15-C14 | 5.00  | 1.58        | 1.43     |
| 38  | 1     | 303  | LUT  | C8-C9   | 4.99  | 1.56        | 1.46     |
| 39  | 5     | 316  | CHL  | C3A-C2A | -4.99 | 1.50        | 1.54     |
| 36  | 5     | 306  | C7Z  | C24-C25 | -4.98 | 1.43        | 1.51     |
| 38  | 6     | 304  | LUT  | C8-C9   | 4.98  | 1.56        | 1.46     |
| 24  | 6     | 306  | BCR  | C23-C22 | 4.97  | 1.56        | 1.46     |
| 38  | 5     | 303  | LUT  | C8-C9   | 4.96  | 1.56        | 1.46     |
| 24  | A     | 844  | BCR  | C15-C14 | 4.95  | 1.58        | 1.43     |
| 38  | 9     | 302  | LUT  | C8-C9   | 4.95  | 1.56        | 1.46     |
| 38  | 7     | 301  | LUT  | C8-C9   | 4.95  | 1.56        | 1.46     |
| 38  | 9     | 301  | LUT  | C8-C9   | 4.95  | 1.56        | 1.46     |
| 38  | 8     | 302  | LUT  | C8-C9   | 4.94  | 1.56        | 1.46     |
| 38  | 3     | 303  | LUT  | C8-C9   | 4.94  | 1.56        | 1.46     |
| 32  | F     | 306  | RRX  | C23-C22 | 4.93  | 1.56        | 1.46     |
| 21  | A     | 801  | CL0  | C3B-C2B | 4.92  | 1.47        | 1.40     |
| 24  | 3     | 304  | BCR  | C15-C14 | 4.91  | 1.58        | 1.43     |
| 24  | 7     | 303  | BCR  | C15-C14 | 4.89  | 1.58        | 1.43     |
| 21  | A     | 801  | CL0  | CHD-C1D | 4.89  | 1.47        | 1.39     |
| 24  | J     | 104  | BCR  | C15-C14 | 4.88  | 1.58        | 1.43     |
| 38  | 4     | 802  | LUT  | C8-C9   | 4.88  | 1.56        | 1.46     |
| 38  | 5     | 302  | LUT  | C8-C9   | 4.88  | 1.56        | 1.46     |
| 24  | 3     | 305  | BCR  | C15-C14 | 4.88  | 1.58        | 1.43     |
| 24  | A     | 848  | BCR  | C15-C14 | 4.87  | 1.58        | 1.43     |
| 24  | 5     | 304  | BCR  | C15-C14 | 4.85  | 1.58        | 1.43     |
| 24  | 6     | 305  | BCR  | C15-C14 | 4.85  | 1.58        | 1.43     |
| 38  | 4     | 803  | LUT  | C8-C9   | 4.85  | 1.56        | 1.46     |
| 24  | B     | 853  | BCR  | C29-C30 | 4.84  | 1.65        | 1.54     |
| 24  | A     | 856  | BCR  | C15-C14 | 4.84  | 1.58        | 1.43     |
| 24  | I     | 4001 | BCR  | C15-C14 | 4.84  | 1.58        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | B     | 853 | BCR  | C19-C18 | 4.84  | 1.56        | 1.46     |
| 24  | 8     | 304 | BCR  | C15-C14 | 4.84  | 1.58        | 1.43     |
| 24  | B     | 849 | BCR  | C15-C14 | 4.83  | 1.58        | 1.43     |
| 24  | 3     | 307 | BCR  | C15-C14 | 4.82  | 1.58        | 1.43     |
| 32  | F     | 306 | RRX  | C24-C25 | 4.82  | 1.61        | 1.45     |
| 24  | F     | 303 | BCR  | C15-C14 | 4.82  | 1.58        | 1.43     |
| 24  | B     | 848 | BCR  | C15-C14 | 4.82  | 1.58        | 1.43     |
| 24  | 4     | 804 | BCR  | C15-C14 | 4.81  | 1.58        | 1.43     |
| 24  | G     | 203 | BCR  | C15-C14 | 4.81  | 1.58        | 1.43     |
| 24  | B     | 845 | BCR  | C15-C14 | 4.81  | 1.58        | 1.43     |
| 38  | 3     | 302 | LUT  | C8-C9   | 4.81  | 1.56        | 1.46     |
| 24  | B     | 846 | BCR  | C15-C14 | 4.80  | 1.58        | 1.43     |
| 24  | 5     | 305 | BCR  | C15-C14 | 4.80  | 1.58        | 1.43     |
| 24  | A     | 845 | BCR  | C15-C14 | 4.80  | 1.58        | 1.43     |
| 24  | A     | 847 | BCR  | C15-C14 | 4.80  | 1.58        | 1.43     |
| 24  | B     | 844 | BCR  | C15-C14 | 4.79  | 1.58        | 1.43     |
| 36  | J     | 105 | C7Z  | C24-C25 | -4.78 | 1.43        | 1.51     |
| 24  | K     | 206 | BCR  | C15-C14 | 4.76  | 1.57        | 1.43     |
| 39  | Z     | 311 | CHL  | C3B-C4B | 4.76  | 1.46        | 1.41     |
| 24  | L     | 204 | BCR  | C15-C14 | 4.76  | 1.57        | 1.43     |
| 24  | 7     | 303 | BCR  | C2-C1   | 4.74  | 1.64        | 1.54     |
| 24  | 7     | 303 | BCR  | C19-C18 | 4.74  | 1.56        | 1.46     |
| 24  | 4     | 804 | BCR  | C2-C1   | 4.73  | 1.64        | 1.54     |
| 24  | A     | 846 | BCR  | C15-C14 | 4.73  | 1.57        | 1.43     |
| 24  | 5     | 305 | BCR  | C19-C18 | 4.73  | 1.56        | 1.46     |
| 24  | J     | 104 | BCR  | C2-C1   | 4.73  | 1.64        | 1.54     |
| 24  | B     | 847 | BCR  | C15-C14 | 4.73  | 1.57        | 1.43     |
| 39  | 7     | 313 | CHL  | C3B-C4B | 4.73  | 1.46        | 1.41     |
| 38  | Z     | 301 | LUT  | C12-C13 | 4.72  | 1.56        | 1.46     |
| 21  | A     | 801 | CL0  | CHD-C4C | 4.72  | 1.48        | 1.39     |
| 24  | 3     | 307 | BCR  | C19-C18 | 4.72  | 1.56        | 1.46     |
| 24  | 3     | 306 | BCR  | C2-C1   | 4.72  | 1.64        | 1.54     |
| 24  | B     | 848 | BCR  | C2-C1   | 4.71  | 1.64        | 1.54     |
| 24  | 8     | 304 | BCR  | C2-C1   | 4.71  | 1.64        | 1.54     |
| 24  | 6     | 306 | BCR  | C15-C14 | 4.70  | 1.57        | 1.43     |
| 38  | 1     | 302 | LUT  | C12-C13 | 4.70  | 1.56        | 1.46     |
| 24  | A     | 848 | BCR  | C19-C18 | 4.70  | 1.56        | 1.46     |
| 39  | 8     | 301 | CHL  | C3B-C4B | 4.70  | 1.46        | 1.41     |
| 24  | A     | 856 | BCR  | C19-C18 | 4.69  | 1.56        | 1.46     |
| 24  | B     | 845 | BCR  | C2-C1   | 4.69  | 1.64        | 1.54     |
| 24  | A     | 847 | BCR  | C2-C1   | 4.69  | 1.64        | 1.54     |
| 24  | B     | 849 | BCR  | C19-C18 | 4.69  | 1.56        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 38  | Z     | 302  | LUT  | C12-C13 | 4.69  | 1.56        | 1.46     |
| 24  | A     | 846  | BCR  | C2-C1   | 4.68  | 1.64        | 1.54     |
| 24  | 6     | 305  | BCR  | C2-C1   | 4.68  | 1.64        | 1.54     |
| 24  | L     | 204  | BCR  | C2-C1   | 4.68  | 1.64        | 1.54     |
| 39  | 4     | 816  | CHL  | C3B-C4B | 4.68  | 1.45        | 1.41     |
| 39  | 4     | 813  | CHL  | C3B-C4B | 4.67  | 1.45        | 1.41     |
| 24  | 3     | 307  | BCR  | C2-C1   | 4.67  | 1.64        | 1.54     |
| 24  | G     | 203  | BCR  | C19-C18 | 4.67  | 1.55        | 1.46     |
| 36  | 5     | 306  | C7Z  | C28-C29 | 4.66  | 1.55        | 1.46     |
| 24  | 3     | 304  | BCR  | C2-C1   | 4.66  | 1.64        | 1.54     |
| 24  | A     | 844  | BCR  | C2-C1   | 4.65  | 1.64        | 1.54     |
| 24  | 4     | 804  | BCR  | C19-C18 | 4.65  | 1.55        | 1.46     |
| 24  | A     | 848  | BCR  | C2-C1   | 4.65  | 1.64        | 1.54     |
| 24  | 8     | 304  | BCR  | C19-C18 | 4.65  | 1.55        | 1.46     |
| 24  | J     | 104  | BCR  | C19-C18 | 4.65  | 1.55        | 1.46     |
| 21  | A     | 801  | CL0  | CHC-C1C | 4.65  | 1.48        | 1.39     |
| 36  | J     | 105  | C7Z  | C28-C29 | 4.65  | 1.55        | 1.46     |
| 38  | 9     | 302  | LUT  | C4-C5   | -4.65 | 1.43        | 1.51     |
| 24  | F     | 303  | BCR  | C19-C18 | 4.64  | 1.55        | 1.46     |
| 38  | 7     | 302  | LUT  | C12-C13 | 4.64  | 1.55        | 1.46     |
| 24  | 3     | 305  | BCR  | C19-C18 | 4.64  | 1.55        | 1.46     |
| 24  | 6     | 306  | BCR  | C2-C1   | 4.64  | 1.64        | 1.54     |
| 38  | 6     | 303  | LUT  | C12-C13 | 4.63  | 1.55        | 1.46     |
| 38  | 1     | 303  | LUT  | C12-C13 | 4.63  | 1.55        | 1.46     |
| 24  | 3     | 306  | BCR  | C19-C18 | 4.63  | 1.55        | 1.46     |
| 24  | 3     | 304  | BCR  | C19-C18 | 4.62  | 1.55        | 1.46     |
| 24  | B     | 853  | BCR  | C2-C1   | 4.62  | 1.64        | 1.54     |
| 36  | 5     | 306  | C7Z  | C31-C30 | 4.62  | 1.57        | 1.43     |
| 38  | 4     | 802  | LUT  | C4-C5   | -4.61 | 1.43        | 1.51     |
| 24  | K     | 206  | BCR  | C19-C18 | 4.60  | 1.55        | 1.46     |
| 24  | A     | 844  | BCR  | C19-C18 | 4.60  | 1.55        | 1.46     |
| 38  | 5     | 303  | LUT  | C12-C13 | 4.60  | 1.55        | 1.46     |
| 24  | B     | 853  | BCR  | C28-C27 | 4.60  | 1.66        | 1.52     |
| 24  | B     | 848  | BCR  | C19-C18 | 4.60  | 1.55        | 1.46     |
| 24  | B     | 845  | BCR  | C19-C18 | 4.60  | 1.55        | 1.46     |
| 38  | 3     | 303  | LUT  | C12-C13 | 4.60  | 1.55        | 1.46     |
| 38  | 8     | 303  | LUT  | C12-C13 | 4.60  | 1.55        | 1.46     |
| 24  | B     | 847  | BCR  | C19-C18 | 4.60  | 1.55        | 1.46     |
| 24  | I     | 4001 | BCR  | C2-C1   | 4.59  | 1.64        | 1.54     |
| 24  | B     | 849  | BCR  | C2-C1   | 4.59  | 1.64        | 1.54     |
| 38  | 7     | 301  | LUT  | C12-C13 | 4.59  | 1.55        | 1.46     |
| 39  | 5     | 321  | CHL  | C3B-C4B | 4.59  | 1.45        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 38  | 4     | 803  | LUT  | C12-C13 | 4.58  | 1.55        | 1.46     |
| 24  | 5     | 304  | BCR  | C2-C1   | 4.58  | 1.64        | 1.54     |
| 24  | A     | 845  | BCR  | C19-C18 | 4.58  | 1.55        | 1.46     |
| 38  | 6     | 304  | LUT  | C12-C13 | 4.58  | 1.55        | 1.46     |
| 24  | A     | 845  | BCR  | C2-C1   | 4.57  | 1.64        | 1.54     |
| 24  | B     | 844  | BCR  | C19-C18 | 4.57  | 1.55        | 1.46     |
| 24  | 5     | 305  | BCR  | C2-C1   | 4.57  | 1.64        | 1.54     |
| 24  | B     | 846  | BCR  | C2-C1   | 4.57  | 1.64        | 1.54     |
| 24  | I     | 4001 | BCR  | C19-C18 | 4.57  | 1.55        | 1.46     |
| 39  | 5     | 316  | CHL  | C3B-C4B | 4.56  | 1.45        | 1.41     |
| 24  | K     | 206  | BCR  | C2-C1   | 4.56  | 1.64        | 1.54     |
| 24  | L     | 204  | BCR  | C19-C18 | 4.56  | 1.55        | 1.46     |
| 24  | 5     | 304  | BCR  | C19-C18 | 4.56  | 1.55        | 1.46     |
| 24  | B     | 846  | BCR  | C19-C18 | 4.55  | 1.55        | 1.46     |
| 24  | 6     | 305  | BCR  | C19-C18 | 4.55  | 1.55        | 1.46     |
| 21  | A     | 801  | CL0  | C3D-C4D | -4.54 | 1.34        | 1.41     |
| 24  | A     | 856  | BCR  | C2-C1   | 4.54  | 1.64        | 1.54     |
| 38  | 7     | 302  | LUT  | C4-C5   | -4.54 | 1.44        | 1.51     |
| 39  | 6     | 315  | CHL  | C3A-C2A | -4.54 | 1.50        | 1.54     |
| 38  | 5     | 302  | LUT  | C12-C13 | 4.53  | 1.55        | 1.46     |
| 24  | B     | 844  | BCR  | C2-C1   | 4.53  | 1.64        | 1.54     |
| 38  | 9     | 302  | LUT  | C12-C13 | 4.53  | 1.55        | 1.46     |
| 38  | 8     | 302  | LUT  | C12-C13 | 4.52  | 1.55        | 1.46     |
| 36  | J     | 105  | C7Z  | C31-C30 | 4.52  | 1.57        | 1.43     |
| 38  | 9     | 301  | LUT  | C12-C13 | 4.52  | 1.55        | 1.46     |
| 38  | 4     | 802  | LUT  | C12-C13 | 4.52  | 1.55        | 1.46     |
| 24  | F     | 303  | BCR  | C2-C1   | 4.51  | 1.64        | 1.54     |
| 39  | 6     | 320  | CHL  | C3B-C4B | 4.51  | 1.45        | 1.41     |
| 24  | B     | 847  | BCR  | C2-C1   | 4.50  | 1.64        | 1.54     |
| 24  | A     | 846  | BCR  | C19-C18 | 4.50  | 1.55        | 1.46     |
| 24  | A     | 847  | BCR  | C19-C18 | 4.49  | 1.55        | 1.46     |
| 38  | 4     | 803  | LUT  | C4-C5   | -4.49 | 1.44        | 1.51     |
| 38  | Z     | 301  | LUT  | C31-C30 | 4.49  | 1.57        | 1.43     |
| 38  | 7     | 301  | LUT  | C4-C5   | -4.49 | 1.44        | 1.51     |
| 38  | Z     | 301  | LUT  | C15-C14 | 4.48  | 1.57        | 1.43     |
| 21  | A     | 801  | CL0  | C3D-C2D | 4.48  | 1.47        | 1.39     |
| 38  | 1     | 302  | LUT  | C15-C14 | 4.48  | 1.57        | 1.43     |
| 38  | 5     | 303  | LUT  | C4-C5   | -4.48 | 1.44        | 1.51     |
| 38  | 3     | 303  | LUT  | C4-C5   | -4.47 | 1.44        | 1.51     |
| 38  | 6     | 304  | LUT  | C4-C5   | -4.47 | 1.44        | 1.51     |
| 38  | 9     | 301  | LUT  | C4-C5   | -4.47 | 1.44        | 1.51     |
| 32  | F     | 306  | RRX  | C12-C13 | 4.47  | 1.55        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 38  | 8     | 303 | LUT  | C4-C5   | -4.47 | 1.44        | 1.51     |
| 39  | 2     | 303 | CHL  | C3A-C2A | -4.47 | 1.50        | 1.54     |
| 38  | Z     | 302 | LUT  | C31-C30 | 4.45  | 1.57        | 1.43     |
| 38  | Z     | 302 | LUT  | C15-C14 | 4.45  | 1.57        | 1.43     |
| 38  | 1     | 303 | LUT  | C15-C14 | 4.45  | 1.57        | 1.43     |
| 24  | 8     | 304 | BCR  | C20-C21 | 4.45  | 1.57        | 1.43     |
| 24  | A     | 856 | BCR  | C20-C21 | 4.45  | 1.57        | 1.43     |
| 38  | Z     | 302 | LUT  | C4-C5   | -4.45 | 1.44        | 1.51     |
| 24  | G     | 203 | BCR  | C2-C1   | 4.45  | 1.64        | 1.54     |
| 39  | 6     | 318 | CHL  | C3B-C4B | 4.44  | 1.45        | 1.41     |
| 38  | 7     | 302 | LUT  | C15-C14 | 4.44  | 1.56        | 1.43     |
| 38  | 5     | 302 | LUT  | C4-C5   | -4.43 | 1.44        | 1.51     |
| 38  | 5     | 303 | LUT  | C31-C30 | 4.43  | 1.56        | 1.43     |
| 39  | 3     | 317 | CHL  | C3B-C4B | 4.43  | 1.45        | 1.41     |
| 38  | 3     | 302 | LUT  | C31-C30 | 4.43  | 1.56        | 1.43     |
| 24  | 3     | 305 | BCR  | C2-C1   | 4.43  | 1.64        | 1.54     |
| 22  | A     | 817 | CLA  | CBB-CAB | 4.43  | 1.51        | 1.30     |
| 24  | 7     | 303 | BCR  | C20-C21 | 4.43  | 1.56        | 1.43     |
| 38  | 5     | 303 | LUT  | C15-C14 | 4.42  | 1.56        | 1.43     |
| 22  | A     | 830 | CLA  | CBB-CAB | 4.42  | 1.51        | 1.30     |
| 38  | 1     | 302 | LUT  | C35-C34 | 4.42  | 1.56        | 1.43     |
| 22  | 8     | 307 | CLA  | CBB-CAB | 4.42  | 1.51        | 1.30     |
| 38  | 8     | 302 | LUT  | C4-C5   | -4.42 | 1.44        | 1.51     |
| 24  | A     | 848 | BCR  | C20-C21 | 4.42  | 1.56        | 1.43     |
| 22  | 5     | 322 | CLA  | CBB-CAB | 4.42  | 1.51        | 1.30     |
| 22  | 6     | 308 | CLA  | CBB-CAB | 4.42  | 1.51        | 1.30     |
| 38  | 3     | 303 | LUT  | C15-C14 | 4.41  | 1.56        | 1.43     |
| 22  | B     | 831 | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | Z     | 306 | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 39  | Z     | 312 | CHL  | C3B-C4B | 4.41  | 1.45        | 1.41     |
| 38  | 3     | 303 | LUT  | C31-C30 | 4.41  | 1.56        | 1.43     |
| 22  | L     | 201 | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | 1     | 308 | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | A     | 808 | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | 8     | 313 | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | 5     | 309 | CLA  | CBB-CAB | 4.41  | 1.51        | 1.30     |
| 22  | B     | 834 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | B     | 808 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | Z     | 310 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | A     | 829 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | Z     | 304 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |
| 22  | B     | 822 | CLA  | CBB-CAB | 4.40  | 1.51        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | 6     | 321 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 4     | 809 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 5     | 318 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 2     | 301 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 7     | 304 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | Z     | 305 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 7     | 310 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 1     | 305 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 1     | 307 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | Z     | 308 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 7     | 311 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 39  | 2     | 303 | CHL  | C3B-C4B | 4.40 | 1.45        | 1.41     |
| 22  | 8     | 310 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 3     | 314 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 38  | 7     | 301 | LUT  | C15-C14 | 4.40 | 1.56        | 1.43     |
| 22  | A     | 820 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 1     | 309 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 8     | 306 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 5     | 307 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | B     | 826 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 38  | 6     | 304 | LUT  | C15-C14 | 4.40 | 1.56        | 1.43     |
| 22  | A     | 821 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | A     | 807 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 38  | 9     | 302 | LUT  | C31-C30 | 4.40 | 1.56        | 1.43     |
| 22  | 3     | 313 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 4     | 810 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 5     | 313 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 9     | 311 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | B     | 838 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 1     | 304 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | A     | 826 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 7     | 314 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | B     | 817 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 9     | 313 | CLA  | CBB-CAB | 4.40 | 1.51        | 1.30     |
| 22  | 6     | 302 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 3     | 309 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 7     | 315 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 5     | 326 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | J     | 103 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 807 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | F     | 305 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 5     | 301 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | 7     | 316 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 5     | 323 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 819 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 823 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 833 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 3     | 322 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 38  | 1     | 302 | LUT  | C31-C30 | 4.39 | 1.56        | 1.43     |
| 22  | 8     | 308 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 6     | 307 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | F     | 302 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 835 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | G     | 201 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 7     | 317 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 825 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 5     | 315 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 820 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 7     | 322 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 5     | 314 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 830 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 2     | 304 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 38  | 8     | 303 | LUT  | C31-C30 | 4.39 | 1.56        | 1.43     |
| 22  | 3     | 310 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 8     | 311 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 4     | 817 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 9     | 308 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 854 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 834 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 6     | 317 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 801 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 810 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 5     | 310 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 828 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 825 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 819 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 835 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 2     | 302 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 841 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | K     | 202 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 1     | 315 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 3     | 312 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 9     | 307 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 804 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | B     | 821 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 5     | 308 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 4     | 815 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 829 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 840 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 1     | 310 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 3     | 311 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 823 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 4     | 812 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 3     | 319 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 831 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | A     | 855 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | F     | 301 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | Z     | 313 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | B     | 836 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 8     | 314 | CLA  | CBB-CAB | 4.39 | 1.51        | 1.30     |
| 22  | 7     | 323 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | B     | 809 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | Z     | 303 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | A     | 832 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | 7     | 309 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | 8     | 316 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | 4     | 818 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | A     | 824 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | G     | 202 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | 7     | 307 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | 1     | 314 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | 7     | 308 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | B     | 827 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | 7     | 312 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | 5     | 312 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 24  | 3     | 307 | BCR  | C20-C21 | 4.38 | 1.56        | 1.43     |
| 22  | 6     | 319 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | A     | 818 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 24  | 3     | 304 | BCR  | C20-C21 | 4.38 | 1.56        | 1.43     |
| 22  | 7     | 324 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 38  | 1     | 303 | LUT  | C31-C30 | 4.38 | 1.56        | 1.43     |
| 22  | B     | 813 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | 3     | 318 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 38  | 8     | 303 | LUT  | C15-C14 | 4.38 | 1.56        | 1.43     |
| 22  | B     | 812 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |
| 22  | A     | 833 | CLA  | CBB-CAB | 4.38 | 1.51        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 832 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 6     | 301 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | A     | 815 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 1     | 313 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 3     | 308 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | A     | 805 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | B     | 842 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | A     | 814 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 24  | B     | 849 | BCR  | C20-C21 | 4.38  | 1.56        | 1.43     |
| 22  | A     | 822 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | L     | 202 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | A     | 802 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 6     | 311 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 38  | 7     | 301 | LUT  | C31-C30 | 4.38  | 1.56        | 1.43     |
| 22  | 3     | 316 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 24  | 4     | 804 | BCR  | C20-C21 | 4.38  | 1.56        | 1.43     |
| 22  | A     | 841 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 1     | 306 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | Z     | 314 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | B     | 818 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 6     | 313 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 39  | 4     | 819 | CHL  | C3B-C4B | 4.38  | 1.45        | 1.41     |
| 22  | B     | 816 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | B     | 839 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | B     | 811 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | A     | 803 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | L     | 203 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 4     | 806 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | B     | 837 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | 7     | 305 | CLA  | CBB-CAB | 4.38  | 1.51        | 1.30     |
| 22  | B     | 814 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 1     | 311 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 6     | 322 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | A     | 839 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | B     | 805 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 6     | 312 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 4     | 807 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 38  | Z     | 301 | LUT  | C35-C34 | 4.37  | 1.56        | 1.43     |
| 22  | B     | 824 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 38  | 3     | 302 | LUT  | C4-C5   | -4.37 | 1.44        | 1.51     |
| 22  | Z     | 307 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | A     | 816 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 4     | 811 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 9     | 306 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 38  | 7     | 302 | LUT  | C31-C30 | 4.37  | 1.56        | 1.43     |
| 38  | 6     | 303 | LUT  | C15-C14 | 4.37  | 1.56        | 1.43     |
| 22  | 3     | 315 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 24  | 3     | 305 | BCR  | C20-C21 | 4.37  | 1.56        | 1.43     |
| 22  | A     | 812 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 6     | 314 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | A     | 809 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | Z     | 316 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 38  | 6     | 304 | LUT  | C31-C30 | 4.37  | 1.56        | 1.43     |
| 24  | B     | 853 | BCR  | C20-C21 | 4.37  | 1.56        | 1.43     |
| 22  | 6     | 309 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 24  | F     | 303 | BCR  | C20-C21 | 4.37  | 1.56        | 1.43     |
| 22  | A     | 840 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 8     | 309 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | 8     | 305 | CLA  | CBB-CAB | 4.37  | 1.51        | 1.30     |
| 22  | B     | 815 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | B     | 828 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 24  | 5     | 304 | BCR  | C20-C21 | 4.36  | 1.56        | 1.43     |
| 22  | Z     | 309 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | F     | 304 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 4     | 805 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | 5     | 311 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | A     | 811 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 24  | 3     | 306 | BCR  | C20-C21 | 4.36  | 1.56        | 1.43     |
| 22  | 5     | 319 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | A     | 842 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | A     | 806 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | Z     | 315 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | A     | 837 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 22  | A     | 813 | CLA  | CBB-CAB | 4.36  | 1.51        | 1.30     |
| 38  | 9     | 301 | LUT  | C15-C14 | 4.36  | 1.56        | 1.43     |
| 22  | 5     | 320 | CLA  | MG-ND   | -4.36 | 1.97        | 2.05     |
| 22  | K     | 203 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 38  | 8     | 302 | LUT  | C15-C14 | 4.35  | 1.56        | 1.43     |
| 22  | A     | 836 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | 7     | 306 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 38  | 6     | 303 | LUT  | C31-C30 | 4.35  | 1.56        | 1.43     |
| 22  | A     | 838 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | B     | 806 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 22  | 4     | 808 | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 810  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 38  | 1     | 303  | LUT  | C4-C5   | -4.35 | 1.44        | 1.51     |
| 38  | 9     | 301  | LUT  | C31-C30 | 4.35  | 1.56        | 1.43     |
| 22  | K     | 204  | CLA  | CBB-CAB | 4.35  | 1.51        | 1.30     |
| 24  | K     | 206  | BCR  | C20-C21 | 4.35  | 1.56        | 1.43     |
| 24  | J     | 104  | BCR  | C20-C21 | 4.34  | 1.56        | 1.43     |
| 22  | K     | 205  | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 38  | 4     | 803  | LUT  | C15-C14 | 4.34  | 1.56        | 1.43     |
| 22  | 9     | 304  | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 38  | 9     | 302  | LUT  | C15-C14 | 4.34  | 1.56        | 1.43     |
| 22  | 6     | 310  | CLA  | CBB-CAB | 4.34  | 1.51        | 1.30     |
| 38  | 1     | 303  | LUT  | C35-C34 | 4.34  | 1.56        | 1.43     |
| 22  | A     | 827  | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 32  | F     | 306  | RRX  | C3-C4   | 4.33  | 1.66        | 1.52     |
| 24  | B     | 847  | BCR  | C20-C21 | 4.33  | 1.56        | 1.43     |
| 32  | F     | 306  | RRX  | C29-C30 | 4.33  | 1.67        | 1.54     |
| 38  | 4     | 802  | LUT  | C31-C30 | 4.33  | 1.56        | 1.43     |
| 24  | B     | 844  | BCR  | C20-C21 | 4.33  | 1.56        | 1.43     |
| 24  | I     | 4001 | BCR  | C20-C21 | 4.33  | 1.56        | 1.43     |
| 38  | Z     | 301  | LUT  | C4-C5   | -4.33 | 1.44        | 1.51     |
| 38  | 5     | 302  | LUT  | C15-C14 | 4.33  | 1.56        | 1.43     |
| 22  | 9     | 305  | CLA  | CBB-CAB | 4.33  | 1.51        | 1.30     |
| 38  | Z     | 302  | LUT  | C35-C34 | 4.33  | 1.56        | 1.43     |
| 24  | B     | 847  | BCR  | C28-C27 | 4.32  | 1.66        | 1.52     |
| 38  | 5     | 303  | LUT  | C35-C34 | 4.32  | 1.56        | 1.43     |
| 38  | 6     | 303  | LUT  | C4-C5   | -4.32 | 1.44        | 1.51     |
| 32  | F     | 306  | RRX  | C11-C10 | 4.32  | 1.56        | 1.43     |
| 38  | 4     | 802  | LUT  | C15-C14 | 4.32  | 1.56        | 1.43     |
| 31  | B     | 852  | DGD  | O1G-C1A | 4.32  | 1.45        | 1.33     |
| 22  | 1     | 316  | CLA  | CBB-CAB | 4.32  | 1.51        | 1.30     |
| 38  | 8     | 302  | LUT  | C31-C30 | 4.32  | 1.56        | 1.43     |
| 38  | 7     | 301  | LUT  | C35-C34 | 4.32  | 1.56        | 1.43     |
| 24  | A     | 856  | BCR  | C28-C27 | 4.32  | 1.66        | 1.52     |
| 38  | 7     | 302  | LUT  | C35-C34 | 4.31  | 1.56        | 1.43     |
| 39  | 6     | 316  | CHL  | C3B-C4B | 4.31  | 1.45        | 1.41     |
| 24  | A     | 844  | BCR  | C28-C27 | 4.31  | 1.66        | 1.52     |
| 24  | A     | 845  | BCR  | C20-C21 | 4.31  | 1.56        | 1.43     |
| 24  | 6     | 305  | BCR  | C20-C21 | 4.31  | 1.56        | 1.43     |
| 24  | L     | 204  | BCR  | C20-C21 | 4.31  | 1.56        | 1.43     |
| 38  | 6     | 304  | LUT  | C35-C34 | 4.31  | 1.56        | 1.43     |
| 24  | J     | 104  | BCR  | C28-C27 | 4.31  | 1.66        | 1.52     |
| 38  | 6     | 303  | LUT  | C35-C34 | 4.31  | 1.56        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | K     | 205  | CLA  | MG-ND   | -4.31 | 1.97        | 2.05     |
| 22  | 9     | 310  | CLA  | CBB-CAB | 4.31  | 1.51        | 1.30     |
| 22  | 9     | 309  | CLA  | CBB-CAB | 4.30  | 1.51        | 1.30     |
| 36  | 5     | 306  | C7Z  | C32-C33 | 4.30  | 1.55        | 1.46     |
| 22  | 3     | 320  | CLA  | CBB-CAB | 4.30  | 1.51        | 1.30     |
| 24  | B     | 845  | BCR  | C20-C21 | 4.30  | 1.56        | 1.43     |
| 24  | A     | 844  | BCR  | C20-C21 | 4.30  | 1.56        | 1.43     |
| 24  | G     | 203  | BCR  | C20-C21 | 4.30  | 1.56        | 1.43     |
| 39  | 3     | 317  | CHL  | C3A-C2A | -4.30 | 1.51        | 1.54     |
| 38  | 4     | 803  | LUT  | C31-C30 | 4.29  | 1.56        | 1.43     |
| 24  | B     | 846  | BCR  | C20-C21 | 4.29  | 1.56        | 1.43     |
| 36  | J     | 105  | C7Z  | C32-C33 | 4.29  | 1.55        | 1.46     |
| 38  | 3     | 302  | LUT  | C12-C13 | 4.29  | 1.55        | 1.46     |
| 24  | A     | 847  | BCR  | C20-C21 | 4.29  | 1.56        | 1.43     |
| 31  | 3     | 301  | DGD  | O1G-C1A | 4.29  | 1.45        | 1.33     |
| 24  | B     | 845  | BCR  | C28-C27 | 4.29  | 1.65        | 1.52     |
| 24  | B     | 848  | BCR  | C20-C21 | 4.29  | 1.56        | 1.43     |
| 24  | L     | 204  | BCR  | C28-C27 | 4.29  | 1.65        | 1.52     |
| 24  | I     | 4001 | BCR  | C28-C27 | 4.28  | 1.65        | 1.52     |
| 24  | 5     | 304  | BCR  | C28-C27 | 4.28  | 1.65        | 1.52     |
| 24  | 5     | 305  | BCR  | C20-C21 | 4.28  | 1.56        | 1.43     |
| 22  | 5     | 320  | CLA  | CBB-CAB | 4.28  | 1.50        | 1.30     |
| 24  | A     | 848  | BCR  | C28-C27 | 4.28  | 1.65        | 1.52     |
| 38  | 8     | 302  | LUT  | C35-C34 | 4.28  | 1.56        | 1.43     |
| 38  | 8     | 303  | LUT  | C35-C34 | 4.27  | 1.56        | 1.43     |
| 38  | 5     | 302  | LUT  | C31-C30 | 4.27  | 1.56        | 1.43     |
| 24  | B     | 849  | BCR  | C28-C27 | 4.27  | 1.65        | 1.52     |
| 24  | A     | 846  | BCR  | C20-C21 | 4.27  | 1.56        | 1.43     |
| 38  | 4     | 803  | LUT  | C35-C34 | 4.27  | 1.56        | 1.43     |
| 38  | 9     | 301  | LUT  | C35-C34 | 4.27  | 1.56        | 1.43     |
| 38  | 3     | 303  | LUT  | C35-C34 | 4.27  | 1.56        | 1.43     |
| 24  | 3     | 305  | BCR  | C28-C27 | 4.26  | 1.65        | 1.52     |
| 38  | 9     | 302  | LUT  | C35-C34 | 4.26  | 1.56        | 1.43     |
| 24  | 6     | 306  | BCR  | C19-C18 | 4.25  | 1.55        | 1.46     |
| 24  | 3     | 306  | BCR  | C28-C27 | 4.25  | 1.65        | 1.52     |
| 24  | A     | 845  | BCR  | C28-C27 | 4.24  | 1.65        | 1.52     |
| 24  | K     | 206  | BCR  | C28-C27 | 4.24  | 1.65        | 1.52     |
| 38  | 4     | 802  | LUT  | C35-C34 | 4.24  | 1.56        | 1.43     |
| 38  | Z     | 301  | LUT  | C7-C6   | 4.23  | 1.59        | 1.45     |
| 24  | A     | 847  | BCR  | C28-C27 | 4.22  | 1.65        | 1.52     |
| 38  | 6     | 303  | LUT  | C7-C6   | 4.22  | 1.59        | 1.45     |
| 38  | 3     | 302  | LUT  | C15-C14 | 4.21  | 1.56        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 39  | 1     | 312 | CHL  | C3B-C4B | 4.21  | 1.45        | 1.41     |
| 24  | B     | 844 | BCR  | C28-C27 | 4.21  | 1.65        | 1.52     |
| 38  | Z     | 301 | LUT  | C28-C29 | 4.20  | 1.54        | 1.46     |
| 38  | 1     | 302 | LUT  | C7-C6   | 4.20  | 1.59        | 1.45     |
| 24  | 5     | 305 | BCR  | C28-C27 | 4.20  | 1.65        | 1.52     |
| 22  | 9     | 303 | CLA  | CBB-CAB | 4.19  | 1.50        | 1.30     |
| 38  | 5     | 302 | LUT  | C35-C34 | 4.18  | 1.56        | 1.43     |
| 24  | 7     | 303 | BCR  | C28-C27 | 4.18  | 1.65        | 1.52     |
| 38  | 7     | 302 | LUT  | C7-C6   | 4.18  | 1.59        | 1.45     |
| 32  | F     | 306 | RRX  | C15-C14 | 4.18  | 1.56        | 1.43     |
| 38  | Z     | 302 | LUT  | C7-C6   | 4.18  | 1.59        | 1.45     |
| 24  | A     | 846 | BCR  | C28-C27 | 4.18  | 1.65        | 1.52     |
| 24  | 4     | 804 | BCR  | C28-C27 | 4.18  | 1.65        | 1.52     |
| 38  | 5     | 303 | LUT  | C7-C6   | 4.17  | 1.59        | 1.45     |
| 38  | 6     | 304 | LUT  | C7-C6   | 4.16  | 1.59        | 1.45     |
| 38  | 3     | 302 | LUT  | C35-C34 | 4.16  | 1.56        | 1.43     |
| 24  | 3     | 307 | BCR  | C28-C27 | 4.16  | 1.65        | 1.52     |
| 24  | 3     | 304 | BCR  | C28-C27 | 4.16  | 1.65        | 1.52     |
| 38  | 9     | 301 | LUT  | C7-C6   | 4.16  | 1.59        | 1.45     |
| 31  | 1     | 319 | DGD  | O1G-C1A | 4.16  | 1.45        | 1.33     |
| 24  | B     | 846 | BCR  | C28-C27 | 4.15  | 1.65        | 1.52     |
| 38  | 5     | 302 | LUT  | C7-C6   | 4.15  | 1.59        | 1.45     |
| 24  | 6     | 306 | BCR  | C20-C21 | 4.15  | 1.56        | 1.43     |
| 38  | 9     | 302 | LUT  | C7-C6   | 4.15  | 1.59        | 1.45     |
| 39  | 6     | 320 | CHL  | C3A-C2A | -4.15 | 1.51        | 1.54     |
| 38  | 8     | 302 | LUT  | C7-C6   | 4.15  | 1.59        | 1.45     |
| 38  | 3     | 303 | LUT  | C7-C6   | 4.15  | 1.59        | 1.45     |
| 24  | F     | 303 | BCR  | C28-C27 | 4.14  | 1.65        | 1.52     |
| 38  | 3     | 302 | LUT  | C28-C29 | 4.14  | 1.54        | 1.46     |
| 39  | 4     | 819 | CHL  | C3A-C2A | -4.14 | 1.51        | 1.54     |
| 38  | 1     | 303 | LUT  | C7-C6   | 4.14  | 1.59        | 1.45     |
| 22  | 1     | 316 | CLA  | MG-ND   | -4.14 | 1.97        | 2.05     |
| 38  | 8     | 303 | LUT  | C7-C6   | 4.14  | 1.59        | 1.45     |
| 38  | 1     | 302 | LUT  | C28-C29 | 4.14  | 1.54        | 1.46     |
| 38  | 7     | 301 | LUT  | C7-C6   | 4.13  | 1.59        | 1.45     |
| 24  | B     | 848 | BCR  | C28-C27 | 4.13  | 1.65        | 1.52     |
| 24  | 6     | 306 | BCR  | C28-C27 | 4.12  | 1.65        | 1.52     |
| 38  | 4     | 803 | LUT  | C7-C6   | 4.12  | 1.59        | 1.45     |
| 36  | 5     | 306 | C7Z  | C22-C21 | 4.12  | 1.67        | 1.54     |
| 32  | F     | 306 | RRX  | C16-C17 | 4.12  | 1.55        | 1.43     |
| 38  | 4     | 802 | LUT  | C7-C6   | 4.11  | 1.59        | 1.45     |
| 24  | G     | 203 | BCR  | C28-C27 | 4.10  | 1.65        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | 8     | 304  | BCR  | C28-C27 | 4.10  | 1.65        | 1.52     |
| 24  | 6     | 305  | BCR  | C28-C27 | 4.09  | 1.65        | 1.52     |
| 38  | 3     | 302  | LUT  | C7-C6   | 4.09  | 1.59        | 1.45     |
| 38  | Z     | 302  | LUT  | C28-C29 | 4.07  | 1.54        | 1.46     |
| 38  | 5     | 303  | LUT  | C28-C29 | 4.05  | 1.54        | 1.46     |
| 39  | 9     | 314  | CHL  | C3B-C4B | 4.05  | 1.45        | 1.41     |
| 38  | 8     | 302  | LUT  | C28-C29 | 4.05  | 1.54        | 1.46     |
| 38  | 1     | 303  | LUT  | C28-C29 | 4.04  | 1.54        | 1.46     |
| 38  | 3     | 303  | LUT  | C28-C29 | 4.04  | 1.54        | 1.46     |
| 32  | F     | 306  | RRX  | C20-C21 | 4.03  | 1.55        | 1.43     |
| 38  | 9     | 302  | LUT  | C28-C29 | 4.03  | 1.54        | 1.46     |
| 38  | 6     | 303  | LUT  | C28-C29 | 4.03  | 1.54        | 1.46     |
| 38  | 8     | 303  | LUT  | C28-C29 | 4.03  | 1.54        | 1.46     |
| 38  | 6     | 304  | LUT  | C28-C29 | 4.03  | 1.54        | 1.46     |
| 38  | 7     | 301  | LUT  | C28-C29 | 4.03  | 1.54        | 1.46     |
| 39  | 6     | 315  | CHL  | C3B-C4B | 4.02  | 1.45        | 1.41     |
| 22  | 9     | 309  | CLA  | MG-ND   | -4.02 | 1.97        | 2.05     |
| 24  | 3     | 306  | BCR  | C11-C10 | 4.02  | 1.55        | 1.43     |
| 38  | 9     | 301  | LUT  | C28-C29 | 4.01  | 1.54        | 1.46     |
| 22  | K     | 205  | CLA  | C1C-NC  | -4.01 | 1.31        | 1.37     |
| 38  | 8     | 302  | LUT  | C21-C26 | 4.01  | 1.67        | 1.56     |
| 24  | 8     | 304  | BCR  | C3-C4   | 4.00  | 1.65        | 1.52     |
| 39  | 7     | 313  | CHL  | C3A-C2A | -4.00 | 1.51        | 1.54     |
| 36  | J     | 105  | C7Z  | C22-C21 | 3.99  | 1.66        | 1.54     |
| 38  | 5     | 302  | LUT  | C28-C29 | 3.99  | 1.54        | 1.46     |
| 22  | 3     | 315  | CLA  | MG-ND   | -3.99 | 1.97        | 2.05     |
| 24  | 3     | 307  | BCR  | C3-C4   | 3.99  | 1.64        | 1.52     |
| 24  | A     | 845  | BCR  | C3-C4   | 3.98  | 1.64        | 1.52     |
| 24  | 5     | 305  | BCR  | C11-C10 | 3.98  | 1.55        | 1.43     |
| 24  | L     | 204  | BCR  | C3-C4   | 3.98  | 1.64        | 1.52     |
| 24  | J     | 104  | BCR  | C3-C4   | 3.98  | 1.64        | 1.52     |
| 24  | 7     | 303  | BCR  | C3-C4   | 3.97  | 1.64        | 1.52     |
| 38  | 1     | 302  | LUT  | C4-C5   | -3.97 | 1.44        | 1.51     |
| 38  | 4     | 803  | LUT  | C28-C29 | 3.97  | 1.54        | 1.46     |
| 38  | 7     | 302  | LUT  | C28-C29 | 3.96  | 1.54        | 1.46     |
| 24  | A     | 848  | BCR  | C3-C4   | 3.96  | 1.64        | 1.52     |
| 24  | B     | 853  | BCR  | C16-C17 | 3.96  | 1.55        | 1.43     |
| 38  | 4     | 802  | LUT  | C28-C29 | 3.95  | 1.54        | 1.46     |
| 22  | 9     | 303  | CLA  | MG-ND   | -3.95 | 1.98        | 2.05     |
| 24  | I     | 4001 | BCR  | C3-C4   | 3.95  | 1.64        | 1.52     |
| 39  | 5     | 321  | CHL  | C1A-CHA | -3.95 | 1.35        | 1.40     |
| 24  | B     | 845  | BCR  | C3-C4   | 3.95  | 1.64        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | J     | 105 | C7Z  | C11-C10 | 3.94  | 1.55        | 1.43     |
| 36  | 5     | 306 | C7Z  | C15-C14 | 3.94  | 1.55        | 1.43     |
| 24  | 3     | 306 | BCR  | C16-C17 | 3.94  | 1.55        | 1.43     |
| 22  | 9     | 304 | CLA  | MG-ND   | -3.94 | 1.98        | 2.05     |
| 24  | A     | 856 | BCR  | C3-C4   | 3.93  | 1.64        | 1.52     |
| 36  | J     | 105 | C7Z  | C15-C14 | 3.93  | 1.55        | 1.43     |
| 38  | Z     | 301 | LUT  | C21-C26 | 3.93  | 1.67        | 1.56     |
| 24  | A     | 844 | BCR  | C16-C17 | 3.92  | 1.55        | 1.43     |
| 38  | 9     | 302 | LUT  | C21-C26 | 3.92  | 1.67        | 1.56     |
| 38  | 9     | 301 | LUT  | C21-C26 | 3.92  | 1.67        | 1.56     |
| 24  | B     | 853 | BCR  | C11-C10 | 3.91  | 1.55        | 1.43     |
| 24  | 6     | 306 | BCR  | C3-C4   | 3.91  | 1.64        | 1.52     |
| 38  | Z     | 302 | LUT  | C21-C26 | 3.91  | 1.67        | 1.56     |
| 24  | B     | 853 | BCR  | C3-C4   | 3.91  | 1.64        | 1.52     |
| 24  | B     | 846 | BCR  | C3-C4   | 3.91  | 1.64        | 1.52     |
| 39  | 4     | 814 | CHL  | C3B-C4B | 3.90  | 1.45        | 1.41     |
| 24  | L     | 204 | BCR  | C11-C10 | 3.90  | 1.55        | 1.43     |
| 36  | 5     | 306 | C7Z  | C27-C26 | 3.90  | 1.58        | 1.45     |
| 24  | 3     | 305 | BCR  | C3-C4   | 3.90  | 1.64        | 1.52     |
| 24  | G     | 203 | BCR  | C3-C4   | 3.90  | 1.64        | 1.52     |
| 24  | 3     | 304 | BCR  | C16-C17 | 3.90  | 1.55        | 1.43     |
| 38  | 8     | 303 | LUT  | C21-C26 | 3.89  | 1.67        | 1.56     |
| 38  | 3     | 303 | LUT  | C21-C26 | 3.89  | 1.67        | 1.56     |
| 24  | B     | 847 | BCR  | C3-C4   | 3.89  | 1.64        | 1.52     |
| 24  | F     | 303 | BCR  | C3-C4   | 3.89  | 1.64        | 1.52     |
| 38  | Z     | 301 | LUT  | C11-C10 | 3.88  | 1.55        | 1.43     |
| 22  | 9     | 305 | CLA  | MG-ND   | -3.88 | 1.98        | 2.05     |
| 24  | G     | 203 | BCR  | C11-C10 | 3.88  | 1.55        | 1.43     |
| 24  | A     | 844 | BCR  | C11-C10 | 3.88  | 1.55        | 1.43     |
| 24  | 3     | 306 | BCR  | C3-C4   | 3.88  | 1.64        | 1.52     |
| 22  | 9     | 310 | CLA  | MG-ND   | -3.88 | 1.98        | 2.05     |
| 24  | 7     | 303 | BCR  | C16-C17 | 3.88  | 1.55        | 1.43     |
| 36  | 5     | 306 | C7Z  | C11-C10 | 3.88  | 1.55        | 1.43     |
| 38  | 6     | 304 | LUT  | C21-C26 | 3.87  | 1.67        | 1.56     |
| 24  | 5     | 305 | BCR  | C3-C4   | 3.87  | 1.64        | 1.52     |
| 24  | A     | 848 | BCR  | C16-C17 | 3.87  | 1.55        | 1.43     |
| 38  | 4     | 803 | LUT  | C21-C26 | 3.87  | 1.67        | 1.56     |
| 39  | 8     | 312 | CHL  | C3B-C4B | 3.87  | 1.45        | 1.41     |
| 38  | 6     | 303 | LUT  | C11-C10 | 3.86  | 1.55        | 1.43     |
| 38  | 1     | 302 | LUT  | C21-C26 | 3.86  | 1.67        | 1.56     |
| 36  | J     | 105 | C7Z  | C27-C26 | 3.86  | 1.58        | 1.45     |
| 38  | 7     | 302 | LUT  | C21-C26 | 3.86  | 1.67        | 1.56     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | A     | 847  | BCR  | C3-C4   | 3.85  | 1.64        | 1.52     |
| 24  | 5     | 304  | BCR  | C3-C4   | 3.85  | 1.64        | 1.52     |
| 24  | A     | 856  | BCR  | C16-C17 | 3.85  | 1.55        | 1.43     |
| 24  | 3     | 305  | BCR  | C16-C17 | 3.85  | 1.55        | 1.43     |
| 22  | 3     | 320  | CLA  | MG-ND   | -3.85 | 1.98        | 2.05     |
| 24  | B     | 849  | BCR  | C11-C10 | 3.85  | 1.55        | 1.43     |
| 39  | 9     | 314  | CHL  | C2A-C3A | -3.85 | 1.51        | 1.54     |
| 24  | B     | 849  | BCR  | C16-C17 | 3.85  | 1.55        | 1.43     |
| 36  | 5     | 306  | C7Z  | C4-C5   | -3.85 | 1.45        | 1.51     |
| 24  | B     | 844  | BCR  | C3-C4   | 3.85  | 1.64        | 1.52     |
| 24  | K     | 206  | BCR  | C3-C4   | 3.84  | 1.64        | 1.52     |
| 38  | Z     | 302  | LUT  | C11-C10 | 3.84  | 1.55        | 1.43     |
| 38  | 5     | 302  | LUT  | C21-C26 | 3.84  | 1.67        | 1.56     |
| 24  | J     | 104  | BCR  | C16-C17 | 3.84  | 1.55        | 1.43     |
| 24  | I     | 4001 | BCR  | C16-C17 | 3.84  | 1.55        | 1.43     |
| 24  | 3     | 307  | BCR  | C16-C17 | 3.83  | 1.55        | 1.43     |
| 24  | F     | 303  | BCR  | C16-C17 | 3.83  | 1.55        | 1.43     |
| 24  | 5     | 305  | BCR  | C16-C17 | 3.83  | 1.55        | 1.43     |
| 24  | B     | 848  | BCR  | C3-C4   | 3.82  | 1.64        | 1.52     |
| 38  | 1     | 302  | LUT  | C11-C10 | 3.82  | 1.55        | 1.43     |
| 38  | 7     | 301  | LUT  | C21-C26 | 3.82  | 1.67        | 1.56     |
| 32  | F     | 306  | RRX  | C7-C6   | 3.82  | 1.58        | 1.45     |
| 24  | B     | 849  | BCR  | C3-C4   | 3.82  | 1.64        | 1.52     |
| 38  | 7     | 301  | LUT  | C11-C10 | 3.82  | 1.55        | 1.43     |
| 24  | A     | 845  | BCR  | C16-C17 | 3.82  | 1.55        | 1.43     |
| 24  | A     | 856  | BCR  | C11-C10 | 3.81  | 1.55        | 1.43     |
| 38  | 9     | 302  | LUT  | C38-C25 | 3.81  | 1.57        | 1.50     |
| 24  | G     | 203  | BCR  | C16-C17 | 3.81  | 1.55        | 1.43     |
| 24  | 4     | 804  | BCR  | C16-C17 | 3.81  | 1.55        | 1.43     |
| 24  | B     | 845  | BCR  | C16-C17 | 3.81  | 1.55        | 1.43     |
| 38  | 7     | 302  | LUT  | C11-C10 | 3.81  | 1.55        | 1.43     |
| 24  | B     | 846  | BCR  | C16-C17 | 3.81  | 1.55        | 1.43     |
| 38  | 1     | 303  | LUT  | C11-C10 | 3.81  | 1.55        | 1.43     |
| 24  | F     | 303  | BCR  | C11-C10 | 3.81  | 1.55        | 1.43     |
| 38  | 5     | 303  | LUT  | C11-C10 | 3.81  | 1.55        | 1.43     |
| 38  | 8     | 303  | LUT  | C11-C10 | 3.81  | 1.55        | 1.43     |
| 24  | A     | 846  | BCR  | C3-C4   | 3.80  | 1.64        | 1.52     |
| 24  | B     | 844  | BCR  | C11-C10 | 3.80  | 1.55        | 1.43     |
| 24  | A     | 848  | BCR  | C11-C10 | 3.80  | 1.55        | 1.43     |
| 24  | K     | 206  | BCR  | C16-C17 | 3.80  | 1.55        | 1.43     |
| 24  | 6     | 305  | BCR  | C16-C17 | 3.80  | 1.55        | 1.43     |
| 24  | J     | 104  | BCR  | C11-C10 | 3.80  | 1.55        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 38  | 3     | 302  | LUT  | C21-C26 | 3.79  | 1.66        | 1.56     |
| 24  | 6     | 305  | BCR  | C3-C4   | 3.79  | 1.64        | 1.52     |
| 38  | 1     | 303  | LUT  | C38-C25 | 3.79  | 1.57        | 1.50     |
| 38  | 1     | 303  | LUT  | C21-C26 | 3.79  | 1.66        | 1.56     |
| 38  | 3     | 303  | LUT  | C11-C10 | 3.79  | 1.54        | 1.43     |
| 38  | 6     | 304  | LUT  | C11-C10 | 3.79  | 1.54        | 1.43     |
| 24  | 7     | 303  | BCR  | C11-C10 | 3.79  | 1.54        | 1.43     |
| 24  | B     | 845  | BCR  | C11-C10 | 3.78  | 1.54        | 1.43     |
| 38  | 9     | 301  | LUT  | C11-C10 | 3.78  | 1.54        | 1.43     |
| 38  | 1     | 302  | LUT  | C19-C9  | 3.78  | 1.58        | 1.50     |
| 24  | 5     | 304  | BCR  | C16-C17 | 3.78  | 1.54        | 1.43     |
| 24  | 8     | 304  | BCR  | C16-C17 | 3.78  | 1.54        | 1.43     |
| 24  | 4     | 804  | BCR  | C11-C10 | 3.78  | 1.54        | 1.43     |
| 39  | 8     | 315  | CHL  | C3B-C4B | 3.78  | 1.45        | 1.41     |
| 24  | B     | 846  | BCR  | C11-C10 | 3.78  | 1.54        | 1.43     |
| 38  | 4     | 802  | LUT  | C21-C26 | 3.78  | 1.66        | 1.56     |
| 24  | 3     | 305  | BCR  | C11-C10 | 3.77  | 1.54        | 1.43     |
| 24  | B     | 844  | BCR  | C16-C17 | 3.77  | 1.54        | 1.43     |
| 38  | 5     | 303  | LUT  | C21-C26 | 3.77  | 1.66        | 1.56     |
| 24  | A     | 856  | BCR  | C24-C25 | 3.77  | 1.58        | 1.45     |
| 24  | 4     | 804  | BCR  | C3-C4   | 3.77  | 1.64        | 1.52     |
| 38  | 9     | 301  | LUT  | C38-C25 | 3.77  | 1.57        | 1.50     |
| 24  | I     | 4001 | BCR  | C11-C10 | 3.77  | 1.54        | 1.43     |
| 24  | L     | 204  | BCR  | C16-C17 | 3.77  | 1.54        | 1.43     |
| 24  | A     | 847  | BCR  | C16-C17 | 3.76  | 1.54        | 1.43     |
| 38  | 8     | 303  | LUT  | C38-C25 | 3.76  | 1.57        | 1.50     |
| 24  | 3     | 304  | BCR  | C11-C10 | 3.76  | 1.54        | 1.43     |
| 32  | F     | 306  | RRX  | C27-C26 | -3.75 | 1.45        | 1.51     |
| 38  | 5     | 302  | LUT  | C11-C10 | 3.75  | 1.54        | 1.43     |
| 38  | 4     | 802  | LUT  | C11-C10 | 3.75  | 1.54        | 1.43     |
| 24  | B     | 848  | BCR  | C16-C17 | 3.75  | 1.54        | 1.43     |
| 24  | 7     | 303  | BCR  | C24-C25 | 3.75  | 1.57        | 1.45     |
| 24  | B     | 847  | BCR  | C16-C17 | 3.75  | 1.54        | 1.43     |
| 38  | 8     | 302  | LUT  | C11-C10 | 3.75  | 1.54        | 1.43     |
| 24  | B     | 844  | BCR  | C24-C25 | 3.75  | 1.57        | 1.45     |
| 38  | 6     | 304  | LUT  | C38-C25 | 3.75  | 1.57        | 1.50     |
| 36  | J     | 105  | C7Z  | C35-C34 | 3.75  | 1.54        | 1.43     |
| 38  | 3     | 302  | LUT  | C19-C9  | 3.74  | 1.58        | 1.50     |
| 24  | 5     | 304  | BCR  | C11-C10 | 3.74  | 1.54        | 1.43     |
| 24  | A     | 845  | BCR  | C24-C25 | 3.74  | 1.57        | 1.45     |
| 36  | 5     | 306  | C7Z  | C35-C34 | 3.74  | 1.54        | 1.43     |
| 24  | 6     | 305  | BCR  | C4-C5   | -3.74 | 1.44        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | A     | 844 | BCR  | C3-C4   | 3.74  | 1.64        | 1.52     |
| 38  | 6     | 303 | LUT  | C21-C26 | 3.74  | 1.66        | 1.56     |
| 24  | A     | 848 | BCR  | C24-C25 | 3.74  | 1.57        | 1.45     |
| 24  | A     | 845 | BCR  | C11-C10 | 3.74  | 1.54        | 1.43     |
| 38  | Z     | 302 | LUT  | C19-C9  | 3.74  | 1.58        | 1.50     |
| 38  | 4     | 803 | LUT  | C11-C10 | 3.74  | 1.54        | 1.43     |
| 31  | B     | 852 | DGD  | CAA-C9A | -3.74 | 1.33        | 1.51     |
| 24  | 3     | 307 | BCR  | C24-C25 | 3.73  | 1.57        | 1.45     |
| 24  | 3     | 306 | BCR  | C24-C25 | 3.73  | 1.57        | 1.45     |
| 24  | 3     | 305 | BCR  | C24-C25 | 3.73  | 1.57        | 1.45     |
| 39  | 4     | 814 | CHL  | C3A-C2A | -3.73 | 1.51        | 1.54     |
| 38  | 7     | 302 | LUT  | C38-C25 | 3.73  | 1.57        | 1.50     |
| 24  | J     | 104 | BCR  | C24-C25 | 3.73  | 1.57        | 1.45     |
| 24  | 8     | 304 | BCR  | C24-C25 | 3.73  | 1.57        | 1.45     |
| 24  | A     | 846 | BCR  | C11-C10 | 3.73  | 1.54        | 1.43     |
| 38  | 4     | 803 | LUT  | C38-C25 | 3.73  | 1.57        | 1.50     |
| 31  | B     | 852 | DGD  | CDB-CCB | -3.73 | 1.33        | 1.51     |
| 24  | 3     | 304 | BCR  | C3-C4   | 3.72  | 1.64        | 1.52     |
| 22  | 1     | 316 | CLA  | C1C-NC  | -3.72 | 1.32        | 1.37     |
| 24  | B     | 847 | BCR  | C11-C10 | 3.72  | 1.54        | 1.43     |
| 31  | B     | 852 | DGD  | CAB-C9B | -3.71 | 1.33        | 1.51     |
| 24  | 6     | 305 | BCR  | C11-C10 | 3.71  | 1.54        | 1.43     |
| 38  | 6     | 303 | LUT  | C19-C9  | 3.71  | 1.58        | 1.50     |
| 38  | 5     | 303 | LUT  | C19-C9  | 3.71  | 1.58        | 1.50     |
| 24  | K     | 206 | BCR  | C11-C10 | 3.71  | 1.54        | 1.43     |
| 38  | 1     | 303 | LUT  | C19-C9  | 3.71  | 1.58        | 1.50     |
| 24  | G     | 203 | BCR  | C24-C25 | 3.71  | 1.57        | 1.45     |
| 38  | 9     | 302 | LUT  | C11-C10 | 3.71  | 1.54        | 1.43     |
| 38  | 9     | 301 | LUT  | C19-C9  | 3.71  | 1.58        | 1.50     |
| 24  | B     | 848 | BCR  | C11-C10 | 3.71  | 1.54        | 1.43     |
| 24  | 3     | 307 | BCR  | C11-C10 | 3.70  | 1.54        | 1.43     |
| 36  | J     | 105 | C7Z  | C2-C1   | 3.70  | 1.65        | 1.54     |
| 24  | 5     | 304 | BCR  | C24-C25 | 3.70  | 1.57        | 1.45     |
| 22  | 3     | 320 | CLA  | C1C-NC  | -3.70 | 1.32        | 1.37     |
| 24  | 6     | 306 | BCR  | C11-C10 | 3.70  | 1.54        | 1.43     |
| 22  | 5     | 320 | CLA  | C1C-NC  | -3.69 | 1.32        | 1.37     |
| 38  | 8     | 302 | LUT  | C38-C25 | 3.69  | 1.57        | 1.50     |
| 38  | 4     | 802 | LUT  | C19-C9  | 3.69  | 1.58        | 1.50     |
| 24  | 3     | 304 | BCR  | C24-C25 | 3.69  | 1.57        | 1.45     |
| 24  | 8     | 304 | BCR  | C11-C10 | 3.69  | 1.54        | 1.43     |
| 36  | J     | 105 | C7Z  | C4-C5   | -3.69 | 1.45        | 1.51     |
| 24  | 5     | 305 | BCR  | C24-C25 | 3.69  | 1.57        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 852 | DGD  | CGB-CFB | -3.69 | 1.33        | 1.51     |
| 31  | 1     | 319 | DGD  | CAA-C9A | -3.69 | 1.33        | 1.51     |
| 38  | 6     | 304 | LUT  | C19-C9  | 3.69  | 1.58        | 1.50     |
| 24  | B     | 849 | BCR  | C24-C25 | 3.69  | 1.57        | 1.45     |
| 24  | 4     | 804 | BCR  | C24-C25 | 3.69  | 1.57        | 1.45     |
| 24  | A     | 847 | BCR  | C11-C10 | 3.69  | 1.54        | 1.43     |
| 24  | A     | 846 | BCR  | C16-C17 | 3.69  | 1.54        | 1.43     |
| 22  | 5     | 313 | CLA  | MG-ND   | -3.68 | 1.98        | 2.05     |
| 24  | L     | 204 | BCR  | C24-C25 | 3.68  | 1.57        | 1.45     |
| 24  | A     | 846 | BCR  | C24-C25 | 3.68  | 1.57        | 1.45     |
| 38  | 4     | 803 | LUT  | C19-C9  | 3.68  | 1.58        | 1.50     |
| 22  | 4     | 806 | CLA  | MG-ND   | -3.68 | 1.98        | 2.05     |
| 24  | B     | 845 | BCR  | C24-C25 | 3.68  | 1.57        | 1.45     |
| 31  | 3     | 301 | DGD  | CAA-C9A | -3.68 | 1.33        | 1.51     |
| 24  | K     | 206 | BCR  | C24-C25 | 3.68  | 1.57        | 1.45     |
| 38  | 5     | 303 | LUT  | C38-C25 | 3.68  | 1.57        | 1.50     |
| 22  | G     | 201 | CLA  | MG-ND   | -3.68 | 1.98        | 2.05     |
| 24  | B     | 846 | BCR  | C27-C26 | -3.68 | 1.44        | 1.51     |
| 22  | Z     | 305 | CLA  | MG-ND   | -3.68 | 1.98        | 2.05     |
| 38  | 7     | 302 | LUT  | C19-C9  | 3.67  | 1.58        | 1.50     |
| 38  | Z     | 302 | LUT  | C38-C25 | 3.67  | 1.57        | 1.50     |
| 22  | 7     | 306 | CLA  | MG-ND   | -3.67 | 1.98        | 2.05     |
| 38  | 5     | 302 | LUT  | C19-C9  | 3.67  | 1.58        | 1.50     |
| 22  | 5     | 320 | CLA  | C4B-NB  | -3.67 | 1.33        | 1.37     |
| 38  | 3     | 303 | LUT  | C19-C9  | 3.67  | 1.58        | 1.50     |
| 24  | 6     | 306 | BCR  | C16-C17 | 3.67  | 1.54        | 1.43     |
| 22  | A     | 820 | CLA  | MG-ND   | -3.67 | 1.98        | 2.05     |
| 22  | B     | 839 | CLA  | MG-ND   | -3.67 | 1.98        | 2.05     |
| 24  | A     | 844 | BCR  | C24-C25 | 3.67  | 1.57        | 1.45     |
| 22  | 9     | 303 | CLA  | C1C-NC  | -3.67 | 1.32        | 1.37     |
| 22  | A     | 816 | CLA  | MG-ND   | -3.67 | 1.98        | 2.05     |
| 22  | Z     | 313 | CLA  | MG-ND   | -3.67 | 1.98        | 2.05     |
| 24  | F     | 303 | BCR  | C24-C25 | 3.67  | 1.57        | 1.45     |
| 38  | 7     | 301 | LUT  | C19-C9  | 3.67  | 1.58        | 1.50     |
| 38  | 9     | 302 | LUT  | C19-C9  | 3.66  | 1.58        | 1.50     |
| 22  | 6     | 312 | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 38  | 5     | 302 | LUT  | C38-C25 | 3.66  | 1.57        | 1.50     |
| 38  | Z     | 301 | LUT  | C19-C9  | 3.66  | 1.58        | 1.50     |
| 22  | K     | 204 | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 22  | 1     | 305 | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 22  | 1     | 311 | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |
| 22  | 5     | 308 | CLA  | MG-ND   | -3.66 | 1.98        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 38  | 9     | 302 | LUT  | C2-C1   | 3.66  | 1.65        | 1.54     |
| 36  | 5     | 306 | C7Z  | C2-C1   | 3.66  | 1.65        | 1.54     |
| 38  | 6     | 303 | LUT  | C38-C25 | 3.66  | 1.57        | 1.50     |
| 24  | J     | 104 | BCR  | C27-C26 | -3.65 | 1.44        | 1.51     |
| 22  | 9     | 303 | CLA  | C4B-NB  | -3.65 | 1.33        | 1.37     |
| 24  | 6     | 305 | BCR  | C24-C25 | 3.65  | 1.57        | 1.45     |
| 24  | B     | 845 | BCR  | C4-C5   | -3.65 | 1.44        | 1.51     |
| 38  | 3     | 302 | LUT  | C11-C10 | 3.65  | 1.54        | 1.43     |
| 38  | 8     | 302 | LUT  | C19-C9  | 3.65  | 1.58        | 1.50     |
| 24  | A     | 847 | BCR  | C24-C25 | 3.65  | 1.57        | 1.45     |
| 22  | 6     | 309 | CLA  | MG-ND   | -3.65 | 1.98        | 2.05     |
| 22  | 8     | 309 | CLA  | MG-ND   | -3.65 | 1.98        | 2.05     |
| 22  | A     | 839 | CLA  | MG-ND   | -3.65 | 1.98        | 2.05     |
| 22  | 6     | 311 | CLA  | MG-ND   | -3.65 | 1.98        | 2.05     |
| 24  | G     | 203 | BCR  | C27-C26 | -3.65 | 1.44        | 1.51     |
| 24  | B     | 847 | BCR  | C24-C25 | 3.64  | 1.57        | 1.45     |
| 22  | 9     | 308 | CLA  | MG-ND   | -3.64 | 1.98        | 2.05     |
| 24  | B     | 845 | BCR  | C27-C26 | -3.64 | 1.44        | 1.51     |
| 38  | 3     | 302 | LUT  | C38-C25 | 3.64  | 1.57        | 1.50     |
| 24  | B     | 848 | BCR  | C24-C25 | 3.64  | 1.57        | 1.45     |
| 24  | 7     | 303 | BCR  | C4-C5   | -3.64 | 1.44        | 1.51     |
| 38  | Z     | 302 | LUT  | C2-C1   | 3.64  | 1.65        | 1.54     |
| 22  | 4     | 818 | CLA  | MG-ND   | -3.64 | 1.98        | 2.05     |
| 24  | L     | 204 | BCR  | C4-C5   | -3.64 | 1.44        | 1.51     |
| 22  | B     | 815 | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 22  | 5     | 309 | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 22  | 4     | 807 | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 22  | B     | 817 | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 38  | 8     | 303 | LUT  | C2-C1   | 3.63  | 1.65        | 1.54     |
| 22  | A     | 836 | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 22  | 5     | 311 | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 22  | K     | 203 | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 22  | 7     | 308 | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 22  | 6     | 302 | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 22  | 6     | 322 | CLA  | MG-ND   | -3.63 | 1.98        | 2.05     |
| 38  | 3     | 303 | LUT  | C38-C25 | 3.63  | 1.57        | 1.50     |
| 24  | 3     | 306 | BCR  | C4-C5   | -3.62 | 1.44        | 1.51     |
| 22  | 1     | 304 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |
| 24  | 3     | 304 | BCR  | C4-C5   | -3.62 | 1.44        | 1.51     |
| 38  | 8     | 303 | LUT  | C19-C9  | 3.62  | 1.58        | 1.50     |
| 22  | A     | 802 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |
| 22  | A     | 842 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 4     | 817 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |
| 22  | B     | 834 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |
| 22  | 1     | 313 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |
| 38  | 4     | 803 | LUT  | C2-C1   | 3.62  | 1.65        | 1.54     |
| 22  | 4     | 808 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |
| 24  | B     | 846 | BCR  | C24-C25 | 3.62  | 1.57        | 1.45     |
| 22  | A     | 835 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |
| 22  | 8     | 306 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |
| 38  | 6     | 304 | LUT  | C2-C1   | 3.62  | 1.65        | 1.54     |
| 22  | 1     | 316 | CLA  | C4B-NB  | -3.62 | 1.33        | 1.37     |
| 22  | 9     | 311 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |
| 24  | 5     | 304 | BCR  | C27-C26 | -3.62 | 1.44        | 1.51     |
| 38  | 3     | 303 | LUT  | C2-C1   | 3.62  | 1.65        | 1.54     |
| 22  | 4     | 809 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | A     | 829 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | K     | 205 | CLA  | C4B-NB  | -3.61 | 1.33        | 1.37     |
| 22  | K     | 202 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | 3     | 309 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | A     | 804 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | 7     | 309 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | 6     | 319 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | B     | 821 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | B     | 822 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | 7     | 305 | CLA  | MG-ND   | -3.61 | 1.98        | 2.05     |
| 22  | 5     | 315 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | A     | 832 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | B     | 806 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | F     | 304 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | 1     | 315 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | 5     | 314 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | 6     | 313 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 38  | 7     | 301 | LUT  | C2-C1   | 3.60  | 1.65        | 1.54     |
| 22  | Z     | 304 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | B     | 841 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | 3     | 310 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | B     | 836 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 24  | 8     | 304 | BCR  | C4-C5   | -3.60 | 1.44        | 1.51     |
| 22  | B     | 807 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | 4     | 812 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | L     | 203 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | 5     | 326 | CLA  | MG-ND   | -3.60 | 1.98        | 2.05     |
| 22  | 8     | 313 | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | B     | 801  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | A     | 831  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | 6     | 310  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | 2     | 302  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | A     | 838  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | A     | 814  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | A     | 854  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | 5     | 310  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | B     | 813  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 24  | A     | 848  | BCR  | C4-C5   | -3.59 | 1.44        | 1.51     |
| 22  | 2     | 301  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | 3     | 315  | CLA  | C1C-NC  | -3.59 | 1.32        | 1.37     |
| 24  | I     | 4001 | BCR  | C24-C25 | 3.59  | 1.57        | 1.45     |
| 38  | 5     | 303  | LUT  | C2-C1   | 3.59  | 1.65        | 1.54     |
| 22  | B     | 808  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | 3     | 308  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | 7     | 322  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | 8     | 305  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 38  | 1     | 302  | LUT  | C38-C25 | 3.59  | 1.57        | 1.50     |
| 22  | B     | 809  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | 3     | 322  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | Z     | 307  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 22  | 6     | 307  | CLA  | MG-ND   | -3.59 | 1.98        | 2.05     |
| 24  | A     | 844  | BCR  | C27-C26 | -3.58 | 1.44        | 1.51     |
| 38  | 1     | 303  | LUT  | C2-C1   | 3.58  | 1.65        | 1.54     |
| 24  | 4     | 804  | BCR  | C4-C5   | -3.58 | 1.44        | 1.51     |
| 22  | J     | 103  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 22  | 8     | 314  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 22  | 5     | 312  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 38  | 7     | 302  | LUT  | C2-C1   | 3.58  | 1.65        | 1.54     |
| 22  | B     | 837  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 22  | 3     | 312  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 24  | 8     | 304  | BCR  | C27-C26 | -3.58 | 1.44        | 1.51     |
| 24  | 3     | 307  | BCR  | C4-C5   | -3.58 | 1.44        | 1.51     |
| 22  | 9     | 313  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 22  | 3     | 314  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 22  | 7     | 314  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 22  | Z     | 315  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 22  | 8     | 310  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 22  | 6     | 317  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 22  | 3     | 319  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |
| 22  | B     | 826  | CLA  | MG-ND   | -3.58 | 1.98        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | 3     | 307  | BCR  | C27-C26 | -3.58 | 1.44        | 1.51     |
| 22  | A     | 817  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | B     | 832  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | A     | 813  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | A     | 821  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | A     | 827  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | 7     | 323  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 24  | A     | 856  | BCR  | C27-C26 | -3.57 | 1.44        | 1.51     |
| 22  | B     | 833  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | 1     | 306  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | Z     | 310  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | 7     | 324  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 38  | 8     | 302  | LUT  | C2-C1   | 3.57  | 1.65        | 1.54     |
| 38  | 4     | 802  | LUT  | C2-C1   | 3.57  | 1.65        | 1.54     |
| 22  | 6     | 308  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 38  | 1     | 302  | LUT  | C2-C1   | 3.57  | 1.65        | 1.54     |
| 22  | 4     | 805  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | 1     | 307  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 38  | Z     | 301  | LUT  | C2-C1   | 3.57  | 1.65        | 1.54     |
| 39  | Z     | 312  | CHL  | CBB-CAB | 3.57  | 1.51        | 1.29     |
| 22  | B     | 828  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | 9     | 306  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | 6     | 321  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 24  | B     | 848  | BCR  | C4-C5   | -3.57 | 1.44        | 1.51     |
| 22  | B     | 823  | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 22  | 7     | 307  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | A     | 809  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | L     | 202  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 39  | 4     | 814  | CHL  | CBB-CAB | 3.56  | 1.51        | 1.29     |
| 22  | 3     | 316  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | 8     | 307  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 38  | 6     | 303  | LUT  | C2-C1   | 3.56  | 1.65        | 1.54     |
| 22  | B     | 824  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | Z     | 303  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 24  | A     | 846  | BCR  | C27-C26 | -3.56 | 1.44        | 1.51     |
| 24  | I     | 4001 | BCR  | C27-C26 | -3.56 | 1.44        | 1.51     |
| 22  | A     | 828  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | A     | 840  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | 4     | 811  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | B     | 829  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | 3     | 311  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | B     | 831  | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 7     | 317 | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | 5     | 307 | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 38  | 5     | 302 | LUT  | C2-C1   | 3.56  | 1.65        | 1.54     |
| 38  | 9     | 301 | LUT  | C2-C1   | 3.56  | 1.65        | 1.54     |
| 22  | B     | 825 | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | B     | 835 | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | B     | 816 | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | Z     | 306 | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | B     | 830 | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 24  | 3     | 304 | BCR  | C27-C26 | -3.56 | 1.44        | 1.51     |
| 24  | 5     | 304 | BCR  | C4-C5   | -3.56 | 1.44        | 1.51     |
| 22  | B     | 811 | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | 7     | 310 | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | 9     | 307 | CLA  | MG-ND   | -3.56 | 1.98        | 2.05     |
| 22  | F     | 305 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 39  | 4     | 816 | CHL  | CBB-CAB | 3.55  | 1.51        | 1.29     |
| 39  | 5     | 317 | CHL  | C3B-C4B | 3.55  | 1.44        | 1.41     |
| 39  | 6     | 318 | CHL  | CBB-CAB | 3.55  | 1.51        | 1.29     |
| 22  | 7     | 304 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 22  | 7     | 316 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 22  | 2     | 304 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 39  | 6     | 316 | CHL  | CBB-CAB | 3.55  | 1.51        | 1.29     |
| 22  | A     | 826 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 22  | B     | 840 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 22  | A     | 815 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 22  | 5     | 301 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 22  | A     | 822 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 22  | A     | 825 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 22  | 1     | 310 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 22  | A     | 812 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 22  | 8     | 311 | CLA  | MG-ND   | -3.55 | 1.98        | 2.05     |
| 39  | 1     | 312 | CHL  | CBB-CAB | 3.54  | 1.51        | 1.29     |
| 24  | K     | 206 | BCR  | C27-C26 | -3.54 | 1.44        | 1.51     |
| 22  | 5     | 322 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 24  | 3     | 305 | BCR  | C27-C26 | -3.54 | 1.44        | 1.51     |
| 22  | A     | 830 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 22  | B     | 810 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 24  | A     | 846 | BCR  | C4-C5   | -3.54 | 1.44        | 1.51     |
| 22  | A     | 818 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 22  | 5     | 323 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 22  | 7     | 312 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 22  | 7     | 315 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | A     | 803 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 22  | 6     | 301 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 39  | 2     | 303 | CHL  | CBB-CAB | 3.54  | 1.51        | 1.29     |
| 39  | 9     | 312 | CHL  | C3B-C4B | 3.54  | 1.44        | 1.41     |
| 24  | K     | 206 | BCR  | C4-C5   | -3.54 | 1.44        | 1.51     |
| 39  | 8     | 312 | CHL  | CBB-CAB | 3.54  | 1.51        | 1.29     |
| 22  | B     | 820 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 24  | 6     | 305 | BCR  | C27-C26 | -3.54 | 1.44        | 1.51     |
| 24  | J     | 104 | BCR  | C4-C5   | -3.54 | 1.44        | 1.51     |
| 22  | A     | 806 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 22  | Z     | 309 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 24  | B     | 853 | BCR  | C4-C5   | -3.53 | 1.44        | 1.51     |
| 22  | 8     | 308 | CLA  | MG-ND   | -3.53 | 1.98        | 2.05     |
| 22  | Z     | 308 | CLA  | MG-ND   | -3.53 | 1.98        | 2.05     |
| 24  | A     | 845 | BCR  | C4-C5   | -3.53 | 1.44        | 1.51     |
| 22  | 4     | 815 | CLA  | MG-ND   | -3.53 | 1.98        | 2.05     |
| 39  | 4     | 813 | CHL  | CBB-CAB | 3.53  | 1.51        | 1.29     |
| 39  | 8     | 315 | CHL  | CBB-CAB | 3.53  | 1.51        | 1.29     |
| 24  | A     | 847 | BCR  | C4-C5   | -3.53 | 1.44        | 1.51     |
| 22  | B     | 812 | CLA  | MG-ND   | -3.53 | 1.98        | 2.05     |
| 22  | G     | 202 | CLA  | MG-ND   | -3.53 | 1.98        | 2.05     |
| 36  | J     | 105 | C7Z  | C21-C26 | -3.53 | 1.49        | 1.53     |
| 22  | B     | 819 | CLA  | MG-ND   | -3.53 | 1.98        | 2.05     |
| 22  | F     | 302 | CLA  | MG-ND   | -3.53 | 1.98        | 2.05     |
| 24  | B     | 848 | BCR  | C27-C26 | -3.53 | 1.44        | 1.51     |
| 39  | 9     | 312 | CHL  | CBB-CAB | 3.53  | 1.51        | 1.29     |
| 22  | 7     | 311 | CLA  | MG-ND   | -3.53 | 1.98        | 2.05     |
| 24  | A     | 844 | BCR  | C4-C5   | -3.53 | 1.44        | 1.51     |
| 24  | 6     | 306 | BCR  | C4-C5   | -3.52 | 1.44        | 1.51     |
| 22  | 6     | 314 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 24  | 6     | 306 | BCR  | C24-C25 | 3.52  | 1.57        | 1.45     |
| 22  | B     | 842 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 22  | A     | 819 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 39  | 5     | 317 | CHL  | CBB-CAB | 3.52  | 1.51        | 1.29     |
| 22  | 1     | 309 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 24  | 6     | 306 | BCR  | C27-C26 | -3.52 | 1.44        | 1.51     |
| 36  | J     | 105 | C7Z  | C18-C5  | 3.52  | 1.56        | 1.50     |
| 22  | Z     | 316 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 22  | A     | 823 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 22  | 3     | 313 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 22  | A     | 824 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 22  | A     | 807 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | A     | 805 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 22  | B     | 805 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 22  | A     | 841 | CLA  | MG-ND   | -3.51 | 1.98        | 2.05     |
| 22  | 5     | 319 | CLA  | MG-ND   | -3.51 | 1.98        | 2.05     |
| 39  | 9     | 314 | CHL  | CBB-CAB | 3.51  | 1.51        | 1.29     |
| 22  | A     | 810 | CLA  | MG-ND   | -3.51 | 1.98        | 2.05     |
| 22  | 4     | 810 | CLA  | MG-ND   | -3.51 | 1.98        | 2.05     |
| 38  | 7     | 301 | LUT  | C38-C25 | 3.51  | 1.57        | 1.50     |
| 22  | A     | 834 | CLA  | MG-ND   | -3.51 | 1.98        | 2.05     |
| 22  | B     | 818 | CLA  | MG-ND   | -3.51 | 1.98        | 2.05     |
| 39  | 3     | 317 | CHL  | CBB-CAB | 3.51  | 1.51        | 1.29     |
| 24  | B     | 847 | BCR  | C4-C5   | -3.50 | 1.44        | 1.51     |
| 22  | 1     | 311 | CLA  | C1C-NC  | -3.50 | 1.32        | 1.37     |
| 22  | A     | 811 | CLA  | MG-ND   | -3.50 | 1.98        | 2.05     |
| 24  | B     | 849 | BCR  | C4-C5   | -3.50 | 1.44        | 1.51     |
| 39  | 4     | 819 | CHL  | CBB-CAB | 3.50  | 1.51        | 1.29     |
| 22  | B     | 814 | CLA  | MG-ND   | -3.50 | 1.98        | 2.05     |
| 22  | A     | 833 | CLA  | MG-ND   | -3.50 | 1.98        | 2.05     |
| 22  | B     | 827 | CLA  | MG-ND   | -3.50 | 1.98        | 2.05     |
| 22  | 8     | 316 | CLA  | MG-ND   | -3.50 | 1.98        | 2.05     |
| 22  | Z     | 314 | CLA  | MG-ND   | -3.49 | 1.98        | 2.05     |
| 39  | 7     | 313 | CHL  | CBB-CAB | 3.49  | 1.51        | 1.29     |
| 24  | 5     | 305 | BCR  | C4-C5   | -3.49 | 1.44        | 1.51     |
| 38  | 8     | 303 | LUT  | C40-C33 | 3.49  | 1.57        | 1.50     |
| 24  | L     | 204 | BCR  | C27-C26 | -3.49 | 1.44        | 1.51     |
| 22  | 5     | 318 | CLA  | MG-ND   | -3.49 | 1.98        | 2.05     |
| 22  | 1     | 308 | CLA  | MG-ND   | -3.49 | 1.98        | 2.05     |
| 39  | 8     | 301 | CHL  | CBB-CAB | 3.49  | 1.51        | 1.29     |
| 22  | 3     | 318 | CLA  | MG-ND   | -3.49 | 1.98        | 2.05     |
| 39  | Z     | 311 | CHL  | CBB-CAB | 3.48  | 1.51        | 1.29     |
| 39  | 6     | 315 | CHL  | CBB-CAB | 3.48  | 1.51        | 1.29     |
| 24  | B     | 844 | BCR  | C27-C26 | -3.48 | 1.44        | 1.51     |
| 39  | 5     | 321 | CHL  | CBB-CAB | 3.48  | 1.51        | 1.29     |
| 22  | A     | 837 | CLA  | MG-ND   | -3.48 | 1.98        | 2.05     |
| 36  | 5     | 306 | C7Z  | C18-C5  | 3.47  | 1.56        | 1.50     |
| 22  | B     | 838 | CLA  | MG-ND   | -3.47 | 1.98        | 2.05     |
| 25  | 3     | 321 | LHG  | O7-C5   | -3.47 | 1.42        | 1.46     |
| 22  | 3     | 315 | CLA  | C4B-NB  | -3.47 | 1.33        | 1.37     |
| 24  | B     | 849 | BCR  | C27-C26 | -3.47 | 1.44        | 1.51     |
| 24  | B     | 844 | BCR  | C4-C5   | -3.47 | 1.44        | 1.51     |
| 24  | B     | 847 | BCR  | C27-C26 | -3.47 | 1.44        | 1.51     |
| 38  | 6     | 304 | LUT  | C40-C33 | 3.47  | 1.57        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 38  | 7     | 302  | LUT  | C40-C33 | 3.47  | 1.57        | 1.50     |
| 38  | 3     | 302  | LUT  | C2-C1   | 3.46  | 1.65        | 1.54     |
| 22  | F     | 301  | CLA  | MG-ND   | -3.46 | 1.98        | 2.05     |
| 24  | B     | 853  | BCR  | C24-C25 | 3.46  | 1.56        | 1.45     |
| 22  | 9     | 305  | CLA  | C1C-NC  | -3.46 | 1.32        | 1.37     |
| 24  | 4     | 804  | BCR  | C27-C26 | -3.46 | 1.44        | 1.51     |
| 38  | 8     | 302  | LUT  | C40-C33 | 3.46  | 1.57        | 1.50     |
| 36  | J     | 105  | C7Z  | C7-C6   | 3.46  | 1.56        | 1.45     |
| 22  | A     | 855  | CLA  | MG-ND   | -3.46 | 1.98        | 2.05     |
| 24  | A     | 848  | BCR  | C27-C26 | -3.46 | 1.44        | 1.51     |
| 24  | I     | 4001 | BCR  | C4-C5   | -3.46 | 1.44        | 1.51     |
| 38  | Z     | 302  | LUT  | C40-C33 | 3.45  | 1.57        | 1.50     |
| 39  | 6     | 320  | CHL  | CBB-CAB | 3.45  | 1.50        | 1.29     |
| 38  | 3     | 303  | LUT  | C40-C33 | 3.45  | 1.57        | 1.50     |
| 38  | 1     | 303  | LUT  | C40-C33 | 3.45  | 1.57        | 1.50     |
| 24  | 3     | 306  | BCR  | C27-C26 | -3.45 | 1.44        | 1.51     |
| 22  | 1     | 314  | CLA  | MG-ND   | -3.45 | 1.99        | 2.05     |
| 38  | 9     | 302  | LUT  | C40-C33 | 3.45  | 1.57        | 1.50     |
| 38  | 7     | 301  | LUT  | C40-C33 | 3.44  | 1.57        | 1.50     |
| 24  | A     | 845  | BCR  | C27-C26 | -3.44 | 1.44        | 1.51     |
| 38  | 5     | 302  | LUT  | C40-C33 | 3.44  | 1.57        | 1.50     |
| 38  | 4     | 802  | LUT  | C40-C33 | 3.44  | 1.57        | 1.50     |
| 38  | 5     | 303  | LUT  | C40-C33 | 3.44  | 1.57        | 1.50     |
| 39  | 5     | 316  | CHL  | CBB-CAB | 3.43  | 1.50        | 1.29     |
| 38  | 9     | 301  | LUT  | C40-C33 | 3.43  | 1.57        | 1.50     |
| 38  | Z     | 301  | LUT  | C40-C33 | 3.42  | 1.57        | 1.50     |
| 38  | Z     | 301  | LUT  | C38-C25 | 3.42  | 1.56        | 1.50     |
| 24  | F     | 303  | BCR  | C4-C5   | -3.42 | 1.44        | 1.51     |
| 38  | 3     | 302  | LUT  | C40-C33 | 3.42  | 1.57        | 1.50     |
| 22  | A     | 808  | CLA  | MG-ND   | -3.42 | 1.99        | 2.05     |
| 22  | 3     | 320  | CLA  | C4B-NB  | -3.42 | 1.33        | 1.37     |
| 39  | 4     | 816  | CHL  | C1A-CHA | -3.41 | 1.36        | 1.40     |
| 38  | 6     | 303  | LUT  | C40-C33 | 3.41  | 1.57        | 1.50     |
| 22  | L     | 201  | CLA  | MG-ND   | -3.41 | 1.99        | 2.05     |
| 24  | B     | 846  | BCR  | C4-C5   | -3.41 | 1.44        | 1.51     |
| 38  | 4     | 802  | LUT  | C38-C25 | 3.41  | 1.56        | 1.50     |
| 27  | A     | 852  | DGA  | OG2-CB1 | 3.40  | 1.43        | 1.34     |
| 22  | 9     | 310  | CLA  | C1C-NC  | -3.40 | 1.32        | 1.37     |
| 32  | F     | 306  | RRX  | C4-C5   | -3.39 | 1.44        | 1.51     |
| 38  | 4     | 803  | LUT  | C40-C33 | 3.39  | 1.57        | 1.50     |
| 36  | 5     | 306  | C7Z  | C7-C6   | 3.39  | 1.56        | 1.45     |
| 38  | 1     | 302  | LUT  | C40-C33 | 3.39  | 1.57        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 38  | 9     | 301 | LUT  | C23-C24 | -3.38 | 1.45        | 1.50     |
| 24  | A     | 847 | BCR  | C27-C26 | -3.38 | 1.44        | 1.51     |
| 36  | 5     | 306 | C7Z  | C21-C26 | -3.37 | 1.49        | 1.53     |
| 24  | A     | 856 | BCR  | C4-C5   | -3.37 | 1.44        | 1.51     |
| 24  | 7     | 303 | BCR  | C27-C26 | -3.37 | 1.44        | 1.51     |
| 38  | Z     | 301 | LUT  | C23-C24 | -3.37 | 1.45        | 1.50     |
| 24  | F     | 303 | BCR  | C27-C26 | -3.36 | 1.44        | 1.51     |
| 39  | Z     | 311 | CHL  | C1A-CHA | -3.35 | 1.36        | 1.40     |
| 36  | J     | 105 | C7Z  | C8-C9   | 3.35  | 1.53        | 1.46     |
| 24  | G     | 203 | BCR  | C4-C5   | -3.35 | 1.44        | 1.51     |
| 22  | 9     | 309 | CLA  | C1C-NC  | -3.34 | 1.32        | 1.37     |
| 24  | 5     | 305 | BCR  | C27-C26 | -3.33 | 1.44        | 1.51     |
| 24  | B     | 853 | BCR  | C27-C26 | -3.33 | 1.44        | 1.51     |
| 22  | 1     | 311 | CLA  | C4B-NB  | -3.31 | 1.33        | 1.37     |
| 22  | 9     | 309 | CLA  | C4B-NB  | -3.31 | 1.33        | 1.37     |
| 22  | 4     | 805 | CLA  | C1C-NC  | -3.31 | 1.32        | 1.37     |
| 22  | 9     | 304 | CLA  | C1C-NC  | -3.30 | 1.32        | 1.37     |
| 38  | 8     | 302 | LUT  | C23-C24 | -3.30 | 1.45        | 1.50     |
| 22  | 8     | 305 | CLA  | C1C-NC  | -3.30 | 1.32        | 1.37     |
| 39  | 6     | 320 | CHL  | C1A-CHA | -3.29 | 1.36        | 1.40     |
| 22  | 9     | 305 | CLA  | C4B-NB  | -3.27 | 1.33        | 1.37     |
| 27  | A     | 852 | DGA  | OG1-CA1 | 3.26  | 1.42        | 1.33     |
| 38  | 4     | 802 | LUT  | C23-C24 | -3.25 | 1.45        | 1.50     |
| 24  | 3     | 305 | BCR  | C4-C5   | -3.24 | 1.45        | 1.51     |
| 38  | 1     | 302 | LUT  | C23-C24 | -3.24 | 1.45        | 1.50     |
| 22  | 1     | 308 | CLA  | C1C-NC  | -3.23 | 1.32        | 1.37     |
| 22  | B     | 815 | CLA  | C1C-NC  | -3.22 | 1.32        | 1.37     |
| 36  | 5     | 306 | C7Z  | C8-C9   | 3.22  | 1.52        | 1.46     |
| 22  | 9     | 310 | CLA  | C4B-NB  | -3.21 | 1.33        | 1.37     |
| 38  | 7     | 301 | LUT  | C23-C24 | -3.19 | 1.45        | 1.50     |
| 22  | G     | 201 | CLA  | C1C-NC  | -3.19 | 1.32        | 1.37     |
| 38  | 3     | 303 | LUT  | C23-C24 | -3.19 | 1.45        | 1.50     |
| 39  | 4     | 819 | CHL  | C1A-CHA | -3.19 | 1.36        | 1.40     |
| 22  | A     | 813 | CLA  | C1C-NC  | -3.18 | 1.32        | 1.37     |
| 22  | Z     | 304 | CLA  | C1C-NC  | -3.17 | 1.32        | 1.37     |
| 22  | 4     | 809 | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 22  | B     | 814 | CLA  | C1C-NC  | -3.16 | 1.32        | 1.37     |
| 38  | 3     | 302 | LUT  | C23-C24 | -3.15 | 1.45        | 1.50     |
| 22  | 6     | 302 | CLA  | C1C-NC  | -3.14 | 1.32        | 1.37     |
| 22  | B     | 818 | CLA  | C1C-NC  | -3.14 | 1.32        | 1.37     |
| 22  | A     | 827 | CLA  | C1C-NC  | -3.14 | 1.32        | 1.37     |
| 39  | 9     | 312 | CHL  | C2C-C3C | 3.14  | 1.39        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 1     | 305 | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | Z     | 303 | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | 8     | 306 | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | 1     | 313 | CLA  | C1C-NC  | -3.13 | 1.33        | 1.37     |
| 22  | Z     | 305 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | 3     | 312 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | Z     | 316 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 39  | Z     | 312 | CHL  | C1A-CHA | -3.12 | 1.36        | 1.40     |
| 38  | Z     | 302 | LUT  | C23-C24 | -3.12 | 1.46        | 1.50     |
| 22  | A     | 805 | CLA  | C1C-NC  | -3.12 | 1.33        | 1.37     |
| 22  | A     | 835 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 22  | 4     | 818 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 22  | A     | 823 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 38  | 6     | 304 | LUT  | C23-C24 | -3.11 | 1.46        | 1.50     |
| 22  | B     | 817 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 38  | 8     | 303 | LUT  | C23-C24 | -3.11 | 1.46        | 1.50     |
| 22  | 3     | 316 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 22  | B     | 830 | CLA  | C1C-NC  | -3.11 | 1.33        | 1.37     |
| 22  | 6     | 301 | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 39  | 1     | 312 | CHL  | C1A-CHA | -3.10 | 1.36        | 1.40     |
| 22  | 2     | 304 | CLA  | C1C-NC  | -3.10 | 1.33        | 1.37     |
| 39  | 4     | 813 | CHL  | C1A-CHA | -3.10 | 1.36        | 1.40     |
| 22  | A     | 812 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 39  | 8     | 315 | CHL  | C3A-C2A | -3.09 | 1.52        | 1.54     |
| 22  | 3     | 311 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | 6     | 307 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | 1     | 304 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | Z     | 313 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | 5     | 314 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | A     | 855 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | 7     | 312 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | 9     | 311 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | 5     | 309 | CLA  | C1C-NC  | -3.09 | 1.33        | 1.37     |
| 22  | A     | 828 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | B     | 827 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | B     | 811 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | 8     | 311 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | 9     | 308 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | 7     | 307 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | A     | 840 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | A     | 806 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | Z     | 309 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | F     | 301 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | K     | 203 | CLA  | C1C-NC  | -3.08 | 1.33        | 1.37     |
| 22  | 8     | 316 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | B     | 821 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | 6     | 311 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | 1     | 307 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | B     | 823 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | 5     | 301 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | G     | 202 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | 7     | 305 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | B     | 834 | CLA  | C1C-NC  | -3.07 | 1.33        | 1.37     |
| 22  | 2     | 302 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | B     | 819 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | 5     | 308 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | A     | 811 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 39  | 8     | 315 | CHL  | C1A-CHA | -3.06 | 1.36        | 1.40     |
| 22  | A     | 803 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | A     | 833 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | 3     | 309 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | J     | 103 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | Z     | 315 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | A     | 821 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | 9     | 306 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | 9     | 313 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | 8     | 305 | CLA  | C4B-NB  | -3.06 | 1.33        | 1.37     |
| 22  | B     | 828 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | 5     | 307 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 22  | 9     | 307 | CLA  | C1C-NC  | -3.06 | 1.33        | 1.37     |
| 39  | 2     | 303 | CHL  | C1A-CHA | -3.05 | 1.36        | 1.40     |
| 22  | A     | 809 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | 2     | 301 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | A     | 824 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | 3     | 308 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | A     | 817 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | A     | 818 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | A     | 820 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | B     | 822 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | F     | 304 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | 3     | 314 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | B     | 832 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | 6     | 313 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | 6     | 314 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 5     | 326 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | L     | 203 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 39  | 8     | 301 | CHL  | C1A-CHA | -3.05 | 1.36        | 1.40     |
| 22  | B     | 809 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | 6     | 317 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | 7     | 308 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | A     | 839 | CLA  | C1C-NC  | -3.05 | 1.33        | 1.37     |
| 22  | A     | 829 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | 4     | 807 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | 7     | 322 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | B     | 825 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | A     | 808 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | 8     | 313 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | 7     | 304 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | 5     | 312 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | A     | 838 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | K     | 202 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | 8     | 309 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | A     | 841 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | 7     | 310 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | Z     | 310 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | A     | 836 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | F     | 302 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | L     | 201 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | 4     | 811 | CLA  | C1C-NC  | -3.04 | 1.33        | 1.37     |
| 22  | 7     | 314 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | B     | 839 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | 4     | 817 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | 5     | 315 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | Z     | 314 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | B     | 836 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | A     | 804 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | A     | 842 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | 5     | 319 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 38  | 7     | 302 | LUT  | C23-C24 | -3.03 | 1.46        | 1.50     |
| 22  | Z     | 307 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | B     | 829 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | 1     | 310 | CLA  | C1C-NC  | -3.03 | 1.33        | 1.37     |
| 22  | 3     | 313 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | 8     | 310 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | A     | 830 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | Z     | 306 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 837 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | 4     | 815 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | B     | 835 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | 7     | 309 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | B     | 805 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | L     | 202 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | 1     | 314 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | 4     | 812 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | 4     | 808 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | A     | 825 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | 3     | 319 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | B     | 831 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | 8     | 314 | CLA  | C1C-NC  | -3.02 | 1.33        | 1.37     |
| 22  | B     | 841 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | A     | 810 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | 8     | 308 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | 5     | 323 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | 5     | 318 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 39  | 5     | 317 | CHL  | C3A-C2A | -3.01 | 1.52        | 1.54     |
| 38  | 5     | 302 | LUT  | C23-C24 | -3.01 | 1.46        | 1.50     |
| 22  | A     | 822 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | B     | 801 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | 5     | 313 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | 6     | 322 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | 1     | 306 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | 7     | 315 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | A     | 832 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | B     | 810 | CLA  | C1C-NC  | -3.01 | 1.33        | 1.37     |
| 22  | B     | 808 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | 3     | 310 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | B     | 807 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | 1     | 309 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | A     | 814 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | 6     | 312 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | A     | 815 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | 7     | 306 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | 4     | 806 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | 7     | 317 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | 7     | 324 | CLA  | C1C-NC  | -3.00 | 1.33        | 1.37     |
| 22  | B     | 840 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | K     | 204 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | 3     | 318 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 39  | 3     | 317 | CHL  | C1A-CHA | -2.99 | 1.36        | 1.40     |
| 22  | A     | 831 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | Z     | 308 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | B     | 833 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | B     | 812 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | 7     | 311 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 39  | 6     | 318 | CHL  | C1A-CHA | -2.99 | 1.36        | 1.40     |
| 22  | 4     | 810 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | A     | 819 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | A     | 802 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | B     | 806 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | 6     | 309 | CLA  | C1C-NC  | -2.99 | 1.33        | 1.37     |
| 22  | F     | 305 | CLA  | C1C-NC  | -2.98 | 1.33        | 1.37     |
| 22  | 3     | 322 | CLA  | C1C-NC  | -2.98 | 1.33        | 1.37     |
| 22  | B     | 838 | CLA  | C1C-NC  | -2.98 | 1.33        | 1.37     |
| 22  | A     | 854 | CLA  | C1C-NC  | -2.98 | 1.33        | 1.37     |
| 22  | A     | 816 | CLA  | C1C-NC  | -2.98 | 1.33        | 1.37     |
| 38  | 4     | 803 | LUT  | C23-C24 | -2.98 | 1.46        | 1.50     |
| 22  | 7     | 323 | CLA  | C1C-NC  | -2.98 | 1.33        | 1.37     |
| 22  | 6     | 308 | CLA  | C1C-NC  | -2.98 | 1.33        | 1.37     |
| 22  | 6     | 321 | CLA  | C1C-NC  | -2.98 | 1.33        | 1.37     |
| 22  | A     | 807 | CLA  | C1C-NC  | -2.97 | 1.33        | 1.37     |
| 22  | 6     | 310 | CLA  | C1C-NC  | -2.97 | 1.33        | 1.37     |
| 22  | 5     | 322 | CLA  | C1C-NC  | -2.97 | 1.33        | 1.37     |
| 22  | 1     | 304 | CLA  | C4B-NB  | -2.97 | 1.34        | 1.37     |
| 22  | 7     | 316 | CLA  | C1C-NC  | -2.97 | 1.33        | 1.37     |
| 22  | B     | 842 | CLA  | C1C-NC  | -2.97 | 1.33        | 1.37     |
| 22  | 5     | 311 | CLA  | C1C-NC  | -2.97 | 1.33        | 1.37     |
| 22  | 5     | 310 | CLA  | C1C-NC  | -2.97 | 1.33        | 1.37     |
| 24  | L     | 204 | BCR  | C34-C9  | 2.97  | 1.56        | 1.50     |
| 22  | Z     | 313 | CLA  | C4B-NB  | -2.97 | 1.34        | 1.37     |
| 22  | A     | 837 | CLA  | C1C-NC  | -2.96 | 1.33        | 1.37     |
| 22  | 4     | 808 | CLA  | C4B-NB  | -2.96 | 1.34        | 1.37     |
| 38  | 9     | 302 | LUT  | C23-C24 | -2.96 | 1.46        | 1.50     |
| 22  | 6     | 307 | CLA  | C4B-NB  | -2.96 | 1.34        | 1.37     |
| 22  | B     | 824 | CLA  | C1C-NC  | -2.95 | 1.33        | 1.37     |
| 22  | B     | 816 | CLA  | C1C-NC  | -2.95 | 1.33        | 1.37     |
| 22  | A     | 834 | CLA  | C1C-NC  | -2.95 | 1.33        | 1.37     |
| 22  | 1     | 313 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |
| 24  | 5     | 305 | BCR  | C34-C9  | 2.95  | 1.56        | 1.50     |
| 22  | B     | 813 | CLA  | C1C-NC  | -2.95 | 1.33        | 1.37     |
| 22  | A     | 836 | CLA  | C4B-NB  | -2.95 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | B     | 853 | BCR  | C34-C9  | 2.95  | 1.56        | 1.50     |
| 22  | 6     | 319 | CLA  | C1C-NC  | -2.95 | 1.33        | 1.37     |
| 22  | A     | 822 | CLA  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 22  | 4     | 818 | CLA  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 22  | B     | 820 | CLA  | C1C-NC  | -2.94 | 1.33        | 1.37     |
| 22  | 8     | 308 | CLA  | C4B-NB  | -2.94 | 1.34        | 1.37     |
| 22  | 1     | 315 | CLA  | C1C-NC  | -2.93 | 1.33        | 1.37     |
| 22  | B     | 815 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 24  | A     | 845 | BCR  | C34-C9  | 2.93  | 1.56        | 1.50     |
| 22  | Z     | 303 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 24  | B     | 853 | BCR  | C7-C6   | 2.93  | 1.55        | 1.45     |
| 22  | B     | 826 | CLA  | C1C-NC  | -2.93 | 1.33        | 1.37     |
| 22  | 9     | 304 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 24  | B     | 849 | BCR  | C34-C9  | 2.93  | 1.56        | 1.50     |
| 22  | A     | 813 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 22  | K     | 202 | CLA  | C4B-NB  | -2.93 | 1.34        | 1.37     |
| 22  | G     | 202 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 22  | 7     | 307 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 24  | B     | 847 | BCR  | C34-C9  | 2.92  | 1.56        | 1.50     |
| 22  | 3     | 308 | CLA  | C4B-NB  | -2.92 | 1.34        | 1.37     |
| 24  | A     | 846 | BCR  | C34-C9  | 2.92  | 1.56        | 1.50     |
| 24  | F     | 303 | BCR  | C34-C9  | 2.92  | 1.56        | 1.50     |
| 38  | 5     | 303 | LUT  | C23-C24 | -2.91 | 1.46        | 1.50     |
| 22  | 1     | 307 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 22  | A     | 842 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 22  | Z     | 306 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 22  | 6     | 317 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 22  | 7     | 309 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 22  | 9     | 306 | CLA  | C4B-NB  | -2.91 | 1.34        | 1.37     |
| 22  | 4     | 805 | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 24  | 5     | 305 | BCR  | C7-C6   | 2.90  | 1.55        | 1.45     |
| 22  | A     | 838 | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 24  | A     | 847 | BCR  | C34-C9  | 2.90  | 1.56        | 1.50     |
| 24  | 5     | 304 | BCR  | C34-C9  | 2.90  | 1.56        | 1.50     |
| 24  | 6     | 306 | BCR  | C34-C9  | 2.90  | 1.56        | 1.50     |
| 22  | 3     | 309 | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 24  | B     | 844 | BCR  | C34-C9  | 2.90  | 1.56        | 1.50     |
| 22  | A     | 835 | CLA  | C4B-NB  | -2.90 | 1.34        | 1.37     |
| 22  | 8     | 307 | CLA  | C1C-NC  | -2.90 | 1.33        | 1.37     |
| 22  | B     | 831 | CLA  | C4B-NB  | -2.89 | 1.34        | 1.37     |
| 22  | 6     | 321 | CLA  | C4B-NB  | -2.89 | 1.34        | 1.37     |
| 22  | 5     | 307 | CLA  | C4B-NB  | -2.89 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | B     | 845  | BCR  | C34-C9  | 2.89  | 1.56        | 1.50     |
| 24  | 3     | 307  | BCR  | C34-C9  | 2.89  | 1.56        | 1.50     |
| 24  | 6     | 305  | BCR  | C34-C9  | 2.89  | 1.56        | 1.50     |
| 22  | 4     | 810  | CLA  | C4B-NB  | -2.89 | 1.34        | 1.37     |
| 22  | A     | 826  | CLA  | C1C-NC  | -2.89 | 1.33        | 1.37     |
| 22  | Z     | 305  | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 22  | Z     | 307  | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 22  | 4     | 817  | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 22  | B     | 842  | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 22  | 6     | 311  | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 22  | A     | 818  | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 22  | A     | 827  | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 22  | B     | 827  | CLA  | C4B-NB  | -2.88 | 1.34        | 1.37     |
| 24  | A     | 856  | BCR  | C34-C9  | 2.88  | 1.56        | 1.50     |
| 24  | I     | 4001 | BCR  | C34-C9  | 2.88  | 1.56        | 1.50     |
| 22  | B     | 836  | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 24  | 3     | 305  | BCR  | C34-C9  | 2.87  | 1.56        | 1.50     |
| 22  | A     | 821  | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 21  | A     | 801  | CL0  | CHB-C4A | -2.87 | 1.35        | 1.38     |
| 22  | A     | 839  | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 22  | 5     | 312  | CLA  | C4B-NB  | -2.87 | 1.34        | 1.37     |
| 38  | 6     | 303  | LUT  | C23-C24 | -2.87 | 1.46        | 1.50     |
| 24  | 3     | 306  | BCR  | C7-C6   | 2.87  | 1.54        | 1.45     |
| 22  | 3     | 311  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 22  | B     | 806  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 22  | 7     | 322  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 22  | K     | 203  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 22  | 8     | 314  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 22  | 5     | 310  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 22  | B     | 809  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 24  | K     | 206  | BCR  | C34-C9  | 2.86  | 1.56        | 1.50     |
| 22  | A     | 831  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 24  | 8     | 304  | BCR  | C34-C9  | 2.86  | 1.56        | 1.50     |
| 22  | A     | 816  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 22  | 3     | 318  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 22  | 4     | 812  | CLA  | C4B-NB  | -2.86 | 1.34        | 1.37     |
| 24  | F     | 303  | BCR  | C7-C6   | 2.86  | 1.54        | 1.45     |
| 24  | J     | 104  | BCR  | C34-C9  | 2.86  | 1.56        | 1.50     |
| 24  | B     | 848  | BCR  | C34-C9  | 2.86  | 1.56        | 1.50     |
| 24  | 3     | 304  | BCR  | C34-C9  | 2.85  | 1.56        | 1.50     |
| 22  | B     | 817  | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 22  | 4     | 815  | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | 4     | 804 | BCR  | C34-C9  | 2.85  | 1.56        | 1.50     |
| 24  | A     | 848 | BCR  | C34-C9  | 2.85  | 1.56        | 1.50     |
| 22  | A     | 832 | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 22  | 9     | 307 | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 22  | A     | 840 | CLA  | C4B-NB  | -2.85 | 1.34        | 1.37     |
| 24  | 7     | 303 | BCR  | C34-C9  | 2.84  | 1.56        | 1.50     |
| 24  | B     | 848 | BCR  | C7-C6   | 2.84  | 1.54        | 1.45     |
| 39  | 6     | 318 | CHL  | C1D-C2D | 2.84  | 1.42        | 1.39     |
| 22  | 8     | 310 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 22  | 6     | 322 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 24  | B     | 844 | BCR  | C7-C6   | 2.84  | 1.54        | 1.45     |
| 22  | A     | 834 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 24  | G     | 203 | BCR  | C34-C9  | 2.84  | 1.56        | 1.50     |
| 22  | B     | 810 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 22  | 8     | 309 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 22  | A     | 830 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 22  | 6     | 312 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 22  | L     | 203 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 22  | 4     | 807 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 22  | B     | 833 | CLA  | C4B-NB  | -2.84 | 1.34        | 1.37     |
| 22  | B     | 841 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | Z     | 315 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | 8     | 313 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | B     | 812 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | B     | 835 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | 7     | 316 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 24  | 3     | 305 | BCR  | C7-C6   | 2.83  | 1.54        | 1.45     |
| 22  | B     | 838 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | 5     | 319 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | A     | 805 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | A     | 804 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | B     | 837 | CLA  | C4B-NB  | -2.83 | 1.34        | 1.37     |
| 22  | 6     | 309 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 22  | 9     | 308 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 22  | B     | 834 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 22  | B     | 839 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 22  | A     | 826 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 22  | 1     | 315 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 22  | J     | 103 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 22  | 7     | 306 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 22  | B     | 822 | CLA  | C4B-NB  | -2.82 | 1.34        | 1.37     |
| 22  | 3     | 313 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 832 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 22  | 5     | 318 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 22  | B     | 824 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 22  | 6     | 310 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 24  | A     | 856 | BCR  | C7-C6   | 2.81  | 1.54        | 1.45     |
| 22  | B     | 825 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 39  | 5     | 321 | CHL  | C1D-C2D | 2.81  | 1.42        | 1.39     |
| 24  | 4     | 804 | BCR  | C7-C6   | 2.81  | 1.54        | 1.45     |
| 22  | B     | 808 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 22  | 7     | 324 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 39  | 6     | 316 | CHL  | C1D-C2D | 2.81  | 1.42        | 1.39     |
| 22  | L     | 202 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 39  | 9     | 312 | CHL  | C1B-C2B | 2.81  | 1.42        | 1.39     |
| 24  | 7     | 303 | BCR  | C7-C6   | 2.81  | 1.54        | 1.45     |
| 22  | F     | 305 | CLA  | C4B-NB  | -2.81 | 1.34        | 1.37     |
| 24  | J     | 104 | BCR  | C7-C6   | 2.80  | 1.54        | 1.45     |
| 24  | B     | 846 | BCR  | C34-C9  | 2.80  | 1.56        | 1.50     |
| 22  | 5     | 311 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 22  | 7     | 304 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 22  | 5     | 323 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 24  | A     | 845 | BCR  | C7-C6   | 2.80  | 1.54        | 1.45     |
| 22  | A     | 815 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 22  | B     | 816 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 22  | K     | 204 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 38  | 8     | 302 | LUT  | O23-C23 | -2.80 | 1.38        | 1.43     |
| 22  | A     | 819 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 22  | 7     | 310 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 24  | 3     | 306 | BCR  | C34-C9  | 2.80  | 1.56        | 1.50     |
| 39  | 1     | 312 | CHL  | C1D-C2D | 2.80  | 1.42        | 1.39     |
| 22  | B     | 820 | CLA  | C4B-NB  | -2.80 | 1.34        | 1.37     |
| 24  | B     | 845 | BCR  | C7-C6   | 2.80  | 1.54        | 1.45     |
| 22  | 6     | 313 | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | A     | 810 | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | A     | 811 | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | A     | 828 | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | A     | 854 | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | 3     | 319 | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | A     | 817 | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 22  | 7     | 308 | CLA  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 24  | B     | 849 | BCR  | C7-C6   | 2.78  | 1.54        | 1.45     |
| 22  | 1     | 306 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 39  | Z     | 312 | CHL  | C1D-C2D | 2.78  | 1.42        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 1     | 314 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 22  | 8     | 307 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 39  | 6     | 315 | CHL  | C1B-C2B | 2.78  | 1.42        | 1.39     |
| 39  | 2     | 303 | CHL  | C1D-C2D | 2.78  | 1.42        | 1.39     |
| 38  | 1     | 302 | LUT  | C18-C5  | 2.78  | 1.55        | 1.50     |
| 22  | B     | 829 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 39  | 9     | 314 | CHL  | C1A-CHA | -2.78 | 1.36        | 1.40     |
| 22  | B     | 813 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 22  | 5     | 308 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 22  | 3     | 310 | CLA  | C4B-NB  | -2.78 | 1.34        | 1.37     |
| 38  | 4     | 802 | LUT  | O23-C23 | -2.77 | 1.38        | 1.43     |
| 38  | 9     | 301 | LUT  | C18-C5  | 2.77  | 1.55        | 1.50     |
| 39  | 1     | 312 | CHL  | C1B-C2B | 2.77  | 1.42        | 1.39     |
| 39  | 4     | 813 | CHL  | CHB-C4A | -2.77 | 1.35        | 1.38     |
| 38  | 6     | 303 | LUT  | C18-C5  | 2.77  | 1.55        | 1.50     |
| 22  | A     | 802 | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 22  | B     | 807 | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 38  | Z     | 301 | LUT  | C18-C5  | 2.77  | 1.55        | 1.50     |
| 39  | 4     | 814 | CHL  | C1B-C2B | 2.77  | 1.42        | 1.39     |
| 22  | 9     | 311 | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 24  | B     | 846 | BCR  | C7-C6   | 2.77  | 1.54        | 1.45     |
| 38  | 4     | 802 | LUT  | C18-C5  | 2.77  | 1.55        | 1.50     |
| 22  | B     | 801 | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 22  | 7     | 323 | CLA  | C4B-NB  | -2.77 | 1.34        | 1.37     |
| 39  | 8     | 301 | CHL  | CHB-C4A | -2.77 | 1.35        | 1.38     |
| 39  | 9     | 314 | CHL  | C1D-C2D | 2.76  | 1.42        | 1.39     |
| 22  | A     | 814 | CLA  | C4B-NB  | -2.76 | 1.34        | 1.37     |
| 38  | 1     | 303 | LUT  | C23-C24 | -2.76 | 1.46        | 1.50     |
| 24  | B     | 853 | BCR  | C36-C18 | 2.76  | 1.56        | 1.50     |
| 39  | 5     | 316 | CHL  | C1D-C2D | 2.76  | 1.42        | 1.39     |
| 39  | 9     | 314 | CHL  | C1B-C2B | 2.76  | 1.42        | 1.39     |
| 24  | B     | 847 | BCR  | C7-C6   | 2.76  | 1.54        | 1.45     |
| 39  | 3     | 317 | CHL  | C1D-C2D | 2.75  | 1.42        | 1.39     |
| 39  | 4     | 816 | CHL  | CHB-C4A | -2.75 | 1.35        | 1.38     |
| 24  | A     | 848 | BCR  | C7-C6   | 2.75  | 1.54        | 1.45     |
| 39  | 8     | 315 | CHL  | C1D-C2D | 2.75  | 1.42        | 1.39     |
| 24  | 6     | 305 | BCR  | C7-C6   | 2.75  | 1.54        | 1.45     |
| 38  | 7     | 301 | LUT  | C18-C5  | 2.75  | 1.55        | 1.50     |
| 41  | 5     | 325 | 3PH  | O21-C2  | -2.75 | 1.40        | 1.46     |
| 22  | 2     | 302 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |
| 39  | 8     | 301 | CHL  | C1D-C2D | 2.75  | 1.42        | 1.39     |
| 22  | A     | 825 | CLA  | C4B-NB  | -2.75 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22  | G     | 201  | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 38  | 9     | 301  | LUT  | O23-C23 | -2.74 | 1.38        | 1.43     |
| 22  | 7     | 314  | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 22  | 5     | 301  | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 39  | 6     | 318  | CHL  | CHB-C4A | -2.74 | 1.35        | 1.38     |
| 39  | 4     | 813  | CHL  | C1B-C2B | 2.74  | 1.42        | 1.39     |
| 24  | G     | 203  | BCR  | C7-C6   | 2.74  | 1.54        | 1.45     |
| 24  | I     | 4001 | BCR  | C7-C6   | 2.74  | 1.54        | 1.45     |
| 22  | 6     | 301  | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 39  | 6     | 320  | CHL  | CHB-C4A | -2.74 | 1.35        | 1.38     |
| 39  | 6     | 318  | CHL  | C1B-C2B | 2.74  | 1.42        | 1.39     |
| 22  | B     | 840  | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 24  | A     | 844  | BCR  | C34-C9  | 2.74  | 1.56        | 1.50     |
| 38  | 5     | 302  | LUT  | C18-C5  | 2.74  | 1.55        | 1.50     |
| 22  | F     | 304  | CLA  | C4B-NB  | -2.74 | 1.34        | 1.37     |
| 39  | 8     | 312  | CHL  | C1B-C2B | 2.73  | 1.42        | 1.39     |
| 39  | 8     | 315  | CHL  | C1B-C2B | 2.73  | 1.42        | 1.39     |
| 22  | B     | 814  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 24  | 3     | 307  | BCR  | C7-C6   | 2.73  | 1.54        | 1.45     |
| 22  | 6     | 302  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 39  | 7     | 313  | CHL  | C1D-C2D | 2.73  | 1.42        | 1.39     |
| 39  | 8     | 312  | CHL  | C1D-C2D | 2.73  | 1.42        | 1.39     |
| 35  | J     | 102  | T7X  | O16-C8  | -2.73 | 1.40        | 1.46     |
| 22  | Z     | 308  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 22  | 5     | 313  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 22  | 5     | 322  | CLA  | C4B-NB  | -2.73 | 1.34        | 1.37     |
| 38  | 3     | 302  | LUT  | C18-C5  | 2.73  | 1.55        | 1.50     |
| 39  | 4     | 816  | CHL  | C1D-C2D | 2.72  | 1.42        | 1.39     |
| 24  | A     | 847  | BCR  | C7-C6   | 2.72  | 1.54        | 1.45     |
| 24  | L     | 204  | BCR  | C7-C6   | 2.72  | 1.54        | 1.45     |
| 22  | 4     | 806  | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 39  | 5     | 316  | CHL  | C1A-CHA | -2.72 | 1.36        | 1.40     |
| 39  | 9     | 312  | CHL  | C1D-C2D | 2.72  | 1.42        | 1.39     |
| 22  | Z     | 304  | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 22  | 2     | 301  | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 22  | 7     | 315  | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 24  | 6     | 306  | BCR  | C7-C6   | 2.72  | 1.54        | 1.45     |
| 24  | 8     | 304  | BCR  | C7-C6   | 2.72  | 1.54        | 1.45     |
| 22  | 7     | 305  | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 39  | 5     | 316  | CHL  | CHB-C4A | -2.72 | 1.35        | 1.38     |
| 39  | 4     | 813  | CHL  | C1D-C2D | 2.72  | 1.42        | 1.39     |
| 24  | A     | 846  | BCR  | C7-C6   | 2.72  | 1.54        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | B     | 826 | CLA  | C4B-NB  | -2.72 | 1.34        | 1.37     |
| 24  | B     | 853 | BCR  | C38-C26 | 2.71  | 1.55        | 1.50     |
| 22  | A     | 855 | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 39  | 6     | 320 | CHL  | C1D-C2D | 2.71  | 1.42        | 1.39     |
| 22  | 8     | 311 | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 39  | 7     | 313 | CHL  | C1A-CHA | -2.71 | 1.36        | 1.40     |
| 38  | 6     | 304 | LUT  | C18-C5  | 2.71  | 1.55        | 1.50     |
| 22  | Z     | 310 | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 22  | A     | 833 | CLA  | C4B-NB  | -2.71 | 1.34        | 1.37     |
| 39  | Z     | 311 | CHL  | C1D-C2D | 2.71  | 1.42        | 1.39     |
| 39  | Z     | 312 | CHL  | C1B-C2B | 2.71  | 1.42        | 1.39     |
| 38  | 5     | 303 | LUT  | O23-C23 | -2.71 | 1.39        | 1.43     |
| 38  | 8     | 302 | LUT  | C18-C5  | 2.71  | 1.55        | 1.50     |
| 22  | B     | 823 | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 22  | 5     | 314 | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 39  | 6     | 316 | CHL  | C1A-CHA | -2.70 | 1.36        | 1.40     |
| 22  | 3     | 322 | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 22  | 4     | 811 | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 22  | 5     | 309 | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 24  | A     | 844 | BCR  | C7-C6   | 2.70  | 1.54        | 1.45     |
| 22  | 1     | 309 | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 39  | 4     | 819 | CHL  | C1D-C2D | 2.70  | 1.42        | 1.39     |
| 24  | 3     | 304 | BCR  | C7-C6   | 2.70  | 1.54        | 1.45     |
| 22  | 5     | 315 | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 22  | B     | 821 | CLA  | C4B-NB  | -2.70 | 1.34        | 1.37     |
| 22  | 5     | 326 | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 22  | 7     | 311 | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 38  | Z     | 301 | LUT  | O23-C23 | -2.69 | 1.39        | 1.43     |
| 39  | 4     | 814 | CHL  | C1D-C2D | 2.69  | 1.42        | 1.39     |
| 24  | 5     | 304 | BCR  | C7-C6   | 2.69  | 1.54        | 1.45     |
| 39  | 7     | 313 | CHL  | CHB-C4A | -2.69 | 1.35        | 1.38     |
| 22  | 3     | 314 | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 39  | 5     | 317 | CHL  | C1D-C2D | 2.69  | 1.42        | 1.39     |
| 39  | 5     | 317 | CHL  | C1B-C2B | 2.69  | 1.42        | 1.39     |
| 24  | K     | 206 | BCR  | C7-C6   | 2.69  | 1.54        | 1.45     |
| 22  | 7     | 312 | CLA  | C4B-NB  | -2.69 | 1.34        | 1.37     |
| 25  | B     | 851 | LHG  | O7-C5   | -2.68 | 1.43        | 1.46     |
| 22  | 7     | 317 | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 22  | 6     | 308 | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 39  | 7     | 313 | CHL  | C1B-C2B | 2.68  | 1.42        | 1.39     |
| 22  | Z     | 316 | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |
| 22  | B     | 819 | CLA  | C4B-NB  | -2.68 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 39  | Z     | 311 | CHL  | C1B-C2B | 2.68  | 1.42        | 1.39     |
| 38  | 3     | 303 | LUT  | O23-C23 | -2.68 | 1.39        | 1.43     |
| 39  | 6     | 316 | CHL  | CHB-C4A | -2.67 | 1.35        | 1.38     |
| 39  | Z     | 312 | CHL  | CHB-C4A | -2.67 | 1.35        | 1.38     |
| 22  | 6     | 319 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 39  | 6     | 315 | CHL  | CHB-C4A | -2.67 | 1.35        | 1.38     |
| 38  | 7     | 301 | LUT  | O23-C23 | -2.67 | 1.39        | 1.43     |
| 39  | Z     | 311 | CHL  | CHB-C4A | -2.67 | 1.35        | 1.38     |
| 22  | A     | 807 | CLA  | C4B-NB  | -2.67 | 1.34        | 1.37     |
| 22  | A     | 806 | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 22  | B     | 811 | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 22  | 1     | 305 | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 39  | 2     | 303 | CHL  | CHB-C4A | -2.66 | 1.35        | 1.38     |
| 39  | 3     | 317 | CHL  | CHB-C4A | -2.66 | 1.35        | 1.38     |
| 39  | 5     | 321 | CHL  | C1B-C2B | 2.66  | 1.42        | 1.39     |
| 22  | 8     | 316 | CLA  | C4B-NB  | -2.66 | 1.34        | 1.37     |
| 38  | 7     | 302 | LUT  | C18-C5  | 2.66  | 1.55        | 1.50     |
| 38  | 3     | 303 | LUT  | C18-C5  | 2.66  | 1.55        | 1.50     |
| 39  | 5     | 316 | CHL  | C1B-C2B | 2.65  | 1.42        | 1.39     |
| 22  | A     | 837 | CLA  | C4B-NB  | -2.65 | 1.34        | 1.37     |
| 39  | 4     | 814 | CHL  | CHB-C4A | -2.65 | 1.35        | 1.38     |
| 38  | 5     | 303 | LUT  | C18-C5  | 2.65  | 1.55        | 1.50     |
| 39  | 6     | 315 | CHL  | C1D-C2D | 2.65  | 1.42        | 1.39     |
| 39  | 9     | 314 | CHL  | CHB-C4A | -2.64 | 1.35        | 1.38     |
| 41  | 7     | 319 | 3PH  | O21-C2  | -2.64 | 1.40        | 1.46     |
| 39  | 5     | 321 | CHL  | CHB-C4A | -2.64 | 1.35        | 1.38     |
| 39  | 8     | 315 | CHL  | CHB-C4A | -2.64 | 1.35        | 1.38     |
| 22  | F     | 301 | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 39  | 4     | 819 | CHL  | CHB-C4A | -2.64 | 1.35        | 1.38     |
| 22  | A     | 841 | CLA  | C4B-NB  | -2.64 | 1.34        | 1.37     |
| 38  | 4     | 803 | LUT  | C18-C5  | 2.64  | 1.55        | 1.50     |
| 38  | 3     | 302 | LUT  | O23-C23 | -2.64 | 1.39        | 1.43     |
| 22  | 2     | 304 | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 22  | B     | 818 | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 22  | 1     | 310 | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 39  | 6     | 316 | CHL  | C1B-C2B | 2.63  | 1.42        | 1.39     |
| 39  | 3     | 317 | CHL  | C1B-C2B | 2.63  | 1.42        | 1.39     |
| 39  | 4     | 819 | CHL  | C1B-C2B | 2.63  | 1.42        | 1.39     |
| 38  | 1     | 303 | LUT  | C18-C5  | 2.63  | 1.55        | 1.50     |
| 38  | Z     | 302 | LUT  | O23-C23 | -2.63 | 1.39        | 1.43     |
| 22  | A     | 809 | CLA  | C4B-NB  | -2.63 | 1.34        | 1.37     |
| 41  | 8     | 320 | 3PH  | O21-C2  | -2.63 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 38  | 6     | 303 | LUT  | O23-C23 | -2.63 | 1.39        | 1.43     |
| 38  | 4     | 803 | LUT  | O23-C23 | -2.63 | 1.39        | 1.43     |
| 39  | 2     | 303 | CHL  | C1B-C2B | 2.63  | 1.42        | 1.39     |
| 22  | B     | 830 | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 38  | 9     | 302 | LUT  | C18-C5  | 2.62  | 1.55        | 1.50     |
| 22  | 3     | 312 | CLA  | C4B-NB  | -2.62 | 1.34        | 1.37     |
| 38  | 1     | 302 | LUT  | O23-C23 | -2.62 | 1.39        | 1.43     |
| 39  | 8     | 312 | CHL  | CHB-C4A | -2.62 | 1.35        | 1.38     |
| 39  | 4     | 816 | CHL  | C1B-C2B | 2.62  | 1.42        | 1.39     |
| 38  | 6     | 304 | LUT  | O23-C23 | -2.62 | 1.39        | 1.43     |
| 22  | 6     | 314 | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 22  | Z     | 309 | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 38  | 1     | 303 | LUT  | O23-C23 | -2.61 | 1.39        | 1.43     |
| 39  | 9     | 312 | CHL  | C1A-CHA | -2.61 | 1.37        | 1.40     |
| 39  | 6     | 320 | CHL  | C1B-C2B | 2.61  | 1.42        | 1.39     |
| 22  | 1     | 308 | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 39  | 8     | 312 | CHL  | C1A-CHA | -2.61 | 1.37        | 1.40     |
| 22  | A     | 820 | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 22  | A     | 803 | CLA  | C4B-NB  | -2.61 | 1.34        | 1.37     |
| 41  | 6     | 324 | 3PH  | O21-C2  | -2.60 | 1.40        | 1.46     |
| 22  | Z     | 314 | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 22  | A     | 823 | CLA  | C4B-NB  | -2.60 | 1.34        | 1.37     |
| 39  | 1     | 312 | CHL  | CHB-C4A | -2.60 | 1.35        | 1.38     |
| 39  | 8     | 301 | CHL  | C1B-C2B | 2.59  | 1.42        | 1.39     |
| 22  | A     | 829 | CLA  | C4B-NB  | -2.59 | 1.34        | 1.37     |
| 22  | 4     | 809 | CLA  | C4B-NB  | -2.59 | 1.34        | 1.37     |
| 38  | 8     | 303 | LUT  | C18-C5  | 2.59  | 1.55        | 1.50     |
| 38  | 5     | 302 | LUT  | O23-C23 | -2.58 | 1.39        | 1.43     |
| 38  | 8     | 303 | LUT  | O23-C23 | -2.58 | 1.39        | 1.43     |
| 38  | 9     | 302 | LUT  | O23-C23 | -2.58 | 1.39        | 1.43     |
| 38  | Z     | 302 | LUT  | C18-C5  | 2.58  | 1.55        | 1.50     |
| 22  | A     | 812 | CLA  | C4B-NB  | -2.57 | 1.34        | 1.37     |
| 22  | B     | 828 | CLA  | C4B-NB  | -2.57 | 1.34        | 1.37     |
| 22  | A     | 824 | CLA  | C4B-NB  | -2.57 | 1.34        | 1.37     |
| 22  | 9     | 313 | CLA  | C4B-NB  | -2.57 | 1.34        | 1.37     |
| 22  | F     | 302 | CLA  | C4B-NB  | -2.55 | 1.34        | 1.37     |
| 22  | B     | 805 | CLA  | C4B-NB  | -2.55 | 1.34        | 1.37     |
| 22  | L     | 201 | CLA  | C4B-NB  | -2.55 | 1.34        | 1.37     |
| 39  | 5     | 317 | CHL  | C1A-CHA | -2.55 | 1.37        | 1.40     |
| 39  | 5     | 317 | CHL  | CHB-C4A | -2.54 | 1.35        | 1.38     |
| 38  | 7     | 302 | LUT  | O23-C23 | -2.54 | 1.39        | 1.43     |
| 22  | 3     | 316 | CLA  | C4B-NB  | -2.52 | 1.34        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 39  | 9     | 312  | CHL  | CHB-C4A | -2.52 | 1.35        | 1.38     |
| 39  | 6     | 318  | CHL  | C2C-C3C | 2.51  | 1.38        | 1.36     |
| 22  | A     | 808  | CLA  | C4B-NB  | -2.51 | 1.34        | 1.37     |
| 22  | 8     | 306  | CLA  | C4B-NB  | -2.51 | 1.34        | 1.37     |
| 24  | 7     | 303  | BCR  | C36-C18 | 2.51  | 1.55        | 1.50     |
| 24  | F     | 303  | BCR  | C36-C18 | 2.50  | 1.55        | 1.50     |
| 24  | 5     | 305  | BCR  | C36-C18 | 2.50  | 1.55        | 1.50     |
| 24  | J     | 104  | BCR  | C36-C18 | 2.49  | 1.55        | 1.50     |
| 24  | B     | 853  | BCR  | C39-C30 | -2.49 | 1.49        | 1.53     |
| 32  | F     | 306  | RRX  | C34-C9  | 2.49  | 1.55        | 1.50     |
| 36  | J     | 105  | C7Z  | C20-C13 | 2.48  | 1.55        | 1.50     |
| 24  | 3     | 307  | BCR  | C36-C18 | 2.47  | 1.55        | 1.50     |
| 24  | B     | 849  | BCR  | C36-C18 | 2.46  | 1.55        | 1.50     |
| 24  | G     | 203  | BCR  | C36-C18 | 2.46  | 1.55        | 1.50     |
| 36  | 5     | 306  | C7Z  | C20-C13 | 2.46  | 1.55        | 1.50     |
| 24  | A     | 848  | BCR  | C36-C18 | 2.46  | 1.55        | 1.50     |
| 24  | 3     | 307  | BCR  | C39-C30 | -2.46 | 1.49        | 1.53     |
| 36  | 5     | 306  | C7Z  | C38-C25 | 2.45  | 1.54        | 1.50     |
| 24  | A     | 856  | BCR  | C36-C18 | 2.45  | 1.55        | 1.50     |
| 24  | I     | 4001 | BCR  | C36-C18 | 2.45  | 1.55        | 1.50     |
| 24  | A     | 847  | BCR  | C36-C18 | 2.45  | 1.55        | 1.50     |
| 24  | 5     | 304  | BCR  | C36-C18 | 2.45  | 1.55        | 1.50     |
| 24  | 3     | 306  | BCR  | C36-C18 | 2.44  | 1.55        | 1.50     |
| 24  | 3     | 305  | BCR  | C36-C18 | 2.44  | 1.55        | 1.50     |
| 24  | 8     | 304  | BCR  | C36-C18 | 2.44  | 1.55        | 1.50     |
| 24  | 6     | 305  | BCR  | C36-C18 | 2.44  | 1.55        | 1.50     |
| 41  | 6     | 324  | 3PH  | O31-C31 | 2.43  | 1.40        | 1.33     |
| 24  | B     | 847  | BCR  | C36-C18 | 2.43  | 1.55        | 1.50     |
| 24  | B     | 845  | BCR  | C36-C18 | 2.43  | 1.55        | 1.50     |
| 24  | K     | 206  | BCR  | C36-C18 | 2.42  | 1.55        | 1.50     |
| 24  | 8     | 304  | BCR  | C39-C30 | -2.42 | 1.49        | 1.53     |
| 24  | 4     | 804  | BCR  | C36-C18 | 2.42  | 1.55        | 1.50     |
| 36  | J     | 105  | C7Z  | C40-C33 | 2.42  | 1.55        | 1.50     |
| 24  | B     | 848  | BCR  | C36-C18 | 2.42  | 1.55        | 1.50     |
| 24  | B     | 846  | BCR  | C36-C18 | 2.42  | 1.55        | 1.50     |
| 39  | 4     | 814  | CHL  | C1A-CHA | -2.42 | 1.37        | 1.40     |
| 36  | J     | 105  | C7Z  | C38-C25 | 2.41  | 1.54        | 1.50     |
| 24  | 6     | 306  | BCR  | C36-C18 | 2.40  | 1.55        | 1.50     |
| 24  | L     | 204  | BCR  | C36-C18 | 2.40  | 1.55        | 1.50     |
| 24  | 3     | 306  | BCR  | C39-C30 | -2.39 | 1.49        | 1.53     |
| 22  | 9     | 305  | CLA  | C1A-CHA | 2.39  | 1.52        | 1.43     |
| 41  | 8     | 320  | 3PH  | O31-C31 | 2.39  | 1.40        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | A     | 844  | BCR  | C36-C18 | 2.39  | 1.55        | 1.50     |
| 24  | A     | 846  | BCR  | C36-C18 | 2.39  | 1.55        | 1.50     |
| 41  | 5     | 325  | 3PH  | O31-C31 | 2.38  | 1.40        | 1.33     |
| 31  | B     | 852  | DGD  | CDA-CCA | -2.37 | 1.33        | 1.50     |
| 36  | 5     | 306  | C7Z  | C40-C33 | 2.37  | 1.55        | 1.50     |
| 35  | J     | 102  | T7X  | O18-C11 | 2.36  | 1.40        | 1.33     |
| 39  | 5     | 316  | CHL  | C3B-C2B | -2.36 | 1.37        | 1.40     |
| 22  | 1     | 308  | CLA  | C1C-C2C | 2.36  | 1.49        | 1.44     |
| 24  | 3     | 304  | BCR  | C36-C18 | 2.35  | 1.55        | 1.50     |
| 39  | 8     | 301  | CHL  | C3B-C2B | -2.35 | 1.37        | 1.40     |
| 24  | A     | 845  | BCR  | C36-C18 | 2.35  | 1.55        | 1.50     |
| 24  | A     | 856  | BCR  | C39-C30 | -2.34 | 1.49        | 1.53     |
| 27  | A     | 852  | DGA  | OG2-CG2 | -2.33 | 1.41        | 1.46     |
| 36  | J     | 105  | C7Z  | C19-C9  | 2.33  | 1.55        | 1.50     |
| 38  | Z     | 301  | LUT  | C26-C27 | 2.32  | 1.53        | 1.50     |
| 24  | B     | 844  | BCR  | C39-C30 | -2.32 | 1.49        | 1.53     |
| 39  | 4     | 813  | CHL  | C2C-C3C | 2.32  | 1.38        | 1.36     |
| 24  | 3     | 304  | BCR  | C39-C30 | -2.31 | 1.49        | 1.53     |
| 24  | K     | 206  | BCR  | C39-C30 | -2.30 | 1.49        | 1.53     |
| 36  | 5     | 306  | C7Z  | C19-C9  | 2.30  | 1.55        | 1.50     |
| 39  | 6     | 315  | CHL  | C1A-CHA | -2.30 | 1.37        | 1.40     |
| 24  | 6     | 305  | BCR  | C39-C30 | -2.30 | 1.49        | 1.53     |
| 24  | A     | 847  | BCR  | C39-C30 | -2.29 | 1.49        | 1.53     |
| 41  | 7     | 319  | 3PH  | O31-C31 | 2.29  | 1.40        | 1.33     |
| 24  | F     | 303  | BCR  | C39-C30 | -2.29 | 1.49        | 1.53     |
| 39  | 9     | 312  | CHL  | C3B-C2B | -2.29 | 1.37        | 1.40     |
| 22  | 3     | 315  | CLA  | C3D-C4D | -2.28 | 1.39        | 1.44     |
| 24  | 5     | 305  | BCR  | C39-C30 | -2.28 | 1.49        | 1.53     |
| 24  | 7     | 303  | BCR  | C39-C30 | -2.27 | 1.49        | 1.53     |
| 24  | L     | 204  | BCR  | C39-C30 | -2.27 | 1.49        | 1.53     |
| 24  | I     | 4001 | BCR  | C38-C26 | 2.27  | 1.54        | 1.50     |
| 24  | 3     | 305  | BCR  | C39-C30 | -2.27 | 1.49        | 1.53     |
| 38  | 1     | 302  | LUT  | C26-C27 | 2.27  | 1.53        | 1.50     |
| 22  | 9     | 303  | CLA  | C3D-C4D | -2.27 | 1.39        | 1.44     |
| 24  | 4     | 804  | BCR  | C39-C30 | -2.26 | 1.49        | 1.53     |
| 22  | K     | 205  | CLA  | C1A-CHA | 2.26  | 1.52        | 1.43     |
| 24  | B     | 845  | BCR  | C39-C30 | -2.26 | 1.49        | 1.53     |
| 24  | 5     | 305  | BCR  | C38-C26 | 2.25  | 1.54        | 1.50     |
| 24  | A     | 846  | BCR  | C39-C30 | -2.25 | 1.49        | 1.53     |
| 24  | B     | 846  | BCR  | C39-C30 | -2.24 | 1.49        | 1.53     |
| 39  | 6     | 320  | CHL  | C3B-C2B | -2.24 | 1.37        | 1.40     |
| 24  | 6     | 306  | BCR  | C39-C30 | -2.24 | 1.49        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 41  | 7     | 319  | 3PH  | O31-C3  | -2.23 | 1.40        | 1.45     |
| 24  | B     | 847  | BCR  | C39-C30 | -2.23 | 1.49        | 1.53     |
| 22  | 3     | 320  | CLA  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 24  | B     | 848  | BCR  | C39-C30 | -2.22 | 1.49        | 1.53     |
| 35  | J     | 102  | T7X  | O18-C9  | -2.22 | 1.40        | 1.45     |
| 24  | J     | 104  | BCR  | C39-C30 | -2.22 | 1.49        | 1.53     |
| 39  | 1     | 312  | CHL  | C2C-C3C | 2.22  | 1.38        | 1.36     |
| 24  | A     | 848  | BCR  | C39-C30 | -2.22 | 1.49        | 1.53     |
| 24  | B     | 849  | BCR  | C39-C30 | -2.22 | 1.49        | 1.53     |
| 24  | A     | 844  | BCR  | C39-C30 | -2.21 | 1.49        | 1.53     |
| 24  | G     | 203  | BCR  | C39-C30 | -2.21 | 1.49        | 1.53     |
| 24  | 8     | 304  | BCR  | C38-C26 | 2.21  | 1.54        | 1.50     |
| 41  | 6     | 324  | 3PH  | O31-C3  | -2.21 | 1.40        | 1.45     |
| 24  | A     | 846  | BCR  | C38-C26 | 2.21  | 1.54        | 1.50     |
| 24  | K     | 206  | BCR  | C38-C26 | 2.21  | 1.54        | 1.50     |
| 32  | F     | 306  | RRX  | C33-C5  | 2.21  | 1.54        | 1.50     |
| 24  | A     | 848  | BCR  | C38-C26 | 2.21  | 1.54        | 1.50     |
| 22  | 1     | 316  | CLA  | C3D-C4D | -2.21 | 1.39        | 1.44     |
| 24  | A     | 845  | BCR  | C39-C30 | -2.21 | 1.49        | 1.53     |
| 39  | 6     | 316  | CHL  | C2C-C3C | 2.20  | 1.38        | 1.36     |
| 24  | I     | 4001 | BCR  | C39-C30 | -2.20 | 1.49        | 1.53     |
| 24  | B     | 853  | BCR  | C37-C22 | 2.20  | 1.55        | 1.50     |
| 24  | 3     | 306  | BCR  | C38-C26 | 2.20  | 1.54        | 1.50     |
| 39  | 9     | 314  | CHL  | C3B-C2B | -2.20 | 1.37        | 1.40     |
| 39  | Z     | 311  | CHL  | C3B-C2B | -2.20 | 1.37        | 1.40     |
| 22  | K     | 205  | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 24  | B     | 847  | BCR  | C38-C26 | 2.20  | 1.54        | 1.50     |
| 41  | 5     | 325  | 3PH  | O31-C3  | -2.20 | 1.40        | 1.45     |
| 24  | B     | 845  | BCR  | C38-C26 | 2.19  | 1.54        | 1.50     |
| 41  | 6     | 324  | 3PH  | O21-C21 | 2.19  | 1.40        | 1.34     |
| 39  | 8     | 312  | CHL  | C2C-C3C | 2.19  | 1.38        | 1.36     |
| 24  | 5     | 304  | BCR  | C39-C30 | -2.19 | 1.49        | 1.53     |
| 24  | B     | 849  | BCR  | C37-C22 | 2.19  | 1.55        | 1.50     |
| 24  | B     | 844  | BCR  | C38-C26 | 2.19  | 1.54        | 1.50     |
| 24  | B     | 848  | BCR  | C38-C26 | 2.19  | 1.54        | 1.50     |
| 24  | 6     | 305  | BCR  | C38-C26 | 2.18  | 1.54        | 1.50     |
| 41  | 8     | 320  | 3PH  | O31-C3  | -2.18 | 1.40        | 1.45     |
| 24  | A     | 844  | BCR  | C38-C26 | 2.18  | 1.54        | 1.50     |
| 24  | B     | 846  | BCR  | C38-C26 | 2.17  | 1.54        | 1.50     |
| 24  | B     | 844  | BCR  | C37-C22 | 2.17  | 1.55        | 1.50     |
| 38  | Z     | 302  | LUT  | C26-C27 | 2.17  | 1.53        | 1.50     |
| 22  | Z     | 306  | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | 3     | 306 | BCR  | C37-C22 | 2.17  | 1.55        | 1.50     |
| 22  | B     | 824 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 24  | A     | 845 | BCR  | C37-C22 | 2.17  | 1.55        | 1.50     |
| 24  | A     | 847 | BCR  | C37-C22 | 2.16  | 1.55        | 1.50     |
| 24  | A     | 847 | BCR  | C38-C26 | 2.16  | 1.54        | 1.50     |
| 24  | 6     | 306 | BCR  | C38-C26 | 2.16  | 1.54        | 1.50     |
| 24  | K     | 206 | BCR  | C37-C22 | 2.16  | 1.55        | 1.50     |
| 38  | 3     | 303 | LUT  | C26-C27 | 2.16  | 1.53        | 1.50     |
| 24  | G     | 203 | BCR  | C37-C22 | 2.16  | 1.55        | 1.50     |
| 41  | 8     | 320 | 3PH  | O21-C21 | 2.15  | 1.40        | 1.34     |
| 41  | 7     | 319 | 3PH  | O21-C21 | 2.15  | 1.40        | 1.34     |
| 24  | L     | 204 | BCR  | C38-C26 | 2.15  | 1.54        | 1.50     |
| 24  | F     | 303 | BCR  | C37-C22 | 2.15  | 1.55        | 1.50     |
| 24  | 3     | 305 | BCR  | C37-C22 | 2.15  | 1.55        | 1.50     |
| 22  | 9     | 305 | CLA  | CAA-C2A | -2.15 | 1.50        | 1.54     |
| 24  | 3     | 307 | BCR  | C38-C26 | 2.14  | 1.54        | 1.50     |
| 24  | 3     | 304 | BCR  | C37-C22 | 2.14  | 1.55        | 1.50     |
| 24  | B     | 845 | BCR  | C37-C22 | 2.14  | 1.55        | 1.50     |
| 24  | 3     | 304 | BCR  | C38-C26 | 2.14  | 1.54        | 1.50     |
| 22  | A     | 826 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 24  | G     | 203 | BCR  | C38-C26 | 2.14  | 1.54        | 1.50     |
| 24  | J     | 104 | BCR  | C38-C26 | 2.14  | 1.54        | 1.50     |
| 24  | A     | 848 | BCR  | C37-C22 | 2.14  | 1.55        | 1.50     |
| 24  | A     | 846 | BCR  | C37-C22 | 2.14  | 1.55        | 1.50     |
| 22  | 1     | 305 | CLA  | C3D-C4D | -2.13 | 1.39        | 1.44     |
| 39  | 8     | 312 | CHL  | CHA-CBD | 2.13  | 1.54        | 1.51     |
| 24  | J     | 104 | BCR  | C37-C22 | 2.13  | 1.55        | 1.50     |
| 22  | 4     | 806 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 22  | 7     | 305 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 22  | 7     | 307 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 22  | 6     | 310 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 38  | 8     | 303 | LUT  | C26-C27 | 2.13  | 1.53        | 1.50     |
| 22  | 6     | 313 | CLA  | C1C-C2C | 2.13  | 1.48        | 1.44     |
| 24  | 3     | 307 | BCR  | C37-C22 | 2.13  | 1.55        | 1.50     |
| 39  | Z     | 311 | CHL  | CHA-CBD | 2.12  | 1.54        | 1.51     |
| 39  | 6     | 316 | CHL  | C3B-C2B | -2.12 | 1.37        | 1.40     |
| 22  | 1     | 311 | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 38  | 6     | 304 | LUT  | C26-C27 | 2.12  | 1.53        | 1.50     |
| 24  | 7     | 303 | BCR  | C37-C22 | 2.12  | 1.55        | 1.50     |
| 22  | B     | 807 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 41  | 5     | 325 | 3PH  | O21-C21 | 2.12  | 1.40        | 1.34     |
| 24  | B     | 849 | BCR  | C38-C26 | 2.12  | 1.54        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 24  | B     | 846  | BCR  | C37-C22 | 2.12  | 1.55        | 1.50     |
| 25  | 1     | 317  | LHG  | O7-C5   | -2.12 | 1.41        | 1.46     |
| 22  | 4     | 815  | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 24  | A     | 845  | BCR  | C38-C26 | 2.12  | 1.54        | 1.50     |
| 24  | 6     | 306  | BCR  | C37-C22 | 2.12  | 1.55        | 1.50     |
| 22  | F     | 302  | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 24  | B     | 848  | BCR  | C37-C22 | 2.11  | 1.55        | 1.50     |
| 24  | I     | 4001 | BCR  | C37-C22 | 2.11  | 1.55        | 1.50     |
| 24  | B     | 847  | BCR  | C37-C22 | 2.11  | 1.55        | 1.50     |
| 22  | B     | 828  | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 22  | 5     | 313  | CLA  | C1A-CHA | 2.11  | 1.51        | 1.43     |
| 24  | 5     | 305  | BCR  | C37-C22 | 2.11  | 1.55        | 1.50     |
| 38  | 9     | 302  | LUT  | C26-C27 | 2.11  | 1.53        | 1.50     |
| 22  | 1     | 313  | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 24  | L     | 204  | BCR  | C37-C22 | 2.11  | 1.55        | 1.50     |
| 24  | A     | 856  | BCR  | C38-C26 | 2.11  | 1.54        | 1.50     |
| 22  | B     | 808  | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 22  | F     | 301  | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 39  | 4     | 814  | CHL  | CHA-CBD | 2.10  | 1.54        | 1.51     |
| 22  | 4     | 811  | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 22  | 5     | 322  | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 38  | Z     | 301  | LUT  | C28-C27 | 2.10  | 1.37        | 1.32     |
| 38  | 7     | 302  | LUT  | C26-C27 | 2.10  | 1.53        | 1.50     |
| 22  | 9     | 309  | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | 5     | 320  | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 22  | J     | 103  | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 22  | 9     | 307  | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 22  | 6     | 309  | CLA  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 39  | 3     | 317  | CHL  | C3B-C2B | -2.09 | 1.37        | 1.40     |
| 24  | F     | 303  | BCR  | C38-C26 | 2.09  | 1.54        | 1.50     |
| 22  | 5     | 310  | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 38  | 5     | 303  | LUT  | C26-C27 | 2.09  | 1.53        | 1.50     |
| 22  | 7     | 307  | CLA  | C3D-C4D | -2.09 | 1.39        | 1.44     |
| 39  | Z     | 312  | CHL  | C2C-C3C | 2.09  | 1.38        | 1.36     |
| 22  | 7     | 322  | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 42  | 7     | 321  | SPH  | C3-C4   | 2.09  | 1.53        | 1.50     |
| 22  | 1     | 315  | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 22  | Z     | 308  | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 39  | 8     | 301  | CHL  | CHA-CBD | 2.09  | 1.54        | 1.51     |
| 39  | 9     | 314  | CHL  | CHA-CBD | 2.09  | 1.54        | 1.51     |
| 22  | 6     | 319  | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 39  | 7     | 313  | CHL  | C3B-C2B | -2.09 | 1.37        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 38  | 8     | 302 | LUT  | C26-C27 | 2.09  | 1.53        | 1.50     |
| 22  | 9     | 310 | CLA  | C1A-CHA | 2.09  | 1.51        | 1.43     |
| 22  | B     | 813 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 22  | A     | 823 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 22  | 7     | 311 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 38  | 7     | 301 | LUT  | C26-C27 | 2.09  | 1.53        | 1.50     |
| 22  | 3     | 318 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | Z     | 314 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | 3     | 310 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 22  | A     | 833 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | A     | 841 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | 7     | 315 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | B     | 825 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | 9     | 304 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 22  | 4     | 805 | CLA  | MG-NC   | 2.08  | 2.11        | 2.06     |
| 24  | 7     | 303 | BCR  | C38-C26 | 2.08  | 1.54        | 1.50     |
| 22  | B     | 805 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | B     | 831 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | 8     | 311 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 38  | 1     | 302 | LUT  | C28-C27 | 2.08  | 1.37        | 1.32     |
| 22  | Z     | 313 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | A     | 834 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 22  | 7     | 308 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 22  | 8     | 307 | CLA  | C1A-CHA | 2.08  | 1.51        | 1.43     |
| 22  | 1     | 307 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 24  | 8     | 304 | BCR  | C37-C22 | 2.08  | 1.55        | 1.50     |
| 22  | 8     | 309 | CLA  | C3D-C4D | -2.08 | 1.39        | 1.44     |
| 39  | 5     | 321 | CHL  | CHA-CBD | 2.08  | 1.54        | 1.51     |
| 22  | L     | 203 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | 7     | 324 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | A     | 812 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | A     | 824 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | 7     | 315 | CLA  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 35  | J     | 102 | T7X  | O16-C10 | 2.07  | 1.40        | 1.34     |
| 24  | 3     | 305 | BCR  | C38-C26 | 2.07  | 1.54        | 1.50     |
| 22  | 9     | 310 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 22  | A     | 818 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | A     | 825 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | B     | 829 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 39  | 5     | 316 | CHL  | C2C-C3C | 2.07  | 1.38        | 1.36     |
| 22  | 7     | 310 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | 6     | 317 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 9     | 305 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 22  | 8     | 306 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 22  | 5     | 314 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 24  | A     | 856 | BCR  | C37-C22 | 2.06  | 1.55        | 1.50     |
| 22  | B     | 837 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | B     | 826 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 5     | 308 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 22  | B     | 801 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 24  | A     | 844 | BCR  | C37-C22 | 2.06  | 1.55        | 1.50     |
| 24  | 4     | 804 | BCR  | C38-C26 | 2.06  | 1.54        | 1.50     |
| 22  | 4     | 807 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 22  | A     | 835 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | B     | 822 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | B     | 823 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 3     | 319 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 8     | 316 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | B     | 838 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 4     | 817 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 9     | 311 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | B     | 833 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 38  | 4     | 802 | LUT  | C26-C27 | 2.06  | 1.53        | 1.50     |
| 22  | 5     | 309 | CLA  | C1A-CHA | 2.06  | 1.51        | 1.43     |
| 22  | A     | 829 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | B     | 820 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 4     | 808 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | B     | 831 | CLA  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 22  | A     | 819 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 3     | 311 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 1     | 304 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | Z     | 309 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 22  | 7     | 308 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | B     | 821 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | 5     | 311 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | 3     | 314 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | 1     | 311 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 22  | B     | 816 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | B     | 836 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 38  | 4     | 803 | LUT  | C26-C27 | 2.05  | 1.53        | 1.50     |
| 22  | 1     | 308 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 22  | 9     | 307 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 22  | 2     | 301 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 22  | 8     | 309 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 39  | 4     | 819 | CHL  | C3B-C2B | -2.05 | 1.37        | 1.40     |
| 22  | A     | 830 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | 8     | 307 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | A     | 816 | CLA  | C1A-CHA | 2.05  | 1.51        | 1.43     |
| 22  | A     | 823 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 22  | A     | 836 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 22  | A     | 809 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | Z     | 306 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 22  | 3     | 308 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 22  | 3     | 316 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 22  | Z     | 304 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 24  | B     | 844 | BCR  | C36-C18 | 2.04  | 1.55        | 1.50     |
| 22  | 1     | 309 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 22  | K     | 202 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 8     | 308 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | Z     | 303 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | A     | 831 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | A     | 806 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 1     | 316 | CLA  | C1A-CHA | 2.04  | 1.51        | 1.43     |
| 22  | B     | 811 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 4     | 809 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 22  | A     | 810 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | B     | 835 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 3     | 322 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | A     | 820 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 1     | 309 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 2     | 304 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | B     | 814 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 22  | B     | 839 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 22  | B     | 806 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 38  | 3     | 302 | LUT  | C28-C27 | 2.04  | 1.37        | 1.32     |
| 22  | A     | 811 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 4     | 806 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 22  | F     | 305 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 5     | 315 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | B     | 809 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 22  | A     | 836 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | 3     | 313 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 22  | A     | 811 | CLA  | C3D-C4D | -2.04 | 1.39        | 1.44     |
| 24  | 4     | 804 | BCR  | C37-C22 | 2.04  | 1.55        | 1.50     |
| 24  | B     | 849 | BCR  | C33-C5  | 2.03  | 1.54        | 1.50     |
| 22  | 4     | 805 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 3     | 309 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | 1     | 310 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 22  | B     | 818 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | 4     | 805 | CLA  | CHD-C1D | 2.03  | 1.42        | 1.38     |
| 22  | Z     | 316 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | A     | 822 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 22  | B     | 835 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | A     | 808 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | A     | 855 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | 6     | 322 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | 6     | 312 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 22  | A     | 807 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | A     | 818 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | Z     | 307 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | A     | 842 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | 7     | 306 | CLA  | C1A-CHA | 2.03  | 1.51        | 1.43     |
| 22  | F     | 305 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | 1     | 307 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 24  | 6     | 305 | BCR  | C37-C22 | 2.03  | 1.54        | 1.50     |
| 22  | 6     | 311 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | 5     | 309 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | 3     | 312 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | B     | 832 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 22  | 5     | 311 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | A     | 839 | CLA  | C3D-C4D | -2.03 | 1.39        | 1.44     |
| 22  | 5     | 307 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | A     | 803 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 24  | 5     | 304 | BCR  | C37-C22 | 2.02  | 1.54        | 1.50     |
| 39  | 7     | 313 | CHL  | CHA-CBD | 2.02  | 1.54        | 1.51     |
| 22  | 6     | 321 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 6     | 310 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 39  | 6     | 318 | CHL  | CHA-CBD | 2.02  | 1.54        | 1.51     |
| 22  | A     | 805 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | Z     | 310 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 8     | 310 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | B     | 817 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | L     | 201 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 7     | 316 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 3     | 322 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | B     | 841 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | A     | 840 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 8     | 316 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | 5     | 320 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 3     | 308 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | A     | 812 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 6     | 307 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 8     | 314 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | A     | 817 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | B     | 823 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 7     | 317 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | F     | 302 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | 5     | 326 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 22  | 4     | 808 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 22  | K     | 203 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 22  | 8     | 313 | CLA  | C1A-CHA | 2.02  | 1.51        | 1.43     |
| 22  | 5     | 313 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | Z     | 315 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | 9     | 306 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | 6     | 301 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | 7     | 304 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | A     | 810 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | G     | 201 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 22  | A     | 809 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | L     | 202 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 38  | 5     | 303 | LUT  | C28-C27 | 2.01  | 1.36        | 1.32     |
| 22  | A     | 814 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | 1     | 306 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | 4     | 811 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 22  | 8     | 305 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | 6     | 312 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | B     | 806 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | G     | 202 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | G     | 202 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | Z     | 303 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 38  | 1     | 303 | LUT  | C26-C27 | 2.01  | 1.53        | 1.50     |
| 22  | A     | 803 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | B     | 828 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | B     | 827 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | 5     | 311 | CLA  | C1A-CHA | 2.01  | 1.51        | 1.43     |
| 38  | 9     | 301 | LUT  | C26-C27 | 2.01  | 1.53        | 1.50     |
| 22  | B     | 830 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | A     | 820 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | Z     | 307 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | B     | 809 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | L     | 202 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 40  | 1     | 318 | SQD  | O47-C45 | -2.01 | 1.41        | 1.46     |
| 22  | 7     | 317 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 38  | 5     | 302 | LUT  | C26-C27 | 2.01  | 1.53        | 1.50     |
| 22  | B     | 807 | CLA  | C3D-C4D | -2.01 | 1.39        | 1.44     |
| 22  | A     | 815 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | B     | 818 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 22  | 5     | 319 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | 7     | 305 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | 8     | 306 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | A     | 839 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 22  | B     | 819 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 22  | 7     | 309 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 22  | 4     | 807 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 39  | 6     | 315 | CHL  | CHA-CBD | 2.00  | 1.54        | 1.51     |
| 22  | A     | 855 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | A     | 827 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 22  | 3     | 310 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 22  | A     | 815 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | B     | 840 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | 1     | 313 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 38  | 9     | 302 | LUT  | C28-C27 | 2.00  | 1.36        | 1.32     |
| 22  | 6     | 307 | CLA  | C1A-CHA | 2.00  | 1.51        | 1.43     |
| 22  | B     | 813 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | B     | 840 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 22  | 1     | 315 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | 8     | 314 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | A     | 822 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 22  | K     | 204 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 39  | 1     | 312 | CHL  | CHA-CBD | 2.00  | 1.54        | 1.51     |
| 22  | 6     | 307 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |

All (5316) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 24  | B     | 848 | BCR  | C23-C22-C21 | 27.34  | 162.01      | 119.01   |
| 24  | B     | 848 | BCR  | C37-C22-C21 | -25.67 | 81.23       | 122.82   |
| 24  | B     | 848 | BCR  | C37-C22-C23 | -24.37 | 80.87       | 118.09   |
| 21  | A     | 801 | CL0  | C1B-CHB-C4A | 14.37  | 130.57      | 121.32   |
| 24  | 3     | 304 | BCR  | C11-C10-C9  | -11.74 | 110.82      | 127.28   |
| 22  | K     | 205 | CLA  | C4A-NA-C1A  | 11.13  | 111.76      | 106.68   |
| 24  | A     | 844 | BCR  | C15-C14-C13 | -10.85 | 112.06      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 9     | 309 | CLA  | C4A-NA-C1A  | 10.80 | 111.61      | 106.68   |
| 22  | 9     | 305 | CLA  | C4A-NA-C1A  | 10.68 | 111.55      | 106.68   |
| 22  | 1     | 311 | CLA  | C4A-NA-C1A  | 10.07 | 111.27      | 106.68   |
| 22  | 3     | 320 | CLA  | C4A-NA-C1A  | 9.68  | 111.10      | 106.68   |
| 24  | 3     | 307 | BCR  | C20-C21-C22 | -9.66 | 113.73      | 127.28   |
| 22  | 9     | 310 | CLA  | C4A-NA-C1A  | 9.57  | 111.05      | 106.68   |
| 24  | 3     | 307 | BCR  | C15-C14-C13 | -9.44 | 114.04      | 127.28   |
| 22  | 8     | 307 | CLA  | C4A-NA-C1A  | 9.38  | 110.96      | 106.68   |
| 22  | 5     | 320 | CLA  | C4A-NA-C1A  | 9.36  | 110.95      | 106.68   |
| 22  | A     | 822 | CLA  | C4A-NA-C1A  | 9.31  | 110.93      | 106.68   |
| 22  | 1     | 316 | CLA  | C4A-NA-C1A  | 9.30  | 110.92      | 106.68   |
| 22  | 3     | 315 | CLA  | C4A-NA-C1A  | 9.27  | 110.91      | 106.68   |
| 24  | A     | 844 | BCR  | C7-C8-C9    | -9.25 | 112.55      | 126.23   |
| 22  | 5     | 323 | CLA  | C4A-NA-C1A  | 9.23  | 110.89      | 106.68   |
| 22  | 6     | 307 | CLA  | C4A-NA-C1A  | 9.21  | 110.88      | 106.68   |
| 22  | 7     | 306 | CLA  | C4A-NA-C1A  | 9.11  | 110.83      | 106.68   |
| 22  | 4     | 807 | CLA  | C4A-NA-C1A  | 9.10  | 110.83      | 106.68   |
| 22  | B     | 815 | CLA  | C4A-NA-C1A  | 9.09  | 110.82      | 106.68   |
| 22  | 9     | 304 | CLA  | C4A-NA-C1A  | 9.09  | 110.82      | 106.68   |
| 22  | A     | 813 | CLA  | C4A-NA-C1A  | 9.05  | 110.81      | 106.68   |
| 22  | 3     | 313 | CLA  | C4A-NA-C1A  | 9.04  | 110.81      | 106.68   |
| 22  | A     | 818 | CLA  | C4A-NA-C1A  | 9.00  | 110.78      | 106.68   |
| 22  | A     | 816 | CLA  | C4A-NA-C1A  | 9.00  | 110.78      | 106.68   |
| 22  | A     | 838 | CLA  | C4A-NA-C1A  | 8.97  | 110.77      | 106.68   |
| 22  | 1     | 309 | CLA  | C4A-NA-C1A  | 8.97  | 110.77      | 106.68   |
| 22  | L     | 201 | CLA  | C4A-NA-C1A  | 8.94  | 110.76      | 106.68   |
| 22  | 7     | 310 | CLA  | C4A-NA-C1A  | 8.93  | 110.75      | 106.68   |
| 22  | 6     | 317 | CLA  | C4A-NA-C1A  | 8.91  | 110.75      | 106.68   |
| 22  | A     | 808 | CLA  | C4A-NA-C1A  | 8.91  | 110.75      | 106.68   |
| 22  | B     | 810 | CLA  | C4A-NA-C1A  | 8.91  | 110.74      | 106.68   |
| 22  | B     | 827 | CLA  | C4A-NA-C1A  | 8.90  | 110.74      | 106.68   |
| 22  | A     | 815 | CLA  | C4A-NA-C1A  | 8.89  | 110.73      | 106.68   |
| 22  | A     | 826 | CLA  | C4A-NA-C1A  | 8.88  | 110.73      | 106.68   |
| 22  | K     | 202 | CLA  | C4A-NA-C1A  | 8.86  | 110.72      | 106.68   |
| 22  | 4     | 815 | CLA  | C4A-NA-C1A  | 8.86  | 110.72      | 106.68   |
| 22  | Z     | 305 | CLA  | C4A-NA-C1A  | 8.86  | 110.72      | 106.68   |
| 24  | B     | 844 | BCR  | C11-C10-C9  | -8.85 | 114.86      | 127.28   |
| 22  | B     | 805 | CLA  | C4A-NA-C1A  | 8.83  | 110.71      | 106.68   |
| 22  | A     | 832 | CLA  | C4A-NA-C1A  | 8.82  | 110.70      | 106.68   |
| 22  | 8     | 305 | CLA  | C4A-NA-C1A  | 8.82  | 110.70      | 106.68   |
| 22  | A     | 827 | CLA  | C4A-NA-C1A  | 8.81  | 110.70      | 106.68   |
| 22  | 7     | 314 | CLA  | C4A-NA-C1A  | 8.81  | 110.70      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22  | 5     | 326 | CLA  | C4A-NA-C1A  | 8.80 | 110.70      | 106.68   |
| 22  | 5     | 309 | CLA  | C4A-NA-C1A  | 8.80 | 110.69      | 106.68   |
| 22  | B     | 817 | CLA  | C4A-NA-C1A  | 8.79 | 110.69      | 106.68   |
| 22  | 7     | 309 | CLA  | C4A-NA-C1A  | 8.78 | 110.69      | 106.68   |
| 22  | 5     | 313 | CLA  | C4A-NA-C1A  | 8.78 | 110.68      | 106.68   |
| 22  | B     | 841 | CLA  | C4A-NA-C1A  | 8.77 | 110.68      | 106.68   |
| 22  | 5     | 318 | CLA  | C4A-NA-C1A  | 8.75 | 110.67      | 106.68   |
| 22  | A     | 817 | CLA  | C4A-NA-C1A  | 8.73 | 110.66      | 106.68   |
| 22  | B     | 833 | CLA  | C4A-NA-C1A  | 8.73 | 110.66      | 106.68   |
| 22  | B     | 834 | CLA  | C4A-NA-C1A  | 8.73 | 110.66      | 106.68   |
| 22  | A     | 839 | CLA  | C4A-NA-C1A  | 8.73 | 110.66      | 106.68   |
| 22  | Z     | 314 | CLA  | C4A-NA-C1A  | 8.73 | 110.66      | 106.68   |
| 22  | 7     | 304 | CLA  | C4A-NA-C1A  | 8.73 | 110.66      | 106.68   |
| 22  | 7     | 315 | CLA  | C4A-NA-C1A  | 8.73 | 110.66      | 106.68   |
| 22  | 4     | 810 | CLA  | C4A-NA-C1A  | 8.73 | 110.66      | 106.68   |
| 22  | A     | 842 | CLA  | C4A-NA-C1A  | 8.71 | 110.65      | 106.68   |
| 22  | B     | 837 | CLA  | C4A-NA-C1A  | 8.70 | 110.65      | 106.68   |
| 22  | B     | 811 | CLA  | C4A-NA-C1A  | 8.70 | 110.65      | 106.68   |
| 22  | 7     | 311 | CLA  | C4A-NA-C1A  | 8.70 | 110.65      | 106.68   |
| 22  | Z     | 313 | CLA  | C4A-NA-C1A  | 8.69 | 110.64      | 106.68   |
| 22  | 6     | 308 | CLA  | C4A-NA-C1A  | 8.69 | 110.64      | 106.68   |
| 22  | 8     | 313 | CLA  | C4A-NA-C1A  | 8.68 | 110.64      | 106.68   |
| 22  | 6     | 313 | CLA  | C4A-NA-C1A  | 8.68 | 110.64      | 106.68   |
| 22  | A     | 807 | CLA  | C4A-NA-C1A  | 8.68 | 110.64      | 106.68   |
| 22  | A     | 812 | CLA  | C4A-NA-C1A  | 8.68 | 110.64      | 106.68   |
| 22  | 3     | 310 | CLA  | C4A-NA-C1A  | 8.68 | 110.64      | 106.68   |
| 22  | 3     | 314 | CLA  | C4A-NA-C1A  | 8.68 | 110.64      | 106.68   |
| 22  | 1     | 304 | CLA  | C4A-NA-C1A  | 8.67 | 110.64      | 106.68   |
| 21  | A     | 801 | CL0  | O2D-CGD-CBD | 8.66 | 120.47      | 110.95   |
| 22  | L     | 203 | CLA  | C4A-NA-C1A  | 8.66 | 110.63      | 106.68   |
| 22  | Z     | 303 | CLA  | C4A-NA-C1A  | 8.66 | 110.63      | 106.68   |
| 22  | 6     | 322 | CLA  | C4A-NA-C1A  | 8.66 | 110.63      | 106.68   |
| 22  | 6     | 309 | CLA  | C4A-NA-C1A  | 8.66 | 110.63      | 106.68   |
| 22  | B     | 813 | CLA  | C4A-NA-C1A  | 8.65 | 110.62      | 106.68   |
| 22  | 1     | 313 | CLA  | C4A-NA-C1A  | 8.65 | 110.62      | 106.68   |
| 22  | 5     | 314 | CLA  | C4A-NA-C1A  | 8.65 | 110.62      | 106.68   |
| 22  | A     | 833 | CLA  | C4A-NA-C1A  | 8.64 | 110.62      | 106.68   |
| 22  | 2     | 304 | CLA  | C4A-NA-C1A  | 8.64 | 110.62      | 106.68   |
| 22  | 8     | 308 | CLA  | C4A-NA-C1A  | 8.64 | 110.62      | 106.68   |
| 22  | 5     | 312 | CLA  | C4A-NA-C1A  | 8.64 | 110.62      | 106.68   |
| 22  | A     | 836 | CLA  | C4A-NA-C1A  | 8.64 | 110.62      | 106.68   |
| 22  | 4     | 811 | CLA  | C4A-NA-C1A  | 8.64 | 110.62      | 106.68   |

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| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 22  | A     | 831 | CLA  | C4A-NA-C1A | 8.63 | 110.62      | 106.68   |
| 22  | A     | 840 | CLA  | C4A-NA-C1A | 8.63 | 110.62      | 106.68   |
| 22  | B     | 819 | CLA  | C4A-NA-C1A | 8.63 | 110.62      | 106.68   |
| 22  | K     | 203 | CLA  | C4A-NA-C1A | 8.63 | 110.62      | 106.68   |
| 22  | Z     | 308 | CLA  | C4A-NA-C1A | 8.63 | 110.61      | 106.68   |
| 22  | 1     | 310 | CLA  | C4A-NA-C1A | 8.62 | 110.61      | 106.68   |
| 22  | A     | 825 | CLA  | C4A-NA-C1A | 8.62 | 110.61      | 106.68   |
| 22  | G     | 201 | CLA  | C4A-NA-C1A | 8.62 | 110.61      | 106.68   |
| 22  | A     | 828 | CLA  | C4A-NA-C1A | 8.61 | 110.61      | 106.68   |
| 22  | 8     | 311 | CLA  | C4A-NA-C1A | 8.61 | 110.61      | 106.68   |
| 22  | F     | 304 | CLA  | C4A-NA-C1A | 8.61 | 110.61      | 106.68   |
| 22  | 1     | 314 | CLA  | C4A-NA-C1A | 8.61 | 110.61      | 106.68   |
| 22  | G     | 202 | CLA  | C4A-NA-C1A | 8.60 | 110.60      | 106.68   |
| 22  | 7     | 324 | CLA  | C4A-NA-C1A | 8.60 | 110.60      | 106.68   |
| 22  | 3     | 318 | CLA  | C4A-NA-C1A | 8.60 | 110.60      | 106.68   |
| 22  | B     | 830 | CLA  | C4A-NA-C1A | 8.59 | 110.60      | 106.68   |
| 22  | 6     | 321 | CLA  | C4A-NA-C1A | 8.59 | 110.60      | 106.68   |
| 22  | A     | 805 | CLA  | C4A-NA-C1A | 8.59 | 110.60      | 106.68   |
| 22  | 3     | 308 | CLA  | C4A-NA-C1A | 8.59 | 110.60      | 106.68   |
| 22  | B     | 826 | CLA  | C4A-NA-C1A | 8.59 | 110.60      | 106.68   |
| 22  | 3     | 311 | CLA  | C4A-NA-C1A | 8.59 | 110.60      | 106.68   |
| 22  | F     | 302 | CLA  | C4A-NA-C1A | 8.58 | 110.59      | 106.68   |
| 22  | A     | 804 | CLA  | C4A-NA-C1A | 8.58 | 110.59      | 106.68   |
| 22  | B     | 842 | CLA  | C4A-NA-C1A | 8.58 | 110.59      | 106.68   |
| 22  | 8     | 316 | CLA  | C4A-NA-C1A | 8.58 | 110.59      | 106.68   |
| 22  | B     | 838 | CLA  | C4A-NA-C1A | 8.57 | 110.59      | 106.68   |
| 22  | 5     | 310 | CLA  | C4A-NA-C1A | 8.57 | 110.59      | 106.68   |
| 22  | 5     | 315 | CLA  | C4A-NA-C1A | 8.57 | 110.59      | 106.68   |
| 22  | A     | 837 | CLA  | C4A-NA-C1A | 8.57 | 110.59      | 106.68   |
| 22  | 1     | 307 | CLA  | C4A-NA-C1A | 8.57 | 110.59      | 106.68   |
| 22  | 6     | 312 | CLA  | C4A-NA-C1A | 8.57 | 110.59      | 106.68   |
| 22  | B     | 818 | CLA  | C4A-NA-C1A | 8.57 | 110.59      | 106.68   |
| 22  | 1     | 315 | CLA  | C4A-NA-C1A | 8.57 | 110.59      | 106.68   |
| 22  | 3     | 319 | CLA  | C4A-NA-C1A | 8.56 | 110.58      | 106.68   |
| 22  | A     | 814 | CLA  | C4A-NA-C1A | 8.55 | 110.58      | 106.68   |
| 22  | 6     | 301 | CLA  | C4A-NA-C1A | 8.55 | 110.58      | 106.68   |
| 22  | B     | 839 | CLA  | C4A-NA-C1A | 8.55 | 110.58      | 106.68   |
| 22  | 7     | 316 | CLA  | C4A-NA-C1A | 8.55 | 110.58      | 106.68   |
| 22  | 5     | 322 | CLA  | C4A-NA-C1A | 8.55 | 110.58      | 106.68   |
| 22  | 5     | 311 | CLA  | C4A-NA-C1A | 8.55 | 110.58      | 106.68   |
| 22  | 4     | 812 | CLA  | C4A-NA-C1A | 8.54 | 110.58      | 106.68   |
| 22  | B     | 820 | CLA  | C4A-NA-C1A | 8.54 | 110.58      | 106.68   |

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| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 22  | B     | 832 | CLA  | C4A-NA-C1A | 8.53 | 110.57      | 106.68   |
| 22  | A     | 830 | CLA  | C4A-NA-C1A | 8.53 | 110.57      | 106.68   |
| 22  | 4     | 818 | CLA  | C4A-NA-C1A | 8.53 | 110.57      | 106.68   |
| 22  | 5     | 307 | CLA  | C4A-NA-C1A | 8.53 | 110.57      | 106.68   |
| 22  | B     | 808 | CLA  | C4A-NA-C1A | 8.52 | 110.57      | 106.68   |
| 22  | 4     | 808 | CLA  | C4A-NA-C1A | 8.51 | 110.56      | 106.68   |
| 22  | A     | 841 | CLA  | C4A-NA-C1A | 8.51 | 110.56      | 106.68   |
| 22  | 2     | 302 | CLA  | C4A-NA-C1A | 8.51 | 110.56      | 106.68   |
| 22  | 6     | 319 | CLA  | C4A-NA-C1A | 8.50 | 110.56      | 106.68   |
| 22  | Z     | 306 | CLA  | C4A-NA-C1A | 8.50 | 110.56      | 106.68   |
| 22  | Z     | 315 | CLA  | C4A-NA-C1A | 8.50 | 110.56      | 106.68   |
| 22  | A     | 802 | CLA  | C4A-NA-C1A | 8.50 | 110.56      | 106.68   |
| 22  | A     | 810 | CLA  | C4A-NA-C1A | 8.50 | 110.56      | 106.68   |
| 22  | B     | 806 | CLA  | C4A-NA-C1A | 8.50 | 110.56      | 106.68   |
| 22  | L     | 202 | CLA  | C4A-NA-C1A | 8.50 | 110.56      | 106.68   |
| 22  | B     | 829 | CLA  | C4A-NA-C1A | 8.49 | 110.55      | 106.68   |
| 22  | A     | 821 | CLA  | C4A-NA-C1A | 8.49 | 110.55      | 106.68   |
| 22  | Z     | 309 | CLA  | C4A-NA-C1A | 8.49 | 110.55      | 106.68   |
| 22  | 5     | 319 | CLA  | C4A-NA-C1A | 8.49 | 110.55      | 106.68   |
| 22  | 9     | 313 | CLA  | C4A-NA-C1A | 8.49 | 110.55      | 106.68   |
| 22  | 9     | 306 | CLA  | C4A-NA-C1A | 8.48 | 110.55      | 106.68   |
| 22  | 1     | 305 | CLA  | C4A-NA-C1A | 8.48 | 110.55      | 106.68   |
| 22  | F     | 301 | CLA  | C4A-NA-C1A | 8.47 | 110.54      | 106.68   |
| 22  | 9     | 311 | CLA  | C4A-NA-C1A | 8.47 | 110.54      | 106.68   |
| 22  | B     | 807 | CLA  | C4A-NA-C1A | 8.47 | 110.54      | 106.68   |
| 22  | A     | 824 | CLA  | C4A-NA-C1A | 8.47 | 110.54      | 106.68   |
| 22  | B     | 840 | CLA  | C4A-NA-C1A | 8.46 | 110.54      | 106.68   |
| 22  | K     | 204 | CLA  | C4A-NA-C1A | 8.45 | 110.53      | 106.68   |
| 22  | Z     | 304 | CLA  | C4A-NA-C1A | 8.45 | 110.53      | 106.68   |
| 22  | A     | 803 | CLA  | C4A-NA-C1A | 8.45 | 110.53      | 106.68   |
| 22  | A     | 854 | CLA  | C4A-NA-C1A | 8.45 | 110.53      | 106.68   |
| 22  | B     | 831 | CLA  | C4A-NA-C1A | 8.45 | 110.53      | 106.68   |
| 22  | 7     | 323 | CLA  | C4A-NA-C1A | 8.43 | 110.53      | 106.68   |
| 22  | 5     | 308 | CLA  | C4A-NA-C1A | 8.43 | 110.53      | 106.68   |
| 22  | A     | 823 | CLA  | C4A-NA-C1A | 8.43 | 110.52      | 106.68   |
| 22  | 4     | 817 | CLA  | C4A-NA-C1A | 8.43 | 110.52      | 106.68   |
| 22  | B     | 835 | CLA  | C4A-NA-C1A | 8.42 | 110.52      | 106.68   |
| 22  | B     | 836 | CLA  | C4A-NA-C1A | 8.42 | 110.52      | 106.68   |
| 22  | 5     | 301 | CLA  | C4A-NA-C1A | 8.42 | 110.52      | 106.68   |
| 22  | 2     | 301 | CLA  | C4A-NA-C1A | 8.41 | 110.52      | 106.68   |
| 22  | B     | 814 | CLA  | C4A-NA-C1A | 8.41 | 110.52      | 106.68   |
| 22  | 3     | 309 | CLA  | C4A-NA-C1A | 8.41 | 110.52      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | 5     | 305 | BCR  | C20-C21-C22 | -8.41 | 115.49      | 127.28   |
| 22  | 6     | 302 | CLA  | C4A-NA-C1A  | 8.41  | 110.51      | 106.68   |
| 22  | B     | 824 | CLA  | C4A-NA-C1A  | 8.40  | 110.51      | 106.68   |
| 22  | B     | 823 | CLA  | C4A-NA-C1A  | 8.40  | 110.51      | 106.68   |
| 22  | 7     | 322 | CLA  | C4A-NA-C1A  | 8.40  | 110.51      | 106.68   |
| 22  | 8     | 309 | CLA  | C4A-NA-C1A  | 8.38  | 110.50      | 106.68   |
| 22  | Z     | 310 | CLA  | C4A-NA-C1A  | 8.37  | 110.50      | 106.68   |
| 22  | J     | 103 | CLA  | C4A-NA-C1A  | 8.37  | 110.50      | 106.68   |
| 22  | A     | 819 | CLA  | C4A-NA-C1A  | 8.37  | 110.50      | 106.68   |
| 22  | 4     | 806 | CLA  | C4A-NA-C1A  | 8.37  | 110.50      | 106.68   |
| 22  | 8     | 314 | CLA  | C4A-NA-C1A  | 8.36  | 110.50      | 106.68   |
| 22  | 9     | 308 | CLA  | C4A-NA-C1A  | 8.36  | 110.50      | 106.68   |
| 22  | 7     | 312 | CLA  | C4A-NA-C1A  | 8.36  | 110.49      | 106.68   |
| 24  | 6     | 306 | BCR  | C24-C23-C22 | -8.36 | 113.87      | 126.23   |
| 22  | A     | 820 | CLA  | C4A-NA-C1A  | 8.35  | 110.49      | 106.68   |
| 22  | A     | 834 | CLA  | C4A-NA-C1A  | 8.34  | 110.49      | 106.68   |
| 22  | F     | 305 | CLA  | C4A-NA-C1A  | 8.34  | 110.49      | 106.68   |
| 22  | B     | 801 | CLA  | C4A-NA-C1A  | 8.34  | 110.48      | 106.68   |
| 22  | 8     | 310 | CLA  | C4A-NA-C1A  | 8.32  | 110.48      | 106.68   |
| 22  | A     | 829 | CLA  | C4A-NA-C1A  | 8.32  | 110.47      | 106.68   |
| 22  | B     | 816 | CLA  | C4A-NA-C1A  | 8.32  | 110.47      | 106.68   |
| 22  | Z     | 316 | CLA  | C4A-NA-C1A  | 8.32  | 110.47      | 106.68   |
| 22  | 7     | 305 | CLA  | C4A-NA-C1A  | 8.32  | 110.47      | 106.68   |
| 22  | B     | 821 | CLA  | C4A-NA-C1A  | 8.31  | 110.47      | 106.68   |
| 22  | 7     | 308 | CLA  | C4A-NA-C1A  | 8.31  | 110.47      | 106.68   |
| 22  | 3     | 316 | CLA  | C4A-NA-C1A  | 8.31  | 110.47      | 106.68   |
| 22  | B     | 812 | CLA  | C4A-NA-C1A  | 8.30  | 110.46      | 106.68   |
| 24  | B     | 848 | BCR  | C20-C21-C22 | -8.29 | 115.65      | 127.28   |
| 22  | A     | 811 | CLA  | C4A-NA-C1A  | 8.29  | 110.46      | 106.68   |
| 22  | A     | 835 | CLA  | C4A-NA-C1A  | 8.27  | 110.45      | 106.68   |
| 22  | B     | 822 | CLA  | C4A-NA-C1A  | 8.27  | 110.45      | 106.68   |
| 22  | 8     | 306 | CLA  | C4A-NA-C1A  | 8.23  | 110.44      | 106.68   |
| 22  | 1     | 306 | CLA  | C4A-NA-C1A  | 8.23  | 110.43      | 106.68   |
| 22  | A     | 855 | CLA  | C4A-NA-C1A  | 8.22  | 110.43      | 106.68   |
| 22  | 6     | 310 | CLA  | C4A-NA-C1A  | 8.21  | 110.42      | 106.68   |
| 22  | 7     | 307 | CLA  | C4A-NA-C1A  | 8.21  | 110.42      | 106.68   |
| 24  | 3     | 304 | BCR  | C7-C8-C9    | -8.21 | 114.10      | 126.23   |
| 22  | 7     | 317 | CLA  | C4A-NA-C1A  | 8.20  | 110.42      | 106.68   |
| 22  | B     | 825 | CLA  | C4A-NA-C1A  | 8.19  | 110.42      | 106.68   |
| 22  | 6     | 314 | CLA  | C4A-NA-C1A  | 8.19  | 110.42      | 106.68   |
| 22  | 3     | 322 | CLA  | C4A-NA-C1A  | 8.18  | 110.41      | 106.68   |
| 22  | B     | 828 | CLA  | C4A-NA-C1A  | 8.17  | 110.41      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 4     | 809  | CLA  | C4A-NA-C1A  | 8.16  | 110.40      | 106.68   |
| 22  | Z     | 307  | CLA  | C4A-NA-C1A  | 8.14  | 110.39      | 106.68   |
| 22  | A     | 806  | CLA  | C4A-NA-C1A  | 8.13  | 110.39      | 106.68   |
| 22  | 6     | 311  | CLA  | C4A-NA-C1A  | 8.13  | 110.39      | 106.68   |
| 22  | 9     | 307  | CLA  | C4A-NA-C1A  | 8.13  | 110.39      | 106.68   |
| 22  | 3     | 312  | CLA  | C4A-NA-C1A  | 8.11  | 110.38      | 106.68   |
| 22  | B     | 809  | CLA  | C4A-NA-C1A  | 8.06  | 110.36      | 106.68   |
| 22  | 1     | 308  | CLA  | C4A-NA-C1A  | 8.04  | 110.35      | 106.68   |
| 22  | 9     | 303  | CLA  | C4A-NA-C1A  | 7.96  | 110.31      | 106.68   |
| 22  | A     | 809  | CLA  | C4A-NA-C1A  | 7.95  | 110.31      | 106.68   |
| 22  | 4     | 805  | CLA  | C4A-NA-C1A  | 7.74  | 110.21      | 106.68   |
| 24  | 6     | 306  | BCR  | C16-C17-C18 | -7.69 | 116.49      | 127.28   |
| 24  | 3     | 307  | BCR  | C24-C23-C22 | -7.64 | 114.93      | 126.23   |
| 24  | 6     | 306  | BCR  | C11-C10-C9  | -7.46 | 116.82      | 127.28   |
| 22  | 9     | 305  | CLA  | CAA-C2A-C3A | -7.42 | 92.94       | 113.00   |
| 24  | 5     | 305  | BCR  | C15-C14-C13 | -7.34 | 116.98      | 127.28   |
| 24  | B     | 847  | BCR  | C15-C14-C13 | -7.27 | 117.09      | 127.28   |
| 24  | I     | 4001 | BCR  | C16-C17-C18 | -7.25 | 117.11      | 127.28   |
| 24  | A     | 846  | BCR  | C15-C14-C13 | -7.24 | 117.12      | 127.28   |
| 32  | F     | 306  | RRX  | C11-C10-C9  | -6.98 | 117.49      | 127.28   |
| 24  | 3     | 304  | BCR  | C15-C16-C17 | -6.69 | 109.82      | 123.52   |
| 24  | 5     | 305  | BCR  | C11-C10-C9  | -6.49 | 118.18      | 127.28   |
| 36  | 5     | 306  | C7Z  | C11-C10-C9  | -6.44 | 118.25      | 127.28   |
| 24  | 3     | 307  | BCR  | C11-C10-C9  | -6.40 | 118.30      | 127.28   |
| 24  | G     | 203  | BCR  | C20-C21-C22 | -6.39 | 118.31      | 127.28   |
| 24  | 5     | 304  | BCR  | C20-C21-C22 | -6.37 | 118.34      | 127.28   |
| 24  | B     | 844  | BCR  | C20-C21-C22 | -6.34 | 118.38      | 127.28   |
| 24  | K     | 206  | BCR  | C11-C10-C9  | -6.31 | 118.43      | 127.28   |
| 24  | B     | 848  | BCR  | C33-C5-C6   | -6.16 | 117.76      | 124.48   |
| 24  | A     | 848  | BCR  | C20-C21-C22 | -6.14 | 118.66      | 127.28   |
| 24  | 6     | 305  | BCR  | C20-C21-C22 | -6.14 | 118.67      | 127.28   |
| 24  | 3     | 307  | BCR  | C38-C26-C25 | -6.14 | 117.78      | 124.48   |
| 24  | A     | 856  | BCR  | C20-C21-C22 | -6.11 | 118.71      | 127.28   |
| 39  | 4     | 816  | CHL  | C1B-CHB-C4A | 6.08  | 125.24      | 121.32   |
| 22  | 9     | 305  | CLA  | O2D-CGD-CBD | 6.08  | 121.86      | 111.23   |
| 22  | 1     | 308  | CLA  | CMD-C2D-C1D | 6.07  | 135.42      | 124.73   |
| 24  | B     | 849  | BCR  | C20-C21-C22 | -6.07 | 118.77      | 127.28   |
| 38  | 5     | 302  | LUT  | C35-C34-C33 | -6.06 | 118.78      | 127.28   |
| 24  | A     | 845  | BCR  | C16-C17-C18 | -6.04 | 118.81      | 127.28   |
| 24  | J     | 104  | BCR  | C27-C26-C25 | -6.03 | 114.55      | 122.70   |
| 39  | 9     | 314  | CHL  | C1B-CHB-C4A | 6.03  | 125.20      | 121.32   |
| 24  | B     | 845  | BCR  | C1-C6-C5    | -6.02 | 114.41      | 122.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | 5     | 304  | BCR  | C16-C17-C18 | -6.02 | 118.83      | 127.28   |
| 24  | B     | 846  | BCR  | C15-C14-C13 | -6.01 | 118.85      | 127.28   |
| 38  | 4     | 803  | LUT  | C35-C34-C33 | -6.00 | 118.86      | 127.28   |
| 39  | 5     | 317  | CHL  | C1B-CHB-C4A | 5.99  | 125.18      | 121.32   |
| 24  | I     | 4001 | BCR  | C24-C23-C22 | -5.97 | 117.41      | 126.23   |
| 24  | 3     | 305  | BCR  | C33-C5-C6   | -5.97 | 117.97      | 124.48   |
| 22  | B     | 831  | CLA  | CMD-C2D-C1D | 5.92  | 135.16      | 124.73   |
| 39  | 7     | 313  | CHL  | C1B-CHB-C4A | 5.91  | 125.13      | 121.32   |
| 38  | 6     | 303  | LUT  | C35-C34-C33 | -5.91 | 118.99      | 127.28   |
| 25  | 3     | 321  | LHG  | O7-C7-O9    | -5.91 | 118.12      | 125.70   |
| 39  | 4     | 814  | CHL  | C1B-CHB-C4A | 5.89  | 125.11      | 121.32   |
| 22  | 6     | 322  | CLA  | O2D-CGD-CBD | 5.88  | 121.51      | 111.23   |
| 24  | F     | 303  | BCR  | C16-C17-C18 | -5.88 | 119.04      | 127.28   |
| 22  | 7     | 307  | CLA  | CMD-C2D-C1D | 5.85  | 135.03      | 124.73   |
| 22  | B     | 835  | CLA  | CMD-C2D-C1D | 5.84  | 135.02      | 124.73   |
| 24  | A     | 847  | BCR  | C38-C26-C25 | -5.84 | 118.11      | 124.48   |
| 22  | 7     | 315  | CLA  | O2D-CGD-CBD | 5.81  | 121.39      | 111.23   |
| 36  | 5     | 306  | C7Z  | C15-C14-C13 | -5.81 | 119.13      | 127.28   |
| 24  | A     | 856  | BCR  | C27-C26-C25 | -5.79 | 114.88      | 122.70   |
| 22  | 5     | 307  | CLA  | CMD-C2D-C1D | 5.77  | 134.89      | 124.73   |
| 39  | 5     | 321  | CHL  | C1B-CHB-C4A | 5.77  | 125.03      | 121.32   |
| 22  | A     | 818  | CLA  | CMD-C2D-C1D | 5.76  | 134.88      | 124.73   |
| 22  | 2     | 301  | CLA  | CMD-C2D-C1D | 5.75  | 134.86      | 124.73   |
| 22  | B     | 838  | CLA  | CMD-C2D-C1D | 5.73  | 134.82      | 124.73   |
| 38  | 4     | 802  | LUT  | C7-C8-C9    | -5.73 | 117.77      | 126.23   |
| 22  | 1     | 309  | CLA  | CMD-C2D-C1D | 5.71  | 134.79      | 124.73   |
| 38  | Z     | 301  | LUT  | C11-C10-C9  | -5.71 | 119.27      | 127.28   |
| 38  | 1     | 302  | LUT  | C11-C10-C9  | -5.70 | 119.29      | 127.28   |
| 22  | B     | 816  | CLA  | CMD-C2D-C1D | 5.70  | 134.76      | 124.73   |
| 22  | B     | 824  | CLA  | CMD-C2D-C1D | 5.68  | 134.74      | 124.73   |
| 32  | F     | 306  | RRX  | C20-C21-C22 | -5.68 | 119.31      | 127.28   |
| 22  | 5     | 323  | CLA  | CMD-C2D-C1D | 5.68  | 134.73      | 124.73   |
| 22  | A     | 825  | CLA  | CMD-C2D-C1D | 5.68  | 134.73      | 124.73   |
| 24  | A     | 848  | BCR  | C7-C8-C9    | -5.68 | 117.84      | 126.23   |
| 24  | 5     | 304  | BCR  | C11-C10-C9  | -5.67 | 119.32      | 127.28   |
| 22  | A     | 811  | CLA  | CMD-C2D-C1D | 5.67  | 134.72      | 124.73   |
| 22  | F     | 304  | CLA  | CMD-C2D-C1D | 5.66  | 134.70      | 124.73   |
| 22  | Z     | 306  | CLA  | CMD-C2D-C1D | 5.66  | 134.69      | 124.73   |
| 24  | A     | 847  | BCR  | C16-C17-C18 | -5.65 | 119.35      | 127.28   |
| 24  | I     | 4001 | BCR  | C30-C25-C26 | -5.65 | 114.91      | 122.64   |
| 22  | A     | 807  | CLA  | CMD-C2D-C1D | 5.65  | 134.68      | 124.73   |
| 22  | B     | 826  | CLA  | CMD-C2D-C1D | 5.65  | 134.68      | 124.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 823  | CLA  | CMD-C2D-C1D | 5.65  | 134.67      | 124.73   |
| 22  | 6     | 309  | CLA  | CMD-C2D-C1D | 5.64  | 134.67      | 124.73   |
| 22  | Z     | 307  | CLA  | CMD-C2D-C1D | 5.64  | 134.67      | 124.73   |
| 22  | B     | 835  | CLA  | O2D-CGD-CBD | 5.64  | 121.09      | 111.23   |
| 22  | A     | 805  | CLA  | CMD-C2D-C1D | 5.64  | 134.65      | 124.73   |
| 22  | 8     | 305  | CLA  | CMD-C2D-C1D | 5.63  | 134.64      | 124.73   |
| 22  | Z     | 303  | CLA  | CMD-C2D-C1D | 5.63  | 134.64      | 124.73   |
| 22  | 1     | 307  | CLA  | CMD-C2D-C1D | 5.62  | 134.63      | 124.73   |
| 22  | B     | 817  | CLA  | O2D-CGD-CBD | 5.62  | 121.05      | 111.23   |
| 22  | A     | 810  | CLA  | CMD-C2D-C1D | 5.61  | 134.61      | 124.73   |
| 24  | I     | 4001 | BCR  | C20-C21-C22 | -5.61 | 119.41      | 127.28   |
| 24  | A     | 846  | BCR  | C11-C10-C9  | -5.60 | 119.42      | 127.28   |
| 22  | 9     | 306  | CLA  | CMD-C2D-C1D | 5.60  | 134.59      | 124.73   |
| 22  | B     | 832  | CLA  | CMD-C2D-C1D | 5.60  | 134.59      | 124.73   |
| 22  | 1     | 315  | CLA  | CMD-C2D-C1D | 5.60  | 134.59      | 124.73   |
| 22  | 5     | 310  | CLA  | CMD-C2D-C1D | 5.60  | 134.59      | 124.73   |
| 22  | 1     | 305  | CLA  | CMD-C2D-C1D | 5.60  | 134.59      | 124.73   |
| 24  | B     | 849  | BCR  | C16-C17-C18 | -5.59 | 119.44      | 127.28   |
| 22  | 2     | 302  | CLA  | O2D-CGD-CBD | 5.59  | 121.01      | 111.23   |
| 22  | B     | 840  | CLA  | CMD-C2D-C1D | 5.59  | 134.57      | 124.73   |
| 22  | 1     | 313  | CLA  | CMD-C2D-C1D | 5.59  | 134.57      | 124.73   |
| 22  | A     | 827  | CLA  | CMD-C2D-C1D | 5.59  | 134.57      | 124.73   |
| 22  | 7     | 323  | CLA  | O2D-CGD-CBD | 5.59  | 121.00      | 111.23   |
| 22  | 3     | 322  | CLA  | CMD-C2D-C1D | 5.58  | 134.56      | 124.73   |
| 22  | B     | 814  | CLA  | CMD-C2D-C1D | 5.58  | 134.56      | 124.73   |
| 22  | B     | 828  | CLA  | CMD-C2D-C1D | 5.58  | 134.56      | 124.73   |
| 22  | 8     | 309  | CLA  | CMD-C2D-C1D | 5.58  | 134.55      | 124.73   |
| 22  | A     | 812  | CLA  | CMD-C2D-C1D | 5.58  | 134.55      | 124.73   |
| 24  | 3     | 306  | BCR  | C1-C6-C5    | -5.58 | 115.02      | 122.64   |
| 22  | A     | 832  | CLA  | CMD-C2D-C1D | 5.58  | 134.55      | 124.73   |
| 22  | 4     | 812  | CLA  | CMD-C2D-C1D | 5.57  | 134.54      | 124.73   |
| 22  | 4     | 809  | CLA  | CMD-C2D-C1D | 5.57  | 134.54      | 124.73   |
| 22  | B     | 818  | CLA  | CMD-C2D-C1D | 5.57  | 134.54      | 124.73   |
| 22  | A     | 809  | CLA  | CMD-C2D-C1D | 5.57  | 134.54      | 124.73   |
| 22  | A     | 839  | CLA  | CMD-C2D-C1D | 5.57  | 134.53      | 124.73   |
| 24  | A     | 845  | BCR  | C15-C14-C13 | -5.57 | 119.47      | 127.28   |
| 22  | 5     | 301  | CLA  | CMD-C2D-C1D | 5.57  | 134.53      | 124.73   |
| 22  | 3     | 313  | CLA  | CMD-C2D-C1D | 5.57  | 134.53      | 124.73   |
| 22  | F     | 305  | CLA  | CMD-C2D-C1D | 5.57  | 134.53      | 124.73   |
| 22  | 3     | 308  | CLA  | CMD-C2D-C1D | 5.57  | 134.53      | 124.73   |
| 22  | A     | 819  | CLA  | CMD-C2D-C1D | 5.56  | 134.53      | 124.73   |
| 22  | 5     | 309  | CLA  | CMD-C2D-C1D | 5.56  | 134.52      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 5     | 308 | CLA  | CMD-C2D-C1D | 5.56  | 134.52      | 124.73   |
| 22  | 6     | 322 | CLA  | CMD-C2D-C1D | 5.56  | 134.52      | 124.73   |
| 22  | 6     | 319 | CLA  | O2D-CGD-CBD | 5.56  | 120.95      | 111.23   |
| 22  | 6     | 310 | CLA  | CMD-C2D-C1D | 5.56  | 134.51      | 124.73   |
| 22  | 3     | 309 | CLA  | CMD-C2D-C1D | 5.56  | 134.51      | 124.73   |
| 24  | B     | 853 | BCR  | C1-C6-C5    | -5.55 | 115.05      | 122.64   |
| 22  | Z     | 308 | CLA  | CMD-C2D-C1D | 5.55  | 134.51      | 124.73   |
| 39  | 3     | 317 | CHL  | C1B-CHB-C4A | 5.55  | 124.89      | 121.32   |
| 22  | A     | 833 | CLA  | CMD-C2D-C1D | 5.55  | 134.50      | 124.73   |
| 22  | 7     | 304 | CLA  | CMD-C2D-C1D | 5.55  | 134.50      | 124.73   |
| 38  | 7     | 301 | LUT  | C35-C34-C33 | -5.55 | 119.50      | 127.28   |
| 22  | 3     | 318 | CLA  | CMD-C2D-C1D | 5.55  | 134.50      | 124.73   |
| 22  | A     | 840 | CLA  | CMD-C2D-C1D | 5.55  | 134.50      | 124.73   |
| 22  | B     | 826 | CLA  | O2D-CGD-CBD | 5.55  | 120.92      | 111.23   |
| 22  | 7     | 323 | CLA  | CMD-C2D-C1D | 5.55  | 134.49      | 124.73   |
| 22  | Z     | 315 | CLA  | CMD-C2D-C1D | 5.54  | 134.49      | 124.73   |
| 38  | 7     | 302 | LUT  | C11-C10-C9  | -5.54 | 119.51      | 127.28   |
| 22  | B     | 815 | CLA  | CMD-C2D-C1D | 5.54  | 134.49      | 124.73   |
| 22  | G     | 201 | CLA  | CMD-C2D-C1D | 5.54  | 134.49      | 124.73   |
| 22  | 7     | 324 | CLA  | CMD-C2D-C1D | 5.54  | 134.48      | 124.73   |
| 22  | A     | 822 | CLA  | CMD-C2D-C1D | 5.54  | 134.48      | 124.73   |
| 22  | A     | 837 | CLA  | CMD-C2D-C1D | 5.54  | 134.48      | 124.73   |
| 22  | B     | 842 | CLA  | CMD-C2D-C1D | 5.54  | 134.48      | 124.73   |
| 22  | B     | 813 | CLA  | CMD-C2D-C1D | 5.54  | 134.48      | 124.73   |
| 22  | Z     | 316 | CLA  | CMD-C2D-C1D | 5.53  | 134.47      | 124.73   |
| 22  | K     | 203 | CLA  | CMD-C2D-C1D | 5.53  | 134.47      | 124.73   |
| 22  | K     | 204 | CLA  | O2A-C1-C2   | 5.53  | 122.16      | 108.99   |
| 22  | G     | 202 | CLA  | CMD-C2D-C1D | 5.53  | 134.47      | 124.73   |
| 22  | L     | 201 | CLA  | CMD-C2D-C1D | 5.53  | 134.47      | 124.73   |
| 22  | B     | 836 | CLA  | CMD-C2D-C1D | 5.53  | 134.47      | 124.73   |
| 32  | F     | 306 | RRX  | C11-C12-C13 | -5.53 | 111.21      | 126.36   |
| 22  | 7     | 309 | CLA  | CMD-C2D-C1D | 5.53  | 134.46      | 124.73   |
| 22  | 7     | 305 | CLA  | CMD-C2D-C1D | 5.53  | 134.46      | 124.73   |
| 22  | B     | 829 | CLA  | CMD-C2D-C1D | 5.52  | 134.46      | 124.73   |
| 22  | B     | 810 | CLA  | CMD-C2D-C1D | 5.52  | 134.45      | 124.73   |
| 22  | B     | 819 | CLA  | CMD-C2D-C1D | 5.52  | 134.45      | 124.73   |
| 32  | F     | 306 | RRX  | C12-C13-C14 | 5.52  | 127.69      | 119.01   |
| 24  | 6     | 305 | BCR  | C11-C10-C9  | -5.52 | 119.54      | 127.28   |
| 22  | 5     | 326 | CLA  | CMD-C2D-C1D | 5.52  | 134.44      | 124.73   |
| 22  | B     | 808 | CLA  | CMD-C2D-C1D | 5.51  | 134.44      | 124.73   |
| 22  | 4     | 810 | CLA  | CMD-C2D-C1D | 5.51  | 134.44      | 124.73   |
| 22  | 8     | 308 | CLA  | CMD-C2D-C1D | 5.51  | 134.44      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 831 | CLA  | CMD-C2D-C1D | 5.51  | 134.43      | 124.73   |
| 39  | 9     | 312 | CHL  | C1B-CHB-C4A | 5.51  | 124.87      | 121.32   |
| 22  | 2     | 302 | CLA  | CMD-C2D-C1D | 5.51  | 134.43      | 124.73   |
| 22  | 3     | 316 | CLA  | CMD-C2D-C1D | 5.51  | 134.43      | 124.73   |
| 22  | 7     | 308 | CLA  | CMD-C2D-C1D | 5.51  | 134.43      | 124.73   |
| 22  | A     | 838 | CLA  | CMD-C2D-C1D | 5.50  | 134.42      | 124.73   |
| 22  | 6     | 312 | CLA  | CMD-C2D-C1D | 5.50  | 134.42      | 124.73   |
| 22  | B     | 825 | CLA  | CMD-C2D-C1D | 5.50  | 134.42      | 124.73   |
| 22  | B     | 833 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | 7     | 314 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | A     | 841 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | A     | 834 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | 6     | 307 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | A     | 802 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | K     | 204 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | B     | 823 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | F     | 301 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | 4     | 817 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | B     | 827 | CLA  | CMD-C2D-C1D | 5.50  | 134.41      | 124.73   |
| 22  | A     | 836 | CLA  | CMD-C2D-C1D | 5.49  | 134.40      | 124.73   |
| 22  | 3     | 319 | CLA  | CMD-C2D-C1D | 5.49  | 134.40      | 124.73   |
| 22  | 5     | 311 | CLA  | CMD-C2D-C1D | 5.49  | 134.40      | 124.73   |
| 22  | 3     | 312 | CLA  | CMD-C2D-C1D | 5.49  | 134.40      | 124.73   |
| 22  | B     | 834 | CLA  | CMD-C2D-C1D | 5.49  | 134.40      | 124.73   |
| 22  | 8     | 307 | CLA  | CMD-C2D-C1D | 5.49  | 134.40      | 124.73   |
| 22  | F     | 302 | CLA  | CMD-C2D-C1D | 5.49  | 134.40      | 124.73   |
| 22  | 4     | 818 | CLA  | CMD-C2D-C1D | 5.49  | 134.40      | 124.73   |
| 22  | Z     | 303 | CLA  | O2D-CGD-CBD | 5.49  | 120.82      | 111.23   |
| 22  | 7     | 312 | CLA  | CMD-C2D-C1D | 5.49  | 134.39      | 124.73   |
| 22  | 5     | 308 | CLA  | O2D-CGD-CBD | 5.48  | 120.82      | 111.23   |
| 22  | A     | 815 | CLA  | CMD-C2D-C1D | 5.48  | 134.39      | 124.73   |
| 24  | B     | 847 | BCR  | C11-C10-C9  | -5.48 | 119.59      | 127.28   |
| 22  | A     | 817 | CLA  | CMD-C2D-C1D | 5.48  | 134.38      | 124.73   |
| 22  | B     | 811 | CLA  | CMD-C2D-C1D | 5.48  | 134.38      | 124.73   |
| 24  | G     | 203 | BCR  | C16-C17-C18 | -5.48 | 119.59      | 127.28   |
| 22  | A     | 821 | CLA  | CMD-C2D-C1D | 5.48  | 134.38      | 124.73   |
| 22  | A     | 813 | CLA  | CMD-C2D-C1D | 5.48  | 134.38      | 124.73   |
| 22  | A     | 855 | CLA  | CMD-C2D-C1D | 5.48  | 134.38      | 124.73   |
| 22  | 9     | 308 | CLA  | CMD-C2D-C1D | 5.48  | 134.37      | 124.73   |
| 22  | B     | 809 | CLA  | CMD-C2D-C1D | 5.48  | 134.37      | 124.73   |
| 22  | 8     | 310 | CLA  | CMD-C2D-C1D | 5.47  | 134.37      | 124.73   |
| 24  | B     | 845 | BCR  | C27-C26-C25 | -5.47 | 115.31      | 122.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 821 | CLA  | CMD-C2D-C1D | 5.47  | 134.36      | 124.73   |
| 22  | 4     | 815 | CLA  | O2D-CGD-CBD | 5.47  | 120.79      | 111.23   |
| 22  | L     | 203 | CLA  | CMD-C2D-C1D | 5.46  | 134.35      | 124.73   |
| 22  | 6     | 301 | CLA  | CMD-C2D-C1D | 5.46  | 134.35      | 124.73   |
| 22  | 6     | 311 | CLA  | CMD-C2D-C1D | 5.46  | 134.35      | 124.73   |
| 24  | G     | 203 | BCR  | C33-C5-C6   | -5.46 | 118.53      | 124.48   |
| 22  | A     | 803 | CLA  | O2D-CGD-CBD | 5.46  | 120.77      | 111.23   |
| 22  | B     | 806 | CLA  | CMD-C2D-C1D | 5.46  | 134.34      | 124.73   |
| 22  | 4     | 808 | CLA  | CMD-C2D-C1D | 5.46  | 134.34      | 124.73   |
| 22  | A     | 816 | CLA  | CMD-C2D-C1D | 5.46  | 134.34      | 124.73   |
| 22  | 5     | 312 | CLA  | CMD-C2D-C1D | 5.45  | 134.33      | 124.73   |
| 22  | 6     | 319 | CLA  | CMD-C2D-C1D | 5.45  | 134.33      | 124.73   |
| 24  | A     | 847 | BCR  | C20-C21-C22 | -5.45 | 119.63      | 127.28   |
| 22  | 7     | 311 | CLA  | CMD-C2D-C1D | 5.45  | 134.33      | 124.73   |
| 22  | J     | 103 | CLA  | CMD-C2D-C1D | 5.45  | 134.33      | 124.73   |
| 22  | 9     | 311 | CLA  | CMD-C2D-C1D | 5.45  | 134.32      | 124.73   |
| 22  | 7     | 316 | CLA  | CMD-C2D-C1D | 5.45  | 134.32      | 124.73   |
| 24  | 7     | 303 | BCR  | C4-C5-C6    | -5.45 | 115.34      | 122.70   |
| 22  | K     | 202 | CLA  | CMD-C2D-C1D | 5.45  | 134.32      | 124.73   |
| 22  | Z     | 307 | CLA  | O2D-CGD-CBD | 5.44  | 120.75      | 111.23   |
| 22  | A     | 803 | CLA  | CMD-C2D-C1D | 5.44  | 134.30      | 124.73   |
| 22  | 1     | 306 | CLA  | CMD-C2D-C1D | 5.44  | 134.30      | 124.73   |
| 22  | 7     | 322 | CLA  | CMD-C2D-C1D | 5.44  | 134.30      | 124.73   |
| 22  | 4     | 806 | CLA  | CMD-C2D-C1D | 5.43  | 134.29      | 124.73   |
| 24  | B     | 846 | BCR  | C24-C23-C22 | -5.43 | 118.20      | 126.23   |
| 22  | B     | 820 | CLA  | CMD-C2D-C1D | 5.43  | 134.28      | 124.73   |
| 22  | A     | 828 | CLA  | CMD-C2D-C1D | 5.42  | 134.28      | 124.73   |
| 22  | 5     | 319 | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.73   |
| 22  | 3     | 310 | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.73   |
| 22  | B     | 839 | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.73   |
| 22  | 4     | 807 | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.73   |
| 24  | 5     | 304 | BCR  | C38-C26-C25 | -5.42 | 118.57      | 124.48   |
| 22  | 7     | 317 | CLA  | CMD-C2D-C1D | 5.42  | 134.27      | 124.73   |
| 22  | A     | 804 | CLA  | O2D-CGD-CBD | 5.41  | 120.69      | 111.23   |
| 39  | 4     | 813 | CHL  | C1B-CHB-C4A | 5.41  | 124.81      | 121.32   |
| 24  | 3     | 307 | BCR  | C15-C16-C17 | -5.41 | 112.45      | 123.52   |
| 22  | 8     | 316 | CLA  | CMD-C2D-C1D | 5.41  | 134.25      | 124.73   |
| 22  | A     | 826 | CLA  | CMD-C2D-C1D | 5.41  | 134.25      | 124.73   |
| 22  | A     | 814 | CLA  | CMD-C2D-C1D | 5.41  | 134.25      | 124.73   |
| 22  | 6     | 314 | CLA  | CMD-C2D-C1D | 5.41  | 134.25      | 124.73   |
| 22  | 4     | 805 | CLA  | CMD-C2D-C1D | 5.41  | 134.25      | 124.73   |
| 22  | A     | 842 | CLA  | CMD-C2D-C1D | 5.41  | 134.25      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 830 | CLA  | CMD-C2D-C1D | 5.40  | 134.25      | 124.73   |
| 24  | K     | 206 | BCR  | C15-C14-C13 | -5.40 | 119.70      | 127.28   |
| 22  | A     | 816 | CLA  | O2D-CGD-CBD | 5.40  | 120.67      | 111.23   |
| 22  | 6     | 308 | CLA  | CMD-C2D-C1D | 5.40  | 134.24      | 124.73   |
| 22  | 1     | 304 | CLA  | CMD-C2D-C1D | 5.40  | 134.24      | 124.73   |
| 22  | 1     | 308 | CLA  | O2D-CGD-CBD | 5.40  | 120.67      | 111.23   |
| 22  | A     | 820 | CLA  | CMD-C2D-C1D | 5.40  | 134.24      | 124.73   |
| 38  | 9     | 302 | LUT  | C35-C34-C33 | -5.40 | 119.71      | 127.28   |
| 22  | B     | 812 | CLA  | CMD-C2D-C1D | 5.40  | 134.23      | 124.73   |
| 22  | 8     | 306 | CLA  | O2D-CGD-CBD | 5.39  | 120.66      | 111.23   |
| 22  | A     | 808 | CLA  | CMD-C2D-C1D | 5.39  | 134.23      | 124.73   |
| 22  | 6     | 321 | CLA  | CMD-C2D-C1D | 5.39  | 134.22      | 124.73   |
| 22  | 8     | 313 | CLA  | CMD-C2D-C1D | 5.39  | 134.22      | 124.73   |
| 22  | A     | 809 | CLA  | O2D-CGD-CBD | 5.39  | 120.65      | 111.23   |
| 22  | A     | 834 | CLA  | O2D-CGD-CBD | 5.38  | 120.64      | 111.23   |
| 22  | A     | 824 | CLA  | CMD-C2D-C1D | 5.38  | 134.21      | 124.73   |
| 22  | 1     | 310 | CLA  | CMD-C2D-C1D | 5.38  | 134.20      | 124.73   |
| 22  | L     | 202 | CLA  | CMD-C2D-C1D | 5.38  | 134.20      | 124.73   |
| 22  | 5     | 318 | CLA  | CMD-C2D-C1D | 5.38  | 134.20      | 124.73   |
| 24  | 3     | 307 | BCR  | C4-C5-C6    | -5.38 | 115.44      | 122.70   |
| 36  | J     | 105 | C7Z  | C27-C28-C29 | -5.37 | 118.28      | 126.23   |
| 22  | B     | 837 | CLA  | CMD-C2D-C1D | 5.37  | 134.19      | 124.73   |
| 22  | 3     | 311 | CLA  | CMD-C2D-C1D | 5.37  | 134.19      | 124.73   |
| 22  | B     | 807 | CLA  | CMD-C2D-C1D | 5.37  | 134.19      | 124.73   |
| 22  | 9     | 307 | CLA  | CMD-C2D-C1D | 5.37  | 134.18      | 124.73   |
| 22  | 5     | 322 | CLA  | CMD-C2D-C1D | 5.36  | 134.17      | 124.73   |
| 38  | 3     | 302 | LUT  | C35-C34-C33 | -5.36 | 119.76      | 127.28   |
| 22  | 8     | 306 | CLA  | CMD-C2D-C1D | 5.36  | 134.17      | 124.73   |
| 22  | A     | 833 | CLA  | O2D-CGD-CBD | 5.36  | 120.60      | 111.23   |
| 22  | A     | 804 | CLA  | CMD-C2D-C1D | 5.36  | 134.16      | 124.73   |
| 22  | 6     | 308 | CLA  | O2D-CGD-CBD | 5.35  | 120.59      | 111.23   |
| 22  | 1     | 314 | CLA  | CMD-C2D-C1D | 5.35  | 134.16      | 124.73   |
| 22  | B     | 831 | CLA  | O2D-CGD-CBD | 5.35  | 120.58      | 111.23   |
| 22  | B     | 820 | CLA  | O2D-CGD-CBD | 5.35  | 120.58      | 111.23   |
| 22  | 9     | 305 | CLA  | CMD-C2D-C1D | 5.35  | 134.15      | 124.73   |
| 22  | A     | 806 | CLA  | CMD-C2D-C1D | 5.35  | 134.14      | 124.73   |
| 22  | B     | 841 | CLA  | CMD-C2D-C1D | 5.34  | 134.13      | 124.73   |
| 36  | J     | 105 | C7Z  | C35-C34-C33 | -5.34 | 119.79      | 127.28   |
| 38  | 8     | 303 | LUT  | C35-C34-C33 | -5.34 | 119.79      | 127.28   |
| 38  | 8     | 302 | LUT  | C35-C34-C33 | -5.34 | 119.79      | 127.28   |
| 24  | 6     | 305 | BCR  | C7-C8-C9    | -5.34 | 118.34      | 126.23   |
| 22  | 9     | 308 | CLA  | O2D-CGD-CBD | 5.34  | 120.56      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 810 | CLA  | O2D-CGD-CBD | 5.33  | 120.55      | 111.23   |
| 22  | 7     | 306 | CLA  | CMD-C2D-C1D | 5.33  | 134.12      | 124.73   |
| 22  | A     | 854 | CLA  | CMD-C2D-C1D | 5.33  | 134.11      | 124.73   |
| 22  | 1     | 311 | CLA  | O2D-CGD-CBD | 5.33  | 120.54      | 111.23   |
| 22  | Z     | 313 | CLA  | O2D-CGD-CBD | 5.33  | 120.54      | 111.23   |
| 22  | 4     | 811 | CLA  | CMD-C2D-C1D | 5.32  | 134.09      | 124.73   |
| 24  | A     | 847 | BCR  | C24-C23-C22 | -5.31 | 118.38      | 126.23   |
| 22  | B     | 805 | CLA  | CMD-C2D-C1D | 5.31  | 134.08      | 124.73   |
| 24  | 7     | 303 | BCR  | C1-C6-C5    | -5.31 | 115.38      | 122.64   |
| 38  | 1     | 302 | LUT  | C1-C6-C5    | -5.31 | 115.38      | 122.64   |
| 22  | 9     | 313 | CLA  | O2D-CGD-CBD | 5.31  | 120.51      | 111.23   |
| 22  | 7     | 307 | CLA  | O2D-CGD-CBD | 5.31  | 120.51      | 111.23   |
| 39  | 5     | 316 | CHL  | C1B-CHB-C4A | 5.31  | 124.74      | 121.32   |
| 24  | A     | 856 | BCR  | C16-C17-C18 | -5.31 | 119.83      | 127.28   |
| 22  | B     | 801 | CLA  | CMD-C2D-C1D | 5.31  | 134.07      | 124.73   |
| 22  | 7     | 305 | CLA  | O2D-CGD-CBD | 5.30  | 120.50      | 111.23   |
| 22  | B     | 834 | CLA  | O2D-CGD-CBD | 5.30  | 120.49      | 111.23   |
| 39  | 6     | 315 | CHL  | C1B-CHB-C4A | 5.30  | 124.73      | 121.32   |
| 22  | B     | 811 | CLA  | O2D-CGD-CBD | 5.30  | 120.49      | 111.23   |
| 22  | B     | 822 | CLA  | CMD-C2D-C1D | 5.29  | 134.05      | 124.73   |
| 22  | B     | 837 | CLA  | O2D-CGD-CBD | 5.29  | 120.48      | 111.23   |
| 22  | Z     | 310 | CLA  | CMD-C2D-C1D | 5.29  | 134.04      | 124.73   |
| 22  | B     | 814 | CLA  | O2D-CGD-CBD | 5.28  | 120.47      | 111.23   |
| 22  | 6     | 314 | CLA  | O2D-CGD-CBD | 5.28  | 120.47      | 111.23   |
| 24  | B     | 853 | BCR  | C7-C8-C9    | -5.28 | 118.42      | 126.23   |
| 24  | 7     | 303 | BCR  | C38-C26-C25 | -5.28 | 118.72      | 124.48   |
| 22  | 5     | 311 | CLA  | O2D-CGD-CBD | 5.28  | 120.46      | 111.23   |
| 38  | 3     | 303 | LUT  | C7-C8-C9    | -5.28 | 118.43      | 126.23   |
| 22  | 3     | 308 | CLA  | O2D-CGD-CBD | 5.27  | 120.45      | 111.23   |
| 39  | 8     | 301 | CHL  | C1B-CHB-C4A | 5.27  | 124.71      | 121.32   |
| 38  | 7     | 302 | LUT  | C15-C14-C13 | -5.27 | 119.89      | 127.28   |
| 22  | B     | 839 | CLA  | O2D-CGD-CBD | 5.27  | 120.44      | 111.23   |
| 22  | 8     | 305 | CLA  | O2D-CGD-CBD | 5.27  | 120.44      | 111.23   |
| 22  | 9     | 313 | CLA  | CMD-C2D-C1D | 5.27  | 134.00      | 124.73   |
| 39  | 4     | 819 | CHL  | C1B-CHB-C4A | 5.27  | 124.71      | 121.32   |
| 22  | 4     | 818 | CLA  | O2D-CGD-CBD | 5.26  | 120.43      | 111.23   |
| 22  | A     | 838 | CLA  | O2D-CGD-CBD | 5.26  | 120.42      | 111.23   |
| 24  | 3     | 306 | BCR  | C15-C14-C13 | -5.26 | 119.91      | 127.28   |
| 22  | 3     | 316 | CLA  | O2D-CGD-CBD | 5.25  | 120.42      | 111.23   |
| 22  | A     | 813 | CLA  | O2D-CGD-CBD | 5.25  | 120.41      | 111.23   |
| 22  | B     | 827 | CLA  | O2D-CGD-CBD | 5.25  | 120.41      | 111.23   |
| 24  | 7     | 303 | BCR  | C11-C10-C9  | -5.25 | 119.91      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 819 | CLA  | O2D-CGD-CBD | 5.25  | 120.41      | 111.23   |
| 38  | 1     | 302 | LUT  | C7-C8-C9    | -5.25 | 118.47      | 126.23   |
| 22  | 5     | 326 | CLA  | O2D-CGD-CBD | 5.25  | 120.41      | 111.23   |
| 22  | 6     | 301 | CLA  | O2D-CGD-CBD | 5.25  | 120.40      | 111.23   |
| 22  | K     | 202 | CLA  | O2D-CGD-CBD | 5.24  | 120.39      | 111.23   |
| 22  | 5     | 313 | CLA  | CMD-C2D-C1D | 5.24  | 133.95      | 124.73   |
| 22  | B     | 822 | CLA  | O2D-CGD-CBD | 5.24  | 120.38      | 111.23   |
| 22  | Z     | 305 | CLA  | O2D-CGD-CBD | 5.23  | 120.38      | 111.23   |
| 22  | F     | 301 | CLA  | O2D-CGD-CBD | 5.22  | 120.36      | 111.23   |
| 22  | 5     | 310 | CLA  | O2D-CGD-CBD | 5.22  | 120.36      | 111.23   |
| 22  | 1     | 313 | CLA  | O2D-CGD-CBD | 5.22  | 120.36      | 111.23   |
| 22  | A     | 835 | CLA  | CMD-C2D-C1D | 5.22  | 133.93      | 124.73   |
| 22  | 9     | 303 | CLA  | CMD-C2D-C1D | 5.22  | 133.93      | 124.73   |
| 22  | B     | 815 | CLA  | O2D-CGD-CBD | 5.22  | 120.36      | 111.23   |
| 22  | G     | 201 | CLA  | O2D-CGD-CBD | 5.22  | 120.35      | 111.23   |
| 24  | 5     | 305 | BCR  | C1-C6-C5    | -5.22 | 115.50      | 122.64   |
| 22  | A     | 839 | CLA  | O2D-CGD-CBD | 5.22  | 120.35      | 111.23   |
| 25  | B     | 851 | LHG  | O7-C7-O9    | -5.22 | 119.01      | 125.70   |
| 22  | A     | 829 | CLA  | CMD-C2D-C1D | 5.22  | 133.91      | 124.73   |
| 32  | F     | 306 | RRX  | C33-C5-C6   | -5.21 | 118.80      | 124.48   |
| 22  | 6     | 312 | CLA  | O2D-CGD-CBD | 5.20  | 120.33      | 111.23   |
| 24  | B     | 848 | BCR  | C7-C8-C9    | -5.20 | 118.54      | 126.23   |
| 22  | A     | 837 | CLA  | O2D-CGD-CBD | 5.20  | 120.33      | 111.23   |
| 22  | 8     | 313 | CLA  | O2D-CGD-CBD | 5.20  | 120.33      | 111.23   |
| 22  | 8     | 314 | CLA  | CMD-C2D-C1D | 5.20  | 133.89      | 124.73   |
| 22  | 9     | 306 | CLA  | O2D-CGD-CBD | 5.20  | 120.32      | 111.23   |
| 22  | B     | 840 | CLA  | O2D-CGD-CBD | 5.19  | 120.31      | 111.23   |
| 22  | B     | 841 | CLA  | O2D-CGD-CBD | 5.19  | 120.31      | 111.23   |
| 39  | Z     | 312 | CHL  | C1B-CHB-C4A | 5.19  | 124.66      | 121.32   |
| 22  | B     | 824 | CLA  | O2D-CGD-CBD | 5.19  | 120.30      | 111.23   |
| 22  | B     | 828 | CLA  | O2D-CGD-CBD | 5.19  | 120.30      | 111.23   |
| 22  | 5     | 314 | CLA  | CMD-C2D-C1D | 5.19  | 133.87      | 124.73   |
| 22  | B     | 832 | CLA  | O2D-CGD-CBD | 5.19  | 120.30      | 111.23   |
| 22  | A     | 808 | CLA  | O2D-CGD-CBD | 5.19  | 120.30      | 111.23   |
| 22  | 4     | 812 | CLA  | O2D-CGD-CBD | 5.19  | 120.30      | 111.23   |
| 22  | A     | 841 | CLA  | O2D-CGD-CBD | 5.18  | 120.29      | 111.23   |
| 22  | 3     | 318 | CLA  | O2D-CGD-CBD | 5.18  | 120.29      | 111.23   |
| 22  | 4     | 817 | CLA  | O2D-CGD-CBD | 5.18  | 120.29      | 111.23   |
| 36  | J     | 105 | C7Z  | C31-C30-C29 | -5.18 | 120.01      | 127.28   |
| 22  | A     | 818 | CLA  | O2D-CGD-CBD | 5.18  | 120.28      | 111.23   |
| 22  | 4     | 808 | CLA  | O2D-CGD-CBD | 5.17  | 120.28      | 111.23   |
| 22  | 7     | 310 | CLA  | CMD-C2D-C1D | 5.17  | 133.84      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 5     | 306 | C7Z  | C35-C34-C33 | -5.17 | 120.02      | 127.28   |
| 22  | 7     | 316 | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 22  | A     | 819 | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 22  | A     | 831 | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 22  | A     | 802 | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 22  | A     | 814 | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 22  | 8     | 307 | CLA  | O2D-CGD-CBD | 5.17  | 120.27      | 111.23   |
| 22  | 7     | 304 | CLA  | O2D-CGD-CBD | 5.16  | 120.26      | 111.23   |
| 22  | B     | 805 | CLA  | O2D-CGD-CBD | 5.16  | 120.25      | 111.23   |
| 22  | G     | 202 | CLA  | O2D-CGD-CBD | 5.16  | 120.25      | 111.23   |
| 22  | 3     | 314 | CLA  | CMD-C2D-C1D | 5.16  | 133.81      | 124.73   |
| 22  | 1     | 305 | CLA  | O2D-CGD-CBD | 5.16  | 120.25      | 111.23   |
| 22  | 4     | 806 | CLA  | O2D-CGD-CBD | 5.16  | 120.25      | 111.23   |
| 22  | 6     | 317 | CLA  | O2D-CGD-CBD | 5.16  | 120.25      | 111.23   |
| 22  | B     | 818 | CLA  | O2D-CGD-CBD | 5.16  | 120.25      | 111.23   |
| 22  | B     | 808 | CLA  | O2D-CGD-CBD | 5.16  | 120.25      | 111.23   |
| 22  | B     | 817 | CLA  | CMD-C2D-C1D | 5.16  | 133.81      | 124.73   |
| 22  | 7     | 314 | CLA  | O2D-CGD-CBD | 5.16  | 120.24      | 111.23   |
| 22  | B     | 830 | CLA  | CMD-C2D-C1D | 5.16  | 133.81      | 124.73   |
| 39  | 8     | 312 | CHL  | C1B-CHB-C4A | 5.15  | 124.64      | 121.32   |
| 39  | 2     | 303 | CHL  | C1B-CHB-C4A | 5.15  | 124.64      | 121.32   |
| 22  | 3     | 319 | CLA  | O2D-CGD-CBD | 5.15  | 120.24      | 111.23   |
| 22  | B     | 806 | CLA  | O2D-CGD-CBD | 5.15  | 120.24      | 111.23   |
| 22  | 3     | 320 | CLA  | CMD-C2D-C1D | 5.15  | 133.80      | 124.73   |
| 24  | F     | 303 | BCR  | C20-C21-C22 | -5.15 | 120.06      | 127.28   |
| 22  | 6     | 302 | CLA  | CMD-C2D-C1D | 5.15  | 133.79      | 124.73   |
| 22  | Z     | 314 | CLA  | CMD-C2D-C1D | 5.14  | 133.79      | 124.73   |
| 22  | 6     | 310 | CLA  | O2D-CGD-CBD | 5.14  | 120.22      | 111.23   |
| 24  | 6     | 306 | BCR  | C38-C26-C25 | -5.14 | 118.87      | 124.48   |
| 38  | 3     | 303 | LUT  | C15-C14-C13 | -5.14 | 120.07      | 127.28   |
| 22  | 4     | 811 | CLA  | O2D-CGD-CBD | 5.14  | 120.22      | 111.23   |
| 22  | 2     | 304 | CLA  | CMD-C2D-C1D | 5.14  | 133.78      | 124.73   |
| 22  | 5     | 319 | CLA  | O2D-CGD-CBD | 5.14  | 120.21      | 111.23   |
| 22  | 3     | 311 | CLA  | O2D-CGD-CBD | 5.14  | 120.21      | 111.23   |
| 39  | Z     | 311 | CHL  | C1B-CHB-C4A | 5.13  | 124.62      | 121.32   |
| 22  | A     | 825 | CLA  | O2D-CGD-CBD | 5.13  | 120.20      | 111.23   |
| 24  | L     | 204 | BCR  | C1-C6-C5    | -5.13 | 115.63      | 122.64   |
| 22  | 3     | 322 | CLA  | O2D-CGD-CBD | 5.13  | 120.19      | 111.23   |
| 22  | 8     | 308 | CLA  | O2D-CGD-CBD | 5.12  | 120.19      | 111.23   |
| 22  | 5     | 315 | CLA  | CMD-C2D-C1D | 5.12  | 133.75      | 124.73   |
| 22  | 8     | 311 | CLA  | CMD-C2D-C1D | 5.12  | 133.74      | 124.73   |
| 22  | A     | 855 | CLA  | O2D-CGD-CBD | 5.12  | 120.18      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 807 | CLA  | O2D-CGD-CBD | 5.12  | 120.17      | 111.23   |
| 22  | 5     | 301 | CLA  | O2D-CGD-CBD | 5.12  | 120.17      | 111.23   |
| 22  | B     | 836 | CLA  | O2D-CGD-CBD | 5.11  | 120.17      | 111.23   |
| 24  | B     | 844 | BCR  | C20-C19-C18 | -5.11 | 112.34      | 126.36   |
| 24  | 6     | 305 | BCR  | C16-C17-C18 | -5.11 | 120.11      | 127.28   |
| 24  | J     | 104 | BCR  | C4-C5-C6    | -5.11 | 115.80      | 122.70   |
| 22  | B     | 816 | CLA  | O2D-CGD-CBD | 5.11  | 120.16      | 111.23   |
| 24  | B     | 849 | BCR  | C7-C8-C9    | -5.11 | 118.68      | 126.23   |
| 24  | 3     | 305 | BCR  | C27-C26-C25 | -5.11 | 115.80      | 122.70   |
| 22  | 3     | 315 | CLA  | O2D-CGD-CBD | 5.11  | 120.16      | 111.23   |
| 22  | A     | 835 | CLA  | O2D-CGD-CBD | 5.11  | 120.16      | 111.23   |
| 22  | Z     | 308 | CLA  | O2D-CGD-CBD | 5.11  | 120.16      | 111.23   |
| 22  | A     | 812 | CLA  | O2D-CGD-CBD | 5.10  | 120.15      | 111.23   |
| 22  | 1     | 309 | CLA  | O2D-CGD-CBD | 5.10  | 120.15      | 111.23   |
| 21  | A     | 801 | CL0  | O2A-CGA-O1A | -5.10 | 110.86      | 123.63   |
| 24  | 8     | 304 | BCR  | C15-C14-C13 | -5.10 | 120.12      | 127.28   |
| 22  | 6     | 317 | CLA  | CMD-C2D-C1D | 5.10  | 133.71      | 124.73   |
| 22  | A     | 805 | CLA  | O2D-CGD-CBD | 5.10  | 120.15      | 111.23   |
| 22  | 5     | 315 | CLA  | O2D-CGD-CBD | 5.10  | 120.15      | 111.23   |
| 24  | A     | 845 | BCR  | C11-C10-C9  | -5.10 | 120.13      | 127.28   |
| 22  | F     | 305 | CLA  | O2D-CGD-CBD | 5.09  | 120.14      | 111.23   |
| 24  | 7     | 303 | BCR  | C20-C21-C22 | -5.09 | 120.14      | 127.28   |
| 22  | Z     | 309 | CLA  | O2D-CGD-CBD | 5.09  | 120.13      | 111.23   |
| 22  | 4     | 809 | CLA  | O2D-CGD-CBD | 5.09  | 120.13      | 111.23   |
| 24  | K     | 206 | BCR  | C20-C21-C22 | -5.09 | 120.14      | 127.28   |
| 22  | A     | 822 | CLA  | O2D-CGD-CBD | 5.09  | 120.13      | 111.23   |
| 22  | B     | 807 | CLA  | O2D-CGD-CBD | 5.09  | 120.13      | 111.23   |
| 24  | A     | 848 | BCR  | C15-C14-C13 | -5.09 | 120.14      | 127.28   |
| 22  | A     | 827 | CLA  | O2D-CGD-CBD | 5.09  | 120.12      | 111.23   |
| 38  | 1     | 303 | LUT  | C35-C34-C33 | -5.09 | 120.14      | 127.28   |
| 22  | 6     | 321 | CLA  | O2D-CGD-CBD | 5.09  | 120.12      | 111.23   |
| 22  | 7     | 309 | CLA  | C1-C2-C3    | -5.09 | 117.86      | 126.20   |
| 24  | 8     | 304 | BCR  | C4-C5-C6    | -5.08 | 115.83      | 122.70   |
| 22  | 5     | 307 | CLA  | O2D-CGD-CBD | 5.08  | 120.11      | 111.23   |
| 24  | 4     | 804 | BCR  | C24-C23-C22 | -5.08 | 118.72      | 126.23   |
| 22  | J     | 103 | CLA  | O2D-CGD-CBD | 5.08  | 120.11      | 111.23   |
| 22  | L     | 202 | CLA  | O2D-CGD-CBD | 5.08  | 120.11      | 111.23   |
| 22  | 7     | 315 | CLA  | CMD-C2D-C1D | 5.08  | 133.67      | 124.73   |
| 24  | A     | 845 | BCR  | C33-C5-C6   | -5.07 | 118.95      | 124.48   |
| 38  | 4     | 803 | LUT  | C7-C8-C9    | -5.07 | 118.73      | 126.23   |
| 22  | 1     | 306 | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 22  | 2     | 304 | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 38  | Z     | 302 | LUT  | C11-C10-C9  | -5.07 | 120.17      | 127.28   |
| 22  | 7     | 324 | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 22  | A     | 806 | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 22  | Z     | 309 | CLA  | CMD-C2D-C1D | 5.07  | 133.65      | 124.73   |
| 22  | 4     | 810 | CLA  | O2D-CGD-CBD | 5.07  | 120.09      | 111.23   |
| 22  | 4     | 815 | CLA  | CMD-C2D-C1D | 5.06  | 133.65      | 124.73   |
| 22  | F     | 302 | CLA  | O2D-CGD-CBD | 5.06  | 120.08      | 111.23   |
| 24  | 4     | 804 | BCR  | C16-C17-C18 | -5.06 | 120.18      | 127.28   |
| 22  | 5     | 314 | CLA  | O2D-CGD-CBD | 5.06  | 120.08      | 111.23   |
| 24  | K     | 206 | BCR  | C16-C17-C18 | -5.06 | 120.18      | 127.28   |
| 22  | 1     | 304 | CLA  | O2D-CGD-CBD | 5.06  | 120.07      | 111.23   |
| 24  | 3     | 306 | BCR  | C30-C25-C26 | -5.06 | 115.72      | 122.64   |
| 22  | 1     | 315 | CLA  | O2D-CGD-CBD | 5.06  | 120.07      | 111.23   |
| 22  | A     | 815 | CLA  | O2D-CGD-CBD | 5.06  | 120.07      | 111.23   |
| 22  | A     | 817 | CLA  | C1-C2-C3    | -5.06 | 117.91      | 126.20   |
| 22  | 3     | 314 | CLA  | O2D-CGD-CBD | 5.06  | 120.07      | 111.23   |
| 22  | A     | 832 | CLA  | O2D-CGD-CBD | 5.05  | 120.07      | 111.23   |
| 24  | B     | 846 | BCR  | C33-C5-C6   | -5.05 | 118.97      | 124.48   |
| 22  | A     | 821 | CLA  | O2D-CGD-CBD | 5.05  | 120.06      | 111.23   |
| 38  | 8     | 302 | LUT  | C18-C5-C6   | -5.05 | 118.97      | 124.48   |
| 24  | A     | 845 | BCR  | C20-C21-C22 | -5.05 | 120.20      | 127.28   |
| 22  | F     | 304 | CLA  | O2D-CGD-CBD | 5.04  | 120.05      | 111.23   |
| 22  | 7     | 322 | CLA  | O2D-CGD-CBD | 5.04  | 120.05      | 111.23   |
| 22  | Z     | 315 | CLA  | O2D-CGD-CBD | 5.04  | 120.04      | 111.23   |
| 22  | 8     | 310 | CLA  | C1-C2-C3    | -5.04 | 117.94      | 126.20   |
| 38  | 9     | 301 | LUT  | C35-C34-C33 | -5.04 | 120.22      | 127.28   |
| 22  | L     | 201 | CLA  | O2D-CGD-CBD | 5.04  | 120.03      | 111.23   |
| 22  | 1     | 307 | CLA  | O2D-CGD-CBD | 5.04  | 120.03      | 111.23   |
| 22  | B     | 842 | CLA  | O2D-CGD-CBD | 5.03  | 120.03      | 111.23   |
| 22  | 8     | 314 | CLA  | O2D-CGD-CBD | 5.03  | 120.03      | 111.23   |
| 34  | F     | 308 | LMG  | O7-C10-C11  | 5.03  | 122.36      | 111.48   |
| 22  | B     | 823 | CLA  | O2D-CGD-CBD | 5.03  | 120.02      | 111.23   |
| 22  | K     | 205 | CLA  | O2D-CGD-CBD | 5.03  | 120.02      | 111.23   |
| 38  | 1     | 303 | LUT  | C7-C8-C9    | -5.03 | 118.80      | 126.23   |
| 22  | 7     | 308 | CLA  | O2D-CGD-CBD | 5.02  | 120.01      | 111.23   |
| 22  | 6     | 313 | CLA  | CMD-C2D-C1D | 5.02  | 133.57      | 124.73   |
| 22  | 1     | 310 | CLA  | O2D-CGD-CBD | 5.02  | 120.01      | 111.23   |
| 24  | B     | 847 | BCR  | C7-C8-C9    | -5.02 | 118.81      | 126.23   |
| 22  | A     | 836 | CLA  | O2D-CGD-CBD | 5.02  | 120.00      | 111.23   |
| 22  | 5     | 309 | CLA  | O2D-CGD-CBD | 5.02  | 120.00      | 111.23   |
| 22  | B     | 833 | CLA  | O2D-CGD-CBD | 5.02  | 120.00      | 111.23   |
| 22  | A     | 820 | CLA  | O2D-CGD-CBD | 5.01  | 120.00      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32  | F     | 306  | RRX  | C1-C6-C5    | -5.01 | 115.79      | 122.64   |
| 22  | 6     | 313  | CLA  | O2D-CGD-CBD | 5.01  | 119.99      | 111.23   |
| 22  | B     | 809  | CLA  | O2D-CGD-CBD | 5.01  | 119.98      | 111.23   |
| 38  | 4     | 802  | LUT  | C35-C34-C33 | -5.00 | 120.26      | 127.28   |
| 22  | Z     | 314  | CLA  | O2D-CGD-CBD | 5.00  | 119.98      | 111.23   |
| 22  | 8     | 310  | CLA  | O2D-CGD-CBD | 5.00  | 119.98      | 111.23   |
| 24  | I     | 4001 | BCR  | C1-C6-C5    | -5.00 | 115.80      | 122.64   |
| 22  | 7     | 312  | CLA  | O2D-CGD-CBD | 5.00  | 119.97      | 111.23   |
| 22  | A     | 817  | CLA  | O2D-CGD-CBD | 5.00  | 119.97      | 111.23   |
| 22  | A     | 830  | CLA  | O2D-CGD-CBD | 4.99  | 119.96      | 111.23   |
| 22  | B     | 813  | CLA  | O2D-CGD-CBD | 4.99  | 119.95      | 111.23   |
| 22  | 5     | 313  | CLA  | O2D-CGD-CBD | 4.99  | 119.95      | 111.23   |
| 38  | 1     | 303  | LUT  | C11-C10-C9  | -4.99 | 120.28      | 127.28   |
| 22  | A     | 828  | CLA  | O2D-CGD-CBD | 4.99  | 119.95      | 111.23   |
| 22  | A     | 823  | CLA  | O2D-CGD-CBD | 4.99  | 119.95      | 111.23   |
| 22  | 7     | 311  | CLA  | O2D-CGD-CBD | 4.99  | 119.95      | 111.23   |
| 22  | 6     | 309  | CLA  | O2D-CGD-CBD | 4.99  | 119.95      | 111.23   |
| 24  | L     | 204  | BCR  | C27-C26-C25 | -4.99 | 115.97      | 122.70   |
| 22  | B     | 838  | CLA  | O2D-CGD-CBD | 4.99  | 119.94      | 111.23   |
| 22  | A     | 824  | CLA  | O2D-CGD-CBD | 4.98  | 119.94      | 111.23   |
| 39  | 6     | 318  | CHL  | C1B-CHB-C4A | 4.98  | 124.53      | 121.32   |
| 22  | A     | 810  | CLA  | O2D-CGD-CBD | 4.98  | 119.93      | 111.23   |
| 24  | 6     | 306  | BCR  | C7-C8-C9    | -4.97 | 118.88      | 126.23   |
| 22  | B     | 801  | CLA  | O2D-CGD-CBD | 4.97  | 119.92      | 111.23   |
| 22  | 3     | 310  | CLA  | O2D-CGD-CBD | 4.97  | 119.92      | 111.23   |
| 22  | Z     | 313  | CLA  | CMD-C2D-C1D | 4.97  | 133.48      | 124.73   |
| 24  | B     | 847  | BCR  | C27-C26-C25 | -4.97 | 115.99      | 122.70   |
| 22  | 6     | 302  | CLA  | O2D-CGD-CBD | 4.97  | 119.91      | 111.23   |
| 24  | A     | 845  | BCR  | C1-C6-C5    | -4.96 | 115.86      | 122.64   |
| 22  | L     | 203  | CLA  | O2D-CGD-CBD | 4.96  | 119.90      | 111.23   |
| 24  | B     | 848  | BCR  | C11-C10-C9  | -4.96 | 120.33      | 127.28   |
| 38  | 6     | 304  | LUT  | C15-C14-C13 | -4.96 | 120.33      | 127.28   |
| 24  | A     | 844  | BCR  | C33-C5-C6   | -4.96 | 119.08      | 124.48   |
| 22  | 9     | 311  | CLA  | O2D-CGD-CBD | 4.95  | 119.89      | 111.23   |
| 22  | Z     | 304  | CLA  | CMD-C2D-C1D | 4.95  | 133.44      | 124.73   |
| 22  | K     | 203  | CLA  | O2D-CGD-CBD | 4.95  | 119.88      | 111.23   |
| 22  | 2     | 301  | CLA  | O2D-CGD-CBD | 4.95  | 119.88      | 111.23   |
| 22  | B     | 821  | CLA  | O2D-CGD-CBD | 4.95  | 119.88      | 111.23   |
| 39  | 6     | 320  | CHL  | C1B-CHB-C4A | 4.95  | 124.50      | 121.32   |
| 24  | K     | 206  | BCR  | C7-C8-C9    | -4.94 | 118.93      | 126.23   |
| 24  | G     | 203  | BCR  | C38-C26-C25 | -4.94 | 119.10      | 124.48   |
| 24  | A     | 844  | BCR  | C38-C26-C25 | -4.94 | 119.10      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | K     | 204 | CLA  | O2D-CGD-CBD | 4.93  | 119.86      | 111.23   |
| 38  | 6     | 304 | LUT  | C35-C34-C33 | -4.93 | 120.36      | 127.28   |
| 24  | J     | 104 | BCR  | C20-C21-C22 | -4.93 | 120.37      | 127.28   |
| 36  | 5     | 306 | C7Z  | C38-C25-C26 | -4.93 | 119.11      | 124.48   |
| 22  | 7     | 309 | CLA  | O2D-CGD-CBD | 4.93  | 119.84      | 111.23   |
| 22  | A     | 842 | CLA  | O2D-CGD-CBD | 4.93  | 119.84      | 111.23   |
| 22  | B     | 829 | CLA  | O2D-CGD-CBD | 4.92  | 119.84      | 111.23   |
| 22  | 5     | 323 | CLA  | O2D-CGD-CBD | 4.92  | 119.83      | 111.23   |
| 24  | 8     | 304 | BCR  | C11-C10-C9  | -4.92 | 120.38      | 127.28   |
| 22  | A     | 854 | CLA  | O2D-CGD-CBD | 4.92  | 119.83      | 111.23   |
| 22  | B     | 812 | CLA  | O2D-CGD-CBD | 4.91  | 119.81      | 111.23   |
| 24  | B     | 846 | BCR  | C7-C8-C9    | -4.91 | 118.98      | 126.23   |
| 38  | 5     | 303 | LUT  | C11-C10-C9  | -4.91 | 120.40      | 127.28   |
| 22  | Z     | 310 | CLA  | O2D-CGD-CBD | 4.90  | 119.80      | 111.23   |
| 22  | 1     | 314 | CLA  | O2D-CGD-CBD | 4.89  | 119.78      | 111.23   |
| 22  | 7     | 306 | CLA  | O2D-CGD-CBD | 4.89  | 119.78      | 111.23   |
| 22  | 6     | 311 | CLA  | O2D-CGD-CBD | 4.89  | 119.78      | 111.23   |
| 22  | Z     | 304 | CLA  | O2D-CGD-CBD | 4.89  | 119.78      | 111.23   |
| 24  | J     | 104 | BCR  | C38-C26-C25 | -4.89 | 119.15      | 124.48   |
| 22  | 8     | 311 | CLA  | O2D-CGD-CBD | 4.89  | 119.77      | 111.23   |
| 24  | 3     | 305 | BCR  | C30-C25-C26 | -4.89 | 115.96      | 122.64   |
| 24  | L     | 204 | BCR  | C4-C5-C6    | -4.89 | 116.10      | 122.70   |
| 38  | Z     | 302 | LUT  | C7-C8-C9    | -4.88 | 119.01      | 126.23   |
| 38  | 6     | 304 | LUT  | C7-C8-C9    | -4.88 | 119.01      | 126.23   |
| 22  | B     | 825 | CLA  | O2D-CGD-CBD | 4.88  | 119.76      | 111.23   |
| 24  | A     | 844 | BCR  | C27-C26-C25 | -4.88 | 116.11      | 122.70   |
| 24  | A     | 856 | BCR  | C38-C26-C25 | -4.88 | 119.16      | 124.48   |
| 38  | 5     | 302 | LUT  | C26-C27-C28 | -4.88 | 116.99      | 124.58   |
| 24  | 8     | 304 | BCR  | C7-C8-C9    | -4.88 | 119.02      | 126.23   |
| 22  | 7     | 317 | CLA  | O2D-CGD-CBD | 4.87  | 119.75      | 111.23   |
| 22  | 3     | 309 | CLA  | O2D-CGD-CBD | 4.87  | 119.75      | 111.23   |
| 38  | Z     | 301 | LUT  | C15-C14-C13 | -4.87 | 120.45      | 127.28   |
| 24  | B     | 845 | BCR  | C16-C17-C18 | -4.87 | 120.45      | 127.28   |
| 22  | 9     | 307 | CLA  | O2D-CGD-CBD | 4.87  | 119.73      | 111.23   |
| 22  | A     | 840 | CLA  | O2D-CGD-CBD | 4.86  | 119.72      | 111.23   |
| 39  | 8     | 315 | CHL  | C1B-CHB-C4A | 4.85  | 124.44      | 121.32   |
| 22  | 6     | 307 | CLA  | O2D-CGD-CBD | 4.85  | 119.71      | 111.23   |
| 39  | 6     | 320 | CHL  | C1C-CHC-C4B | 4.85  | 133.41      | 116.07   |
| 24  | 6     | 305 | BCR  | C24-C23-C22 | -4.85 | 119.07      | 126.23   |
| 24  | 5     | 305 | BCR  | C38-C26-C25 | -4.84 | 119.20      | 124.48   |
| 24  | A     | 844 | BCR  | C15-C16-C17 | -4.84 | 113.61      | 123.52   |
| 24  | B     | 853 | BCR  | C20-C21-C22 | -4.84 | 120.49      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | 8     | 315 | CHL  | C1C-CHC-C4B | 4.84  | 133.38      | 116.07   |
| 39  | 4     | 819 | CHL  | C1C-CHC-C4B | 4.84  | 133.38      | 116.07   |
| 38  | 7     | 302 | LUT  | C7-C8-C9    | -4.83 | 119.09      | 126.23   |
| 39  | 6     | 316 | CHL  | C1B-CHB-C4A | 4.83  | 124.43      | 121.32   |
| 22  | A     | 826 | CLA  | O2D-CGD-CBD | 4.83  | 119.67      | 111.23   |
| 39  | 6     | 318 | CHL  | C1C-CHC-C4B | 4.83  | 133.34      | 116.07   |
| 22  | 9     | 310 | CLA  | O2D-CGD-CBD | 4.83  | 119.67      | 111.23   |
| 22  | 8     | 316 | CLA  | O2D-CGD-CBD | 4.82  | 119.66      | 111.23   |
| 24  | 7     | 303 | BCR  | C15-C14-C13 | -4.82 | 120.52      | 127.28   |
| 22  | 8     | 309 | CLA  | O2D-CGD-CBD | 4.81  | 119.64      | 111.23   |
| 22  | 5     | 312 | CLA  | O2D-CGD-CBD | 4.81  | 119.64      | 111.23   |
| 36  | J     | 105 | C7Z  | C11-C10-C9  | -4.81 | 120.53      | 127.28   |
| 39  | 9     | 312 | CHL  | C1C-CHC-C4B | 4.81  | 133.28      | 116.07   |
| 39  | 6     | 316 | CHL  | C1C-CHC-C4B | 4.81  | 133.27      | 116.07   |
| 22  | Z     | 316 | CLA  | O2D-CGD-CBD | 4.81  | 119.63      | 111.23   |
| 39  | 1     | 312 | CHL  | C1C-CHC-C4B | 4.81  | 133.27      | 116.07   |
| 39  | 4     | 816 | CHL  | C1C-CHC-C4B | 4.80  | 133.26      | 116.07   |
| 38  | 5     | 303 | LUT  | C15-C14-C13 | -4.80 | 120.54      | 127.28   |
| 22  | 1     | 316 | CLA  | CMD-C2D-C1D | 4.80  | 133.18      | 124.73   |
| 24  | 3     | 307 | BCR  | C7-C8-C9    | -4.80 | 119.13      | 126.23   |
| 38  | 5     | 302 | LUT  | C18-C5-C6   | -4.80 | 119.25      | 124.48   |
| 39  | Z     | 311 | CHL  | C1C-CHC-C4B | 4.79  | 133.22      | 116.07   |
| 22  | Z     | 306 | CLA  | O2D-CGD-CBD | 4.79  | 119.61      | 111.23   |
| 24  | 4     | 804 | BCR  | C38-C26-C25 | -4.79 | 119.26      | 124.48   |
| 39  | 6     | 315 | CHL  | C1C-CHC-C4B | 4.79  | 133.21      | 116.07   |
| 38  | 5     | 303 | LUT  | C7-C8-C9    | -4.79 | 119.15      | 126.23   |
| 22  | 9     | 304 | CLA  | O2D-CGD-CBD | 4.79  | 119.60      | 111.23   |
| 24  | L     | 204 | BCR  | C38-C26-C25 | -4.78 | 119.26      | 124.48   |
| 38  | 3     | 302 | LUT  | C11-C10-C9  | -4.78 | 120.57      | 127.28   |
| 24  | 4     | 804 | BCR  | C15-C14-C13 | -4.78 | 120.58      | 127.28   |
| 22  | 1     | 306 | CLA  | C1-C2-C3    | -4.78 | 118.37      | 126.20   |
| 39  | 2     | 303 | CHL  | C1C-CHC-C4B | 4.78  | 133.16      | 116.07   |
| 22  | A     | 829 | CLA  | O2D-CGD-CBD | 4.78  | 119.58      | 111.23   |
| 38  | 7     | 302 | LUT  | C26-C27-C28 | -4.77 | 117.16      | 124.58   |
| 22  | A     | 811 | CLA  | O2D-CGD-CBD | 4.76  | 119.55      | 111.23   |
| 24  | B     | 844 | BCR  | C33-C5-C6   | -4.76 | 119.29      | 124.48   |
| 39  | 8     | 312 | CHL  | C1C-CHC-C4B | 4.76  | 133.10      | 116.07   |
| 39  | 5     | 321 | CHL  | C1C-CHC-C4B | 4.76  | 133.09      | 116.07   |
| 22  | 5     | 322 | CLA  | O2D-CGD-CBD | 4.75  | 119.54      | 111.23   |
| 39  | Z     | 312 | CHL  | C1C-CHC-C4B | 4.75  | 133.08      | 116.07   |
| 22  | 3     | 313 | CLA  | O2D-CGD-CBD | 4.75  | 119.54      | 111.23   |
| 22  | 3     | 312 | CLA  | O2D-CGD-CBD | 4.75  | 119.53      | 111.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 38  | 4     | 802 | LUT  | C15-C14-C13 | -4.75 | 120.62      | 127.28   |
| 24  | B     | 853 | BCR  | C27-C26-C25 | -4.75 | 116.29      | 122.70   |
| 22  | 9     | 304 | CLA  | CMD-C2D-C1D | 4.74  | 133.08      | 124.73   |
| 39  | 4     | 813 | CHL  | C1C-CHC-C4B | 4.74  | 133.03      | 116.07   |
| 24  | 6     | 305 | BCR  | C38-C26-C25 | -4.73 | 119.32      | 124.48   |
| 38  | Z     | 302 | LUT  | C15-C14-C13 | -4.73 | 120.64      | 127.28   |
| 38  | 3     | 302 | LUT  | C7-C8-C9    | -4.73 | 119.24      | 126.23   |
| 24  | 3     | 305 | BCR  | C38-C26-C25 | -4.73 | 119.33      | 124.48   |
| 24  | A     | 856 | BCR  | C33-C5-C6   | -4.72 | 119.34      | 124.48   |
| 36  | 5     | 306 | C7Z  | C7-C8-C9    | -4.72 | 119.26      | 126.23   |
| 24  | 8     | 304 | BCR  | C16-C17-C18 | -4.71 | 120.67      | 127.28   |
| 38  | 7     | 302 | LUT  | C35-C34-C33 | -4.71 | 120.68      | 127.28   |
| 39  | 5     | 316 | CHL  | C1C-CHC-C4B | 4.71  | 132.91      | 116.07   |
| 24  | A     | 848 | BCR  | C1-C6-C5    | -4.71 | 116.21      | 122.64   |
| 24  | 3     | 305 | BCR  | C24-C23-C22 | -4.71 | 119.27      | 126.23   |
| 39  | 9     | 312 | CHL  | CMA-C3A-C4A | 4.70  | 124.75      | 114.61   |
| 39  | 1     | 312 | CHL  | C1B-CHB-C4A | 4.70  | 124.35      | 121.32   |
| 39  | 3     | 317 | CHL  | C1C-CHC-C4B | 4.70  | 132.89      | 116.07   |
| 24  | B     | 844 | BCR  | C7-C8-C9    | -4.70 | 119.28      | 126.23   |
| 22  | B     | 830 | CLA  | O2D-CGD-CBD | 4.69  | 119.43      | 111.23   |
| 24  | A     | 844 | BCR  | C12-C13-C14 | 4.69  | 126.39      | 119.01   |
| 24  | F     | 303 | BCR  | C33-C5-C6   | -4.69 | 119.37      | 124.48   |
| 39  | 8     | 301 | CHL  | C1C-CHC-C4B | 4.69  | 132.84      | 116.07   |
| 39  | 7     | 313 | CHL  | C1C-CHC-C4B | 4.69  | 132.84      | 116.07   |
| 39  | 5     | 317 | CHL  | C1C-CHC-C4B | 4.68  | 132.82      | 116.07   |
| 39  | 4     | 814 | CHL  | C1C-CHC-C4B | 4.68  | 132.81      | 116.07   |
| 31  | 1     | 319 | DGD  | O2G-C1B-C2B | 4.68  | 121.60      | 111.48   |
| 22  | B     | 813 | CLA  | C1-C2-C3    | -4.68 | 118.54      | 126.20   |
| 22  | Z     | 305 | CLA  | CMD-C2D-C1D | 4.67  | 132.96      | 124.73   |
| 24  | B     | 844 | BCR  | C11-C12-C13 | -4.67 | 113.56      | 126.36   |
| 24  | K     | 206 | BCR  | C30-C25-C26 | -4.66 | 116.27      | 122.64   |
| 24  | B     | 849 | BCR  | C38-C26-C25 | -4.66 | 119.40      | 124.48   |
| 24  | A     | 844 | BCR  | C8-C9-C10   | 4.66  | 126.33      | 119.01   |
| 24  | J     | 104 | BCR  | C33-C5-C6   | -4.65 | 119.41      | 124.48   |
| 39  | 9     | 314 | CHL  | C1C-CHC-C4B | 4.65  | 132.71      | 116.07   |
| 38  | 3     | 303 | LUT  | C11-C10-C9  | -4.65 | 120.76      | 127.28   |
| 38  | 4     | 803 | LUT  | C11-C10-C9  | -4.64 | 120.77      | 127.28   |
| 24  | 5     | 304 | BCR  | C24-C23-C22 | -4.64 | 119.37      | 126.23   |
| 38  | 9     | 301 | LUT  | C7-C8-C9    | -4.64 | 119.38      | 126.23   |
| 24  | A     | 856 | BCR  | C1-C6-C5    | -4.64 | 116.30      | 122.64   |
| 24  | B     | 844 | BCR  | C19-C18-C17 | 4.64  | 126.30      | 119.01   |
| 38  | 6     | 303 | LUT  | C26-C27-C28 | -4.64 | 117.37      | 124.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 5     | 318 | CLA  | O2D-CGD-CBD | 4.63  | 119.33      | 111.23   |
| 24  | 3     | 306 | BCR  | C27-C26-C25 | -4.63 | 116.45      | 122.70   |
| 38  | 1     | 303 | LUT  | C15-C14-C13 | -4.63 | 120.79      | 127.28   |
| 22  | B     | 837 | CLA  | C1-C2-C3    | -4.63 | 118.62      | 126.20   |
| 38  | 4     | 803 | LUT  | C26-C27-C28 | -4.62 | 117.38      | 124.58   |
| 22  | 1     | 311 | CLA  | CMD-C2D-C1D | 4.62  | 132.86      | 124.73   |
| 38  | 9     | 301 | LUT  | C31-C30-C29 | -4.62 | 120.80      | 127.28   |
| 24  | A     | 856 | BCR  | C24-C23-C22 | -4.62 | 119.41      | 126.23   |
| 22  | 5     | 307 | CLA  | C1-C2-C3    | -4.62 | 118.63      | 126.20   |
| 24  | J     | 104 | BCR  | C1-C6-C5    | -4.61 | 116.33      | 122.64   |
| 24  | 3     | 306 | BCR  | C16-C17-C18 | -4.61 | 120.81      | 127.28   |
| 24  | 5     | 305 | BCR  | C15-C16-C17 | -4.61 | 114.09      | 123.52   |
| 24  | B     | 848 | BCR  | C38-C26-C25 | -4.60 | 119.46      | 124.48   |
| 22  | 4     | 807 | CLA  | O2D-CGD-CBD | 4.60  | 119.27      | 111.23   |
| 24  | A     | 856 | BCR  | C15-C14-C13 | -4.60 | 120.83      | 127.28   |
| 24  | A     | 844 | BCR  | C20-C21-C22 | -4.59 | 120.83      | 127.28   |
| 24  | A     | 846 | BCR  | C24-C23-C22 | -4.59 | 119.44      | 126.23   |
| 24  | 5     | 305 | BCR  | C33-C5-C6   | -4.59 | 119.48      | 124.48   |
| 24  | B     | 845 | BCR  | C38-C26-C25 | -4.59 | 119.48      | 124.48   |
| 24  | B     | 848 | BCR  | C24-C23-C22 | -4.59 | 119.45      | 126.23   |
| 22  | 4     | 806 | CLA  | C1-C2-C3    | -4.58 | 118.69      | 126.20   |
| 38  | Z     | 302 | LUT  | C35-C34-C33 | -4.58 | 120.85      | 127.28   |
| 38  | 5     | 303 | LUT  | C35-C34-C33 | -4.58 | 120.85      | 127.28   |
| 22  | K     | 203 | CLA  | C1-C2-C3    | -4.58 | 118.69      | 126.20   |
| 24  | 3     | 304 | BCR  | C33-C5-C6   | -4.58 | 119.49      | 124.48   |
| 31  | 3     | 301 | DGD  | O2G-C1B-C2B | 4.57  | 121.37      | 111.48   |
| 24  | G     | 203 | BCR  | C15-C14-C13 | -4.57 | 120.87      | 127.28   |
| 38  | Z     | 301 | LUT  | C35-C34-C33 | -4.57 | 120.87      | 127.28   |
| 24  | 3     | 304 | BCR  | C27-C26-C25 | -4.56 | 116.54      | 122.70   |
| 24  | B     | 847 | BCR  | C33-C5-C6   | -4.56 | 119.51      | 124.48   |
| 32  | F     | 306 | RRX  | C7-C8-C9    | -4.55 | 119.50      | 126.23   |
| 22  | 7     | 310 | CLA  | C1-C2-C3    | -4.55 | 118.75      | 126.20   |
| 24  | 8     | 304 | BCR  | C33-C5-C6   | -4.55 | 119.52      | 124.48   |
| 22  | 7     | 306 | CLA  | C1-C2-C3    | -4.53 | 118.77      | 126.20   |
| 24  | A     | 846 | BCR  | C7-C8-C9    | -4.53 | 119.54      | 126.23   |
| 24  | G     | 203 | BCR  | C27-C26-C25 | -4.52 | 116.60      | 122.70   |
| 22  | 3     | 320 | CLA  | O2D-CGD-CBD | 4.52  | 119.13      | 111.23   |
| 24  | B     | 847 | BCR  | C38-C26-C25 | -4.51 | 119.56      | 124.48   |
| 24  | A     | 848 | BCR  | C4-C5-C6    | -4.50 | 116.62      | 122.70   |
| 22  | 9     | 306 | CLA  | C1-C2-C3    | -4.50 | 118.82      | 126.20   |
| 24  | 5     | 304 | BCR  | C30-C25-C26 | -4.50 | 116.49      | 122.64   |
| 22  | A     | 806 | CLA  | C1-C2-C3    | -4.50 | 118.83      | 126.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | B     | 853  | BCR  | C16-C17-C18 | -4.50 | 120.97      | 127.28   |
| 24  | B     | 845  | BCR  | C4-C5-C6    | -4.50 | 116.63      | 122.70   |
| 22  | 1     | 316  | CLA  | O2D-CGD-CBD | 4.49  | 119.08      | 111.23   |
| 22  | A     | 814  | CLA  | C1-C2-C3    | -4.49 | 118.84      | 126.20   |
| 24  | A     | 847  | BCR  | C7-C8-C9    | -4.49 | 119.59      | 126.23   |
| 24  | B     | 844  | BCR  | C38-C26-C25 | -4.49 | 119.59      | 124.48   |
| 22  | 6     | 319  | CLA  | C1-C2-C3    | -4.47 | 118.87      | 126.20   |
| 22  | 9     | 310  | CLA  | CMD-C2D-C1D | 4.47  | 132.60      | 124.73   |
| 22  | B     | 835  | CLA  | C1-C2-C3    | -4.47 | 119.53      | 126.76   |
| 38  | 4     | 802  | LUT  | C11-C10-C9  | -4.47 | 121.02      | 127.28   |
| 24  | 7     | 303  | BCR  | C16-C17-C18 | -4.46 | 121.02      | 127.28   |
| 22  | Z     | 307  | CLA  | C1-C2-C3    | -4.46 | 118.89      | 126.20   |
| 24  | 8     | 304  | BCR  | C24-C23-C22 | -4.46 | 119.64      | 126.23   |
| 24  | B     | 846  | BCR  | C16-C17-C18 | -4.46 | 121.03      | 127.28   |
| 24  | 4     | 804  | BCR  | C20-C21-C22 | -4.45 | 121.04      | 127.28   |
| 24  | 8     | 304  | BCR  | C1-C6-C5    | -4.45 | 116.56      | 122.64   |
| 24  | I     | 4001 | BCR  | C4-C5-C6    | -4.44 | 116.70      | 122.70   |
| 24  | I     | 4001 | BCR  | C27-C26-C25 | -4.44 | 116.71      | 122.70   |
| 25  | B     | 803  | LHG  | O7-C7-C8    | 4.44  | 121.08      | 111.48   |
| 24  | F     | 303  | BCR  | C38-C26-C25 | -4.44 | 119.64      | 124.48   |
| 24  | L     | 204  | BCR  | C33-C5-C6   | -4.43 | 119.65      | 124.48   |
| 38  | 1     | 302  | LUT  | C35-C34-C33 | -4.43 | 121.07      | 127.28   |
| 22  | 4     | 805  | CLA  | O2D-CGD-CBD | 4.43  | 118.97      | 111.23   |
| 21  | A     | 801  | CL0  | CHA-C1A-C2A | -4.42 | 122.92      | 133.31   |
| 22  | 7     | 317  | CLA  | C1-C2-C3    | -4.42 | 118.95      | 126.20   |
| 38  | 7     | 301  | LUT  | C15-C14-C13 | -4.42 | 121.08      | 127.28   |
| 38  | 1     | 303  | LUT  | C26-C27-C28 | -4.41 | 117.71      | 124.58   |
| 22  | A     | 825  | CLA  | C1-C2-C3    | -4.41 | 118.97      | 126.20   |
| 24  | 3     | 307  | BCR  | C27-C26-C25 | -4.41 | 116.75      | 122.70   |
| 36  | 5     | 306  | C7Z  | C1-C6-C5    | -4.41 | 116.61      | 122.64   |
| 24  | B     | 853  | BCR  | C38-C26-C25 | -4.41 | 119.68      | 124.48   |
| 24  | L     | 204  | BCR  | C30-C25-C26 | -4.41 | 116.62      | 122.64   |
| 22  | 7     | 310  | CLA  | O2D-CGD-CBD | 4.41  | 118.93      | 111.23   |
| 24  | B     | 845  | BCR  | C11-C10-C9  | -4.40 | 121.10      | 127.28   |
| 24  | A     | 846  | BCR  | C33-C5-C6   | -4.40 | 119.68      | 124.48   |
| 25  | 6     | 323  | LHG  | O7-C7-C8    | 4.40  | 121.00      | 111.48   |
| 24  | L     | 204  | BCR  | C16-C17-C18 | -4.40 | 121.11      | 127.28   |
| 22  | 5     | 320  | CLA  | CMD-C2D-C1D | 4.40  | 132.47      | 124.73   |
| 24  | I     | 4001 | BCR  | C7-C8-C9    | -4.40 | 119.73      | 126.23   |
| 24  | 3     | 307  | BCR  | C1-C6-C5    | -4.39 | 116.63      | 122.64   |
| 24  | 6     | 305  | BCR  | C15-C14-C13 | -4.39 | 121.12      | 127.28   |
| 22  | 9     | 303  | CLA  | O2D-CGD-CBD | 4.38  | 118.89      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 1     | 308  | CLA  | C1-C2-C3    | -4.38 | 119.02      | 126.20   |
| 22  | A     | 828  | CLA  | C1-C2-C3    | -4.38 | 119.02      | 126.20   |
| 24  | 3     | 304  | BCR  | C12-C13-C14 | -4.37 | 112.14      | 119.01   |
| 24  | B     | 845  | BCR  | C15-C14-C13 | -4.36 | 121.16      | 127.28   |
| 24  | I     | 4001 | BCR  | C11-C10-C9  | -4.36 | 121.17      | 127.28   |
| 24  | 3     | 307  | BCR  | C33-C5-C6   | -4.35 | 119.74      | 124.48   |
| 24  | 3     | 306  | BCR  | C4-C5-C6    | -4.35 | 116.83      | 122.70   |
| 24  | A     | 848  | BCR  | C30-C25-C26 | -4.34 | 116.70      | 122.64   |
| 22  | B     | 810  | CLA  | C1-C2-C3    | -4.34 | 119.08      | 126.20   |
| 24  | F     | 303  | BCR  | C24-C23-C22 | -4.33 | 119.82      | 126.23   |
| 24  | L     | 204  | BCR  | C15-C14-C13 | -4.33 | 121.20      | 127.28   |
| 38  | 7     | 301  | LUT  | C7-C8-C9    | -4.33 | 119.83      | 126.23   |
| 24  | B     | 848  | BCR  | C16-C17-C18 | -4.32 | 121.22      | 127.28   |
| 24  | A     | 846  | BCR  | C20-C21-C22 | -4.32 | 121.22      | 127.28   |
| 24  | A     | 844  | BCR  | C30-C25-C26 | -4.32 | 116.73      | 122.64   |
| 22  | 1     | 307  | CLA  | C1-C2-C3    | -4.32 | 119.12      | 126.20   |
| 22  | 7     | 307  | CLA  | C1-C2-C3    | -4.31 | 119.13      | 126.20   |
| 36  | J     | 105  | C7Z  | C18-C5-C6   | -4.31 | 119.78      | 124.48   |
| 22  | 4     | 807  | CLA  | C1-C2-C3    | -4.31 | 119.14      | 126.20   |
| 39  | 8     | 301  | CHL  | C1-C2-C3    | -4.30 | 119.15      | 126.20   |
| 39  | 5     | 321  | CHL  | CHA-C1A-C2A | -4.30 | 123.21      | 133.31   |
| 24  | K     | 206  | BCR  | C24-C23-C22 | -4.30 | 119.88      | 126.23   |
| 38  | 4     | 803  | LUT  | C18-C5-C6   | -4.30 | 119.80      | 124.48   |
| 22  | B     | 824  | CLA  | C1-C2-C3    | -4.29 | 119.16      | 126.20   |
| 22  | B     | 825  | CLA  | C1-C2-C3    | -4.29 | 119.16      | 126.20   |
| 38  | 8     | 303  | LUT  | C21-C26-C27 | -4.29 | 107.89      | 112.83   |
| 33  | 4     | 822  | LMT  | C1B-O1B-C4' | -4.29 | 107.81      | 117.98   |
| 24  | A     | 856  | BCR  | C11-C10-C9  | -4.29 | 121.26      | 127.28   |
| 36  | J     | 105  | C7Z  | C1-C6-C5    | -4.29 | 116.78      | 122.64   |
| 21  | A     | 801  | CL0  | O2A-CGA-CBA | 4.28  | 124.88      | 111.83   |
| 24  | A     | 846  | BCR  | C38-C26-C25 | -4.27 | 119.82      | 124.48   |
| 24  | 5     | 304  | BCR  | C33-C5-C6   | -4.27 | 119.83      | 124.48   |
| 39  | 1     | 312  | CHL  | CHA-C1A-C2A | -4.27 | 123.29      | 133.31   |
| 39  | 8     | 315  | CHL  | CHA-C1A-C2A | -4.27 | 123.29      | 133.31   |
| 24  | 6     | 306  | BCR  | C4-C5-C6    | -4.26 | 116.94      | 122.70   |
| 38  | Z     | 302  | LUT  | C18-C5-C6   | -4.25 | 119.84      | 124.48   |
| 22  | L     | 203  | CLA  | C1-C2-C3    | -4.25 | 119.88      | 126.76   |
| 22  | 7     | 305  | CLA  | C1-C2-C3    | -4.25 | 119.88      | 126.76   |
| 24  | B     | 849  | BCR  | C24-C23-C22 | -4.25 | 119.95      | 126.23   |
| 24  | 8     | 304  | BCR  | C29-C30-C25 | 4.25  | 116.61      | 110.44   |
| 25  | 1     | 317  | LHG  | O7-C7-C8    | 4.25  | 120.67      | 111.48   |
| 24  | B     | 849  | BCR  | C27-C26-C25 | -4.25 | 116.97      | 122.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | Z     | 317 | LHG  | O7-C7-C8    | 4.25  | 120.67      | 111.48   |
| 22  | B     | 841 | CLA  | C1-C2-C3    | -4.25 | 119.24      | 126.20   |
| 22  | 4     | 810 | CLA  | C1-C2-C3    | -4.24 | 119.90      | 126.76   |
| 22  | 3     | 312 | CLA  | C1-C2-C3    | -4.24 | 119.25      | 126.20   |
| 38  | 1     | 303 | LUT  | C18-C5-C6   | -4.24 | 119.86      | 124.48   |
| 38  | 5     | 303 | LUT  | C26-C27-C28 | -4.24 | 117.98      | 124.58   |
| 22  | 5     | 313 | CLA  | C1-C2-C3    | -4.23 | 119.26      | 126.20   |
| 38  | Z     | 301 | LUT  | C1-C6-C5    | -4.23 | 116.86      | 122.64   |
| 36  | J     | 105 | C7Z  | C38-C25-C26 | -4.23 | 119.87      | 124.48   |
| 22  | 2     | 301 | CLA  | C1-C2-C3    | -4.23 | 119.27      | 126.20   |
| 38  | 7     | 301 | LUT  | C11-C10-C9  | -4.23 | 121.35      | 127.28   |
| 24  | B     | 845 | BCR  | C7-C8-C9    | -4.22 | 119.99      | 126.23   |
| 38  | 4     | 803 | LUT  | C1-C6-C5    | -4.22 | 116.87      | 122.64   |
| 22  | A     | 826 | CLA  | C1-C2-C3    | -4.22 | 119.94      | 126.76   |
| 36  | 5     | 306 | C7Z  | C31-C30-C29 | -4.22 | 121.36      | 127.28   |
| 22  | 7     | 304 | CLA  | O2A-C1-C2   | 4.22  | 124.34      | 108.11   |
| 38  | 3     | 302 | LUT  | C18-C5-C6   | -4.22 | 119.88      | 124.48   |
| 38  | 6     | 304 | LUT  | C21-C26-C27 | -4.22 | 107.98      | 112.83   |
| 38  | 6     | 304 | LUT  | C11-C10-C9  | -4.21 | 121.38      | 127.28   |
| 22  | Z     | 316 | CLA  | C1-C2-C3    | -4.20 | 119.31      | 126.20   |
| 24  | B     | 845 | BCR  | C30-C25-C26 | -4.20 | 116.90      | 122.64   |
| 24  | 8     | 304 | BCR  | C20-C21-C22 | -4.19 | 121.40      | 127.28   |
| 22  | 9     | 309 | CLA  | CMD-C2D-C1D | 4.19  | 132.11      | 124.73   |
| 24  | 6     | 306 | BCR  | C33-C5-C6   | -4.19 | 119.91      | 124.48   |
| 24  | A     | 856 | BCR  | C30-C25-C26 | -4.19 | 116.91      | 122.64   |
| 22  | 3     | 315 | CLA  | CMD-C2D-C1D | 4.19  | 132.10      | 124.73   |
| 38  | 4     | 803 | LUT  | C15-C14-C13 | -4.19 | 121.41      | 127.28   |
| 38  | 8     | 303 | LUT  | C18-C5-C6   | -4.18 | 119.92      | 124.48   |
| 24  | A     | 844 | BCR  | C10-C11-C12 | -4.18 | 111.09      | 123.20   |
| 24  | A     | 845 | BCR  | C4-C5-C6    | -4.18 | 117.06      | 122.70   |
| 24  | A     | 847 | BCR  | C15-C14-C13 | -4.17 | 121.43      | 127.28   |
| 24  | L     | 204 | BCR  | C24-C23-C22 | -4.16 | 120.07      | 126.23   |
| 24  | G     | 203 | BCR  | C1-C6-C5    | -4.16 | 116.95      | 122.64   |
| 22  | 4     | 815 | CLA  | C1-C2-C3    | -4.15 | 120.05      | 126.76   |
| 22  | B     | 839 | CLA  | C1-C2-C3    | -4.15 | 119.40      | 126.20   |
| 24  | 6     | 306 | BCR  | C27-C26-C25 | -4.15 | 117.10      | 122.70   |
| 22  | 8     | 305 | CLA  | C1-C2-C3    | -4.15 | 119.40      | 126.20   |
| 24  | A     | 847 | BCR  | C11-C10-C9  | -4.15 | 121.46      | 127.28   |
| 22  | 7     | 315 | CLA  | C1-C2-C3    | -4.15 | 120.05      | 126.76   |
| 36  | 5     | 306 | C7Z  | C27-C28-C29 | -4.14 | 120.10      | 126.23   |
| 39  | Z     | 311 | CHL  | CHA-C1A-C2A | -4.14 | 123.58      | 133.31   |
| 24  | A     | 847 | BCR  | C4-C5-C6    | -4.14 | 117.11      | 122.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | 6     | 305 | BCR  | C4-C5-C6    | -4.14 | 117.11      | 122.70   |
| 24  | 3     | 306 | BCR  | C38-C26-C25 | -4.13 | 119.97      | 124.48   |
| 24  | 3     | 306 | BCR  | C7-C8-C9    | -4.13 | 120.12      | 126.23   |
| 22  | 7     | 314 | CLA  | C1-C2-C3    | -4.13 | 120.09      | 126.76   |
| 24  | 5     | 304 | BCR  | C4-C5-C6    | -4.12 | 117.13      | 122.70   |
| 22  | Z     | 308 | CLA  | C1-C2-C3    | -4.12 | 119.45      | 126.20   |
| 22  | 6     | 309 | CLA  | C1-C2-C3    | -4.11 | 119.46      | 126.20   |
| 22  | 5     | 309 | CLA  | C1-C2-C3    | -4.11 | 119.46      | 126.20   |
| 22  | F     | 301 | CLA  | C1-C2-C3    | -4.11 | 119.46      | 126.20   |
| 22  | 6     | 317 | CLA  | C1-C2-C3    | -4.11 | 120.11      | 126.76   |
| 24  | 6     | 306 | BCR  | C15-C14-C13 | -4.11 | 121.52      | 127.28   |
| 39  | Z     | 312 | CHL  | CHA-C1A-C2A | -4.11 | 123.66      | 133.31   |
| 39  | 8     | 301 | CHL  | CHA-C1A-C2A | -4.09 | 123.70      | 133.31   |
| 24  | B     | 847 | BCR  | C30-C25-C26 | -4.09 | 117.05      | 122.64   |
| 22  | B     | 821 | CLA  | C1-C2-C3    | -4.09 | 119.50      | 126.20   |
| 22  | 9     | 303 | CLA  | O2A-C1-C2   | 4.08  | 123.81      | 108.11   |
| 24  | J     | 104 | BCR  | C30-C25-C26 | -4.08 | 117.06      | 122.64   |
| 38  | 3     | 303 | LUT  | C18-C5-C6   | -4.08 | 120.04      | 124.48   |
| 25  | A     | 850 | LHG  | O7-C7-C8    | 4.07  | 120.30      | 111.48   |
| 38  | 8     | 303 | LUT  | C1-C6-C5    | -4.07 | 117.07      | 122.64   |
| 39  | 3     | 317 | CHL  | CHA-C1A-C2A | -4.07 | 123.75      | 133.31   |
| 24  | 5     | 304 | BCR  | C27-C26-C25 | -4.06 | 117.21      | 122.70   |
| 41  | 5     | 325 | 3PH  | O21-C21-C22 | 4.06  | 120.27      | 111.48   |
| 25  | 7     | 318 | LHG  | O7-C7-C8    | 4.06  | 120.26      | 111.48   |
| 39  | 6     | 318 | CHL  | CHA-C1A-C2A | -4.06 | 123.78      | 133.31   |
| 38  | 9     | 301 | LUT  | C11-C10-C9  | -4.05 | 121.60      | 127.28   |
| 24  | 3     | 304 | BCR  | C38-C26-C25 | -4.05 | 120.07      | 124.48   |
| 22  | A     | 841 | CLA  | C1-C2-C3    | -4.04 | 119.58      | 126.20   |
| 24  | 7     | 303 | BCR  | C24-C23-C22 | -4.04 | 120.26      | 126.23   |
| 24  | 6     | 306 | BCR  | C11-C12-C13 | -4.04 | 115.29      | 126.36   |
| 22  | 5     | 319 | CLA  | C1-C2-C3    | -4.04 | 119.58      | 126.20   |
| 39  | 6     | 320 | CHL  | CHA-C1A-C2A | -4.03 | 123.84      | 133.31   |
| 22  | 3     | 308 | CLA  | C1-C2-C3    | -4.03 | 119.60      | 126.20   |
| 38  | 8     | 302 | LUT  | C26-C27-C28 | -4.03 | 118.31      | 124.58   |
| 22  | 9     | 308 | CLA  | C1-C2-C3    | -4.03 | 120.25      | 126.76   |
| 22  | A     | 816 | CLA  | C1-C2-C3    | -4.03 | 119.60      | 126.20   |
| 24  | 3     | 304 | BCR  | C8-C9-C10   | 4.03  | 125.34      | 119.01   |
| 38  | 4     | 803 | LUT  | C21-C26-C27 | -4.02 | 108.20      | 112.83   |
| 39  | 2     | 303 | CHL  | CHA-C1A-C2A | -4.02 | 123.86      | 133.31   |
| 24  | B     | 853 | BCR  | C33-C5-C6   | -4.02 | 120.10      | 124.48   |
| 24  | B     | 847 | BCR  | C24-C23-C22 | -4.02 | 120.29      | 126.23   |
| 22  | 9     | 313 | CLA  | C1-C2-C3    | -4.02 | 120.26      | 126.76   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32  | F     | 306  | RRX  | C16-C15-C14 | -4.02 | 115.30      | 123.52   |
| 24  | 3     | 304  | BCR  | C2-C1-C6    | 4.01  | 116.27      | 110.44   |
| 22  | A     | 830  | CLA  | C1-C2-C3    | -4.01 | 119.63      | 126.20   |
| 24  | A     | 844  | BCR  | C24-C23-C22 | -4.01 | 120.31      | 126.23   |
| 24  | A     | 844  | BCR  | C1-C6-C5    | -4.00 | 117.17      | 122.64   |
| 39  | 4     | 813  | CHL  | CHA-C1A-C2A | -4.00 | 123.91      | 133.31   |
| 39  | 4     | 819  | CHL  | CHA-C1A-C2A | -4.00 | 123.91      | 133.31   |
| 39  | 6     | 316  | CHL  | CHA-C1A-C2A | -4.00 | 123.91      | 133.31   |
| 38  | 5     | 302  | LUT  | C7-C8-C9    | -4.00 | 120.32      | 126.23   |
| 32  | F     | 306  | RRX  | C38-C26-C25 | -4.00 | 120.12      | 124.48   |
| 39  | 4     | 816  | CHL  | CHA-C1A-C2A | -4.00 | 123.92      | 133.31   |
| 24  | I     | 4001 | BCR  | C33-C5-C6   | -4.00 | 120.12      | 124.48   |
| 22  | 8     | 311  | CLA  | C1-C2-C3    | -4.00 | 120.30      | 126.76   |
| 25  | B     | 850  | LHG  | O7-C7-C8    | 3.99  | 120.12      | 111.48   |
| 22  | 9     | 309  | CLA  | O2D-CGD-CBD | 3.99  | 118.21      | 111.23   |
| 36  | 5     | 306  | C7Z  | C18-C5-C6   | -3.99 | 120.13      | 124.48   |
| 24  | K     | 206  | BCR  | C4-C5-C6    | -3.99 | 117.32      | 122.70   |
| 38  | 8     | 302  | LUT  | C21-C26-C27 | -3.98 | 108.25      | 112.83   |
| 22  | A     | 808  | CLA  | C1-C2-C3    | -3.98 | 119.67      | 126.20   |
| 22  | 7     | 322  | CLA  | C1-C2-C3    | -3.98 | 119.67      | 126.20   |
| 24  | 3     | 307  | BCR  | C30-C25-C26 | -3.98 | 117.20      | 122.64   |
| 22  | 5     | 310  | CLA  | C1-C2-C3    | -3.98 | 119.68      | 126.20   |
| 22  | B     | 809  | CLA  | C1-C2-C3    | -3.98 | 119.68      | 126.20   |
| 21  | A     | 801  | CL0  | C1C-CHC-C4B | 3.98  | 130.29      | 116.07   |
| 27  | A     | 852  | DGA  | CDB-CCB-CBB | -3.97 | 80.39       | 115.25   |
| 22  | A     | 831  | CLA  | C1-C2-C3    | -3.97 | 120.33      | 126.76   |
| 22  | 6     | 302  | CLA  | C1-C2-C3    | -3.97 | 119.69      | 126.20   |
| 38  | 9     | 302  | LUT  | C15-C14-C13 | -3.97 | 121.71      | 127.28   |
| 22  | 4     | 818  | CLA  | O2A-C1-C2   | 3.97  | 123.38      | 108.11   |
| 22  | 5     | 308  | CLA  | C1-C2-C3    | -3.97 | 119.70      | 126.20   |
| 22  | A     | 842  | CLA  | C1-C2-C3    | -3.97 | 119.70      | 126.20   |
| 21  | A     | 801  | CL0  | C1-C2-C3    | -3.96 | 119.70      | 126.20   |
| 24  | A     | 845  | BCR  | C38-C26-C25 | -3.96 | 120.16      | 124.48   |
| 24  | 6     | 305  | BCR  | C33-C5-C6   | -3.96 | 120.16      | 124.48   |
| 22  | B     | 828  | CLA  | C1-C2-C3    | -3.96 | 119.70      | 126.20   |
| 39  | 8     | 312  | CHL  | CHA-C1A-C2A | -3.96 | 124.01      | 133.31   |
| 34  | J     | 101  | LMG  | O7-C10-C11  | 3.96  | 120.05      | 111.48   |
| 25  | A     | 849  | LHG  | O7-C7-C8    | 3.96  | 120.04      | 111.48   |
| 24  | 3     | 307  | BCR  | C11-C12-C13 | -3.95 | 115.53      | 126.36   |
| 22  | 7     | 312  | CLA  | C1-C2-C3    | -3.95 | 119.72      | 126.20   |
| 38  | 6     | 304  | LUT  | C26-C27-C28 | -3.95 | 118.44      | 124.58   |
| 22  | B     | 815  | CLA  | C1-C2-C3    | -3.95 | 119.73      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | 4     | 814 | CHL  | CHA-C1A-C2A | -3.94 | 124.05      | 133.31   |
| 22  | G     | 201 | CLA  | C1-C2-C3    | -3.94 | 120.39      | 126.76   |
| 38  | 5     | 303 | LUT  | C18-C5-C6   | -3.94 | 120.18      | 124.48   |
| 39  | 6     | 318 | CHL  | C1-C2-C3    | -3.94 | 119.75      | 126.20   |
| 22  | A     | 809 | CLA  | C1-C2-C3    | -3.94 | 119.75      | 126.20   |
| 24  | J     | 104 | BCR  | C24-C23-C22 | -3.93 | 120.41      | 126.23   |
| 24  | F     | 303 | BCR  | C11-C12-C13 | -3.93 | 115.59      | 126.36   |
| 38  | 6     | 304 | LUT  | C18-C5-C6   | -3.93 | 120.20      | 124.48   |
| 24  | K     | 206 | BCR  | C33-C5-C6   | -3.93 | 120.20      | 124.48   |
| 22  | 7     | 308 | CLA  | C1-C2-C3    | -3.93 | 119.76      | 126.20   |
| 22  | B     | 830 | CLA  | C1-C2-C3    | -3.93 | 119.76      | 126.20   |
| 22  | A     | 802 | CLA  | O2A-C1-C2   | 3.93  | 123.22      | 108.11   |
| 24  | 7     | 303 | BCR  | C33-C5-C6   | -3.92 | 120.20      | 124.48   |
| 24  | A     | 845 | BCR  | C30-C25-C26 | -3.92 | 117.28      | 122.64   |
| 24  | B     | 853 | BCR  | C24-C23-C22 | -3.92 | 120.44      | 126.23   |
| 22  | 8     | 307 | CLA  | C1-C2-C3    | -3.92 | 119.78      | 126.20   |
| 22  | 5     | 309 | CLA  | O2A-C1-C2   | 3.92  | 123.17      | 108.11   |
| 41  | 6     | 324 | 3PH  | O21-C21-C22 | 3.91  | 119.95      | 111.48   |
| 22  | A     | 840 | CLA  | C1-C2-C3    | -3.91 | 119.78      | 126.20   |
| 38  | 4     | 802 | LUT  | C26-C27-C28 | -3.91 | 118.49      | 124.58   |
| 39  | 7     | 313 | CHL  | CHA-C1A-C2A | -3.91 | 124.14      | 133.31   |
| 22  | 7     | 304 | CLA  | C1-C2-C3    | -3.91 | 119.80      | 126.20   |
| 38  | 1     | 303 | LUT  | C31-C30-C29 | -3.90 | 121.81      | 127.28   |
| 24  | B     | 853 | BCR  | C38-C26-C27 | 3.90  | 121.90      | 113.60   |
| 22  | 5     | 312 | CLA  | C1-C2-C3    | -3.89 | 120.46      | 126.76   |
| 38  | Z     | 302 | LUT  | C21-C26-C27 | -3.89 | 108.35      | 112.83   |
| 22  | 1     | 310 | CLA  | C1-C2-C3    | -3.89 | 119.83      | 126.20   |
| 39  | 9     | 312 | CHL  | C1-O2A-CGA  | 3.89  | 126.06      | 116.65   |
| 24  | B     | 846 | BCR  | C20-C21-C22 | -3.89 | 121.83      | 127.28   |
| 39  | 5     | 317 | CHL  | CHA-C1A-C2A | -3.88 | 124.19      | 133.31   |
| 22  | 6     | 308 | CLA  | C1-C2-C3    | -3.88 | 119.84      | 126.20   |
| 22  | 8     | 308 | CLA  | C1-C2-C3    | -3.88 | 119.84      | 126.20   |
| 24  | 3     | 304 | BCR  | C16-C15-C14 | 3.88  | 131.46      | 123.52   |
| 24  | A     | 848 | BCR  | C27-C26-C25 | -3.88 | 117.47      | 122.70   |
| 39  | 5     | 316 | CHL  | CHA-C1A-C2A | -3.87 | 124.22      | 133.31   |
| 24  | A     | 847 | BCR  | C33-C5-C6   | -3.87 | 120.26      | 124.48   |
| 22  | A     | 803 | CLA  | C1-C2-C3    | -3.87 | 119.86      | 126.20   |
| 38  | 8     | 303 | LUT  | C26-C27-C28 | -3.87 | 118.56      | 124.58   |
| 22  | Z     | 309 | CLA  | C1-C2-C3    | -3.87 | 119.86      | 126.20   |
| 22  | B     | 818 | CLA  | C1-C2-C3    | -3.86 | 119.87      | 126.20   |
| 39  | 6     | 320 | CHL  | C1A-CHA-C4D | 3.86  | 125.43      | 118.98   |
| 22  | 8     | 310 | CLA  | O2A-C1-C2   | 3.86  | 122.97      | 108.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24  | B     | 846  | BCR  | C15-C16-C17 | -3.86 | 115.62      | 123.52   |
| 39  | 8     | 315  | CHL  | C1A-CHA-C4D | 3.86  | 125.42      | 118.98   |
| 22  | 4     | 818  | CLA  | C1-C2-C3    | -3.85 | 119.89      | 126.20   |
| 38  | 6     | 304  | LUT  | C31-C30-C29 | -3.85 | 121.88      | 127.28   |
| 22  | B     | 827  | CLA  | C1-C2-C3    | -3.85 | 119.89      | 126.20   |
| 22  | 6     | 311  | CLA  | C1-C2-C3    | -3.84 | 119.90      | 126.20   |
| 22  | 3     | 314  | CLA  | O2A-C1-C2   | 3.84  | 122.90      | 108.11   |
| 25  | 4     | 820  | LHG  | O7-C7-C8    | 3.84  | 119.79      | 111.48   |
| 22  | A     | 838  | CLA  | C1-C2-C3    | -3.84 | 119.91      | 126.20   |
| 38  | 7     | 301  | LUT  | C26-C27-C28 | -3.84 | 118.60      | 124.58   |
| 39  | 9     | 314  | CHL  | C3D-C4D-CHA | 3.84  | 114.37      | 108.54   |
| 24  | L     | 204  | BCR  | C7-C8-C9    | -3.83 | 120.56      | 126.23   |
| 38  | 8     | 303  | LUT  | C11-C10-C9  | -3.83 | 121.90      | 127.28   |
| 38  | Z     | 301  | LUT  | C7-C8-C9    | -3.83 | 120.57      | 126.23   |
| 22  | A     | 807  | CLA  | C1-C2-C3    | -3.83 | 119.92      | 126.20   |
| 22  | 4     | 812  | CLA  | C1-C2-C3    | -3.83 | 119.92      | 126.20   |
| 24  | A     | 845  | BCR  | C7-C8-C9    | -3.83 | 120.57      | 126.23   |
| 24  | I     | 4001 | BCR  | C38-C26-C27 | 3.83  | 121.76      | 113.60   |
| 39  | 5     | 316  | CHL  | C3D-C4D-CHA | 3.82  | 114.35      | 108.54   |
| 22  | 1     | 309  | CLA  | C1-C2-C3    | -3.82 | 119.93      | 126.20   |
| 22  | B     | 832  | CLA  | C1-C2-C3    | -3.82 | 120.58      | 126.76   |
| 24  | A     | 846  | BCR  | C16-C17-C18 | -3.82 | 121.92      | 127.28   |
| 24  | B     | 846  | BCR  | C29-C30-C25 | 3.82  | 115.98      | 110.44   |
| 32  | F     | 306  | RRX  | C4-C5-C6    | -3.82 | 117.55      | 122.70   |
| 39  | 9     | 312  | CHL  | C3D-C4D-CHA | 3.81  | 114.34      | 108.54   |
| 38  | 6     | 303  | LUT  | C18-C5-C6   | -3.81 | 120.33      | 124.48   |
| 24  | 3     | 304  | BCR  | C15-C14-C13 | 3.81  | 132.62      | 127.28   |
| 38  | 1     | 302  | LUT  | C15-C14-C13 | -3.81 | 121.94      | 127.28   |
| 38  | 9     | 302  | LUT  | C26-C27-C28 | -3.80 | 118.67      | 124.58   |
| 22  | 5     | 322  | CLA  | C1-C2-C3    | -3.80 | 119.97      | 126.20   |
| 22  | A     | 822  | CLA  | C1-C2-C3    | -3.79 | 119.98      | 126.20   |
| 22  | Z     | 310  | CLA  | C1-C2-C3    | -3.79 | 120.62      | 126.76   |
| 39  | 4     | 819  | CHL  | C1A-CHA-C4D | 3.79  | 125.31      | 118.98   |
| 21  | A     | 801  | CL0  | CBC-CAC-C3C | -3.79 | 107.45      | 112.87   |
| 39  | 2     | 303  | CHL  | C3D-C4D-CHA | 3.79  | 114.30      | 108.54   |
| 24  | A     | 845  | BCR  | C27-C26-C25 | -3.78 | 117.59      | 122.70   |
| 35  | J     | 102  | T7X  | O16-C10-C12 | 3.78  | 119.66      | 111.48   |
| 39  | 4     | 814  | CHL  | C3D-C4D-CHA | 3.78  | 114.28      | 108.54   |
| 39  | 6     | 315  | CHL  | C3D-C4D-CHA | 3.78  | 114.28      | 108.54   |
| 24  | B     | 849  | BCR  | C15-C14-C13 | -3.77 | 121.98      | 127.28   |
| 38  | 3     | 303  | LUT  | C35-C34-C33 | -3.77 | 121.99      | 127.28   |
| 24  | A     | 846  | BCR  | C4-C5-C6    | -3.77 | 117.61      | 122.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | 8     | 301 | CHL  | C3D-C4D-CHA | 3.77  | 114.27      | 108.54   |
| 25  | 5     | 324 | LHG  | O7-C7-C8    | 3.77  | 119.64      | 111.48   |
| 22  | B     | 834 | CLA  | C1-C2-C3    | -3.77 | 120.02      | 126.20   |
| 24  | B     | 844 | BCR  | C12-C13-C14 | 3.77  | 124.94      | 119.01   |
| 22  | 7     | 323 | CLA  | O2A-C1-C2   | 3.77  | 122.61      | 108.11   |
| 22  | 7     | 324 | CLA  | O2A-C1-C2   | 3.77  | 122.61      | 108.11   |
| 22  | A     | 818 | CLA  | C1-C2-C3    | -3.76 | 120.03      | 126.20   |
| 39  | 9     | 312 | CHL  | CHA-C1A-C2A | -3.76 | 124.47      | 133.31   |
| 24  | B     | 846 | BCR  | C4-C5-C6    | -3.76 | 117.62      | 122.70   |
| 39  | 5     | 317 | CHL  | C3D-C4D-CHA | 3.76  | 114.25      | 108.54   |
| 22  | 6     | 309 | CLA  | CAA-C2A-C3A | -3.76 | 102.84      | 113.00   |
| 22  | 8     | 309 | CLA  | C1-C2-C3    | -3.76 | 120.04      | 126.20   |
| 22  | 5     | 313 | CLA  | O2A-C1-C2   | 3.76  | 122.56      | 108.11   |
| 24  | B     | 844 | BCR  | C4-C5-C6    | -3.75 | 117.63      | 122.70   |
| 24  | 3     | 304 | BCR  | C35-C13-C12 | 3.74  | 123.81      | 118.09   |
| 24  | K     | 206 | BCR  | C38-C26-C25 | -3.74 | 120.40      | 124.48   |
| 38  | Z     | 302 | LUT  | C31-C30-C29 | -3.74 | 122.03      | 127.28   |
| 38  | 3     | 302 | LUT  | C31-C30-C29 | -3.74 | 122.03      | 127.28   |
| 39  | Z     | 311 | CHL  | C3D-C4D-CHA | 3.74  | 114.23      | 108.54   |
| 39  | 6     | 315 | CHL  | CHA-C1A-C2A | -3.74 | 124.53      | 133.31   |
| 22  | 4     | 811 | CLA  | O2A-C1-C2   | 3.74  | 122.50      | 108.11   |
| 24  | J     | 104 | BCR  | C11-C10-C9  | -3.74 | 122.03      | 127.28   |
| 22  | 1     | 306 | CLA  | O2A-C1-C2   | 3.74  | 122.49      | 108.11   |
| 22  | 6     | 309 | CLA  | O2A-C1-C2   | 3.74  | 122.49      | 108.11   |
| 22  | Z     | 313 | CLA  | O2A-C1-C2   | 3.73  | 122.48      | 108.11   |
| 22  | 3     | 310 | CLA  | CAA-C2A-C3A | -3.73 | 102.92      | 113.00   |
| 22  | 9     | 306 | CLA  | O2A-C1-C2   | 3.73  | 122.44      | 108.11   |
| 22  | A     | 818 | CLA  | O2A-C1-C2   | 3.72  | 122.44      | 108.11   |
| 24  | 4     | 804 | BCR  | C2-C1-C6    | 3.72  | 115.85      | 110.44   |
| 24  | 5     | 304 | BCR  | C1-C6-C5    | -3.72 | 117.55      | 122.64   |
| 38  | Z     | 302 | LUT  | C26-C27-C28 | -3.72 | 118.79      | 124.58   |
| 22  | 3     | 310 | CLA  | C1-C2-C3    | -3.72 | 120.10      | 126.20   |
| 39  | 2     | 303 | CHL  | C1A-CHA-C4D | 3.72  | 125.19      | 118.98   |
| 22  | 8     | 313 | CLA  | C1-C2-C3    | -3.72 | 120.74      | 126.76   |
| 38  | 4     | 802 | LUT  | C31-C30-C29 | -3.72 | 122.06      | 127.28   |
| 24  | B     | 848 | BCR  | C15-C16-C17 | -3.72 | 115.91      | 123.52   |
| 22  | B     | 822 | CLA  | C1-C2-C3    | -3.72 | 120.11      | 126.20   |
| 27  | A     | 852 | DGA  | OG2-CB1-CB2 | 3.72  | 119.52      | 111.48   |
| 39  | 8     | 312 | CHL  | C3D-C4D-CHA | 3.72  | 114.19      | 108.54   |
| 22  | B     | 805 | CLA  | C1-C2-C3    | -3.72 | 120.11      | 126.20   |
| 22  | B     | 806 | CLA  | C1-C2-C3    | -3.71 | 120.11      | 126.20   |
| 24  | 4     | 804 | BCR  | C11-C10-C9  | -3.71 | 122.07      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 816 | CLA  | C1-C2-C3    | -3.71 | 120.12      | 126.20   |
| 24  | A     | 846 | BCR  | C15-C16-C17 | -3.71 | 115.93      | 123.52   |
| 39  | 6     | 316 | CHL  | C3D-C4D-CHA | 3.71  | 114.17      | 108.54   |
| 22  | 5     | 320 | CLA  | O2D-CGD-CBD | 3.70  | 117.71      | 111.23   |
| 24  | J     | 104 | BCR  | C15-C14-C13 | -3.70 | 122.09      | 127.28   |
| 22  | A     | 814 | CLA  | O2A-C1-C2   | 3.70  | 122.35      | 108.11   |
| 22  | 1     | 313 | CLA  | O2A-C1-C2   | 3.70  | 122.35      | 108.11   |
| 38  | 9     | 301 | LUT  | C26-C27-C28 | -3.69 | 118.83      | 124.58   |
| 22  | B     | 829 | CLA  | C1-C2-C3    | -3.69 | 120.15      | 126.20   |
| 22  | A     | 823 | CLA  | C1-C2-C3    | -3.69 | 120.16      | 126.20   |
| 25  | 4     | 821 | LHG  | O7-C7-C8    | 3.69  | 119.46      | 111.48   |
| 24  | A     | 844 | BCR  | C35-C13-C14 | -3.69 | 116.84      | 122.82   |
| 38  | 4     | 802 | LUT  | C21-C26-C27 | -3.68 | 108.59      | 112.83   |
| 39  | 8     | 315 | CHL  | C3D-C4D-CHA | 3.68  | 114.14      | 108.54   |
| 39  | 7     | 313 | CHL  | C3D-C4D-CHA | 3.68  | 114.14      | 108.54   |
| 39  | Z     | 311 | CHL  | C1-C2-C3    | -3.68 | 120.81      | 126.76   |
| 22  | A     | 815 | CLA  | C1-C2-C3    | -3.68 | 120.17      | 126.20   |
| 24  | L     | 204 | BCR  | C20-C21-C22 | -3.68 | 122.12      | 127.28   |
| 22  | 5     | 319 | CLA  | O2A-C1-C2   | 3.68  | 122.26      | 108.11   |
| 39  | 6     | 318 | CHL  | C3D-C4D-CHA | 3.68  | 114.13      | 108.54   |
| 38  | 7     | 302 | LUT  | C18-C5-C6   | -3.67 | 120.47      | 124.48   |
| 24  | F     | 303 | BCR  | C1-C6-C5    | -3.67 | 117.62      | 122.64   |
| 39  | 1     | 312 | CHL  | C3D-C4D-CHA | 3.67  | 114.12      | 108.54   |
| 24  | 5     | 304 | BCR  | C8-C7-C6    | -3.67 | 117.19      | 127.00   |
| 22  | 5     | 301 | CLA  | O2A-C1-C2   | 3.67  | 122.23      | 108.11   |
| 24  | B     | 847 | BCR  | C20-C21-C22 | -3.67 | 122.13      | 127.28   |
| 24  | J     | 104 | BCR  | C7-C8-C9    | -3.67 | 120.81      | 126.23   |
| 38  | 9     | 301 | LUT  | C18-C5-C6   | -3.67 | 120.48      | 124.48   |
| 22  | A     | 841 | CLA  | O2A-C1-C2   | 3.67  | 122.22      | 108.11   |
| 22  | B     | 813 | CLA  | O2A-C1-C2   | 3.66  | 122.20      | 108.11   |
| 38  | Z     | 301 | LUT  | C26-C27-C28 | -3.66 | 118.88      | 124.58   |
| 22  | 5     | 315 | CLA  | C1-C2-C3    | -3.66 | 120.20      | 126.20   |
| 38  | 1     | 302 | LUT  | C26-C27-C28 | -3.66 | 118.88      | 124.58   |
| 39  | 3     | 317 | CHL  | C3D-C4D-CHA | 3.66  | 114.10      | 108.54   |
| 22  | 3     | 311 | CLA  | C1-C2-C3    | -3.66 | 120.20      | 126.20   |
| 24  | G     | 203 | BCR  | C29-C30-C25 | 3.66  | 115.75      | 110.44   |
| 22  | B     | 842 | CLA  | C1-C2-C3    | -3.66 | 120.20      | 126.20   |
| 24  | 6     | 305 | BCR  | C29-C30-C25 | 3.66  | 115.75      | 110.44   |
| 22  | B     | 831 | CLA  | C1-C2-C3    | -3.65 | 120.21      | 126.20   |
| 38  | 9     | 302 | LUT  | C31-C30-C29 | -3.65 | 122.16      | 127.28   |
| 22  | 5     | 320 | CLA  | C2C-C1C-NC  | 3.65  | 113.82      | 109.98   |
| 39  | 6     | 316 | CHL  | C1A-CHA-C4D | 3.65  | 125.07      | 118.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 6     | 313 | CLA  | C1-C2-C3    | -3.65 | 120.22      | 126.20   |
| 24  | K     | 206 | BCR  | C27-C26-C25 | -3.65 | 117.78      | 122.70   |
| 24  | 5     | 305 | BCR  | C24-C23-C22 | -3.64 | 120.84      | 126.23   |
| 39  | 6     | 320 | CHL  | C3D-C4D-CHA | 3.64  | 114.08      | 108.54   |
| 24  | J     | 104 | BCR  | C16-C17-C18 | -3.64 | 122.17      | 127.28   |
| 22  | B     | 829 | CLA  | O2A-C1-C2   | 3.64  | 122.10      | 108.11   |
| 24  | B     | 849 | BCR  | C1-C6-C5    | -3.64 | 117.67      | 122.64   |
| 39  | Z     | 312 | CHL  | C3D-C4D-CHA | 3.64  | 114.07      | 108.54   |
| 22  | Z     | 303 | CLA  | C1-C2-C3    | -3.64 | 120.24      | 126.20   |
| 22  | A     | 810 | CLA  | O2A-C1-C2   | 3.64  | 122.10      | 108.11   |
| 38  | 5     | 302 | LUT  | C11-C10-C9  | -3.63 | 122.18      | 127.28   |
| 24  | K     | 206 | BCR  | C1-C6-C5    | -3.63 | 117.67      | 122.64   |
| 24  | B     | 849 | BCR  | C15-C16-C17 | -3.63 | 116.09      | 123.52   |
| 24  | B     | 845 | BCR  | C24-C23-C22 | -3.63 | 120.86      | 126.23   |
| 22  | 9     | 305 | CLA  | C1-C2-C3    | -3.63 | 120.25      | 126.20   |
| 39  | 4     | 813 | CHL  | C3D-C4D-CHA | 3.63  | 114.05      | 108.54   |
| 22  | A     | 817 | CLA  | O2A-C1-C2   | 3.62  | 122.06      | 108.11   |
| 38  | 3     | 302 | LUT  | C15-C14-C13 | -3.62 | 122.20      | 127.28   |
| 25  | 8     | 317 | LHG  | O7-C7-C8    | 3.62  | 119.32      | 111.48   |
| 24  | 3     | 305 | BCR  | C11-C12-C13 | -3.62 | 116.43      | 126.36   |
| 22  | 9     | 310 | CLA  | O2D-CGD-O1D | -3.62 | 116.80      | 123.85   |
| 41  | 7     | 319 | 3PH  | O21-C21-C22 | 3.62  | 119.30      | 111.48   |
| 22  | F     | 302 | CLA  | C1-C2-C3    | -3.62 | 120.27      | 126.20   |
| 24  | B     | 844 | BCR  | C27-C26-C25 | -3.62 | 117.82      | 122.70   |
| 22  | 3     | 318 | CLA  | C1-C2-C3    | -3.61 | 120.28      | 126.20   |
| 22  | 7     | 307 | CLA  | O2A-C1-C2   | 3.61  | 122.00      | 108.11   |
| 39  | 6     | 315 | CHL  | C1A-CHA-C4D | 3.61  | 125.00      | 118.98   |
| 22  | 6     | 301 | CLA  | C1-C2-C3    | -3.60 | 120.30      | 126.20   |
| 24  | A     | 846 | BCR  | C29-C30-C25 | 3.60  | 115.67      | 110.44   |
| 39  | 4     | 819 | CHL  | C3D-C4D-CHA | 3.60  | 114.01      | 108.54   |
| 24  | 6     | 306 | BCR  | C20-C21-C22 | -3.60 | 122.23      | 127.28   |
| 22  | 5     | 322 | CLA  | O2A-C1-C2   | 3.59  | 121.94      | 108.11   |
| 24  | 5     | 304 | BCR  | C11-C12-C13 | -3.59 | 116.51      | 126.36   |
| 22  | 6     | 319 | CLA  | O2A-C1-C2   | 3.59  | 121.94      | 108.11   |
| 22  | 4     | 808 | CLA  | C1-C2-C3    | -3.59 | 120.31      | 126.20   |
| 24  | A     | 845 | BCR  | C24-C23-C22 | -3.59 | 120.92      | 126.23   |
| 22  | 5     | 309 | CLA  | CAA-C2A-C3A | -3.59 | 103.30      | 113.00   |
| 39  | 1     | 312 | CHL  | C1A-CHA-C4D | 3.59  | 124.97      | 118.98   |
| 22  | A     | 838 | CLA  | O2A-C1-C2   | 3.58  | 121.90      | 108.11   |
| 24  | B     | 847 | BCR  | C15-C16-C17 | -3.58 | 116.19      | 123.52   |
| 24  | F     | 303 | BCR  | C15-C14-C13 | -3.58 | 122.26      | 127.28   |
| 22  | B     | 841 | CLA  | O2A-C1-C2   | 3.58  | 121.88      | 108.11   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | 6     | 318 | CHL  | C1A-CHA-C4D | 3.58  | 124.95      | 118.98   |
| 39  | 5     | 321 | CHL  | C3D-C4D-CHA | 3.57  | 113.97      | 108.54   |
| 22  | 3     | 315 | CLA  | O2D-CGD-O1D | -3.57 | 116.89      | 123.85   |
| 24  | B     | 853 | BCR  | C4-C5-C6    | -3.57 | 117.88      | 122.70   |
| 22  | A     | 822 | CLA  | O2A-C1-C2   | 3.57  | 121.85      | 108.11   |
| 22  | L     | 202 | CLA  | C1-C2-C3    | -3.57 | 120.35      | 126.20   |
| 22  | 6     | 312 | CLA  | C1-C2-C3    | -3.57 | 120.35      | 126.20   |
| 22  | A     | 829 | CLA  | O2A-C1-C2   | 3.57  | 121.83      | 108.11   |
| 22  | B     | 809 | CLA  | O2A-C1-C2   | 3.57  | 121.83      | 108.11   |
| 22  | 1     | 310 | CLA  | O2A-C1-C2   | 3.56  | 121.83      | 108.11   |
| 22  | 1     | 304 | CLA  | C1-C2-C3    | -3.56 | 120.36      | 126.20   |
| 22  | 9     | 307 | CLA  | C1-C2-C3    | -3.56 | 120.36      | 126.20   |
| 39  | Z     | 312 | CHL  | C1A-CHA-C4D | 3.56  | 124.93      | 118.98   |
| 22  | 6     | 301 | CLA  | O2A-C1-C2   | 3.56  | 121.82      | 108.11   |
| 22  | 8     | 307 | CLA  | O2A-C1-C2   | 3.56  | 121.80      | 108.11   |
| 22  | L     | 201 | CLA  | C1-C2-C3    | -3.56 | 120.37      | 126.20   |
| 39  | 4     | 816 | CHL  | C3D-C4D-CHA | 3.55  | 113.94      | 108.54   |
| 38  | 3     | 302 | LUT  | C26-C27-C28 | -3.55 | 119.05      | 124.58   |
| 39  | 5     | 316 | CHL  | C1A-CHA-C4D | 3.55  | 124.91      | 118.98   |
| 22  | K     | 205 | CLA  | O2A-C1-C2   | 3.55  | 121.78      | 108.11   |
| 22  | A     | 833 | CLA  | C1-C2-C3    | -3.55 | 120.38      | 126.20   |
| 38  | 7     | 302 | LUT  | C21-C26-C27 | -3.55 | 108.74      | 112.83   |
| 38  | 9     | 302 | LUT  | C18-C5-C6   | -3.55 | 120.61      | 124.48   |
| 22  | 1     | 308 | CLA  | O2A-C1-C2   | 3.55  | 121.76      | 108.11   |
| 31  | B     | 852 | DGD  | O2G-C1B-C2B | 3.55  | 119.16      | 111.48   |
| 22  | F     | 304 | CLA  | O2A-C1-C2   | 3.55  | 121.75      | 108.11   |
| 22  | A     | 830 | CLA  | O2A-C1-C2   | 3.54  | 121.74      | 108.11   |
| 22  | 4     | 806 | CLA  | O2A-C1-C2   | 3.54  | 121.74      | 108.11   |
| 22  | 5     | 310 | CLA  | O2A-C1-C2   | 3.54  | 121.74      | 108.11   |
| 39  | 4     | 814 | CHL  | C1-C2-C3    | -3.54 | 121.03      | 126.76   |
| 22  | G     | 201 | CLA  | O2A-C1-C2   | 3.54  | 121.72      | 108.11   |
| 39  | 8     | 312 | CHL  | C1A-CHA-C4D | 3.54  | 124.88      | 118.98   |
| 22  | B     | 815 | CLA  | O2A-C1-C2   | 3.53  | 121.71      | 108.11   |
| 24  | B     | 846 | BCR  | C38-C26-C25 | -3.53 | 120.63      | 124.48   |
| 24  | B     | 848 | BCR  | C15-C14-C13 | -3.53 | 122.32      | 127.28   |
| 22  | A     | 839 | CLA  | C1-C2-C3    | -3.53 | 120.41      | 126.20   |
| 24  | 3     | 306 | BCR  | C33-C5-C6   | -3.53 | 120.63      | 124.48   |
| 39  | 9     | 314 | CHL  | C1A-CHA-C4D | 3.53  | 124.87      | 118.98   |
| 24  | B     | 844 | BCR  | C1-C6-C5    | -3.53 | 117.81      | 122.64   |
| 22  | 9     | 303 | CLA  | CAA-C2A-C3A | -3.53 | 103.47      | 113.00   |
| 32  | F     | 306 | RRX  | C16-C17-C18 | -3.53 | 122.33      | 127.28   |
| 39  | 4     | 813 | CHL  | C1A-CHA-C4D | 3.52  | 124.86      | 118.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 38  | 6     | 303 | LUT  | C1-C6-C5    | -3.52 | 117.83      | 122.64   |
| 38  | 8     | 303 | LUT  | C7-C8-C9    | -3.52 | 121.03      | 126.23   |
| 22  | 8     | 309 | CLA  | O2A-C1-C2   | 3.52  | 121.64      | 108.11   |
| 38  | 5     | 302 | LUT  | C21-C26-C27 | -3.51 | 108.79      | 112.83   |
| 22  | 8     | 306 | CLA  | C1-C2-C3    | -3.51 | 120.44      | 126.20   |
| 24  | 3     | 304 | BCR  | C24-C23-C22 | -3.51 | 121.04      | 126.23   |
| 24  | A     | 856 | BCR  | C4-C5-C6    | -3.51 | 117.96      | 122.70   |
| 22  | B     | 828 | CLA  | O2A-C1-C2   | 3.51  | 121.61      | 108.11   |
| 38  | Z     | 302 | LUT  | C1-C6-C5    | -3.50 | 117.85      | 122.64   |
| 39  | 3     | 317 | CHL  | C1A-CHA-C4D | 3.50  | 124.83      | 118.98   |
| 22  | 3     | 308 | CLA  | O2A-C1-C2   | 3.50  | 121.58      | 108.11   |
| 22  | B     | 806 | CLA  | O2A-C1-C2   | 3.50  | 121.58      | 108.11   |
| 22  | Z     | 314 | CLA  | O2A-C1-C2   | 3.50  | 121.58      | 108.11   |
| 22  | 1     | 316 | CLA  | C2C-C1C-NC  | 3.50  | 113.66      | 109.98   |
| 22  | B     | 814 | CLA  | O2A-C1-C2   | 3.50  | 121.58      | 108.11   |
| 22  | 6     | 310 | CLA  | C1-C2-C3    | -3.50 | 120.47      | 126.20   |
| 22  | F     | 301 | CLA  | O2A-C1-C2   | 3.50  | 121.57      | 108.11   |
| 24  | B     | 849 | BCR  | C30-C25-C26 | -3.50 | 117.86      | 122.64   |
| 22  | Z     | 308 | CLA  | O2A-C1-C2   | 3.50  | 121.56      | 108.11   |
| 22  | B     | 811 | CLA  | O2A-C1-C2   | 3.50  | 121.56      | 108.11   |
| 22  | B     | 833 | CLA  | C1-C2-C3    | -3.49 | 120.47      | 126.20   |
| 22  | 9     | 307 | CLA  | O2A-C1-C2   | 3.49  | 121.54      | 108.11   |
| 22  | B     | 830 | CLA  | O2A-C1-C2   | 3.49  | 121.54      | 108.11   |
| 22  | B     | 831 | CLA  | O2A-C1-C2   | 3.49  | 121.53      | 108.11   |
| 22  | B     | 837 | CLA  | O2A-C1-C2   | 3.49  | 121.53      | 108.11   |
| 22  | B     | 835 | CLA  | O2A-C1-C2   | 3.49  | 121.52      | 108.11   |
| 39  | 4     | 816 | CHL  | C1A-CHA-C4D | 3.49  | 124.80      | 118.98   |
| 38  | 5     | 303 | LUT  | C1-C6-C5    | -3.48 | 117.87      | 122.64   |
| 22  | A     | 840 | CLA  | O2A-C1-C2   | 3.48  | 121.52      | 108.11   |
| 24  | G     | 203 | BCR  | C11-C12-C13 | -3.48 | 116.82      | 126.36   |
| 24  | A     | 848 | BCR  | C33-C5-C4   | 3.48  | 121.02      | 113.60   |
| 22  | B     | 839 | CLA  | O2A-C1-C2   | 3.48  | 121.49      | 108.11   |
| 22  | B     | 823 | CLA  | C1-C2-C3    | -3.47 | 120.50      | 126.20   |
| 38  | 3     | 303 | LUT  | C31-C30-C29 | -3.47 | 122.41      | 127.28   |
| 22  | 3     | 310 | CLA  | O2A-C1-C2   | 3.47  | 121.47      | 108.11   |
| 22  | A     | 855 | CLA  | C1-C2-C3    | -3.47 | 120.52      | 126.20   |
| 38  | 9     | 302 | LUT  | C11-C10-C9  | -3.47 | 122.42      | 127.28   |
| 22  | 2     | 301 | CLA  | O2A-C1-C2   | 3.46  | 121.44      | 108.11   |
| 24  | 4     | 804 | BCR  | C7-C8-C9    | -3.46 | 121.11      | 126.23   |
| 22  | 7     | 309 | CLA  | O2A-C1-C2   | 3.46  | 121.43      | 108.11   |
| 22  | 7     | 308 | CLA  | O2A-C1-C2   | 3.46  | 121.43      | 108.11   |
| 22  | A     | 810 | CLA  | C1-C2-C3    | -3.46 | 120.53      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 824 | CLA  | O2A-C1-C2   | 3.46  | 121.41      | 108.11   |
| 22  | 6     | 313 | CLA  | O2A-C1-C2   | 3.46  | 121.41      | 108.11   |
| 22  | B     | 816 | CLA  | O2A-C1-C2   | 3.46  | 121.41      | 108.11   |
| 22  | A     | 827 | CLA  | C1-C2-C3    | -3.46 | 120.53      | 126.20   |
| 22  | 3     | 318 | CLA  | O2A-C1-C2   | 3.45  | 121.40      | 108.11   |
| 22  | B     | 812 | CLA  | O2A-C1-C2   | 3.45  | 121.40      | 108.11   |
| 38  | 4     | 803 | LUT  | C31-C30-C29 | -3.45 | 122.44      | 127.28   |
| 22  | 6     | 311 | CLA  | O2A-C1-C2   | 3.45  | 121.40      | 108.11   |
| 22  | 7     | 305 | CLA  | O2A-C1-C2   | 3.45  | 121.39      | 108.11   |
| 22  | A     | 812 | CLA  | C1-C2-C3    | -3.45 | 120.54      | 126.20   |
| 24  | B     | 848 | BCR  | C11-C12-C13 | -3.45 | 116.90      | 126.36   |
| 22  | A     | 826 | CLA  | O2A-C1-C2   | 3.45  | 121.39      | 108.11   |
| 22  | B     | 810 | CLA  | O2A-C1-C2   | 3.45  | 121.39      | 108.11   |
| 38  | 1     | 302 | LUT  | C18-C5-C4   | 3.45  | 120.77      | 114.42   |
| 38  | 4     | 802 | LUT  | C18-C5-C6   | -3.45 | 120.72      | 124.48   |
| 22  | 7     | 317 | CLA  | O2A-C1-C2   | 3.45  | 121.38      | 108.11   |
| 22  | 5     | 308 | CLA  | O2A-C1-C2   | 3.45  | 121.38      | 108.11   |
| 22  | L     | 203 | CLA  | O2A-C1-C2   | 3.45  | 121.37      | 108.11   |
| 21  | A     | 801 | CL0  | O2A-C1-C2   | 3.45  | 121.37      | 108.11   |
| 22  | B     | 811 | CLA  | C1-C2-C3    | -3.44 | 120.55      | 126.20   |
| 22  | 3     | 315 | CLA  | C3B-C4B-NB  | -3.44 | 107.46      | 110.53   |
| 22  | Z     | 305 | CLA  | C1-C2-C3    | -3.44 | 120.56      | 126.20   |
| 22  | A     | 819 | CLA  | C1-C2-C3    | -3.44 | 120.56      | 126.20   |
| 38  | 5     | 303 | LUT  | C31-C30-C29 | -3.44 | 122.45      | 127.28   |
| 22  | 3     | 322 | CLA  | O2A-C1-C2   | 3.44  | 121.34      | 108.11   |
| 39  | Z     | 311 | CHL  | C1A-CHA-C4D | 3.44  | 124.72      | 118.98   |
| 39  | 5     | 321 | CHL  | C1A-CHA-C4D | 3.44  | 124.71      | 118.98   |
| 22  | 1     | 308 | CLA  | C1D-ND-C4D  | -3.43 | 103.90      | 106.31   |
| 22  | 6     | 314 | CLA  | C1-C2-C3    | -3.43 | 120.57      | 126.20   |
| 22  | A     | 842 | CLA  | O2A-C1-C2   | 3.43  | 121.31      | 108.11   |
| 24  | A     | 848 | BCR  | C38-C26-C25 | -3.43 | 120.74      | 124.48   |
| 22  | A     | 837 | CLA  | C1-C2-C3    | -3.43 | 120.58      | 126.20   |
| 24  | 5     | 305 | BCR  | C4-C5-C6    | -3.42 | 118.08      | 122.70   |
| 22  | 6     | 322 | CLA  | O2A-C1-C2   | 3.42  | 121.28      | 108.11   |
| 22  | B     | 819 | CLA  | C1-C2-C3    | -3.42 | 120.59      | 126.20   |
| 22  | 4     | 815 | CLA  | O2A-C1-C2   | 3.42  | 121.27      | 108.11   |
| 24  | B     | 846 | BCR  | C38-C26-C27 | 3.42  | 120.89      | 113.60   |
| 38  | 3     | 303 | LUT  | C26-C27-C28 | -3.41 | 119.27      | 124.58   |
| 22  | B     | 826 | CLA  | O2A-C1-C2   | 3.41  | 121.25      | 108.11   |
| 24  | G     | 203 | BCR  | C24-C23-C22 | -3.41 | 121.19      | 126.23   |
| 24  | 3     | 305 | BCR  | C20-C21-C22 | -3.41 | 122.50      | 127.28   |
| 22  | 5     | 301 | CLA  | C1-C2-C3    | -3.41 | 120.61      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 6     | 317 | CLA  | O2A-C1-C2   | 3.41  | 121.22      | 108.11   |
| 22  | 9     | 309 | CLA  | O2A-C1-C2   | 3.40  | 121.21      | 108.11   |
| 22  | A     | 815 | CLA  | O2A-C1-C2   | 3.40  | 121.20      | 108.11   |
| 22  | A     | 855 | CLA  | O2A-C1-C2   | 3.40  | 121.19      | 108.11   |
| 22  | B     | 818 | CLA  | O2A-C1-C2   | 3.40  | 121.19      | 108.11   |
| 22  | 9     | 313 | CLA  | O2A-C1-C2   | 3.40  | 121.18      | 108.11   |
| 39  | 5     | 317 | CHL  | C1A-CHA-C4D | 3.40  | 124.65      | 118.98   |
| 22  | 4     | 807 | CLA  | O2A-C1-C2   | 3.40  | 121.18      | 108.11   |
| 22  | A     | 834 | CLA  | C1-C2-C3    | -3.39 | 120.64      | 126.20   |
| 39  | 4     | 814 | CHL  | C1A-CHA-C4D | 3.39  | 124.64      | 118.98   |
| 22  | 8     | 308 | CLA  | O2A-C1-C2   | 3.39  | 121.16      | 108.11   |
| 22  | A     | 805 | CLA  | C1-C2-C3    | -3.39 | 120.64      | 126.20   |
| 22  | 6     | 312 | CLA  | O2A-C1-C2   | 3.39  | 121.16      | 108.11   |
| 32  | F     | 306 | RRX  | C24-C23-C22 | -3.39 | 121.22      | 126.23   |
| 22  | A     | 839 | CLA  | O2A-C1-C2   | 3.39  | 121.14      | 108.11   |
| 39  | 8     | 301 | CHL  | C1A-CHA-C4D | 3.39  | 124.63      | 118.98   |
| 22  | B     | 819 | CLA  | O2A-C1-C2   | 3.38  | 121.13      | 108.11   |
| 39  | 7     | 313 | CHL  | C1A-CHA-C4D | 3.38  | 124.63      | 118.98   |
| 22  | 9     | 303 | CLA  | C1D-ND-C4D  | -3.38 | 103.94      | 106.31   |
| 24  | 6     | 305 | BCR  | C15-C16-C17 | -3.38 | 116.60      | 123.52   |
| 38  | 1     | 303 | LUT  | C1-C6-C5    | -3.38 | 118.01      | 122.64   |
| 22  | A     | 816 | CLA  | O2A-C1-C2   | 3.38  | 121.12      | 108.11   |
| 22  | 1     | 308 | CLA  | C3B-C4B-NB  | -3.38 | 107.51      | 110.53   |
| 24  | A     | 847 | BCR  | C1-C6-C5    | -3.38 | 118.02      | 122.64   |
| 22  | Z     | 316 | CLA  | O2A-C1-C2   | 3.38  | 121.12      | 108.11   |
| 38  | 7     | 301 | LUT  | C21-C26-C27 | -3.38 | 108.94      | 112.83   |
| 22  | A     | 835 | CLA  | O2A-C1-C2   | 3.38  | 121.11      | 108.11   |
| 24  | A     | 848 | BCR  | C16-C17-C18 | -3.37 | 122.55      | 127.28   |
| 22  | 3     | 319 | CLA  | O2A-C1-C2   | 3.37  | 121.09      | 108.11   |
| 38  | 9     | 302 | LUT  | C21-C26-C27 | -3.37 | 108.95      | 112.83   |
| 22  | B     | 840 | CLA  | C1-C2-C3    | -3.37 | 120.67      | 126.20   |
| 22  | B     | 817 | CLA  | C1-C2-C3    | -3.37 | 120.68      | 126.20   |
| 22  | 1     | 314 | CLA  | O2A-C1-C2   | 3.37  | 121.06      | 108.11   |
| 39  | 4     | 813 | CHL  | C1-C2-C3    | -3.36 | 121.32      | 126.76   |
| 24  | B     | 853 | BCR  | C30-C25-C26 | -3.36 | 118.04      | 122.64   |
| 22  | A     | 809 | CLA  | O2A-C1-C2   | 3.36  | 121.02      | 108.11   |
| 24  | B     | 846 | BCR  | C1-C6-C5    | -3.35 | 118.06      | 122.64   |
| 22  | B     | 808 | CLA  | O2A-C1-C2   | 3.35  | 120.99      | 108.11   |
| 24  | 6     | 305 | BCR  | C11-C12-C13 | -3.35 | 117.19      | 126.36   |
| 22  | B     | 812 | CLA  | C1-C2-C3    | -3.35 | 120.71      | 126.20   |
| 22  | 6     | 322 | CLA  | C1-C2-C3    | -3.35 | 120.72      | 126.20   |
| 22  | B     | 840 | CLA  | O2A-C1-C2   | 3.34  | 120.98      | 108.11   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | 3     | 305 | BCR  | C15-C14-C13 | -3.34 | 122.59      | 127.28   |
| 38  | Z     | 301 | LUT  | C18-C5-C4   | 3.34  | 120.57      | 114.42   |
| 22  | B     | 805 | CLA  | O2A-C1-C2   | 3.34  | 120.97      | 108.11   |
| 22  | A     | 803 | CLA  | O2A-C1-C2   | 3.34  | 120.96      | 108.11   |
| 22  | 7     | 314 | CLA  | O2A-C1-C2   | 3.34  | 120.96      | 108.11   |
| 22  | 3     | 312 | CLA  | O2A-C1-C2   | 3.34  | 120.96      | 108.11   |
| 22  | Z     | 307 | CLA  | O2A-C1-C2   | 3.34  | 120.95      | 108.11   |
| 22  | A     | 836 | CLA  | C1-C2-C3    | -3.34 | 120.73      | 126.20   |
| 22  | L     | 202 | CLA  | O2A-C1-C2   | 3.33  | 120.94      | 108.11   |
| 22  | 6     | 314 | CLA  | O2A-C1-C2   | 3.33  | 120.94      | 108.11   |
| 38  | 8     | 302 | LUT  | C15-C14-C13 | -3.33 | 122.60      | 127.28   |
| 24  | A     | 848 | BCR  | C38-C26-C27 | 3.33  | 120.70      | 113.60   |
| 39  | 5     | 321 | CHL  | CMA-C3A-C4A | 3.33  | 121.79      | 114.61   |
| 22  | 6     | 302 | CLA  | O2A-C1-C2   | 3.33  | 120.93      | 108.11   |
| 24  | 4     | 804 | BCR  | C30-C25-C26 | -3.33 | 118.08      | 122.64   |
| 22  | 9     | 303 | CLA  | C3B-C4B-NB  | -3.33 | 107.56      | 110.53   |
| 38  | 5     | 302 | LUT  | C35-C15-C14 | -3.33 | 116.71      | 123.52   |
| 22  | B     | 827 | CLA  | O2A-C1-C2   | 3.33  | 120.90      | 108.11   |
| 24  | B     | 845 | BCR  | C20-C21-C22 | -3.32 | 122.62      | 127.28   |
| 22  | 1     | 307 | CLA  | O2A-C1-C2   | 3.32  | 120.90      | 108.11   |
| 22  | 3     | 319 | CLA  | C1-C2-C3    | -3.32 | 120.75      | 126.20   |
| 36  | J     | 105 | C7Z  | C31-C32-C33 | -3.32 | 117.26      | 126.36   |
| 38  | 8     | 303 | LUT  | C15-C14-C13 | -3.31 | 122.63      | 127.28   |
| 24  | 6     | 306 | BCR  | C1-C6-C5    | -3.31 | 118.11      | 122.64   |
| 22  | 1     | 314 | CLA  | C1-C2-C3    | -3.31 | 120.77      | 126.20   |
| 24  | 3     | 304 | BCR  | C34-C9-C10  | -3.31 | 117.45      | 122.82   |
| 38  | 8     | 302 | LUT  | C11-C10-C9  | -3.31 | 122.64      | 127.28   |
| 22  | 7     | 306 | CLA  | O2A-C1-C2   | 3.30  | 120.82      | 108.11   |
| 22  | Z     | 314 | CLA  | C1-C2-C3    | -3.30 | 120.78      | 126.20   |
| 22  | Z     | 309 | CLA  | O2A-C1-C2   | 3.30  | 120.82      | 108.11   |
| 22  | 3     | 313 | CLA  | C1-C2-C3    | -3.30 | 120.79      | 126.20   |
| 22  | 6     | 308 | CLA  | O2A-C1-C2   | 3.30  | 120.80      | 108.11   |
| 24  | B     | 844 | BCR  | C30-C25-C26 | -3.30 | 118.13      | 122.64   |
| 39  | Z     | 311 | CHL  | C3C-C4C-NC  | -3.29 | 106.60      | 114.65   |
| 22  | L     | 201 | CLA  | O2A-C1-C2   | 3.29  | 120.78      | 108.11   |
| 24  | 3     | 306 | BCR  | C24-C23-C22 | -3.29 | 121.36      | 126.23   |
| 22  | B     | 821 | CLA  | O2A-C1-C2   | 3.29  | 120.77      | 108.11   |
| 22  | A     | 805 | CLA  | O2A-C1-C2   | 3.29  | 120.77      | 108.11   |
| 22  | K     | 203 | CLA  | O2A-C1-C2   | 3.29  | 120.76      | 108.11   |
| 22  | A     | 825 | CLA  | O2A-C1-C2   | 3.29  | 120.76      | 108.11   |
| 22  | B     | 825 | CLA  | O2A-C1-C2   | 3.29  | 120.75      | 108.11   |
| 22  | 3     | 316 | CLA  | C1-C2-C3    | -3.28 | 120.81      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 822 | CLA  | O2A-C1-C2   | 3.28  | 120.74      | 108.11   |
| 24  | B     | 845 | BCR  | C33-C5-C4   | 3.28  | 120.59      | 113.60   |
| 24  | A     | 848 | BCR  | C24-C23-C22 | -3.28 | 121.39      | 126.23   |
| 38  | 9     | 302 | LUT  | C7-C8-C9    | -3.28 | 121.39      | 126.23   |
| 22  | K     | 205 | CLA  | C2C-C1C-NC  | 3.28  | 113.42      | 109.98   |
| 22  | 4     | 805 | CLA  | CMA-C3A-C4A | 3.27  | 120.57      | 111.77   |
| 36  | 5     | 306 | C7Z  | C21-C26-C25 | -3.27 | 118.16      | 122.64   |
| 24  | 8     | 304 | BCR  | C38-C26-C27 | 3.27  | 120.57      | 113.60   |
| 22  | 6     | 307 | CLA  | O2A-C1-C2   | 3.27  | 120.69      | 108.11   |
| 22  | 4     | 810 | CLA  | O2A-C1-C2   | 3.27  | 120.69      | 108.11   |
| 22  | 9     | 308 | CLA  | O2A-C1-C2   | 3.27  | 120.69      | 108.11   |
| 24  | L     | 204 | BCR  | C11-C10-C9  | -3.27 | 122.70      | 127.28   |
| 38  | 8     | 302 | LUT  | C7-C8-C9    | -3.27 | 121.40      | 126.23   |
| 22  | A     | 834 | CLA  | O2A-C1-C2   | 3.27  | 120.68      | 108.11   |
| 22  | 7     | 310 | CLA  | O2A-C1-C2   | 3.26  | 120.67      | 108.11   |
| 24  | G     | 203 | BCR  | C7-C8-C9    | -3.26 | 121.41      | 126.23   |
| 22  | 4     | 811 | CLA  | C1-C2-C3    | -3.26 | 120.86      | 126.20   |
| 22  | B     | 842 | CLA  | O2A-C1-C2   | 3.26  | 120.65      | 108.11   |
| 22  | Z     | 305 | CLA  | O2A-C1-C2   | 3.26  | 120.64      | 108.11   |
| 22  | 9     | 303 | CLA  | O2A-CGA-CBA | 3.25  | 121.76      | 111.83   |
| 22  | A     | 823 | CLA  | C3B-C4B-NB  | -3.25 | 107.63      | 110.53   |
| 22  | 1     | 304 | CLA  | O2A-C1-C2   | 3.25  | 120.62      | 108.11   |
| 24  | A     | 844 | BCR  | C4-C5-C6    | -3.25 | 118.31      | 122.70   |
| 22  | A     | 819 | CLA  | O2A-C1-C2   | 3.25  | 120.61      | 108.11   |
| 22  | A     | 813 | CLA  | C1-C2-C3    | -3.25 | 120.88      | 126.20   |
| 22  | A     | 854 | CLA  | O2A-C1-C2   | 3.25  | 120.60      | 108.11   |
| 22  | B     | 833 | CLA  | O2A-C1-C2   | 3.25  | 120.60      | 108.11   |
| 39  | 2     | 303 | CHL  | C1-C2-C3    | -3.24 | 121.51      | 126.76   |
| 22  | A     | 833 | CLA  | O2A-C1-C2   | 3.24  | 120.59      | 108.11   |
| 22  | A     | 811 | CLA  | C1-C2-C3    | -3.24 | 120.89      | 126.20   |
| 22  | 5     | 318 | CLA  | O2A-C1-C2   | 3.24  | 120.57      | 108.11   |
| 22  | B     | 808 | CLA  | C1-C2-C3    | -3.24 | 120.89      | 126.20   |
| 22  | 7     | 315 | CLA  | O2A-C1-C2   | 3.24  | 120.57      | 108.11   |
| 22  | 6     | 310 | CLA  | O2A-C1-C2   | 3.24  | 120.57      | 108.11   |
| 22  | 7     | 312 | CLA  | O2A-C1-C2   | 3.24  | 120.56      | 108.11   |
| 22  | B     | 834 | CLA  | O2A-C1-C2   | 3.24  | 120.56      | 108.11   |
| 39  | 5     | 317 | CHL  | C1-C2-C3    | -3.24 | 121.53      | 126.76   |
| 22  | B     | 814 | CLA  | C1-C2-C3    | -3.24 | 120.89      | 126.20   |
| 24  | K     | 206 | BCR  | C38-C26-C27 | 3.23  | 120.49      | 113.60   |
| 22  | 7     | 322 | CLA  | O2A-C1-C2   | 3.23  | 120.55      | 108.11   |
| 22  | A     | 817 | CLA  | CMA-C3A-C4A | 3.23  | 120.46      | 111.77   |
| 22  | A     | 806 | CLA  | O2A-C1-C2   | 3.23  | 120.54      | 108.11   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | K     | 205 | CLA  | C1-C2-C3    | -3.23 | 120.91      | 126.20   |
| 24  | G     | 203 | BCR  | C8-C7-C6    | -3.23 | 118.37      | 127.00   |
| 38  | 9     | 301 | LUT  | C15-C14-C13 | -3.23 | 122.75      | 127.28   |
| 22  | 5     | 326 | CLA  | C1-C2-C3    | -3.23 | 120.91      | 126.20   |
| 22  | A     | 854 | CLA  | C1-C2-C3    | -3.22 | 120.92      | 126.20   |
| 38  | 8     | 302 | LUT  | C31-C30-C29 | -3.22 | 122.76      | 127.28   |
| 22  | A     | 823 | CLA  | O2A-C1-C2   | 3.22  | 120.50      | 108.11   |
| 22  | 8     | 313 | CLA  | O2A-C1-C2   | 3.22  | 120.50      | 108.11   |
| 38  | 3     | 303 | LUT  | C1-C6-C5    | -3.22 | 118.24      | 122.64   |
| 22  | 8     | 306 | CLA  | O2A-C1-C2   | 3.22  | 120.49      | 108.11   |
| 24  | B     | 844 | BCR  | C24-C23-C22 | -3.22 | 121.48      | 126.23   |
| 24  | 8     | 304 | BCR  | C38-C26-C25 | -3.22 | 120.97      | 124.48   |
| 24  | A     | 846 | BCR  | C27-C26-C25 | -3.21 | 118.36      | 122.70   |
| 24  | 8     | 304 | BCR  | C27-C26-C25 | -3.21 | 118.36      | 122.70   |
| 22  | 8     | 311 | CLA  | O2A-C1-C2   | 3.21  | 120.48      | 108.11   |
| 38  | 8     | 303 | LUT  | C31-C30-C29 | -3.21 | 122.77      | 127.28   |
| 24  | B     | 849 | BCR  | C33-C5-C6   | -3.21 | 120.98      | 124.48   |
| 22  | Z     | 303 | CLA  | O2A-C1-C2   | 3.21  | 120.46      | 108.11   |
| 22  | 3     | 313 | CLA  | C1D-ND-C4D  | -3.21 | 104.06      | 106.31   |
| 38  | 6     | 304 | LUT  | C1-C6-C5    | -3.21 | 118.25      | 122.64   |
| 22  | 5     | 312 | CLA  | O2A-C1-C2   | 3.21  | 120.46      | 108.11   |
| 39  | 3     | 317 | CHL  | C3C-C4C-NC  | -3.21 | 106.81      | 114.65   |
| 22  | A     | 837 | CLA  | O2A-C1-C2   | 3.21  | 120.44      | 108.11   |
| 22  | A     | 821 | CLA  | O2A-C1-C2   | 3.20  | 120.43      | 108.11   |
| 22  | B     | 801 | CLA  | O2A-C1-C2   | 3.20  | 120.43      | 108.11   |
| 24  | 5     | 304 | BCR  | C15-C16-C17 | -3.20 | 116.97      | 123.52   |
| 24  | 5     | 305 | BCR  | C36-C18-C19 | 3.20  | 122.97      | 118.09   |
| 22  | 5     | 311 | CLA  | O2A-C1-C2   | 3.20  | 120.42      | 108.11   |
| 22  | 9     | 305 | CLA  | O2A-C1-C2   | 3.20  | 120.42      | 108.11   |
| 22  | A     | 802 | CLA  | C1-C2-C3    | -3.20 | 120.96      | 126.20   |
| 22  | 5     | 315 | CLA  | O2A-C1-C2   | 3.20  | 120.41      | 108.11   |
| 22  | 9     | 310 | CLA  | C3B-C4B-NB  | -3.20 | 107.68      | 110.53   |
| 22  | A     | 808 | CLA  | O2A-C1-C2   | 3.19  | 120.40      | 108.11   |
| 22  | 4     | 808 | CLA  | O2A-C1-C2   | 3.19  | 120.40      | 108.11   |
| 22  | A     | 823 | CLA  | C1D-ND-C4D  | -3.19 | 104.07      | 106.31   |
| 22  | A     | 811 | CLA  | O2A-C1-C2   | 3.19  | 120.38      | 108.11   |
| 22  | 5     | 320 | CLA  | C1-C2-C3    | -3.19 | 121.60      | 126.76   |
| 24  | A     | 848 | BCR  | C20-C19-C18 | -3.19 | 117.62      | 126.36   |
| 22  | A     | 811 | CLA  | C3B-C4B-NB  | -3.19 | 107.68      | 110.53   |
| 24  | A     | 848 | BCR  | C33-C5-C6   | -3.19 | 121.01      | 124.48   |
| 22  | A     | 831 | CLA  | O2A-C1-C2   | 3.19  | 120.36      | 108.11   |
| 39  | 8     | 301 | CHL  | C3C-C4C-NC  | -3.18 | 106.87      | 114.65   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 813 | CLA  | O2A-C1-C2   | 3.18  | 120.35      | 108.11   |
| 22  | 3     | 316 | CLA  | O2A-C1-C2   | 3.18  | 120.34      | 108.11   |
| 22  | B     | 815 | CLA  | CMA-C3A-C4A | 3.18  | 120.31      | 111.77   |
| 22  | A     | 828 | CLA  | O2A-C1-C2   | 3.18  | 120.34      | 108.11   |
| 22  | B     | 832 | CLA  | O2A-C1-C2   | 3.18  | 120.33      | 108.11   |
| 22  | 3     | 311 | CLA  | O2A-C1-C2   | 3.18  | 120.33      | 108.11   |
| 22  | 9     | 305 | CLA  | CMA-C3A-C4A | 3.18  | 120.31      | 111.77   |
| 22  | 5     | 320 | CLA  | O2A-C1-C2   | 3.18  | 120.33      | 108.11   |
| 22  | 4     | 809 | CLA  | O2A-C1-C2   | 3.18  | 120.33      | 108.11   |
| 22  | 2     | 301 | CLA  | CMA-C3A-C4A | 3.17  | 120.30      | 111.77   |
| 24  | A     | 844 | BCR  | C34-C9-C10  | -3.17 | 117.68      | 122.82   |
| 22  | 3     | 313 | CLA  | O2A-C1-C2   | 3.17  | 120.31      | 108.11   |
| 38  | 7     | 301 | LUT  | C31-C30-C29 | -3.17 | 122.83      | 127.28   |
| 22  | 9     | 303 | CLA  | C4B-CHC-C1C | 3.17  | 133.70      | 126.25   |
| 22  | A     | 820 | CLA  | O2A-C1-C2   | 3.17  | 120.31      | 108.11   |
| 24  | B     | 847 | BCR  | C4-C5-C6    | -3.17 | 118.42      | 122.70   |
| 24  | B     | 849 | BCR  | C11-C10-C9  | -3.17 | 122.84      | 127.28   |
| 24  | B     | 846 | BCR  | C27-C26-C25 | -3.17 | 118.43      | 122.70   |
| 39  | 3     | 317 | CHL  | C1-C2-C3    | -3.16 | 121.01      | 126.20   |
| 24  | 6     | 305 | BCR  | C27-C26-C25 | -3.16 | 118.43      | 122.70   |
| 22  | A     | 827 | CLA  | O2A-C1-C2   | 3.16  | 120.28      | 108.11   |
| 24  | A     | 846 | BCR  | C1-C6-C5    | -3.16 | 118.32      | 122.64   |
| 32  | F     | 306 | RRX  | C35-C13-C14 | -3.16 | 117.70      | 122.82   |
| 22  | 5     | 315 | CLA  | C3B-C4B-NB  | -3.16 | 107.71      | 110.53   |
| 24  | B     | 847 | BCR  | C11-C12-C13 | -3.16 | 117.71      | 126.36   |
| 22  | Z     | 310 | CLA  | O2A-C1-C2   | 3.15  | 120.25      | 108.11   |
| 22  | 8     | 305 | CLA  | O2A-C1-C2   | 3.15  | 120.24      | 108.11   |
| 24  | 3     | 305 | BCR  | C1-C6-C5    | -3.15 | 118.33      | 122.64   |
| 22  | 8     | 311 | CLA  | C3B-C4B-NB  | -3.15 | 107.72      | 110.53   |
| 24  | B     | 849 | BCR  | C4-C5-C6    | -3.15 | 118.45      | 122.70   |
| 24  | A     | 844 | BCR  | C2-C1-C6    | 3.14  | 115.00      | 110.44   |
| 22  | 4     | 806 | CLA  | C3B-C4B-NB  | -3.14 | 107.73      | 110.53   |
| 25  | 9     | 315 | LHG  | O7-C7-C8    | 3.14  | 118.27      | 111.48   |
| 22  | 1     | 309 | CLA  | O2A-C1-C2   | 3.14  | 120.19      | 108.11   |
| 22  | A     | 812 | CLA  | O2A-C1-C2   | 3.14  | 120.18      | 108.11   |
| 22  | Z     | 307 | CLA  | CMA-C3A-C4A | 3.14  | 120.20      | 111.77   |
| 22  | 6     | 310 | CLA  | C3B-C4B-NB  | -3.13 | 107.73      | 110.53   |
| 22  | F     | 302 | CLA  | O2A-C1-C2   | 3.13  | 120.17      | 108.11   |
| 22  | A     | 824 | CLA  | O2A-C1-C2   | 3.13  | 120.17      | 108.11   |
| 22  | A     | 836 | CLA  | O2A-C1-C2   | 3.13  | 120.16      | 108.11   |
| 24  | A     | 845 | BCR  | C38-C26-C27 | 3.13  | 120.27      | 113.60   |
| 22  | A     | 841 | CLA  | C3B-C4B-NB  | -3.13 | 107.74      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 5     | 306 | C7Z  | C11-C12-C13 | -3.13 | 117.78      | 126.36   |
| 22  | 1     | 313 | CLA  | C1-C2-C3    | -3.13 | 121.07      | 126.20   |
| 22  | B     | 823 | CLA  | C3B-C4B-NB  | -3.13 | 107.74      | 110.53   |
| 22  | 4     | 809 | CLA  | C1-C2-C3    | -3.13 | 121.08      | 126.20   |
| 22  | A     | 825 | CLA  | CMA-C3A-C4A | 3.12  | 120.17      | 111.77   |
| 24  | 3     | 307 | BCR  | C36-C18-C19 | 3.12  | 122.86      | 118.09   |
| 39  | 6     | 316 | CHL  | C1-C2-C3    | -3.12 | 121.71      | 126.76   |
| 38  | 7     | 301 | LUT  | C18-C5-C6   | -3.12 | 121.08      | 124.48   |
| 22  | 1     | 307 | CLA  | CMA-C3A-C4A | 3.12  | 120.16      | 111.77   |
| 22  | 8     | 305 | CLA  | CMA-C3A-C4A | 3.12  | 120.16      | 111.77   |
| 22  | B     | 811 | CLA  | CMA-C3A-C4A | 3.12  | 120.16      | 111.77   |
| 22  | 6     | 314 | CLA  | CMA-C3A-C4A | 3.12  | 120.16      | 111.77   |
| 38  | 6     | 303 | LUT  | C11-C10-C9  | -3.12 | 122.90      | 127.28   |
| 39  | 5     | 321 | CHL  | C3C-C4C-NC  | -3.12 | 107.03      | 114.65   |
| 24  | 7     | 303 | BCR  | C33-C5-C4   | 3.12  | 120.24      | 113.60   |
| 22  | 3     | 310 | CLA  | CMA-C3A-C4A | 3.12  | 120.15      | 111.77   |
| 38  | 7     | 301 | LUT  | C18-C5-C4   | 3.12  | 120.15      | 114.42   |
| 22  | A     | 807 | CLA  | O2A-C1-C2   | 3.11  | 120.09      | 108.11   |
| 22  | A     | 835 | CLA  | C1-C2-C3    | -3.11 | 121.10      | 126.20   |
| 22  | A     | 816 | CLA  | CMA-C3A-C4A | 3.11  | 120.14      | 111.77   |
| 24  | B     | 847 | BCR  | C16-C17-C18 | -3.11 | 122.91      | 127.28   |
| 22  | 9     | 308 | CLA  | CMA-C3A-C4A | 3.11  | 120.14      | 111.77   |
| 38  | 1     | 302 | LUT  | C18-C5-C6   | -3.11 | 121.09      | 124.48   |
| 39  | 9     | 312 | CHL  | C1A-CHA-C4D | 3.11  | 124.17      | 118.98   |
| 38  | 5     | 302 | LUT  | C1-C6-C5    | -3.11 | 118.39      | 122.64   |
| 22  | A     | 824 | CLA  | C3B-C4B-NB  | -3.11 | 107.76      | 110.53   |
| 22  | 9     | 307 | CLA  | CMA-C3A-C4A | 3.10  | 120.11      | 111.77   |
| 22  | 9     | 303 | CLA  | C1-C2-C3    | -3.10 | 121.11      | 126.20   |
| 22  | 6     | 301 | CLA  | C3B-C4B-NB  | -3.10 | 107.76      | 110.53   |
| 22  | A     | 809 | CLA  | C3B-C4B-NB  | -3.10 | 107.76      | 110.53   |
| 22  | 9     | 305 | CLA  | C2A-C1A-CHA | 3.10  | 129.25      | 123.87   |
| 22  | 9     | 305 | CLA  | C2C-C1C-NC  | 3.10  | 113.23      | 109.98   |
| 24  | 7     | 303 | BCR  | C7-C8-C9    | -3.10 | 121.66      | 126.23   |
| 22  | 7     | 304 | CLA  | CMA-C3A-C4A | 3.10  | 120.09      | 111.77   |
| 39  | 4     | 819 | CHL  | C3C-C4C-NC  | -3.09 | 107.09      | 114.65   |
| 39  | 4     | 816 | CHL  | C3C-C4C-NC  | -3.09 | 107.09      | 114.65   |
| 22  | 5     | 320 | CLA  | O2D-CGD-O1D | -3.09 | 117.84      | 123.85   |
| 24  | 3     | 304 | BCR  | C29-C30-C25 | 3.09  | 114.92      | 110.44   |
| 24  | L     | 204 | BCR  | C33-C5-C4   | 3.09  | 120.18      | 113.60   |
| 24  | 6     | 306 | BCR  | C21-C20-C19 | -3.08 | 114.27      | 123.20   |
| 22  | B     | 826 | CLA  | C1-C2-C3    | -3.08 | 121.15      | 126.20   |
| 24  | 4     | 804 | BCR  | C33-C5-C6   | -3.08 | 121.12      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 1     | 311 | CLA  | C2C-C1C-NC  | 3.08  | 113.22      | 109.98   |
| 22  | F     | 304 | CLA  | C1-C2-C3    | -3.08 | 121.16      | 126.20   |
| 39  | 4     | 814 | CHL  | C3C-C4C-NC  | -3.07 | 107.14      | 114.65   |
| 22  | Z     | 316 | CLA  | C3B-C4B-NB  | -3.07 | 107.79      | 110.53   |
| 38  | 9     | 301 | LUT  | C1-C6-C5    | -3.07 | 118.44      | 122.64   |
| 22  | B     | 825 | CLA  | CMA-C3A-C4A | 3.07  | 120.02      | 111.77   |
| 39  | 8     | 312 | CHL  | C1-C2-C3    | -3.07 | 121.17      | 126.20   |
| 39  | 6     | 320 | CHL  | C3C-C4C-NC  | -3.07 | 107.15      | 114.65   |
| 22  | A     | 806 | CLA  | C3B-C4B-NB  | -3.07 | 107.79      | 110.53   |
| 24  | 4     | 804 | BCR  | C33-C5-C4   | 3.07  | 120.14      | 113.60   |
| 22  | 8     | 306 | CLA  | C3B-C4B-NB  | -3.07 | 107.79      | 110.53   |
| 22  | Z     | 306 | CLA  | C1-C2-C3    | -3.07 | 121.17      | 126.20   |
| 24  | B     | 853 | BCR  | C11-C10-C9  | -3.06 | 122.98      | 127.28   |
| 39  | 2     | 303 | CHL  | C3C-C4C-NC  | -3.06 | 107.17      | 114.65   |
| 22  | 7     | 305 | CLA  | CMA-C3A-C4A | 3.06  | 119.99      | 111.77   |
| 22  | 4     | 805 | CLA  | C2C-C1C-NC  | 3.06  | 113.19      | 109.98   |
| 24  | 4     | 804 | BCR  | C29-C30-C25 | 3.06  | 114.88      | 110.44   |
| 22  | B     | 835 | CLA  | C1D-ND-C4D  | -3.05 | 104.17      | 106.31   |
| 22  | K     | 205 | CLA  | CMD-C2D-C1D | 3.05  | 130.11      | 124.73   |
| 22  | A     | 813 | CLA  | C2C-C1C-NC  | 3.05  | 113.19      | 109.98   |
| 36  | 5     | 306 | C7Z  | C18-C5-C4   | 3.05  | 120.03      | 114.42   |
| 22  | Z     | 309 | CLA  | C3B-C4B-NB  | -3.05 | 107.81      | 110.53   |
| 22  | K     | 204 | CLA  | CMA-C3A-C4A | 3.05  | 119.97      | 111.77   |
| 22  | B     | 828 | CLA  | C3B-C4B-NB  | -3.05 | 107.81      | 110.53   |
| 22  | 5     | 307 | CLA  | O2A-C1-C2   | 3.05  | 119.84      | 108.11   |
| 24  | 3     | 305 | BCR  | C16-C17-C18 | -3.05 | 123.00      | 127.28   |
| 24  | 3     | 306 | BCR  | C20-C21-C22 | -3.04 | 123.01      | 127.28   |
| 23  | A     | 843 | PQN  | C11-C12-C13 | -3.04 | 121.59      | 126.83   |
| 22  | 2     | 304 | CLA  | C3B-C4B-NB  | -3.04 | 107.81      | 110.53   |
| 22  | A     | 812 | CLA  | C3B-C4B-NB  | -3.04 | 107.81      | 110.53   |
| 22  | B     | 838 | CLA  | O2A-C1-C2   | 3.04  | 119.81      | 108.11   |
| 39  | 6     | 315 | CHL  | C1-O2A-CGA  | 3.04  | 124.01      | 116.65   |
| 39  | 8     | 315 | CHL  | C3C-C4C-NC  | -3.04 | 107.22      | 114.65   |
| 22  | A     | 805 | CLA  | CMA-C3A-C4A | 3.04  | 119.94      | 111.77   |
| 22  | L     | 201 | CLA  | C1D-ND-C4D  | -3.04 | 104.18      | 106.31   |
| 22  | A     | 807 | CLA  | C3B-C4B-NB  | -3.04 | 107.82      | 110.53   |
| 38  | 7     | 302 | LUT  | C31-C30-C29 | -3.04 | 123.02      | 127.28   |
| 24  | B     | 853 | BCR  | C23-C24-C25 | -3.04 | 118.89      | 127.00   |
| 22  | 4     | 812 | CLA  | O2A-C1-C2   | 3.04  | 119.79      | 108.11   |
| 22  | A     | 855 | CLA  | C3B-C4B-NB  | -3.03 | 107.82      | 110.53   |
| 23  | B     | 843 | PQN  | C14-C13-C15 | 3.03  | 120.50      | 115.23   |
| 39  | 6     | 315 | CHL  | C3C-C4C-NC  | -3.03 | 107.24      | 114.65   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 7     | 324 | CLA  | C1-C2-C3    | -3.03 | 121.23      | 126.20   |
| 39  | 7     | 313 | CHL  | C3C-C4C-NC  | -3.03 | 107.24      | 114.65   |
| 22  | B     | 818 | CLA  | C3B-C4B-NB  | -3.03 | 107.82      | 110.53   |
| 22  | 6     | 313 | CLA  | C3B-C4B-NB  | -3.03 | 107.82      | 110.53   |
| 25  | 4     | 821 | LHG  | C5-O7-C7    | -3.03 | 110.54      | 117.80   |
| 22  | K     | 202 | CLA  | CMA-C3A-C4A | 3.03  | 119.92      | 111.77   |
| 22  | F     | 301 | CLA  | C3B-C4B-NB  | -3.03 | 107.83      | 110.53   |
| 22  | 5     | 326 | CLA  | C3B-C4B-NB  | -3.03 | 107.83      | 110.53   |
| 22  | B     | 824 | CLA  | C3B-C4B-NB  | -3.03 | 107.83      | 110.53   |
| 22  | K     | 204 | CLA  | C3B-C4B-NB  | -3.03 | 107.83      | 110.53   |
| 22  | B     | 817 | CLA  | O2A-C1-C2   | 3.03  | 119.75      | 108.11   |
| 22  | B     | 820 | CLA  | O2A-C1-C2   | 3.03  | 119.75      | 108.11   |
| 39  | 9     | 314 | CHL  | C3C-C4C-NC  | -3.02 | 107.26      | 114.65   |
| 22  | A     | 829 | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 22  | A     | 820 | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 22  | 2     | 304 | CLA  | CMA-C3A-C4A | 3.02  | 119.89      | 111.77   |
| 22  | 5     | 315 | CLA  | CMA-C3A-C4A | 3.02  | 119.89      | 111.77   |
| 22  | 7     | 305 | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 22  | 7     | 304 | CLA  | C1D-ND-C4D  | -3.02 | 104.19      | 106.31   |
| 22  | A     | 822 | CLA  | CMA-C3A-C4A | 3.02  | 119.88      | 111.77   |
| 22  | 3     | 322 | CLA  | C1-C2-C3    | -3.02 | 121.25      | 126.20   |
| 36  | J     | 105 | C7Z  | C8-C7-C6    | -3.02 | 118.94      | 127.00   |
| 22  | A     | 832 | CLA  | C1-C2-C3    | -3.01 | 121.26      | 126.20   |
| 22  | 9     | 311 | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 22  | B     | 823 | CLA  | O2A-C1-C2   | 3.01  | 119.71      | 108.11   |
| 36  | J     | 105 | C7Z  | C38-C25-C24 | 3.01  | 119.96      | 114.42   |
| 22  | B     | 830 | CLA  | CMA-C3A-C4A | 3.01  | 119.87      | 111.77   |
| 22  | 7     | 306 | CLA  | C2C-C1C-NC  | 3.01  | 113.15      | 109.98   |
| 22  | 1     | 308 | CLA  | C1C-C2C-C3C | -3.01 | 103.81      | 106.98   |
| 22  | 5     | 314 | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 22  | A     | 841 | CLA  | C1D-ND-C4D  | -3.01 | 104.20      | 106.31   |
| 22  | B     | 823 | CLA  | CMA-C3A-C4A | 3.01  | 119.86      | 111.77   |
| 38  | 8     | 302 | LUT  | C8-C7-C6    | -3.01 | 118.96      | 127.00   |
| 22  | A     | 823 | CLA  | CMA-C3A-C4A | 3.01  | 119.86      | 111.77   |
| 22  | 2     | 301 | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 38  | 1     | 302 | LUT  | C31-C30-C29 | -3.01 | 123.06      | 127.28   |
| 22  | F     | 302 | CLA  | CMA-C3A-C4A | 3.01  | 119.86      | 111.77   |
| 24  | 6     | 305 | BCR  | C2-C1-C6    | 3.01  | 114.81      | 110.44   |
| 22  | 1     | 306 | CLA  | CMA-C3A-C4A | 3.01  | 119.85      | 111.77   |
| 24  | 3     | 307 | BCR  | C23-C22-C21 | 3.01  | 123.74      | 119.01   |
| 39  | 1     | 312 | CHL  | C3C-C4C-NC  | -3.01 | 107.30      | 114.65   |
| 22  | A     | 818 | CLA  | C1D-ND-C4D  | -3.01 | 104.20      | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 818 | CLA  | C1D-ND-C4D  | -3.01 | 104.20      | 106.31   |
| 22  | Z     | 304 | CLA  | C3B-C4B-NB  | -3.01 | 107.85      | 110.53   |
| 22  | 5     | 309 | CLA  | CMA-C3A-C4A | 3.00  | 119.85      | 111.77   |
| 22  | B     | 824 | CLA  | C1D-ND-C4D  | -3.00 | 104.21      | 106.31   |
| 22  | A     | 829 | CLA  | C1-C2-C3    | -3.00 | 121.28      | 126.20   |
| 22  | 3     | 314 | CLA  | C3B-C4B-NB  | -3.00 | 107.85      | 110.53   |
| 22  | 4     | 811 | CLA  | C3B-C4B-NB  | -3.00 | 107.85      | 110.53   |
| 22  | B     | 807 | CLA  | CMA-C3A-C4A | 3.00  | 119.83      | 111.77   |
| 22  | B     | 823 | CLA  | C1D-ND-C4D  | -3.00 | 104.21      | 106.31   |
| 22  | 7     | 311 | CLA  | C1D-ND-C4D  | -3.00 | 104.21      | 106.31   |
| 22  | A     | 838 | CLA  | CMA-C3A-C4A | 3.00  | 119.83      | 111.77   |
| 22  | 5     | 326 | CLA  | O2A-C1-C2   | 3.00  | 119.65      | 108.11   |
| 39  | 5     | 317 | CHL  | C3C-C4C-NC  | -3.00 | 107.32      | 114.65   |
| 22  | B     | 811 | CLA  | C1D-ND-C4D  | -3.00 | 104.21      | 106.31   |
| 22  | 6     | 309 | CLA  | CMA-C3A-C4A | 3.00  | 119.83      | 111.77   |
| 38  | 4     | 803 | LUT  | C18-C5-C4   | 3.00  | 119.93      | 114.42   |
| 22  | 5     | 319 | CLA  | C3B-C4B-NB  | -3.00 | 107.86      | 110.53   |
| 22  | F     | 302 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 22  | 8     | 316 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 39  | Z     | 312 | CHL  | C3C-C4C-NC  | -2.99 | 107.33      | 114.65   |
| 22  | A     | 830 | CLA  | CMA-C3A-C4A | 2.99  | 119.82      | 111.77   |
| 22  | A     | 818 | CLA  | CMA-C3A-C4A | 2.99  | 119.82      | 111.77   |
| 22  | A     | 829 | CLA  | CMA-C3A-C4A | 2.99  | 119.81      | 111.77   |
| 36  | J     | 105 | C7Z  | C35-C15-C14 | -2.99 | 117.40      | 123.52   |
| 22  | B     | 821 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 22  | 6     | 321 | CLA  | CMA-C3A-C4A | 2.99  | 119.81      | 111.77   |
| 22  | Z     | 308 | CLA  | C1D-ND-C4D  | -2.99 | 104.21      | 106.31   |
| 22  | 9     | 310 | CLA  | CMA-C3A-C4A | 2.99  | 119.81      | 111.77   |
| 39  | 8     | 312 | CHL  | C3C-C4C-NC  | -2.99 | 107.34      | 114.65   |
| 22  | B     | 810 | CLA  | CMA-C3A-C4A | 2.99  | 119.81      | 111.77   |
| 22  | A     | 805 | CLA  | C1D-ND-C4D  | -2.99 | 104.22      | 106.31   |
| 22  | A     | 837 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 22  | 7     | 314 | CLA  | CMA-C3A-C4A | 2.99  | 119.80      | 111.77   |
| 22  | F     | 304 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 22  | B     | 815 | CLA  | C2C-C1C-NC  | 2.99  | 113.12      | 109.98   |
| 22  | 4     | 815 | CLA  | CMA-C3A-C4A | 2.99  | 119.80      | 111.77   |
| 24  | 3     | 306 | BCR  | C11-C12-C13 | -2.99 | 118.18      | 126.36   |
| 22  | 9     | 313 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 24  | 5     | 305 | BCR  | C23-C24-C25 | -2.98 | 119.03      | 127.00   |
| 22  | B     | 836 | CLA  | CMA-C3A-C4A | 2.98  | 119.79      | 111.77   |
| 39  | 6     | 316 | CHL  | C1-O2A-CGA  | 2.98  | 123.87      | 116.65   |
| 22  | 7     | 306 | CLA  | CMA-C3A-C4A | 2.98  | 119.79      | 111.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 9     | 305 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 22  | G     | 201 | CLA  | C2C-C1C-NC  | 2.98  | 113.11      | 109.98   |
| 22  | 7     | 317 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 22  | A     | 803 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 22  | 7     | 312 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 22  | Z     | 306 | CLA  | O2A-C1-C2   | 2.98  | 119.56      | 108.11   |
| 22  | A     | 810 | CLA  | CMA-C3A-C4A | 2.98  | 119.77      | 111.77   |
| 22  | A     | 819 | CLA  | CMA-C3A-C4A | 2.98  | 119.77      | 111.77   |
| 22  | 5     | 313 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 22  | 3     | 322 | CLA  | CMA-C3A-C4A | 2.97  | 119.77      | 111.77   |
| 39  | 6     | 316 | CHL  | C3C-C4C-NC  | -2.97 | 107.38      | 114.65   |
| 22  | 9     | 309 | CLA  | C2C-C1C-NC  | 2.97  | 113.11      | 109.98   |
| 22  | A     | 855 | CLA  | CMA-C3A-C4A | 2.97  | 119.76      | 111.77   |
| 22  | 1     | 304 | CLA  | CMA-C3A-C4A | 2.97  | 119.75      | 111.77   |
| 24  | 4     | 804 | BCR  | C4-C5-C6    | -2.97 | 118.69      | 122.70   |
| 22  | 9     | 304 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 22  | B     | 837 | CLA  | CMA-C3A-C4A | 2.97  | 119.75      | 111.77   |
| 22  | 7     | 310 | CLA  | CMA-C3A-C4A | 2.97  | 119.75      | 111.77   |
| 22  | 7     | 311 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 22  | B     | 820 | CLA  | CMA-C3A-C4A | 2.96  | 119.73      | 111.77   |
| 36  | J     | 105 | C7Z  | C15-C14-C13 | -2.96 | 123.13      | 127.28   |
| 22  | 9     | 304 | CLA  | C2D-C1D-ND  | 2.96  | 113.06      | 110.13   |
| 22  | 9     | 313 | CLA  | CMA-C3A-C4A | 2.96  | 119.73      | 111.77   |
| 24  | F     | 303 | BCR  | C8-C7-C6    | -2.96 | 119.09      | 127.00   |
| 22  | Z     | 315 | CLA  | CMA-C3A-C4A | 2.96  | 119.72      | 111.77   |
| 22  | 3     | 308 | CLA  | CMA-C3A-C4A | 2.96  | 119.72      | 111.77   |
| 22  | Z     | 310 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 24  | B     | 845 | BCR  | C23-C24-C25 | -2.96 | 119.10      | 127.00   |
| 22  | B     | 813 | CLA  | CMA-C3A-C4A | 2.95  | 119.71      | 111.77   |
| 22  | B     | 840 | CLA  | CMA-C3A-C4A | 2.95  | 119.71      | 111.77   |
| 22  | 1     | 311 | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 22  | 1     | 309 | CLA  | C1D-ND-C4D  | -2.95 | 104.24      | 106.31   |
| 39  | 4     | 813 | CHL  | C3C-C4C-NC  | -2.95 | 107.43      | 114.65   |
| 22  | 4     | 812 | CLA  | CMA-C3A-C4A | 2.95  | 119.71      | 111.77   |
| 25  | 4     | 820 | LHG  | O8-C23-C24  | 2.95  | 120.84      | 111.83   |
| 22  | A     | 824 | CLA  | C1D-ND-C4D  | -2.95 | 104.24      | 106.31   |
| 39  | 5     | 316 | CHL  | C3C-C4C-NC  | -2.95 | 107.43      | 114.65   |
| 22  | 4     | 806 | CLA  | CMA-C3A-C4A | 2.95  | 119.71      | 111.77   |
| 22  | 3     | 318 | CLA  | C1D-ND-C4D  | -2.95 | 104.24      | 106.31   |
| 22  | Z     | 315 | CLA  | C2C-C1C-NC  | 2.95  | 113.08      | 109.98   |
| 22  | 4     | 807 | CLA  | C2C-C1C-NC  | 2.95  | 113.08      | 109.98   |
| 22  | A     | 833 | CLA  | CMA-C3A-C4A | 2.95  | 119.70      | 111.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 9     | 309 | CLA  | C1C-C2C-C3C | -2.95 | 103.88      | 106.98   |
| 22  | 3     | 312 | CLA  | C1D-ND-C4D  | -2.95 | 104.24      | 106.31   |
| 22  | B     | 814 | CLA  | C3B-C4B-NB  | -2.95 | 107.90      | 110.53   |
| 39  | 6     | 318 | CHL  | C3C-C4C-NC  | -2.95 | 107.44      | 114.65   |
| 22  | 1     | 315 | CLA  | CMA-C3A-C4A | 2.95  | 119.69      | 111.77   |
| 22  | A     | 809 | CLA  | CMA-C3A-C4A | 2.95  | 119.69      | 111.77   |
| 22  | 4     | 805 | CLA  | O2A-C1-C2   | 2.94  | 119.44      | 108.11   |
| 22  | J     | 103 | CLA  | CMA-C3A-C4A | 2.94  | 119.69      | 111.77   |
| 22  | 5     | 313 | CLA  | C2C-C1C-NC  | 2.94  | 113.08      | 109.98   |
| 22  | 8     | 311 | CLA  | CMA-C3A-C4A | 2.94  | 119.69      | 111.77   |
| 22  | 3     | 316 | CLA  | C3B-C4B-NB  | -2.94 | 107.90      | 110.53   |
| 22  | 9     | 313 | CLA  | C1D-ND-C4D  | -2.94 | 104.25      | 106.31   |
| 22  | 8     | 306 | CLA  | CMA-C3A-C4A | 2.94  | 119.68      | 111.77   |
| 22  | B     | 833 | CLA  | CMA-C3A-C4A | 2.94  | 119.68      | 111.77   |
| 22  | B     | 820 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 22  | 3     | 320 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 22  | A     | 824 | CLA  | CMA-C3A-C4A | 2.94  | 119.67      | 111.77   |
| 22  | 5     | 314 | CLA  | CMA-C3A-C4A | 2.94  | 119.67      | 111.77   |
| 22  | B     | 805 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 22  | 3     | 322 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 22  | 7     | 315 | CLA  | CMA-C3A-C4A | 2.94  | 119.67      | 111.77   |
| 22  | Z     | 309 | CLA  | C1D-ND-C4D  | -2.94 | 104.25      | 106.31   |
| 22  | Z     | 316 | CLA  | C1D-ND-C4D  | -2.94 | 104.25      | 106.31   |
| 22  | Z     | 314 | CLA  | C3B-C4B-NB  | -2.94 | 107.91      | 110.53   |
| 22  | A     | 802 | CLA  | CMA-C3A-C4A | 2.94  | 119.67      | 111.77   |
| 22  | Z     | 310 | CLA  | CMA-C3A-C4A | 2.94  | 119.67      | 111.77   |
| 22  | 5     | 318 | CLA  | CMA-C3A-C4A | 2.94  | 119.66      | 111.77   |
| 24  | A     | 856 | BCR  | C7-C8-C9    | -2.94 | 121.89      | 126.23   |
| 24  | B     | 847 | BCR  | C23-C24-C25 | -2.93 | 119.16      | 127.00   |
| 22  | Z     | 304 | CLA  | CMA-C3A-C4A | 2.93  | 119.66      | 111.77   |
| 22  | 1     | 311 | CLA  | C1C-C2C-C3C | -2.93 | 103.89      | 106.98   |
| 22  | B     | 824 | CLA  | CMA-C3A-C4A | 2.93  | 119.66      | 111.77   |
| 22  | B     | 806 | CLA  | CMA-C3A-C4A | 2.93  | 119.65      | 111.77   |
| 22  | 3     | 313 | CLA  | C1C-C2C-C3C | -2.93 | 103.90      | 106.98   |
| 22  | B     | 805 | CLA  | C1D-ND-C4D  | -2.93 | 104.25      | 106.31   |
| 22  | 2     | 302 | CLA  | CMA-C3A-C4A | 2.93  | 119.65      | 111.77   |
| 22  | 3     | 312 | CLA  | C3B-C4B-NB  | -2.93 | 107.91      | 110.53   |
| 38  | Z     | 301 | LUT  | C11-C12-C13 | -2.93 | 118.33      | 126.36   |
| 22  | B     | 842 | CLA  | CMA-C3A-C4A | 2.93  | 119.65      | 111.77   |
| 22  | 5     | 311 | CLA  | C1-C2-C3    | -2.93 | 121.40      | 126.20   |
| 24  | 4     | 804 | BCR  | C27-C26-C25 | -2.93 | 118.75      | 122.70   |
| 22  | 5     | 307 | CLA  | CMA-C3A-C4A | 2.93  | 119.64      | 111.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | L     | 202 | CLA  | CMA-C3A-C4A | 2.93  | 119.64      | 111.77   |
| 22  | Z     | 313 | CLA  | CMA-C3A-C4A | 2.93  | 119.64      | 111.77   |
| 24  | 6     | 306 | BCR  | C33-C5-C4   | 2.93  | 119.84      | 113.60   |
| 22  | B     | 808 | CLA  | C1D-ND-C4D  | -2.93 | 104.26      | 106.31   |
| 22  | 9     | 309 | CLA  | C3B-C4B-NB  | -2.93 | 107.92      | 110.53   |
| 22  | 4     | 811 | CLA  | CMA-C3A-C4A | 2.93  | 119.64      | 111.77   |
| 24  | F     | 303 | BCR  | C29-C30-C25 | 2.93  | 114.69      | 110.44   |
| 22  | A     | 837 | CLA  | CMA-C3A-C4A | 2.93  | 119.64      | 111.77   |
| 24  | F     | 303 | BCR  | C38-C26-C27 | 2.92  | 119.83      | 113.60   |
| 22  | A     | 803 | CLA  | C1D-ND-C4D  | -2.92 | 104.26      | 106.31   |
| 22  | A     | 809 | CLA  | C1D-ND-C4D  | -2.92 | 104.26      | 106.31   |
| 22  | A     | 812 | CLA  | C1D-ND-C4D  | -2.92 | 104.26      | 106.31   |
| 22  | 5     | 323 | CLA  | CMA-C3A-C4A | 2.92  | 119.62      | 111.77   |
| 22  | 9     | 311 | CLA  | CMA-C3A-C4A | 2.92  | 119.62      | 111.77   |
| 22  | 4     | 818 | CLA  | C1-O2A-CGA  | 2.92  | 123.72      | 116.65   |
| 25  | 4     | 821 | LHG  | O8-C23-C24  | 2.92  | 120.73      | 111.83   |
| 22  | 7     | 309 | CLA  | C1D-ND-C4D  | -2.92 | 104.26      | 106.31   |
| 22  | A     | 812 | CLA  | CMA-C3A-C4A | 2.92  | 119.62      | 111.77   |
| 22  | Z     | 309 | CLA  | CMA-C3A-C4A | 2.92  | 119.62      | 111.77   |
| 22  | 1     | 313 | CLA  | CMA-C3A-C4A | 2.92  | 119.61      | 111.77   |
| 22  | A     | 816 | CLA  | C2C-C1C-NC  | 2.92  | 113.05      | 109.98   |
| 24  | B     | 844 | BCR  | C34-C9-C10  | -2.92 | 118.09      | 122.82   |
| 22  | B     | 830 | CLA  | C3B-C4B-NB  | -2.92 | 107.93      | 110.53   |
| 22  | 4     | 809 | CLA  | C3B-C4B-NB  | -2.92 | 107.93      | 110.53   |
| 24  | A     | 844 | BCR  | C23-C24-C25 | -2.92 | 119.21      | 127.00   |
| 22  | 1     | 310 | CLA  | C3B-C4B-NB  | -2.92 | 107.93      | 110.53   |
| 22  | 2     | 302 | CLA  | C3B-C4B-NB  | -2.92 | 107.93      | 110.53   |
| 22  | A     | 814 | CLA  | CMA-C3A-C4A | 2.92  | 119.61      | 111.77   |
| 22  | 6     | 314 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 24  | K     | 206 | BCR  | C11-C12-C13 | -2.91 | 118.37      | 126.36   |
| 22  | L     | 202 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 22  | A     | 803 | CLA  | CMA-C3A-C4A | 2.91  | 119.60      | 111.77   |
| 22  | 4     | 808 | CLA  | CMA-C3A-C4A | 2.91  | 119.60      | 111.77   |
| 22  | B     | 814 | CLA  | C1D-ND-C4D  | -2.91 | 104.27      | 106.31   |
| 22  | 4     | 807 | CLA  | CMA-C3A-C4A | 2.91  | 119.59      | 111.77   |
| 22  | A     | 833 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 36  | J     | 105 | C7Z  | C18-C5-C4   | 2.91  | 119.77      | 114.42   |
| 22  | B     | 838 | CLA  | CMA-C3A-C4A | 2.91  | 119.59      | 111.77   |
| 22  | 1     | 310 | CLA  | CMA-C3A-C4A | 2.91  | 119.59      | 111.77   |
| 22  | 6     | 302 | CLA  | C3B-C4B-NB  | -2.91 | 107.94      | 110.53   |
| 22  | 3     | 312 | CLA  | CMA-C3A-C4A | 2.91  | 119.58      | 111.77   |
| 22  | Z     | 314 | CLA  | C1D-ND-C4D  | -2.91 | 104.27      | 106.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 2     | 301  | CLA  | C1D-ND-C4D  | -2.90 | 104.27      | 106.31   |
| 22  | 1     | 316  | CLA  | O2A-C1-C2   | 2.90  | 119.28      | 108.11   |
| 34  | F     | 308  | LMG  | C9-C8-C7    | -2.90 | 105.01      | 111.78   |
| 22  | B     | 829  | CLA  | CMA-C3A-C4A | 2.90  | 119.58      | 111.77   |
| 22  | 6     | 313  | CLA  | CMA-C3A-C4A | 2.90  | 119.58      | 111.77   |
| 22  | 9     | 310  | CLA  | C2D-C1D-ND  | 2.90  | 113.00      | 110.13   |
| 22  | 7     | 324  | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 22  | 7     | 307  | CLA  | CMA-C3A-C4A | 2.90  | 119.57      | 111.77   |
| 22  | A     | 813  | CLA  | CMA-C3A-C4A | 2.90  | 119.57      | 111.77   |
| 24  | I     | 4001 | BCR  | C20-C19-C18 | -2.90 | 118.41      | 126.36   |
| 24  | I     | 4001 | BCR  | C33-C5-C4   | 2.90  | 119.78      | 113.60   |
| 38  | 1     | 302  | LUT  | C21-C26-C27 | -2.90 | 109.49      | 112.83   |
| 22  | Z     | 306  | CLA  | C1D-ND-C4D  | -2.90 | 104.28      | 106.31   |
| 24  | 3     | 306  | BCR  | C23-C24-C25 | -2.90 | 119.26      | 127.00   |
| 22  | 5     | 319  | CLA  | C1C-C2C-C3C | -2.90 | 103.93      | 106.98   |
| 22  | A     | 832  | CLA  | CMA-C3A-C4A | 2.90  | 119.56      | 111.77   |
| 22  | 3     | 314  | CLA  | CMA-C3A-C4A | 2.90  | 119.56      | 111.77   |
| 22  | 8     | 316  | CLA  | CMA-C3A-C4A | 2.90  | 119.56      | 111.77   |
| 22  | A     | 837  | CLA  | C1D-ND-C4D  | -2.90 | 104.28      | 106.31   |
| 22  | Z     | 307  | CLA  | C1D-ND-C4D  | -2.90 | 104.28      | 106.31   |
| 31  | B     | 852  | DGD  | C2G-O2G-C1B | -2.90 | 110.86      | 117.80   |
| 24  | G     | 203  | BCR  | C23-C24-C25 | -2.90 | 119.26      | 127.00   |
| 22  | 3     | 315  | CLA  | CMA-C3A-C4A | 2.89  | 119.55      | 111.77   |
| 22  | B     | 832  | CLA  | C1D-ND-C4D  | -2.89 | 104.28      | 106.31   |
| 22  | 7     | 307  | CLA  | C1D-ND-C4D  | -2.89 | 104.28      | 106.31   |
| 22  | 4     | 817  | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 22  | 7     | 309  | CLA  | CMA-C3A-C4A | 2.89  | 119.55      | 111.77   |
| 22  | A     | 842  | CLA  | C2C-C1C-NC  | 2.89  | 113.02      | 109.98   |
| 23  | B     | 843  | PQN  | C11-C12-C13 | -2.89 | 121.85      | 126.83   |
| 22  | B     | 807  | CLA  | C1D-ND-C4D  | -2.89 | 104.28      | 106.31   |
| 22  | 6     | 301  | CLA  | C1D-ND-C4D  | -2.89 | 104.28      | 106.31   |
| 24  | 3     | 304  | BCR  | C21-C20-C19 | -2.89 | 114.82      | 123.20   |
| 24  | F     | 303  | BCR  | C4-C5-C6    | -2.89 | 118.80      | 122.70   |
| 38  | 6     | 303  | LUT  | C7-C8-C9    | -2.89 | 121.96      | 126.23   |
| 22  | A     | 821  | CLA  | C1-C2-C3    | -2.89 | 121.46      | 126.20   |
| 24  | 5     | 305  | BCR  | C33-C5-C4   | 2.89  | 119.76      | 113.60   |
| 38  | 3     | 303  | LUT  | C21-C26-C27 | -2.89 | 109.50      | 112.83   |
| 22  | B     | 828  | CLA  | CMA-C3A-C4A | 2.89  | 119.54      | 111.77   |
| 24  | B     | 848  | BCR  | C30-C25-C26 | -2.89 | 118.69      | 122.64   |
| 22  | A     | 811  | CLA  | C1D-ND-C4D  | -2.89 | 104.28      | 106.31   |
| 22  | 7     | 310  | CLA  | C1D-ND-C4D  | -2.89 | 104.28      | 106.31   |
| 22  | B     | 831  | CLA  | CMA-C3A-C4A | 2.89  | 119.53      | 111.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | Z     | 306 | CLA  | CMA-C3A-C4A | 2.89  | 119.53      | 111.77   |
| 22  | 7     | 314 | CLA  | C1D-ND-C4D  | -2.89 | 104.29      | 106.31   |
| 22  | B     | 834 | CLA  | C2C-C1C-NC  | 2.89  | 113.01      | 109.98   |
| 22  | Z     | 303 | CLA  | CMA-C3A-C4A | 2.89  | 119.53      | 111.77   |
| 38  | 5     | 303 | LUT  | C21-C26-C27 | -2.89 | 109.51      | 112.83   |
| 22  | B     | 838 | CLA  | C1D-ND-C4D  | -2.89 | 104.29      | 106.31   |
| 22  | 6     | 310 | CLA  | C1D-ND-C4D  | -2.89 | 104.29      | 106.31   |
| 22  | 5     | 323 | CLA  | C1D-ND-C4D  | -2.88 | 104.29      | 106.31   |
| 22  | A     | 808 | CLA  | CMA-C3A-C4A | 2.88  | 119.53      | 111.77   |
| 22  | B     | 811 | CLA  | C3B-C4B-NB  | -2.88 | 107.95      | 110.53   |
| 22  | J     | 103 | CLA  | C1D-ND-C4D  | -2.88 | 104.29      | 106.31   |
| 22  | L     | 202 | CLA  | C1D-ND-C4D  | -2.88 | 104.29      | 106.31   |
| 22  | A     | 834 | CLA  | CMA-C3A-C4A | 2.88  | 119.52      | 111.77   |
| 22  | B     | 819 | CLA  | CMA-C3A-C4A | 2.88  | 119.52      | 111.77   |
| 22  | B     | 830 | CLA  | C1D-ND-C4D  | -2.88 | 104.29      | 106.31   |
| 22  | Z     | 305 | CLA  | CMA-C3A-C4A | 2.88  | 119.52      | 111.77   |
| 22  | 1     | 305 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 22  | 5     | 320 | CLA  | C1C-C2C-C3C | -2.88 | 103.95      | 106.98   |
| 22  | Z     | 303 | CLA  | C1D-ND-C4D  | -2.88 | 104.29      | 106.31   |
| 38  | 6     | 303 | LUT  | C35-C15-C14 | -2.88 | 117.63      | 123.52   |
| 25  | 5     | 324 | LHG  | O8-C23-C24  | 2.88  | 120.61      | 111.83   |
| 22  | A     | 842 | CLA  | CMA-C3A-C4A | 2.88  | 119.51      | 111.77   |
| 22  | Z     | 314 | CLA  | CMA-C3A-C4A | 2.88  | 119.51      | 111.77   |
| 22  | B     | 839 | CLA  | C2C-C1C-NC  | 2.88  | 113.00      | 109.98   |
| 22  | B     | 807 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 24  | 3     | 307 | BCR  | C33-C5-C4   | 2.88  | 119.73      | 113.60   |
| 24  | B     | 847 | BCR  | C38-C26-C27 | 2.88  | 119.73      | 113.60   |
| 22  | L     | 203 | CLA  | CMA-C3A-C4A | 2.88  | 119.50      | 111.77   |
| 24  | 5     | 304 | BCR  | C38-C26-C27 | 2.88  | 119.73      | 113.60   |
| 22  | 5     | 310 | CLA  | CMA-C3A-C4A | 2.87  | 119.50      | 111.77   |
| 22  | A     | 814 | CLA  | C2C-C1C-NC  | 2.87  | 113.00      | 109.98   |
| 22  | Z     | 310 | CLA  | C1D-ND-C4D  | -2.87 | 104.30      | 106.31   |
| 22  | 9     | 303 | CLA  | CBA-CAA-C2A | 2.87  | 122.34      | 113.79   |
| 22  | 5     | 313 | CLA  | CMA-C3A-C4A | 2.87  | 119.49      | 111.77   |
| 22  | A     | 807 | CLA  | CMA-C3A-C4A | 2.87  | 119.49      | 111.77   |
| 22  | 4     | 818 | CLA  | CMA-C3A-C4A | 2.87  | 119.49      | 111.77   |
| 22  | A     | 802 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 22  | 8     | 313 | CLA  | C1D-ND-C4D  | -2.87 | 104.30      | 106.31   |
| 22  | K     | 203 | CLA  | C2C-C1C-NC  | 2.87  | 113.00      | 109.98   |
| 24  | 5     | 305 | BCR  | C27-C26-C25 | -2.87 | 118.82      | 122.70   |
| 22  | 7     | 308 | CLA  | CMA-C3A-C4A | 2.87  | 119.49      | 111.77   |
| 22  | 6     | 319 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 38  | 8     | 303 | LUT  | C8-C7-C6    | -2.87 | 119.33      | 127.00   |
| 22  | 9     | 308 | CLA  | C2C-C1C-NC  | 2.87  | 113.00      | 109.98   |
| 22  | 5     | 318 | CLA  | C1D-ND-C4D  | -2.87 | 104.30      | 106.31   |
| 22  | L     | 201 | CLA  | CMA-C3A-C4A | 2.87  | 119.49      | 111.77   |
| 22  | B     | 801 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 22  | 4     | 817 | CLA  | CMA-C3A-C4A | 2.87  | 119.49      | 111.77   |
| 23  | A     | 843 | PQN  | C14-C13-C15 | 2.87  | 120.21      | 115.23   |
| 22  | K     | 203 | CLA  | CMA-C3A-C4A | 2.87  | 119.48      | 111.77   |
| 22  | 5     | 320 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 22  | A     | 839 | CLA  | CMA-C3A-C4A | 2.87  | 119.48      | 111.77   |
| 22  | Z     | 306 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 22  | 1     | 313 | CLA  | C1C-C2C-C3C | -2.87 | 103.96      | 106.98   |
| 22  | 6     | 301 | CLA  | CMA-C3A-C4A | 2.87  | 119.48      | 111.77   |
| 22  | B     | 813 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 22  | 5     | 301 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 24  | 8     | 304 | BCR  | C33-C5-C4   | 2.87  | 119.71      | 113.60   |
| 22  | 5     | 301 | CLA  | CMA-C3A-C4A | 2.87  | 119.48      | 111.77   |
| 22  | 6     | 309 | CLA  | O2A-CGA-CBA | 2.86  | 120.57      | 111.83   |
| 22  | 1     | 308 | CLA  | CMA-C3A-C4A | 2.86  | 119.47      | 111.77   |
| 22  | 5     | 322 | CLA  | CMA-C3A-C4A | 2.86  | 119.47      | 111.77   |
| 22  | B     | 801 | CLA  | C1-C2-C3    | -2.86 | 121.50      | 126.20   |
| 38  | 9     | 302 | LUT  | C8-C7-C6    | -2.86 | 119.35      | 127.00   |
| 22  | A     | 833 | CLA  | C1D-ND-C4D  | -2.86 | 104.30      | 106.31   |
| 22  | Z     | 304 | CLA  | C1D-ND-C4D  | -2.86 | 104.30      | 106.31   |
| 22  | B     | 810 | CLA  | C2C-C1C-NC  | 2.86  | 112.99      | 109.98   |
| 38  | 3     | 302 | LUT  | C18-C5-C4   | 2.86  | 119.68      | 114.42   |
| 22  | A     | 854 | CLA  | O2A-CGA-CBA | 2.86  | 120.56      | 111.83   |
| 24  | L     | 204 | BCR  | C15-C16-C17 | -2.86 | 117.66      | 123.52   |
| 38  | 7     | 302 | LUT  | C1-C6-C5    | -2.86 | 118.73      | 122.64   |
| 22  | A     | 820 | CLA  | CMA-C3A-C4A | 2.86  | 119.46      | 111.77   |
| 38  | 1     | 303 | LUT  | C18-C5-C4   | 2.86  | 119.68      | 114.42   |
| 24  | B     | 849 | BCR  | C33-C5-C4   | 2.86  | 119.69      | 113.60   |
| 22  | B     | 819 | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 39  | 7     | 313 | CHL  | C1-O2A-CGA  | 2.86  | 123.57      | 116.65   |
| 22  | 9     | 305 | CLA  | C1D-ND-C4D  | -2.86 | 104.31      | 106.31   |
| 22  | 7     | 323 | CLA  | CMA-C3A-C4A | 2.86  | 119.45      | 111.77   |
| 22  | 1     | 314 | CLA  | CMA-C3A-C4A | 2.86  | 119.45      | 111.77   |
| 22  | 6     | 312 | CLA  | CMA-C3A-C4A | 2.86  | 119.45      | 111.77   |
| 22  | B     | 841 | CLA  | CMA-C3A-C4A | 2.86  | 119.45      | 111.77   |
| 22  | 8     | 306 | CLA  | C1D-ND-C4D  | -2.86 | 104.31      | 106.31   |
| 22  | Z     | 305 | CLA  | C2C-C1C-NC  | 2.86  | 112.98      | 109.98   |
| 38  | 1     | 302 | LUT  | C11-C12-C13 | -2.85 | 118.53      | 126.36   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 6     | 308  | CLA  | C1D-ND-C4D  | -2.85 | 104.31      | 106.31   |
| 22  | A     | 817  | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 22  | L     | 201  | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 22  | 7     | 315  | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 22  | A     | 840  | CLA  | CMA-C3A-C4A | 2.85  | 119.44      | 111.77   |
| 24  | I     | 4001 | BCR  | C38-C26-C25 | -2.85 | 121.37      | 124.48   |
| 22  | 6     | 314  | CLA  | C2C-C1C-NC  | 2.85  | 112.98      | 109.98   |
| 22  | 9     | 303  | CLA  | C2D-C1D-ND  | 2.85  | 112.95      | 110.13   |
| 24  | B     | 844  | BCR  | C15-C16-C17 | -2.85 | 117.68      | 123.52   |
| 22  | B     | 841  | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 22  | 4     | 809  | CLA  | CMA-C3A-C4A | 2.85  | 119.43      | 111.77   |
| 22  | 7     | 305  | CLA  | C1D-ND-C4D  | -2.85 | 104.31      | 106.31   |
| 22  | 6     | 313  | CLA  | C1D-ND-C4D  | -2.85 | 104.31      | 106.31   |
| 22  | B     | 818  | CLA  | CMA-C3A-C4A | 2.85  | 119.43      | 111.77   |
| 22  | 1     | 313  | CLA  | C1D-ND-C4D  | -2.85 | 104.31      | 106.31   |
| 38  | 9     | 302  | LUT  | C18-C5-C4   | 2.85  | 119.66      | 114.42   |
| 22  | Z     | 315  | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 22  | 3     | 318  | CLA  | CMA-C3A-C4A | 2.85  | 119.42      | 111.77   |
| 22  | Z     | 313  | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 24  | 3     | 307  | BCR  | C12-C13-C14 | 2.84  | 123.48      | 119.01   |
| 22  | A     | 838  | CLA  | C1D-ND-C4D  | -2.84 | 104.32      | 106.31   |
| 22  | 6     | 312  | CLA  | C2C-C1C-NC  | 2.84  | 112.97      | 109.98   |
| 22  | F     | 302  | CLA  | C1C-C2C-C3C | -2.84 | 103.99      | 106.98   |
| 24  | L     | 204  | BCR  | C8-C7-C6    | -2.84 | 119.40      | 127.00   |
| 22  | B     | 806  | CLA  | C2C-C1C-NC  | 2.84  | 112.97      | 109.98   |
| 22  | F     | 301  | CLA  | CMA-C3A-C4A | 2.84  | 119.41      | 111.77   |
| 22  | 7     | 311  | CLA  | CMA-C3A-C4A | 2.84  | 119.41      | 111.77   |
| 22  | 5     | 323  | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 22  | 7     | 312  | CLA  | C1D-ND-C4D  | -2.84 | 104.32      | 106.31   |
| 22  | 7     | 324  | CLA  | CMA-C3A-C4A | 2.84  | 119.41      | 111.77   |
| 22  | 4     | 808  | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 24  | B     | 844  | BCR  | C36-C18-C17 | -2.84 | 118.21      | 122.82   |
| 22  | F     | 302  | CLA  | C1D-ND-C4D  | -2.84 | 104.32      | 106.31   |
| 22  | B     | 842  | CLA  | C1C-C2C-C3C | -2.84 | 103.99      | 106.98   |
| 22  | A     | 806  | CLA  | CMA-C3A-C4A | 2.84  | 119.41      | 111.77   |
| 22  | B     | 820  | CLA  | C1-C2-C3    | -2.84 | 121.55      | 126.20   |
| 22  | 9     | 304  | CLA  | C2C-C1C-NC  | 2.84  | 112.96      | 109.98   |
| 22  | B     | 808  | CLA  | CMA-C3A-C4A | 2.84  | 119.40      | 111.77   |
| 22  | 5     | 309  | CLA  | C3B-C4B-NB  | -2.84 | 108.00      | 110.53   |
| 22  | A     | 836  | CLA  | C1D-ND-C4D  | -2.84 | 104.32      | 106.31   |
| 22  | A     | 839  | CLA  | C2C-C1C-NC  | 2.84  | 112.96      | 109.98   |
| 22  | 7     | 316  | CLA  | C3B-C4B-NB  | -2.84 | 108.00      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 5     | 309 | CLA  | C2C-C1C-NC  | 2.84  | 112.96      | 109.98   |
| 22  | B     | 816 | CLA  | CMA-C3A-C4A | 2.84  | 119.39      | 111.77   |
| 24  | B     | 848 | BCR  | C2-C1-C6    | 2.83  | 114.56      | 110.44   |
| 22  | 6     | 319 | CLA  | CMA-C3A-C4A | 2.83  | 119.39      | 111.77   |
| 22  | A     | 827 | CLA  | CMA-C3A-C4A | 2.83  | 119.39      | 111.77   |
| 22  | A     | 808 | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 22  | 8     | 309 | CLA  | CMA-C3A-C4A | 2.83  | 119.38      | 111.77   |
| 22  | A     | 807 | CLA  | C1D-ND-C4D  | -2.83 | 104.33      | 106.31   |
| 22  | A     | 828 | CLA  | C1D-ND-C4D  | -2.83 | 104.33      | 106.31   |
| 22  | A     | 840 | CLA  | C1C-C2C-C3C | -2.83 | 104.00      | 106.98   |
| 22  | A     | 822 | CLA  | C2C-C1C-NC  | 2.83  | 112.95      | 109.98   |
| 22  | 3     | 316 | CLA  | CMA-C3A-C4A | 2.83  | 119.38      | 111.77   |
| 22  | A     | 854 | CLA  | C3B-C4B-NB  | -2.83 | 108.01      | 110.53   |
| 24  | 6     | 305 | BCR  | C33-C5-C4   | 2.83  | 119.62      | 113.60   |
| 22  | 2     | 302 | CLA  | C1D-ND-C4D  | -2.83 | 104.33      | 106.31   |
| 22  | 8     | 310 | CLA  | CMA-C3A-C4A | 2.83  | 119.37      | 111.77   |
| 22  | 4     | 815 | CLA  | C3B-C4B-NB  | -2.83 | 108.01      | 110.53   |
| 24  | 3     | 304 | BCR  | C23-C24-C25 | -2.82 | 119.45      | 127.00   |
| 22  | 4     | 812 | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 22  | 6     | 309 | CLA  | C2C-C1C-NC  | 2.82  | 112.95      | 109.98   |
| 22  | B     | 819 | CLA  | C1D-ND-C4D  | -2.82 | 104.33      | 106.31   |
| 22  | 3     | 308 | CLA  | C1D-ND-C4D  | -2.82 | 104.33      | 106.31   |
| 22  | 4     | 812 | CLA  | C2C-C1C-NC  | 2.82  | 112.95      | 109.98   |
| 22  | B     | 822 | CLA  | CMA-C3A-C4A | 2.82  | 119.36      | 111.77   |
| 22  | A     | 817 | CLA  | C2C-C1C-NC  | 2.82  | 112.95      | 109.98   |
| 22  | B     | 811 | CLA  | C2C-C1C-NC  | 2.82  | 112.95      | 109.98   |
| 22  | 6     | 311 | CLA  | C2C-C1C-NC  | 2.82  | 112.95      | 109.98   |
| 22  | A     | 823 | CLA  | C4B-CHC-C1C | 2.82  | 132.88      | 126.25   |
| 38  | 3     | 303 | LUT  | C18-C5-C4   | 2.82  | 119.61      | 114.42   |
| 22  | 3     | 319 | CLA  | C1C-C2C-C3C | -2.82 | 104.01      | 106.98   |
| 22  | 1     | 307 | CLA  | C1D-ND-C4D  | -2.82 | 104.33      | 106.31   |
| 22  | 5     | 310 | CLA  | C1D-ND-C4D  | -2.82 | 104.33      | 106.31   |
| 22  | K     | 204 | CLA  | C2C-C1C-NC  | 2.82  | 112.94      | 109.98   |
| 22  | 9     | 303 | CLA  | CMA-C3A-C4A | 2.82  | 119.35      | 111.77   |
| 22  | 5     | 318 | CLA  | C1-C2-C3    | -2.82 | 121.58      | 126.20   |
| 22  | A     | 810 | CLA  | C1D-ND-C4D  | -2.82 | 104.33      | 106.31   |
| 22  | 4     | 818 | CLA  | C3B-C4B-NB  | -2.82 | 108.02      | 110.53   |
| 22  | 5     | 319 | CLA  | C2C-C1C-NC  | 2.82  | 112.94      | 109.98   |
| 38  | 7     | 301 | LUT  | C1-C6-C5    | -2.82 | 118.79      | 122.64   |
| 22  | 7     | 312 | CLA  | CMA-C3A-C4A | 2.82  | 119.34      | 111.77   |
| 38  | 9     | 301 | LUT  | C18-C5-C4   | 2.82  | 119.60      | 114.42   |
| 22  | 3     | 310 | CLA  | C2C-C1C-NC  | 2.82  | 112.94      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 4     | 809 | CLA  | C1D-ND-C4D  | -2.82 | 104.34      | 106.31   |
| 22  | 4     | 810 | CLA  | C1D-ND-C4D  | -2.82 | 104.34      | 106.31   |
| 22  | 6     | 317 | CLA  | CMA-C3A-C4A | 2.82  | 119.34      | 111.77   |
| 22  | 6     | 311 | CLA  | C1C-C2C-C3C | -2.82 | 104.02      | 106.98   |
| 22  | 6     | 314 | CLA  | C1C-C2C-C3C | -2.82 | 104.02      | 106.98   |
| 22  | 4     | 818 | CLA  | O2A-CGA-CBA | 2.81  | 120.42      | 111.83   |
| 22  | F     | 301 | CLA  | C1D-ND-C4D  | -2.81 | 104.34      | 106.31   |
| 22  | 1     | 310 | CLA  | C2C-C1C-NC  | 2.81  | 112.94      | 109.98   |
| 22  | 8     | 308 | CLA  | C1D-ND-C4D  | -2.81 | 104.34      | 106.31   |
| 38  | 6     | 304 | LUT  | C18-C5-C4   | 2.81  | 119.59      | 114.42   |
| 22  | B     | 806 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 22  | B     | 822 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 38  | 6     | 304 | LUT  | C11-C12-C13 | -2.81 | 118.66      | 126.36   |
| 22  | 6     | 307 | CLA  | C1-C2-C3    | -2.81 | 121.59      | 126.20   |
| 22  | 7     | 310 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 22  | F     | 305 | CLA  | CMA-C3A-C4A | 2.81  | 119.32      | 111.77   |
| 22  | 9     | 305 | CLA  | O2A-CGA-CBA | 2.81  | 120.40      | 111.83   |
| 22  | A     | 811 | CLA  | CMA-C3A-C4A | 2.81  | 119.32      | 111.77   |
| 22  | 5     | 301 | CLA  | C1D-ND-C4D  | -2.81 | 104.34      | 106.31   |
| 22  | 5     | 307 | CLA  | C1D-ND-C4D  | -2.81 | 104.34      | 106.31   |
| 22  | 4     | 807 | CLA  | C1C-C2C-C3C | -2.81 | 104.03      | 106.98   |
| 38  | 5     | 302 | LUT  | C30-C31-C32 | -2.81 | 115.07      | 123.20   |
| 22  | 7     | 306 | CLA  | C1C-C2C-C3C | -2.81 | 104.03      | 106.98   |
| 24  | 3     | 307 | BCR  | C35-C13-C14 | -2.81 | 118.27      | 122.82   |
| 22  | 8     | 307 | CLA  | C2C-C1C-NC  | 2.81  | 112.93      | 109.98   |
| 22  | B     | 826 | CLA  | O2A-CGA-CBA | 2.81  | 120.39      | 111.83   |
| 24  | 3     | 306 | BCR  | C33-C5-C4   | 2.81  | 119.58      | 113.60   |
| 22  | B     | 813 | CLA  | C1D-ND-C4D  | -2.80 | 104.34      | 106.31   |
| 22  | 7     | 322 | CLA  | C1D-ND-C4D  | -2.80 | 104.34      | 106.31   |
| 22  | 6     | 302 | CLA  | CMA-C3A-C4A | 2.80  | 119.31      | 111.77   |
| 24  | A     | 848 | BCR  | C23-C24-C25 | -2.80 | 119.51      | 127.00   |
| 24  | B     | 844 | BCR  | C23-C24-C25 | -2.80 | 119.51      | 127.00   |
| 22  | 1     | 309 | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 24  | B     | 848 | BCR  | C27-C26-C25 | -2.80 | 118.92      | 122.70   |
| 22  | 5     | 326 | CLA  | CMA-C3A-C4A | 2.80  | 119.31      | 111.77   |
| 22  | B     | 816 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 22  | 8     | 309 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 25  | 6     | 323 | LHG  | O8-C23-C24  | 2.80  | 120.38      | 111.83   |
| 22  | 8     | 311 | CLA  | C1D-ND-C4D  | -2.80 | 104.34      | 106.31   |
| 22  | 3     | 319 | CLA  | C2C-C1C-NC  | 2.80  | 112.92      | 109.98   |
| 24  | 6     | 306 | BCR  | C30-C25-C26 | -2.80 | 118.81      | 122.64   |
| 24  | B     | 848 | BCR  | C38-C26-C27 | 2.80  | 119.57      | 113.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 826 | CLA  | C1D-ND-C4D  | -2.80 | 104.35      | 106.31   |
| 22  | 4     | 808 | CLA  | C1D-ND-C4D  | -2.80 | 104.35      | 106.31   |
| 22  | 3     | 312 | CLA  | C2C-C1C-NC  | 2.80  | 112.92      | 109.98   |
| 39  | 9     | 314 | CHL  | CMA-C3A-C2A | 2.80  | 122.65      | 116.23   |
| 22  | 4     | 818 | CLA  | C1D-ND-C4D  | -2.80 | 104.35      | 106.31   |
| 22  | B     | 842 | CLA  | C2C-C1C-NC  | 2.80  | 112.92      | 109.98   |
| 22  | A     | 808 | CLA  | C1C-C2C-C3C | -2.80 | 104.04      | 106.98   |
| 24  | B     | 853 | BCR  | C33-C5-C4   | 2.80  | 119.56      | 113.60   |
| 24  | A     | 856 | BCR  | C8-C7-C6    | -2.80 | 119.52      | 127.00   |
| 22  | 2     | 304 | CLA  | C1D-ND-C4D  | -2.80 | 104.35      | 106.31   |
| 22  | A     | 842 | CLA  | C1C-C2C-C3C | -2.80 | 104.04      | 106.98   |
| 22  | 9     | 305 | CLA  | C1C-C2C-C3C | -2.80 | 104.04      | 106.98   |
| 22  | A     | 832 | CLA  | C1D-ND-C4D  | -2.79 | 104.35      | 106.31   |
| 22  | 7     | 304 | CLA  | C1C-C2C-C3C | -2.79 | 104.04      | 106.98   |
| 22  | 3     | 314 | CLA  | C1-C2-C3    | -2.79 | 121.62      | 126.20   |
| 24  | 3     | 304 | BCR  | C1-C6-C5    | -2.79 | 118.82      | 122.64   |
| 22  | A     | 806 | CLA  | C1D-ND-C4D  | -2.79 | 104.35      | 106.31   |
| 22  | F     | 304 | CLA  | C1D-ND-C4D  | -2.79 | 104.35      | 106.31   |
| 22  | Z     | 305 | CLA  | C1C-C2C-C3C | -2.79 | 104.04      | 106.98   |
| 22  | A     | 827 | CLA  | C2C-C1C-NC  | 2.79  | 112.92      | 109.98   |
| 22  | Z     | 315 | CLA  | C1C-C2C-C3C | -2.79 | 104.04      | 106.98   |
| 25  | 6     | 323 | LHG  | C5-O7-C7    | -2.79 | 111.11      | 117.80   |
| 39  | 9     | 312 | CHL  | C4D-CHA-CBD | -2.79 | 106.15      | 108.97   |
| 22  | A     | 815 | CLA  | C1D-ND-C4D  | -2.79 | 104.35      | 106.31   |
| 22  | K     | 204 | CLA  | C1D-ND-C4D  | -2.79 | 104.35      | 106.31   |
| 38  | 6     | 303 | LUT  | C15-C14-C13 | -2.79 | 123.36      | 127.28   |
| 22  | 1     | 314 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 22  | 8     | 314 | CLA  | CMA-C3A-C4A | 2.79  | 119.27      | 111.77   |
| 22  | B     | 823 | CLA  | C4B-CHC-C1C | 2.79  | 132.81      | 126.25   |
| 22  | L     | 203 | CLA  | C1D-ND-C4D  | -2.79 | 104.36      | 106.31   |
| 22  | 4     | 809 | CLA  | C2C-C1C-NC  | 2.79  | 112.91      | 109.98   |
| 22  | 8     | 313 | CLA  | CMA-C3A-C4A | 2.79  | 119.27      | 111.77   |
| 22  | 7     | 323 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 38  | 9     | 301 | LUT  | C27-C28-C29 | -2.79 | 120.33      | 126.32   |
| 22  | 6     | 302 | CLA  | C2C-C1C-NC  | 2.79  | 112.91      | 109.98   |
| 22  | B     | 810 | CLA  | C1C-C2C-C3C | -2.79 | 104.05      | 106.98   |
| 22  | A     | 826 | CLA  | CMA-C3A-C4A | 2.79  | 119.26      | 111.77   |
| 22  | 7     | 310 | CLA  | C1C-C2C-C3C | -2.79 | 104.05      | 106.98   |
| 22  | 7     | 308 | CLA  | C1D-ND-C4D  | -2.79 | 104.36      | 106.31   |
| 24  | A     | 848 | BCR  | C11-C10-C9  | -2.79 | 123.37      | 127.28   |
| 22  | A     | 808 | CLA  | C1D-ND-C4D  | -2.78 | 104.36      | 106.31   |
| 22  | A     | 827 | CLA  | C1D-ND-C4D  | -2.78 | 104.36      | 106.31   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | A     | 829  | CLA  | C1D-ND-C4D  | -2.78 | 104.36      | 106.31   |
| 22  | 3     | 319  | CLA  | C1D-ND-C4D  | -2.78 | 104.36      | 106.31   |
| 22  | 8     | 314  | CLA  | C3B-C4B-NB  | -2.78 | 108.04      | 110.53   |
| 39  | 4     | 814  | CHL  | C1-O2A-CGA  | 2.78  | 123.39      | 116.65   |
| 24  | B     | 847  | BCR  | C1-C6-C5    | -2.78 | 118.83      | 122.64   |
| 22  | 5     | 314  | CLA  | C1D-ND-C4D  | -2.78 | 104.36      | 106.31   |
| 24  | 5     | 304  | BCR  | C15-C14-C13 | -2.78 | 123.38      | 127.28   |
| 22  | B     | 812  | CLA  | C2C-C1C-NC  | 2.78  | 112.91      | 109.98   |
| 22  | 8     | 305  | CLA  | C2C-C1C-NC  | 2.78  | 112.91      | 109.98   |
| 22  | 9     | 310  | CLA  | C1D-ND-C4D  | -2.78 | 104.36      | 106.31   |
| 22  | 1     | 305  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 22  | 7     | 312  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 22  | 4     | 808  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 22  | B     | 817  | CLA  | C1D-ND-C4D  | -2.78 | 104.36      | 106.31   |
| 22  | Z     | 307  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 22  | B     | 832  | CLA  | CMA-C3A-C4A | 2.78  | 119.25      | 111.77   |
| 24  | A     | 846  | BCR  | C33-C5-C4   | 2.78  | 119.52      | 113.60   |
| 22  | A     | 802  | CLA  | C1D-ND-C4D  | -2.78 | 104.36      | 106.31   |
| 24  | 8     | 304  | BCR  | C11-C12-C13 | -2.78 | 118.74      | 126.36   |
| 22  | A     | 838  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 22  | 3     | 320  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 22  | 5     | 323  | CLA  | C1C-C2C-C3C | -2.78 | 104.06      | 106.98   |
| 22  | B     | 833  | CLA  | C1D-ND-C4D  | -2.78 | 104.36      | 106.31   |
| 22  | A     | 808  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 38  | 8     | 302  | LUT  | C35-C15-C14 | -2.78 | 117.84      | 123.52   |
| 22  | B     | 817  | CLA  | CMA-C3A-C4A | 2.78  | 119.23      | 111.77   |
| 22  | 2     | 304  | CLA  | C2C-C1C-NC  | 2.78  | 112.90      | 109.98   |
| 22  | 1     | 308  | CLA  | CMD-C2D-C3D | -2.78 | 121.33      | 127.69   |
| 22  | 1     | 304  | CLA  | C1D-ND-C4D  | -2.77 | 104.36      | 106.31   |
| 22  | 6     | 322  | CLA  | C2C-C1C-NC  | 2.77  | 112.90      | 109.98   |
| 22  | B     | 832  | CLA  | C3B-C4B-NB  | -2.77 | 108.05      | 110.53   |
| 22  | 5     | 311  | CLA  | C3B-C4B-NB  | -2.77 | 108.05      | 110.53   |
| 22  | B     | 825  | CLA  | C1D-ND-C4D  | -2.77 | 104.37      | 106.31   |
| 22  | Z     | 307  | CLA  | C1C-C2C-C3C | -2.77 | 104.06      | 106.98   |
| 22  | 4     | 817  | CLA  | CAA-C2A-C3A | -2.77 | 109.87      | 116.23   |
| 22  | B     | 805  | CLA  | CMA-C3A-C4A | 2.77  | 119.23      | 111.77   |
| 39  | 6     | 315  | CHL  | C4D-CHA-CBD | -2.77 | 106.17      | 108.97   |
| 21  | A     | 801  | CL0  | O1D-CGD-CBD | -2.77 | 120.52      | 124.72   |
| 24  | I     | 4001 | BCR  | C15-C14-C13 | -2.77 | 123.39      | 127.28   |
| 22  | 3     | 316  | CLA  | C2C-C1C-NC  | 2.77  | 112.89      | 109.98   |
| 22  | A     | 814  | CLA  | C1C-C2C-C3C | -2.77 | 104.06      | 106.98   |
| 22  | A     | 839  | CLA  | C1D-ND-C4D  | -2.77 | 104.37      | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 4     | 815 | CLA  | C1D-ND-C4D  | -2.77 | 104.37      | 106.31   |
| 22  | Z     | 313 | CLA  | C2C-C1C-NC  | 2.77  | 112.89      | 109.98   |
| 22  | 8     | 307 | CLA  | C1C-C2C-C3C | -2.77 | 104.07      | 106.98   |
| 36  | J     | 105 | C7Z  | C21-C26-C25 | -2.77 | 118.85      | 122.64   |
| 22  | A     | 841 | CLA  | CMA-C3A-C4A | 2.77  | 119.22      | 111.77   |
| 22  | 6     | 308 | CLA  | C1C-C2C-C3C | -2.77 | 104.07      | 106.98   |
| 22  | A     | 828 | CLA  | CMA-C3A-C4A | 2.77  | 119.21      | 111.77   |
| 24  | A     | 847 | BCR  | C15-C16-C17 | -2.77 | 117.86      | 123.52   |
| 22  | 4     | 811 | CLA  | O2A-CGA-CBA | 2.77  | 120.27      | 111.83   |
| 22  | A     | 835 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 22  | A     | 829 | CLA  | C2C-C1C-NC  | 2.77  | 112.89      | 109.98   |
| 22  | A     | 820 | CLA  | C1D-ND-C4D  | -2.77 | 104.37      | 106.31   |
| 22  | B     | 831 | CLA  | C1D-ND-C4D  | -2.77 | 104.37      | 106.31   |
| 22  | 6     | 317 | CLA  | C1D-ND-C4D  | -2.77 | 104.37      | 106.31   |
| 24  | 6     | 305 | BCR  | C1-C6-C5    | -2.77 | 118.86      | 122.64   |
| 22  | 6     | 308 | CLA  | CMA-C3A-C4A | 2.77  | 119.21      | 111.77   |
| 22  | A     | 831 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 22  | B     | 829 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 22  | 8     | 308 | CLA  | CMA-C3A-C4A | 2.77  | 119.21      | 111.77   |
| 25  | 1     | 317 | LHG  | O8-C23-C24  | 2.77  | 120.27      | 111.83   |
| 22  | B     | 827 | CLA  | C2C-C1C-NC  | 2.76  | 112.89      | 109.98   |
| 22  | G     | 201 | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 24  | B     | 853 | BCR  | C30-C25-C24 | 2.76  | 123.15      | 115.65   |
| 22  | B     | 813 | CLA  | C2C-C1C-NC  | 2.76  | 112.89      | 109.98   |
| 22  | 7     | 310 | CLA  | C2C-C1C-NC  | 2.76  | 112.89      | 109.98   |
| 22  | 3     | 316 | CLA  | C1D-ND-C4D  | -2.76 | 104.37      | 106.31   |
| 22  | B     | 820 | CLA  | C2C-C1C-NC  | 2.76  | 112.88      | 109.98   |
| 22  | 2     | 302 | CLA  | C2C-C1C-NC  | 2.76  | 112.88      | 109.98   |
| 24  | 7     | 303 | BCR  | C29-C30-C25 | 2.76  | 114.45      | 110.44   |
| 22  | J     | 103 | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 22  | B     | 829 | CLA  | C2C-C1C-NC  | 2.76  | 112.88      | 109.98   |
| 22  | B     | 814 | CLA  | C4B-CHC-C1C | 2.76  | 132.74      | 126.25   |
| 24  | B     | 845 | BCR  | C38-C26-C27 | 2.76  | 119.48      | 113.60   |
| 22  | B     | 834 | CLA  | C1C-C2C-C3C | -2.76 | 104.08      | 106.98   |
| 22  | B     | 836 | CLA  | C1D-ND-C4D  | -2.76 | 104.38      | 106.31   |
| 22  | Z     | 305 | CLA  | C1D-ND-C4D  | -2.76 | 104.38      | 106.31   |
| 24  | A     | 844 | BCR  | C38-C26-C27 | 2.76  | 119.48      | 113.60   |
| 22  | 9     | 306 | CLA  | CMA-C3A-C4A | 2.76  | 119.19      | 111.77   |
| 22  | A     | 832 | CLA  | O2A-C1-C2   | 2.76  | 118.73      | 108.11   |
| 22  | 9     | 311 | CLA  | C1D-ND-C4D  | -2.76 | 104.38      | 106.31   |
| 22  | 5     | 309 | CLA  | O2A-CGA-CBA | 2.76  | 120.25      | 111.83   |
| 38  | 6     | 303 | LUT  | C8-C7-C6    | -2.76 | 119.63      | 127.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | 9     | 312 | CHL  | C3C-C4C-NC  | -2.76 | 107.91      | 114.65   |
| 22  | L     | 202 | CLA  | C1C-C2C-C3C | -2.76 | 104.08      | 106.98   |
| 22  | 5     | 313 | CLA  | C1C-C2C-C3C | -2.76 | 104.08      | 106.98   |
| 22  | 6     | 322 | CLA  | C1C-C2C-C3C | -2.76 | 104.08      | 106.98   |
| 38  | 8     | 302 | LUT  | C1-C6-C5    | -2.76 | 118.87      | 122.64   |
| 22  | 5     | 322 | CLA  | C1D-ND-C4D  | -2.76 | 104.38      | 106.31   |
| 24  | 3     | 306 | BCR  | C38-C26-C27 | 2.76  | 119.47      | 113.60   |
| 22  | 1     | 314 | CLA  | C1C-C2C-C3C | -2.76 | 104.08      | 106.98   |
| 22  | A     | 840 | CLA  | C2C-C1C-NC  | 2.76  | 112.88      | 109.98   |
| 22  | 3     | 315 | CLA  | C2D-C1D-ND  | 2.76  | 112.85      | 110.13   |
| 22  | 1     | 306 | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |
| 22  | 7     | 323 | CLA  | C2C-C1C-NC  | 2.75  | 112.88      | 109.98   |
| 24  | A     | 844 | BCR  | C16-C17-C18 | -2.75 | 123.42      | 127.28   |
| 24  | B     | 853 | BCR  | C2-C1-C6    | 2.75  | 114.44      | 110.44   |
| 22  | 3     | 311 | CLA  | C1D-ND-C4D  | -2.75 | 104.38      | 106.31   |
| 22  | A     | 802 | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 24  | 3     | 305 | BCR  | C20-C19-C18 | -2.75 | 118.81      | 126.36   |
| 24  | 6     | 305 | BCR  | C38-C26-C27 | 2.75  | 119.46      | 113.60   |
| 22  | 6     | 307 | CLA  | CMA-C3A-C4A | 2.75  | 119.17      | 111.77   |
| 22  | A     | 820 | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 22  | 5     | 314 | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 38  | 3     | 303 | LUT  | C15-C35-C34 | -2.75 | 117.89      | 123.52   |
| 22  | Z     | 314 | CLA  | C1C-C2C-C3C | -2.75 | 104.09      | 106.98   |
| 22  | A     | 819 | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 22  | A     | 837 | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 22  | 9     | 304 | CLA  | C1D-ND-C4D  | -2.75 | 104.38      | 106.31   |
| 22  | 3     | 315 | CLA  | CAA-C2A-C3A | -2.75 | 105.57      | 113.00   |
| 22  | F     | 304 | CLA  | O2A-CGA-CBA | 2.75  | 120.22      | 111.83   |
| 22  | A     | 838 | CLA  | C1C-C2C-C3C | -2.75 | 104.09      | 106.98   |
| 22  | 6     | 307 | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 22  | B     | 809 | CLA  | C1C-C2C-C3C | -2.75 | 104.09      | 106.98   |
| 22  | 1     | 315 | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 22  | 9     | 308 | CLA  | C1C-C2C-C3C | -2.75 | 104.09      | 106.98   |
| 22  | 9     | 310 | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 22  | 8     | 307 | CLA  | O2D-CGD-O1D | -2.75 | 118.50      | 123.85   |
| 22  | A     | 835 | CLA  | C1D-ND-C4D  | -2.75 | 104.39      | 106.31   |
| 22  | B     | 841 | CLA  | C1D-ND-C4D  | -2.75 | 104.39      | 106.31   |
| 22  | 4     | 812 | CLA  | C1D-ND-C4D  | -2.75 | 104.39      | 106.31   |
| 22  | 7     | 305 | CLA  | C1C-C2C-C3C | -2.75 | 104.09      | 106.98   |
| 22  | A     | 806 | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 22  | B     | 833 | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |
| 22  | 7     | 305 | CLA  | C2C-C1C-NC  | 2.75  | 112.87      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 831 | CLA  | C1D-ND-C4D  | -2.74 | 104.39      | 106.31   |
| 22  | A     | 855 | CLA  | C1D-ND-C4D  | -2.74 | 104.39      | 106.31   |
| 22  | A     | 802 | CLA  | C1C-C2C-C3C | -2.74 | 104.09      | 106.98   |
| 22  | A     | 816 | CLA  | C1C-C2C-C3C | -2.74 | 104.09      | 106.98   |
| 22  | B     | 811 | CLA  | C1C-C2C-C3C | -2.74 | 104.09      | 106.98   |
| 22  | 4     | 809 | CLA  | C4B-CHC-C1C | 2.74  | 132.70      | 126.25   |
| 22  | A     | 830 | CLA  | O2D-CGD-O1D | -2.74 | 118.51      | 123.85   |
| 22  | A     | 809 | CLA  | C6-C5-C3    | -2.74 | 106.78      | 113.47   |
| 22  | Z     | 316 | CLA  | C4B-CHC-C1C | 2.74  | 132.70      | 126.25   |
| 22  | 7     | 323 | CLA  | C1C-C2C-C3C | -2.74 | 104.09      | 106.98   |
| 22  | 3     | 314 | CLA  | C2C-C1C-NC  | 2.74  | 112.86      | 109.98   |
| 22  | 1     | 308 | CLA  | C4B-CHC-C1C | 2.74  | 132.70      | 126.25   |
| 22  | B     | 839 | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | 3     | 312 | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | 7     | 312 | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | A     | 804 | CLA  | C2C-C1C-NC  | 2.74  | 112.86      | 109.98   |
| 22  | 4     | 811 | CLA  | C1D-ND-C4D  | -2.74 | 104.39      | 106.31   |
| 22  | B     | 834 | CLA  | CMA-C3A-C4A | 2.74  | 119.14      | 111.77   |
| 22  | 8     | 306 | CLA  | C4B-CHC-C1C | 2.74  | 132.69      | 126.25   |
| 22  | K     | 203 | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 23  | A     | 843 | PQN  | C2M-C2-C3   | -2.74 | 119.95      | 124.45   |
| 24  | 3     | 304 | BCR  | C30-C25-C26 | -2.74 | 118.89      | 122.64   |
| 22  | 7     | 314 | CLA  | C3B-C4B-NB  | -2.74 | 108.08      | 110.53   |
| 24  | A     | 845 | BCR  | C23-C24-C25 | -2.74 | 119.68      | 127.00   |
| 22  | B     | 812 | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | 4     | 812 | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | 9     | 309 | CLA  | C2D-C1D-ND  | 2.74  | 112.84      | 110.13   |
| 24  | 3     | 304 | BCR  | C4-C5-C6    | -2.74 | 119.00      | 122.70   |
| 22  | 7     | 316 | CLA  | C1D-ND-C4D  | -2.74 | 104.39      | 106.31   |
| 22  | 8     | 310 | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 22  | Z     | 310 | CLA  | C2C-C1C-NC  | 2.74  | 112.86      | 109.98   |
| 22  | 8     | 309 | CLA  | C1D-ND-C4D  | -2.74 | 104.39      | 106.31   |
| 22  | B     | 840 | CLA  | C2C-C1C-NC  | 2.74  | 112.86      | 109.98   |
| 38  | 6     | 303 | LUT  | C22-C23-C24 | 2.74  | 115.25      | 111.18   |
| 22  | A     | 828 | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 22  | A     | 836 | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 22  | A     | 839 | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | Z     | 313 | CLA  | C1C-C2C-C3C | -2.74 | 104.10      | 106.98   |
| 22  | F     | 305 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 22  | 7     | 322 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 22  | B     | 841 | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |
| 22  | 5     | 311 | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 820 | CLA  | C4B-CHC-C1C | 2.73  | 132.68      | 126.25   |
| 22  | 8     | 313 | CLA  | C1C-C2C-C3C | -2.73 | 104.11      | 106.98   |
| 22  | 8     | 311 | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |
| 22  | B     | 806 | CLA  | C1C-C2C-C3C | -2.73 | 104.11      | 106.98   |
| 24  | A     | 846 | BCR  | C2-C1-C6    | 2.73  | 114.41      | 110.44   |
| 22  | 8     | 308 | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |
| 22  | 5     | 301 | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |
| 22  | A     | 812 | CLA  | C4B-CHC-C1C | 2.73  | 132.67      | 126.25   |
| 22  | A     | 825 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 22  | 3     | 310 | CLA  | C1C-C2C-C3C | -2.73 | 104.11      | 106.98   |
| 22  | 2     | 301 | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |
| 22  | B     | 839 | CLA  | C1D-ND-C4D  | -2.73 | 104.40      | 106.31   |
| 22  | 6     | 302 | CLA  | C1D-ND-C4D  | -2.73 | 104.40      | 106.31   |
| 22  | B     | 837 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 22  | B     | 813 | CLA  | C1C-C2C-C3C | -2.73 | 104.11      | 106.98   |
| 22  | 3     | 309 | CLA  | C1D-ND-C4D  | -2.73 | 104.40      | 106.31   |
| 22  | 1     | 304 | CLA  | C1C-C2C-C3C | -2.73 | 104.11      | 106.98   |
| 38  | Z     | 301 | LUT  | C21-C26-C27 | -2.73 | 109.69      | 112.83   |
| 22  | 4     | 808 | CLA  | C1C-C2C-C3C | -2.73 | 104.11      | 106.98   |
| 22  | F     | 304 | CLA  | C2C-C1C-NC  | 2.73  | 112.85      | 109.98   |
| 22  | A     | 854 | CLA  | C1D-ND-C4D  | -2.73 | 104.40      | 106.31   |
| 22  | A     | 807 | CLA  | C2C-C1C-NC  | 2.73  | 112.84      | 109.98   |
| 22  | 1     | 305 | CLA  | CMA-C3A-C4A | 2.73  | 119.10      | 111.77   |
| 22  | G     | 201 | CLA  | C4B-CHC-C1C | 2.73  | 132.66      | 126.25   |
| 40  | 1     | 318 | SQD  | O7-S-C6     | -2.73 | 102.69      | 106.76   |
| 22  | B     | 809 | CLA  | C1D-ND-C4D  | -2.73 | 104.40      | 106.31   |
| 22  | 6     | 321 | CLA  | C1D-ND-C4D  | -2.73 | 104.40      | 106.31   |
| 22  | 6     | 309 | CLA  | C1C-C2C-C3C | -2.72 | 104.11      | 106.98   |
| 22  | A     | 809 | CLA  | C4B-CHC-C1C | 2.72  | 132.65      | 126.25   |
| 22  | 7     | 323 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 22  | K     | 204 | CLA  | C1C-C2C-C3C | -2.72 | 104.11      | 106.98   |
| 22  | 3     | 320 | CLA  | C1C-C2C-C3C | -2.72 | 104.11      | 106.98   |
| 22  | 6     | 302 | CLA  | C1C-C2C-C3C | -2.72 | 104.11      | 106.98   |
| 22  | 3     | 322 | CLA  | C2C-C1C-NC  | 2.72  | 112.84      | 109.98   |
| 22  | 9     | 311 | CLA  | C2C-C1C-NC  | 2.72  | 112.84      | 109.98   |
| 21  | A     | 801 | CL0  | CMC-C2C-C1C | 2.72  | 129.63      | 124.73   |
| 22  | B     | 821 | CLA  | C1D-ND-C4D  | -2.72 | 104.40      | 106.31   |
| 22  | 8     | 316 | CLA  | C1D-ND-C4D  | -2.72 | 104.40      | 106.31   |
| 22  | B     | 811 | CLA  | C4B-CHC-C1C | 2.72  | 132.65      | 126.25   |
| 22  | 6     | 321 | CLA  | C2C-C1C-NC  | 2.72  | 112.84      | 109.98   |
| 22  | B     | 829 | CLA  | C1D-ND-C4D  | -2.72 | 104.40      | 106.31   |
| 22  | 8     | 307 | CLA  | C1D-ND-C4D  | -2.72 | 104.40      | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 817 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 22  | 1     | 313 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 22  | 1     | 306 | CLA  | C2C-C1C-NC  | 2.72  | 112.84      | 109.98   |
| 22  | 6     | 313 | CLA  | C2C-C1C-NC  | 2.72  | 112.84      | 109.98   |
| 22  | 7     | 316 | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 41  | 7     | 319 | 3PH  | O31-C31-C32 | 2.72  | 120.13      | 111.83   |
| 22  | B     | 828 | CLA  | C1D-ND-C4D  | -2.72 | 104.40      | 106.31   |
| 22  | 1     | 310 | CLA  | C4B-CHC-C1C | 2.72  | 132.64      | 126.25   |
| 22  | 1     | 309 | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 22  | 8     | 314 | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 22  | 7     | 304 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 22  | A     | 824 | CLA  | C4B-CHC-C1C | 2.72  | 132.64      | 126.25   |
| 22  | 5     | 315 | CLA  | C1D-ND-C4D  | -2.72 | 104.40      | 106.31   |
| 22  | B     | 827 | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 22  | 1     | 304 | CLA  | C2C-C1C-NC  | 2.72  | 112.84      | 109.98   |
| 22  | L     | 203 | CLA  | C2C-C1C-NC  | 2.72  | 112.84      | 109.98   |
| 22  | 9     | 306 | CLA  | C1D-ND-C4D  | -2.72 | 104.41      | 106.31   |
| 22  | A     | 808 | CLA  | C4B-CHC-C1C | 2.72  | 132.64      | 126.25   |
| 22  | 8     | 310 | CLA  | C1C-C2C-C3C | -2.72 | 104.12      | 106.98   |
| 24  | B     | 848 | BCR  | C33-C5-C4   | 2.72  | 119.39      | 113.60   |
| 22  | 8     | 305 | CLA  | C1D-ND-C4D  | -2.72 | 104.41      | 106.31   |
| 22  | A     | 827 | CLA  | C3B-C4B-NB  | -2.72 | 108.11      | 110.53   |
| 22  | B     | 812 | CLA  | CMA-C3A-C4A | 2.72  | 119.07      | 111.77   |
| 22  | A     | 837 | CLA  | C4B-CHC-C1C | 2.72  | 132.63      | 126.25   |
| 22  | A     | 818 | CLA  | C3B-C4B-NB  | -2.72 | 108.11      | 110.53   |
| 22  | F     | 305 | CLA  | C1D-ND-C4D  | -2.72 | 104.41      | 106.31   |
| 22  | 1     | 315 | CLA  | C1D-ND-C4D  | -2.72 | 104.41      | 106.31   |
| 22  | 5     | 309 | CLA  | C1D-ND-C4D  | -2.72 | 104.41      | 106.31   |
| 22  | Z     | 306 | CLA  | C4B-CHC-C1C | 2.71  | 132.63      | 126.25   |
| 22  | 3     | 311 | CLA  | CMA-C3A-C4A | 2.71  | 119.07      | 111.77   |
| 22  | B     | 821 | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 22  | A     | 840 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | B     | 840 | CLA  | C1D-ND-C4D  | -2.71 | 104.41      | 106.31   |
| 22  | 5     | 309 | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 22  | B     | 827 | CLA  | CMA-C3A-C4A | 2.71  | 119.07      | 111.77   |
| 21  | A     | 801 | CL0  | C4-C3-C5    | 2.71  | 119.94      | 115.23   |
| 22  | 7     | 309 | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 24  | 3     | 307 | BCR  | C19-C18-C17 | -2.71 | 114.74      | 119.01   |
| 22  | 4     | 805 | CLA  | O2A-CGA-CBA | 2.71  | 120.11      | 111.83   |
| 22  | 9     | 307 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | 5     | 311 | CLA  | CMA-C3A-C4A | 2.71  | 119.06      | 111.77   |
| 22  | A     | 836 | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 5     | 307 | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 22  | B     | 809 | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 22  | 3     | 310 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | 7     | 306 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | Z     | 309 | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 22  | Z     | 304 | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 22  | A     | 811 | CLA  | C4B-CHC-C1C | 2.71  | 132.62      | 126.25   |
| 22  | B     | 805 | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 22  | B     | 830 | CLA  | C4B-CHC-C1C | 2.71  | 132.62      | 126.25   |
| 22  | A     | 830 | CLA  | C1D-ND-C4D  | -2.71 | 104.41      | 106.31   |
| 22  | B     | 816 | CLA  | C1D-ND-C4D  | -2.71 | 104.41      | 106.31   |
| 22  | 5     | 315 | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 22  | K     | 202 | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 22  | 5     | 312 | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 22  | 3     | 319 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | A     | 825 | CLA  | C1D-ND-C4D  | -2.71 | 104.41      | 106.31   |
| 22  | 3     | 314 | CLA  | C1D-ND-C4D  | -2.71 | 104.41      | 106.31   |
| 22  | B     | 821 | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 22  | 6     | 317 | CLA  | C2C-C1C-NC  | 2.71  | 112.83      | 109.98   |
| 22  | 7     | 307 | CLA  | C4B-CHC-C1C | 2.71  | 132.61      | 126.25   |
| 24  | B     | 849 | BCR  | C2-C1-C6    | 2.71  | 114.37      | 110.44   |
| 22  | B     | 825 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | B     | 826 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | B     | 841 | CLA  | C1C-C2C-C3C | -2.71 | 104.13      | 106.98   |
| 32  | F     | 306 | RRX  | C38-C26-C27 | 2.71  | 119.40      | 114.42   |
| 22  | 3     | 315 | CLA  | C1D-ND-C4D  | -2.71 | 104.41      | 106.31   |
| 22  | Z     | 308 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | 3     | 318 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | B     | 837 | CLA  | C2C-C1C-NC  | 2.71  | 112.82      | 109.98   |
| 22  | 1     | 307 | CLA  | C2C-C1C-NC  | 2.71  | 112.82      | 109.98   |
| 22  | B     | 809 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | 6     | 321 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 22  | F     | 304 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 8     | 314 | CLA  | C2C-C1C-NC  | 2.70  | 112.82      | 109.98   |
| 22  | 6     | 307 | CLA  | C1D-ND-C4D  | -2.70 | 104.42      | 106.31   |
| 22  | A     | 807 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 8     | 311 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 5     | 311 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 4     | 811 | CLA  | C2C-C1C-NC  | 2.70  | 112.82      | 109.98   |
| 22  | B     | 821 | CLA  | CMA-C3A-C4A | 2.70  | 119.04      | 111.77   |
| 22  | 2     | 304 | CLA  | C4B-CHC-C1C | 2.70  | 132.60      | 126.25   |
| 22  | 8     | 310 | CLA  | C2C-C1C-NC  | 2.70  | 112.82      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 4     | 810 | CLA  | C2C-C1C-NC  | 2.70  | 112.82      | 109.98   |
| 22  | B     | 831 | CLA  | CMD-C2D-C3D | -2.70 | 121.49      | 127.69   |
| 24  | 7     | 303 | BCR  | C15-C16-C17 | -2.70 | 117.99      | 123.52   |
| 22  | A     | 806 | CLA  | C4B-CHC-C1C | 2.70  | 132.60      | 126.25   |
| 22  | A     | 832 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 9     | 311 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 1     | 313 | CLA  | C2C-C1C-NC  | 2.70  | 112.82      | 109.98   |
| 34  | F     | 308 | LMG  | O8-C28-C29  | 2.70  | 120.07      | 111.83   |
| 22  | B     | 838 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 6     | 307 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | 7     | 324 | CLA  | C2C-C1C-NC  | 2.70  | 112.82      | 109.98   |
| 22  | A     | 831 | CLA  | CMA-C3A-C4A | 2.70  | 119.03      | 111.77   |
| 24  | B     | 846 | BCR  | C11-C10-C9  | -2.70 | 123.49      | 127.28   |
| 24  | 3     | 304 | BCR  | C10-C11-C12 | 2.70  | 131.02      | 123.20   |
| 25  | 8     | 317 | LHG  | O8-C23-C24  | 2.70  | 120.06      | 111.83   |
| 22  | A     | 832 | CLA  | C2C-C1C-NC  | 2.70  | 112.82      | 109.98   |
| 22  | 6     | 301 | CLA  | C2C-C1C-NC  | 2.70  | 112.82      | 109.98   |
| 22  | 7     | 307 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 22  | 1     | 309 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 22  | B     | 840 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | A     | 834 | CLA  | C1D-ND-C4D  | -2.70 | 104.42      | 106.31   |
| 22  | 4     | 817 | CLA  | C1D-ND-C4D  | -2.70 | 104.42      | 106.31   |
| 22  | 6     | 319 | CLA  | C1D-ND-C4D  | -2.70 | 104.42      | 106.31   |
| 22  | B     | 831 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 22  | Z     | 305 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 22  | A     | 825 | CLA  | C2C-C1C-NC  | 2.70  | 112.81      | 109.98   |
| 22  | 7     | 304 | CLA  | C2C-C1C-NC  | 2.70  | 112.81      | 109.98   |
| 22  | 1     | 305 | CLA  | C4B-CHC-C1C | 2.70  | 132.59      | 126.25   |
| 22  | 8     | 307 | CLA  | CMA-C3A-C4A | 2.70  | 119.02      | 111.77   |
| 22  | 3     | 316 | CLA  | C4B-CHC-C1C | 2.70  | 132.59      | 126.25   |
| 22  | 8     | 308 | CLA  | C1C-C2C-C3C | -2.70 | 104.14      | 106.98   |
| 22  | B     | 840 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 24  | A     | 844 | BCR  | C33-C5-C4   | 2.69  | 119.34      | 113.60   |
| 25  | B     | 850 | LHG  | C5-O7-C7    | -2.69 | 111.35      | 117.80   |
| 22  | 5     | 301 | CLA  | C1C-C2C-C3C | -2.69 | 104.15      | 106.98   |
| 25  | Z     | 317 | LHG  | O8-C23-C24  | 2.69  | 120.05      | 111.83   |
| 24  | K     | 206 | BCR  | C33-C5-C4   | 2.69  | 119.34      | 113.60   |
| 22  | 9     | 306 | CLA  | C2C-C1C-NC  | 2.69  | 112.81      | 109.98   |
| 36  | J     | 105 | C7Z  | C7-C8-C9    | -2.69 | 122.25      | 126.23   |
| 22  | 6     | 314 | CLA  | C4B-CHC-C1C | 2.69  | 132.58      | 126.25   |
| 22  | 8     | 309 | CLA  | C2C-C1C-NC  | 2.69  | 112.81      | 109.98   |
| 22  | 8     | 313 | CLA  | C2C-C1C-NC  | 2.69  | 112.81      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 5     | 326 | CLA  | C2C-C1C-NC  | 2.69  | 112.81      | 109.98   |
| 24  | A     | 846 | BCR  | C8-C7-C6    | -2.69 | 119.81      | 127.00   |
| 22  | Z     | 304 | CLA  | C4B-CHC-C1C | 2.69  | 132.58      | 126.25   |
| 22  | 8     | 310 | CLA  | C1D-ND-C4D  | -2.69 | 104.42      | 106.31   |
| 22  | B     | 842 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 22  | Z     | 313 | CLA  | C4B-CHC-C1C | 2.69  | 132.58      | 126.25   |
| 22  | 7     | 312 | CLA  | C4B-CHC-C1C | 2.69  | 132.57      | 126.25   |
| 22  | 7     | 317 | CLA  | C1D-ND-C4D  | -2.69 | 104.42      | 106.31   |
| 22  | B     | 805 | CLA  | C4B-CHC-C1C | 2.69  | 132.57      | 126.25   |
| 24  | 7     | 303 | BCR  | C8-C7-C6    | -2.69 | 119.81      | 127.00   |
| 22  | A     | 824 | CLA  | C1-C2-C3    | -2.69 | 121.79      | 126.20   |
| 22  | A     | 806 | CLA  | C1C-C2C-C3C | -2.69 | 104.15      | 106.98   |
| 22  | 3     | 316 | CLA  | C1C-C2C-C3C | -2.69 | 104.15      | 106.98   |
| 22  | L     | 201 | CLA  | C2C-C1C-NC  | 2.69  | 112.81      | 109.98   |
| 22  | 5     | 307 | CLA  | C2C-C1C-NC  | 2.69  | 112.81      | 109.98   |
| 22  | 5     | 322 | CLA  | C2C-C1C-NC  | 2.69  | 112.81      | 109.98   |
| 22  | 5     | 307 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 22  | A     | 833 | CLA  | C1C-C2C-C3C | -2.69 | 104.15      | 106.98   |
| 22  | 7     | 307 | CLA  | C1C-C2C-C3C | -2.69 | 104.15      | 106.98   |
| 22  | Z     | 307 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 22  | F     | 302 | CLA  | C4B-CHC-C1C | 2.69  | 132.57      | 126.25   |
| 22  | 3     | 322 | CLA  | C1D-ND-C4D  | -2.69 | 104.43      | 106.31   |
| 22  | 7     | 323 | CLA  | C1D-ND-C4D  | -2.69 | 104.43      | 106.31   |
| 25  | 9     | 315 | LHG  | O8-C23-C24  | 2.69  | 120.03      | 111.83   |
| 22  | A     | 803 | CLA  | C4B-CHC-C1C | 2.69  | 132.57      | 126.25   |
| 24  | 6     | 306 | BCR  | C16-C15-C14 | -2.69 | 118.02      | 123.52   |
| 24  | A     | 856 | BCR  | C38-C26-C27 | 2.69  | 119.33      | 113.60   |
| 22  | 7     | 308 | CLA  | C2C-C1C-NC  | 2.69  | 112.80      | 109.98   |
| 22  | Z     | 313 | CLA  | C1D-ND-C4D  | -2.69 | 104.43      | 106.31   |
| 22  | 9     | 308 | CLA  | C1D-ND-C4D  | -2.69 | 104.43      | 106.31   |
| 22  | 1     | 316 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 22  | 5     | 312 | CLA  | C1C-C2C-C3C | -2.69 | 104.16      | 106.98   |
| 22  | 6     | 310 | CLA  | CMA-C3A-C4A | 2.69  | 118.99      | 111.77   |
| 22  | A     | 831 | CLA  | C2C-C1C-NC  | 2.69  | 112.80      | 109.98   |
| 22  | B     | 826 | CLA  | C1D-ND-C4D  | -2.69 | 104.43      | 106.31   |
| 22  | 6     | 314 | CLA  | C1D-ND-C4D  | -2.69 | 104.43      | 106.31   |
| 22  | 9     | 304 | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | A     | 821 | CLA  | C2C-C1C-NC  | 2.68  | 112.80      | 109.98   |
| 22  | Z     | 313 | CLA  | C1-C2-C3    | -2.68 | 121.80      | 126.20   |
| 22  | 5     | 309 | CLA  | C4B-CHC-C1C | 2.68  | 132.56      | 126.25   |
| 22  | 1     | 316 | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | 9     | 313 | CLA  | C2C-C1C-NC  | 2.68  | 112.80      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | Z     | 316 | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | B     | 810 | CLA  | C1D-ND-C4D  | -2.68 | 104.43      | 106.31   |
| 22  | B     | 827 | CLA  | C1D-ND-C4D  | -2.68 | 104.43      | 106.31   |
| 22  | B     | 820 | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | 1     | 315 | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | Z     | 308 | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | A     | 818 | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | 4     | 810 | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | 5     | 326 | CLA  | C1D-ND-C4D  | -2.68 | 104.43      | 106.31   |
| 22  | 9     | 313 | CLA  | C4B-CHC-C1C | 2.68  | 132.55      | 126.25   |
| 22  | A     | 839 | CLA  | C3B-C4B-NB  | -2.68 | 108.14      | 110.53   |
| 38  | 7     | 302 | LUT  | C18-C5-C4   | 2.68  | 119.35      | 114.42   |
| 25  | A     | 850 | LHG  | O8-C23-C24  | 2.68  | 120.01      | 111.83   |
| 22  | B     | 832 | CLA  | C2C-C1C-NC  | 2.68  | 112.80      | 109.98   |
| 22  | J     | 103 | CLA  | C2C-C1C-NC  | 2.68  | 112.80      | 109.98   |
| 39  | 8     | 315 | CHL  | C1-O2A-CGA  | 2.68  | 123.14      | 116.65   |
| 22  | B     | 835 | CLA  | C3B-C4B-NB  | -2.68 | 108.14      | 110.53   |
| 22  | 5     | 310 | CLA  | C3B-C4B-NB  | -2.68 | 108.14      | 110.53   |
| 22  | G     | 202 | CLA  | C1D-ND-C4D  | -2.68 | 104.43      | 106.31   |
| 22  | G     | 201 | CLA  | C1C-C2C-C3C | -2.68 | 104.16      | 106.98   |
| 22  | 9     | 306 | CLA  | C4B-CHC-C1C | 2.68  | 132.55      | 126.25   |
| 22  | 6     | 308 | CLA  | C2C-C1C-NC  | 2.68  | 112.80      | 109.98   |
| 22  | 1     | 306 | CLA  | C1D-ND-C4D  | -2.68 | 104.43      | 106.31   |
| 22  | 7     | 324 | CLA  | C1D-ND-C4D  | -2.68 | 104.43      | 106.31   |
| 38  | 7     | 302 | LUT  | C11-C12-C13 | -2.68 | 119.02      | 126.36   |
| 24  | G     | 203 | BCR  | C33-C5-C4   | 2.68  | 119.31      | 113.60   |
| 22  | B     | 830 | CLA  | C2C-C1C-NC  | 2.68  | 112.79      | 109.98   |
| 22  | L     | 201 | CLA  | C1C-C2C-C3C | -2.68 | 104.17      | 106.98   |
| 22  | 4     | 817 | CLA  | C1C-C2C-C3C | -2.68 | 104.17      | 106.98   |
| 22  | 5     | 310 | CLA  | C1C-C2C-C3C | -2.68 | 104.17      | 106.98   |
| 22  | 9     | 307 | CLA  | C2C-C1C-NC  | 2.68  | 112.79      | 109.98   |
| 22  | A     | 804 | CLA  | C3B-C4B-NB  | -2.68 | 108.14      | 110.53   |
| 31  | B     | 852 | DGD  | O1G-C1A-C2A | 2.67  | 119.99      | 111.83   |
| 22  | J     | 103 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | 5     | 314 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 38  | 9     | 301 | LUT  | C21-C26-C27 | -2.67 | 109.75      | 112.83   |
| 22  | 1     | 314 | CLA  | C1D-ND-C4D  | -2.67 | 104.44      | 106.31   |
| 22  | L     | 203 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | 6     | 313 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | 2     | 301 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | 3     | 322 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | 7     | 309 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 7     | 324 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | A     | 824 | CLA  | C2C-C1C-NC  | 2.67  | 112.79      | 109.98   |
| 22  | 4     | 805 | CLA  | C4B-CHC-C1C | 2.67  | 132.53      | 126.25   |
| 36  | 5     | 306 | C7Z  | C28-C27-C26 | -2.67 | 119.86      | 127.00   |
| 22  | 6     | 312 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | F     | 301 | CLA  | C2C-C1C-NC  | 2.67  | 112.79      | 109.98   |
| 22  | Z     | 309 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | 3     | 308 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | B     | 831 | CLA  | C2C-C1C-NC  | 2.67  | 112.79      | 109.98   |
| 24  | J     | 104 | BCR  | C20-C19-C18 | -2.67 | 119.04      | 126.36   |
| 22  | B     | 801 | CLA  | C1D-ND-C4D  | -2.67 | 104.44      | 106.31   |
| 22  | B     | 839 | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |
| 22  | A     | 826 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | B     | 801 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | B     | 831 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | 4     | 809 | CLA  | C1C-C2C-C3C | -2.67 | 104.17      | 106.98   |
| 22  | B     | 828 | CLA  | C4B-CHC-C1C | 2.67  | 132.52      | 126.25   |
| 22  | A     | 810 | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |
| 22  | A     | 840 | CLA  | C1D-ND-C4D  | -2.67 | 104.44      | 106.31   |
| 22  | 3     | 312 | CLA  | C4B-CHC-C1C | 2.67  | 132.52      | 126.25   |
| 22  | A     | 805 | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |
| 22  | 1     | 307 | CLA  | C4B-CHC-C1C | 2.67  | 132.52      | 126.25   |
| 22  | 4     | 811 | CLA  | C4B-CHC-C1C | 2.67  | 132.52      | 126.25   |
| 22  | 8     | 305 | CLA  | C4B-CHC-C1C | 2.67  | 132.52      | 126.25   |
| 22  | 3     | 308 | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |
| 22  | B     | 833 | CLA  | C1C-C2C-C3C | -2.67 | 104.18      | 106.98   |
| 22  | B     | 826 | CLA  | C2C-C1C-NC  | 2.67  | 112.78      | 109.98   |
| 22  | 4     | 806 | CLA  | C2C-C1C-NC  | 2.67  | 112.78      | 109.98   |
| 22  | A     | 819 | CLA  | C1D-ND-C4D  | -2.67 | 104.44      | 106.31   |
| 22  | A     | 841 | CLA  | C4B-CHC-C1C | 2.67  | 132.51      | 126.25   |
| 24  | B     | 848 | BCR  | C1-C6-C5    | -2.67 | 118.99      | 122.64   |
| 22  | 3     | 314 | CLA  | C1C-C2C-C3C | -2.67 | 104.18      | 106.98   |
| 32  | F     | 306 | RRX  | C23-C24-C25 | -2.66 | 119.88      | 127.00   |
| 22  | F     | 302 | CLA  | C2C-C1C-NC  | 2.66  | 112.78      | 109.98   |
| 22  | 8     | 314 | CLA  | C1D-ND-C4D  | -2.66 | 104.44      | 106.31   |
| 22  | F     | 301 | CLA  | C1C-C2C-C3C | -2.66 | 104.18      | 106.98   |
| 22  | 7     | 308 | CLA  | C1C-C2C-C3C | -2.66 | 104.18      | 106.98   |
| 22  | 5     | 322 | CLA  | C1C-C2C-C3C | -2.66 | 104.18      | 106.98   |
| 22  | B     | 826 | CLA  | CMA-C3A-C4A | 2.66  | 118.93      | 111.77   |
| 22  | B     | 810 | CLA  | C3B-C4B-NB  | -2.66 | 108.15      | 110.53   |
| 22  | 5     | 320 | CLA  | CMA-C3A-C4A | 2.66  | 118.93      | 111.77   |
| 22  | B     | 822 | CLA  | C1D-ND-C4D  | -2.66 | 104.44      | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 827 | CLA  | C1C-C2C-C3C | -2.66 | 104.18      | 106.98   |
| 22  | 7     | 323 | CLA  | C1-C2-C3    | -2.66 | 121.84      | 126.20   |
| 25  | B     | 803 | LHG  | O8-C23-C24  | 2.66  | 119.95      | 111.83   |
| 38  | Z     | 301 | LUT  | C18-C5-C6   | -2.66 | 121.58      | 124.48   |
| 22  | 3     | 318 | CLA  | C1C-C2C-C3C | -2.66 | 104.18      | 106.98   |
| 22  | B     | 818 | CLA  | C4B-CHC-C1C | 2.66  | 132.50      | 126.25   |
| 22  | Z     | 314 | CLA  | C2C-C1C-NC  | 2.66  | 112.78      | 109.98   |
| 22  | 8     | 316 | CLA  | C2C-C1C-NC  | 2.66  | 112.78      | 109.98   |
| 22  | 3     | 309 | CLA  | CMA-C3A-C4A | 2.66  | 118.92      | 111.77   |
| 22  | L     | 203 | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 22  | 6     | 311 | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 22  | B     | 819 | CLA  | C1C-C2C-C3C | -2.66 | 104.18      | 106.98   |
| 22  | 3     | 308 | CLA  | O2A-CGA-CBA | 2.66  | 119.94      | 111.83   |
| 32  | F     | 306 | RRX  | C2-C1-C6    | 2.66  | 114.30      | 110.44   |
| 22  | Z     | 304 | CLA  | C1C-C2C-C3C | -2.66 | 104.18      | 106.98   |
| 22  | A     | 818 | CLA  | C2C-C1C-NC  | 2.66  | 112.78      | 109.98   |
| 22  | 7     | 311 | CLA  | C2C-C1C-NC  | 2.66  | 112.78      | 109.98   |
| 22  | L     | 201 | CLA  | C4B-CHC-C1C | 2.66  | 132.50      | 126.25   |
| 22  | 5     | 326 | CLA  | C4B-CHC-C1C | 2.66  | 132.50      | 126.25   |
| 38  | 8     | 303 | LUT  | C18-C5-C4   | 2.66  | 119.31      | 114.42   |
| 22  | 6     | 310 | CLA  | C4B-CHC-C1C | 2.66  | 132.50      | 126.25   |
| 22  | 4     | 806 | CLA  | C1C-C2C-C3C | -2.66 | 104.18      | 106.98   |
| 22  | F     | 301 | CLA  | C4B-CHC-C1C | 2.66  | 132.50      | 126.25   |
| 22  | 5     | 308 | CLA  | C1D-ND-C4D  | -2.66 | 104.45      | 106.31   |
| 22  | B     | 809 | CLA  | CMA-C3A-C4A | 2.66  | 118.92      | 111.77   |
| 22  | 6     | 311 | CLA  | CMA-C3A-C4A | 2.66  | 118.92      | 111.77   |
| 22  | 2     | 304 | CLA  | C1C-C2C-C3C | -2.66 | 104.19      | 106.98   |
| 22  | A     | 830 | CLA  | C2C-C1C-NC  | 2.66  | 112.77      | 109.98   |
| 22  | K     | 202 | CLA  | C1D-ND-C4D  | -2.66 | 104.45      | 106.31   |
| 22  | 6     | 321 | CLA  | C1C-C2C-C3C | -2.66 | 104.19      | 106.98   |
| 22  | A     | 828 | CLA  | C2C-C1C-NC  | 2.66  | 112.77      | 109.98   |
| 22  | 3     | 320 | CLA  | C2D-C1D-ND  | 2.66  | 112.75      | 110.13   |
| 22  | Z     | 307 | CLA  | O2D-CGD-O1D | -2.66 | 118.68      | 123.85   |
| 24  | 3     | 305 | BCR  | C7-C8-C9    | -2.66 | 122.31      | 126.23   |
| 22  | A     | 815 | CLA  | CMA-C3A-C4A | 2.66  | 118.91      | 111.77   |
| 22  | B     | 805 | CLA  | C2C-C1C-NC  | 2.66  | 112.77      | 109.98   |
| 22  | L     | 202 | CLA  | C2C-C1C-NC  | 2.66  | 112.77      | 109.98   |
| 22  | 7     | 314 | CLA  | C2C-C1C-NC  | 2.66  | 112.77      | 109.98   |
| 22  | Z     | 310 | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | A     | 836 | CLA  | C2C-C1C-NC  | 2.65  | 112.77      | 109.98   |
| 22  | B     | 817 | CLA  | O2D-CGD-O1D | -2.65 | 118.68      | 123.85   |
| 22  | 8     | 311 | CLA  | C4B-CHC-C1C | 2.65  | 132.49      | 126.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 821 | CLA  | C1D-ND-C4D  | -2.65 | 104.45      | 106.31   |
| 22  | 1     | 307 | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | 5     | 308 | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | Z     | 303 | CLA  | C4B-CHC-C1C | 2.65  | 132.49      | 126.25   |
| 22  | 7     | 324 | CLA  | O2A-CGA-CBA | 2.65  | 119.92      | 111.83   |
| 22  | B     | 835 | CLA  | CMA-C3A-C4A | 2.65  | 118.90      | 111.77   |
| 22  | 5     | 308 | CLA  | C2C-C1C-NC  | 2.65  | 112.77      | 109.98   |
| 22  | 2     | 301 | CLA  | C4B-CHC-C1C | 2.65  | 132.48      | 126.25   |
| 24  | B     | 848 | BCR  | C4-C5-C6    | -2.65 | 119.12      | 122.70   |
| 22  | 3     | 311 | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | 9     | 306 | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | B     | 838 | CLA  | C2C-C1C-NC  | 2.65  | 112.77      | 109.98   |
| 22  | 7     | 309 | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 22  | 7     | 315 | CLA  | C1C-C2C-C3C | -2.65 | 104.19      | 106.98   |
| 22  | A     | 826 | CLA  | C2C-C1C-NC  | 2.65  | 112.77      | 109.98   |
| 22  | 3     | 308 | CLA  | C2C-C1C-NC  | 2.65  | 112.77      | 109.98   |
| 22  | 5     | 323 | CLA  | C2C-C1C-NC  | 2.65  | 112.77      | 109.98   |
| 22  | A     | 815 | CLA  | C2C-C1C-NC  | 2.65  | 112.76      | 109.98   |
| 22  | 7     | 317 | CLA  | C2C-C1C-NC  | 2.65  | 112.76      | 109.98   |
| 22  | B     | 819 | CLA  | C2C-C1C-NC  | 2.65  | 112.76      | 109.98   |
| 22  | A     | 835 | CLA  | C1C-C2C-C3C | -2.65 | 104.20      | 106.98   |
| 22  | 1     | 305 | CLA  | C1C-C2C-C3C | -2.65 | 104.20      | 106.98   |
| 22  | Z     | 316 | CLA  | C2C-C1C-NC  | 2.65  | 112.76      | 109.98   |
| 22  | 7     | 307 | CLA  | C2C-C1C-NC  | 2.65  | 112.76      | 109.98   |
| 22  | A     | 855 | CLA  | C4B-CHC-C1C | 2.65  | 132.47      | 126.25   |
| 22  | 7     | 311 | CLA  | C1C-C2C-C3C | -2.65 | 104.20      | 106.98   |
| 22  | 6     | 301 | CLA  | C1C-C2C-C3C | -2.65 | 104.20      | 106.98   |
| 22  | A     | 834 | CLA  | C2C-C1C-NC  | 2.65  | 112.76      | 109.98   |
| 22  | A     | 842 | CLA  | C1D-ND-C4D  | -2.65 | 104.46      | 106.31   |
| 38  | 3     | 302 | LUT  | C8-C7-C6    | -2.65 | 119.93      | 127.00   |
| 22  | 1     | 306 | CLA  | C1C-C2C-C3C | -2.65 | 104.20      | 106.98   |
| 24  | A     | 856 | BCR  | C20-C19-C18 | -2.64 | 119.11      | 126.36   |
| 24  | 5     | 304 | BCR  | C33-C5-C4   | 2.64  | 119.23      | 113.60   |
| 22  | 7     | 315 | CLA  | O2D-CGD-O1D | -2.64 | 118.70      | 123.85   |
| 22  | G     | 202 | CLA  | CMA-C3A-C4A | 2.64  | 118.88      | 111.77   |
| 22  | 8     | 313 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 22  | A     | 834 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 22  | B     | 808 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 24  | A     | 856 | BCR  | C33-C5-C4   | 2.64  | 119.23      | 113.60   |
| 22  | B     | 817 | CLA  | C1C-C2C-C3C | -2.64 | 104.20      | 106.98   |
| 22  | A     | 822 | CLA  | O2D-CGD-O1D | -2.64 | 118.70      | 123.85   |
| 24  | 3     | 305 | BCR  | C8-C7-C6    | -2.64 | 119.94      | 127.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 5     | 315 | CLA  | C4B-CHC-C1C | 2.64  | 132.46      | 126.25   |
| 22  | 4     | 815 | CLA  | O2D-CGD-O1D | -2.64 | 118.71      | 123.85   |
| 22  | A     | 835 | CLA  | O2A-CGA-CBA | 2.64  | 119.89      | 111.83   |
| 22  | B     | 836 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 22  | G     | 202 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 22  | 8     | 316 | CLA  | C4B-CHC-C1C | 2.64  | 132.46      | 126.25   |
| 22  | 4     | 805 | CLA  | C1-C2-C3    | -2.64 | 121.87      | 126.20   |
| 22  | A     | 842 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 22  | B     | 828 | CLA  | C1C-C2C-C3C | -2.64 | 104.20      | 106.98   |
| 24  | 5     | 305 | BCR  | C8-C9-C10   | 2.64  | 123.16      | 119.01   |
| 22  | 5     | 310 | CLA  | C4B-CHC-C1C | 2.64  | 132.45      | 126.25   |
| 22  | K     | 203 | CLA  | C1D-ND-C4D  | -2.64 | 104.46      | 106.31   |
| 22  | 8     | 308 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 22  | A     | 819 | CLA  | C2C-C1C-NC  | 2.64  | 112.75      | 109.98   |
| 22  | 1     | 309 | CLA  | C2C-C1C-NC  | 2.64  | 112.75      | 109.98   |
| 24  | B     | 849 | BCR  | C38-C26-C27 | 2.64  | 119.22      | 113.60   |
| 22  | 5     | 314 | CLA  | C4B-CHC-C1C | 2.64  | 132.45      | 126.25   |
| 22  | 1     | 305 | CLA  | C1D-ND-C4D  | -2.64 | 104.46      | 106.31   |
| 22  | 9     | 310 | CLA  | C1C-C2C-C3C | -2.64 | 104.21      | 106.98   |
| 22  | B     | 817 | CLA  | C2C-C1C-NC  | 2.64  | 112.75      | 109.98   |
| 22  | 1     | 314 | CLA  | C2C-C1C-NC  | 2.64  | 112.75      | 109.98   |
| 22  | 7     | 316 | CLA  | C2C-C1C-NC  | 2.64  | 112.75      | 109.98   |
| 22  | 4     | 808 | CLA  | C4B-CHC-C1C | 2.64  | 132.44      | 126.25   |
| 22  | 5     | 322 | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 22  | B     | 835 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | 9     | 307 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | A     | 809 | CLA  | C2C-C1C-NC  | 2.63  | 112.75      | 109.98   |
| 22  | 3     | 311 | CLA  | C2C-C1C-NC  | 2.63  | 112.75      | 109.98   |
| 22  | B     | 813 | CLA  | O2D-CGD-O1D | -2.63 | 118.72      | 123.85   |
| 22  | A     | 841 | CLA  | O2A-CGA-CBA | 2.63  | 119.87      | 111.83   |
| 24  | 3     | 307 | BCR  | C37-C22-C21 | -2.63 | 118.55      | 122.82   |
| 22  | Z     | 303 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | A     | 828 | CLA  | O2A-CGA-CBA | 2.63  | 119.86      | 111.83   |
| 22  | A     | 854 | CLA  | C2C-C1C-NC  | 2.63  | 112.75      | 109.98   |
| 22  | 7     | 322 | CLA  | CMA-C3A-C4A | 2.63  | 118.85      | 111.77   |
| 38  | 5     | 302 | LUT  | C8-C7-C6    | -2.63 | 119.96      | 127.00   |
| 22  | Z     | 303 | CLA  | O1D-CGD-CBD | -2.63 | 119.33      | 124.52   |
| 22  | 4     | 818 | CLA  | C2C-C1C-NC  | 2.63  | 112.75      | 109.98   |
| 22  | 5     | 310 | CLA  | C2C-C1C-NC  | 2.63  | 112.75      | 109.98   |
| 22  | 9     | 306 | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 22  | 3     | 314 | CLA  | C4B-CHC-C1C | 2.63  | 132.44      | 126.25   |
| 22  | A     | 821 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 837 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | A     | 841 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | 6     | 319 | CLA  | C2C-C1C-NC  | 2.63  | 112.75      | 109.98   |
| 22  | K     | 205 | CLA  | O2D-CGD-O1D | -2.63 | 118.73      | 123.85   |
| 24  | G     | 203 | BCR  | C30-C25-C26 | -2.63 | 119.04      | 122.64   |
| 22  | A     | 834 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | K     | 205 | CLA  | C2D-C1D-ND  | 2.63  | 112.73      | 110.13   |
| 22  | 1     | 310 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | 3     | 309 | CLA  | C1C-C2C-C3C | -2.63 | 104.21      | 106.98   |
| 22  | 1     | 315 | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 22  | 8     | 309 | CLA  | C1C-C2C-C3C | -2.63 | 104.22      | 106.98   |
| 22  | 6     | 317 | CLA  | C1C-C2C-C3C | -2.63 | 104.22      | 106.98   |
| 22  | B     | 837 | CLA  | C1C-C2C-C3C | -2.63 | 104.22      | 106.98   |
| 38  | 4     | 802 | LUT  | C18-C5-C4   | 2.63  | 119.25      | 114.42   |
| 22  | 4     | 818 | CLA  | C4B-CHC-C1C | 2.63  | 132.43      | 126.25   |
| 22  | B     | 838 | CLA  | C3B-C4B-NB  | -2.63 | 108.19      | 110.53   |
| 22  | 4     | 817 | CLA  | C2C-C1C-NC  | 2.63  | 112.74      | 109.98   |
| 22  | 6     | 312 | CLA  | C1D-ND-C4D  | -2.63 | 104.47      | 106.31   |
| 22  | 3     | 309 | CLA  | C2C-C1C-NC  | 2.63  | 112.74      | 109.98   |
| 22  | 3     | 311 | CLA  | C3B-C4B-NB  | -2.63 | 108.19      | 110.53   |
| 22  | 7     | 317 | CLA  | CMA-C3A-C4A | 2.63  | 118.83      | 111.77   |
| 22  | 7     | 315 | CLA  | C2C-C1C-NC  | 2.62  | 112.74      | 109.98   |
| 22  | 5     | 319 | CLA  | CMA-C3A-C4A | 2.62  | 118.83      | 111.77   |
| 22  | 4     | 811 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 22  | 4     | 810 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 22  | 6     | 308 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 22  | B     | 829 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 38  | 6     | 303 | LUT  | C18-C5-C4   | 2.62  | 119.24      | 114.42   |
| 24  | 5     | 304 | BCR  | C7-C8-C9    | -2.62 | 122.36      | 126.23   |
| 22  | 3     | 308 | CLA  | C4B-CHC-C1C | 2.62  | 132.41      | 126.25   |
| 22  | 1     | 311 | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |
| 22  | 3     | 319 | CLA  | CMA-C3A-C4A | 2.62  | 118.82      | 111.77   |
| 22  | A     | 819 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 22  | 5     | 320 | CLA  | C2A-C1A-CHA | 2.62  | 128.42      | 123.87   |
| 22  | A     | 829 | CLA  | C4B-CHC-C1C | 2.62  | 132.41      | 126.25   |
| 24  | J     | 104 | BCR  | C33-C5-C4   | 2.62  | 119.18      | 113.60   |
| 22  | A     | 822 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 22  | B     | 808 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 22  | Z     | 306 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |
| 24  | J     | 104 | BCR  | C23-C24-C25 | -2.62 | 120.00      | 127.00   |
| 22  | 1     | 310 | CLA  | C1D-ND-C4D  | -2.62 | 104.47      | 106.31   |
| 22  | A     | 820 | CLA  | C1C-C2C-C3C | -2.62 | 104.22      | 106.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 1     | 307 | CLA  | O2A-CGA-CBA | 2.62  | 119.82      | 111.83   |
| 22  | A     | 815 | CLA  | C1C-C2C-C3C | -2.62 | 104.23      | 106.98   |
| 22  | A     | 817 | CLA  | C1C-C2C-C3C | -2.62 | 104.23      | 106.98   |
| 22  | F     | 305 | CLA  | C2C-C1C-NC  | 2.62  | 112.73      | 109.98   |
| 22  | 9     | 306 | CLA  | O2A-CGA-CBA | 2.62  | 119.82      | 111.83   |
| 22  | 1     | 304 | CLA  | C4B-CHC-C1C | 2.62  | 132.40      | 126.25   |
| 22  | 8     | 316 | CLA  | C1C-C2C-C3C | -2.62 | 104.23      | 106.98   |
| 22  | 9     | 310 | CLA  | C4B-CHC-C1C | 2.62  | 132.40      | 126.25   |
| 22  | G     | 202 | CLA  | C2C-C1C-NC  | 2.62  | 112.73      | 109.98   |
| 22  | 5     | 311 | CLA  | C1D-ND-C4D  | -2.62 | 104.48      | 106.31   |
| 22  | A     | 809 | CLA  | O2A-CGA-CBA | 2.62  | 119.81      | 111.83   |
| 22  | G     | 202 | CLA  | C1C-C2C-C3C | -2.62 | 104.23      | 106.98   |
| 22  | A     | 804 | CLA  | C1C-C2C-C3C | -2.62 | 104.23      | 106.98   |
| 24  | B     | 848 | BCR  | C23-C24-C25 | -2.62 | 120.01      | 127.00   |
| 22  | F     | 304 | CLA  | CMA-C3A-C4A | 2.62  | 118.80      | 111.77   |
| 22  | 4     | 815 | CLA  | C1C-C2C-C3C | -2.61 | 104.23      | 106.98   |
| 22  | 3     | 322 | CLA  | C4B-CHC-C1C | 2.61  | 132.40      | 126.25   |
| 22  | 8     | 308 | CLA  | C4B-CHC-C1C | 2.61  | 132.40      | 126.25   |
| 22  | F     | 305 | CLA  | C1C-C2C-C3C | -2.61 | 104.23      | 106.98   |
| 24  | 5     | 305 | BCR  | C8-C7-C6    | -2.61 | 120.02      | 127.00   |
| 22  | G     | 201 | CLA  | CMA-C3A-C4A | 2.61  | 118.79      | 111.77   |
| 24  | J     | 104 | BCR  | C38-C26-C27 | 2.61  | 119.16      | 113.60   |
| 22  | A     | 810 | CLA  | C1C-C2C-C3C | -2.61 | 104.23      | 106.98   |
| 39  | 9     | 314 | CHL  | C4D-CHA-CBD | -2.61 | 106.33      | 108.97   |
| 24  | 4     | 804 | BCR  | C15-C16-C17 | -2.61 | 118.18      | 123.52   |
| 22  | A     | 813 | CLA  | C1C-C2C-C3C | -2.61 | 104.23      | 106.98   |
| 22  | B     | 806 | CLA  | C1D-ND-C4D  | -2.61 | 104.48      | 106.31   |
| 22  | A     | 807 | CLA  | C4B-CHC-C1C | 2.61  | 132.38      | 126.25   |
| 22  | 6     | 302 | CLA  | C4B-CHC-C1C | 2.61  | 132.38      | 126.25   |
| 22  | K     | 205 | CLA  | C2A-C1A-CHA | 2.61  | 128.39      | 123.87   |
| 22  | 5     | 326 | CLA  | C1C-C2C-C3C | -2.61 | 104.24      | 106.98   |
| 24  | A     | 847 | BCR  | C2-C1-C6    | 2.61  | 114.23      | 110.44   |
| 22  | Z     | 309 | CLA  | C4B-CHC-C1C | 2.61  | 132.38      | 126.25   |
| 22  | B     | 820 | CLA  | C1D-ND-C4D  | -2.61 | 104.48      | 106.31   |
| 22  | 7     | 312 | CLA  | O2A-CGA-CBA | 2.61  | 119.78      | 111.83   |
| 22  | 6     | 322 | CLA  | O2D-CGD-O1D | -2.61 | 118.78      | 123.85   |
| 22  | A     | 820 | CLA  | C1-C2-C3    | -2.61 | 121.93      | 126.20   |
| 22  | A     | 803 | CLA  | C1C-C2C-C3C | -2.61 | 104.24      | 106.98   |
| 22  | 5     | 312 | CLA  | CMA-C3A-C4A | 2.61  | 118.78      | 111.77   |
| 22  | 1     | 307 | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 22  | Z     | 316 | CLA  | CMA-C3A-C4A | 2.61  | 118.78      | 111.77   |
| 22  | B     | 834 | CLA  | C1D-ND-C4D  | -2.61 | 104.48      | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 831 | CLA  | C1C-C2C-C3C | -2.61 | 104.24      | 106.98   |
| 22  | 2     | 302 | CLA  | C1C-C2C-C3C | -2.60 | 104.24      | 106.98   |
| 22  | 4     | 806 | CLA  | C1D-ND-C4D  | -2.60 | 104.48      | 106.31   |
| 22  | Z     | 303 | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 22  | B     | 823 | CLA  | C2C-C1C-NC  | 2.60  | 112.72      | 109.98   |
| 22  | 8     | 306 | CLA  | C2C-C1C-NC  | 2.60  | 112.72      | 109.98   |
| 22  | 9     | 311 | CLA  | C4B-CHC-C1C | 2.60  | 132.37      | 126.25   |
| 22  | A     | 814 | CLA  | C1D-ND-C4D  | -2.60 | 104.49      | 106.31   |
| 22  | 4     | 807 | CLA  | C1D-ND-C4D  | -2.60 | 104.49      | 106.31   |
| 38  | 3     | 302 | LUT  | C1-C6-C5    | -2.60 | 119.08      | 122.64   |
| 22  | B     | 814 | CLA  | C2C-C1C-NC  | 2.60  | 112.72      | 109.98   |
| 22  | B     | 830 | CLA  | C1C-C2C-C3C | -2.60 | 104.24      | 106.98   |
| 24  | F     | 303 | BCR  | C33-C5-C4   | 2.60  | 119.14      | 113.60   |
| 22  | 6     | 301 | CLA  | C4B-CHC-C1C | 2.60  | 132.36      | 126.25   |
| 22  | B     | 816 | CLA  | C2C-C1C-NC  | 2.60  | 112.71      | 109.98   |
| 22  | B     | 822 | CLA  | C2C-C1C-NC  | 2.60  | 112.71      | 109.98   |
| 23  | A     | 843 | PQN  | C11-C3-C2   | -2.60 | 120.43      | 124.89   |
| 22  | B     | 825 | CLA  | C2C-C1C-NC  | 2.60  | 112.71      | 109.98   |
| 22  | Z     | 309 | CLA  | O2A-CGA-CBA | 2.60  | 119.76      | 111.83   |
| 22  | A     | 829 | CLA  | C1C-C2C-C3C | -2.60 | 104.25      | 106.98   |
| 22  | 1     | 308 | CLA  | O2D-CGD-O1D | -2.60 | 118.79      | 123.85   |
| 22  | 7     | 317 | CLA  | C4B-CHC-C1C | 2.60  | 132.35      | 126.25   |
| 22  | B     | 815 | CLA  | C1D-ND-C4D  | -2.60 | 104.49      | 106.31   |
| 22  | 9     | 309 | CLA  | C1D-ND-C4D  | -2.60 | 104.49      | 106.31   |
| 22  | A     | 825 | CLA  | C1C-C2C-C3C | -2.60 | 104.25      | 106.98   |
| 22  | B     | 814 | CLA  | O2D-CGD-O1D | -2.60 | 118.79      | 123.85   |
| 22  | Z     | 303 | CLA  | C2C-C1C-NC  | 2.60  | 112.71      | 109.98   |
| 22  | B     | 815 | CLA  | C4B-CHC-C1C | 2.60  | 132.35      | 126.25   |
| 22  | A     | 855 | CLA  | C2C-C1C-NC  | 2.60  | 112.71      | 109.98   |
| 22  | 9     | 305 | CLA  | C2D-C1D-ND  | 2.59  | 112.69      | 110.13   |
| 22  | A     | 816 | CLA  | C3B-C4B-NB  | -2.59 | 108.21      | 110.53   |
| 22  | 9     | 313 | CLA  | C1C-C2C-C3C | -2.59 | 104.25      | 106.98   |
| 22  | 7     | 316 | CLA  | CMA-C3A-C4A | 2.59  | 118.74      | 111.77   |
| 22  | A     | 820 | CLA  | C6-C5-C3    | -2.59 | 107.15      | 113.47   |
| 24  | G     | 203 | BCR  | C20-C19-C18 | -2.59 | 119.25      | 126.36   |
| 22  | A     | 826 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 22  | K     | 202 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 22  | K     | 203 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 22  | 3     | 313 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 22  | 6     | 312 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 22  | A     | 809 | CLA  | C1C-C2C-C3C | -2.59 | 104.25      | 106.98   |
| 22  | A     | 804 | CLA  | C1D-ND-C4D  | -2.59 | 104.49      | 106.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 825 | CLA  | C1C-C2C-C3C | -2.59 | 104.25      | 106.98   |
| 22  | B     | 826 | CLA  | C1C-C2C-C3C | -2.59 | 104.25      | 106.98   |
| 22  | Z     | 314 | CLA  | C4B-CHC-C1C | 2.59  | 132.34      | 126.25   |
| 22  | G     | 201 | CLA  | CHA-C4D-ND  | 2.59  | 137.90      | 132.55   |
| 22  | Z     | 310 | CLA  | C4B-CHC-C1C | 2.59  | 132.34      | 126.25   |
| 22  | A     | 824 | CLA  | C1C-C2C-C3C | -2.59 | 104.25      | 106.98   |
| 38  | 1     | 303 | LUT  | C11-C12-C13 | -2.59 | 119.26      | 126.36   |
| 22  | 3     | 313 | CLA  | C2D-C1D-ND  | 2.59  | 112.69      | 110.13   |
| 22  | K     | 205 | CLA  | CMA-C3A-C2A | 2.59  | 124.00      | 113.98   |
| 22  | 7     | 314 | CLA  | C1C-C2C-C3C | -2.59 | 104.26      | 106.98   |
| 22  | 9     | 304 | CLA  | C4B-CHC-C1C | 2.59  | 132.34      | 126.25   |
| 22  | A     | 810 | CLA  | C2C-C1C-NC  | 2.59  | 112.70      | 109.98   |
| 22  | 5     | 315 | CLA  | C2C-C1C-NC  | 2.59  | 112.70      | 109.98   |
| 22  | 1     | 316 | CLA  | CHA-C4D-ND  | 2.59  | 137.89      | 132.55   |
| 36  | 5     | 306 | C7Z  | C8-C7-C6    | -2.59 | 120.08      | 127.00   |
| 22  | 6     | 317 | CLA  | C4B-CHC-C1C | 2.59  | 132.33      | 126.25   |
| 22  | B     | 814 | CLA  | CMA-C3A-C4A | 2.59  | 118.73      | 111.77   |
| 22  | B     | 816 | CLA  | C1C-C2C-C3C | -2.59 | 104.26      | 106.98   |
| 24  | A     | 856 | BCR  | C29-C30-C25 | 2.59  | 114.20      | 110.44   |
| 22  | 9     | 304 | CLA  | CHA-C4D-ND  | 2.59  | 137.88      | 132.55   |
| 22  | A     | 854 | CLA  | C1C-C2C-C3C | -2.59 | 104.26      | 106.98   |
| 39  | 6     | 316 | CHL  | CMA-C3A-C4A | 2.59  | 120.18      | 114.61   |
| 22  | 6     | 307 | CLA  | O2A-CGA-CBA | 2.58  | 119.72      | 111.83   |
| 22  | 6     | 310 | CLA  | C1C-C2C-C3C | -2.58 | 104.26      | 106.98   |
| 22  | A     | 835 | CLA  | C2C-C1C-NC  | 2.58  | 112.70      | 109.98   |
| 22  | 5     | 301 | CLA  | C4B-CHC-C1C | 2.58  | 132.32      | 126.25   |
| 22  | 6     | 307 | CLA  | C4B-CHC-C1C | 2.58  | 132.32      | 126.25   |
| 22  | A     | 803 | CLA  | C2C-C1C-NC  | 2.58  | 112.69      | 109.98   |
| 22  | Z     | 308 | CLA  | C2C-C1C-NC  | 2.58  | 112.69      | 109.98   |
| 22  | A     | 811 | CLA  | O2A-CGA-CBA | 2.58  | 119.71      | 111.83   |
| 22  | B     | 836 | CLA  | C1C-C2C-C3C | -2.58 | 104.26      | 106.98   |
| 22  | B     | 835 | CLA  | C2C-C1C-NC  | 2.58  | 112.69      | 109.98   |
| 24  | A     | 845 | BCR  | C33-C5-C4   | 2.58  | 119.10      | 113.60   |
| 22  | B     | 819 | CLA  | C4B-CHC-C1C | 2.58  | 132.32      | 126.25   |
| 24  | B     | 844 | BCR  | C8-C9-C10   | 2.58  | 123.07      | 119.01   |
| 24  | G     | 203 | BCR  | C38-C26-C27 | 2.58  | 119.10      | 113.60   |
| 22  | 3     | 315 | CLA  | C4B-CHC-C1C | 2.58  | 132.32      | 126.25   |
| 22  | A     | 805 | CLA  | C2C-C1C-NC  | 2.58  | 112.69      | 109.98   |
| 22  | 5     | 313 | CLA  | C4B-CHC-C1C | 2.58  | 132.31      | 126.25   |
| 22  | 5     | 312 | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 22  | 4     | 806 | CLA  | CHA-C4D-ND  | 2.58  | 137.87      | 132.55   |
| 24  | B     | 844 | BCR  | C15-C14-C13 | -2.58 | 123.66      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | 8     | 315 | CHL  | C4D-CHA-CBD | -2.58 | 106.37      | 108.97   |
| 22  | 6     | 319 | CLA  | C4B-CHC-C1C | 2.58  | 132.31      | 126.25   |
| 24  | B     | 846 | BCR  | C10-C11-C12 | -2.58 | 115.73      | 123.20   |
| 39  | 1     | 312 | CHL  | CMA-C3A-C4A | 2.58  | 120.16      | 114.61   |
| 36  | 5     | 306 | C7Z  | C24-C25-C26 | -2.58 | 115.47      | 120.76   |
| 22  | 3     | 311 | CLA  | C4B-CHC-C1C | 2.58  | 132.30      | 126.25   |
| 22  | 5     | 312 | CLA  | C1D-ND-C4D  | -2.58 | 104.50      | 106.31   |
| 22  | 2     | 302 | CLA  | C4B-CHC-C1C | 2.57  | 132.30      | 126.25   |
| 22  | 7     | 322 | CLA  | C1C-C2C-C3C | -2.57 | 104.27      | 106.98   |
| 24  | 8     | 304 | BCR  | C8-C7-C6    | -2.57 | 120.12      | 127.00   |
| 22  | A     | 854 | CLA  | CMA-C3A-C4A | 2.57  | 118.69      | 111.77   |
| 22  | A     | 833 | CLA  | C2C-C1C-NC  | 2.57  | 112.68      | 109.98   |
| 22  | 7     | 306 | CLA  | C1D-ND-C4D  | -2.57 | 104.51      | 106.31   |
| 38  | 3     | 302 | LUT  | C35-C15-C14 | -2.57 | 118.26      | 123.52   |
| 22  | A     | 832 | CLA  | C6-C5-C3    | -2.57 | 107.20      | 113.47   |
| 22  | 6     | 308 | CLA  | O2D-CGD-O1D | -2.57 | 118.84      | 123.85   |
| 22  | B     | 831 | CLA  | C4B-CHC-C1C | 2.57  | 132.29      | 126.25   |
| 22  | L     | 202 | CLA  | C4B-CHC-C1C | 2.57  | 132.29      | 126.25   |
| 39  | 5     | 316 | CHL  | C1-C2-C3    | -2.57 | 121.99      | 126.20   |
| 22  | 5     | 318 | CLA  | C1C-C2C-C3C | -2.57 | 104.28      | 106.98   |
| 22  | B     | 835 | CLA  | C4B-CHC-C1C | 2.57  | 132.29      | 126.25   |
| 22  | B     | 837 | CLA  | C1D-ND-C4D  | -2.57 | 104.51      | 106.31   |
| 22  | A     | 812 | CLA  | C2C-C1C-NC  | 2.57  | 112.68      | 109.98   |
| 24  | 7     | 303 | BCR  | C30-C25-C26 | -2.57 | 119.13      | 122.64   |
| 22  | A     | 812 | CLA  | O2D-CGD-O1D | -2.57 | 118.85      | 123.85   |
| 22  | K     | 202 | CLA  | C1C-C2C-C3C | -2.57 | 104.28      | 106.98   |
| 24  | B     | 844 | BCR  | C38-C26-C27 | 2.57  | 119.07      | 113.60   |
| 24  | 6     | 305 | BCR  | C23-C24-C25 | -2.57 | 120.14      | 127.00   |
| 22  | A     | 841 | CLA  | C2C-C1C-NC  | 2.57  | 112.68      | 109.98   |
| 22  | 5     | 319 | CLA  | C1D-ND-C4D  | -2.57 | 104.51      | 106.31   |
| 24  | 3     | 307 | BCR  | C8-C7-C6    | -2.57 | 120.14      | 127.00   |
| 22  | A     | 816 | CLA  | O2A-CGA-CBA | 2.57  | 119.66      | 111.83   |
| 24  | A     | 847 | BCR  | C27-C26-C25 | -2.56 | 119.24      | 122.70   |
| 22  | B     | 821 | CLA  | C4B-CHC-C1C | 2.56  | 132.28      | 126.25   |
| 22  | A     | 833 | CLA  | C4B-CHC-C1C | 2.56  | 132.28      | 126.25   |
| 22  | A     | 855 | CLA  | C1C-C2C-C3C | -2.56 | 104.28      | 106.98   |
| 22  | A     | 813 | CLA  | C1D-ND-C4D  | -2.56 | 104.51      | 106.31   |
| 22  | B     | 828 | CLA  | C2C-C1C-NC  | 2.56  | 112.67      | 109.98   |
| 22  | 9     | 303 | CLA  | O2D-CGD-O1D | -2.56 | 118.86      | 123.85   |
| 24  | 3     | 304 | BCR  | C38-C26-C27 | 2.56  | 119.06      | 113.60   |
| 22  | 1     | 316 | CLA  | CHA-C1A-NA  | -2.56 | 120.59      | 126.39   |
| 22  | 7     | 308 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 839 | CLA  | CMA-C3A-C4A | 2.56  | 118.66      | 111.77   |
| 22  | K     | 205 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 22  | A     | 813 | CLA  | C4B-CHC-C1C | 2.56  | 132.27      | 126.25   |
| 22  | 7     | 315 | CLA  | C1D-ND-C4D  | -2.56 | 104.52      | 106.31   |
| 22  | 5     | 318 | CLA  | C2C-C1C-NC  | 2.56  | 112.67      | 109.98   |
| 24  | A     | 845 | BCR  | C8-C7-C6    | -2.56 | 120.16      | 127.00   |
| 22  | B     | 807 | CLA  | C1C-C2C-C3C | -2.56 | 104.29      | 106.98   |
| 36  | 5     | 306 | C7Z  | C38-C25-C24 | 2.56  | 119.13      | 114.42   |
| 22  | B     | 825 | CLA  | O2A-CGA-CBA | 2.56  | 119.64      | 111.83   |
| 24  | B     | 853 | BCR  | C36-C18-C17 | -2.56 | 118.67      | 122.82   |
| 22  | B     | 824 | CLA  | C4B-CHC-C1C | 2.56  | 132.27      | 126.25   |
| 22  | 6     | 314 | CLA  | O2D-CGD-O1D | -2.56 | 118.87      | 123.85   |
| 24  | 3     | 304 | BCR  | C7-C6-C5    | -2.56 | 115.66      | 121.56   |
| 39  | 8     | 315 | CHL  | C1-C2-C3    | -2.56 | 122.01      | 126.20   |
| 22  | A     | 811 | CLA  | C1C-C2C-C3C | -2.56 | 104.29      | 106.98   |
| 22  | 5     | 320 | CLA  | C4B-CHC-C1C | 2.56  | 132.26      | 126.25   |
| 22  | 7     | 322 | CLA  | C4B-CHC-C1C | 2.56  | 132.26      | 126.25   |
| 39  | 6     | 318 | CHL  | C4D-CHA-CBD | -2.56 | 106.39      | 108.97   |
| 24  | 7     | 303 | BCR  | C1-C6-C7    | 2.56  | 122.58      | 115.65   |
| 24  | K     | 206 | BCR  | C15-C16-C17 | -2.56 | 118.29      | 123.52   |
| 22  | B     | 808 | CLA  | C2C-C1C-NC  | 2.56  | 112.67      | 109.98   |
| 22  | B     | 831 | CLA  | CHA-C4D-ND  | 2.56  | 137.82      | 132.55   |
| 22  | 5     | 313 | CLA  | CHA-C4D-ND  | 2.56  | 137.82      | 132.55   |
| 22  | B     | 832 | CLA  | C1C-C2C-C3C | -2.55 | 104.29      | 106.98   |
| 22  | A     | 835 | CLA  | C4B-CHC-C1C | 2.55  | 132.25      | 126.25   |
| 22  | J     | 103 | CLA  | C4B-CHC-C1C | 2.55  | 132.25      | 126.25   |
| 22  | A     | 811 | CLA  | C2C-C1C-NC  | 2.55  | 112.67      | 109.98   |
| 24  | J     | 104 | BCR  | C8-C7-C6    | -2.55 | 120.17      | 127.00   |
| 22  | A     | 814 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 24  | A     | 847 | BCR  | C8-C7-C6    | -2.55 | 120.18      | 127.00   |
| 38  | Z     | 302 | LUT  | C11-C12-C13 | -2.55 | 119.36      | 126.36   |
| 22  | 9     | 304 | CLA  | CHA-C1A-NA  | -2.55 | 120.61      | 126.39   |
| 24  | B     | 848 | BCR  | C1-C6-C7    | 2.55  | 122.57      | 115.65   |
| 22  | A     | 830 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 22  | 6     | 312 | CLA  | O2A-CGA-CBA | 2.55  | 119.61      | 111.83   |
| 22  | 3     | 310 | CLA  | O2A-CGA-CBA | 2.55  | 119.61      | 111.83   |
| 22  | 6     | 309 | CLA  | CHA-C4D-ND  | 2.55  | 137.81      | 132.55   |
| 22  | 5     | 308 | CLA  | CHA-C4D-ND  | 2.55  | 137.81      | 132.55   |
| 22  | 7     | 311 | CLA  | C4B-CHC-C1C | 2.55  | 132.24      | 126.25   |
| 22  | 7     | 305 | CLA  | O2D-CGD-O1D | -2.55 | 118.89      | 123.85   |
| 22  | 6     | 322 | CLA  | CMA-C3A-C4A | 2.55  | 118.62      | 111.77   |
| 39  | 4     | 819 | CHL  | C4D-CHA-CBD | -2.55 | 106.40      | 108.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 6     | 310 | CLA  | C2C-C1C-NC  | 2.55  | 112.66      | 109.98   |
| 22  | 3     | 310 | CLA  | C1D-ND-C4D  | -2.55 | 104.52      | 106.31   |
| 31  | 3     | 301 | DGD  | O1G-C1A-C2A | 2.55  | 119.60      | 111.83   |
| 22  | 7     | 307 | CLA  | CMD-C2D-C3D | -2.55 | 121.85      | 127.69   |
| 24  | 3     | 304 | BCR  | C33-C5-C4   | 2.55  | 119.03      | 113.60   |
| 22  | 8     | 306 | CLA  | C1C-C2C-C3C | -2.55 | 104.30      | 106.98   |
| 22  | B     | 832 | CLA  | C4B-CHC-C1C | 2.55  | 132.24      | 126.25   |
| 22  | A     | 828 | CLA  | C1C-C2C-C3C | -2.55 | 104.30      | 106.98   |
| 22  | 4     | 805 | CLA  | C1C-C2C-C3C | -2.55 | 104.30      | 106.98   |
| 22  | 3     | 309 | CLA  | C3B-C4B-NB  | -2.55 | 108.26      | 110.53   |
| 22  | 8     | 307 | CLA  | C3B-C4B-NB  | -2.55 | 108.26      | 110.53   |
| 22  | 4     | 809 | CLA  | CHA-C4D-ND  | 2.54  | 137.80      | 132.55   |
| 22  | 2     | 301 | CLA  | CMD-C2D-C3D | -2.54 | 121.86      | 127.69   |
| 22  | 5     | 318 | CLA  | C3B-C4B-NB  | -2.54 | 108.26      | 110.53   |
| 22  | 1     | 308 | CLA  | CHD-C1D-ND  | -2.54 | 121.22      | 124.80   |
| 22  | A     | 830 | CLA  | C4B-CHC-C1C | 2.54  | 132.23      | 126.25   |
| 22  | A     | 819 | CLA  | C4B-CHC-C1C | 2.54  | 132.22      | 126.25   |
| 22  | 7     | 304 | CLA  | C4B-CHC-C1C | 2.54  | 132.22      | 126.25   |
| 22  | B     | 836 | CLA  | C2C-C1C-NC  | 2.54  | 112.65      | 109.98   |
| 22  | 5     | 308 | CLA  | O2D-CGD-O1D | -2.54 | 118.90      | 123.85   |
| 41  | 5     | 325 | 3PH  | O31-C31-C32 | 2.54  | 119.58      | 111.83   |
| 22  | 1     | 313 | CLA  | C4B-CHC-C1C | 2.54  | 132.22      | 126.25   |
| 22  | F     | 304 | CLA  | CHA-C4D-ND  | 2.54  | 137.79      | 132.55   |
| 38  | 3     | 303 | LUT  | C27-C28-C29 | -2.54 | 120.86      | 126.32   |
| 24  | L     | 204 | BCR  | C23-C24-C25 | -2.54 | 120.21      | 127.00   |
| 22  | 9     | 307 | CLA  | C1D-ND-C4D  | -2.54 | 104.53      | 106.31   |
| 22  | A     | 834 | CLA  | C4B-CHC-C1C | 2.54  | 132.22      | 126.25   |
| 22  | B     | 842 | CLA  | C1D-ND-C4D  | -2.54 | 104.53      | 106.31   |
| 22  | 5     | 326 | CLA  | CHA-C4D-ND  | 2.54  | 137.79      | 132.55   |
| 39  | 2     | 303 | CHL  | C4D-CHA-CBD | -2.54 | 106.41      | 108.97   |
| 24  | A     | 847 | BCR  | C33-C5-C4   | 2.54  | 119.01      | 113.60   |
| 22  | 6     | 322 | CLA  | CHA-C4D-ND  | 2.54  | 137.78      | 132.55   |
| 22  | A     | 830 | CLA  | C1C-C2C-C3C | -2.54 | 104.31      | 106.98   |
| 22  | A     | 826 | CLA  | C4B-CHC-C1C | 2.54  | 132.21      | 126.25   |
| 22  | F     | 304 | CLA  | C4B-CHC-C1C | 2.54  | 132.21      | 126.25   |
| 22  | 4     | 815 | CLA  | C2C-C1C-NC  | 2.54  | 112.65      | 109.98   |
| 24  | F     | 303 | BCR  | C23-C24-C25 | -2.54 | 120.22      | 127.00   |
| 22  | 9     | 309 | CLA  | CHA-C4D-ND  | 2.54  | 137.78      | 132.55   |
| 22  | A     | 832 | CLA  | C3B-C4B-NB  | -2.54 | 108.27      | 110.53   |
| 38  | Z     | 302 | LUT  | C18-C5-C4   | 2.54  | 119.08      | 114.42   |
| 22  | B     | 807 | CLA  | C4B-CHC-C1C | 2.53  | 132.21      | 126.25   |
| 22  | B     | 808 | CLA  | O2A-CGA-CBA | 2.53  | 119.56      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 1     | 309 | CLA  | CMA-C3A-C4A | 2.53  | 118.59      | 111.77   |
| 22  | A     | 803 | CLA  | O2A-CGA-CBA | 2.53  | 119.56      | 111.83   |
| 22  | Z     | 307 | CLA  | C4B-CHC-C1C | 2.53  | 132.21      | 126.25   |
| 22  | 1     | 305 | CLA  | CHA-C4D-ND  | 2.53  | 137.78      | 132.55   |
| 22  | 1     | 304 | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 22  | 6     | 322 | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 22  | A     | 834 | CLA  | O2D-CGD-O1D | -2.53 | 118.92      | 123.85   |
| 22  | 1     | 315 | CLA  | C4B-CHC-C1C | 2.53  | 132.21      | 126.25   |
| 22  | B     | 835 | CLA  | CMD-C2D-C3D | -2.53 | 121.88      | 127.69   |
| 22  | 7     | 317 | CLA  | C1C-C2C-C3C | -2.53 | 104.32      | 106.98   |
| 22  | A     | 804 | CLA  | C4B-CHC-C1C | 2.53  | 132.20      | 126.25   |
| 22  | A     | 810 | CLA  | C4B-CHC-C1C | 2.53  | 132.20      | 126.25   |
| 22  | A     | 838 | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 22  | 3     | 318 | CLA  | C2C-C1C-NC  | 2.53  | 112.64      | 109.98   |
| 25  | A     | 849 | LHG  | O8-C23-C24  | 2.53  | 119.56      | 111.83   |
| 24  | 3     | 307 | BCR  | C29-C30-C25 | 2.53  | 114.12      | 110.44   |
| 22  | 6     | 311 | CLA  | C1D-ND-C4D  | -2.53 | 104.54      | 106.31   |
| 22  | 5     | 311 | CLA  | C4B-CHC-C1C | 2.53  | 132.20      | 126.25   |
| 22  | 7     | 308 | CLA  | CHA-C4D-ND  | 2.53  | 137.77      | 132.55   |
| 22  | A     | 812 | CLA  | C1C-C2C-C3C | -2.53 | 104.32      | 106.98   |
| 22  | 6     | 313 | CLA  | C4B-CHC-C1C | 2.53  | 132.20      | 126.25   |
| 22  | B     | 826 | CLA  | CHA-C4D-ND  | 2.53  | 137.77      | 132.55   |
| 22  | B     | 822 | CLA  | C1C-C2C-C3C | -2.53 | 104.32      | 106.98   |
| 22  | 8     | 310 | CLA  | C4B-CHC-C1C | 2.53  | 132.20      | 126.25   |
| 22  | B     | 812 | CLA  | C1D-ND-C4D  | -2.53 | 104.54      | 106.31   |
| 22  | 9     | 309 | CLA  | O2A-CGA-CBA | 2.53  | 119.55      | 111.83   |
| 22  | 6     | 310 | CLA  | O2A-CGA-CBA | 2.53  | 119.55      | 111.83   |
| 24  | B     | 847 | BCR  | C2-C1-C6    | 2.53  | 114.11      | 110.44   |
| 22  | F     | 305 | CLA  | C4B-CHC-C1C | 2.53  | 132.19      | 126.25   |
| 22  | 8     | 305 | CLA  | C1C-C2C-C3C | -2.53 | 104.32      | 106.98   |
| 22  | 3     | 315 | CLA  | CHA-C4D-ND  | 2.53  | 137.76      | 132.55   |
| 22  | 3     | 320 | CLA  | C1D-ND-C4D  | -2.53 | 104.54      | 106.31   |
| 22  | B     | 812 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 22  | 9     | 307 | CLA  | C4B-CHC-C1C | 2.52  | 132.18      | 126.25   |
| 38  | 5     | 303 | LUT  | C18-C5-C4   | 2.52  | 119.06      | 114.42   |
| 22  | A     | 805 | CLA  | C4B-CHC-C1C | 2.52  | 132.18      | 126.25   |
| 24  | 3     | 305 | BCR  | C38-C26-C27 | 2.52  | 118.98      | 113.60   |
| 24  | B     | 844 | BCR  | C33-C5-C4   | 2.52  | 118.98      | 113.60   |
| 22  | A     | 818 | CLA  | C4B-CHC-C1C | 2.52  | 132.18      | 126.25   |
| 22  | Z     | 315 | CLA  | C1D-ND-C4D  | -2.52 | 104.54      | 106.31   |
| 22  | 5     | 320 | CLA  | CHA-C1A-NA  | -2.52 | 120.68      | 126.39   |
| 22  | 4     | 810 | CLA  | CMA-C3A-C4A | 2.52  | 118.55      | 111.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | 4     | 804 | BCR  | C8-C7-C6    | -2.52 | 120.26      | 127.00   |
| 22  | K     | 202 | CLA  | C4B-CHC-C1C | 2.52  | 132.18      | 126.25   |
| 38  | 7     | 301 | LUT  | C27-C28-C29 | -2.52 | 120.90      | 126.32   |
| 22  | 3     | 314 | CLA  | C1-O2A-CGA  | 2.52  | 122.75      | 116.65   |
| 22  | 6     | 317 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 22  | 3     | 313 | CLA  | C2C-C1C-NC  | 2.52  | 112.63      | 109.98   |
| 22  | B     | 834 | CLA  | O2A-CGA-CBA | 2.52  | 119.52      | 111.83   |
| 22  | 6     | 307 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 22  | 8     | 305 | CLA  | O1D-CGD-CBD | -2.52 | 119.55      | 124.52   |
| 22  | B     | 842 | CLA  | C4B-CHC-C1C | 2.52  | 132.17      | 126.25   |
| 22  | B     | 838 | CLA  | CMD-C2D-C3D | -2.52 | 121.91      | 127.69   |
| 33  | 4     | 801 | LMT  | C1B-O1B-C4' | -2.52 | 112.01      | 117.98   |
| 23  | B     | 843 | PQN  | C11-C3-C2   | -2.52 | 120.57      | 124.89   |
| 22  | A     | 822 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 22  | 9     | 305 | CLA  | CAA-CBA-CGA | -2.52 | 106.06      | 113.21   |
| 25  | 5     | 324 | LHG  | C5-O7-C7    | -2.52 | 111.77      | 117.80   |
| 22  | 5     | 311 | CLA  | CHA-C4D-ND  | 2.52  | 137.74      | 132.55   |
| 22  | B     | 801 | CLA  | C2C-C1C-NC  | 2.52  | 112.62      | 109.98   |
| 22  | B     | 838 | CLA  | C4B-CHC-C1C | 2.52  | 132.16      | 126.25   |
| 22  | 8     | 309 | CLA  | C4B-CHC-C1C | 2.52  | 132.16      | 126.25   |
| 22  | 7     | 314 | CLA  | O2A-CGA-CBA | 2.52  | 119.51      | 111.83   |
| 22  | B     | 827 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 22  | B     | 841 | CLA  | C4B-CHC-C1C | 2.52  | 132.16      | 126.25   |
| 22  | 9     | 304 | CLA  | O2D-CGD-O1D | -2.52 | 118.95      | 123.85   |
| 39  | 8     | 312 | CHL  | C4D-CHA-CBD | -2.52 | 106.43      | 108.97   |
| 39  | 4     | 816 | CHL  | C4D-CHA-CBD | -2.52 | 106.43      | 108.97   |
| 22  | B     | 837 | CLA  | C4B-CHC-C1C | 2.51  | 132.16      | 126.25   |
| 22  | A     | 815 | CLA  | C3B-C4B-NB  | -2.51 | 108.28      | 110.53   |
| 22  | 7     | 304 | CLA  | C1-O2A-CGA  | 2.51  | 122.74      | 116.65   |
| 24  | B     | 846 | BCR  | C34-C9-C10  | -2.51 | 118.74      | 122.82   |
| 22  | B     | 833 | CLA  | C3B-C4B-NB  | -2.51 | 108.29      | 110.53   |
| 22  | B     | 813 | CLA  | C4B-CHC-C1C | 2.51  | 132.16      | 126.25   |
| 22  | B     | 813 | CLA  | CHA-C4D-ND  | 2.51  | 137.74      | 132.55   |
| 22  | 5     | 307 | CLA  | C4B-CHC-C1C | 2.51  | 132.16      | 126.25   |
| 22  | A     | 840 | CLA  | C4B-CHC-C1C | 2.51  | 132.16      | 126.25   |
| 22  | 7     | 322 | CLA  | C2C-C1C-NC  | 2.51  | 112.62      | 109.98   |
| 39  | 5     | 317 | CHL  | C4D-CHA-CBD | -2.51 | 106.43      | 108.97   |
| 22  | 9     | 310 | CLA  | CHA-C4D-ND  | 2.51  | 137.73      | 132.55   |
| 22  | A     | 805 | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |
| 22  | A     | 822 | CLA  | O2A-CGA-CBA | 2.51  | 119.49      | 111.83   |
| 22  | 8     | 306 | CLA  | CHA-C4D-ND  | 2.51  | 137.73      | 132.55   |
| 22  | 6     | 309 | CLA  | C3B-C4B-NB  | -2.51 | 108.29      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 817 | CLA  | CHA-C4D-ND  | 2.51  | 137.73      | 132.55   |
| 22  | 7     | 315 | CLA  | CHA-C4D-ND  | 2.51  | 137.73      | 132.55   |
| 22  | B     | 834 | CLA  | CHA-C4D-ND  | 2.51  | 137.73      | 132.55   |
| 22  | 7     | 308 | CLA  | C4B-CHC-C1C | 2.51  | 132.15      | 126.25   |
| 38  | 3     | 303 | LUT  | C30-C31-C32 | -2.51 | 115.93      | 123.20   |
| 24  | F     | 303 | BCR  | C20-C19-C18 | -2.51 | 119.48      | 126.36   |
| 22  | A     | 823 | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |
| 22  | 6     | 319 | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |
| 22  | 1     | 310 | CLA  | CHA-C4D-ND  | 2.51  | 137.72      | 132.55   |
| 24  | A     | 856 | BCR  | C15-C16-C17 | -2.51 | 118.39      | 123.52   |
| 22  | 7     | 324 | CLA  | C4B-CHC-C1C | 2.51  | 132.15      | 126.25   |
| 22  | B     | 823 | CLA  | C1C-C2C-C3C | -2.51 | 104.34      | 106.98   |
| 22  | 9     | 307 | CLA  | O2D-CGD-O1D | -2.51 | 118.97      | 123.85   |
| 22  | 4     | 809 | CLA  | O2A-CGA-CBA | 2.51  | 119.48      | 111.83   |
| 24  | B     | 845 | BCR  | C30-C25-C24 | 2.51  | 122.45      | 115.65   |
| 24  | A     | 844 | BCR  | C7-C6-C5    | -2.51 | 115.78      | 121.56   |
| 22  | 3     | 309 | CLA  | C4B-CHC-C1C | 2.51  | 132.14      | 126.25   |
| 22  | 3     | 318 | CLA  | C4B-CHC-C1C | 2.51  | 132.14      | 126.25   |
| 22  | 4     | 806 | CLA  | C4B-CHC-C1C | 2.51  | 132.14      | 126.25   |
| 22  | A     | 807 | CLA  | CHA-C4D-ND  | 2.51  | 137.72      | 132.55   |
| 24  | B     | 853 | BCR  | C20-C19-C18 | -2.51 | 119.49      | 126.36   |
| 22  | A     | 822 | CLA  | C4B-CHC-C1C | 2.51  | 132.14      | 126.25   |
| 22  | 6     | 321 | CLA  | C4B-CHC-C1C | 2.51  | 132.14      | 126.25   |
| 22  | 4     | 810 | CLA  | C4B-CHC-C1C | 2.51  | 132.14      | 126.25   |
| 22  | A     | 816 | CLA  | CHA-C4D-ND  | 2.51  | 137.72      | 132.55   |
| 22  | 1     | 306 | CLA  | O2A-CGA-CBA | 2.50  | 119.47      | 111.83   |
| 39  | 4     | 813 | CHL  | C4D-CHA-CBD | -2.50 | 106.44      | 108.97   |
| 22  | 3     | 320 | CLA  | CHA-C4D-ND  | 2.50  | 137.72      | 132.55   |
| 22  | B     | 835 | CLA  | CHD-C1D-ND  | -2.50 | 121.28      | 124.80   |
| 22  | 9     | 309 | CLA  | CMA-C3A-C4A | 2.50  | 118.50      | 111.77   |
| 22  | 5     | 308 | CLA  | C3B-C4B-NB  | -2.50 | 108.30      | 110.53   |
| 22  | 8     | 309 | CLA  | CHA-C4D-ND  | 2.50  | 137.71      | 132.55   |
| 22  | 6     | 312 | CLA  | CHA-C4D-ND  | 2.50  | 137.71      | 132.55   |
| 22  | 1     | 316 | CLA  | C1-C2-C3    | -2.50 | 122.10      | 126.20   |
| 32  | F     | 306 | RRX  | C30-C25-C26 | -2.50 | 119.22      | 122.64   |
| 22  | 7     | 315 | CLA  | C4B-CHC-C1C | 2.50  | 132.13      | 126.25   |
| 22  | 5     | 307 | CLA  | CMD-C2D-C3D | -2.50 | 121.95      | 127.69   |
| 24  | K     | 206 | BCR  | C8-C7-C6    | -2.50 | 120.32      | 127.00   |
| 22  | 3     | 312 | CLA  | O2A-CGA-CBA | 2.50  | 119.46      | 111.83   |
| 22  | 3     | 311 | CLA  | O2A-CGA-CBA | 2.50  | 119.46      | 111.83   |
| 22  | 4     | 811 | CLA  | CHA-C4D-ND  | 2.50  | 137.71      | 132.55   |
| 22  | 2     | 302 | CLA  | O2D-CGD-O1D | -2.50 | 118.98      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | 6     | 320 | CHL  | C4D-CHA-CBD | -2.50 | 106.45      | 108.97   |
| 22  | Z     | 306 | CLA  | C2C-C1C-NC  | 2.50  | 112.61      | 109.98   |
| 22  | 9     | 303 | CLA  | C6-C5-C3    | -2.50 | 107.38      | 113.47   |
| 22  | L     | 203 | CLA  | C4B-CHC-C1C | 2.50  | 132.12      | 126.25   |
| 22  | 1     | 304 | CLA  | O2A-CGA-CBA | 2.50  | 119.45      | 111.83   |
| 22  | 1     | 314 | CLA  | C4B-CHC-C1C | 2.50  | 132.12      | 126.25   |
| 22  | B     | 814 | CLA  | C1C-C2C-C3C | -2.50 | 104.35      | 106.98   |
| 22  | B     | 822 | CLA  | C4B-CHC-C1C | 2.50  | 132.12      | 126.25   |
| 22  | 4     | 817 | CLA  | C4B-CHC-C1C | 2.50  | 132.12      | 126.25   |
| 38  | 9     | 301 | LUT  | C35-C15-C14 | -2.50 | 118.41      | 123.52   |
| 22  | B     | 827 | CLA  | C4B-CHC-C1C | 2.50  | 132.12      | 126.25   |
| 22  | 4     | 812 | CLA  | C4B-CHC-C1C | 2.50  | 132.12      | 126.25   |
| 22  | 5     | 311 | CLA  | O2A-CGA-CBA | 2.50  | 119.45      | 111.83   |
| 22  | B     | 828 | CLA  | CHA-C4D-ND  | 2.50  | 137.70      | 132.55   |
| 24  | A     | 846 | BCR  | C23-C24-C25 | -2.50 | 120.33      | 127.00   |
| 22  | A     | 812 | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 22  | K     | 202 | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 22  | 1     | 316 | CLA  | C4B-CHC-C1C | 2.49  | 132.11      | 126.25   |
| 22  | B     | 815 | CLA  | C1C-C2C-C3C | -2.49 | 104.36      | 106.98   |
| 22  | Z     | 306 | CLA  | O2A-CGA-CBA | 2.49  | 119.44      | 111.83   |
| 22  | B     | 808 | CLA  | C4B-CHC-C1C | 2.49  | 132.11      | 126.25   |
| 22  | Z     | 306 | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 22  | B     | 835 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 22  | 6     | 307 | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 24  | A     | 847 | BCR  | C11-C12-C13 | -2.49 | 119.53      | 126.36   |
| 22  | 7     | 323 | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 22  | 6     | 301 | CLA  | C6-C5-C3    | -2.49 | 107.40      | 113.47   |
| 22  | 5     | 318 | CLA  | C4B-CHC-C1C | 2.49  | 132.11      | 126.25   |
| 22  | B     | 810 | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 22  | 1     | 309 | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 24  | 6     | 306 | BCR  | C37-C22-C23 | 2.49  | 121.89      | 118.09   |
| 41  | 8     | 320 | 3PH  | O21-C21-C22 | 2.49  | 120.08      | 110.93   |
| 22  | K     | 205 | CLA  | CHA-C4D-ND  | 2.49  | 137.69      | 132.55   |
| 22  | A     | 823 | CLA  | C2C-C1C-NC  | 2.49  | 112.60      | 109.98   |
| 22  | B     | 831 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 41  | 6     | 324 | 3PH  | O31-C31-C32 | 2.49  | 119.43      | 111.83   |
| 22  | B     | 816 | CLA  | C4B-CHC-C1C | 2.49  | 132.10      | 126.25   |
| 22  | 5     | 322 | CLA  | C4B-CHC-C1C | 2.49  | 132.10      | 126.25   |
| 22  | B     | 827 | CLA  | O2A-CGA-CBA | 2.49  | 119.42      | 111.83   |
| 22  | B     | 841 | CLA  | O2A-CGA-CBA | 2.49  | 119.42      | 111.83   |
| 22  | B     | 840 | CLA  | O2D-CGD-O1D | -2.49 | 119.00      | 123.85   |
| 22  | 9     | 304 | CLA  | C3D-C2D-C1D | -2.49 | 102.44      | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 1     | 313  | CLA  | CHA-C4D-ND  | 2.49  | 137.68      | 132.55   |
| 24  | I     | 4001 | BCR  | C8-C7-C6    | -2.49 | 120.35      | 127.00   |
| 22  | B     | 816  | CLA  | CMD-C2D-C3D | -2.49 | 121.98      | 127.69   |
| 22  | 8     | 314  | CLA  | C4B-CHC-C1C | 2.49  | 132.10      | 126.25   |
| 22  | A     | 804  | CLA  | CHA-C4D-ND  | 2.49  | 137.68      | 132.55   |
| 39  | 5     | 316  | CHL  | C4D-CHA-CBD | -2.49 | 106.46      | 108.97   |
| 38  | 5     | 303  | LUT  | C11-C12-C13 | -2.49 | 119.55      | 126.36   |
| 22  | 1     | 315  | CLA  | CHA-C4D-ND  | 2.49  | 137.68      | 132.55   |
| 22  | Z     | 313  | CLA  | CHA-C4D-ND  | 2.49  | 137.68      | 132.55   |
| 22  | A     | 821  | CLA  | C3B-C4B-NB  | -2.49 | 108.31      | 110.53   |
| 22  | 6     | 322  | CLA  | C1D-ND-C4D  | -2.49 | 104.57      | 106.31   |
| 22  | K     | 203  | CLA  | CHA-C4D-ND  | 2.49  | 137.68      | 132.55   |
| 22  | 7     | 324  | CLA  | CHA-C4D-ND  | 2.49  | 137.68      | 132.55   |
| 22  | 4     | 818  | CLA  | C1C-C2C-C3C | -2.49 | 104.37      | 106.98   |
| 24  | 6     | 306  | BCR  | C29-C30-C25 | 2.49  | 114.05      | 110.44   |
| 22  | A     | 827  | CLA  | C4B-CHC-C1C | 2.49  | 132.09      | 126.25   |
| 22  | A     | 831  | CLA  | C4B-CHC-C1C | 2.49  | 132.09      | 126.25   |
| 22  | Z     | 315  | CLA  | C4B-CHC-C1C | 2.49  | 132.09      | 126.25   |
| 22  | 3     | 313  | CLA  | CMA-C3A-C4A | 2.49  | 118.45      | 111.77   |
| 21  | A     | 801  | CL0  | O2D-CGD-O1D | -2.48 | 119.01      | 123.85   |
| 22  | B     | 836  | CLA  | C4B-CHC-C1C | 2.48  | 132.09      | 126.25   |
| 22  | 4     | 815  | CLA  | C4B-CHC-C1C | 2.48  | 132.09      | 126.25   |
| 35  | J     | 102  | T7X  | O18-C11-C31 | 2.48  | 119.41      | 111.83   |
| 22  | B     | 825  | CLA  | C4B-CHC-C1C | 2.48  | 132.09      | 126.25   |
| 22  | 3     | 320  | CLA  | C4B-CHC-C1C | 2.48  | 132.09      | 126.25   |
| 22  | 6     | 309  | CLA  | C4B-CHC-C1C | 2.48  | 132.09      | 126.25   |
| 22  | 5     | 312  | CLA  | CHA-C4D-ND  | 2.48  | 137.67      | 132.55   |
| 22  | 6     | 309  | CLA  | CHA-C1A-NA  | -2.48 | 120.77      | 126.39   |
| 22  | A     | 818  | CLA  | O2A-CGA-CBA | 2.48  | 119.41      | 111.83   |
| 38  | 6     | 303  | LUT  | C30-C31-C32 | -2.48 | 116.01      | 123.20   |
| 22  | Z     | 307  | CLA  | O2A-CGA-CBA | 2.48  | 119.41      | 111.83   |
| 22  | B     | 805  | CLA  | CHA-C4D-ND  | 2.48  | 137.67      | 132.55   |
| 22  | 5     | 312  | CLA  | C4B-CHC-C1C | 2.48  | 132.08      | 126.25   |
| 22  | A     | 804  | CLA  | CMA-C3A-C4A | 2.48  | 118.44      | 111.77   |
| 22  | B     | 834  | CLA  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 22  | 6     | 312  | CLA  | C4B-CHC-C1C | 2.48  | 132.08      | 126.25   |
| 39  | 8     | 312  | CHL  | C1-O2A-CGA  | 2.48  | 122.65      | 116.65   |
| 38  | 3     | 302  | LUT  | C27-C28-C29 | -2.48 | 120.99      | 126.32   |
| 22  | 6     | 301  | CLA  | O2A-CGA-CBA | 2.48  | 119.40      | 111.83   |
| 22  | 4     | 805  | CLA  | O2D-CGD-O1D | -2.48 | 119.02      | 123.85   |
| 22  | 5     | 309  | CLA  | CHA-C4D-ND  | 2.48  | 137.66      | 132.55   |
| 22  | A     | 838  | CLA  | C4B-CHC-C1C | 2.48  | 132.07      | 126.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | 8     | 304 | BCR  | C23-C24-C25 | -2.48 | 120.38      | 127.00   |
| 22  | 5     | 311 | CLA  | O2D-CGD-O1D | -2.48 | 119.03      | 123.85   |
| 22  | 3     | 309 | CLA  | CHA-C4D-ND  | 2.48  | 137.66      | 132.55   |
| 22  | B     | 826 | CLA  | O2D-CGD-O1D | -2.48 | 119.03      | 123.85   |
| 22  | 1     | 309 | CLA  | C4B-CHC-C1C | 2.48  | 132.07      | 126.25   |
| 22  | Z     | 308 | CLA  | C4B-CHC-C1C | 2.48  | 132.07      | 126.25   |
| 22  | 6     | 308 | CLA  | O2A-CGA-CBA | 2.48  | 119.39      | 111.83   |
| 24  | K     | 206 | BCR  | C23-C24-C25 | -2.48 | 120.39      | 127.00   |
| 22  | 1     | 306 | CLA  | C4B-CHC-C1C | 2.48  | 132.07      | 126.25   |
| 22  | B     | 806 | CLA  | CHA-C4D-ND  | 2.48  | 137.66      | 132.55   |
| 25  | A     | 849 | LHG  | C5-O7-C7    | -2.47 | 111.87      | 117.80   |
| 22  | A     | 833 | CLA  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 22  | 9     | 313 | CLA  | O2A-CGA-CBA | 2.47  | 119.38      | 111.83   |
| 22  | 4     | 805 | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | B     | 810 | CLA  | C4B-CHC-C1C | 2.47  | 132.06      | 126.25   |
| 22  | 3     | 320 | CLA  | CHA-C1A-NA  | -2.47 | 120.79      | 126.39   |
| 22  | B     | 826 | CLA  | C4B-CHC-C1C | 2.47  | 132.06      | 126.25   |
| 22  | A     | 826 | CLA  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 22  | 5     | 320 | CLA  | C1-O2A-CGA  | 2.47  | 122.64      | 116.65   |
| 22  | 7     | 306 | CLA  | CHA-C1A-NA  | -2.47 | 120.79      | 126.39   |
| 22  | 4     | 806 | CLA  | O2D-CGD-O1D | -2.47 | 119.03      | 123.85   |
| 22  | A     | 821 | CLA  | C4B-CHC-C1C | 2.47  | 132.06      | 126.25   |
| 22  | 9     | 307 | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 24  | B     | 853 | BCR  | C34-C9-C10  | -2.47 | 118.81      | 122.82   |
| 22  | A     | 820 | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | B     | 834 | CLA  | C3B-C4B-NB  | -2.47 | 108.32      | 110.53   |
| 22  | B     | 820 | CLA  | C4B-CHC-C1C | 2.47  | 132.06      | 126.25   |
| 22  | B     | 829 | CLA  | C4B-CHC-C1C | 2.47  | 132.06      | 126.25   |
| 22  | 3     | 312 | CLA  | O2D-CGD-O1D | -2.47 | 119.04      | 123.85   |
| 39  | 4     | 813 | CHL  | C1-O2A-CGA  | 2.47  | 122.63      | 116.65   |
| 22  | A     | 826 | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | Z     | 303 | CLA  | O2A-CGA-CBA | 2.47  | 119.37      | 111.83   |
| 39  | Z     | 311 | CHL  | CMA-C3A-C4A | 2.47  | 119.93      | 114.61   |
| 22  | A     | 827 | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | 3     | 312 | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | 5     | 307 | CLA  | CHA-C4D-ND  | 2.47  | 137.65      | 132.55   |
| 22  | 9     | 308 | CLA  | C3B-C4B-NB  | -2.47 | 108.33      | 110.53   |
| 22  | A     | 802 | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 22  | A     | 836 | CLA  | C4B-CHC-C1C | 2.47  | 132.05      | 126.25   |
| 24  | A     | 846 | BCR  | C38-C26-C27 | 2.47  | 118.86      | 113.60   |
| 22  | B     | 809 | CLA  | C4B-CHC-C1C | 2.47  | 132.05      | 126.25   |
| 22  | A     | 806 | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 816 | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 22  | G     | 202 | CLA  | C4B-CHC-C1C | 2.47  | 132.05      | 126.25   |
| 22  | B     | 818 | CLA  | O2A-CGA-CBA | 2.47  | 119.36      | 111.83   |
| 22  | A     | 804 | CLA  | O2D-CGD-O1D | -2.47 | 119.05      | 123.85   |
| 22  | A     | 828 | CLA  | C4B-CHC-C1C | 2.47  | 132.05      | 126.25   |
| 22  | A     | 818 | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 22  | B     | 837 | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 22  | 6     | 308 | CLA  | C4B-CHC-C1C | 2.47  | 132.05      | 126.25   |
| 22  | 3     | 322 | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 22  | F     | 302 | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 22  | 5     | 310 | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 25  | 7     | 318 | LHG  | C5-O7-C7    | -2.47 | 111.89      | 117.80   |
| 22  | A     | 825 | CLA  | CHA-C4D-ND  | 2.47  | 137.64      | 132.55   |
| 22  | 5     | 320 | CLA  | C2D-C1D-ND  | 2.47  | 112.57      | 110.13   |
| 22  | 9     | 305 | CLA  | CHA-C4D-ND  | 2.47  | 137.63      | 132.55   |
| 22  | 7     | 304 | CLA  | CHD-C1D-ND  | -2.46 | 121.33      | 124.80   |
| 22  | B     | 827 | CLA  | O2D-CGD-O1D | -2.46 | 119.05      | 123.85   |
| 22  | Z     | 305 | CLA  | C4B-CHC-C1C | 2.46  | 132.04      | 126.25   |
| 22  | 7     | 304 | CLA  | O2A-CGA-CBA | 2.46  | 119.35      | 111.83   |
| 22  | B     | 842 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | 7     | 312 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | A     | 840 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | Z     | 303 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | 3     | 316 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | A     | 813 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | 6     | 311 | CLA  | C4B-CHC-C1C | 2.46  | 132.04      | 126.25   |
| 22  | A     | 837 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | G     | 201 | CLA  | C1D-ND-C4D  | -2.46 | 104.58      | 106.31   |
| 22  | A     | 833 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | B     | 807 | CLA  | C2C-C1C-NC  | 2.46  | 112.57      | 109.98   |
| 22  | 4     | 810 | CLA  | CHA-C4D-ND  | 2.46  | 137.63      | 132.55   |
| 22  | 1     | 309 | CLA  | CMD-C2D-C3D | -2.46 | 122.05      | 127.69   |
| 22  | 3     | 310 | CLA  | CHA-C1A-NA  | -2.46 | 120.82      | 126.39   |
| 22  | B     | 840 | CLA  | C4B-CHC-C1C | 2.46  | 132.03      | 126.25   |
| 24  | 6     | 306 | BCR  | C8-C7-C6    | -2.46 | 120.43      | 127.00   |
| 22  | 4     | 807 | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | 7     | 309 | CLA  | C4B-CHC-C1C | 2.46  | 132.03      | 126.25   |
| 22  | 7     | 309 | CLA  | O2A-CGA-CBA | 2.46  | 119.33      | 111.83   |
| 22  | B     | 824 | CLA  | O2A-CGA-CBA | 2.46  | 119.33      | 111.83   |
| 34  | J     | 101 | LMG  | C8-O7-C10   | -2.46 | 111.91      | 117.80   |
| 22  | 5     | 315 | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | A     | 821 | CLA  | O2A-CGA-CBA | 2.46  | 119.33      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 839 | CLA  | O2A-CGA-CBA | 2.46  | 119.33      | 111.83   |
| 22  | 7     | 311 | CLA  | C2D-C1D-ND  | 2.46  | 112.56      | 110.13   |
| 25  | 7     | 318 | LHG  | O8-C23-C24  | 2.46  | 119.33      | 111.83   |
| 22  | 9     | 306 | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 24  | 3     | 304 | BCR  | C36-C18-C19 | 2.46  | 121.84      | 118.09   |
| 22  | A     | 842 | CLA  | C4B-CHC-C1C | 2.46  | 132.02      | 126.25   |
| 22  | 7     | 305 | CLA  | C4B-CHC-C1C | 2.46  | 132.02      | 126.25   |
| 22  | F     | 302 | CLA  | O2A-CGA-CBA | 2.46  | 119.33      | 111.83   |
| 22  | A     | 830 | CLA  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 22  | B     | 812 | CLA  | C4B-CHC-C1C | 2.46  | 132.02      | 126.25   |
| 39  | 4     | 814 | CHL  | C4D-CHA-CBD | -2.46 | 106.49      | 108.97   |
| 22  | B     | 834 | CLA  | C4B-CHC-C1C | 2.46  | 132.02      | 126.25   |
| 22  | 6     | 308 | CLA  | C2D-C1D-ND  | 2.46  | 112.56      | 110.13   |
| 22  | B     | 833 | CLA  | C4B-CHC-C1C | 2.45  | 132.02      | 126.25   |
| 22  | A     | 839 | CLA  | CHA-C4D-ND  | 2.45  | 137.61      | 132.55   |
| 22  | B     | 824 | CLA  | C2D-C1D-ND  | 2.45  | 112.55      | 110.13   |
| 22  | A     | 854 | CLA  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 22  | B     | 818 | CLA  | C2C-C1C-NC  | 2.45  | 112.56      | 109.98   |
| 22  | A     | 842 | CLA  | O2D-CGD-O1D | -2.45 | 119.08      | 123.85   |
| 22  | 3     | 310 | CLA  | C4B-CHC-C1C | 2.45  | 132.01      | 126.25   |
| 22  | L     | 201 | CLA  | CHA-C4D-ND  | 2.45  | 137.61      | 132.55   |
| 22  | 3     | 320 | CLA  | CMA-C3A-C4A | 2.45  | 118.36      | 111.77   |
| 22  | A     | 839 | CLA  | O2A-CGA-CBA | 2.45  | 119.31      | 111.83   |
| 22  | 8     | 307 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | 5     | 323 | CLA  | C4B-CHC-C1C | 2.45  | 132.01      | 126.25   |
| 38  | 6     | 304 | LUT  | C15-C35-C34 | -2.45 | 118.51      | 123.52   |
| 22  | 6     | 309 | CLA  | C1D-ND-C4D  | -2.45 | 104.59      | 106.31   |
| 22  | B     | 827 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | F     | 305 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | B     | 826 | CLA  | CMD-C2D-C3D | -2.45 | 122.07      | 127.69   |
| 22  | A     | 836 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | 3     | 308 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 27  | A     | 852 | DGA  | OG1-CA1-CA2 | 2.45  | 119.30      | 111.83   |
| 22  | 5     | 322 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 38  | 3     | 302 | LUT  | C21-C26-C27 | -2.45 | 110.01      | 112.83   |
| 22  | A     | 839 | CLA  | C4B-CHC-C1C | 2.45  | 132.00      | 126.25   |
| 22  | A     | 815 | CLA  | C4B-CHC-C1C | 2.45  | 132.00      | 126.25   |
| 22  | 9     | 311 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | A     | 819 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | K     | 203 | CLA  | C4B-CHC-C1C | 2.45  | 132.00      | 126.25   |
| 22  | A     | 815 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | 1     | 307 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 3     | 310 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | A     | 819 | CLA  | O2D-CGD-O1D | -2.45 | 119.09      | 123.85   |
| 22  | B     | 838 | CLA  | C1-C2-C3    | -2.45 | 122.19      | 126.20   |
| 22  | B     | 819 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | B     | 820 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | 6     | 301 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | 6     | 314 | CLA  | CHA-C4D-ND  | 2.45  | 137.60      | 132.55   |
| 22  | L     | 201 | CLA  | C2D-C1D-ND  | 2.45  | 112.55      | 110.13   |
| 22  | 7     | 306 | CLA  | CHA-C4D-ND  | 2.45  | 137.59      | 132.55   |
| 22  | B     | 809 | CLA  | O2A-CGA-CBA | 2.45  | 119.29      | 111.83   |
| 22  | B     | 811 | CLA  | CHA-C4D-ND  | 2.45  | 137.59      | 132.55   |
| 22  | 8     | 310 | CLA  | CHA-C4D-ND  | 2.45  | 137.59      | 132.55   |
| 22  | 5     | 322 | CLA  | O2A-CGA-CBA | 2.45  | 119.29      | 111.83   |
| 24  | 3     | 306 | BCR  | C8-C7-C6    | -2.44 | 120.47      | 127.00   |
| 22  | B     | 814 | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 22  | 7     | 306 | CLA  | C4B-CHC-C1C | 2.44  | 132.00      | 126.25   |
| 22  | F     | 301 | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 22  | 8     | 313 | CLA  | C4B-CHC-C1C | 2.44  | 131.99      | 126.25   |
| 22  | A     | 814 | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 24  | 3     | 305 | BCR  | C1-C6-C7    | 2.44  | 122.28      | 115.65   |
| 38  | 6     | 303 | LUT  | C11-C12-C13 | -2.44 | 119.67      | 126.36   |
| 22  | B     | 817 | CLA  | C4B-CHC-C1C | 2.44  | 131.99      | 126.25   |
| 22  | 7     | 310 | CLA  | C4B-CHC-C1C | 2.44  | 131.99      | 126.25   |
| 22  | B     | 818 | CLA  | C1C-C2C-C3C | -2.44 | 104.41      | 106.98   |
| 22  | 8     | 309 | CLA  | O2A-CGA-CBA | 2.44  | 119.28      | 111.83   |
| 22  | A     | 821 | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 22  | B     | 817 | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 22  | A     | 825 | CLA  | C4B-CHC-C1C | 2.44  | 131.99      | 126.25   |
| 22  | B     | 836 | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 24  | A     | 848 | BCR  | C34-C9-C10  | -2.44 | 118.86      | 122.82   |
| 22  | 5     | 308 | CLA  | CMA-C3A-C4A | 2.44  | 118.33      | 111.77   |
| 22  | A     | 833 | CLA  | O2A-CGA-CBA | 2.44  | 119.28      | 111.83   |
| 25  | Z     | 317 | LHG  | C5-O7-C7    | -2.44 | 111.95      | 117.80   |
| 22  | 3     | 314 | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 22  | 2     | 301 | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 22  | 8     | 313 | CLA  | O2D-CGD-O1D | -2.44 | 119.10      | 123.85   |
| 22  | B     | 806 | CLA  | O2A-CGA-CBA | 2.44  | 119.28      | 111.83   |
| 38  | 4     | 803 | LUT  | C11-C12-C13 | -2.44 | 119.67      | 126.36   |
| 22  | A     | 855 | CLA  | CHA-C4D-ND  | 2.44  | 137.59      | 132.55   |
| 22  | A     | 803 | CLA  | O2D-CGD-O1D | -2.44 | 119.10      | 123.85   |
| 22  | 6     | 311 | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | 1     | 311 | CLA  | C4B-CHC-C1C | 2.44  | 131.99      | 126.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | G     | 202 | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | B     | 833 | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | B     | 840 | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | A     | 832 | CLA  | C4B-CHC-C1C | 2.44  | 131.98      | 126.25   |
| 22  | 7     | 311 | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | B     | 815 | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | 2     | 302 | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | 4     | 807 | CLA  | C4B-CHC-C1C | 2.44  | 131.98      | 126.25   |
| 22  | 6     | 302 | CLA  | O2D-CGD-O1D | -2.44 | 119.10      | 123.85   |
| 22  | 6     | 322 | CLA  | O1D-CGD-CBD | -2.44 | 119.71      | 124.52   |
| 22  | L     | 203 | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | K     | 204 | CLA  | C4B-CHC-C1C | 2.44  | 131.98      | 126.25   |
| 22  | 1     | 308 | CLA  | CHA-C4D-ND  | 2.44  | 137.58      | 132.55   |
| 22  | A     | 836 | CLA  | CMA-C3A-C4A | 2.44  | 118.32      | 111.77   |
| 22  | Z     | 306 | CLA  | C6-C5-C3    | -2.44 | 107.53      | 113.47   |
| 22  | 5     | 319 | CLA  | C4B-CHC-C1C | 2.44  | 131.98      | 126.25   |
| 22  | 3     | 319 | CLA  | C4B-CHC-C1C | 2.44  | 131.98      | 126.25   |
| 22  | B     | 841 | CLA  | O2D-CGD-O1D | -2.44 | 119.11      | 123.85   |
| 22  | A     | 854 | CLA  | CHA-C4D-ND  | 2.44  | 137.57      | 132.55   |
| 22  | A     | 802 | CLA  | C4B-CHC-C1C | 2.44  | 131.97      | 126.25   |
| 22  | 4     | 815 | CLA  | CHA-C4D-ND  | 2.44  | 137.57      | 132.55   |
| 22  | 6     | 319 | CLA  | CHA-C4D-ND  | 2.44  | 137.57      | 132.55   |
| 22  | A     | 813 | CLA  | O2A-CGA-CBA | 2.44  | 119.26      | 111.83   |
| 22  | A     | 811 | CLA  | CHA-C4D-ND  | 2.44  | 137.57      | 132.55   |
| 22  | 5     | 320 | CLA  | CHA-C4D-ND  | 2.43  | 137.57      | 132.55   |
| 22  | 7     | 316 | CLA  | C4B-CHC-C1C | 2.43  | 131.97      | 126.25   |
| 22  | 6     | 319 | CLA  | O2D-CGD-O1D | -2.43 | 119.11      | 123.85   |
| 22  | Z     | 306 | CLA  | CMD-C2D-C3D | -2.43 | 122.11      | 127.69   |
| 22  | 7     | 309 | CLA  | C2D-C1D-ND  | 2.43  | 112.53      | 110.13   |
| 22  | A     | 814 | CLA  | C4B-CHC-C1C | 2.43  | 131.97      | 126.25   |
| 22  | B     | 838 | CLA  | CHA-C4D-ND  | 2.43  | 137.57      | 132.55   |
| 22  | Z     | 315 | CLA  | CHA-C4D-ND  | 2.43  | 137.57      | 132.55   |
| 22  | A     | 805 | CLA  | CHD-C1D-ND  | -2.43 | 121.38      | 124.80   |
| 22  | A     | 822 | CLA  | CHA-C4D-ND  | 2.43  | 137.57      | 132.55   |
| 22  | A     | 831 | CLA  | CHA-C4D-ND  | 2.43  | 137.57      | 132.55   |
| 24  | F     | 303 | BCR  | C30-C25-C26 | -2.43 | 119.31      | 122.64   |
| 22  | A     | 828 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | A     | 832 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | 3     | 319 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | B     | 820 | CLA  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |
| 22  | 5     | 310 | CLA  | CMD-C2D-C3D | -2.43 | 122.11      | 127.69   |
| 22  | 4     | 817 | CLA  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 842 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | B     | 816 | CLA  | O2A-CGA-CBA | 2.43  | 119.24      | 111.83   |
| 22  | A     | 808 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | 7     | 307 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | B     | 841 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | 8     | 316 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | 6     | 322 | CLA  | C4B-CHC-C1C | 2.43  | 131.96      | 126.25   |
| 22  | 7     | 316 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | Z     | 309 | CLA  | C2D-C1D-ND  | 2.43  | 112.53      | 110.13   |
| 22  | B     | 801 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | Z     | 305 | CLA  | O2A-CGA-CBA | 2.43  | 119.23      | 111.83   |
| 22  | Z     | 307 | CLA  | CMD-C2D-C3D | -2.43 | 122.12      | 127.69   |
| 22  | 6     | 307 | CLA  | O2D-CGD-O1D | -2.43 | 119.12      | 123.85   |
| 22  | 4     | 805 | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 22  | 7     | 305 | CLA  | CHA-C4D-ND  | 2.43  | 137.56      | 132.55   |
| 22  | A     | 842 | CLA  | O2A-CGA-CBA | 2.43  | 119.23      | 111.83   |
| 22  | F     | 301 | CLA  | C6-C5-C3    | -2.43 | 107.56      | 113.47   |
| 22  | B     | 839 | CLA  | C4B-CHC-C1C | 2.43  | 131.95      | 126.25   |
| 22  | 3     | 316 | CLA  | O2D-CGD-O1D | -2.43 | 119.13      | 123.85   |
| 22  | 8     | 311 | CLA  | CHA-C4D-ND  | 2.43  | 137.55      | 132.55   |
| 22  | 8     | 313 | CLA  | CHA-C4D-ND  | 2.43  | 137.55      | 132.55   |
| 22  | 6     | 309 | CLA  | CMD-C2D-C3D | -2.43 | 122.13      | 127.69   |
| 22  | B     | 809 | CLA  | CHA-C4D-ND  | 2.43  | 137.55      | 132.55   |
| 22  | Z     | 307 | CLA  | CHA-C4D-ND  | 2.43  | 137.55      | 132.55   |
| 24  | 7     | 303 | BCR  | C23-C24-C25 | -2.43 | 120.52      | 127.00   |
| 22  | 1     | 311 | CLA  | CHA-C4D-ND  | 2.42  | 137.55      | 132.55   |
| 22  | 6     | 302 | CLA  | CHA-C4D-ND  | 2.42  | 137.55      | 132.55   |
| 22  | A     | 829 | CLA  | CHA-C4D-ND  | 2.42  | 137.55      | 132.55   |
| 22  | 4     | 812 | CLA  | O2D-CGD-O1D | -2.42 | 119.13      | 123.85   |
| 22  | B     | 806 | CLA  | C4B-CHC-C1C | 2.42  | 131.95      | 126.25   |
| 22  | 8     | 305 | CLA  | CMD-C2D-C3D | -2.42 | 122.13      | 127.69   |
| 22  | 4     | 817 | CLA  | CHA-C4D-ND  | 2.42  | 137.55      | 132.55   |
| 22  | B     | 829 | CLA  | O2A-CGA-CBA | 2.42  | 119.22      | 111.83   |
| 22  | B     | 818 | CLA  | CHA-C4D-ND  | 2.42  | 137.55      | 132.55   |
| 22  | B     | 821 | CLA  | CHA-C4D-ND  | 2.42  | 137.55      | 132.55   |
| 22  | B     | 835 | CLA  | CHA-C4D-ND  | 2.42  | 137.55      | 132.55   |
| 22  | B     | 825 | CLA  | CAA-CBA-CGA | -2.42 | 106.33      | 113.21   |
| 22  | Z     | 309 | CLA  | O2D-CGD-O1D | -2.42 | 119.13      | 123.85   |
| 22  | A     | 838 | CLA  | O2A-CGA-CBA | 2.42  | 119.22      | 111.83   |
| 22  | 4     | 807 | CLA  | CHA-C1A-NA  | -2.42 | 120.91      | 126.39   |
| 22  | Z     | 308 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | A     | 816 | CLA  | C4B-CHC-C1C | 2.42  | 131.94      | 126.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 1     | 306 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | 3     | 313 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | 9     | 313 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | 7     | 323 | CLA  | C4B-CHC-C1C | 2.42  | 131.94      | 126.25   |
| 22  | 6     | 317 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | 6     | 321 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | 7     | 324 | CLA  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 22  | 8     | 307 | CLA  | C4B-CHC-C1C | 2.42  | 131.94      | 126.25   |
| 22  | 1     | 304 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | 5     | 323 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | B     | 839 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | A     | 818 | CLA  | CMD-C2D-C3D | -2.42 | 122.14      | 127.69   |
| 22  | B     | 824 | CLA  | C1C-C2C-C3C | -2.42 | 104.44      | 106.98   |
| 24  | A     | 856 | BCR  | C29-C28-C27 | 2.42  | 116.59      | 111.28   |
| 22  | 6     | 317 | CLA  | O2A-CGA-CBA | 2.42  | 119.21      | 111.83   |
| 22  | 1     | 308 | CLA  | C2D-C1D-ND  | 2.42  | 112.52      | 110.13   |
| 22  | 3     | 313 | CLA  | CHD-C1D-ND  | -2.42 | 121.40      | 124.80   |
| 22  | A     | 838 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | B     | 808 | CLA  | CHA-C4D-ND  | 2.42  | 137.54      | 132.55   |
| 22  | B     | 801 | CLA  | C4B-CHC-C1C | 2.42  | 131.93      | 126.25   |
| 22  | A     | 820 | CLA  | O2A-CGA-CBA | 2.42  | 119.20      | 111.83   |
| 22  | 9     | 308 | CLA  | CHA-C4D-ND  | 2.42  | 137.53      | 132.55   |
| 22  | A     | 805 | CLA  | O2A-CGA-CBA | 2.42  | 119.20      | 111.83   |
| 22  | A     | 816 | CLA  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 22  | B     | 837 | CLA  | O2D-CGD-O1D | -2.42 | 119.14      | 123.85   |
| 24  | 5     | 304 | BCR  | C23-C24-C25 | -2.42 | 120.54      | 127.00   |
| 22  | A     | 810 | CLA  | CHA-C4D-ND  | 2.42  | 137.53      | 132.55   |
| 22  | 5     | 307 | CLA  | O1D-CGD-CBD | -2.41 | 119.75      | 124.52   |
| 22  | 3     | 311 | CLA  | CHA-C4D-ND  | 2.41  | 137.53      | 132.55   |
| 22  | 8     | 311 | CLA  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 22  | 9     | 308 | CLA  | C4B-CHC-C1C | 2.41  | 131.93      | 126.25   |
| 22  | B     | 840 | CLA  | O2A-CGA-CBA | 2.41  | 119.20      | 111.83   |
| 22  | 7     | 307 | CLA  | CHD-C1D-ND  | -2.41 | 121.41      | 124.80   |
| 22  | 7     | 316 | CLA  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 22  | B     | 822 | CLA  | CHA-C4D-ND  | 2.41  | 137.53      | 132.55   |
| 22  | A     | 835 | CLA  | CMA-C3A-C4A | 2.41  | 118.26      | 111.77   |
| 22  | B     | 814 | CLA  | CMD-C2D-C3D | -2.41 | 122.15      | 127.69   |
| 22  | 4     | 818 | CLA  | CHA-C4D-ND  | 2.41  | 137.53      | 132.55   |
| 22  | 8     | 308 | CLA  | CHA-C4D-ND  | 2.41  | 137.53      | 132.55   |
| 22  | 4     | 812 | CLA  | CHA-C4D-ND  | 2.41  | 137.53      | 132.55   |
| 22  | B     | 828 | CLA  | O2D-CGD-O1D | -2.41 | 119.15      | 123.85   |
| 22  | 5     | 318 | CLA  | CHA-C4D-ND  | 2.41  | 137.53      | 132.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 801 | CLA  | O2A-CGA-CBA | 2.41  | 119.19      | 111.83   |
| 22  | B     | 812 | CLA  | CHA-C4D-ND  | 2.41  | 137.53      | 132.55   |
| 22  | 7     | 322 | CLA  | CHA-C4D-ND  | 2.41  | 137.53      | 132.55   |
| 22  | A     | 854 | CLA  | C4B-CHC-C1C | 2.41  | 131.92      | 126.25   |
| 39  | 6     | 316 | CHL  | C4D-CHA-CBD | -2.41 | 106.54      | 108.97   |
| 22  | 7     | 305 | CLA  | C2D-C1D-ND  | 2.41  | 112.51      | 110.13   |
| 22  | 5     | 308 | CLA  | C4B-CHC-C1C | 2.41  | 131.92      | 126.25   |
| 22  | Z     | 310 | CLA  | O2A-CGA-CBA | 2.41  | 119.19      | 111.83   |
| 22  | 5     | 314 | CLA  | CHA-C4D-ND  | 2.41  | 137.52      | 132.55   |
| 24  | B     | 844 | BCR  | C35-C13-C14 | -2.41 | 118.91      | 122.82   |
| 22  | 8     | 314 | CLA  | CHA-C4D-ND  | 2.41  | 137.52      | 132.55   |
| 22  | A     | 805 | CLA  | C2D-C1D-ND  | 2.41  | 112.51      | 110.13   |
| 22  | B     | 805 | CLA  | C2D-C1D-ND  | 2.41  | 112.51      | 110.13   |
| 22  | A     | 816 | CLA  | C1D-ND-C4D  | -2.41 | 104.62      | 106.31   |
| 22  | 9     | 309 | CLA  | C4B-CHC-C1C | 2.41  | 131.91      | 126.25   |
| 22  | 7     | 304 | CLA  | CAA-C2A-C3A | -2.41 | 106.49      | 113.00   |
| 22  | 7     | 317 | CLA  | CHA-C4D-ND  | 2.41  | 137.52      | 132.55   |
| 22  | A     | 823 | CLA  | CHA-C4D-ND  | 2.41  | 137.52      | 132.55   |
| 22  | B     | 824 | CLA  | CHA-C4D-ND  | 2.41  | 137.52      | 132.55   |
| 22  | 3     | 313 | CLA  | C4B-CHC-C1C | 2.41  | 131.91      | 126.25   |
| 22  | 4     | 810 | CLA  | O2A-CGA-CBA | 2.41  | 119.17      | 111.83   |
| 22  | A     | 834 | CLA  | CHA-C4D-ND  | 2.41  | 137.51      | 132.55   |
| 22  | 7     | 304 | CLA  | C2D-C1D-ND  | 2.41  | 112.51      | 110.13   |
| 22  | B     | 819 | CLA  | O2A-CGA-CBA | 2.41  | 119.17      | 111.83   |
| 22  | B     | 832 | CLA  | CHA-C4D-ND  | 2.41  | 137.51      | 132.55   |
| 23  | B     | 843 | PQN  | C2M-C2-C3   | -2.41 | 120.50      | 124.45   |
| 38  | 5     | 302 | LUT  | C18-C5-C4   | 2.41  | 118.84      | 114.42   |
| 22  | 1     | 313 | CLA  | C2D-C1D-ND  | 2.41  | 112.51      | 110.13   |
| 22  | J     | 103 | CLA  | CHA-C4D-ND  | 2.41  | 137.51      | 132.55   |
| 22  | 7     | 314 | CLA  | CHA-C4D-ND  | 2.41  | 137.51      | 132.55   |
| 22  | 6     | 310 | CLA  | CHA-C4D-ND  | 2.41  | 137.51      | 132.55   |
| 22  | 6     | 313 | CLA  | CHA-C4D-ND  | 2.41  | 137.51      | 132.55   |
| 22  | A     | 807 | CLA  | CMD-C2D-C3D | -2.40 | 122.17      | 127.69   |
| 22  | 7     | 322 | CLA  | C2D-C1D-ND  | 2.40  | 112.51      | 110.13   |
| 22  | A     | 803 | CLA  | CHA-C4D-ND  | 2.40  | 137.51      | 132.55   |
| 22  | A     | 823 | CLA  | CMD-C2D-C3D | -2.40 | 122.17      | 127.69   |
| 22  | 6     | 314 | CLA  | O2A-CGA-CBA | 2.40  | 119.16      | 111.83   |
| 22  | 6     | 313 | CLA  | O2A-CGA-CBA | 2.40  | 119.16      | 111.83   |
| 22  | 4     | 811 | CLA  | O2D-CGD-O1D | -2.40 | 119.17      | 123.85   |
| 24  | 4     | 804 | BCR  | C38-C26-C27 | 2.40  | 118.72      | 113.60   |
| 22  | A     | 839 | CLA  | O2D-CGD-O1D | -2.40 | 119.17      | 123.85   |
| 22  | 8     | 305 | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | A     | 847 | BCR  | C30-C25-C26 | -2.40 | 119.35      | 122.64   |
| 22  | G     | 202 | CLA  | CHD-C1D-ND  | -2.40 | 121.42      | 124.80   |
| 22  | Z     | 316 | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 22  | B     | 807 | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 22  | 5     | 319 | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 22  | 8     | 306 | CLA  | O2D-CGD-O1D | -2.40 | 119.18      | 123.85   |
| 22  | A     | 835 | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 22  | 1     | 309 | CLA  | O2A-CGA-CBA | 2.40  | 119.15      | 111.83   |
| 22  | 1     | 315 | CLA  | CMD-C2D-C3D | -2.40 | 122.19      | 127.69   |
| 22  | 4     | 805 | CLA  | CMD-C2D-C3D | -2.40 | 122.19      | 127.69   |
| 22  | B     | 823 | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 22  | 3     | 318 | CLA  | CHA-C4D-ND  | 2.40  | 137.50      | 132.55   |
| 22  | 8     | 311 | CLA  | O2A-CGA-CBA | 2.40  | 119.15      | 111.83   |
| 22  | B     | 801 | CLA  | CMA-C3A-C4A | 2.40  | 118.22      | 111.77   |
| 41  | 8     | 320 | 3PH  | O31-C31-C32 | 2.40  | 119.15      | 111.83   |
| 22  | 7     | 315 | CLA  | CAA-C2A-C3A | -2.40 | 106.52      | 113.00   |
| 22  | B     | 815 | CLA  | O2A-CGA-CBA | 2.40  | 119.14      | 111.83   |
| 22  | B     | 825 | CLA  | CHA-C4D-ND  | 2.40  | 137.49      | 132.55   |
| 22  | 6     | 308 | CLA  | CHA-C4D-ND  | 2.40  | 137.49      | 132.55   |
| 22  | 7     | 308 | CLA  | O2A-CGA-CBA | 2.40  | 119.14      | 111.83   |
| 22  | 7     | 323 | CLA  | O2A-CGA-CBA | 2.40  | 119.14      | 111.83   |
| 22  | K     | 204 | CLA  | CHA-C4D-ND  | 2.40  | 137.49      | 132.55   |
| 39  | 7     | 313 | CHL  | C4D-CHA-CBD | -2.40 | 106.55      | 108.97   |
| 22  | A     | 825 | CLA  | CMD-C2D-C3D | -2.40 | 122.19      | 127.69   |
| 22  | Z     | 313 | CLA  | O2D-CGD-O1D | -2.40 | 119.19      | 123.85   |
| 22  | 6     | 302 | CLA  | O2A-CGA-CBA | 2.40  | 119.14      | 111.83   |
| 22  | A     | 841 | CLA  | CHA-C4D-ND  | 2.40  | 137.49      | 132.55   |
| 22  | 5     | 301 | CLA  | CHA-C4D-ND  | 2.40  | 137.49      | 132.55   |
| 22  | F     | 304 | CLA  | CMD-C2D-C3D | -2.40 | 122.20      | 127.69   |
| 22  | 4     | 807 | CLA  | C3B-C4B-NB  | -2.39 | 108.39      | 110.53   |
| 22  | L     | 202 | CLA  | CHA-C4D-ND  | 2.39  | 137.49      | 132.55   |
| 21  | A     | 801 | CL0  | CMB-C2B-C3B | 2.39  | 129.47      | 124.68   |
| 24  | B     | 848 | BCR  | C29-C30-C25 | 2.39  | 113.92      | 110.44   |
| 24  | B     | 849 | BCR  | C23-C24-C25 | -2.39 | 120.60      | 127.00   |
| 24  | B     | 846 | BCR  | C33-C5-C4   | 2.39  | 118.70      | 113.60   |
| 22  | B     | 810 | CLA  | O2D-CGD-O1D | -2.39 | 119.19      | 123.85   |
| 39  | 2     | 303 | CHL  | C1-O2A-CGA  | 2.39  | 122.44      | 116.65   |
| 22  | A     | 806 | CLA  | O2D-CGD-O1D | -2.39 | 119.19      | 123.85   |
| 22  | 1     | 316 | CLA  | C2D-C1D-ND  | 2.39  | 112.49      | 110.13   |
| 22  | Z     | 307 | CLA  | CHD-C1D-ND  | -2.39 | 121.44      | 124.80   |
| 22  | 7     | 324 | CLA  | C1-O2A-CGA  | 2.39  | 122.44      | 116.65   |
| 22  | B     | 830 | CLA  | CHA-C4D-ND  | 2.39  | 137.48      | 132.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | Z     | 314 | CLA  | CHA-C4D-ND  | 2.39  | 137.48      | 132.55   |
| 36  | J     | 105 | C7Z  | C11-C12-C13 | -2.39 | 119.81      | 126.36   |
| 38  | Z     | 301 | LUT  | C31-C30-C29 | -2.39 | 123.93      | 127.28   |
| 22  | 3     | 319 | CLA  | O2A-CGA-CBA | 2.39  | 119.11      | 111.83   |
| 22  | 1     | 311 | CLA  | CMA-C3A-C4A | 2.39  | 118.19      | 111.77   |
| 22  | 9     | 308 | CLA  | O2D-CGD-O1D | -2.39 | 119.20      | 123.85   |
| 39  | 8     | 312 | CHL  | CMA-C3A-C4A | 2.39  | 119.75      | 114.61   |
| 22  | A     | 823 | CLA  | O2A-CGA-CBA | 2.39  | 119.11      | 111.83   |
| 22  | 4     | 808 | CLA  | CHA-C4D-ND  | 2.39  | 137.47      | 132.55   |
| 22  | 4     | 806 | CLA  | O2A-CGA-CBA | 2.39  | 119.11      | 111.83   |
| 22  | 7     | 310 | CLA  | C2D-C1D-ND  | 2.39  | 112.49      | 110.13   |
| 22  | 2     | 304 | CLA  | CHA-C4D-ND  | 2.39  | 137.47      | 132.55   |
| 22  | 1     | 316 | CLA  | C2A-C1A-CHA | 2.38  | 128.00      | 123.87   |
| 22  | B     | 832 | CLA  | CMD-C2D-C3D | -2.38 | 122.22      | 127.69   |
| 22  | A     | 838 | CLA  | O2D-CGD-O1D | -2.38 | 119.21      | 123.85   |
| 22  | 3     | 318 | CLA  | CHD-C1D-ND  | -2.38 | 121.45      | 124.80   |
| 24  | B     | 848 | BCR  | C7-C6-C5    | -2.38 | 116.06      | 121.56   |
| 24  | B     | 849 | BCR  | C29-C30-C25 | 2.38  | 113.90      | 110.44   |
| 22  | 5     | 307 | CLA  | CHD-C1D-ND  | -2.38 | 121.45      | 124.80   |
| 22  | 3     | 314 | CLA  | O2D-CGD-O1D | -2.38 | 119.21      | 123.85   |
| 39  | 6     | 318 | CHL  | CMA-C3A-C4A | 2.38  | 119.74      | 114.61   |
| 22  | 5     | 313 | CLA  | CHA-C1A-NA  | -2.38 | 121.00      | 126.39   |
| 36  | 5     | 306 | C7Z  | C4-C5-C6    | -2.38 | 115.87      | 120.76   |
| 22  | 7     | 314 | CLA  | C4B-CHC-C1C | 2.38  | 131.84      | 126.25   |
| 22  | A     | 834 | CLA  | O2A-CGA-CBA | 2.38  | 119.09      | 111.83   |
| 22  | 1     | 307 | CLA  | CMD-C2D-C3D | -2.38 | 122.23      | 127.69   |
| 22  | A     | 812 | CLA  | C2D-C1D-ND  | 2.38  | 112.48      | 110.13   |
| 38  | 8     | 303 | LUT  | C35-C15-C14 | -2.38 | 118.65      | 123.52   |
| 22  | K     | 204 | CLA  | CHD-C1D-ND  | -2.38 | 121.45      | 124.80   |
| 22  | F     | 304 | CLA  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 22  | 9     | 303 | CLA  | C3D-C2D-C1D | -2.38 | 102.58      | 105.83   |
| 22  | A     | 818 | CLA  | C2D-C1D-ND  | 2.38  | 112.48      | 110.13   |
| 22  | 5     | 322 | CLA  | C2D-C1D-ND  | 2.38  | 112.48      | 110.13   |
| 24  | 3     | 307 | BCR  | C1-C6-C7    | 2.38  | 122.10      | 115.65   |
| 22  | 1     | 313 | CLA  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 22  | 1     | 316 | CLA  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 22  | F     | 302 | CLA  | C2D-C1D-ND  | 2.38  | 112.48      | 110.13   |
| 22  | A     | 822 | CLA  | C1D-ND-C4D  | -2.38 | 104.64      | 106.31   |
| 22  | 1     | 309 | CLA  | CAA-CBA-CGA | -2.38 | 106.46      | 113.21   |
| 22  | A     | 805 | CLA  | CHA-C4D-ND  | 2.38  | 137.45      | 132.55   |
| 22  | 9     | 313 | CLA  | O2D-CGD-O1D | -2.38 | 119.22      | 123.85   |
| 39  | 7     | 313 | CHL  | C1-C2-C3    | -2.38 | 122.31      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 824 | CLA  | CHA-C4D-ND  | 2.38  | 137.45      | 132.55   |
| 24  | A     | 845 | BCR  | C11-C12-C13 | -2.37 | 119.85      | 126.36   |
| 22  | A     | 819 | CLA  | CMD-C2D-C3D | -2.37 | 122.25      | 127.69   |
| 22  | G     | 202 | CLA  | O2D-CGD-O1D | -2.37 | 119.23      | 123.85   |
| 22  | 5     | 326 | CLA  | C2D-C1D-ND  | 2.37  | 112.47      | 110.13   |
| 22  | 9     | 303 | CLA  | CHA-C1A-NA  | -2.37 | 121.02      | 126.39   |
| 22  | A     | 808 | CLA  | O2D-CGD-O1D | -2.37 | 119.23      | 123.85   |
| 22  | A     | 814 | CLA  | O2A-CGA-CBA | 2.37  | 119.07      | 111.83   |
| 22  | B     | 829 | CLA  | CHA-C4D-ND  | 2.37  | 137.44      | 132.55   |
| 22  | 5     | 319 | CLA  | O2D-CGD-O1D | -2.37 | 119.23      | 123.85   |
| 22  | Z     | 304 | CLA  | CHA-C4D-ND  | 2.37  | 137.44      | 132.55   |
| 22  | Z     | 308 | CLA  | CHD-C1D-ND  | -2.37 | 121.47      | 124.80   |
| 22  | A     | 810 | CLA  | CMD-C2D-C3D | -2.37 | 122.25      | 127.69   |
| 24  | 7     | 303 | BCR  | C27-C26-C25 | -2.37 | 119.50      | 122.70   |
| 22  | A     | 837 | CLA  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 22  | 5     | 326 | CLA  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 22  | A     | 824 | CLA  | C6-C5-C3    | -2.37 | 107.70      | 113.47   |
| 22  | 8     | 305 | CLA  | C3B-C4B-NB  | -2.37 | 108.42      | 110.53   |
| 22  | B     | 823 | CLA  | O2A-CGA-CBA | 2.37  | 119.05      | 111.83   |
| 22  | G     | 201 | CLA  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 38  | 1     | 303 | LUT  | C22-C23-C24 | 2.37  | 114.70      | 111.18   |
| 22  | A     | 831 | CLA  | O2A-CGA-CBA | 2.37  | 119.05      | 111.83   |
| 22  | 3     | 308 | CLA  | CMD-C2D-C3D | -2.37 | 122.26      | 127.69   |
| 22  | A     | 827 | CLA  | C2D-C1D-ND  | 2.37  | 112.47      | 110.13   |
| 22  | B     | 824 | CLA  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 22  | 1     | 315 | CLA  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 22  | F     | 301 | CLA  | C2D-C1D-ND  | 2.37  | 112.47      | 110.13   |
| 24  | F     | 303 | BCR  | C27-C26-C25 | -2.37 | 119.51      | 122.70   |
| 22  | A     | 802 | CLA  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |
| 22  | B     | 838 | CLA  | CHD-C1D-ND  | -2.36 | 121.47      | 124.80   |
| 22  | A     | 833 | CLA  | C2D-C1D-ND  | 2.36  | 112.47      | 110.13   |
| 22  | Z     | 313 | CLA  | C2D-C1D-ND  | 2.36  | 112.47      | 110.13   |
| 22  | A     | 840 | CLA  | O2A-CGA-CBA | 2.36  | 119.04      | 111.83   |
| 22  | B     | 813 | CLA  | O2A-CGA-CBA | 2.36  | 119.04      | 111.83   |
| 22  | 5     | 323 | CLA  | CMD-C2D-C3D | -2.36 | 122.27      | 127.69   |
| 24  | 6     | 306 | BCR  | C35-C13-C12 | 2.36  | 121.70      | 118.09   |
| 31  | 1     | 319 | DGD  | O6D-C5D-C6D | 2.36  | 111.38      | 106.69   |
| 38  | 7     | 301 | LUT  | C8-C7-C6    | -2.36 | 120.69      | 127.00   |
| 22  | 3     | 308 | CLA  | O1D-CGD-CBD | -2.36 | 119.86      | 124.52   |
| 22  | B     | 801 | CLA  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |
| 22  | J     | 103 | CLA  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |
| 22  | 4     | 808 | CLA  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 811 | CLA  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |
| 22  | Z     | 310 | CLA  | CHA-C4D-ND  | 2.36  | 137.42      | 132.55   |
| 22  | A     | 841 | CLA  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |
| 22  | 7     | 311 | CLA  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |
| 22  | A     | 811 | CLA  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |
| 22  | 7     | 307 | CLA  | O2D-CGD-O1D | -2.36 | 119.25      | 123.85   |
| 22  | Z     | 309 | CLA  | CHA-C4D-ND  | 2.36  | 137.42      | 132.55   |
| 22  | 7     | 309 | CLA  | CHA-C4D-ND  | 2.36  | 137.42      | 132.55   |
| 22  | 2     | 304 | CLA  | C2D-C1D-ND  | 2.36  | 112.46      | 110.13   |
| 39  | 8     | 301 | CHL  | CMA-C3A-C4A | 2.36  | 119.69      | 114.61   |
| 22  | Z     | 303 | CLA  | C2D-C1D-ND  | 2.36  | 112.46      | 110.13   |
| 22  | 3     | 315 | CLA  | C1C-C2C-C3C | -2.36 | 104.50      | 106.98   |
| 22  | A     | 812 | CLA  | O2A-CGA-CBA | 2.36  | 119.02      | 111.83   |
| 22  | 1     | 307 | CLA  | O2D-CGD-O1D | -2.36 | 119.26      | 123.85   |
| 24  | L     | 204 | BCR  | C38-C26-C27 | 2.36  | 118.62      | 113.60   |
| 39  | Z     | 311 | CHL  | C1-O2A-CGA  | 2.36  | 122.35      | 116.65   |
| 22  | B     | 808 | CLA  | O2D-CGD-O1D | -2.36 | 119.26      | 123.85   |
| 22  | F     | 305 | CLA  | CMD-C2D-C3D | -2.36 | 122.29      | 127.69   |
| 22  | A     | 809 | CLA  | CHA-C4D-ND  | 2.35  | 137.41      | 132.55   |
| 22  | 1     | 314 | CLA  | CHD-C1D-ND  | -2.35 | 121.49      | 124.80   |
| 22  | Z     | 316 | CLA  | O2A-CGA-CBA | 2.35  | 119.01      | 111.83   |
| 24  | 6     | 306 | BCR  | C38-C26-C27 | 2.35  | 118.62      | 113.60   |
| 22  | A     | 826 | CLA  | O2A-CGA-CBA | 2.35  | 119.01      | 111.83   |
| 22  | K     | 204 | CLA  | O2A-CGA-CBA | 2.35  | 119.01      | 111.83   |
| 22  | B     | 806 | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 22  | Z     | 305 | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 22  | A     | 839 | CLA  | CMD-C2D-C3D | -2.35 | 122.29      | 127.69   |
| 22  | A     | 840 | CLA  | CMD-C2D-C3D | -2.35 | 122.29      | 127.69   |
| 22  | B     | 822 | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 32  | F     | 306 | RRX  | C33-C5-C4   | 2.35  | 118.61      | 113.60   |
| 22  | B     | 812 | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 22  | A     | 817 | CLA  | O2A-CGA-CBA | 2.35  | 119.00      | 111.83   |
| 22  | 5     | 323 | CLA  | CHD-C1D-ND  | -2.35 | 121.50      | 124.80   |
| 22  | 6     | 310 | CLA  | CHD-C1D-ND  | -2.35 | 121.50      | 124.80   |
| 22  | 5     | 315 | CLA  | C2D-C1D-ND  | 2.35  | 112.45      | 110.13   |
| 22  | 3     | 320 | CLA  | C3D-C2D-C1D | -2.35 | 102.62      | 105.83   |
| 22  | 7     | 312 | CLA  | O2D-CGD-O1D | -2.35 | 119.27      | 123.85   |
| 24  | B     | 845 | BCR  | C8-C7-C6    | -2.35 | 120.72      | 127.00   |
| 22  | A     | 817 | CLA  | C4B-CHC-C1C | 2.35  | 131.77      | 126.25   |
| 22  | A     | 811 | CLA  | CMD-C2D-C3D | -2.35 | 122.30      | 127.69   |
| 22  | B     | 818 | CLA  | C2D-C1D-ND  | 2.35  | 112.45      | 110.13   |
| 22  | Z     | 308 | CLA  | C2D-C1D-ND  | 2.35  | 112.45      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | B     | 847 | BCR  | C8-C7-C6    | -2.35 | 120.73      | 127.00   |
| 22  | Z     | 315 | CLA  | O2D-CGD-O1D | -2.35 | 119.28      | 123.85   |
| 22  | 5     | 309 | CLA  | CHA-C1A-NA  | -2.35 | 121.08      | 126.39   |
| 22  | 6     | 307 | CLA  | CMD-C2D-C3D | -2.35 | 122.31      | 127.69   |
| 22  | 1     | 308 | CLA  | C2C-C1C-NC  | 2.35  | 112.45      | 109.98   |
| 22  | 1     | 311 | CLA  | C1D-ND-C4D  | -2.35 | 104.67      | 106.31   |
| 22  | 9     | 305 | CLA  | CHA-C1A-NA  | -2.35 | 121.08      | 126.39   |
| 22  | 7     | 308 | CLA  | O2D-CGD-O1D | -2.35 | 119.28      | 123.85   |
| 22  | A     | 806 | CLA  | O2A-CGA-CBA | 2.35  | 118.99      | 111.83   |
| 22  | 3     | 322 | CLA  | CMD-C2D-C3D | -2.35 | 122.31      | 127.69   |
| 22  | B     | 812 | CLA  | O2A-CGA-CBA | 2.35  | 118.99      | 111.83   |
| 22  | 3     | 322 | CLA  | O2D-CGD-O1D | -2.35 | 119.28      | 123.85   |
| 22  | 5     | 326 | CLA  | CHA-C1A-NA  | -2.34 | 121.08      | 126.39   |
| 22  | Z     | 305 | CLA  | C2D-C1D-ND  | 2.34  | 112.45      | 110.13   |
| 22  | B     | 824 | CLA  | CHD-C1D-ND  | -2.34 | 121.50      | 124.80   |
| 22  | 3     | 319 | CLA  | O2D-CGD-O1D | -2.34 | 119.29      | 123.85   |
| 24  | B     | 845 | BCR  | C11-C12-C13 | -2.34 | 119.94      | 126.36   |
| 22  | B     | 819 | CLA  | O2D-CGD-O1D | -2.34 | 119.29      | 123.85   |
| 22  | 4     | 805 | CLA  | CHD-C1D-ND  | -2.34 | 121.50      | 124.80   |
| 22  | A     | 824 | CLA  | C2D-C1D-ND  | 2.34  | 112.44      | 110.13   |
| 22  | 5     | 314 | CLA  | O2D-CGD-O1D | -2.34 | 119.29      | 123.85   |
| 24  | 5     | 305 | BCR  | C1-C6-C7    | 2.34  | 122.00      | 115.65   |
| 22  | Z     | 314 | CLA  | C2D-C1D-ND  | 2.34  | 112.44      | 110.13   |
| 22  | 9     | 305 | CLA  | C4B-CHC-C1C | 2.34  | 131.75      | 126.25   |
| 22  | 7     | 304 | CLA  | CHA-C4D-ND  | 2.34  | 137.38      | 132.55   |
| 22  | B     | 840 | CLA  | CMD-C2D-C3D | -2.34 | 122.32      | 127.69   |
| 22  | 3     | 308 | CLA  | CHD-C1D-ND  | -2.34 | 121.51      | 124.80   |
| 22  | Z     | 304 | CLA  | C2D-C1D-ND  | 2.34  | 112.44      | 110.13   |
| 22  | A     | 823 | CLA  | C2D-C1D-ND  | 2.34  | 112.44      | 110.13   |
| 22  | Z     | 314 | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 22  | B     | 824 | CLA  | C2C-C1C-NC  | 2.34  | 112.44      | 109.98   |
| 22  | 7     | 310 | CLA  | CHA-C4D-ND  | 2.34  | 137.37      | 132.55   |
| 22  | Z     | 310 | CLA  | C2D-C1D-ND  | 2.34  | 112.44      | 110.13   |
| 22  | A     | 836 | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 22  | A     | 813 | CLA  | C3B-C4B-NB  | -2.34 | 108.44      | 110.53   |
| 39  | 5     | 316 | CHL  | CMA-C3A-C2A | 2.34  | 123.16      | 114.13   |
| 22  | 1     | 306 | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 22  | 7     | 312 | CLA  | C2D-C1D-ND  | 2.34  | 112.44      | 110.13   |
| 22  | 8     | 316 | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 22  | 9     | 306 | CLA  | CMD-C2D-C3D | -2.34 | 122.33      | 127.69   |
| 22  | 7     | 315 | CLA  | O1D-CGD-CBD | -2.34 | 119.91      | 124.52   |
| 22  | 5     | 301 | CLA  | CHD-C1D-ND  | -2.34 | 121.51      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 813 | CLA  | C2D-C1D-ND  | 2.34  | 112.44      | 110.13   |
| 22  | 3     | 318 | CLA  | O2D-CGD-O1D | -2.34 | 119.30      | 123.85   |
| 22  | 8     | 307 | CLA  | CHA-C1A-NA  | -2.34 | 121.10      | 126.39   |
| 22  | B     | 805 | CLA  | O2A-CGA-CBA | 2.34  | 118.95      | 111.83   |
| 22  | 6     | 322 | CLA  | CMD-C2D-C3D | -2.34 | 122.33      | 127.69   |
| 22  | 4     | 807 | CLA  | C2D-C1D-ND  | 2.34  | 112.44      | 110.13   |
| 22  | 2     | 301 | CLA  | CHD-C1D-ND  | -2.33 | 121.52      | 124.80   |
| 24  | 7     | 303 | BCR  | C11-C12-C13 | -2.33 | 119.96      | 126.36   |
| 22  | 5     | 313 | CLA  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 22  | B     | 809 | CLA  | CHD-C1D-ND  | -2.33 | 121.52      | 124.80   |
| 22  | A     | 816 | CLA  | CHA-C1A-NA  | -2.33 | 121.11      | 126.39   |
| 21  | A     | 801 | CL0  | C4D-ND-C1D  | -2.33 | 103.45      | 105.22   |
| 22  | A     | 821 | CLA  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 22  | 6     | 301 | CLA  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 22  | L     | 203 | CLA  | O2A-CGA-CBA | 2.33  | 118.95      | 111.83   |
| 22  | 7     | 305 | CLA  | CHD-C1D-ND  | -2.33 | 121.52      | 124.80   |
| 22  | 4     | 811 | CLA  | C2D-C1D-ND  | 2.33  | 112.43      | 110.13   |
| 38  | 3     | 303 | LUT  | C11-C12-C13 | -2.33 | 119.97      | 126.36   |
| 22  | A     | 807 | CLA  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 22  | 6     | 317 | CLA  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 22  | B     | 835 | CLA  | O1D-CGD-CBD | -2.33 | 119.92      | 124.52   |
| 24  | A     | 846 | BCR  | C36-C18-C19 | 2.33  | 121.65      | 118.09   |
| 22  | A     | 828 | CLA  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 38  | 4     | 802 | LUT  | C11-C12-C13 | -2.33 | 119.97      | 126.36   |
| 22  | B     | 839 | CLA  | O1D-CGD-CBD | -2.33 | 119.92      | 124.52   |
| 24  | G     | 203 | BCR  | C16-C15-C14 | -2.33 | 118.75      | 123.52   |
| 22  | B     | 814 | CLA  | O2A-CGA-CBA | 2.33  | 118.94      | 111.83   |
| 35  | J     | 102 | T7X  | C12-C13-C14 | -2.33 | 108.26      | 113.35   |
| 22  | 5     | 315 | CLA  | O2D-CGD-O1D | -2.33 | 119.32      | 123.85   |
| 22  | K     | 205 | CLA  | C1D-ND-C4D  | -2.33 | 104.68      | 106.31   |
| 22  | K     | 205 | CLA  | CHA-C1A-NA  | -2.33 | 121.12      | 126.39   |
| 22  | B     | 824 | CLA  | CMD-C2D-C3D | -2.33 | 122.35      | 127.69   |
| 22  | K     | 202 | CLA  | O2D-CGD-O1D | -2.33 | 119.32      | 123.85   |
| 38  | 4     | 802 | LUT  | C1-C6-C5    | -2.33 | 119.46      | 122.64   |
| 22  | B     | 806 | CLA  | CHD-C1D-ND  | -2.33 | 121.53      | 124.80   |
| 22  | B     | 815 | CLA  | O2D-CGD-O1D | -2.33 | 119.32      | 123.85   |
| 22  | F     | 305 | CLA  | O2D-CGD-O1D | -2.33 | 119.32      | 123.85   |
| 22  | 3     | 315 | CLA  | C2C-C1C-NC  | 2.33  | 112.42      | 109.98   |
| 22  | 5     | 309 | CLA  | C2D-C1D-ND  | 2.32  | 112.43      | 110.13   |
| 22  | 6     | 313 | CLA  | O2D-CGD-O1D | -2.32 | 119.32      | 123.85   |
| 22  | 6     | 311 | CLA  | O2D-CGD-O1D | -2.32 | 119.32      | 123.85   |
| 22  | 1     | 307 | CLA  | CHD-C1D-ND  | -2.32 | 121.53      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 3     | 318 | CLA  | C2D-C1D-ND  | 2.32  | 112.43      | 110.13   |
| 22  | A     | 837 | CLA  | CMD-C2D-C3D | -2.32 | 122.36      | 127.69   |
| 24  | 3     | 307 | BCR  | C21-C20-C19 | 2.32  | 129.93      | 123.20   |
| 22  | B     | 816 | CLA  | O2D-CGD-O1D | -2.32 | 119.33      | 123.85   |
| 22  | A     | 803 | CLA  | C2D-C1D-ND  | 2.32  | 112.42      | 110.13   |
| 22  | 5     | 301 | CLA  | O2A-CGA-CBA | 2.32  | 118.91      | 111.83   |
| 22  | 1     | 314 | CLA  | CHA-C4D-ND  | 2.32  | 137.34      | 132.55   |
| 22  | 6     | 319 | CLA  | O1D-CGD-CBD | -2.32 | 119.94      | 124.52   |
| 36  | 5     | 306 | C7Z  | C31-C32-C33 | -2.32 | 120.00      | 126.36   |
| 22  | B     | 842 | CLA  | CMD-C2D-C3D | -2.32 | 122.37      | 127.69   |
| 22  | 4     | 810 | CLA  | CMD-C2D-C3D | -2.32 | 122.37      | 127.69   |
| 22  | B     | 841 | CLA  | C2D-C1D-ND  | 2.32  | 112.42      | 110.13   |
| 24  | 3     | 305 | BCR  | C33-C5-C4   | 2.32  | 118.54      | 113.60   |
| 38  | 4     | 802 | LUT  | C15-C35-C34 | -2.32 | 118.77      | 123.52   |
| 22  | A     | 802 | CLA  | CHD-C1D-ND  | -2.32 | 121.54      | 124.80   |
| 24  | 8     | 304 | BCR  | C30-C25-C26 | -2.32 | 119.47      | 122.64   |
| 22  | K     | 204 | CLA  | C2D-C1D-ND  | 2.32  | 112.42      | 110.13   |
| 22  | A     | 810 | CLA  | CHD-C1D-ND  | -2.32 | 121.54      | 124.80   |
| 22  | J     | 103 | CLA  | C2D-C1D-ND  | 2.32  | 112.42      | 110.13   |
| 22  | 5     | 323 | CLA  | C2D-C1D-ND  | 2.32  | 112.42      | 110.13   |
| 22  | A     | 823 | CLA  | C11-C12-C13 | -2.32 | 108.26      | 115.97   |
| 38  | 7     | 301 | LUT  | C11-C12-C13 | -2.32 | 120.01      | 126.36   |
| 22  | B     | 830 | CLA  | C2D-C1D-ND  | 2.32  | 112.42      | 110.13   |
| 22  | 2     | 302 | CLA  | C2D-C1D-ND  | 2.32  | 112.42      | 110.13   |
| 22  | 8     | 310 | CLA  | O2D-CGD-O1D | -2.32 | 119.34      | 123.85   |
| 22  | L     | 201 | CLA  | O2A-CGA-CBA | 2.32  | 118.90      | 111.83   |
| 22  | 7     | 305 | CLA  | O2A-CGA-CBA | 2.32  | 118.90      | 111.83   |
| 22  | B     | 811 | CLA  | C2D-C1D-ND  | 2.32  | 112.42      | 110.13   |
| 22  | 6     | 317 | CLA  | C2D-C1D-ND  | 2.32  | 112.42      | 110.13   |
| 22  | 3     | 316 | CLA  | O2A-CGA-CBA | 2.32  | 118.90      | 111.83   |
| 22  | B     | 815 | CLA  | CMD-C2D-C3D | -2.32 | 122.38      | 127.69   |
| 22  | 9     | 306 | CLA  | O2D-CGD-O1D | -2.32 | 119.34      | 123.85   |
| 22  | K     | 205 | CLA  | C4B-CHC-C1C | 2.32  | 131.69      | 126.25   |
| 22  | 6     | 311 | CLA  | CHD-C1D-ND  | -2.32 | 121.54      | 124.80   |
| 22  | B     | 818 | CLA  | CMD-C2D-C3D | -2.31 | 122.38      | 127.69   |
| 22  | 4     | 818 | CLA  | O1D-CGD-CBD | -2.31 | 119.95      | 124.52   |
| 22  | 8     | 306 | CLA  | CMD-C2D-C3D | -2.31 | 122.38      | 127.69   |
| 22  | 8     | 313 | CLA  | C2D-C1D-ND  | 2.31  | 112.42      | 110.13   |
| 25  | A     | 850 | LHG  | C5-O7-C7    | -2.31 | 112.26      | 117.80   |
| 22  | A     | 855 | CLA  | O2D-CGD-O1D | -2.31 | 119.34      | 123.85   |
| 22  | B     | 807 | CLA  | O2D-CGD-O1D | -2.31 | 119.34      | 123.85   |
| 22  | 3     | 310 | CLA  | O2D-CGD-O1D | -2.31 | 119.34      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | B     | 847 | BCR  | C33-C5-C4   | 2.31  | 118.53      | 113.60   |
| 22  | Z     | 303 | CLA  | CHD-C1D-ND  | -2.31 | 121.55      | 124.80   |
| 22  | 3     | 316 | CLA  | CMD-C2D-C3D | -2.31 | 122.39      | 127.69   |
| 22  | 3     | 322 | CLA  | CHD-C1D-ND  | -2.31 | 121.55      | 124.80   |
| 22  | A     | 809 | CLA  | O2D-CGD-O1D | -2.31 | 119.35      | 123.85   |
| 22  | A     | 839 | CLA  | CHD-C1D-ND  | -2.31 | 121.55      | 124.80   |
| 22  | B     | 832 | CLA  | CHD-C1D-ND  | -2.31 | 121.55      | 124.80   |
| 22  | A     | 832 | CLA  | CMD-C2D-C3D | -2.31 | 122.39      | 127.69   |
| 22  | Z     | 316 | CLA  | CMD-C2D-C3D | -2.31 | 122.39      | 127.69   |
| 24  | A     | 856 | BCR  | C37-C22-C21 | -2.31 | 119.07      | 122.82   |
| 22  | 5     | 301 | CLA  | O2D-CGD-O1D | -2.31 | 119.35      | 123.85   |
| 22  | 1     | 311 | CLA  | CHA-C1A-NA  | -2.31 | 121.16      | 126.39   |
| 22  | L     | 201 | CLA  | O2D-CGD-O1D | -2.31 | 119.35      | 123.85   |
| 22  | B     | 817 | CLA  | C2D-C1D-ND  | 2.31  | 112.41      | 110.13   |
| 24  | G     | 203 | BCR  | C4-C5-C6    | -2.31 | 119.58      | 122.70   |
| 22  | Z     | 303 | CLA  | CMD-C2D-C3D | -2.31 | 122.39      | 127.69   |
| 22  | A     | 839 | CLA  | CAA-CBA-CGA | -2.31 | 106.65      | 113.21   |
| 22  | A     | 813 | CLA  | O2D-CGD-O1D | -2.31 | 119.35      | 123.85   |
| 22  | Z     | 308 | CLA  | CMA-C3A-C4A | 2.31  | 117.98      | 111.77   |
| 24  | 5     | 305 | BCR  | C37-C22-C21 | -2.31 | 119.08      | 122.82   |
| 22  | B     | 821 | CLA  | CHD-C1D-ND  | -2.31 | 121.56      | 124.80   |
| 22  | A     | 823 | CLA  | CHD-C1D-ND  | -2.31 | 121.56      | 124.80   |
| 22  | 8     | 307 | CLA  | C2D-C1D-ND  | 2.31  | 112.41      | 110.13   |
| 22  | 4     | 815 | CLA  | C2D-C1D-ND  | 2.31  | 112.41      | 110.13   |
| 36  | J     | 105 | C7Z  | C28-C27-C26 | -2.31 | 120.84      | 127.00   |
| 22  | 3     | 319 | CLA  | CHD-C1D-ND  | -2.31 | 121.56      | 124.80   |
| 24  | B     | 847 | BCR  | C21-C20-C19 | -2.31 | 116.52      | 123.20   |
| 25  | 4     | 820 | LHG  | C5-O7-C7    | -2.31 | 112.28      | 117.80   |
| 22  | 8     | 308 | CLA  | C2D-C1D-ND  | 2.31  | 112.41      | 110.13   |
| 22  | A     | 817 | CLA  | O2D-CGD-O1D | -2.31 | 119.36      | 123.85   |
| 22  | 6     | 311 | CLA  | O2A-CGA-CBA | 2.30  | 118.86      | 111.83   |
| 38  | 5     | 302 | LUT  | C20-C13-C12 | 2.30  | 121.61      | 118.09   |
| 39  | 3     | 317 | CHL  | C4D-CHA-CBD | -2.30 | 106.64      | 108.97   |
| 22  | 6     | 312 | CLA  | O2D-CGD-O1D | -2.30 | 119.36      | 123.85   |
| 22  | 3     | 322 | CLA  | O2A-CGA-CBA | 2.30  | 118.86      | 111.83   |
| 22  | A     | 821 | CLA  | CMA-C3A-C4A | 2.30  | 117.97      | 111.77   |
| 22  | B     | 828 | CLA  | CHA-C1A-NA  | -2.30 | 121.17      | 126.39   |
| 22  | Z     | 315 | CLA  | CMD-C2D-C3D | -2.30 | 122.41      | 127.69   |
| 22  | 6     | 310 | CLA  | CMD-C2D-C3D | -2.30 | 122.41      | 127.69   |
| 24  | B     | 853 | BCR  | C15-C14-C13 | -2.30 | 124.05      | 127.28   |
| 22  | A     | 809 | CLA  | CMD-C2D-C3D | -2.30 | 122.41      | 127.69   |
| 22  | A     | 808 | CLA  | C2D-C1D-ND  | 2.30  | 112.41      | 110.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 809 | CLA  | CMD-C2D-C3D | -2.30 | 122.41      | 127.69   |
| 22  | 5     | 308 | CLA  | O2A-CGA-CBA | 2.30  | 118.85      | 111.83   |
| 22  | B     | 801 | CLA  | CHD-C1D-ND  | -2.30 | 121.56      | 124.80   |
| 22  | B     | 828 | CLA  | C2D-C1D-ND  | 2.30  | 112.40      | 110.13   |
| 22  | 6     | 302 | CLA  | C2D-C1D-ND  | 2.30  | 112.40      | 110.13   |
| 22  | 4     | 805 | CLA  | CHA-C1A-NA  | -2.30 | 121.18      | 126.39   |
| 22  | 1     | 305 | CLA  | O2D-CGD-O1D | -2.30 | 119.37      | 123.85   |
| 24  | 6     | 305 | BCR  | C8-C7-C6    | -2.30 | 120.85      | 127.00   |
| 22  | B     | 811 | CLA  | CMD-C2D-C3D | -2.30 | 122.41      | 127.69   |
| 22  | 5     | 301 | CLA  | CMD-C2D-C3D | -2.30 | 122.41      | 127.69   |
| 22  | A     | 820 | CLA  | O2D-CGD-O1D | -2.30 | 119.37      | 123.85   |
| 22  | Z     | 316 | CLA  | CHD-C1D-ND  | -2.30 | 121.56      | 124.80   |
| 22  | A     | 814 | CLA  | O2D-CGD-O1D | -2.30 | 119.37      | 123.85   |
| 22  | A     | 831 | CLA  | O2D-CGD-O1D | -2.30 | 119.37      | 123.85   |
| 22  | B     | 836 | CLA  | CHD-C1D-ND  | -2.30 | 121.57      | 124.80   |
| 24  | A     | 847 | BCR  | C23-C24-C25 | -2.30 | 120.86      | 127.00   |
| 22  | 3     | 309 | CLA  | O2D-CGD-O1D | -2.30 | 119.37      | 123.85   |
| 22  | A     | 802 | CLA  | C1-O2A-CGA  | 2.30  | 122.22      | 116.65   |
| 22  | 7     | 311 | CLA  | CHD-C1D-ND  | -2.30 | 121.57      | 124.80   |
| 39  | 5     | 321 | CHL  | C4D-CHA-CBD | -2.30 | 106.65      | 108.97   |
| 22  | A     | 809 | CLA  | C2D-C1D-ND  | 2.30  | 112.40      | 110.13   |
| 22  | B     | 819 | CLA  | C2D-C1D-ND  | 2.30  | 112.40      | 110.13   |
| 22  | B     | 823 | CLA  | C2D-C1D-ND  | 2.30  | 112.40      | 110.13   |
| 22  | 9     | 311 | CLA  | C2D-C1D-ND  | 2.30  | 112.40      | 110.13   |
| 22  | 5     | 311 | CLA  | CHA-C1A-NA  | -2.30 | 121.19      | 126.39   |
| 22  | A     | 821 | CLA  | CMD-C2D-C3D | -2.30 | 122.42      | 127.69   |
| 22  | Z     | 308 | CLA  | CMD-C2D-C3D | -2.30 | 122.42      | 127.69   |
| 22  | 5     | 326 | CLA  | CAA-C2A-C3A | -2.30 | 106.79      | 113.00   |
| 22  | B     | 836 | CLA  | C2D-C1D-ND  | 2.30  | 112.40      | 110.13   |
| 22  | 5     | 311 | CLA  | C2D-C1D-ND  | 2.30  | 112.40      | 110.13   |
| 22  | A     | 832 | CLA  | O2D-CGD-O1D | -2.30 | 119.38      | 123.85   |
| 38  | 9     | 301 | LUT  | C8-C7-C6    | -2.30 | 120.86      | 127.00   |
| 22  | A     | 812 | CLA  | CMD-C2D-C3D | -2.30 | 122.42      | 127.69   |
| 22  | B     | 808 | CLA  | CHD-C1D-ND  | -2.30 | 121.57      | 124.80   |
| 22  | 7     | 314 | CLA  | CHD-C1D-ND  | -2.30 | 121.57      | 124.80   |
| 22  | 8     | 306 | CLA  | O2A-CGA-CBA | 2.30  | 118.84      | 111.83   |
| 22  | 4     | 812 | CLA  | C2D-C1D-ND  | 2.30  | 112.40      | 110.13   |
| 22  | 8     | 309 | CLA  | CMD-C2D-C3D | -2.30 | 122.42      | 127.69   |
| 22  | A     | 811 | CLA  | C2D-C1D-ND  | 2.29  | 112.40      | 110.13   |
| 22  | A     | 841 | CLA  | C2D-C1D-ND  | 2.29  | 112.40      | 110.13   |
| 22  | 6     | 321 | CLA  | O2D-CGD-O1D | -2.29 | 119.38      | 123.85   |
| 31  | 3     | 301 | DGD  | C2G-O2G-C1B | -2.29 | 112.31      | 117.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 38  | 4     | 802 | LUT  | C27-C28-C29 | -2.29 | 121.39      | 126.32   |
| 22  | A     | 855 | CLA  | CMD-C2D-C3D | -2.29 | 122.43      | 127.69   |
| 22  | B     | 807 | CLA  | C2D-C1D-ND  | 2.29  | 112.40      | 110.13   |
| 22  | B     | 808 | CLA  | C2D-C1D-ND  | 2.29  | 112.40      | 110.13   |
| 22  | 7     | 323 | CLA  | CMD-C2D-C3D | -2.29 | 122.43      | 127.69   |
| 22  | A     | 825 | CLA  | O2D-CGD-O1D | -2.29 | 119.39      | 123.85   |
| 22  | 8     | 310 | CLA  | CHD-C1D-ND  | -2.29 | 121.58      | 124.80   |
| 22  | A     | 854 | CLA  | CHD-C1D-ND  | -2.29 | 121.58      | 124.80   |
| 22  | A     | 829 | CLA  | C2D-C1D-ND  | 2.29  | 112.39      | 110.13   |
| 22  | 3     | 309 | CLA  | C2D-C1D-ND  | 2.29  | 112.39      | 110.13   |
| 22  | A     | 802 | CLA  | CMD-C2D-C3D | -2.29 | 122.43      | 127.69   |
| 22  | 3     | 318 | CLA  | CMD-C2D-C3D | -2.29 | 122.43      | 127.69   |
| 22  | L     | 203 | CLA  | O2D-CGD-O1D | -2.29 | 119.39      | 123.85   |
| 22  | 1     | 305 | CLA  | CMD-C2D-C3D | -2.29 | 122.44      | 127.69   |
| 22  | B     | 825 | CLA  | CHD-C1D-ND  | -2.29 | 121.58      | 124.80   |
| 22  | 4     | 809 | CLA  | O2D-CGD-O1D | -2.29 | 119.39      | 123.85   |
| 22  | B     | 833 | CLA  | O2A-CGA-CBA | 2.29  | 118.82      | 111.83   |
| 22  | A     | 841 | CLA  | CMD-C2D-C3D | -2.29 | 122.44      | 127.69   |
| 22  | A     | 838 | CLA  | C2D-C1D-ND  | 2.29  | 112.39      | 110.13   |
| 40  | 1     | 318 | SQD  | O3-C3-C2    | -2.29 | 104.98      | 110.38   |
| 22  | 2     | 301 | CLA  | O2D-CGD-O1D | -2.29 | 119.39      | 123.85   |
| 24  | G     | 203 | BCR  | C11-C10-C9  | -2.29 | 124.07      | 127.28   |
| 22  | 1     | 310 | CLA  | O2D-CGD-O1D | -2.29 | 119.39      | 123.85   |
| 22  | 7     | 322 | CLA  | O2D-CGD-O1D | -2.29 | 119.39      | 123.85   |
| 22  | A     | 826 | CLA  | C2D-C1D-ND  | 2.29  | 112.39      | 110.13   |
| 22  | A     | 814 | CLA  | CHA-C1A-NA  | -2.29 | 121.21      | 126.39   |
| 38  | 8     | 302 | LUT  | C18-C5-C4   | 2.29  | 118.63      | 114.42   |
| 22  | A     | 809 | CLA  | O1D-CGD-CBD | -2.29 | 120.01      | 124.52   |
| 22  | 7     | 316 | CLA  | C2D-C1D-ND  | 2.29  | 112.39      | 110.13   |
| 22  | 4     | 809 | CLA  | C2D-C1D-ND  | 2.29  | 112.39      | 110.13   |
| 22  | 7     | 324 | CLA  | CMD-C2D-C3D | -2.29 | 122.44      | 127.69   |
| 22  | 3     | 312 | CLA  | C2D-C1D-ND  | 2.29  | 112.39      | 110.13   |
| 22  | 9     | 310 | CLA  | CHA-C1A-NA  | -2.29 | 121.21      | 126.39   |
| 22  | A     | 818 | CLA  | O2D-CGD-O1D | -2.29 | 119.40      | 123.85   |
| 22  | A     | 822 | CLA  | CMD-C2D-C3D | -2.29 | 122.45      | 127.69   |
| 22  | 2     | 302 | CLA  | O1D-CGD-CBD | -2.29 | 120.01      | 124.52   |
| 39  | 6     | 316 | CHL  | CMA-C3A-C2A | 2.28  | 122.95      | 114.13   |
| 22  | Z     | 310 | CLA  | CHD-C1D-ND  | -2.28 | 121.59      | 124.80   |
| 22  | Z     | 306 | CLA  | O2D-CGD-O1D | -2.28 | 119.40      | 123.85   |
| 24  | B     | 846 | BCR  | C8-C9-C10   | 2.28  | 122.60      | 119.01   |
| 22  | B     | 821 | CLA  | CMD-C2D-C3D | -2.28 | 122.45      | 127.69   |
| 22  | Z     | 308 | CLA  | O2D-CGD-O1D | -2.28 | 119.40      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 819 | CLA  | CHD-C1D-ND  | -2.28 | 121.59      | 124.80   |
| 22  | 8     | 305 | CLA  | CHD-C1D-ND  | -2.28 | 121.59      | 124.80   |
| 22  | 3     | 311 | CLA  | C2D-C1D-ND  | 2.28  | 112.39      | 110.13   |
| 22  | 3     | 319 | CLA  | CMD-C2D-C3D | -2.28 | 122.45      | 127.69   |
| 22  | 7     | 314 | CLA  | CMD-C2D-C3D | -2.28 | 122.45      | 127.69   |
| 22  | A     | 831 | CLA  | CMD-C2D-C3D | -2.28 | 122.46      | 127.69   |
| 22  | B     | 831 | CLA  | O2A-CGA-CBA | 2.28  | 118.79      | 111.83   |
| 24  | 5     | 304 | BCR  | C21-C20-C19 | -2.28 | 116.59      | 123.20   |
| 22  | A     | 810 | CLA  | O2D-CGD-O1D | -2.28 | 119.41      | 123.85   |
| 22  | 5     | 314 | CLA  | C2D-C1D-ND  | 2.28  | 112.38      | 110.13   |
| 22  | A     | 837 | CLA  | CHD-C1D-ND  | -2.28 | 121.59      | 124.80   |
| 22  | G     | 201 | CLA  | CHA-C1A-NA  | -2.28 | 121.22      | 126.39   |
| 38  | 8     | 303 | LUT  | C27-C28-C29 | -2.28 | 121.42      | 126.32   |
| 22  | 8     | 308 | CLA  | O2D-CGD-O1D | -2.28 | 119.41      | 123.85   |
| 22  | B     | 801 | CLA  | CHA-C1A-NA  | -2.28 | 121.23      | 126.39   |
| 22  | A     | 823 | CLA  | O2D-CGD-O1D | -2.28 | 119.41      | 123.85   |
| 22  | A     | 809 | CLA  | CHD-C1D-ND  | -2.28 | 121.59      | 124.80   |
| 22  | A     | 815 | CLA  | O2D-CGD-O1D | -2.28 | 119.41      | 123.85   |
| 22  | 5     | 318 | CLA  | C2D-C1D-ND  | 2.28  | 112.38      | 110.13   |
| 22  | 9     | 313 | CLA  | C2D-C1D-ND  | 2.28  | 112.38      | 110.13   |
| 22  | B     | 806 | CLA  | CMD-C2D-C3D | -2.28 | 122.46      | 127.69   |
| 22  | A     | 838 | CLA  | CMD-C2D-C3D | -2.28 | 122.46      | 127.69   |
| 22  | A     | 824 | CLA  | O2D-CGD-O1D | -2.28 | 119.42      | 123.85   |
| 22  | 1     | 311 | CLA  | C2D-C1D-ND  | 2.28  | 112.38      | 110.13   |
| 22  | B     | 808 | CLA  | CMD-C2D-C3D | -2.28 | 122.47      | 127.69   |
| 22  | A     | 819 | CLA  | CHD-C1D-ND  | -2.28 | 121.60      | 124.80   |
| 24  | 3     | 305 | BCR  | C11-C10-C9  | -2.28 | 124.08      | 127.28   |
| 22  | B     | 825 | CLA  | C2D-C1D-ND  | 2.28  | 112.38      | 110.13   |
| 22  | 4     | 817 | CLA  | C2D-C1D-ND  | 2.28  | 112.38      | 110.13   |
| 22  | 1     | 309 | CLA  | CHD-C1D-ND  | -2.28 | 121.60      | 124.80   |
| 22  | 8     | 313 | CLA  | CHD-C1D-ND  | -2.28 | 121.60      | 124.80   |
| 32  | F     | 306 | RRX  | C35-C13-C12 | -2.28 | 114.61      | 118.09   |
| 22  | 5     | 310 | CLA  | O2D-CGD-O1D | -2.28 | 119.42      | 123.85   |
| 22  | A     | 805 | CLA  | CMD-C2D-C3D | -2.28 | 122.47      | 127.69   |
| 22  | 7     | 308 | CLA  | CMD-C2D-C3D | -2.28 | 122.47      | 127.69   |
| 22  | 8     | 310 | CLA  | CMD-C2D-C3D | -2.28 | 122.47      | 127.69   |
| 31  | 1     | 319 | DGD  | O2G-C1B-O1B | -2.28 | 118.39      | 123.70   |
| 22  | 1     | 304 | CLA  | O1D-CGD-CBD | -2.28 | 120.03      | 124.52   |
| 22  | 6     | 301 | CLA  | C2D-C1D-ND  | 2.28  | 112.38      | 110.13   |
| 22  | 1     | 313 | CLA  | CMD-C2D-C3D | -2.28 | 122.47      | 127.69   |
| 22  | 1     | 308 | CLA  | O2A-CGA-CBA | 2.28  | 118.77      | 111.83   |
| 22  | A     | 832 | CLA  | CHD-C1D-ND  | -2.27 | 121.60      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 840 | CLA  | CHD-C1D-ND  | -2.27 | 121.60      | 124.80   |
| 22  | 8     | 308 | CLA  | CHD-C1D-ND  | -2.27 | 121.60      | 124.80   |
| 22  | G     | 202 | CLA  | CMD-C2D-C3D | -2.27 | 122.47      | 127.69   |
| 22  | B     | 821 | CLA  | O2A-CGA-CBA | 2.27  | 118.77      | 111.83   |
| 22  | 3     | 318 | CLA  | O2A-CGA-CBA | 2.27  | 118.77      | 111.83   |
| 22  | 4     | 809 | CLA  | CMD-C2D-C3D | -2.27 | 122.47      | 127.69   |
| 22  | 5     | 301 | CLA  | C2D-C1D-ND  | 2.27  | 112.38      | 110.13   |
| 22  | B     | 818 | CLA  | O2D-CGD-O1D | -2.27 | 119.42      | 123.85   |
| 22  | B     | 829 | CLA  | CMD-C2D-C3D | -2.27 | 122.47      | 127.69   |
| 22  | A     | 836 | CLA  | CHD-C1D-ND  | -2.27 | 121.60      | 124.80   |
| 22  | Z     | 316 | CLA  | C2D-C1D-ND  | 2.27  | 112.38      | 110.13   |
| 21  | A     | 801 | CL0  | C4C-CHD-C1D | 2.27  | 124.20      | 116.07   |
| 22  | 7     | 309 | CLA  | CHD-C1D-ND  | -2.27 | 121.60      | 124.80   |
| 22  | 8     | 308 | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 22  | 5     | 319 | CLA  | O2A-CGA-CBA | 2.27  | 118.76      | 111.83   |
| 22  | 7     | 323 | CLA  | C2D-C1D-ND  | 2.27  | 112.38      | 110.13   |
| 22  | A     | 811 | CLA  | CHD-C1D-ND  | -2.27 | 121.61      | 124.80   |
| 22  | B     | 829 | CLA  | CHD-C1D-ND  | -2.27 | 121.61      | 124.80   |
| 22  | 6     | 322 | CLA  | O2A-CGA-CBA | 2.27  | 118.76      | 111.83   |
| 22  | B     | 823 | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 22  | Z     | 305 | CLA  | CHA-C4D-ND  | 2.27  | 137.24      | 132.55   |
| 24  | 5     | 305 | BCR  | C35-C13-C14 | -2.27 | 119.14      | 122.82   |
| 22  | 6     | 310 | CLA  | O2D-CGD-O1D | -2.27 | 119.43      | 123.85   |
| 22  | 1     | 310 | CLA  | CHA-C1A-NA  | -2.27 | 121.25      | 126.39   |
| 22  | B     | 810 | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 22  | 4     | 812 | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 38  | 5     | 302 | LUT  | C39-C29-C28 | 2.27  | 121.56      | 118.09   |
| 22  | B     | 839 | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 22  | 7     | 304 | CLA  | CMD-C2D-C3D | -2.27 | 122.48      | 127.69   |
| 22  | A     | 816 | CLA  | CAA-CBA-CGA | -2.27 | 106.76      | 113.21   |
| 22  | 9     | 303 | CLA  | CHA-C4D-ND  | 2.27  | 137.23      | 132.55   |
| 22  | 1     | 316 | CLA  | C3D-C2D-C1D | -2.27 | 102.73      | 105.83   |
| 22  | K     | 203 | CLA  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |
| 22  | 4     | 808 | CLA  | CHD-C1D-ND  | -2.27 | 121.61      | 124.80   |
| 22  | 8     | 311 | CLA  | C2D-C1D-ND  | 2.27  | 112.37      | 110.13   |
| 22  | A     | 818 | CLA  | CHD-C1D-ND  | -2.27 | 121.61      | 124.80   |
| 22  | 6     | 309 | CLA  | O2D-CGD-O1D | -2.27 | 119.43      | 123.85   |
| 24  | K     | 206 | BCR  | C29-C30-C25 | 2.27  | 113.73      | 110.44   |
| 22  | 6     | 310 | CLA  | C2D-C1D-ND  | 2.27  | 112.37      | 110.13   |
| 22  | B     | 839 | CLA  | CHD-C1D-ND  | -2.27 | 121.61      | 124.80   |
| 22  | B     | 826 | CLA  | O1D-CGD-CBD | -2.27 | 120.05      | 124.52   |
| 22  | A     | 817 | CLA  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 5     | 308 | CLA  | C2D-C1D-ND  | 2.27  | 112.37      | 110.13   |
| 39  | Z     | 312 | CHL  | CMA-C3A-C4A | 2.27  | 119.49      | 114.61   |
| 22  | L     | 203 | CLA  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |
| 22  | A     | 815 | CLA  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |
| 22  | A     | 833 | CLA  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |
| 22  | 5     | 309 | CLA  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |
| 22  | B     | 830 | CLA  | O2A-CGA-CBA | 2.27  | 118.74      | 111.83   |
| 22  | A     | 813 | CLA  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |
| 22  | L     | 201 | CLA  | CMD-C2D-C3D | -2.27 | 122.49      | 127.69   |
| 24  | 5     | 305 | BCR  | C19-C18-C17 | -2.27 | 115.45      | 119.01   |
| 22  | 7     | 314 | CLA  | C2D-C1D-ND  | 2.26  | 112.37      | 110.13   |
| 22  | 4     | 818 | CLA  | C2D-C1D-ND  | 2.26  | 112.37      | 110.13   |
| 22  | B     | 833 | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 22  | 7     | 306 | CLA  | O2D-CGD-O1D | -2.26 | 119.44      | 123.85   |
| 22  | 6     | 312 | CLA  | CMD-C2D-C3D | -2.26 | 122.50      | 127.69   |
| 31  | 3     | 301 | DGD  | O2G-C1B-O1B | -2.26 | 118.41      | 123.70   |
| 22  | B     | 835 | CLA  | C2D-C1D-ND  | 2.26  | 112.37      | 110.13   |
| 22  | 4     | 808 | CLA  | C2D-C1D-ND  | 2.26  | 112.37      | 110.13   |
| 22  | 5     | 315 | CLA  | CHA-C1A-NA  | -2.26 | 121.27      | 126.39   |
| 22  | B     | 827 | CLA  | CMD-C2D-C3D | -2.26 | 122.50      | 127.69   |
| 22  | B     | 836 | CLA  | O2D-CGD-O1D | -2.26 | 119.44      | 123.85   |
| 22  | 1     | 313 | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 22  | 3     | 309 | CLA  | CMD-C2D-C3D | -2.26 | 122.50      | 127.69   |
| 22  | B     | 809 | CLA  | O2D-CGD-O1D | -2.26 | 119.44      | 123.85   |
| 38  | 6     | 303 | LUT  | C21-C26-C27 | -2.26 | 110.22      | 112.83   |
| 39  | 5     | 317 | CHL  | C1-O2A-CGA  | 2.26  | 122.13      | 116.65   |
| 22  | B     | 825 | CLA  | O2D-CGD-O1D | -2.26 | 119.44      | 123.85   |
| 22  | A     | 837 | CLA  | C2D-C1D-ND  | 2.26  | 112.36      | 110.13   |
| 22  | B     | 833 | CLA  | C2D-C1D-ND  | 2.26  | 112.36      | 110.13   |
| 22  | B     | 838 | CLA  | O2A-CGA-CBA | 2.26  | 118.73      | 111.83   |
| 22  | B     | 813 | CLA  | CMD-C2D-C3D | -2.26 | 122.50      | 127.69   |
| 22  | B     | 807 | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 24  | J     | 104 | BCR  | C30-C25-C24 | 2.26  | 121.78      | 115.65   |
| 22  | B     | 825 | CLA  | CMD-C2D-C3D | -2.26 | 122.51      | 127.69   |
| 22  | 4     | 810 | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 22  | 5     | 318 | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 22  | 5     | 323 | CLA  | O2D-CGD-O1D | -2.26 | 119.45      | 123.85   |
| 22  | 6     | 308 | CLA  | CAA-CBA-CGA | -2.26 | 106.79      | 113.21   |
| 22  | 8     | 316 | CLA  | CMD-C2D-C3D | -2.26 | 122.51      | 127.69   |
| 38  | 4     | 803 | LUT  | C8-C7-C6    | -2.26 | 120.96      | 127.00   |
| 24  | A     | 856 | BCR  | C10-C11-C12 | -2.26 | 116.65      | 123.20   |
| 22  | 8     | 308 | CLA  | O2A-CGA-CBA | 2.26  | 118.72      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | 5     | 308  | CLA  | CHD-C1D-ND  | -2.26 | 121.62      | 124.80   |
| 22  | F     | 302  | CLA  | O2D-CGD-O1D | -2.26 | 119.45      | 123.85   |
| 22  | B     | 828  | CLA  | CMD-C2D-C3D | -2.26 | 122.51      | 127.69   |
| 22  | B     | 821  | CLA  | O2D-CGD-O1D | -2.26 | 119.45      | 123.85   |
| 22  | A     | 831  | CLA  | CHD-C1D-ND  | -2.26 | 121.63      | 124.80   |
| 22  | 7     | 312  | CLA  | CHD-C1D-ND  | -2.26 | 121.63      | 124.80   |
| 24  | I     | 4001 | BCR  | C23-C24-C25 | -2.26 | 120.97      | 127.00   |
| 22  | B     | 818  | CLA  | CHD-C1D-ND  | -2.26 | 121.63      | 124.80   |
| 22  | L     | 203  | CLA  | CHD-C1D-ND  | -2.26 | 121.63      | 124.80   |
| 22  | B     | 833  | CLA  | O2D-CGD-O1D | -2.26 | 119.46      | 123.85   |
| 22  | B     | 829  | CLA  | C2D-C1D-ND  | 2.26  | 112.36      | 110.13   |
| 22  | B     | 823  | CLA  | CHD-C1D-ND  | -2.26 | 121.63      | 124.80   |
| 24  | B     | 846  | BCR  | C23-C24-C25 | -2.25 | 120.97      | 127.00   |
| 22  | A     | 834  | CLA  | C2D-C1D-ND  | 2.25  | 112.36      | 110.13   |
| 22  | A     | 836  | CLA  | C2D-C1D-ND  | 2.25  | 112.36      | 110.13   |
| 22  | 7     | 315  | CLA  | C2D-C1D-ND  | 2.25  | 112.36      | 110.13   |
| 22  | B     | 842  | CLA  | O2D-CGD-O1D | -2.25 | 119.46      | 123.85   |
| 22  | 4     | 812  | CLA  | CHD-C1D-ND  | -2.25 | 121.63      | 124.80   |
| 22  | A     | 836  | CLA  | CMD-C2D-C3D | -2.25 | 122.52      | 127.69   |
| 22  | 8     | 307  | CLA  | CMD-C2D-C3D | -2.25 | 122.52      | 127.69   |
| 22  | 4     | 806  | CLA  | C2D-C1D-ND  | 2.25  | 112.36      | 110.13   |
| 22  | B     | 832  | CLA  | O2A-CGA-CBA | 2.25  | 118.70      | 111.83   |
| 22  | 5     | 310  | CLA  | O2A-CGA-CBA | 2.25  | 118.70      | 111.83   |
| 22  | 3     | 313  | CLA  | CMD-C2D-C3D | -2.25 | 122.52      | 127.69   |
| 22  | A     | 828  | CLA  | CHD-C1D-ND  | -2.25 | 121.63      | 124.80   |
| 22  | B     | 820  | CLA  | CMD-C2D-C3D | -2.25 | 122.52      | 127.69   |
| 39  | 8     | 301  | CHL  | CMA-C3A-C2A | 2.25  | 122.83      | 114.13   |
| 22  | A     | 802  | CLA  | O2A-CGA-CBA | 2.25  | 118.70      | 111.83   |
| 22  | 4     | 808  | CLA  | O2A-CGA-CBA | 2.25  | 118.70      | 111.83   |
| 22  | 5     | 318  | CLA  | O2A-CGA-CBA | 2.25  | 118.70      | 111.83   |
| 22  | 5     | 319  | CLA  | CHD-C1D-ND  | -2.25 | 121.63      | 124.80   |
| 22  | 4     | 818  | CLA  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 22  | G     | 202  | CLA  | C2D-C1D-ND  | 2.25  | 112.35      | 110.13   |
| 22  | B     | 833  | CLA  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 22  | 4     | 812  | CLA  | O2A-CGA-CBA | 2.25  | 118.70      | 111.83   |
| 22  | 9     | 306  | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |
| 22  | 5     | 309  | CLA  | O2D-CGD-O1D | -2.25 | 119.47      | 123.85   |
| 22  | 6     | 311  | CLA  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 22  | 2     | 302  | CLA  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 22  | A     | 828  | CLA  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 22  | 6     | 301  | CLA  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 22  | A     | 821  | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 9     | 303 | CLA  | C1-O2A-CGA  | 2.25  | 122.09      | 116.65   |
| 22  | F     | 301 | CLA  | O2A-CGA-CBA | 2.25  | 118.69      | 111.83   |
| 22  | A     | 805 | CLA  | O2D-CGD-O1D | -2.25 | 119.47      | 123.85   |
| 22  | Z     | 313 | CLA  | C6-C5-C3    | -2.25 | 107.99      | 113.47   |
| 22  | L     | 201 | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |
| 22  | A     | 830 | CLA  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 22  | 3     | 312 | CLA  | CMD-C2D-C3D | -2.25 | 122.53      | 127.69   |
| 22  | 9     | 307 | CLA  | O2A-CGA-CBA | 2.25  | 118.69      | 111.83   |
| 22  | 7     | 322 | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |
| 22  | 6     | 319 | CLA  | C2D-C1D-ND  | 2.25  | 112.35      | 110.13   |
| 22  | A     | 830 | CLA  | O2A-CGA-CBA | 2.25  | 118.68      | 111.83   |
| 22  | A     | 835 | CLA  | C2D-C1D-ND  | 2.25  | 112.35      | 110.13   |
| 22  | K     | 202 | CLA  | C2D-C1D-ND  | 2.25  | 112.35      | 110.13   |
| 22  | A     | 825 | CLA  | CHD-C1D-ND  | -2.25 | 121.64      | 124.80   |
| 22  | 2     | 301 | CLA  | O2A-CGA-CBA | 2.24  | 118.68      | 111.83   |
| 22  | B     | 819 | CLA  | CMD-C2D-C3D | -2.24 | 122.54      | 127.69   |
| 22  | B     | 836 | CLA  | CMD-C2D-C3D | -2.24 | 122.54      | 127.69   |
| 22  | 6     | 312 | CLA  | C2D-C1D-ND  | 2.24  | 112.35      | 110.13   |
| 22  | 9     | 308 | CLA  | CMD-C2D-C3D | -2.24 | 122.54      | 127.69   |
| 22  | A     | 832 | CLA  | C2D-C1D-ND  | 2.24  | 112.35      | 110.13   |
| 22  | 1     | 304 | CLA  | C2D-C1D-ND  | 2.24  | 112.35      | 110.13   |
| 22  | 9     | 305 | CLA  | O1D-CGD-CBD | -2.24 | 120.09      | 124.52   |
| 22  | A     | 835 | CLA  | CHD-C1D-ND  | -2.24 | 121.65      | 124.80   |
| 22  | Z     | 316 | CLA  | O2D-CGD-O1D | -2.24 | 119.48      | 123.85   |
| 22  | 4     | 811 | CLA  | CHA-C1A-NA  | -2.24 | 121.31      | 126.39   |
| 22  | B     | 805 | CLA  | O2D-CGD-O1D | -2.24 | 119.48      | 123.85   |
| 22  | A     | 834 | CLA  | CMD-C2D-C3D | -2.24 | 122.55      | 127.69   |
| 22  | L     | 202 | CLA  | CMD-C2D-C3D | -2.24 | 122.55      | 127.69   |
| 22  | A     | 831 | CLA  | C2D-C1D-ND  | 2.24  | 112.34      | 110.13   |
| 22  | B     | 827 | CLA  | C2D-C1D-ND  | 2.24  | 112.34      | 110.13   |
| 22  | F     | 301 | CLA  | O1D-CGD-CBD | -2.24 | 120.10      | 124.52   |
| 22  | 5     | 312 | CLA  | CMD-C2D-C3D | -2.24 | 122.55      | 127.69   |
| 22  | B     | 832 | CLA  | O2D-CGD-O1D | -2.24 | 119.49      | 123.85   |
| 22  | 7     | 317 | CLA  | CHD-C1D-ND  | -2.24 | 121.65      | 124.80   |
| 24  | 8     | 304 | BCR  | C2-C1-C6    | 2.24  | 113.69      | 110.44   |
| 24  | 4     | 804 | BCR  | C23-C24-C25 | -2.24 | 121.01      | 127.00   |
| 22  | K     | 203 | CLA  | C2D-C1D-ND  | 2.24  | 112.34      | 110.13   |
| 22  | K     | 203 | CLA  | CHA-C1A-NA  | -2.24 | 121.32      | 126.39   |
| 22  | 4     | 806 | CLA  | CHA-C1A-NA  | -2.24 | 121.32      | 126.39   |
| 22  | F     | 305 | CLA  | CHD-C1D-ND  | -2.24 | 121.65      | 124.80   |
| 22  | 4     | 817 | CLA  | CMD-C2D-C3D | -2.24 | 122.55      | 127.69   |
| 22  | B     | 835 | CLA  | O2A-CGA-CBA | 2.24  | 118.66      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 5     | 313 | CLA  | C1D-ND-C4D  | -2.24 | 104.74      | 106.31   |
| 38  | 8     | 303 | LUT  | C30-C31-C32 | -2.24 | 116.71      | 123.20   |
| 22  | B     | 827 | CLA  | CHD-C1D-ND  | -2.24 | 121.65      | 124.80   |
| 22  | B     | 801 | CLA  | C2D-C1D-ND  | 2.24  | 112.34      | 110.13   |
| 22  | B     | 810 | CLA  | C2D-C1D-ND  | 2.24  | 112.34      | 110.13   |
| 22  | B     | 832 | CLA  | C2D-C1D-ND  | 2.24  | 112.34      | 110.13   |
| 24  | B     | 845 | BCR  | C15-C16-C17 | -2.24 | 118.94      | 123.52   |
| 22  | B     | 820 | CLA  | O2A-CGA-CBA | 2.24  | 118.66      | 111.83   |
| 22  | B     | 828 | CLA  | O2A-CGA-CBA | 2.24  | 118.66      | 111.83   |
| 22  | 1     | 310 | CLA  | O2A-CGA-CBA | 2.24  | 118.66      | 111.83   |
| 22  | 3     | 310 | CLA  | C6-C7-C8    | -2.24 | 108.53      | 115.97   |
| 22  | A     | 807 | CLA  | C2D-C1D-ND  | 2.24  | 112.34      | 110.13   |
| 22  | A     | 834 | CLA  | CHD-C1D-ND  | -2.24 | 121.66      | 124.80   |
| 22  | 7     | 317 | CLA  | O2A-CGA-CBA | 2.24  | 118.65      | 111.83   |
| 22  | A     | 827 | CLA  | CMD-C2D-C3D | -2.24 | 122.56      | 127.69   |
| 22  | 6     | 314 | CLA  | CHD-C1D-ND  | -2.24 | 121.66      | 124.80   |
| 22  | B     | 834 | CLA  | C2D-C1D-ND  | 2.23  | 112.34      | 110.13   |
| 22  | B     | 834 | CLA  | CMD-C2D-C3D | -2.23 | 122.56      | 127.69   |
| 22  | A     | 802 | CLA  | C2D-C1D-ND  | 2.23  | 112.34      | 110.13   |
| 22  | G     | 201 | CLA  | C2D-C1D-ND  | 2.23  | 112.34      | 110.13   |
| 22  | A     | 812 | CLA  | CHA-C1A-NA  | -2.23 | 121.33      | 126.39   |
| 22  | 9     | 311 | CLA  | CHA-C1A-NA  | -2.23 | 121.33      | 126.39   |
| 22  | A     | 827 | CLA  | O2A-CGA-CBA | 2.23  | 118.64      | 111.83   |
| 22  | K     | 204 | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 22  | A     | 820 | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 22  | 7     | 317 | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 22  | B     | 816 | CLA  | CHD-C1D-ND  | -2.23 | 121.66      | 124.80   |
| 22  | B     | 829 | CLA  | C6-C5-C3    | -2.23 | 108.03      | 113.47   |
| 22  | J     | 103 | CLA  | CHD-C1D-ND  | -2.23 | 121.66      | 124.80   |
| 22  | 5     | 310 | CLA  | CHD-C1D-ND  | -2.23 | 121.66      | 124.80   |
| 22  | 9     | 308 | CLA  | CHD-C1D-ND  | -2.23 | 121.66      | 124.80   |
| 22  | A     | 842 | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 24  | J     | 104 | BCR  | C1-C6-C7    | 2.23  | 121.70      | 115.65   |
| 24  | 5     | 304 | BCR  | C37-C22-C21 | -2.23 | 119.20      | 122.82   |
| 22  | F     | 301 | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 22  | 5     | 308 | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 22  | 8     | 309 | CLA  | C2D-C1D-ND  | 2.23  | 112.33      | 110.13   |
| 22  | A     | 804 | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 22  | G     | 201 | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 22  | 3     | 309 | CLA  | CHD-C1D-ND  | -2.23 | 121.66      | 124.80   |
| 22  | 7     | 324 | CLA  | CHD-C1D-ND  | -2.23 | 121.66      | 124.80   |
| 25  | 1     | 317 | LHG  | O7-C7-O9    | -2.23 | 118.49      | 123.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 835 | CLA  | O2D-CGD-O1D | -2.23 | 119.51      | 123.85   |
| 22  | 7     | 312 | CLA  | CHA-C1A-NA  | -2.23 | 121.34      | 126.39   |
| 22  | 7     | 309 | CLA  | CMD-C2D-C3D | -2.23 | 122.58      | 127.69   |
| 22  | 6     | 319 | CLA  | CMD-C2D-C3D | -2.23 | 122.58      | 127.69   |
| 22  | A     | 842 | CLA  | CHD-C1D-ND  | -2.23 | 121.67      | 124.80   |
| 22  | Z     | 315 | CLA  | CHD-C1D-ND  | -2.23 | 121.67      | 124.80   |
| 38  | 6     | 304 | LUT  | C8-C7-C6    | -2.23 | 121.05      | 127.00   |
| 22  | 1     | 306 | CLA  | CHD-C1D-ND  | -2.23 | 121.67      | 124.80   |
| 22  | L     | 202 | CLA  | C2D-C1D-ND  | 2.23  | 112.33      | 110.13   |
| 22  | 7     | 324 | CLA  | C2D-C1D-ND  | 2.23  | 112.33      | 110.13   |
| 22  | B     | 842 | CLA  | CHA-C1A-NA  | -2.23 | 121.35      | 126.39   |
| 22  | B     | 815 | CLA  | C3B-C4B-NB  | -2.23 | 108.54      | 110.53   |
| 22  | F     | 304 | CLA  | C2D-C1D-ND  | 2.23  | 112.33      | 110.13   |
| 22  | 6     | 321 | CLA  | CHD-C1D-ND  | -2.23 | 121.67      | 124.80   |
| 34  | J     | 101 | LMG  | O8-C28-C29  | 2.23  | 118.62      | 111.83   |
| 22  | 6     | 321 | CLA  | CMD-C2D-C3D | -2.23 | 122.58      | 127.69   |
| 22  | A     | 808 | CLA  | CHD-C1D-ND  | -2.23 | 121.67      | 124.80   |
| 22  | B     | 822 | CLA  | C2D-C1D-ND  | 2.23  | 112.33      | 110.13   |
| 22  | 3     | 319 | CLA  | C2D-C1D-ND  | 2.23  | 112.33      | 110.13   |
| 22  | A     | 816 | CLA  | CMD-C2D-C3D | -2.23 | 122.58      | 127.69   |
| 24  | B     | 846 | BCR  | C8-C7-C6    | -2.23 | 121.05      | 127.00   |
| 34  | F     | 308 | LMG  | O6-C1-C2    | -2.23 | 105.80      | 110.37   |
| 22  | 3     | 311 | CLA  | O2D-CGD-O1D | -2.23 | 119.52      | 123.85   |
| 22  | F     | 304 | CLA  | CHA-C1A-NA  | -2.22 | 121.35      | 126.39   |
| 22  | A     | 855 | CLA  | CHD-C1D-ND  | -2.22 | 121.67      | 124.80   |
| 22  | A     | 803 | CLA  | O1D-CGD-CBD | -2.22 | 120.13      | 124.52   |
| 22  | 1     | 309 | CLA  | C2D-C1D-ND  | 2.22  | 112.33      | 110.13   |
| 22  | 7     | 308 | CLA  | C2D-C1D-ND  | 2.22  | 112.33      | 110.13   |
| 22  | 6     | 314 | CLA  | CMD-C2D-C3D | -2.22 | 122.59      | 127.69   |
| 22  | B     | 831 | CLA  | CHD-C1D-ND  | -2.22 | 121.67      | 124.80   |
| 22  | L     | 202 | CLA  | O2D-CGD-O1D | -2.22 | 119.52      | 123.85   |
| 22  | 9     | 306 | CLA  | C2D-C1D-ND  | 2.22  | 112.33      | 110.13   |
| 22  | J     | 103 | CLA  | CMD-C2D-C3D | -2.22 | 122.59      | 127.69   |
| 22  | A     | 803 | CLA  | CHD-C1D-ND  | -2.22 | 121.67      | 124.80   |
| 22  | A     | 810 | CLA  | O2A-CGA-CBA | 2.22  | 118.61      | 111.83   |
| 22  | A     | 803 | CLA  | CMD-C2D-C3D | -2.22 | 122.59      | 127.69   |
| 22  | 7     | 312 | CLA  | CMD-C2D-C3D | -2.22 | 122.59      | 127.69   |
| 22  | 9     | 313 | CLA  | CHD-C1D-ND  | -2.22 | 121.68      | 124.80   |
| 24  | A     | 848 | BCR  | C36-C18-C17 | -2.22 | 119.22      | 122.82   |
| 22  | A     | 814 | CLA  | CHD-C1D-ND  | -2.22 | 121.68      | 124.80   |
| 22  | A     | 815 | CLA  | C2D-C1D-ND  | 2.22  | 112.32      | 110.13   |
| 22  | 7     | 306 | CLA  | O2A-CGA-CBA | 2.22  | 118.61      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 8     | 314 | CLA  | O2D-CGD-O1D | -2.22 | 119.53      | 123.85   |
| 22  | K     | 202 | CLA  | CMD-C2D-C3D | -2.22 | 122.60      | 127.69   |
| 22  | A     | 806 | CLA  | C2D-C1D-ND  | 2.22  | 112.32      | 110.13   |
| 22  | 5     | 312 | CLA  | CHD-C1D-ND  | -2.22 | 121.68      | 124.80   |
| 22  | B     | 810 | CLA  | C6-C5-C3    | -2.22 | 108.06      | 113.47   |
| 22  | 6     | 308 | CLA  | CHD-C1D-ND  | -2.22 | 121.68      | 124.80   |
| 39  | 4     | 816 | CHL  | CMA-C3A-C4A | 2.22  | 119.39      | 114.61   |
| 22  | Z     | 310 | CLA  | CHA-C1A-NA  | -2.22 | 121.37      | 126.39   |
| 22  | A     | 826 | CLA  | CMD-C2D-C3D | -2.22 | 122.60      | 127.69   |
| 22  | F     | 301 | CLA  | O2D-CGD-O1D | -2.22 | 119.53      | 123.85   |
| 22  | 4     | 810 | CLA  | O2D-CGD-O1D | -2.22 | 119.53      | 123.85   |
| 22  | B     | 828 | CLA  | CHD-C1D-ND  | -2.22 | 121.68      | 124.80   |
| 22  | 7     | 306 | CLA  | C2D-C1D-ND  | 2.22  | 112.32      | 110.13   |
| 22  | 7     | 316 | CLA  | CMD-C2D-C3D | -2.22 | 122.61      | 127.69   |
| 22  | 4     | 807 | CLA  | CAA-C2A-C3A | -2.22 | 107.01      | 113.00   |
| 22  | A     | 838 | CLA  | CHD-C1D-ND  | -2.22 | 121.69      | 124.80   |
| 22  | 9     | 310 | CLA  | C3D-C2D-C1D | -2.22 | 102.81      | 105.83   |
| 22  | 9     | 307 | CLA  | CMD-C2D-C3D | -2.22 | 122.61      | 127.69   |
| 22  | 7     | 315 | CLA  | O2A-CGA-CBA | 2.22  | 118.59      | 111.83   |
| 22  | B     | 812 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | B     | 813 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | 7     | 323 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | 5     | 319 | CLA  | C2D-C1D-ND  | 2.21  | 112.32      | 110.13   |
| 22  | 9     | 305 | CLA  | C3B-C4B-NB  | -2.21 | 108.55      | 110.53   |
| 22  | 9     | 305 | CLA  | C3A-C2A-C1A | 2.21  | 104.65      | 101.34   |
| 22  | 1     | 306 | CLA  | CMD-C2D-C3D | -2.21 | 122.61      | 127.69   |
| 22  | 6     | 313 | CLA  | C2D-C1D-ND  | 2.21  | 112.32      | 110.13   |
| 22  | A     | 820 | CLA  | C2D-C1D-ND  | 2.21  | 112.31      | 110.13   |
| 22  | 4     | 808 | CLA  | CMD-C2D-C3D | -2.21 | 122.62      | 127.69   |
| 22  | A     | 825 | CLA  | C2D-C1D-ND  | 2.21  | 112.31      | 110.13   |
| 22  | 3     | 314 | CLA  | C2D-C1D-ND  | 2.21  | 112.31      | 110.13   |
| 22  | 7     | 304 | CLA  | O1D-CGD-CBD | -2.21 | 120.16      | 124.52   |
| 22  | 3     | 310 | CLA  | CMD-C2D-C3D | -2.21 | 122.62      | 127.69   |
| 22  | A     | 841 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | 4     | 817 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | 4     | 818 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | 7     | 316 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | A     | 836 | CLA  | C6-C5-C3    | -2.21 | 108.09      | 113.47   |
| 22  | 7     | 322 | CLA  | CHA-C1A-NA  | -2.21 | 121.39      | 126.39   |
| 24  | 3     | 304 | BCR  | C19-C18-C17 | -2.21 | 115.53      | 119.01   |
| 22  | A     | 825 | CLA  | O2A-CGA-CBA | 2.21  | 118.57      | 111.83   |
| 22  | B     | 814 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 814 | CLA  | C2D-C1D-ND  | 2.21  | 112.31      | 110.13   |
| 22  | 1     | 310 | CLA  | CMD-C2D-C3D | -2.21 | 122.62      | 127.69   |
| 22  | 8     | 306 | CLA  | O1D-CGD-CBD | -2.21 | 120.16      | 124.52   |
| 22  | A     | 820 | CLA  | CHA-C1A-NA  | -2.21 | 121.39      | 126.39   |
| 22  | B     | 842 | CLA  | CHD-C1D-ND  | -2.21 | 121.69      | 124.80   |
| 22  | L     | 203 | CLA  | C2D-C1D-ND  | 2.21  | 112.31      | 110.13   |
| 22  | A     | 817 | CLA  | C1D-ND-C4D  | -2.21 | 104.76      | 106.31   |
| 39  | 1     | 312 | CHL  | C4D-CHA-CBD | -2.21 | 106.74      | 108.97   |
| 24  | 5     | 305 | BCR  | C38-C26-C27 | 2.21  | 118.30      | 113.60   |
| 22  | 7     | 323 | CLA  | CAA-CBA-CGA | -2.21 | 106.94      | 113.21   |
| 22  | B     | 826 | CLA  | CHD-C1D-ND  | -2.21 | 121.70      | 124.80   |
| 22  | 1     | 304 | CLA  | CHD-C1D-ND  | -2.21 | 121.70      | 124.80   |
| 24  | 4     | 804 | BCR  | C1-C6-C5    | -2.21 | 119.62      | 122.64   |
| 22  | 1     | 304 | CLA  | CMD-C2D-C3D | -2.21 | 122.63      | 127.69   |
| 38  | 6     | 303 | LUT  | C38-C25-C24 | -2.21 | 118.14      | 123.36   |
| 22  | F     | 302 | CLA  | CMD-C2D-C3D | -2.21 | 122.63      | 127.69   |
| 22  | F     | 301 | CLA  | CHD-C1D-ND  | -2.20 | 121.70      | 124.80   |
| 22  | 6     | 312 | CLA  | CHD-C1D-ND  | -2.20 | 121.70      | 124.80   |
| 22  | 6     | 311 | CLA  | CHA-C1A-NA  | -2.20 | 121.40      | 126.39   |
| 22  | 9     | 311 | CLA  | CMD-C2D-C3D | -2.20 | 122.64      | 127.69   |
| 22  | 9     | 303 | CLA  | CHD-C1D-ND  | -2.20 | 121.70      | 124.80   |
| 22  | B     | 823 | CLA  | CAA-CBA-CGA | -2.20 | 106.95      | 113.21   |
| 39  | Z     | 311 | CHL  | C4C-CHD-C1D | 2.20  | 123.95      | 116.07   |
| 22  | 5     | 326 | CLA  | CMD-C2D-C3D | -2.20 | 122.64      | 127.69   |
| 22  | B     | 815 | CLA  | CHD-C1D-ND  | -2.20 | 121.70      | 124.80   |
| 38  | 1     | 302 | LUT  | C19-C9-C10  | -2.20 | 119.25      | 122.82   |
| 22  | B     | 812 | CLA  | CMD-C2D-C3D | -2.20 | 122.64      | 127.69   |
| 22  | A     | 840 | CLA  | O2D-CGD-O1D | -2.20 | 119.56      | 123.85   |
| 22  | A     | 828 | CLA  | C2D-C1D-ND  | 2.20  | 112.31      | 110.13   |
| 22  | 3     | 310 | CLA  | C2D-C1D-ND  | 2.20  | 112.31      | 110.13   |
| 22  | A     | 816 | CLA  | O1D-CGD-CBD | -2.20 | 120.18      | 124.52   |
| 22  | A     | 808 | CLA  | CMD-C2D-C3D | -2.20 | 122.64      | 127.69   |
| 22  | A     | 807 | CLA  | CHD-C1D-ND  | -2.20 | 121.70      | 124.80   |
| 22  | L     | 202 | CLA  | CHD-C1D-ND  | -2.20 | 121.70      | 124.80   |
| 22  | A     | 815 | CLA  | O2A-CGA-CBA | 2.20  | 118.54      | 111.83   |
| 22  | 1     | 314 | CLA  | CMD-C2D-C3D | -2.20 | 122.64      | 127.69   |
| 22  | 5     | 311 | CLA  | CMD-C2D-C3D | -2.20 | 122.64      | 127.69   |
| 22  | 7     | 314 | CLA  | O2D-CGD-O1D | -2.20 | 119.57      | 123.85   |
| 22  | 4     | 810 | CLA  | C2D-C1D-ND  | 2.20  | 112.30      | 110.13   |
| 22  | 6     | 322 | CLA  | CHD-C1D-ND  | -2.20 | 121.71      | 124.80   |
| 22  | F     | 304 | CLA  | C1-O2A-CGA  | 2.20  | 121.97      | 116.65   |
| 24  | B     | 845 | BCR  | C2-C1-C6    | 2.20  | 113.63      | 110.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 8     | 313 | CLA  | CMD-C2D-C3D | -2.20 | 122.65      | 127.69   |
| 22  | A     | 833 | CLA  | CHD-C1D-ND  | -2.20 | 121.71      | 124.80   |
| 22  | A     | 804 | CLA  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 22  | A     | 811 | CLA  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 22  | A     | 823 | CLA  | C6-C5-C3    | -2.20 | 108.11      | 113.47   |
| 22  | 7     | 322 | CLA  | O2A-CGA-CBA | 2.20  | 118.54      | 111.83   |
| 22  | 4     | 809 | CLA  | CHA-C1A-NA  | -2.20 | 121.41      | 126.39   |
| 22  | 2     | 304 | CLA  | O2D-CGD-O1D | -2.20 | 119.57      | 123.85   |
| 22  | K     | 203 | CLA  | O2D-CGD-O1D | -2.20 | 119.57      | 123.85   |
| 38  | 3     | 302 | LUT  | C11-C12-C13 | -2.20 | 120.34      | 126.36   |
| 22  | Z     | 306 | CLA  | CHD-C1D-ND  | -2.20 | 121.71      | 124.80   |
| 33  | 4     | 822 | LMT  | C1B-O5B-C5B | 2.20  | 118.01      | 113.72   |
| 22  | A     | 854 | CLA  | C2D-C1D-ND  | 2.20  | 112.30      | 110.13   |
| 22  | 9     | 308 | CLA  | C2D-C1D-ND  | 2.20  | 112.30      | 110.13   |
| 22  | 8     | 310 | CLA  | O2A-CGA-CBA | 2.20  | 118.53      | 111.83   |
| 24  | A     | 844 | BCR  | C21-C20-C19 | -2.20 | 116.84      | 123.20   |
| 22  | 4     | 805 | CLA  | C1D-ND-C4D  | -2.19 | 104.77      | 106.31   |
| 22  | 7     | 314 | CLA  | O1D-CGD-CBD | -2.19 | 120.19      | 124.52   |
| 22  | Z     | 304 | CLA  | O2D-CGD-O1D | -2.19 | 119.58      | 123.85   |
| 22  | 8     | 309 | CLA  | CHD-C1D-ND  | -2.19 | 121.71      | 124.80   |
| 22  | A     | 830 | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | K     | 203 | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | A     | 832 | CLA  | O2A-CGA-CBA | 2.19  | 118.52      | 111.83   |
| 38  | 1     | 303 | LUT  | C21-C26-C27 | -2.19 | 110.30      | 112.83   |
| 22  | A     | 813 | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | A     | 840 | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | 3     | 316 | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | A     | 854 | CLA  | CMD-C2D-C3D | -2.19 | 122.66      | 127.69   |
| 22  | 6     | 301 | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | 1     | 305 | CLA  | C2D-C1D-ND  | 2.19  | 112.30      | 110.13   |
| 22  | 5     | 315 | CLA  | O2A-CGA-CBA | 2.19  | 118.52      | 111.83   |
| 22  | Z     | 313 | CLA  | CHA-C1A-NA  | -2.19 | 121.43      | 126.39   |
| 22  | A     | 814 | CLA  | CMD-C2D-C3D | -2.19 | 122.66      | 127.69   |
| 22  | B     | 837 | CLA  | CMD-C2D-C3D | -2.19 | 122.66      | 127.69   |
| 22  | 7     | 304 | CLA  | O2D-CGD-O1D | -2.19 | 119.58      | 123.85   |
| 22  | 6     | 321 | CLA  | C2D-C1D-ND  | 2.19  | 112.29      | 110.13   |
| 22  | 2     | 302 | CLA  | CHA-C1A-NA  | -2.19 | 121.43      | 126.39   |
| 22  | 5     | 318 | CLA  | CMD-C2D-C3D | -2.19 | 122.67      | 127.69   |
| 25  | B     | 803 | LHG  | O7-C7-O9    | -2.19 | 118.58      | 123.70   |
| 22  | 7     | 305 | CLA  | CMD-C2D-C3D | -2.19 | 122.67      | 127.69   |
| 22  | 4     | 815 | CLA  | O2A-CGA-CBA | 2.19  | 118.51      | 111.83   |
| 22  | 1     | 314 | CLA  | O2A-CGA-CBA | 2.19  | 118.51      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 38  | 9     | 302 | LUT  | C11-C12-C13 | -2.19 | 120.36      | 126.36   |
| 22  | 3     | 311 | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | 5     | 309 | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | K     | 205 | CLA  | CMA-C3A-C4A | 2.19  | 117.65      | 111.77   |
| 22  | 1     | 305 | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 22  | A     | 831 | CLA  | CHA-C1A-NA  | -2.19 | 121.44      | 126.39   |
| 22  | B     | 829 | CLA  | CHA-C1A-NA  | -2.19 | 121.44      | 126.39   |
| 31  | 1     | 319 | DGD  | O1G-C1A-C2A | 2.19  | 118.50      | 111.83   |
| 22  | 7     | 309 | CLA  | O2D-CGD-O1D | -2.19 | 119.59      | 123.85   |
| 22  | A     | 827 | CLA  | CHD-C1D-ND  | -2.19 | 121.73      | 124.80   |
| 22  | Z     | 308 | CLA  | CHA-C1A-NA  | -2.19 | 121.44      | 126.39   |
| 39  | 2     | 303 | CHL  | CMA-C3A-C2A | 2.19  | 122.57      | 114.13   |
| 22  | J     | 103 | CLA  | CHA-C1A-NA  | -2.19 | 121.44      | 126.39   |
| 22  | Z     | 306 | CLA  | C2D-C1D-ND  | 2.18  | 112.29      | 110.13   |
| 22  | 3     | 316 | CLA  | C2D-C1D-ND  | 2.18  | 112.29      | 110.13   |
| 22  | 3     | 320 | CLA  | C2A-C1A-CHA | 2.18  | 127.66      | 123.87   |
| 22  | A     | 806 | CLA  | CMD-C2D-C3D | -2.18 | 122.68      | 127.69   |
| 22  | 7     | 311 | CLA  | CMD-C2D-C3D | -2.18 | 122.68      | 127.69   |
| 22  | B     | 832 | CLA  | O1D-CGD-CBD | -2.18 | 120.21      | 124.52   |
| 25  | 9     | 315 | LHG  | C9-C8-C7    | -2.18 | 105.69      | 113.69   |
| 38  | Z     | 301 | LUT  | C19-C9-C10  | -2.18 | 119.28      | 122.82   |
| 22  | 8     | 316 | CLA  | CHD-C1D-ND  | -2.18 | 121.73      | 124.80   |
| 22  | Z     | 309 | CLA  | C6-C5-C3    | -2.18 | 108.15      | 113.47   |
| 22  | Z     | 307 | CLA  | CAA-CBA-CGA | -2.18 | 107.01      | 113.21   |
| 22  | B     | 840 | CLA  | C2D-C1D-ND  | 2.18  | 112.29      | 110.13   |
| 22  | K     | 204 | CLA  | CHA-C1A-NA  | -2.18 | 121.45      | 126.39   |
| 22  | B     | 829 | CLA  | O2D-CGD-O1D | -2.18 | 119.60      | 123.85   |
| 22  | 9     | 304 | CLA  | C2A-C1A-CHA | 2.18  | 127.65      | 123.87   |
| 22  | A     | 827 | CLA  | O2D-CGD-O1D | -2.18 | 119.60      | 123.85   |
| 22  | B     | 820 | CLA  | CHD-C1D-ND  | -2.18 | 121.73      | 124.80   |
| 22  | 8     | 305 | CLA  | O2A-CGA-CBA | 2.18  | 118.49      | 111.83   |
| 22  | B     | 810 | CLA  | CHD-C1D-ND  | -2.18 | 121.73      | 124.80   |
| 22  | B     | 841 | CLA  | CHD-C1D-ND  | -2.18 | 121.73      | 124.80   |
| 22  | A     | 824 | CLA  | CMD-C2D-C3D | -2.18 | 122.69      | 127.69   |
| 22  | 5     | 310 | CLA  | O1D-CGD-CBD | -2.18 | 120.22      | 124.52   |
| 24  | A     | 845 | BCR  | C29-C30-C25 | 2.18  | 113.61      | 110.44   |
| 22  | A     | 809 | CLA  | CHA-C1A-NA  | -2.18 | 121.45      | 126.39   |
| 22  | 7     | 316 | CLA  | CHA-C1A-NA  | -2.18 | 121.45      | 126.39   |
| 39  | Z     | 312 | CHL  | C4D-CHA-CBD | -2.18 | 106.77      | 108.97   |
| 22  | 8     | 309 | CLA  | O2D-CGD-O1D | -2.18 | 119.61      | 123.85   |
| 22  | 1     | 306 | CLA  | C2D-C1D-ND  | 2.18  | 112.28      | 110.13   |
| 22  | 7     | 310 | CLA  | CHA-C1A-NA  | -2.18 | 121.46      | 126.39   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 806 | CLA  | CHD-C1D-ND  | -2.18 | 121.74      | 124.80   |
| 22  | 6     | 319 | CLA  | CHD-C1D-ND  | -2.18 | 121.74      | 124.80   |
| 22  | B     | 838 | CLA  | O2D-CGD-O1D | -2.18 | 119.61      | 123.85   |
| 22  | 1     | 313 | CLA  | O2A-CGA-CBA | 2.18  | 118.48      | 111.83   |
| 24  | A     | 856 | BCR  | C30-C25-C24 | 2.18  | 121.56      | 115.65   |
| 22  | 1     | 315 | CLA  | CHD-C1D-ND  | -2.18 | 121.74      | 124.80   |
| 22  | 4     | 806 | CLA  | CMD-C2D-C3D | -2.18 | 122.70      | 127.69   |
| 22  | K     | 202 | CLA  | CHD-C1D-ND  | -2.18 | 121.74      | 124.80   |
| 22  | 5     | 312 | CLA  | O2A-CGA-CBA | 2.18  | 118.47      | 111.83   |
| 22  | 1     | 310 | CLA  | C2D-C1D-ND  | 2.18  | 112.28      | 110.13   |
| 22  | 4     | 818 | CLA  | O2D-CGD-O1D | -2.18 | 119.61      | 123.85   |
| 22  | 4     | 818 | CLA  | CHA-C1A-NA  | -2.17 | 121.47      | 126.39   |
| 22  | A     | 813 | CLA  | CHA-C1A-NA  | -2.17 | 121.47      | 126.39   |
| 22  | B     | 810 | CLA  | CHA-C1A-NA  | -2.17 | 121.47      | 126.39   |
| 22  | 5     | 319 | CLA  | CMD-C2D-C3D | -2.17 | 122.70      | 127.69   |
| 24  | A     | 848 | BCR  | C8-C9-C10   | 2.17  | 122.43      | 119.01   |
| 22  | 7     | 307 | CLA  | O1D-CGD-CBD | -2.17 | 120.23      | 124.52   |
| 22  | A     | 826 | CLA  | CHD-C1D-ND  | -2.17 | 121.74      | 124.80   |
| 22  | A     | 815 | CLA  | CHD-C1D-ND  | -2.17 | 121.75      | 124.80   |
| 22  | 8     | 314 | CLA  | C2D-C1D-ND  | 2.17  | 112.28      | 110.13   |
| 22  | 3     | 322 | CLA  | CHA-C1A-NA  | -2.17 | 121.47      | 126.39   |
| 22  | 5     | 322 | CLA  | CHA-C1A-NA  | -2.17 | 121.47      | 126.39   |
| 22  | A     | 813 | CLA  | O1D-CGD-CBD | -2.17 | 120.23      | 124.52   |
| 22  | Z     | 315 | CLA  | CHA-C1A-NA  | -2.17 | 121.47      | 126.39   |
| 22  | A     | 810 | CLA  | C2D-C1D-ND  | 2.17  | 112.28      | 110.13   |
| 22  | 6     | 308 | CLA  | C3D-C2D-C1D | -2.17 | 102.87      | 105.83   |
| 22  | 7     | 306 | CLA  | C6-C5-C3    | -2.17 | 108.18      | 113.47   |
| 22  | A     | 824 | CLA  | CHD-C1D-ND  | -2.17 | 121.75      | 124.80   |
| 22  | 9     | 308 | CLA  | O1D-CGD-CBD | -2.17 | 120.24      | 124.52   |
| 22  | A     | 827 | CLA  | C3D-C2D-C1D | -2.17 | 102.87      | 105.83   |
| 22  | B     | 834 | CLA  | CHA-C1A-NA  | -2.17 | 121.48      | 126.39   |
| 22  | 8     | 305 | CLA  | C6-C5-C3    | -2.17 | 108.18      | 113.47   |
| 24  | 3     | 305 | BCR  | C29-C30-C25 | 2.17  | 113.59      | 110.44   |
| 22  | 5     | 307 | CLA  | O2A-CGA-CBA | 2.17  | 118.45      | 111.83   |
| 22  | 6     | 312 | CLA  | CHA-C1A-NA  | -2.17 | 121.48      | 126.39   |
| 22  | B     | 842 | CLA  | O2A-CGA-CBA | 2.17  | 118.45      | 111.83   |
| 22  | A     | 836 | CLA  | CHA-C1A-NA  | -2.17 | 121.48      | 126.39   |
| 22  | A     | 855 | CLA  | C2D-C1D-ND  | 2.17  | 112.27      | 110.13   |
| 22  | A     | 825 | CLA  | CHA-C1A-NA  | -2.17 | 121.48      | 126.39   |
| 22  | 3     | 312 | CLA  | CHA-C1A-NA  | -2.17 | 121.48      | 126.39   |
| 22  | 7     | 305 | CLA  | C3D-C2D-C1D | -2.17 | 102.87      | 105.83   |
| 24  | B     | 845 | BCR  | C33-C5-C6   | -2.17 | 122.12      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 837 | CLA  | C2D-C1D-ND  | 2.17  | 112.27      | 110.13   |
| 22  | 3     | 319 | CLA  | CHA-C1A-NA  | -2.17 | 121.49      | 126.39   |
| 38  | 1     | 303 | LUT  | C8-C7-C6    | -2.17 | 121.21      | 127.00   |
| 22  | B     | 839 | CLA  | O2D-CGD-O1D | -2.16 | 119.63      | 123.85   |
| 24  | K     | 206 | BCR  | C2-C1-C6    | 2.16  | 113.58      | 110.44   |
| 22  | B     | 824 | CLA  | CHA-C1A-NA  | -2.16 | 121.49      | 126.39   |
| 22  | 5     | 312 | CLA  | C2D-C1D-ND  | 2.16  | 112.27      | 110.13   |
| 22  | 5     | 315 | CLA  | C6-C5-C3    | -2.16 | 108.20      | 113.47   |
| 22  | B     | 807 | CLA  | CMD-C2D-C3D | -2.16 | 122.73      | 127.69   |
| 22  | 7     | 322 | CLA  | CMD-C2D-C3D | -2.16 | 122.73      | 127.69   |
| 22  | A     | 805 | CLA  | C3D-C2D-C1D | -2.16 | 102.88      | 105.83   |
| 22  | 4     | 812 | CLA  | CHA-C1A-NA  | -2.16 | 121.49      | 126.39   |
| 22  | 3     | 311 | CLA  | CMD-C2D-C3D | -2.16 | 122.73      | 127.69   |
| 22  | 3     | 310 | CLA  | CAA-CBA-CGA | -2.16 | 107.06      | 113.21   |
| 22  | B     | 806 | CLA  | CHA-C1A-NA  | -2.16 | 121.49      | 126.39   |
| 22  | 8     | 314 | CLA  | CHA-C1A-NA  | -2.16 | 121.49      | 126.39   |
| 22  | 8     | 314 | CLA  | CHD-C1D-ND  | -2.16 | 121.76      | 124.80   |
| 22  | 2     | 302 | CLA  | CHD-C1D-ND  | -2.16 | 121.76      | 124.80   |
| 22  | 5     | 322 | CLA  | O2D-CGD-O1D | -2.16 | 119.64      | 123.85   |
| 22  | 5     | 313 | CLA  | OBD-CAD-C3D | -2.16 | 123.36      | 128.42   |
| 22  | Z     | 314 | CLA  | O2A-CGA-CBA | 2.16  | 118.43      | 111.83   |
| 22  | 5     | 320 | CLA  | C3D-C2D-C1D | -2.16 | 102.88      | 105.83   |
| 22  | 8     | 310 | CLA  | C2D-C1D-ND  | 2.16  | 112.27      | 110.13   |
| 22  | A     | 813 | CLA  | C6-C5-C3    | -2.16 | 108.20      | 113.47   |
| 22  | B     | 839 | CLA  | CHA-C1A-NA  | -2.16 | 121.50      | 126.39   |
| 22  | 9     | 311 | CLA  | O2D-CGD-O1D | -2.16 | 119.64      | 123.85   |
| 22  | 8     | 313 | CLA  | O2A-CGA-CBA | 2.16  | 118.42      | 111.83   |
| 38  | Z     | 302 | LUT  | C27-C28-C29 | -2.16 | 121.68      | 126.32   |
| 22  | Z     | 314 | CLA  | CHD-C1D-ND  | -2.16 | 121.76      | 124.80   |
| 22  | A     | 830 | CLA  | C2D-C1D-ND  | 2.16  | 112.26      | 110.13   |
| 22  | 1     | 307 | CLA  | C2D-C1D-ND  | 2.16  | 112.26      | 110.13   |
| 22  | A     | 808 | CLA  | O2A-CGA-CBA | 2.16  | 118.42      | 111.83   |
| 22  | A     | 827 | CLA  | CHA-C1A-NA  | -2.16 | 121.50      | 126.39   |
| 22  | B     | 834 | CLA  | CHD-C1D-ND  | -2.16 | 121.76      | 124.80   |
| 22  | B     | 810 | CLA  | O1D-CGD-CBD | -2.16 | 120.26      | 124.52   |
| 22  | A     | 804 | CLA  | O1D-CGD-CBD | -2.16 | 120.26      | 124.52   |
| 22  | A     | 855 | CLA  | O2A-CGA-CBA | 2.16  | 118.42      | 111.83   |
| 22  | B     | 819 | CLA  | C6-C5-C3    | -2.16 | 108.21      | 113.47   |
| 38  | 8     | 302 | LUT  | C30-C31-C32 | -2.16 | 116.94      | 123.20   |
| 38  | 1     | 303 | LUT  | C27-C28-C29 | -2.16 | 121.68      | 126.32   |
| 22  | B     | 837 | CLA  | O2A-CGA-CBA | 2.16  | 118.42      | 111.83   |
| 22  | B     | 805 | CLA  | O1D-CGD-CBD | -2.16 | 120.26      | 124.52   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 811  | CLA  | O1D-CGD-CBD | -2.16 | 120.26      | 124.52   |
| 22  | A     | 839  | CLA  | C2D-C1D-ND  | 2.16  | 112.26      | 110.13   |
| 22  | B     | 823  | CLA  | O2D-CGD-O1D | -2.16 | 119.65      | 123.85   |
| 22  | Z     | 313  | CLA  | O2A-CGA-CBA | 2.16  | 118.41      | 111.83   |
| 24  | 3     | 307  | BCR  | C38-C26-C27 | 2.16  | 118.19      | 113.60   |
| 22  | B     | 813  | CLA  | C6-C5-C3    | -2.16 | 108.21      | 113.47   |
| 22  | 9     | 313  | CLA  | O1D-CGD-CBD | -2.16 | 120.26      | 124.52   |
| 22  | A     | 840  | CLA  | CHA-C1A-NA  | -2.16 | 121.51      | 126.39   |
| 22  | 4     | 807  | CLA  | CMD-C2D-C3D | -2.16 | 122.74      | 127.69   |
| 22  | 7     | 307  | CLA  | C6-C5-C3    | -2.16 | 108.22      | 113.47   |
| 22  | B     | 805  | CLA  | CHD-C1D-ND  | -2.16 | 121.77      | 124.80   |
| 22  | 5     | 322  | CLA  | CHD-C1D-ND  | -2.16 | 121.77      | 124.80   |
| 38  | Z     | 301  | LUT  | C8-C7-C6    | -2.16 | 121.24      | 127.00   |
| 39  | 6     | 318  | CHL  | CMA-C3A-C2A | 2.16  | 122.45      | 114.13   |
| 22  | B     | 817  | CLA  | O1D-CGD-CBD | -2.16 | 120.27      | 124.52   |
| 22  | B     | 840  | CLA  | CHA-C1A-NA  | -2.16 | 121.51      | 126.39   |
| 22  | 3     | 312  | CLA  | CHD-C1D-ND  | -2.15 | 121.77      | 124.80   |
| 22  | 2     | 304  | CLA  | CHD-C1D-ND  | -2.15 | 121.77      | 124.80   |
| 22  | B     | 837  | CLA  | CHD-C1D-ND  | -2.15 | 121.77      | 124.80   |
| 22  | B     | 810  | CLA  | CAA-CBA-CGA | -2.15 | 107.09      | 113.21   |
| 24  | 3     | 305  | BCR  | C23-C24-C25 | -2.15 | 121.24      | 127.00   |
| 22  | A     | 835  | CLA  | CHA-C1A-NA  | -2.15 | 121.51      | 126.39   |
| 24  | L     | 204  | BCR  | C29-C30-C25 | 2.15  | 113.57      | 110.44   |
| 22  | A     | 833  | CLA  | CHA-C1A-NA  | -2.15 | 121.52      | 126.39   |
| 22  | A     | 827  | CLA  | O1D-CGD-CBD | -2.15 | 120.27      | 124.52   |
| 22  | A     | 821  | CLA  | C2D-C1D-ND  | 2.15  | 112.26      | 110.13   |
| 22  | 7     | 317  | CLA  | CHA-C1A-NA  | -2.15 | 121.52      | 126.39   |
| 25  | 4     | 820  | LHG  | O7-C7-O9    | -2.15 | 118.67      | 123.70   |
| 22  | Z     | 313  | CLA  | O1D-CGD-CBD | -2.15 | 120.27      | 124.52   |
| 32  | F     | 306  | RRX  | C36-C18-C17 | -2.15 | 119.33      | 122.82   |
| 38  | 9     | 302  | LUT  | C30-C31-C32 | -2.15 | 116.97      | 123.20   |
| 39  | Z     | 311  | CHL  | C4D-CHA-CBD | -2.15 | 106.80      | 108.97   |
| 24  | I     | 4001 | BCR  | C36-C18-C17 | -2.15 | 119.33      | 122.82   |
| 22  | 1     | 305  | CLA  | OBD-CAD-C3D | -2.15 | 123.39      | 128.42   |
| 22  | 3     | 311  | CLA  | O1D-CGD-CBD | -2.15 | 120.28      | 124.52   |
| 22  | 5     | 308  | CLA  | O1D-CGD-CBD | -2.15 | 120.28      | 124.52   |
| 22  | B     | 811  | CLA  | CHD-C1D-ND  | -2.15 | 121.78      | 124.80   |
| 22  | 7     | 310  | CLA  | CHD-C1D-ND  | -2.15 | 121.78      | 124.80   |
| 22  | 3     | 311  | CLA  | CHA-C1A-NA  | -2.15 | 121.52      | 126.39   |
| 22  | Z     | 307  | CLA  | C2D-C1D-ND  | 2.15  | 112.25      | 110.13   |
| 22  | 7     | 317  | CLA  | C2D-C1D-ND  | 2.15  | 112.25      | 110.13   |
| 24  | 3     | 306  | BCR  | C2-C1-C6    | 2.15  | 113.56      | 110.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 7     | 306 | CLA  | CMD-C2D-C3D | -2.15 | 122.76      | 127.69   |
| 22  | A     | 821 | CLA  | CHA-C1A-NA  | -2.15 | 121.53      | 126.39   |
| 22  | B     | 836 | CLA  | CHA-C1A-NA  | -2.15 | 121.53      | 126.39   |
| 22  | B     | 839 | CLA  | C2D-C1D-ND  | 2.15  | 112.25      | 110.13   |
| 24  | 6     | 305 | BCR  | C21-C20-C19 | -2.15 | 116.98      | 123.20   |
| 22  | 7     | 309 | CLA  | CAA-CBA-CGA | -2.15 | 107.11      | 113.21   |
| 24  | 5     | 305 | BCR  | C10-C11-C12 | -2.15 | 116.98      | 123.20   |
| 22  | A     | 816 | CLA  | C2D-C1D-ND  | 2.15  | 112.25      | 110.13   |
| 39  | 9     | 312 | CHL  | CMD-C2D-C3D | 2.15  | 128.97      | 124.68   |
| 22  | K     | 202 | CLA  | O1D-CGD-CBD | -2.15 | 120.29      | 124.52   |
| 22  | A     | 829 | CLA  | CHA-C1A-NA  | -2.15 | 121.53      | 126.39   |
| 22  | A     | 854 | CLA  | CHA-C1A-NA  | -2.15 | 121.53      | 126.39   |
| 22  | B     | 820 | CLA  | CHA-C1A-NA  | -2.15 | 121.53      | 126.39   |
| 22  | F     | 302 | CLA  | CHD-C1D-ND  | -2.14 | 121.78      | 124.80   |
| 33  | G     | 204 | LMT  | C1B-O1B-C4' | -2.14 | 112.89      | 117.98   |
| 22  | A     | 813 | CLA  | C2D-C1D-ND  | 2.14  | 112.25      | 110.13   |
| 22  | 3     | 322 | CLA  | C2D-C1D-ND  | 2.14  | 112.25      | 110.13   |
| 38  | 7     | 302 | LUT  | C15-C35-C34 | -2.14 | 119.13      | 123.52   |
| 22  | 6     | 301 | CLA  | O1D-CGD-CBD | -2.14 | 120.29      | 124.52   |
| 22  | F     | 302 | CLA  | CHA-C1A-NA  | -2.14 | 121.54      | 126.39   |
| 22  | 3     | 309 | CLA  | CHA-C1A-NA  | -2.14 | 121.54      | 126.39   |
| 39  | 9     | 312 | CHL  | CMA-C3A-C2A | 2.14  | 122.41      | 114.13   |
| 22  | 5     | 310 | CLA  | C2D-C1D-ND  | 2.14  | 112.25      | 110.13   |
| 22  | 2     | 301 | CLA  | C6-C5-C3    | -2.14 | 108.25      | 113.47   |
| 22  | 6     | 319 | CLA  | CHA-C1A-NA  | -2.14 | 121.54      | 126.39   |
| 22  | 8     | 316 | CLA  | C2D-C1D-ND  | 2.14  | 112.25      | 110.13   |
| 22  | 7     | 308 | CLA  | CHA-C1A-NA  | -2.14 | 121.54      | 126.39   |
| 22  | 3     | 313 | CLA  | O2A-CGA-CBA | 2.14  | 118.36      | 111.83   |
| 38  | 5     | 303 | LUT  | C8-C7-C6    | -2.14 | 121.28      | 127.00   |
| 22  | B     | 824 | CLA  | C3D-C2D-C1D | -2.14 | 102.91      | 105.83   |
| 22  | 5     | 308 | CLA  | C3D-C2D-C1D | -2.14 | 102.91      | 105.83   |
| 22  | B     | 821 | CLA  | C2D-C1D-ND  | 2.14  | 112.25      | 110.13   |
| 22  | B     | 826 | CLA  | C2D-C1D-ND  | 2.14  | 112.25      | 110.13   |
| 39  | 8     | 301 | CHL  | C4D-CHA-CBD | -2.14 | 106.81      | 108.97   |
| 24  | 3     | 307 | BCR  | C30-C25-C24 | 2.14  | 121.45      | 115.65   |
| 22  | B     | 815 | CLA  | C2D-C1D-ND  | 2.14  | 112.24      | 110.13   |
| 22  | 1     | 315 | CLA  | C2D-C1D-ND  | 2.14  | 112.24      | 110.13   |
| 22  | 8     | 306 | CLA  | C2D-C1D-ND  | 2.14  | 112.24      | 110.13   |
| 39  | Z     | 312 | CHL  | CMA-C3A-C2A | 2.14  | 122.39      | 114.13   |
| 22  | B     | 801 | CLA  | CMD-C2D-C3D | -2.14 | 122.78      | 127.69   |
| 22  | B     | 822 | CLA  | CMD-C2D-C3D | -2.14 | 122.78      | 127.69   |
| 22  | G     | 201 | CLA  | O2A-CGA-CBA | 2.14  | 118.36      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | 5     | 305 | BCR  | C29-C30-C25 | 2.14  | 113.55      | 110.44   |
| 22  | 3     | 316 | CLA  | CHA-C1A-NA  | -2.14 | 121.55      | 126.39   |
| 22  | 1     | 315 | CLA  | CHA-C1A-NA  | -2.14 | 121.55      | 126.39   |
| 22  | B     | 814 | CLA  | C2D-C1D-ND  | 2.14  | 112.24      | 110.13   |
| 22  | A     | 855 | CLA  | CHA-C1A-NA  | -2.14 | 121.55      | 126.39   |
| 38  | 8     | 302 | LUT  | C27-C28-C29 | -2.14 | 121.72      | 126.32   |
| 22  | 9     | 311 | CLA  | CHD-C1D-ND  | -2.14 | 121.79      | 124.80   |
| 22  | B     | 820 | CLA  | O1D-CGD-CBD | -2.14 | 120.30      | 124.52   |
| 22  | B     | 819 | CLA  | O1D-CGD-CBD | -2.14 | 120.30      | 124.52   |
| 22  | 6     | 301 | CLA  | CHA-C1A-NA  | -2.14 | 121.55      | 126.39   |
| 22  | B     | 816 | CLA  | CHA-C1A-NA  | -2.14 | 121.55      | 126.39   |
| 22  | 3     | 308 | CLA  | C2D-C1D-ND  | 2.14  | 112.24      | 110.13   |
| 23  | A     | 843 | PQN  | C12-C11-C3  | -2.13 | 106.82      | 112.08   |
| 22  | 1     | 314 | CLA  | C2D-C1D-ND  | 2.13  | 112.24      | 110.13   |
| 22  | 5     | 322 | CLA  | CMD-C2D-C3D | -2.13 | 122.79      | 127.69   |
| 22  | 3     | 308 | CLA  | O2D-CGD-O1D | -2.13 | 119.69      | 123.85   |
| 22  | 5     | 326 | CLA  | C3D-C2D-C1D | -2.13 | 102.92      | 105.83   |
| 22  | 6     | 312 | CLA  | O1D-CGD-CBD | -2.13 | 120.31      | 124.52   |
| 22  | A     | 842 | CLA  | CHA-C1A-NA  | -2.13 | 121.56      | 126.39   |
| 22  | K     | 202 | CLA  | CHA-C1A-NA  | -2.13 | 121.56      | 126.39   |
| 22  | 9     | 306 | CLA  | CHA-C1A-NA  | -2.13 | 121.56      | 126.39   |
| 22  | 5     | 314 | CLA  | CHD-C1D-ND  | -2.13 | 121.80      | 124.80   |
| 22  | 8     | 310 | CLA  | CAA-C2A-C3A | -2.13 | 107.23      | 113.00   |
| 22  | 7     | 307 | CLA  | C2D-C1D-ND  | 2.13  | 112.24      | 110.13   |
| 22  | 8     | 311 | CLA  | CHD-C1D-ND  | -2.13 | 121.80      | 124.80   |
| 22  | B     | 841 | CLA  | CMD-C2D-C3D | -2.13 | 122.80      | 127.69   |
| 22  | 7     | 323 | CLA  | C1-O2A-CGA  | 2.13  | 121.81      | 116.65   |
| 22  | 6     | 321 | CLA  | CHA-C1A-NA  | -2.13 | 121.56      | 126.39   |
| 22  | A     | 842 | CLA  | C2D-C1D-ND  | 2.13  | 112.23      | 110.13   |
| 22  | B     | 838 | CLA  | C2D-C1D-ND  | 2.13  | 112.23      | 110.13   |
| 22  | 6     | 314 | CLA  | C2D-C1D-ND  | 2.13  | 112.23      | 110.13   |
| 22  | 7     | 324 | CLA  | CHA-C1A-NA  | -2.13 | 121.57      | 126.39   |
| 22  | 1     | 304 | CLA  | CHA-C1A-NA  | -2.13 | 121.57      | 126.39   |
| 22  | B     | 806 | CLA  | C2D-C1D-ND  | 2.13  | 112.23      | 110.13   |
| 22  | B     | 842 | CLA  | C2D-C1D-ND  | 2.13  | 112.23      | 110.13   |
| 22  | Z     | 308 | CLA  | O2A-CGA-CBA | 2.13  | 118.33      | 111.83   |
| 22  | B     | 812 | CLA  | CHA-C1A-NA  | -2.13 | 121.57      | 126.39   |
| 22  | 4     | 810 | CLA  | CHA-C1A-NA  | -2.13 | 121.57      | 126.39   |
| 22  | A     | 804 | CLA  | CHD-C1D-ND  | -2.13 | 121.81      | 124.80   |
| 38  | 5     | 303 | LUT  | C15-C35-C34 | -2.13 | 119.16      | 123.52   |
| 36  | J     | 105 | C7Z  | C4-C5-C6    | -2.13 | 116.39      | 120.76   |
| 22  | B     | 811 | CLA  | CHA-C1A-NA  | -2.13 | 121.57      | 126.39   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 9     | 308 | CLA  | CHA-C1A-NA  | -2.13 | 121.57      | 126.39   |
| 39  | 4     | 813 | CHL  | CMA-C3A-C4A | 2.13  | 119.20      | 114.61   |
| 22  | 7     | 317 | CLA  | O2D-CGD-O1D | -2.13 | 119.71      | 123.85   |
| 22  | 6     | 311 | CLA  | C2D-C1D-ND  | 2.13  | 112.23      | 110.13   |
| 22  | B     | 815 | CLA  | O1D-CGD-CBD | -2.13 | 120.32      | 124.52   |
| 22  | A     | 819 | CLA  | O2A-CGA-CBA | 2.13  | 118.32      | 111.83   |
| 22  | K     | 205 | CLA  | C1C-C2C-C3C | -2.13 | 104.74      | 106.98   |
| 38  | 6     | 303 | LUT  | C39-C29-C28 | 2.13  | 121.34      | 118.09   |
| 22  | A     | 822 | CLA  | CHD-C1D-ND  | -2.13 | 121.81      | 124.80   |
| 22  | A     | 818 | CLA  | O1D-CGD-CBD | -2.13 | 120.33      | 124.52   |
| 22  | B     | 828 | CLA  | C3D-C2D-C1D | -2.13 | 102.93      | 105.83   |
| 22  | B     | 823 | CLA  | O1D-CGD-CBD | -2.13 | 120.33      | 124.52   |
| 22  | 6     | 302 | CLA  | CHA-C1A-NA  | -2.13 | 121.58      | 126.39   |
| 22  | 9     | 307 | CLA  | CHA-C1A-NA  | -2.12 | 121.58      | 126.39   |
| 22  | 9     | 313 | CLA  | CMD-C2D-C3D | -2.12 | 122.82      | 127.69   |
| 22  | A     | 824 | CLA  | O2A-CGA-CBA | 2.12  | 118.31      | 111.83   |
| 22  | 3     | 311 | CLA  | C6-C5-C3    | -2.12 | 108.30      | 113.47   |
| 22  | B     | 833 | CLA  | CHA-C1A-NA  | -2.12 | 121.58      | 126.39   |
| 22  | 9     | 307 | CLA  | CHD-C1D-ND  | -2.12 | 121.81      | 124.80   |
| 38  | 1     | 302 | LUT  | C30-C31-C32 | -2.12 | 117.05      | 123.20   |
| 22  | B     | 812 | CLA  | C2D-C1D-ND  | 2.12  | 112.23      | 110.13   |
| 22  | F     | 305 | CLA  | C2D-C1D-ND  | 2.12  | 112.23      | 110.13   |
| 22  | A     | 835 | CLA  | O1D-CGD-CBD | -2.12 | 120.33      | 124.52   |
| 22  | B     | 818 | CLA  | O1D-CGD-CBD | -2.12 | 120.33      | 124.52   |
| 22  | B     | 819 | CLA  | CHA-C1A-NA  | -2.12 | 121.58      | 126.39   |
| 22  | 7     | 311 | CLA  | CHA-C1A-NA  | -2.12 | 121.58      | 126.39   |
| 22  | 5     | 308 | CLA  | CHA-C1A-NA  | -2.12 | 121.58      | 126.39   |
| 22  | 2     | 304 | CLA  | O1D-CGD-CBD | -2.12 | 120.33      | 124.52   |
| 22  | B     | 807 | CLA  | CHA-C1A-NA  | -2.12 | 121.59      | 126.39   |
| 22  | 9     | 313 | CLA  | CHA-C1A-NA  | -2.12 | 121.59      | 126.39   |
| 24  | 3     | 304 | BCR  | C20-C21-C22 | -2.12 | 124.31      | 127.28   |
| 22  | 5     | 319 | CLA  | CHA-C1A-NA  | -2.12 | 121.59      | 126.39   |
| 22  | 7     | 310 | CLA  | O2A-CGA-CBA | 2.12  | 118.30      | 111.83   |
| 22  | 1     | 313 | CLA  | CHA-C1A-NA  | -2.12 | 121.59      | 126.39   |
| 22  | Z     | 310 | CLA  | O2D-CGD-O1D | -2.12 | 119.72      | 123.85   |
| 22  | A     | 802 | CLA  | CHA-C1A-NA  | -2.12 | 121.59      | 126.39   |
| 22  | B     | 815 | CLA  | CHA-C1A-NA  | -2.12 | 121.59      | 126.39   |
| 22  | B     | 822 | CLA  | CHD-C1D-ND  | -2.12 | 121.82      | 124.80   |
| 22  | 9     | 306 | CLA  | O1D-CGD-CBD | -2.12 | 120.34      | 124.52   |
| 22  | L     | 202 | CLA  | O2A-CGA-CBA | 2.12  | 118.29      | 111.83   |
| 38  | 1     | 302 | LUT  | C27-C28-C29 | -2.12 | 121.77      | 126.32   |
| 22  | A     | 807 | CLA  | CHA-C1A-NA  | -2.12 | 121.60      | 126.39   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | G     | 201  | CLA  | C3D-C2D-C1D | -2.12 | 102.94      | 105.83   |
| 39  | 6     | 318  | CHL  | C1-O2A-CGA  | 2.12  | 121.78      | 116.65   |
| 24  | 5     | 305  | BCR  | C7-C8-C9    | -2.12 | 123.10      | 126.23   |
| 22  | A     | 824  | CLA  | CHA-C1A-NA  | -2.12 | 121.60      | 126.39   |
| 22  | 4     | 809  | CLA  | CHD-C1D-ND  | -2.12 | 121.83      | 124.80   |
| 22  | 5     | 313  | CLA  | C2D-C1D-ND  | 2.12  | 112.22      | 110.13   |
| 22  | Z     | 305  | CLA  | O1D-CGD-CBD | -2.12 | 120.34      | 124.52   |
| 22  | 3     | 315  | CLA  | OBD-CAD-C3D | -2.11 | 123.47      | 128.42   |
| 22  | A     | 840  | CLA  | C2D-C1D-ND  | 2.11  | 112.22      | 110.13   |
| 22  | Z     | 315  | CLA  | C2D-C1D-ND  | 2.11  | 112.22      | 110.13   |
| 22  | A     | 827  | CLA  | C1-O2A-CGA  | 2.11  | 121.77      | 116.65   |
| 22  | B     | 805  | CLA  | CHA-C1A-NA  | -2.11 | 121.60      | 126.39   |
| 22  | B     | 822  | CLA  | O1D-CGD-CBD | -2.11 | 120.35      | 124.52   |
| 22  | K     | 204  | CLA  | O1D-CGD-CBD | -2.11 | 120.35      | 124.52   |
| 38  | 6     | 303  | LUT  | C31-C30-C29 | -2.11 | 124.31      | 127.28   |
| 22  | 3     | 313  | CLA  | C3D-C2D-C1D | -2.11 | 102.95      | 105.83   |
| 22  | 6     | 310  | CLA  | O1D-CGD-CBD | -2.11 | 120.35      | 124.52   |
| 22  | 5     | 326  | CLA  | O1D-CGD-CBD | -2.11 | 120.35      | 124.52   |
| 39  | 9     | 314  | CHL  | CMD-C2D-C3D | 2.11  | 128.91      | 124.68   |
| 22  | 7     | 308  | CLA  | CHD-C1D-ND  | -2.11 | 121.83      | 124.80   |
| 24  | I     | 4001 | BCR  | C10-C11-C12 | -2.11 | 117.08      | 123.20   |
| 38  | 7     | 302  | LUT  | C8-C7-C6    | -2.11 | 121.36      | 127.00   |
| 22  | B     | 813  | CLA  | CHA-C1A-NA  | -2.11 | 121.61      | 126.39   |
| 22  | B     | 809  | CLA  | C2D-C1D-ND  | 2.11  | 112.22      | 110.13   |
| 24  | 5     | 305  | BCR  | C7-C6-C5    | -2.11 | 116.69      | 121.56   |
| 21  | A     | 801  | CL0  | C4C-C3C-C2C | -2.11 | 105.03      | 113.37   |
| 24  | A     | 847  | BCR  | C38-C26-C27 | 2.11  | 118.10      | 113.60   |
| 22  | Z     | 305  | CLA  | CHD-C1D-ND  | -2.11 | 121.83      | 124.80   |
| 22  | A     | 837  | CLA  | O2A-CGA-CBA | 2.11  | 118.27      | 111.83   |
| 22  | B     | 805  | CLA  | CMD-C2D-C3D | -2.11 | 122.85      | 127.69   |
| 22  | 9     | 309  | CLA  | CHA-C1A-NA  | -2.11 | 121.61      | 126.39   |
| 22  | B     | 822  | CLA  | CHA-C1A-NA  | -2.11 | 121.61      | 126.39   |
| 22  | B     | 811  | CLA  | CAA-C2A-C3A | -2.11 | 107.30      | 113.00   |
| 22  | B     | 821  | CLA  | CHA-C1A-NA  | -2.11 | 121.61      | 126.39   |
| 22  | 4     | 811  | CLA  | CMD-C2D-C3D | -2.11 | 122.85      | 127.69   |
| 22  | A     | 814  | CLA  | O1D-CGD-CBD | -2.11 | 120.36      | 124.52   |
| 22  | A     | 810  | CLA  | CHA-C1A-NA  | -2.11 | 121.61      | 126.39   |
| 22  | 5     | 311  | CLA  | C3D-C2D-C1D | -2.11 | 102.95      | 105.83   |
| 22  | A     | 841  | CLA  | C1-O2A-CGA  | 2.11  | 121.75      | 116.65   |
| 22  | B     | 820  | CLA  | C2D-C1D-ND  | 2.11  | 112.21      | 110.13   |
| 22  | 6     | 322  | CLA  | C2D-C1D-ND  | 2.11  | 112.21      | 110.13   |
| 22  | A     | 837  | CLA  | CHA-C1A-NA  | -2.11 | 121.62      | 126.39   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | A     | 831 | CLA  | O1D-CGD-CBD | -2.11 | 120.36      | 124.52   |
| 39  | 8     | 312 | CHL  | CMA-C3A-C2A | 2.11  | 122.27      | 114.13   |
| 39  | 5     | 316 | CHL  | C1-O2A-CGA  | 2.11  | 121.75      | 116.65   |
| 38  | 3     | 303 | LUT  | C40-C33-C32 | 2.11  | 121.31      | 118.09   |
| 22  | 7     | 315 | CLA  | CHA-C1A-NA  | -2.11 | 121.62      | 126.39   |
| 22  | A     | 804 | CLA  | C2D-C1D-ND  | 2.11  | 112.21      | 110.13   |
| 22  | 6     | 307 | CLA  | CHA-C1A-NA  | -2.11 | 121.62      | 126.39   |
| 22  | F     | 301 | CLA  | CHA-C1A-NA  | -2.11 | 121.62      | 126.39   |
| 22  | K     | 203 | CLA  | O2A-CGA-CBA | 2.11  | 118.26      | 111.83   |
| 22  | Z     | 309 | CLA  | CHD-C1D-ND  | -2.11 | 121.84      | 124.80   |
| 22  | A     | 833 | CLA  | O1D-CGD-CBD | -2.11 | 120.36      | 124.52   |
| 22  | 1     | 313 | CLA  | C3D-C2D-C1D | -2.11 | 102.96      | 105.83   |
| 39  | 1     | 312 | CHL  | CMA-C3A-C2A | 2.10  | 122.26      | 114.13   |
| 22  | 7     | 317 | CLA  | C6-C5-C3    | -2.10 | 108.34      | 113.47   |
| 22  | 2     | 301 | CLA  | C2D-C1D-ND  | 2.10  | 112.21      | 110.13   |
| 22  | B     | 811 | CLA  | O2A-CGA-CBA | 2.10  | 118.25      | 111.83   |
| 24  | 3     | 304 | BCR  | C11-C12-C13 | 2.10  | 132.13      | 126.36   |
| 39  | 8     | 301 | CHL  | C4C-CHD-C1D | 2.10  | 123.60      | 116.07   |
| 22  | 4     | 810 | CLA  | CAA-CBA-CGA | -2.10 | 107.23      | 113.21   |
| 22  | 4     | 811 | CLA  | CHD-C1D-ND  | -2.10 | 121.84      | 124.80   |
| 22  | 1     | 316 | CLA  | CMA-C3A-C4A | 2.10  | 117.43      | 111.77   |
| 22  | A     | 838 | CLA  | O1D-CGD-CBD | -2.10 | 120.37      | 124.52   |
| 22  | A     | 803 | CLA  | CHA-C1A-NA  | -2.10 | 121.63      | 126.39   |
| 22  | 7     | 309 | CLA  | C3D-C2D-C1D | -2.10 | 102.96      | 105.83   |
| 22  | 5     | 313 | CLA  | CAA-C2A-C3A | -2.10 | 107.32      | 113.00   |
| 22  | A     | 834 | CLA  | CHA-C1A-NA  | -2.10 | 121.63      | 126.39   |
| 22  | B     | 835 | CLA  | CHA-C1A-NA  | -2.10 | 121.63      | 126.39   |
| 22  | L     | 202 | CLA  | O1D-CGD-CBD | -2.10 | 120.37      | 124.52   |
| 22  | B     | 806 | CLA  | C6-C5-C3    | -2.10 | 108.35      | 113.47   |
| 22  | A     | 815 | CLA  | CHA-C1A-NA  | -2.10 | 121.63      | 126.39   |
| 22  | 6     | 322 | CLA  | CHA-C1A-NA  | -2.10 | 121.63      | 126.39   |
| 22  | 6     | 307 | CLA  | C2D-C1D-ND  | 2.10  | 112.20      | 110.13   |
| 22  | B     | 837 | CLA  | O1D-CGD-CBD | -2.10 | 120.38      | 124.52   |
| 22  | 9     | 305 | CLA  | CMD-C2D-C3D | -2.10 | 122.87      | 127.69   |
| 22  | B     | 826 | CLA  | CHA-C1A-NA  | -2.10 | 121.64      | 126.39   |
| 22  | Z     | 316 | CLA  | CHA-C1A-NA  | -2.10 | 121.64      | 126.39   |
| 22  | 8     | 311 | CLA  | CMD-C2D-C3D | -2.10 | 122.87      | 127.69   |
| 22  | A     | 841 | CLA  | CHA-C1A-NA  | -2.10 | 121.64      | 126.39   |
| 22  | L     | 201 | CLA  | CHA-C1A-NA  | -2.10 | 121.64      | 126.39   |
| 22  | 4     | 817 | CLA  | CHA-C1A-NA  | -2.10 | 121.64      | 126.39   |
| 22  | B     | 841 | CLA  | C6-C5-C3    | -2.10 | 108.35      | 113.47   |
| 39  | 5     | 316 | CHL  | CMD-C2D-C3D | 2.10  | 128.88      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 4     | 807 | CLA  | CHD-C1D-ND  | -2.10 | 121.85      | 124.80   |
| 22  | 4     | 810 | CLA  | O1D-CGD-CBD | -2.10 | 120.38      | 124.52   |
| 22  | A     | 805 | CLA  | O1D-CGD-CBD | -2.10 | 120.38      | 124.52   |
| 22  | 5     | 307 | CLA  | C2D-C1D-ND  | 2.10  | 112.20      | 110.13   |
| 39  | 6     | 315 | CHL  | CMA-C3A-C2A | 2.10  | 122.23      | 114.13   |
| 22  | 1     | 305 | CLA  | O1D-CGD-CBD | -2.10 | 120.38      | 124.52   |
| 38  | 1     | 302 | LUT  | C38-C25-C24 | -2.10 | 118.40      | 123.36   |
| 22  | F     | 302 | CLA  | C3D-C2D-C1D | -2.10 | 102.97      | 105.83   |
| 22  | 5     | 307 | CLA  | CHA-C1A-NA  | -2.10 | 121.65      | 126.39   |
| 22  | Z     | 303 | CLA  | C3D-C2D-C1D | -2.09 | 102.97      | 105.83   |
| 22  | 7     | 322 | CLA  | C3D-C2D-C1D | -2.09 | 102.97      | 105.83   |
| 24  | B     | 847 | BCR  | C35-C13-C14 | -2.09 | 119.42      | 122.82   |
| 22  | 6     | 307 | CLA  | CHD-C1D-ND  | -2.09 | 121.86      | 124.80   |
| 22  | A     | 806 | CLA  | C6-C5-C3    | -2.09 | 108.37      | 113.47   |
| 22  | B     | 836 | CLA  | O1D-CGD-CBD | -2.09 | 120.39      | 124.52   |
| 24  | 3     | 307 | BCR  | C34-C9-C10  | -2.09 | 119.42      | 122.82   |
| 22  | 4     | 812 | CLA  | C3D-C2D-C1D | -2.09 | 102.97      | 105.83   |
| 22  | A     | 829 | CLA  | CMD-C2D-C3D | -2.09 | 122.89      | 127.69   |
| 39  | 4     | 813 | CHL  | CMA-C3A-C2A | 2.09  | 122.21      | 114.13   |
| 22  | F     | 302 | CLA  | C6-C5-C3    | -2.09 | 108.37      | 113.47   |
| 22  | K     | 204 | CLA  | O2D-CGD-O1D | -2.09 | 119.77      | 123.85   |
| 22  | 1     | 305 | CLA  | C3D-C2D-C1D | -2.09 | 102.97      | 105.83   |
| 22  | L     | 202 | CLA  | CHA-C1A-NA  | -2.09 | 121.65      | 126.39   |
| 24  | 5     | 304 | BCR  | C1-C6-C7    | 2.09  | 121.33      | 115.65   |
| 22  | 5     | 301 | CLA  | CHA-C1A-NA  | -2.09 | 121.65      | 126.39   |
| 22  | 7     | 309 | CLA  | CHA-C1A-NA  | -2.09 | 121.65      | 126.39   |
| 22  | 6     | 308 | CLA  | CMD-C2D-C3D | -2.09 | 122.89      | 127.69   |
| 22  | Z     | 314 | CLA  | CHA-C1A-NA  | -2.09 | 121.66      | 126.39   |
| 22  | 1     | 314 | CLA  | O1D-CGD-CBD | -2.09 | 120.39      | 124.52   |
| 33  | G     | 204 | LMT  | C1'-O5'-C5' | -2.09 | 109.64      | 113.72   |
| 22  | 1     | 305 | CLA  | CHA-C1A-NA  | -2.09 | 121.66      | 126.39   |
| 22  | A     | 829 | CLA  | CHD-C1D-ND  | -2.09 | 121.86      | 124.80   |
| 22  | Z     | 304 | CLA  | CHD-C1D-ND  | -2.09 | 121.86      | 124.80   |
| 22  | 5     | 326 | CLA  | CHD-C1D-ND  | -2.09 | 121.86      | 124.80   |
| 22  | A     | 830 | CLA  | CHA-C1A-NA  | -2.09 | 121.66      | 126.39   |
| 22  | B     | 841 | CLA  | CHA-C1A-NA  | -2.09 | 121.66      | 126.39   |
| 22  | A     | 818 | CLA  | C3D-C2D-C1D | -2.09 | 102.98      | 105.83   |
| 22  | B     | 830 | CLA  | CHD-C1D-ND  | -2.09 | 121.86      | 124.80   |
| 22  | 6     | 302 | CLA  | CHD-C1D-ND  | -2.09 | 121.86      | 124.80   |
| 24  | A     | 846 | BCR  | C11-C12-C13 | -2.09 | 120.64      | 126.36   |
| 22  | Z     | 309 | CLA  | CHA-C1A-NA  | -2.09 | 121.66      | 126.39   |
| 22  | A     | 811 | CLA  | C3D-C2D-C1D | -2.09 | 102.98      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 8     | 309 | CLA  | CHA-C1A-NA  | -2.09 | 121.66      | 126.39   |
| 22  | F     | 304 | CLA  | CHD-C1D-ND  | -2.09 | 121.86      | 124.80   |
| 22  | 9     | 305 | CLA  | C3D-C2D-C1D | -2.09 | 102.98      | 105.83   |
| 22  | B     | 831 | CLA  | CHA-C1A-NA  | -2.09 | 121.66      | 126.39   |
| 22  | 8     | 308 | CLA  | O1D-CGD-CBD | -2.09 | 120.40      | 124.52   |
| 22  | 4     | 809 | CLA  | C3D-C2D-C1D | -2.09 | 102.98      | 105.83   |
| 22  | 5     | 309 | CLA  | C3D-C2D-C1D | -2.09 | 102.98      | 105.83   |
| 22  | A     | 820 | CLA  | CHD-C1D-ND  | -2.09 | 121.87      | 124.80   |
| 22  | 5     | 310 | CLA  | CHA-C1A-NA  | -2.09 | 121.67      | 126.39   |
| 22  | A     | 819 | CLA  | C2D-C1D-ND  | 2.09  | 112.19      | 110.13   |
| 22  | B     | 815 | CLA  | CAC-C3C-C4C | 2.09  | 127.50      | 124.79   |
| 22  | G     | 201 | CLA  | O1D-CGD-CBD | -2.09 | 120.41      | 124.52   |
| 22  | 6     | 310 | CLA  | CHA-C1A-NA  | -2.09 | 121.67      | 126.39   |
| 22  | 8     | 310 | CLA  | CHA-C1A-NA  | -2.08 | 121.67      | 126.39   |
| 22  | 5     | 312 | CLA  | O2D-CGD-O1D | -2.08 | 119.79      | 123.85   |
| 22  | 4     | 807 | CLA  | C3D-C2D-C1D | -2.08 | 102.99      | 105.83   |
| 22  | 9     | 308 | CLA  | O2A-CGA-CBA | 2.08  | 118.19      | 111.83   |
| 22  | A     | 836 | CLA  | O2A-CGA-CBA | 2.08  | 118.19      | 111.83   |
| 22  | A     | 812 | CLA  | CHD-C1D-ND  | -2.08 | 121.87      | 124.80   |
| 22  | 3     | 309 | CLA  | C3D-C2D-C1D | -2.08 | 102.99      | 105.83   |
| 22  | 8     | 313 | CLA  | CHA-C1A-NA  | -2.08 | 121.67      | 126.39   |
| 22  | A     | 835 | CLA  | CMD-C2D-C3D | -2.08 | 122.91      | 127.69   |
| 22  | 7     | 305 | CLA  | CHA-C1A-NA  | -2.08 | 121.67      | 126.39   |
| 22  | 7     | 311 | CLA  | C3D-C2D-C1D | -2.08 | 102.99      | 105.83   |
| 39  | 8     | 315 | CHL  | CMD-C2D-C3D | 2.08  | 128.84      | 124.68   |
| 22  | 3     | 318 | CLA  | O1D-CGD-CBD | -2.08 | 120.41      | 124.52   |
| 39  | 8     | 312 | CHL  | CMD-C2D-C3D | 2.08  | 128.84      | 124.68   |
| 22  | B     | 831 | CLA  | O1D-CGD-CBD | -2.08 | 120.41      | 124.52   |
| 22  | Z     | 310 | CLA  | CMD-C2D-C3D | -2.08 | 122.92      | 127.69   |
| 22  | 8     | 314 | CLA  | CMD-C2D-C3D | -2.08 | 122.92      | 127.69   |
| 22  | A     | 822 | CLA  | C2D-C1D-ND  | 2.08  | 112.19      | 110.13   |
| 22  | 1     | 307 | CLA  | CHA-C1A-NA  | -2.08 | 121.68      | 126.39   |
| 38  | 8     | 303 | LUT  | C20-C13-C12 | 2.08  | 121.27      | 118.09   |
| 22  | A     | 825 | CLA  | O1D-CGD-CBD | -2.08 | 120.42      | 124.52   |
| 22  | F     | 302 | CLA  | CAA-CBA-CGA | -2.08 | 107.30      | 113.21   |
| 22  | B     | 836 | CLA  | C3D-C2D-C1D | -2.08 | 102.99      | 105.83   |
| 22  | 9     | 310 | CLA  | OBD-CAD-C3D | -2.08 | 123.56      | 128.42   |
| 22  | A     | 826 | CLA  | CHA-C1A-NA  | -2.08 | 121.68      | 126.39   |
| 22  | 1     | 313 | CLA  | O1D-CGD-CBD | -2.08 | 120.42      | 124.52   |
| 22  | B     | 823 | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |
| 22  | B     | 837 | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |
| 22  | 1     | 306 | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 1     | 314 | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |
| 22  | 1     | 310 | CLA  | CHD-C1D-ND  | -2.08 | 121.88      | 124.80   |
| 22  | 5     | 312 | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |
| 22  | 5     | 318 | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |
| 22  | 4     | 808 | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |
| 22  | 3     | 314 | CLA  | CMD-C2D-C3D | -2.08 | 122.93      | 127.69   |
| 39  | Z     | 312 | CHL  | CMD-C2D-C3D | 2.08  | 128.83      | 124.68   |
| 39  | 6     | 316 | CHL  | CMD-C2D-C3D | 2.08  | 128.83      | 124.68   |
| 22  | Z     | 306 | CLA  | CHA-C1A-NA  | -2.08 | 121.69      | 126.39   |
| 22  | A     | 839 | CLA  | CHA-C1A-NA  | -2.07 | 121.69      | 126.39   |
| 39  | 9     | 312 | CHL  | C4C-CHD-C1D | 2.07  | 123.49      | 116.07   |
| 24  | 3     | 306 | BCR  | C35-C13-C14 | -2.07 | 119.46      | 122.82   |
| 22  | B     | 808 | CLA  | CHA-C1A-NA  | -2.07 | 121.69      | 126.39   |
| 22  | B     | 830 | CLA  | O2D-CGD-O1D | -2.07 | 119.81      | 123.85   |
| 22  | A     | 832 | CLA  | CHA-C1A-NA  | -2.07 | 121.70      | 126.39   |
| 22  | 8     | 306 | CLA  | CHA-C1A-NA  | -2.07 | 121.70      | 126.39   |
| 22  | 5     | 311 | CLA  | CHD-C1D-ND  | -2.07 | 121.89      | 124.80   |
| 22  | 5     | 323 | CLA  | C3D-C2D-C1D | -2.07 | 103.00      | 105.83   |
| 38  | 6     | 304 | LUT  | C27-C28-C29 | -2.07 | 121.87      | 126.32   |
| 22  | A     | 838 | CLA  | CHA-C1A-NA  | -2.07 | 121.70      | 126.39   |
| 22  | A     | 833 | CLA  | C3D-C2D-C1D | -2.07 | 103.00      | 105.83   |
| 24  | A     | 848 | BCR  | C8-C7-C6    | -2.07 | 121.47      | 127.00   |
| 22  | A     | 837 | CLA  | O1D-CGD-CBD | -2.07 | 120.44      | 124.52   |
| 22  | B     | 819 | CLA  | C3D-C2D-C1D | -2.07 | 103.01      | 105.83   |
| 22  | B     | 816 | CLA  | C2D-C1D-ND  | 2.07  | 112.17      | 110.13   |
| 39  | 1     | 312 | CHL  | CMD-C2D-C3D | 2.07  | 128.82      | 124.68   |
| 22  | 7     | 314 | CLA  | CHA-C1A-NA  | -2.07 | 121.71      | 126.39   |
| 22  | 8     | 316 | CLA  | CHA-C1A-NA  | -2.07 | 121.71      | 126.39   |
| 22  | 1     | 314 | CLA  | O2D-CGD-O1D | -2.07 | 119.82      | 123.85   |
| 38  | 8     | 303 | LUT  | C11-C12-C13 | -2.07 | 120.69      | 126.36   |
| 22  | A     | 817 | CLA  | CHA-C1A-NA  | -2.07 | 121.71      | 126.39   |
| 22  | B     | 827 | CLA  | CHA-C1A-NA  | -2.07 | 121.71      | 126.39   |
| 39  | 6     | 315 | CHL  | CMD-C2D-C3D | 2.07  | 128.82      | 124.68   |
| 39  | 2     | 303 | CHL  | CMD-C2D-C3D | 2.07  | 128.82      | 124.68   |
| 22  | Z     | 308 | CLA  | O1D-CGD-CBD | -2.07 | 120.44      | 124.52   |
| 22  | 6     | 309 | CLA  | CHD-C1D-ND  | -2.07 | 121.89      | 124.80   |
| 22  | A     | 818 | CLA  | C1-O2A-CGA  | 2.07  | 121.66      | 116.65   |
| 22  | A     | 805 | CLA  | C6-C5-C3    | -2.07 | 108.43      | 113.47   |
| 22  | A     | 829 | CLA  | O2A-CGA-CBA | 2.07  | 118.14      | 111.83   |
| 22  | 4     | 806 | CLA  | C3D-C2D-C1D | -2.07 | 103.01      | 105.83   |
| 22  | A     | 834 | CLA  | O1D-CGD-CBD | -2.07 | 120.44      | 124.52   |
| 39  | 8     | 301 | CHL  | CMD-C2D-C3D | 2.07  | 128.81      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 6     | 317 | CLA  | O1D-CGD-CBD | -2.07 | 120.44      | 124.52   |
| 24  | 4     | 804 | BCR  | C21-C20-C19 | -2.07 | 117.21      | 123.20   |
| 22  | 8     | 314 | CLA  | O1D-CGD-CBD | -2.07 | 120.44      | 124.52   |
| 24  | A     | 845 | BCR  | C36-C18-C17 | -2.07 | 119.47      | 122.82   |
| 22  | 6     | 317 | CLA  | CHA-C1A-NA  | -2.07 | 121.71      | 126.39   |
| 22  | 3     | 320 | CLA  | CHD-C1D-ND  | -2.07 | 121.90      | 124.80   |
| 22  | A     | 829 | CLA  | O2D-CGD-O1D | -2.07 | 119.83      | 123.85   |
| 22  | B     | 838 | CLA  | O1D-CGD-CBD | -2.07 | 120.44      | 124.52   |
| 22  | 7     | 312 | CLA  | C3D-C2D-C1D | -2.06 | 103.01      | 105.83   |
| 22  | 3     | 310 | CLA  | CHD-C1D-ND  | -2.06 | 121.90      | 124.80   |
| 22  | 6     | 312 | CLA  | CAA-C2A-C3A | -2.06 | 107.42      | 113.00   |
| 24  | J     | 104 | BCR  | C16-C15-C14 | -2.06 | 119.30      | 123.52   |
| 38  | Z     | 302 | LUT  | C8-C7-C6    | -2.06 | 121.49      | 127.00   |
| 22  | 7     | 304 | CLA  | C3D-C2D-C1D | -2.06 | 103.02      | 105.83   |
| 22  | 5     | 314 | CLA  | CHA-C1A-NA  | -2.06 | 121.72      | 126.39   |
| 22  | B     | 824 | CLA  | O1D-CGD-CBD | -2.06 | 120.45      | 124.52   |
| 22  | B     | 813 | CLA  | C3D-C2D-C1D | -2.06 | 103.02      | 105.83   |
| 22  | F     | 305 | CLA  | CHA-C1A-NA  | -2.06 | 121.73      | 126.39   |
| 22  | A     | 841 | CLA  | O1D-CGD-CBD | -2.06 | 120.46      | 124.52   |
| 22  | 3     | 316 | CLA  | O1D-CGD-CBD | -2.06 | 120.46      | 124.52   |
| 22  | G     | 202 | CLA  | CHA-C1A-NA  | -2.06 | 121.73      | 126.39   |
| 22  | 2     | 304 | CLA  | CHA-C1A-NA  | -2.06 | 121.73      | 126.39   |
| 22  | Z     | 307 | CLA  | OBD-CAD-C3D | -2.06 | 123.60      | 128.42   |
| 22  | F     | 301 | CLA  | C3D-C2D-C1D | -2.06 | 103.02      | 105.83   |
| 22  | K     | 204 | CLA  | C3D-C2D-C1D | -2.06 | 103.02      | 105.83   |
| 22  | 8     | 309 | CLA  | C3D-C2D-C1D | -2.06 | 103.02      | 105.83   |
| 38  | 9     | 302 | LUT  | C27-C28-C29 | -2.06 | 121.89      | 126.32   |
| 39  | 3     | 317 | CHL  | C4C-CHD-C1D | 2.06  | 123.44      | 116.07   |
| 22  | B     | 822 | CLA  | O2A-CGA-CBA | 2.06  | 118.11      | 111.83   |
| 22  | 5     | 319 | CLA  | C3D-C2D-C1D | -2.06 | 103.02      | 105.83   |
| 22  | 3     | 314 | CLA  | CHD-C1D-ND  | -2.06 | 121.91      | 124.80   |
| 22  | 8     | 305 | CLA  | C2D-C1D-ND  | 2.06  | 112.16      | 110.13   |
| 22  | 3     | 318 | CLA  | C6-C7-C8    | -2.06 | 109.12      | 115.97   |
| 22  | 6     | 313 | CLA  | CHA-C1A-NA  | -2.06 | 121.73      | 126.39   |
| 22  | 6     | 314 | CLA  | CHA-C1A-NA  | -2.06 | 121.73      | 126.39   |
| 39  | 7     | 313 | CHL  | CMD-C2D-C3D | 2.06  | 128.79      | 124.68   |
| 24  | B     | 849 | BCR  | C8-C7-C6    | -2.06 | 121.50      | 127.00   |
| 22  | 9     | 307 | CLA  | C2D-C1D-ND  | 2.06  | 112.16      | 110.13   |
| 22  | A     | 806 | CLA  | CHA-C1A-NA  | -2.06 | 121.74      | 126.39   |
| 22  | 9     | 309 | CLA  | C1-O2A-CGA  | 2.06  | 121.63      | 116.65   |
| 39  | Z     | 311 | CHL  | CMA-C3A-C2A | 2.06  | 122.07      | 114.13   |
| 38  | 5     | 303 | LUT  | C22-C23-C24 | 2.06  | 114.24      | 111.18   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | A     | 844 | BCR  | C29-C30-C25 | 2.05  | 113.42      | 110.44   |
| 22  | F     | 302 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | 5     | 314 | CLA  | CMD-C2D-C3D | -2.05 | 122.98      | 127.69   |
| 39  | 5     | 316 | CHL  | CMA-C3A-C4A | 2.05  | 119.04      | 114.61   |
| 22  | A     | 833 | CLA  | C6-C5-C3    | -2.05 | 108.46      | 113.47   |
| 22  | 9     | 311 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | 9     | 309 | CLA  | C2A-C1A-CHA | 2.05  | 127.43      | 123.87   |
| 22  | Z     | 303 | CLA  | O2D-CGD-O1D | -2.05 | 119.85      | 123.85   |
| 24  | 7     | 303 | BCR  | C38-C26-C27 | 2.05  | 117.97      | 113.60   |
| 24  | B     | 847 | BCR  | C36-C18-C19 | 2.05  | 121.22      | 118.09   |
| 22  | 8     | 308 | CLA  | CHA-C1A-NA  | -2.05 | 121.74      | 126.39   |
| 22  | A     | 816 | CLA  | CHD-C1D-ND  | -2.05 | 121.91      | 124.80   |
| 22  | A     | 817 | CLA  | CHD-C1D-ND  | -2.05 | 121.91      | 124.80   |
| 22  | B     | 817 | CLA  | CHD-C1D-ND  | -2.05 | 121.91      | 124.80   |
| 22  | G     | 201 | CLA  | CHD-C1D-ND  | -2.05 | 121.91      | 124.80   |
| 22  | A     | 808 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | A     | 812 | CLA  | C3D-C2D-C1D | -2.05 | 103.03      | 105.83   |
| 39  | 3     | 317 | CHL  | CMD-C2D-C3D | 2.05  | 128.78      | 124.68   |
| 22  | 4     | 808 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | L     | 203 | CLA  | CHA-C1A-NA  | -2.05 | 121.75      | 126.39   |
| 39  | 4     | 814 | CHL  | CMD-C2D-C3D | 2.05  | 128.78      | 124.68   |
| 34  | F     | 308 | LMG  | O7-C8-C9    | 2.05  | 115.70      | 108.34   |
| 22  | B     | 830 | CLA  | CMD-C2D-C3D | -2.05 | 122.99      | 127.69   |
| 22  | 3     | 319 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | 6     | 309 | CLA  | C2D-C1D-ND  | 2.05  | 112.16      | 110.13   |
| 22  | A     | 839 | CLA  | O1D-CGD-CBD | -2.05 | 120.47      | 124.52   |
| 22  | Z     | 314 | CLA  | CMD-C2D-C3D | -2.05 | 122.99      | 127.69   |
| 22  | Z     | 310 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 22  | G     | 201 | CLA  | OBD-CAD-C3D | -2.05 | 123.63      | 128.42   |
| 22  | 5     | 301 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 22  | Z     | 303 | CLA  | CHA-C1A-NA  | -2.05 | 121.75      | 126.39   |
| 22  | 4     | 815 | CLA  | CHD-C1D-ND  | -2.05 | 121.92      | 124.80   |
| 22  | A     | 855 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 38  | 5     | 302 | LUT  | C15-C14-C13 | -2.05 | 124.41      | 127.28   |
| 22  | 5     | 313 | CLA  | CMD-C2D-C3D | -2.05 | 122.99      | 127.69   |
| 22  | 6     | 302 | CLA  | C6-C5-C3    | -2.05 | 108.48      | 113.47   |
| 22  | B     | 834 | CLA  | C3D-C2D-C1D | -2.05 | 103.04      | 105.83   |
| 22  | 5     | 322 | CLA  | C3D-C2D-C1D | -2.05 | 103.04      | 105.83   |
| 22  | 6     | 313 | CLA  | CMD-C2D-C3D | -2.05 | 123.00      | 127.69   |
| 22  | 4     | 809 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 39  | 6     | 320 | CHL  | CMD-C2D-C3D | 2.05  | 128.77      | 124.68   |
| 22  | A     | 834 | CLA  | C3D-C2D-C1D | -2.05 | 103.04      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | L     | 201 | CLA  | C3D-C2D-C1D | -2.05 | 103.04      | 105.83   |
| 22  | 9     | 311 | CLA  | C3D-C2D-C1D | -2.05 | 103.04      | 105.83   |
| 22  | A     | 802 | CLA  | O1D-CGD-CBD | -2.05 | 120.48      | 124.52   |
| 24  | A     | 845 | BCR  | C20-C19-C18 | -2.05 | 120.75      | 126.36   |
| 22  | B     | 830 | CLA  | CHA-C1A-NA  | -2.05 | 121.76      | 126.39   |
| 22  | 4     | 817 | CLA  | C3D-C2D-C1D | -2.05 | 103.04      | 105.83   |
| 38  | 8     | 302 | LUT  | C39-C29-C28 | 2.05  | 121.21      | 118.09   |
| 22  | K     | 203 | CLA  | C3D-C2D-C1D | -2.04 | 103.04      | 105.83   |
| 22  | B     | 817 | CLA  | CMD-C2D-C3D | -2.04 | 123.00      | 127.69   |
| 23  | A     | 843 | PQN  | C16-C17-C18 | -2.04 | 109.17      | 115.97   |
| 22  | B     | 834 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 38  | 9     | 302 | LUT  | C35-C15-C14 | -2.04 | 119.34      | 123.52   |
| 22  | Z     | 310 | CLA  | C3D-C2D-C1D | -2.04 | 103.04      | 105.83   |
| 39  | 5     | 316 | CHL  | C4C-CHD-C1D | 2.04  | 123.38      | 116.07   |
| 22  | Z     | 304 | CLA  | CHA-C1A-NA  | -2.04 | 121.77      | 126.39   |
| 22  | B     | 808 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 22  | 6     | 308 | CLA  | CHA-C1A-NA  | -2.04 | 121.77      | 126.39   |
| 38  | 7     | 301 | LUT  | C15-C35-C34 | -2.04 | 119.34      | 123.52   |
| 22  | 4     | 808 | CLA  | C3D-C2D-C1D | -2.04 | 103.05      | 105.83   |
| 22  | 2     | 302 | CLA  | C3D-C2D-C1D | -2.04 | 103.05      | 105.83   |
| 22  | B     | 806 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 22  | 6     | 321 | CLA  | O1D-CGD-CBD | -2.04 | 120.49      | 124.52   |
| 22  | B     | 805 | CLA  | C6-C5-C3    | -2.04 | 108.50      | 113.47   |
| 22  | 4     | 815 | CLA  | O1D-CGD-CBD | -2.04 | 120.50      | 124.52   |
| 22  | 8     | 307 | CLA  | CHD-C1D-ND  | -2.04 | 121.94      | 124.80   |
| 22  | A     | 819 | CLA  | CHA-C1A-NA  | -2.04 | 121.78      | 126.39   |
| 22  | A     | 819 | CLA  | C6-C5-C3    | -2.04 | 108.51      | 113.47   |
| 24  | A     | 845 | BCR  | C16-C15-C14 | -2.04 | 119.35      | 123.52   |
| 39  | 1     | 312 | CHL  | C1-O2A-CGA  | 2.04  | 122.45      | 116.67   |
| 39  | Z     | 311 | CHL  | CMD-C2D-C3D | 2.04  | 128.75      | 124.68   |
| 38  | 4     | 803 | LUT  | C15-C35-C34 | -2.04 | 119.36      | 123.52   |
| 22  | 5     | 301 | CLA  | C3D-C2D-C1D | -2.03 | 103.05      | 105.83   |
| 24  | 8     | 304 | BCR  | C15-C16-C17 | -2.03 | 119.36      | 123.52   |
| 38  | 6     | 304 | LUT  | C4-C5-C6    | -2.03 | 116.58      | 120.76   |
| 22  | 5     | 313 | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 22  | 6     | 317 | CLA  | CHD-C1D-ND  | -2.03 | 121.94      | 124.80   |
| 22  | 5     | 318 | CLA  | O2D-CGD-O1D | -2.03 | 119.89      | 123.85   |
| 22  | 2     | 304 | CLA  | O2A-CGA-CBA | 2.03  | 119.82      | 112.14   |
| 22  | B     | 842 | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 22  | A     | 809 | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 24  | A     | 845 | BCR  | C15-C16-C17 | -2.03 | 119.36      | 123.52   |
| 22  | 9     | 313 | CLA  | CAA-CBA-CGA | -2.03 | 107.44      | 113.21   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | B     | 833  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 22  | 3     | 308  | CLA  | CHA-C1A-NA  | -2.03 | 121.79      | 126.39   |
| 22  | A     | 807  | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 22  | 4     | 811  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 22  | 7     | 315  | CLA  | CHD-C1D-ND  | -2.03 | 121.94      | 124.80   |
| 22  | A     | 815  | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 22  | B     | 816  | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 22  | 5     | 311  | CLA  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 22  | 3     | 314  | CLA  | CHA-C1A-NA  | -2.03 | 121.79      | 126.39   |
| 22  | 1     | 304  | CLA  | O2D-CGD-O1D | -2.03 | 119.90      | 123.85   |
| 22  | G     | 202  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 39  | 4     | 813  | CHL  | CMD-C2D-C3D | 2.03  | 128.74      | 124.68   |
| 39  | 6     | 318  | CHL  | C4C-CHD-C1D | 2.03  | 123.33      | 116.07   |
| 39  | 4     | 813  | CHL  | C4C-CHD-C1D | 2.03  | 123.33      | 116.07   |
| 39  | 5     | 317  | CHL  | CMD-C2D-C3D | 2.03  | 128.74      | 124.68   |
| 22  | B     | 810  | CLA  | C6-C7-C8    | -2.03 | 109.22      | 115.97   |
| 22  | 3     | 312  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 22  | 4     | 807  | CLA  | O2A-CGA-CBA | 2.03  | 118.02      | 111.83   |
| 39  | 3     | 317  | CHL  | C1-O2A-CGA  | 2.03  | 121.56      | 116.65   |
| 24  | 4     | 804  | BCR  | C11-C12-C13 | -2.03 | 120.80      | 126.36   |
| 22  | B     | 823  | CLA  | C6-C5-C3    | -2.03 | 108.53      | 113.47   |
| 22  | 9     | 306  | CLA  | C1-O2A-CGA  | 2.03  | 121.56      | 116.65   |
| 22  | B     | 810  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 22  | G     | 202  | CLA  | O1D-CGD-CBD | -2.03 | 120.52      | 124.52   |
| 33  | 4     | 822  | LMT  | O5B-C5B-C4B | -2.03 | 106.05      | 109.70   |
| 22  | A     | 832  | CLA  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 39  | 4     | 816  | CHL  | CMD-C2D-C3D | 2.03  | 128.73      | 124.68   |
| 22  | 3     | 322  | CLA  | O1D-CGD-CBD | -2.03 | 120.52      | 124.52   |
| 38  | 7     | 302  | LUT  | C19-C9-C10  | -2.03 | 119.53      | 122.82   |
| 22  | 3     | 313  | CLA  | O2D-CGD-O1D | -2.03 | 119.90      | 123.85   |
| 24  | L     | 204  | BCR  | C21-C20-C19 | -2.03 | 117.33      | 123.20   |
| 39  | 4     | 816  | CHL  | C1-O2A-CGA  | 2.03  | 122.56      | 116.07   |
| 24  | I     | 4001 | BCR  | C16-C15-C14 | -2.03 | 119.38      | 123.52   |
| 22  | B     | 829  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | B     | 841  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 38  | 7     | 301  | LUT  | C30-C31-C32 | -2.02 | 117.33      | 123.20   |
| 22  | B     | 807  | CLA  | O1D-CGD-CBD | -2.02 | 120.53      | 124.52   |
| 22  | B     | 805  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | 3     | 318  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | 7     | 316  | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | A     | 807  | CLA  | O2A-CGA-CBA | 2.02  | 118.01      | 111.83   |
| 22  | 5     | 315  | CLA  | CHD-C1D-ND  | -2.02 | 121.95      | 124.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 39  | 6     | 318 | CHL  | CMD-C2D-C3D | 2.02  | 128.73      | 124.68   |
| 38  | 4     | 802 | LUT  | C30-C31-C32 | -2.02 | 117.34      | 123.20   |
| 22  | B     | 809 | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 22  | 5     | 323 | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 24  | 6     | 306 | BCR  | C34-C9-C10  | -2.02 | 119.54      | 122.82   |
| 22  | 5     | 309 | CLA  | O1D-CGD-CBD | -2.02 | 120.53      | 124.52   |
| 22  | 4     | 806 | CLA  | CHD-C1D-ND  | -2.02 | 121.96      | 124.80   |
| 22  | A     | 808 | CLA  | CHA-C1A-NA  | -2.02 | 121.81      | 126.39   |
| 24  | B     | 844 | BCR  | C8-C7-C6    | -2.02 | 121.60      | 127.00   |
| 22  | A     | 822 | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | B     | 827 | CLA  | O1D-CGD-CBD | -2.02 | 120.53      | 124.52   |
| 38  | Z     | 301 | LUT  | C30-C31-C32 | -2.02 | 117.35      | 123.20   |
| 22  | 7     | 310 | CLA  | C3D-C2D-C1D | -2.02 | 103.07      | 105.83   |
| 22  | B     | 832 | CLA  | CHA-C1A-NA  | -2.02 | 121.82      | 126.39   |
| 22  | Z     | 308 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 22  | 7     | 324 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 22  | 6     | 309 | CLA  | C2A-C1A-CHA | 2.02  | 127.37      | 123.87   |
| 22  | 5     | 315 | CLA  | O1D-CGD-CBD | -2.02 | 120.54      | 124.52   |
| 22  | B     | 825 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 42  | 7     | 321 | SPH  | C3-C4-C5    | -2.02 | 120.51      | 124.69   |
| 22  | 1     | 308 | CLA  | O1D-CGD-CBD | -2.02 | 120.54      | 124.52   |
| 22  | 1     | 313 | CLA  | OBD-CAD-C3D | -2.02 | 123.70      | 128.42   |
| 22  | A     | 836 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 22  | 7     | 323 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 22  | 9     | 306 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 22  | 4     | 818 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 22  | 5     | 309 | CLA  | C6-C5-C3    | -2.02 | 108.55      | 113.47   |
| 33  | 4     | 822 | LMT  | O1B-C1B-C2B | 2.02  | 113.05      | 108.09   |
| 24  | 8     | 304 | BCR  | C39-C30-C25 | -2.02 | 107.08      | 110.24   |
| 39  | 7     | 313 | CHL  | C4C-CHD-C1D | 2.02  | 123.28      | 116.07   |
| 22  | 3     | 313 | CLA  | CHA-C1A-NA  | -2.02 | 121.82      | 126.39   |
| 22  | A     | 825 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 22  | 6     | 310 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 39  | 5     | 317 | CHL  | C4C-CHD-C1D | 2.02  | 123.28      | 116.07   |
| 22  | A     | 818 | CLA  | CHA-C1A-NA  | -2.02 | 121.83      | 126.39   |
| 38  | 4     | 803 | LUT  | C30-C31-C32 | -2.02 | 117.36      | 123.20   |
| 22  | A     | 816 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 22  | B     | 828 | CLA  | O1D-CGD-CBD | -2.02 | 120.54      | 124.52   |
| 22  | F     | 305 | CLA  | O1D-CGD-CBD | -2.02 | 120.54      | 124.52   |
| 22  | 7     | 317 | CLA  | O1D-CGD-CBD | -2.02 | 120.54      | 124.52   |
| 22  | 6     | 317 | CLA  | CMD-C2D-C3D | -2.02 | 123.07      | 127.69   |
| 22  | B     | 833 | CLA  | O1D-CGD-CBD | -2.02 | 120.54      | 124.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | B     | 818 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 22  | J     | 103 | CLA  | C3D-C2D-C1D | -2.02 | 103.08      | 105.83   |
| 24  | 5     | 305 | BCR  | C30-C25-C26 | -2.02 | 119.88      | 122.64   |
| 22  | K     | 202 | CLA  | C3D-C2D-C1D | -2.01 | 103.08      | 105.83   |
| 22  | 6     | 312 | CLA  | C3D-C2D-C1D | -2.01 | 103.08      | 105.83   |
| 22  | B     | 814 | CLA  | CHA-C1A-NA  | -2.01 | 121.83      | 126.39   |
| 22  | K     | 203 | CLA  | O1D-CGD-CBD | -2.01 | 120.55      | 124.52   |
| 22  | 8     | 307 | CLA  | C3D-C2D-C1D | -2.01 | 103.08      | 105.83   |
| 38  | 8     | 302 | LUT  | C20-C13-C12 | 2.01  | 121.16      | 118.09   |
| 25  | 6     | 323 | LHG  | O7-C7-O9    | -2.01 | 119.00      | 123.70   |
| 22  | 1     | 306 | CLA  | C3D-C2D-C1D | -2.01 | 103.08      | 105.83   |
| 22  | 3     | 311 | CLA  | C3D-C2D-C1D | -2.01 | 103.08      | 105.83   |
| 39  | 6     | 320 | CHL  | CMA-C3A-C2A | 2.01  | 121.90      | 114.13   |
| 22  | 9     | 308 | CLA  | C3D-C2D-C1D | -2.01 | 103.08      | 105.83   |
| 22  | B     | 825 | CLA  | CHA-C1A-NA  | -2.01 | 121.84      | 126.39   |
| 24  | 3     | 307 | BCR  | C24-C25-C26 | -2.01 | 116.92      | 121.56   |
| 22  | A     | 814 | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | B     | 807 | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | Z     | 313 | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | 8     | 308 | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | 5     | 319 | CLA  | O1D-CGD-CBD | -2.01 | 120.55      | 124.52   |
| 22  | 6     | 308 | CLA  | O1D-CGD-CBD | -2.01 | 120.55      | 124.52   |
| 22  | 3     | 318 | CLA  | CHA-C1A-NA  | -2.01 | 121.84      | 126.39   |
| 22  | 6     | 319 | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | 4     | 807 | CLA  | O2D-CGD-O1D | -2.01 | 119.94      | 123.85   |
| 39  | 4     | 814 | CHL  | C4C-CHD-C1D | 2.01  | 123.26      | 116.07   |
| 22  | B     | 826 | CLA  | C16-C15-C13 | -2.01 | 109.29      | 115.97   |
| 22  | A     | 832 | CLA  | O1D-CGD-CBD | -2.01 | 120.56      | 124.52   |
| 39  | 5     | 321 | CHL  | CMD-C2D-C3D | 2.01  | 128.70      | 124.68   |
| 38  | 7     | 302 | LUT  | C30-C31-C32 | -2.01 | 117.38      | 123.20   |
| 38  | 3     | 303 | LUT  | C8-C7-C6    | -2.01 | 121.63      | 127.00   |
| 22  | 3     | 318 | CLA  | C11-C10-C8  | -2.01 | 109.29      | 115.97   |
| 22  | 3     | 313 | CLA  | O1D-CGD-CBD | -2.01 | 120.56      | 124.52   |
| 22  | 7     | 322 | CLA  | O1D-CGD-CBD | -2.01 | 120.56      | 124.52   |
| 22  | B     | 829 | CLA  | O1D-CGD-CBD | -2.01 | 120.56      | 124.52   |
| 22  | 7     | 310 | CLA  | CMD-C2D-C3D | -2.01 | 123.09      | 127.69   |
| 39  | 9     | 314 | CHL  | C4C-CHD-C1D | 2.01  | 123.25      | 116.07   |
| 22  | 7     | 323 | CLA  | CHA-C1A-NA  | -2.01 | 121.85      | 126.39   |
| 22  | B     | 808 | CLA  | C3D-C2D-C1D | -2.01 | 103.09      | 105.83   |
| 22  | 6     | 313 | CLA  | CHD-C1D-ND  | -2.00 | 121.98      | 124.80   |
| 22  | 5     | 315 | CLA  | C3D-C2D-C1D | -2.00 | 103.09      | 105.83   |
| 22  | B     | 809 | CLA  | O1D-CGD-CBD | -2.00 | 120.56      | 124.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | 4     | 815 | CLA  | CHA-C1A-NA  | -2.00 | 121.85      | 126.39   |
| 22  | B     | 827 | CLA  | C3D-C2D-C1D | -2.00 | 103.10      | 105.83   |
| 22  | 6     | 302 | CLA  | C3D-C2D-C1D | -2.00 | 103.10      | 105.83   |
| 22  | 1     | 316 | CLA  | C1D-ND-C4D  | -2.00 | 104.91      | 106.31   |
| 22  | A     | 836 | CLA  | CAA-C2A-C3A | -2.00 | 107.58      | 113.00   |
| 22  | 7     | 309 | CLA  | O1D-CGD-CBD | -2.00 | 120.57      | 124.52   |
| 22  | 7     | 306 | CLA  | CHD-C1D-ND  | -2.00 | 121.98      | 124.80   |
| 22  | 8     | 305 | CLA  | CHA-C1A-NA  | -2.00 | 121.86      | 126.39   |
| 39  | 4     | 819 | CHL  | CMA-C3A-C2A | 2.00  | 121.86      | 114.13   |
| 22  | A     | 822 | CLA  | CHA-C1A-NA  | -2.00 | 121.86      | 126.39   |
| 22  | B     | 817 | CLA  | CHA-C1A-NA  | -2.00 | 121.86      | 126.39   |
| 38  | 9     | 301 | LUT  | C31-C32-C33 | -2.00 | 120.88      | 126.36   |
| 22  | 5     | 312 | CLA  | O1D-CGD-CBD | -2.00 | 120.57      | 124.52   |
| 39  | 4     | 819 | CHL  | CMD-C2D-C3D | 2.00  | 128.68      | 124.68   |
| 22  | 4     | 812 | CLA  | O1D-CGD-CBD | -2.00 | 120.57      | 124.52   |
| 38  | 3     | 302 | LUT  | C22-C23-C24 | 2.00  | 114.16      | 111.18   |
| 22  | 7     | 308 | CLA  | C3D-C2D-C1D | -2.00 | 103.10      | 105.83   |

All (283) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21  | A     | 801 | CL0  | ND   |
| 21  | A     | 801 | CL0  | NC   |
| 21  | A     | 801 | CL0  | NA   |
| 22  | A     | 802 | CLA  | ND   |
| 22  | A     | 803 | CLA  | ND   |
| 22  | A     | 804 | CLA  | ND   |
| 22  | A     | 805 | CLA  | ND   |
| 22  | A     | 806 | CLA  | ND   |
| 22  | A     | 807 | CLA  | ND   |
| 22  | A     | 808 | CLA  | ND   |
| 22  | A     | 809 | CLA  | ND   |
| 22  | A     | 810 | CLA  | ND   |
| 22  | A     | 811 | CLA  | ND   |
| 22  | A     | 812 | CLA  | ND   |
| 22  | A     | 813 | CLA  | ND   |
| 22  | A     | 814 | CLA  | ND   |
| 22  | A     | 815 | CLA  | ND   |
| 22  | A     | 816 | CLA  | ND   |
| 22  | A     | 817 | CLA  | ND   |
| 22  | A     | 818 | CLA  | ND   |
| 22  | A     | 819 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | A     | 820 | CLA  | ND   |
| 22  | A     | 821 | CLA  | ND   |
| 22  | A     | 822 | CLA  | ND   |
| 22  | A     | 823 | CLA  | ND   |
| 22  | A     | 824 | CLA  | ND   |
| 22  | A     | 825 | CLA  | ND   |
| 22  | A     | 826 | CLA  | ND   |
| 22  | A     | 827 | CLA  | ND   |
| 22  | A     | 828 | CLA  | ND   |
| 22  | A     | 829 | CLA  | ND   |
| 22  | A     | 830 | CLA  | ND   |
| 22  | A     | 831 | CLA  | ND   |
| 22  | A     | 832 | CLA  | ND   |
| 22  | A     | 833 | CLA  | ND   |
| 22  | A     | 834 | CLA  | ND   |
| 22  | A     | 835 | CLA  | ND   |
| 22  | A     | 836 | CLA  | ND   |
| 22  | A     | 837 | CLA  | ND   |
| 22  | A     | 838 | CLA  | ND   |
| 22  | A     | 839 | CLA  | ND   |
| 22  | A     | 840 | CLA  | ND   |
| 22  | A     | 841 | CLA  | ND   |
| 22  | A     | 842 | CLA  | ND   |
| 22  | A     | 854 | CLA  | ND   |
| 22  | A     | 855 | CLA  | ND   |
| 22  | B     | 801 | CLA  | ND   |
| 22  | B     | 805 | CLA  | ND   |
| 22  | B     | 806 | CLA  | ND   |
| 22  | B     | 807 | CLA  | ND   |
| 22  | B     | 808 | CLA  | ND   |
| 22  | B     | 809 | CLA  | ND   |
| 22  | B     | 810 | CLA  | ND   |
| 22  | B     | 811 | CLA  | ND   |
| 22  | B     | 812 | CLA  | ND   |
| 22  | B     | 812 | CLA  | C13  |
| 22  | B     | 813 | CLA  | ND   |
| 22  | B     | 814 | CLA  | ND   |
| 22  | B     | 815 | CLA  | ND   |
| 22  | B     | 816 | CLA  | ND   |
| 22  | B     | 817 | CLA  | ND   |
| 22  | B     | 818 | CLA  | ND   |
| 22  | B     | 819 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | B     | 820 | CLA  | ND   |
| 22  | B     | 821 | CLA  | ND   |
| 22  | B     | 822 | CLA  | ND   |
| 22  | B     | 823 | CLA  | ND   |
| 22  | B     | 824 | CLA  | ND   |
| 22  | B     | 825 | CLA  | ND   |
| 22  | B     | 826 | CLA  | ND   |
| 22  | B     | 827 | CLA  | ND   |
| 22  | B     | 828 | CLA  | ND   |
| 22  | B     | 829 | CLA  | ND   |
| 22  | B     | 830 | CLA  | ND   |
| 22  | B     | 831 | CLA  | ND   |
| 22  | B     | 832 | CLA  | ND   |
| 22  | B     | 833 | CLA  | ND   |
| 22  | B     | 834 | CLA  | ND   |
| 22  | B     | 835 | CLA  | ND   |
| 22  | B     | 836 | CLA  | ND   |
| 22  | B     | 837 | CLA  | ND   |
| 22  | B     | 838 | CLA  | ND   |
| 22  | B     | 839 | CLA  | ND   |
| 22  | B     | 840 | CLA  | ND   |
| 22  | B     | 841 | CLA  | ND   |
| 22  | B     | 842 | CLA  | ND   |
| 22  | F     | 301 | CLA  | ND   |
| 22  | F     | 302 | CLA  | ND   |
| 22  | F     | 304 | CLA  | ND   |
| 22  | F     | 305 | CLA  | ND   |
| 22  | G     | 201 | CLA  | ND   |
| 22  | G     | 202 | CLA  | ND   |
| 22  | J     | 103 | CLA  | ND   |
| 22  | K     | 202 | CLA  | ND   |
| 22  | K     | 203 | CLA  | ND   |
| 22  | K     | 204 | CLA  | ND   |
| 22  | K     | 205 | CLA  | ND   |
| 22  | L     | 201 | CLA  | ND   |
| 22  | L     | 202 | CLA  | ND   |
| 22  | L     | 203 | CLA  | ND   |
| 22  | 1     | 304 | CLA  | ND   |
| 22  | 1     | 305 | CLA  | ND   |
| 22  | 1     | 306 | CLA  | ND   |
| 22  | 1     | 307 | CLA  | ND   |
| 22  | 1     | 308 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | 1     | 309 | CLA  | ND   |
| 22  | 1     | 310 | CLA  | ND   |
| 22  | 1     | 311 | CLA  | ND   |
| 22  | 1     | 313 | CLA  | ND   |
| 22  | 1     | 314 | CLA  | ND   |
| 22  | 1     | 315 | CLA  | ND   |
| 22  | 1     | 316 | CLA  | ND   |
| 22  | Z     | 303 | CLA  | ND   |
| 22  | Z     | 304 | CLA  | ND   |
| 22  | Z     | 305 | CLA  | ND   |
| 22  | Z     | 306 | CLA  | ND   |
| 22  | Z     | 307 | CLA  | ND   |
| 22  | Z     | 308 | CLA  | ND   |
| 22  | Z     | 309 | CLA  | ND   |
| 22  | Z     | 310 | CLA  | ND   |
| 22  | Z     | 313 | CLA  | ND   |
| 22  | Z     | 314 | CLA  | ND   |
| 22  | Z     | 315 | CLA  | ND   |
| 22  | Z     | 316 | CLA  | ND   |
| 22  | 3     | 308 | CLA  | ND   |
| 22  | 3     | 309 | CLA  | ND   |
| 22  | 3     | 310 | CLA  | ND   |
| 22  | 3     | 311 | CLA  | ND   |
| 22  | 3     | 312 | CLA  | ND   |
| 22  | 3     | 313 | CLA  | ND   |
| 22  | 3     | 314 | CLA  | ND   |
| 22  | 3     | 315 | CLA  | ND   |
| 22  | 3     | 316 | CLA  | ND   |
| 22  | 3     | 318 | CLA  | ND   |
| 22  | 3     | 319 | CLA  | ND   |
| 22  | 3     | 320 | CLA  | ND   |
| 22  | 3     | 322 | CLA  | ND   |
| 22  | 7     | 304 | CLA  | ND   |
| 22  | 7     | 305 | CLA  | ND   |
| 22  | 7     | 306 | CLA  | ND   |
| 22  | 7     | 307 | CLA  | ND   |
| 22  | 7     | 308 | CLA  | ND   |
| 22  | 7     | 309 | CLA  | ND   |
| 22  | 7     | 310 | CLA  | ND   |
| 22  | 7     | 311 | CLA  | ND   |
| 22  | 7     | 312 | CLA  | ND   |
| 22  | 7     | 314 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | 7     | 315 | CLA  | ND   |
| 22  | 7     | 316 | CLA  | ND   |
| 22  | 7     | 317 | CLA  | ND   |
| 22  | 7     | 322 | CLA  | ND   |
| 22  | 7     | 323 | CLA  | ND   |
| 22  | 7     | 324 | CLA  | ND   |
| 22  | 8     | 305 | CLA  | ND   |
| 22  | 8     | 306 | CLA  | ND   |
| 22  | 8     | 307 | CLA  | ND   |
| 22  | 8     | 308 | CLA  | ND   |
| 22  | 8     | 309 | CLA  | ND   |
| 22  | 8     | 310 | CLA  | ND   |
| 22  | 8     | 311 | CLA  | ND   |
| 22  | 8     | 313 | CLA  | ND   |
| 22  | 8     | 314 | CLA  | ND   |
| 22  | 8     | 316 | CLA  | ND   |
| 22  | 4     | 805 | CLA  | ND   |
| 22  | 4     | 806 | CLA  | ND   |
| 22  | 4     | 807 | CLA  | ND   |
| 22  | 4     | 808 | CLA  | ND   |
| 22  | 4     | 809 | CLA  | ND   |
| 22  | 4     | 810 | CLA  | ND   |
| 22  | 4     | 811 | CLA  | ND   |
| 22  | 4     | 812 | CLA  | ND   |
| 22  | 4     | 815 | CLA  | ND   |
| 22  | 4     | 817 | CLA  | ND   |
| 22  | 4     | 818 | CLA  | ND   |
| 22  | 5     | 301 | CLA  | ND   |
| 22  | 5     | 307 | CLA  | ND   |
| 22  | 5     | 308 | CLA  | ND   |
| 22  | 5     | 309 | CLA  | ND   |
| 22  | 5     | 310 | CLA  | ND   |
| 22  | 5     | 311 | CLA  | ND   |
| 22  | 5     | 312 | CLA  | ND   |
| 22  | 5     | 313 | CLA  | ND   |
| 22  | 5     | 314 | CLA  | ND   |
| 22  | 5     | 315 | CLA  | ND   |
| 22  | 5     | 318 | CLA  | ND   |
| 22  | 5     | 319 | CLA  | ND   |
| 22  | 5     | 320 | CLA  | ND   |
| 22  | 5     | 322 | CLA  | ND   |
| 22  | 5     | 323 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22  | 5     | 326 | CLA  | ND   |
| 22  | 6     | 301 | CLA  | ND   |
| 22  | 6     | 302 | CLA  | ND   |
| 22  | 6     | 307 | CLA  | ND   |
| 22  | 6     | 308 | CLA  | ND   |
| 22  | 6     | 309 | CLA  | ND   |
| 22  | 6     | 310 | CLA  | ND   |
| 22  | 6     | 311 | CLA  | ND   |
| 22  | 6     | 312 | CLA  | ND   |
| 22  | 6     | 313 | CLA  | ND   |
| 22  | 6     | 314 | CLA  | ND   |
| 22  | 6     | 317 | CLA  | ND   |
| 22  | 6     | 319 | CLA  | ND   |
| 22  | 6     | 321 | CLA  | ND   |
| 22  | 6     | 322 | CLA  | ND   |
| 22  | 9     | 303 | CLA  | ND   |
| 22  | 9     | 304 | CLA  | ND   |
| 22  | 9     | 305 | CLA  | ND   |
| 22  | 9     | 306 | CLA  | ND   |
| 22  | 9     | 307 | CLA  | ND   |
| 22  | 9     | 308 | CLA  | ND   |
| 22  | 9     | 309 | CLA  | ND   |
| 22  | 9     | 310 | CLA  | ND   |
| 22  | 9     | 311 | CLA  | ND   |
| 22  | 9     | 313 | CLA  | ND   |
| 22  | 2     | 301 | CLA  | ND   |
| 22  | 2     | 302 | CLA  | ND   |
| 22  | 2     | 304 | CLA  | ND   |
| 39  | 1     | 312 | CHL  | ND   |
| 39  | 1     | 312 | CHL  | NC   |
| 39  | 1     | 312 | CHL  | NA   |
| 39  | Z     | 311 | CHL  | ND   |
| 39  | Z     | 311 | CHL  | NC   |
| 39  | Z     | 311 | CHL  | NA   |
| 39  | Z     | 312 | CHL  | ND   |
| 39  | Z     | 312 | CHL  | NC   |
| 39  | Z     | 312 | CHL  | NA   |
| 39  | 3     | 317 | CHL  | ND   |
| 39  | 3     | 317 | CHL  | NC   |
| 39  | 3     | 317 | CHL  | NA   |
| 39  | 7     | 313 | CHL  | ND   |
| 39  | 7     | 313 | CHL  | NC   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 39  | 7     | 313 | CHL  | NA   |
| 39  | 8     | 301 | CHL  | ND   |
| 39  | 8     | 301 | CHL  | NC   |
| 39  | 8     | 301 | CHL  | NA   |
| 39  | 8     | 312 | CHL  | ND   |
| 39  | 8     | 312 | CHL  | NC   |
| 39  | 8     | 312 | CHL  | NA   |
| 39  | 8     | 315 | CHL  | ND   |
| 39  | 8     | 315 | CHL  | NC   |
| 39  | 8     | 315 | CHL  | NA   |
| 39  | 4     | 813 | CHL  | ND   |
| 39  | 4     | 813 | CHL  | NC   |
| 39  | 4     | 813 | CHL  | NA   |
| 39  | 4     | 814 | CHL  | ND   |
| 39  | 4     | 814 | CHL  | NC   |
| 39  | 4     | 814 | CHL  | NA   |
| 39  | 4     | 816 | CHL  | ND   |
| 39  | 4     | 816 | CHL  | NC   |
| 39  | 4     | 816 | CHL  | NA   |
| 39  | 4     | 819 | CHL  | ND   |
| 39  | 4     | 819 | CHL  | NC   |
| 39  | 4     | 819 | CHL  | NA   |
| 39  | 5     | 316 | CHL  | ND   |
| 39  | 5     | 316 | CHL  | NC   |
| 39  | 5     | 316 | CHL  | NA   |
| 39  | 5     | 317 | CHL  | ND   |
| 39  | 5     | 317 | CHL  | NC   |
| 39  | 5     | 317 | CHL  | NA   |
| 39  | 5     | 321 | CHL  | ND   |
| 39  | 5     | 321 | CHL  | NC   |
| 39  | 5     | 321 | CHL  | NA   |
| 39  | 6     | 315 | CHL  | ND   |
| 39  | 6     | 315 | CHL  | NC   |
| 39  | 6     | 315 | CHL  | NA   |
| 39  | 6     | 316 | CHL  | ND   |
| 39  | 6     | 316 | CHL  | NC   |
| 39  | 6     | 316 | CHL  | NA   |
| 39  | 6     | 318 | CHL  | ND   |
| 39  | 6     | 318 | CHL  | NC   |
| 39  | 6     | 318 | CHL  | NA   |
| 39  | 6     | 320 | CHL  | ND   |
| 39  | 6     | 320 | CHL  | NC   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 39  | 6     | 320 | CHL  | NA   |
| 39  | 9     | 312 | CHL  | ND   |
| 39  | 9     | 312 | CHL  | NC   |
| 39  | 9     | 312 | CHL  | NA   |
| 39  | 9     | 314 | CHL  | ND   |
| 39  | 9     | 314 | CHL  | NC   |
| 39  | 9     | 314 | CHL  | NA   |
| 39  | 2     | 303 | CHL  | ND   |
| 39  | 2     | 303 | CHL  | NC   |
| 39  | 2     | 303 | CHL  | NA   |

All (3783) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | A     | 801 | CL0  | CHA-CBD-CGD-O1D |
| 22  | A     | 802 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 802 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 803 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 803 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 803 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 804 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 805 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 806 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 806 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 806 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 806 | CLA  | CHA-CBD-CGD-O1D |
| 22  | A     | 806 | CLA  | CHA-CBD-CGD-O2D |
| 22  | A     | 806 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 807 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 807 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 807 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 807 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 808 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 808 | CLA  | CHA-CBD-CGD-O1D |
| 22  | A     | 808 | CLA  | CHA-CBD-CGD-O2D |
| 22  | A     | 810 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 811 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 811 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 812 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 812 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 814 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 22  | A     | 814 | CLA  | CHA-CBD-CGD-O2D |
| 22  | A     | 815 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 815 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 815 | CLA  | CHA-CBD-CGD-O1D |
| 22  | A     | 815 | CLA  | CHA-CBD-CGD-O2D |
| 22  | A     | 816 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 816 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 817 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 818 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 818 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 820 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 821 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 822 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 822 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 822 | CLA  | CAD-CBD-CGD-O1D |
| 22  | A     | 822 | CLA  | CAD-CBD-CGD-O2D |
| 22  | A     | 823 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 825 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 825 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 825 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 826 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 826 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 827 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 827 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 828 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 828 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 828 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 829 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 829 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 830 | CLA  | CAD-CBD-CGD-O1D |
| 22  | A     | 830 | CLA  | CAD-CBD-CGD-O2D |
| 22  | A     | 831 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 832 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 832 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 833 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 833 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 833 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 834 | CLA  | CHA-CBD-CGD-O1D |
| 22  | A     | 834 | CLA  | CHA-CBD-CGD-O2D |
| 22  | A     | 835 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 835 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 835 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 836 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 838 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 838 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 839 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 839 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 840 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 840 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 841 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 842 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 842 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 842 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 854 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 854 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 855 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 855 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 801 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 805 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 806 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 807 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 808 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 810 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 810 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 811 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 811 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 811 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 811 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 812 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 812 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 812 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 812 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 812 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 813 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 813 | CLA  | CAD-CBD-CGD-O1D |
| 22  | B     | 813 | CLA  | CAD-CBD-CGD-O2D |
| 22  | B     | 814 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 815 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 816 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 817 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 817 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 817 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 819 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 821 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 821 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 822 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 822 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 822 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 822 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 824 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 825 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 826 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 826 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 827 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 827 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 827 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 829 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 830 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 831 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 831 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 832 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 833 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 834 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 834 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 834 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 835 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 835 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 835 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 836 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 837 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 837 | CLA  | CHA-CBD-CGD-O1D |
| 22  | B     | 837 | CLA  | CHA-CBD-CGD-O2D |
| 22  | B     | 841 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 841 | CLA  | C11-C10-C8-C9   |
| 22  | F     | 301 | CLA  | C1A-C2A-CAA-CBA |
| 22  | F     | 301 | CLA  | C3A-C2A-CAA-CBA |
| 22  | F     | 302 | CLA  | C2-C1-O2A-CGA   |
| 22  | F     | 302 | CLA  | CBD-CGD-O2D-CED |
| 22  | F     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 22  | F     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 22  | F     | 304 | CLA  | O1A-CGA-O2A-C1  |
| 22  | F     | 304 | CLA  | CAD-CBD-CGD-O1D |
| 22  | F     | 304 | CLA  | CAD-CBD-CGD-O2D |
| 22  | F     | 305 | CLA  | C1A-C2A-CAA-CBA |
| 22  | F     | 305 | CLA  | C3A-C2A-CAA-CBA |
| 22  | G     | 202 | CLA  | C1A-C2A-CAA-CBA |
| 22  | G     | 202 | CLA  | C3A-C2A-CAA-CBA |
| 22  | G     | 202 | CLA  | CHA-CBD-CGD-O1D |
| 22  | G     | 202 | CLA  | CHA-CBD-CGD-O2D |
| 22  | J     | 103 | CLA  | C1A-C2A-CAA-CBA |
| 22  | K     | 204 | CLA  | C2B-C3B-CAB-CBB |
| 22  | K     | 204 | CLA  | C4B-C3B-CAB-CBB |
| 22  | K     | 205 | CLA  | C2B-C3B-CAB-CBB |
| 22  | K     | 205 | CLA  | C4B-C3B-CAB-CBB |
| 22  | K     | 205 | CLA  | CBD-CGD-O2D-CED |
| 22  | L     | 201 | CLA  | C1A-C2A-CAA-CBA |
| 22  | L     | 201 | CLA  | CHA-CBD-CGD-O1D |
| 22  | L     | 201 | CLA  | CHA-CBD-CGD-O2D |
| 22  | L     | 202 | CLA  | C1A-C2A-CAA-CBA |
| 22  | L     | 202 | CLA  | C3A-C2A-CAA-CBA |
| 22  | L     | 203 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 305 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 1     | 305 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 1     | 306 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 307 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 308 | CLA  | C2-C1-O2A-CGA   |
| 22  | 1     | 308 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 1     | 308 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 1     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 309 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 311 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 311 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 1     | 313 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 314 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 316 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 1     | 316 | CLA  | C4B-C3B-CAB-CBB |
| 22  | Z     | 303 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Z     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 303 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 22  | Z     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 22  | Z     | 305 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 306 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Z     | 306 | CLA  | CHA-CBD-CGD-O1D |
| 22  | Z     | 306 | CLA  | CHA-CBD-CGD-O2D |
| 22  | Z     | 307 | CLA  | CHA-CBD-CGD-O1D |
| 22  | Z     | 307 | CLA  | CHA-CBD-CGD-O2D |
| 22  | Z     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 308 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 310 | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 314 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Z     | 314 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 315 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 316 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 316 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 316 | CLA  | C11-C10-C8-C9   |
| 22  | 3     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 309 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 310 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 311 | CLA  | C6-C7-C8-C9     |
| 22  | 3     | 311 | CLA  | C11-C10-C8-C7   |
| 22  | 3     | 312 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 3     | 313 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 314 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 315 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 3     | 315 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 316 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 316 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 318 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 319 | CLA  | C4-C3-C5-C6     |
| 22  | 3     | 320 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 3     | 320 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 304 | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 305 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 305 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 305 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 306 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 306 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 307 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 309 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 310 | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 312 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 312 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 314 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 315 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 7     | 315 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 7     | 316 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 316 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 317 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 317 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 317 | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 323 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 323 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 323 | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 323 | CLA  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 7     | 323 | CLA  | CAD-CBD-CGD-O2D |
| 22  | 7     | 324 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 324 | CLA  | C2-C1-O2A-CGA   |
| 22  | 8     | 305 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 305 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 305 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 307 | CLA  | CAD-CBD-CGD-O2D |
| 22  | 8     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 309 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 310 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 313 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 316 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 316 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 805 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 805 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 806 | CLA  | C2-C1-O2A-CGA   |
| 22  | 4     | 806 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 4     | 806 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 807 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 808 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 809 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 809 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 809 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 811 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 811 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 815 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 815 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 4     | 815 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 4     | 815 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 818 | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 301 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 307 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 308 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 5     | 308 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 309 | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 310 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 310 | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 315 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 315 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 315 | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 318 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 319 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 319 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 319 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 319 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 320 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 320 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 320 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 5     | 320 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 5     | 320 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 322 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 322 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 323 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 326 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 326 | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 301 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 301 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 302 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 302 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 302 | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 307 | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 308 | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 311 | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 312 | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 312 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 6     | 312 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 6     | 317 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 317 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 6     | 317 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 317 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 6     | 317 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 6     | 319 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 319 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 6     | 319 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 6     | 321 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 321 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 321 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 322 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 322 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 322 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 6     | 322 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 9     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 305 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 9     | 305 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 9     | 307 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 9     | 307 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 9     | 308 | CLA  | C2-C1-O2A-CGA   |
| 22  | 9     | 308 | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 309 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 9     | 309 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 9     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 9     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 9     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 311 | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 2     | 301 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 2     | 301 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 2     | 302 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 2     | 302 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 2     | 302 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 2     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 2     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 2     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 24  | A     | 844 | BCR  | C5-C6-C7-C8     |
| 24  | A     | 844 | BCR  | C21-C22-C23-C24 |
| 24  | A     | 845 | BCR  | C7-C8-C9-C34    |
| 24  | A     | 845 | BCR  | C21-C22-C23-C24 |
| 24  | A     | 845 | BCR  | C37-C22-C23-C24 |
| 24  | A     | 846 | BCR  | C7-C8-C9-C10    |
| 24  | A     | 846 | BCR  | C7-C8-C9-C34    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | A     | 847 | BCR  | C1-C6-C7-C8     |
| 24  | A     | 847 | BCR  | C11-C12-C13-C14 |
| 24  | A     | 847 | BCR  | C11-C12-C13-C35 |
| 24  | A     | 847 | BCR  | C13-C14-C15-C16 |
| 24  | A     | 847 | BCR  | C19-C20-C21-C22 |
| 24  | A     | 847 | BCR  | C23-C24-C25-C26 |
| 24  | A     | 848 | BCR  | C15-C16-C17-C18 |
| 24  | A     | 848 | BCR  | C17-C18-C19-C20 |
| 24  | A     | 848 | BCR  | C36-C18-C19-C20 |
| 24  | A     | 848 | BCR  | C21-C22-C23-C24 |
| 24  | A     | 848 | BCR  | C37-C22-C23-C24 |
| 24  | A     | 856 | BCR  | C1-C6-C7-C8     |
| 24  | A     | 856 | BCR  | C9-C10-C11-C12  |
| 24  | A     | 856 | BCR  | C11-C12-C13-C14 |
| 24  | A     | 856 | BCR  | C11-C12-C13-C35 |
| 24  | A     | 856 | BCR  | C17-C18-C19-C20 |
| 24  | B     | 844 | BCR  | C7-C8-C9-C34    |
| 24  | B     | 845 | BCR  | C7-C8-C9-C10    |
| 24  | B     | 845 | BCR  | C7-C8-C9-C34    |
| 24  | B     | 845 | BCR  | C9-C10-C11-C12  |
| 24  | B     | 845 | BCR  | C11-C12-C13-C14 |
| 24  | B     | 846 | BCR  | C11-C12-C13-C14 |
| 24  | B     | 846 | BCR  | C11-C12-C13-C35 |
| 24  | B     | 846 | BCR  | C15-C16-C17-C18 |
| 24  | B     | 846 | BCR  | C17-C18-C19-C20 |
| 24  | B     | 846 | BCR  | C36-C18-C19-C20 |
| 24  | B     | 846 | BCR  | C21-C22-C23-C24 |
| 24  | B     | 846 | BCR  | C37-C22-C23-C24 |
| 24  | B     | 847 | BCR  | C11-C12-C13-C14 |
| 24  | B     | 847 | BCR  | C17-C18-C19-C20 |
| 24  | B     | 848 | BCR  | C1-C6-C7-C8     |
| 24  | B     | 848 | BCR  | C5-C6-C7-C8     |
| 24  | B     | 848 | BCR  | C11-C12-C13-C14 |
| 24  | B     | 848 | BCR  | C11-C12-C13-C35 |
| 24  | B     | 848 | BCR  | C13-C14-C15-C16 |
| 24  | B     | 848 | BCR  | C21-C22-C23-C24 |
| 24  | B     | 848 | BCR  | C37-C22-C23-C24 |
| 24  | B     | 849 | BCR  | C9-C10-C11-C12  |
| 24  | B     | 849 | BCR  | C11-C12-C13-C14 |
| 24  | B     | 849 | BCR  | C11-C12-C13-C35 |
| 24  | B     | 849 | BCR  | C36-C18-C19-C20 |
| 24  | B     | 849 | BCR  | C21-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 24  | B     | 849  | BCR  | C37-C22-C23-C24 |
| 24  | B     | 853  | BCR  | C7-C8-C9-C10    |
| 24  | B     | 853  | BCR  | C19-C20-C21-C22 |
| 24  | F     | 303  | BCR  | C1-C6-C7-C8     |
| 24  | F     | 303  | BCR  | C9-C10-C11-C12  |
| 24  | F     | 303  | BCR  | C11-C12-C13-C14 |
| 24  | F     | 303  | BCR  | C11-C12-C13-C35 |
| 24  | F     | 303  | BCR  | C13-C14-C15-C16 |
| 24  | F     | 303  | BCR  | C17-C18-C19-C20 |
| 24  | F     | 303  | BCR  | C36-C18-C19-C20 |
| 24  | F     | 303  | BCR  | C19-C20-C21-C22 |
| 24  | G     | 203  | BCR  | C7-C8-C9-C10    |
| 24  | I     | 4001 | BCR  | C5-C6-C7-C8     |
| 24  | I     | 4001 | BCR  | C17-C18-C19-C20 |
| 24  | I     | 4001 | BCR  | C36-C18-C19-C20 |
| 24  | I     | 4001 | BCR  | C19-C20-C21-C22 |
| 24  | I     | 4001 | BCR  | C21-C22-C23-C24 |
| 24  | I     | 4001 | BCR  | C37-C22-C23-C24 |
| 24  | J     | 104  | BCR  | C11-C12-C13-C14 |
| 24  | J     | 104  | BCR  | C11-C12-C13-C35 |
| 24  | J     | 104  | BCR  | C17-C18-C19-C20 |
| 24  | J     | 104  | BCR  | C36-C18-C19-C20 |
| 24  | K     | 206  | BCR  | C7-C8-C9-C10    |
| 24  | K     | 206  | BCR  | C7-C8-C9-C34    |
| 24  | K     | 206  | BCR  | C19-C20-C21-C22 |
| 24  | K     | 206  | BCR  | C23-C24-C25-C26 |
| 24  | L     | 204  | BCR  | C7-C8-C9-C10    |
| 24  | L     | 204  | BCR  | C13-C14-C15-C16 |
| 24  | L     | 204  | BCR  | C15-C16-C17-C18 |
| 24  | L     | 204  | BCR  | C36-C18-C19-C20 |
| 24  | L     | 204  | BCR  | C19-C20-C21-C22 |
| 24  | L     | 204  | BCR  | C21-C22-C23-C24 |
| 24  | L     | 204  | BCR  | C37-C22-C23-C24 |
| 24  | 3     | 304  | BCR  | C7-C8-C9-C10    |
| 24  | 3     | 304  | BCR  | C13-C14-C15-C16 |
| 24  | 3     | 304  | BCR  | C17-C18-C19-C20 |
| 24  | 3     | 305  | BCR  | C1-C6-C7-C8     |
| 24  | 3     | 305  | BCR  | C5-C6-C7-C8     |
| 24  | 3     | 305  | BCR  | C9-C10-C11-C12  |
| 24  | 3     | 305  | BCR  | C11-C12-C13-C14 |
| 24  | 3     | 305  | BCR  | C11-C12-C13-C35 |
| 24  | 3     | 305  | BCR  | C19-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | 3     | 306 | BCR  | C11-C12-C13-C14 |
| 24  | 3     | 306 | BCR  | C11-C12-C13-C35 |
| 24  | 3     | 306 | BCR  | C17-C18-C19-C20 |
| 24  | 3     | 306 | BCR  | C19-C20-C21-C22 |
| 24  | 3     | 306 | BCR  | C21-C22-C23-C24 |
| 24  | 3     | 306 | BCR  | C37-C22-C23-C24 |
| 24  | 3     | 307 | BCR  | C11-C12-C13-C14 |
| 24  | 3     | 307 | BCR  | C11-C12-C13-C35 |
| 24  | 3     | 307 | BCR  | C17-C18-C19-C20 |
| 24  | 3     | 307 | BCR  | C36-C18-C19-C20 |
| 24  | 3     | 307 | BCR  | C23-C24-C25-C26 |
| 24  | 7     | 303 | BCR  | C7-C8-C9-C10    |
| 24  | 7     | 303 | BCR  | C7-C8-C9-C34    |
| 24  | 7     | 303 | BCR  | C11-C12-C13-C14 |
| 24  | 7     | 303 | BCR  | C11-C12-C13-C35 |
| 24  | 7     | 303 | BCR  | C13-C14-C15-C16 |
| 24  | 7     | 303 | BCR  | C23-C24-C25-C26 |
| 24  | 8     | 304 | BCR  | C11-C12-C13-C14 |
| 24  | 8     | 304 | BCR  | C11-C12-C13-C35 |
| 24  | 8     | 304 | BCR  | C13-C14-C15-C16 |
| 24  | 4     | 804 | BCR  | C7-C8-C9-C10    |
| 24  | 4     | 804 | BCR  | C7-C8-C9-C34    |
| 24  | 4     | 804 | BCR  | C9-C10-C11-C12  |
| 24  | 4     | 804 | BCR  | C23-C24-C25-C26 |
| 24  | 5     | 304 | BCR  | C7-C8-C9-C10    |
| 24  | 5     | 304 | BCR  | C7-C8-C9-C34    |
| 24  | 5     | 304 | BCR  | C11-C12-C13-C14 |
| 24  | 5     | 304 | BCR  | C11-C12-C13-C35 |
| 24  | 5     | 304 | BCR  | C13-C14-C15-C16 |
| 24  | 5     | 304 | BCR  | C23-C24-C25-C26 |
| 24  | 5     | 305 | BCR  | C5-C6-C7-C8     |
| 24  | 5     | 305 | BCR  | C9-C10-C11-C12  |
| 24  | 5     | 305 | BCR  | C17-C18-C19-C20 |
| 24  | 6     | 305 | BCR  | C11-C12-C13-C14 |
| 24  | 6     | 305 | BCR  | C11-C12-C13-C35 |
| 24  | 6     | 306 | BCR  | C1-C6-C7-C8     |
| 24  | 6     | 306 | BCR  | C5-C6-C7-C8     |
| 24  | 6     | 306 | BCR  | C7-C8-C9-C34    |
| 24  | 6     | 306 | BCR  | C23-C24-C25-C26 |
| 25  | A     | 849 | LHG  | C3-O3-P-O6      |
| 25  | A     | 849 | LHG  | C4-O6-P-O4      |
| 25  | A     | 849 | LHG  | C4-O6-P-O5      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | A     | 850 | LHG  | O1-C1-C2-C3     |
| 25  | A     | 850 | LHG  | C1-C2-C3-O3     |
| 25  | A     | 850 | LHG  | C4-O6-P-O3      |
| 25  | A     | 850 | LHG  | C4-O6-P-O5      |
| 25  | B     | 803 | LHG  | C3-O3-P-O6      |
| 25  | B     | 803 | LHG  | O9-C7-O7-C5     |
| 25  | B     | 803 | LHG  | C8-C7-O7-C5     |
| 25  | B     | 850 | LHG  | C3-O3-P-O4      |
| 25  | B     | 850 | LHG  | C3-O3-P-O6      |
| 25  | B     | 850 | LHG  | O9-C7-O7-C5     |
| 25  | B     | 851 | LHG  | O1-C1-C2-O2     |
| 25  | B     | 851 | LHG  | C3-O3-P-O5      |
| 25  | B     | 851 | LHG  | O9-C7-O7-C5     |
| 25  | 1     | 317 | LHG  | C8-C7-O7-C5     |
| 25  | Z     | 317 | LHG  | O1-C1-C2-O2     |
| 25  | Z     | 317 | LHG  | C4-O6-P-O3      |
| 25  | 3     | 321 | LHG  | O9-C7-O7-C5     |
| 25  | 7     | 318 | LHG  | C1-C2-C3-O3     |
| 25  | 7     | 318 | LHG  | C4-O6-P-O3      |
| 25  | 7     | 318 | LHG  | C4-O6-P-O4      |
| 25  | 8     | 317 | LHG  | O1-C1-C2-C3     |
| 25  | 8     | 317 | LHG  | C4-O6-P-O4      |
| 25  | 4     | 820 | LHG  | C3-O3-P-O4      |
| 25  | 4     | 820 | LHG  | C4-O6-P-O3      |
| 25  | 4     | 820 | LHG  | C8-C7-O7-C5     |
| 25  | 5     | 324 | LHG  | O1-C1-C2-O2     |
| 25  | 6     | 323 | LHG  | O1-C1-C2-O2     |
| 25  | 6     | 323 | LHG  | C3-O3-P-O5      |
| 25  | 6     | 323 | LHG  | C4-O6-P-O4      |
| 25  | 6     | 323 | LHG  | C4-O6-P-O5      |
| 25  | 6     | 323 | LHG  | C24-C23-O8-C6   |
| 25  | 9     | 315 | LHG  | C3-O3-P-O4      |
| 25  | 9     | 315 | LHG  | C3-O3-P-O6      |
| 25  | 9     | 315 | LHG  | C4-O6-P-O3      |
| 27  | A     | 852 | DGA  | CA2-CA1-OG1-CG1 |
| 27  | A     | 852 | DGA  | OA1-CA1-OG1-CG1 |
| 31  | B     | 852 | DGD  | O1B-C1B-O2G-C2G |
| 31  | 1     | 319 | DGD  | C2A-C1A-O1G-C1G |
| 31  | 1     | 319 | DGD  | O1A-C1A-O1G-C1G |
| 31  | 1     | 319 | DGD  | C2B-C1B-O2G-C2G |
| 31  | 1     | 319 | DGD  | O1B-C1B-O2G-C2G |
| 31  | 1     | 319 | DGD  | O6E-C1E-O5D-C6D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 3     | 301 | DGD  | C2B-C1B-O2G-C2G |
| 31  | 3     | 301 | DGD  | O1B-C1B-O2G-C2G |
| 32  | F     | 306 | RRX  | C7-C8-C9-C10    |
| 32  | F     | 306 | RRX  | C5-C6-C7-C8     |
| 33  | G     | 204 | LMT  | C2'-C1'-O1'-C1  |
| 33  | G     | 204 | LMT  | O5'-C1'-O1'-C1  |
| 33  | 1     | 301 | LMT  | C2-C1-O1'-C1'   |
| 34  | F     | 308 | LMG  | C11-C10-O7-C8   |
| 36  | J     | 105 | C7Z  | C5-C6-C7-C8     |
| 36  | J     | 105 | C7Z  | C7-C8-C9-C10    |
| 36  | J     | 105 | C7Z  | C31-C32-C33-C34 |
| 36  | J     | 105 | C7Z  | C31-C32-C33-C40 |
| 36  | 5     | 306 | C7Z  | C11-C12-C13-C14 |
| 36  | 5     | 306 | C7Z  | C31-C32-C33-C40 |
| 38  | 1     | 302 | LUT  | C11-C12-C13-C14 |
| 38  | 1     | 302 | LUT  | C27-C28-C29-C30 |
| 38  | 1     | 302 | LUT  | C31-C32-C33-C34 |
| 38  | 1     | 303 | LUT  | C11-C12-C13-C14 |
| 38  | 1     | 303 | LUT  | C31-C32-C33-C34 |
| 38  | 1     | 303 | LUT  | C31-C32-C33-C40 |
| 38  | Z     | 301 | LUT  | C11-C12-C13-C14 |
| 38  | Z     | 301 | LUT  | C11-C12-C13-C20 |
| 38  | Z     | 302 | LUT  | C7-C8-C9-C10    |
| 38  | Z     | 302 | LUT  | C11-C12-C13-C14 |
| 38  | 3     | 302 | LUT  | C11-C12-C13-C14 |
| 38  | 3     | 302 | LUT  | C31-C32-C33-C34 |
| 38  | 3     | 303 | LUT  | C11-C12-C13-C14 |
| 38  | 7     | 301 | LUT  | C11-C12-C13-C14 |
| 38  | 7     | 301 | LUT  | C11-C12-C13-C20 |
| 38  | 7     | 301 | LUT  | C31-C32-C33-C34 |
| 38  | 7     | 301 | LUT  | C31-C32-C33-C40 |
| 38  | 7     | 302 | LUT  | C7-C8-C9-C10    |
| 38  | 8     | 302 | LUT  | C11-C12-C13-C14 |
| 38  | 8     | 302 | LUT  | C11-C12-C13-C20 |
| 38  | 8     | 302 | LUT  | C27-C28-C29-C30 |
| 38  | 8     | 303 | LUT  | C11-C12-C13-C14 |
| 38  | 8     | 303 | LUT  | C11-C12-C13-C20 |
| 38  | 4     | 802 | LUT  | C5-C6-C7-C8     |
| 38  | 4     | 802 | LUT  | C7-C8-C9-C10    |
| 38  | 4     | 802 | LUT  | C7-C8-C9-C19    |
| 38  | 4     | 802 | LUT  | C31-C32-C33-C34 |
| 38  | 4     | 802 | LUT  | C31-C32-C33-C40 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 38  | 4     | 803 | LUT  | C11-C12-C13-C14 |
| 38  | 5     | 302 | LUT  | C7-C8-C9-C19    |
| 38  | 5     | 302 | LUT  | C11-C12-C13-C14 |
| 38  | 5     | 302 | LUT  | C11-C12-C13-C20 |
| 38  | 5     | 302 | LUT  | C31-C32-C33-C34 |
| 38  | 5     | 303 | LUT  | C11-C12-C13-C14 |
| 38  | 6     | 303 | LUT  | C7-C8-C9-C10    |
| 38  | 6     | 303 | LUT  | C7-C8-C9-C19    |
| 38  | 6     | 303 | LUT  | C11-C12-C13-C14 |
| 38  | 6     | 303 | LUT  | C11-C12-C13-C20 |
| 38  | 6     | 304 | LUT  | C11-C12-C13-C14 |
| 38  | 9     | 301 | LUT  | C11-C12-C13-C14 |
| 38  | 9     | 301 | LUT  | C11-C12-C13-C20 |
| 38  | 9     | 301 | LUT  | C31-C32-C33-C34 |
| 38  | 9     | 301 | LUT  | C31-C32-C33-C40 |
| 38  | 9     | 302 | LUT  | C7-C8-C9-C10    |
| 38  | 9     | 302 | LUT  | C11-C12-C13-C20 |
| 39  | Z     | 311 | CHL  | C4C-C3C-CAC-CBC |
| 39  | Z     | 312 | CHL  | CBD-CGD-O2D-CED |
| 39  | 8     | 312 | CHL  | CBD-CGD-O2D-CED |
| 39  | 4     | 814 | CHL  | CBD-CGD-O2D-CED |
| 39  | 4     | 816 | CHL  | C1A-C2A-CAA-CBA |
| 39  | 5     | 317 | CHL  | C3A-C2A-CAA-CBA |
| 39  | 5     | 321 | CHL  | C3A-C2A-CAA-CBA |
| 39  | 6     | 316 | CHL  | C3A-C2A-CAA-CBA |
| 39  | 6     | 316 | CHL  | CBA-CGA-O2A-C1  |
| 39  | 6     | 316 | CHL  | O1A-CGA-O2A-C1  |
| 39  | 6     | 318 | CHL  | CBD-CGD-O2D-CED |
| 39  | 9     | 312 | CHL  | C4C-C3C-CAC-CBC |
| 39  | 9     | 312 | CHL  | CBD-CGD-O2D-CED |
| 39  | 2     | 303 | CHL  | CBD-CGD-O2D-CED |
| 40  | 1     | 318 | SQD  | O5-C5-C6-S      |
| 41  | 7     | 319 | 3PH  | C22-C21-O21-C2  |
| 41  | 8     | 320 | 3PH  | C1-O11-P-O13    |
| 41  | 8     | 320 | 3PH  | C1-O11-P-O14    |
| 41  | 8     | 320 | 3PH  | C2-C1-O11-P     |
| 41  | 5     | 325 | 3PH  | O22-C21-O21-C2  |
| 41  | 5     | 325 | 3PH  | C22-C21-O21-C2  |
| 41  | 6     | 324 | 3PH  | C22-C21-O21-C2  |
| 42  | 7     | 320 | SPH  | O1-C1-C2-N2     |
| 42  | 7     | 321 | SPH  | C1-C2-C3-O3     |
| 42  | 7     | 321 | SPH  | C1-C2-C3-C4     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 42  | 7     | 321 | SPH  | N2-C2-C3-O3     |
| 42  | 7     | 321 | SPH  | N2-C2-C3-C4     |
| 43  | 8     | 319 | LPX  | C4-C3-O1-P1     |
| 43  | 8     | 319 | LPX  | C2-C1-O2-P1     |
| 22  | B     | 809 | CLA  | O1D-CGD-O2D-CED |
| 22  | F     | 302 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 315 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 315 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 308 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 306 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 309 | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 316 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 818 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 319 | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 302 | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 308 | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 311 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 310 | CLA  | O1D-CGD-O2D-CED |
| 33  | F     | 307 | LMT  | O5B-C1B-O1B-C4' |
| 22  | A     | 811 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 823 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 825 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 842 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 805 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 829 | CLA  | O1D-CGD-O2D-CED |
| 22  | J     | 103 | CLA  | O1D-CGD-O2D-CED |
| 22  | K     | 204 | CLA  | O1D-CGD-O2D-CED |
| 22  | L     | 203 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 309 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 314 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 308 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 312 | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 310 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 809 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 817 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 309 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 315 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 303 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 802 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 804 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 808 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 809 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 814 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 819 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 821 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 825 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 832 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 834 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 836 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 838 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 807 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 809 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 818 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 819 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 820 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 821 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 823 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 827 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 828 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 829 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 836 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 840 | CLA  | CBD-CGD-O2D-CED |
| 22  | F     | 301 | CLA  | CBD-CGD-O2D-CED |
| 22  | F     | 304 | CLA  | CBD-CGD-O2D-CED |
| 22  | F     | 305 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 201 | CLA  | CBD-CGD-O2D-CED |
| 22  | G     | 202 | CLA  | CBD-CGD-O2D-CED |
| 22  | J     | 103 | CLA  | CBD-CGD-O2D-CED |
| 22  | K     | 204 | CLA  | CBD-CGD-O2D-CED |
| 22  | L     | 203 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 309 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 311 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 315 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 316 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 306 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 307 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 313 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 308 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 314 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 318 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 319 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 320 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 304 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 308 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 7     | 315 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 324 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 307 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 309 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 316 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 806 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 812 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 817 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 818 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 309 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 319 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 322 | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 308 | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 309 | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 317 | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 322 | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 303 | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 304 | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 305 | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 307 | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 310 | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 313 | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 301 | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 302 | CLA  | CBD-CGD-O2D-CED |
| 39  | 7     | 313 | CHL  | CBD-CGD-O2D-CED |
| 39  | 4     | 813 | CHL  | CBD-CGD-O2D-CED |
| 33  | F     | 307 | LMT  | C2B-C1B-O1B-C4' |
| 22  | A     | 816 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 826 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 831 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 841 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 855 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 808 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 814 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 823 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 832 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 839 | CLA  | O1A-CGA-O2A-C1  |
| 22  | K     | 204 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 315 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 7     | 322 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 307 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 9     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 6     | 323 | LHG  | O10-C23-O8-C6   |
| 34  | J     | 101 | LMG  | O10-C28-O8-C9   |
| 39  | 5     | 316 | CHL  | O1A-CGA-O2A-C1  |
| 39  | 9     | 312 | CHL  | O1A-CGA-O2A-C1  |
| 22  | K     | 202 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 316 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 2     | 304 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 827 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 305 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 314 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 316 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 310 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 320 | CLA  | O1D-CGD-O2D-CED |
| 22  | K     | 202 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 315 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 315 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 316 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 802 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 821 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 832 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 828 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 836 | CLA  | O1D-CGD-O2D-CED |
| 22  | F     | 301 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 319 | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 301 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 816 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 841 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 805 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 812 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 839 | CLA  | CBA-CGA-O2A-C1  |
| 22  | K     | 204 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 315 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 7     | 322 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 812 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 34  | J     | 101 | LMG  | C29-C28-O8-C9   |
| 39  | 9     | 312 | CHL  | CBA-CGA-O2A-C1  |
| 22  | B     | 811 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 304 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 306 | CLA  | CBD-CGD-O2D-CED |
| 22  | 9     | 306 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 807 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 812 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 814 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 815 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 819 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 821 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 822 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 823 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 827 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 837 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 819 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 821 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 834 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 307 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 307 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 3     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 324 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 305 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 810 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 812 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 818 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 301 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 9     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 40  | 1     | 318 | SQD  | O10-C23-O48-C46 |
| 41  | 7     | 319 | 3PH  | O32-C31-O31-C3  |
| 22  | B     | 812 | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 308 | CLA  | C8-C10-C11-C12  |
| 22  | 1     | 311 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 1     | 315 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 315 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 3     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 321 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 9     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 39  | Z     | 311 | CHL  | C2C-C3C-CAC-CBC |
| 39  | 9     | 312 | CHL  | C2C-C3C-CAC-CBC |
| 22  | A     | 818 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 820 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 801 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 806 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 841 | CLA  | O1D-CGD-O2D-CED |
| 22  | F     | 304 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 306 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 316 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 303 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 312 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 315 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 324 | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 317 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 313 | CLA  | O1D-CGD-O2D-CED |
| 39  | 6     | 318 | CHL  | O1D-CGD-O2D-CED |
| 22  | A     | 817 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 828 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 808 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 812 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 824 | CLA  | O1D-CGD-O2D-CED |
| 22  | K     | 205 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 313 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 316 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 305 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 316 | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 305 | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 313 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 815 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 301 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 323 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 326 | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 307 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 308 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 311 | CLA  | O1D-CGD-O2D-CED |
| 39  | Z     | 312 | CHL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 39  | 8     | 312 | CHL  | O1D-CGD-O2D-CED |
| 25  | 3     | 321 | LHG  | C24-C23-O8-C6   |
| 22  | B     | 811 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 838 | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 306 | CLA  | C5-C6-C7-C8     |
| 23  | A     | 843 | PQN  | C18-C20-C21-C22 |
| 22  | A     | 812 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 305 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 307 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 811 | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 301 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 306 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 1     | 317 | LHG  | O9-C7-O7-C5     |
| 34  | F     | 308 | LMG  | O9-C10-O7-C8    |
| 34  | J     | 101 | LMG  | O9-C10-O7-C8    |
| 41  | 7     | 319 | 3PH  | O22-C21-O21-C2  |
| 41  | 6     | 324 | 3PH  | O22-C21-O21-C2  |
| 22  | B     | 831 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 802 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 805 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 818 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 820 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 855 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 801 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 816 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 819 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 827 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 828 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 829 | CLA  | C3-C5-C6-C7     |
| 22  | F     | 302 | CLA  | C3-C5-C6-C7     |
| 22  | L     | 202 | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 314 | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 306 | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 307 | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 314 | CLA  | C3-C5-C6-C7     |
| 22  | 8     | 307 | CLA  | C3-C5-C6-C7     |
| 22  | 8     | 310 | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 315 | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 322 | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 311 | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 313 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 9     | 305 | CLA  | C3-C5-C6-C7     |
| 31  | 3     | 301 | DGD  | C2G-C1G-O1G-C1A |
| 22  | B     | 814 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 819 | CLA  | O1D-CGD-O2D-CED |
| 39  | 9     | 312 | CHL  | O1D-CGD-O2D-CED |
| 22  | A     | 807 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 808 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 814 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 821 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 823 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 831 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 837 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 855 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 808 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 813 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 814 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 823 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 831 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 832 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 307 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 316 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 316 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 324 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 305 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 810 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 818 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 301 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 307 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 326 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 26  | A     | 851 | NKP  | CAL-CAK-OAJ-CAI |
| 39  | 5     | 316 | CHL  | CBA-CGA-O2A-C1  |
| 40  | 1     | 318 | SQD  | C24-C23-O48-C46 |
| 41  | 7     | 319 | 3PH  | C32-C31-O31-C3  |
| 22  | A     | 803 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 830 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 831 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 841 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 813 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 817 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 833 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 834 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 837 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 842 | CLA  | CBD-CGD-O2D-CED |
| 22  | K     | 202 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 308 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 311 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 805 | CLA  | CBD-CGD-O2D-CED |
| 22  | 4     | 808 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 307 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 311 | CLA  | CBD-CGD-O2D-CED |
| 39  | 5     | 316 | CHL  | CBD-CGD-O2D-CED |
| 39  | 6     | 315 | CHL  | CBD-CGD-O2D-CED |
| 25  | B     | 850 | LHG  | C8-C7-O7-C5     |
| 31  | B     | 852 | DGD  | C2B-C1B-O2G-C2G |
| 34  | J     | 101 | LMG  | C11-C10-O7-C8   |
| 22  | A     | 807 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 816 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 833 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 855 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 816 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 821 | CLA  | O1D-CGD-O2D-CED |
| 22  | F     | 305 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 201 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 308 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 313 | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 309 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 308 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 304 | CLA  | O1D-CGD-O2D-CED |
| 39  | 2     | 303 | CHL  | O1D-CGD-O2D-CED |
| 22  | 8     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 835 | CLA  | O1D-CGD-O2D-CED |
| 39  | 4     | 814 | CHL  | O1D-CGD-O2D-CED |
| 22  | A     | 817 | CLA  | C4-C3-C5-C6     |
| 22  | K     | 205 | CLA  | C4-C3-C5-C6     |
| 22  | 4     | 808 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 817 | CLA  | C2-C3-C5-C6     |
| 22  | K     | 205 | CLA  | C2-C3-C5-C6     |
| 22  | 3     | 319 | CLA  | C2-C3-C5-C6     |
| 22  | 4     | 808 | CLA  | C2-C3-C5-C6     |
| 25  | B     | 850 | LHG  | C24-C23-O8-C6   |
| 25  | B     | 851 | LHG  | C24-C23-O8-C6   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 3     | 320 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 311 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 840 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 318 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 322 | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 309 | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 322 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 810 | CLA  | C8-C10-C11-C12  |
| 22  | 6     | 308 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 836 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 840 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 803 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 812 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 828 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 836 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 841 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 815 | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 313 | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 313 | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 308 | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 310 | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 312 | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 312 | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 324 | CLA  | C3-C5-C6-C7     |
| 22  | 8     | 308 | CLA  | C3-C5-C6-C7     |
| 22  | 9     | 307 | CLA  | C3-C5-C6-C7     |
| 39  | 4     | 813 | CHL  | O1D-CGD-O2D-CED |
| 22  | A     | 812 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 815 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 819 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 822 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 827 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 828 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 832 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 819 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 820 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 821 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 834 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 840 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 304 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 22  | 1     | 306  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 310  | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 307  | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 310  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 308  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 310  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 312  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 311  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 301  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 311  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 313  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 306  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 309  | CLA  | CBA-CGA-O2A-C1  |
| 39  | 2     | 303  | CHL  | CBA-CGA-O2A-C1  |
| 31  | B     | 852  | DGD  | C8A-C9A-CAA-CBA |
| 24  | A     | 845  | BCR  | C9-C10-C11-C12  |
| 24  | A     | 845  | BCR  | C19-C20-C21-C22 |
| 24  | A     | 846  | BCR  | C9-C10-C11-C12  |
| 24  | A     | 846  | BCR  | C15-C16-C17-C18 |
| 24  | B     | 848  | BCR  | C15-C16-C17-C18 |
| 24  | B     | 849  | BCR  | C19-C20-C21-C22 |
| 24  | B     | 853  | BCR  | C15-C16-C17-C18 |
| 24  | G     | 203  | BCR  | C19-C20-C21-C22 |
| 24  | I     | 4001 | BCR  | C13-C14-C15-C16 |
| 24  | J     | 104  | BCR  | C19-C20-C21-C22 |
| 24  | K     | 206  | BCR  | C15-C16-C17-C18 |
| 24  | L     | 204  | BCR  | C9-C10-C11-C12  |
| 24  | 7     | 303  | BCR  | C9-C10-C11-C12  |
| 24  | 7     | 303  | BCR  | C19-C20-C21-C22 |
| 24  | 4     | 804  | BCR  | C13-C14-C15-C16 |
| 24  | 5     | 304  | BCR  | C9-C10-C11-C12  |
| 24  | 6     | 305  | BCR  | C9-C10-C11-C12  |
| 24  | 6     | 305  | BCR  | C13-C14-C15-C16 |
| 24  | 6     | 306  | BCR  | C13-C14-C15-C16 |
| 24  | 6     | 306  | BCR  | C19-C20-C21-C22 |
| 36  | 5     | 306  | C7Z  | C29-C30-C31-C32 |
| 22  | A     | 828  | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 842  | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 820  | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 831 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 304 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 306 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 3     | 316 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 806 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 322 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 301 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 9     | 306 | CLA  | O1A-CGA-O2A-C1  |
| 26  | A     | 851 | NKP  | OAE-CAK-OAJ-CAI |
| 39  | 7     | 313 | CHL  | O1A-CGA-O2A-C1  |
| 39  | 2     | 303 | CHL  | O1A-CGA-O2A-C1  |
| 25  | 4     | 820 | LHG  | O9-C7-O7-C5     |
| 22  | G     | 202 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 306 | CLA  | O1D-CGD-O2D-CED |
| 22  | 3     | 320 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 814 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 831 | CLA  | C5-C6-C7-C8     |
| 22  | 3     | 320 | CLA  | O1A-CGA-O2A-C1  |
| 25  | Z     | 317 | LHG  | C11-C12-C13-C14 |
| 31  | 3     | 301 | DGD  | C8A-C9A-CAA-CBA |
| 22  | A     | 804 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 809 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 812 | CLA  | O1D-CGD-O2D-CED |
| 21  | A     | 801 | CL0  | C3-C5-C6-C7     |
| 22  | A     | 809 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 816 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 821 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 810 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 822 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 823 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 825 | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 308 | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 319 | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 318 | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 302 | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 309 | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 319 | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 322 | CLA  | C3-C5-C6-C7     |
| 22  | 2     | 301 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 826 | CLA  | CBD-CGD-O2D-CED |
| 25  | A     | 849 | LHG  | O2-C2-C3-O3     |
| 25  | A     | 850 | LHG  | O2-C2-C3-O3     |
| 25  | B     | 803 | LHG  | O2-C2-C3-O3     |
| 25  | B     | 850 | LHG  | O2-C2-C3-O3     |
| 25  | 3     | 321 | LHG  | O2-C2-C3-O3     |
| 25  | 9     | 315 | LHG  | O2-C2-C3-O3     |
| 22  | A     | 838 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 818 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 307 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 304 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 806 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 307 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 833 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 836 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 839 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 816 | CLA  | CBA-CGA-O2A-C1  |
| 22  | F     | 302 | CLA  | CBA-CGA-O2A-C1  |
| 22  | Z     | 306 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 4     | 808 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 39  | 7     | 313 | CHL  | CBA-CGA-O2A-C1  |
| 22  | A     | 808 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 833 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 3     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 326 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 33  | G     | 204 | LMT  | C4'-C5'-C6'-O6' |
| 25  | Z     | 317 | LHG  | C23-C24-C25-C26 |
| 22  | A     | 814 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 311 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 315 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 815 | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 825 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 304 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 310 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 310 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 314 | CLA  | CBD-CGD-O2D-CED |
| 39  | 6     | 316 | CHL  | CBD-CGD-O2D-CED |
| 25  | 7     | 318 | LHG  | C8-C7-O7-C5     |
| 35  | J     | 102 | T7X  | C12-C10-O16-C8  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 816 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 820 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 309 | CLA  | O1D-CGD-O2D-CED |
| 39  | 7     | 313 | CHL  | O1D-CGD-O2D-CED |
| 22  | A     | 807 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 814 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 821 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 838 | CLA  | C3-C5-C6-C7     |
| 22  | F     | 301 | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 322 | CLA  | C3-C5-C6-C7     |
| 22  | 4     | 812 | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 301 | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 310 | CLA  | C3-C5-C6-C7     |
| 22  | L     | 201 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 313 | CLA  | CBD-CGD-O2D-CED |
| 22  | 2     | 304 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 808 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 834 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 836 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 807 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 823 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 304 | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 307 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 305 | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 302 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 842 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 833 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 322 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 839 | CLA  | O1A-CGA-O2A-C1  |
| 22  | F     | 302 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 808 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 819 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 807 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 825 | CLA  | C8-C10-C11-C12  |
| 26  | A     | 851 | NKP  | CAH-CAG-OAF-PAC |
| 22  | A     | 842 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 839 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 1     | 307 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 833 | CLA  | O1A-CGA-O2A-C1  |
| 22  | L     | 203 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 310 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 33  | F     | 307  | LMT  | O5'-C1'-O1'-C1  |
| 33  | 1     | 301  | LMT  | O5'-C1'-O1'-C1  |
| 22  | A     | 840  | CLA  | CBA-CGA-O2A-C1  |
| 22  | L     | 203  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 317  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 310  | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 308  | CLA  | CBA-CGA-O2A-C1  |
| 39  | 6     | 315  | CHL  | CBA-CGA-O2A-C1  |
| 22  | B     | 822  | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 838  | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 322  | CLA  | CBD-CGD-O2D-CED |
| 22  | 6     | 310  | CLA  | CBD-CGD-O2D-CED |
| 25  | 3     | 321  | LHG  | O10-C23-O8-C6   |
| 22  | G     | 202  | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 811  | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 305  | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 306  | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 301  | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 306  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 810  | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 323  | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 314  | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 817  | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 310  | CLA  | C3-C5-C6-C7     |
| 24  | A     | 847  | BCR  | C15-C16-C17-C18 |
| 24  | A     | 856  | BCR  | C13-C14-C15-C16 |
| 24  | A     | 856  | BCR  | C19-C20-C21-C22 |
| 24  | B     | 845  | BCR  | C15-C16-C17-C18 |
| 24  | B     | 845  | BCR  | C19-C20-C21-C22 |
| 24  | I     | 4001 | BCR  | C15-C16-C17-C18 |
| 24  | 7     | 303  | BCR  | C15-C16-C17-C18 |
| 24  | 8     | 304  | BCR  | C15-C16-C17-C18 |
| 24  | 8     | 304  | BCR  | C19-C20-C21-C22 |
| 24  | 4     | 804  | BCR  | C15-C16-C17-C18 |
| 24  | 4     | 804  | BCR  | C19-C20-C21-C22 |
| 24  | 6     | 306  | BCR  | C15-C16-C17-C18 |
| 22  | 9     | 308  | CLA  | O1A-CGA-O2A-C1  |
| 35  | J     | 102  | T7X  | O17-C10-O16-C8  |
| 25  | B     | 803  | LHG  | C1-C2-C3-O3     |
| 25  | 4     | 820  | LHG  | C1-C2-C3-O3     |
| 25  | 5     | 324  | LHG  | C1-C2-C3-O3     |
| 25  | 6     | 323  | LHG  | C1-C2-C3-O3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 810 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 834 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 809 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 22  | K     | 205 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 5     | 319 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 307 | CLA  | CBA-CGA-O2A-C1  |
| 25  | 5     | 324 | LHG  | C24-C23-O8-C6   |
| 39  | 8     | 315 | CHL  | CBA-CGA-O2A-C1  |
| 22  | 1     | 310 | CLA  | CBD-CGD-O2D-CED |
| 22  | 5     | 313 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 812 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 805 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 808 | CLA  | O1D-CGD-O2D-CED |
| 22  | 4     | 811 | CLA  | O1D-CGD-O2D-CED |
| 22  | 9     | 307 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 834 | CLA  | O1D-CGD-O2D-CED |
| 41  | 6     | 324 | 3PH  | C22-C23-C24-C25 |
| 22  | 3     | 314 | CLA  | C4-C3-C5-C6     |
| 22  | 3     | 314 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 817 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 830 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 811 | CLA  | C3-C5-C6-C7     |
| 22  | 9     | 306 | CLA  | C3-C5-C6-C7     |
| 39  | 9     | 312 | CHL  | C3-C5-C6-C7     |
| 22  | A     | 837 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 802 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 803 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 807 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 808 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 812 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 812 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 814 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 815 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 816 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 818 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 818 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 820 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 823 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 823 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 830 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 832 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 834 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 835 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 838 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 854 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 855 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 801 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 809 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 813 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 815 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 818 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 819 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 820 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 824 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 825 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 828 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 829 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 830 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 833 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 842 | CLA  | C11-C10-C8-C9   |
| 22  | F     | 304 | CLA  | C6-C7-C8-C9     |
| 22  | L     | 202 | CLA  | C11-C12-C13-C14 |
| 22  | 1     | 304 | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 306 | CLA  | C11-C12-C13-C14 |
| 22  | 1     | 307 | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 309 | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 310 | CLA  | C11-C10-C8-C9   |
| 22  | 1     | 313 | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 316 | CLA  | C11-C10-C8-C9   |
| 22  | Z     | 303 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 313 | CLA  | C6-C7-C8-C9     |
| 22  | 3     | 312 | CLA  | C11-C10-C8-C9   |
| 22  | 3     | 314 | CLA  | C11-C10-C8-C9   |
| 22  | 3     | 318 | CLA  | C6-C7-C8-C9     |
| 22  | 3     | 322 | CLA  | C6-C7-C8-C9     |
| 22  | 3     | 322 | CLA  | C11-C10-C8-C9   |
| 22  | 3     | 322 | CLA  | C11-C12-C13-C14 |
| 22  | 7     | 304 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 7     | 307 | CLA  | C11-C10-C8-C9   |
| 22  | 7     | 312 | CLA  | C11-C10-C8-C9   |
| 22  | 7     | 324 | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 324 | CLA  | C11-C10-C8-C9   |
| 22  | 8     | 308 | CLA  | C6-C7-C8-C9     |
| 22  | 4     | 807 | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 313 | CLA  | C11-C10-C8-C9   |
| 22  | 5     | 318 | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 322 | CLA  | C11-C10-C8-C9   |
| 22  | 6     | 307 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 312 | CLA  | C6-C7-C8-C9     |
| 22  | 9     | 305 | CLA  | C6-C7-C8-C9     |
| 39  | 3     | 317 | CHL  | C11-C10-C8-C9   |
| 39  | 5     | 316 | CHL  | C14-C13-C15-C16 |
| 22  | B     | 817 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 833 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 842 | CLA  | O1D-CGD-O2D-CED |
| 39  | 6     | 315 | CHL  | O1D-CGD-O2D-CED |
| 33  | F     | 307 | LMT  | C2'-C1'-O1'-C1  |
| 33  | 1     | 301 | LMT  | C2'-C1'-O1'-C1  |
| 25  | 4     | 820 | LHG  | O2-C2-C3-O3     |
| 43  | 8     | 319 | LPX  | O1-C3-C4-O5     |
| 22  | A     | 841 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 311 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 311 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 834 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 840 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 817 | CLA  | O1A-CGA-O2A-C1  |
| 22  | K     | 205 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 1     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 837 | CLA  | O1D-CGD-O2D-CED |
| 24  | A     | 844 | BCR  | C11-C12-C13-C35 |
| 24  | A     | 844 | BCR  | C36-C18-C19-C20 |
| 24  | A     | 844 | BCR  | C37-C22-C23-C24 |
| 24  | A     | 846 | BCR  | C11-C12-C13-C35 |
| 24  | A     | 847 | BCR  | C7-C8-C9-C34    |
| 24  | A     | 847 | BCR  | C36-C18-C19-C20 |
| 24  | A     | 848 | BCR  | C11-C12-C13-C35 |
| 24  | A     | 856 | BCR  | C7-C8-C9-C34    |
| 24  | A     | 856 | BCR  | C36-C18-C19-C20 |
| 24  | A     | 856 | BCR  | C37-C22-C23-C24 |
| 24  | B     | 845 | BCR  | C11-C12-C13-C35 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 24  | B     | 845  | BCR  | C36-C18-C19-C20 |
| 24  | B     | 846  | BCR  | C7-C8-C9-C34    |
| 24  | B     | 847  | BCR  | C11-C12-C13-C35 |
| 24  | B     | 847  | BCR  | C36-C18-C19-C20 |
| 24  | B     | 848  | BCR  | C7-C8-C9-C34    |
| 24  | B     | 853  | BCR  | C7-C8-C9-C34    |
| 24  | B     | 853  | BCR  | C11-C12-C13-C35 |
| 24  | B     | 853  | BCR  | C36-C18-C19-C20 |
| 24  | B     | 853  | BCR  | C37-C22-C23-C24 |
| 24  | F     | 303  | BCR  | C37-C22-C23-C24 |
| 24  | G     | 203  | BCR  | C7-C8-C9-C34    |
| 24  | G     | 203  | BCR  | C37-C22-C23-C24 |
| 24  | I     | 4001 | BCR  | C7-C8-C9-C34    |
| 24  | I     | 4001 | BCR  | C11-C12-C13-C35 |
| 24  | J     | 104  | BCR  | C7-C8-C9-C34    |
| 24  | K     | 206  | BCR  | C11-C12-C13-C35 |
| 24  | K     | 206  | BCR  | C37-C22-C23-C24 |
| 24  | L     | 204  | BCR  | C7-C8-C9-C34    |
| 24  | 3     | 304  | BCR  | C7-C8-C9-C34    |
| 24  | 3     | 304  | BCR  | C36-C18-C19-C20 |
| 24  | 3     | 304  | BCR  | C37-C22-C23-C24 |
| 24  | 3     | 305  | BCR  | C7-C8-C9-C34    |
| 24  | 3     | 305  | BCR  | C37-C22-C23-C24 |
| 24  | 3     | 306  | BCR  | C36-C18-C19-C20 |
| 24  | 3     | 307  | BCR  | C7-C8-C9-C34    |
| 24  | 3     | 307  | BCR  | C37-C22-C23-C24 |
| 24  | 7     | 303  | BCR  | C36-C18-C19-C20 |
| 24  | 4     | 804  | BCR  | C36-C18-C19-C20 |
| 24  | 5     | 304  | BCR  | C36-C18-C19-C20 |
| 24  | 5     | 305  | BCR  | C36-C18-C19-C20 |
| 24  | 5     | 305  | BCR  | C37-C22-C23-C24 |
| 24  | 6     | 305  | BCR  | C7-C8-C9-C34    |
| 24  | 6     | 305  | BCR  | C36-C18-C19-C20 |
| 24  | 6     | 306  | BCR  | C11-C12-C13-C35 |
| 24  | 6     | 306  | BCR  | C36-C18-C19-C20 |
| 32  | F     | 306  | RRX  | C7-C8-C9-C34    |
| 36  | J     | 105  | C7Z  | C7-C8-C9-C19    |
| 36  | J     | 105  | C7Z  | C11-C12-C13-C20 |
| 36  | 5     | 306  | C7Z  | C7-C8-C9-C19    |
| 36  | 5     | 306  | C7Z  | C11-C12-C13-C20 |
| 36  | 5     | 306  | C7Z  | C27-C28-C29-C39 |
| 38  | 1     | 302  | LUT  | C11-C12-C13-C20 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 38  | 1     | 302  | LUT  | C27-C28-C29-C39 |
| 38  | 1     | 302  | LUT  | C31-C32-C33-C40 |
| 38  | 1     | 303  | LUT  | C11-C12-C13-C20 |
| 38  | Z     | 302  | LUT  | C11-C12-C13-C20 |
| 38  | 3     | 302  | LUT  | C11-C12-C13-C20 |
| 38  | 3     | 302  | LUT  | C31-C32-C33-C40 |
| 38  | 3     | 303  | LUT  | C7-C8-C9-C19    |
| 38  | 3     | 303  | LUT  | C11-C12-C13-C20 |
| 38  | 8     | 302  | LUT  | C27-C28-C29-C39 |
| 38  | 4     | 803  | LUT  | C11-C12-C13-C20 |
| 38  | 5     | 302  | LUT  | C31-C32-C33-C40 |
| 38  | 5     | 303  | LUT  | C7-C8-C9-C19    |
| 38  | 5     | 303  | LUT  | C11-C12-C13-C20 |
| 38  | 6     | 303  | LUT  | C31-C32-C33-C40 |
| 38  | 6     | 304  | LUT  | C11-C12-C13-C20 |
| 38  | 9     | 302  | LUT  | C7-C8-C9-C19    |
| 33  | G     | 204  | LMT  | O5'-C5'-C6'-O6' |
| 24  | A     | 844  | BCR  | C11-C12-C13-C14 |
| 24  | A     | 844  | BCR  | C17-C18-C19-C20 |
| 24  | A     | 845  | BCR  | C7-C8-C9-C10    |
| 24  | A     | 846  | BCR  | C11-C12-C13-C14 |
| 24  | A     | 847  | BCR  | C17-C18-C19-C20 |
| 24  | A     | 856  | BCR  | C7-C8-C9-C10    |
| 24  | A     | 856  | BCR  | C21-C22-C23-C24 |
| 24  | B     | 844  | BCR  | C7-C8-C9-C10    |
| 24  | B     | 845  | BCR  | C21-C22-C23-C24 |
| 24  | B     | 848  | BCR  | C7-C8-C9-C10    |
| 24  | B     | 849  | BCR  | C17-C18-C19-C20 |
| 24  | B     | 853  | BCR  | C11-C12-C13-C14 |
| 24  | B     | 853  | BCR  | C21-C22-C23-C24 |
| 24  | F     | 303  | BCR  | C21-C22-C23-C24 |
| 24  | G     | 203  | BCR  | C21-C22-C23-C24 |
| 24  | I     | 4001 | BCR  | C7-C8-C9-C10    |
| 24  | I     | 4001 | BCR  | C11-C12-C13-C14 |
| 24  | J     | 104  | BCR  | C7-C8-C9-C10    |
| 24  | K     | 206  | BCR  | C21-C22-C23-C24 |
| 24  | L     | 204  | BCR  | C11-C12-C13-C14 |
| 24  | L     | 204  | BCR  | C17-C18-C19-C20 |
| 24  | 3     | 304  | BCR  | C21-C22-C23-C24 |
| 24  | 3     | 305  | BCR  | C7-C8-C9-C10    |
| 24  | 3     | 305  | BCR  | C17-C18-C19-C20 |
| 24  | 3     | 305  | BCR  | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | 3     | 307 | BCR  | C7-C8-C9-C10    |
| 24  | 3     | 307 | BCR  | C21-C22-C23-C24 |
| 24  | 7     | 303 | BCR  | C17-C18-C19-C20 |
| 24  | 4     | 804 | BCR  | C11-C12-C13-C14 |
| 24  | 4     | 804 | BCR  | C17-C18-C19-C20 |
| 24  | 5     | 304 | BCR  | C17-C18-C19-C20 |
| 24  | 6     | 305 | BCR  | C7-C8-C9-C10    |
| 24  | 6     | 305 | BCR  | C17-C18-C19-C20 |
| 24  | 6     | 306 | BCR  | C7-C8-C9-C10    |
| 24  | 6     | 306 | BCR  | C11-C12-C13-C14 |
| 24  | 6     | 306 | BCR  | C17-C18-C19-C20 |
| 36  | J     | 105 | C7Z  | C11-C12-C13-C14 |
| 36  | 5     | 306 | C7Z  | C7-C8-C9-C10    |
| 36  | 5     | 306 | C7Z  | C31-C32-C33-C34 |
| 36  | 5     | 306 | C7Z  | C27-C28-C29-C30 |
| 38  | 1     | 302 | LUT  | C7-C8-C9-C10    |
| 38  | 3     | 303 | LUT  | C7-C8-C9-C10    |
| 38  | 5     | 302 | LUT  | C7-C8-C9-C10    |
| 38  | 5     | 303 | LUT  | C7-C8-C9-C10    |
| 38  | 9     | 302 | LUT  | C11-C12-C13-C14 |
| 22  | B     | 839 | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 303 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 316 | CLA  | C3-C5-C6-C7     |
| 22  | 8     | 309 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 4     | 806 | CLA  | C2A-CAA-CBA-CGA |
| 25  | 6     | 323 | LHG  | C7-C8-C9-C10    |
| 22  | B     | 809 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 39  | 8     | 315 | CHL  | O1A-CGA-O2A-C1  |
| 22  | K     | 203 | CLA  | C3-C5-C6-C7     |
| 25  | 7     | 318 | LHG  | O9-C7-O7-C5     |
| 22  | A     | 840 | CLA  | CBD-CGD-O2D-CED |
| 22  | 3     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 303 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 832 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 838 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 839 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 806 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 825 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 831 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 1     | 314 | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 310 | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 316 | CLA  | C2-C1-O2A-CGA   |
| 22  | 8     | 310 | CLA  | C2-C1-O2A-CGA   |
| 22  | 8     | 311 | CLA  | C2-C1-O2A-CGA   |
| 22  | 4     | 810 | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 302 | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 307 | CLA  | C2-C1-O2A-CGA   |
| 25  | 8     | 317 | LHG  | C25-C26-C27-C28 |
| 25  | B     | 850 | LHG  | O10-C23-O8-C6   |
| 25  | B     | 851 | LHG  | O10-C23-O8-C6   |
| 22  | A     | 830 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 831 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 806 | CLA  | CBD-CGD-O2D-CED |
| 22  | 1     | 306 | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 314 | CLA  | C8-C10-C11-C12  |
| 25  | 7     | 318 | LHG  | O1-C1-C2-O2     |
| 22  | A     | 834 | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 307 | CLA  | C3-C5-C6-C7     |
| 22  | 6     | 310 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 810 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 839 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 806 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 820 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 827 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 841 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 815 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 819 | CLA  | C11-C10-C8-C7   |
| 22  | L     | 201 | CLA  | C6-C7-C8-C10    |
| 22  | Z     | 309 | CLA  | C6-C7-C8-C10    |
| 22  | 3     | 314 | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 312 | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 317 | CLA  | C6-C7-C8-C10    |
| 22  | 8     | 310 | CLA  | C11-C10-C8-C7   |
| 22  | 6     | 302 | CLA  | C6-C7-C8-C10    |
| 22  | 6     | 319 | CLA  | C6-C7-C8-C10    |
| 22  | 9     | 306 | CLA  | C11-C10-C8-C7   |
| 39  | 8     | 315 | CHL  | C11-C10-C8-C7   |
| 39  | 9     | 312 | CHL  | C12-C13-C15-C16 |
| 22  | 5     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 24  | A     | 844 | BCR  | C15-C16-C17-C18 |
| 24  | A     | 848 | BCR  | C13-C14-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 24  | B     | 845  | BCR  | C13-C14-C15-C16 |
| 24  | B     | 847  | BCR  | C9-C10-C11-C12  |
| 24  | B     | 849  | BCR  | C13-C14-C15-C16 |
| 24  | B     | 853  | BCR  | C13-C14-C15-C16 |
| 24  | I     | 4001 | BCR  | C9-C10-C11-C12  |
| 24  | J     | 104  | BCR  | C13-C14-C15-C16 |
| 24  | J     | 104  | BCR  | C15-C16-C17-C18 |
| 24  | 3     | 306  | BCR  | C13-C14-C15-C16 |
| 24  | 5     | 304  | BCR  | C15-C16-C17-C18 |
| 24  | 6     | 305  | BCR  | C15-C16-C17-C18 |
| 38  | 6     | 303  | LUT  | C9-C10-C11-C12  |
| 38  | 6     | 304  | LUT  | C9-C10-C11-C12  |
| 22  | 5     | 307  | CLA  | O1D-CGD-O2D-CED |
| 39  | 5     | 316  | CHL  | O1D-CGD-O2D-CED |
| 22  | B     | 808  | CLA  | C3-C5-C6-C7     |
| 22  | B     | 814  | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 309  | CLA  | C3-C5-C6-C7     |
| 22  | B     | 818  | CLA  | C10-C11-C12-C13 |
| 22  | 5     | 310  | CLA  | C5-C6-C7-C8     |
| 25  | A     | 850  | LHG  | C23-C24-C25-C26 |
| 25  | 8     | 317  | LHG  | C23-C24-C25-C26 |
| 25  | 6     | 323  | LHG  | C23-C24-C25-C26 |
| 22  | 5     | 319  | CLA  | O1A-CGA-O2A-C1  |
| 25  | 5     | 324  | LHG  | O10-C23-O8-C6   |
| 22  | 7     | 307  | CLA  | CBD-CGD-O2D-CED |
| 22  | B     | 813  | CLA  | O1D-CGD-O2D-CED |
| 22  | K     | 202  | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 818  | CLA  | C5-C6-C7-C8     |
| 22  | 9     | 303  | CLA  | C10-C11-C12-C13 |
| 22  | A     | 855  | CLA  | C2A-CAA-CBA-CGA |
| 22  | K     | 204  | CLA  | C2A-CAA-CBA-CGA |
| 22  | K     | 205  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 315  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 320  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 4     | 806  | CLA  | C3-C5-C6-C7     |
| 22  | 4     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 5     | 313  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 5     | 318  | CLA  | C2A-CAA-CBA-CGA |
| 22  | 9     | 305  | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 819  | CLA  | C8-C10-C11-C12  |
| 22  | B     | 805  | CLA  | C5-C6-C7-C8     |
| 22  | B     | 829  | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | F     | 304 | CLA  | C5-C6-C7-C8     |
| 22  | 3     | 313 | CLA  | C10-C11-C12-C13 |
| 22  | 7     | 306 | CLA  | C8-C10-C11-C12  |
| 22  | 9     | 303 | CLA  | C5-C6-C7-C8     |
| 25  | A     | 849 | LHG  | C23-C24-C25-C26 |
| 25  | A     | 850 | LHG  | C7-C8-C9-C10    |
| 25  | 4     | 820 | LHG  | C23-C24-C25-C26 |
| 34  | F     | 308 | LMG  | C10-C11-C12-C13 |
| 22  | 1     | 308 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 815 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 854 | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 307 | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 309 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 803 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 819 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 825 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 828 | CLA  | C10-C11-C12-C13 |
| 22  | 1     | 316 | CLA  | C10-C11-C12-C13 |
| 22  | 3     | 312 | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 306 | CLA  | C10-C11-C12-C13 |
| 22  | 6     | 312 | CLA  | C5-C6-C7-C8     |
| 22  | 9     | 305 | CLA  | C5-C6-C7-C8     |
| 25  | B     | 851 | LHG  | O2-C2-C3-O3     |
| 25  | Z     | 317 | LHG  | O2-C2-C3-O3     |
| 25  | 7     | 318 | LHG  | O2-C2-C3-O3     |
| 25  | 8     | 317 | LHG  | O2-C2-C3-O3     |
| 25  | 5     | 324 | LHG  | O2-C2-C3-O3     |
| 25  | 6     | 323 | LHG  | O2-C2-C3-O3     |
| 33  | 4     | 822 | LMT  | O1'-C1-C2-C3    |
| 22  | A     | 830 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 310 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 839 | CLA  | CBD-CGD-O2D-CED |
| 22  | 7     | 317 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 39  | 6     | 315 | CHL  | O1A-CGA-O2A-C1  |
| 25  | B     | 803 | LHG  | C23-C24-C25-C26 |
| 27  | A     | 852 | DGA  | CA7-CA8-CA9-CAA |
| 22  | A     | 808 | CLA  | C3-C5-C6-C7     |
| 22  | 8     | 311 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 306 | CLA  | C8-C10-C11-C12  |
| 22  | 9     | 305 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 5     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 25  | B     | 803 | LHG  | C7-C8-C9-C10    |
| 25  | 1     | 317 | LHG  | C23-C24-C25-C26 |
| 25  | Z     | 317 | LHG  | C7-C8-C9-C10    |
| 22  | A     | 815 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 826 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 310 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 841 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 3     | 301 | DGD  | C2A-C1A-O1G-C1G |
| 25  | 4     | 821 | LHG  | C8-C7-O7-C5     |
| 41  | 8     | 320 | 3PH  | C3A-C3B-C3C-C3D |
| 22  | 3     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 9     | 303 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 8     | 309 | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 309 | CLA  | C3-C5-C6-C7     |
| 25  | 5     | 324 | LHG  | C11-C10-C9-C8   |
| 24  | A     | 844 | BCR  | C19-C20-C21-C22 |
| 24  | A     | 847 | BCR  | C9-C10-C11-C12  |
| 24  | A     | 848 | BCR  | C19-C20-C21-C22 |
| 24  | A     | 856 | BCR  | C15-C16-C17-C18 |
| 24  | B     | 848 | BCR  | C9-C10-C11-C12  |
| 24  | B     | 849 | BCR  | C15-C16-C17-C18 |
| 24  | F     | 303 | BCR  | C15-C16-C17-C18 |
| 24  | 5     | 304 | BCR  | C19-C20-C21-C22 |
| 24  | 6     | 305 | BCR  | C19-C20-C21-C22 |
| 38  | 4     | 802 | LUT  | C9-C10-C11-C12  |
| 22  | L     | 202 | CLA  | C8-C10-C11-C12  |
| 25  | 5     | 324 | LHG  | C7-C8-C9-C10    |
| 25  | 9     | 315 | LHG  | C23-C24-C25-C26 |
| 25  | 4     | 821 | LHG  | O9-C7-O7-C5     |
| 25  | A     | 849 | LHG  | C1-C2-C3-O3     |
| 25  | B     | 850 | LHG  | C1-C2-C3-O3     |
| 25  | B     | 851 | LHG  | C1-C2-C3-O3     |
| 25  | Z     | 317 | LHG  | C1-C2-C3-O3     |
| 25  | 8     | 317 | LHG  | C1-C2-C3-O3     |
| 22  | A     | 824 | CLA  | C2A-CAA-CBA-CGA |
| 22  | F     | 304 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 1     | 306 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 9     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 805 | CLA  | CBA-CGA-O2A-C1  |
| 22  | G     | 201 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | 4     | 820 | LHG  | C24-C23-O8-C6   |
| 25  | 4     | 821 | LHG  | C24-C23-O8-C6   |
| 25  | 7     | 318 | LHG  | C11-C10-C9-C8   |
| 22  | A     | 825 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 840 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 801 | CLA  | C13-C15-C16-C17 |
| 22  | Z     | 309 | CLA  | C5-C6-C7-C8     |
| 22  | 3     | 313 | CLA  | C8-C10-C11-C12  |
| 22  | 1     | 304 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 314 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 827 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 855 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 806 | CLA  | C8-C10-C11-C12  |
| 22  | Z     | 303 | CLA  | C5-C6-C7-C8     |
| 22  | 8     | 307 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 806 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 820 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 825 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 828 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 817 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 830 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 841 | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 323 | CLA  | C13-C15-C16-C17 |
| 22  | 5     | 315 | CLA  | C8-C10-C11-C12  |
| 22  | 6     | 307 | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 322 | CLA  | C8-C10-C11-C12  |
| 22  | 2     | 304 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 323 | CLA  | CBA-CGA-O2A-C1  |
| 22  | L     | 201 | CLA  | O1D-CGD-O2D-CED |
| 22  | Z     | 310 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 202 | CLA  | O1A-CGA-O2A-C1  |
| 22  | K     | 205 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 825 | CLA  | O1D-CGD-O2D-CED |
| 39  | 6     | 316 | CHL  | O1D-CGD-O2D-CED |
| 25  | 1     | 317 | LHG  | O2-C2-C3-O3     |
| 22  | A     | 811 | CLA  | CBA-CGA-O2A-C1  |
| 25  | B     | 803 | LHG  | C24-C23-O8-C6   |
| 25  | 9     | 315 | LHG  | C24-C23-O8-C6   |
| 22  | B     | 823 | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 311 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 313 | CLA  | C6-C7-C8-C10    |
| 22  | 2     | 301 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 830 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 310 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 323 | CLA  | C3-C5-C6-C7     |
| 25  | 5     | 324 | LHG  | C23-C24-C25-C26 |
| 24  | A     | 845 | BCR  | C36-C18-C19-C20 |
| 24  | A     | 846 | BCR  | C36-C18-C19-C20 |
| 24  | A     | 846 | BCR  | C37-C22-C23-C24 |
| 24  | B     | 845 | BCR  | C37-C22-C23-C24 |
| 24  | B     | 848 | BCR  | C36-C18-C19-C20 |
| 24  | B     | 849 | BCR  | C7-C8-C9-C34    |
| 24  | F     | 303 | BCR  | C7-C8-C9-C34    |
| 24  | G     | 203 | BCR  | C36-C18-C19-C20 |
| 24  | J     | 104 | BCR  | C37-C22-C23-C24 |
| 24  | K     | 206 | BCR  | C36-C18-C19-C20 |
| 24  | L     | 204 | BCR  | C11-C12-C13-C35 |
| 24  | 3     | 305 | BCR  | C36-C18-C19-C20 |
| 24  | 8     | 304 | BCR  | C7-C8-C9-C34    |
| 24  | 8     | 304 | BCR  | C36-C18-C19-C20 |
| 24  | 8     | 304 | BCR  | C37-C22-C23-C24 |
| 24  | 4     | 804 | BCR  | C11-C12-C13-C35 |
| 24  | 5     | 305 | BCR  | C11-C12-C13-C35 |
| 24  | 6     | 306 | BCR  | C37-C22-C23-C24 |
| 25  | 3     | 321 | LHG  | C2-C3-O3-P      |
| 32  | F     | 306 | RRX  | C37-C22-C23-C24 |
| 32  | F     | 306 | RRX  | C36-C18-C19-C20 |
| 38  | 1     | 302 | LUT  | C7-C8-C9-C19    |
| 38  | 1     | 303 | LUT  | C7-C8-C9-C19    |
| 38  | Z     | 302 | LUT  | C7-C8-C9-C19    |
| 38  | 7     | 301 | LUT  | C7-C8-C9-C19    |
| 38  | 7     | 302 | LUT  | C7-C8-C9-C19    |
| 38  | 7     | 302 | LUT  | C11-C12-C13-C20 |
| 38  | 4     | 803 | LUT  | C7-C8-C9-C19    |
| 38  | 5     | 302 | LUT  | C27-C28-C29-C39 |
| 38  | 6     | 304 | LUT  | C7-C8-C9-C19    |
| 42  | 7     | 320 | SPH  | C12-C13-C14-C15 |
| 24  | A     | 845 | BCR  | C17-C18-C19-C20 |
| 24  | A     | 846 | BCR  | C17-C18-C19-C20 |
| 24  | A     | 846 | BCR  | C21-C22-C23-C24 |
| 24  | A     | 847 | BCR  | C7-C8-C9-C10    |
| 24  | A     | 848 | BCR  | C11-C12-C13-C14 |
| 24  | B     | 845 | BCR  | C17-C18-C19-C20 |
| 24  | B     | 846 | BCR  | C7-C8-C9-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | B     | 848 | BCR  | C17-C18-C19-C20 |
| 24  | B     | 849 | BCR  | C7-C8-C9-C10    |
| 24  | F     | 303 | BCR  | C7-C8-C9-C10    |
| 24  | G     | 203 | BCR  | C17-C18-C19-C20 |
| 24  | J     | 104 | BCR  | C21-C22-C23-C24 |
| 24  | K     | 206 | BCR  | C11-C12-C13-C14 |
| 24  | K     | 206 | BCR  | C17-C18-C19-C20 |
| 24  | 8     | 304 | BCR  | C7-C8-C9-C10    |
| 24  | 8     | 304 | BCR  | C17-C18-C19-C20 |
| 24  | 8     | 304 | BCR  | C21-C22-C23-C24 |
| 24  | 5     | 305 | BCR  | C11-C12-C13-C14 |
| 24  | 5     | 305 | BCR  | C21-C22-C23-C24 |
| 24  | 6     | 306 | BCR  | C21-C22-C23-C24 |
| 32  | F     | 306 | RRX  | C21-C22-C23-C24 |
| 32  | F     | 306 | RRX  | C17-C18-C19-C20 |
| 36  | J     | 105 | C7Z  | C27-C28-C29-C30 |
| 38  | 1     | 303 | LUT  | C7-C8-C9-C10    |
| 38  | 7     | 301 | LUT  | C7-C8-C9-C10    |
| 38  | 4     | 803 | LUT  | C7-C8-C9-C10    |
| 38  | 6     | 304 | LUT  | C7-C8-C9-C10    |
| 25  | 4     | 820 | LHG  | C9-C10-C11-C12  |
| 22  | A     | 809 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 840 | CLA  | C2A-CAA-CBA-CGA |
| 22  | Z     | 306 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 313 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 7     | 323 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 8     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 5     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 9     | 306 | CLA  | C2A-CAA-CBA-CGA |
| 39  | 4     | 814 | CHL  | C2A-CAA-CBA-CGA |
| 25  | A     | 849 | LHG  | O1-C1-C2-C3     |
| 25  | B     | 803 | LHG  | O1-C1-C2-C3     |
| 25  | B     | 850 | LHG  | O1-C1-C2-C3     |
| 25  | B     | 851 | LHG  | O1-C1-C2-C3     |
| 25  | Z     | 317 | LHG  | O1-C1-C2-C3     |
| 25  | 7     | 318 | LHG  | O1-C1-C2-C3     |
| 25  | 4     | 820 | LHG  | O1-C1-C2-C3     |
| 25  | 4     | 821 | LHG  | O1-C1-C2-C3     |
| 25  | 5     | 324 | LHG  | O1-C1-C2-C3     |
| 25  | 6     | 323 | LHG  | O1-C1-C2-C3     |
| 25  | 7     | 318 | LHG  | C7-C8-C9-C10    |
| 22  | Z     | 313 | CLA  | O2A-C1-C2-C3    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | A     | 852 | DGA  | CCA-CDA-CEA-CFA |
| 24  | G     | 203 | BCR  | C9-C10-C11-C12  |
| 22  | 3     | 319 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 311 | CLA  | C6-C7-C8-C10    |
| 22  | 3     | 313 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 827 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 833 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 833 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 834 | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 317 | CLA  | C3-C5-C6-C7     |
| 22  | 8     | 305 | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 322 | CLA  | C13-C15-C16-C17 |
| 23  | A     | 843 | PQN  | C25-C26-C27-C28 |
| 22  | 4     | 807 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 818 | CLA  | CBA-CGA-O2A-C1  |
| 22  | L     | 201 | CLA  | CBA-CGA-O2A-C1  |
| 22  | L     | 202 | CLA  | CBA-CGA-O2A-C1  |
| 25  | A     | 850 | LHG  | C24-C23-O8-C6   |
| 22  | A     | 832 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 830 | CLA  | C5-C6-C7-C8     |
| 22  | 1     | 316 | CLA  | C8-C10-C11-C12  |
| 27  | A     | 852 | DGA  | CB1-CB2-CB3-CB4 |
| 22  | A     | 805 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 820 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 822 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 808 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 820 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 823 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 829 | CLA  | C2-C1-O2A-CGA   |
| 22  | F     | 301 | CLA  | C2-C1-O2A-CGA   |
| 22  | F     | 304 | CLA  | C2-C1-O2A-CGA   |
| 22  | G     | 201 | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 313 | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 314 | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 314 | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 319 | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 322 | CLA  | C2-C1-O2A-CGA   |
| 22  | 9     | 303 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 812 | CLA  | C6-C7-C8-C9     |
| 22  | K     | 205 | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 322 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 4     | 812 | CLA  | C6-C7-C8-C10    |
| 31  | 3     | 301 | DGD  | O1A-C1A-O1G-C1G |
| 22  | A     | 807 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 822 | CLA  | O1D-CGD-O2D-CED |
| 25  | 4     | 820 | LHG  | C11-C12-C13-C14 |
| 33  | 4     | 822 | LMT  | C6-C7-C8-C9     |
| 40  | 1     | 318 | SQD  | C11-C10-C9-C8   |
| 41  | 7     | 319 | 3PH  | C37-C38-C39-C3A |
| 22  | 3     | 318 | CLA  | C5-C6-C7-C8     |
| 25  | 8     | 317 | LHG  | C11-C12-C13-C14 |
| 22  | 5     | 318 | CLA  | CBA-CGA-O2A-C1  |
| 25  | 1     | 317 | LHG  | C11-C12-C13-C14 |
| 27  | A     | 852 | DGA  | CB9-CAB-CBB-CCB |
| 25  | B     | 803 | LHG  | O1-C1-C2-O2     |
| 25  | B     | 850 | LHG  | O1-C1-C2-O2     |
| 25  | 8     | 317 | LHG  | O1-C1-C2-O2     |
| 25  | 4     | 821 | LHG  | O1-C1-C2-O2     |
| 25  | A     | 849 | LHG  | C11-C12-C13-C14 |
| 25  | A     | 849 | LHG  | C13-C14-C15-C16 |
| 25  | 4     | 821 | LHG  | C11-C12-C13-C14 |
| 22  | B     | 838 | CLA  | O1D-CGD-O2D-CED |
| 22  | 6     | 310 | CLA  | O1D-CGD-O2D-CED |
| 22  | 5     | 323 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 6     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 25  | 9     | 315 | LHG  | C7-C8-C9-C10    |
| 25  | A     | 850 | LHG  | C13-C14-C15-C16 |
| 25  | 1     | 317 | LHG  | C27-C28-C29-C30 |
| 22  | A     | 836 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 836 | CLA  | C6-C7-C8-C10    |
| 22  | 3     | 319 | CLA  | C6-C7-C8-C10    |
| 22  | 6     | 311 | CLA  | C6-C7-C8-C9     |
| 22  | 9     | 307 | CLA  | C6-C7-C8-C9     |
| 22  | 9     | 307 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 320 | CLA  | C2A-CAA-CBA-CGA |
| 39  | 4     | 813 | CHL  | C2A-CAA-CBA-CGA |
| 39  | 5     | 317 | CHL  | C2A-CAA-CBA-CGA |
| 27  | A     | 852 | DGA  | CA6-CA7-CA8-CA9 |
| 22  | 8     | 308 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 809 | CLA  | C5-C6-C7-C8     |
| 39  | 8     | 315 | CHL  | C10-C11-C12-C13 |
| 25  | 1     | 317 | LHG  | C16-C17-C18-C19 |
| 22  | A     | 805 | CLA  | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 810 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 811 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 823 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 829 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 838 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 801 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 809 | CLA  | C11-C10-C8-C7   |
| 22  | 8     | 307 | CLA  | C11-C12-C13-C15 |
| 22  | 5     | 308 | CLA  | C6-C7-C8-C10    |
| 22  | 6     | 322 | CLA  | C11-C10-C8-C7   |
| 23  | B     | 843 | PQN  | C17-C18-C20-C21 |
| 22  | A     | 805 | CLA  | C5-C6-C7-C8     |
| 22  | 1     | 304 | CLA  | C5-C6-C7-C8     |
| 25  | 1     | 317 | LHG  | C12-C13-C14-C15 |
| 41  | 8     | 320 | 3PH  | C36-C37-C38-C39 |
| 22  | A     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 802 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 803 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 811 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 813 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 816 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 825 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 837 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 808 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 815 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 836 | CLA  | C3A-C2A-CAA-CBA |
| 22  | K     | 202 | CLA  | C3A-C2A-CAA-CBA |
| 22  | K     | 205 | CLA  | C3A-C2A-CAA-CBA |
| 22  | L     | 201 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 310 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 1     | 315 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Z     | 315 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 315 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 306 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 306 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 307 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 8     | 314 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 807 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 314 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 326 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 6     | 307 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 9     | 303 | CLA  | C3A-C2A-CAA-CBA |
| 39  | 4     | 816 | CHL  | C3A-C2A-CAA-CBA |
| 22  | 3     | 322 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 838 | CLA  | C10-C11-C12-C13 |
| 22  | 1     | 307 | CLA  | C5-C6-C7-C8     |
| 22  | 4     | 808 | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 311 | CLA  | C5-C6-C7-C8     |
| 25  | B     | 850 | LHG  | C7-C8-C9-C10    |
| 24  | B     | 847 | BCR  | C15-C16-C17-C18 |
| 24  | G     | 203 | BCR  | C15-C16-C17-C18 |
| 24  | 3     | 306 | BCR  | C15-C16-C17-C18 |
| 24  | 5     | 305 | BCR  | C15-C16-C17-C18 |
| 32  | F     | 306 | RRX  | C19-C20-C21-C22 |
| 22  | A     | 822 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 307 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 841 | CLA  | O1A-CGA-O2A-C1  |
| 22  | G     | 201 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 4     | 820 | LHG  | O10-C23-O8-C6   |
| 25  | 4     | 821 | LHG  | O10-C23-O8-C6   |
| 22  | 6     | 319 | CLA  | CBD-CGD-O2D-CED |
| 25  | 1     | 317 | LHG  | C10-C11-C12-C13 |
| 22  | B     | 825 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 835 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 7     | 305 | CLA  | CBA-CGA-O2A-C1  |
| 39  | 3     | 317 | CHL  | CBA-CGA-O2A-C1  |
| 25  | 4     | 821 | LHG  | C4-C5-C6-O8     |
| 25  | 8     | 317 | LHG  | C11-C10-C9-C8   |
| 25  | 5     | 324 | LHG  | C28-C29-C30-C31 |
| 22  | A     | 813 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 840 | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 307 | CLA  | C3-C5-C6-C7     |
| 23  | B     | 843 | PQN  | C23-C25-C26-C27 |
| 25  | A     | 850 | LHG  | C11-C12-C13-C14 |
| 25  | Z     | 317 | LHG  | C13-C14-C15-C16 |
| 25  | Z     | 317 | LHG  | C26-C27-C28-C29 |
| 25  | 4     | 820 | LHG  | C29-C30-C31-C32 |
| 22  | A     | 818 | CLA  | O1A-CGA-O2A-C1  |
| 25  | B     | 803 | LHG  | O10-C23-O8-C6   |
| 25  | 9     | 315 | LHG  | O10-C23-O8-C6   |
| 25  | B     | 803 | LHG  | C11-C10-C9-C8   |
| 25  | 7     | 318 | LHG  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | 4     | 820 | LHG  | C33-C34-C35-C36 |
| 25  | 4     | 820 | LHG  | C28-C29-C30-C31 |
| 22  | A     | 810 | CLA  | O1D-CGD-O2D-CED |
| 25  | 4     | 820 | LHG  | C34-C35-C36-C37 |
| 22  | K     | 205 | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 322 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 326 | CLA  | C6-C7-C8-C9     |
| 25  | 8     | 317 | LHG  | C7-C8-C9-C10    |
| 22  | L     | 202 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 3     | 315 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 24  | A     | 844 | BCR  | C1-C6-C7-C8     |
| 24  | A     | 844 | BCR  | C23-C24-C25-C26 |
| 24  | A     | 845 | BCR  | C1-C6-C7-C8     |
| 24  | A     | 845 | BCR  | C23-C24-C25-C26 |
| 24  | A     | 846 | BCR  | C5-C6-C7-C8     |
| 24  | A     | 846 | BCR  | C23-C24-C25-C26 |
| 24  | A     | 847 | BCR  | C5-C6-C7-C8     |
| 24  | A     | 847 | BCR  | C23-C24-C25-C30 |
| 24  | A     | 848 | BCR  | C23-C24-C25-C30 |
| 24  | A     | 856 | BCR  | C23-C24-C25-C26 |
| 24  | B     | 845 | BCR  | C1-C6-C7-C8     |
| 24  | B     | 845 | BCR  | C5-C6-C7-C8     |
| 24  | B     | 847 | BCR  | C23-C24-C25-C26 |
| 24  | B     | 848 | BCR  | C23-C24-C25-C26 |
| 24  | B     | 853 | BCR  | C23-C24-C25-C30 |
| 24  | F     | 303 | BCR  | C5-C6-C7-C8     |
| 24  | G     | 203 | BCR  | C1-C6-C7-C8     |
| 24  | G     | 203 | BCR  | C23-C24-C25-C30 |
| 24  | J     | 104 | BCR  | C1-C6-C7-C8     |
| 24  | J     | 104 | BCR  | C23-C24-C25-C30 |
| 24  | L     | 204 | BCR  | C5-C6-C7-C8     |
| 24  | 3     | 306 | BCR  | C1-C6-C7-C8     |
| 24  | 7     | 303 | BCR  | C1-C6-C7-C8     |
| 24  | 7     | 303 | BCR  | C23-C24-C25-C30 |
| 24  | 4     | 804 | BCR  | C23-C24-C25-C30 |
| 24  | 5     | 304 | BCR  | C23-C24-C25-C30 |
| 24  | 5     | 305 | BCR  | C1-C6-C7-C8     |
| 32  | F     | 306 | RRX  | C1-C6-C7-C8     |
| 36  | 5     | 306 | C7Z  | C1-C6-C7-C8     |
| 36  | 5     | 306 | C7Z  | C21-C26-C27-C28 |
| 38  | 7     | 301 | LUT  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 38  | 4     | 802 | LUT  | C1-C6-C7-C8     |
| 25  | 9     | 315 | LHG  | C11-C10-C9-C8   |
| 35  | J     | 102 | T7X  | C31-C11-O18-C9  |
| 22  | A     | 802 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 826 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 811 | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 311 | CLA  | C3-C5-C6-C7     |
| 41  | 7     | 319 | 3PH  | C22-C23-C24-C25 |
| 22  | 8     | 314 | CLA  | O1D-CGD-O2D-CED |
| 33  | 4     | 822 | LMT  | C1-C2-C3-C4     |
| 22  | B     | 813 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 6     | 319 | CLA  | C2A-CAA-CBA-CGA |
| 39  | 1     | 312 | CHL  | C2A-CAA-CBA-CGA |
| 39  | Z     | 312 | CHL  | C2A-CAA-CBA-CGA |
| 39  | 6     | 316 | CHL  | C2A-CAA-CBA-CGA |
| 22  | B     | 801 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 814 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 827 | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 302 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 811 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 825 | CLA  | O1A-CGA-O2A-C1  |
| 22  | L     | 201 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 5     | 318 | CLA  | O1A-CGA-O2A-C1  |
| 25  | A     | 850 | LHG  | O10-C23-O8-C6   |
| 22  | 9     | 305 | CLA  | C4-C3-C5-C6     |
| 39  | 9     | 312 | CHL  | C4-C3-C5-C6     |
| 25  | 6     | 323 | LHG  | C25-C26-C27-C28 |
| 28  | A     | 853 | OCA  | C4-C5-C6-C7     |
| 22  | A     | 815 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 820 | CLA  | C8-C10-C11-C12  |
| 22  | 5     | 301 | CLA  | C5-C6-C7-C8     |
| 25  | 4     | 821 | LHG  | C9-C10-C11-C12  |
| 22  | 8     | 306 | CLA  | CBA-CGA-O2A-C1  |
| 25  | Z     | 317 | LHG  | C24-C23-O8-C6   |
| 22  | 4     | 805 | CLA  | C6-C7-C8-C9     |
| 25  | 4     | 821 | LHG  | C11-C10-C9-C8   |
| 41  | 7     | 319 | 3PH  | C27-C28-C29-C2A |
| 34  | F     | 308 | LMG  | C29-C30-C31-C32 |
| 42  | 7     | 320 | SPH  | C4-C5-C6-C7     |
| 22  | 5     | 307 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 831 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 826 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 302 | CLA  | CBA-CGA-O2A-C1  |
| 24  | A     | 846 | BCR  | C19-C20-C21-C22 |
| 24  | B     | 846 | BCR  | C13-C14-C15-C16 |
| 36  | 5     | 306 | C7Z  | C13-C14-C15-C35 |
| 38  | 7     | 301 | LUT  | C9-C10-C11-C12  |
| 22  | B     | 823 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 842 | CLA  | C16-C17-C18-C20 |
| 22  | 5     | 311 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 319 | CLA  | C6-C7-C8-C9     |
| 25  | 6     | 323 | LHG  | C8-C7-O7-C5     |
| 41  | 8     | 320 | 3PH  | C22-C21-O21-C2  |
| 22  | B     | 829 | CLA  | C8-C10-C11-C12  |
| 25  | 1     | 317 | LHG  | C9-C10-C11-C12  |
| 26  | A     | 851 | NKP  | CAP-CAQ-CAR-CAS |
| 31  | B     | 852 | DGD  | C3A-C4A-C5A-C6A |
| 41  | 7     | 319 | 3PH  | C24-C25-C26-C27 |
| 24  | B     | 847 | BCR  | C7-C8-C9-C34    |
| 36  | J     | 105 | C7Z  | C27-C28-C29-C39 |
| 38  | Z     | 301 | LUT  | C7-C8-C9-C19    |
| 22  | B     | 809 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 820 | CLA  | C3-C5-C6-C7     |
| 24  | B     | 853 | BCR  | C17-C18-C19-C20 |
| 38  | Z     | 301 | LUT  | C7-C8-C9-C10    |
| 38  | 6     | 303 | LUT  | C31-C32-C33-C34 |
| 31  | 3     | 301 | DGD  | C2G-C3G-O3G-C1D |
| 22  | B     | 840 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 822 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 812 | CLA  | C6-C7-C8-C10    |
| 22  | Z     | 309 | CLA  | C11-C12-C13-C15 |
| 22  | 5     | 319 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 326 | CLA  | C6-C7-C8-C10    |
| 22  | 2     | 301 | CLA  | C6-C7-C8-C10    |
| 39  | 6     | 318 | CHL  | C4-C3-C5-C6     |
| 25  | 8     | 317 | LHG  | C28-C29-C30-C31 |
| 27  | A     | 852 | DGA  | CB7-CB8-CB9-CAB |
| 41  | 7     | 319 | 3PH  | C25-C26-C27-C28 |
| 22  | A     | 834 | CLA  | C5-C6-C7-C8     |
| 25  | 9     | 315 | LHG  | C26-C27-C28-C29 |
| 22  | B     | 835 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 7     | 305 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 305 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 1     | 313 | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 317 | CLA  | C5-C6-C7-C8     |
| 27  | A     | 852 | DGA  | CA4-CA5-CA6-CA7 |
| 25  | 7     | 318 | LHG  | C9-C10-C11-C12  |
| 22  | A     | 806 | CLA  | C5-C6-C7-C8     |
| 22  | Z     | 313 | CLA  | C8-C10-C11-C12  |
| 22  | 1     | 308 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 309 | CLA  | C11-C12-C13-C14 |
| 35  | J     | 102 | T7X  | O19-C11-O18-C9  |
| 39  | 3     | 317 | CHL  | O1A-CGA-O2A-C1  |
| 25  | A     | 850 | LHG  | C34-C35-C36-C37 |
| 25  | 7     | 318 | LHG  | C11-C12-C13-C14 |
| 25  | 6     | 323 | LHG  | C9-C10-C11-C12  |
| 33  | 4     | 822 | LMT  | C3-C4-C5-C6     |
| 31  | 1     | 319 | DGD  | C1B-C2B-C3B-C4B |
| 22  | 1     | 307 | CLA  | C8-C10-C11-C12  |
| 33  | G     | 204 | LMT  | O5B-C5B-C6B-O6B |
| 22  | A     | 824 | CLA  | C3-C5-C6-C7     |
| 22  | B     | 817 | CLA  | C3-C5-C6-C7     |
| 22  | F     | 304 | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 309 | CLA  | C3-C5-C6-C7     |
| 22  | 4     | 807 | CLA  | C3-C5-C6-C7     |
| 25  | A     | 850 | LHG  | O7-C5-C6-O8     |
| 25  | 4     | 821 | LHG  | O7-C5-C6-O8     |
| 25  | 5     | 324 | LHG  | O7-C5-C6-O8     |
| 22  | B     | 811 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 309 | CLA  | C5-C6-C7-C8     |
| 22  | 1     | 310 | CLA  | O1D-CGD-O2D-CED |
| 22  | 7     | 323 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 811 | CLA  | C2-C1-O2A-CGA   |
| 22  | 1     | 313 | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 307 | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 313 | CLA  | O1D-CGD-O2D-CED |
| 25  | B     | 851 | LHG  | C2-C3-O3-P      |
| 25  | 5     | 324 | LHG  | C11-C12-C13-C14 |
| 25  | 6     | 323 | LHG  | C28-C29-C30-C31 |
| 27  | A     | 852 | DGA  | CB5-CB6-CB7-CB8 |
| 22  | A     | 814 | CLA  | C4-C3-C5-C6     |
| 39  | 8     | 315 | CHL  | C4-C3-C5-C6     |
| 39  | 6     | 315 | CHL  | C4-C3-C5-C6     |
| 22  | A     | 819 | CLA  | C3-C5-C6-C7     |
| 22  | Z     | 308 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 828 | CLA  | C2-C3-C5-C6     |
| 41  | 8     | 320 | 3PH  | O22-C21-O21-C2  |
| 25  | 1     | 317 | LHG  | C1-C2-C3-O3     |
| 25  | Z     | 317 | LHG  | C9-C10-C11-C12  |
| 25  | 6     | 323 | LHG  | C29-C30-C31-C32 |
| 33  | 4     | 822 | LMT  | C7-C8-C9-C10    |
| 42  | 7     | 321 | SPH  | C10-C11-C12-C13 |
| 22  | A     | 826 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 815 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 831 | CLA  | C2A-CAA-CBA-CGA |
| 22  | Z     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 318 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 4     | 815 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 6     | 307 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 1     | 319 | DGD  | O6E-C5E-C6E-O5E |
| 22  | A     | 840 | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 310 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 806 | CLA  | O1D-CGD-O2D-CED |
| 25  | 4     | 820 | LHG  | C30-C31-C32-C33 |
| 22  | F     | 301 | CLA  | C8-C10-C11-C12  |
| 22  | 1     | 316 | CLA  | C15-C16-C17-C18 |
| 22  | 5     | 307 | CLA  | C5-C6-C7-C8     |
| 25  | A     | 850 | LHG  | O1-C1-C2-O2     |
| 22  | 8     | 306 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 3     | 318 | CLA  | C3-C5-C6-C7     |
| 22  | 5     | 308 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 804 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 805 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 808 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 809 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 810 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 813 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 815 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 22  | A     | 837 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 809 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 813 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 816 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 817 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 823 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 825 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 827 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 829 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 832 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 834 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 837 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 839 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 840 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 841 | CLA  | C1A-C2A-CAA-CBA |
| 22  | B     | 842 | CLA  | C1A-C2A-CAA-CBA |
| 22  | F     | 302 | CLA  | C1A-C2A-CAA-CBA |
| 22  | K     | 202 | CLA  | C1A-C2A-CAA-CBA |
| 22  | K     | 203 | CLA  | C1A-C2A-CAA-CBA |
| 22  | K     | 205 | CLA  | C1A-C2A-CAA-CBA |
| 22  | L     | 203 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 303 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 306 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 318 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 3     | 322 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 312 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 322 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 324 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 306 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 8     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 808 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 811 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 4     | 815 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 311 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 5     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 318 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 312 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 317 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 319 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 2     | 301 | CLA  | C1A-C2A-CAA-CBA |
| 25  | Z     | 317 | LHG  | C28-C29-C30-C31 |
| 35  | J     | 102 | T7X  | C25-C26-C27-C28 |
| 42  | 7     | 320 | SPH  | C5-C6-C7-C8     |
| 22  | B     | 811 | CLA  | O1A-CGA-O2A-C1  |
| 41  | 6     | 324 | 3PH  | C24-C25-C26-C27 |
| 22  | A     | 835 | CLA  | C5-C6-C7-C8     |
| 25  | A     | 850 | LHG  | O6-C4-C5-C6     |
| 25  | 8     | 317 | LHG  | O6-C4-C5-C6     |
| 25  | 5     | 324 | LHG  | O6-C4-C5-C6     |
| 25  | 6     | 323 | LHG  | O9-C7-O7-C5     |
| 22  | 1     | 316 | CLA  | C3-C5-C6-C7     |
| 21  | A     | 801 | CL0  | C6-C7-C8-C10    |
| 22  | A     | 807 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 813 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 815 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 821 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 830 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 832 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 855 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 855 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 801 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 805 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 808 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 820 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 821 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 824 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 838 | CLA  | C12-C13-C15-C16 |
| 22  | F     | 301 | CLA  | C6-C7-C8-C10    |
| 22  | F     | 302 | CLA  | C6-C7-C8-C10    |
| 22  | F     | 304 | CLA  | C11-C12-C13-C15 |
| 22  | L     | 201 | CLA  | C11-C10-C8-C7   |
| 22  | 1     | 306 | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 310 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 1     | 314 | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 314 | CLA  | C11-C10-C8-C7   |
| 22  | 1     | 316 | CLA  | C11-C10-C8-C7   |
| 22  | Z     | 306 | CLA  | C6-C7-C8-C10    |
| 22  | Z     | 308 | CLA  | C6-C7-C8-C10    |
| 22  | Z     | 316 | CLA  | C6-C7-C8-C10    |
| 22  | Z     | 316 | CLA  | C11-C12-C13-C15 |
| 22  | 3     | 308 | CLA  | C6-C7-C8-C10    |
| 22  | 3     | 313 | CLA  | C11-C12-C13-C15 |
| 22  | 3     | 314 | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 307 | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 324 | CLA  | C11-C10-C8-C7   |
| 22  | 8     | 305 | CLA  | C6-C7-C8-C10    |
| 22  | 8     | 307 | CLA  | C6-C7-C8-C10    |
| 22  | 8     | 309 | CLA  | C6-C7-C8-C10    |
| 22  | 8     | 309 | CLA  | C11-C12-C13-C15 |
| 22  | 4     | 805 | CLA  | C11-C10-C8-C7   |
| 22  | 4     | 807 | CLA  | C11-C10-C8-C7   |
| 22  | 5     | 301 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 309 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 310 | CLA  | C11-C10-C8-C7   |
| 22  | 5     | 315 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 322 | CLA  | C11-C10-C8-C7   |
| 22  | 6     | 314 | CLA  | C11-C12-C13-C15 |
| 22  | 9     | 306 | CLA  | C6-C7-C8-C10    |
| 23  | A     | 843 | PQN  | C17-C18-C20-C21 |
| 23  | B     | 843 | PQN  | C21-C22-C23-C25 |
| 39  | 3     | 317 | CHL  | C11-C10-C8-C7   |
| 41  | 6     | 324 | 3PH  | C27-C28-C29-C2A |
| 22  | B     | 842 | CLA  | C16-C17-C18-C19 |
| 22  | A     | 805 | CLA  | C15-C16-C17-C18 |
| 22  | A     | 808 | CLA  | C8-C10-C11-C12  |
| 25  | Z     | 317 | LHG  | O10-C23-O8-C6   |
| 33  | F     | 307 | LMT  | O5'-C5'-C6'-O6' |
| 22  | 7     | 316 | CLA  | C3A-C2A-CAA-CBA |
| 21  | A     | 801 | CL0  | CBA-CGA-O2A-C1  |
| 25  | 8     | 317 | LHG  | C24-C23-O8-C6   |
| 22  | 3     | 310 | CLA  | C5-C6-C7-C8     |
| 25  | A     | 849 | LHG  | C7-C8-C9-C10    |
| 22  | A     | 828 | CLA  | C4-C3-C5-C6     |
| 22  | F     | 304 | CLA  | C2-C3-C5-C6     |
| 39  | 3     | 317 | CHL  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 41  | 7     | 319 | 3PH  | C3C-C3D-C3E-C3F |
| 25  | 4     | 821 | LHG  | C10-C11-C12-C13 |
| 25  | 6     | 323 | LHG  | C12-C13-C14-C15 |
| 25  | 4     | 821 | LHG  | C23-C24-C25-C26 |
| 22  | 5     | 311 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 808 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 842 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 830 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 7     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 6     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 21  | A     | 801 | CL0  | C6-C7-C8-C9     |
| 22  | A     | 811 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 820 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 828 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 832 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 855 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 801 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 841 | CLA  | C6-C7-C8-C9     |
| 22  | F     | 301 | CLA  | C6-C7-C8-C9     |
| 22  | 1     | 314 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 306 | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 323 | CLA  | C11-C12-C13-C14 |
| 22  | 8     | 309 | CLA  | C11-C12-C13-C14 |
| 22  | 4     | 805 | CLA  | C11-C10-C8-C9   |
| 22  | 4     | 807 | CLA  | C11-C10-C8-C9   |
| 22  | 5     | 307 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 301 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 302 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 310 | CLA  | C6-C7-C8-C9     |
| 34  | F     | 308 | LMG  | C12-C13-C14-C15 |
| 22  | A     | 820 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 305 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 6     | 302 | CLA  | O1A-CGA-O2A-C1  |
| 22  | A     | 837 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 828 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 834 | CLA  | C8-C10-C11-C12  |
| 33  | F     | 307 | LMT  | O5B-C5B-C6B-O6B |
| 22  | B     | 839 | CLA  | O1D-CGD-O2D-CED |
| 25  | 3     | 321 | LHG  | C4-C5-C6-O8     |
| 25  | 7     | 318 | LHG  | C4-C5-C6-O8     |
| 25  | 6     | 323 | LHG  | C4-C5-C6-O8     |
| 31  | B     | 852 | DGD  | O1G-C1G-C2G-C3G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 812 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 829 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 842 | CLA  | C5-C6-C7-C8     |
| 22  | Z     | 309 | CLA  | C8-C10-C11-C12  |
| 39  | 3     | 317 | CHL  | C8-C10-C11-C12  |
| 27  | A     | 852 | DGA  | CB3-CB4-CB5-CB6 |
| 22  | A     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 1     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 33  | 1     | 301 | LMT  | O5'-C5'-C6'-O6' |
| 33  | 4     | 801 | LMT  | O5'-C5'-C6'-O6' |
| 25  | A     | 850 | LHG  | C28-C29-C30-C31 |
| 33  | F     | 307 | LMT  | C2-C3-C4-C5     |
| 41  | 7     | 319 | 3PH  | C3A-C3B-C3C-C3D |
| 21  | A     | 801 | CL0  | CHA-CBD-CGD-O2D |
| 39  | 2     | 303 | CHL  | CHA-CBD-CGD-O1D |
| 39  | 2     | 303 | CHL  | CHA-CBD-CGD-O2D |
| 22  | B     | 826 | CLA  | O1A-CGA-O2A-C1  |
| 22  | F     | 304 | CLA  | C4-C3-C5-C6     |
| 39  | 8     | 315 | CHL  | C2-C3-C5-C6     |
| 22  | B     | 822 | CLA  | C5-C6-C7-C8     |
| 22  | Z     | 306 | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 310 | CLA  | C8-C10-C11-C12  |
| 24  | G     | 203 | BCR  | C11-C12-C13-C35 |
| 24  | 7     | 303 | BCR  | C37-C22-C23-C24 |
| 24  | 4     | 804 | BCR  | C37-C22-C23-C24 |
| 24  | 5     | 304 | BCR  | C37-C22-C23-C24 |
| 24  | 5     | 305 | BCR  | C7-C8-C9-C34    |
| 38  | 8     | 302 | LUT  | C31-C32-C33-C40 |
| 42  | 7     | 321 | SPH  | C2-C3-C4-C5     |
| 22  | B     | 817 | CLA  | C8-C10-C11-C12  |
| 25  | 9     | 315 | LHG  | C9-C10-C11-C12  |
| 24  | B     | 847 | BCR  | C7-C8-C9-C10    |
| 24  | 7     | 303 | BCR  | C21-C22-C23-C24 |
| 24  | 4     | 804 | BCR  | C21-C22-C23-C24 |
| 24  | 5     | 305 | BCR  | C7-C8-C9-C10    |
| 21  | A     | 801 | CL0  | O1A-CGA-O2A-C1  |
| 22  | 1     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 805 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 823 | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 310 | CLA  | C13-C15-C16-C17 |
| 22  | 8     | 309 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 821 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 814 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 824 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 5     | 323 | CLA  | O1A-CGA-O2A-C1  |
| 33  | 4     | 822 | LMT  | O5B-C5B-C6B-O6B |
| 22  | A     | 838 | CLA  | C5-C6-C7-C8     |
| 22  | 5     | 313 | CLA  | C10-C11-C12-C13 |
| 41  | 6     | 324 | 3PH  | C21-C22-C23-C24 |
| 22  | 1     | 313 | CLA  | O2A-C1-C2-C3    |
| 22  | 6     | 313 | CLA  | O2A-C1-C2-C3    |
| 25  | 7     | 318 | LHG  | C29-C30-C31-C32 |
| 22  | B     | 813 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 818 | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 317 | CLA  | C8-C10-C11-C12  |
| 24  | K     | 206 | BCR  | C13-C14-C15-C16 |
| 24  | 8     | 304 | BCR  | C9-C10-C11-C12  |
| 25  | A     | 850 | LHG  | C33-C34-C35-C36 |
| 25  | 8     | 317 | LHG  | O10-C23-O8-C6   |
| 35  | J     | 102 | T7X  | O13-C7-C8-O16   |
| 22  | A     | 823 | CLA  | C8-C10-C11-C12  |
| 22  | K     | 205 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 813 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 3     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 9     | 305 | CLA  | O1A-CGA-O2A-C1  |
| 25  | B     | 803 | LHG  | C9-C10-C11-C12  |
| 41  | 7     | 319 | 3PH  | C39-C3A-C3B-C3C |
| 39  | 3     | 317 | CHL  | C4-C3-C5-C6     |
| 22  | B     | 815 | CLA  | C2-C3-C5-C6     |
| 22  | 9     | 305 | CLA  | C2-C3-C5-C6     |
| 25  | 5     | 324 | LHG  | C13-C14-C15-C16 |
| 22  | K     | 203 | CLA  | C6-C7-C8-C9     |
| 41  | 8     | 320 | 3PH  | C35-C36-C37-C38 |
| 22  | A     | 817 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 6     | 307 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 7     | 318 | LHG  | O7-C5-C6-O8     |
| 25  | 8     | 317 | LHG  | O7-C5-C6-O8     |
| 25  | B     | 803 | LHG  | C10-C11-C12-C13 |
| 22  | B     | 842 | CLA  | CBA-CGA-O2A-C1  |
| 22  | L     | 202 | CLA  | C5-C6-C7-C8     |
| 22  | 3     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 39  | 8     | 312 | CHL  | C2A-CAA-CBA-CGA |
| 42  | 7     | 321 | SPH  | C4-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | K     | 205 | CLA  | C2-C1-O2A-CGA   |
| 25  | 7     | 318 | LHG  | C26-C27-C28-C29 |
| 22  | Z     | 303 | CLA  | C8-C10-C11-C12  |
| 25  | 1     | 317 | LHG  | C24-C23-O8-C6   |
| 34  | F     | 308 | LMG  | C15-C16-C17-C18 |
| 22  | A     | 806 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 854 | CLA  | C5-C6-C7-C8     |
| 22  | Z     | 316 | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 310 | CLA  | C15-C16-C17-C18 |
| 22  | 4     | 805 | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 307 | CLA  | O1D-CGD-O2D-CED |
| 24  | 3     | 306 | BCR  | C9-C10-C11-C12  |
| 22  | B     | 815 | CLA  | C4-C3-C5-C6     |
| 26  | A     | 851 | NKP  | OBC-CAH-CAI-OAJ |
| 25  | 4     | 820 | LHG  | C31-C32-C33-C34 |
| 41  | 5     | 325 | 3PH  | C22-C23-C24-C25 |
| 22  | 7     | 308 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 805 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 813 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 838 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 841 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 855 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 805 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 816 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 821 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 828 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 828 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 840 | CLA  | C6-C7-C8-C9     |
| 22  | F     | 302 | CLA  | C11-C12-C13-C14 |
| 22  | L     | 201 | CLA  | C6-C7-C8-C9     |
| 22  | L     | 201 | CLA  | C11-C10-C8-C9   |
| 22  | L     | 202 | CLA  | C11-C10-C8-C9   |
| 22  | 1     | 314 | CLA  | C11-C10-C8-C9   |
| 22  | 1     | 316 | CLA  | C11-C12-C13-C14 |
| 22  | Z     | 308 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 309 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 316 | CLA  | C6-C7-C8-C9     |
| 22  | 3     | 308 | CLA  | C6-C7-C8-C9     |
| 22  | 3     | 314 | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 307 | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 308 | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 312 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 8     | 305 | CLA  | C6-C7-C8-C9     |
| 22  | 8     | 307 | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 301 | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 308 | CLA  | C6-C7-C8-C9     |
| 22  | 5     | 309 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 319 | CLA  | C6-C7-C8-C9     |
| 22  | 9     | 306 | CLA  | C6-C7-C8-C9     |
| 23  | A     | 843 | PQN  | C19-C18-C20-C21 |
| 39  | 8     | 315 | CHL  | C11-C10-C8-C9   |
| 39  | 9     | 312 | CHL  | C11-C12-C13-C14 |
| 22  | A     | 839 | CLA  | O1D-CGD-O2D-CED |
| 26  | 8     | 318 | NKP  | CAH-CAG-OAF-PAC |
| 25  | B     | 803 | LHG  | C11-C12-C13-C14 |
| 22  | A     | 820 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 315 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 805 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 812 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 818 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 9     | 303 | CLA  | C4B-C3B-CAB-CBB |
| 21  | A     | 801 | CL0  | C5-C6-C7-C8     |
| 22  | A     | 830 | CLA  | C5-C6-C7-C8     |
| 22  | 5     | 308 | CLA  | C8-C10-C11-C12  |
| 25  | 8     | 317 | LHG  | C13-C14-C15-C16 |
| 22  | K     | 203 | CLA  | C6-C7-C8-C10    |
| 28  | A     | 853 | OCA  | C5-C6-C7-C8     |
| 22  | 1     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 7     | 324 | CLA  | C2A-CAA-CBA-CGA |
| 22  | L     | 201 | CLA  | C3-C5-C6-C7     |
| 27  | A     | 852 | DGA  | CA1-CA2-CA3-CA4 |
| 25  | Z     | 317 | LHG  | O6-C4-C5-C6     |
| 25  | 7     | 318 | LHG  | O6-C4-C5-C6     |
| 41  | 6     | 324 | 3PH  | O11-C1-C2-C3    |
| 25  | 4     | 820 | LHG  | O8-C23-C24-C25  |
| 22  | A     | 802 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 806 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 811 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 812 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 817 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 820 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 823 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 828 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | A     | 828 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 854 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 855 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 811 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 816 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 821 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 825 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 828 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 840 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 841 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 841 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 842 | CLA  | C6-C7-C8-C10    |
| 22  | L     | 202 | CLA  | C11-C10-C8-C7   |
| 22  | 1     | 306 | CLA  | C11-C10-C8-C7   |
| 22  | 1     | 316 | CLA  | C11-C12-C13-C15 |
| 22  | 3     | 311 | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 304 | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 307 | CLA  | C11-C12-C13-C15 |
| 22  | 7     | 310 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 307 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 318 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 322 | CLA  | C6-C7-C8-C10    |
| 22  | 6     | 301 | CLA  | C6-C7-C8-C10    |
| 22  | 6     | 310 | CLA  | C6-C7-C8-C10    |
| 25  | 1     | 317 | LHG  | C31-C32-C33-C34 |
| 22  | 4     | 812 | CLA  | C6-C7-C8-C9     |
| 25  | 6     | 323 | LHG  | C19-C20-C21-C22 |
| 21  | A     | 801 | CL0  | C3A-C2A-CAA-CBA |
| 22  | B     | 809 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 824 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 826 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Z     | 310 | CLA  | C3A-C2A-CAA-CBA |
| 39  | Z     | 311 | CHL  | C3A-C2A-CAA-CBA |
| 39  | 8     | 315 | CHL  | C3A-C2A-CAA-CBA |
| 22  | 4     | 807 | CLA  | C5-C6-C7-C8     |
| 25  | 4     | 820 | LHG  | C15-C16-C17-C18 |
| 22  | B     | 826 | CLA  | C8-C10-C11-C12  |
| 39  | Z     | 312 | CHL  | CBA-CGA-O2A-C1  |
| 24  | 3     | 304 | BCR  | C19-C20-C21-C22 |
| 24  | 6     | 306 | BCR  | C9-C10-C11-C12  |
| 38  | Z     | 301 | LUT  | C9-C10-C11-C12  |
| 24  | B     | 844 | BCR  | C37-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | A     | 852 | DGA  | CA8-CA9-CAA-CBA |
| 22  | 3     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 24  | A     | 847 | BCR  | C21-C22-C23-C24 |
| 24  | 5     | 304 | BCR  | C21-C22-C23-C24 |
| 25  | 6     | 323 | LHG  | C35-C36-C37-C38 |
| 22  | K     | 204 | CLA  | O2A-C1-C2-C3    |
| 22  | A     | 816 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 835 | CLA  | C2A-CAA-CBA-CGA |
| 39  | 7     | 313 | CHL  | C2A-CAA-CBA-CGA |
| 25  | A     | 850 | LHG  | C4-C5-C6-O8     |
| 25  | B     | 851 | LHG  | C4-C5-C6-O8     |
| 25  | 1     | 317 | LHG  | C4-C5-C6-O8     |
| 25  | Z     | 317 | LHG  | C4-C5-C6-O8     |
| 25  | 5     | 324 | LHG  | C4-C5-C6-O8     |
| 31  | 3     | 301 | DGD  | O1G-C1G-C2G-C3G |
| 34  | F     | 308 | LMG  | C7-C8-C9-O8     |
| 40  | 1     | 318 | SQD  | C44-C45-C46-O48 |
| 23  | A     | 843 | PQN  | C13-C15-C16-C17 |
| 25  | 8     | 317 | LHG  | C9-C10-C11-C12  |
| 22  | 1     | 308 | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 310 | CLA  | C11-C12-C13-C15 |
| 39  | 8     | 315 | CHL  | C8-C10-C11-C12  |
| 22  | A     | 813 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 3     | 301 | DGD  | C3A-C4A-C5A-C6A |
| 39  | 8     | 315 | CHL  | C1A-C2A-CAA-CBA |
| 25  | A     | 849 | LHG  | C16-C17-C18-C19 |
| 25  | Z     | 317 | LHG  | C31-C32-C33-C34 |
| 22  | A     | 830 | CLA  | C8-C10-C11-C12  |
| 41  | 6     | 324 | 3PH  | C25-C26-C27-C28 |
| 22  | A     | 820 | CLA  | C11-C12-C13-C15 |
| 25  | A     | 850 | LHG  | O6-C4-C5-O7     |
| 25  | B     | 850 | LHG  | O6-C4-C5-O7     |
| 25  | Z     | 317 | LHG  | O6-C4-C5-O7     |
| 25  | 8     | 317 | LHG  | O6-C4-C5-O7     |
| 22  | 3     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 24  | A     | 856 | BCR  | C23-C24-C25-C30 |
| 24  | B     | 844 | BCR  | C1-C6-C7-C8     |
| 24  | B     | 846 | BCR  | C1-C6-C7-C8     |
| 24  | B     | 849 | BCR  | C23-C24-C25-C30 |
| 24  | K     | 206 | BCR  | C23-C24-C25-C30 |
| 24  | 3     | 304 | BCR  | C5-C6-C7-C8     |
| 24  | 3     | 305 | BCR  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | 6     | 305 | BCR  | C1-C6-C7-C8     |
| 24  | 6     | 306 | BCR  | C23-C24-C25-C30 |
| 36  | J     | 105 | C7Z  | C1-C6-C7-C8     |
| 38  | 8     | 303 | LUT  | C5-C6-C7-C8     |
| 38  | 4     | 803 | LUT  | C1-C6-C7-C8     |
| 38  | 5     | 303 | LUT  | C1-C6-C7-C8     |
| 22  | 1     | 314 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 810 | CLA  | C11-C10-C8-C9   |
| 22  | 5     | 301 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 822 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 854 | CLA  | C8-C10-C11-C12  |
| 22  | L     | 202 | CLA  | CBD-CGD-O2D-CED |
| 22  | Z     | 307 | CLA  | C6-C7-C8-C10    |
| 22  | Z     | 308 | CLA  | C8-C10-C11-C12  |
| 25  | A     | 849 | LHG  | O7-C5-C6-O8     |
| 25  | 6     | 323 | LHG  | O7-C5-C6-O8     |
| 31  | 1     | 319 | DGD  | O2G-C2G-C3G-O3G |
| 40  | 1     | 318 | SQD  | O6-C44-C45-O47  |
| 40  | 1     | 318 | SQD  | O47-C45-C46-O48 |
| 35  | J     | 102 | T7X  | C18-C19-C20-C21 |
| 35  | J     | 102 | T7X  | C22-C23-C24-C25 |
| 22  | 3     | 308 | CLA  | C8-C10-C11-C12  |
| 22  | 8     | 308 | CLA  | C8-C10-C11-C12  |
| 22  | 6     | 313 | CLA  | C6-C7-C8-C9     |
| 22  | 2     | 301 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 805 | CLA  | C11-C12-C13-C14 |
| 22  | F     | 302 | CLA  | C6-C7-C8-C9     |
| 22  | F     | 302 | CLA  | C11-C10-C8-C9   |
| 22  | 1     | 306 | CLA  | C11-C10-C8-C9   |
| 22  | 7     | 309 | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 310 | CLA  | C11-C10-C8-C9   |
| 22  | 8     | 309 | CLA  | C6-C7-C8-C9     |
| 22  | 4     | 808 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 314 | CLA  | C11-C12-C13-C14 |
| 22  | 6     | 319 | CLA  | C11-C12-C13-C14 |
| 23  | B     | 843 | PQN  | C21-C22-C23-C24 |
| 22  | B     | 824 | CLA  | C11-C12-C13-C14 |
| 22  | 4     | 811 | CLA  | C6-C7-C8-C9     |
| 22  | 4     | 811 | CLA  | C6-C7-C8-C10    |
| 23  | A     | 843 | PQN  | C26-C27-C28-C30 |
| 25  | 6     | 323 | LHG  | C11-C12-C13-C14 |
| 34  | J     | 101 | LMG  | C2-C1-O1-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 6     | 309 | CLA  | CAA-CBA-CGA-O2A |
| 39  | Z     | 311 | CHL  | C2A-CAA-CBA-CGA |
| 39  | 8     | 301 | CHL  | C2A-CAA-CBA-CGA |
| 22  | 5     | 309 | CLA  | C5-C6-C7-C8     |
| 25  | A     | 849 | LHG  | O1-C1-C2-O2     |
| 22  | Z     | 316 | CLA  | C3-C5-C6-C7     |
| 24  | 3     | 307 | BCR  | C19-C20-C21-C22 |
| 22  | A     | 820 | CLA  | C11-C12-C13-C14 |
| 22  | 1     | 310 | CLA  | C11-C12-C13-C14 |
| 39  | 3     | 317 | CHL  | CBD-CGD-O2D-CED |
| 22  | A     | 812 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 819 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 821 | CLA  | C8-C10-C11-C12  |
| 25  | 4     | 821 | LHG  | C7-C8-C9-C10    |
| 25  | 9     | 315 | LHG  | C24-C25-C26-C27 |
| 22  | 6     | 314 | CLA  | C10-C11-C12-C13 |
| 25  | 3     | 321 | LHG  | C1-C2-C3-O3     |
| 25  | 9     | 315 | LHG  | C1-C2-C3-O3     |
| 22  | B     | 842 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 812 | CLA  | C3-C5-C6-C7     |
| 25  | Z     | 317 | LHG  | C25-C26-C27-C28 |
| 22  | 3     | 318 | CLA  | C8-C10-C11-C12  |
| 25  | B     | 803 | LHG  | O6-C4-C5-C6     |
| 25  | B     | 850 | LHG  | O6-C4-C5-C6     |
| 25  | 6     | 323 | LHG  | O6-C4-C5-C6     |
| 22  | A     | 809 | CLA  | C6-C7-C8-C9     |
| 26  | 8     | 318 | NKP  | CAS-CAT-CAU-CAV |
| 35  | J     | 102 | T7X  | C24-C25-C26-C27 |
| 22  | B     | 824 | CLA  | C5-C6-C7-C8     |
| 24  | A     | 847 | BCR  | C37-C22-C23-C24 |
| 24  | 6     | 305 | BCR  | C37-C22-C23-C24 |
| 38  | Z     | 301 | LUT  | C27-C28-C29-C39 |
| 22  | A     | 803 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 808 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 808 | CLA  | C12-C13-C15-C16 |
| 22  | A     | 812 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 813 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 815 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 816 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 830 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 833 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 834 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 806 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 814 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 815 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 826 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 827 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 833 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 840 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 842 | CLA  | C11-C10-C8-C7   |
| 22  | F     | 302 | CLA  | C11-C10-C8-C7   |
| 22  | 1     | 309 | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 313 | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 304 | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 308 | CLA  | C11-C12-C13-C15 |
| 22  | 7     | 309 | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 310 | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 317 | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 324 | CLA  | C6-C7-C8-C10    |
| 22  | 8     | 308 | CLA  | C11-C10-C8-C7   |
| 22  | 4     | 807 | CLA  | C6-C7-C8-C10    |
| 22  | 6     | 312 | CLA  | C6-C7-C8-C10    |
| 22  | 6     | 319 | CLA  | C11-C12-C13-C15 |
| 39  | 5     | 316 | CHL  | C12-C13-C15-C16 |
| 25  | 4     | 820 | LHG  | C13-C14-C15-C16 |
| 25  | B     | 803 | LHG  | C25-C26-C27-C28 |
| 22  | A     | 825 | CLA  | C13-C15-C16-C17 |
| 22  | 7     | 310 | CLA  | C5-C6-C7-C8     |
| 24  | G     | 203 | BCR  | C11-C12-C13-C14 |
| 24  | 6     | 305 | BCR  | C21-C22-C23-C24 |
| 38  | 7     | 302 | LUT  | C11-C12-C13-C14 |
| 38  | 8     | 302 | LUT  | C31-C32-C33-C34 |
| 38  | 5     | 302 | LUT  | C27-C28-C29-C30 |
| 22  | 1     | 316 | CLA  | CBA-CGA-O2A-C1  |
| 22  | 8     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 26  | 8     | 318 | NKP  | CAL-CAK-OAJ-CAI |
| 39  | 8     | 312 | CHL  | CBA-CGA-O2A-C1  |
| 39  | Z     | 312 | CHL  | O1A-CGA-O2A-C1  |
| 31  | B     | 852 | DGD  | C5D-C6D-O5D-C1E |
| 31  | 1     | 319 | DGD  | C1A-C2A-C3A-C4A |
| 22  | K     | 203 | CLA  | C5-C6-C7-C8     |
| 22  | K     | 202 | CLA  | C2A-CAA-CBA-CGA |
| 39  | 5     | 316 | CHL  | C2A-CAA-CBA-CGA |
| 39  | 6     | 318 | CHL  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 39  | 2     | 303 | CHL  | C2A-CAA-CBA-CGA |
| 22  | 7     | 309 | CLA  | C11-C10-C8-C9   |
| 27  | A     | 852 | DGA  | CA2-CA3-CA4-CA5 |
| 22  | 1     | 316 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 801 | CLA  | C5-C6-C7-C8     |
| 25  | A     | 849 | LHG  | C24-C23-O8-C6   |
| 22  | A     | 829 | CLA  | O2A-C1-C2-C3    |
| 22  | L     | 202 | CLA  | O2A-C1-C2-C3    |
| 25  | 7     | 318 | LHG  | C12-C13-C14-C15 |
| 24  | G     | 203 | BCR  | C13-C14-C15-C16 |
| 39  | 5     | 321 | CHL  | CBD-CGD-O2D-CED |
| 25  | 6     | 323 | LHG  | C31-C32-C33-C34 |
| 25  | 1     | 317 | LHG  | O10-C23-O8-C6   |
| 22  | 1     | 306 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 813 | CLA  | C13-C15-C16-C17 |
| 22  | 1     | 316 | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 319 | CLA  | O1D-CGD-O2D-CED |
| 25  | 7     | 318 | LHG  | O6-C4-C5-O7     |
| 25  | 5     | 324 | LHG  | O6-C4-C5-O7     |
| 25  | 6     | 323 | LHG  | C30-C31-C32-C33 |
| 40  | 1     | 318 | SQD  | O6-C44-C45-C46  |
| 22  | 5     | 319 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 842 | CLA  | CAA-CBA-CGA-O2A |
| 39  | 6     | 315 | CHL  | C2-C3-C5-C6     |
| 25  | 1     | 317 | LHG  | C15-C16-C17-C18 |
| 22  | A     | 805 | CLA  | C8-C10-C11-C12  |
| 25  | 6     | 323 | LHG  | C10-C11-C12-C13 |
| 22  | 6     | 301 | CLA  | C3-C5-C6-C7     |
| 25  | B     | 850 | LHG  | O7-C5-C6-O8     |
| 25  | B     | 851 | LHG  | O7-C5-C6-O8     |
| 25  | Z     | 317 | LHG  | O7-C5-C6-O8     |
| 25  | 3     | 321 | LHG  | O7-C5-C6-O8     |
| 31  | B     | 852 | DGD  | O1G-C1G-C2G-O2G |
| 31  | 3     | 301 | DGD  | O1G-C1G-C2G-O2G |
| 34  | F     | 308 | LMG  | O1-C7-C8-O7     |
| 34  | F     | 308 | LMG  | O7-C8-C9-O8     |
| 22  | A     | 824 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 805 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 833 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 806 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 808 | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 317 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 7     | 317 | CLA  | C11-C10-C8-C9   |
| 22  | 5     | 322 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 312 | CLA  | C11-C12-C13-C14 |
| 39  | 9     | 312 | CHL  | C14-C13-C15-C16 |
| 22  | B     | 820 | CLA  | C11-C12-C13-C14 |
| 22  | Z     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 42  | 7     | 321 | SPH  | C12-C13-C14-C15 |
| 25  | Z     | 317 | LHG  | C30-C31-C32-C33 |
| 22  | A     | 806 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 828 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 809 | CLA  | C8-C10-C11-C12  |
| 22  | 4     | 808 | CLA  | C8-C10-C11-C12  |
| 22  | 6     | 301 | CLA  | C5-C6-C7-C8     |
| 21  | A     | 801 | CL0  | CAA-CBA-CGA-O2A |
| 22  | Z     | 316 | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 315 | CLA  | C2-C1-O2A-CGA   |
| 22  | 4     | 808 | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 301 | CLA  | C2-C1-O2A-CGA   |
| 22  | 9     | 307 | CLA  | C2-C1-O2A-CGA   |
| 22  | 9     | 313 | CLA  | C2-C1-O2A-CGA   |
| 22  | B     | 824 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 825 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 828 | CLA  | C8-C10-C11-C12  |
| 41  | 8     | 320 | 3PH  | C3B-C3C-C3D-C3E |
| 22  | Z     | 309 | CLA  | C10-C11-C12-C13 |
| 22  | L     | 202 | CLA  | C2A-CAA-CBA-CGA |
| 40  | 1     | 318 | SQD  | C10-C11-C12-C13 |
| 22  | 7     | 304 | CLA  | C11-C12-C13-C15 |
| 23  | A     | 843 | PQN  | C26-C27-C28-C29 |
| 22  | Z     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 26  | 8     | 318 | NKP  | OAE-CAK-OAJ-CAI |
| 33  | F     | 307 | LMT  | C1-C2-C3-C4     |
| 22  | A     | 838 | CLA  | C3-C5-C6-C7     |
| 39  | 6     | 315 | CHL  | C4C-C3C-CAC-CBC |
| 40  | 1     | 318 | SQD  | C4-C5-C6-S      |
| 27  | A     | 852 | DGA  | CA9-CAA-CBA-CCA |
| 25  | 4     | 820 | LHG  | O1-C1-C2-O2     |
| 22  | 1     | 310 | CLA  | C3-C5-C6-C7     |
| 22  | 3     | 313 | CLA  | C3-C5-C6-C7     |
| 38  | 3     | 303 | LUT  | C31-C32-C33-C40 |
| 38  | 4     | 802 | LUT  | C11-C12-C13-C20 |
| 22  | B     | 808 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 1     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 1     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 7     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 9     | 304 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 324 | CLA  | C4-C3-C5-C6     |
| 22  | 1     | 316 | CLA  | C13-C15-C16-C17 |
| 22  | 5     | 309 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 807 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 821 | CLA  | C2A-CAA-CBA-CGA |
| 25  | A     | 849 | LHG  | O6-C4-C5-C6     |
| 35  | J     | 102 | T7X  | O13-C7-C8-C9    |
| 41  | 7     | 319 | 3PH  | O11-C1-C2-C3    |
| 22  | 4     | 810 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 827 | CLA  | C15-C16-C17-C18 |
| 22  | 7     | 309 | CLA  | C5-C6-C7-C8     |
| 25  | 6     | 323 | LHG  | C34-C35-C36-C37 |
| 22  | A     | 802 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 805 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 807 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 808 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 814 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 814 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 818 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 818 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 835 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 835 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 840 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 854 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 801 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 809 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 813 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 816 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 820 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 825 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 826 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 829 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 830 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 833 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 834 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 838 | CLA  | C11-C12-C13-C15 |
| 22  | F     | 301 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 1     | 304 | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 307 | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 307 | CLA  | C11-C10-C8-C7   |
| 22  | 1     | 309 | CLA  | C11-C10-C8-C7   |
| 22  | Z     | 303 | CLA  | C6-C7-C8-C10    |
| 22  | Z     | 306 | CLA  | C11-C10-C8-C7   |
| 22  | Z     | 309 | CLA  | C11-C10-C8-C7   |
| 22  | Z     | 316 | CLA  | C12-C13-C15-C16 |
| 22  | 3     | 308 | CLA  | C11-C12-C13-C15 |
| 22  | 3     | 318 | CLA  | C6-C7-C8-C10    |
| 22  | 3     | 322 | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 306 | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 306 | CLA  | C11-C12-C13-C15 |
| 22  | 7     | 308 | CLA  | C11-C10-C8-C7   |
| 22  | 8     | 305 | CLA  | C11-C10-C8-C7   |
| 22  | 8     | 310 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 308 | CLA  | C11-C12-C13-C15 |
| 22  | 5     | 315 | CLA  | C11-C12-C13-C15 |
| 22  | 6     | 301 | CLA  | C11-C10-C8-C7   |
| 22  | 6     | 302 | CLA  | C11-C10-C8-C7   |
| 22  | 6     | 309 | CLA  | C6-C7-C8-C10    |
| 22  | 6     | 310 | CLA  | C11-C10-C8-C7   |
| 22  | 6     | 310 | CLA  | C11-C12-C13-C15 |
| 22  | 6     | 319 | CLA  | C11-C10-C8-C7   |
| 22  | 9     | 303 | CLA  | C11-C10-C8-C7   |
| 23  | B     | 843 | PQN  | C16-C17-C18-C20 |
| 22  | B     | 841 | CLA  | C8-C10-C11-C12  |
| 41  | 7     | 319 | 3PH  | C33-C34-C35-C36 |
| 26  | 8     | 318 | NKP  | CAQ-CAR-CAS-CAT |
| 22  | 8     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 25  | A     | 849 | LHG  | O10-C23-O8-C6   |
| 39  | 8     | 312 | CHL  | O1A-CGA-O2A-C1  |
| 25  | 6     | 323 | LHG  | C2-C3-O3-P      |
| 22  | A     | 822 | CLA  | C4-C3-C5-C6     |
| 22  | 1     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 312 | CLA  | C3A-C2A-CAA-CBA |
| 39  | Z     | 312 | CHL  | C3A-C2A-CAA-CBA |
| 22  | B     | 820 | CLA  | C11-C12-C13-C15 |
| 22  | Z     | 306 | CLA  | C11-C12-C13-C15 |
| 22  | F     | 302 | CLA  | C13-C15-C16-C17 |
| 25  | A     | 849 | LHG  | O6-C4-C5-O7     |
| 25  | B     | 803 | LHG  | O6-C4-C5-O7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | B     | 851 | LHG  | O6-C4-C5-O7     |
| 25  | 6     | 323 | LHG  | O6-C4-C5-O7     |
| 41  | 7     | 319 | 3PH  | O11-C1-C2-O21   |
| 41  | 6     | 324 | 3PH  | O11-C1-C2-O21   |
| 22  | A     | 817 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 828 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 830 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 814 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 821 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 826 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 826 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 827 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 833 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 838 | CLA  | C14-C13-C15-C16 |
| 22  | B     | 842 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 316 | CLA  | C14-C13-C15-C16 |
| 22  | 3     | 310 | CLA  | C6-C7-C8-C9     |
| 22  | 7     | 308 | CLA  | C11-C12-C13-C14 |
| 22  | 7     | 323 | CLA  | C11-C10-C8-C9   |
| 22  | 8     | 308 | CLA  | C11-C10-C8-C9   |
| 26  | A     | 851 | NKP  | CAG-CAH-CAI-OAJ |
| 25  | A     | 849 | LHG  | C11-C10-C9-C8   |
| 25  | 6     | 323 | LHG  | C11-C10-C9-C8   |
| 24  | 3     | 305 | BCR  | C15-C16-C17-C18 |
| 38  | 4     | 803 | LUT  | C9-C10-C11-C12  |
| 38  | 4     | 803 | LUT  | C33-C34-C35-C15 |
| 22  | 3     | 310 | CLA  | C8-C10-C11-C12  |
| 25  | 1     | 317 | LHG  | O7-C5-C6-O8     |
| 25  | 4     | 820 | LHG  | O7-C5-C6-O8     |
| 22  | A     | 840 | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 308 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 816 | CLA  | C11-C10-C8-C9   |
| 25  | B     | 850 | LHG  | C4-C5-C6-O8     |
| 25  | 4     | 820 | LHG  | C4-C5-C6-O8     |
| 25  | 9     | 315 | LHG  | C4-C5-C6-O8     |
| 31  | 1     | 319 | DGD  | C1G-C2G-C3G-O3G |
| 34  | F     | 308 | LMG  | O1-C7-C8-C9     |
| 22  | B     | 842 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 813 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 824 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 826 | CLA  | CAD-CBD-CGD-O2D |
| 22  | 1     | 309 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 9     | 305 | CLA  | CAD-CBD-CGD-O2D |
| 39  | Z     | 311 | CHL  | CAD-CBD-CGD-O2D |
| 39  | 8     | 301 | CHL  | CAD-CBD-CGD-O2D |
| 22  | 1     | 308 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 809 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 813 | CLA  | C2A-CAA-CBA-CGA |
| 39  | 3     | 317 | CHL  | C2A-CAA-CBA-CGA |
| 25  | 5     | 324 | LHG  | C26-C27-C28-C29 |
| 22  | 6     | 312 | CLA  | C15-C16-C17-C18 |
| 25  | A     | 850 | LHG  | C30-C31-C32-C33 |
| 22  | A     | 826 | CLA  | CAD-CBD-CGD-O1D |
| 22  | K     | 205 | CLA  | CAD-CBD-CGD-O1D |
| 22  | 1     | 307 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 1     | 307 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 1     | 309 | CLA  | CAD-CBD-CGD-O1D |
| 22  | 1     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 8     | 307 | CLA  | CAD-CBD-CGD-O1D |
| 22  | 8     | 309 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 8     | 309 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 4     | 808 | CLA  | CHA-CBD-CGD-O1D |
| 22  | 4     | 808 | CLA  | CHA-CBD-CGD-O2D |
| 22  | 9     | 305 | CLA  | CAD-CBD-CGD-O1D |
| 25  | A     | 849 | LHG  | C3-O3-P-O5      |
| 25  | A     | 849 | LHG  | C4-O6-P-O3      |
| 25  | A     | 850 | LHG  | C4-O6-P-O4      |
| 25  | B     | 803 | LHG  | C3-O3-P-O5      |
| 25  | B     | 850 | LHG  | C4-O6-P-O5      |
| 25  | B     | 851 | LHG  | C3-O3-P-O6      |
| 25  | 8     | 317 | LHG  | C4-O6-P-O3      |
| 25  | 4     | 820 | LHG  | C3-O3-P-O6      |
| 25  | 4     | 820 | LHG  | C4-O6-P-O5      |
| 25  | 5     | 324 | LHG  | C3-O3-P-O4      |
| 25  | 5     | 324 | LHG  | C3-O3-P-O5      |
| 25  | 5     | 324 | LHG  | C3-O3-P-O6      |
| 25  | 5     | 324 | LHG  | C4-O6-P-O5      |
| 25  | 6     | 323 | LHG  | C4-O6-P-O3      |
| 25  | 9     | 315 | LHG  | C4-O6-P-O5      |
| 38  | 8     | 302 | LUT  | C9-C10-C11-C12  |
| 38  | 5     | 302 | LUT  | C9-C10-C11-C12  |
| 39  | Z     | 311 | CHL  | CAD-CBD-CGD-O1D |
| 39  | 3     | 317 | CHL  | CHA-CBD-CGD-O1D |
| 39  | 3     | 317 | CHL  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 39  | 8     | 301 | CHL  | CAD-CBD-CGD-O1D |
| 39  | 8     | 315 | CHL  | CHA-CBD-CGD-O1D |
| 39  | 8     | 315 | CHL  | CHA-CBD-CGD-O2D |
| 39  | 4     | 819 | CHL  | CHA-CBD-CGD-O1D |
| 39  | 4     | 819 | CHL  | CHA-CBD-CGD-O2D |
| 39  | 5     | 316 | CHL  | CHA-CBD-CGD-O1D |
| 39  | 5     | 316 | CHL  | CHA-CBD-CGD-O2D |
| 39  | 5     | 317 | CHL  | CHA-CBD-CGD-O1D |
| 39  | 5     | 317 | CHL  | CHA-CBD-CGD-O2D |
| 39  | 5     | 321 | CHL  | CHA-CBD-CGD-O1D |
| 39  | 5     | 321 | CHL  | CHA-CBD-CGD-O2D |
| 39  | 6     | 316 | CHL  | CHA-CBD-CGD-O1D |
| 39  | 6     | 316 | CHL  | CHA-CBD-CGD-O2D |
| 39  | 6     | 320 | CHL  | CHA-CBD-CGD-O1D |
| 39  | 6     | 320 | CHL  | CHA-CBD-CGD-O2D |
| 39  | 9     | 314 | CHL  | CHA-CBD-CGD-O1D |
| 39  | 9     | 314 | CHL  | CHA-CBD-CGD-O2D |
| 43  | 8     | 319 | LPX  | C1-O2-P1-O4     |
| 22  | 5     | 323 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 9     | 303 | CLA  | C2B-C3B-CAB-CBB |
| 24  | B     | 845 | BCR  | C23-C24-C25-C30 |
| 39  | 9     | 312 | CHL  | C2-C3-C5-C6     |
| 25  | 7     | 318 | LHG  | C5-C4-O6-P      |
| 25  | 5     | 324 | LHG  | C5-C4-O6-P      |
| 35  | J     | 102 | T7X  | C8-C7-O13-P1    |
| 38  | 4     | 802 | LUT  | C11-C12-C13-C14 |
| 22  | A     | 802 | CLA  | O1A-CGA-O2A-C1  |
| 22  | 4     | 810 | CLA  | O1D-CGD-O2D-CED |
| 22  | 1     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 39  | 6     | 315 | CHL  | C2A-CAA-CBA-CGA |
| 25  | 7     | 318 | LHG  | C30-C31-C32-C33 |
| 22  | 7     | 324 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 810 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 813 | CLA  | C11-C10-C8-C7   |
| 22  | Z     | 305 | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 309 | CLA  | C11-C10-C8-C7   |
| 22  | 5     | 301 | CLA  | C11-C10-C8-C7   |
| 22  | 5     | 309 | CLA  | C11-C10-C8-C7   |
| 34  | F     | 308 | LMG  | C9-C8-O7-C10    |
| 24  | B     | 848 | BCR  | C18-C19-C20-C21 |
| 24  | 3     | 304 | BCR  | C10-C11-C12-C13 |
| 24  | 3     | 307 | BCR  | C18-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | 5     | 305 | BCR  | C18-C19-C20-C21 |
| 22  | A     | 838 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 3     | 311 | CLA  | C8-C10-C11-C12  |
| 22  | 5     | 313 | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 307 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 814 | CLA  | C2-C3-C5-C6     |
| 36  | J     | 105 | C7Z  | C29-C30-C31-C32 |
| 22  | F     | 304 | CLA  | C16-C17-C18-C20 |
| 22  | 8     | 310 | CLA  | C11-C12-C13-C15 |
| 41  | 8     | 320 | 3PH  | O22-C21-C22-C23 |
| 27  | A     | 852 | DGA  | CBB-CCB-CDB-CEB |
| 25  | B     | 851 | LHG  | O6-C4-C5-C6     |
| 22  | A     | 805 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 819 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 833 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 835 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 840 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 811 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 818 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 822 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 831 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 305 | CLA  | C6-C7-C8-C9     |
| 22  | Z     | 306 | CLA  | C11-C10-C8-C9   |
| 22  | Z     | 309 | CLA  | C11-C10-C8-C9   |
| 22  | 7     | 304 | CLA  | C11-C10-C8-C9   |
| 22  | 7     | 307 | CLA  | C11-C12-C13-C14 |
| 22  | 7     | 308 | CLA  | C11-C10-C8-C9   |
| 22  | 5     | 308 | CLA  | C11-C12-C13-C14 |
| 22  | 6     | 301 | CLA  | C11-C10-C8-C9   |
| 22  | 6     | 302 | CLA  | C11-C10-C8-C9   |
| 39  | 5     | 316 | CHL  | C6-C7-C8-C9     |
| 22  | A     | 819 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 823 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 824 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 825 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 833 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 817 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 822 | CLA  | C6-C7-C8-C10    |
| 22  | L     | 202 | CLA  | C11-C12-C13-C15 |
| 22  | 1     | 304 | CLA  | C11-C12-C13-C15 |
| 22  | 1     | 306 | CLA  | C11-C12-C13-C15 |
| 22  | Z     | 305 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 3     | 322 | CLA  | C11-C10-C8-C7   |
| 22  | 7     | 312 | CLA  | C11-C10-C8-C7   |
| 25  | 6     | 323 | LHG  | C13-C14-C15-C16 |
| 22  | L     | 202 | CLA  | O1D-CGD-O2D-CED |
| 41  | 5     | 325 | 3PH  | O11-C1-C2-O21   |
| 22  | A     | 807 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 805 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 835 | CLA  | CBD-CGD-O2D-CED |
| 39  | 6     | 318 | CHL  | C2-C3-C5-C6     |
| 25  | A     | 850 | LHG  | C27-C28-C29-C30 |
| 25  | 9     | 315 | LHG  | O7-C5-C6-O8     |
| 22  | B     | 842 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 6     | 302 | CLA  | CAA-CBA-CGA-O2A |
| 24  | B     | 847 | BCR  | C13-C14-C15-C16 |
| 38  | 5     | 303 | LUT  | C9-C10-C11-C12  |
| 22  | A     | 805 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 8     | 316 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 811 | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 312 | CLA  | C8-C10-C11-C12  |
| 39  | 3     | 317 | CHL  | O1D-CGD-O2D-CED |
| 22  | 1     | 316 | CLA  | C2-C1-O2A-CGA   |
| 22  | 4     | 815 | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 309 | CLA  | C4-C3-C5-C6     |
| 25  | 8     | 317 | LHG  | C29-C30-C31-C32 |
| 42  | 7     | 321 | SPH  | C14-C15-C16-C17 |
| 25  | 8     | 317 | LHG  | C4-C5-C6-O8     |
| 25  | B     | 803 | LHG  | C26-C27-C28-C29 |
| 38  | 6     | 303 | LUT  | C27-C28-C29-C39 |
| 22  | Z     | 306 | CLA  | C11-C12-C13-C14 |
| 22  | 6     | 309 | CLA  | C16-C17-C18-C19 |
| 22  | 6     | 312 | CLA  | O1D-CGD-O2D-CED |
| 22  | A     | 854 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 805 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 810 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 812 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 825 | CLA  | C2A-CAA-CBA-CGA |
| 22  | Z     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 24  | A     | 845 | BCR  | C15-C16-C17-C18 |
| 24  | 3     | 307 | BCR  | C15-C16-C17-C18 |
| 22  | 6     | 307 | CLA  | C11-C12-C13-C15 |
| 25  | 7     | 318 | LHG  | C10-C11-C12-C13 |
| 31  | 1     | 319 | DGD  | C6A-C7A-C8A-C9A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 8     | 307 | CLA  | O1A-CGA-O2A-C1  |
| 41  | 8     | 320 | 3PH  | O21-C21-C22-C23 |
| 22  | 4     | 808 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 826 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 827 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 830 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 834 | CLA  | C11-C10-C8-C9   |
| 22  | F     | 301 | CLA  | C11-C10-C8-C9   |
| 22  | L     | 202 | CLA  | C14-C13-C15-C16 |
| 22  | 8     | 310 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 309 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 314 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 319 | CLA  | C11-C10-C8-C9   |
| 22  | 8     | 307 | CLA  | CBA-CGA-O2A-C1  |
| 22  | B     | 835 | CLA  | O1D-CGD-O2D-CED |
| 39  | 5     | 321 | CHL  | O1D-CGD-O2D-CED |
| 22  | B     | 821 | CLA  | C13-C15-C16-C17 |
| 22  | 4     | 807 | CLA  | C16-C17-C18-C20 |
| 22  | Z     | 313 | CLA  | C5-C6-C7-C8     |
| 22  | 7     | 309 | CLA  | C2-C3-C5-C6     |
| 26  | A     | 851 | NKP  | CAQ-CAR-CAS-CAT |
| 38  | 7     | 302 | LUT  | C9-C10-C11-C12  |
| 39  | 4     | 816 | CHL  | CBD-CGD-O2D-CED |
| 22  | A     | 802 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 810 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 821 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 819 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 828 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 831 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 834 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 838 | CLA  | C6-C7-C8-C10    |
| 22  | 1     | 310 | CLA  | C6-C7-C8-C10    |
| 22  | Z     | 308 | CLA  | C11-C10-C8-C7   |
| 22  | 5     | 308 | CLA  | C11-C10-C8-C7   |
| 22  | 6     | 322 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 816 | CLA  | C5-C6-C7-C8     |
| 22  | 6     | 312 | CLA  | CBD-CGD-O2D-CED |
| 42  | 7     | 320 | SPH  | C11-C10-C9-C8   |
| 22  | B     | 824 | CLA  | C3-C5-C6-C7     |
| 22  | 7     | 304 | CLA  | C3-C5-C6-C7     |
| 22  | F     | 302 | CLA  | C8-C10-C11-C12  |
| 22  | 6     | 302 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 7     | 324 | CLA  | C11-C12-C13-C14 |
| 22  | 3     | 313 | CLA  | C13-C15-C16-C17 |
| 22  | Z     | 316 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 5     | 309 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 6     | 309 | CLA  | C3A-C2A-CAA-CBA |
| 39  | 4     | 814 | CHL  | C3A-C2A-CAA-CBA |
| 22  | B     | 817 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 820 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 804 | CLA  | CAA-CBA-CGA-O1A |
| 24  | A     | 844 | BCR  | C11-C10-C9-C34  |
| 24  | A     | 845 | BCR  | C35-C13-C14-C15 |
| 24  | A     | 848 | BCR  | C11-C10-C9-C34  |
| 24  | A     | 848 | BCR  | C16-C17-C18-C36 |
| 24  | B     | 844 | BCR  | C35-C13-C14-C15 |
| 24  | B     | 844 | BCR  | C16-C17-C18-C36 |
| 24  | B     | 846 | BCR  | C11-C10-C9-C34  |
| 24  | B     | 846 | BCR  | C20-C21-C22-C37 |
| 24  | B     | 848 | BCR  | C20-C21-C22-C37 |
| 24  | B     | 853 | BCR  | C11-C10-C9-C34  |
| 32  | F     | 306 | RRX  | C16-C17-C18-C36 |
| 32  | F     | 306 | RRX  | C35-C13-C14-C15 |
| 32  | F     | 306 | RRX  | C11-C10-C9-C34  |
| 22  | A     | 802 | CLA  | C8-C10-C11-C12  |
| 31  | 1     | 319 | DGD  | O6D-C5D-C6D-O5D |
| 42  | 7     | 320 | SPH  | C10-C11-C12-C13 |
| 41  | 7     | 319 | 3PH  | C34-C35-C36-C37 |
| 22  | B     | 801 | CLA  | C2-C1-O2A-CGA   |
| 22  | 3     | 312 | CLA  | C2-C1-O2A-CGA   |
| 22  | 4     | 812 | CLA  | C2-C1-O2A-CGA   |
| 22  | 5     | 315 | CLA  | C2-C1-O2A-CGA   |
| 22  | 6     | 301 | CLA  | C2-C1-O2A-CGA   |
| 24  | A     | 848 | BCR  | C9-C10-C11-C12  |
| 24  | 3     | 306 | BCR  | C7-C8-C9-C34    |
| 22  | 1     | 305 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 5     | 315 | CLA  | C15-C16-C17-C18 |
| 25  | 8     | 317 | LHG  | C26-C27-C28-C29 |
| 25  | 5     | 324 | LHG  | C25-C26-C27-C28 |
| 22  | 5     | 318 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 842 | CLA  | C2-C3-C5-C6     |
| 26  | A     | 851 | NKP  | OAF-CAG-CAH-CAI |
| 22  | A     | 824 | CLA  | O1D-CGD-O2D-CED |
| 22  | 8     | 305 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 5     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 25  | A     | 849 | LHG  | C4-C5-C6-O8     |
| 22  | A     | 810 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 824 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 828 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 821 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 834 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 838 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 838 | CLA  | C11-C12-C13-C14 |
| 22  | 1     | 304 | CLA  | C14-C13-C15-C16 |
| 22  | 1     | 307 | CLA  | C11-C10-C8-C9   |
| 22  | 7     | 306 | CLA  | C11-C10-C8-C9   |
| 22  | 7     | 306 | CLA  | C11-C12-C13-C14 |
| 22  | 8     | 309 | CLA  | C11-C10-C8-C9   |
| 22  | 6     | 310 | CLA  | C11-C10-C8-C9   |
| 22  | 6     | 314 | CLA  | C11-C10-C8-C9   |
| 22  | 6     | 322 | CLA  | C6-C7-C8-C9     |
| 22  | 9     | 306 | CLA  | C11-C10-C8-C9   |
| 39  | 5     | 316 | CHL  | C11-C12-C13-C14 |
| 25  | 6     | 323 | LHG  | C33-C34-C35-C36 |
| 22  | 3     | 308 | CLA  | C15-C16-C17-C18 |
| 22  | 3     | 312 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 826 | CLA  | CAA-CBA-CGA-O2A |
| 34  | J     | 101 | LMG  | C9-C8-O7-C10    |
| 21  | A     | 801 | CL0  | C1A-C2A-CAA-CBA |
| 22  | 7     | 312 | CLA  | C11-C12-C13-C14 |
| 22  | 6     | 309 | CLA  | C16-C17-C18-C20 |
| 22  | 8     | 308 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 834 | CLA  | C1A-C2A-CAA-CBA |
| 22  | Z     | 316 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 5     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 24  | A     | 844 | BCR  | C11-C10-C9-C8   |
| 24  | A     | 845 | BCR  | C12-C13-C14-C15 |
| 24  | A     | 848 | BCR  | C11-C10-C9-C8   |
| 24  | A     | 848 | BCR  | C16-C17-C18-C19 |
| 24  | B     | 844 | BCR  | C12-C13-C14-C15 |
| 24  | B     | 844 | BCR  | C16-C17-C18-C19 |
| 24  | B     | 846 | BCR  | C11-C10-C9-C8   |
| 24  | B     | 846 | BCR  | C20-C21-C22-C23 |
| 24  | B     | 853 | BCR  | C11-C10-C9-C8   |
| 32  | F     | 306 | RRX  | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | F     | 306 | RRX  | C12-C13-C14-C15 |
| 32  | F     | 306 | RRX  | C11-C10-C9-C8   |
| 22  | 1     | 305 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 833 | CLA  | C8-C10-C11-C12  |
| 22  | 6     | 319 | CLA  | C8-C10-C11-C12  |
| 31  | B     | 852 | DGD  | O1A-C1A-O1G-C1G |
| 22  | 4     | 818 | CLA  | C2B-C3B-CAB-CBB |
| 24  | A     | 856 | BCR  | C5-C6-C7-C8     |
| 24  | B     | 846 | BCR  | C23-C24-C25-C26 |
| 24  | B     | 853 | BCR  | C23-C24-C25-C26 |
| 24  | F     | 303 | BCR  | C23-C24-C25-C26 |
| 24  | J     | 104 | BCR  | C23-C24-C25-C26 |
| 24  | 3     | 307 | BCR  | C23-C24-C25-C30 |
| 38  | 3     | 303 | LUT  | C1-C6-C7-C8     |
| 27  | A     | 852 | DGA  | CBB-CAB-CB9-CB8 |
| 25  | 3     | 321 | LHG  | C5-C4-O6-P      |
| 26  | 8     | 318 | NKP  | CAR-CAS-CAT-CAU |
| 42  | 7     | 320 | SPH  | C7-C8-C9-C10    |
| 22  | B     | 822 | CLA  | C11-C10-C8-C9   |
| 22  | Z     | 305 | CLA  | C11-C10-C8-C9   |
| 42  | 7     | 321 | SPH  | O1-C1-C2-N2     |
| 22  | A     | 822 | CLA  | C2-C3-C5-C6     |
| 40  | 1     | 318 | SQD  | C7-C8-C9-C10    |
| 22  | B     | 807 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Z     | 304 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 9     | 310 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 5     | 308 | CLA  | C5-C6-C7-C8     |
| 21  | A     | 801 | CL0  | C11-C12-C13-C15 |
| 22  | A     | 825 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 830 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 832 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 832 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 838 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 840 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 805 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 809 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 818 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 827 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 831 | CLA  | C11-C10-C8-C7   |
| 22  | L     | 202 | CLA  | C12-C13-C15-C16 |
| 22  | Z     | 313 | CLA  | C6-C7-C8-C10    |
| 22  | 7     | 323 | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 5     | 307 | CLA  | C11-C10-C8-C7   |
| 22  | 6     | 309 | CLA  | C11-C10-C8-C7   |
| 22  | 6     | 309 | CLA  | C11-C12-C13-C15 |
| 22  | 6     | 314 | CLA  | C6-C7-C8-C10    |
| 39  | 3     | 317 | CHL  | C6-C7-C8-C10    |
| 28  | A     | 853 | OCA  | C3-C4-C5-C6     |
| 22  | 6     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 7     | 322 | CLA  | C5-C6-C7-C8     |
| 25  | 6     | 323 | LHG  | C14-C15-C16-C17 |
| 35  | J     | 102 | T7X  | C16-C17-C18-C19 |
| 25  | 4     | 820 | LHG  | C25-C26-C27-C28 |
| 22  | 8     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 804 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Z     | 316 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 816 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 822 | CLA  | C11-C10-C8-C7   |
| 24  | B     | 844 | BCR  | C11-C12-C13-C35 |
| 38  | Z     | 302 | LUT  | C31-C32-C33-C40 |
| 25  | A     | 849 | LHG  | C10-C11-C12-C13 |
| 22  | Z     | 304 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 811 | CLA  | C15-C16-C17-C18 |
| 40  | 1     | 318 | SQD  | C24-C25-C26-C27 |
| 25  | 1     | 317 | LHG  | C17-C18-C19-C20 |
| 22  | A     | 808 | CLA  | C5-C6-C7-C8     |
| 22  | B     | 807 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 9     | 310 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 814 | CLA  | C11-C12-C13-C15 |
| 22  | 1     | 307 | CLA  | C11-C12-C13-C15 |
| 22  | 7     | 323 | CLA  | C16-C17-C18-C20 |
| 22  | B     | 806 | CLA  | CBA-CGA-O2A-C1  |
| 33  | G     | 204 | LMT  | C5-C6-C7-C8     |
| 22  | A     | 823 | CLA  | C3-C5-C6-C7     |
| 22  | 1     | 310 | CLA  | C2C-C3C-CAC-CBC |
| 22  | A     | 802 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 814 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 810 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 817 | CLA  | C6-C7-C8-C9     |
| 22  | 8     | 310 | CLA  | C11-C10-C8-C9   |
| 22  | 6     | 310 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 835 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 838 | CLA  | C8-C10-C11-C12  |
| 22  | A     | 811 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | B     | 831 | CLA  | C8-C10-C11-C12  |
| 22  | 3     | 314 | CLA  | C5-C6-C7-C8     |
| 22  | 9     | 304 | CLA  | CAA-CBA-CGA-O2A |
| 42  | 7     | 320 | SPH  | O1-C1-C2-C3     |
| 27  | A     | 852 | DGA  | CB6-CB7-CB8-CB9 |
| 25  | 4     | 820 | LHG  | O10-C23-C24-C25 |
| 22  | 6     | 301 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 813 | CLA  | C11-C10-C8-C9   |
| 22  | 5     | 309 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 828 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 5     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 27  | A     | 852 | DGA  | CAA-CBA-CCA-CDA |
| 39  | 4     | 816 | CHL  | O1D-CGD-O2D-CED |
| 22  | A     | 805 | CLA  | C2A-CAA-CBA-CGA |
| 22  | B     | 809 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 3     | 314 | CLA  | C11-C12-C13-C15 |
| 22  | 6     | 307 | CLA  | C11-C12-C13-C14 |
| 41  | 6     | 324 | 3PH  | C29-C2A-C2B-C2C |
| 22  | 2     | 304 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 820 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 841 | CLA  | C4-C3-C5-C6     |
| 22  | 5     | 310 | CLA  | C4-C3-C5-C6     |
| 22  | 5     | 311 | CLA  | C4-C3-C5-C6     |
| 26  | A     | 851 | NKP  | CAN-CAO-CAP-CAQ |
| 42  | 7     | 320 | SPH  | C13-C14-C15-C16 |
| 22  | 4     | 808 | CLA  | C11-C12-C13-C14 |
| 22  | Z     | 316 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 841 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 310 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 807 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 834 | CLA  | CAA-CBA-CGA-O2A |
| 41  | 6     | 324 | 3PH  | O21-C21-C22-C23 |
| 22  | 6     | 301 | CLA  | C11-C12-C13-C15 |
| 42  | 7     | 321 | SPH  | C5-C6-C7-C8     |
| 39  | 9     | 312 | CHL  | CHA-CBD-CGD-O1D |
| 22  | 6     | 322 | CLA  | O1A-CGA-O2A-C1  |
| 22  | Z     | 310 | CLA  | CAA-CBA-CGA-O2A |
| 39  | 6     | 318 | CHL  | O1A-CGA-O2A-C1  |
| 22  | A     | 808 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 809 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 815 | CLA  | CAA-CBA-CGA-O2A |
| 22  | L     | 201 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 42  | 7     | 321 | SPH  | C13-C14-C15-C16 |
| 22  | A     | 824 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 810 | CLA  | C6-C7-C8-C10    |
| 25  | 6     | 323 | LHG  | C16-C17-C18-C19 |
| 42  | 7     | 320 | SPH  | C11-C12-C13-C14 |
| 22  | B     | 833 | CLA  | C13-C15-C16-C17 |
| 22  | B     | 806 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 810 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 9     | 304 | CLA  | CAA-CBA-CGA-O1A |
| 38  | 3     | 303 | LUT  | C31-C32-C33-C34 |
| 22  | A     | 840 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 814 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 816 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 818 | CLA  | C6-C7-C8-C9     |
| 22  | 3     | 308 | CLA  | C11-C12-C13-C14 |
| 22  | 3     | 311 | CLA  | C11-C10-C8-C9   |
| 22  | 5     | 315 | CLA  | C11-C12-C13-C14 |
| 31  | 1     | 319 | DGD  | C2G-C3G-O3G-C1D |
| 41  | 8     | 320 | 3PH  | C1-O11-P-O12    |
| 25  | A     | 850 | LHG  | C9-C10-C11-C12  |
| 22  | B     | 822 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 7     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 4     | 805 | CLA  | C2A-CAA-CBA-CGA |
| 25  | A     | 850 | LHG  | C11-C10-C9-C8   |
| 25  | A     | 850 | LHG  | C25-C26-C27-C28 |
| 22  | A     | 834 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 807 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 838 | CLA  | C3A-C2A-CAA-CBA |
| 22  | F     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 22  | Z     | 308 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 2     | 302 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 2     | 302 | CLA  | CAA-CBA-CGA-O2A |
| 25  | 8     | 317 | LHG  | C24-C25-C26-C27 |
| 34  | F     | 308 | LMG  | O10-C28-O8-C9   |
| 22  | 7     | 306 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 852 | DGD  | C9B-CAB-CBB-CCB |
| 22  | L     | 203 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 810 | CLA  | O2A-C1-C2-C3    |
| 22  | A     | 839 | CLA  | O2A-C1-C2-C3    |
| 22  | 7     | 324 | CLA  | C10-C11-C12-C13 |
| 22  | A     | 820 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 6     | 309 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 852 | DGD  | C2A-C1A-O1G-C1G |
| 34  | F     | 308 | LMG  | C29-C28-O8-C9   |
| 39  | 6     | 318 | CHL  | CBA-CGA-O2A-C1  |
| 22  | 1     | 313 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 825 | CLA  | C16-C17-C18-C20 |
| 22  | 5     | 307 | CLA  | C11-C12-C13-C15 |
| 25  | B     | 803 | LHG  | C2-C3-O3-P      |
| 22  | F     | 304 | CLA  | C8-C10-C11-C12  |
| 22  | 7     | 324 | CLA  | C8-C10-C11-C12  |
| 22  | B     | 808 | CLA  | C8-C10-C11-C12  |
| 41  | 8     | 320 | 3PH  | C38-C39-C3A-C3B |
| 22  | Z     | 309 | CLA  | O1D-CGD-O2D-CED |
| 22  | 2     | 302 | CLA  | CAA-CBA-CGA-O1A |
| 36  | J     | 105 | C7Z  | C33-C34-C35-C15 |
| 25  | 8     | 317 | LHG  | C30-C31-C32-C33 |
| 25  | Z     | 317 | LHG  | C24-C25-C26-C27 |
| 22  | 7     | 304 | CLA  | C8-C10-C11-C12  |
| 22  | 3     | 322 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 7     | 312 | CLA  | CAA-CBA-CGA-O2A |
| 35  | J     | 102 | T7X  | O16-C8-C9-O18   |
| 22  | A     | 802 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 808 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 808 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 811 | CLA  | C14-C13-C15-C16 |
| 22  | A     | 827 | CLA  | C11-C12-C13-C14 |
| 22  | A     | 854 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 817 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 825 | CLA  | C11-C10-C8-C9   |
| 22  | 1     | 309 | CLA  | C11-C10-C8-C9   |
| 22  | 1     | 314 | CLA  | C14-C13-C15-C16 |
| 22  | 1     | 316 | CLA  | C14-C13-C15-C16 |
| 22  | 8     | 305 | CLA  | C11-C10-C8-C9   |
| 22  | 6     | 322 | CLA  | C11-C10-C8-C9   |
| 22  | 9     | 303 | CLA  | C11-C10-C8-C9   |
| 23  | B     | 843 | PQN  | C16-C17-C18-C19 |
| 23  | B     | 843 | PQN  | C19-C18-C20-C21 |
| 22  | A     | 807 | CLA  | CAA-CBA-CGA-O2A |
| 41  | 5     | 325 | 3PH  | O11-C1-C2-C3    |
| 24  | B     | 844 | BCR  | C21-C22-C23-C24 |
| 38  | Z     | 301 | LUT  | C27-C28-C29-C30 |
| 25  | A     | 850 | LHG  | C35-C36-C37-C38 |
| 25  | 1     | 317 | LHG  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 7     | 324 | CLA  | C2-C3-C5-C6     |
| 22  | 7     | 317 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 803 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 803 | CLA  | C11-C12-C13-C15 |
| 22  | A     | 827 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 840 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 817 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 818 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 826 | CLA  | C12-C13-C15-C16 |
| 22  | B     | 827 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 833 | CLA  | C11-C12-C13-C15 |
| 22  | 1     | 316 | CLA  | C12-C13-C15-C16 |
| 22  | Z     | 316 | CLA  | C11-C10-C8-C7   |
| 22  | 3     | 310 | CLA  | C11-C10-C8-C7   |
| 22  | 3     | 312 | CLA  | C11-C10-C8-C7   |
| 22  | 3     | 313 | CLA  | C11-C10-C8-C7   |
| 22  | 3     | 322 | CLA  | C11-C12-C13-C15 |
| 22  | 7     | 307 | CLA  | C11-C10-C8-C7   |
| 22  | 5     | 310 | CLA  | C6-C7-C8-C10    |
| 22  | 5     | 313 | CLA  | C11-C10-C8-C7   |
| 22  | 5     | 318 | CLA  | C11-C12-C13-C15 |
| 39  | 9     | 312 | CHL  | C11-C12-C13-C15 |
| 22  | 1     | 304 | CLA  | C8-C10-C11-C12  |
| 22  | Z     | 305 | CLA  | C5-C6-C7-C8     |
| 25  | A     | 850 | LHG  | C12-C13-C14-C15 |
| 22  | B     | 841 | CLA  | C2B-C3B-CAB-CBB |
| 22  | Z     | 315 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 7     | 310 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 4     | 805 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 4     | 812 | CLA  | C2B-C3B-CAB-CBB |
| 22  | 6     | 308 | CLA  | C2B-C3B-CAB-CBB |
| 24  | B     | 847 | BCR  | C23-C24-C25-C30 |
| 24  | G     | 203 | BCR  | C23-C24-C25-C26 |
| 36  | 5     | 306 | C7Z  | C25-C26-C27-C28 |
| 38  | 1     | 302 | LUT  | C1-C6-C7-C8     |
| 38  | Z     | 302 | LUT  | C1-C6-C7-C8     |
| 38  | 8     | 302 | LUT  | C5-C6-C7-C8     |
| 38  | 6     | 304 | LUT  | C1-C6-C7-C8     |
| 22  | B     | 818 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 3     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 25  | A     | 849 | LHG  | O7-C7-C8-C9     |
| 25  | 1     | 317 | LHG  | O8-C23-C24-C25  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 3     | 301 | DGD  | O1G-C1A-C2A-C3A |
| 22  | A     | 816 | CLA  | C2-C1-O2A-CGA   |
| 22  | Z     | 303 | CLA  | C2-C1-O2A-CGA   |
| 39  | 5     | 316 | CHL  | C8-C10-C11-C12  |
| 25  | A     | 850 | LHG  | C2-C3-O3-P      |
| 22  | A     | 812 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 4     | 806 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 9     | 306 | CLA  | CAA-CBA-CGA-O2A |
| 25  | 7     | 318 | LHG  | C25-C26-C27-C28 |
| 22  | A     | 837 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 5     | 323 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 834 | CLA  | C2-C3-C5-C6     |
| 22  | L     | 202 | CLA  | C2-C3-C5-C6     |
| 22  | 3     | 312 | CLA  | C2-C3-C5-C6     |
| 22  | 5     | 311 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 833 | CLA  | C8-C10-C11-C12  |
| 39  | 8     | 301 | CHL  | O1A-CGA-O2A-C1  |
| 22  | 5     | 310 | CLA  | C8-C10-C11-C12  |
| 34  | F     | 308 | LMG  | C13-C14-C15-C16 |
| 22  | 1     | 306 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 835 | CLA  | C3-C5-C6-C7     |
| 22  | A     | 821 | CLA  | C16-C17-C18-C20 |
| 23  | B     | 843 | PQN  | C26-C27-C28-C29 |
| 22  | A     | 815 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 3     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 24  | B     | 846 | BCR  | C9-C10-C11-C12  |
| 24  | B     | 853 | BCR  | C9-C10-C11-C12  |
| 42  | 7     | 320 | SPH  | C6-C7-C8-C9     |
| 22  | L     | 202 | CLA  | C4-C3-C5-C6     |
| 22  | 3     | 312 | CLA  | C4-C3-C5-C6     |
| 22  | B     | 824 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 8     | 309 | CLA  | CAA-CBA-CGA-O2A |
| 39  | 6     | 315 | CHL  | C6-C7-C8-C10    |
| 22  | B     | 820 | CLA  | C2A-CAA-CBA-CGA |
| 22  | A     | 811 | CLA  | C13-C15-C16-C17 |
| 22  | 4     | 808 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 805 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 809 | CLA  | C11-C12-C13-C14 |
| 22  | B     | 811 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 824 | CLA  | C6-C7-C8-C9     |
| 22  | B     | 831 | CLA  | C11-C10-C8-C9   |
| 22  | 1     | 304 | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 3     | 313 | CLA  | C11-C10-C8-C9   |
| 22  | 5     | 307 | CLA  | C11-C10-C8-C9   |
| 22  | K     | 203 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 7     | 324 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 8     | 316 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 9     | 305 | CLA  | CAA-CBA-CGA-O2A |
| 25  | Z     | 317 | LHG  | O8-C23-C24-C25  |
| 25  | 9     | 315 | LHG  | O7-C7-C8-C9     |
| 25  | 9     | 315 | LHG  | O8-C23-C24-C25  |
| 34  | F     | 308 | LMG  | O7-C10-C11-C12  |
| 27  | A     | 852 | DGA  | OG1-CG1-CG2-CG3 |
| 22  | Z     | 303 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 22  | F     | 304 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 7     | 311 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 4     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 22  | 6     | 313 | CLA  | C4B-C3B-CAB-CBB |
| 22  | 3     | 322 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 810 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 813 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 820 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 855 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 823 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 825 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Z     | 305 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 4     | 805 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 4     | 818 | CLA  | CAA-CBA-CGA-O2A |
| 24  | B     | 844 | BCR  | C11-C12-C13-C14 |
| 24  | 3     | 306 | BCR  | C7-C8-C9-C10    |
| 38  | Z     | 302 | LUT  | C31-C32-C33-C34 |
| 38  | 6     | 303 | LUT  | C27-C28-C29-C30 |
| 38  | 4     | 803 | LUT  | C13-C14-C15-C35 |
| 22  | 1     | 310 | CLA  | C10-C11-C12-C13 |
| 22  | B     | 814 | CLA  | C11-C12-C13-C14 |
| 22  | Z     | 306 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 811 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 812 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 814 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 817 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 6     | 317 | CLA  | CAA-CBA-CGA-O2A |
| 35  | J     | 102 | T7X  | O18-C11-C31-C32 |
| 39  | 4     | 814 | CHL  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | 1     | 317 | LHG  | C24-C25-C26-C27 |
| 27  | A     | 852 | DGA  | CB4-CB5-CB6-CB7 |
| 27  | A     | 852 | DGA  | CDA-CEA-CFA-CGA |
| 22  | 6     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 824 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 837 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 834 | CLA  | C13-C15-C16-C17 |
| 22  | 7     | 314 | CLA  | O1D-CGD-O2D-CED |
| 22  | B     | 829 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 817 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 836 | CLA  | C2-C1-O2A-CGA   |
| 22  | 7     | 308 | CLA  | C2-C1-O2A-CGA   |
| 22  | 4     | 811 | CLA  | C2-C1-O2A-CGA   |
| 22  | 9     | 309 | CLA  | C2-C1-O2A-CGA   |
| 21  | A     | 801 | CL0  | C11-C10-C8-C7   |
| 22  | A     | 810 | CLA  | C11-C10-C8-C7   |
| 22  | A     | 812 | CLA  | C11-C12-C13-C15 |
| 22  | B     | 808 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 811 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 814 | CLA  | C6-C7-C8-C10    |
| 22  | B     | 829 | CLA  | C11-C10-C8-C7   |
| 22  | B     | 830 | CLA  | C6-C7-C8-C10    |
| 22  | F     | 304 | CLA  | C6-C7-C8-C10    |
| 22  | L     | 201 | CLA  | C11-C12-C13-C15 |
| 22  | 7     | 323 | CLA  | C6-C7-C8-C10    |
| 22  | 8     | 308 | CLA  | C11-C12-C13-C15 |
| 22  | 9     | 305 | CLA  | C6-C7-C8-C10    |
| 22  | 6     | 322 | CLA  | CBA-CGA-O2A-C1  |
| 22  | A     | 814 | CLA  | C5-C6-C7-C8     |
| 22  | A     | 824 | CLA  | C5-C6-C7-C8     |
| 22  | 1     | 307 | CLA  | C11-C12-C13-C14 |
| 22  | 7     | 312 | CLA  | C11-C12-C13-C15 |
| 25  | Z     | 317 | LHG  | C29-C30-C31-C32 |
| 22  | A     | 827 | CLA  | CAA-CBA-CGA-O2A |
| 25  | 8     | 317 | LHG  | O7-C7-C8-C9     |
| 25  | Z     | 317 | LHG  | C11-C10-C9-C8   |
| 22  | 1     | 310 | CLA  | C4C-C3C-CAC-CBC |
| 22  | A     | 834 | CLA  | C2A-CAA-CBA-CGA |
| 22  | 6     | 301 | CLA  | C2A-CAA-CBA-CGA |
| 25  | A     | 849 | LHG  | O9-C7-O7-C5     |
| 22  | 6     | 310 | CLA  | C16-C17-C18-C19 |
| 22  | B     | 828 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | 4     | 820 | LHG  | C5-C4-O6-P      |
| 22  | A     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 824 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 836 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 841 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 806 | CLA  | C3A-C2A-CAA-CBA |
| 22  | B     | 831 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 3     | 316 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 310 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 7     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 806 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 4     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 22  | 9     | 305 | CLA  | C3A-C2A-CAA-CBA |
| 22  | A     | 815 | CLA  | CAA-CBA-CGA-O1A |
| 22  | A     | 837 | CLA  | CAA-CBA-CGA-O1A |
| 22  | L     | 201 | CLA  | C8-C10-C11-C12  |
| 22  | 8     | 308 | CLA  | O1D-CGD-O2D-CED |
| 22  | G     | 201 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 5     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 39  | Z     | 311 | CHL  | CAA-CBA-CGA-O2A |
| 39  | 4     | 813 | CHL  | CAA-CBA-CGA-O2A |
| 22  | Z     | 309 | CLA  | CBD-CGD-O2D-CED |
| 22  | 8     | 308 | CLA  | CBD-CGD-O2D-CED |
| 22  | A     | 832 | CLA  | C15-C16-C17-C18 |
| 23  | B     | 843 | PQN  | C20-C21-C22-C23 |
| 21  | A     | 801 | CL0  | CAA-CBA-CGA-O1A |
| 22  | A     | 842 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 5     | 309 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 9     | 305 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 9     | 309 | CLA  | O1D-CGD-O2D-CED |
| 39  | 8     | 312 | CHL  | CAA-CBA-CGA-O2A |
| 39  | 5     | 317 | CHL  | CAA-CBA-CGA-O2A |
| 39  | 6     | 316 | CHL  | CAA-CBA-CGA-O2A |
| 39  | 2     | 303 | CHL  | CAA-CBA-CGA-O2A |
| 37  | K     | 201 | DAO  | C7-C8-C9-C10    |
| 22  | A     | 803 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 824 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 825 | CLA  | C11-C10-C8-C9   |
| 22  | A     | 827 | CLA  | C6-C7-C8-C9     |
| 22  | A     | 840 | CLA  | C11-C12-C13-C14 |
| 22  | Z     | 308 | CLA  | C11-C10-C8-C9   |
| 22  | 7     | 306 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | 7     | 323 | CLA  | C6-C7-C8-C9     |
| 22  | 6     | 309 | CLA  | C11-C10-C8-C9   |
| 22  | B     | 822 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 837 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 814 | CLA  | C5-C6-C7-C8     |
| 38  | 3     | 303 | LUT  | C13-C14-C15-C35 |
| 22  | B     | 833 | CLA  | C4-C3-C5-C6     |
| 22  | A     | 807 | CLA  | CAA-CBA-CGA-O1A |
| 22  | A     | 812 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 1     | 306 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 3     | 308 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 3     | 322 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 4     | 806 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 5     | 323 | CLA  | CAA-CBA-CGA-O1A |
| 31  | B     | 852 | DGD  | C5B-C6B-C7B-C8B |
| 22  | Z     | 306 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 829 | CLA  | C2-C3-C5-C6     |
| 22  | A     | 820 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 8     | 309 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 8     | 316 | CLA  | CAA-CBA-CGA-O1A |
| 25  | 1     | 317 | LHG  | O10-C23-C24-C25 |
| 25  | 9     | 315 | LHG  | O10-C23-C24-C25 |
| 22  | F     | 302 | CLA  | C10-C11-C12-C13 |
| 38  | 7     | 301 | LUT  | C27-C28-C29-C30 |
| 22  | K     | 203 | CLA  | CAA-CBA-CGA-O1A |
| 33  | G     | 204 | LMT  | C3'-C4'-O1B-C1B |
| 34  | J     | 101 | LMG  | C8-C7-O1-C1     |
| 27  | A     | 852 | DGA  | OG1-CG1-CG2-OG2 |
| 22  | A     | 811 | CLA  | CAA-CBA-CGA-O1A |
| 22  | A     | 855 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 4     | 805 | CLA  | CAA-CBA-CGA-O1A |
| 25  | A     | 849 | LHG  | O9-C7-C8-C9     |
| 25  | Z     | 317 | LHG  | O10-C23-C24-C25 |
| 31  | 3     | 301 | DGD  | O1A-C1A-C2A-C3A |
| 22  | A     | 814 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 3     | 316 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 8     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 39  | 6     | 315 | CHL  | C6-C7-C8-C9     |
| 41  | 7     | 319 | 3PH  | C1-C2-C3-O31    |
| 22  | A     | 810 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 814 | CLA  | CAA-CBA-CGA-O1A |
| 22  | Z     | 305 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | 9     | 315 | LHG  | O9-C7-C8-C9     |
| 39  | 4     | 814 | CHL  | CAA-CBA-CGA-O1A |
| 22  | B     | 806 | CLA  | C5-C6-C7-C8     |
| 22  | K     | 204 | CLA  | CAA-CBA-CGA-O2A |
| 25  | 6     | 323 | LHG  | O7-C7-C8-C9     |
| 39  | 1     | 312 | CHL  | CAA-CBA-CGA-O2A |
| 39  | Z     | 312 | CHL  | CAA-CBA-CGA-O2A |
| 22  | 6     | 309 | CLA  | C15-C16-C17-C18 |
| 22  | B     | 824 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 7     | 324 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 9     | 306 | CLA  | CAA-CBA-CGA-O1A |
| 35  | J     | 102 | T7X  | O19-C11-C31-C32 |
| 33  | G     | 204 | LMT  | C5'-C4'-O1B-C1B |
| 22  | K     | 204 | CLA  | CAD-CBD-CGD-O2D |
| 22  | 8     | 309 | CLA  | CAD-CBD-CGD-O2D |
| 22  | F     | 304 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 8     | 306 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 5     | 310 | CLA  | CAA-CBA-CGA-O2A |
| 40  | 1     | 318 | SQD  | C27-C28-C29-C30 |
| 22  | 3     | 314 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 4     | 818 | CLA  | CAA-CBA-CGA-O1A |
| 34  | F     | 308 | LMG  | O9-C10-C11-C12  |
| 22  | A     | 832 | CLA  | C10-C11-C12-C13 |
| 22  | 1     | 314 | CLA  | C13-C15-C16-C17 |
| 21  | A     | 801 | CL0  | C2-C1-O2A-CGA   |
| 22  | B     | 816 | CLA  | C2-C1-O2A-CGA   |
| 22  | A     | 827 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 812 | CLA  | CAA-CBA-CGA-O1A |
| 22  | Z     | 315 | CLA  | CAA-CBA-CGA-O2A |
| 39  | 5     | 316 | CHL  | CAA-CBA-CGA-O2A |
| 22  | B     | 817 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 6     | 314 | CLA  | CAA-CBA-CGA-O1A |
| 22  | 6     | 317 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 840 | CLA  | C5-C6-C7-C8     |
| 41  | 7     | 319 | 3PH  | C21-C22-C23-C24 |
| 22  | B     | 824 | CLA  | C6-C7-C8-C10    |
| 22  | A     | 823 | CLA  | CAA-CBA-CGA-O2A |
| 22  | A     | 831 | CLA  | CAA-CBA-CGA-O2A |
| 22  | B     | 831 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 1     | 315 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 5     | 318 | CLA  | CAA-CBA-CGA-O2A |
| 22  | 9     | 308 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | F     | 304 | CLA  | C13-C15-C16-C17 |
| 22  | A     | 814 | CLA  | C11-C12-C13-C15 |
| 22  | 6     | 312 | CLA  | C16-C17-C18-C20 |
| 22  | A     | 813 | CLA  | CAA-CBA-CGA-O1A |
| 22  | B     | 823 | CLA  | CAA-CBA-CGA-O1A |
| 25  | 8     | 317 | LHG  | O9-C7-C8-C9     |
| 39  | Z     | 311 | CHL  | CAA-CBA-CGA-O1A |
| 39  | 2     | 303 | CHL  | CAA-CBA-CGA-O1A |
| 33  | F     | 307 | LMT  | C5-C6-C7-C8     |
| 22  | B     | 839 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Z     | 303 | CLA  | CAA-CBA-CGA-O2A |
| 22  | Z     | 309 | CLA  | CAA-CBA-CGA-O2A |
| 25  | 4     | 821 | LHG  | O7-C7-C8-C9     |
| 26  | 8     | 318 | NKP  | OAJ-CAK-CAL-CAM |
| 22  | 3     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 22  | B     | 811 | CLA  | C8-C10-C11-C12  |
| 25  | 6     | 323 | LHG  | O9-C7-C8-C9     |

There are no ring outliers.

328 monomers are involved in 2929 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | 7     | 303 | BCR  | 14      | 0            |
| 24  | A     | 846 | BCR  | 11      | 0            |
| 22  | 1     | 314 | CLA  | 19      | 0            |
| 39  | 8     | 312 | CHL  | 14      | 0            |
| 25  | 3     | 321 | LHG  | 1       | 0            |
| 25  | B     | 803 | LHG  | 8       | 0            |
| 24  | B     | 848 | BCR  | 15      | 0            |
| 22  | A     | 815 | CLA  | 18      | 0            |
| 22  | A     | 803 | CLA  | 7       | 0            |
| 22  | 3     | 314 | CLA  | 12      | 0            |
| 22  | Z     | 307 | CLA  | 10      | 0            |
| 22  | B     | 830 | CLA  | 15      | 0            |
| 38  | 5     | 302 | LUT  | 16      | 0            |
| 22  | 3     | 315 | CLA  | 8       | 0            |
| 22  | 1     | 305 | CLA  | 10      | 0            |
| 22  | 7     | 314 | CLA  | 3       | 0            |
| 38  | Z     | 302 | LUT  | 13      | 0            |
| 38  | 1     | 302 | LUT  | 8       | 0            |
| 22  | 5     | 320 | CLA  | 11      | 0            |
| 22  | A     | 807 | CLA  | 15      | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | B     | 846 | BCR  | 12      | 0            |
| 22  | 7     | 324 | CLA  | 4       | 0            |
| 22  | 4     | 805 | CLA  | 17      | 0            |
| 22  | 8     | 309 | CLA  | 14      | 0            |
| 22  | B     | 810 | CLA  | 13      | 0            |
| 22  | B     | 812 | CLA  | 14      | 0            |
| 22  | 1     | 308 | CLA  | 19      | 0            |
| 26  | A     | 851 | NKP  | 3       | 0            |
| 24  | B     | 853 | BCR  | 20      | 0            |
| 22  | 6     | 307 | CLA  | 20      | 0            |
| 22  | B     | 832 | CLA  | 9       | 0            |
| 24  | 3     | 305 | BCR  | 15      | 0            |
| 42  | 7     | 320 | SPH  | 4       | 0            |
| 22  | K     | 203 | CLA  | 9       | 0            |
| 25  | 5     | 324 | LHG  | 7       | 0            |
| 22  | Z     | 314 | CLA  | 6       | 0            |
| 39  | 7     | 313 | CHL  | 9       | 0            |
| 22  | K     | 205 | CLA  | 4       | 0            |
| 22  | 3     | 309 | CLA  | 7       | 0            |
| 22  | 5     | 315 | CLA  | 19      | 0            |
| 24  | A     | 845 | BCR  | 20      | 0            |
| 38  | 8     | 302 | LUT  | 16      | 0            |
| 22  | B     | 833 | CLA  | 12      | 0            |
| 22  | Z     | 315 | CLA  | 10      | 0            |
| 39  | 4     | 814 | CHL  | 5       | 0            |
| 22  | 7     | 304 | CLA  | 10      | 0            |
| 22  | A     | 826 | CLA  | 7       | 0            |
| 22  | G     | 201 | CLA  | 12      | 0            |
| 22  | 6     | 312 | CLA  | 13      | 0            |
| 22  | A     | 827 | CLA  | 17      | 0            |
| 22  | 4     | 810 | CLA  | 17      | 0            |
| 22  | 8     | 316 | CLA  | 3       | 0            |
| 22  | 3     | 310 | CLA  | 7       | 0            |
| 22  | 5     | 318 | CLA  | 18      | 0            |
| 22  | A     | 828 | CLA  | 14      | 0            |
| 22  | A     | 802 | CLA  | 12      | 0            |
| 22  | A     | 834 | CLA  | 10      | 0            |
| 22  | 8     | 313 | CLA  | 9       | 0            |
| 22  | 3     | 312 | CLA  | 24      | 0            |
| 22  | 2     | 304 | CLA  | 9       | 0            |
| 39  | 5     | 321 | CHL  | 6       | 0            |
| 22  | 7     | 312 | CLA  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | 5     | 308 | CLA  | 23      | 0            |
| 39  | 4     | 819 | CHL  | 9       | 0            |
| 22  | B     | 808 | CLA  | 13      | 0            |
| 22  | B     | 828 | CLA  | 20      | 0            |
| 22  | 7     | 306 | CLA  | 11      | 0            |
| 38  | 7     | 302 | LUT  | 15      | 0            |
| 22  | 1     | 310 | CLA  | 10      | 0            |
| 22  | A     | 840 | CLA  | 13      | 0            |
| 22  | 6     | 311 | CLA  | 10      | 0            |
| 38  | 4     | 802 | LUT  | 15      | 0            |
| 22  | 6     | 321 | CLA  | 6       | 0            |
| 22  | 7     | 308 | CLA  | 12      | 0            |
| 24  | 5     | 305 | BCR  | 10      | 0            |
| 22  | B     | 809 | CLA  | 13      | 0            |
| 25  | Z     | 317 | LHG  | 9       | 0            |
| 35  | J     | 102 | T7X  | 2       | 0            |
| 22  | 6     | 302 | CLA  | 16      | 0            |
| 24  | A     | 856 | BCR  | 24      | 0            |
| 22  | A     | 813 | CLA  | 18      | 0            |
| 39  | 6     | 318 | CHL  | 12      | 0            |
| 22  | 5     | 311 | CLA  | 13      | 0            |
| 38  | 3     | 303 | LUT  | 18      | 0            |
| 22  | 8     | 306 | CLA  | 14      | 0            |
| 22  | Z     | 316 | CLA  | 15      | 0            |
| 25  | 7     | 318 | LHG  | 10      | 0            |
| 25  | 4     | 820 | LHG  | 15      | 0            |
| 22  | 6     | 313 | CLA  | 6       | 0            |
| 22  | 4     | 808 | CLA  | 15      | 0            |
| 22  | 5     | 319 | CLA  | 13      | 0            |
| 22  | 7     | 315 | CLA  | 10      | 0            |
| 22  | B     | 826 | CLA  | 12      | 0            |
| 33  | 4     | 801 | LMT  | 7       | 0            |
| 38  | 1     | 303 | LUT  | 18      | 0            |
| 22  | B     | 834 | CLA  | 11      | 0            |
| 22  | B     | 839 | CLA  | 16      | 0            |
| 22  | B     | 824 | CLA  | 18      | 0            |
| 22  | 3     | 313 | CLA  | 22      | 0            |
| 39  | 6     | 316 | CHL  | 11      | 0            |
| 42  | 7     | 321 | SPH  | 8       | 0            |
| 22  | A     | 842 | CLA  | 6       | 0            |
| 22  | 8     | 311 | CLA  | 14      | 0            |
| 38  | 7     | 301 | LUT  | 14      | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | A     | 838 | CLA  | 7       | 0            |
| 22  | 4     | 806 | CLA  | 8       | 0            |
| 22  | G     | 202 | CLA  | 14      | 0            |
| 22  | B     | 814 | CLA  | 16      | 0            |
| 22  | A     | 819 | CLA  | 8       | 0            |
| 22  | 1     | 307 | CLA  | 17      | 0            |
| 33  | F     | 307 | LMT  | 5       | 0            |
| 37  | K     | 201 | DAO  | 8       | 0            |
| 22  | 4     | 817 | CLA  | 4       | 0            |
| 22  | B     | 831 | CLA  | 10      | 0            |
| 22  | 1     | 304 | CLA  | 14      | 0            |
| 38  | 9     | 302 | LUT  | 17      | 0            |
| 22  | 5     | 314 | CLA  | 7       | 0            |
| 22  | B     | 825 | CLA  | 21      | 0            |
| 22  | 9     | 313 | CLA  | 17      | 0            |
| 22  | 9     | 308 | CLA  | 9       | 0            |
| 22  | B     | 820 | CLA  | 11      | 0            |
| 21  | A     | 801 | CL0  | 7       | 0            |
| 22  | Z     | 313 | CLA  | 23      | 0            |
| 22  | A     | 804 | CLA  | 14      | 0            |
| 22  | A     | 817 | CLA  | 14      | 0            |
| 22  | A     | 812 | CLA  | 24      | 0            |
| 22  | K     | 204 | CLA  | 6       | 0            |
| 22  | L     | 202 | CLA  | 16      | 0            |
| 22  | B     | 806 | CLA  | 19      | 0            |
| 29  | C     | 101 | SF4  | 3       | 0            |
| 24  | F     | 303 | BCR  | 14      | 0            |
| 41  | 5     | 325 | 3PH  | 3       | 0            |
| 22  | B     | 842 | CLA  | 24      | 0            |
| 29  | B     | 802 | SF4  | 8       | 0            |
| 40  | 1     | 318 | SQD  | 12      | 0            |
| 22  | 5     | 310 | CLA  | 13      | 0            |
| 22  | 7     | 309 | CLA  | 9       | 0            |
| 39  | 5     | 316 | CHL  | 17      | 0            |
| 22  | 7     | 307 | CLA  | 18      | 0            |
| 34  | F     | 308 | LMG  | 1       | 0            |
| 38  | 9     | 301 | LUT  | 16      | 0            |
| 22  | 3     | 308 | CLA  | 18      | 0            |
| 22  | B     | 841 | CLA  | 15      | 0            |
| 22  | B     | 829 | CLA  | 12      | 0            |
| 25  | B     | 850 | LHG  | 4       | 0            |
| 24  | 3     | 306 | BCR  | 14      | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | A     | 820 | CLA  | 8       | 0            |
| 22  | A     | 818 | CLA  | 11      | 0            |
| 22  | 1     | 306 | CLA  | 8       | 0            |
| 22  | A     | 835 | CLA  | 15      | 0            |
| 24  | A     | 847 | BCR  | 14      | 0            |
| 25  | A     | 850 | LHG  | 8       | 0            |
| 22  | A     | 816 | CLA  | 23      | 0            |
| 24  | 5     | 304 | BCR  | 20      | 0            |
| 22  | Z     | 308 | CLA  | 12      | 0            |
| 22  | B     | 836 | CLA  | 7       | 0            |
| 22  | B     | 835 | CLA  | 10      | 0            |
| 39  | 1     | 312 | CHL  | 8       | 0            |
| 22  | 8     | 305 | CLA  | 24      | 0            |
| 22  | 3     | 318 | CLA  | 18      | 0            |
| 22  | B     | 840 | CLA  | 16      | 0            |
| 22  | 6     | 309 | CLA  | 21      | 0            |
| 27  | A     | 852 | DGA  | 20      | 0            |
| 22  | 1     | 315 | CLA  | 4       | 0            |
| 24  | B     | 845 | BCR  | 9       | 0            |
| 22  | B     | 821 | CLA  | 13      | 0            |
| 22  | 4     | 811 | CLA  | 6       | 0            |
| 22  | B     | 827 | CLA  | 23      | 0            |
| 22  | 6     | 308 | CLA  | 15      | 0            |
| 25  | A     | 849 | LHG  | 5       | 0            |
| 22  | A     | 821 | CLA  | 24      | 0            |
| 23  | B     | 843 | PQN  | 5       | 0            |
| 25  | 1     | 317 | LHG  | 8       | 0            |
| 38  | 8     | 303 | LUT  | 12      | 0            |
| 22  | A     | 837 | CLA  | 9       | 0            |
| 29  | C     | 102 | SF4  | 5       | 0            |
| 22  | 2     | 301 | CLA  | 17      | 0            |
| 22  | 9     | 305 | CLA  | 6       | 0            |
| 22  | Z     | 310 | CLA  | 2       | 0            |
| 38  | 6     | 303 | LUT  | 11      | 0            |
| 22  | 3     | 322 | CLA  | 15      | 0            |
| 22  | 3     | 319 | CLA  | 5       | 0            |
| 41  | 6     | 324 | 3PH  | 5       | 0            |
| 22  | A     | 831 | CLA  | 5       | 0            |
| 22  | 7     | 305 | CLA  | 6       | 0            |
| 22  | 4     | 812 | CLA  | 4       | 0            |
| 39  | 3     | 317 | CHL  | 14      | 0            |
| 22  | 4     | 815 | CLA  | 12      | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22  | B     | 813  | CLA  | 7       | 0            |
| 22  | 5     | 322  | CLA  | 10      | 0            |
| 22  | 8     | 314  | CLA  | 6       | 0            |
| 22  | 5     | 313  | CLA  | 12      | 0            |
| 22  | 5     | 323  | CLA  | 9       | 0            |
| 24  | 6     | 306  | BCR  | 16      | 0            |
| 22  | Z     | 304  | CLA  | 19      | 0            |
| 22  | 1     | 313  | CLA  | 12      | 0            |
| 38  | 3     | 302  | LUT  | 10      | 0            |
| 22  | 8     | 310  | CLA  | 12      | 0            |
| 22  | 4     | 807  | CLA  | 12      | 0            |
| 22  | 7     | 316  | CLA  | 8       | 0            |
| 24  | B     | 849  | BCR  | 9       | 0            |
| 22  | A     | 805  | CLA  | 15      | 0            |
| 22  | 4     | 809  | CLA  | 5       | 0            |
| 39  | 2     | 303  | CHL  | 8       | 0            |
| 22  | 3     | 316  | CLA  | 12      | 0            |
| 22  | A     | 811  | CLA  | 15      | 0            |
| 22  | 7     | 323  | CLA  | 16      | 0            |
| 22  | L     | 201  | CLA  | 15      | 0            |
| 22  | 5     | 312  | CLA  | 8       | 0            |
| 39  | Z     | 311  | CHL  | 11      | 0            |
| 22  | B     | 811  | CLA  | 21      | 0            |
| 22  | 6     | 317  | CLA  | 11      | 0            |
| 24  | I     | 4001 | BCR  | 12      | 0            |
| 22  | 5     | 301  | CLA  | 12      | 0            |
| 22  | B     | 838  | CLA  | 14      | 0            |
| 39  | 8     | 315  | CHL  | 21      | 0            |
| 24  | 3     | 307  | BCR  | 19      | 0            |
| 31  | 3     | 301  | DGD  | 21      | 0            |
| 22  | B     | 819  | CLA  | 15      | 0            |
| 22  | A     | 810  | CLA  | 20      | 0            |
| 24  | 8     | 304  | BCR  | 14      | 0            |
| 22  | 2     | 302  | CLA  | 5       | 0            |
| 22  | 9     | 306  | CLA  | 15      | 0            |
| 24  | J     | 104  | BCR  | 18      | 0            |
| 24  | B     | 844  | BCR  | 20      | 0            |
| 39  | 5     | 317  | CHL  | 8       | 0            |
| 25  | 6     | 323  | LHG  | 11      | 0            |
| 33  | 1     | 301  | LMT  | 7       | 0            |
| 22  | 7     | 322  | CLA  | 15      | 0            |
| 22  | L     | 203  | CLA  | 6       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 43  | 8     | 319 | LPX  | 7       | 0            |
| 38  | 4     | 803 | LUT  | 19      | 0            |
| 22  | B     | 817 | CLA  | 17      | 0            |
| 41  | 7     | 319 | 3PH  | 14      | 0            |
| 22  | A     | 832 | CLA  | 13      | 0            |
| 39  | 4     | 813 | CHL  | 12      | 0            |
| 22  | A     | 814 | CLA  | 23      | 0            |
| 22  | B     | 823 | CLA  | 14      | 0            |
| 22  | 9     | 303 | CLA  | 6       | 0            |
| 22  | 9     | 310 | CLA  | 1       | 0            |
| 24  | 6     | 305 | BCR  | 19      | 0            |
| 22  | A     | 808 | CLA  | 14      | 0            |
| 22  | F     | 301 | CLA  | 8       | 0            |
| 25  | 4     | 821 | LHG  | 4       | 0            |
| 22  | 5     | 309 | CLA  | 13      | 0            |
| 39  | 4     | 816 | CHL  | 21      | 0            |
| 22  | F     | 305 | CLA  | 9       | 0            |
| 22  | 9     | 304 | CLA  | 2       | 0            |
| 22  | K     | 202 | CLA  | 9       | 0            |
| 22  | A     | 806 | CLA  | 10      | 0            |
| 22  | A     | 833 | CLA  | 18      | 0            |
| 22  | J     | 103 | CLA  | 1       | 0            |
| 22  | B     | 818 | CLA  | 13      | 0            |
| 24  | B     | 847 | BCR  | 20      | 0            |
| 22  | B     | 815 | CLA  | 23      | 0            |
| 22  | 6     | 314 | CLA  | 17      | 0            |
| 22  | B     | 807 | CLA  | 8       | 0            |
| 22  | A     | 809 | CLA  | 15      | 0            |
| 22  | Z     | 306 | CLA  | 16      | 0            |
| 24  | 4     | 804 | BCR  | 26      | 0            |
| 23  | A     | 843 | PQN  | 10      | 0            |
| 22  | A     | 822 | CLA  | 26      | 0            |
| 22  | 1     | 309 | CLA  | 4       | 0            |
| 22  | A     | 839 | CLA  | 8       | 0            |
| 22  | A     | 824 | CLA  | 16      | 0            |
| 22  | B     | 805 | CLA  | 11      | 0            |
| 22  | 8     | 308 | CLA  | 11      | 0            |
| 32  | F     | 306 | RRX  | 19      | 0            |
| 38  | 6     | 304 | LUT  | 13      | 0            |
| 38  | 5     | 303 | LUT  | 16      | 0            |
| 22  | 9     | 307 | CLA  | 8       | 0            |
| 22  | B     | 822 | CLA  | 11      | 0            |

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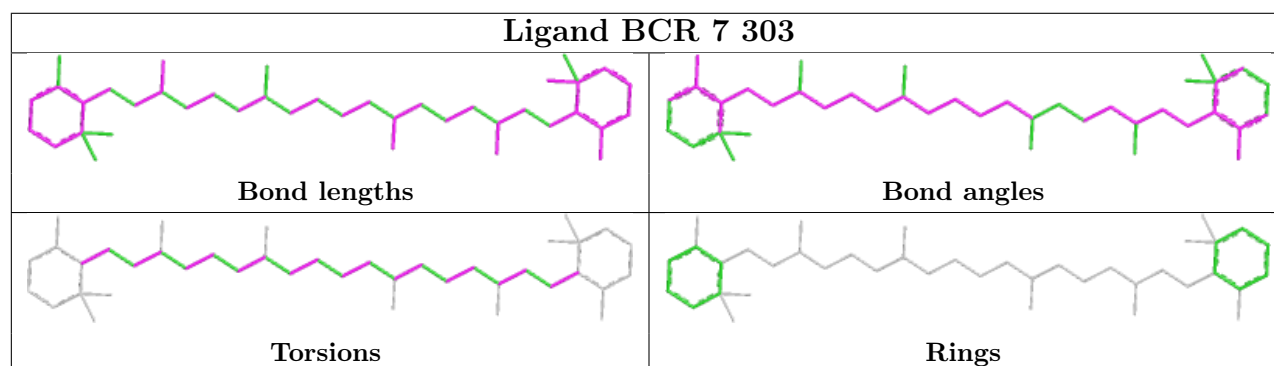
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | G     | 203 | BCR  | 12      | 0            |
| 22  | 7     | 311 | CLA  | 1       | 0            |
| 22  | F     | 302 | CLA  | 16      | 0            |
| 39  | 6     | 315 | CHL  | 21      | 0            |
| 24  | 3     | 304 | BCR  | 13      | 0            |
| 24  | A     | 848 | BCR  | 7       | 0            |
| 25  | B     | 851 | LHG  | 3       | 0            |
| 22  | 1     | 316 | CLA  | 5       | 0            |
| 31  | 1     | 319 | DGD  | 10      | 0            |
| 41  | 8     | 320 | 3PH  | 4       | 0            |
| 24  | A     | 844 | BCR  | 30      | 0            |
| 31  | B     | 852 | DGD  | 17      | 0            |
| 22  | 7     | 317 | CLA  | 4       | 0            |
| 33  | G     | 204 | LMT  | 10      | 0            |
| 24  | L     | 204 | BCR  | 17      | 0            |
| 38  | Z     | 301 | LUT  | 23      | 0            |
| 26  | 8     | 318 | NKP  | 7       | 0            |
| 39  | 6     | 320 | CHL  | 13      | 0            |
| 22  | 4     | 818 | CLA  | 9       | 0            |
| 25  | 9     | 315 | LHG  | 2       | 0            |
| 22  | A     | 854 | CLA  | 10      | 0            |
| 22  | Z     | 303 | CLA  | 29      | 0            |
| 22  | B     | 816 | CLA  | 12      | 0            |
| 39  | 9     | 314 | CHL  | 13      | 0            |
| 25  | 8     | 317 | LHG  | 7       | 0            |
| 22  | 7     | 310 | CLA  | 13      | 0            |
| 22  | B     | 801 | CLA  | 13      | 0            |
| 34  | J     | 101 | LMG  | 10      | 0            |
| 39  | 8     | 301 | CHL  | 11      | 0            |
| 22  | A     | 825 | CLA  | 18      | 0            |
| 22  | B     | 837 | CLA  | 1       | 0            |
| 22  | 6     | 310 | CLA  | 15      | 0            |
| 22  | A     | 823 | CLA  | 28      | 0            |
| 22  | 3     | 320 | CLA  | 10      | 0            |
| 22  | A     | 830 | CLA  | 9       | 0            |
| 22  | 5     | 307 | CLA  | 24      | 0            |
| 22  | 6     | 301 | CLA  | 20      | 0            |
| 24  | K     | 206 | BCR  | 12      | 0            |
| 22  | A     | 841 | CLA  | 16      | 0            |
| 22  | A     | 829 | CLA  | 16      | 0            |
| 36  | 5     | 306 | C7Z  | 1       | 0            |
| 22  | F     | 304 | CLA  | 27      | 0            |

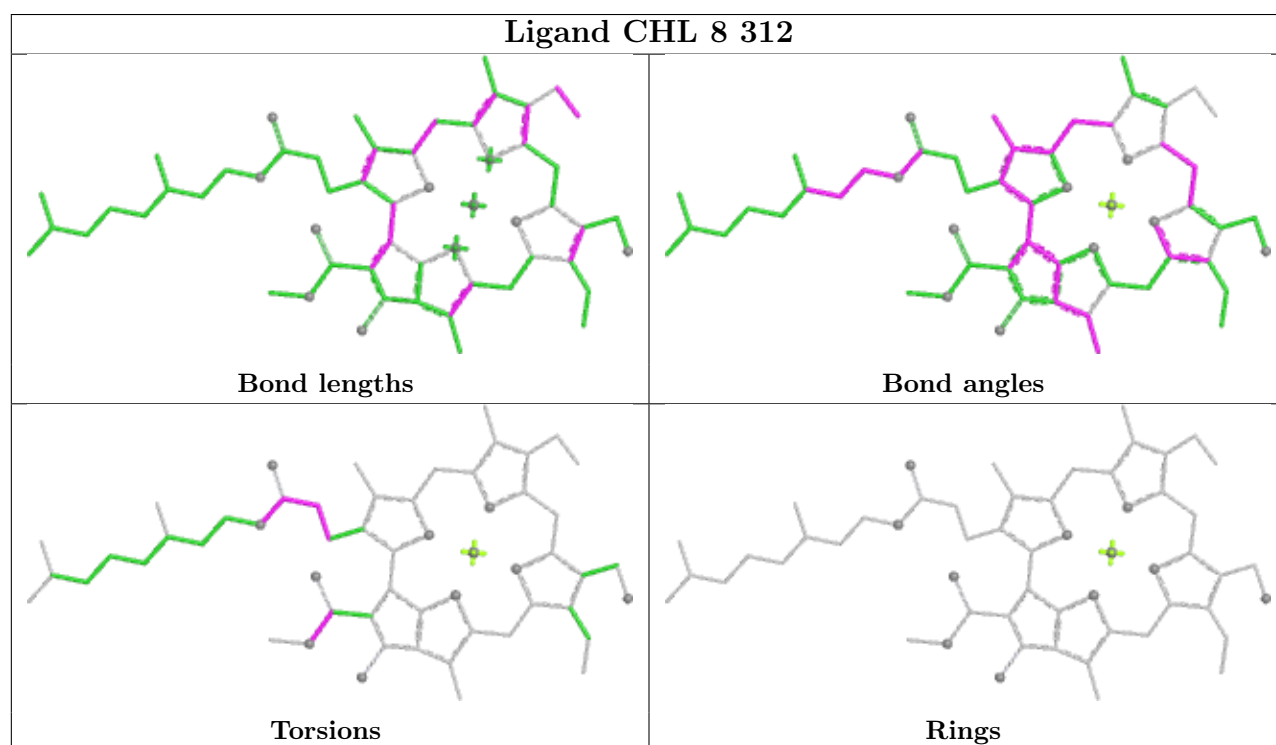
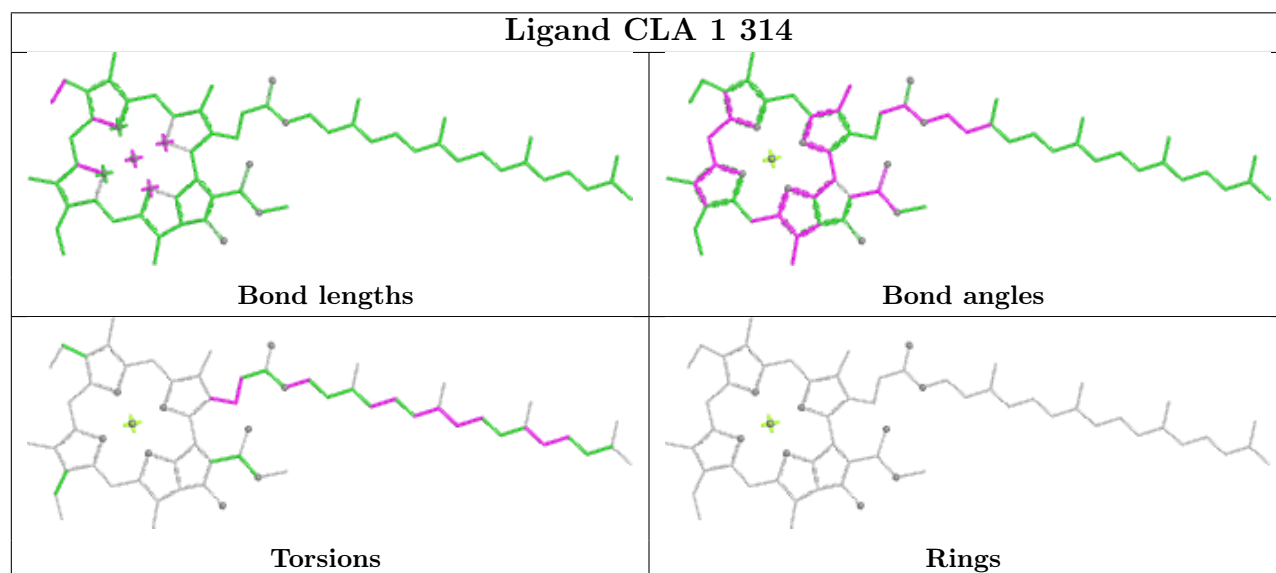
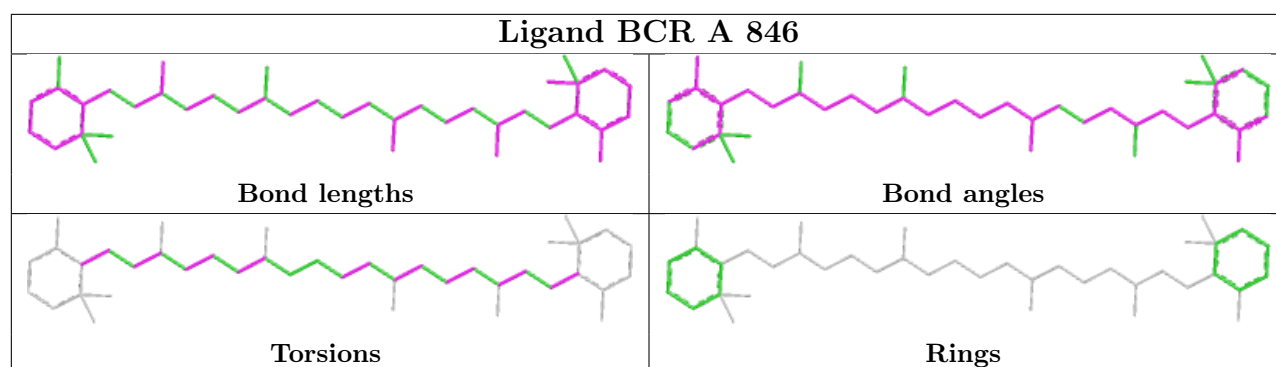
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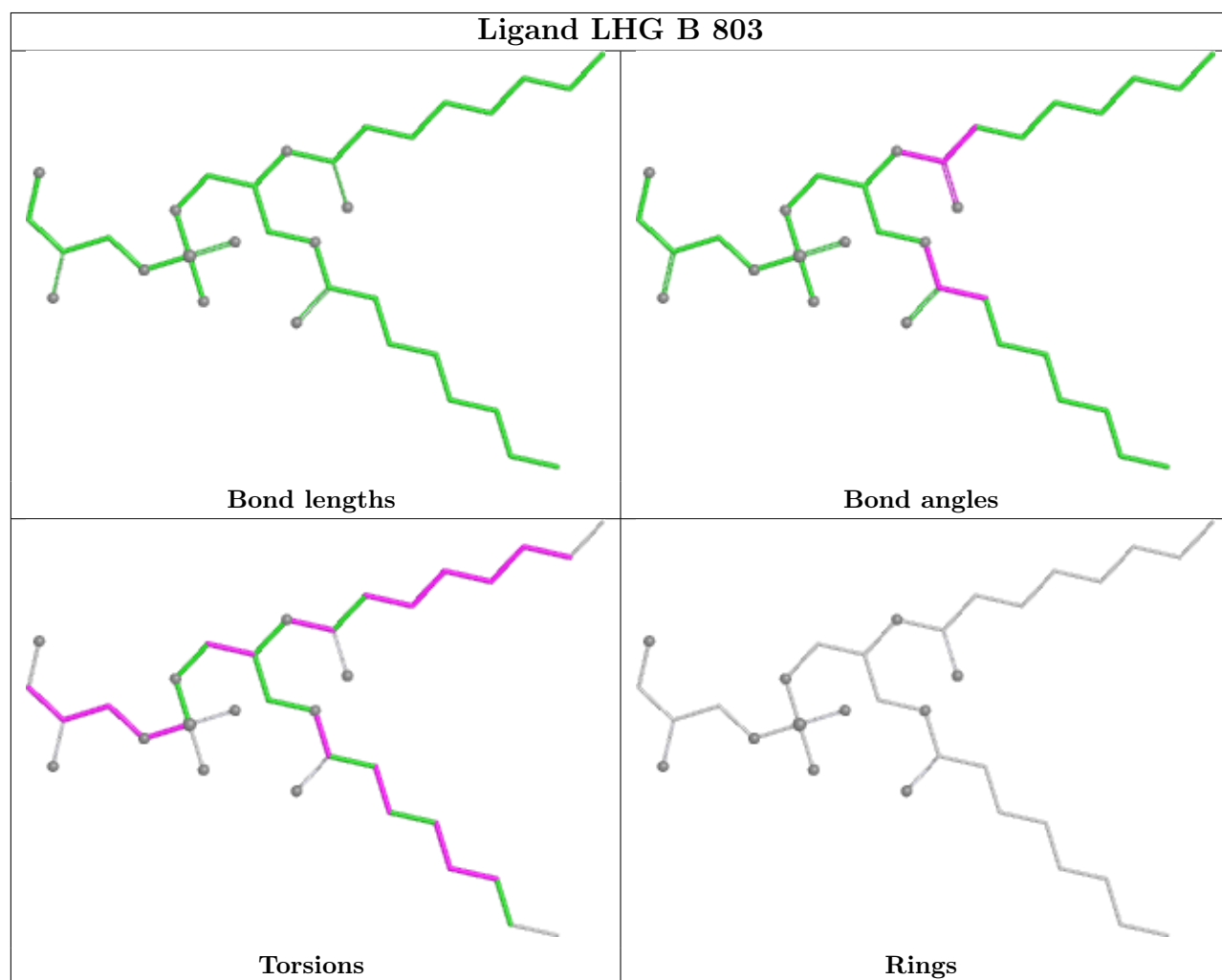
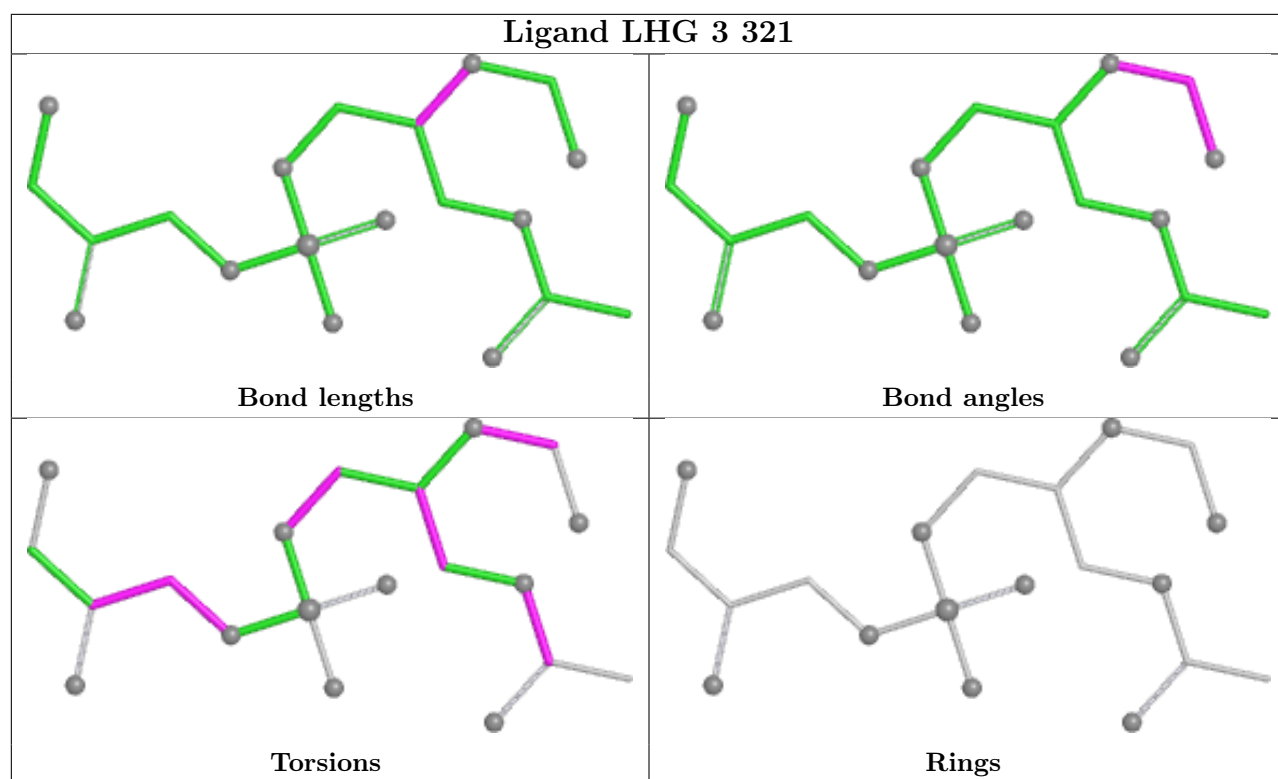
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 39  | Z     | 312 | CHL  | 12      | 0            |
| 33  | 4     | 822 | LMT  | 2       | 0            |
| 39  | 9     | 312 | CHL  | 24      | 0            |
| 22  | 6     | 322 | CLA  | 17      | 0            |
| 22  | A     | 836 | CLA  | 13      | 0            |
| 22  | A     | 855 | CLA  | 14      | 0            |
| 36  | J     | 105 | C7Z  | 2       | 0            |
| 22  | 9     | 311 | CLA  | 5       | 0            |
| 22  | Z     | 305 | CLA  | 14      | 0            |
| 22  | 5     | 326 | CLA  | 17      | 0            |
| 22  | 8     | 307 | CLA  | 15      | 0            |
| 22  | 3     | 311 | CLA  | 14      | 0            |
| 22  | Z     | 309 | CLA  | 21      | 0            |
| 22  | 6     | 319 | CLA  | 11      | 0            |

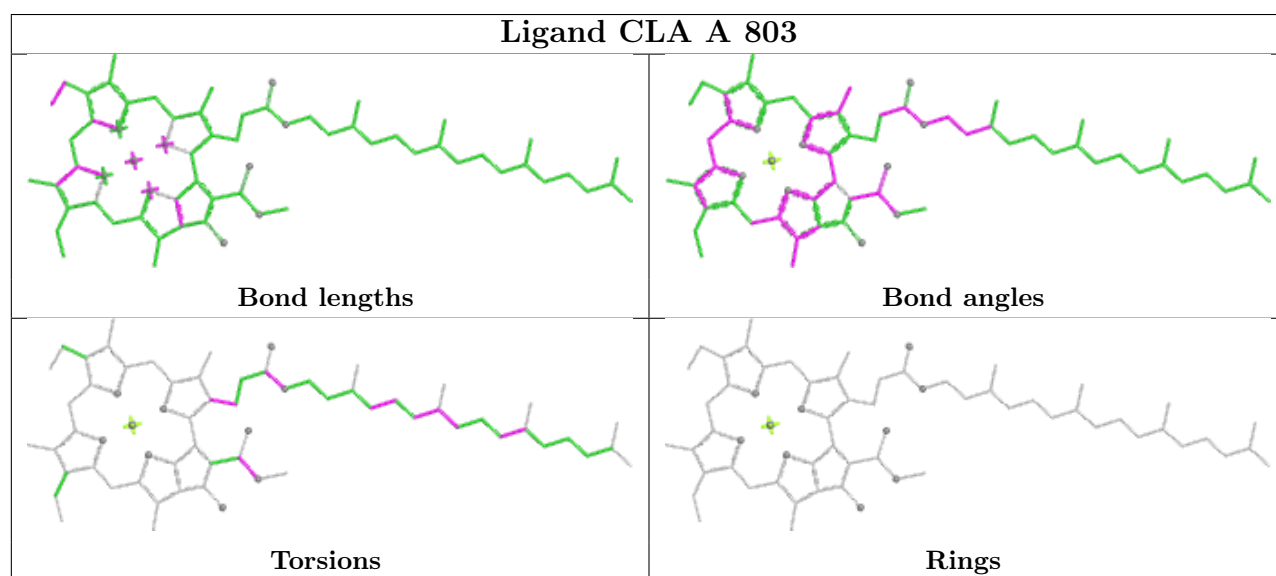
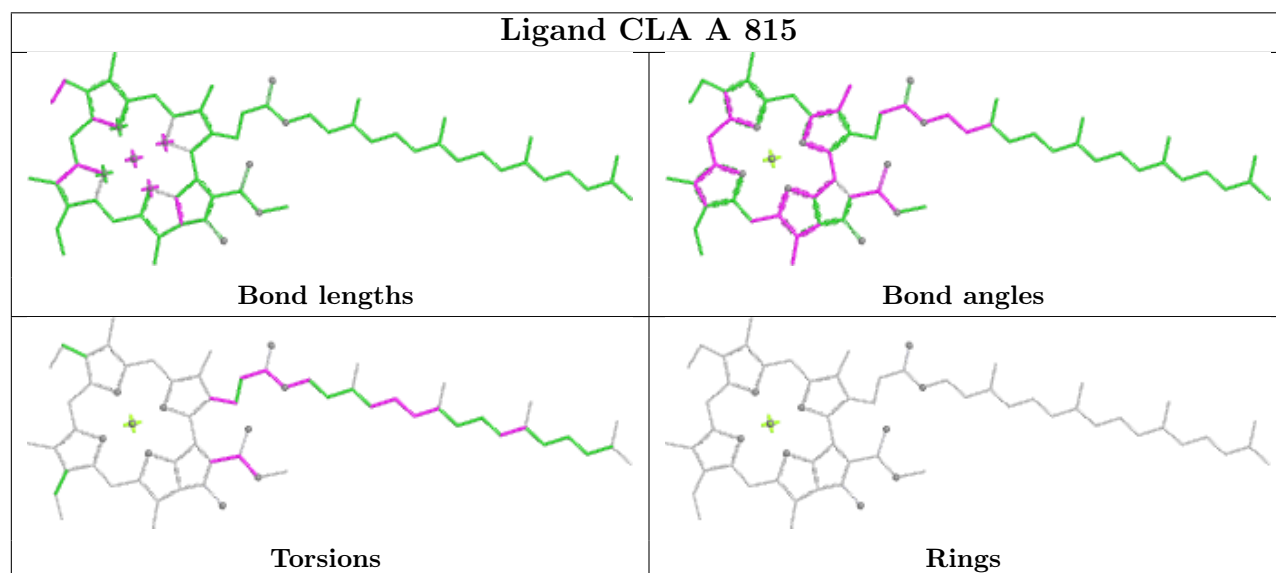
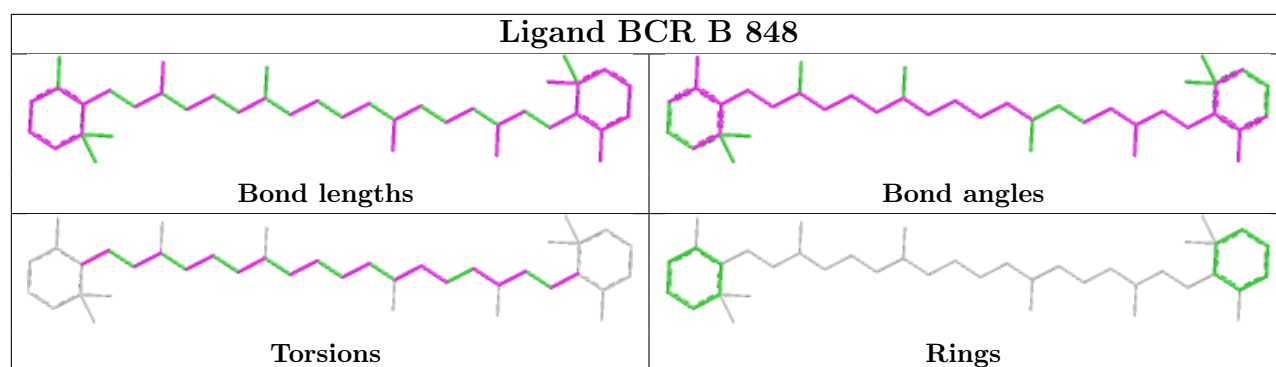
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



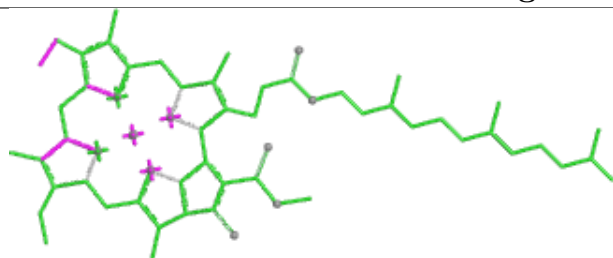




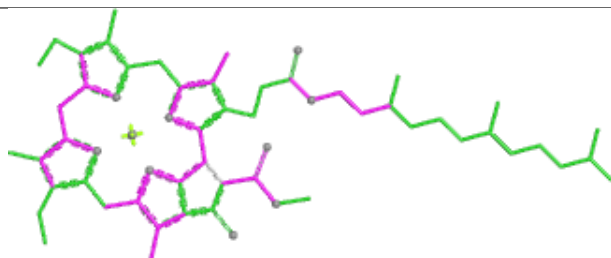




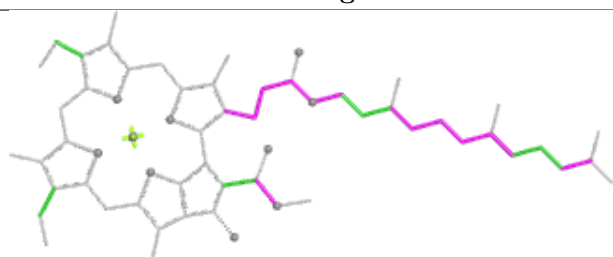
## Ligand CLA 3 314



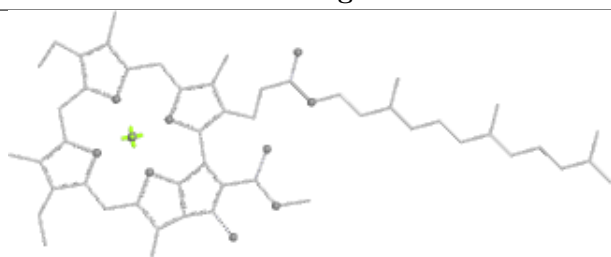
Bond lengths



Bond angles

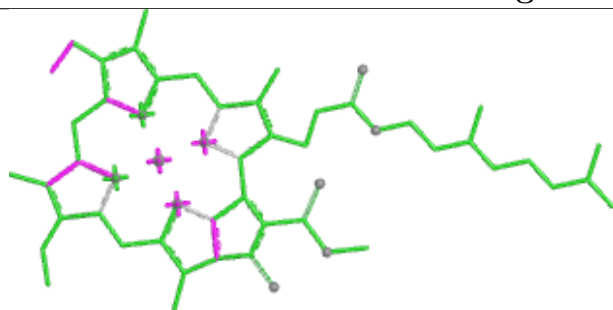


Torsions

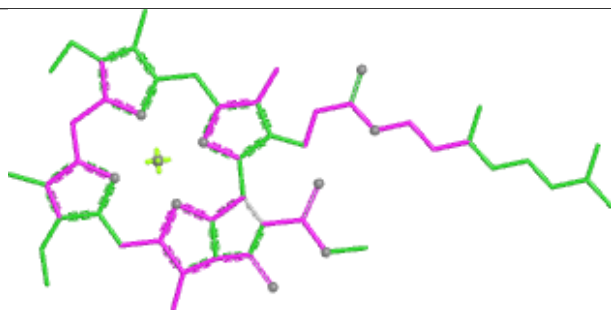


Rings

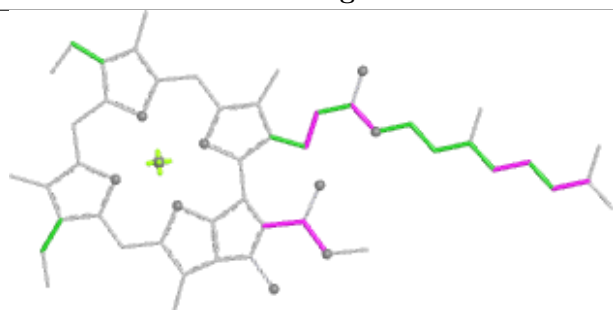
## Ligand CLA Z 307



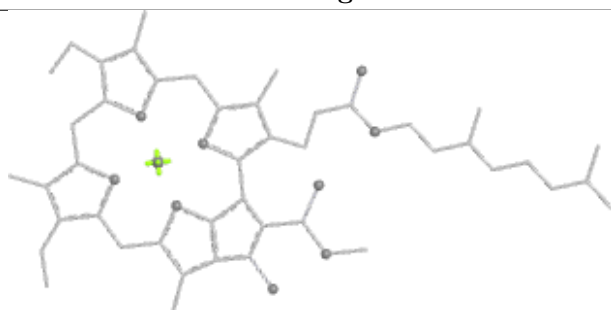
Bond lengths



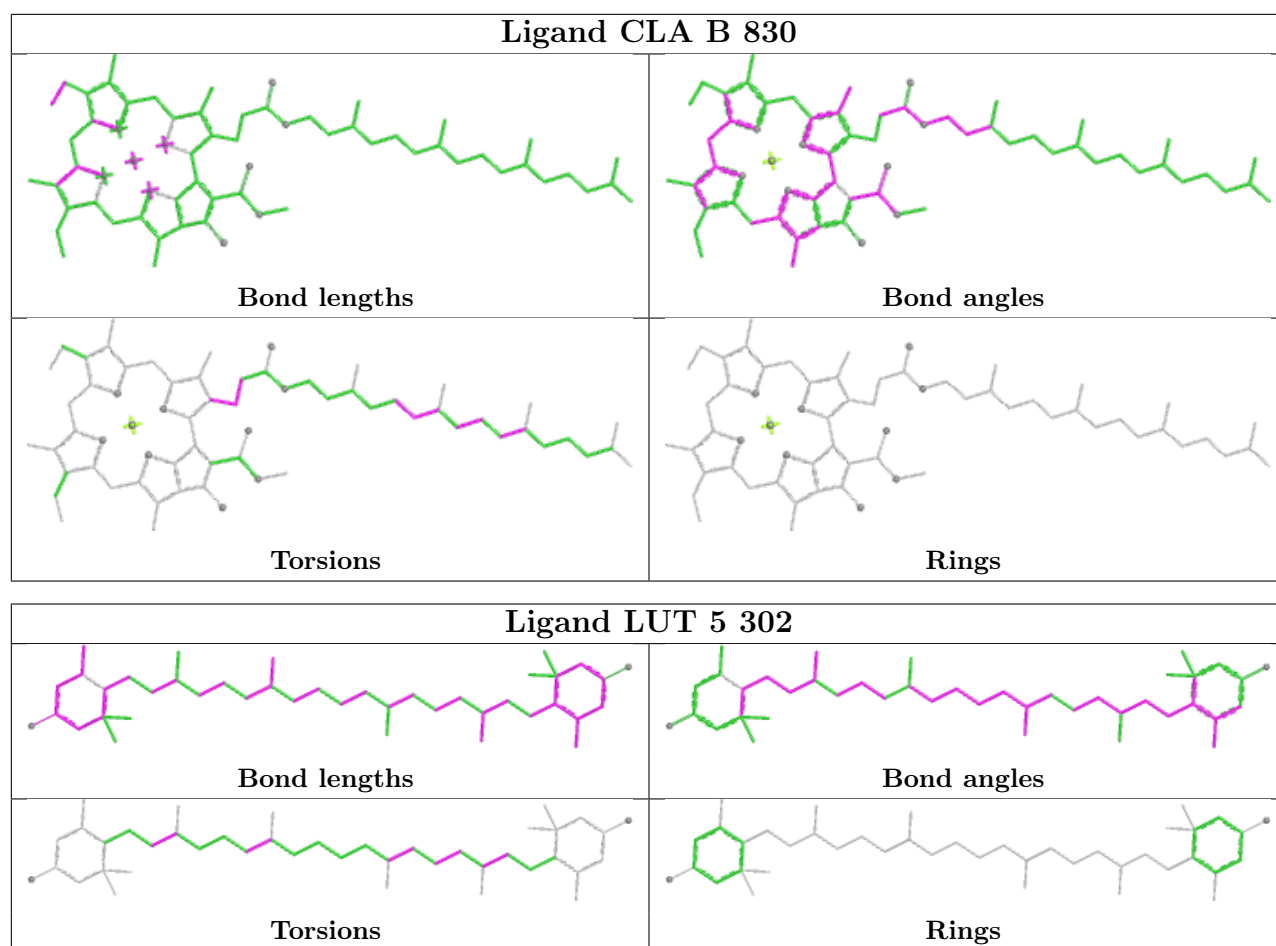
Bond angles



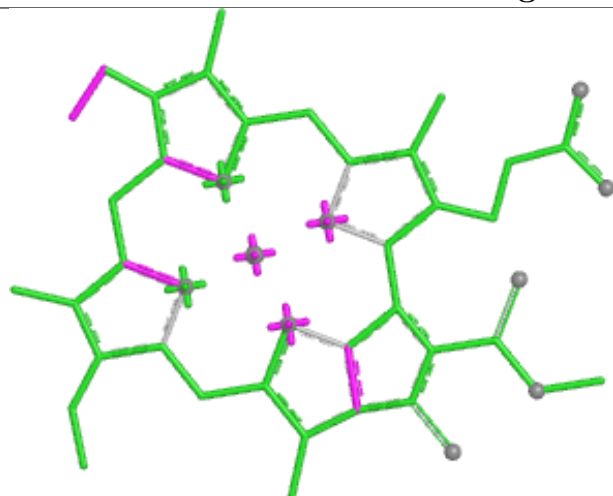
Torsions



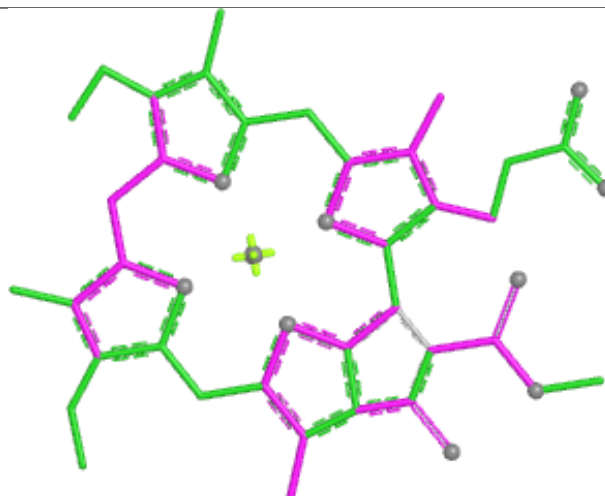
Rings



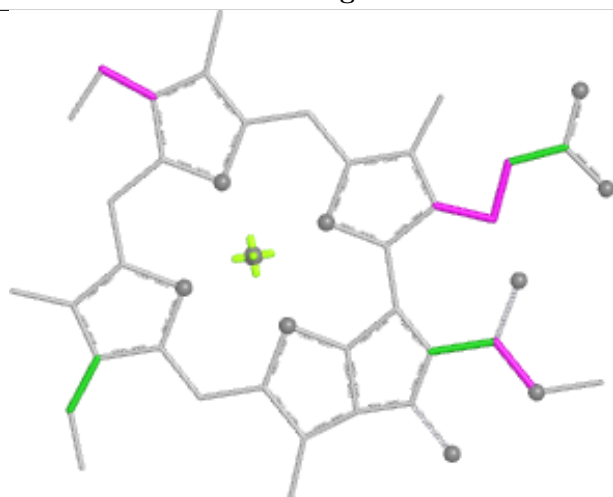
## Ligand CLA 3 315



Bond lengths



Bond angles

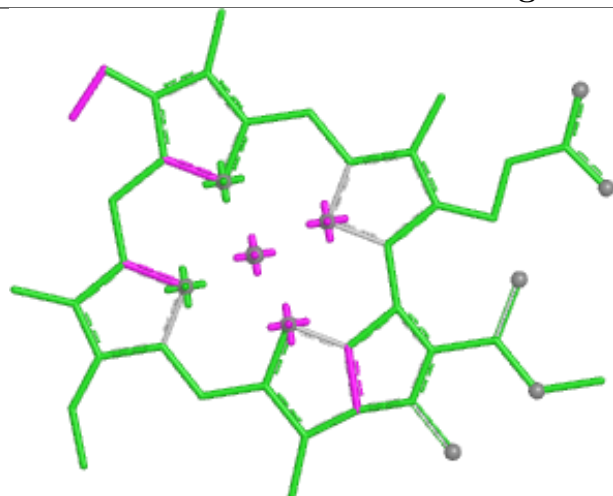


Torsions

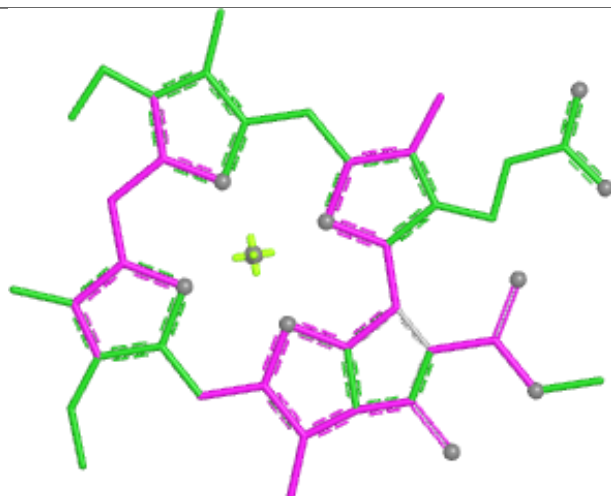


Rings

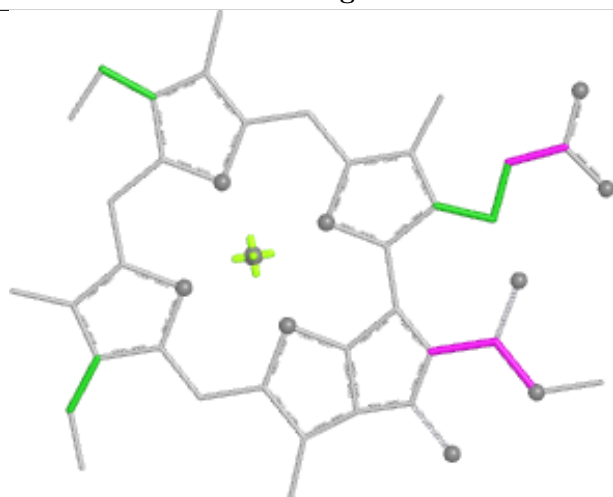
## Ligand CLA 1 305



Bond lengths



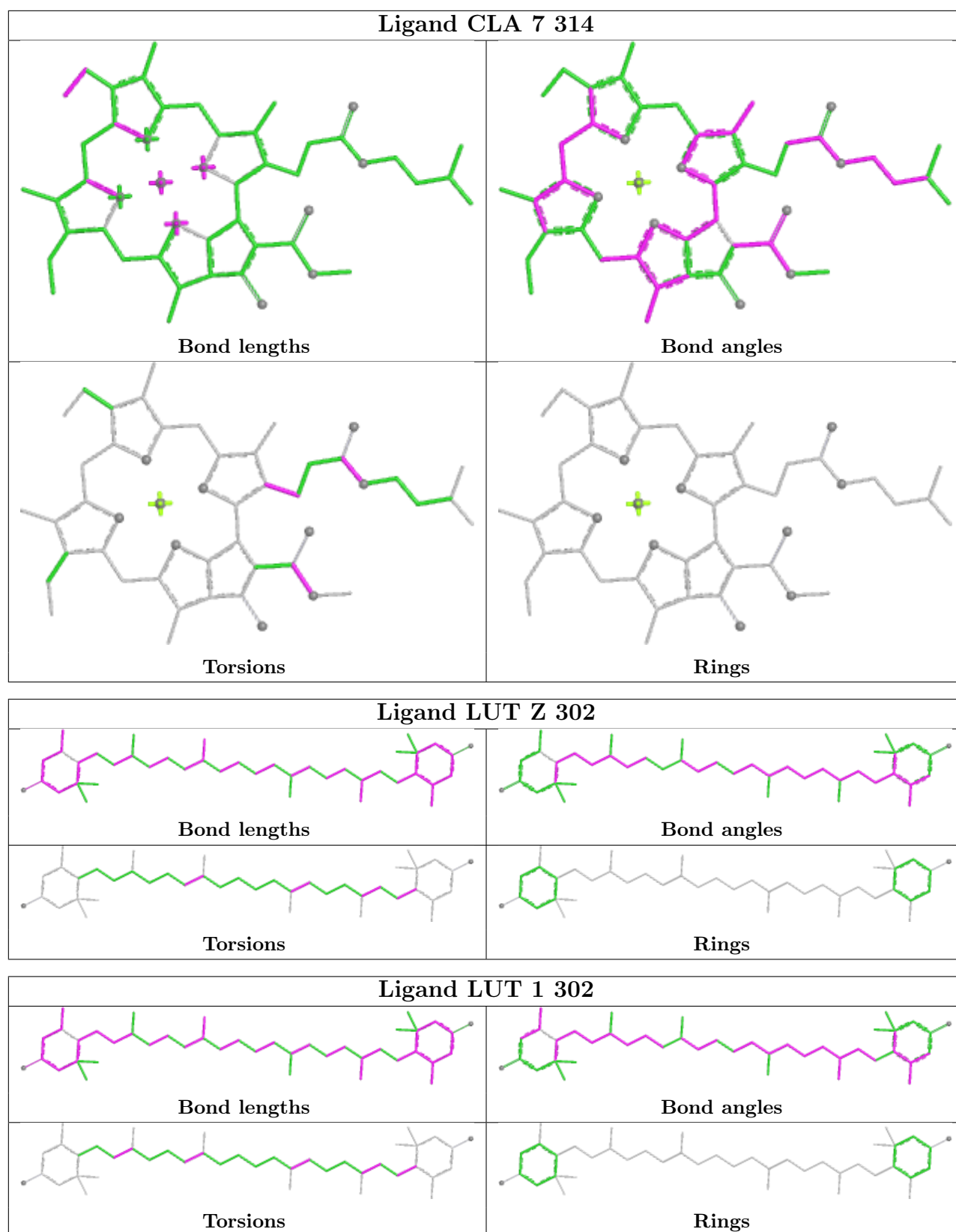
Bond angles



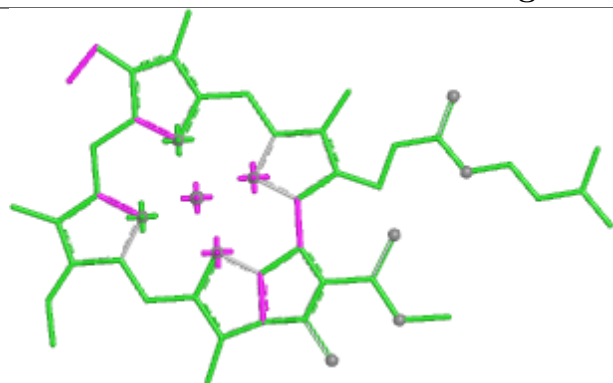
Torsions



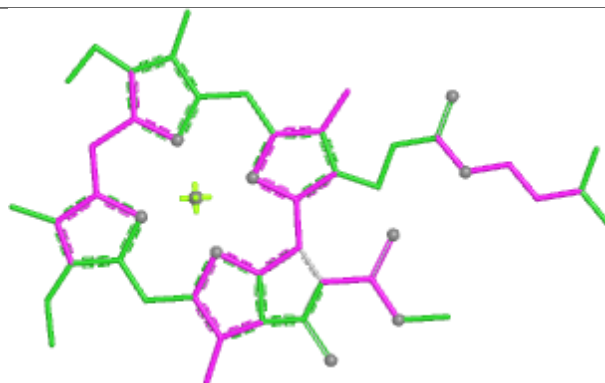
Rings



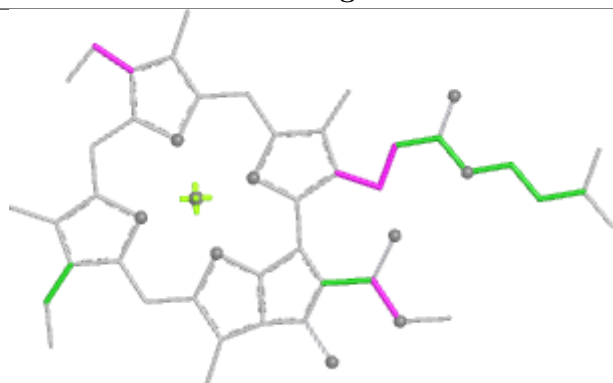
## Ligand CLA 5 320



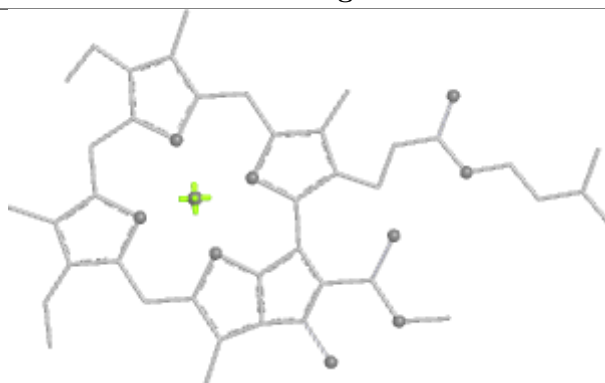
Bond lengths



Bond angles

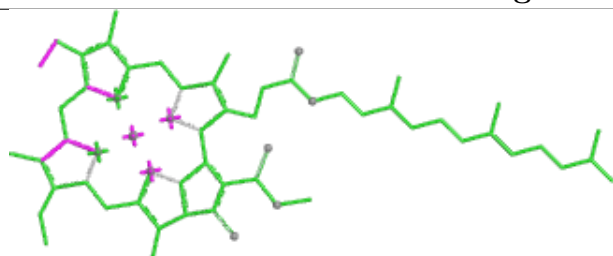


Torsions

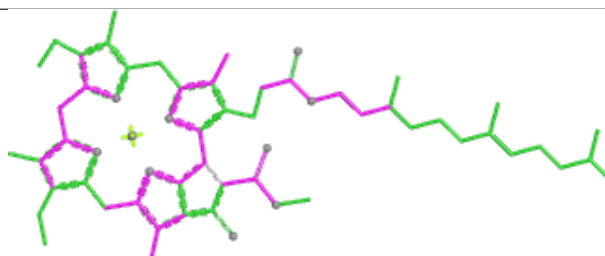


Rings

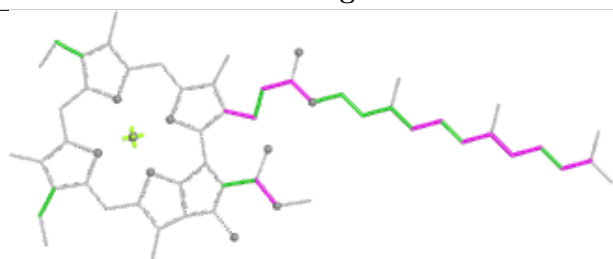
## Ligand CLA A 807



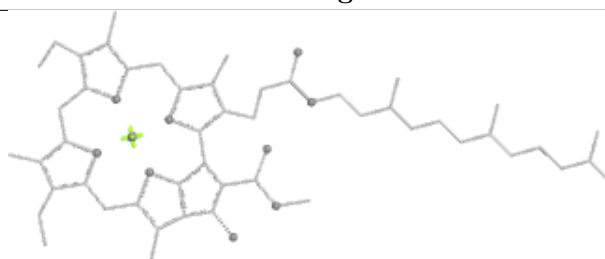
Bond lengths



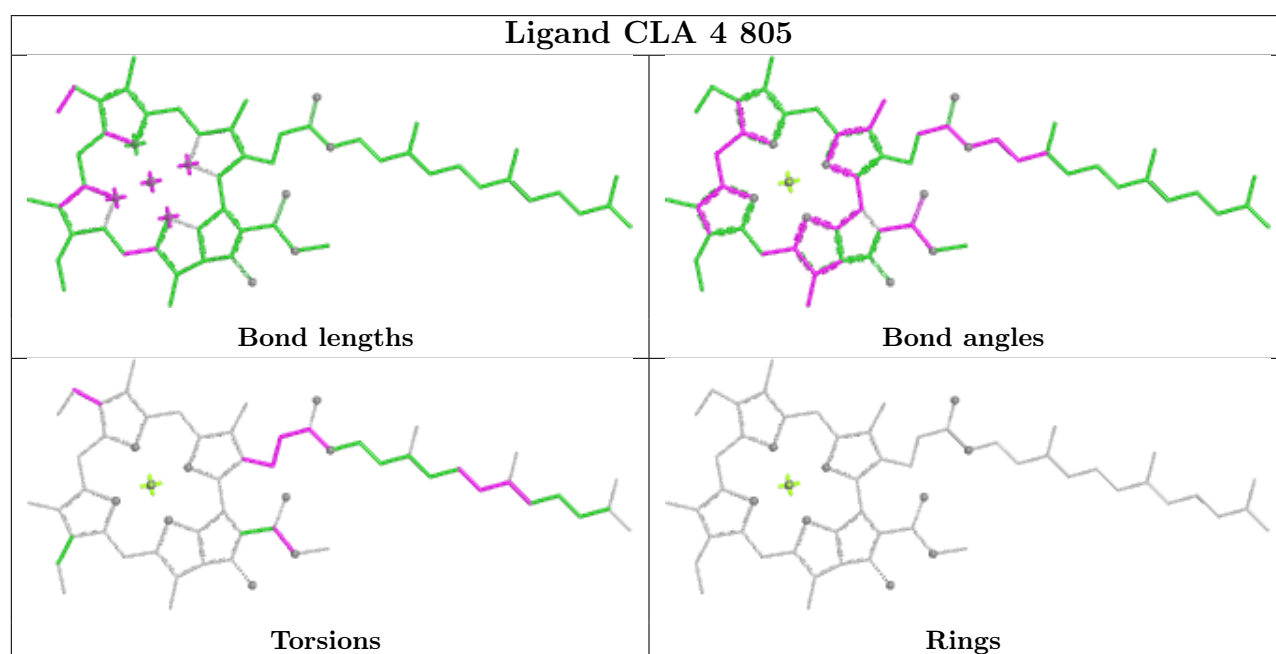
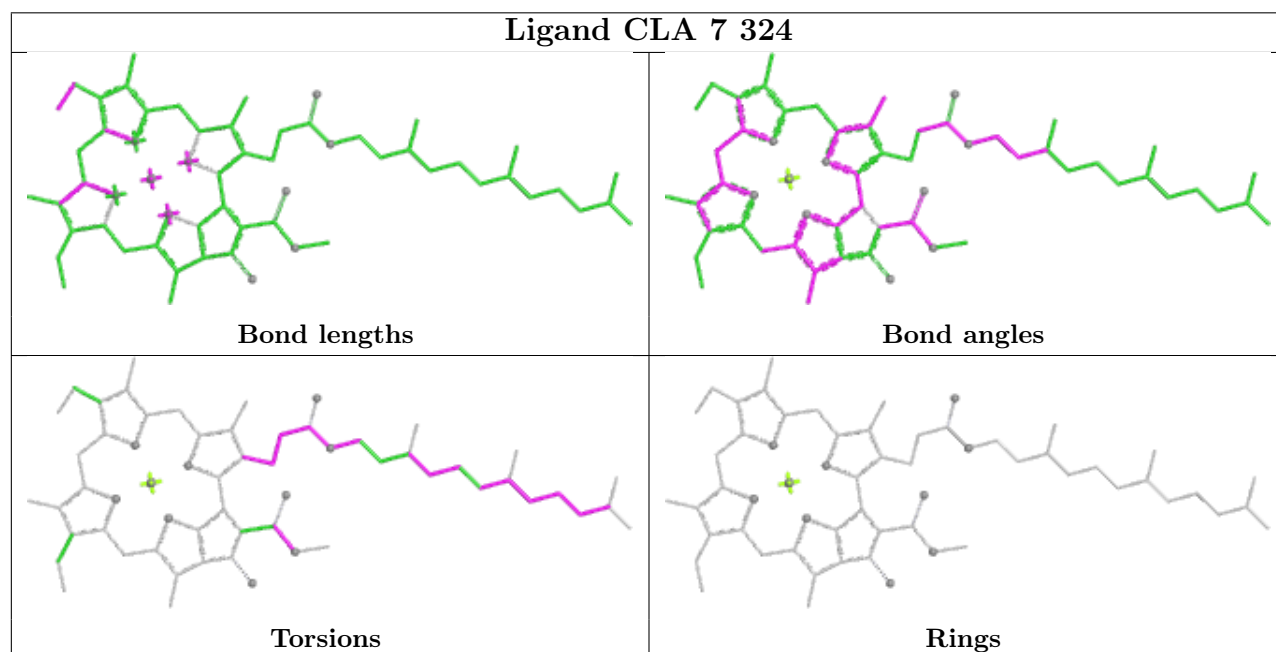
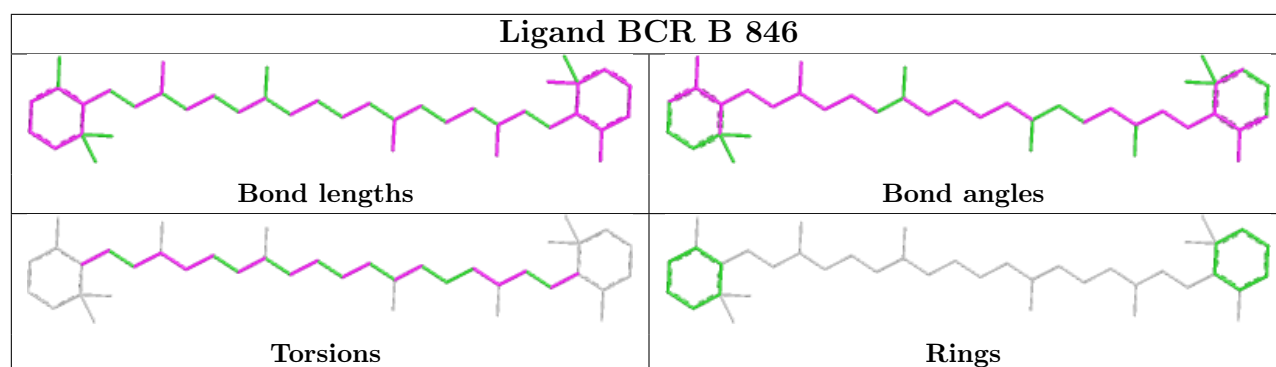
Bond angles



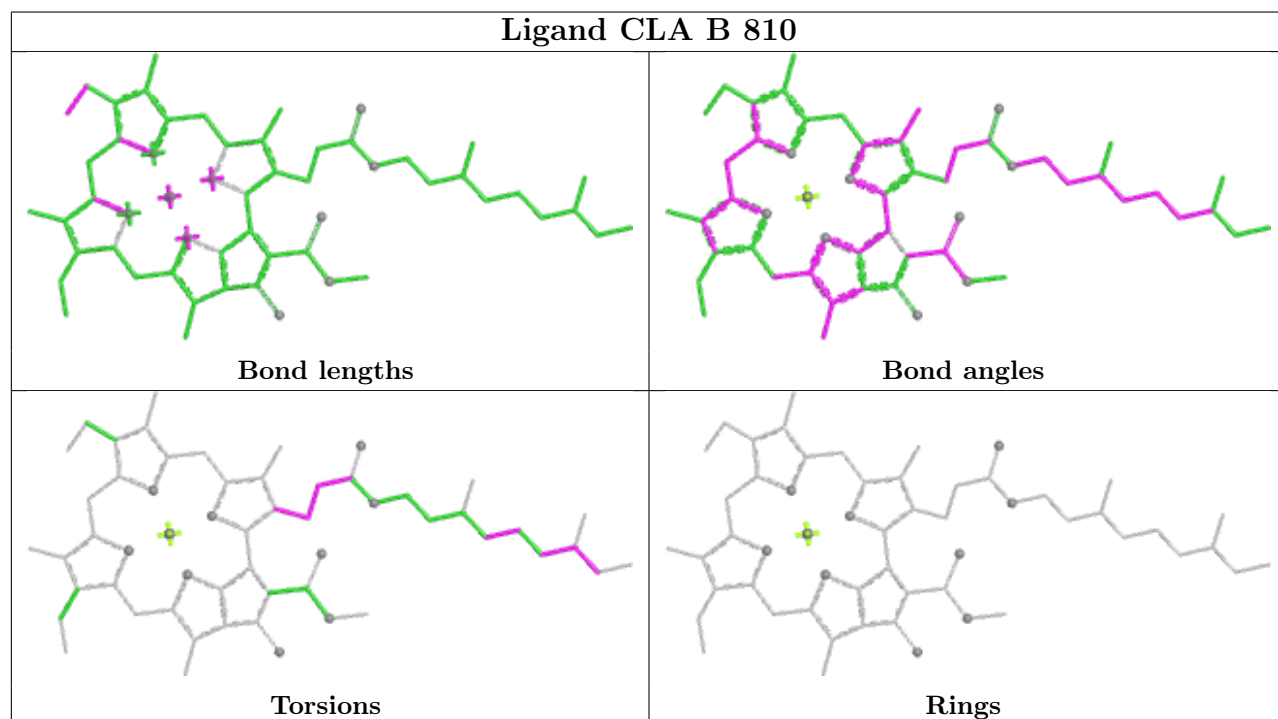
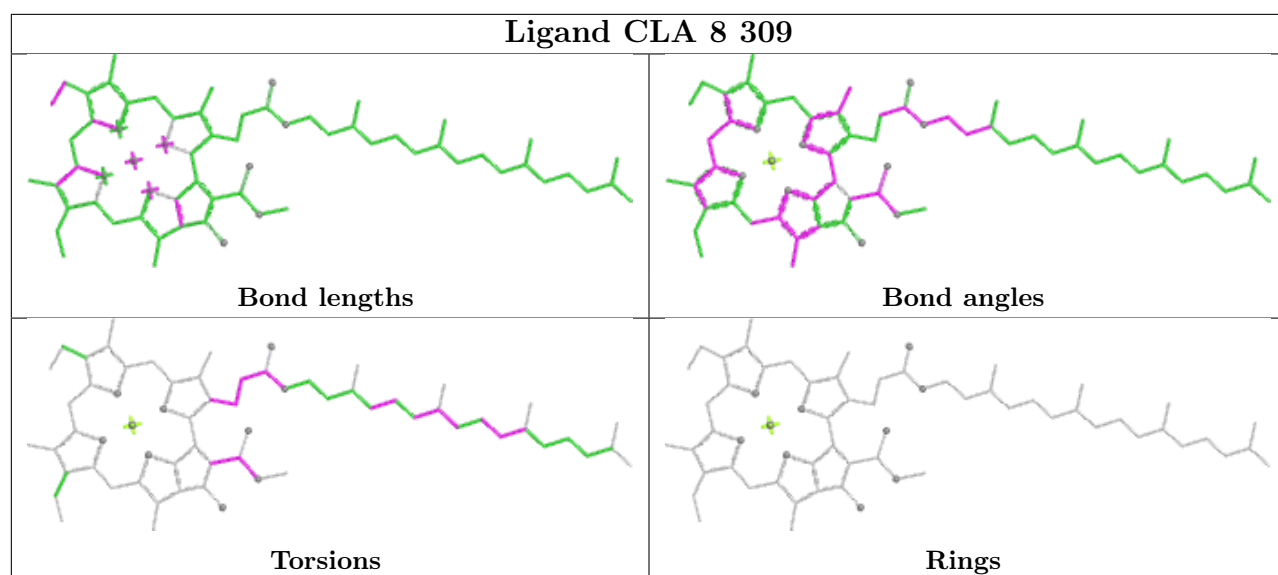
Torsions

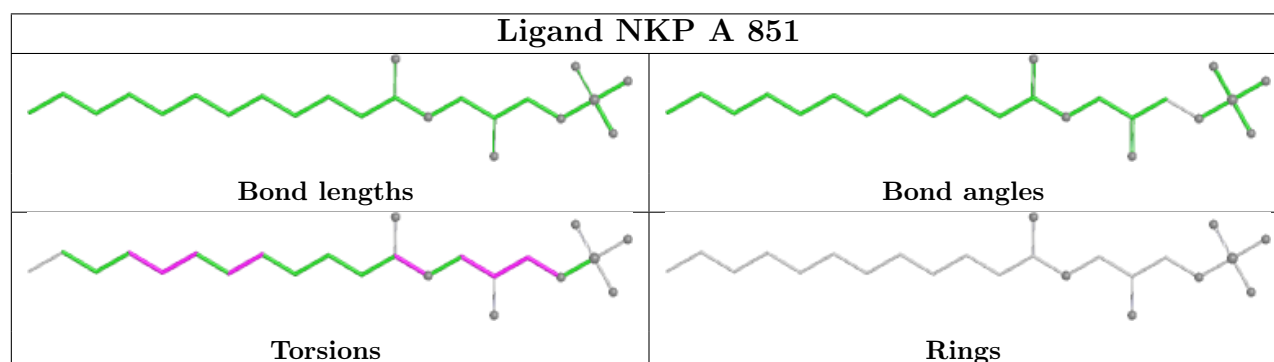
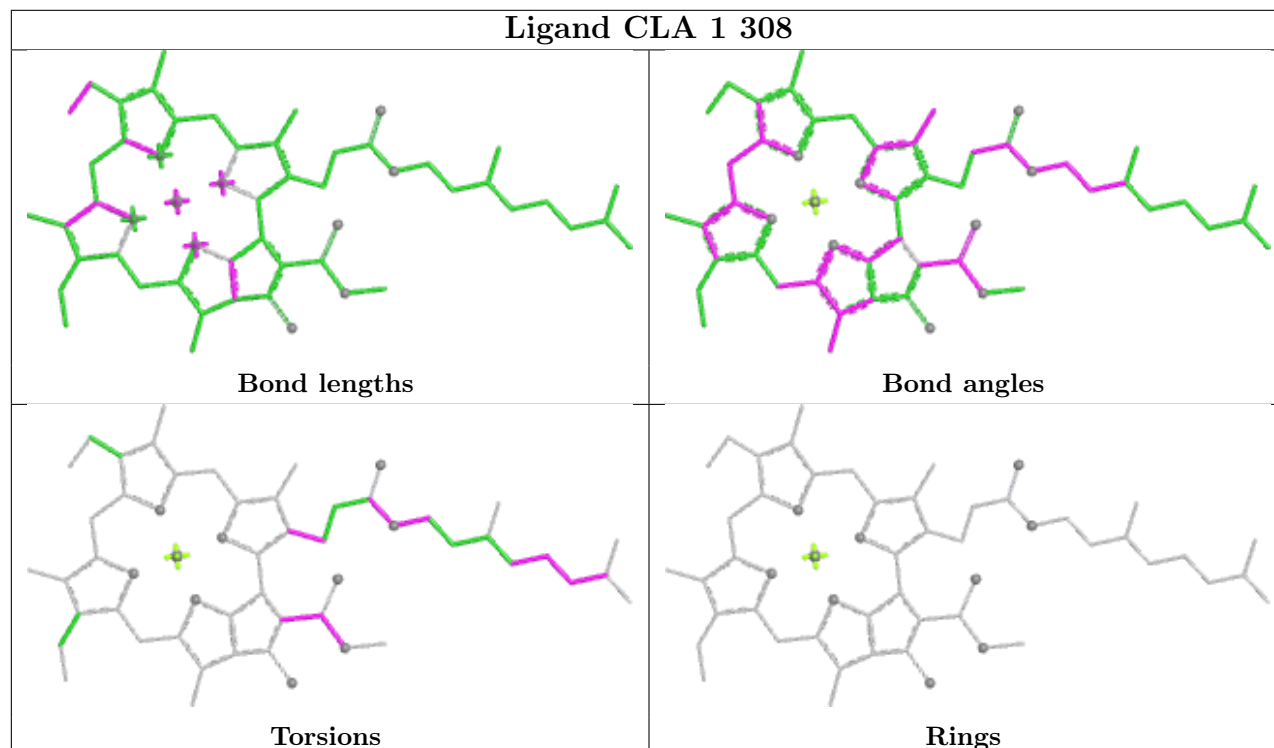
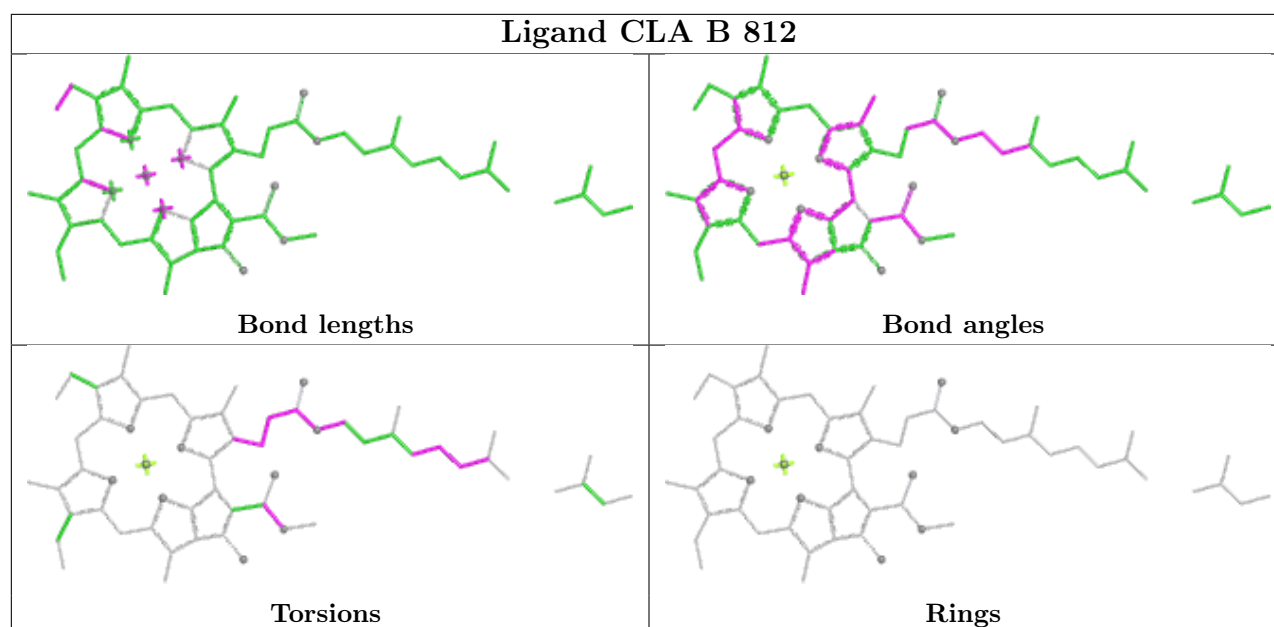


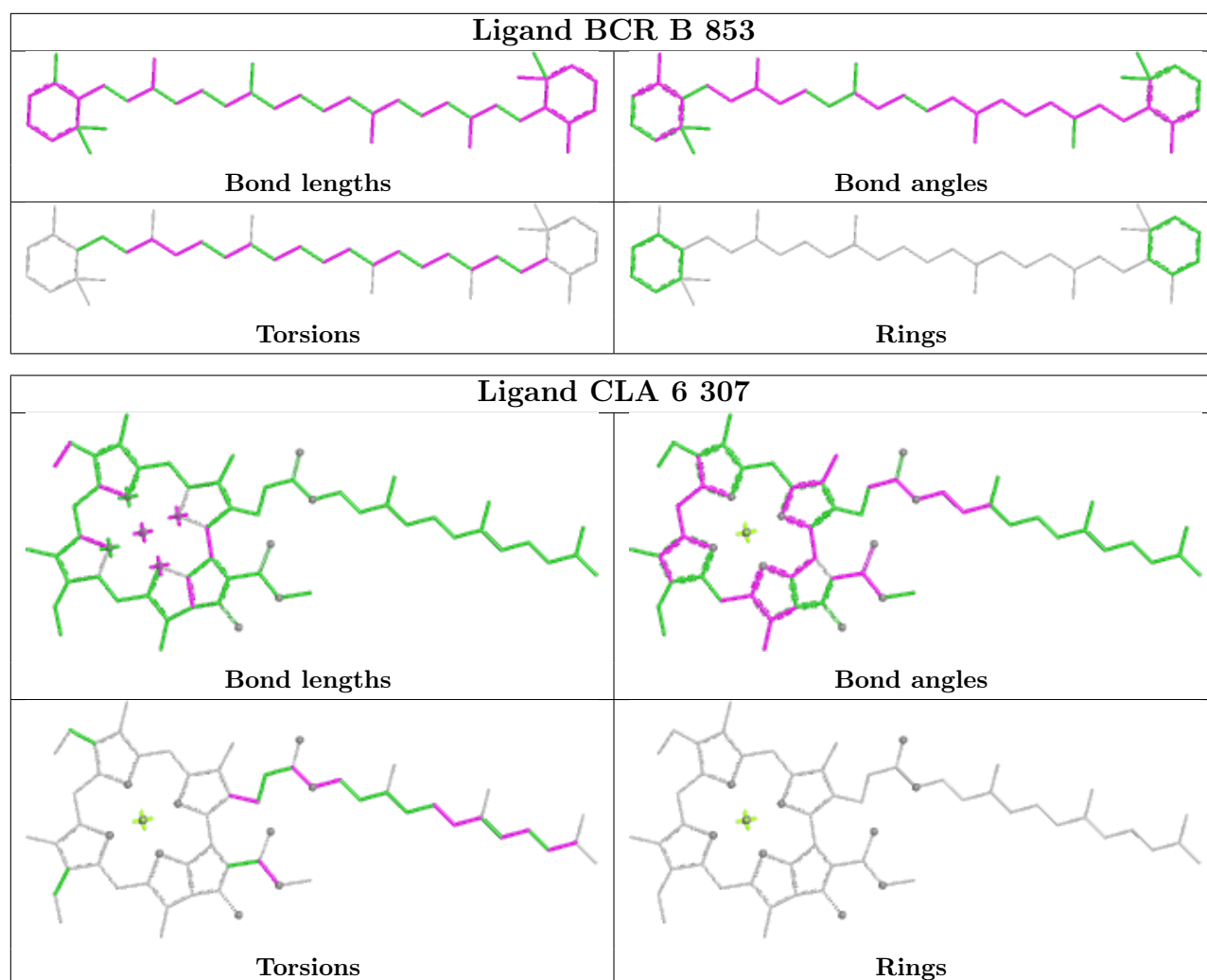
Rings

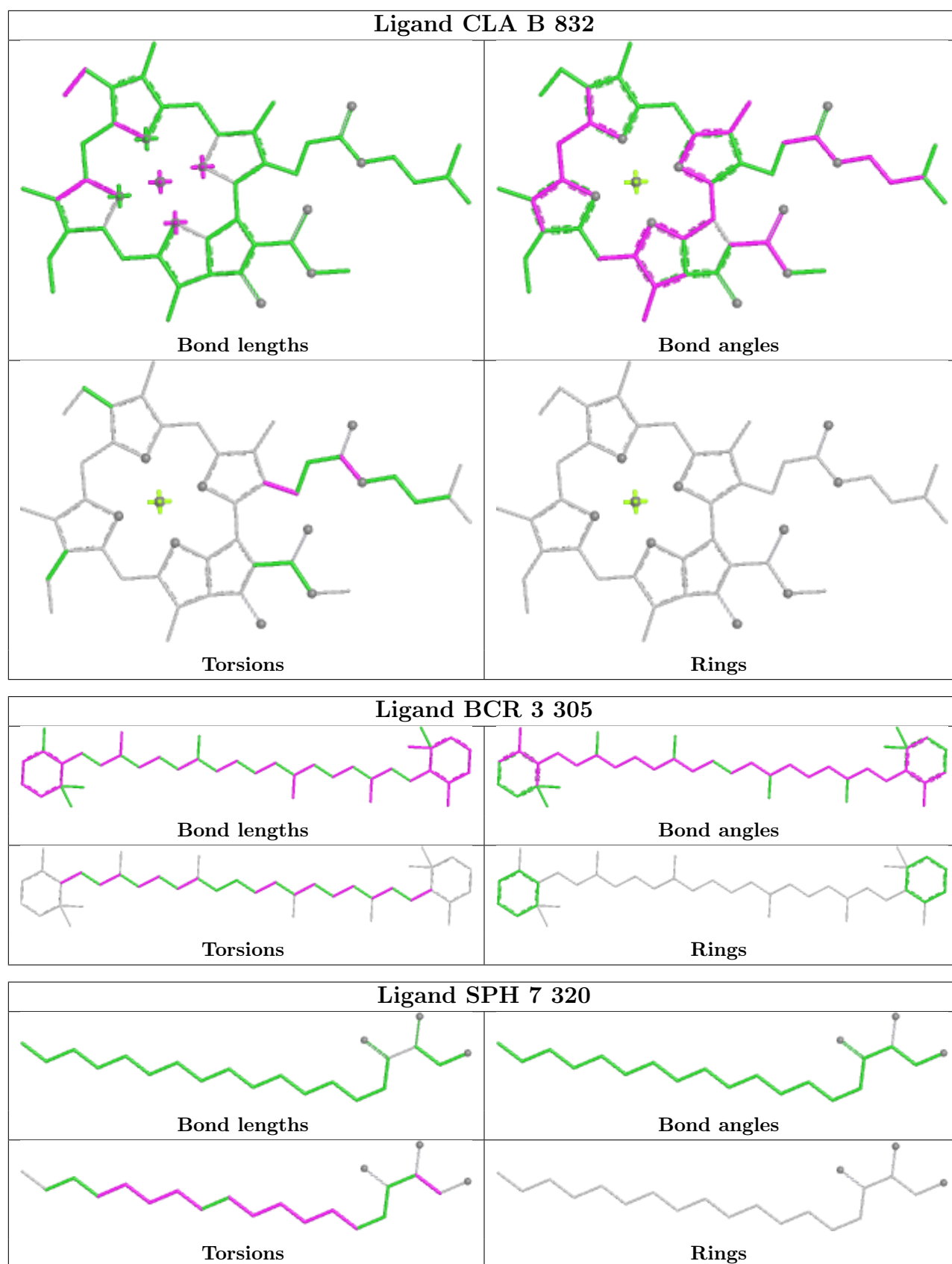


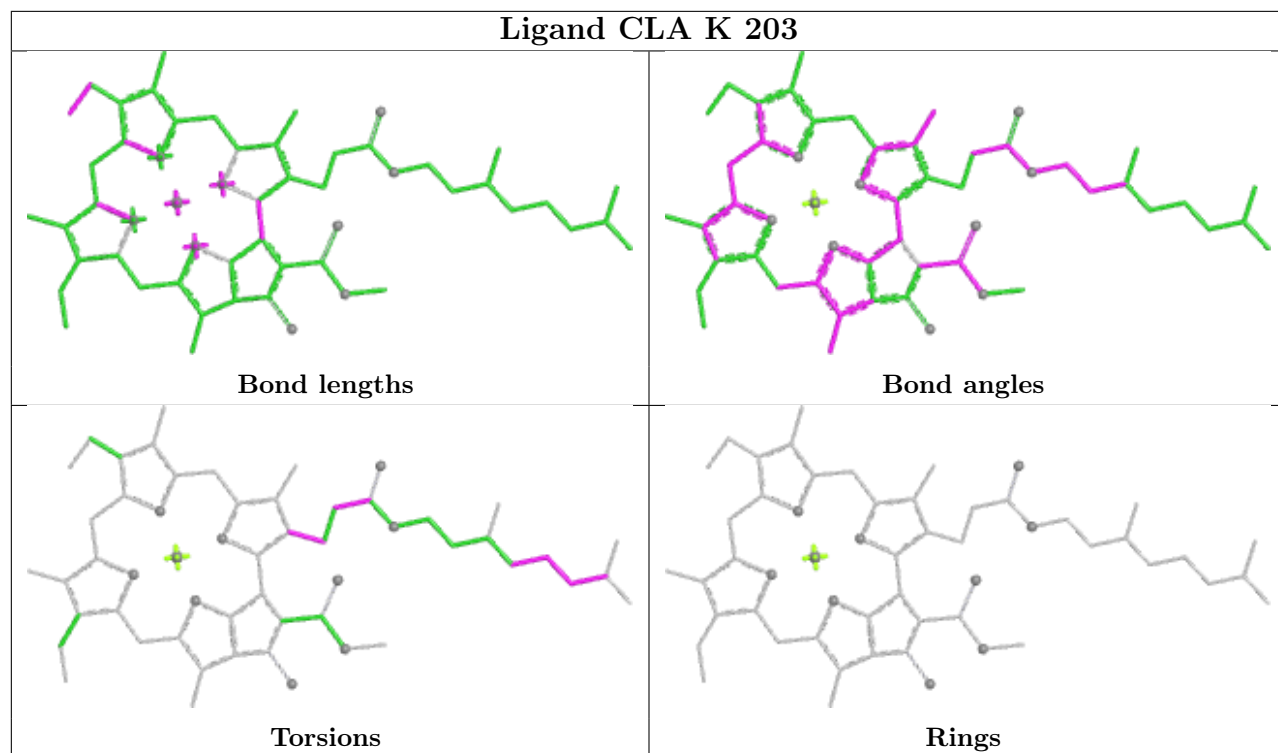


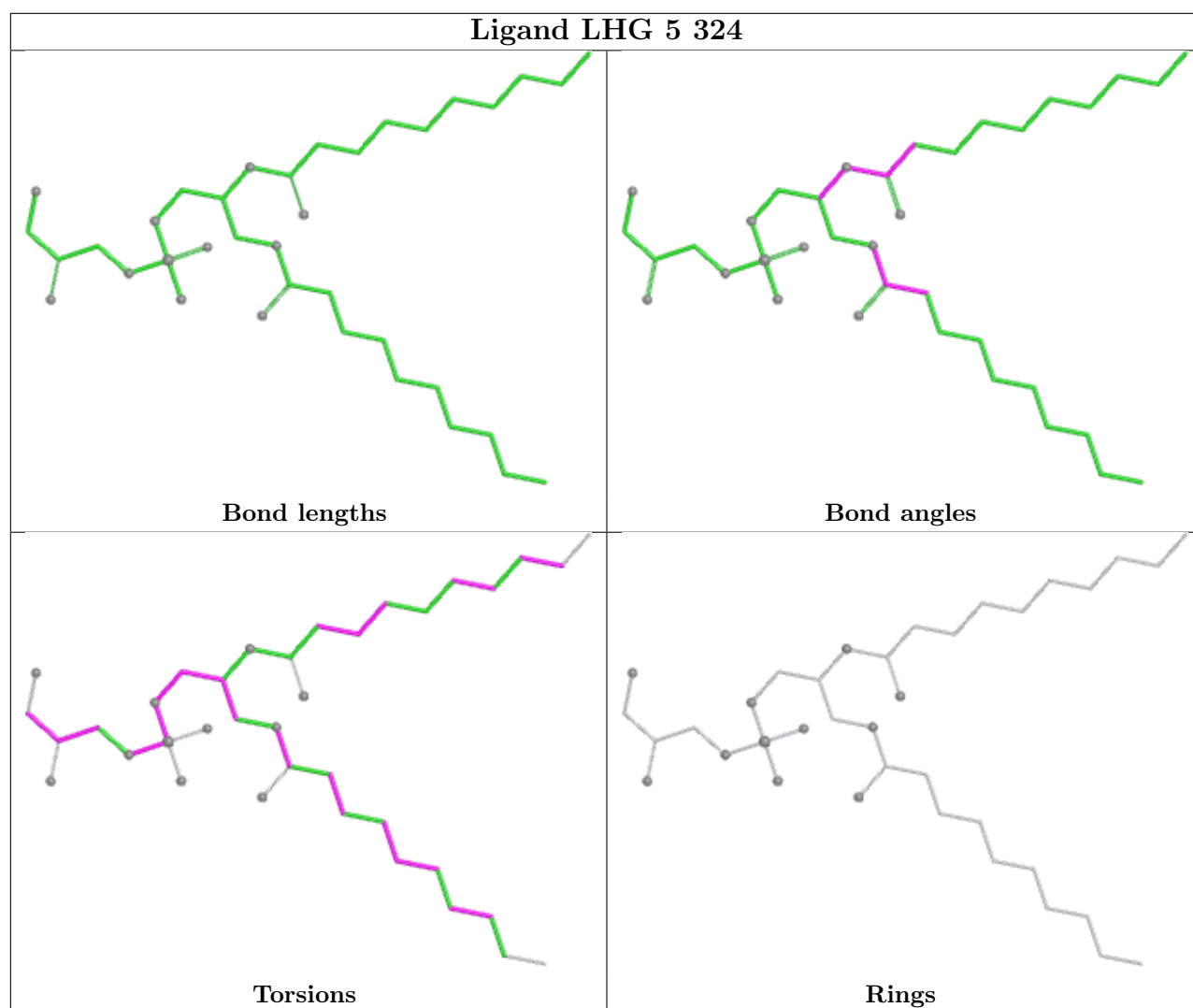




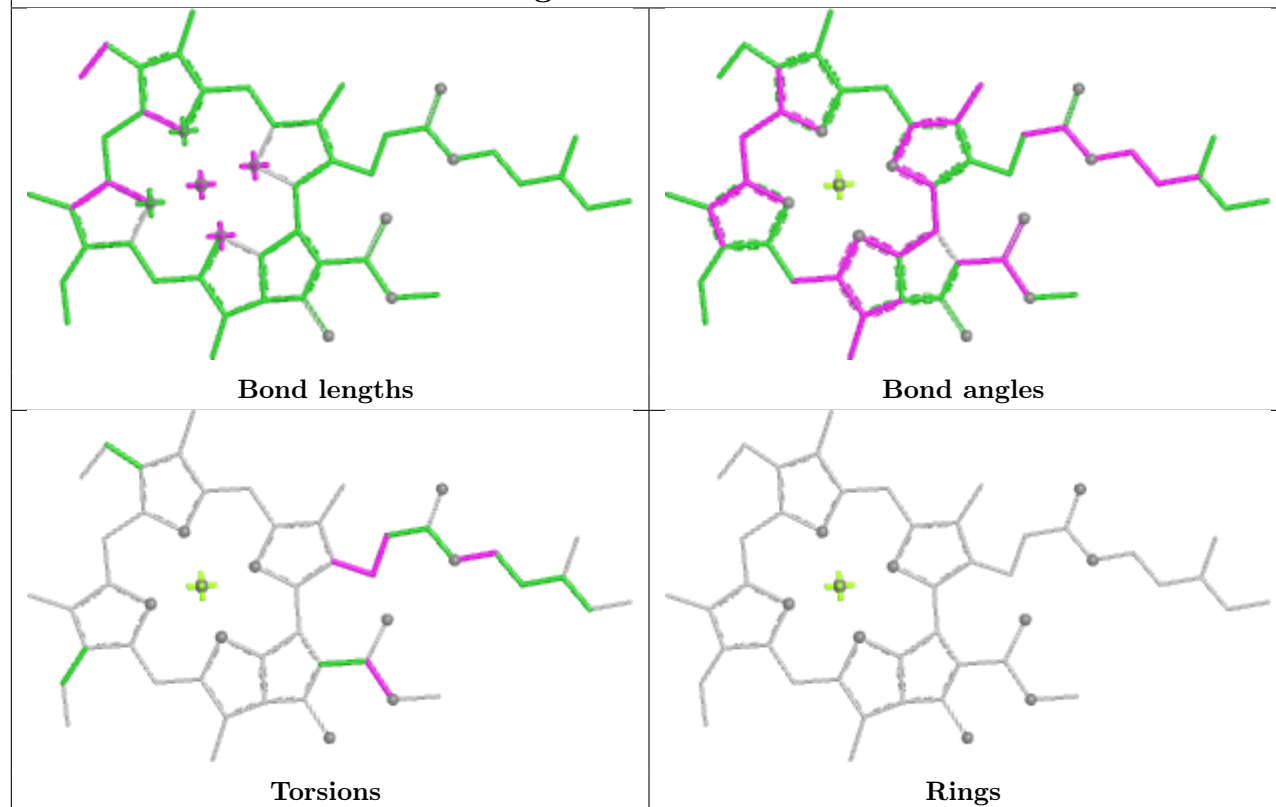




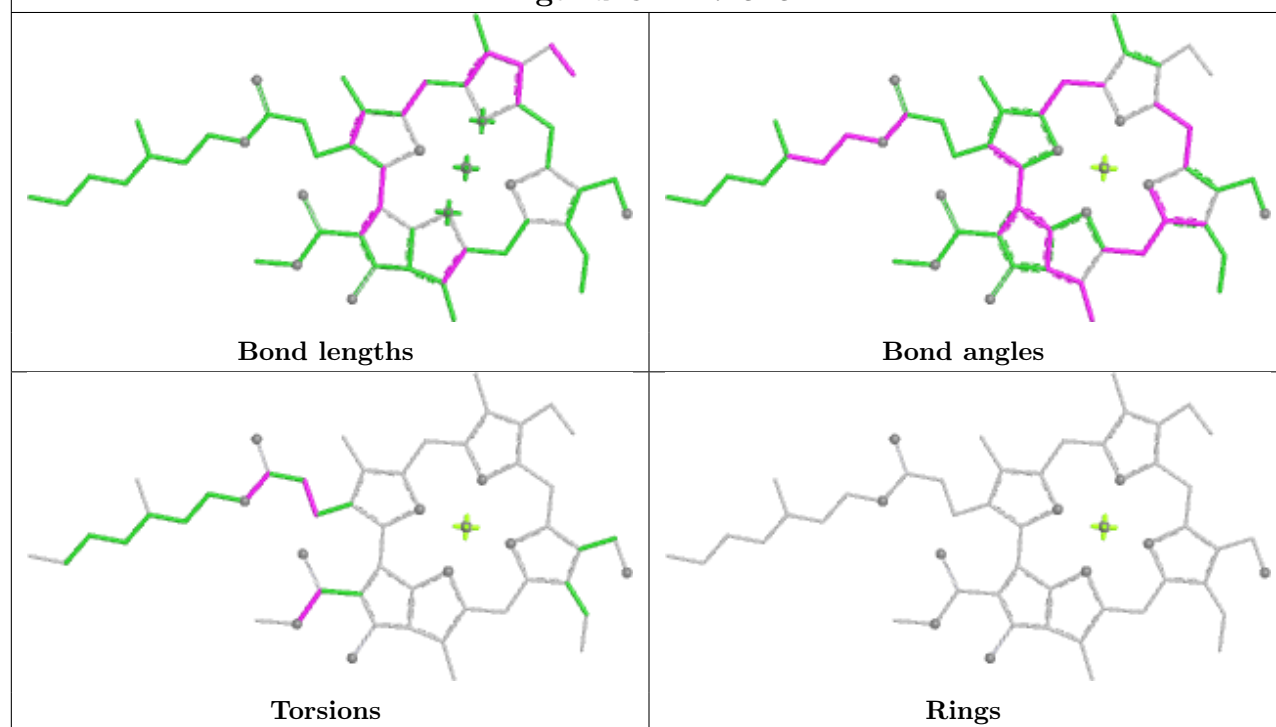


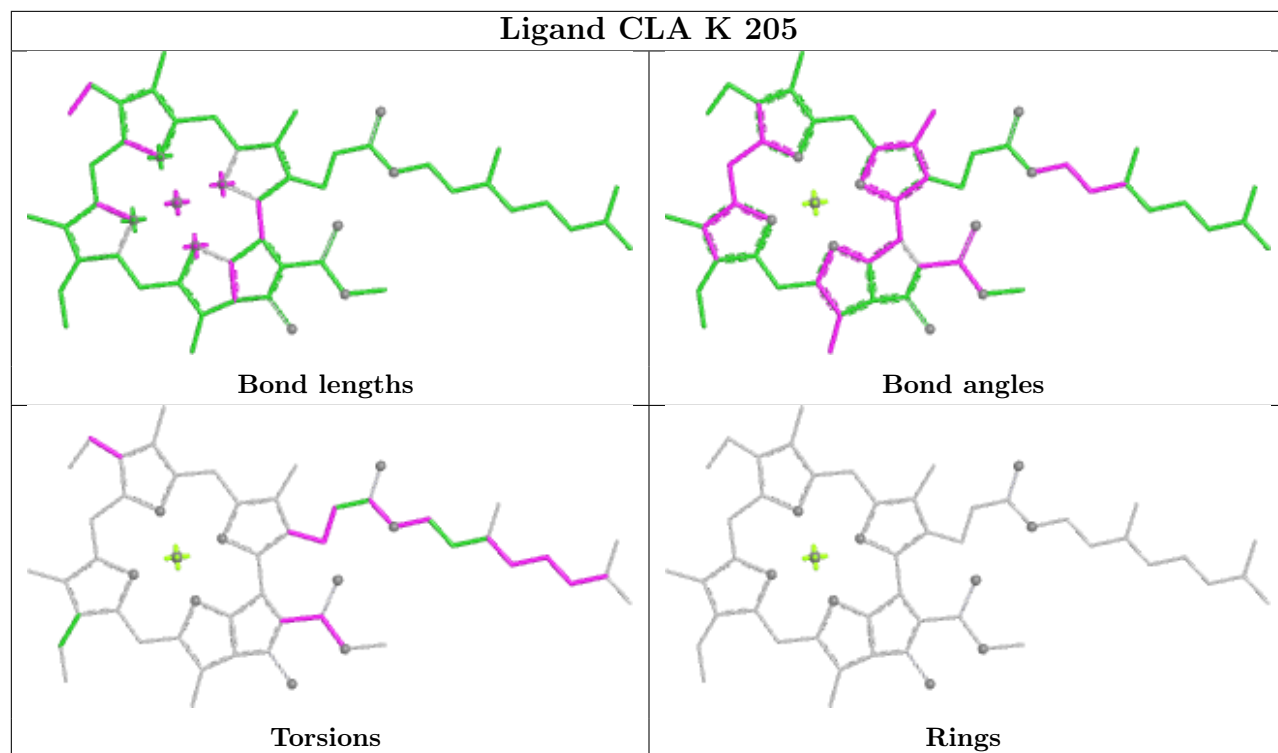


## Ligand CLA Z 314



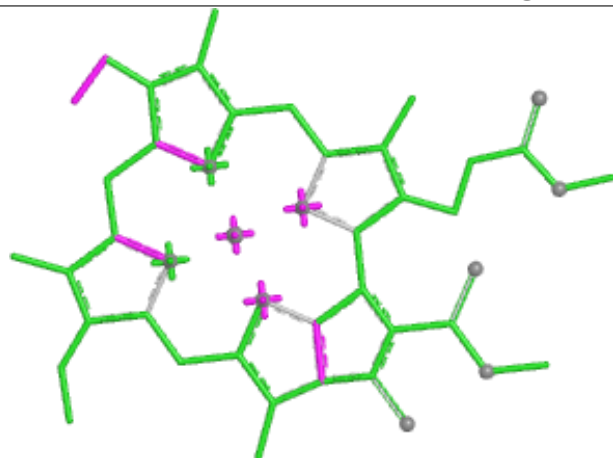
## Ligand CHL 7 313



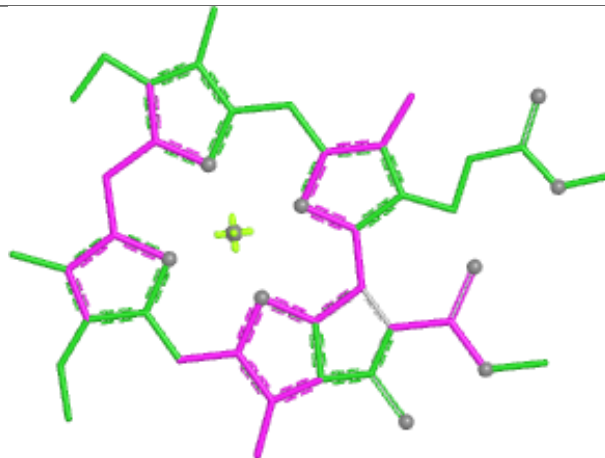




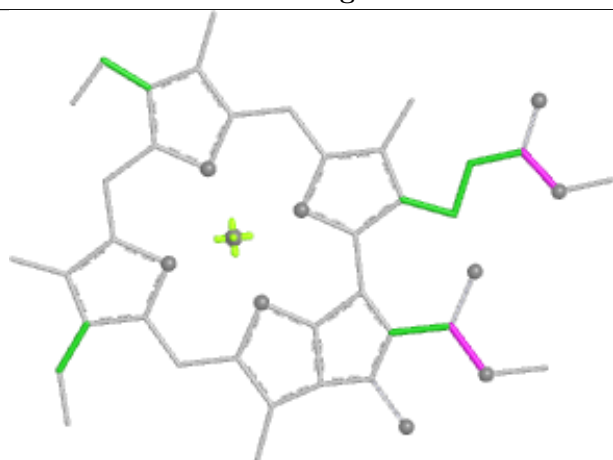
## Ligand CLA 3 309



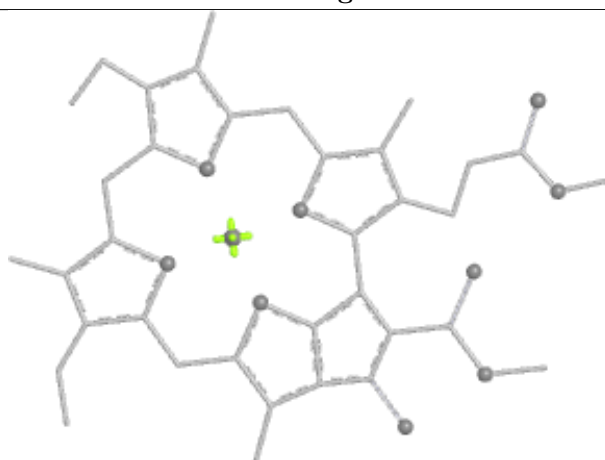
Bond lengths



Bond angles

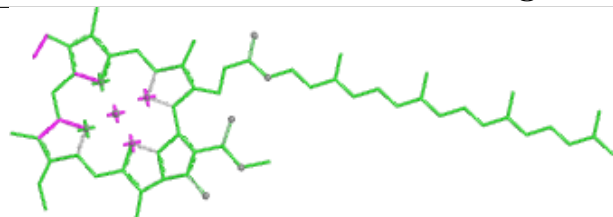


Torsions

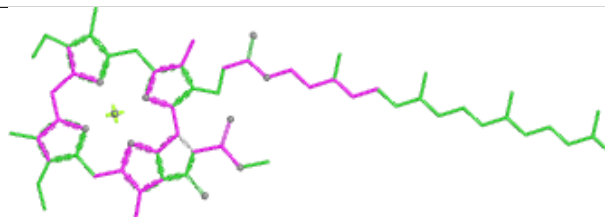


Rings

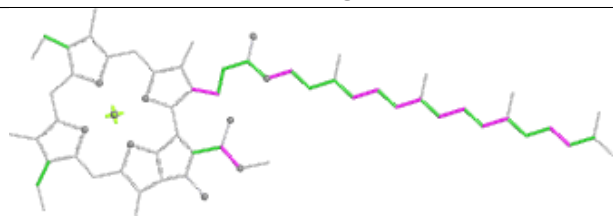
## Ligand CLA 5 315



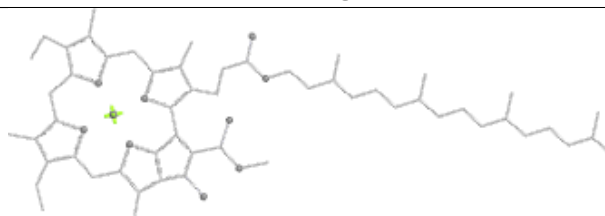
Bond lengths



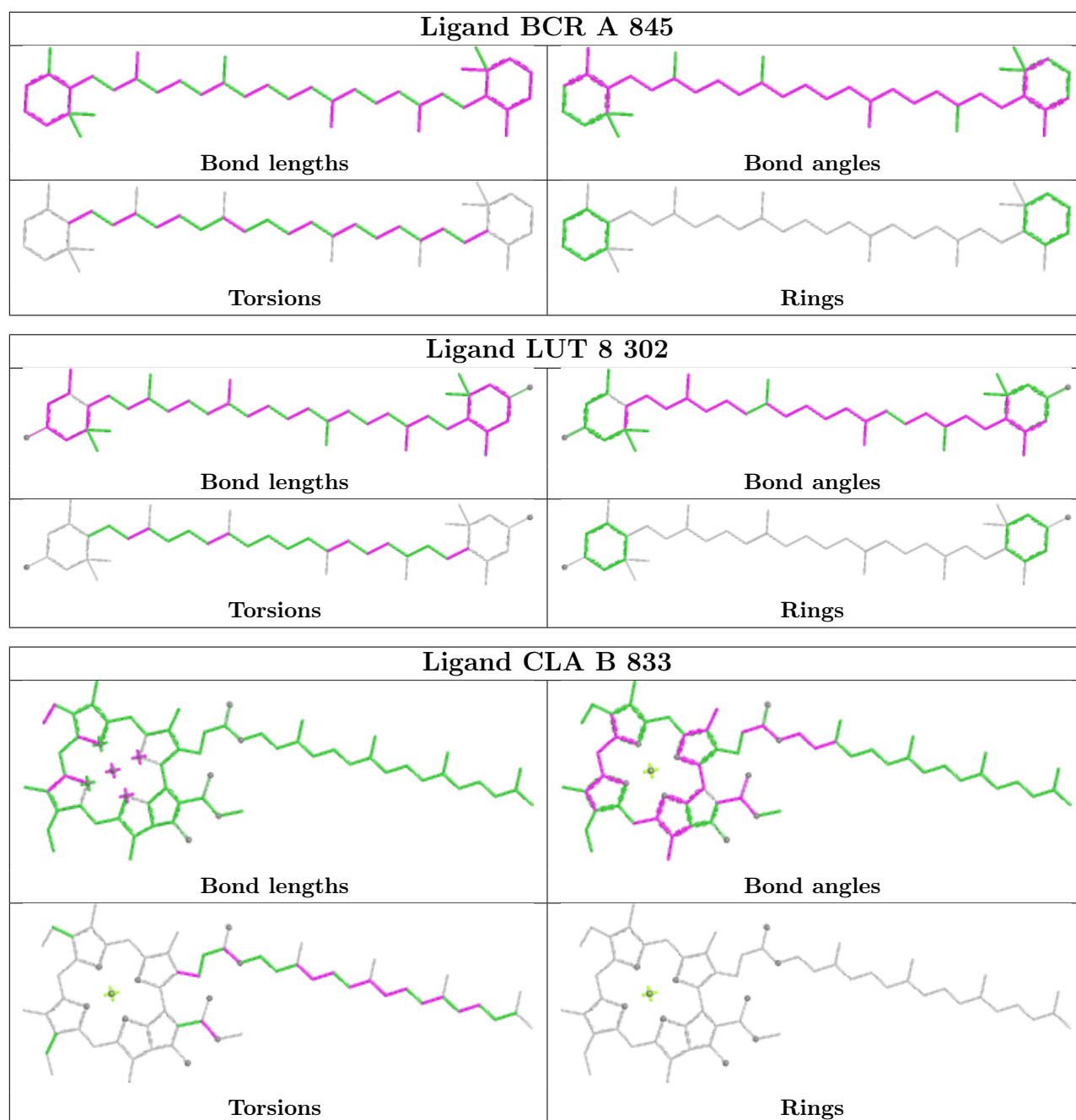
Bond angles



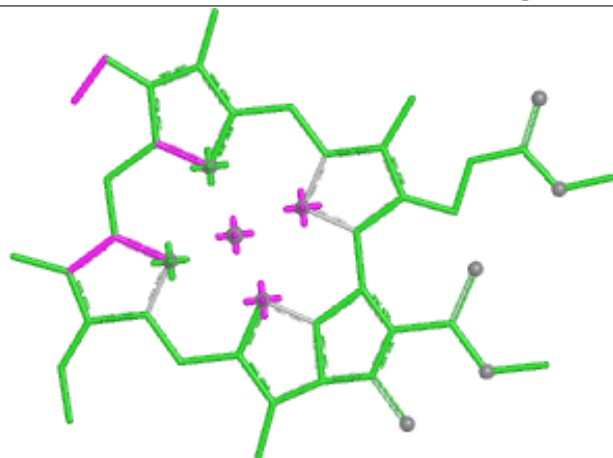
Torsions



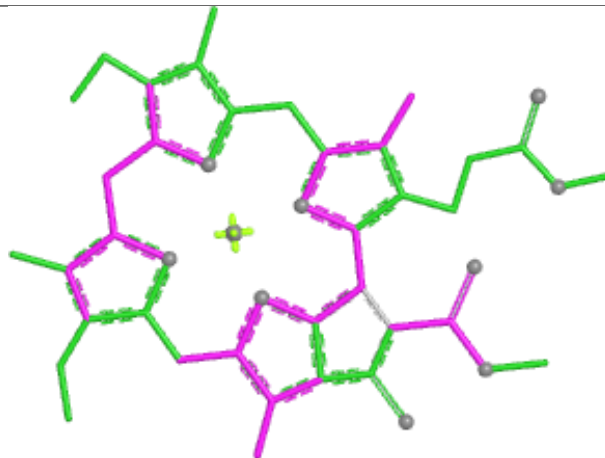
Rings



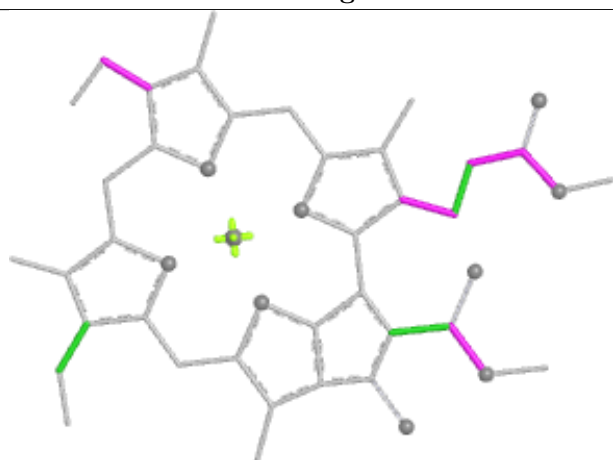
## Ligand CLA Z 315



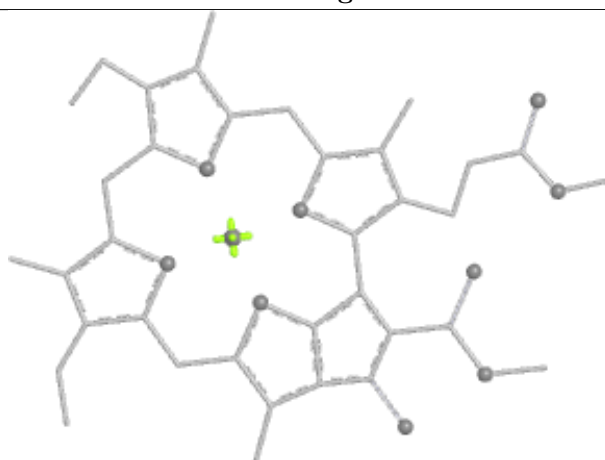
Bond lengths



Bond angles

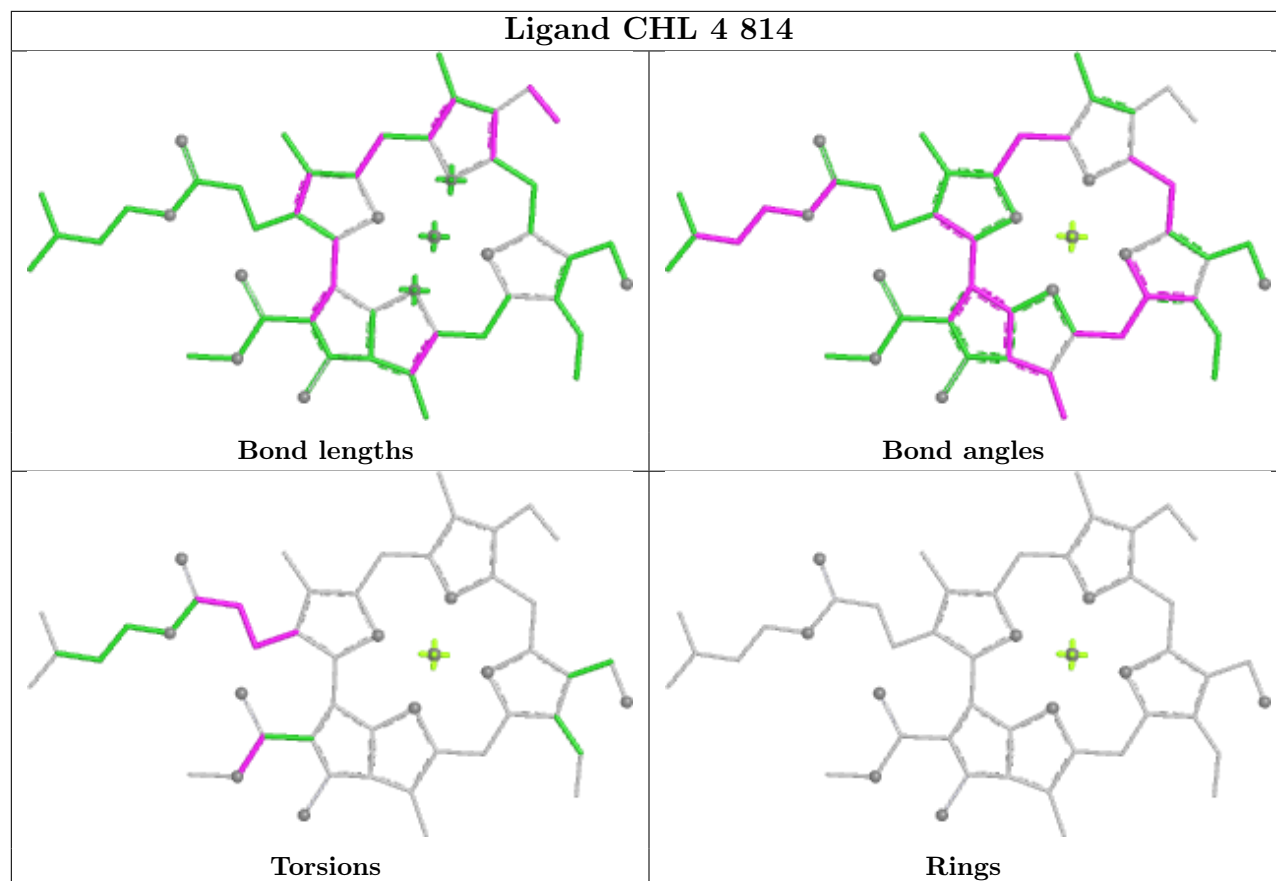


Torsions

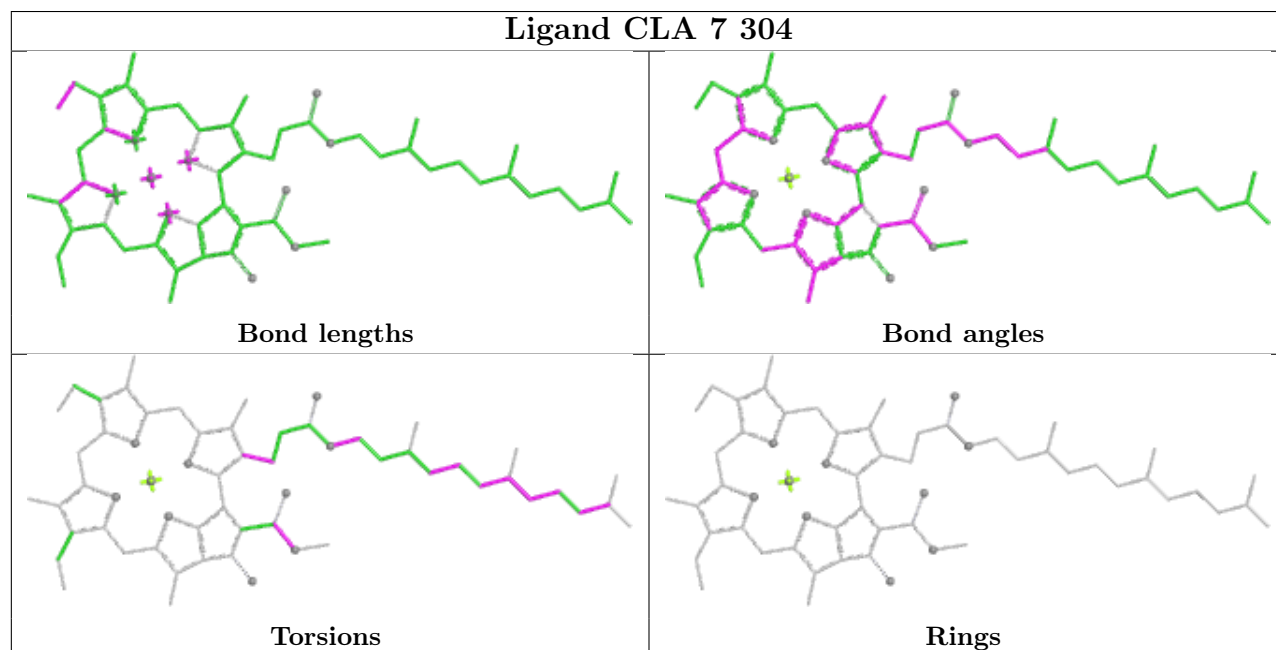


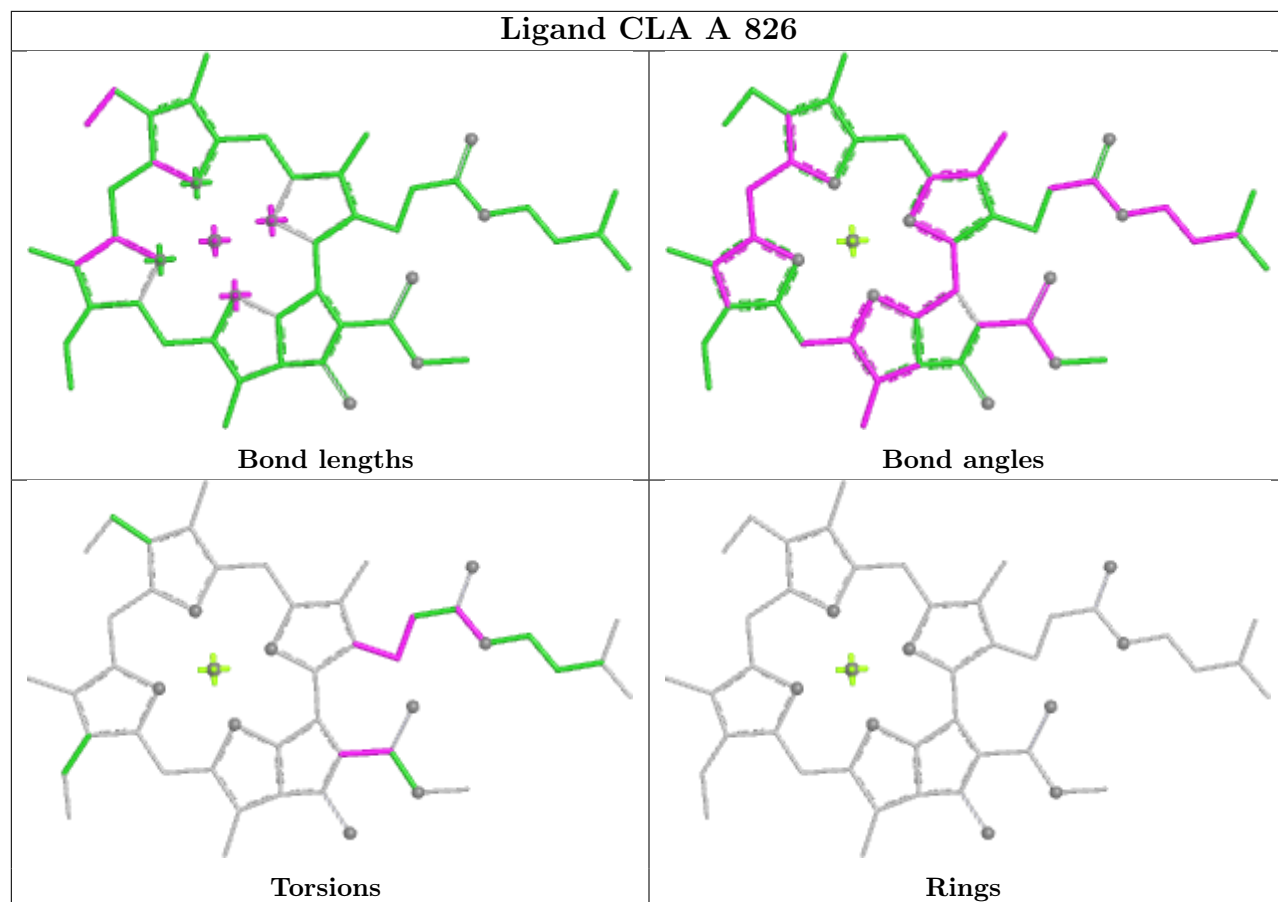
Rings

## Ligand CHL 4 814

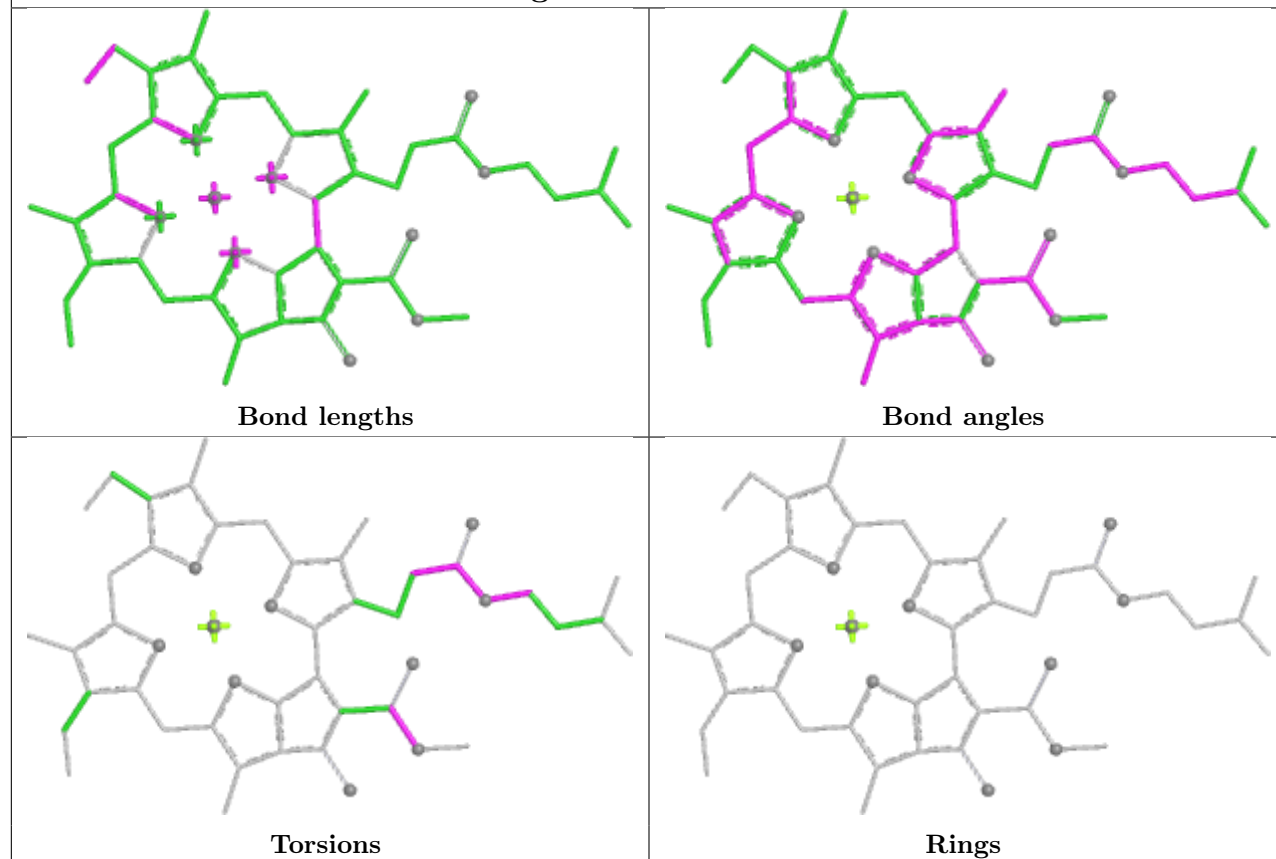


## Ligand CLA 7 304

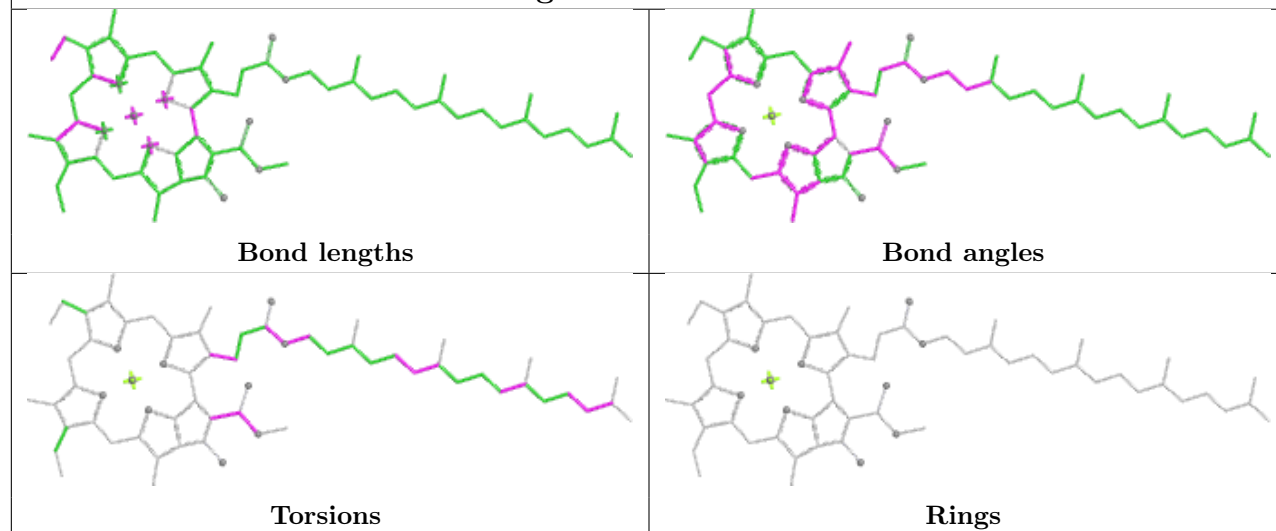




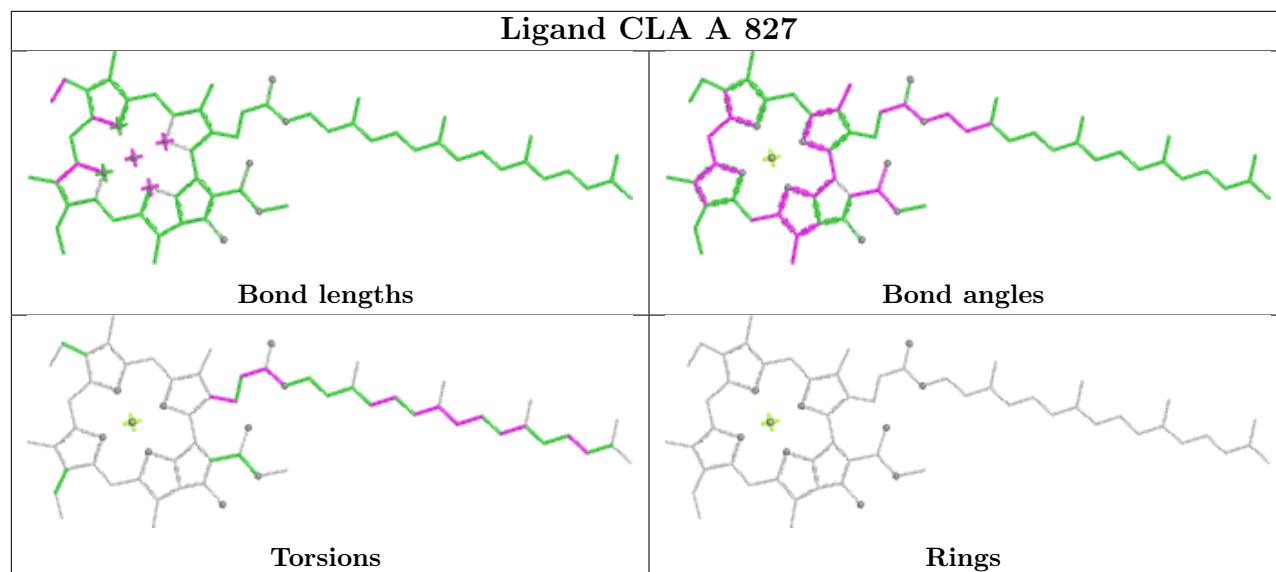
## Ligand CLA G 201



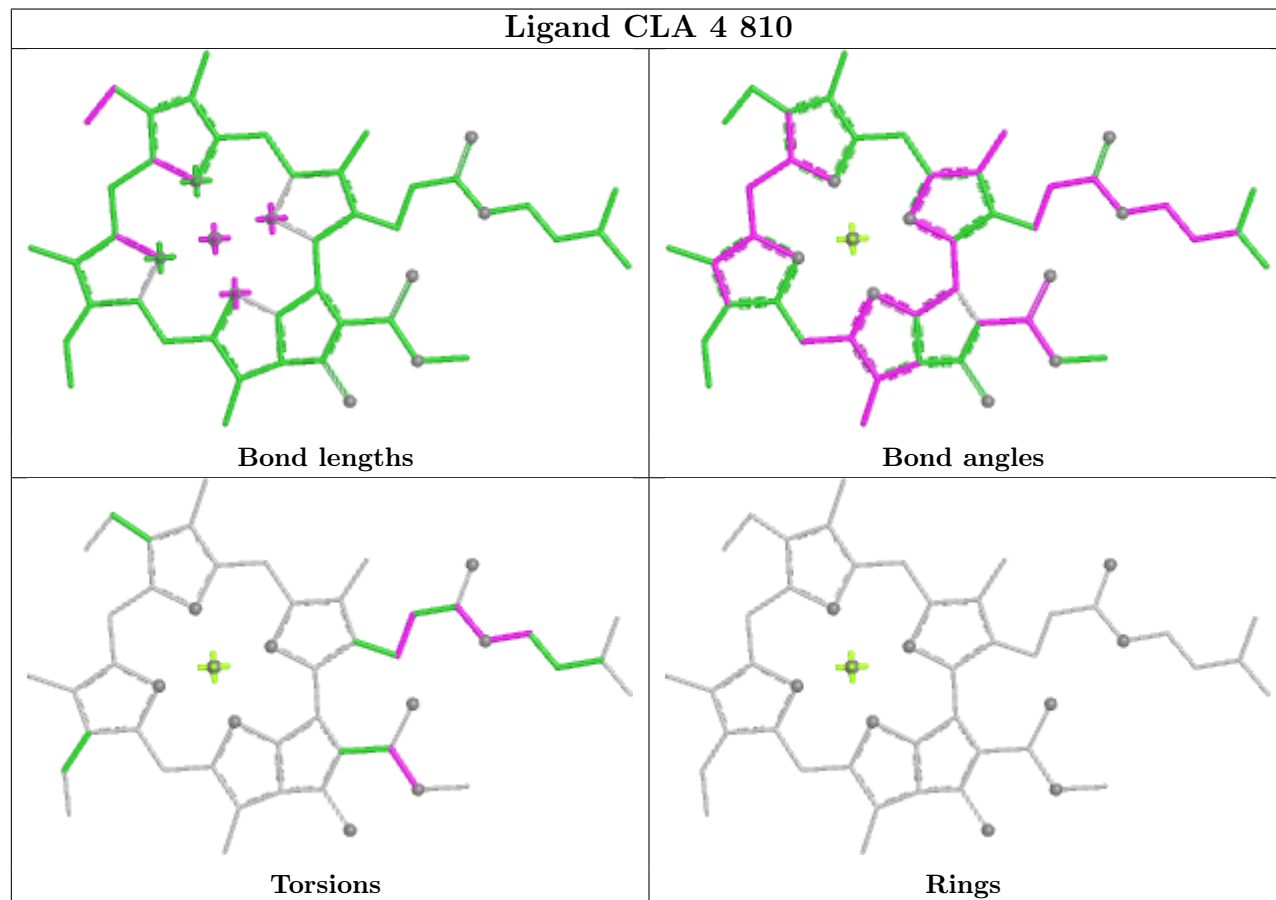
## Ligand CLA 6 312



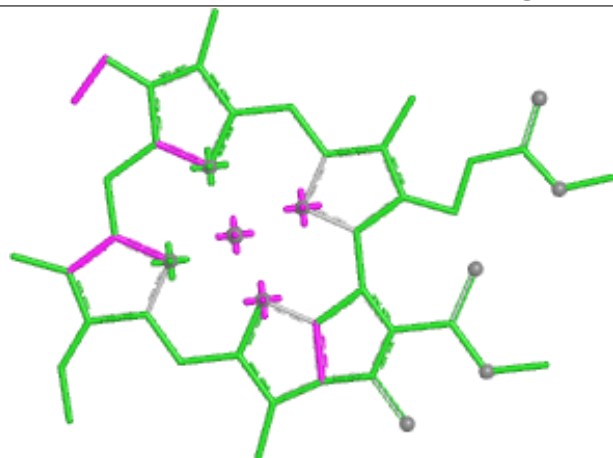
## Ligand CLA A 827



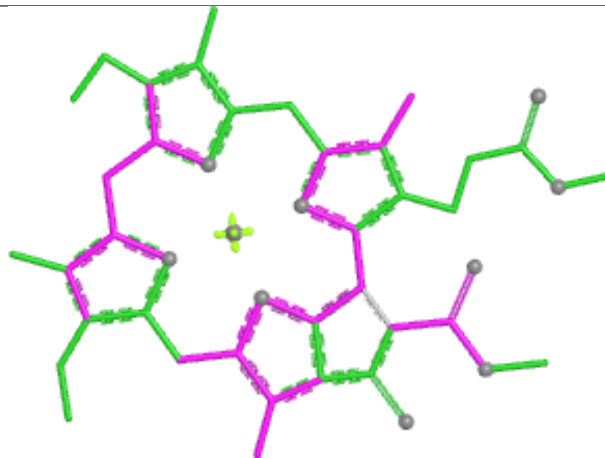
## Ligand CLA 4 810



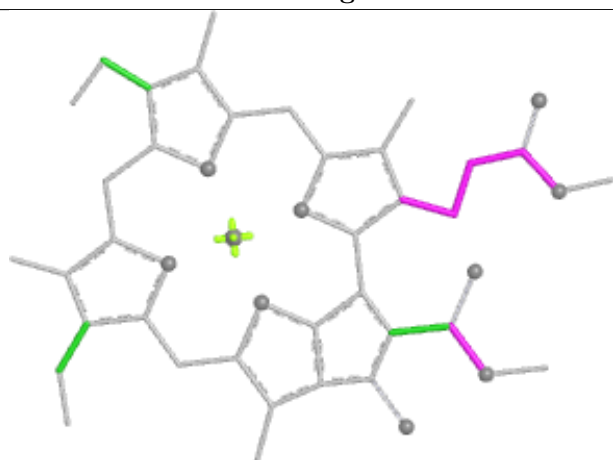
## Ligand CLA 8 316



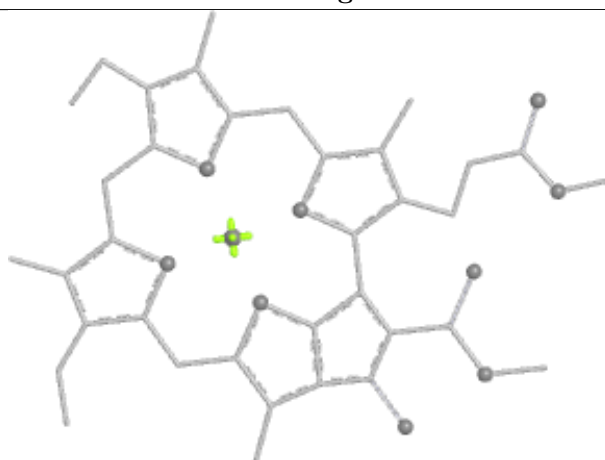
Bond lengths



Bond angles

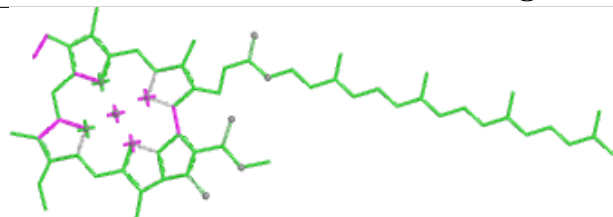


Torsions

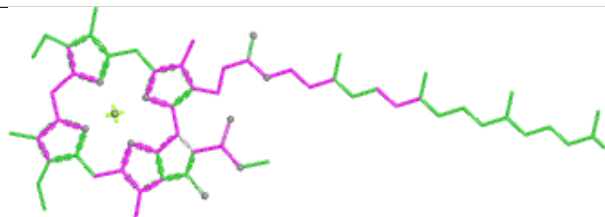


Rings

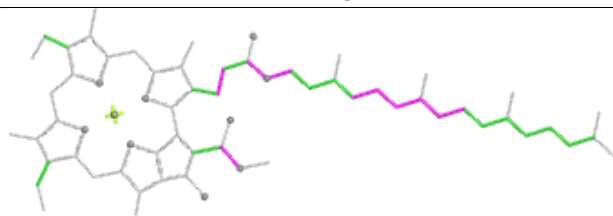
## Ligand CLA 3 310



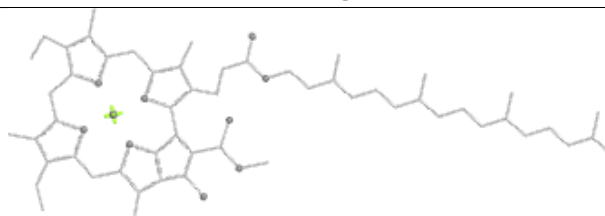
Bond lengths



Bond angles

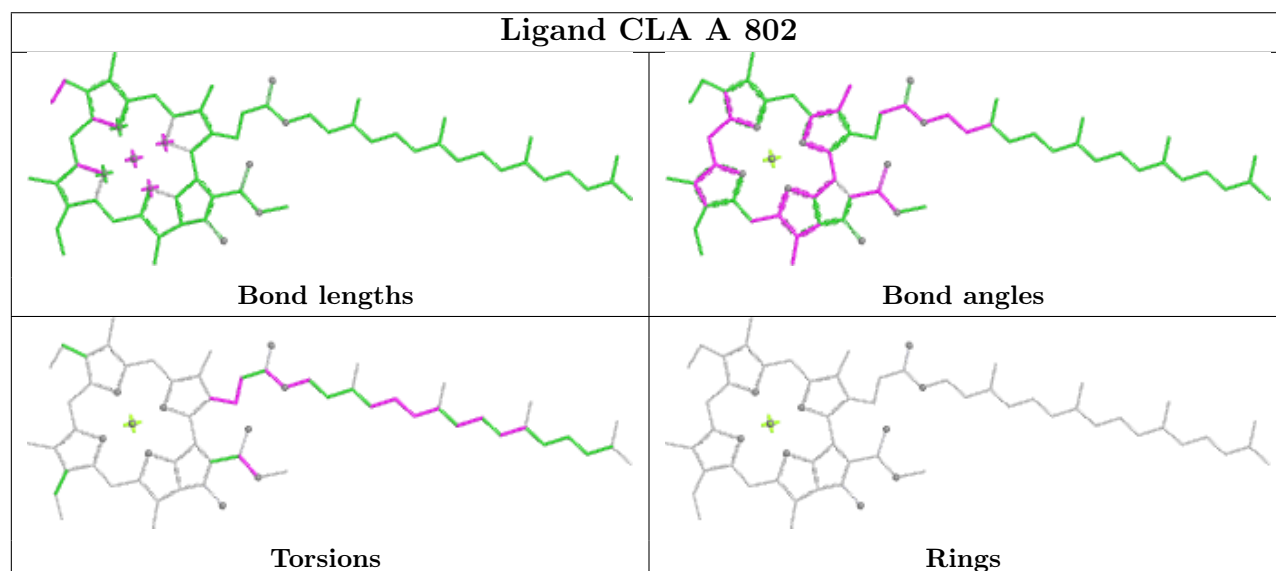
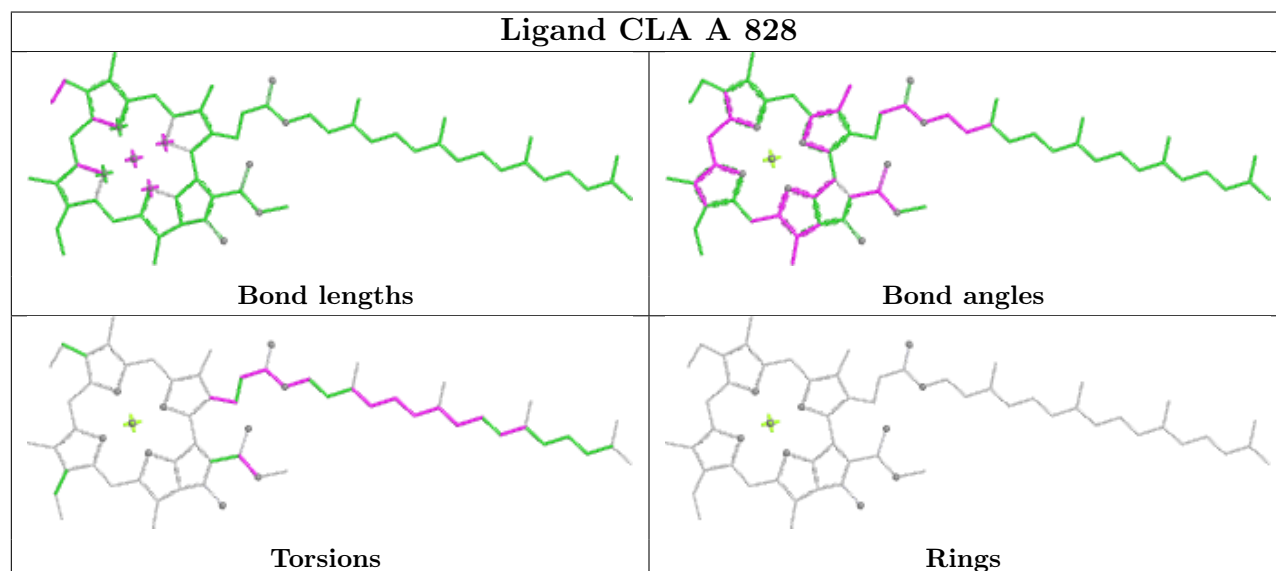
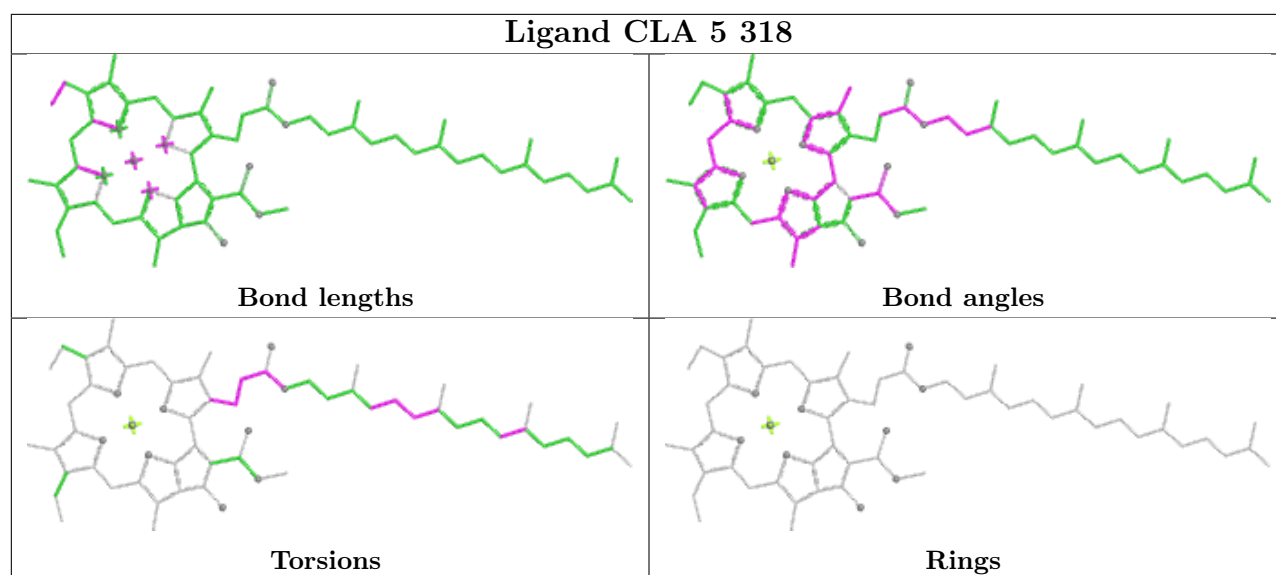


Torsions

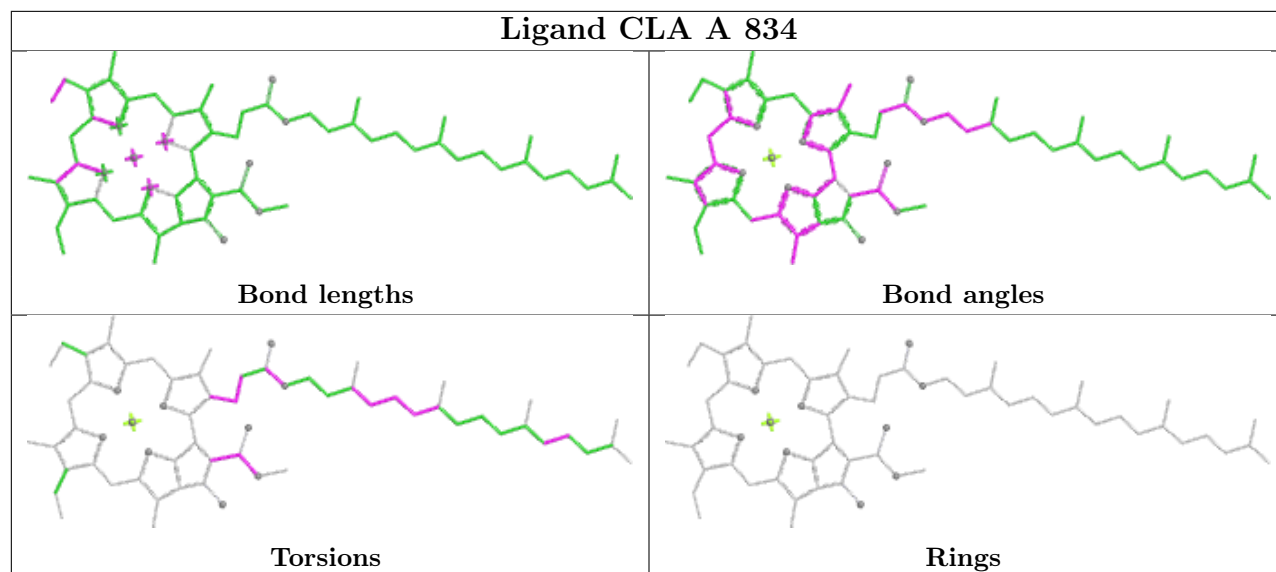


Rings

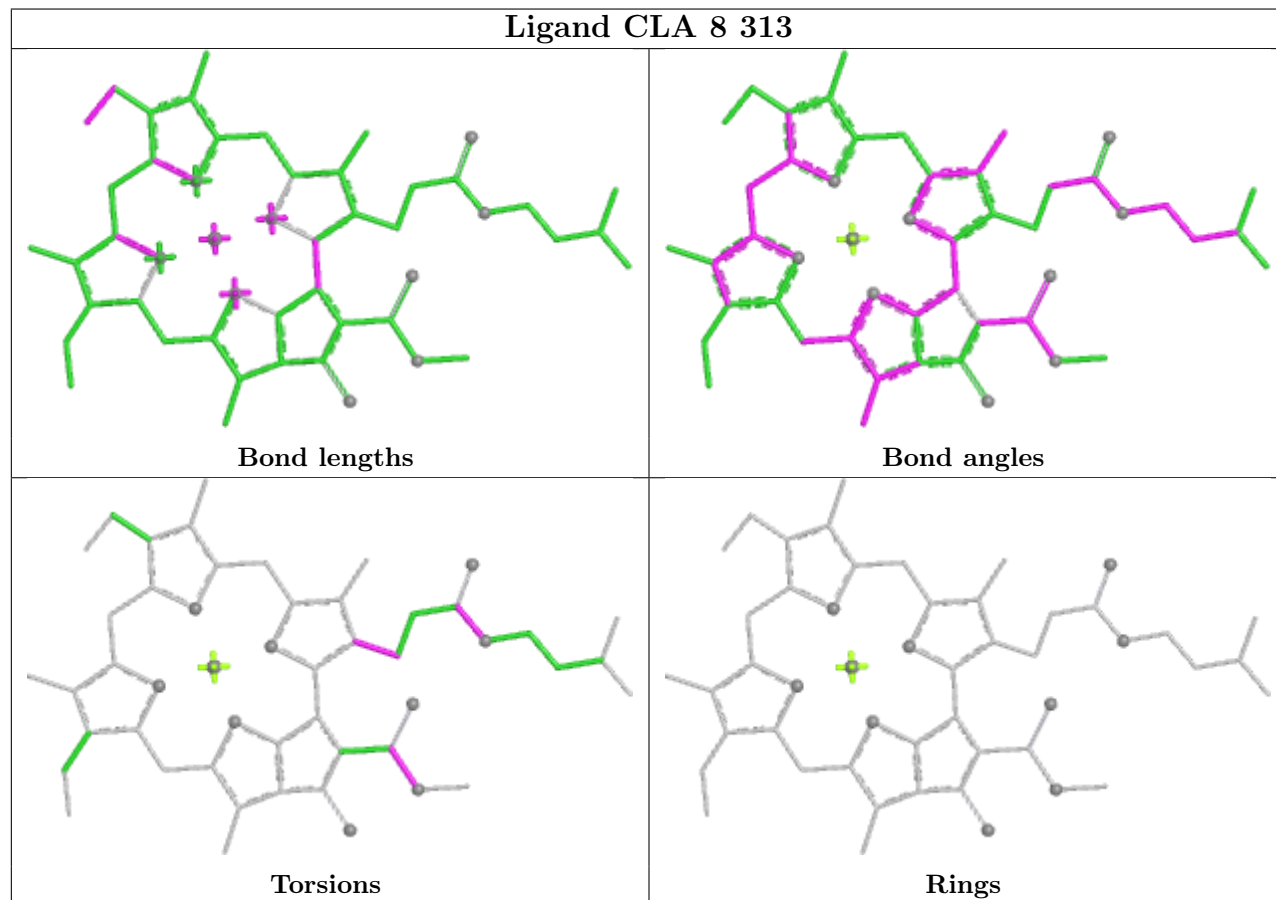




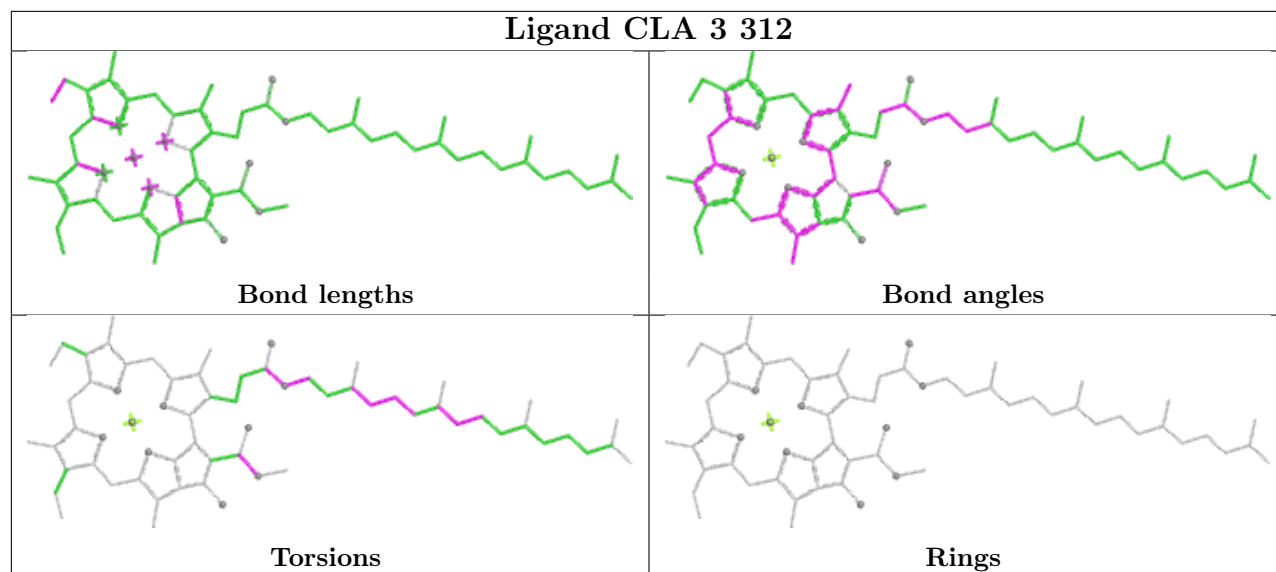
## Ligand CLA A 834



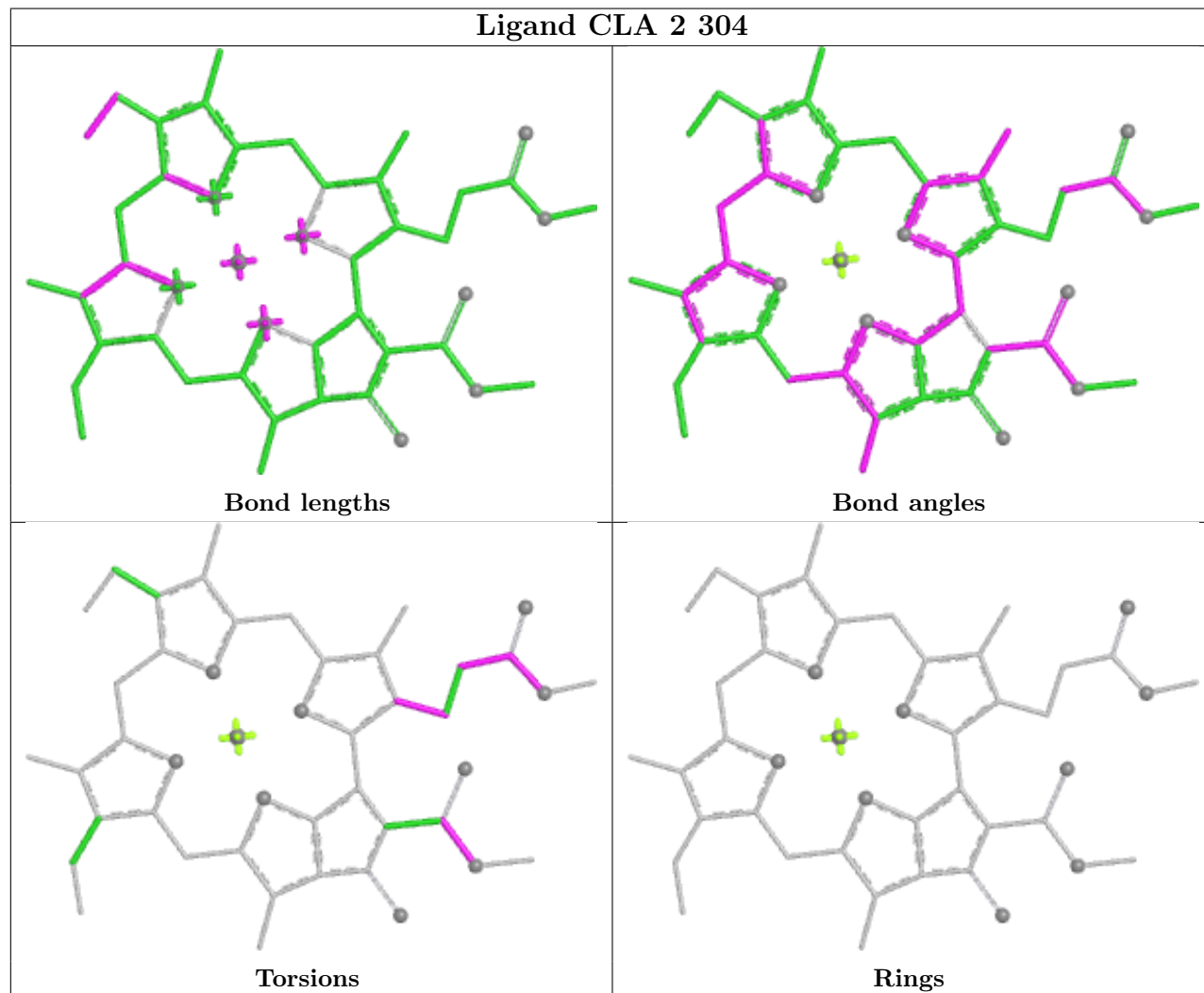
## Ligand CLA 8 313



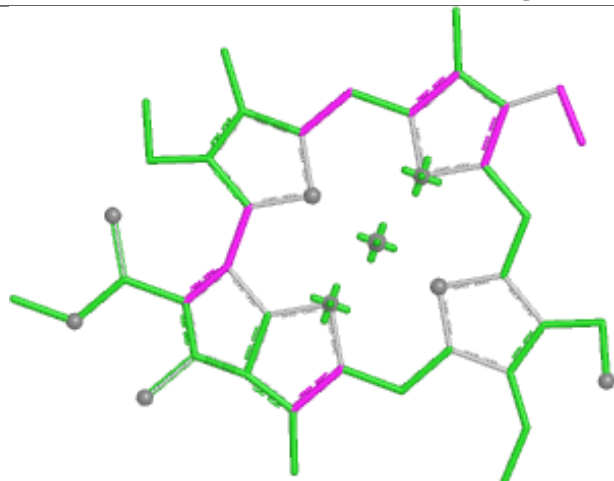
## Ligand CLA 3 312



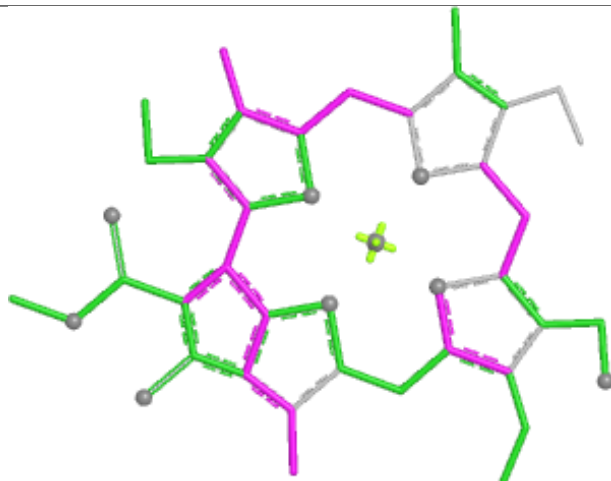
## Ligand CLA 2 304



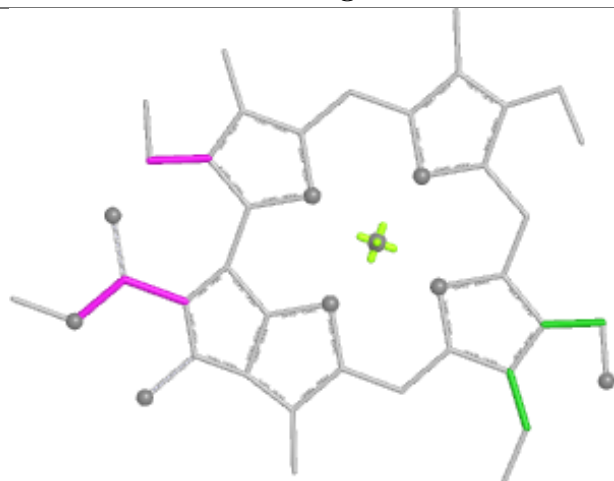
## Ligand CHL 5 321



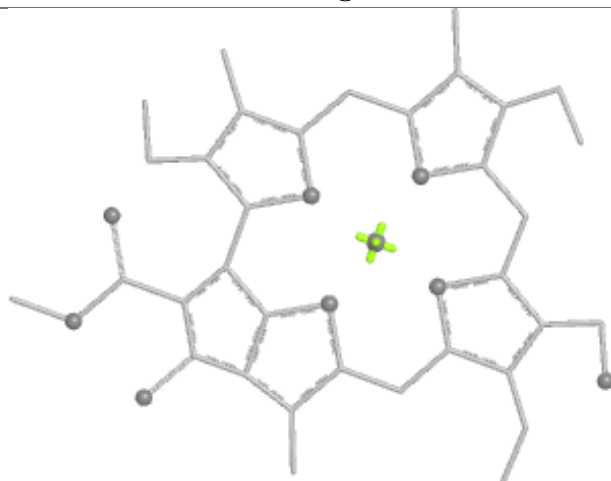
Bond lengths



Bond angles

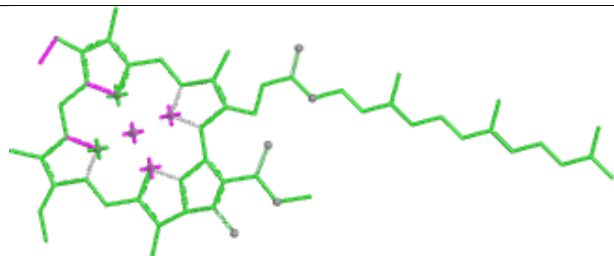


Torsions

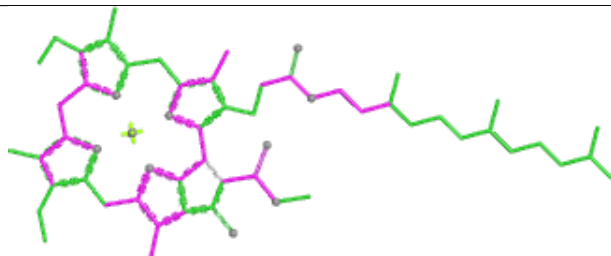


Rings

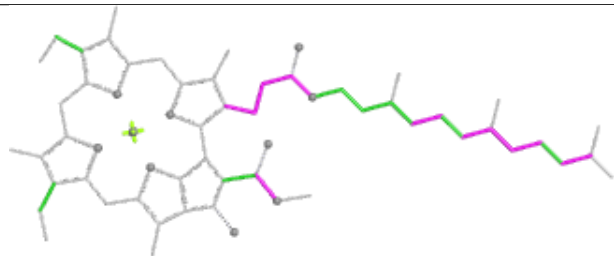
## Ligand CLA 7 312



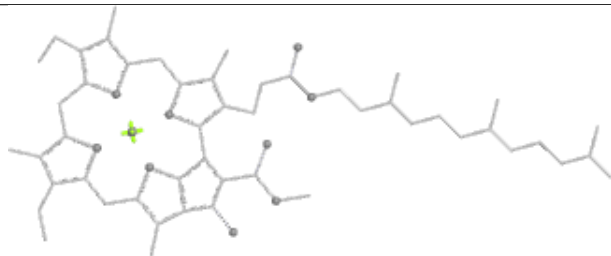
Bond lengths



Bond angles

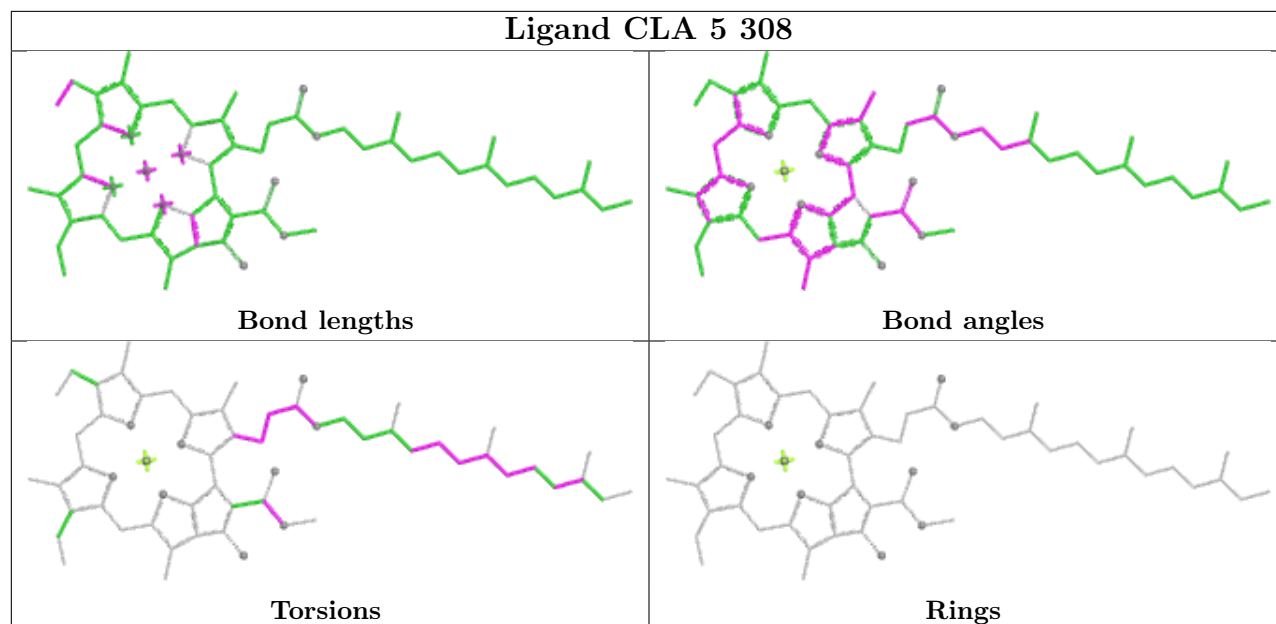


Torsions

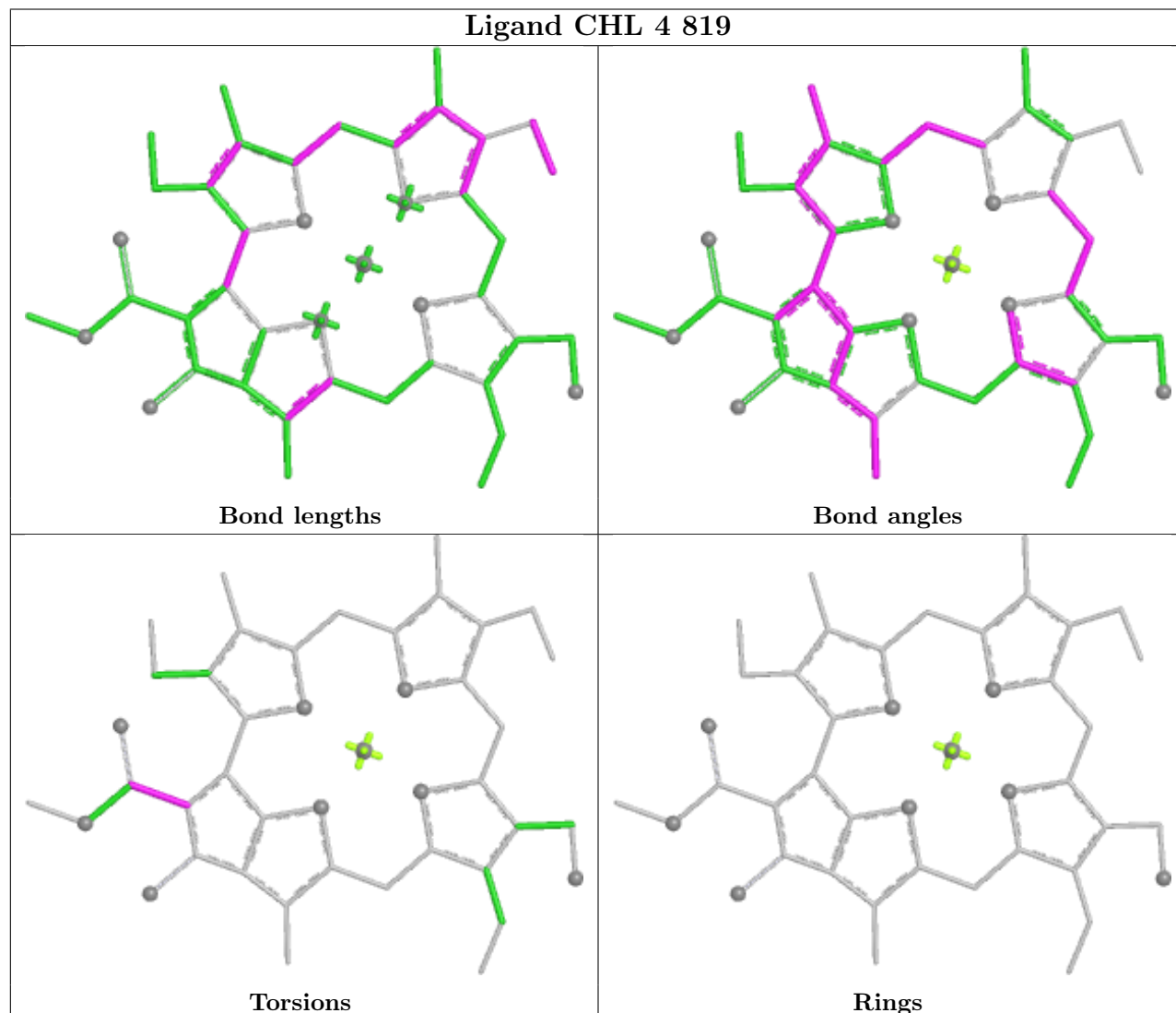


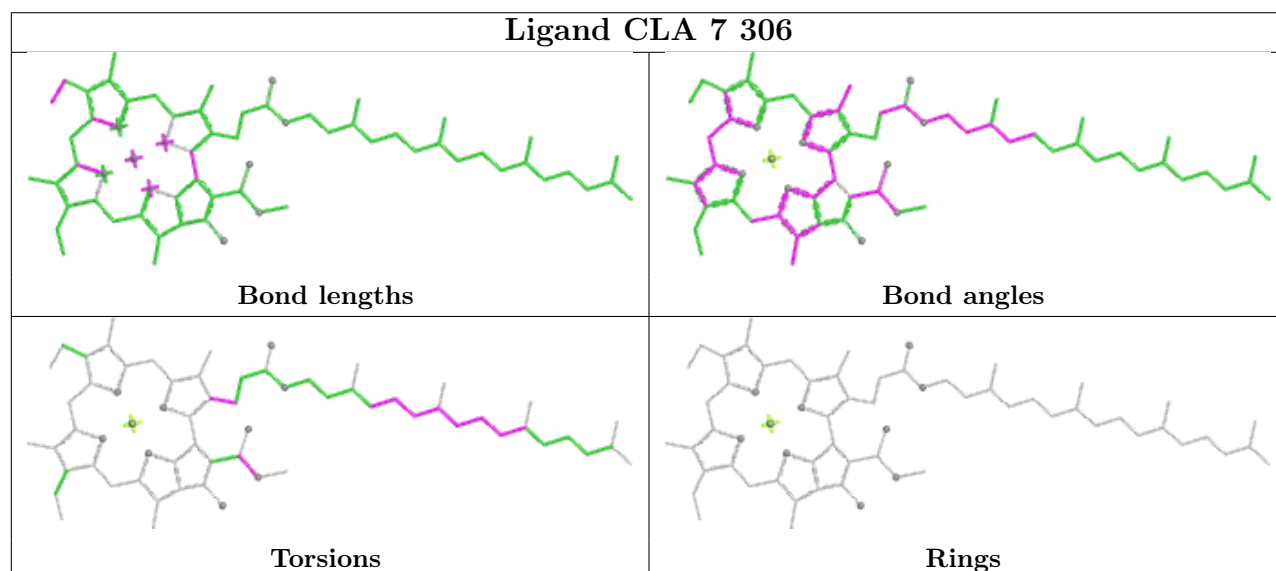
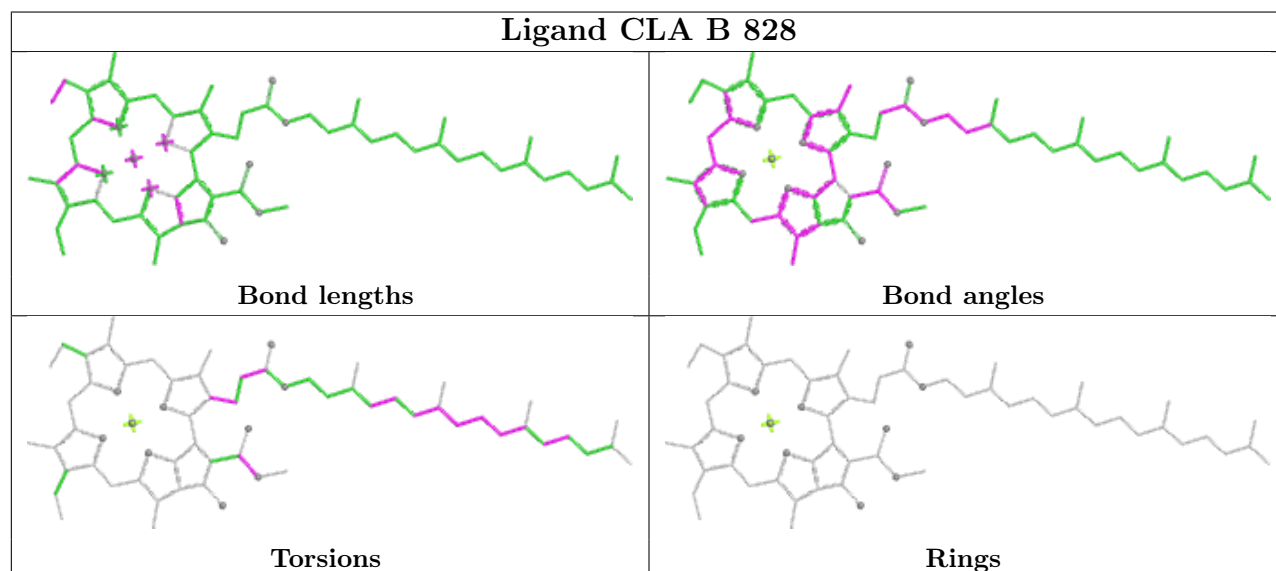
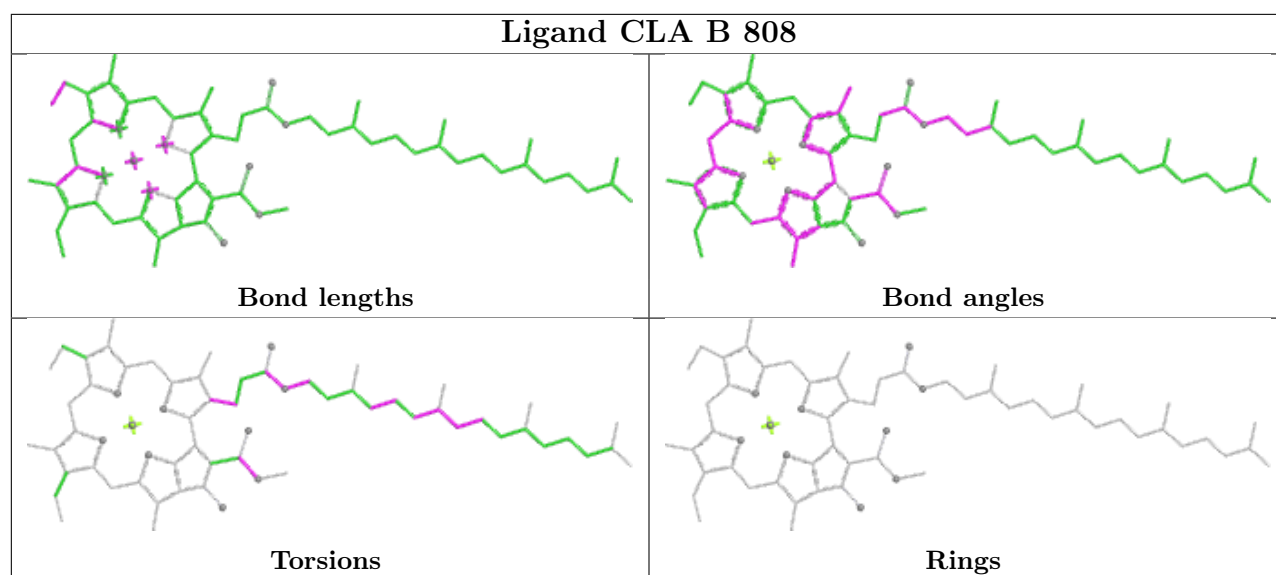
Rings

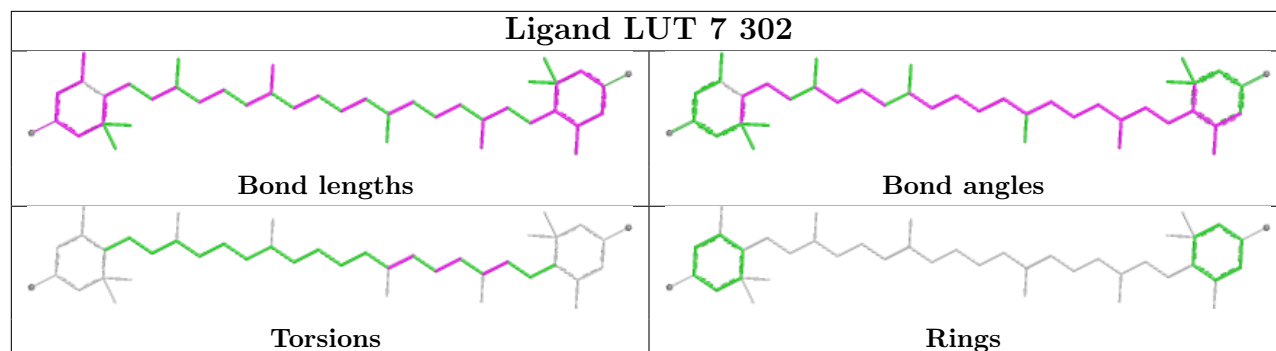
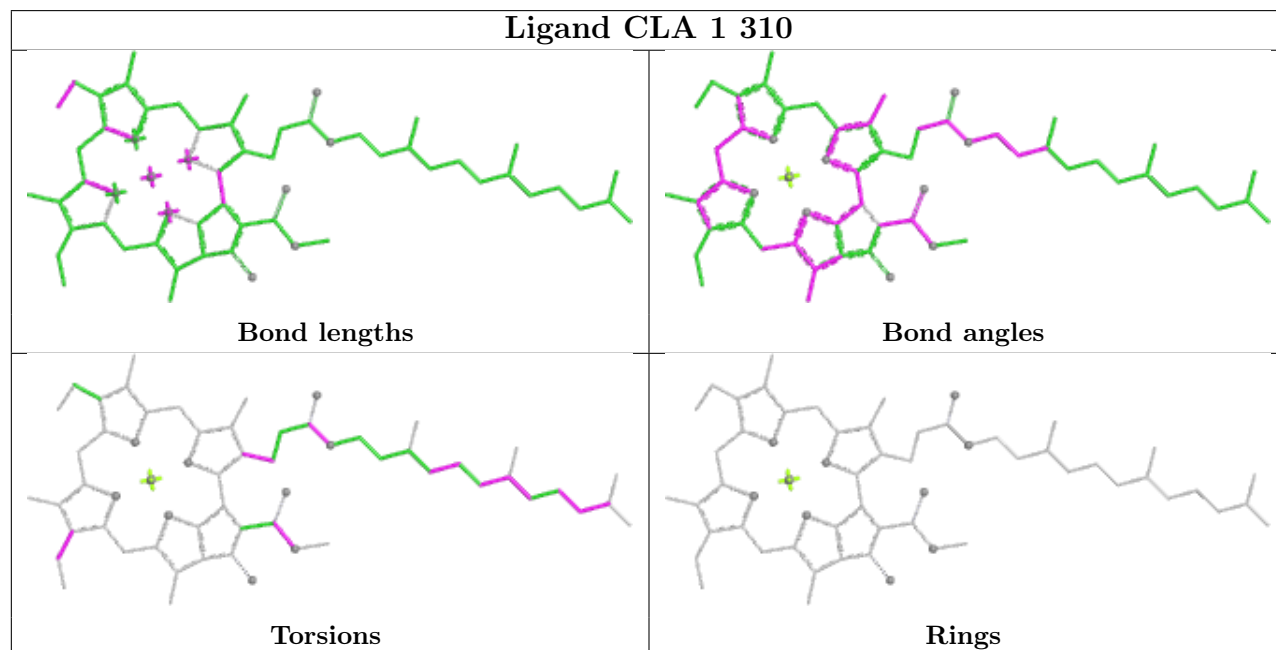
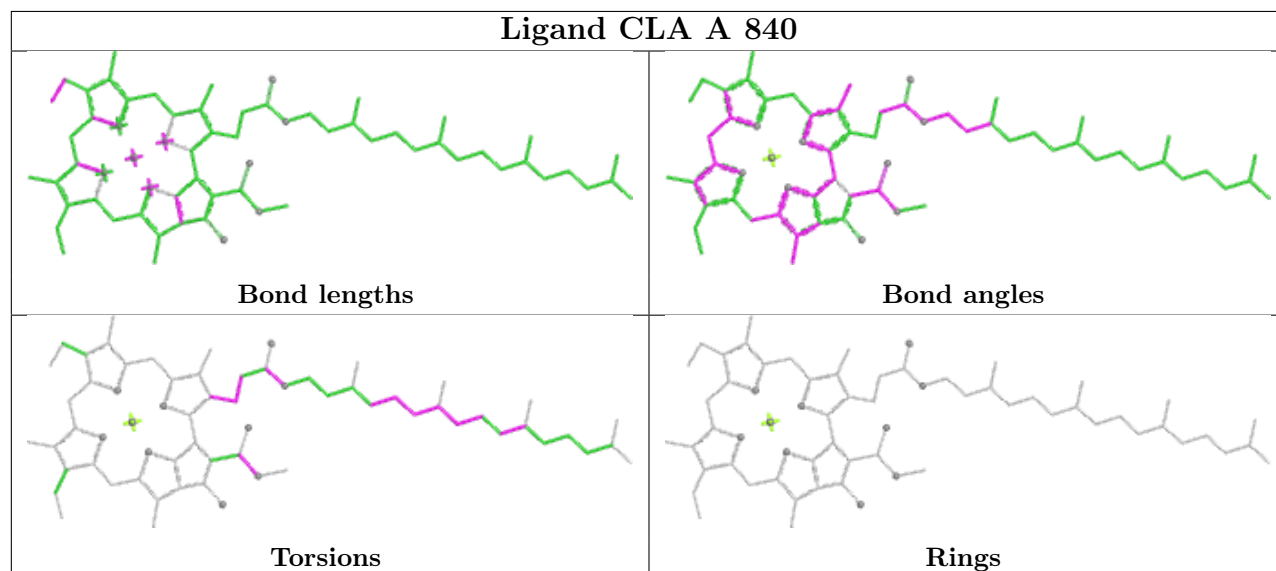
## Ligand CLA 5 308

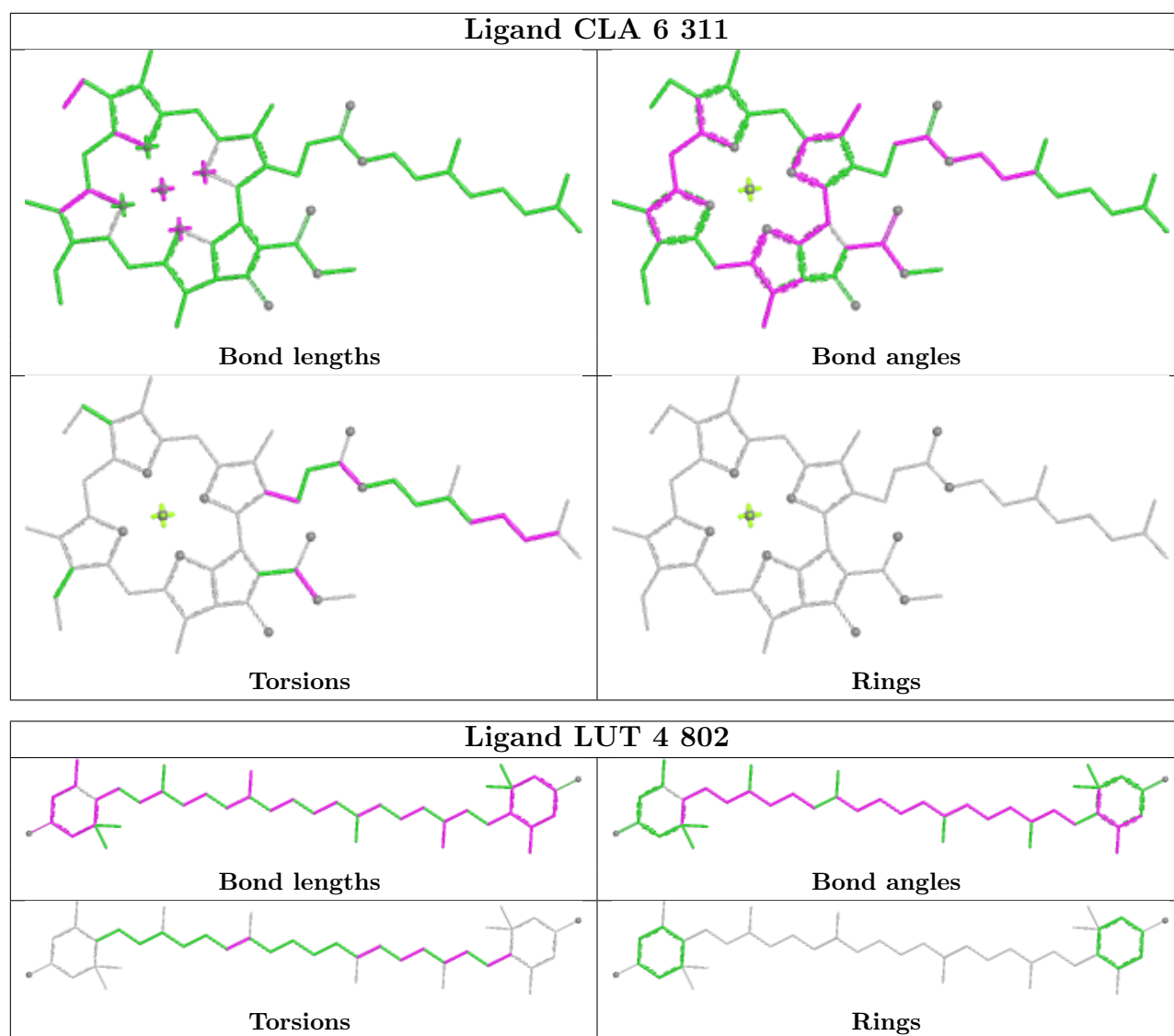


## Ligand CHL 4 819



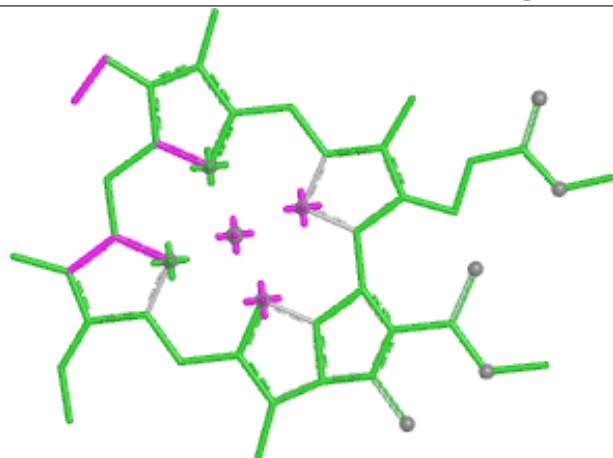


**Ligand LUT 7 302****Ligand CLA 1 310****Ligand CLA A 840**

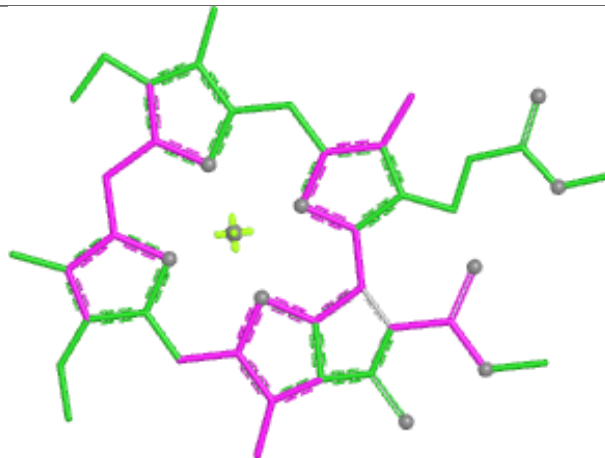




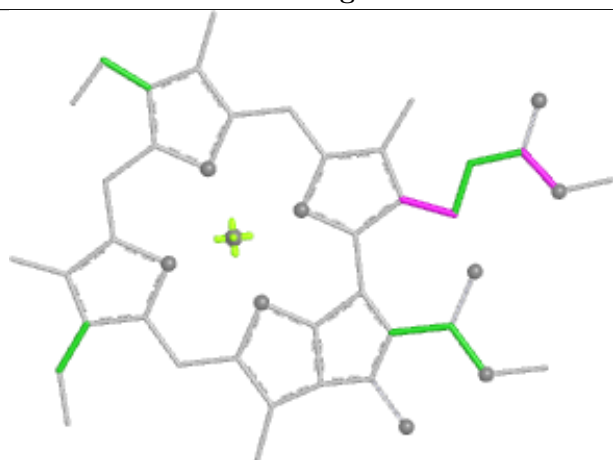
## Ligand CLA 6 321



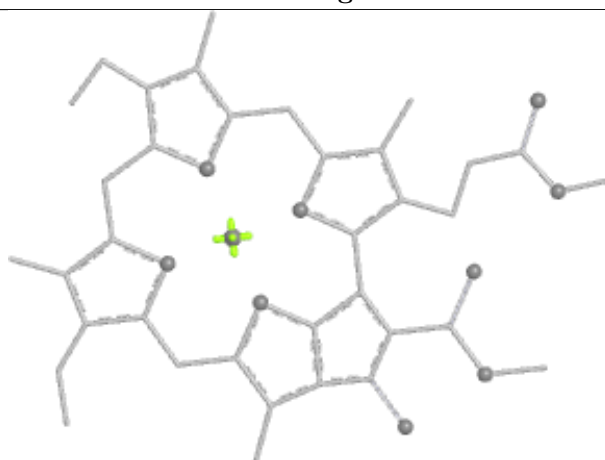
Bond lengths



Bond angles

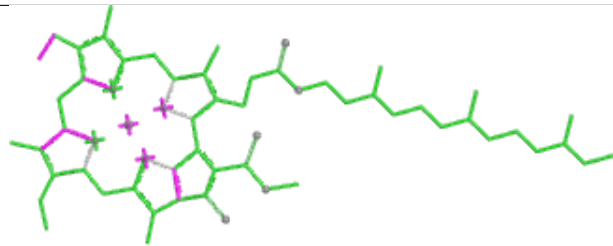


Torsions

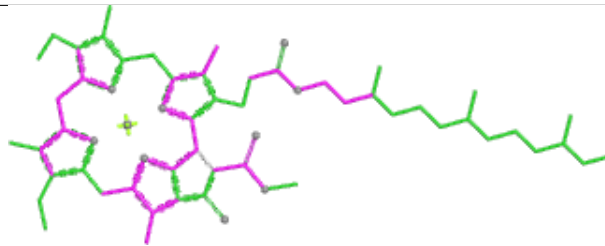


Rings

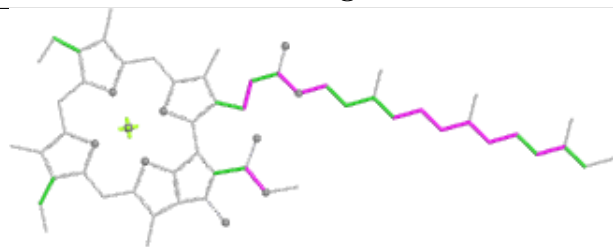
## Ligand CLA 7 308



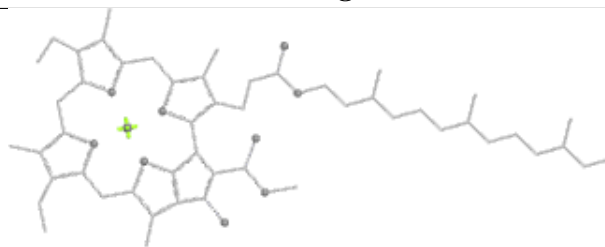
Bond lengths



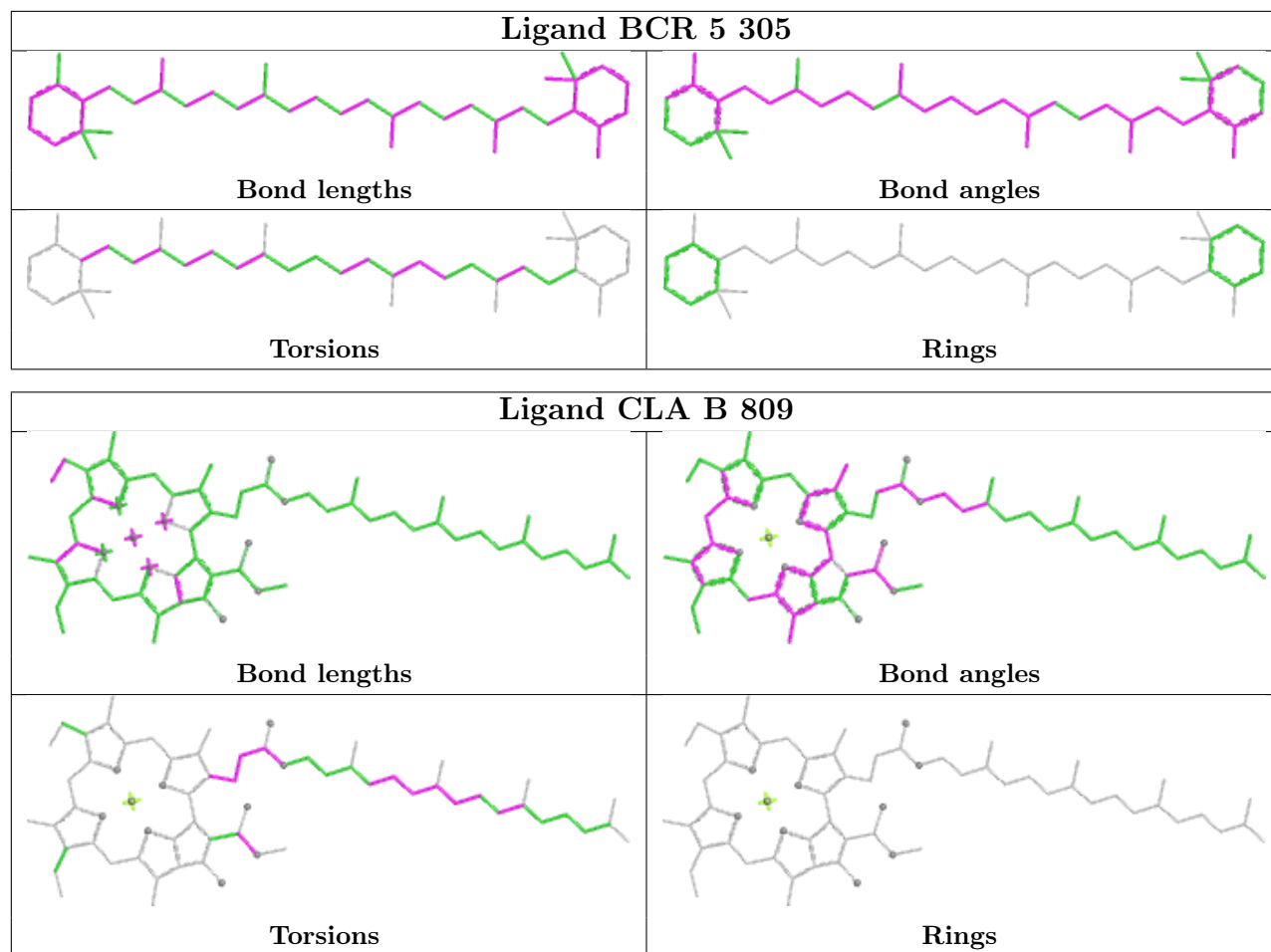
Bond angles

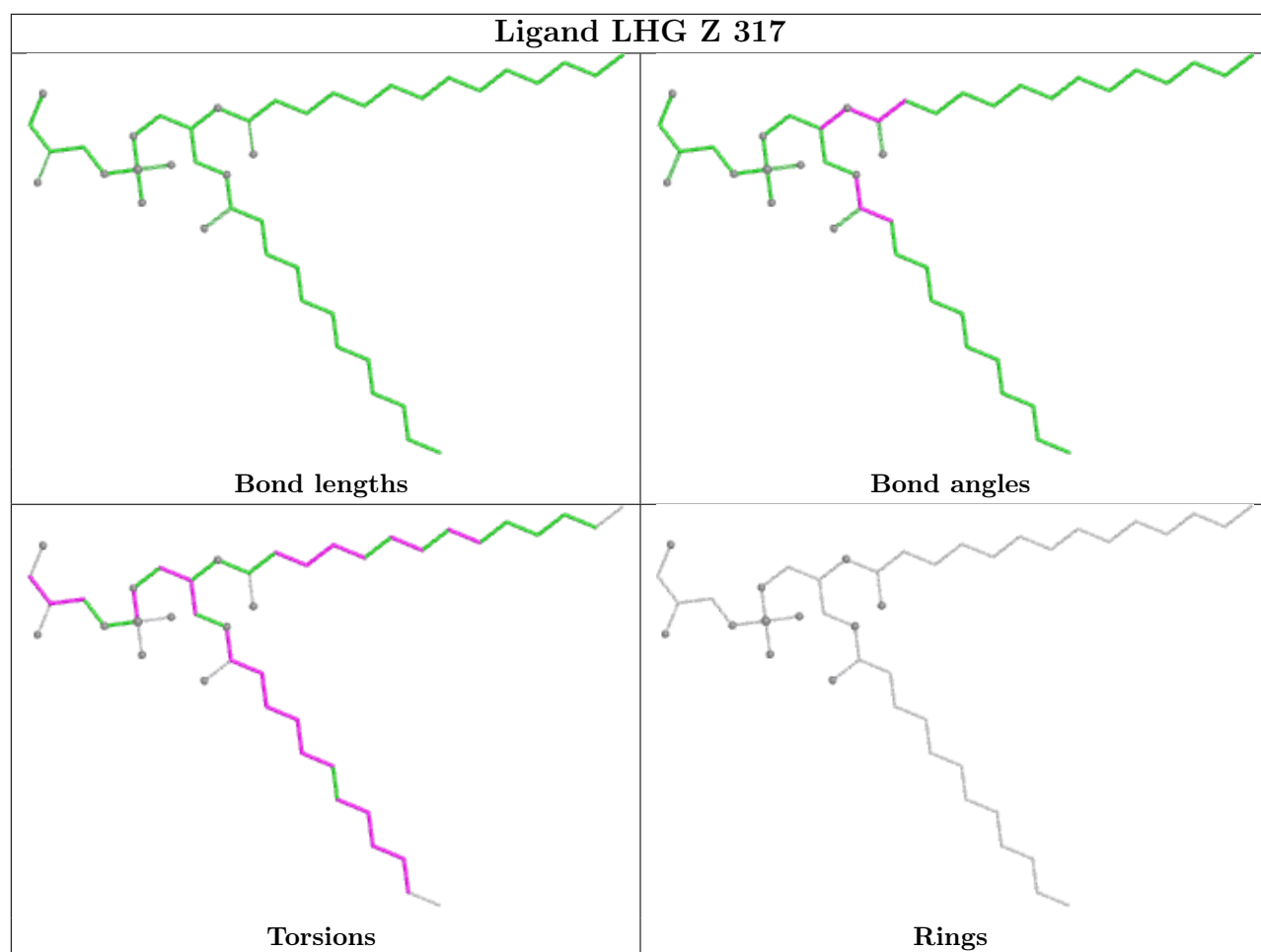


Torsions

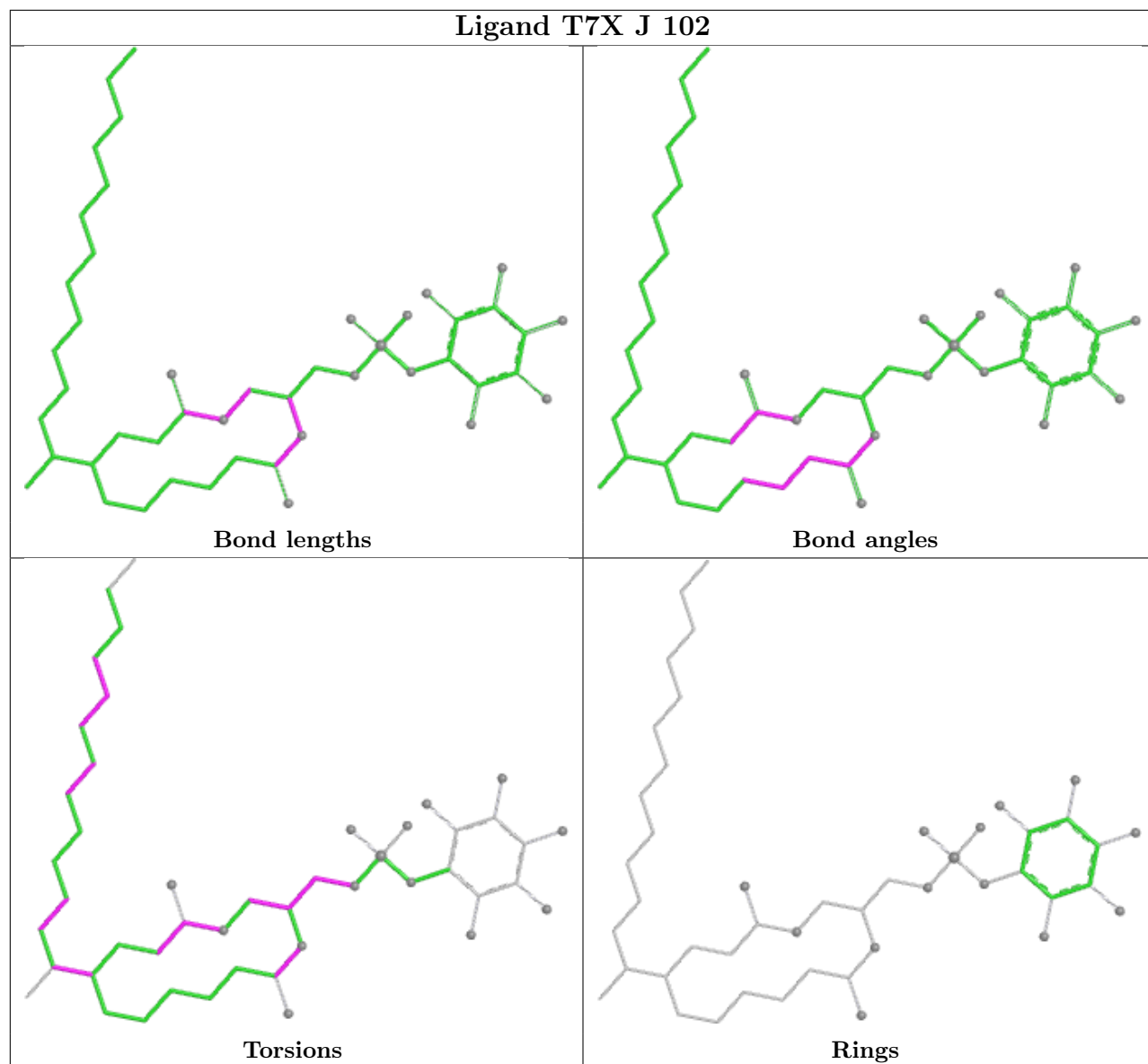


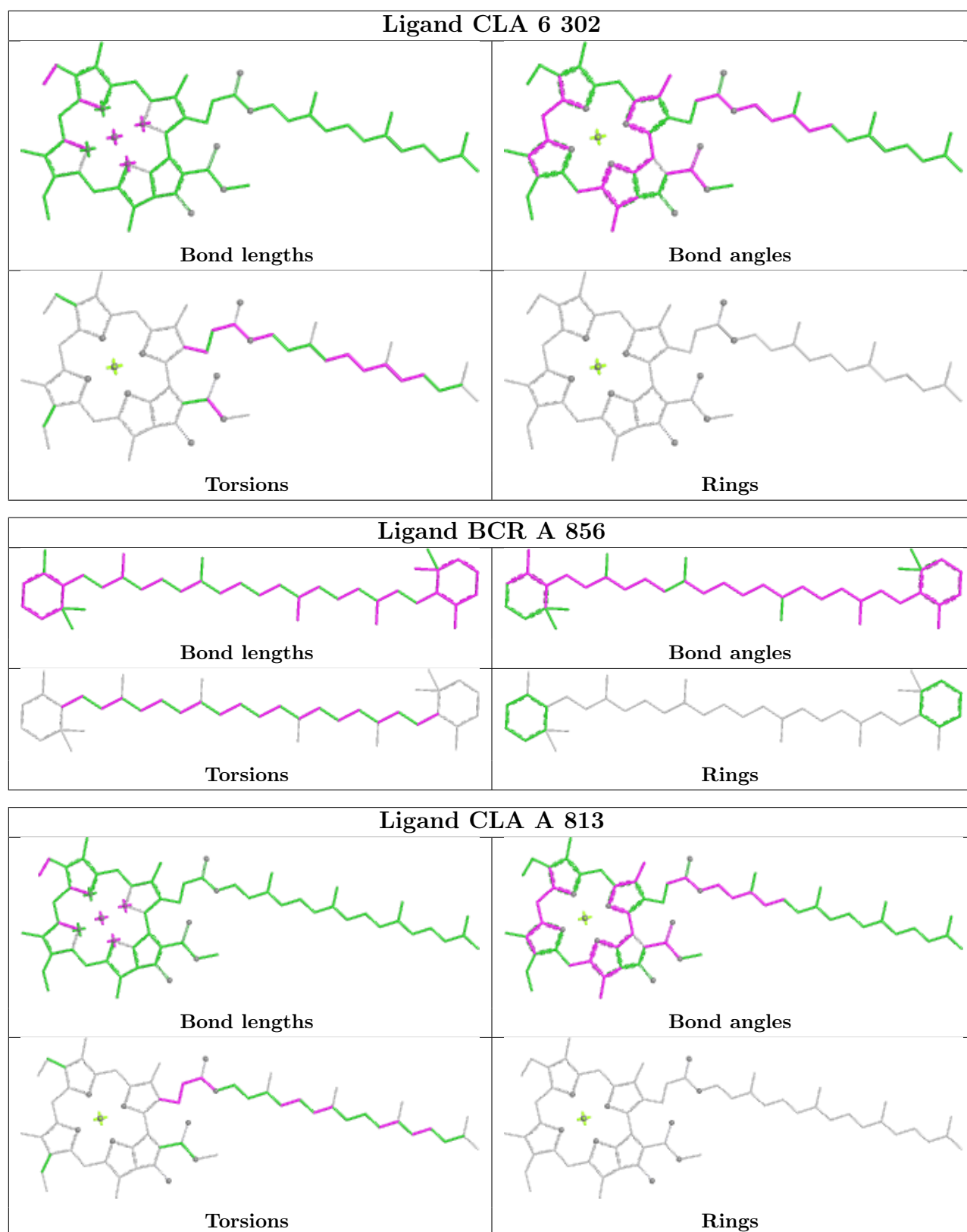
Rings



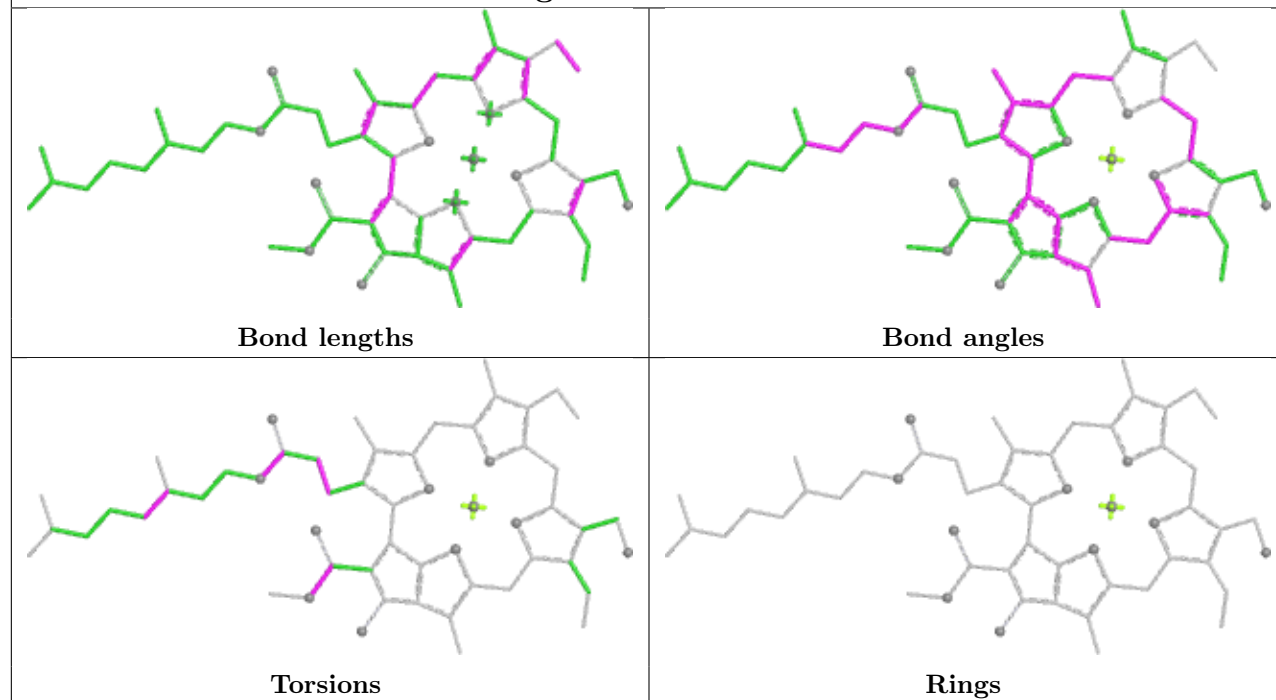


## Ligand T7X J 102

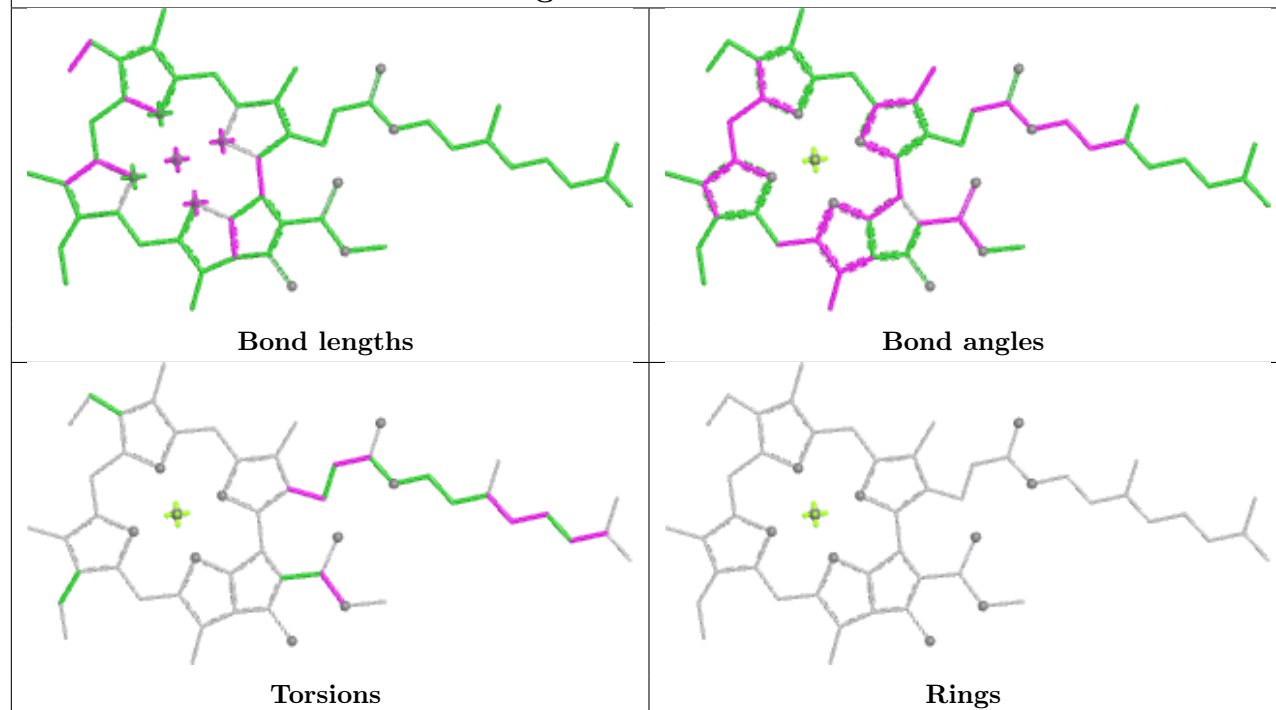




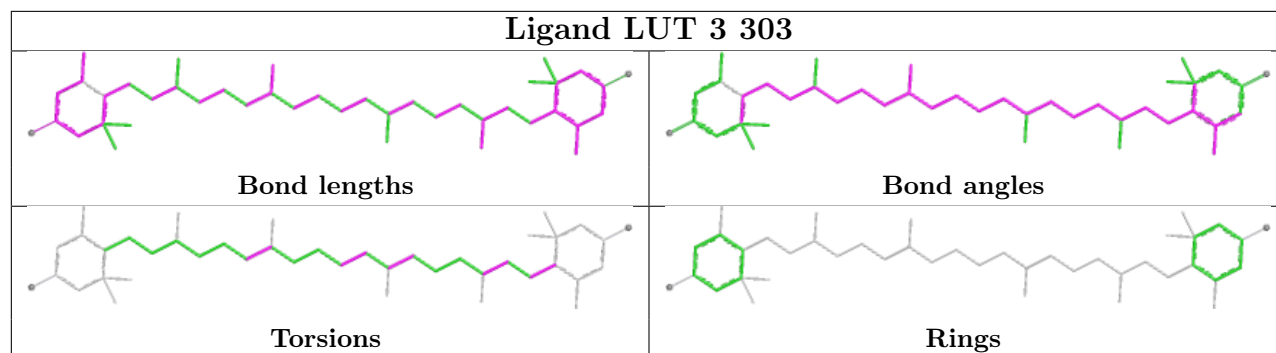
## Ligand CHL 6 318



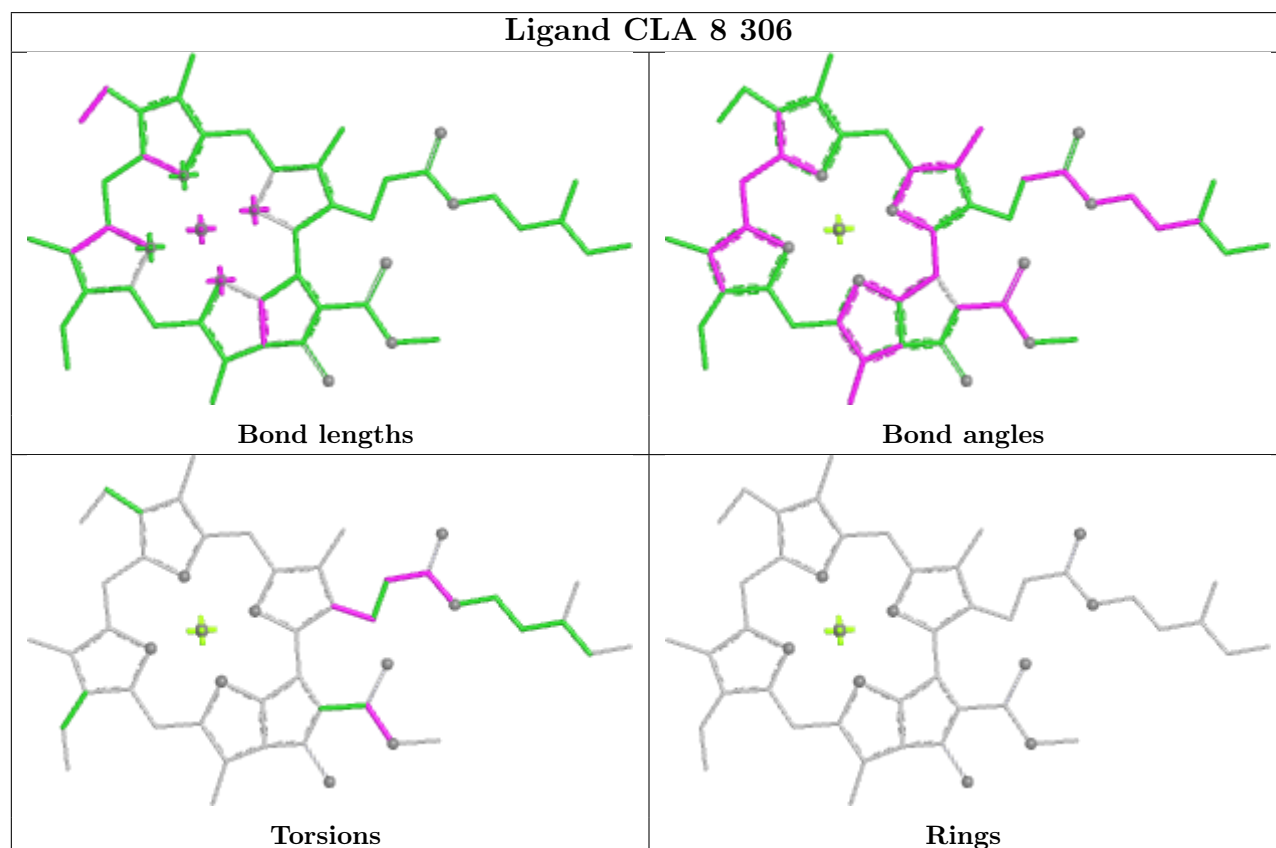
## Ligand CLA 5 311



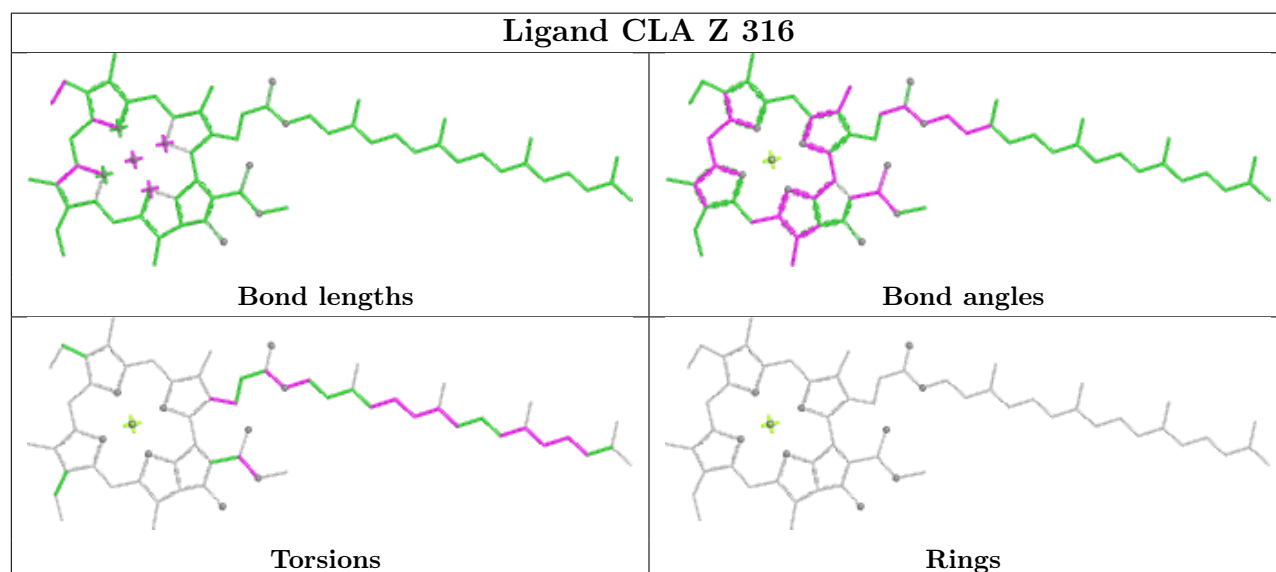
## Ligand LUT 3 303

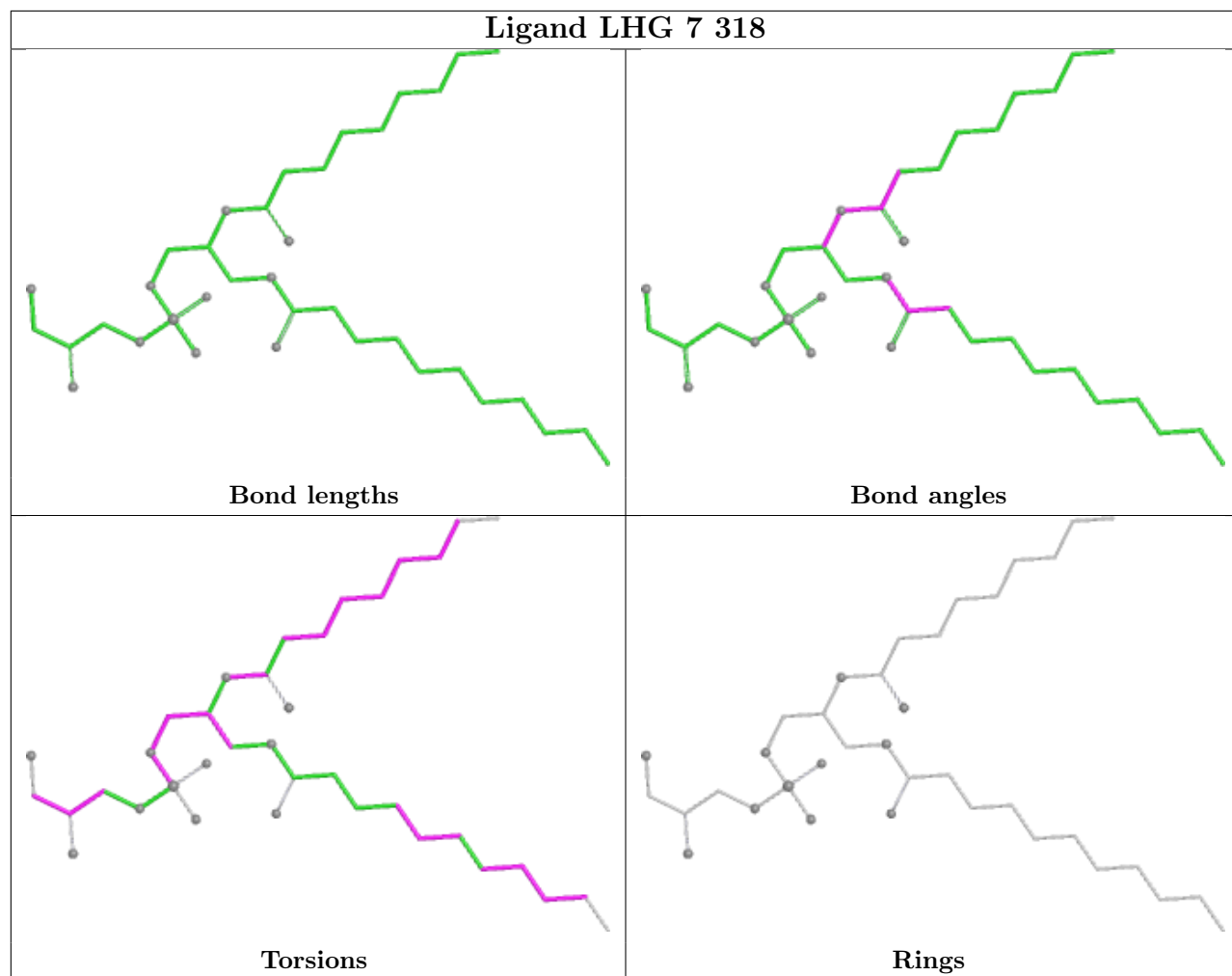


## Ligand CLA 8 306

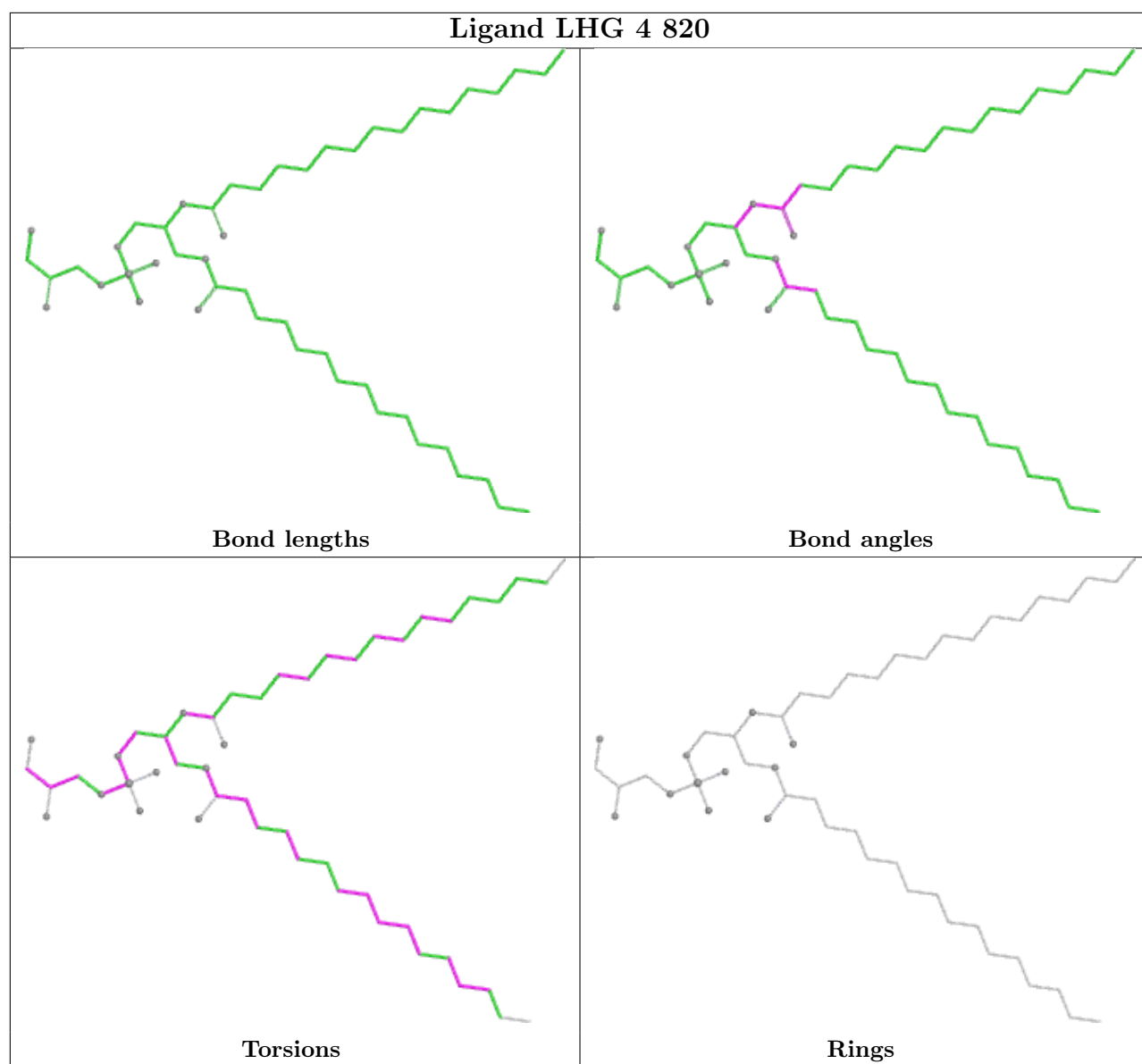


## Ligand CLA Z 316

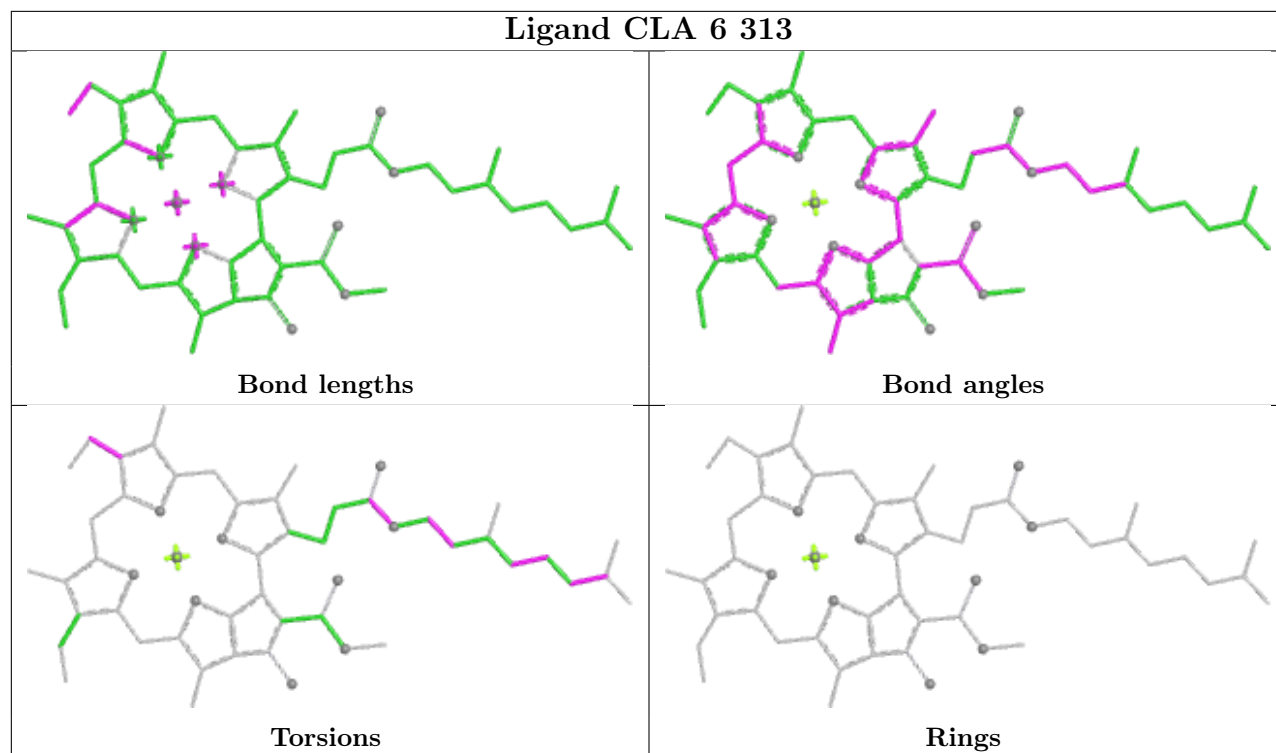




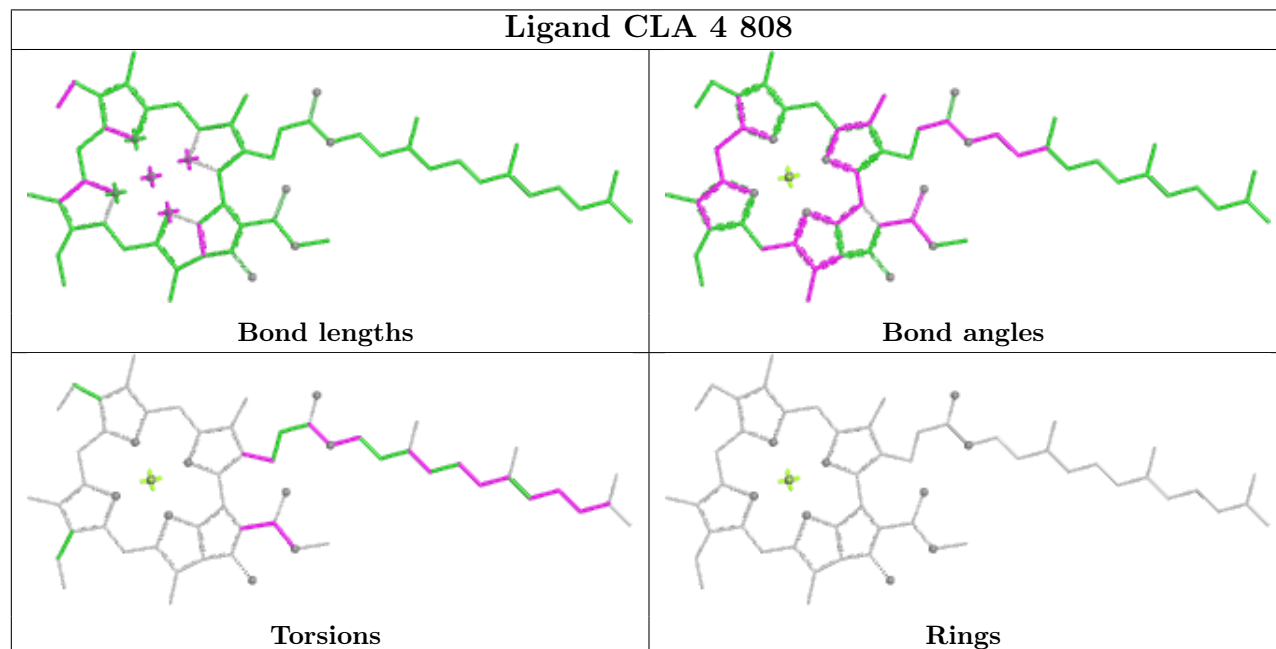




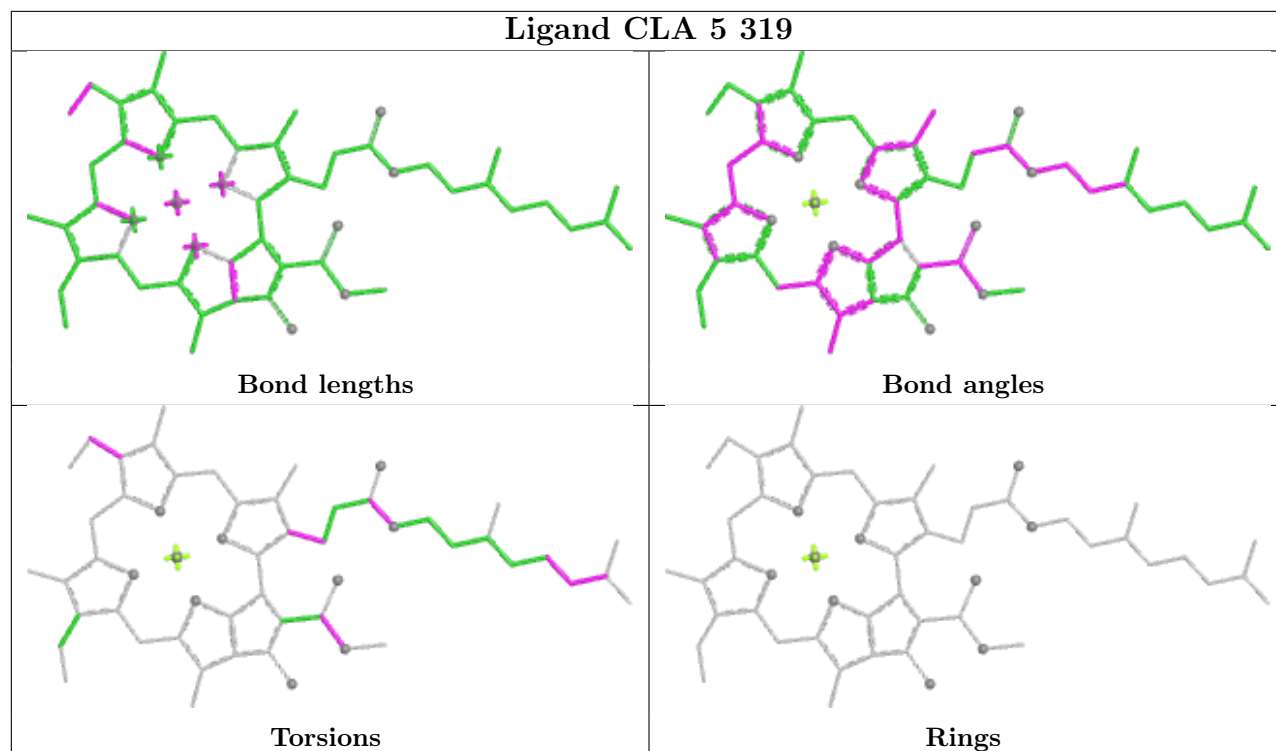
## Ligand CLA 6 313



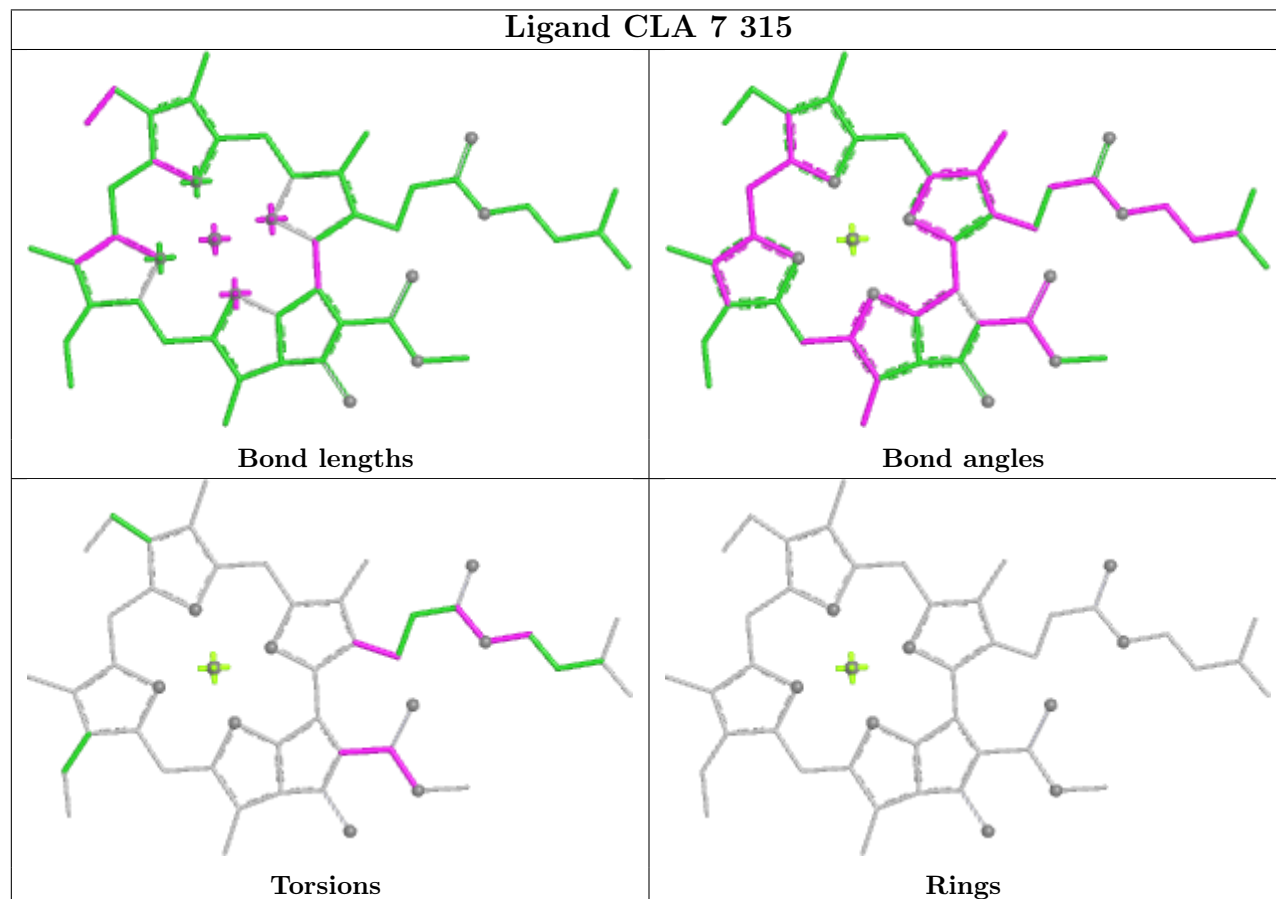
## Ligand CLA 4 808

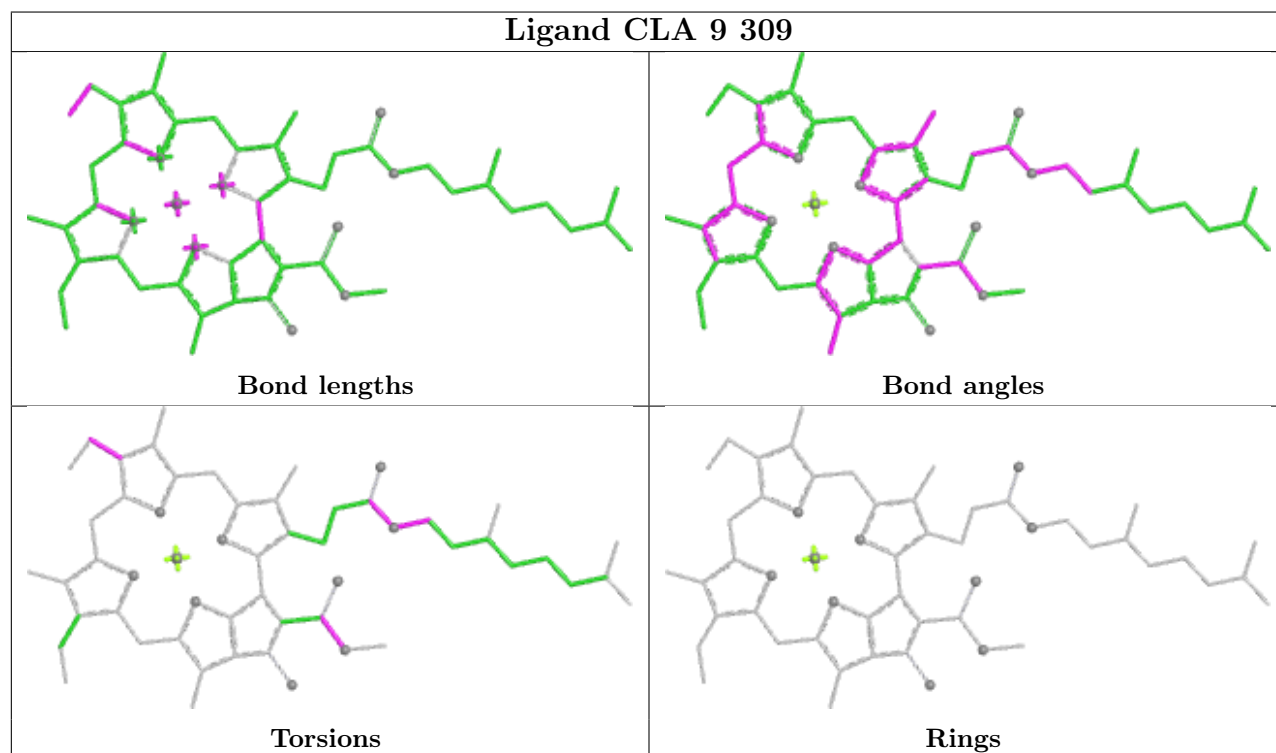
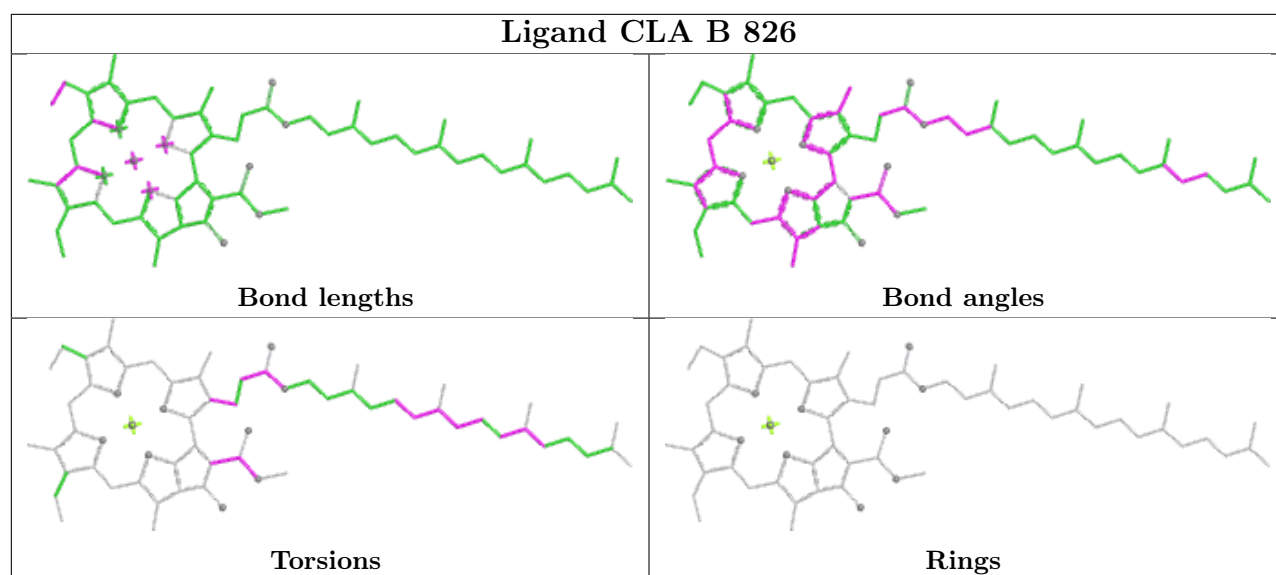


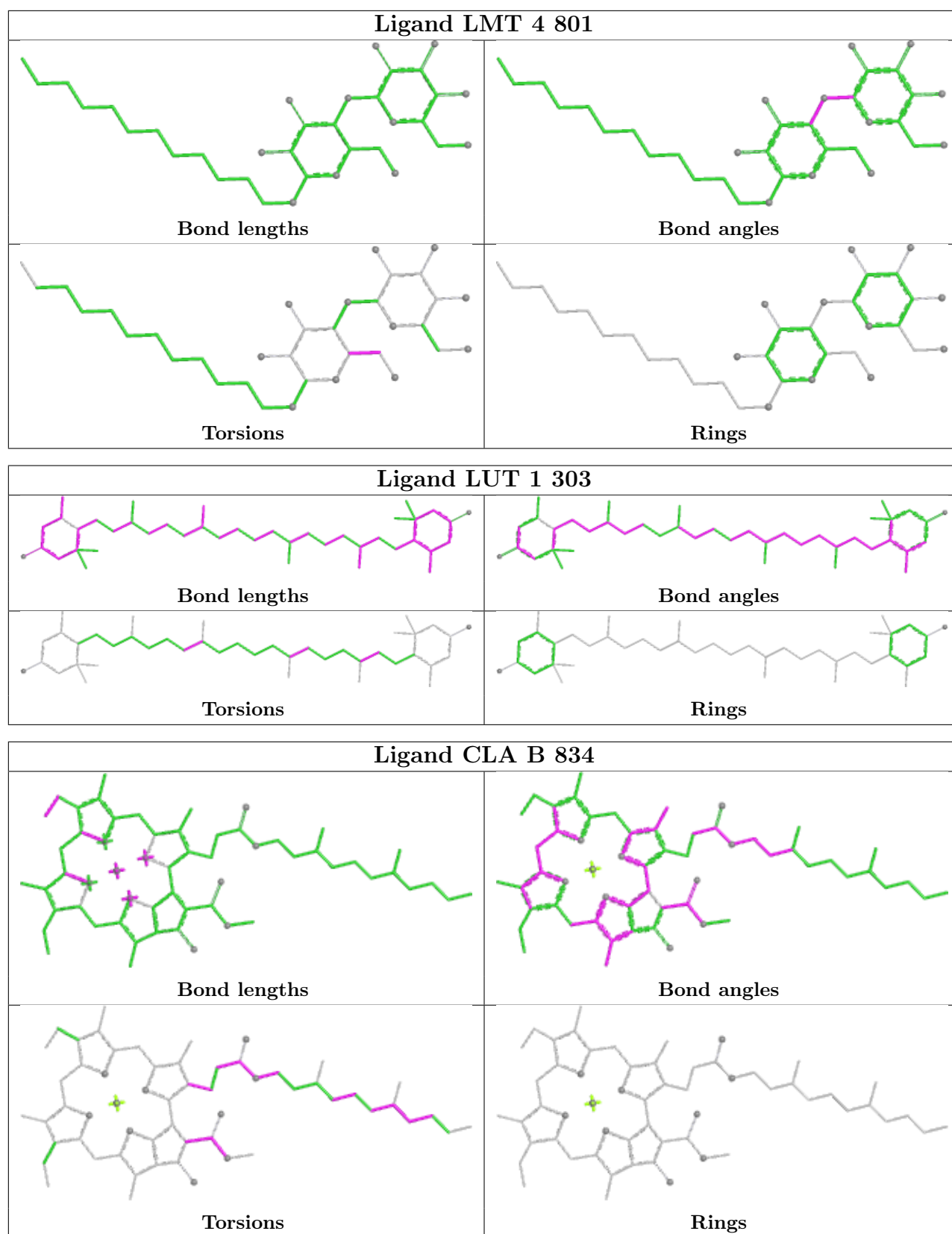
## Ligand CLA 5 319

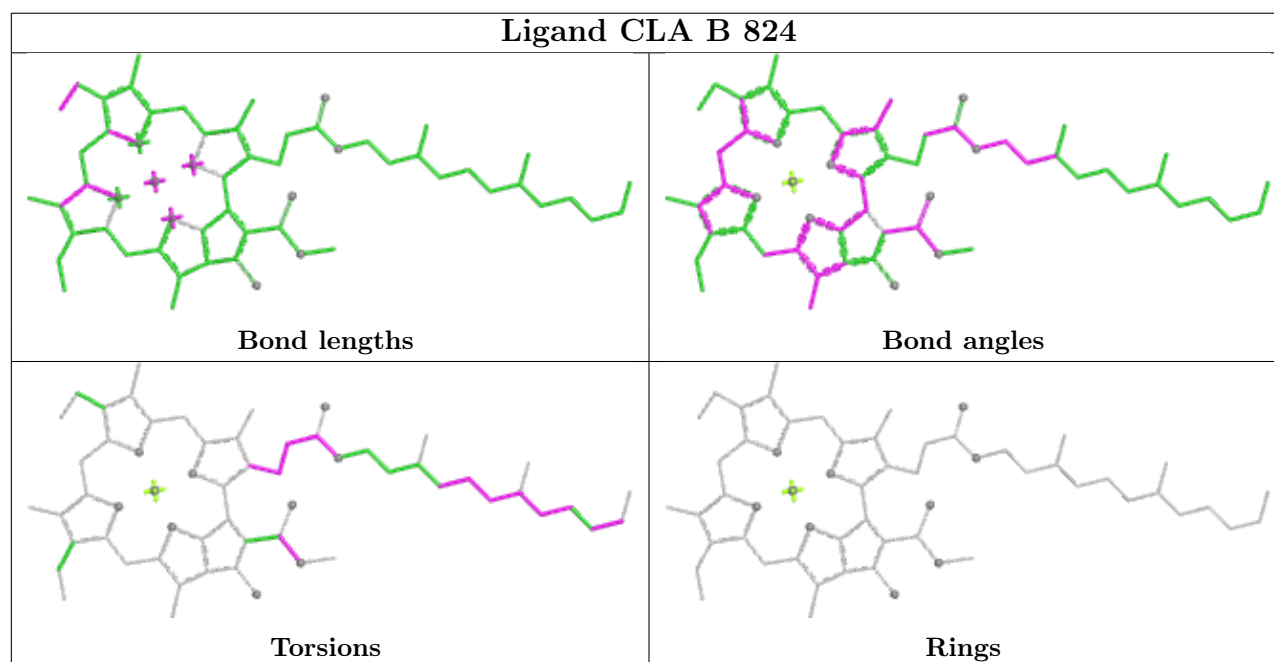
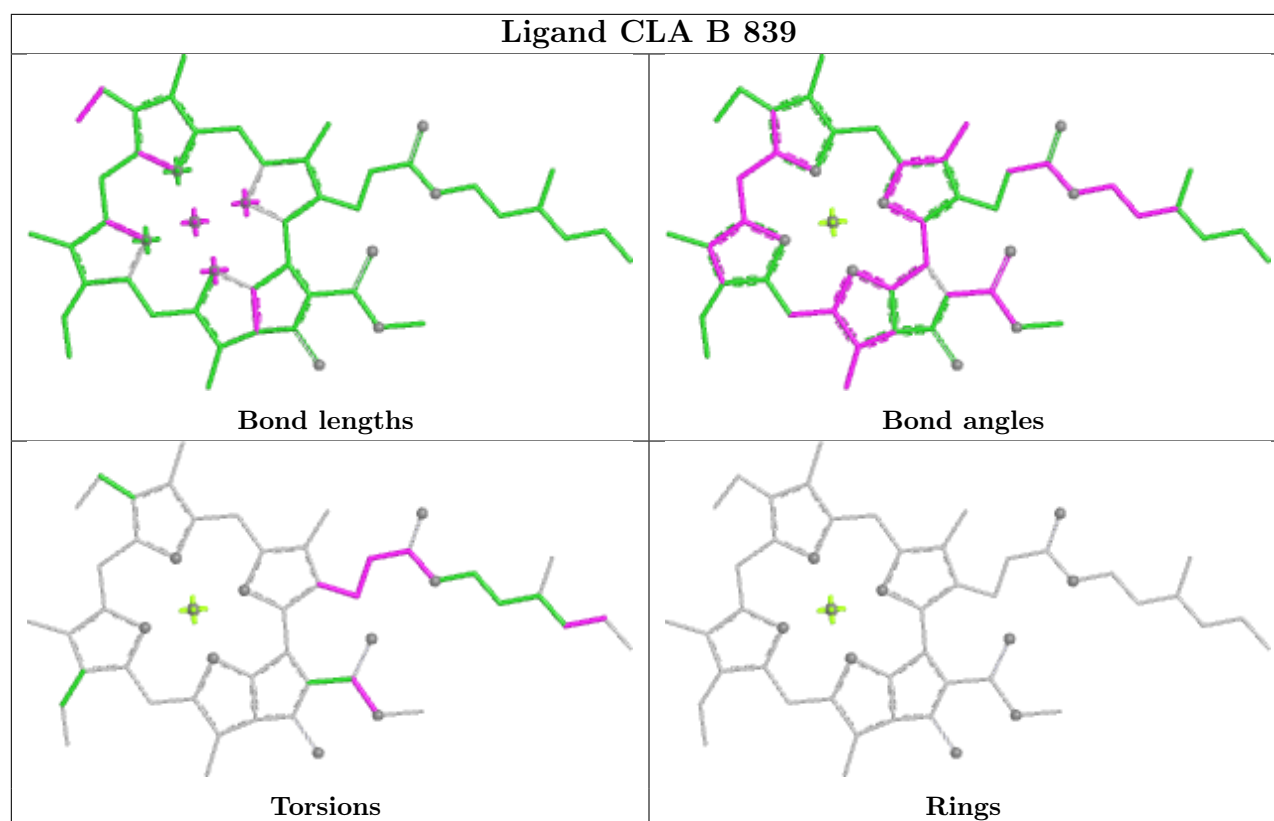


## Ligand CLA 7 315

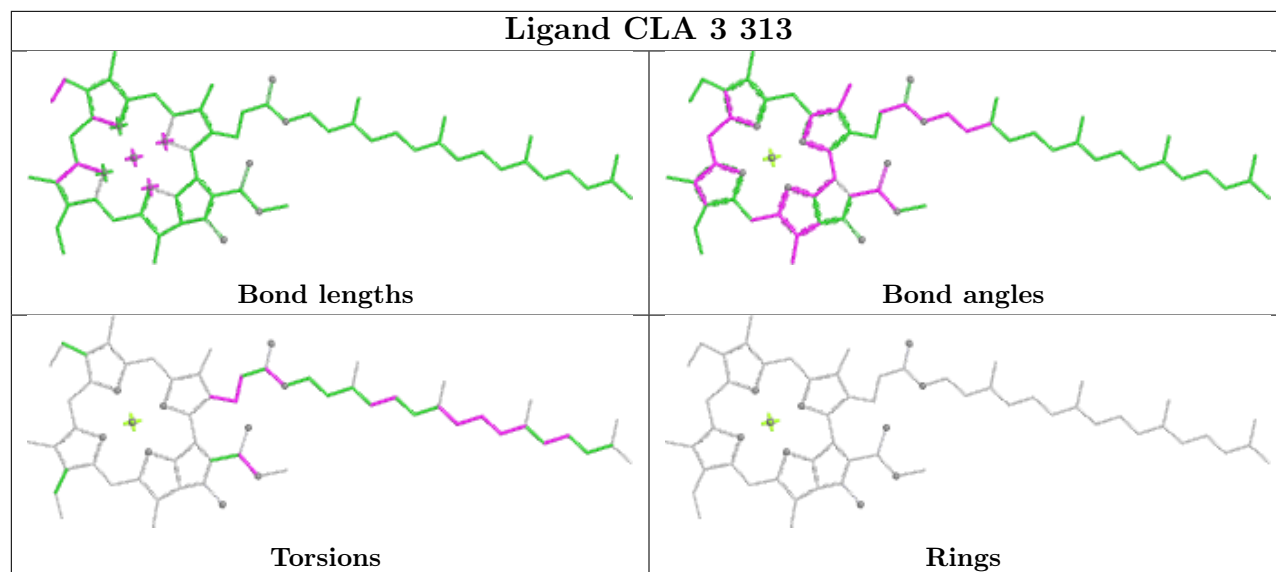




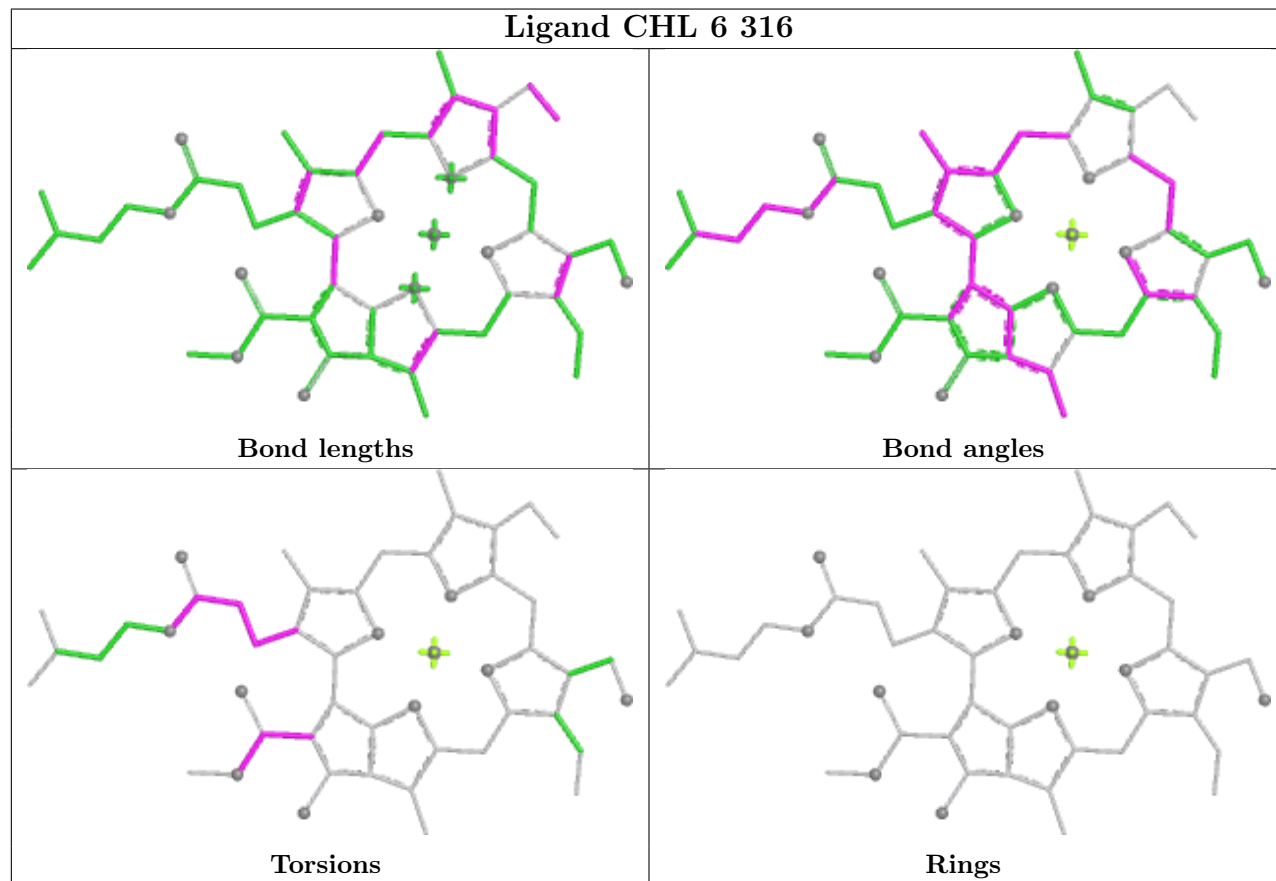


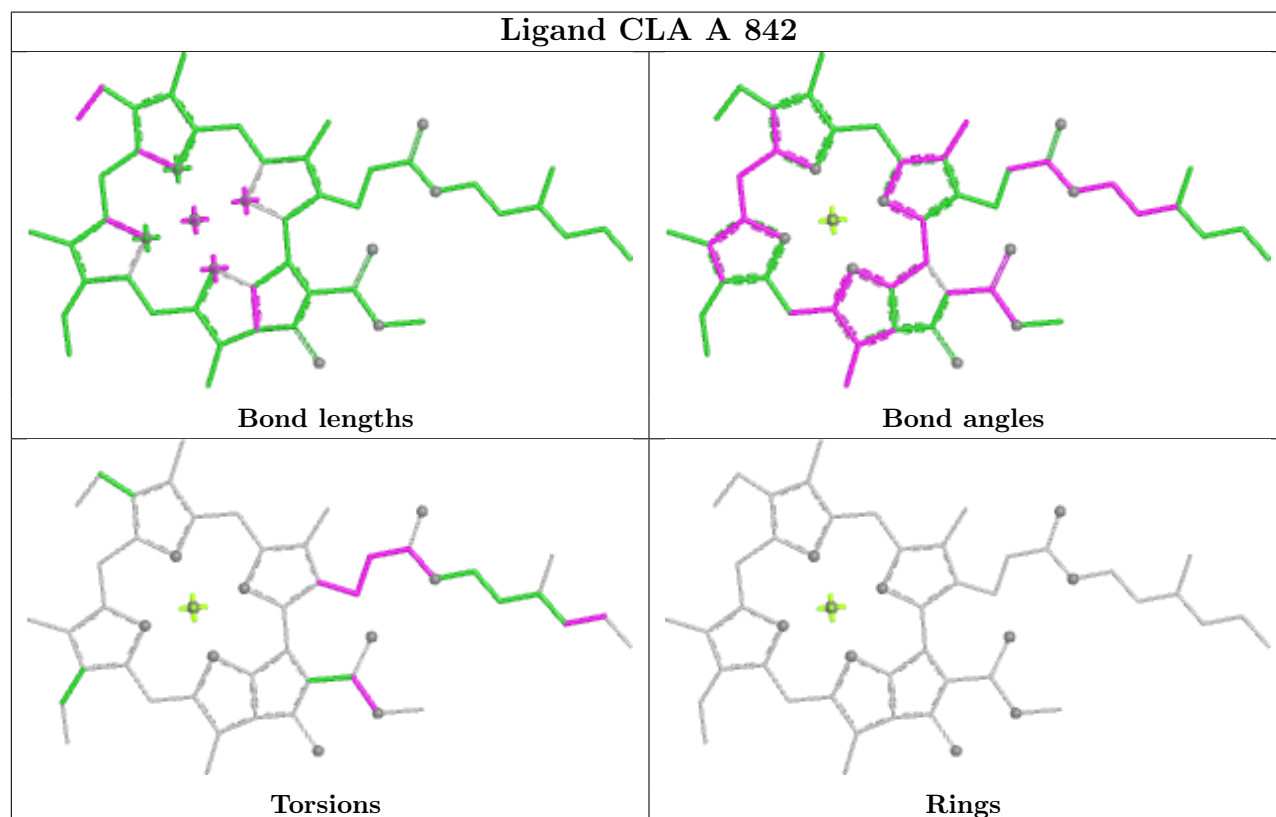
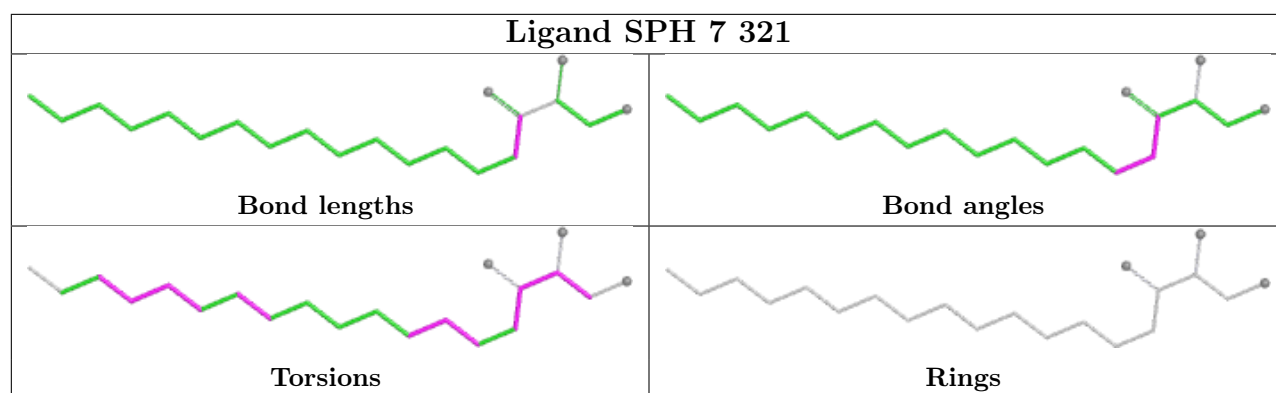


## Ligand CLA 3 313



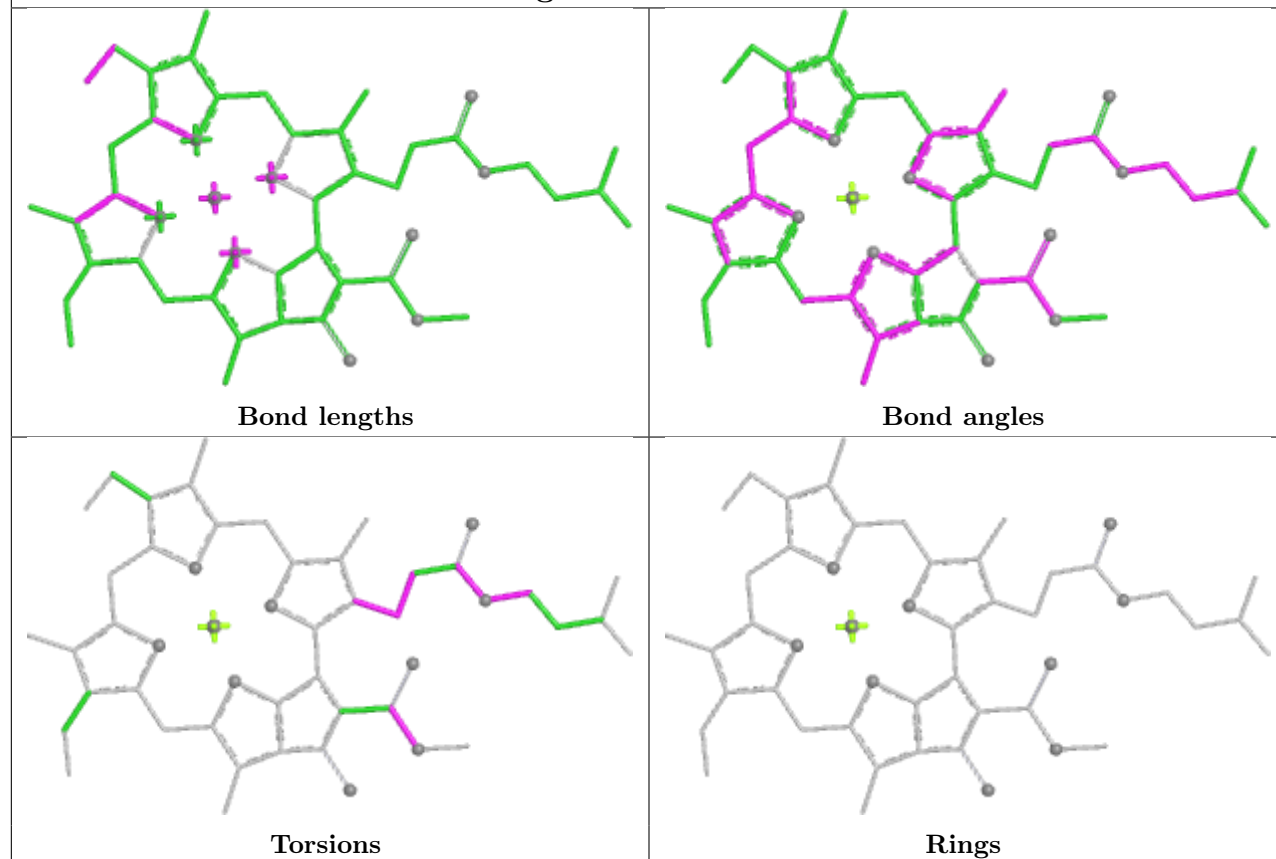
## Ligand CHL 6 316



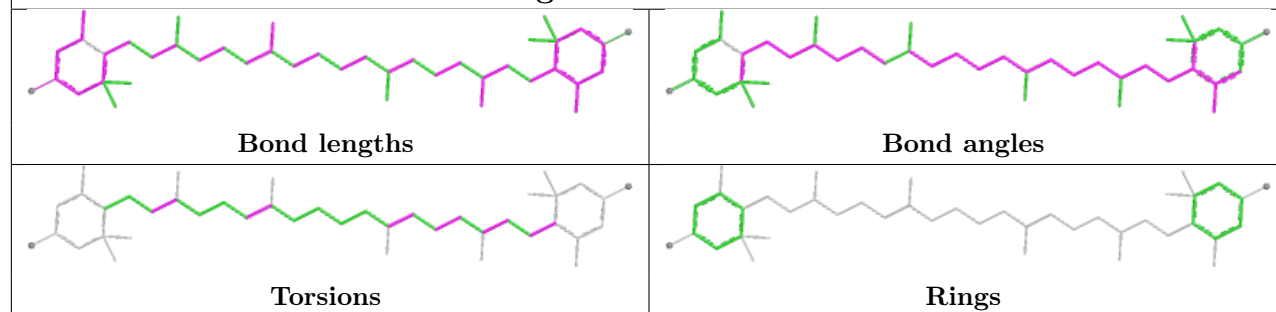


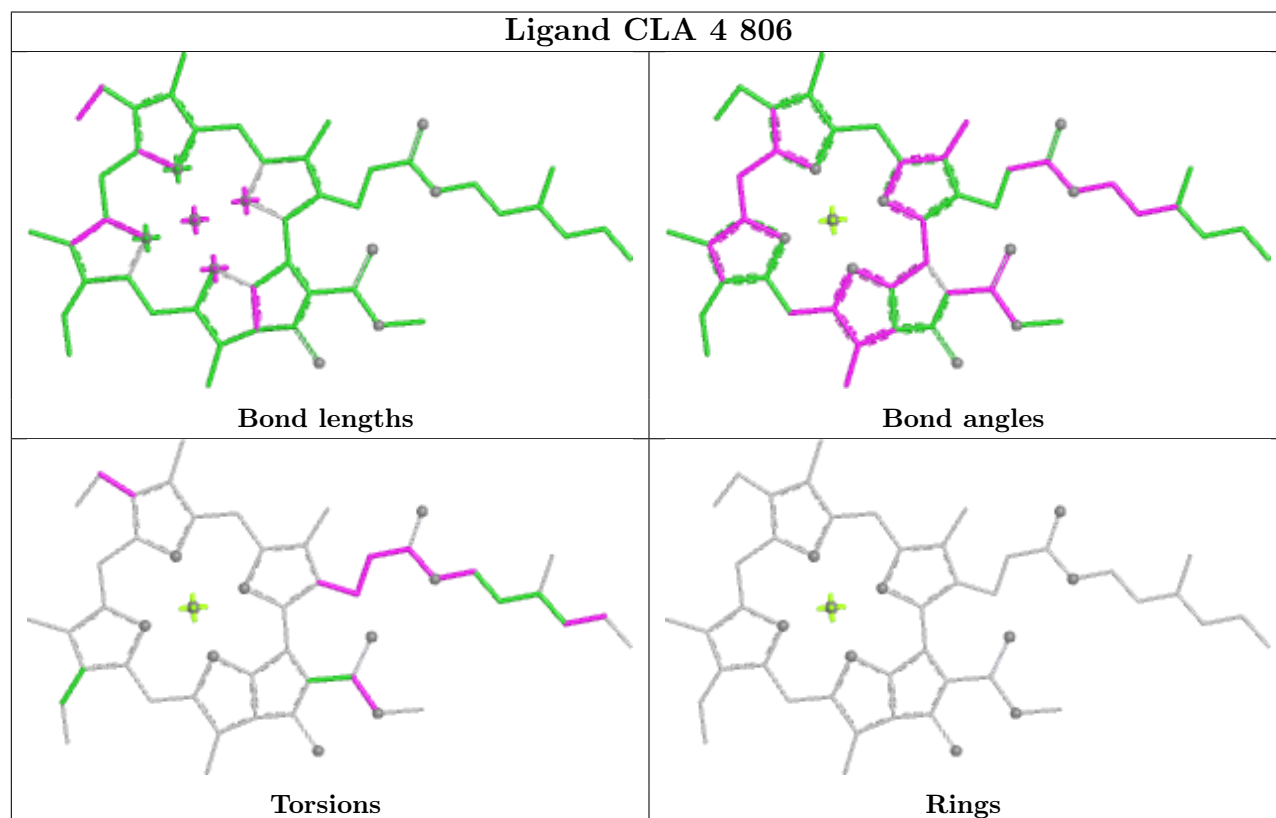
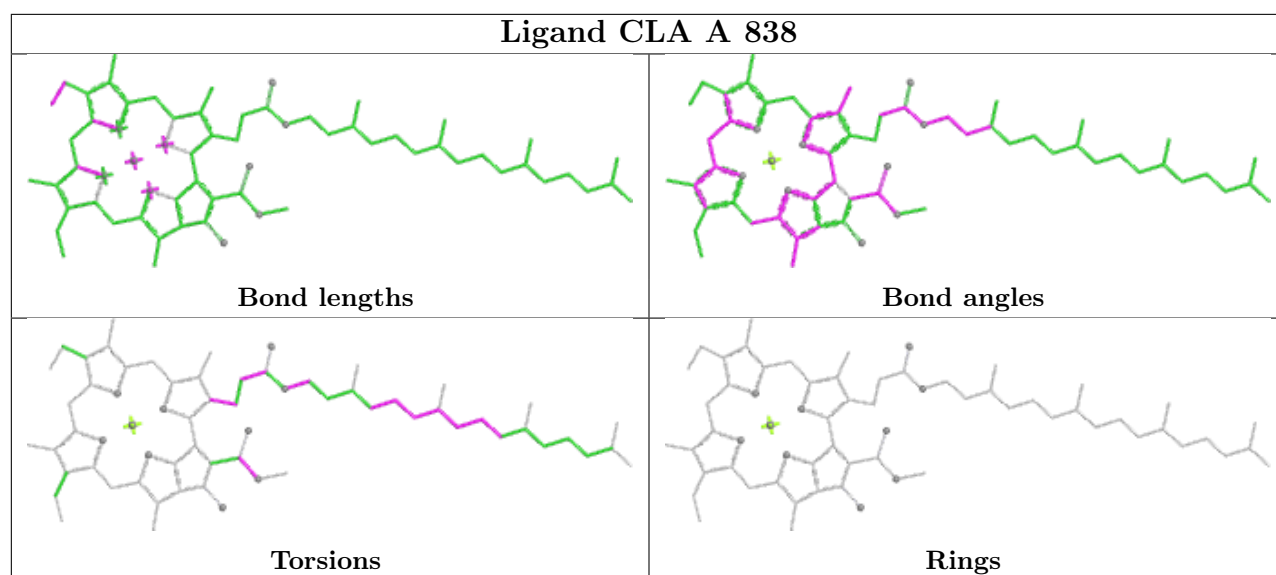


## Ligand CLA 8 311

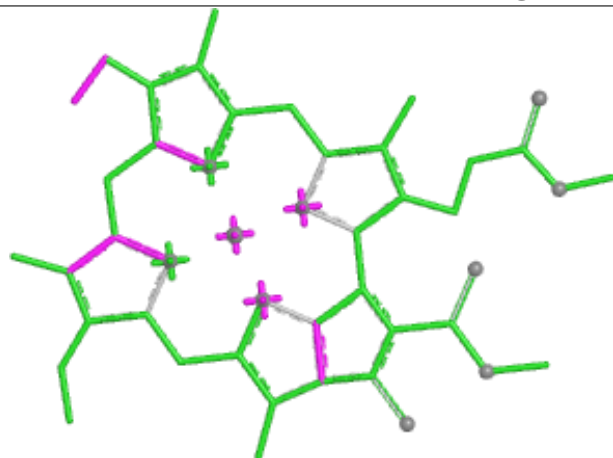


## Ligand LUT 7 301

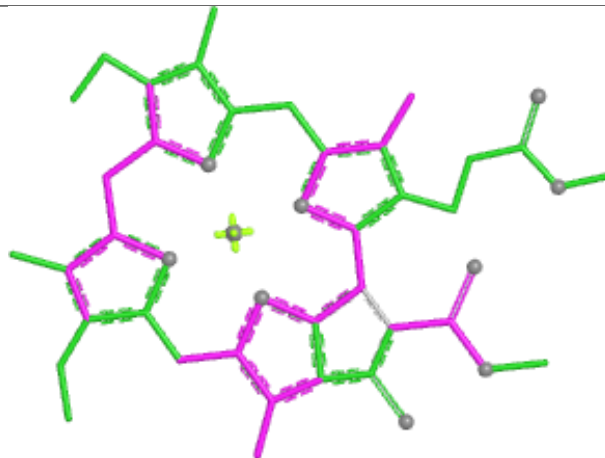




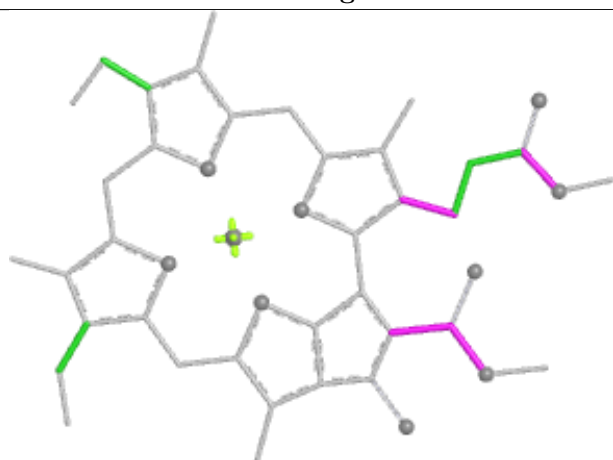
## Ligand CLA G 202



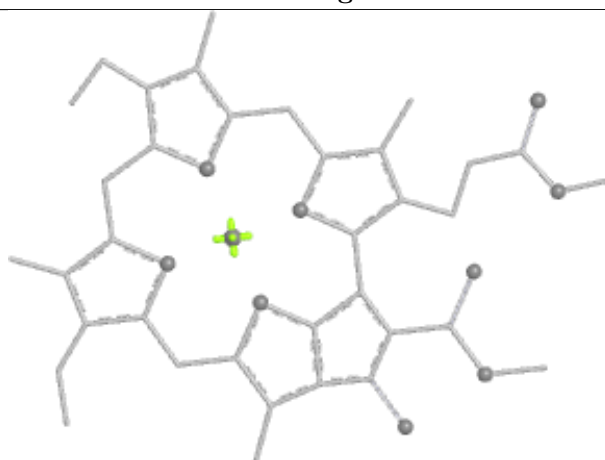
Bond lengths



Bond angles

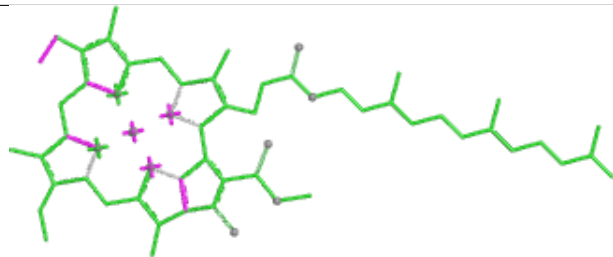


Torsions

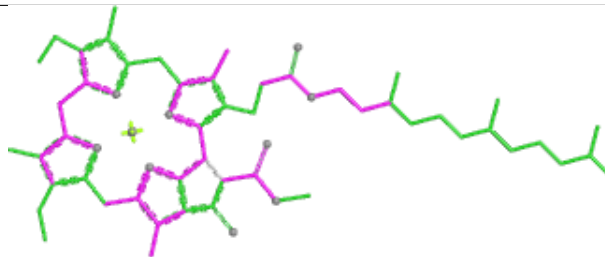


Rings

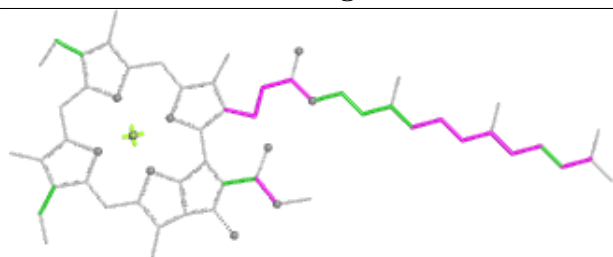
## Ligand CLA B 814



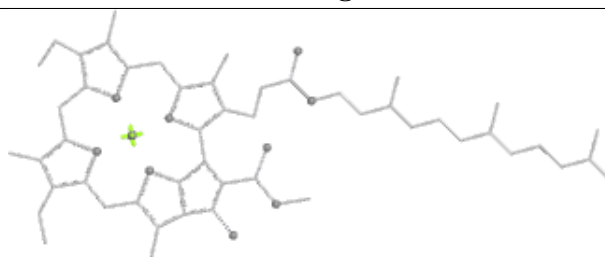
Bond lengths



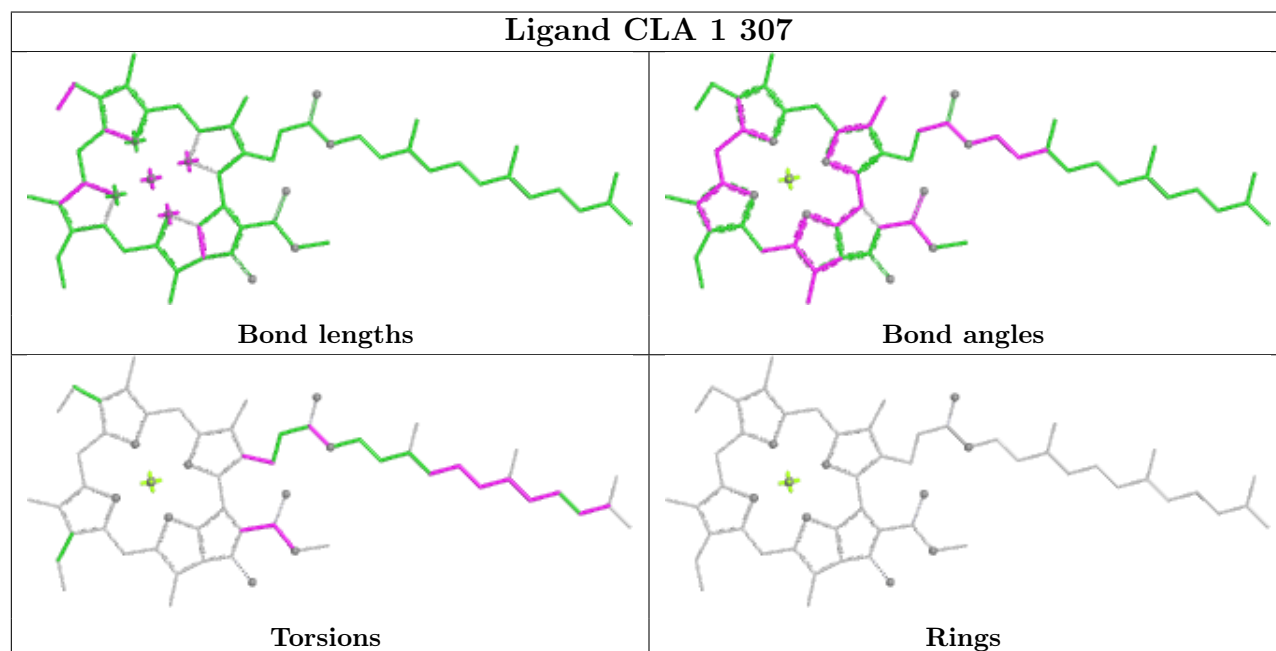
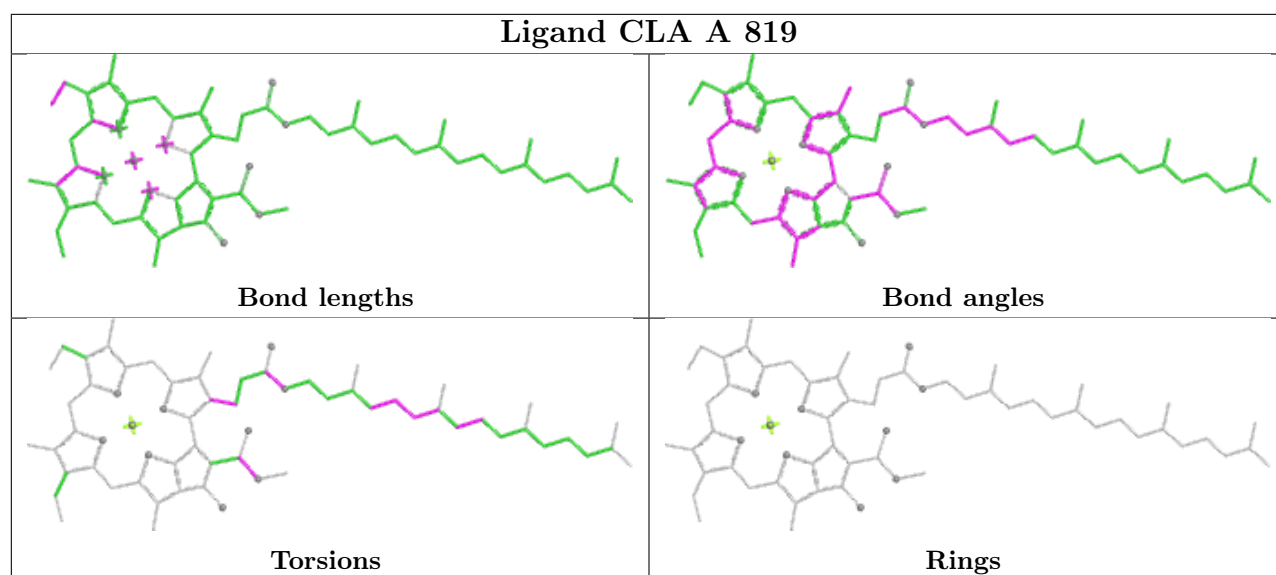
Bond angles

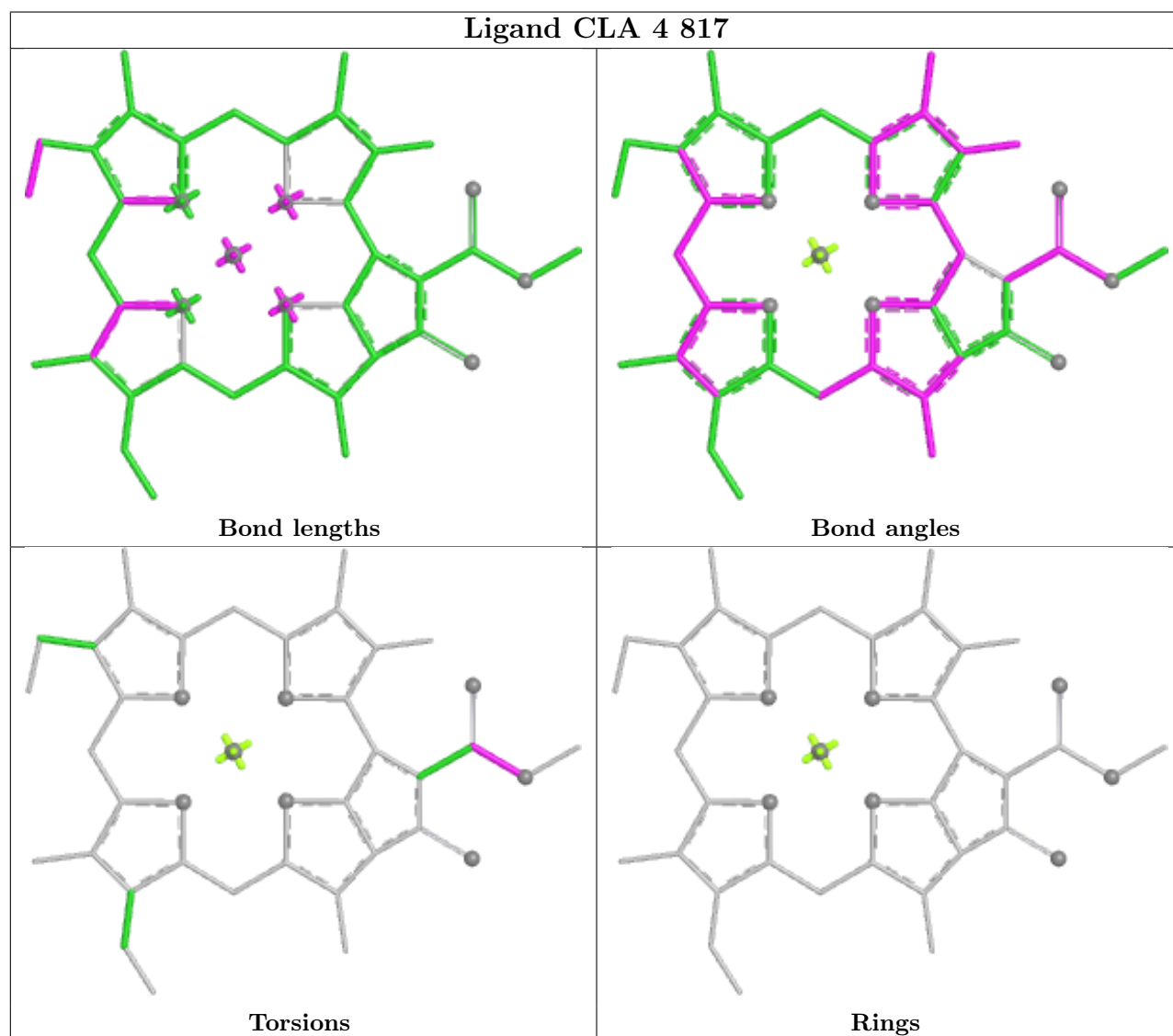
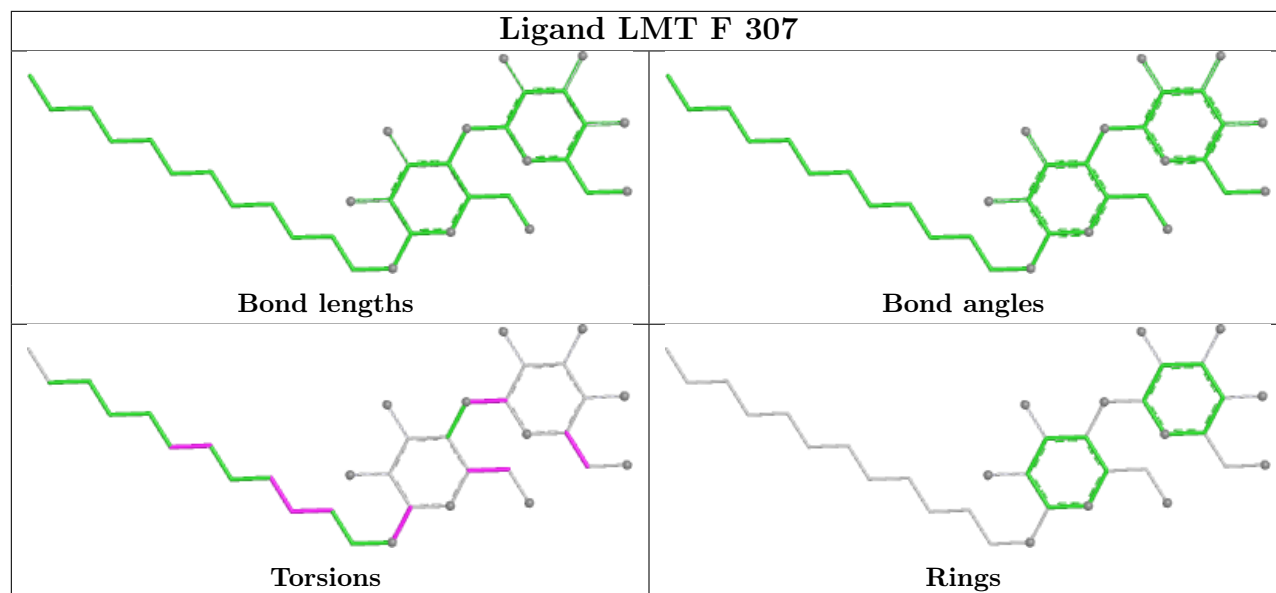


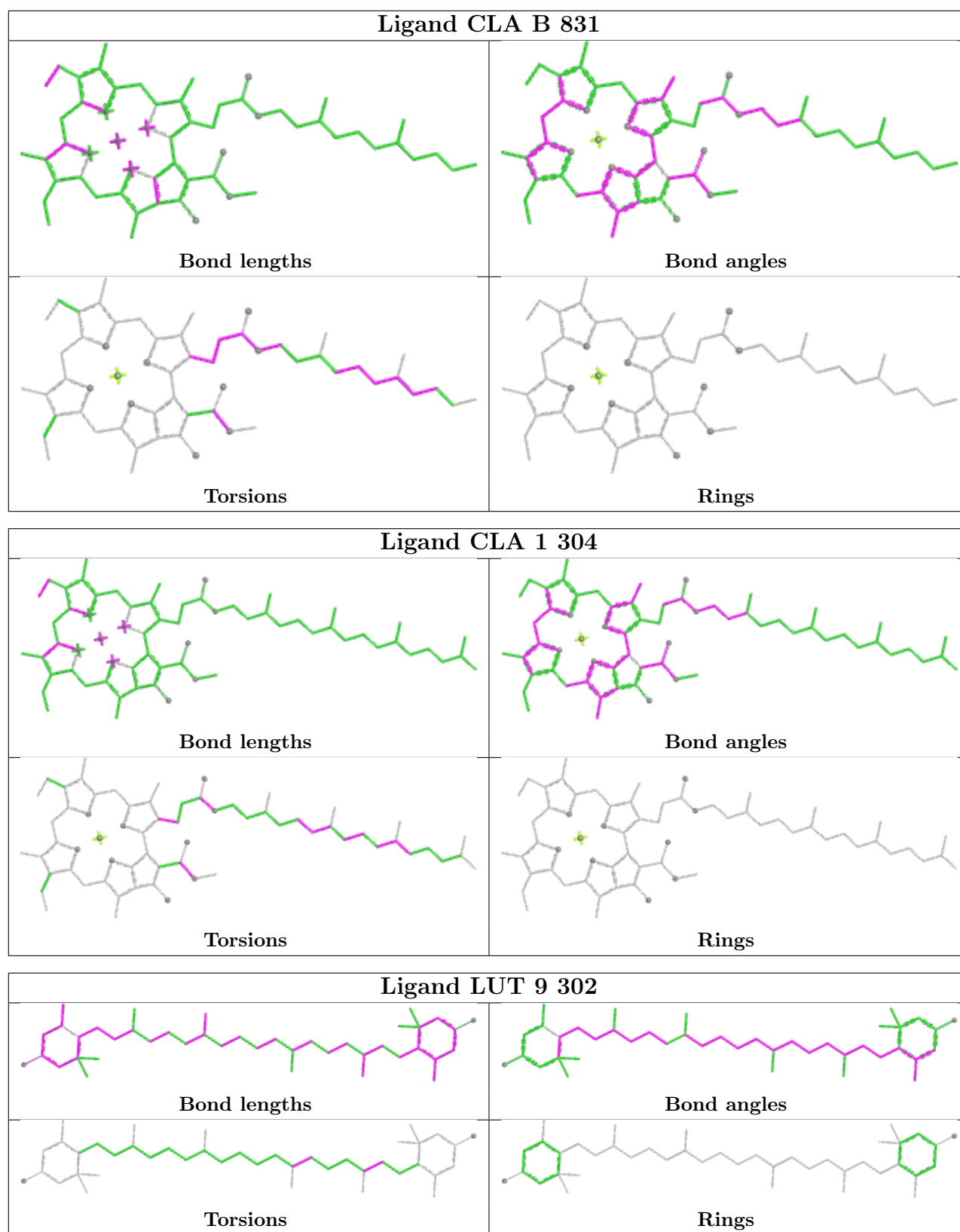
Torsions



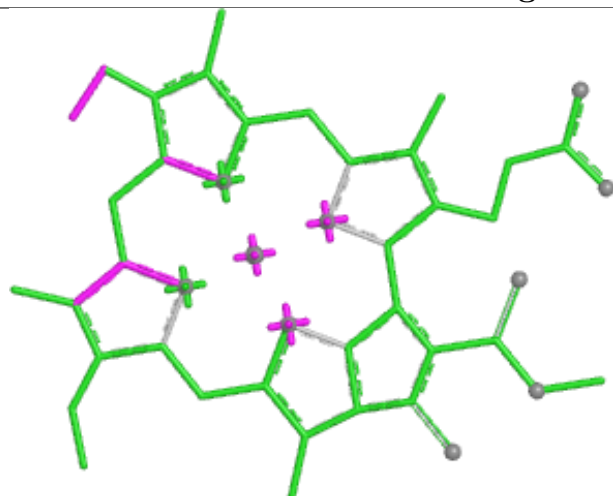
Rings



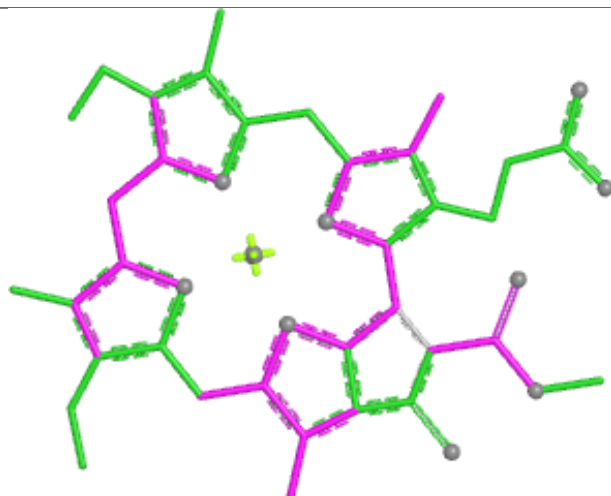




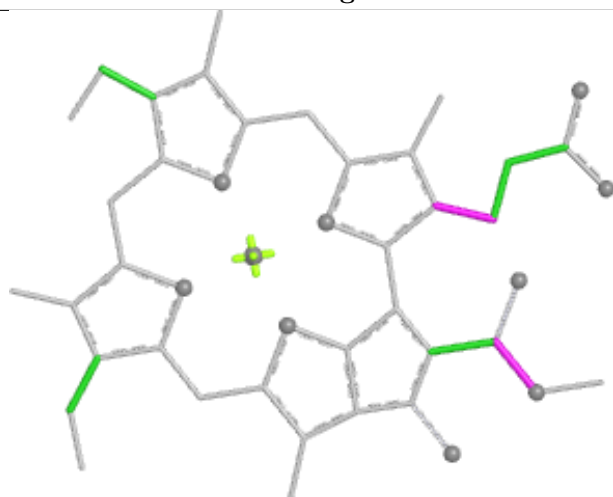
## Ligand CLA 5 314



Bond lengths



Bond angles

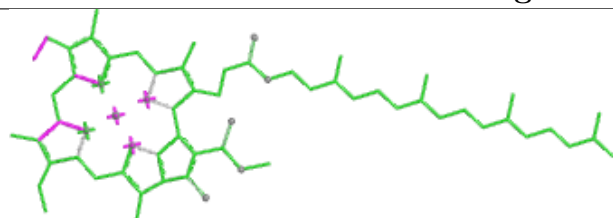


Torsions

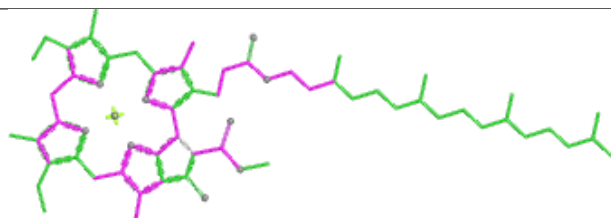


Rings

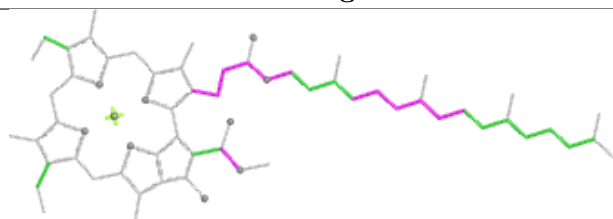
## Ligand CLA B 825



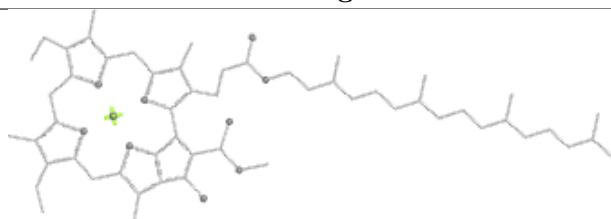
Bond lengths



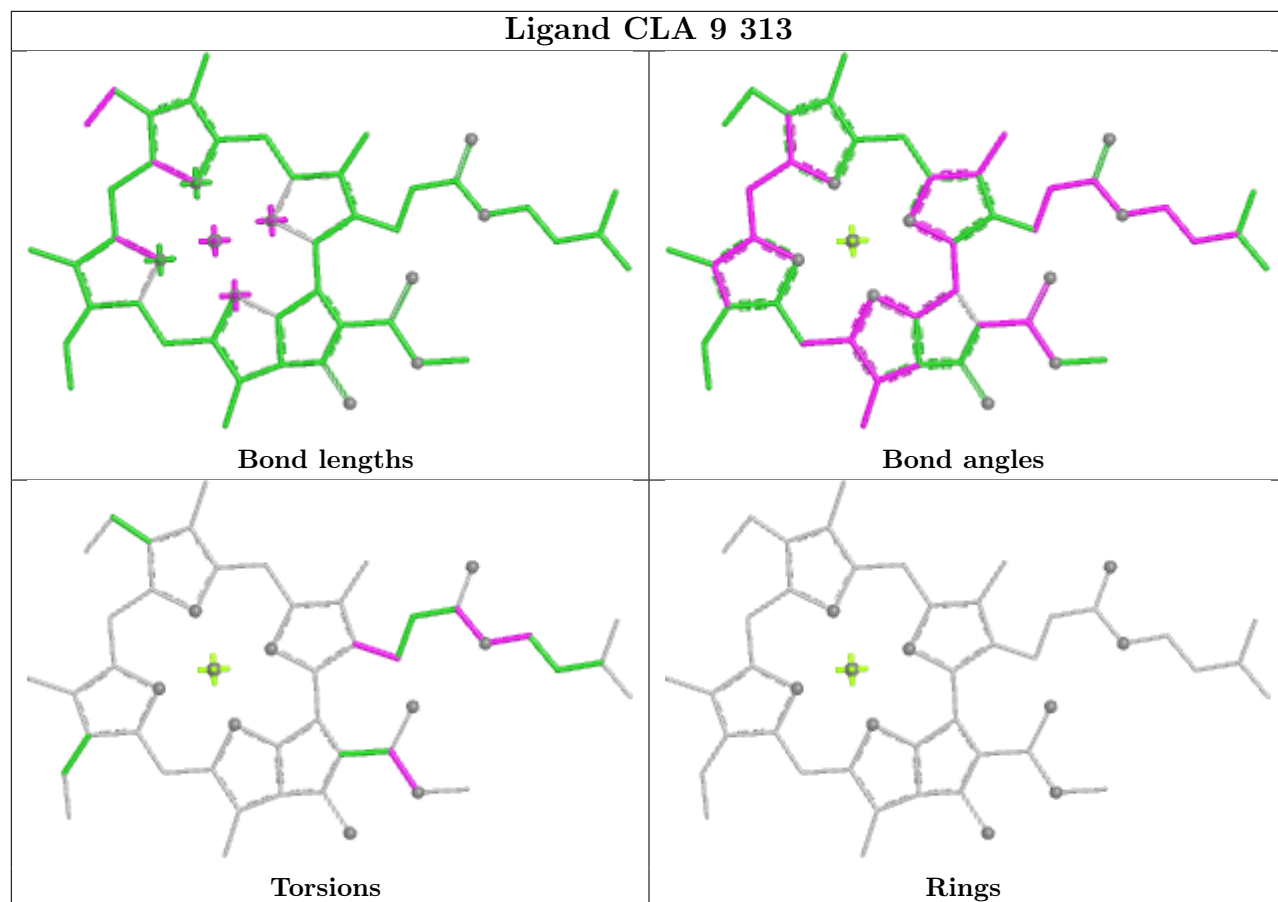
Bond angles



Torsions

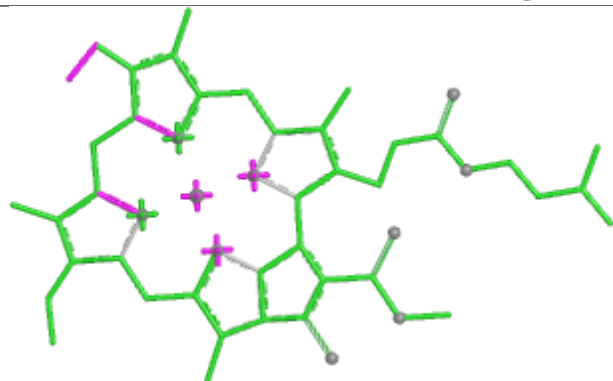


Rings

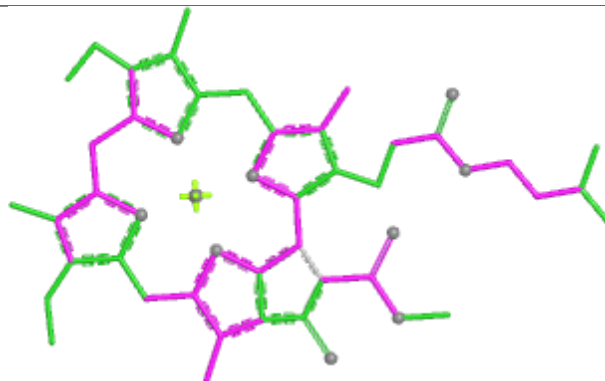




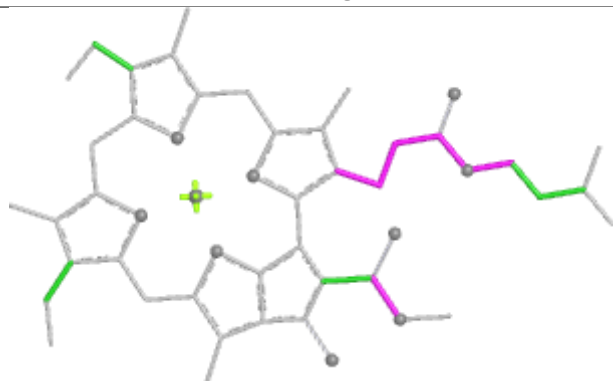
## Ligand CLA 9 308



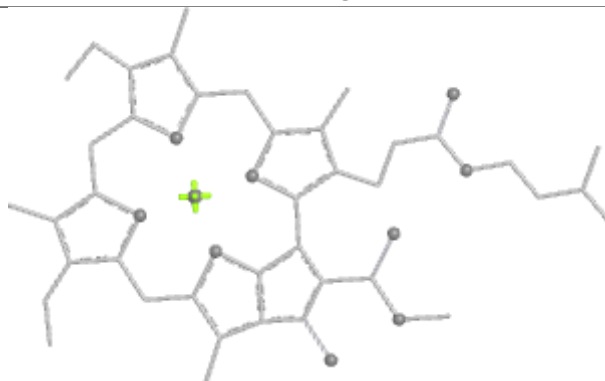
Bond lengths



Bond angles

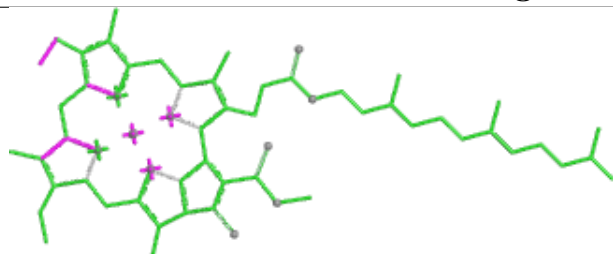


Torsions

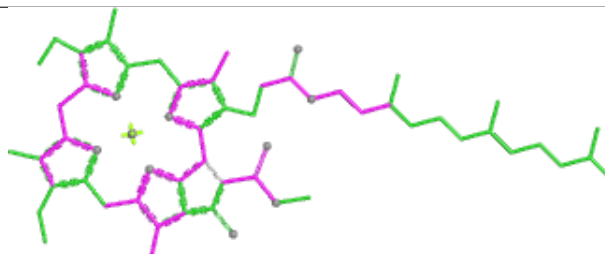


Rings

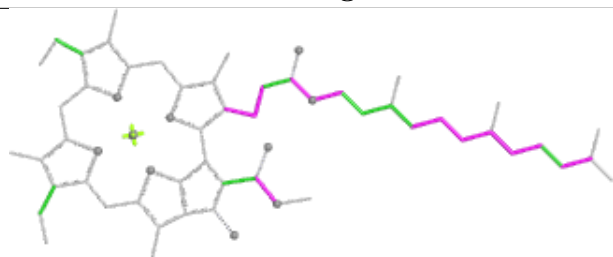
## Ligand CLA B 820



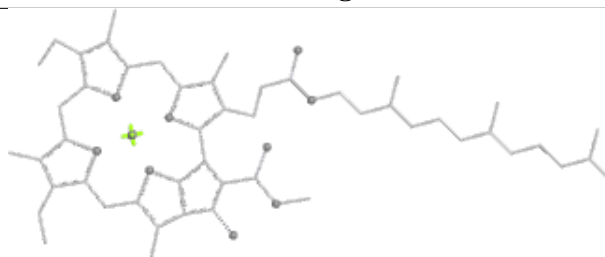
Bond lengths



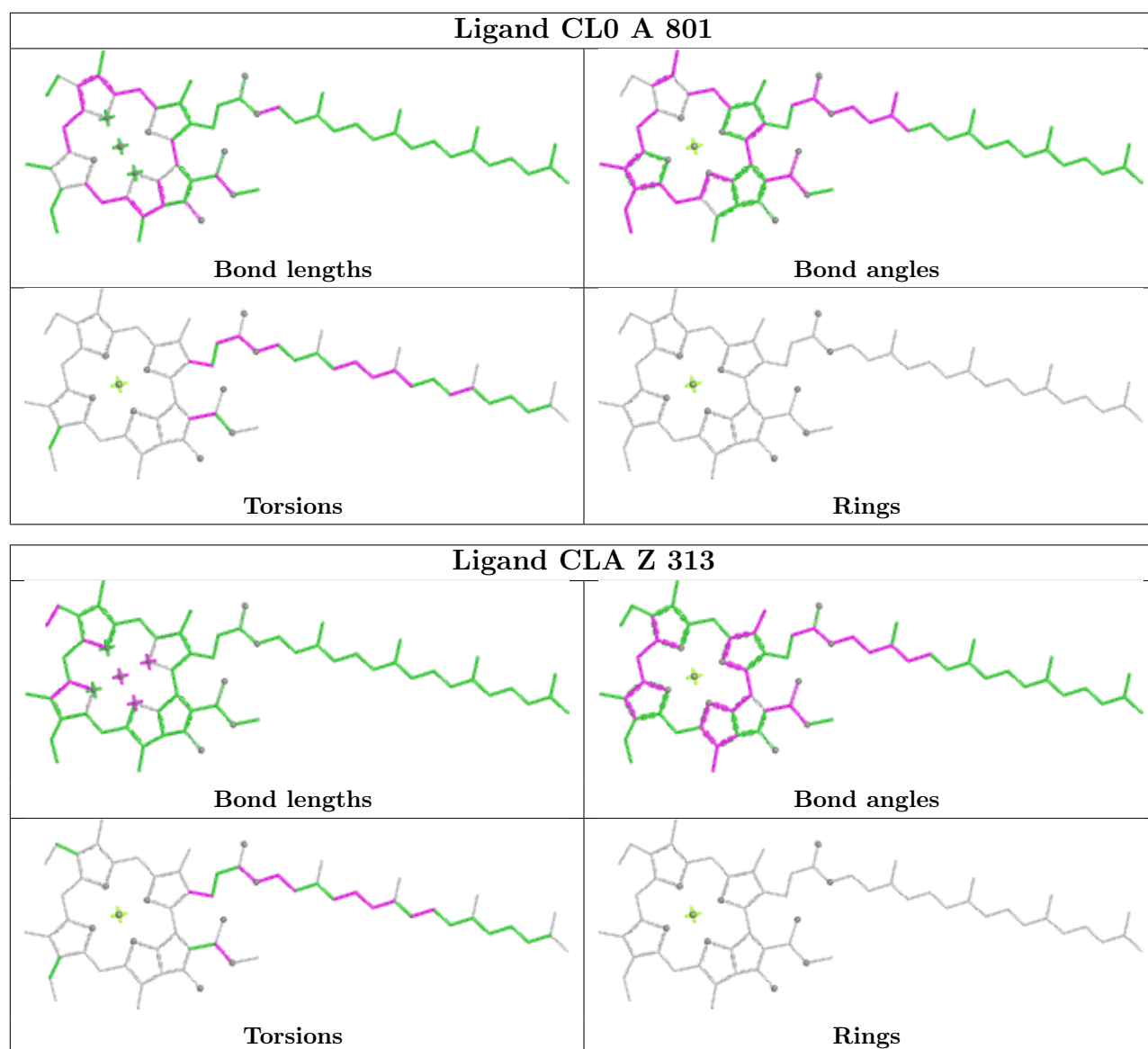
Bond angles



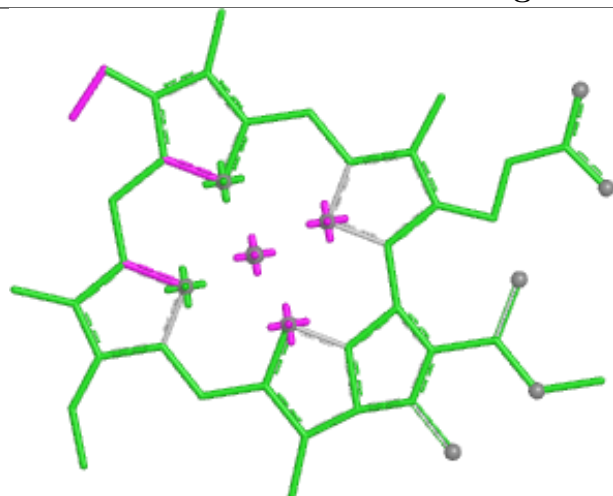
Torsions



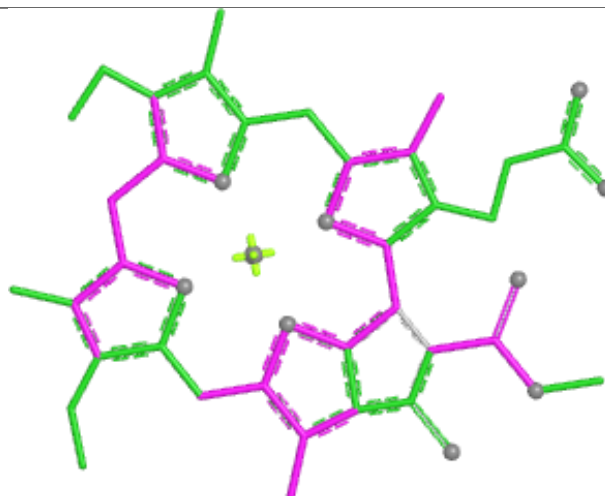
Rings



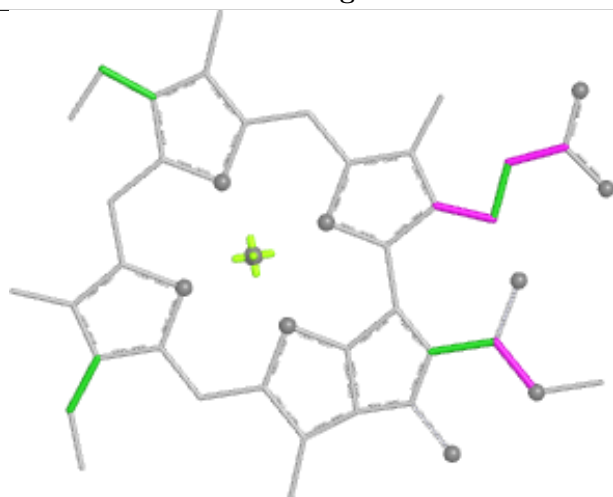
## Ligand CLA A 804



Bond lengths



Bond angles

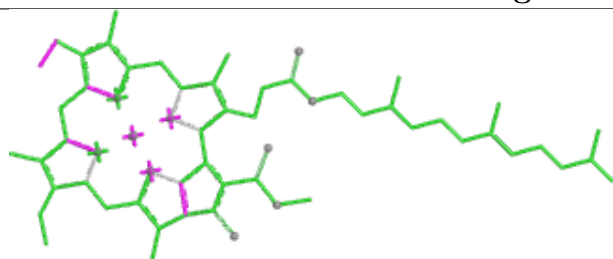


Torsions

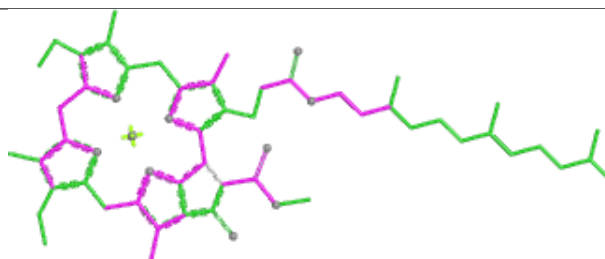


Rings

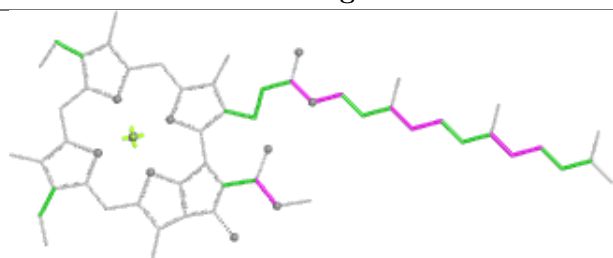
## Ligand CLA A 817



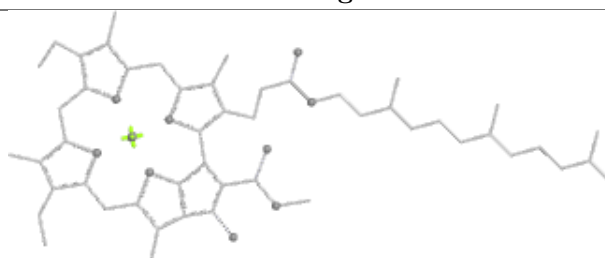
Bond lengths



Bond angles

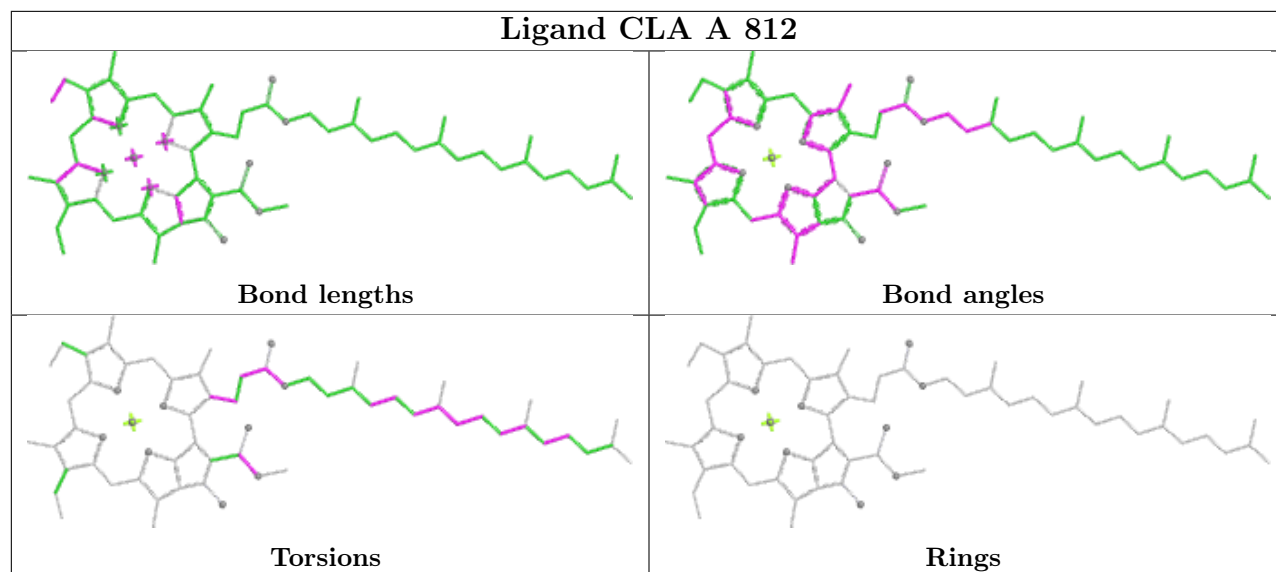


Torsions

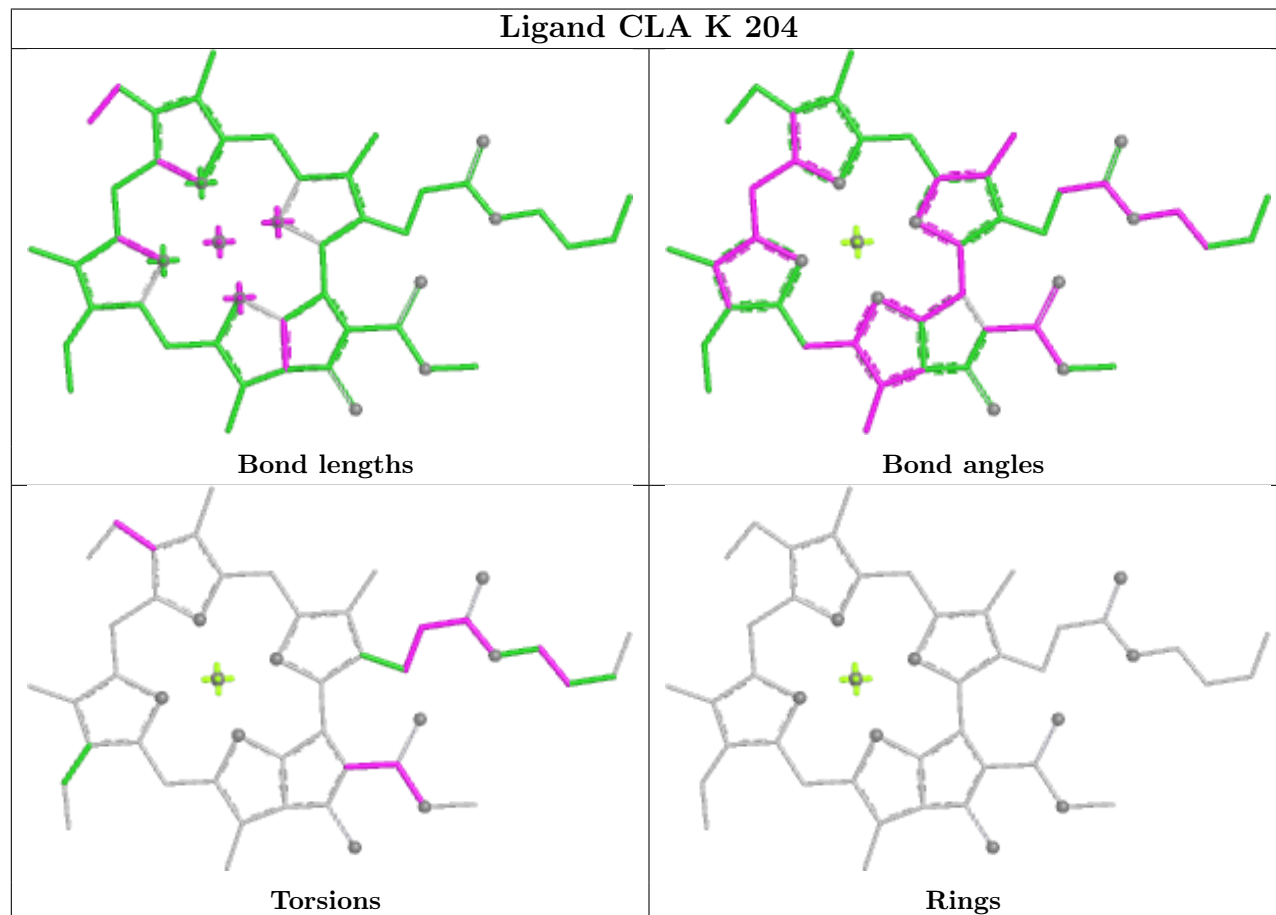


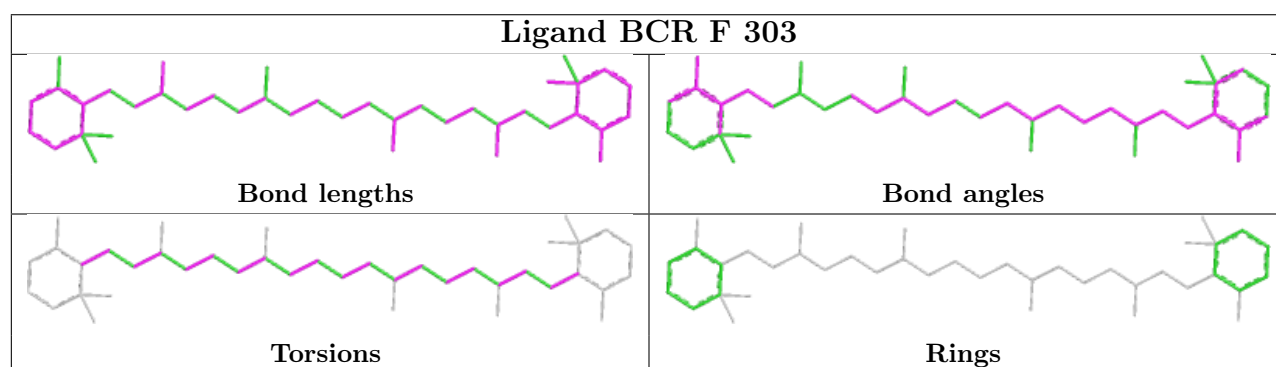
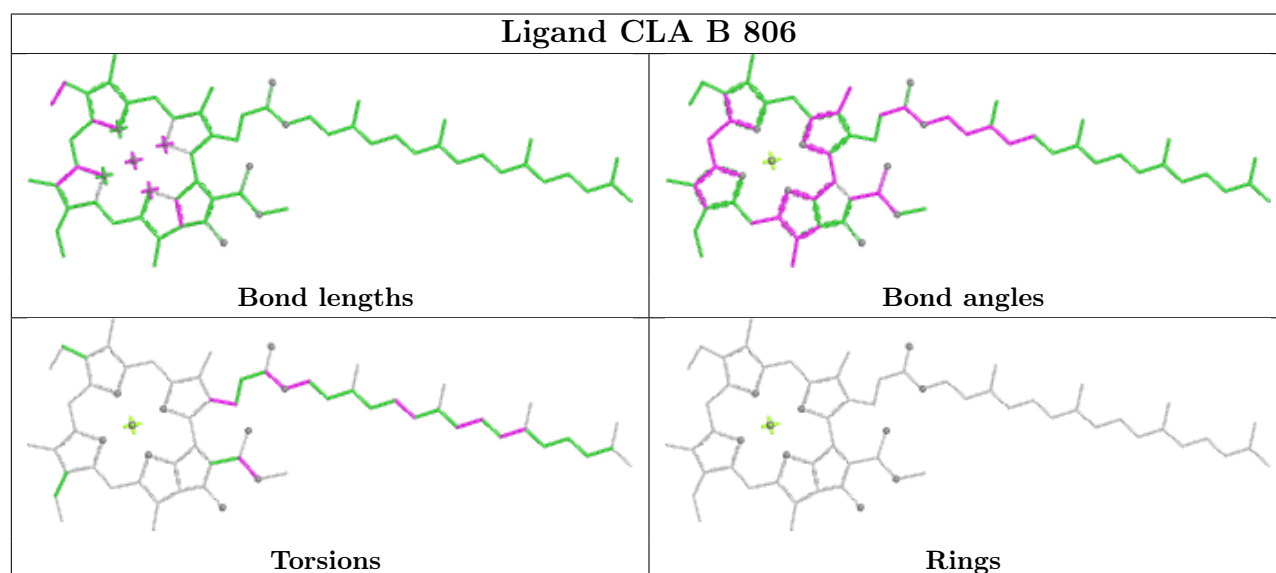
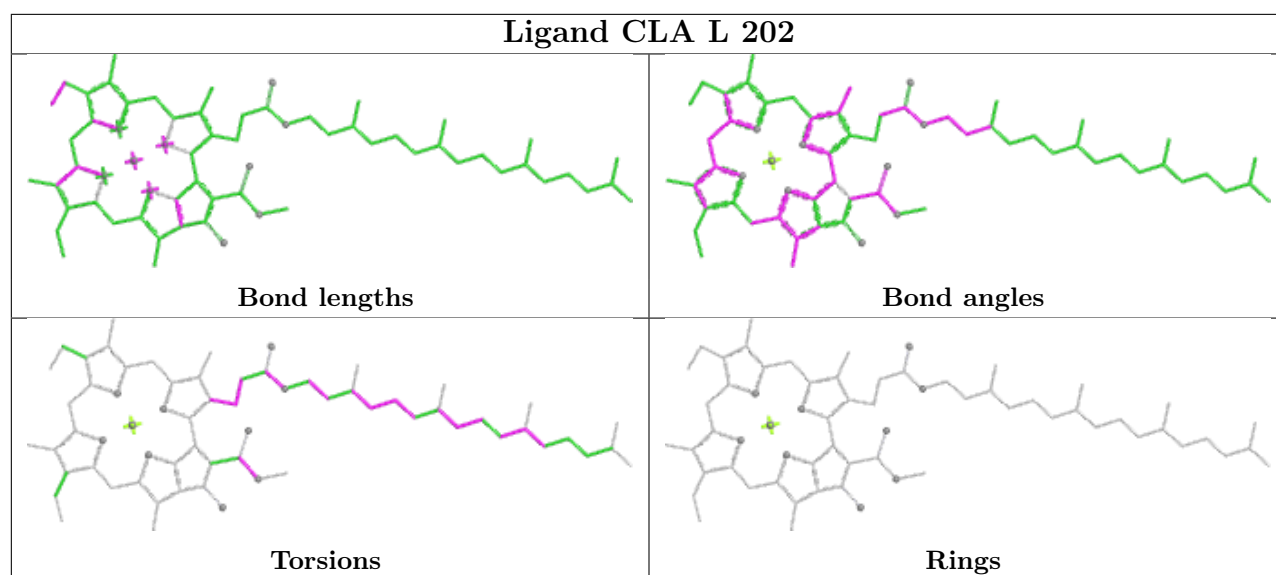
Rings

## Ligand CLA A 812

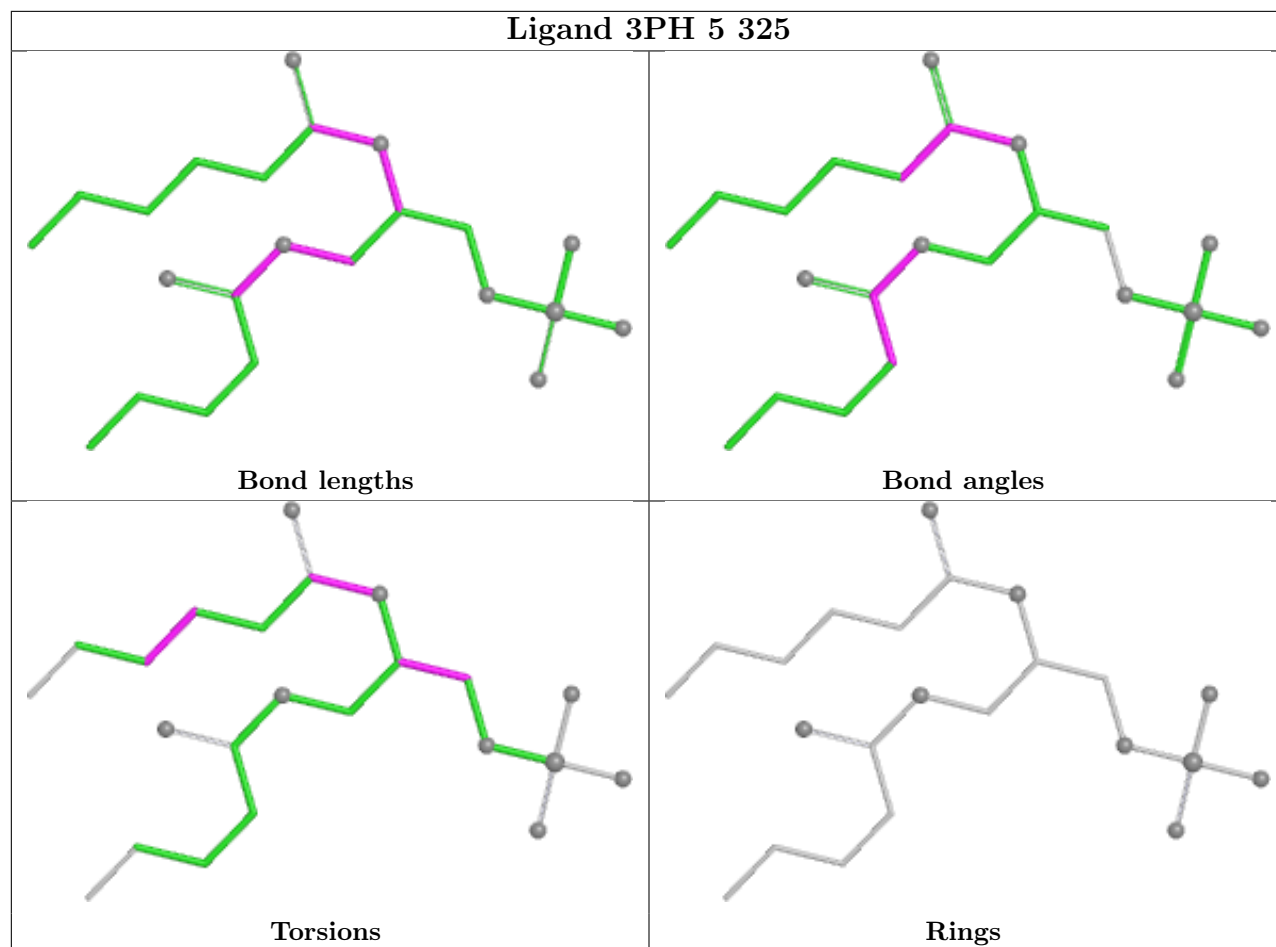


## Ligand CLA K 204

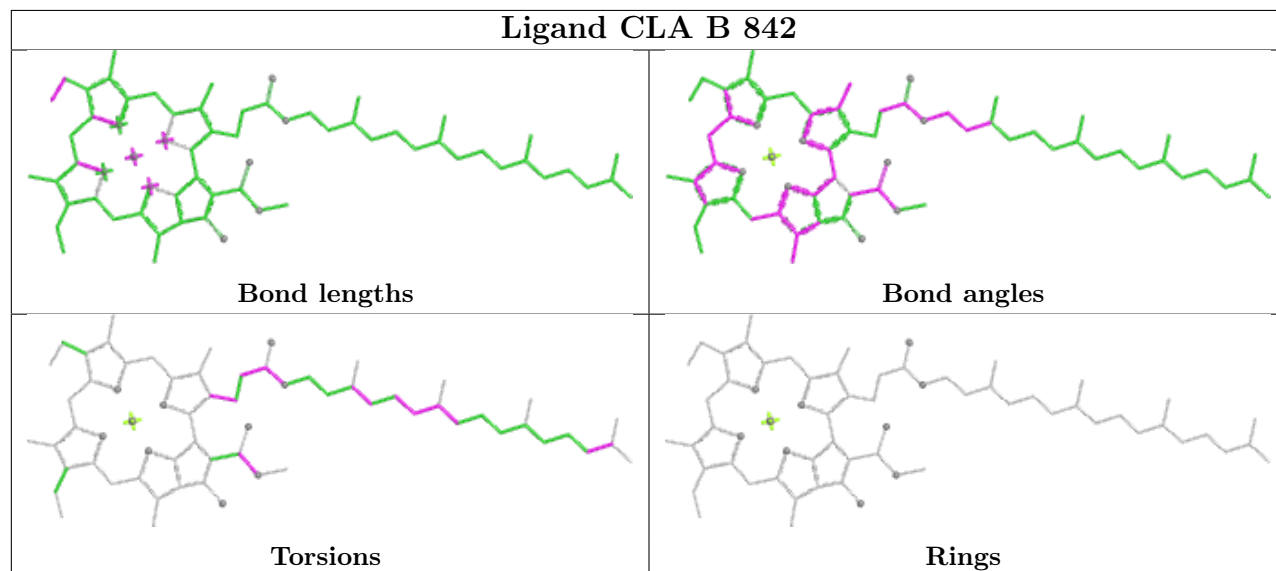


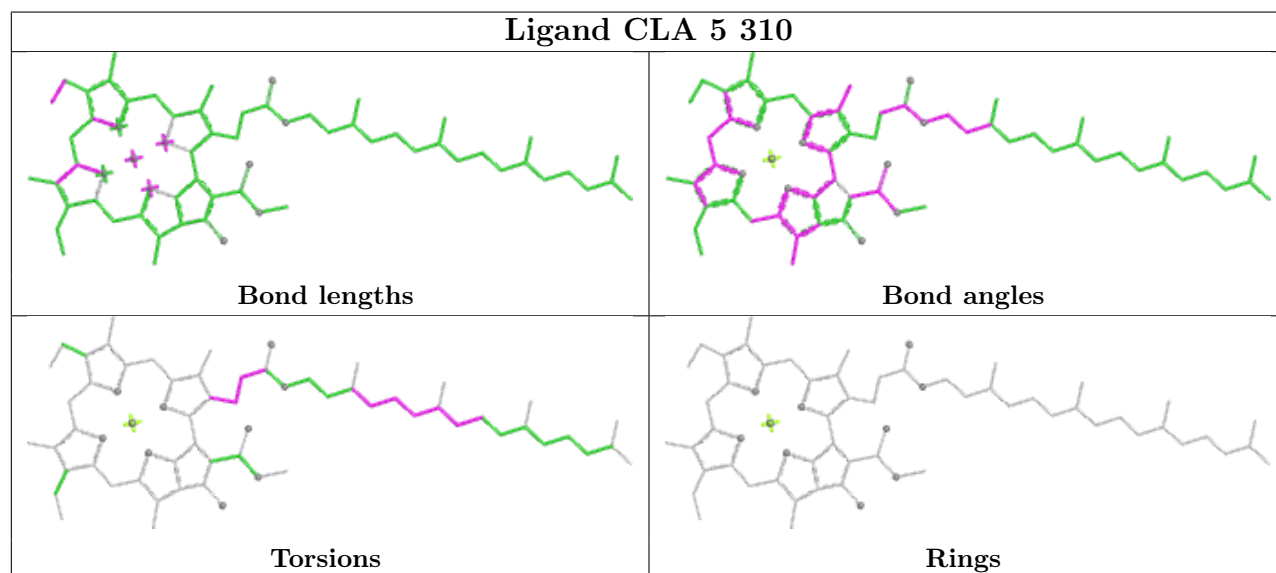
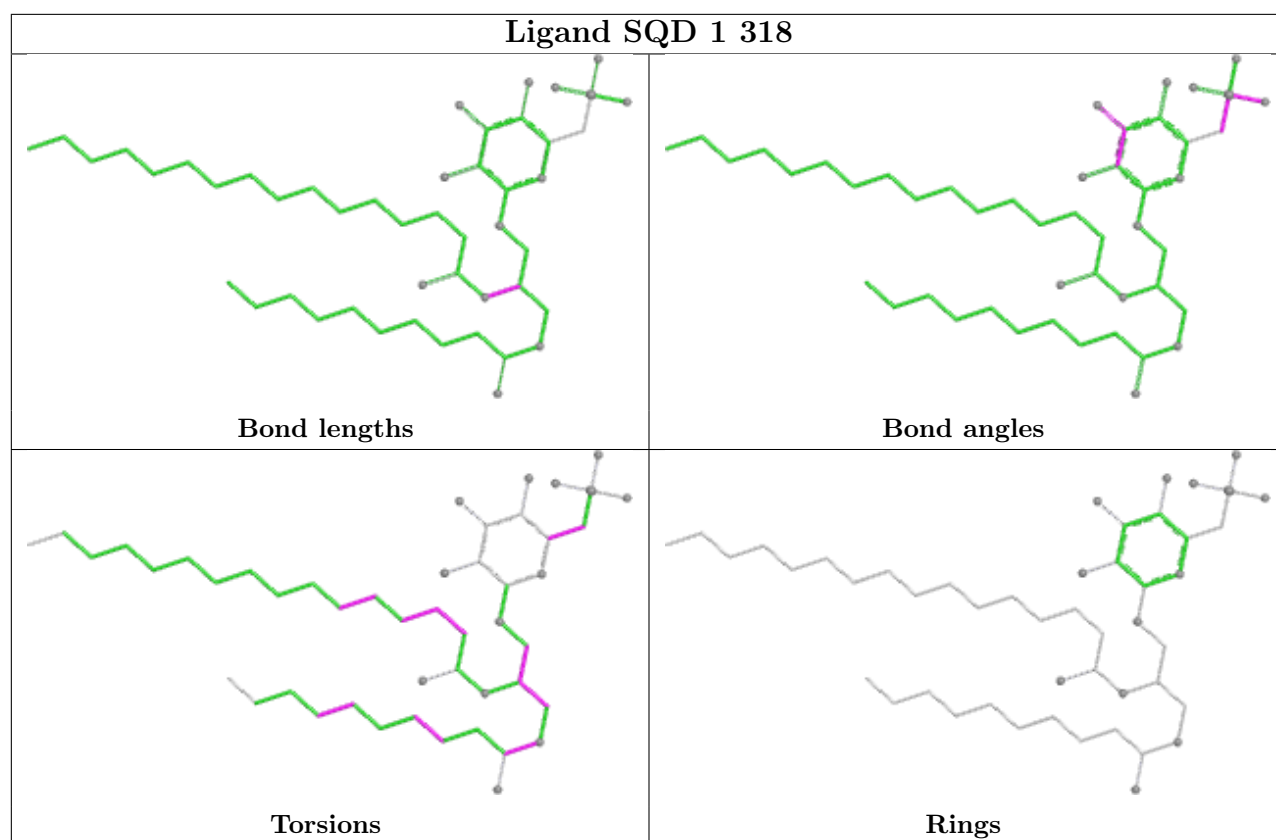


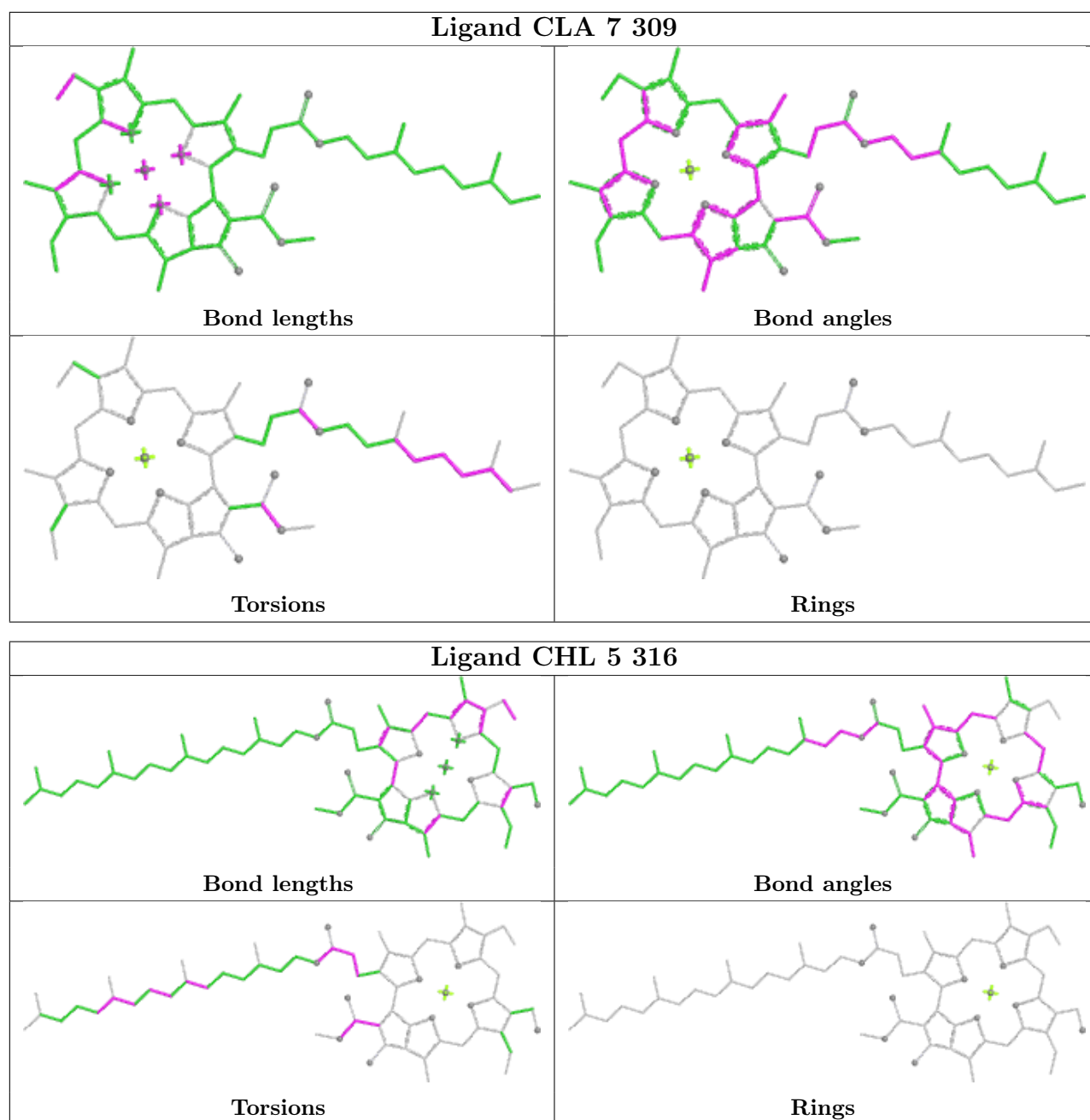
## Ligand 3PH 5 325



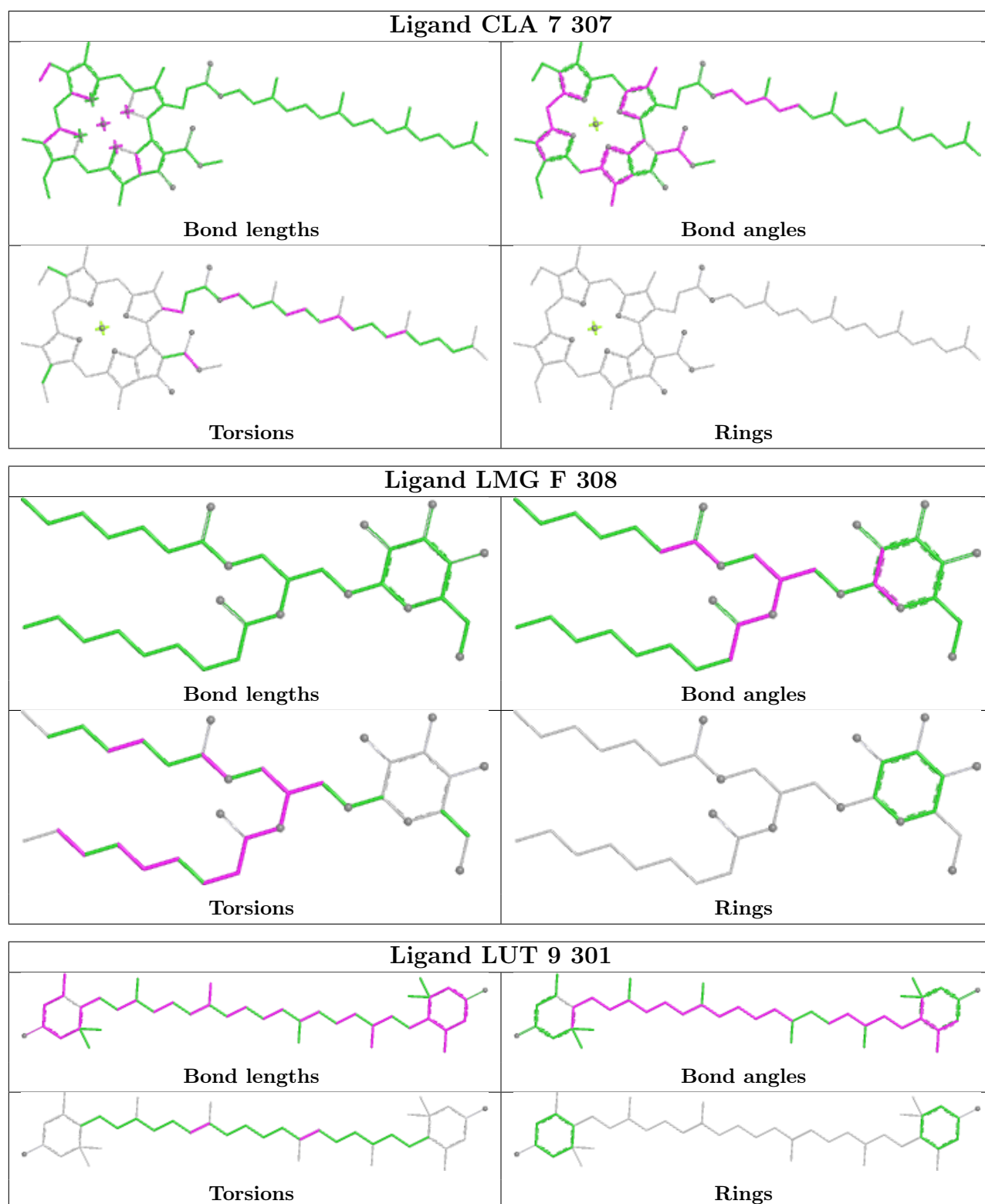
## Ligand CLA B 842

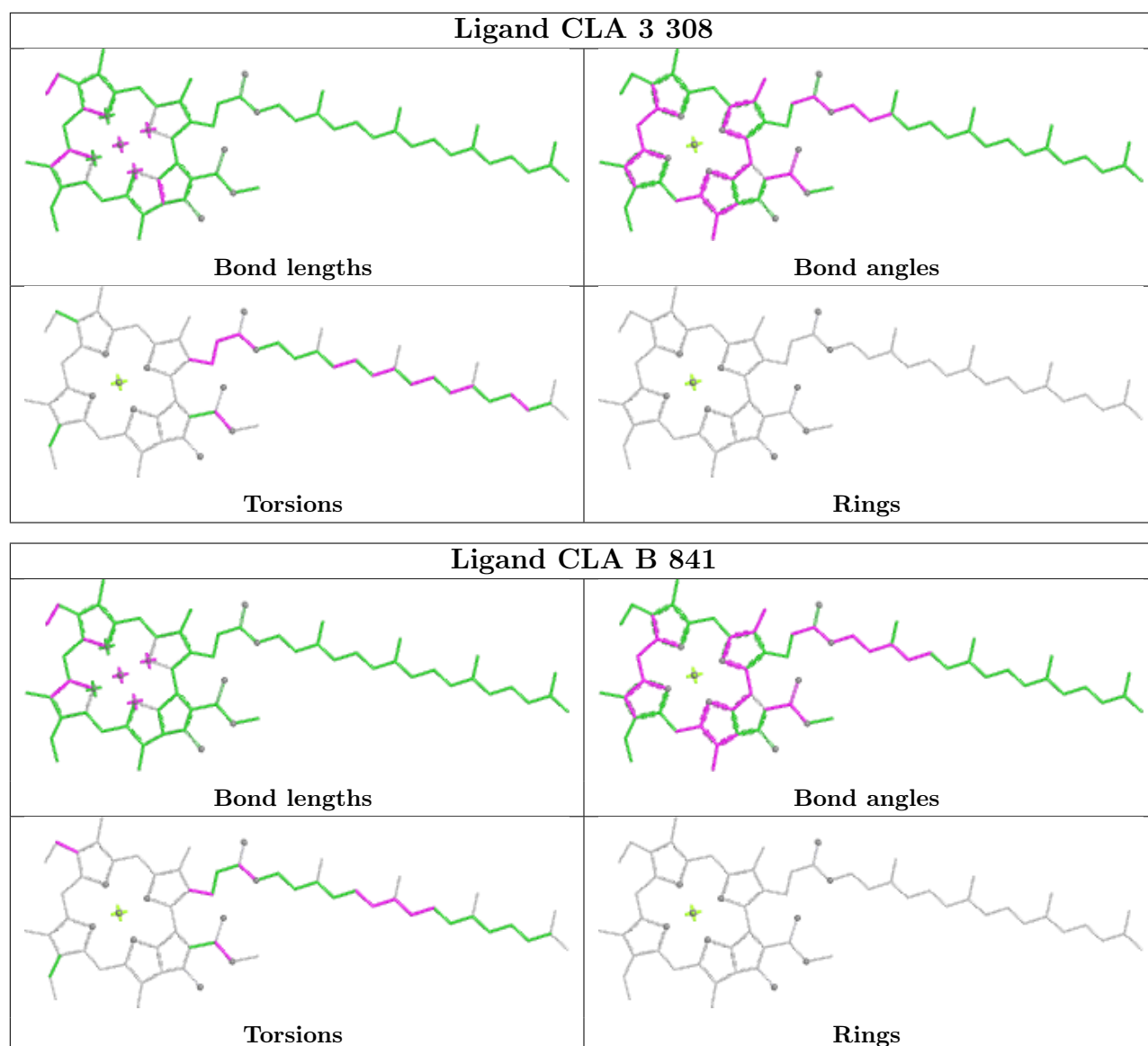


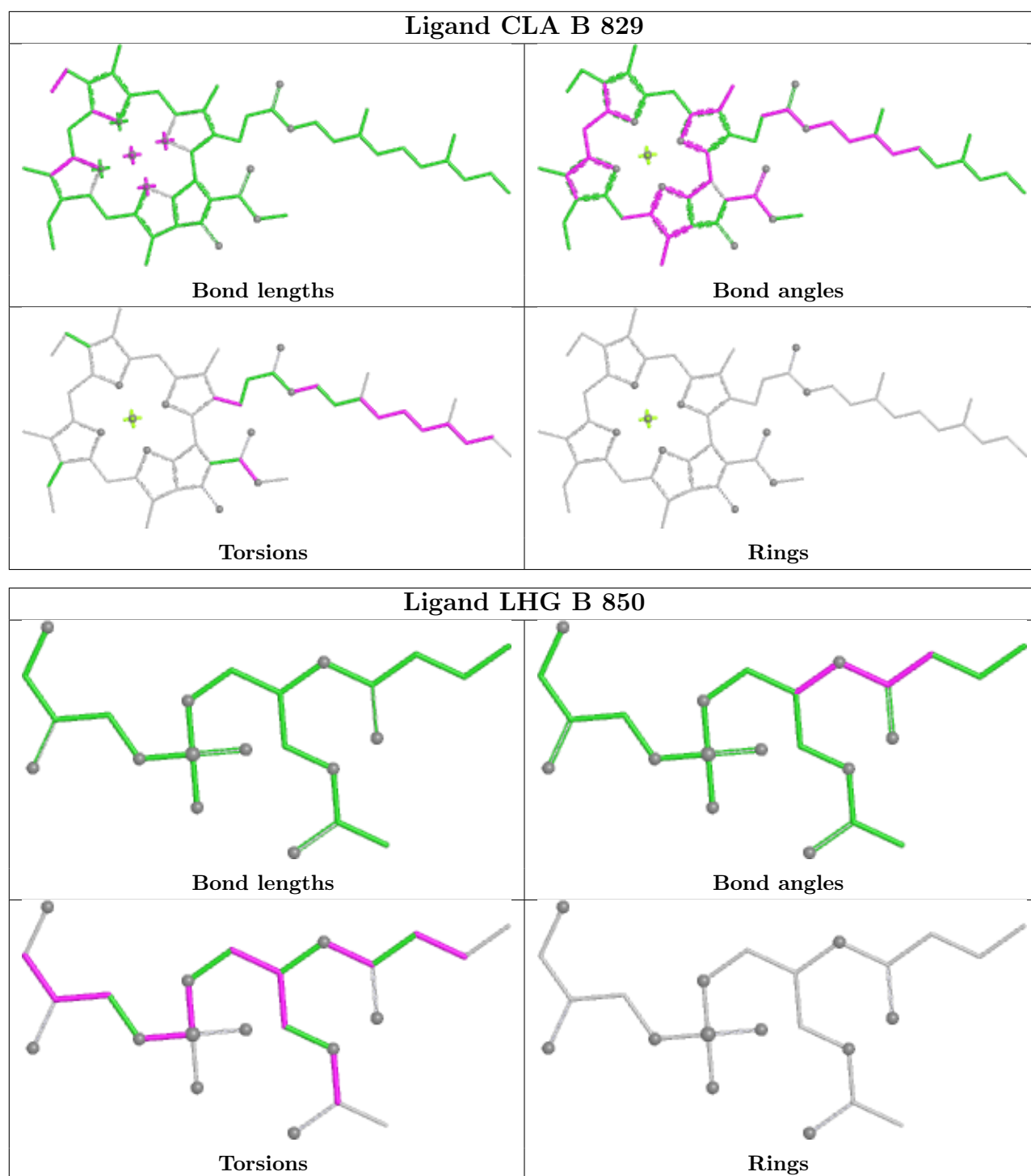


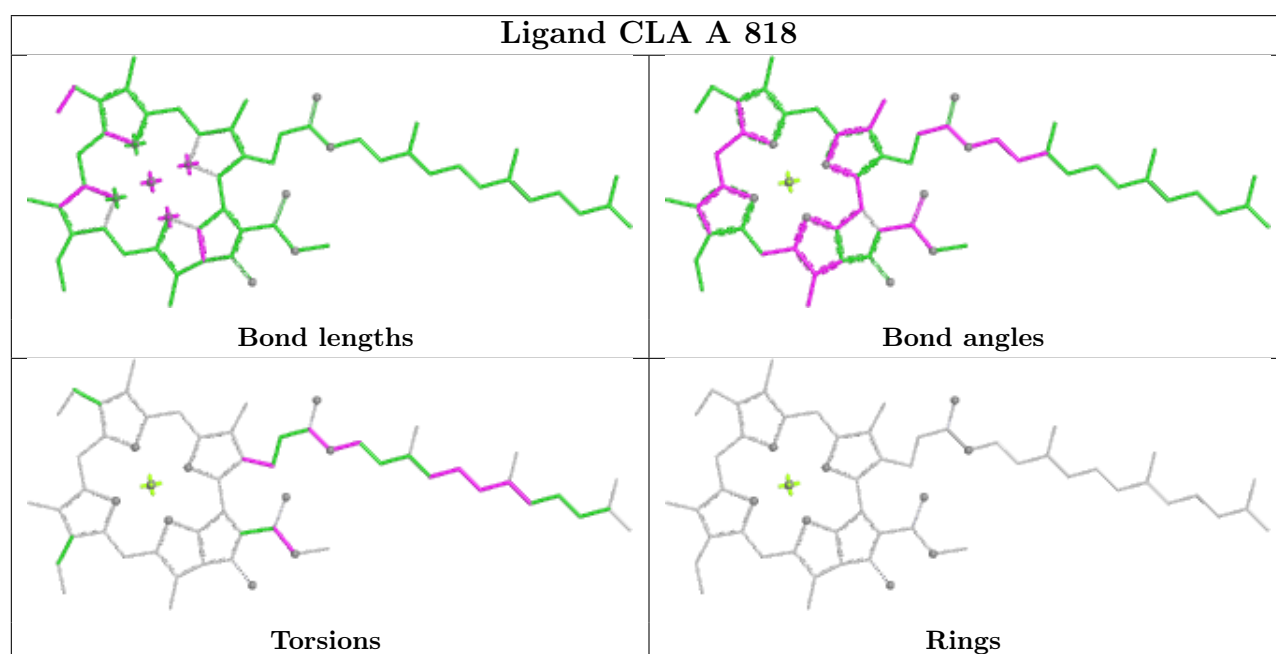
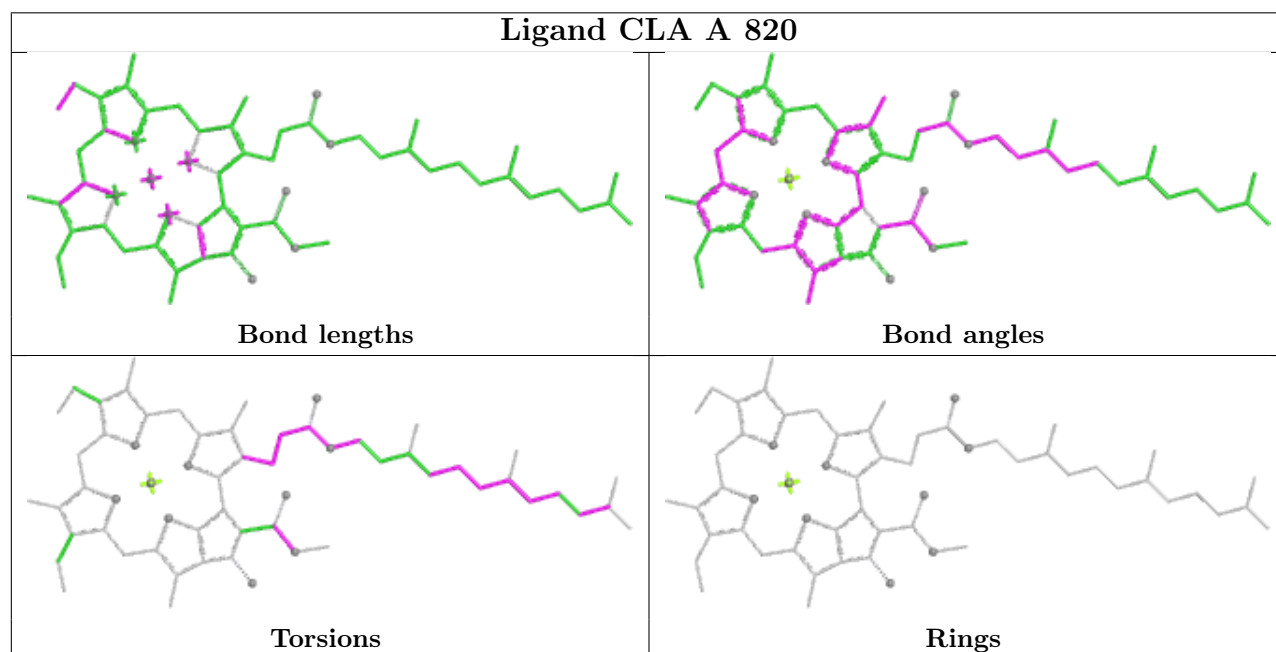
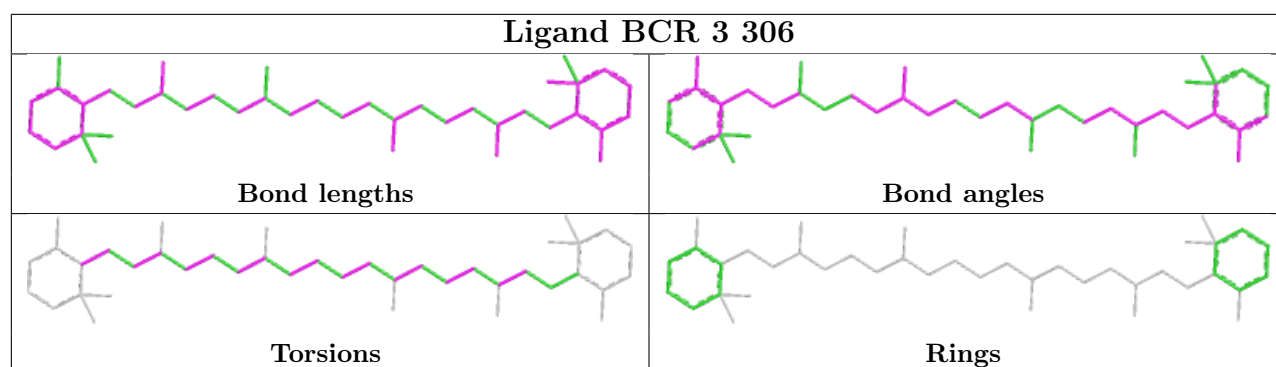


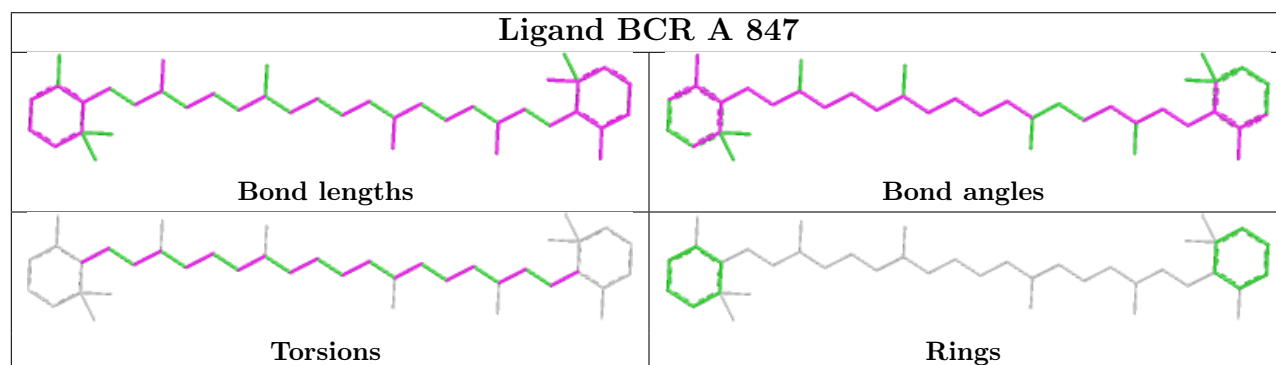
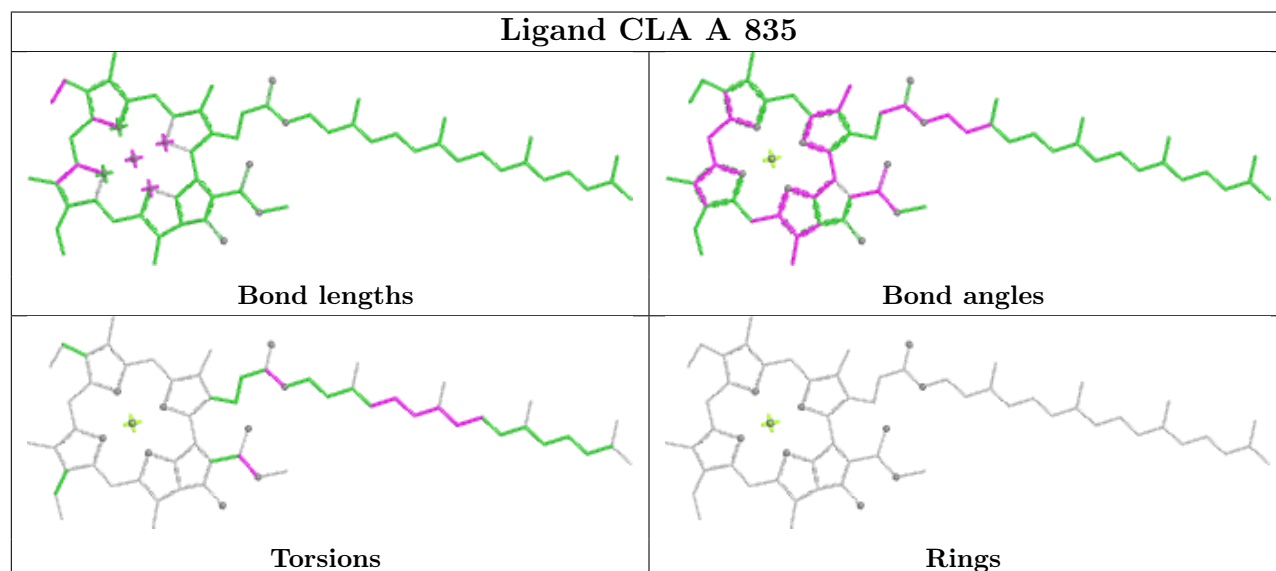
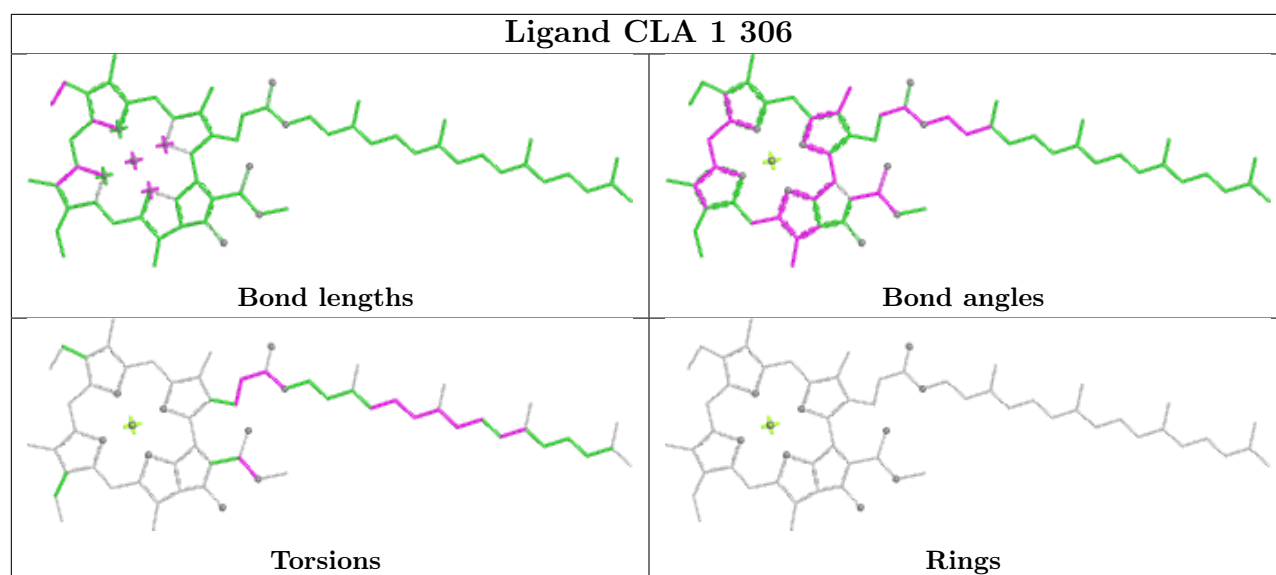


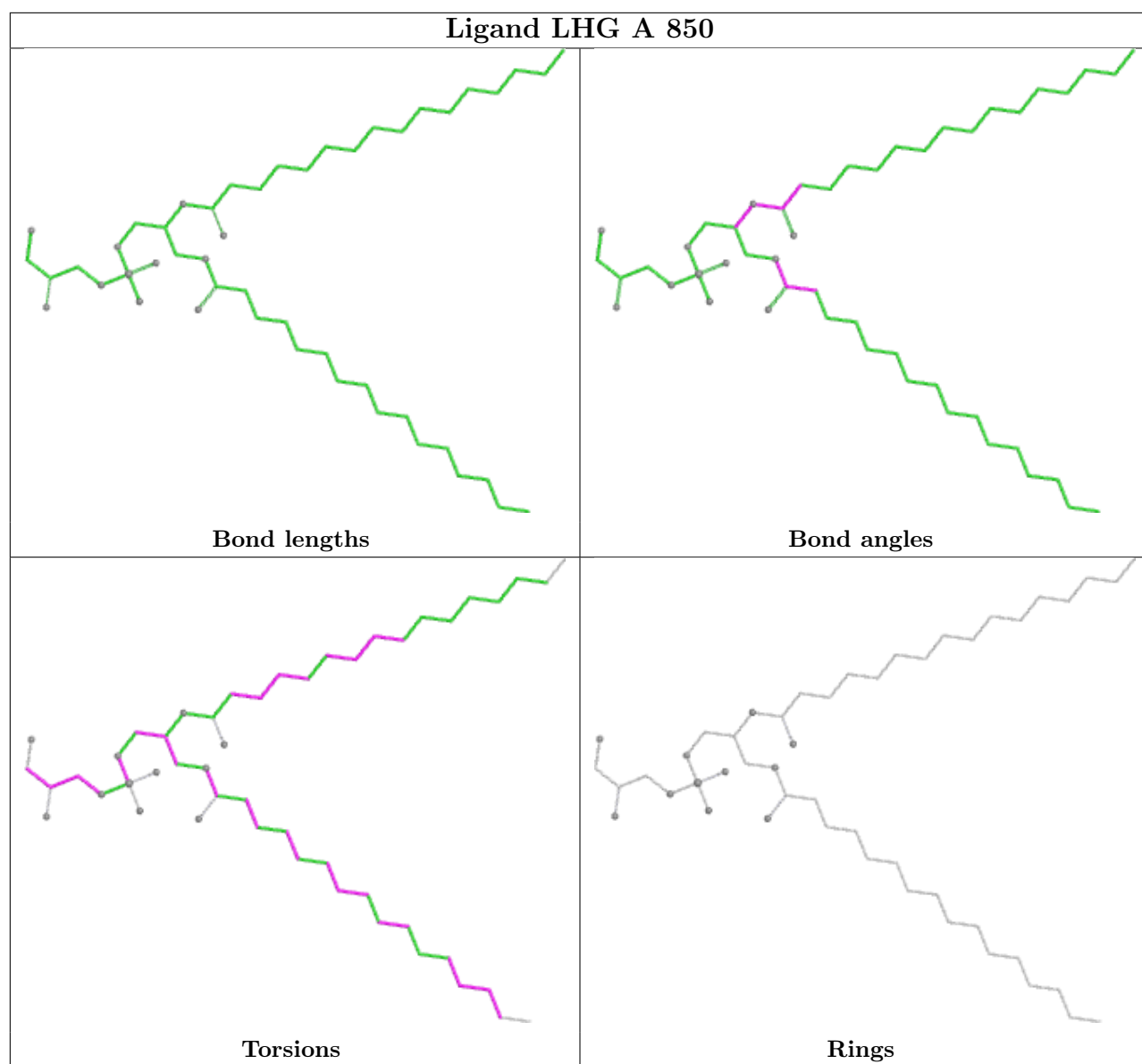


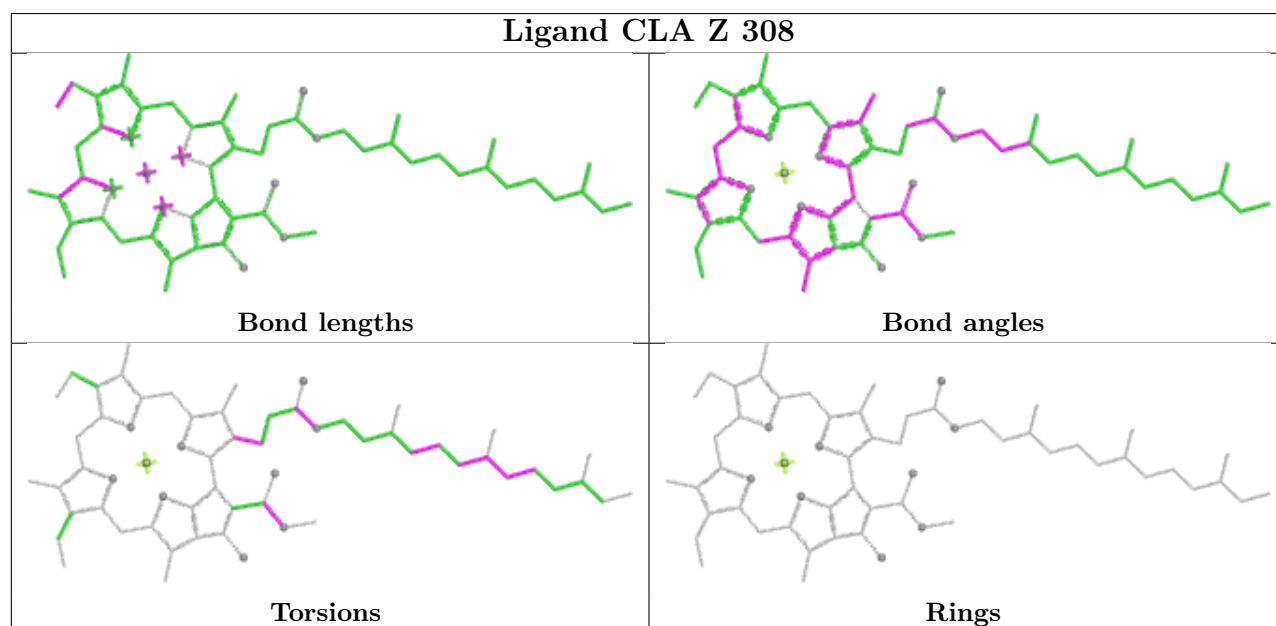
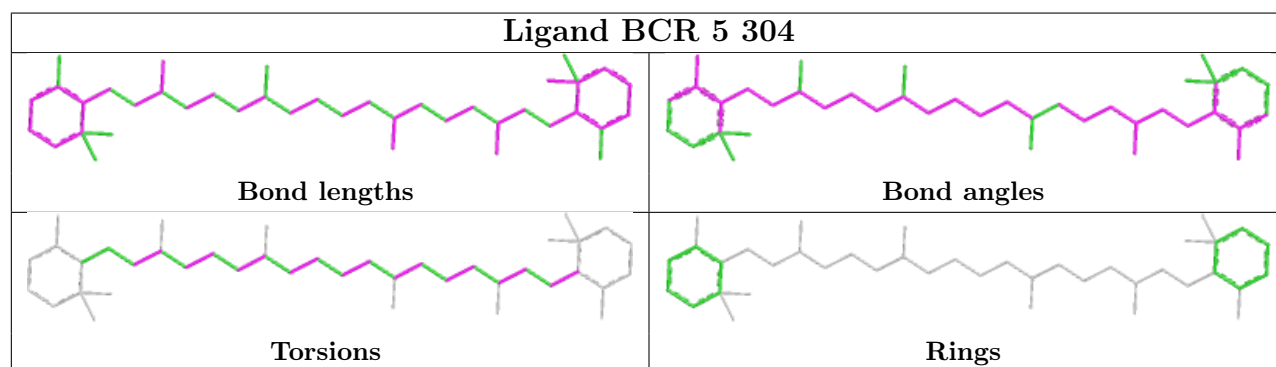
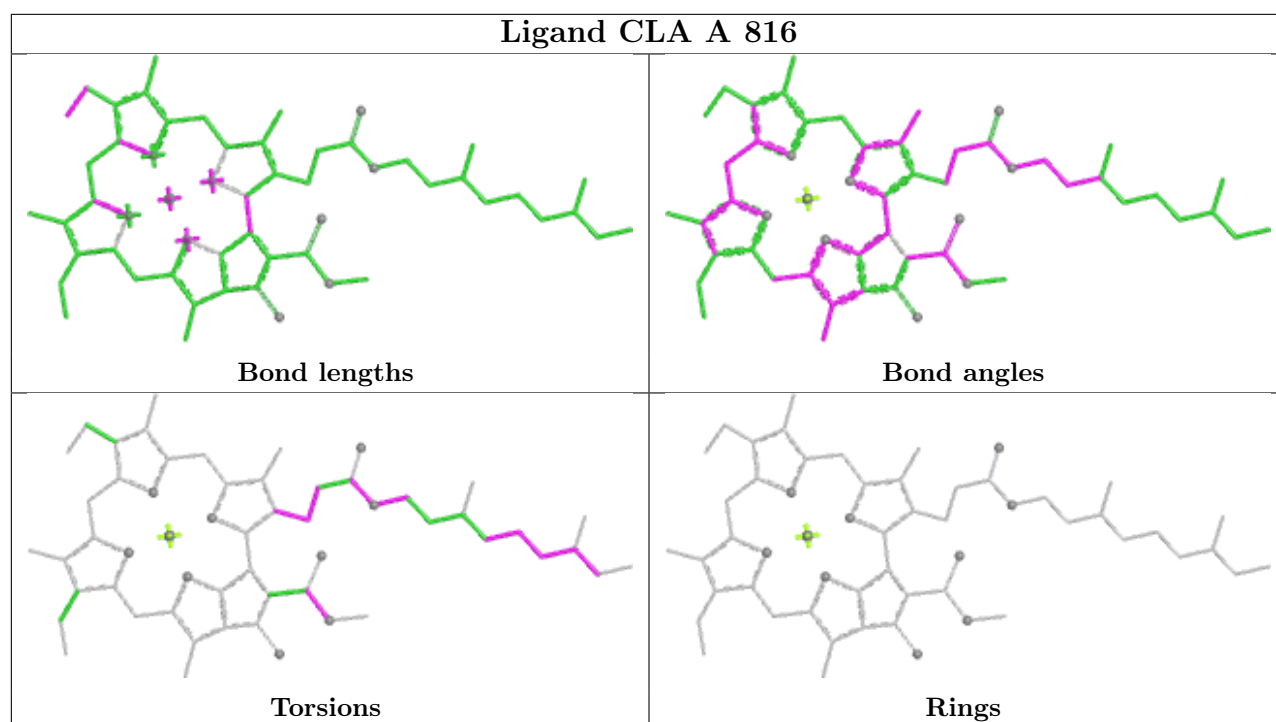


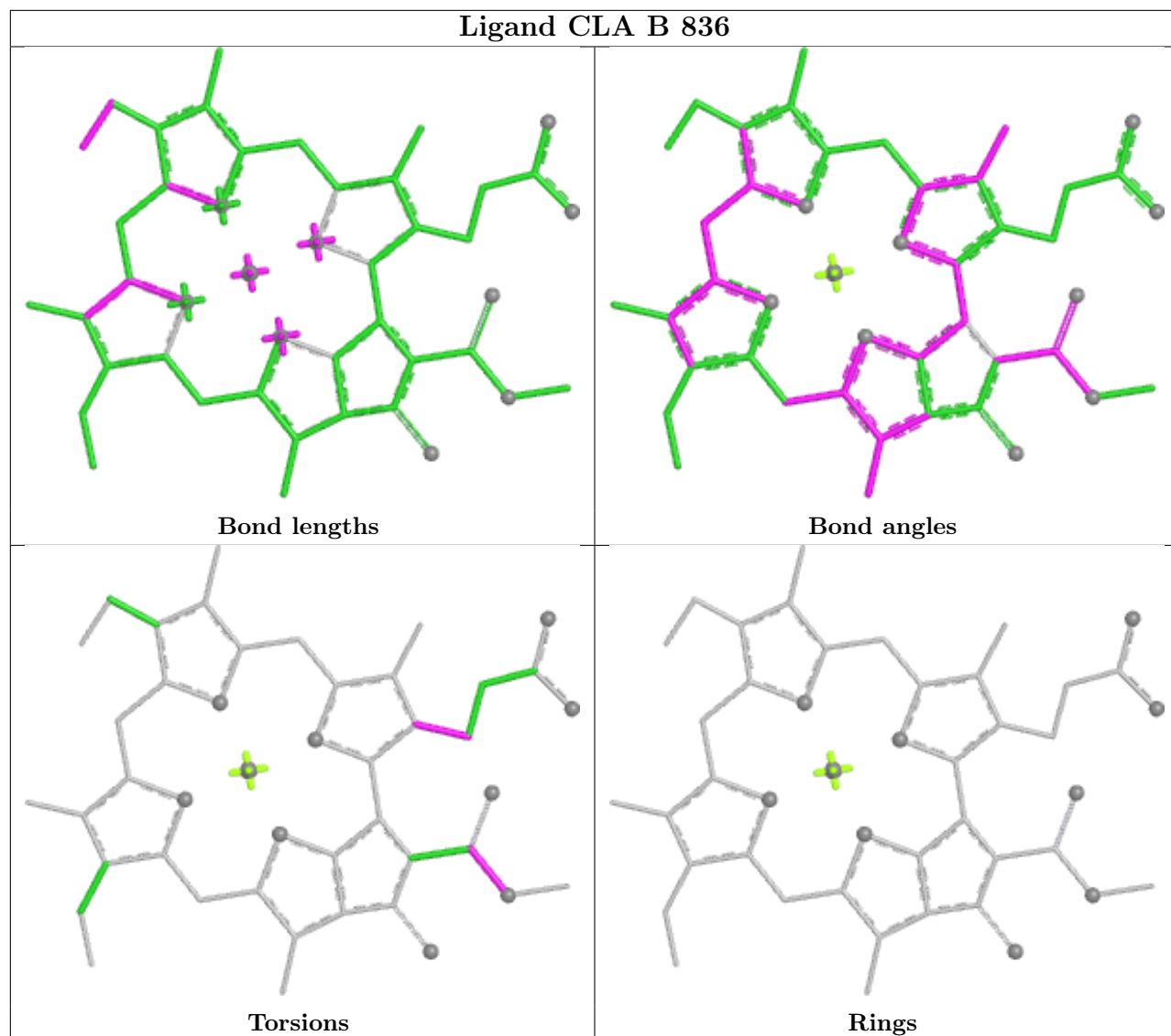




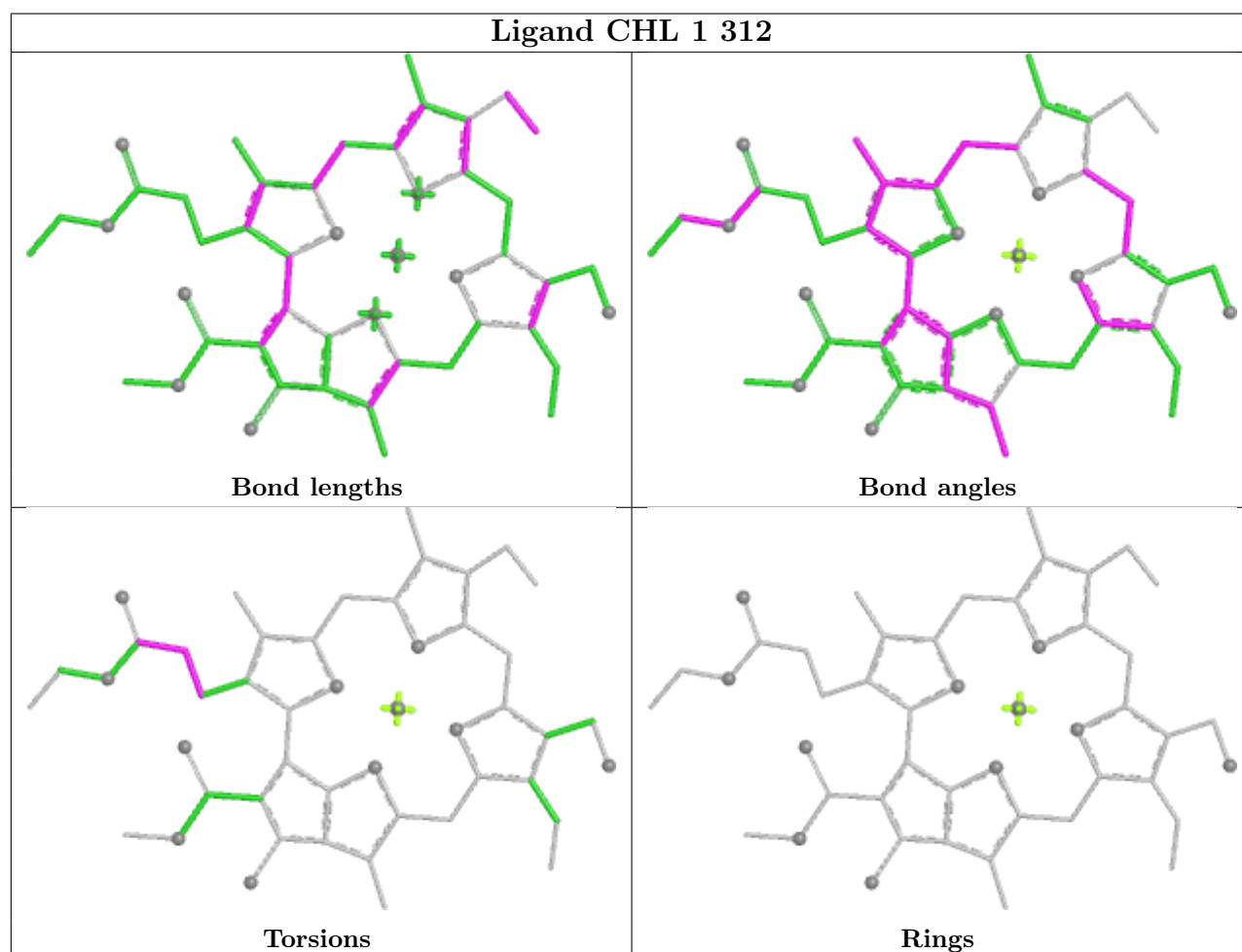
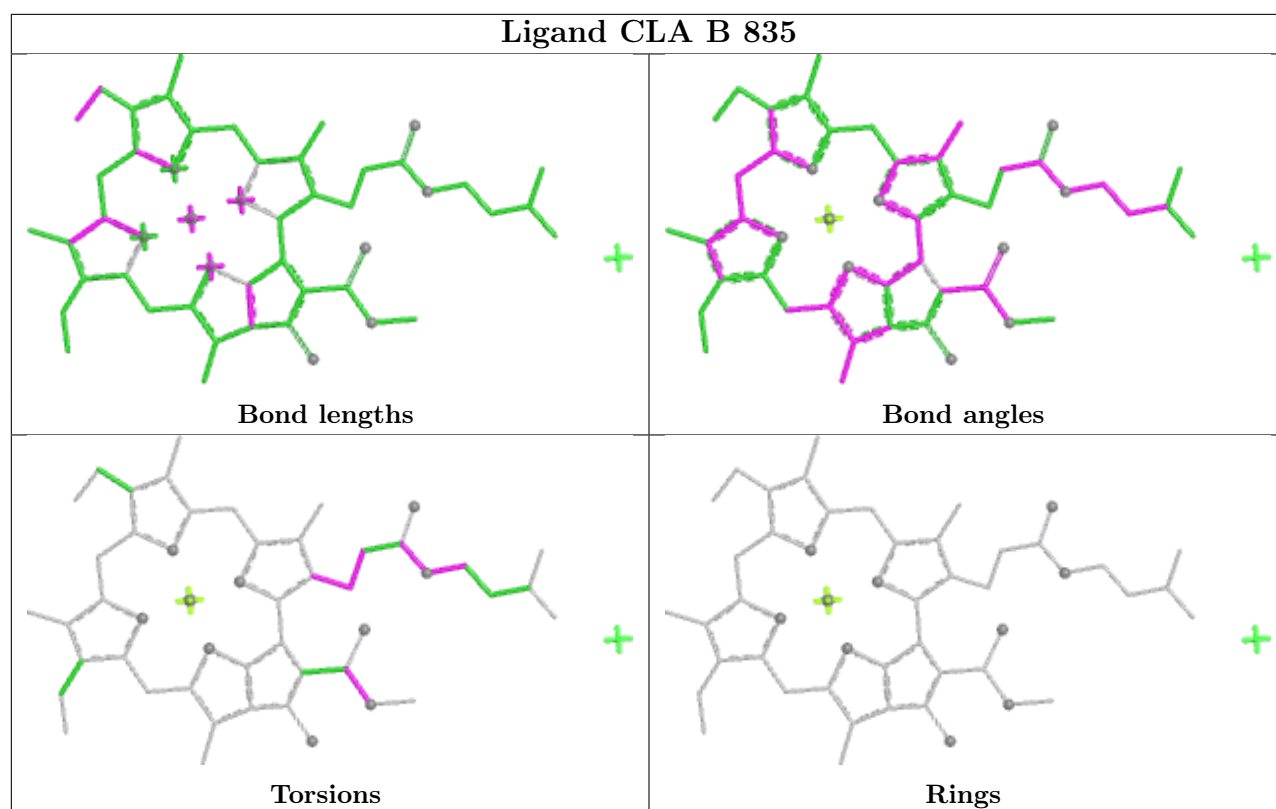




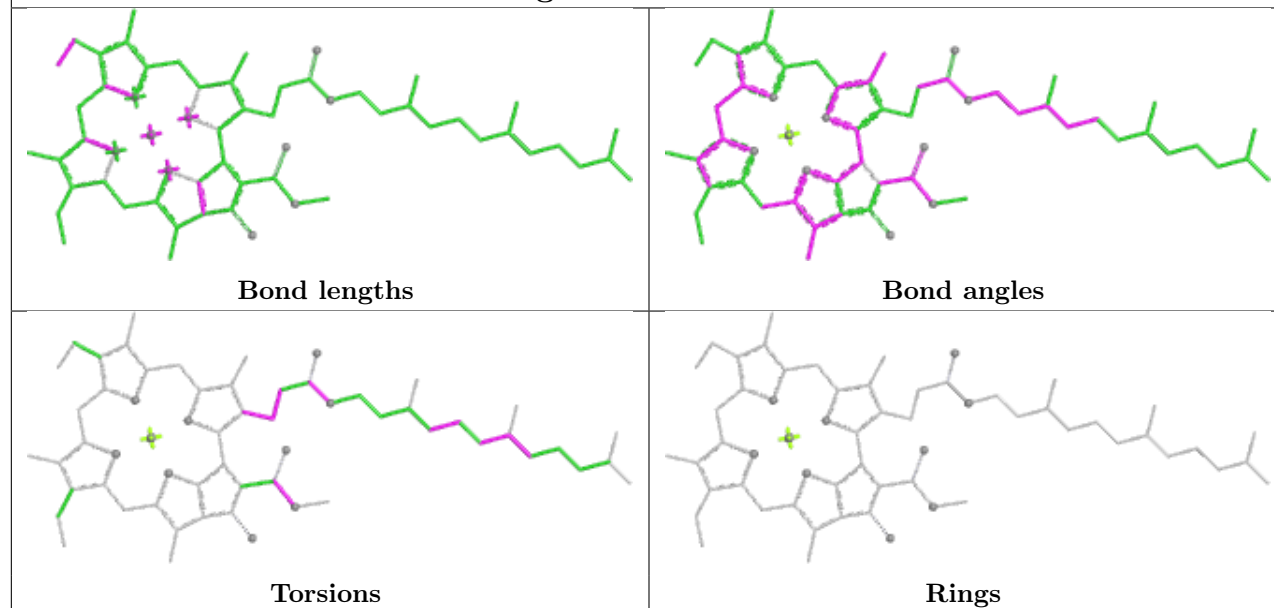




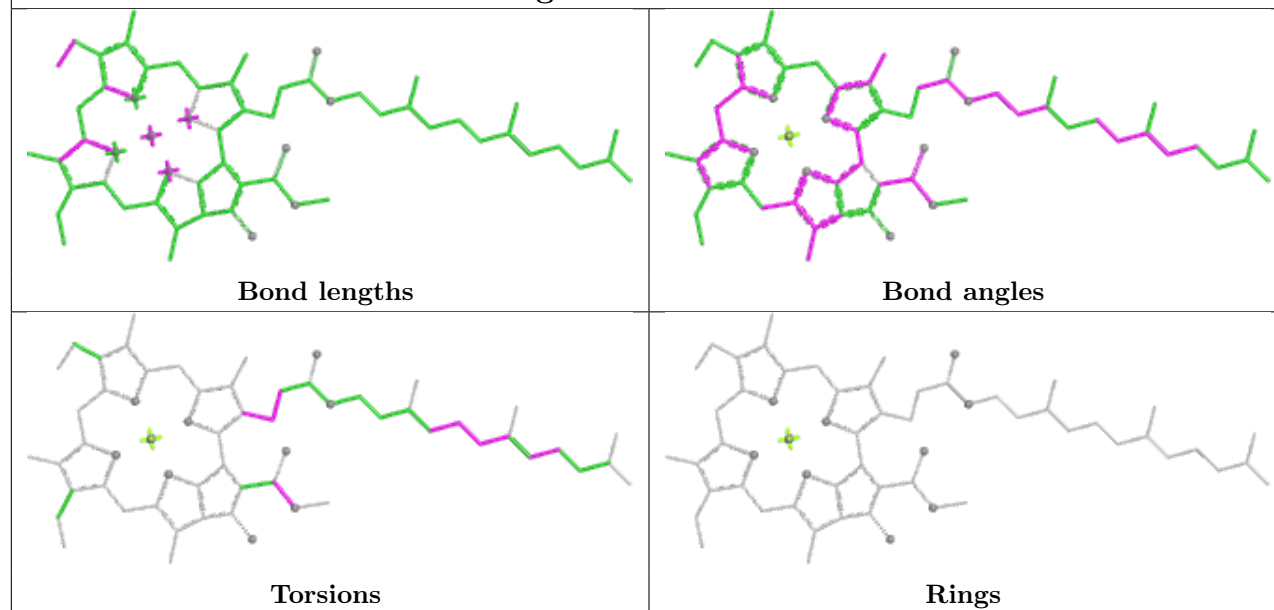


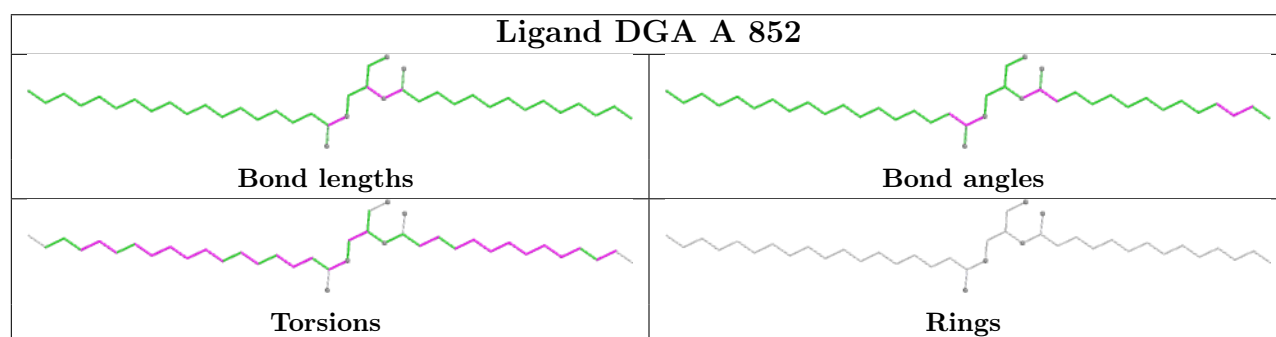
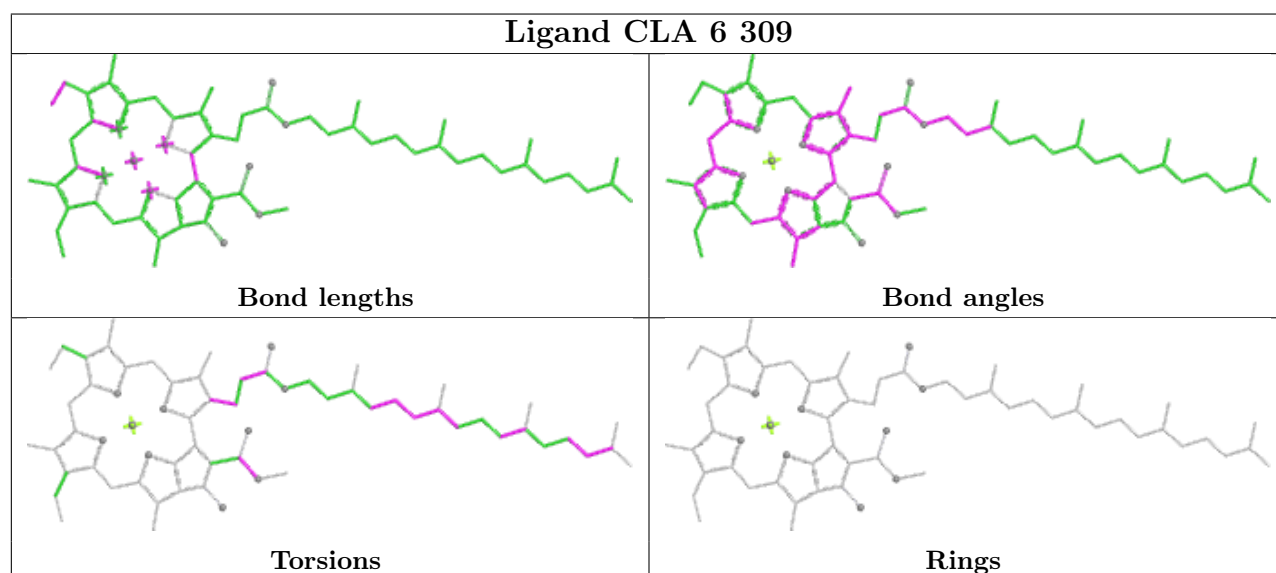
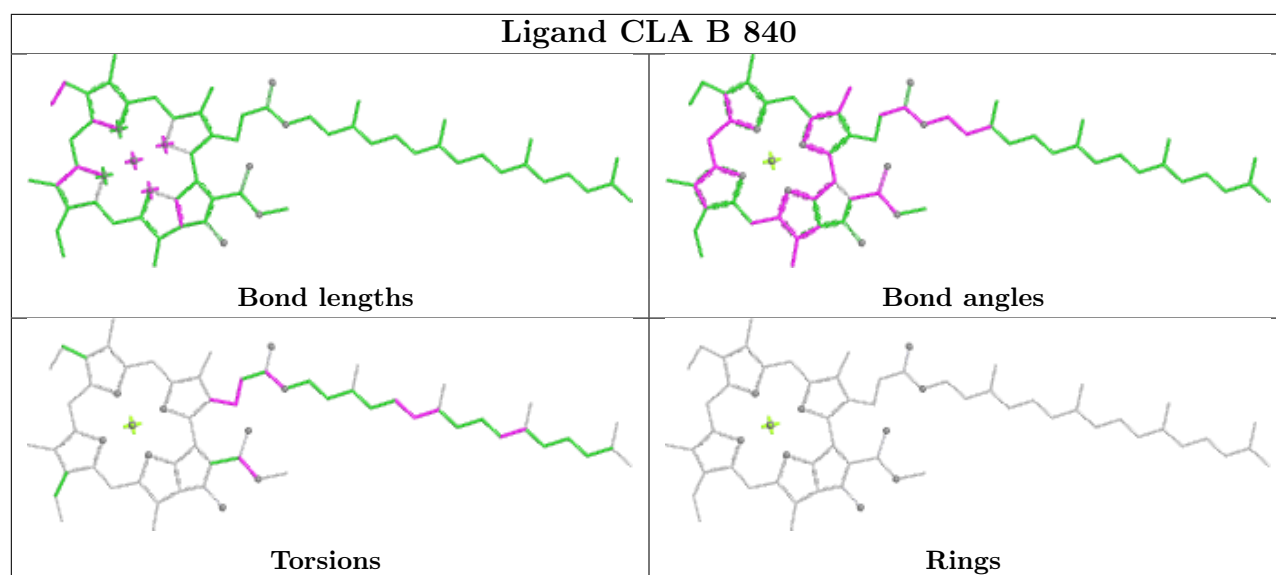


## Ligand CLA 8 305

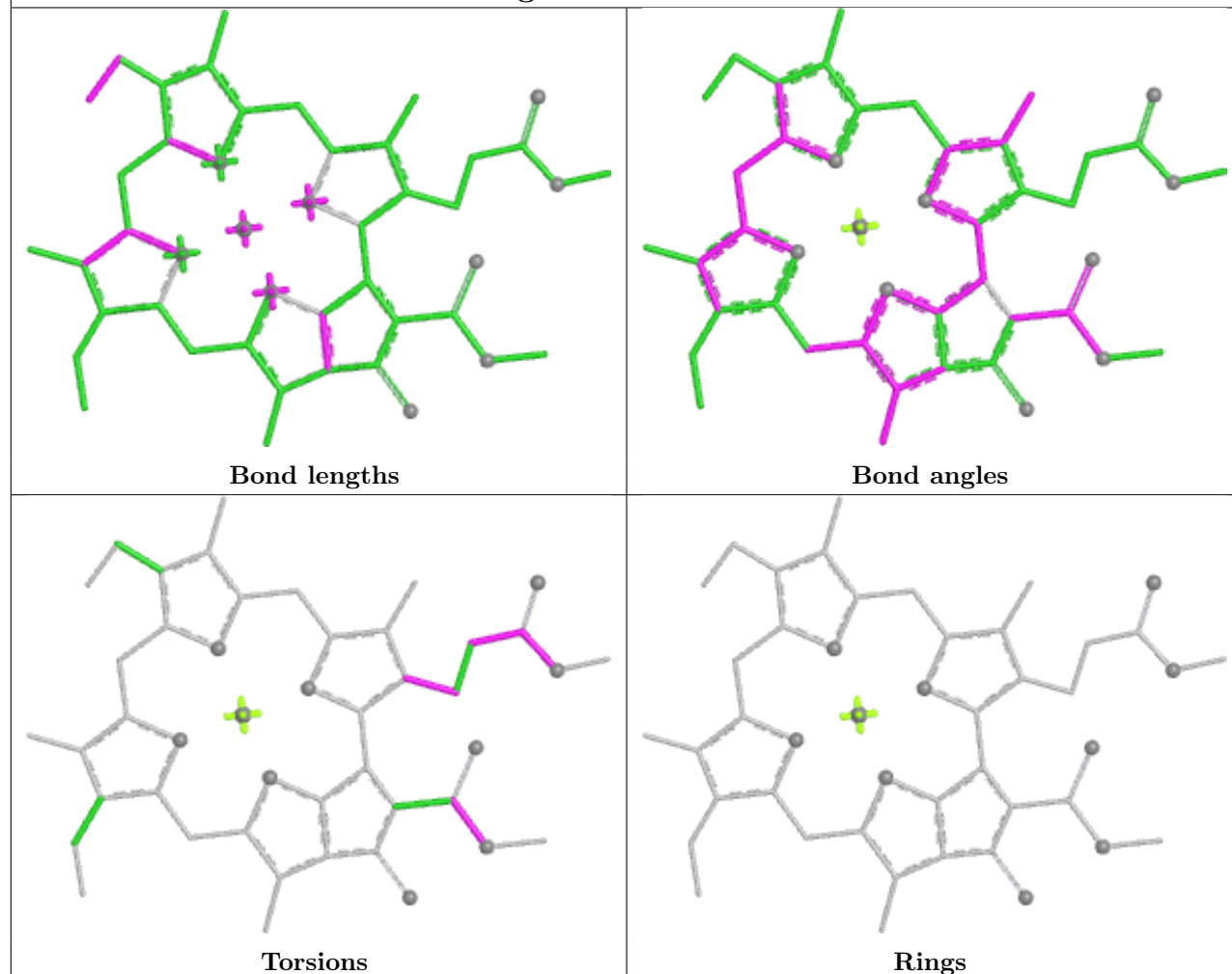


## Ligand CLA 3 318

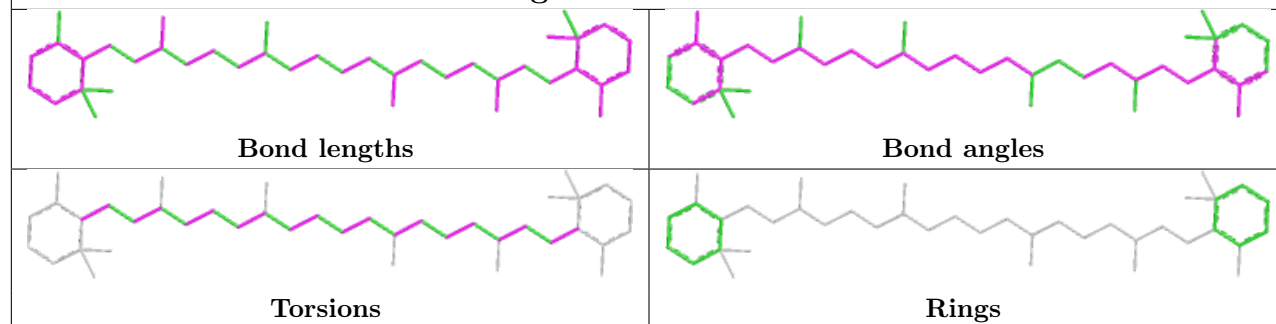


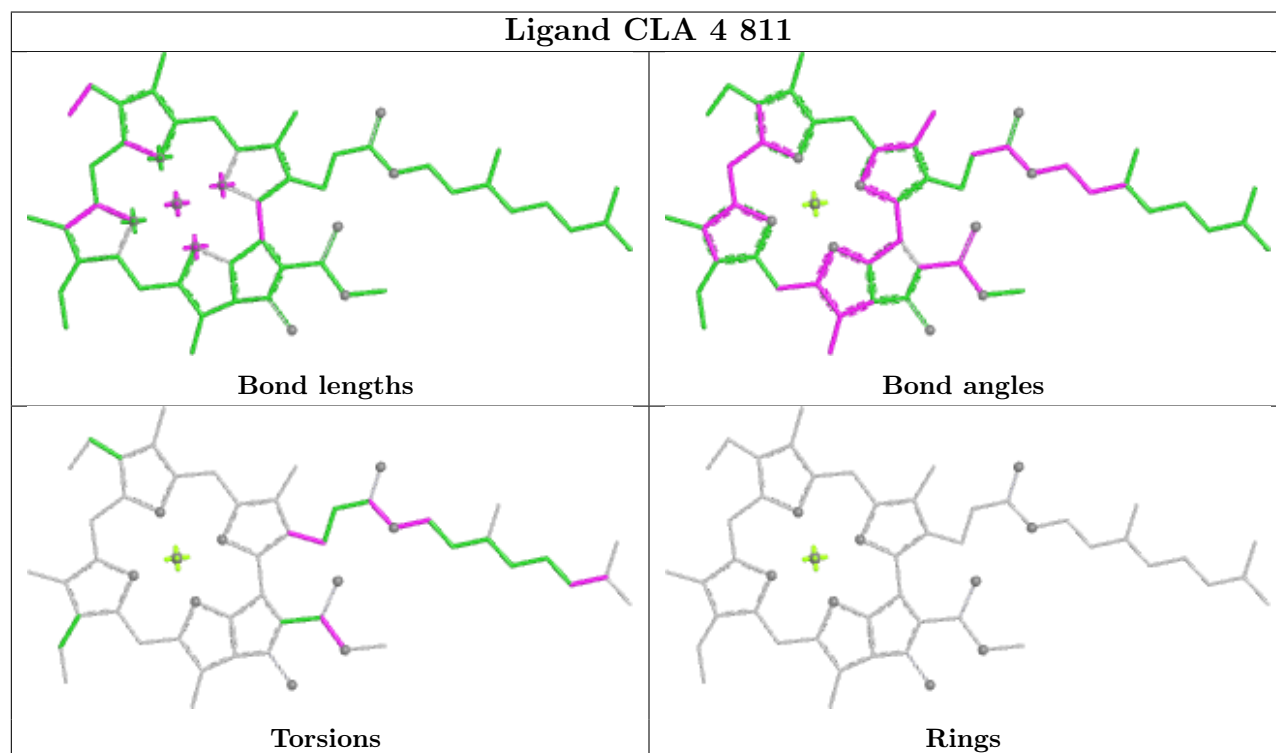
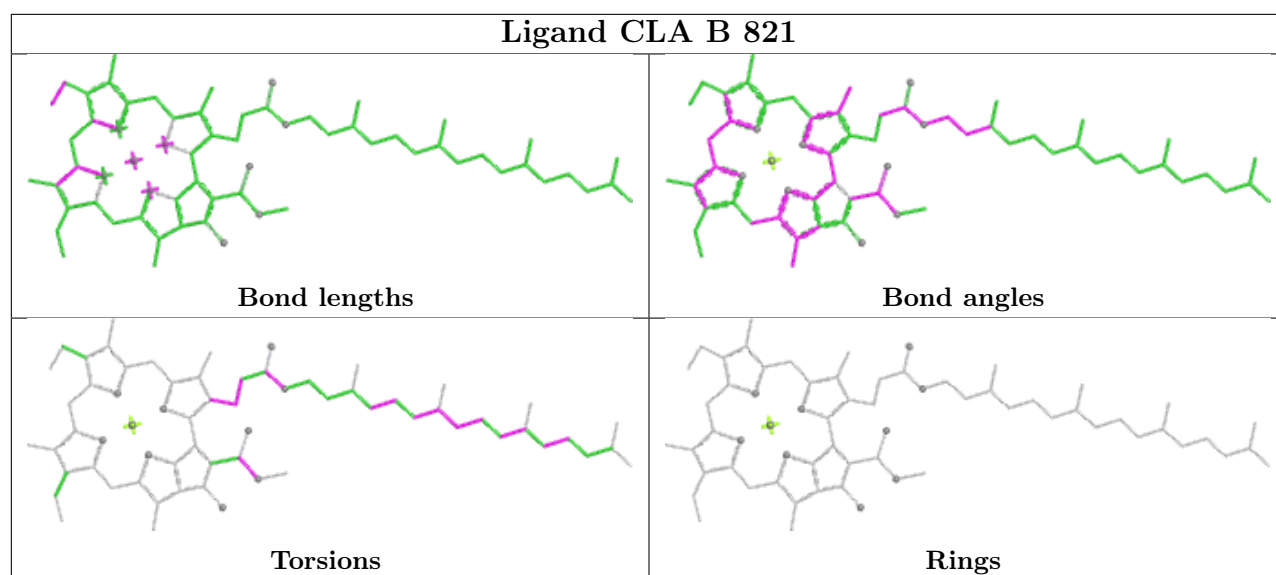


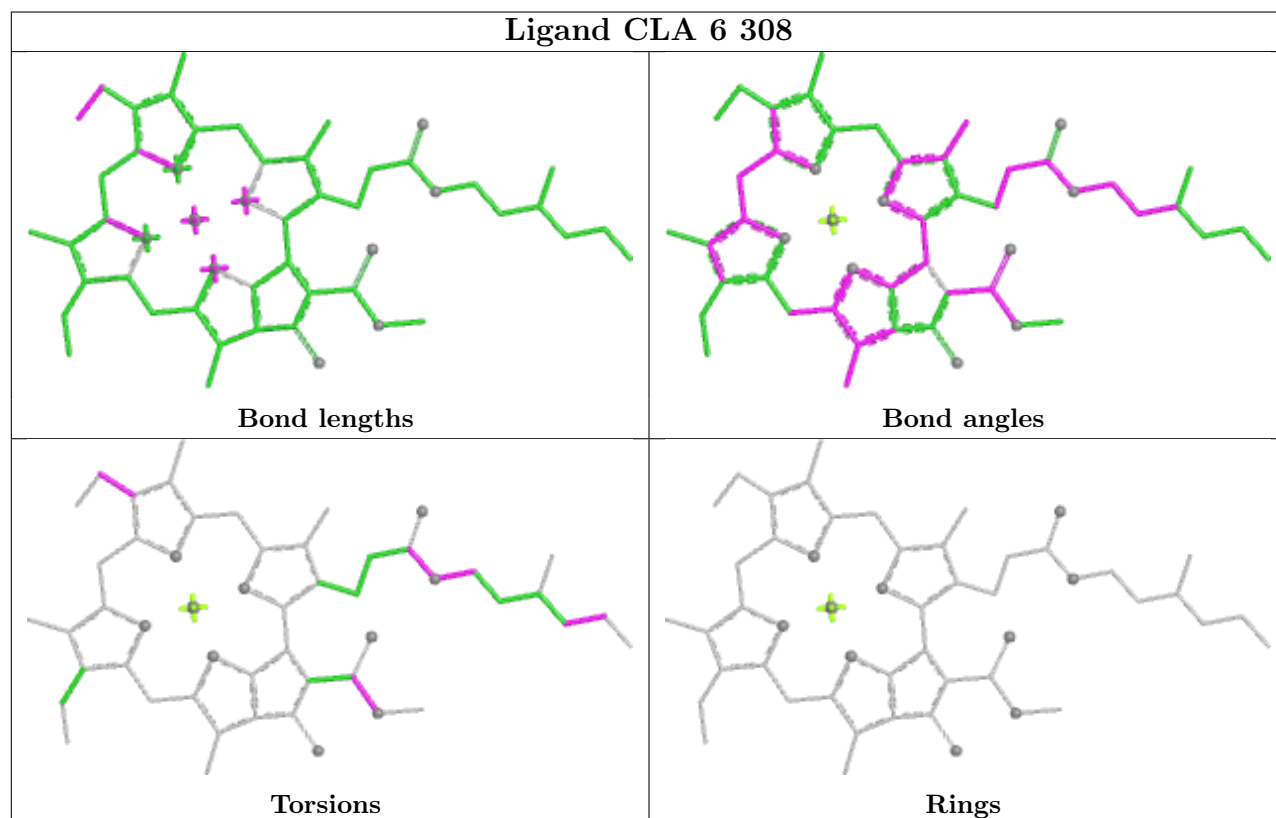
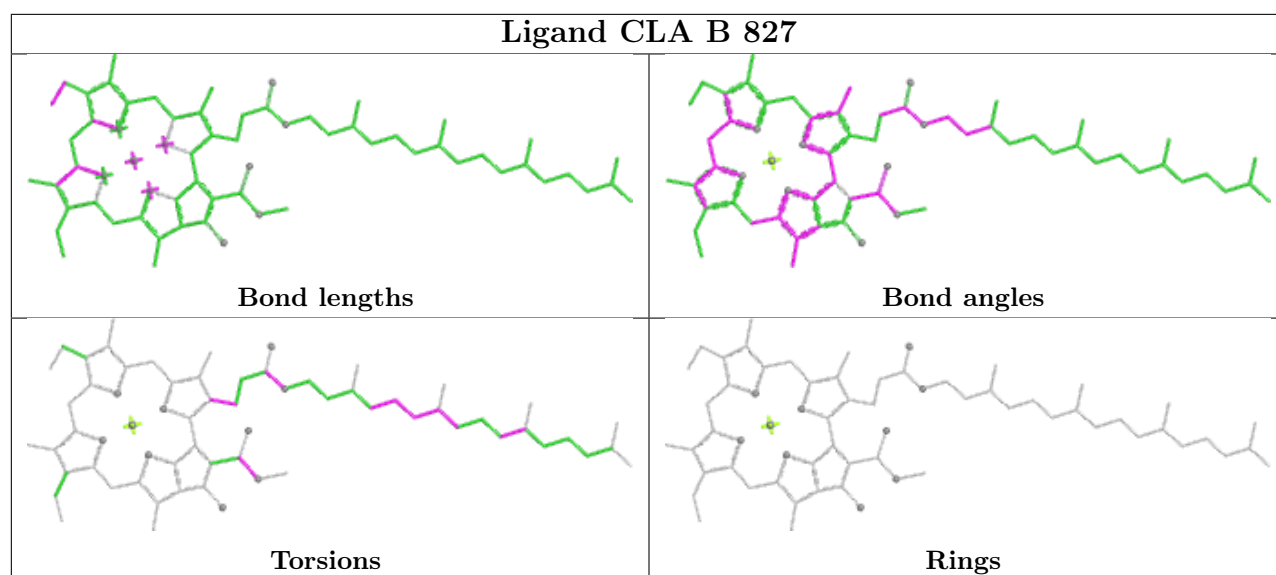
## Ligand CLA 1 315

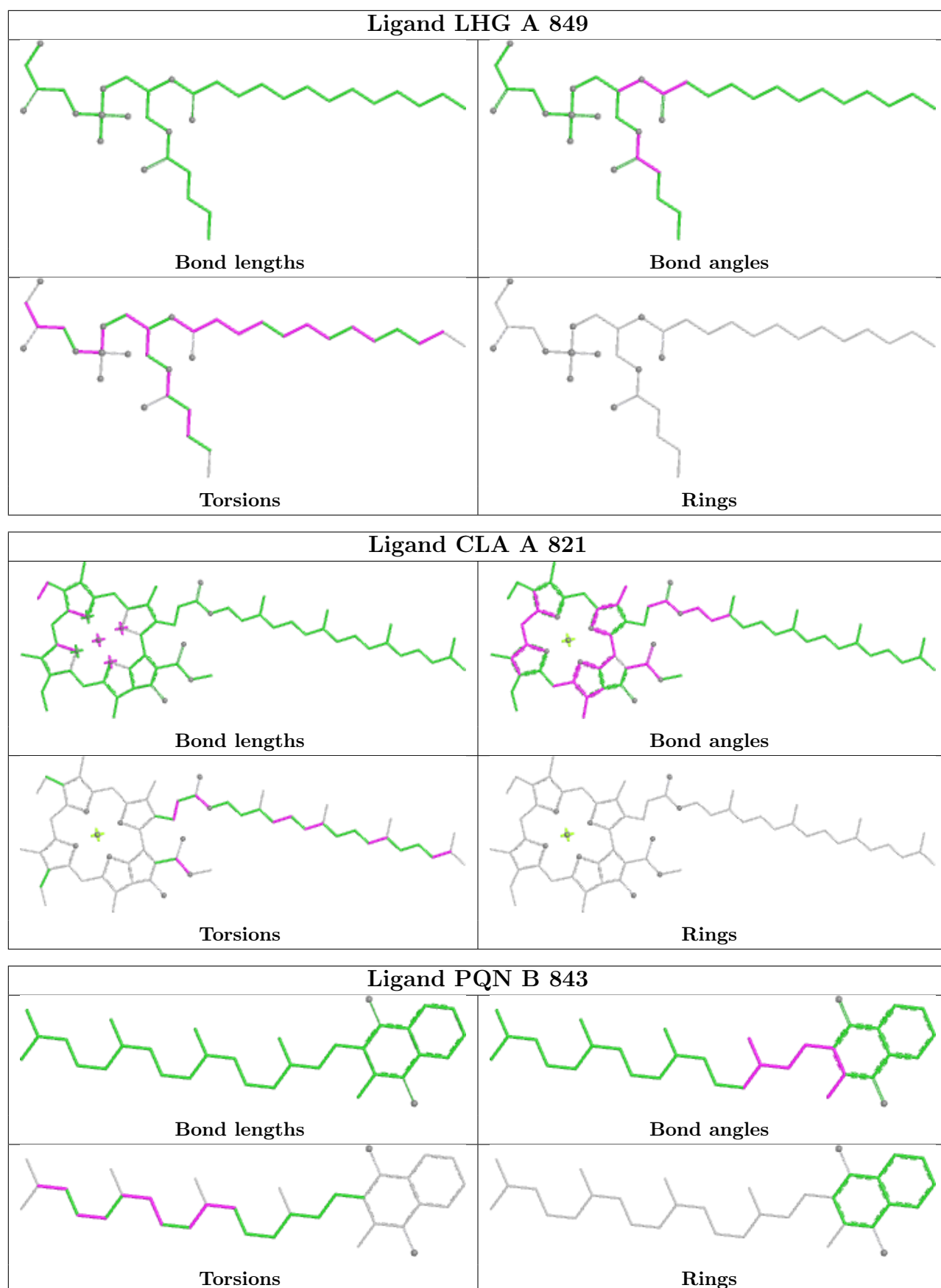


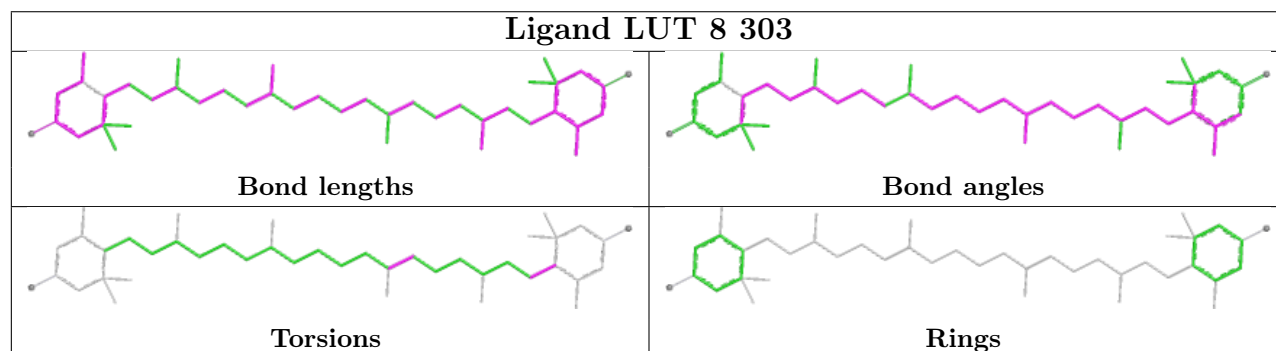
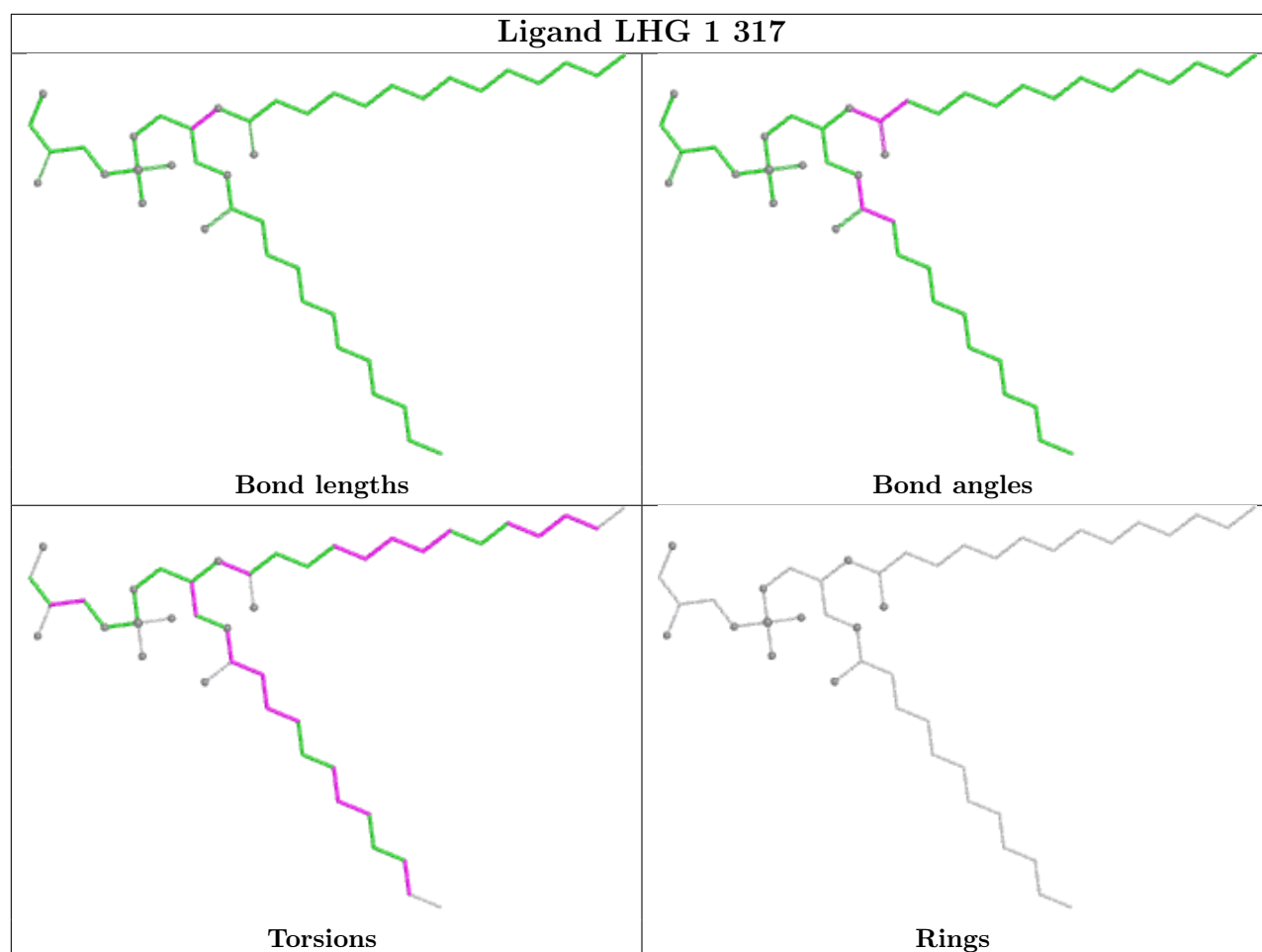
## Ligand BCR B 845





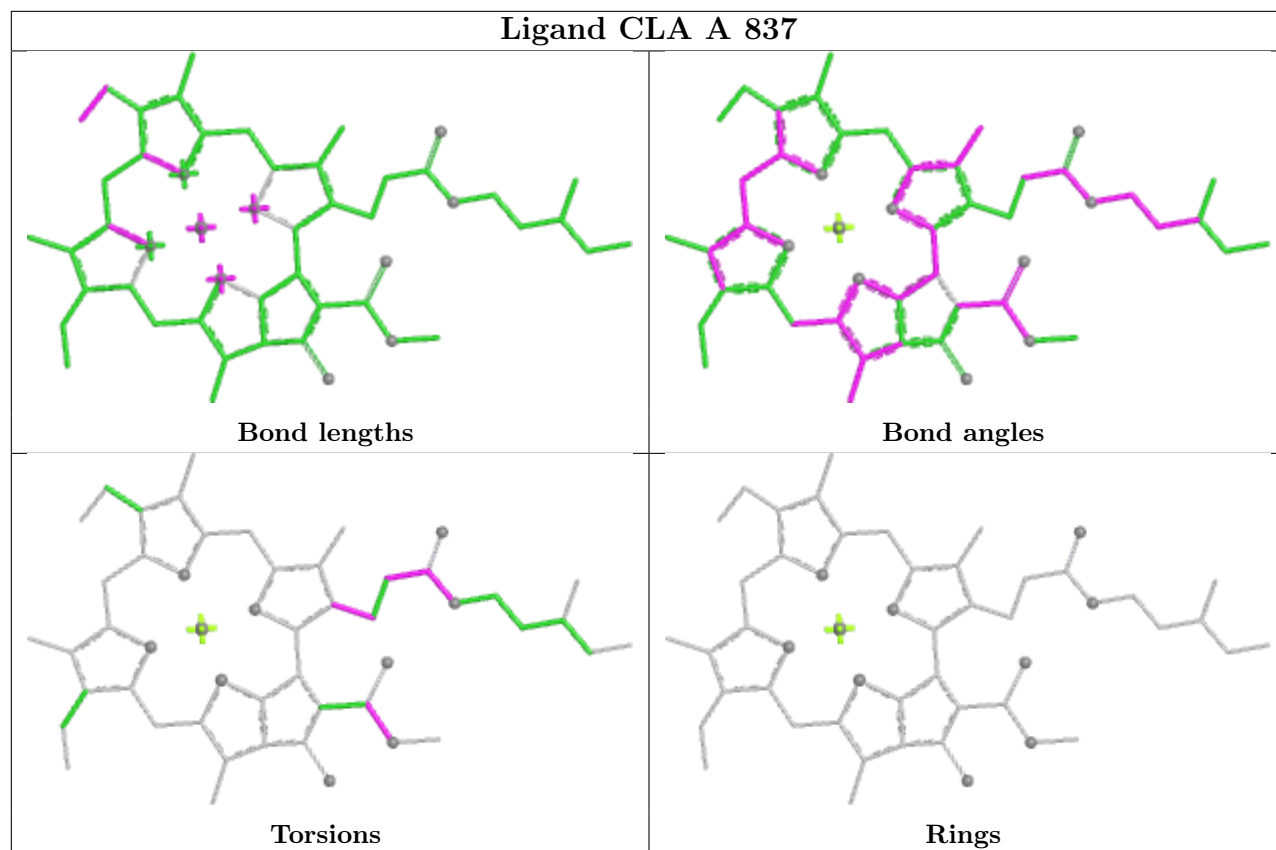




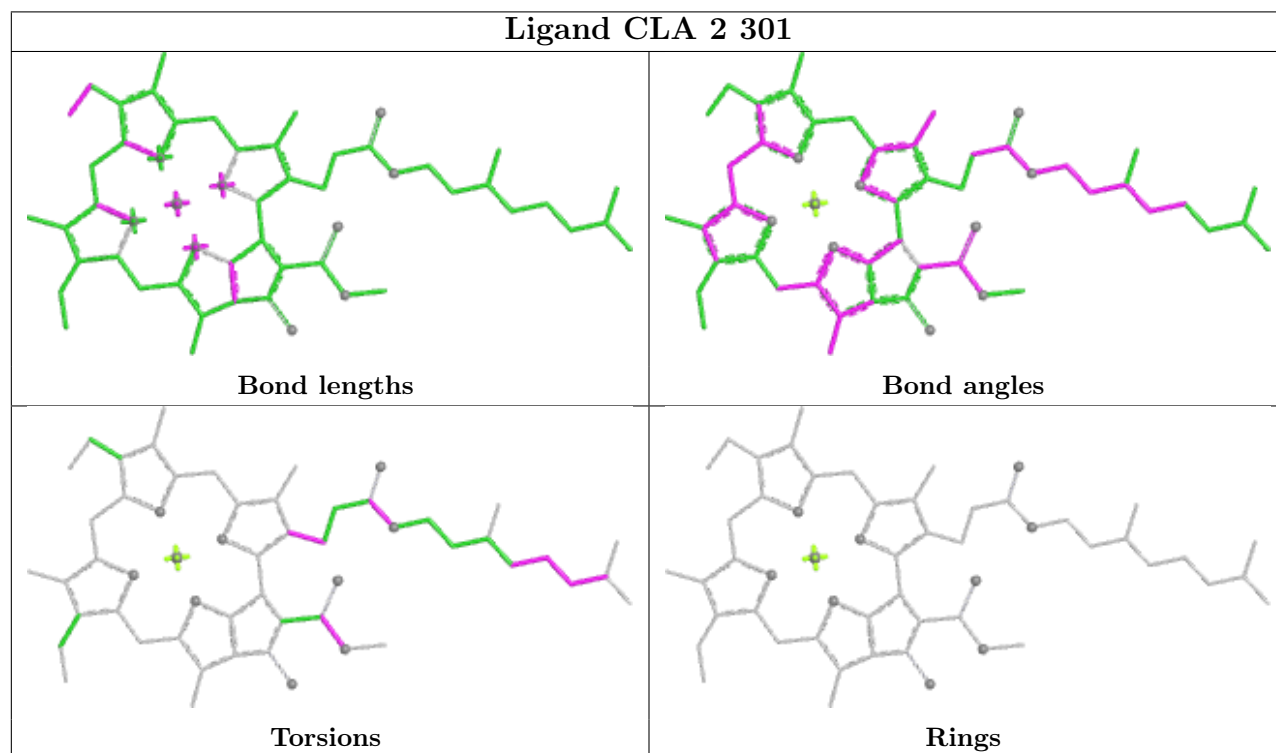




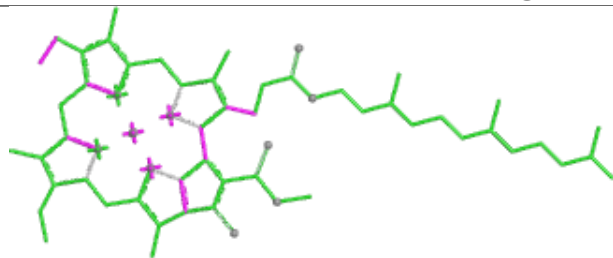
## Ligand CLA A 837



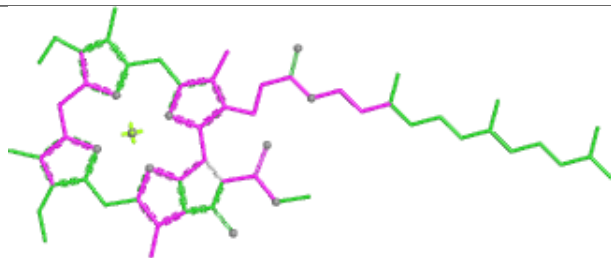
## Ligand CLA 2 301



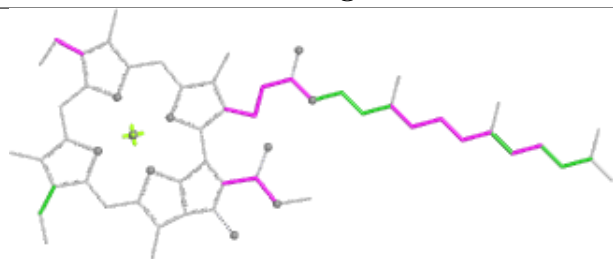
## Ligand CLA 9 305



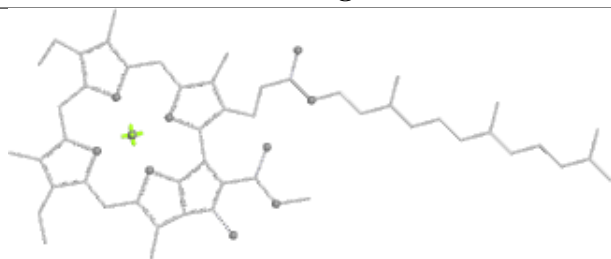
Bond lengths



Bond angles

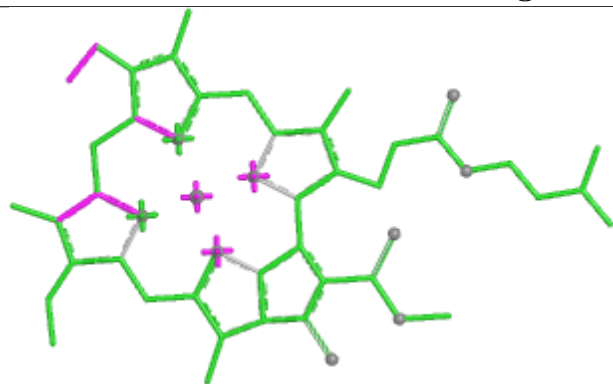


Torsions

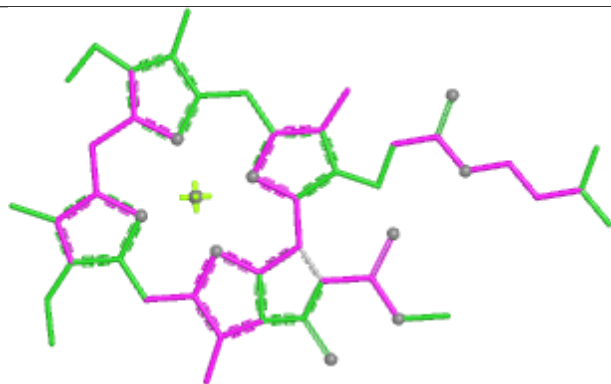


Rings

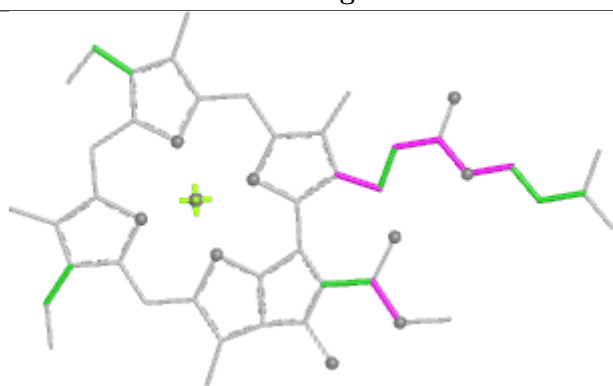
## Ligand CLA Z 310



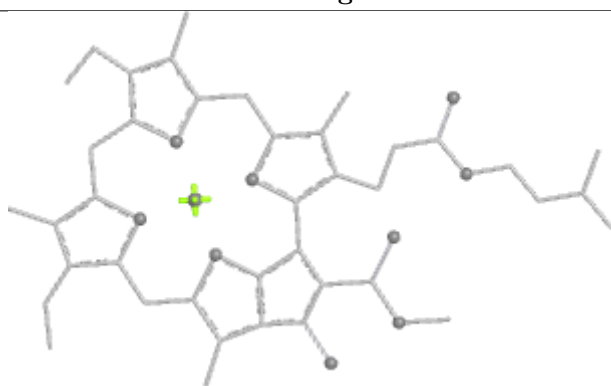
Bond lengths



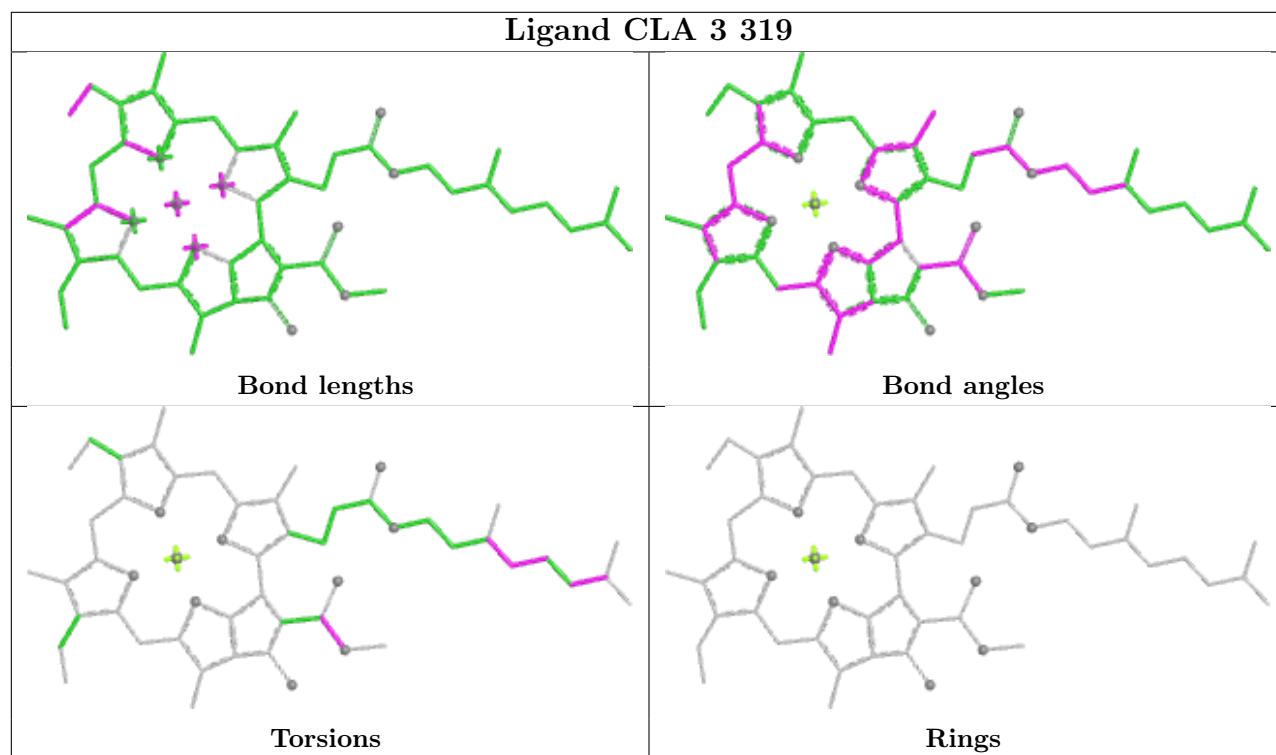
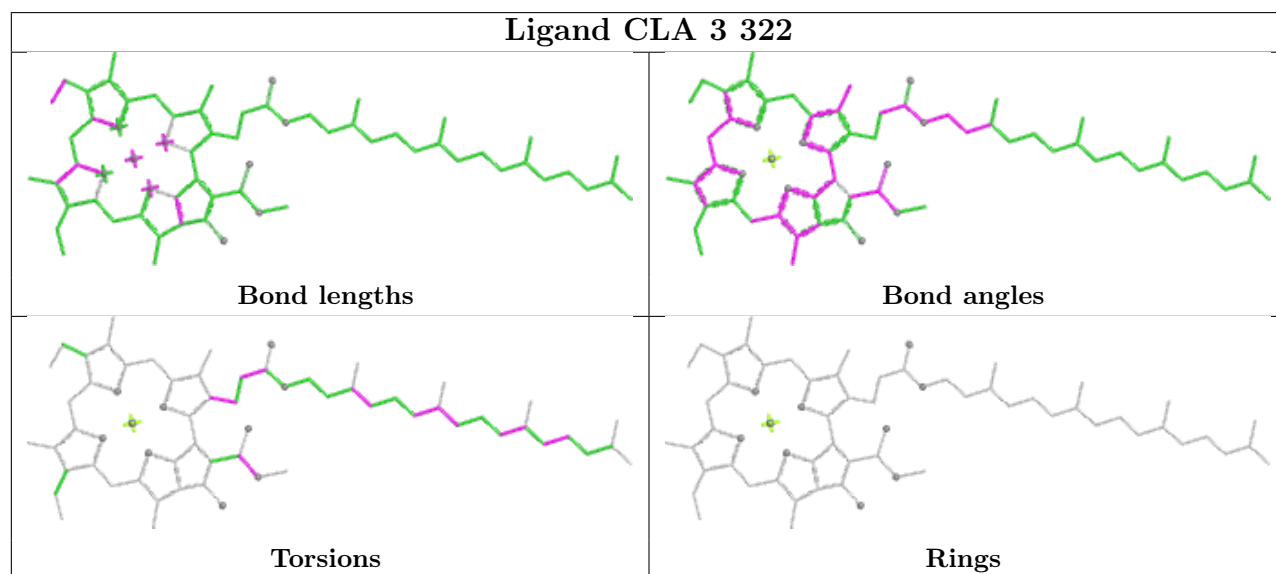
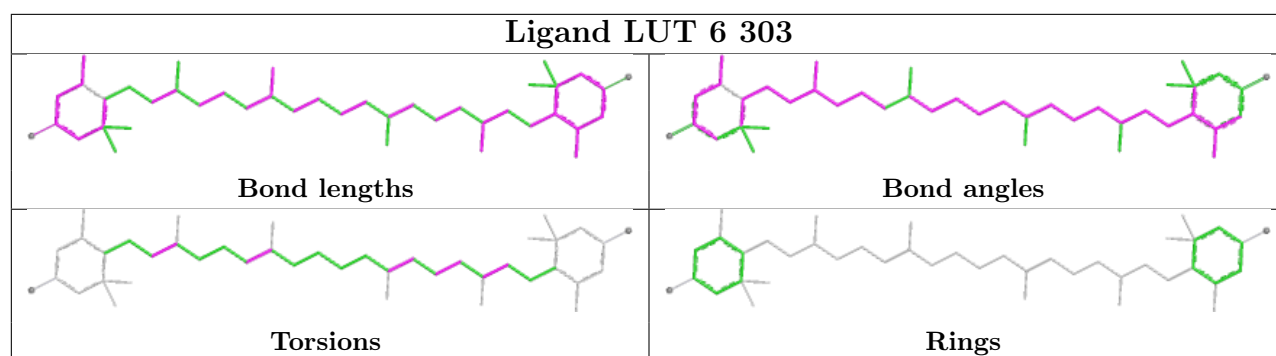
Bond angles

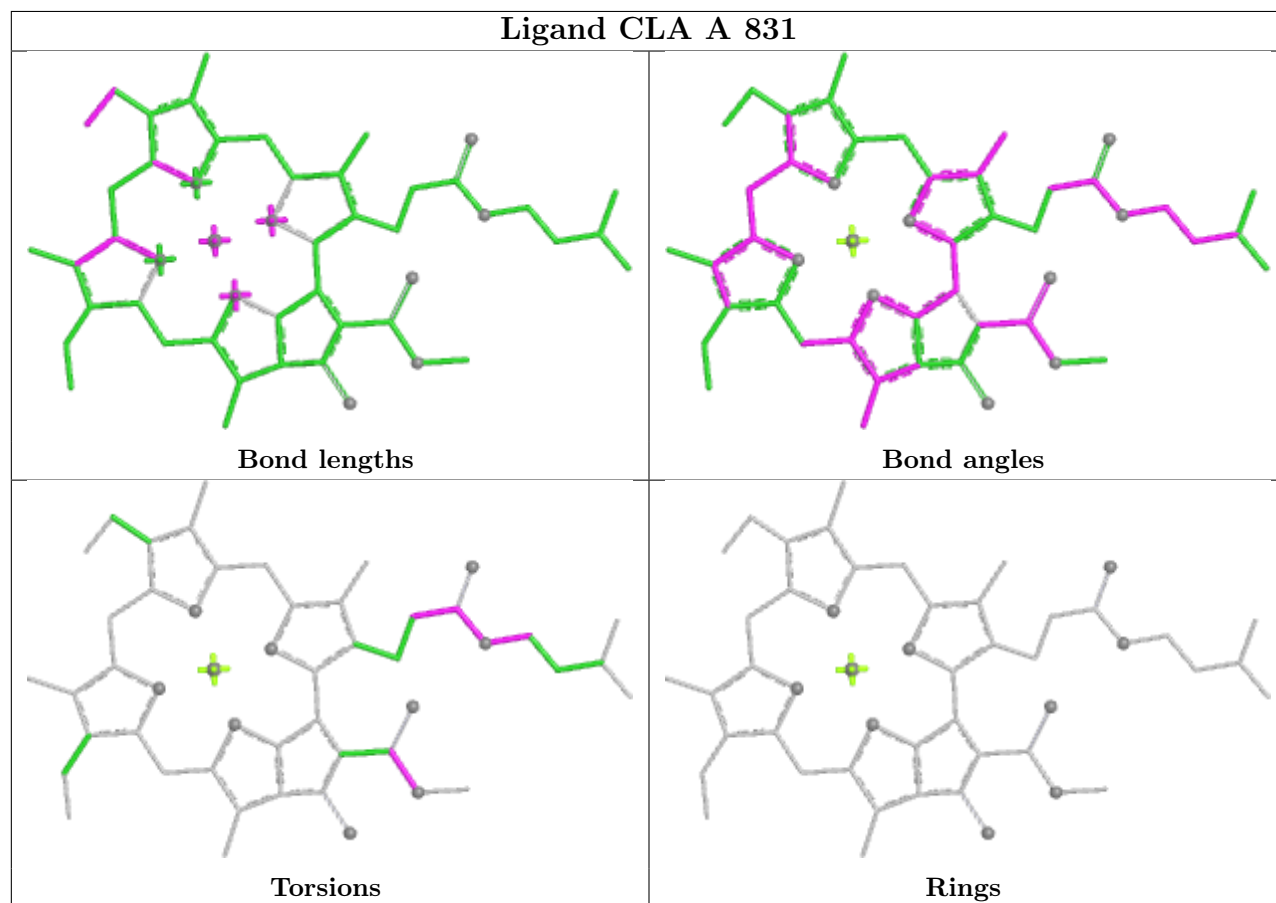
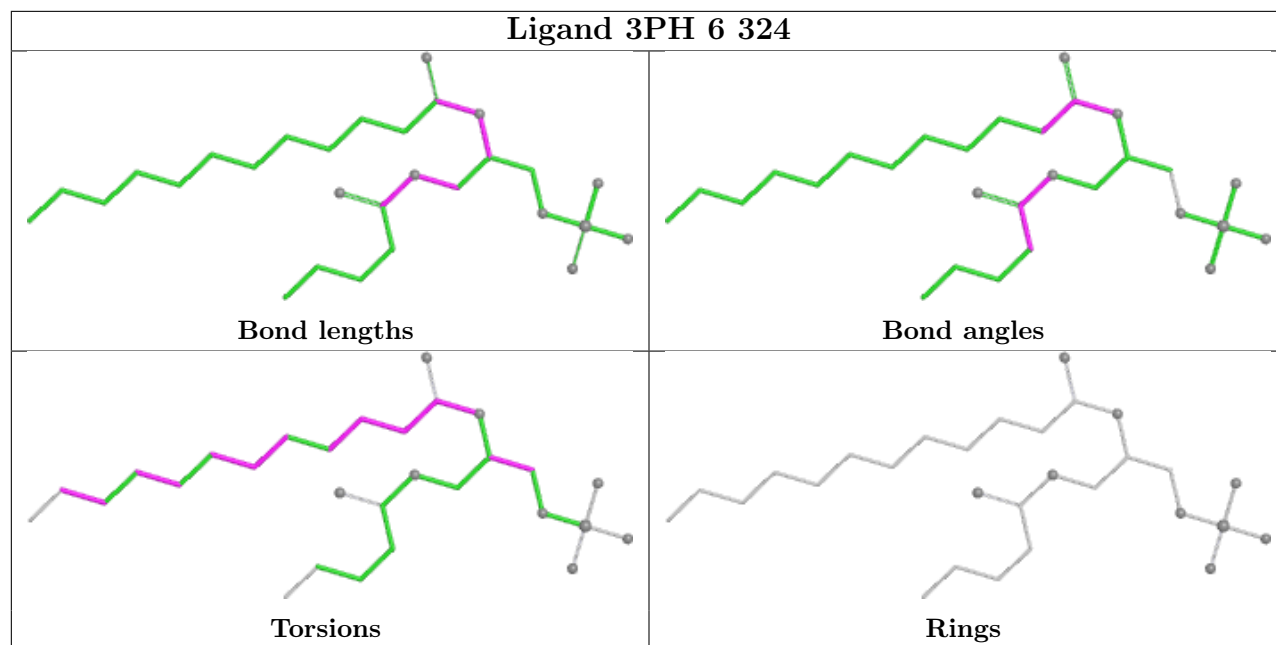


Torsions

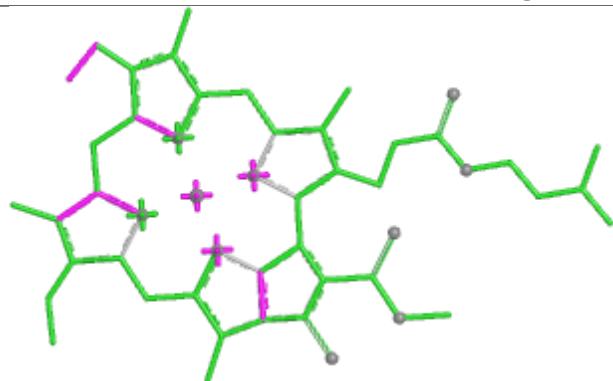


Rings

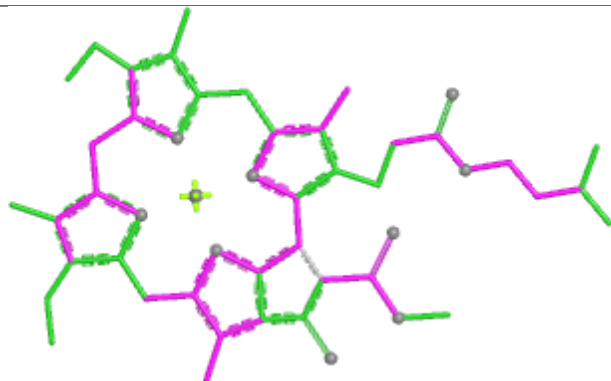




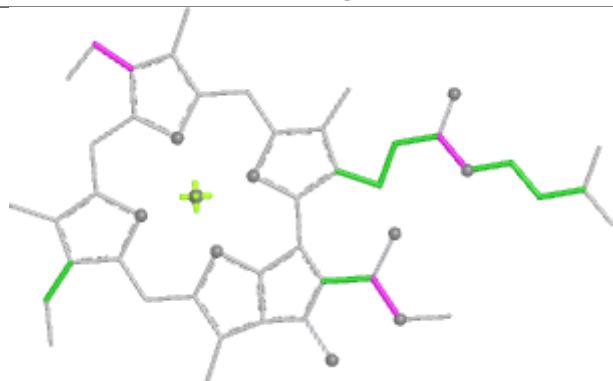
## Ligand CLA 7 305



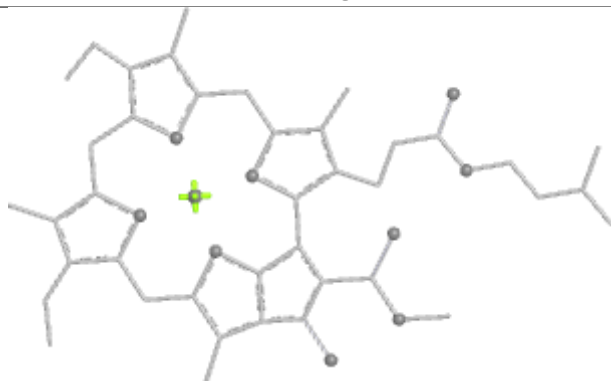
Bond lengths



Bond angles

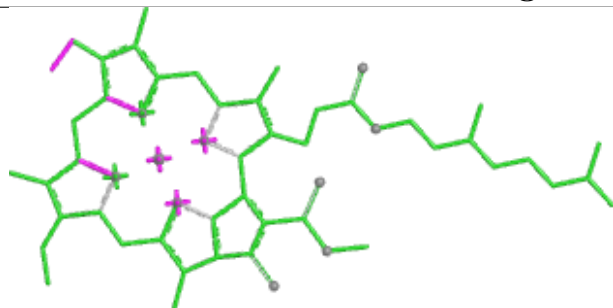


Torsions

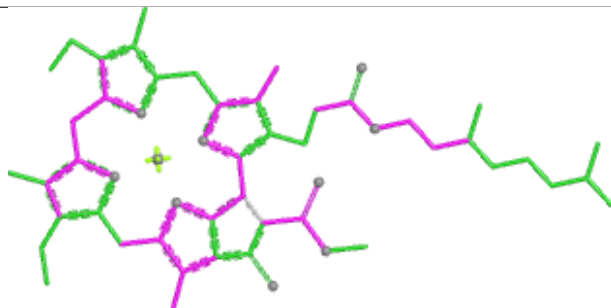


Rings

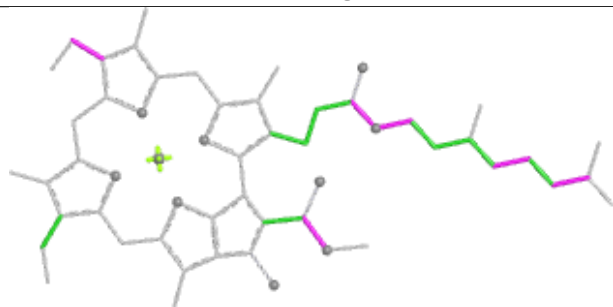
## Ligand CLA 4 812



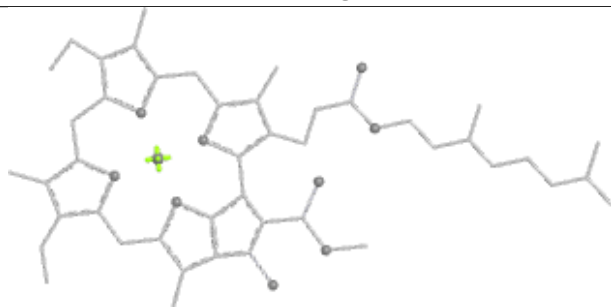
Bond lengths



Bond angles

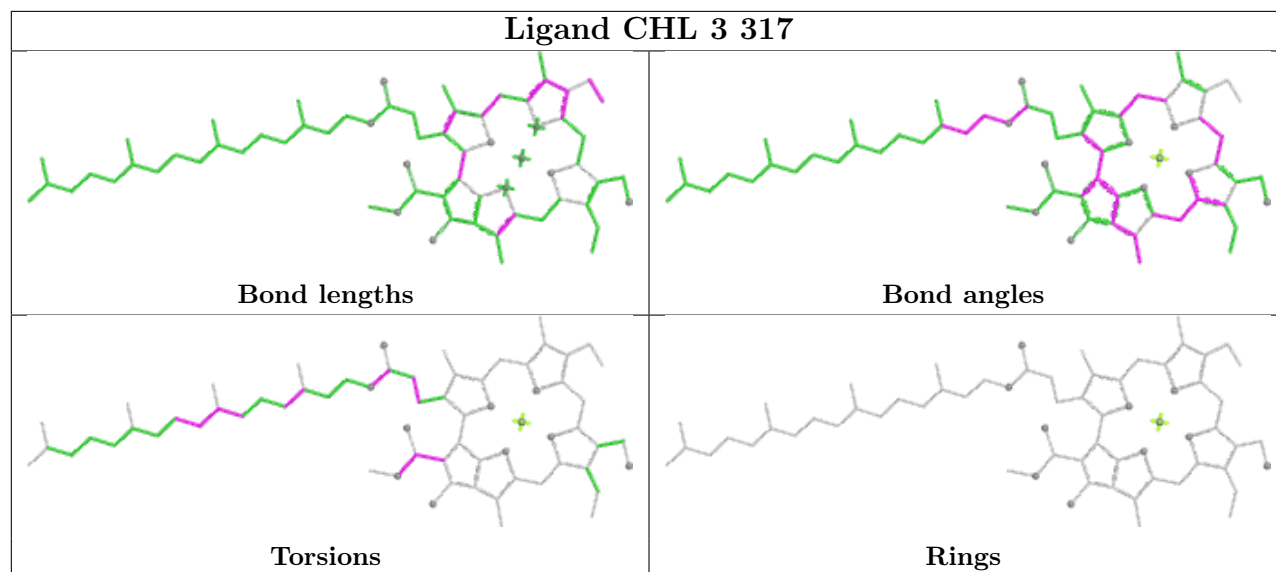


Torsions

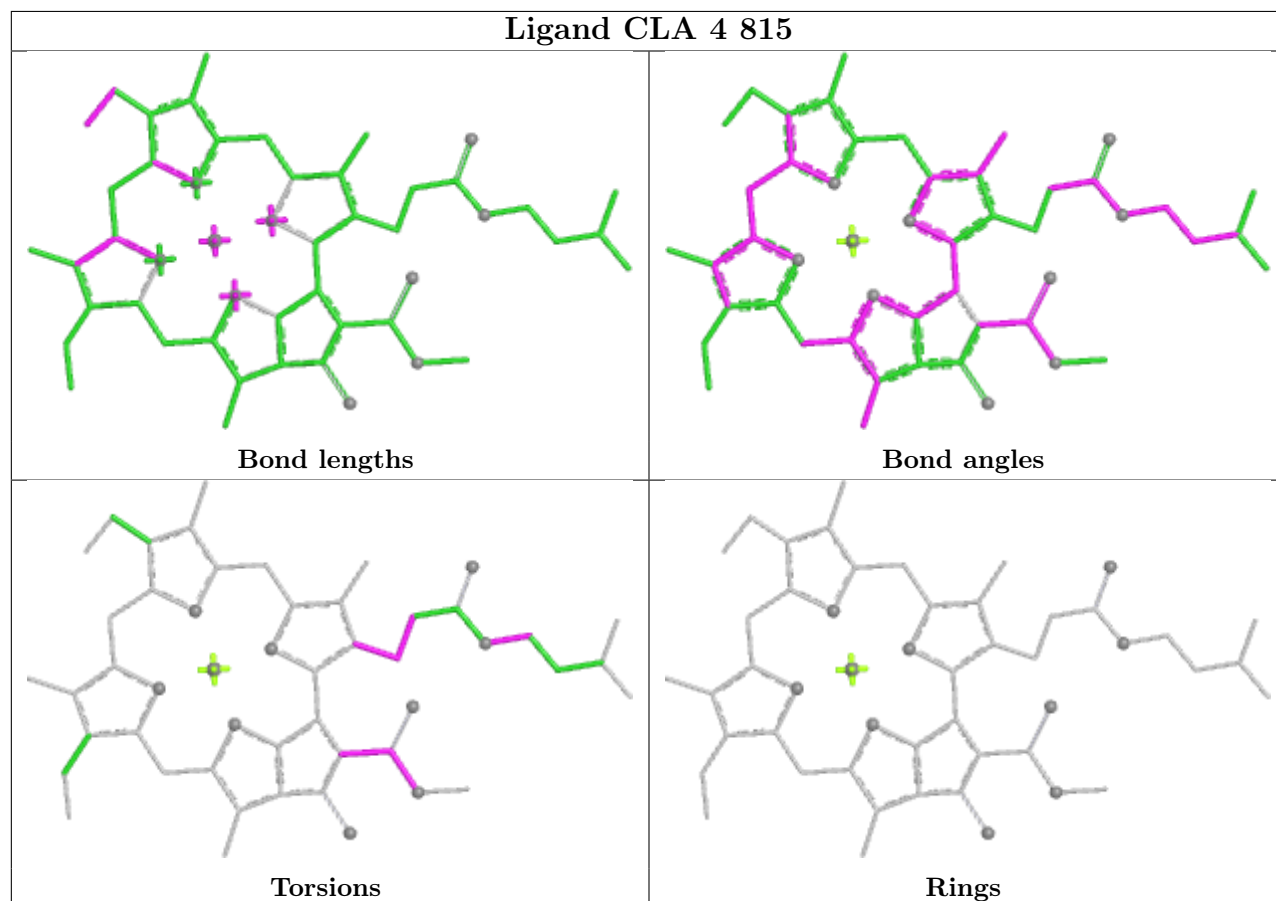


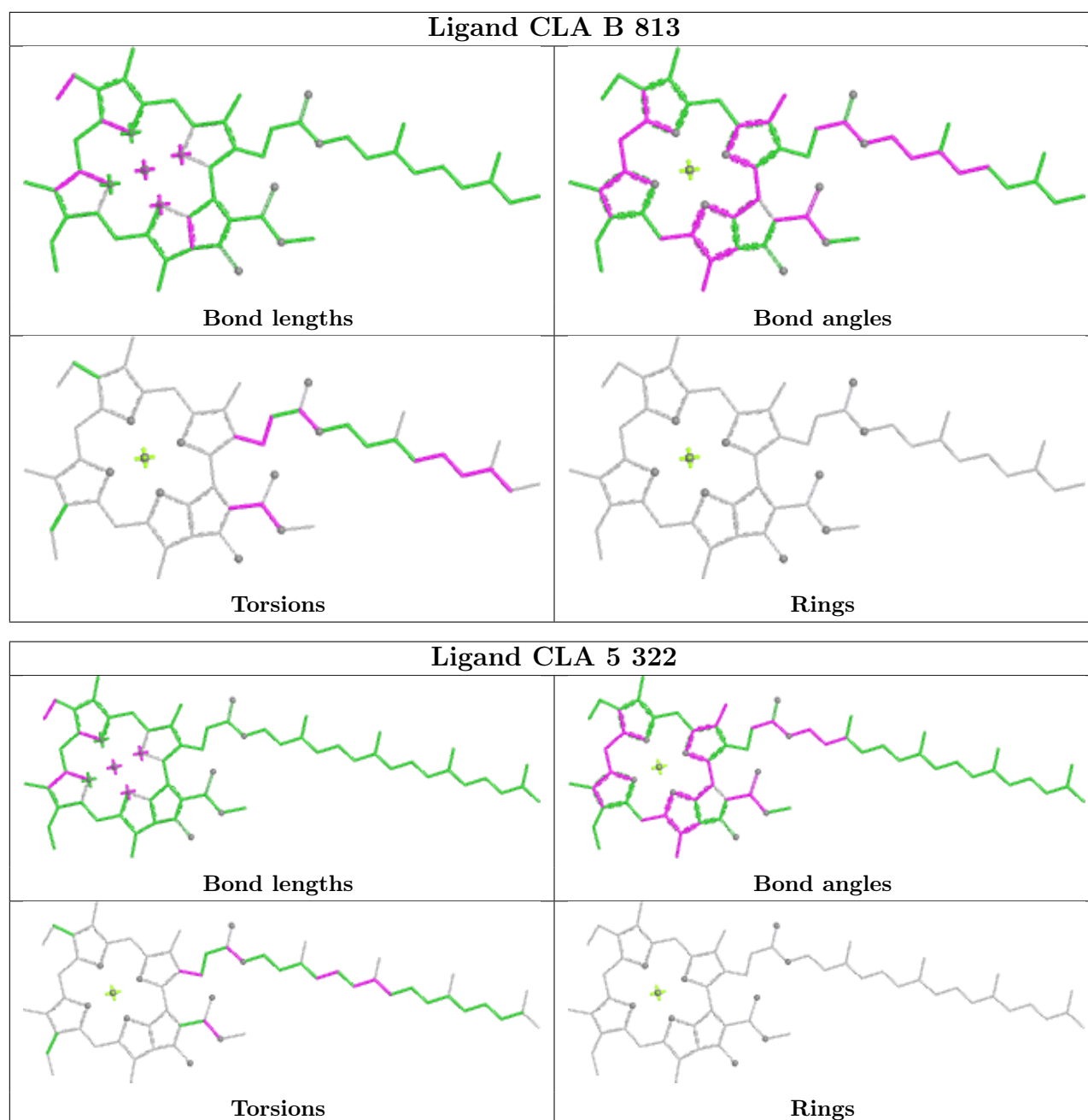
Rings

## Ligand CHL 3 317

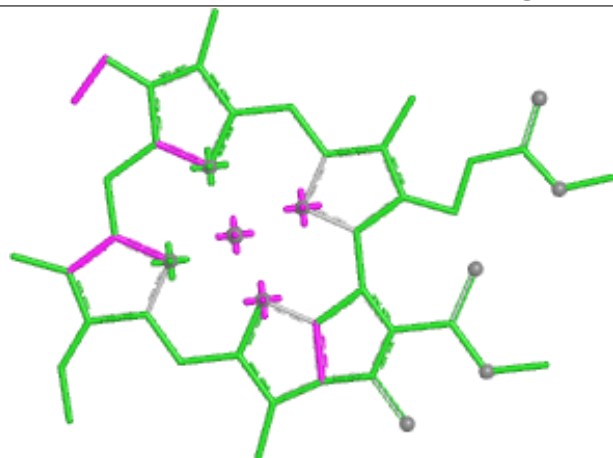


## Ligand CLA 4 815

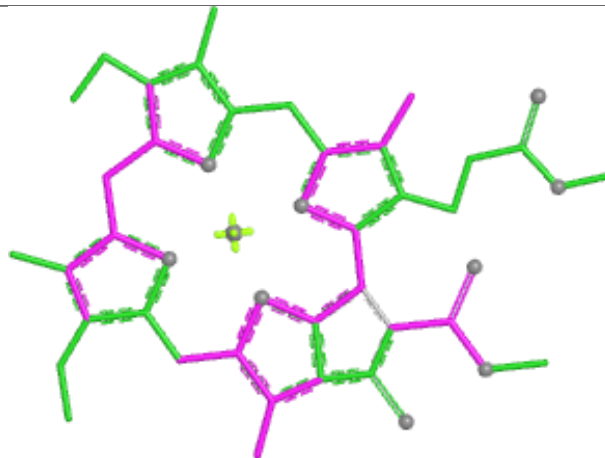




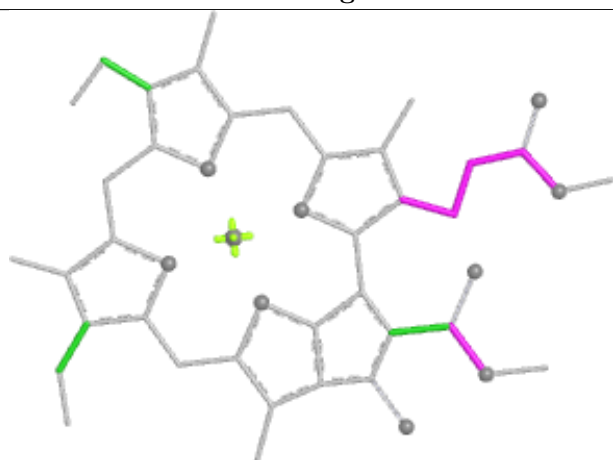
## Ligand CLA 8 314



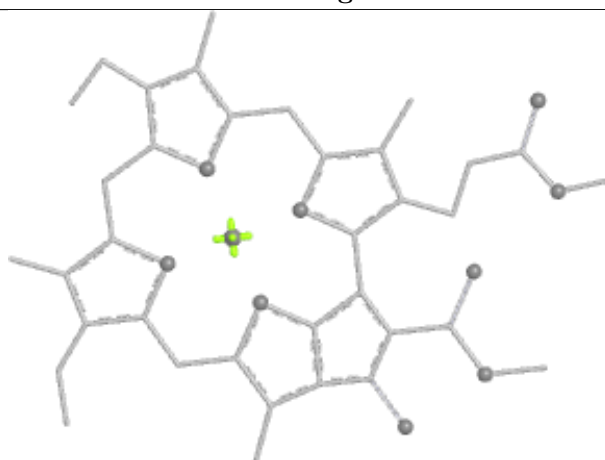
Bond lengths



Bond angles

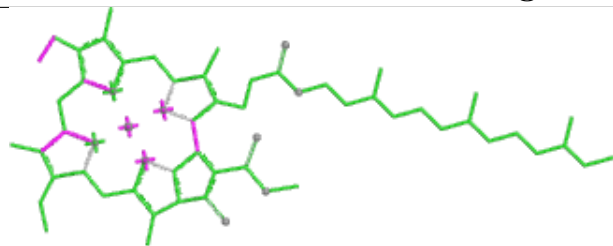


Torsions

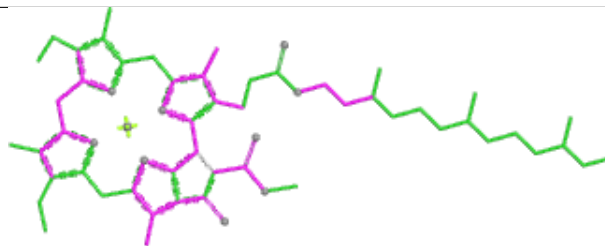


Rings

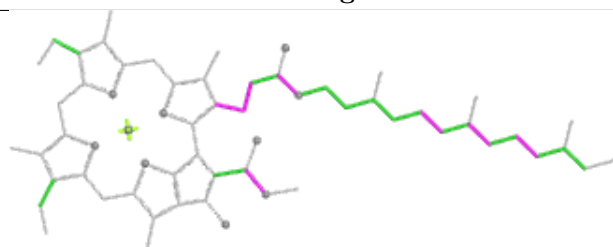
## Ligand CLA 5 313



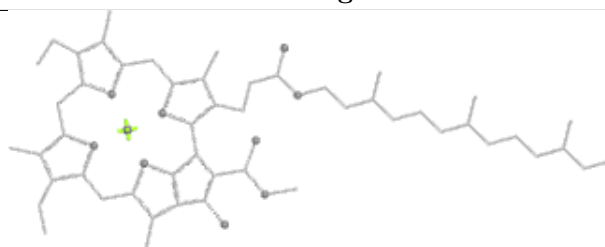
Bond lengths



Bond angles



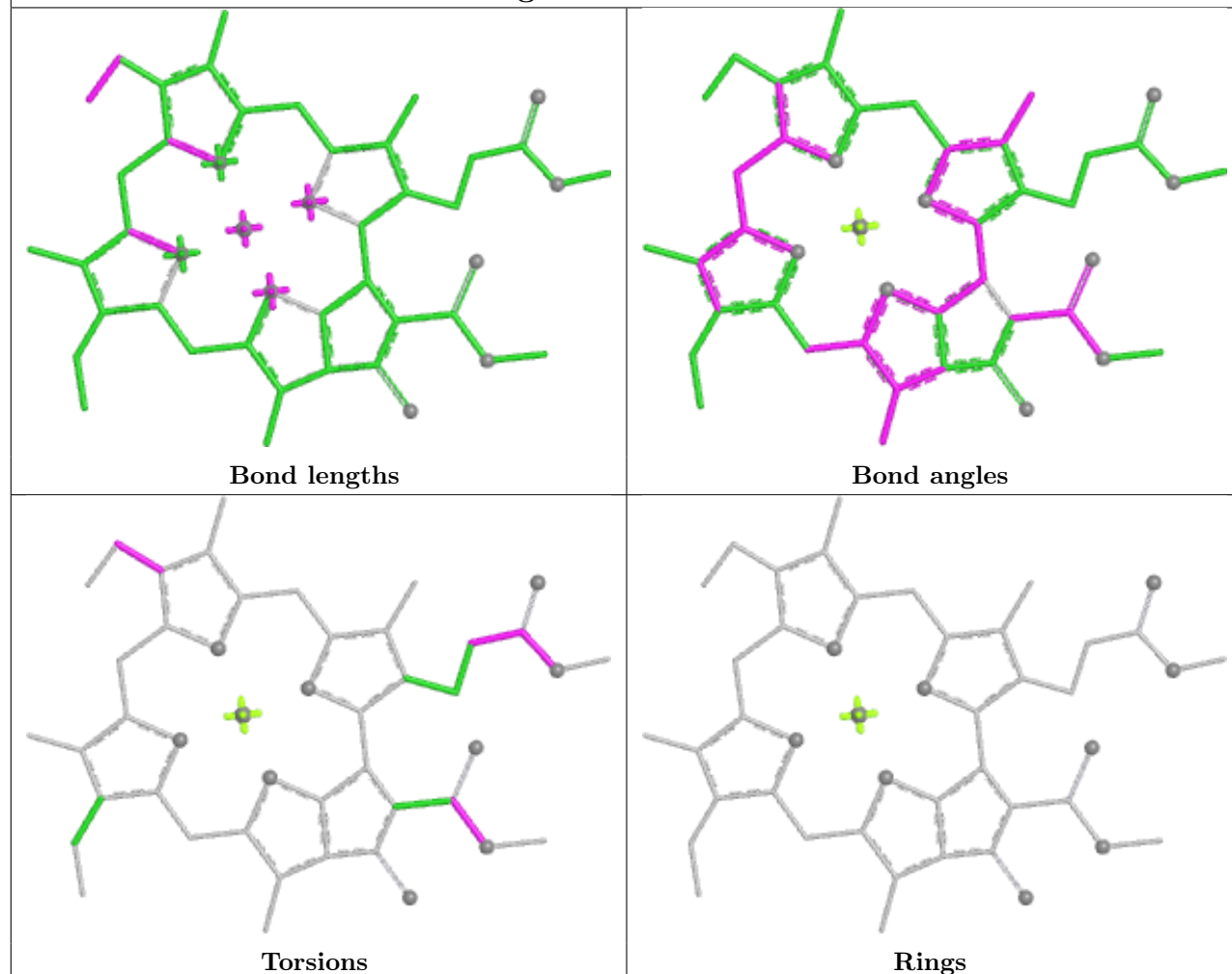
Torsions



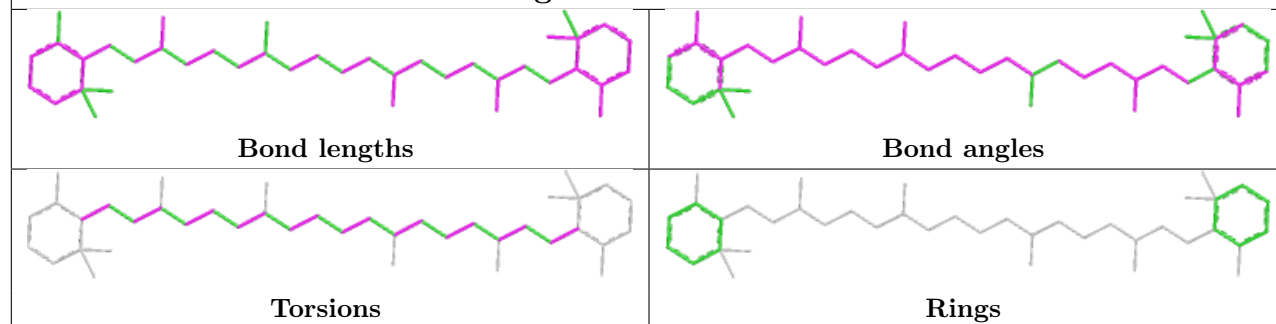
Rings



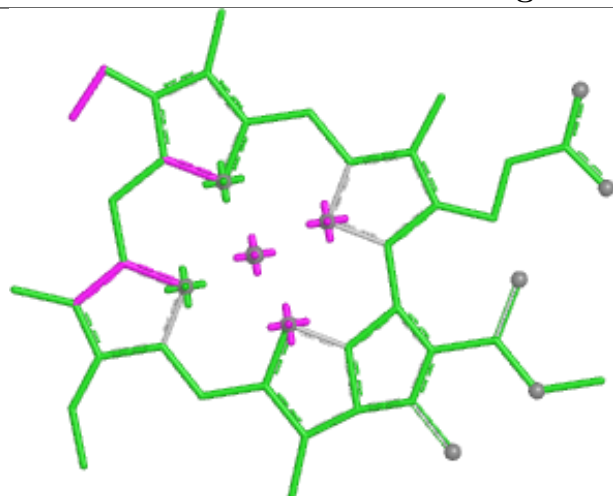
## Ligand CLA 5 323



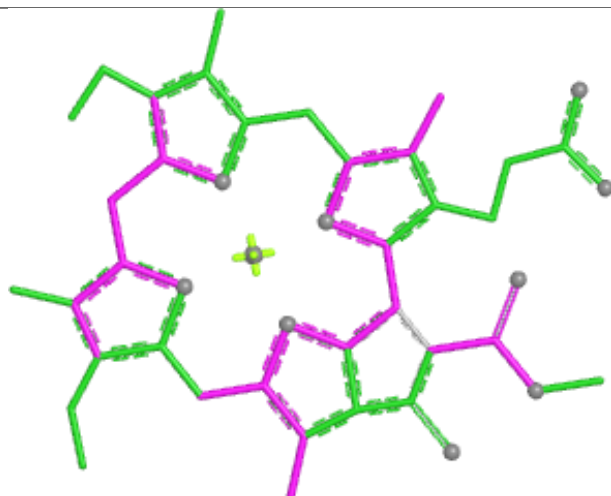
## Ligand BCR 6 306



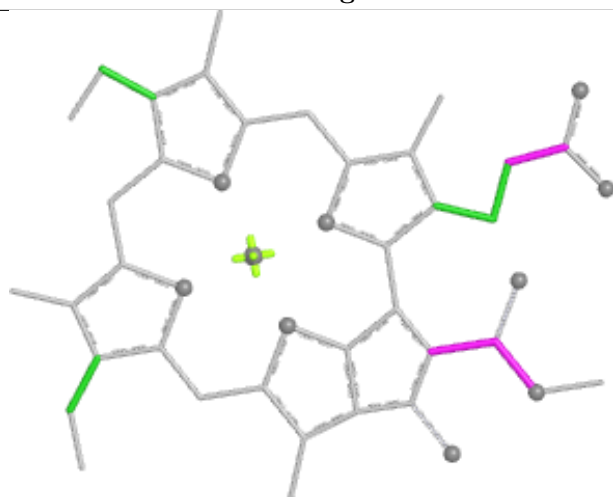
## Ligand CLA Z 304



Bond lengths



Bond angles

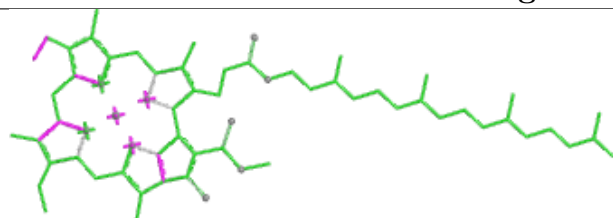


Torsions

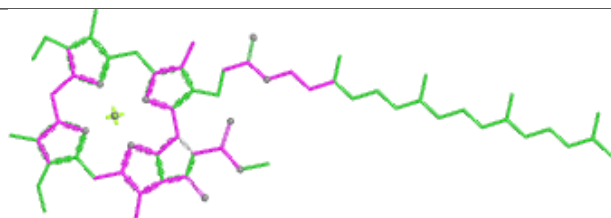


Rings

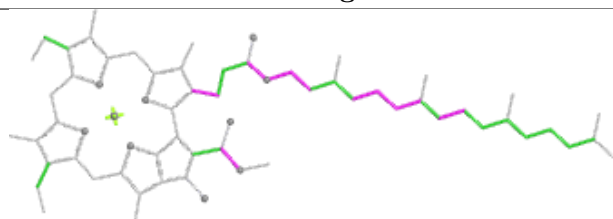
## Ligand CLA 1 313



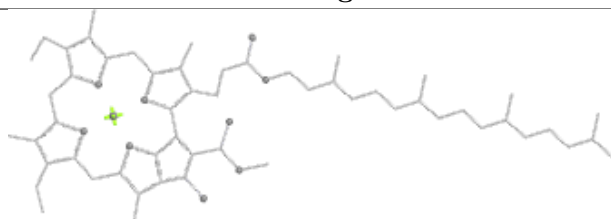
Bond lengths



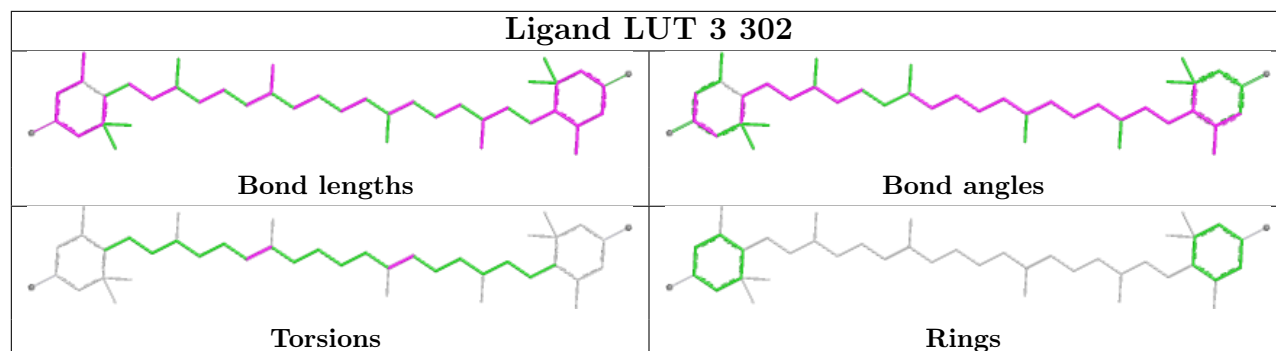
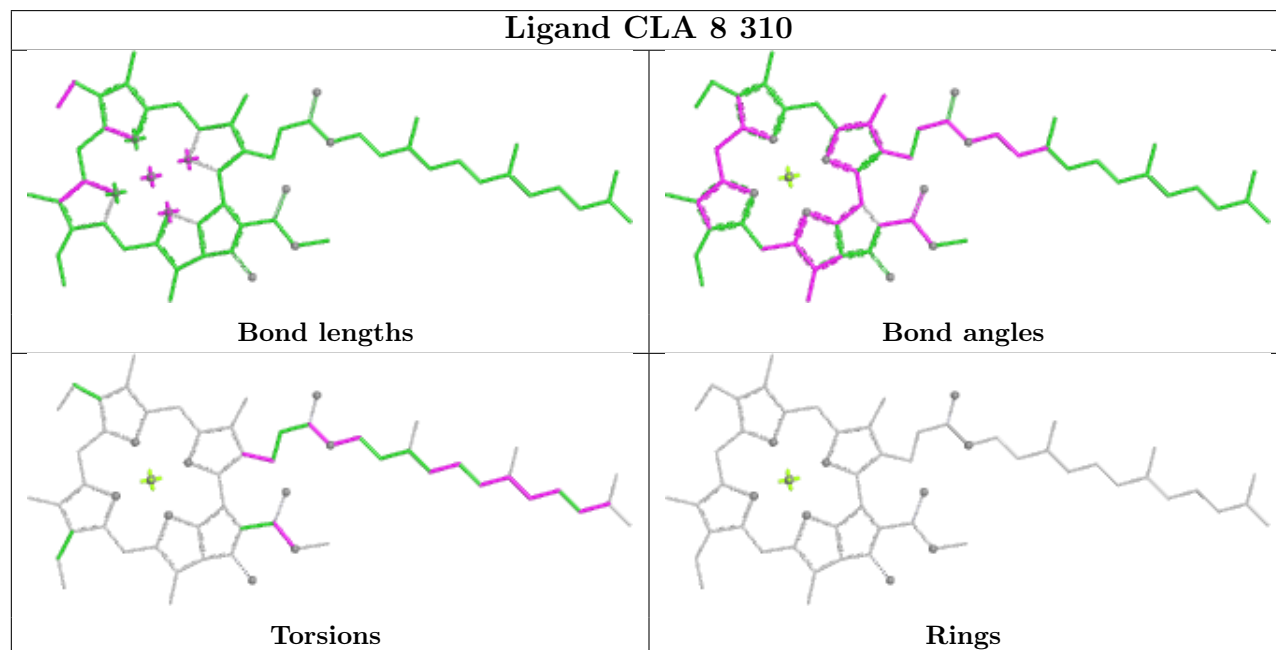
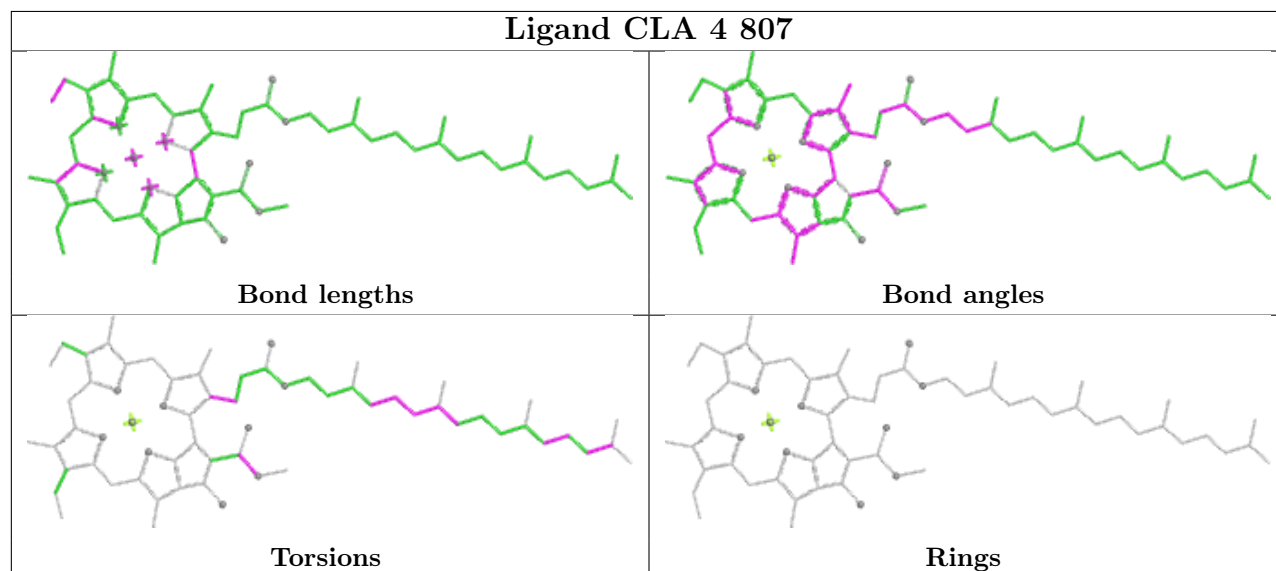
Bond angles



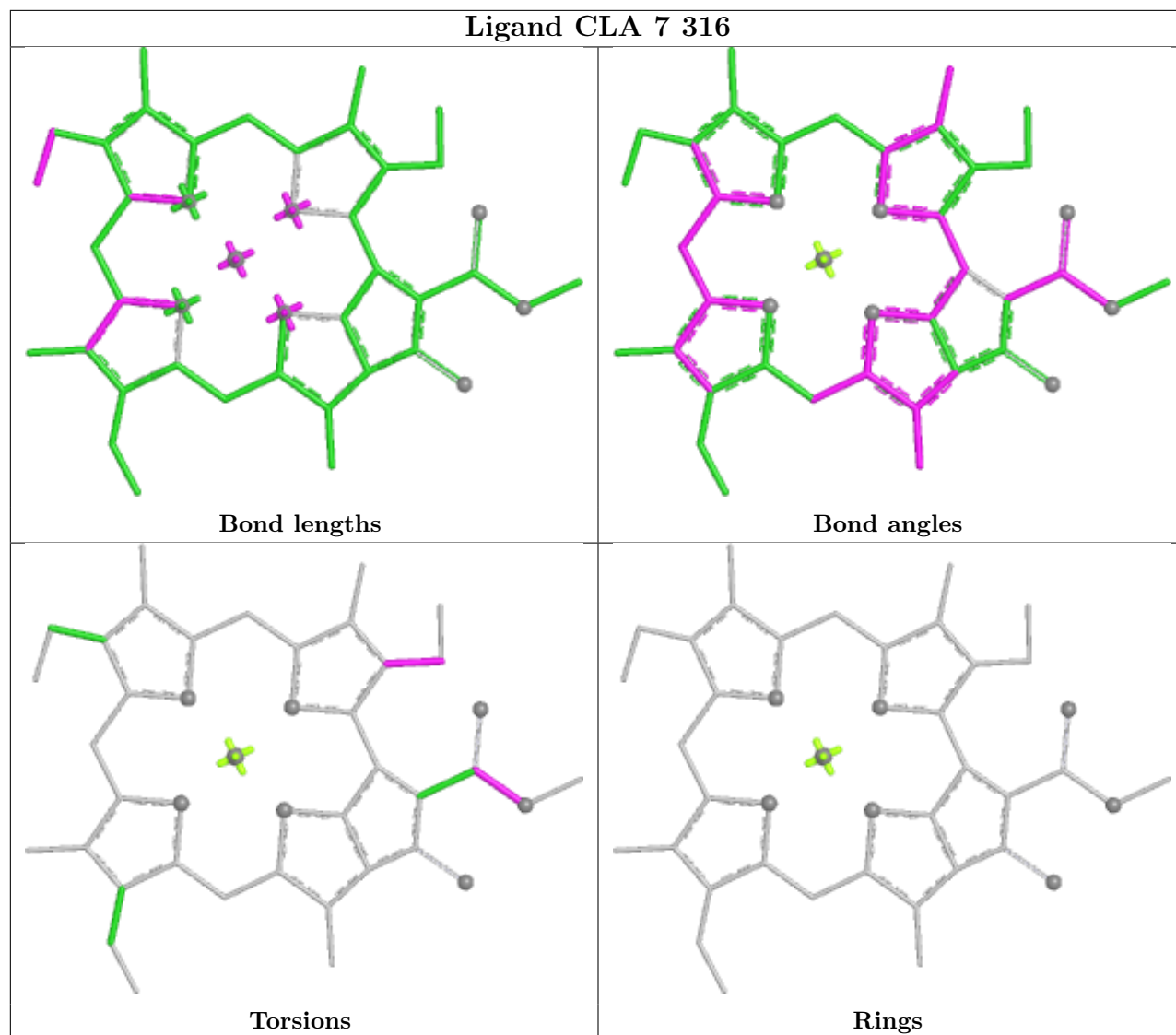
Torsions



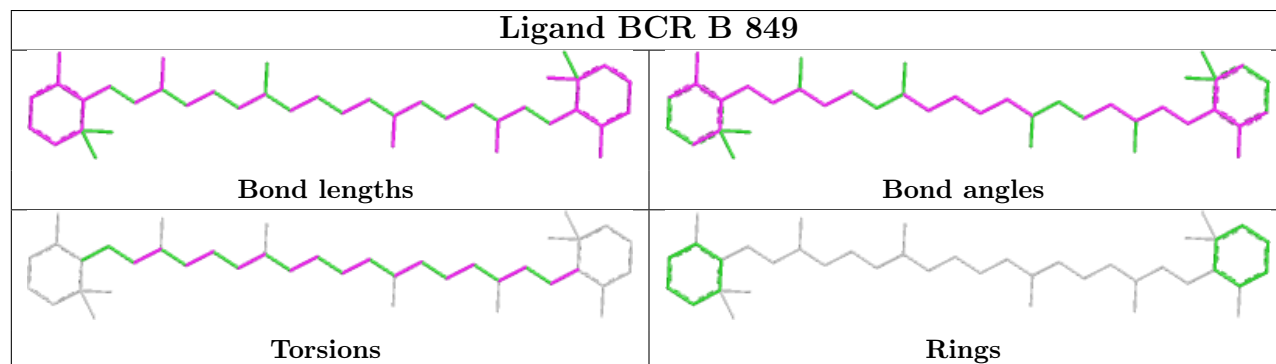
Rings

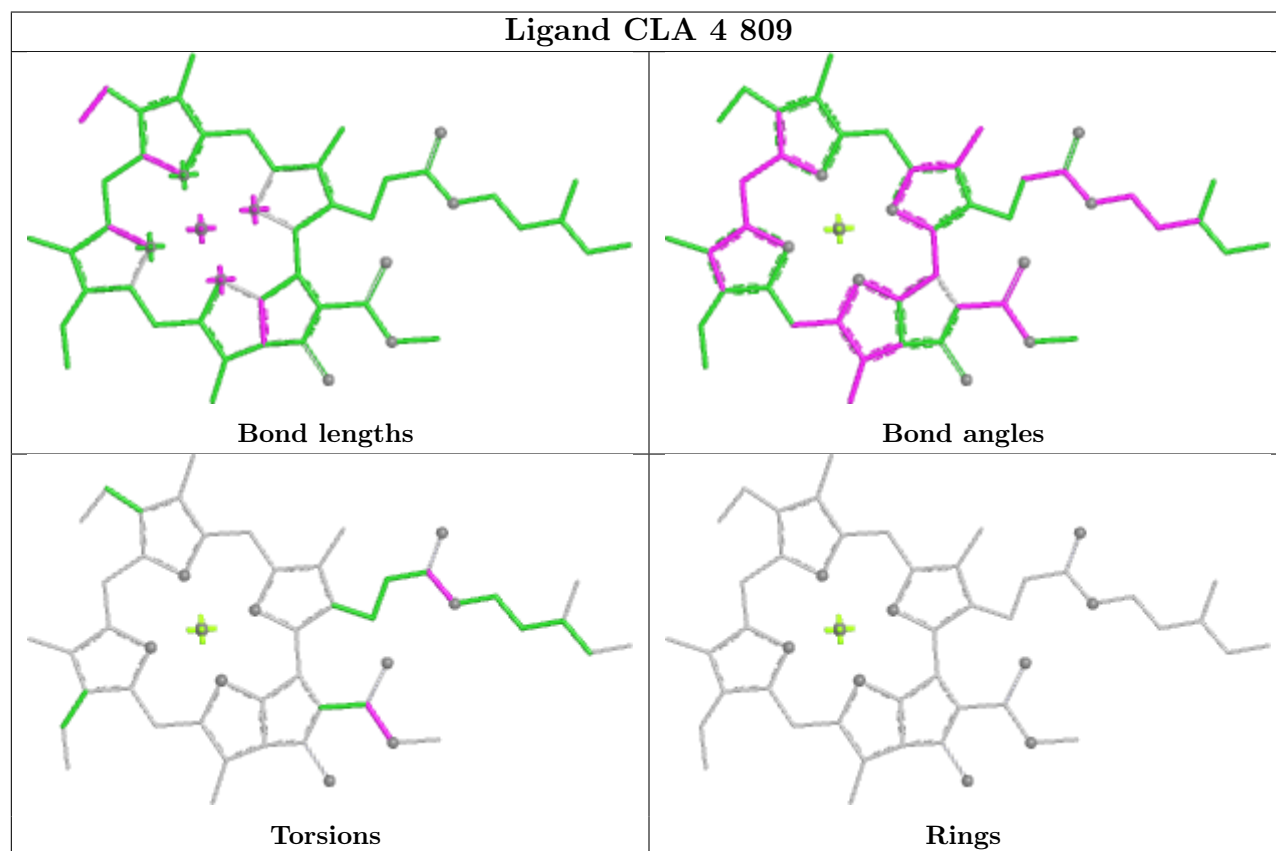
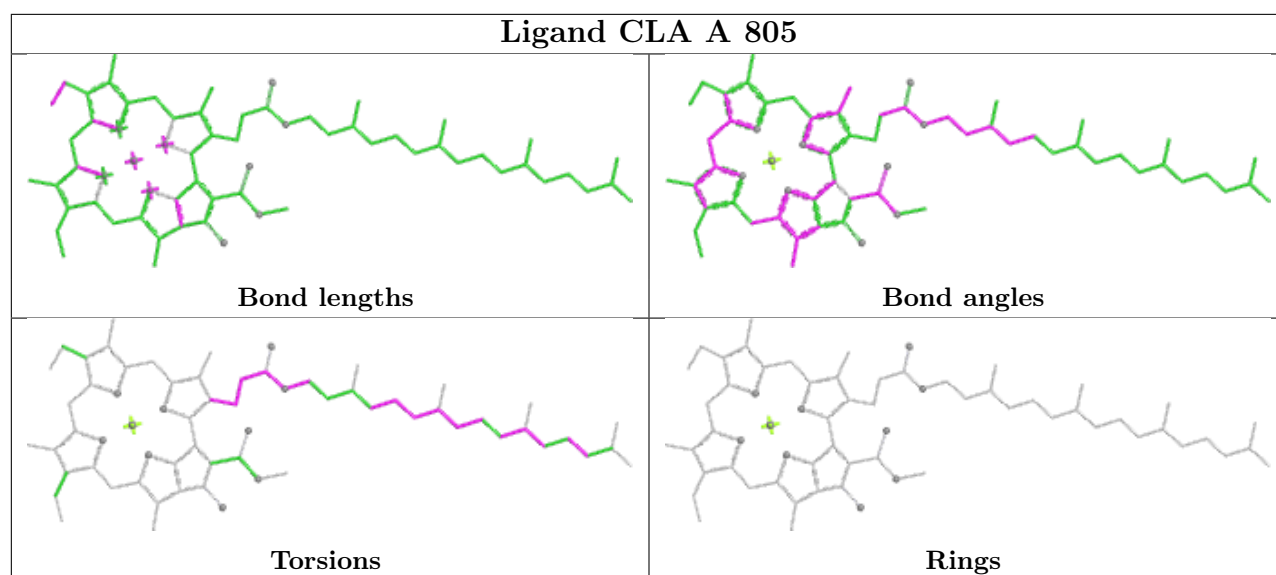
**Ligand LUT 3 302****Ligand CLA 8 310****Ligand CLA 4 807**

## Ligand CLA 7 316

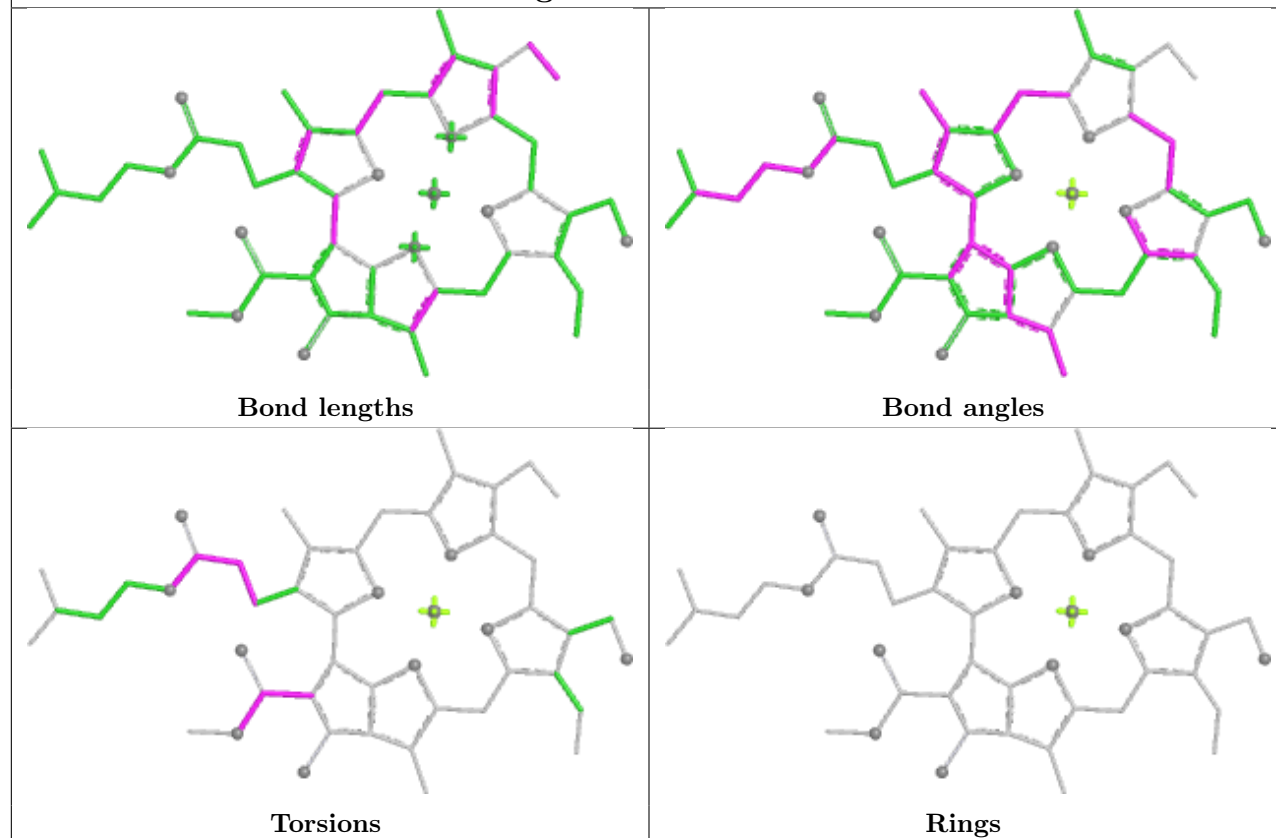


## Ligand BCR B 849

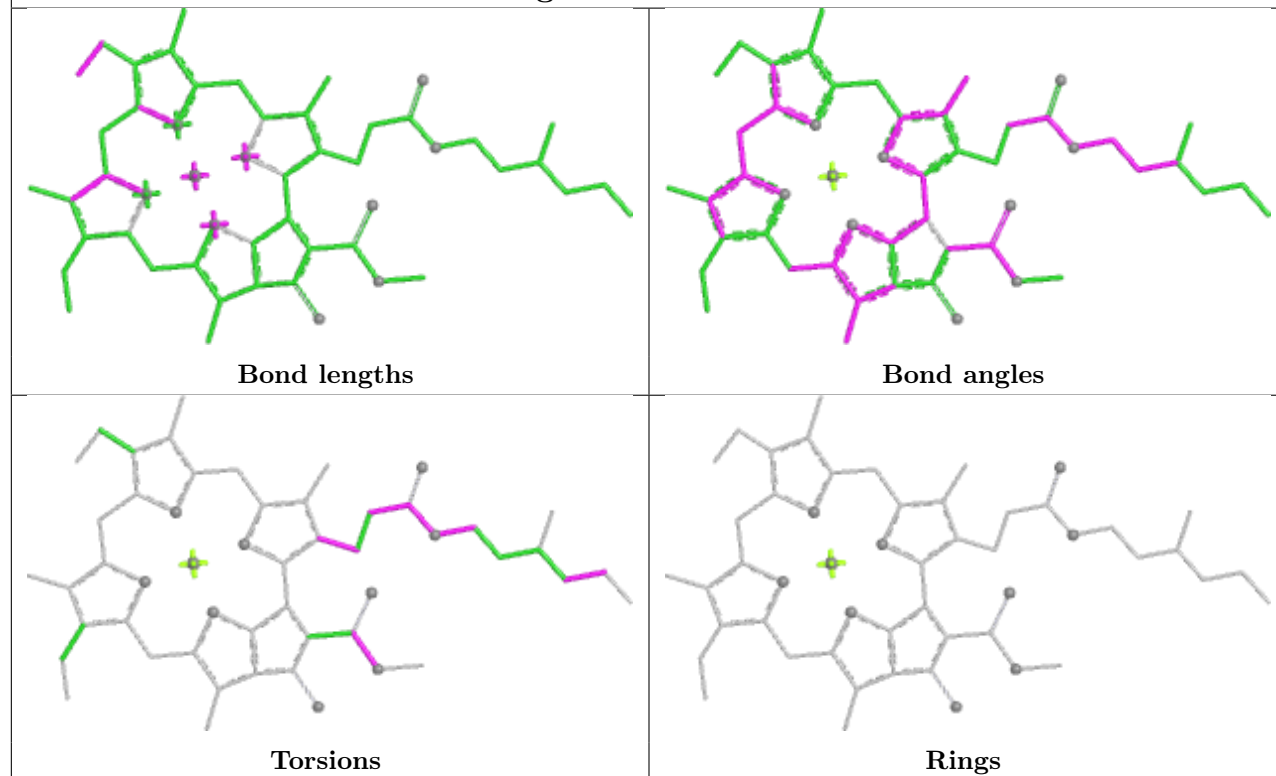




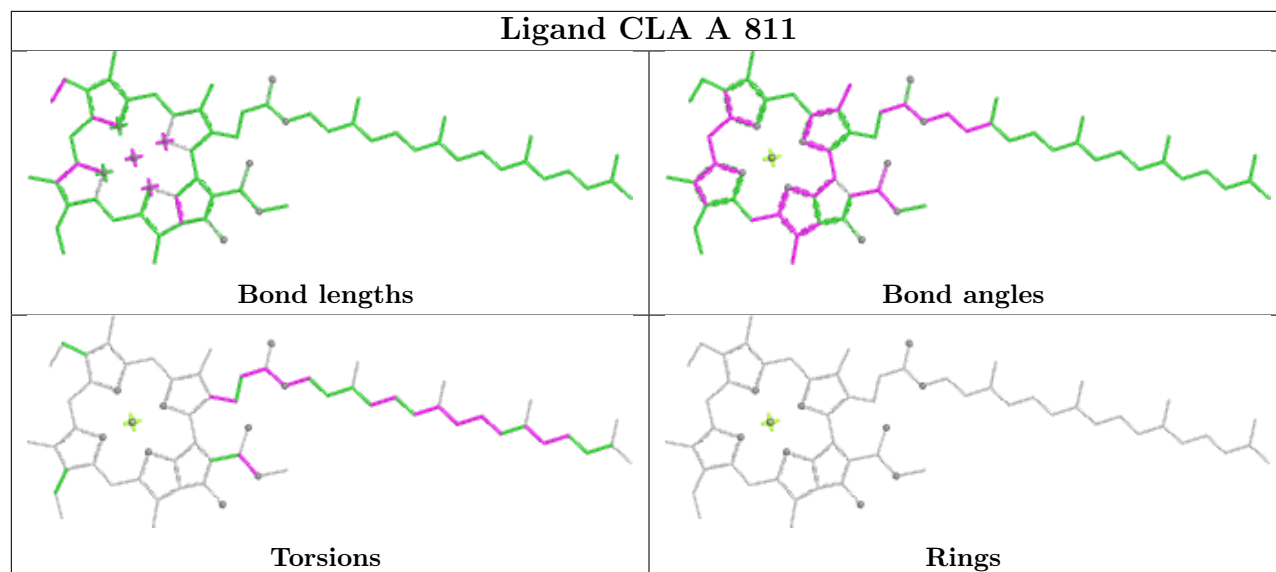
## Ligand CHL 2 303



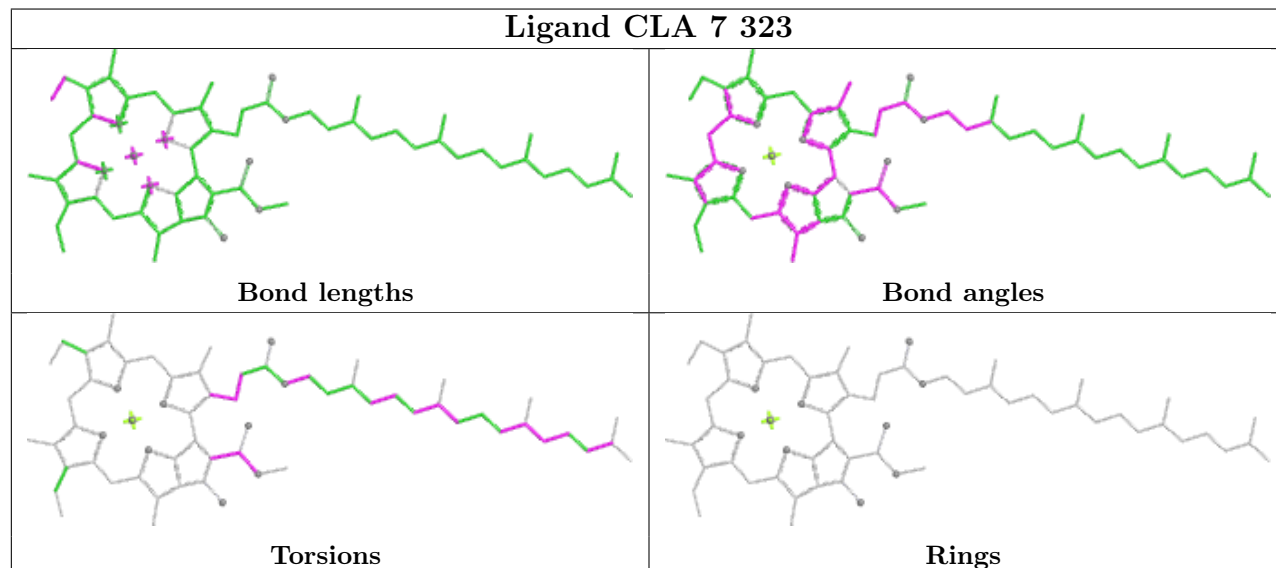
## Ligand CLA 3 316



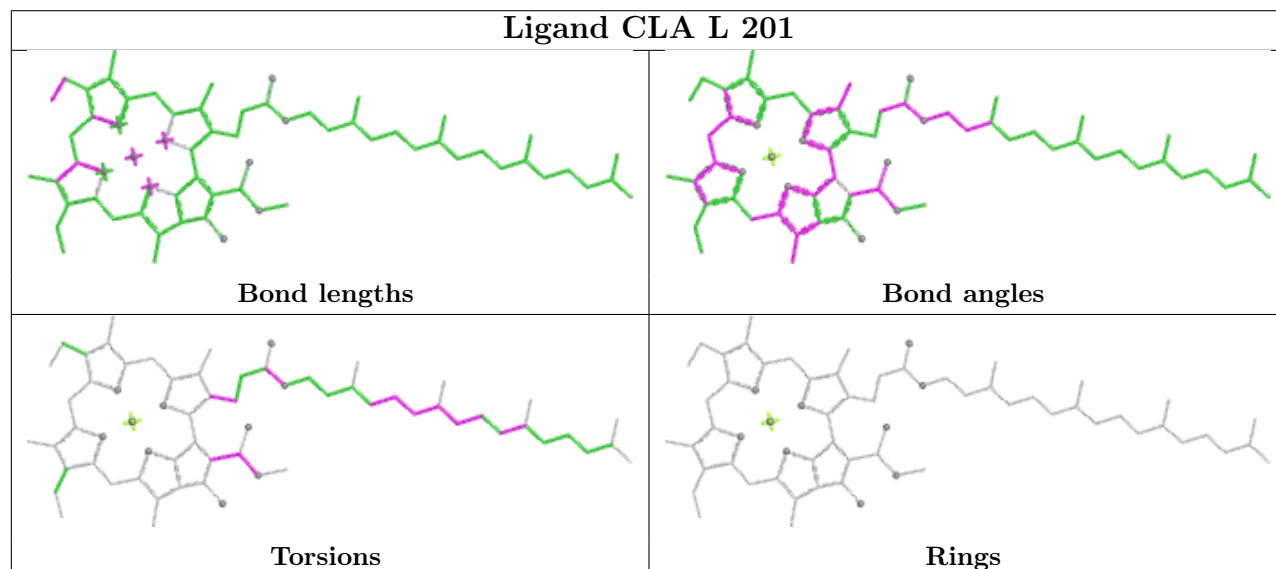
## Ligand CLA A 811



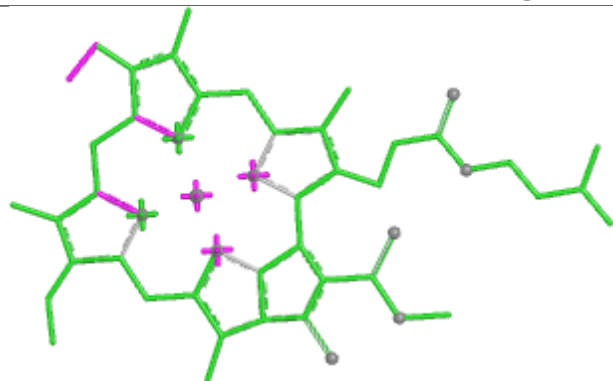
## Ligand CLA 7 323



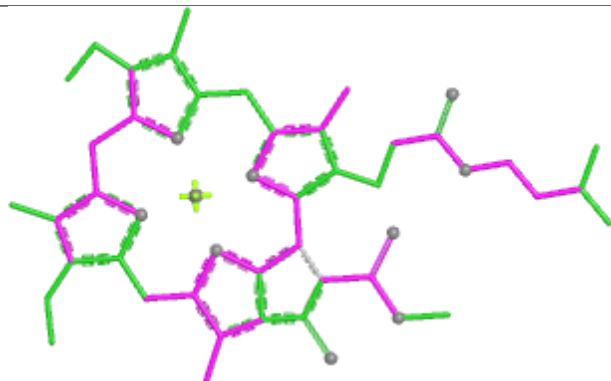
## Ligand CLA L 201



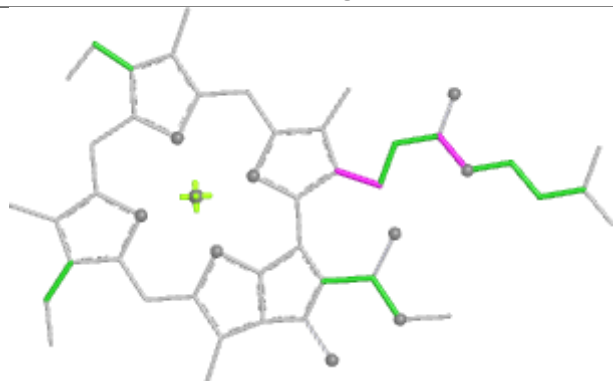
## Ligand CLA 5 312



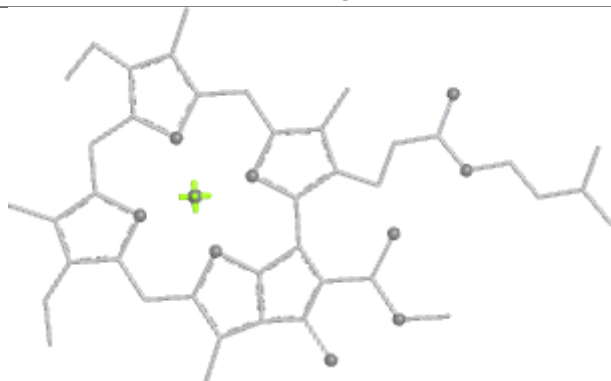
Bond lengths



Bond angles

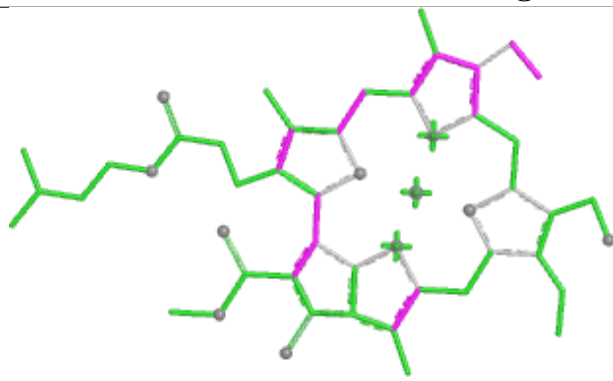


Torsions

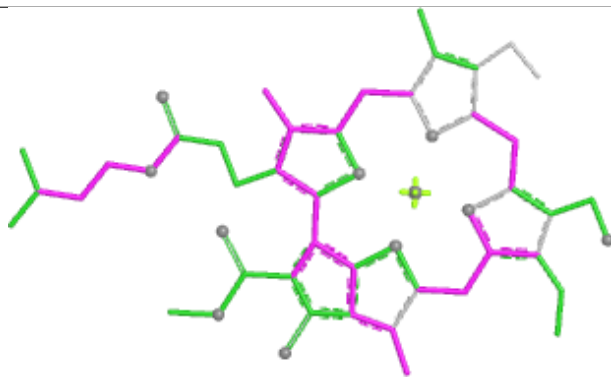


Rings

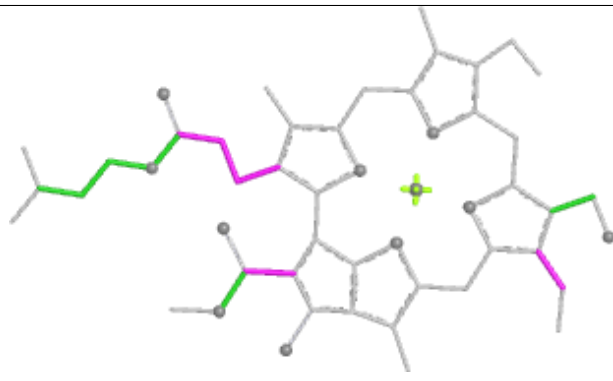
## Ligand CHL Z 311



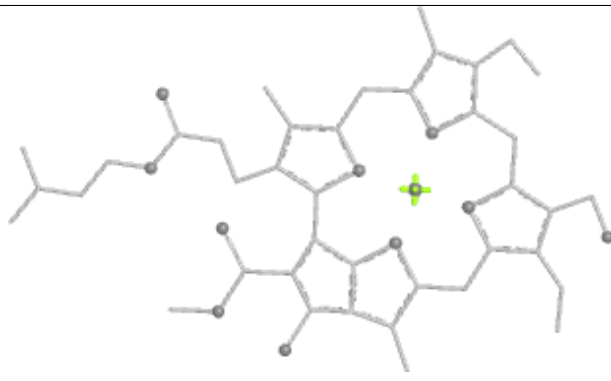
Bond lengths



Bond angles

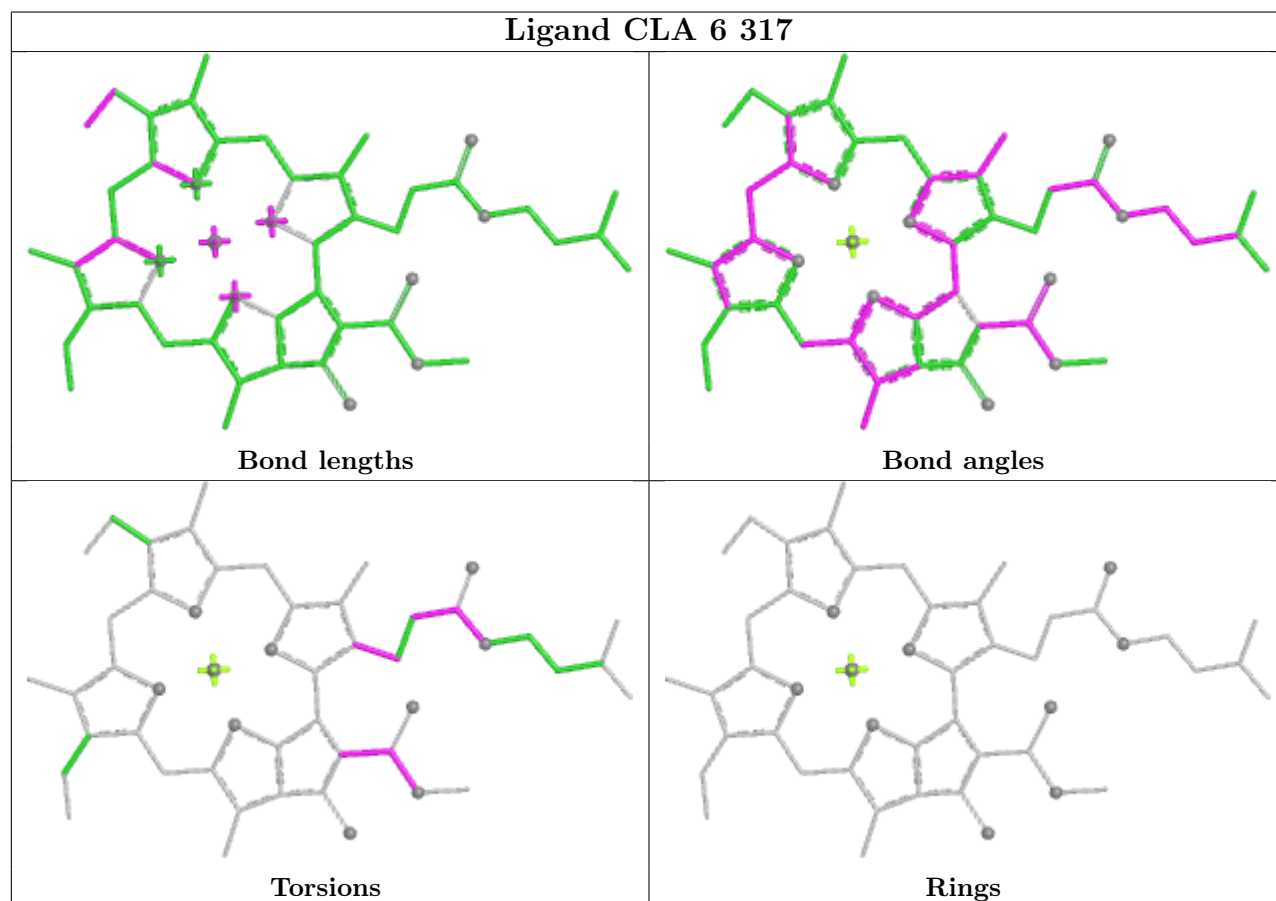
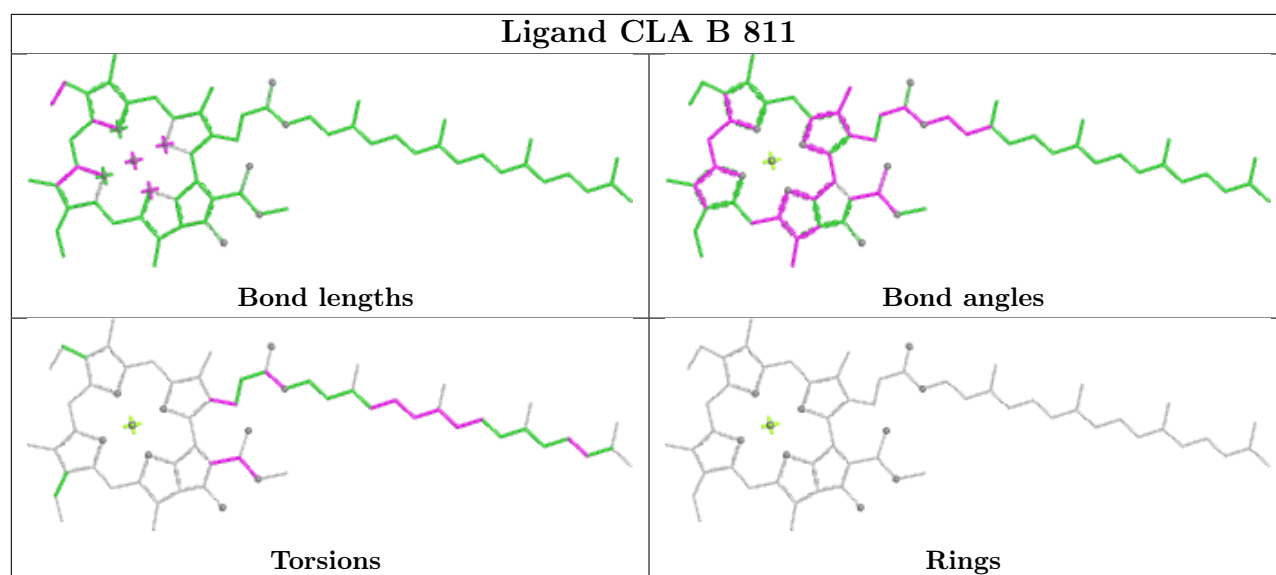


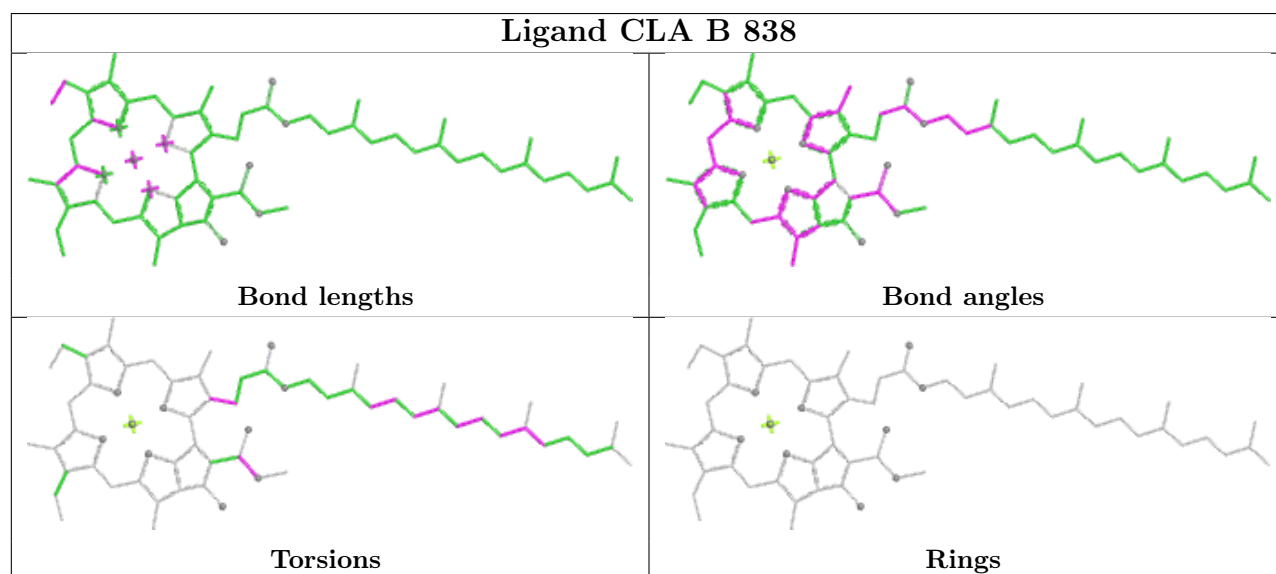
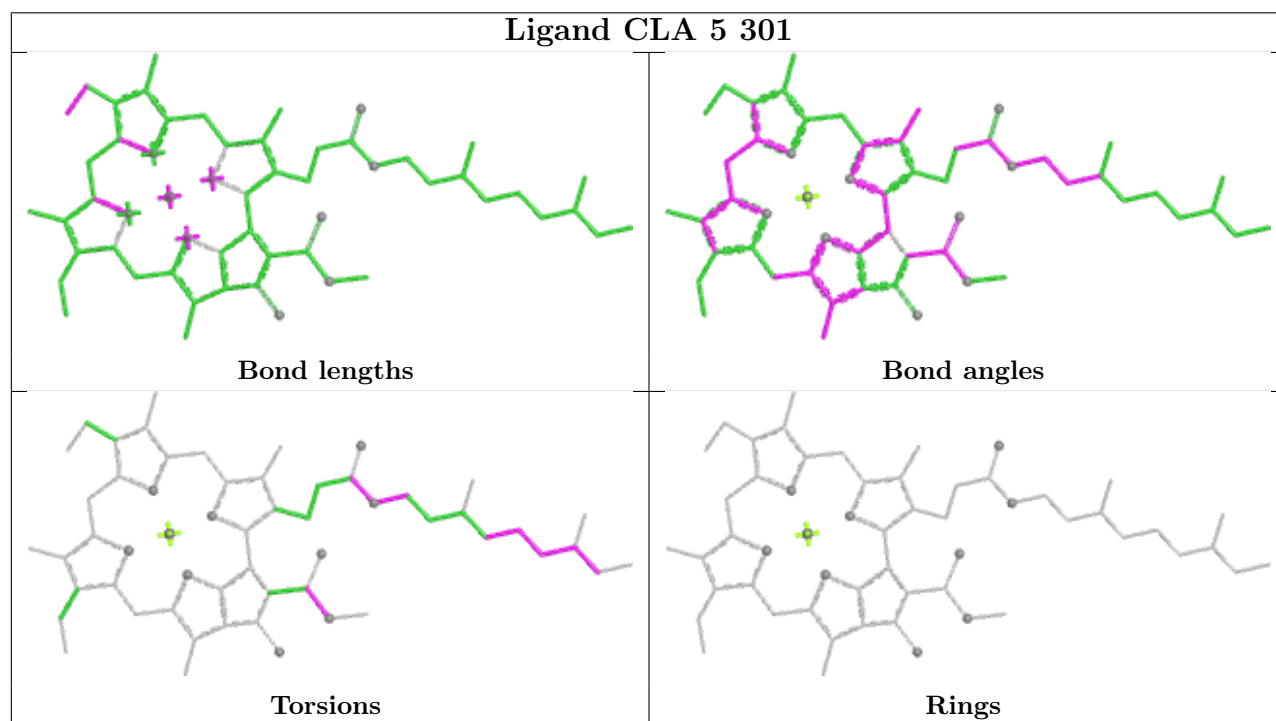
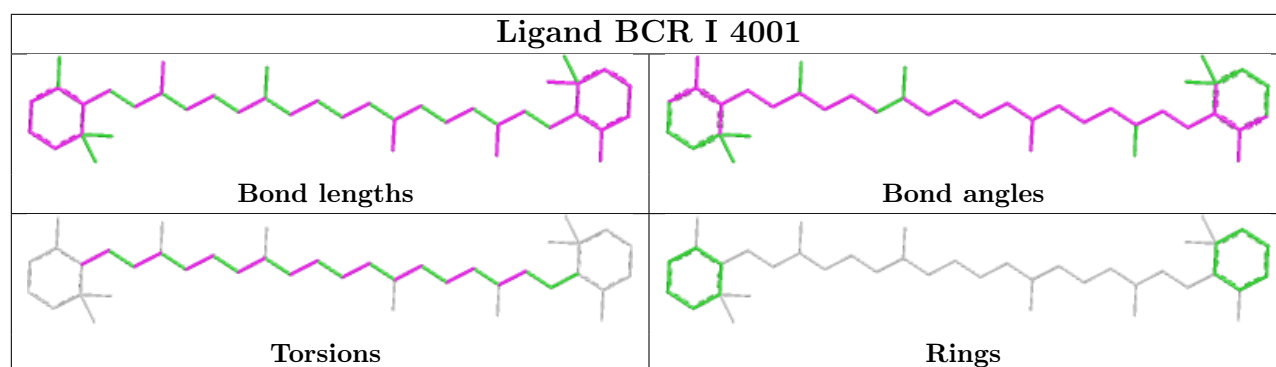
Torsions

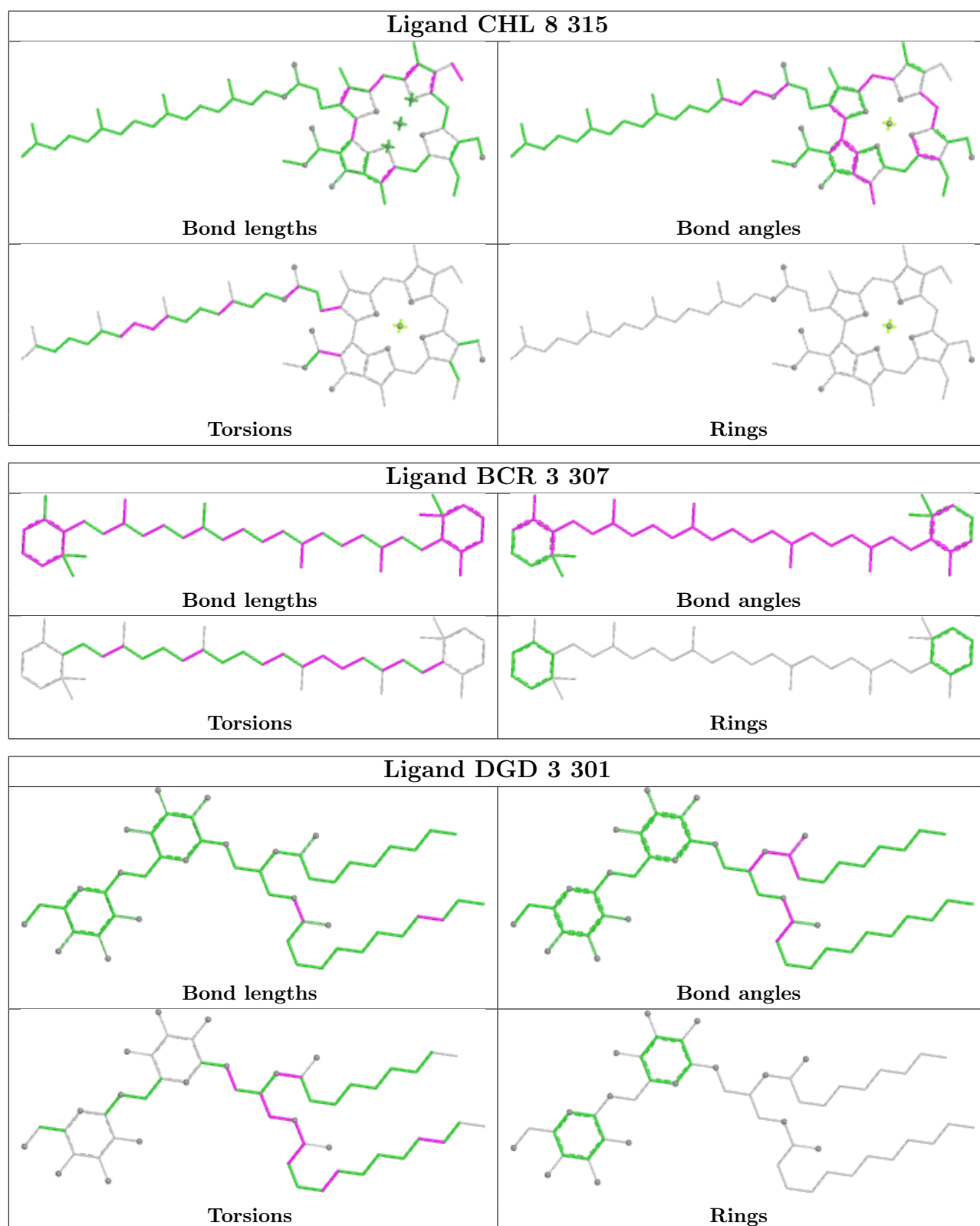


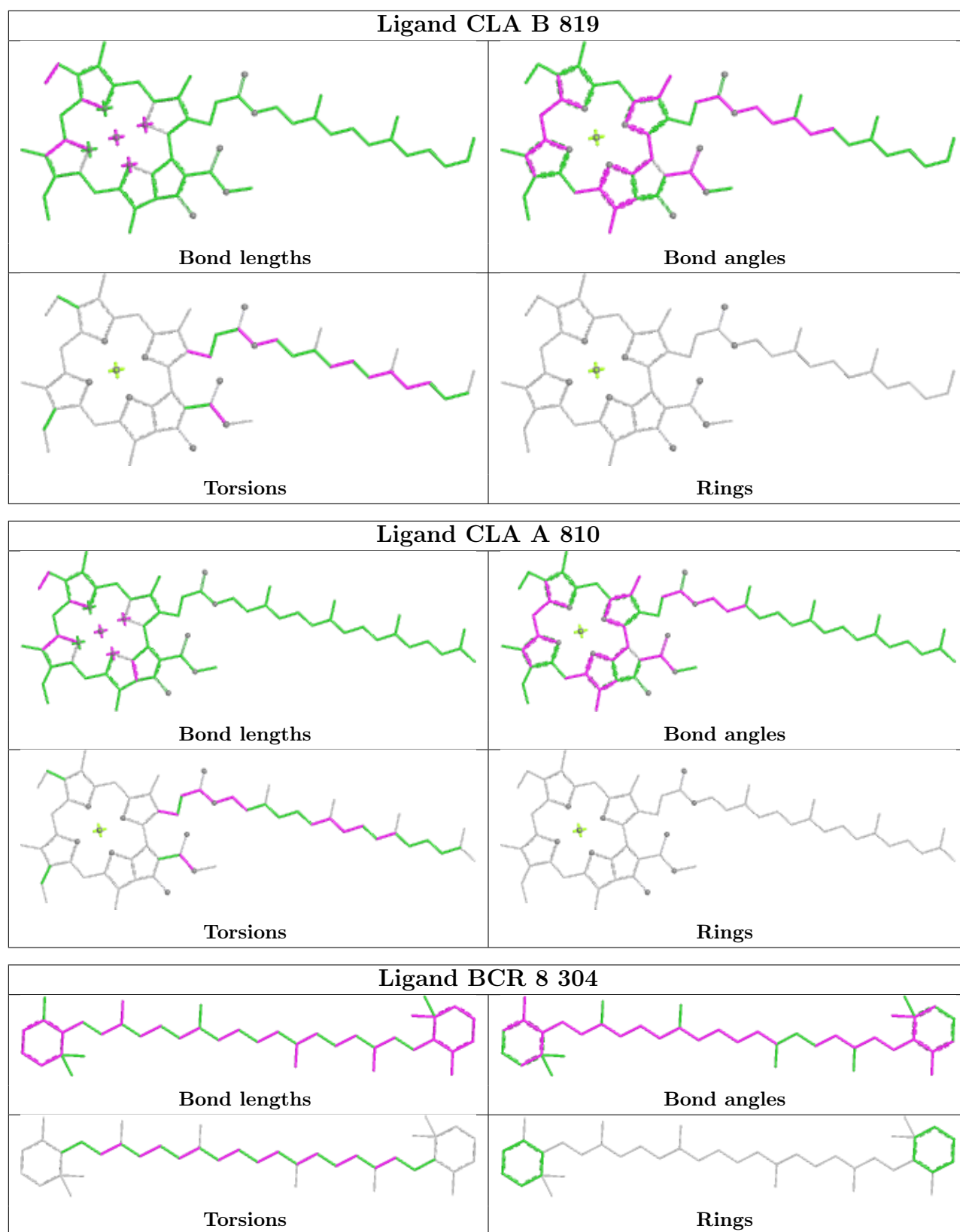
Rings



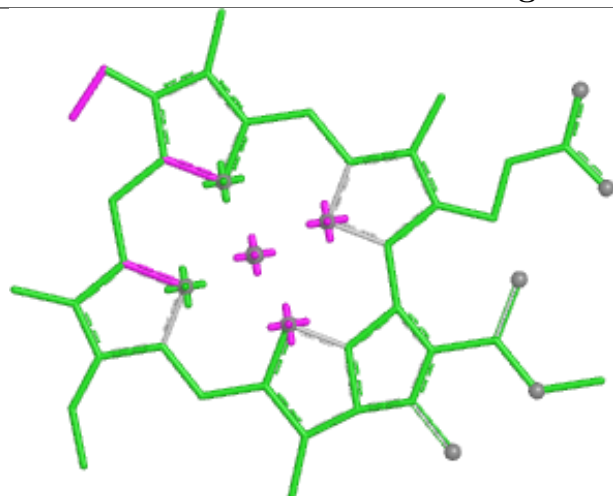




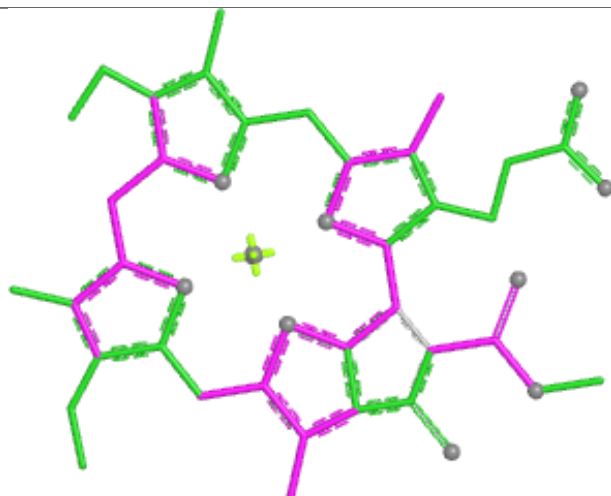




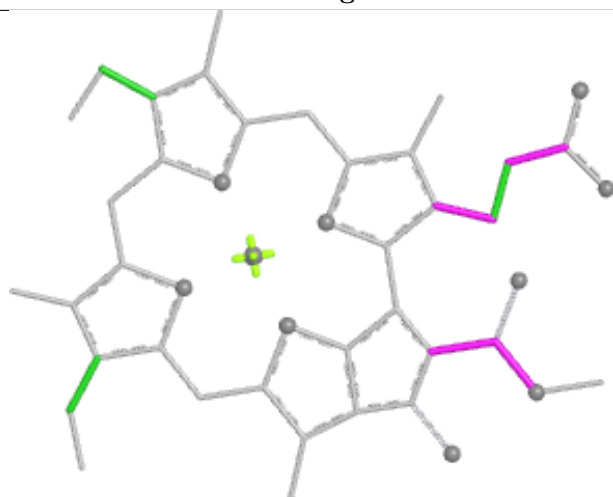
## Ligand CLA 2 302



Bond lengths



Bond angles

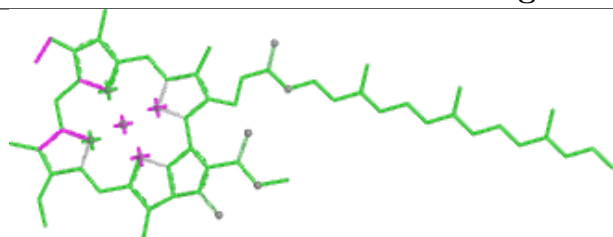


Torsions

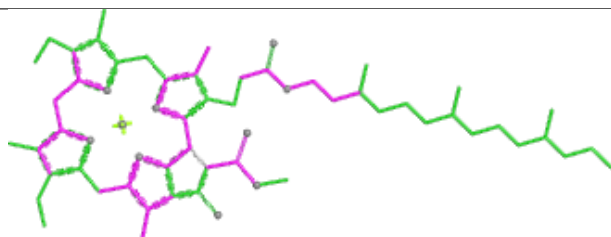


Rings

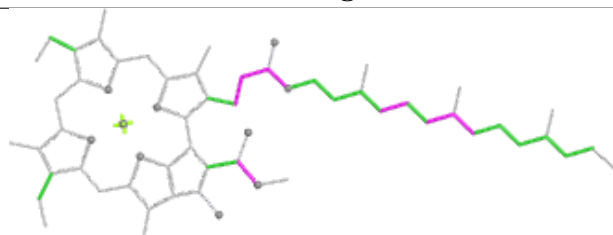
## Ligand CLA 9 306



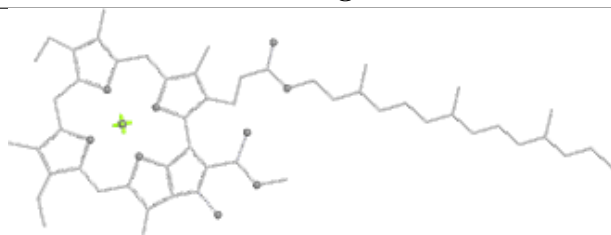
Bond lengths



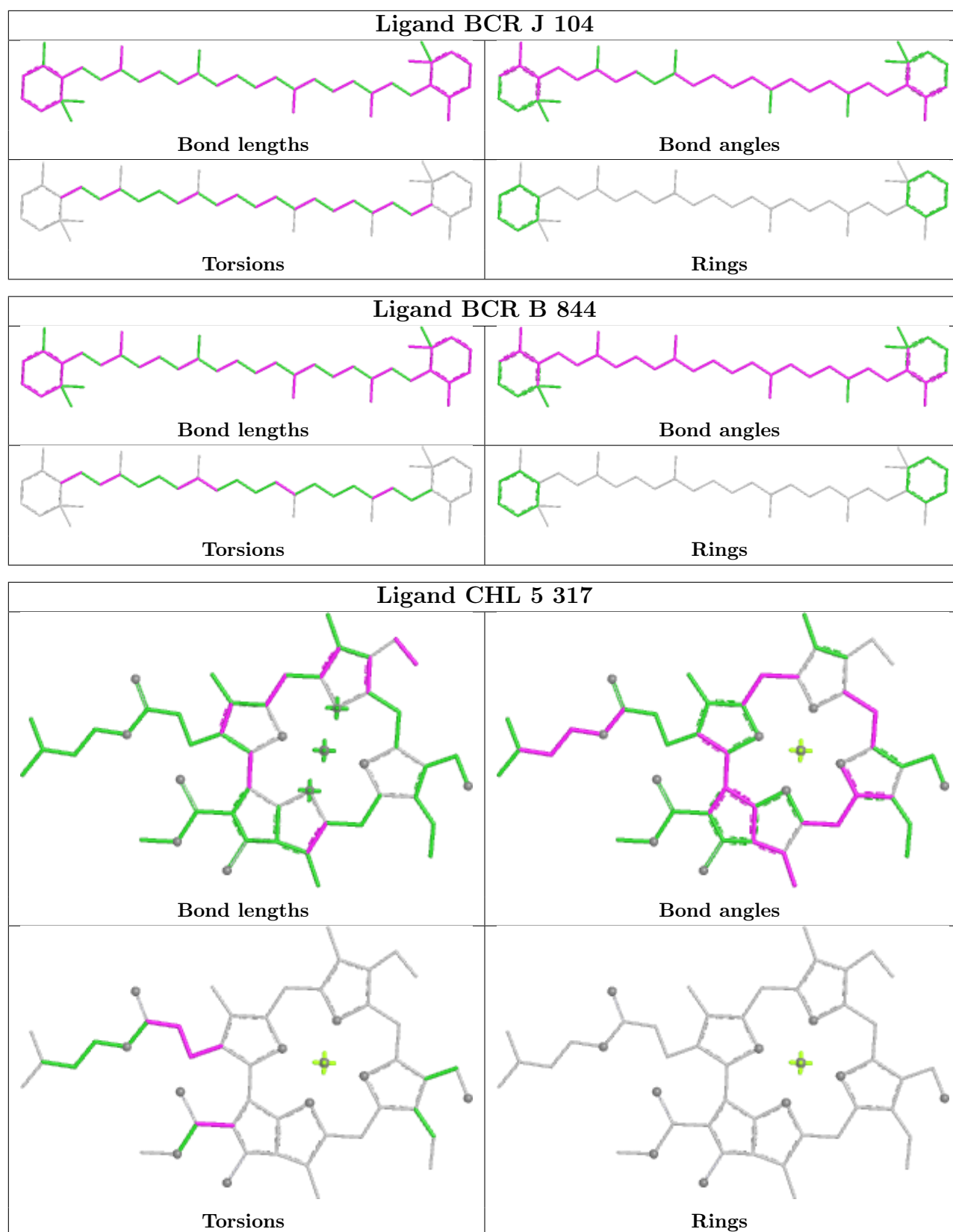
Bond angles



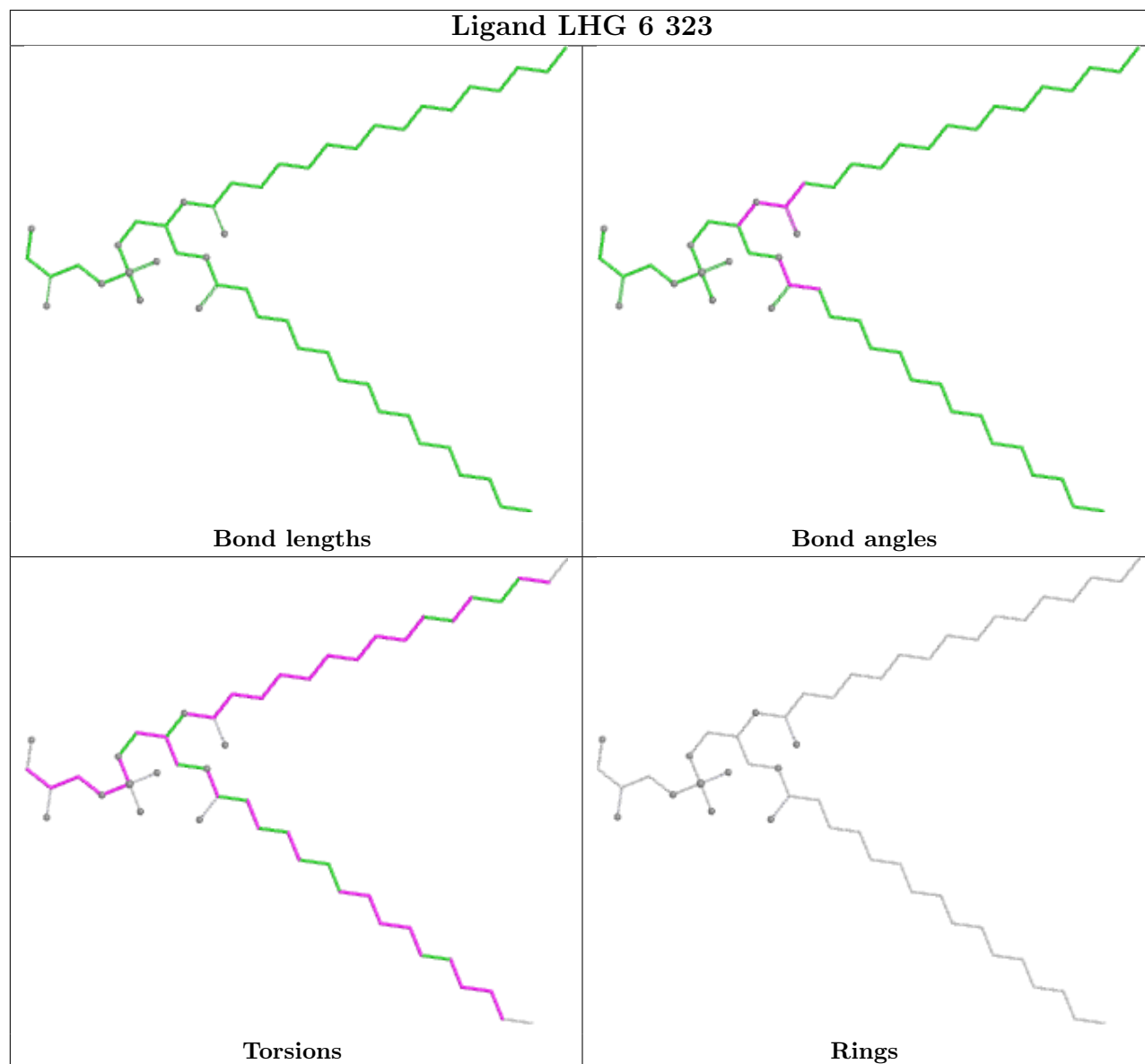
Torsions



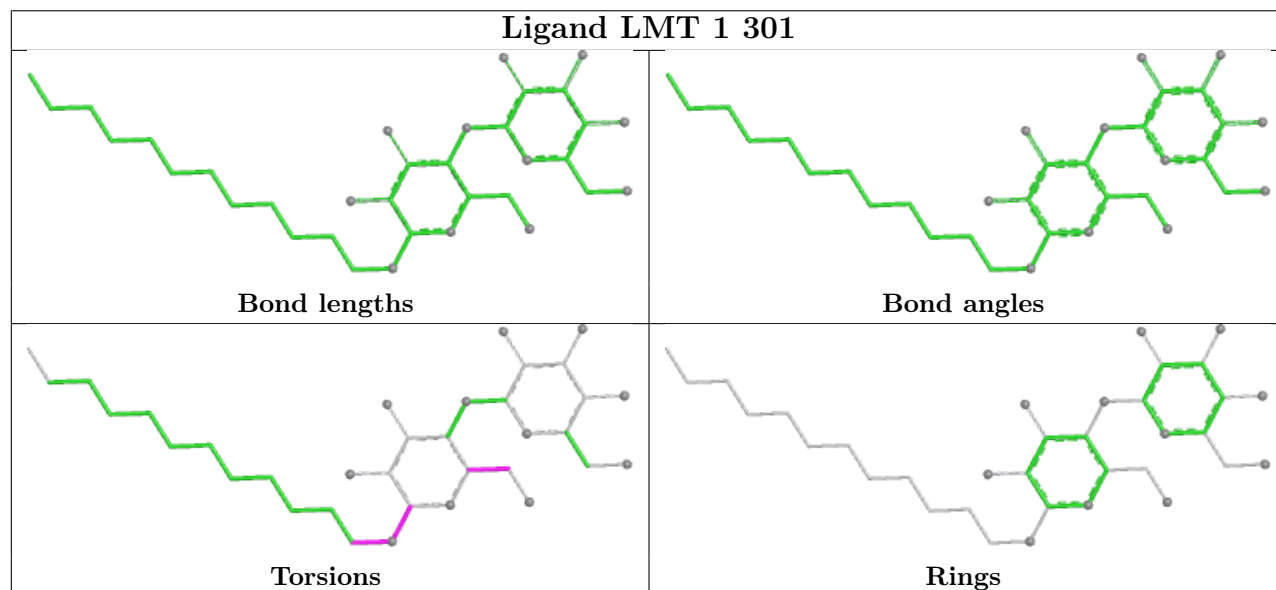
Rings



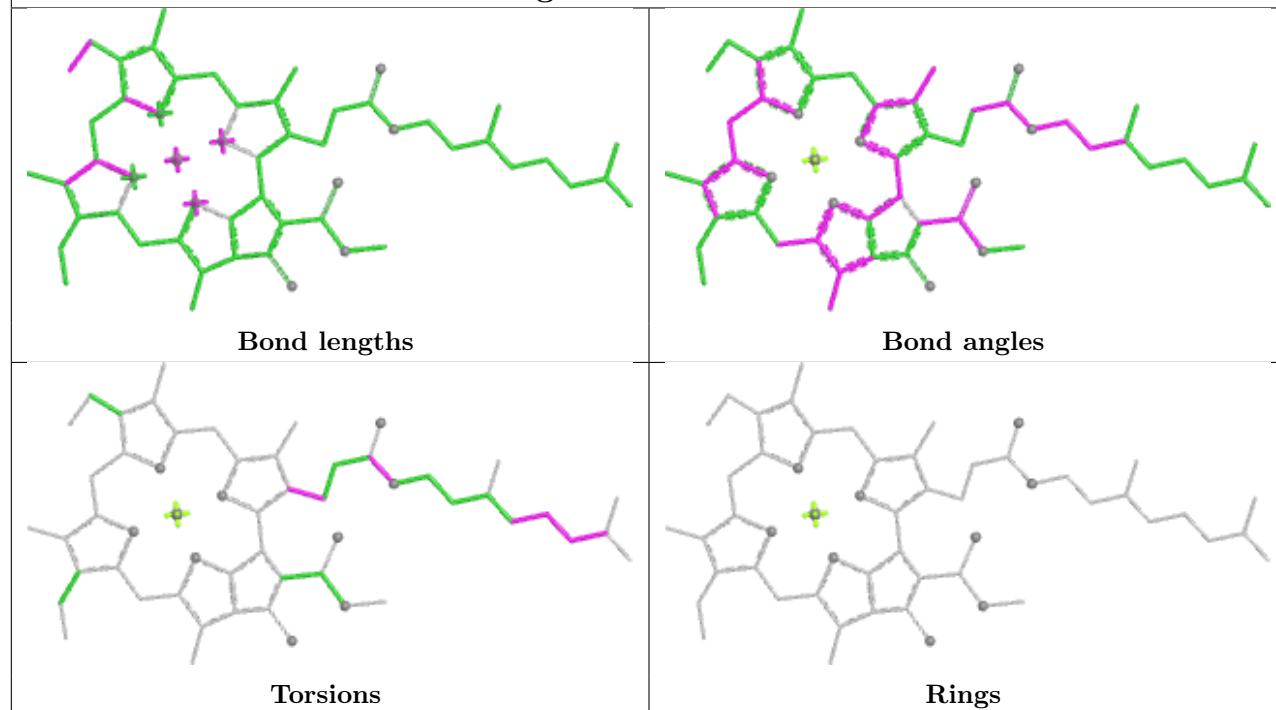
## Ligand LHG 6 323



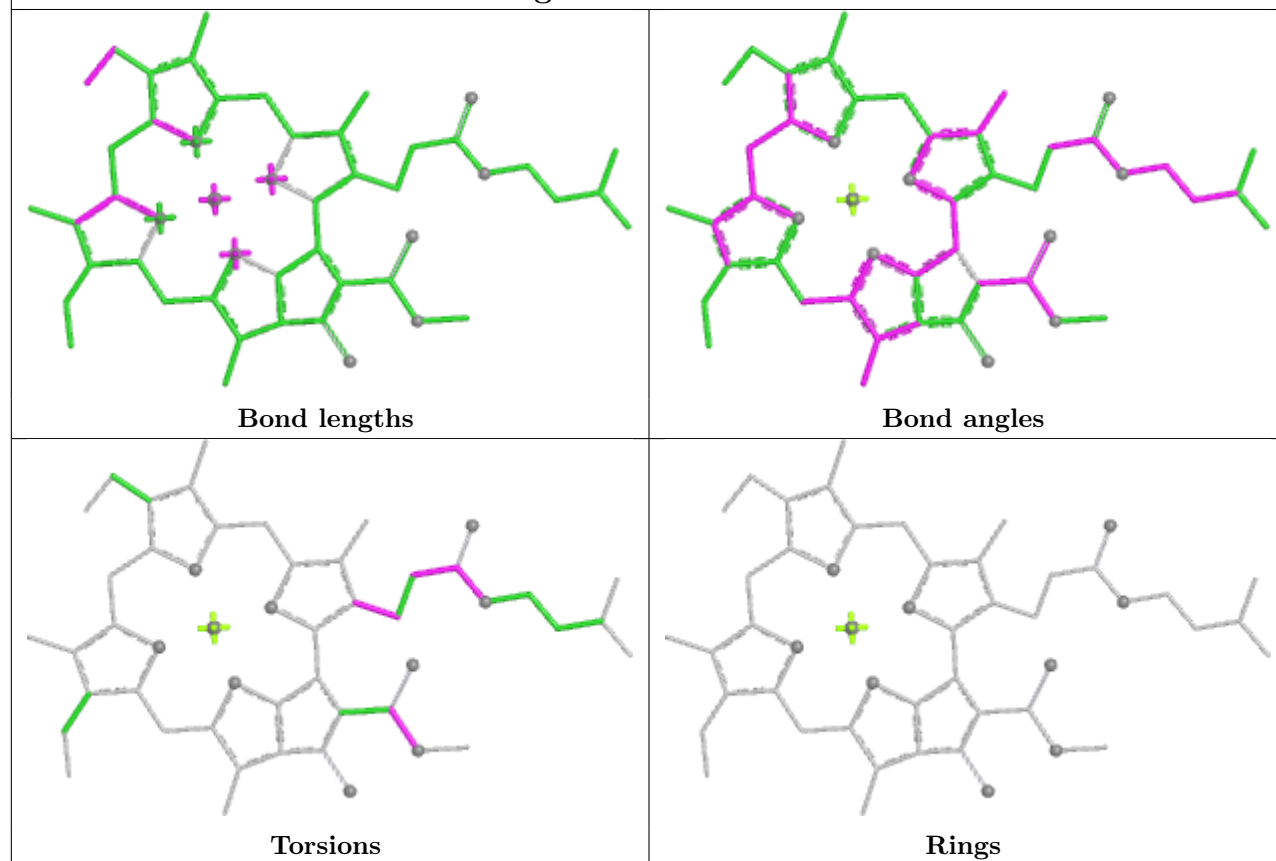
## Ligand LMT 1 301



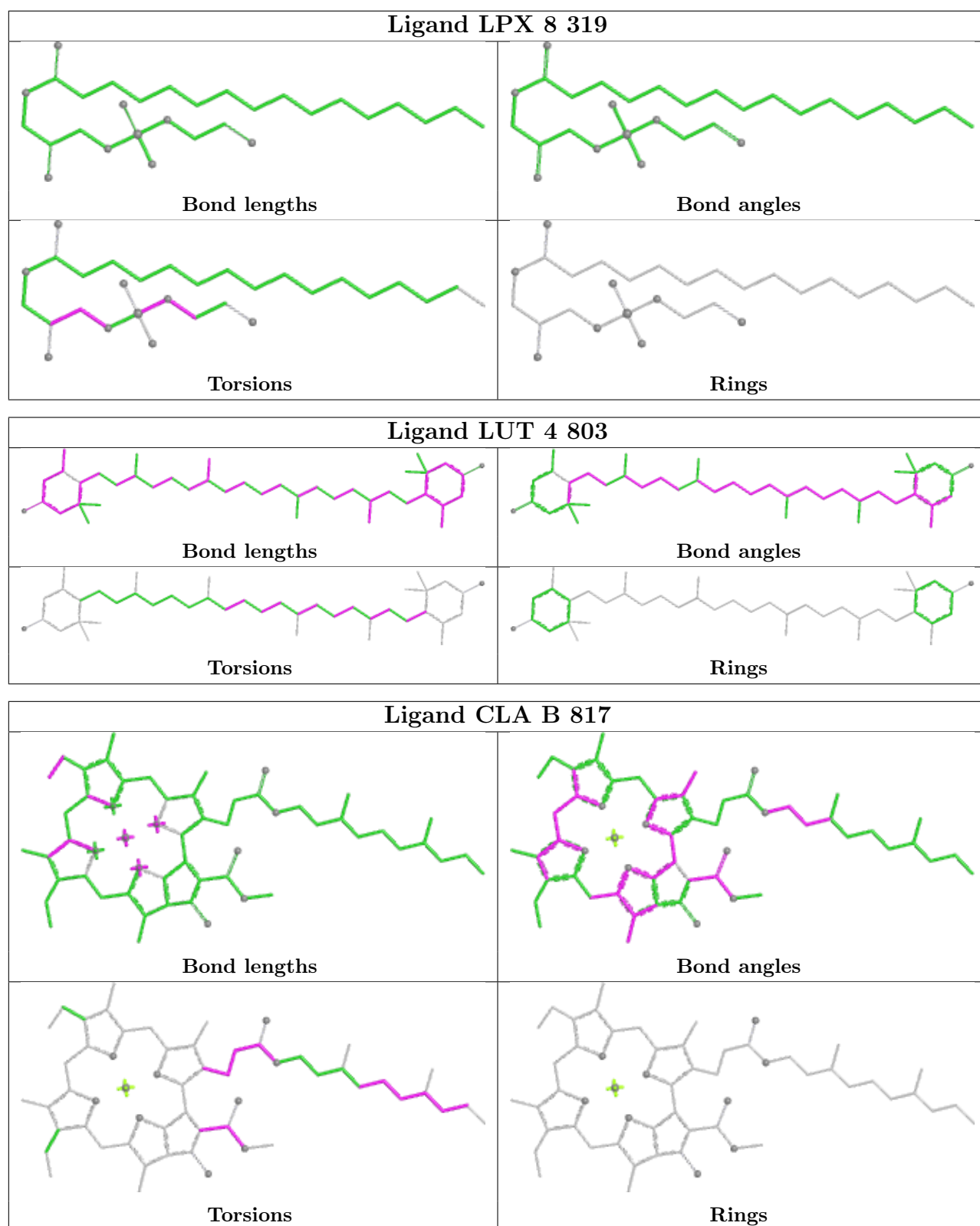
## Ligand CLA 7 322

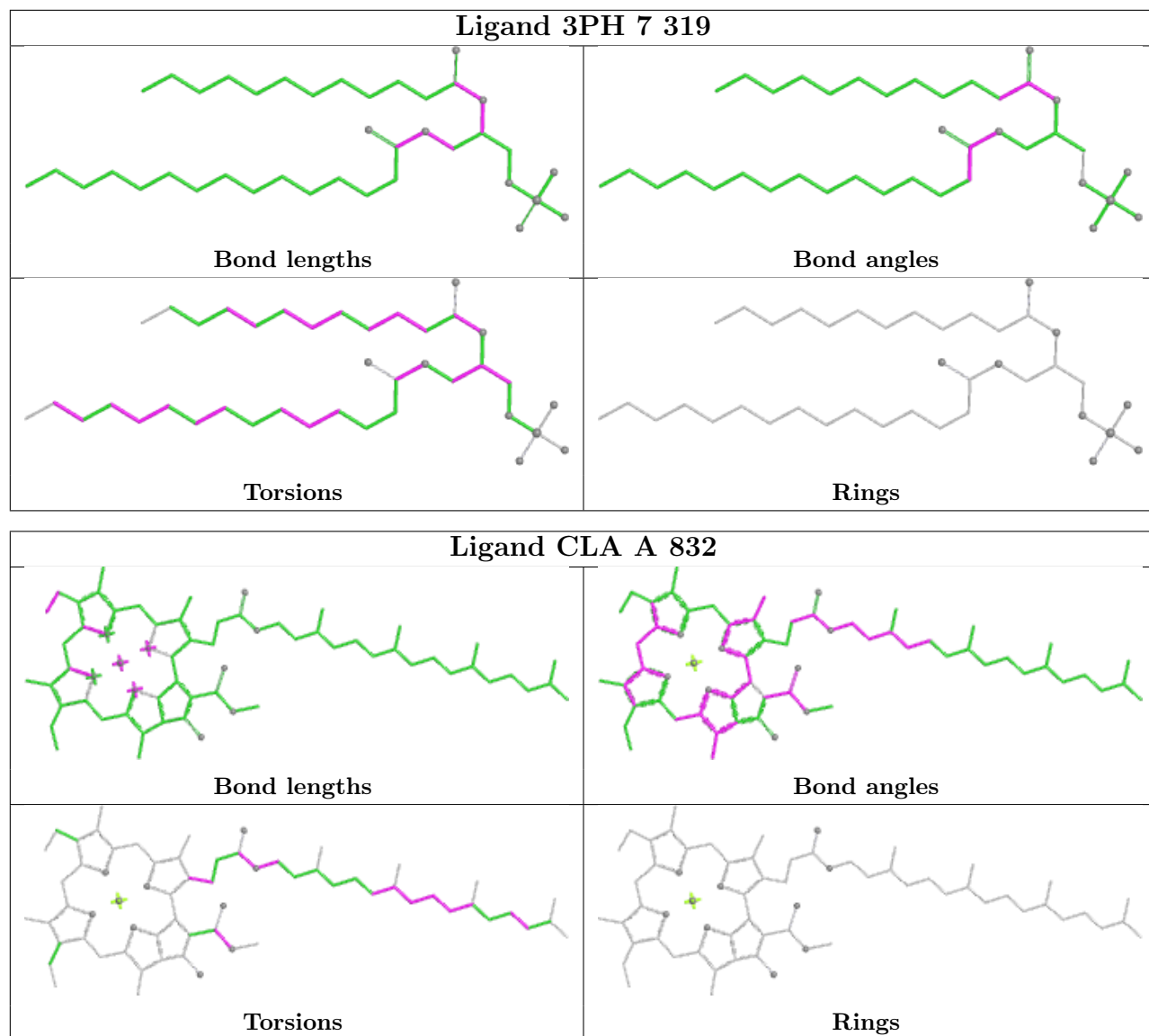


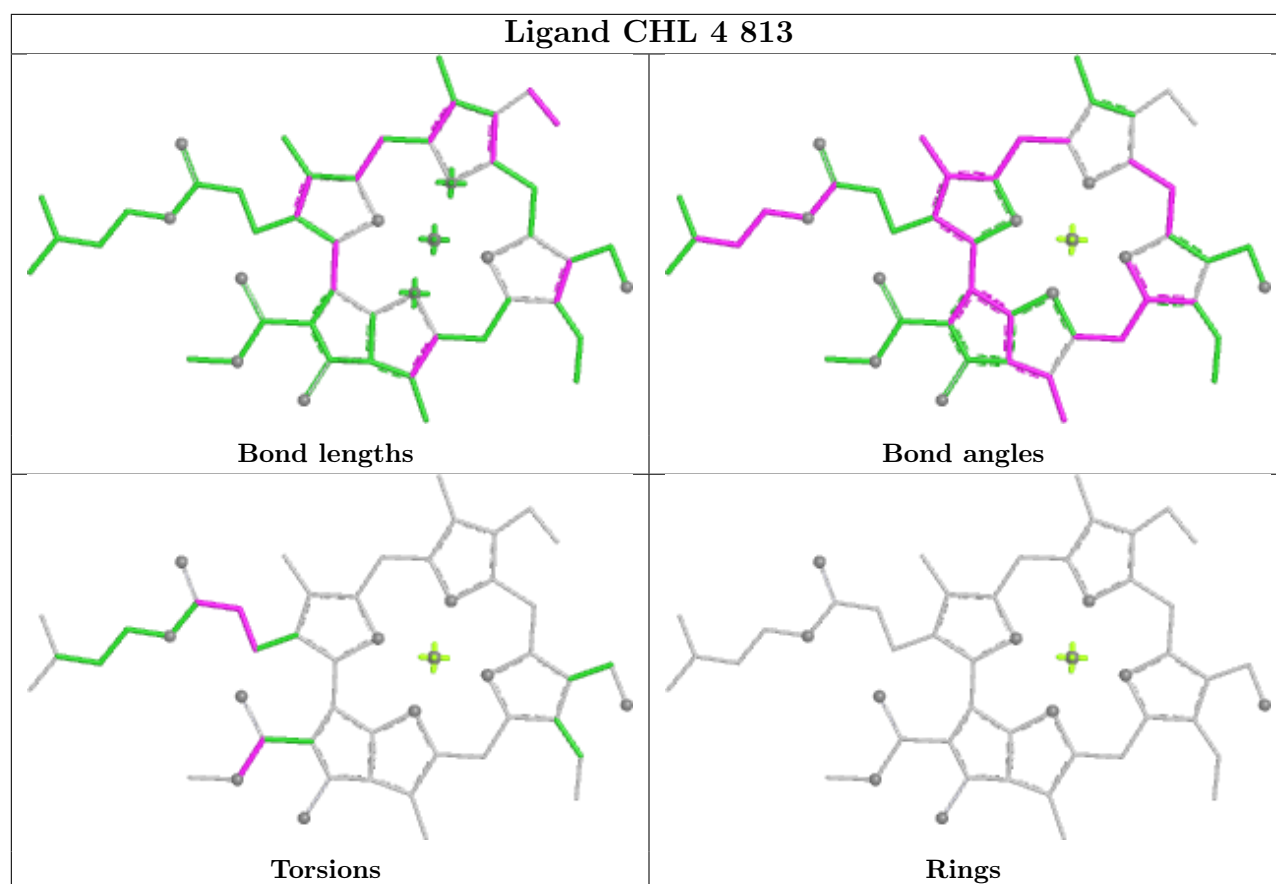
## Ligand CLA L 203



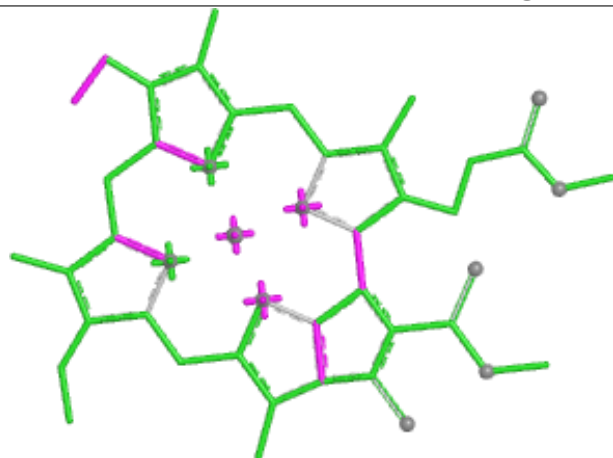




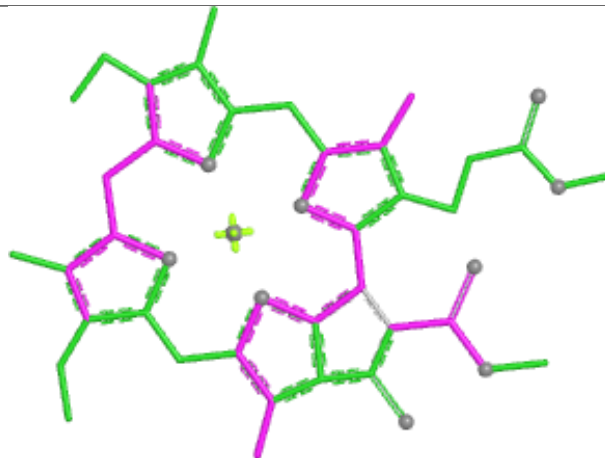




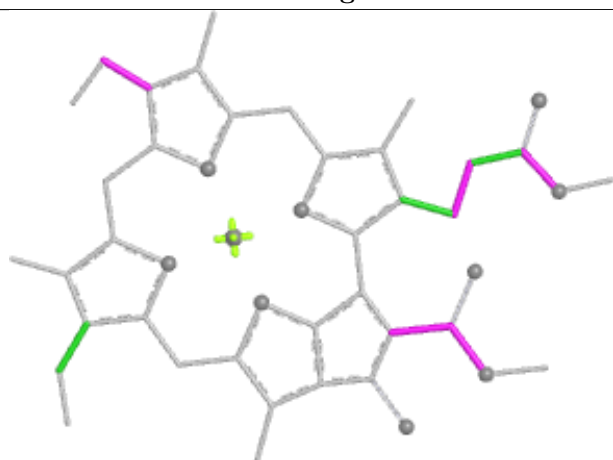
## Ligand CLA 1 311



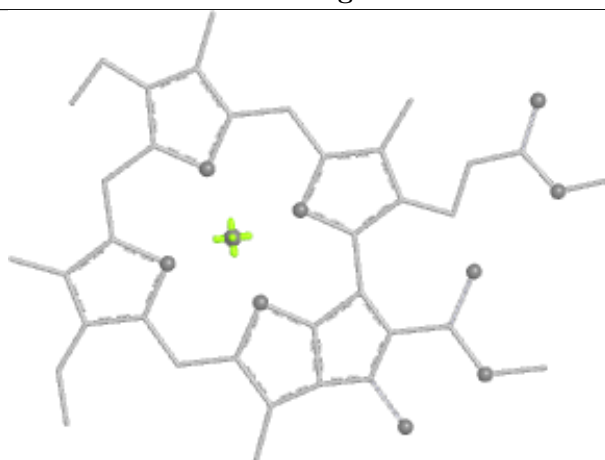
Bond lengths



Bond angles

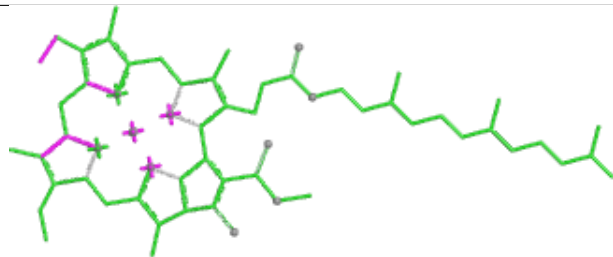


Torsions

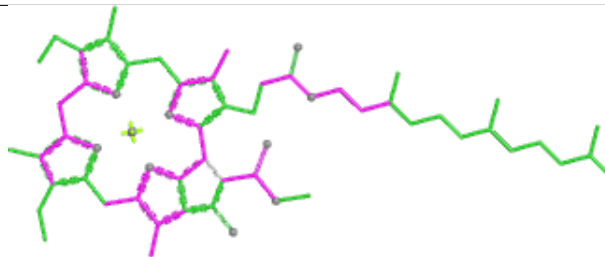


Rings

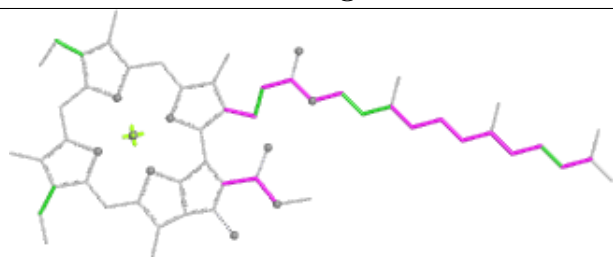
## Ligand CLA A 814



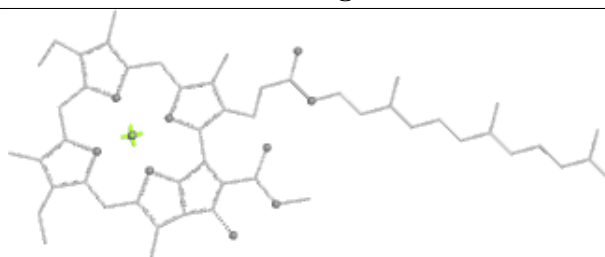
Bond lengths



Bond angles

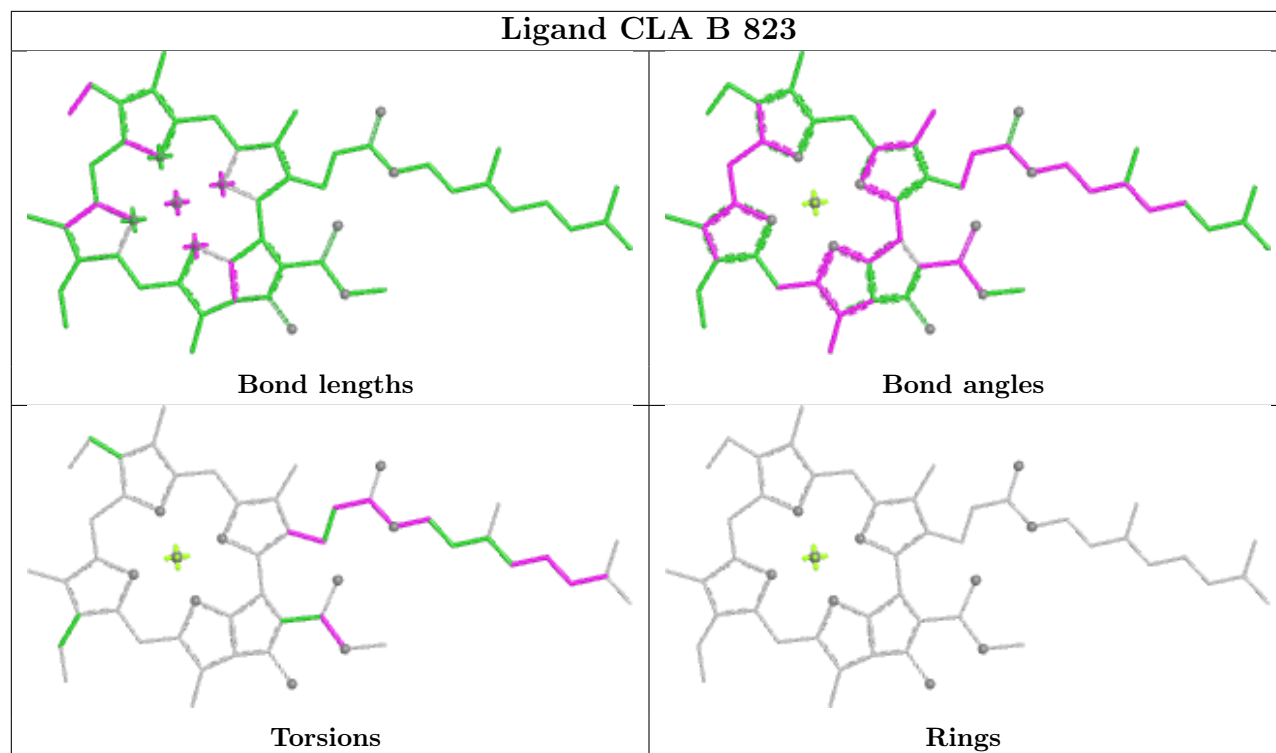


Torsions

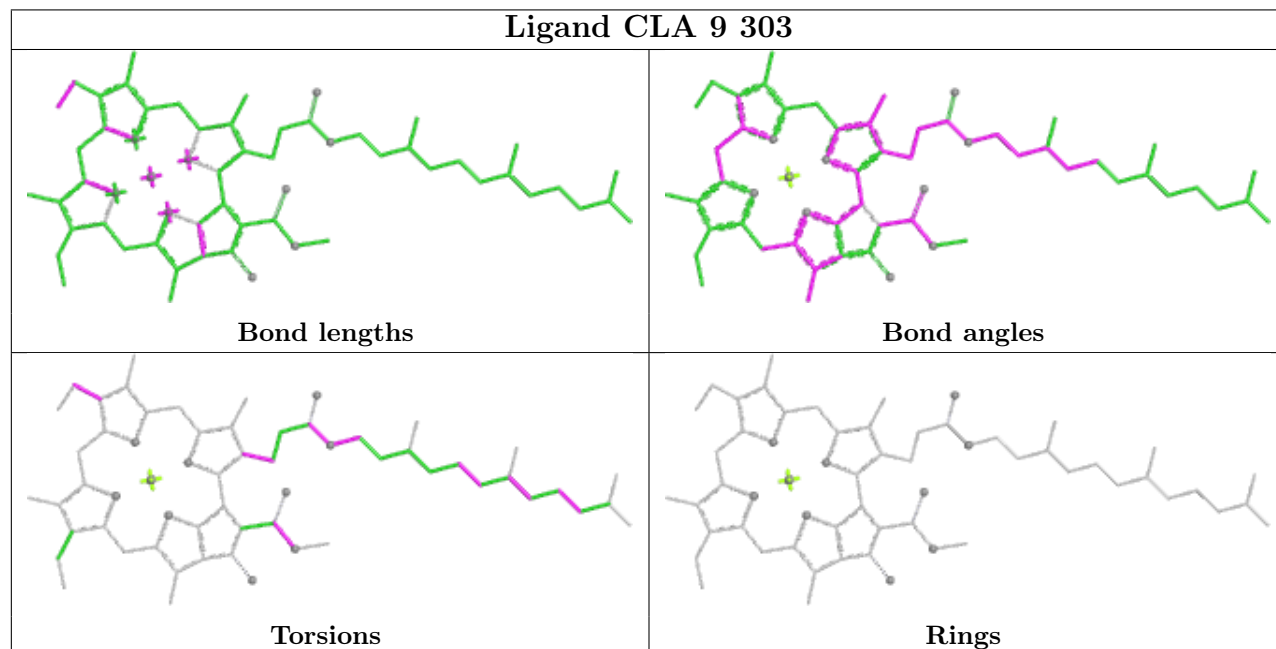


Rings

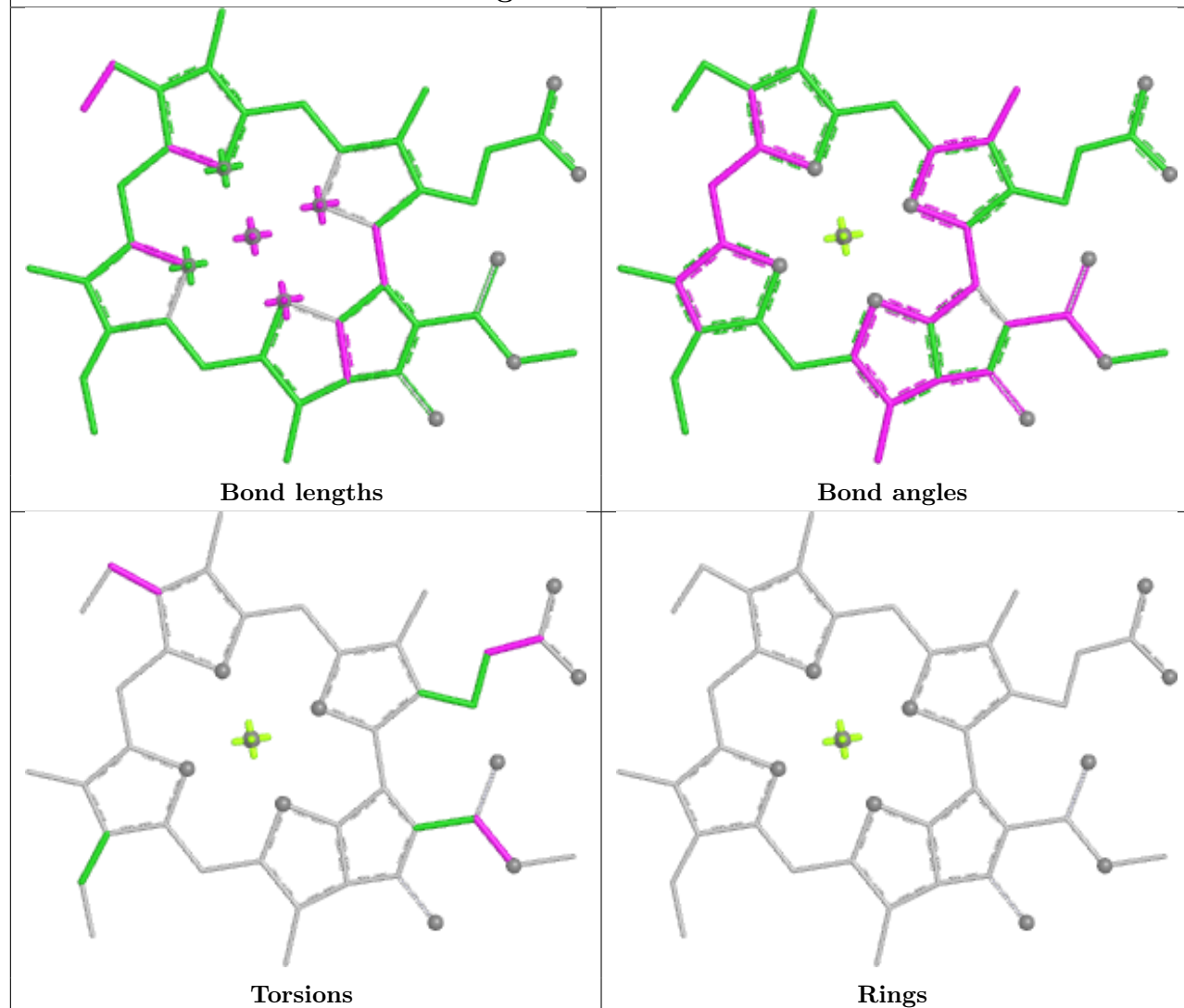
## Ligand CLA B 823



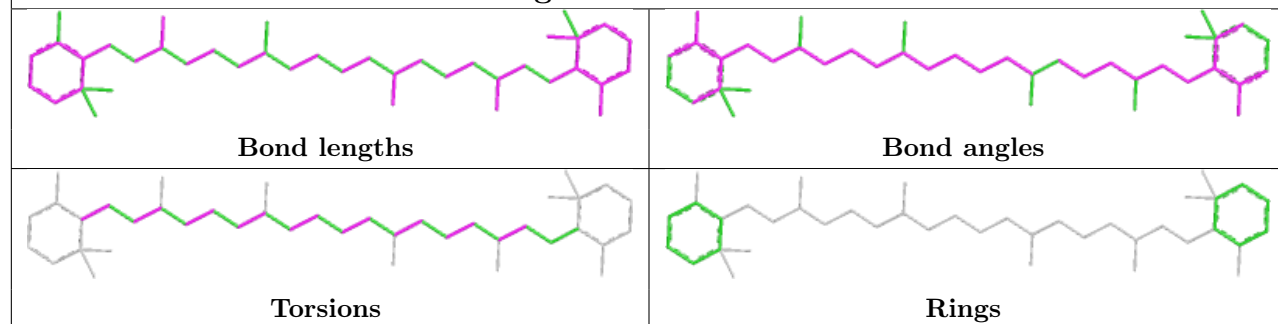
## Ligand CLA 9 303

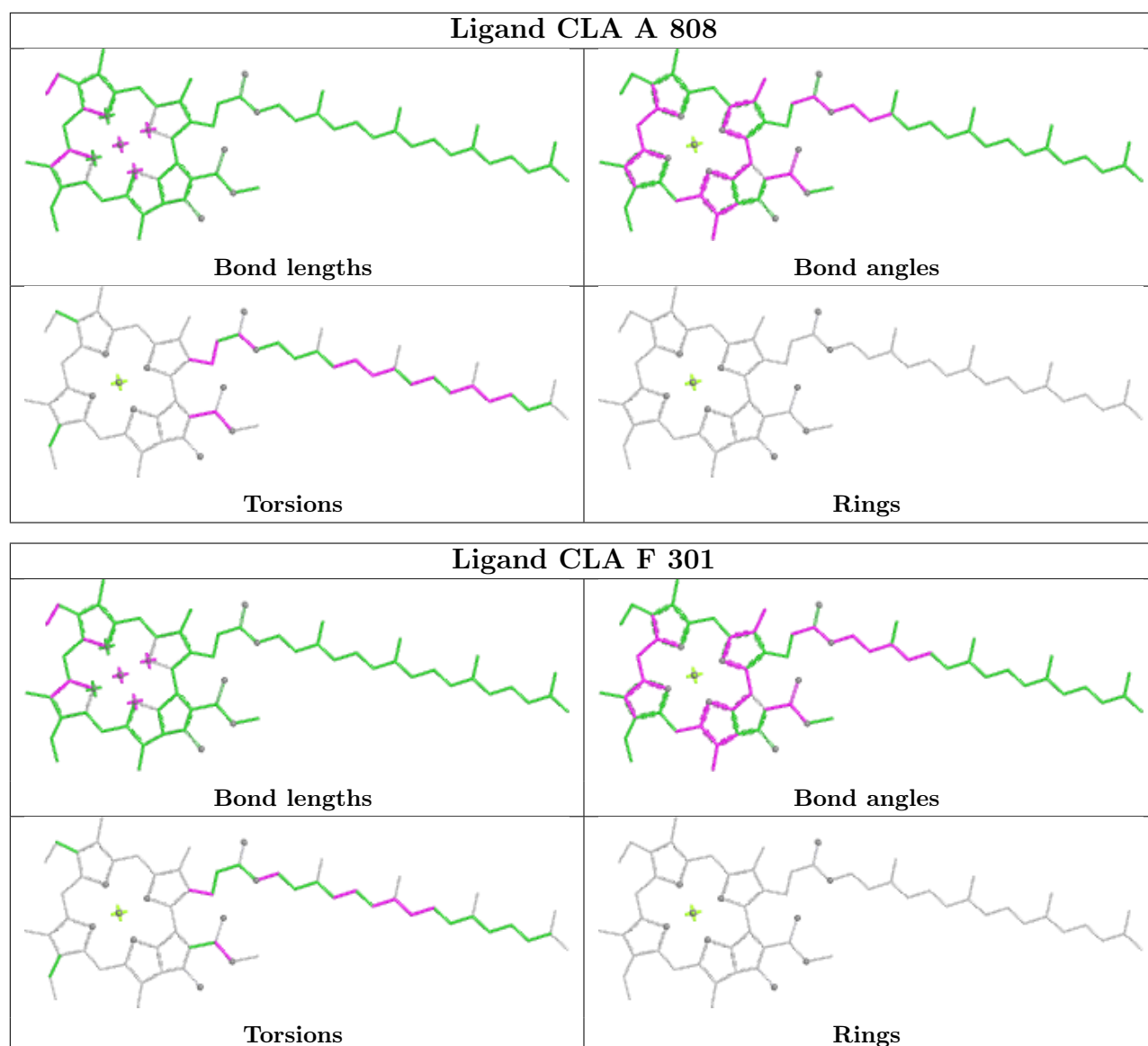


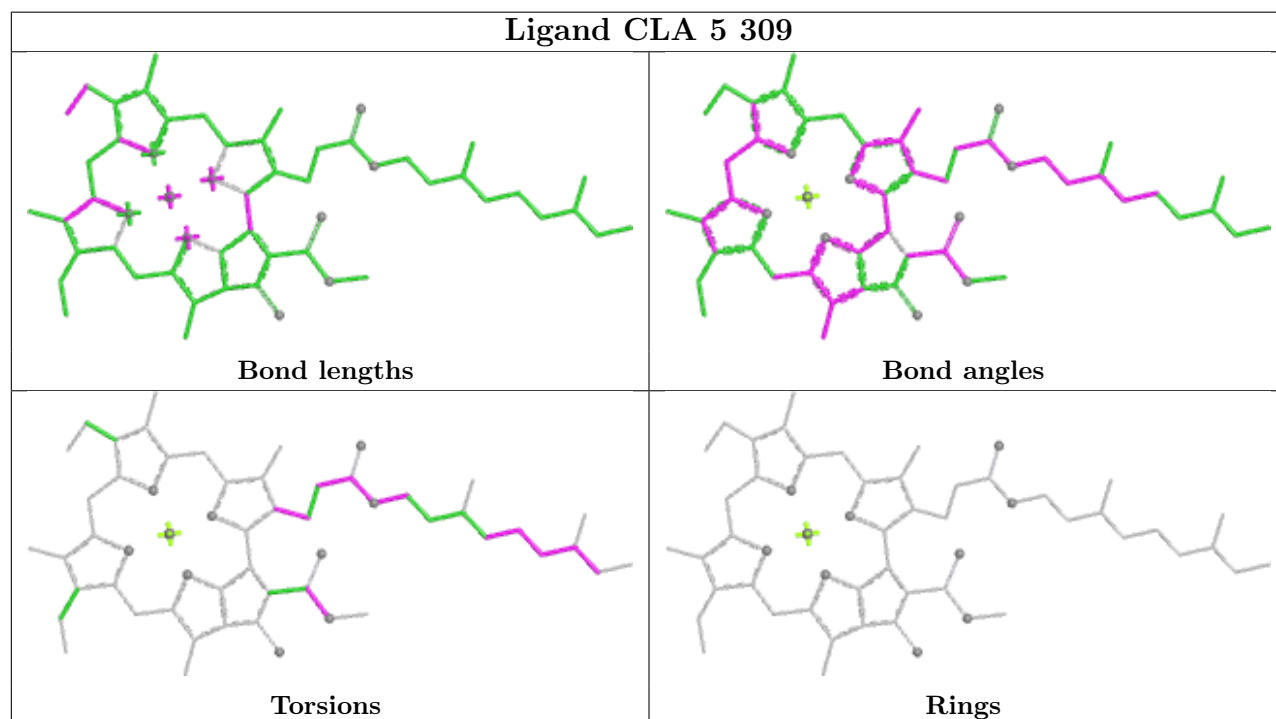
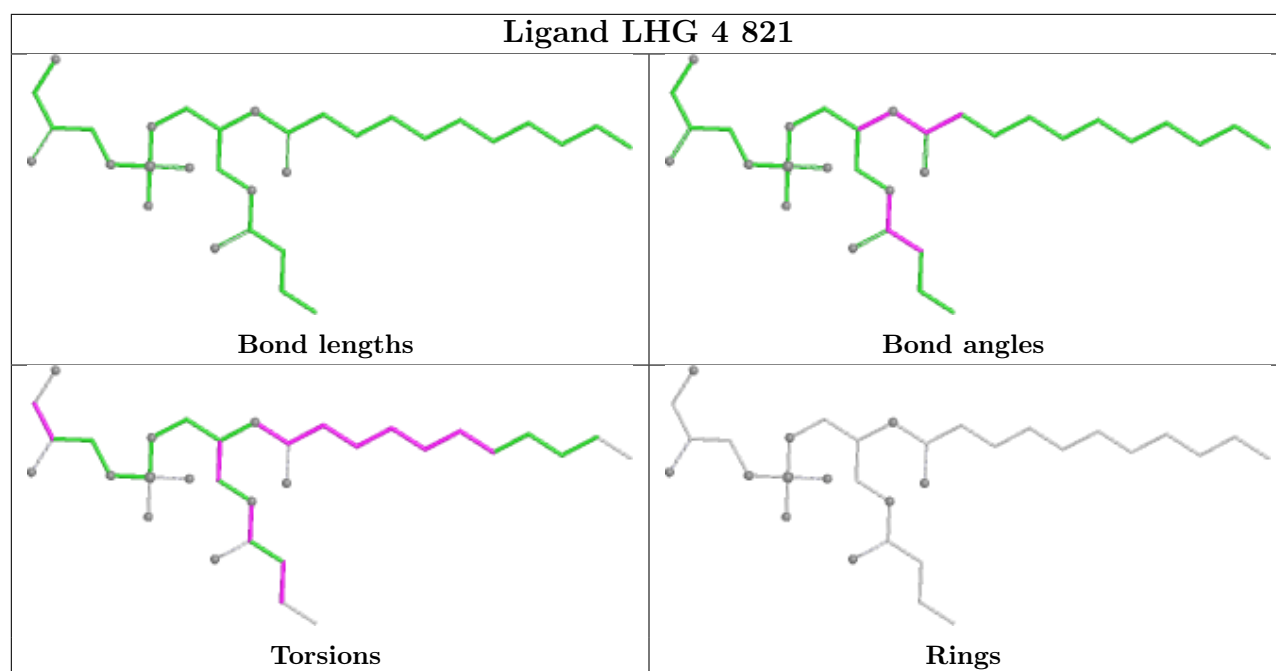
## Ligand CLA 9 310



## Ligand BCR 6 305

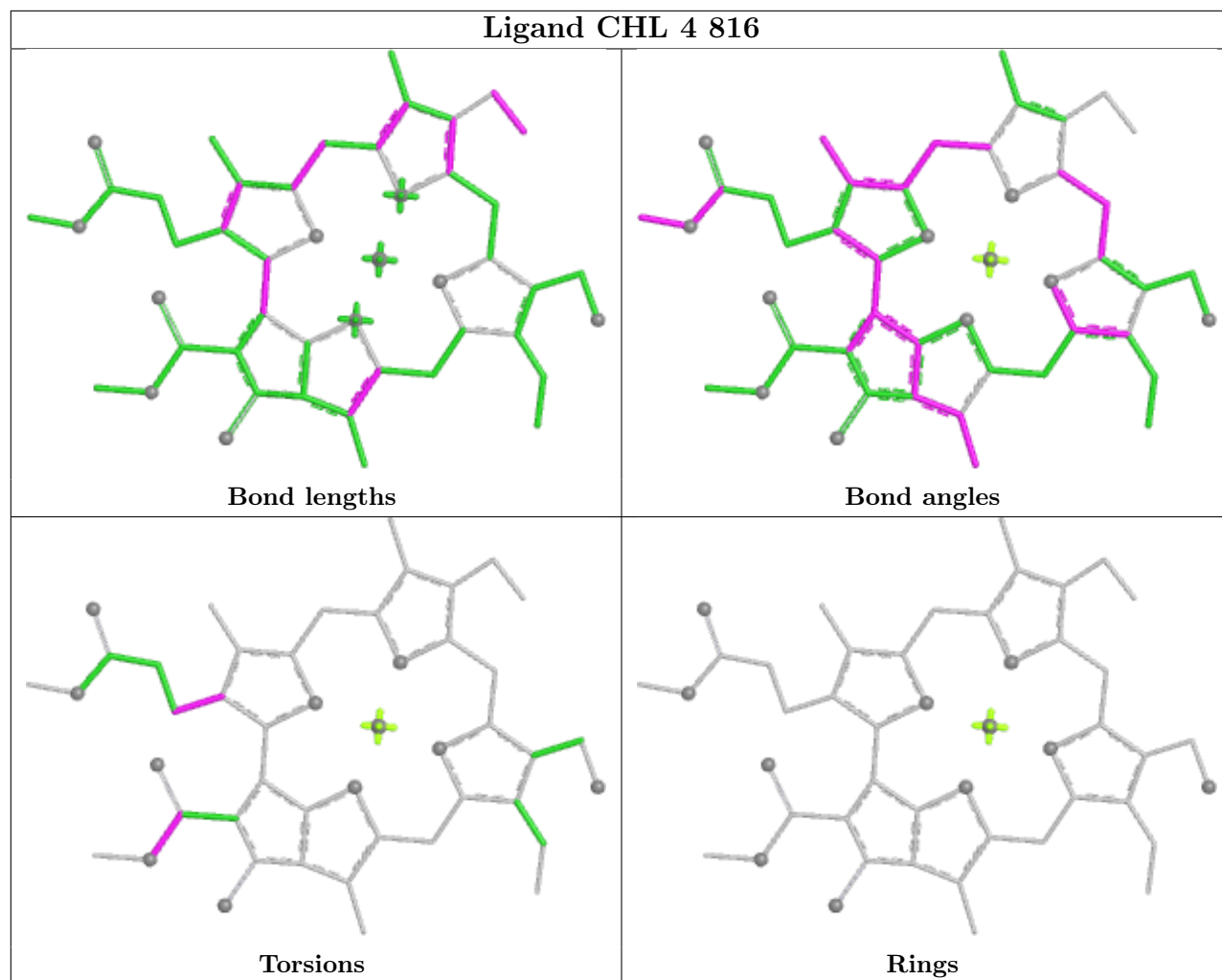




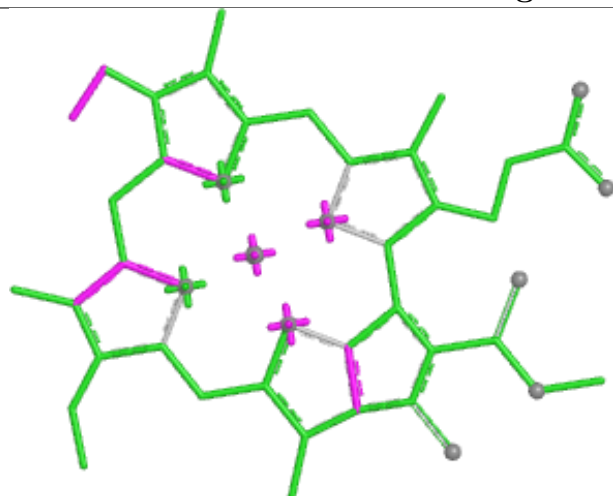




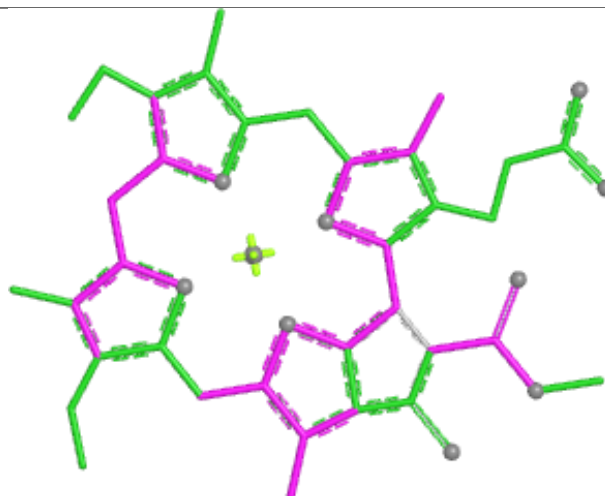
## Ligand CHL 4 816



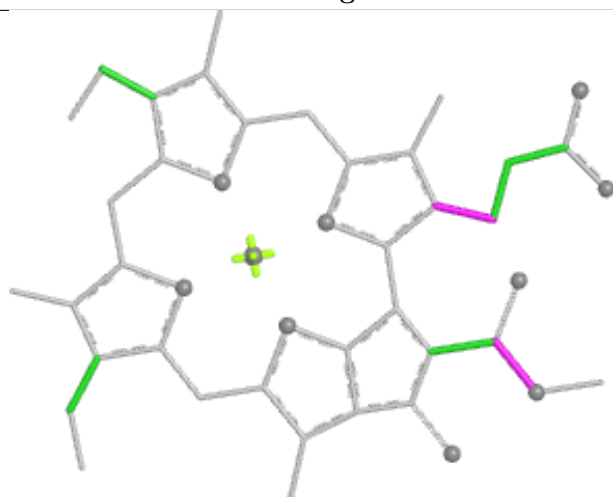
## Ligand CLA F 305



Bond lengths



Bond angles

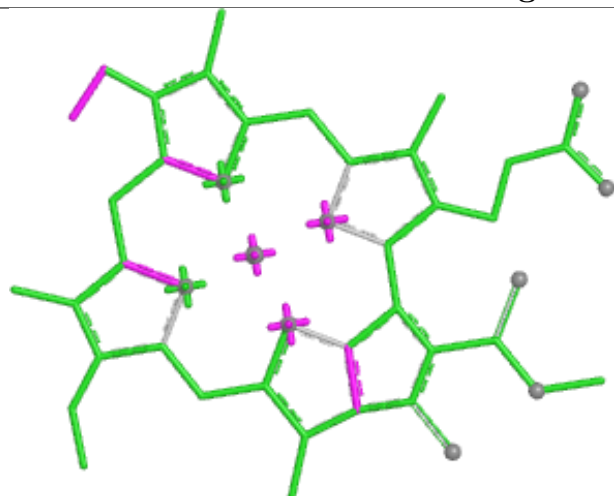


Torsions

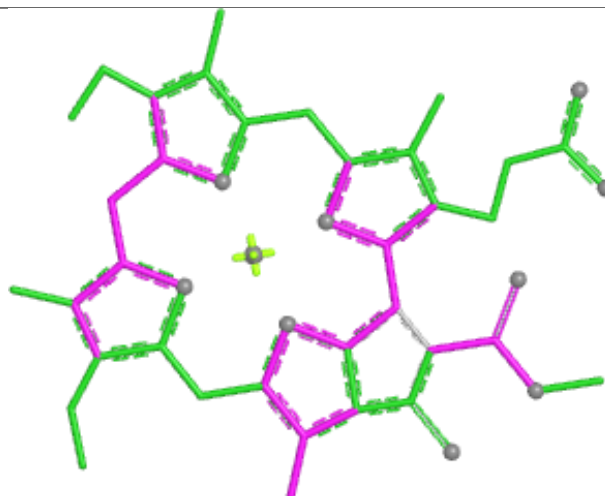


Rings

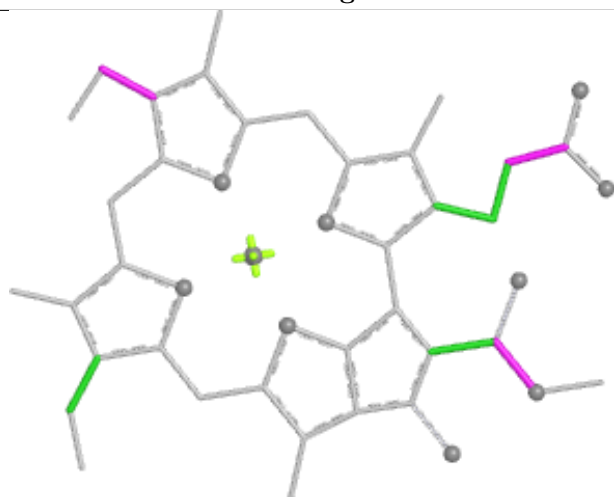
## Ligand CLA 9 304



Bond lengths



Bond angles

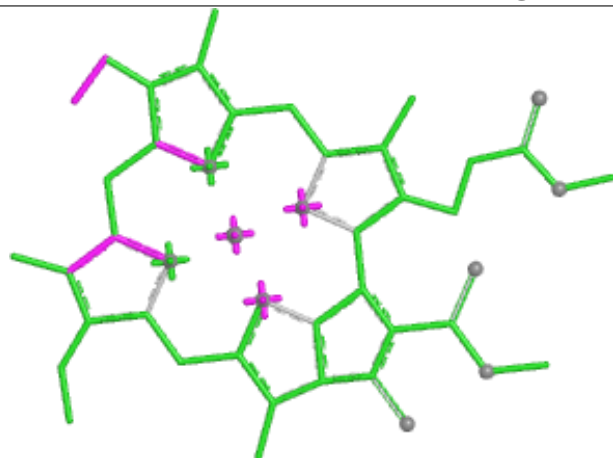


Torsions

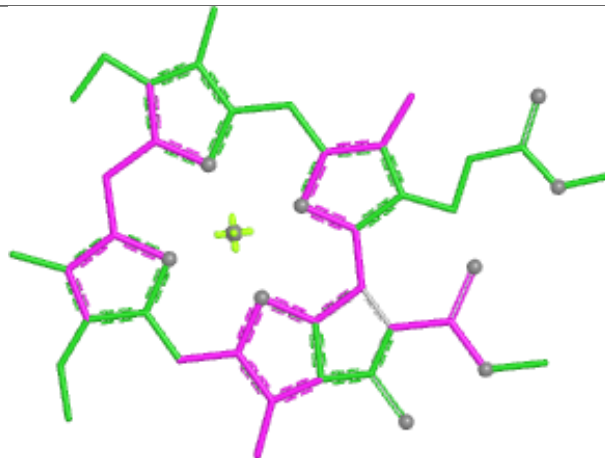


Rings

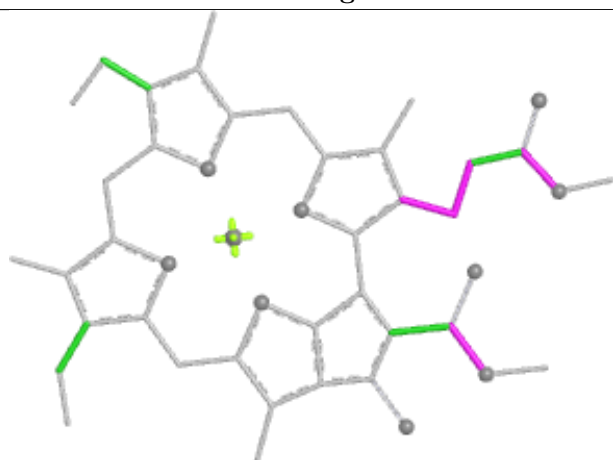
## Ligand CLA K 202



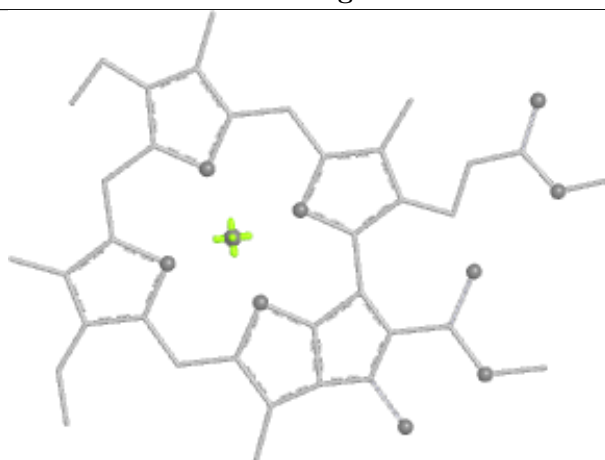
Bond lengths



Bond angles

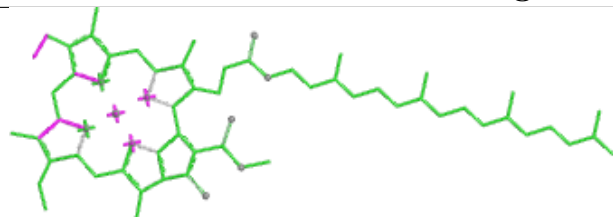


Torsions

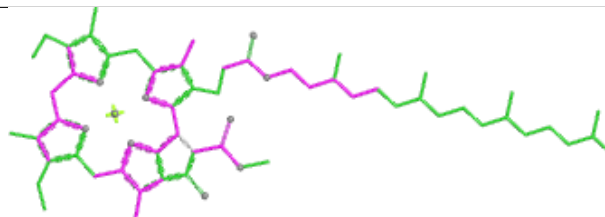


Rings

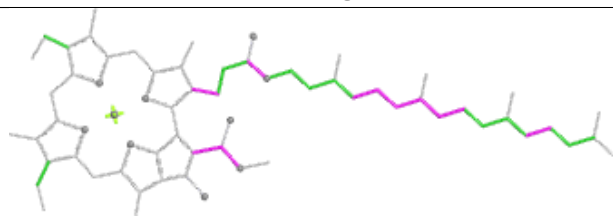
## Ligand CLA A 806



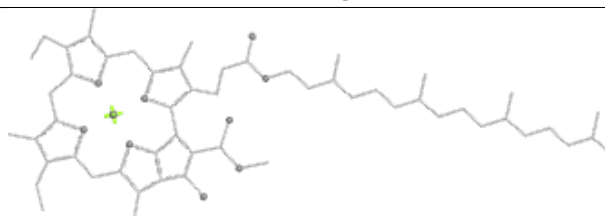
Bond lengths



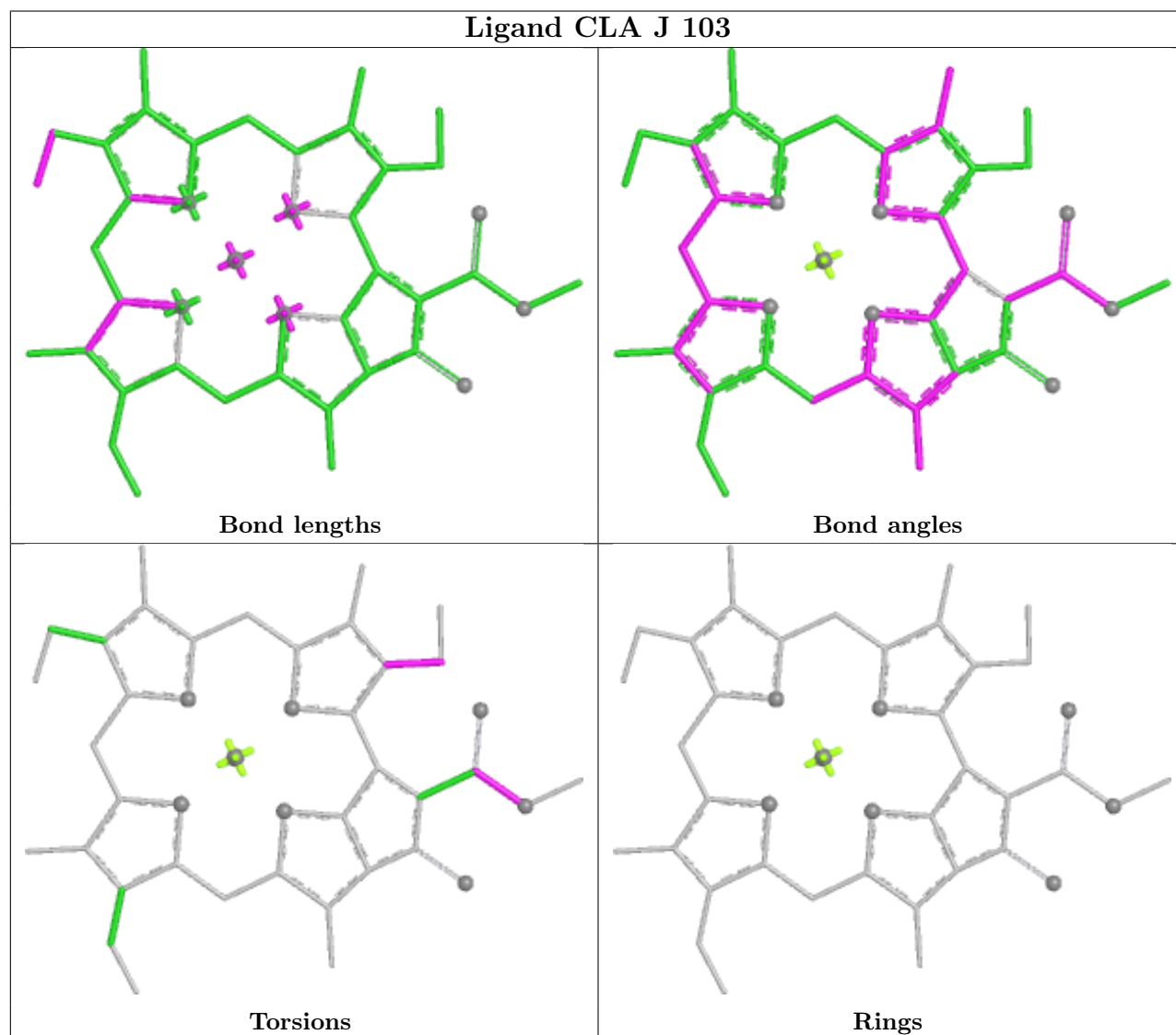
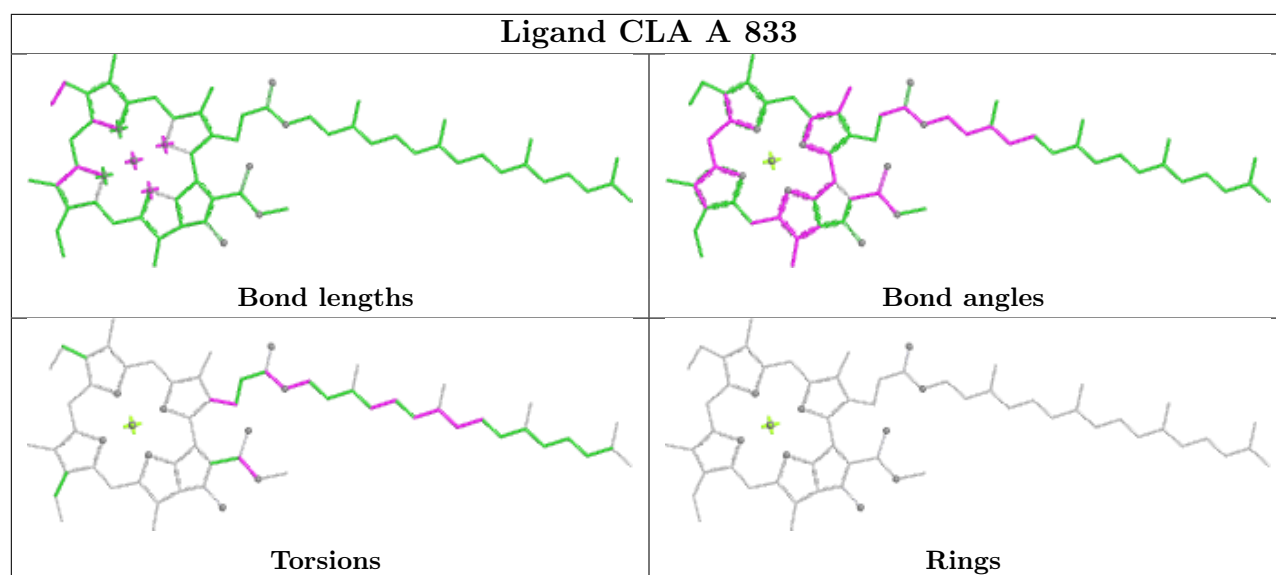
Bond angles

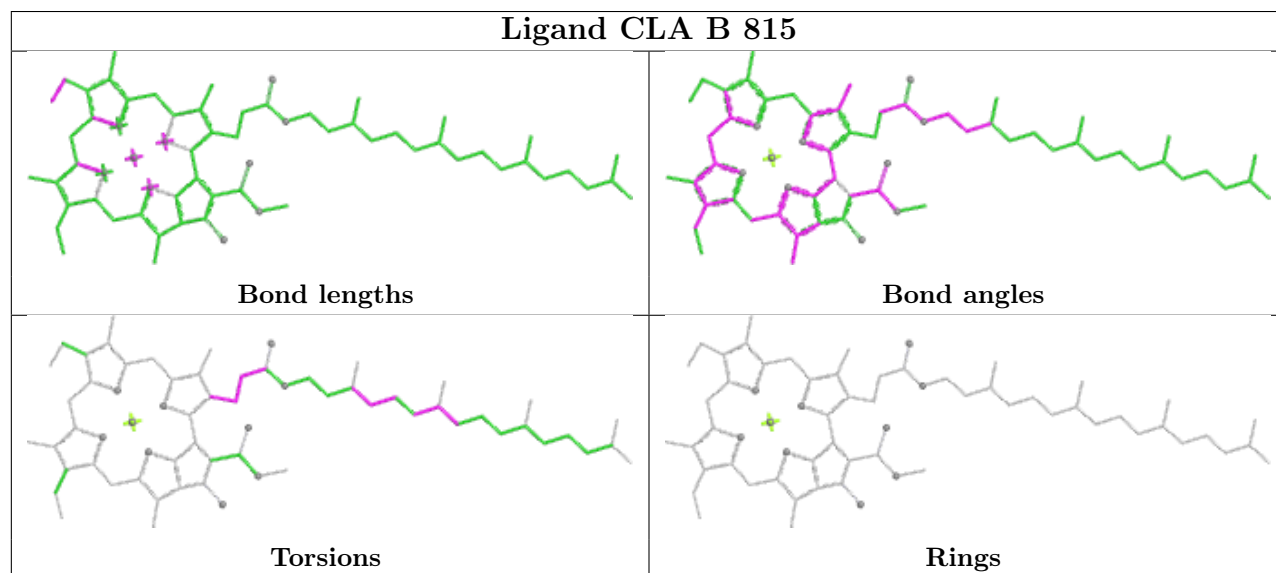
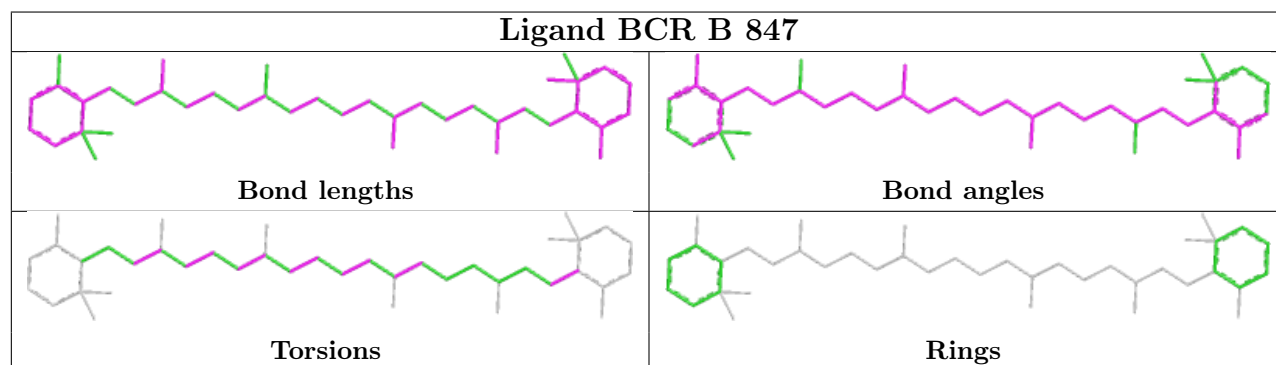
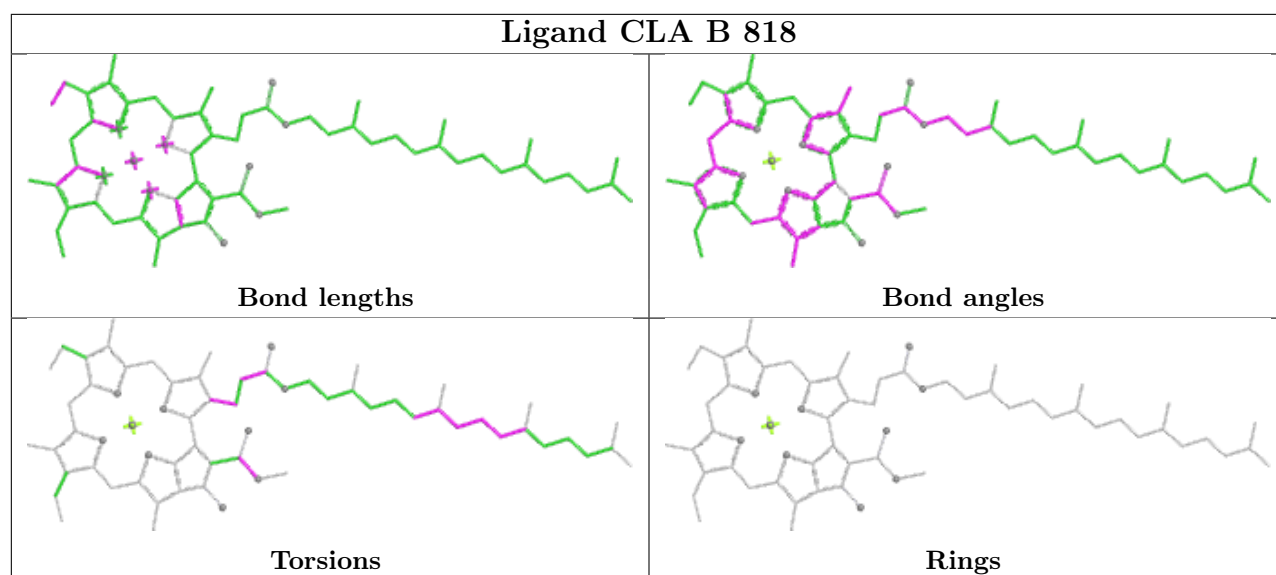


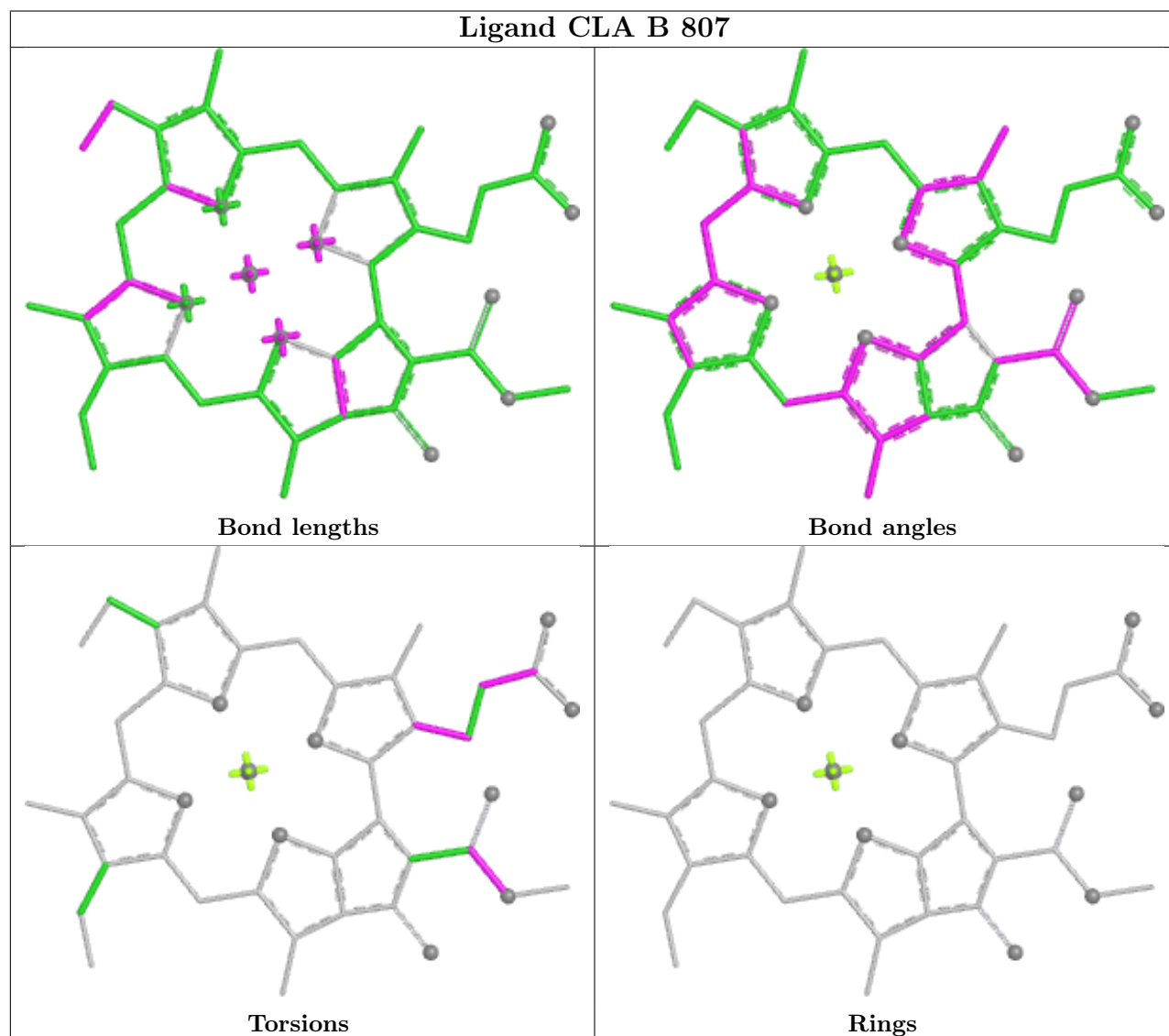
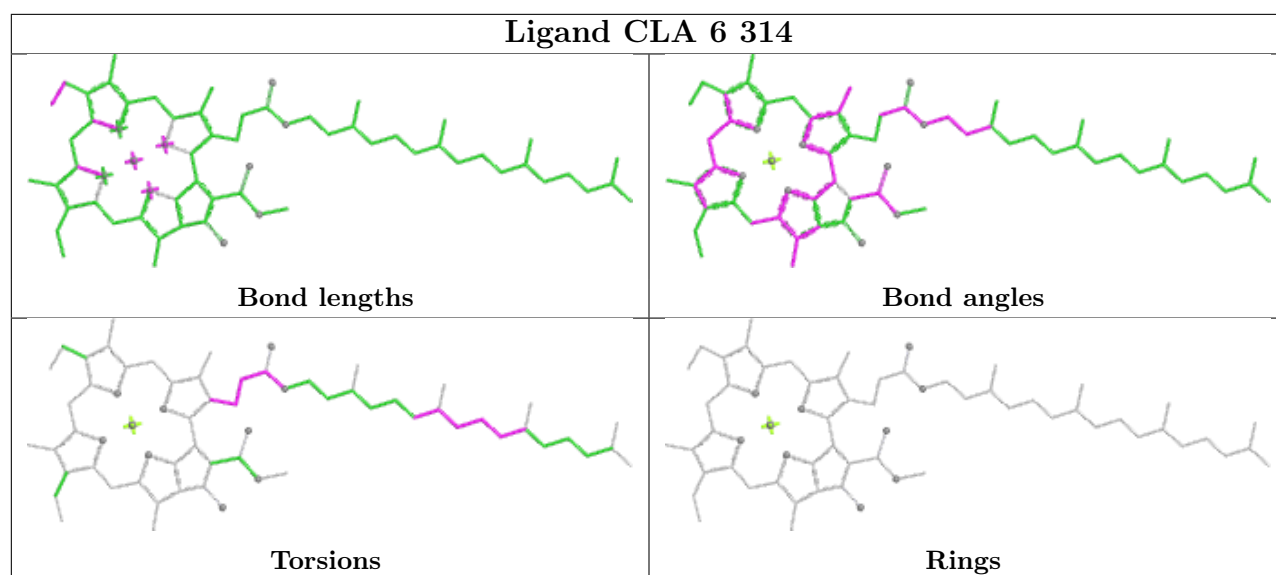
Torsions

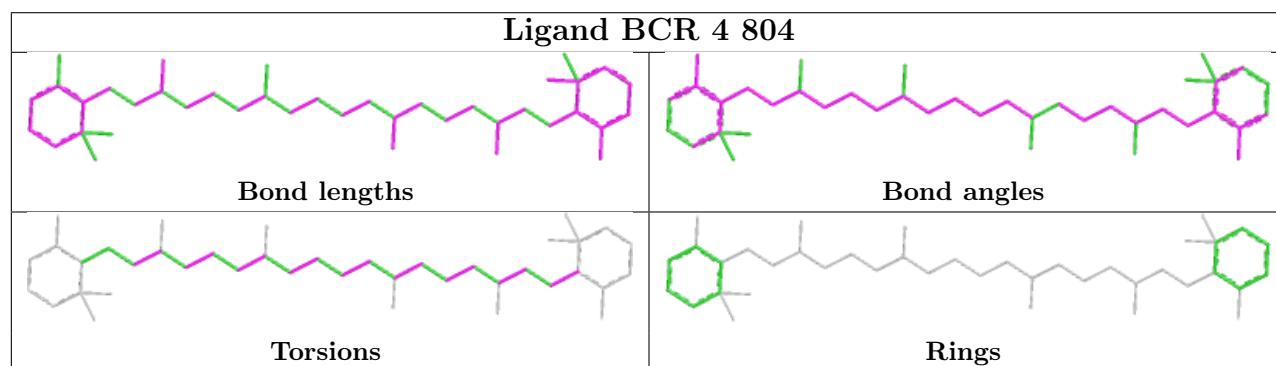
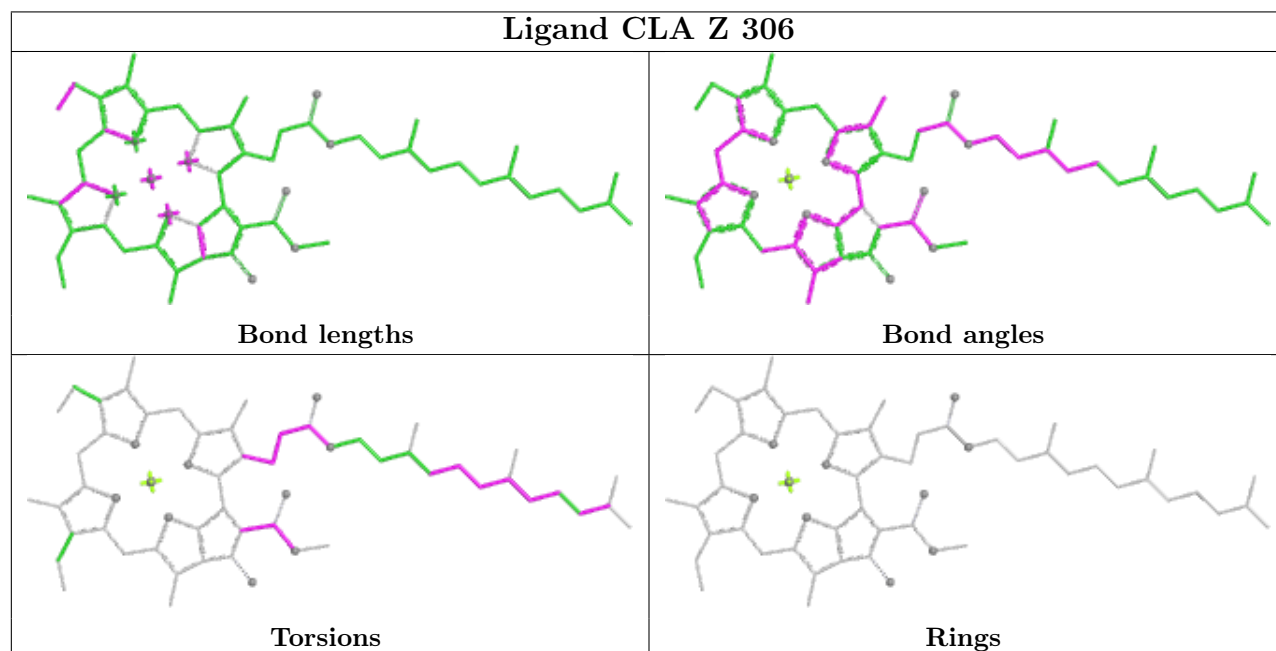
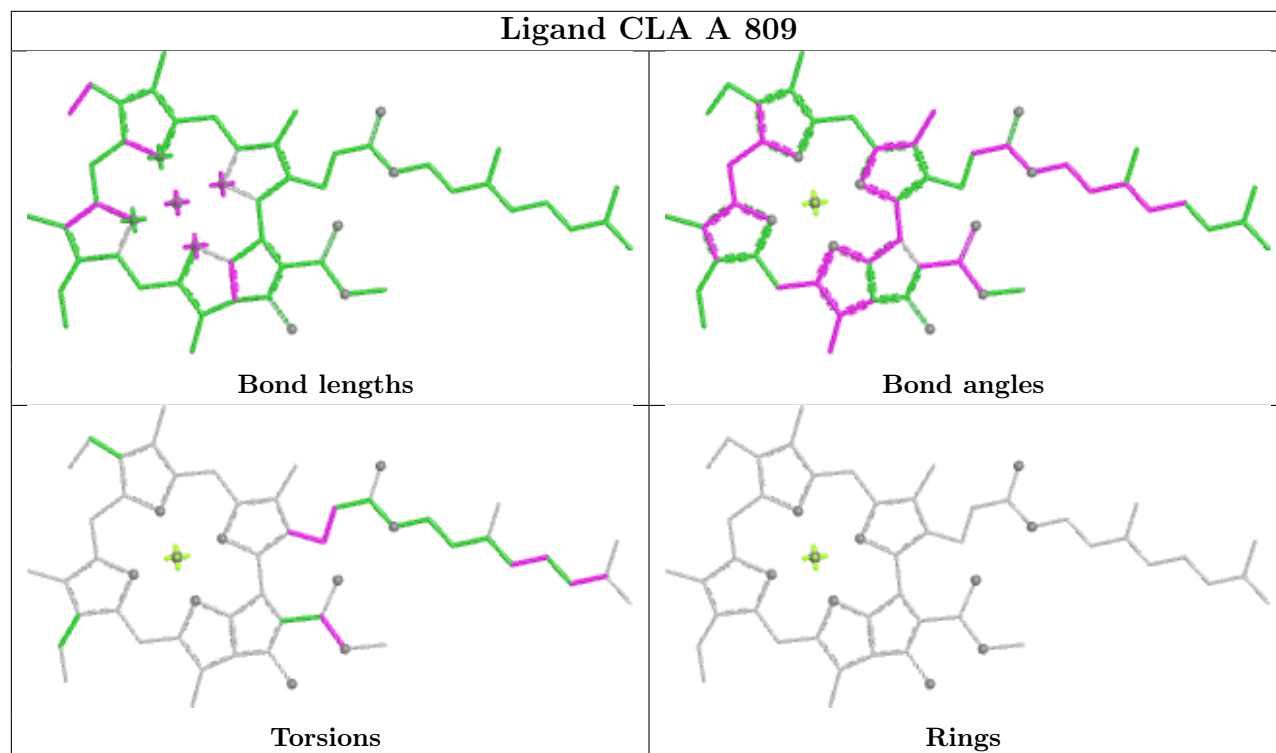


Rings

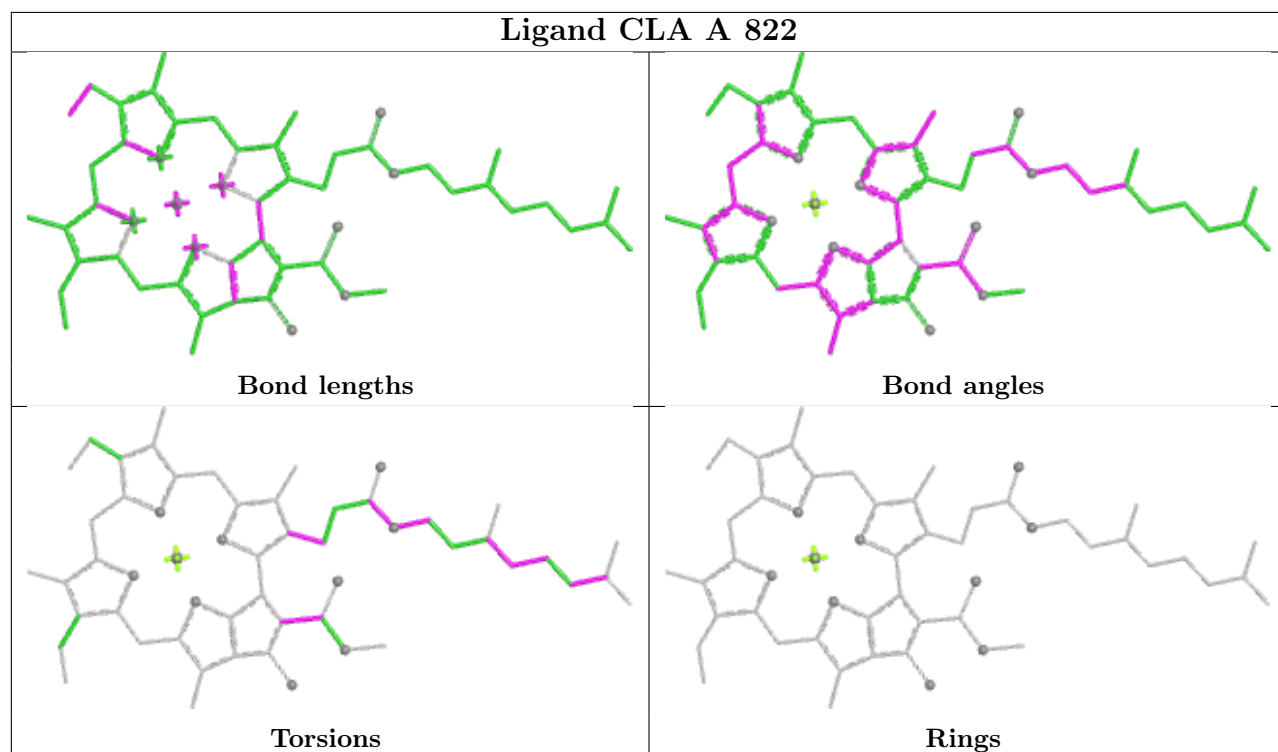
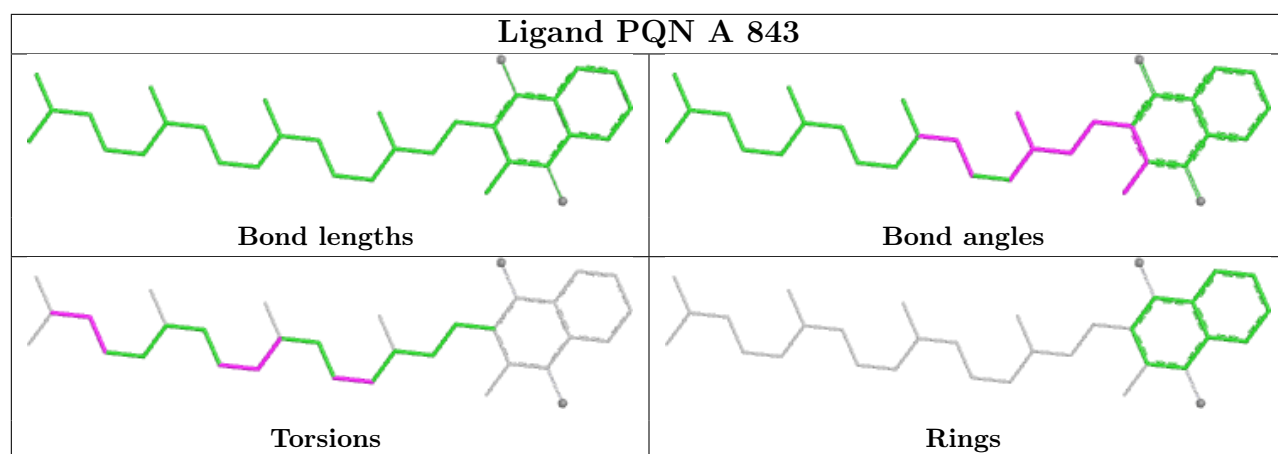




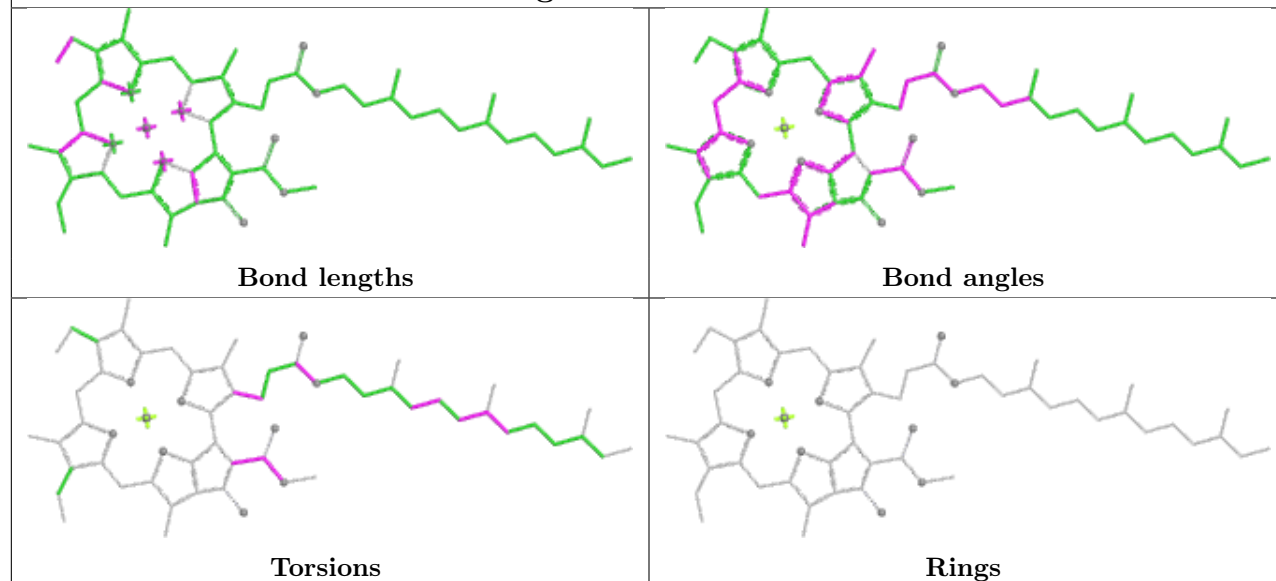




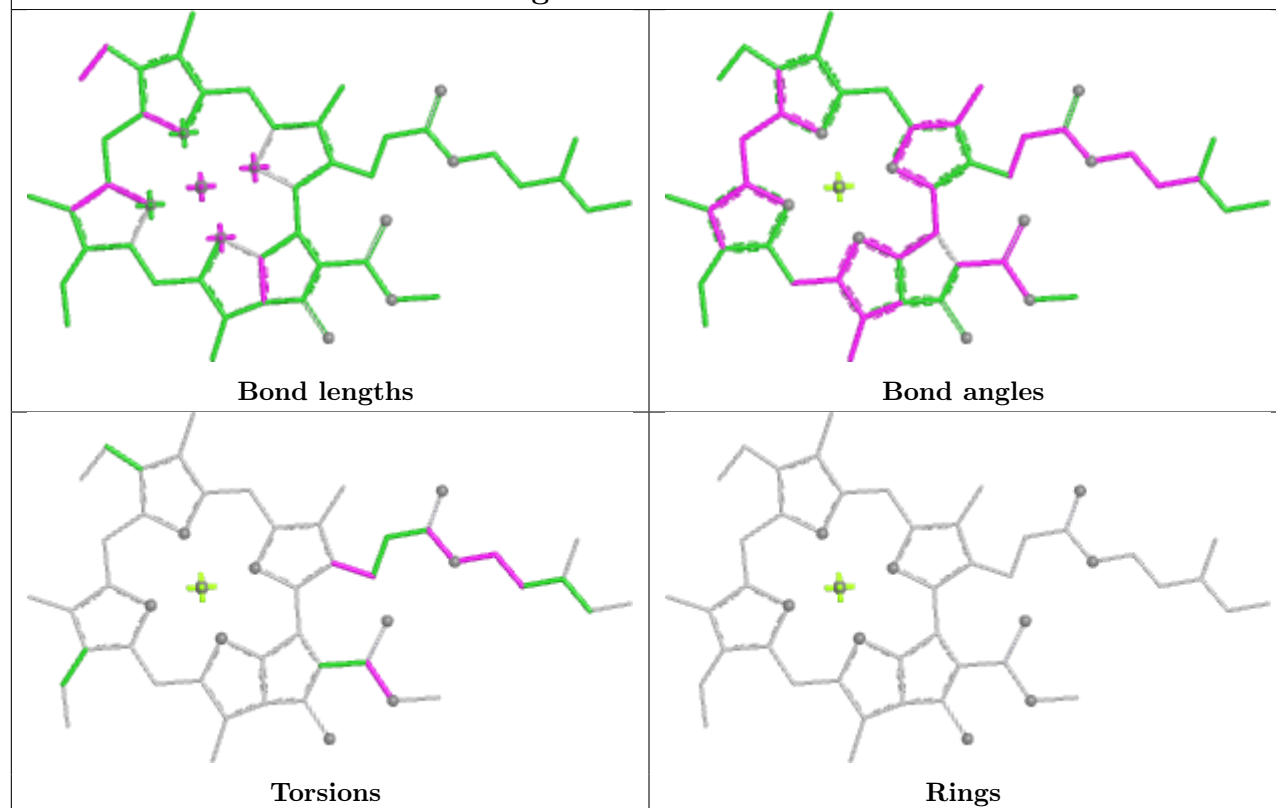


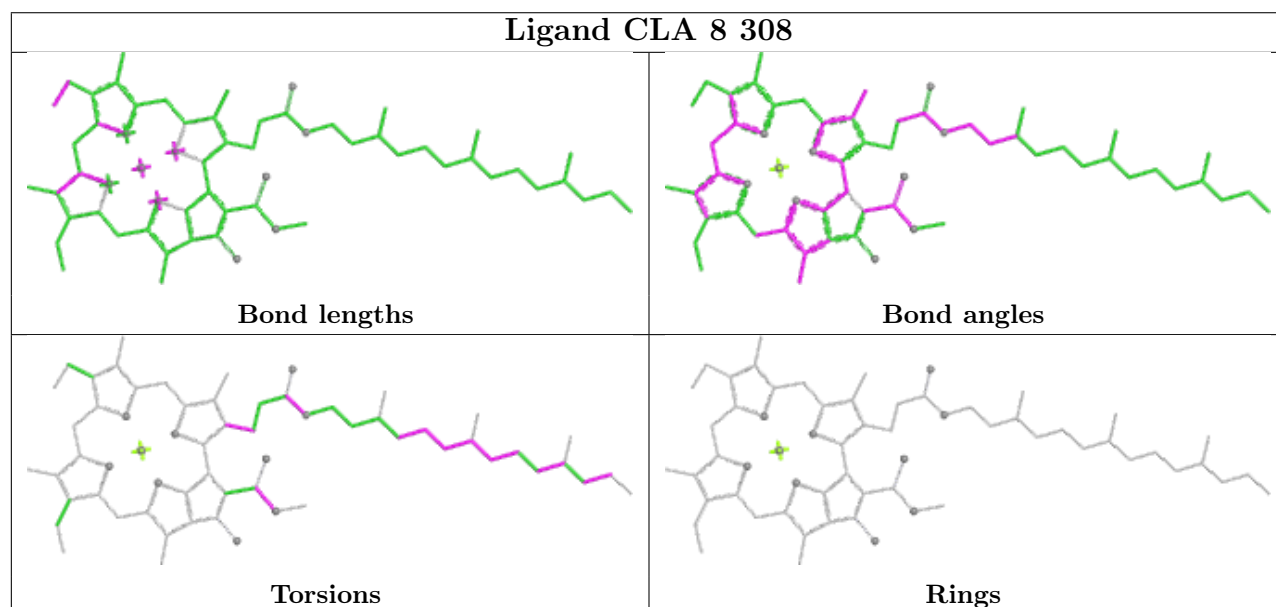
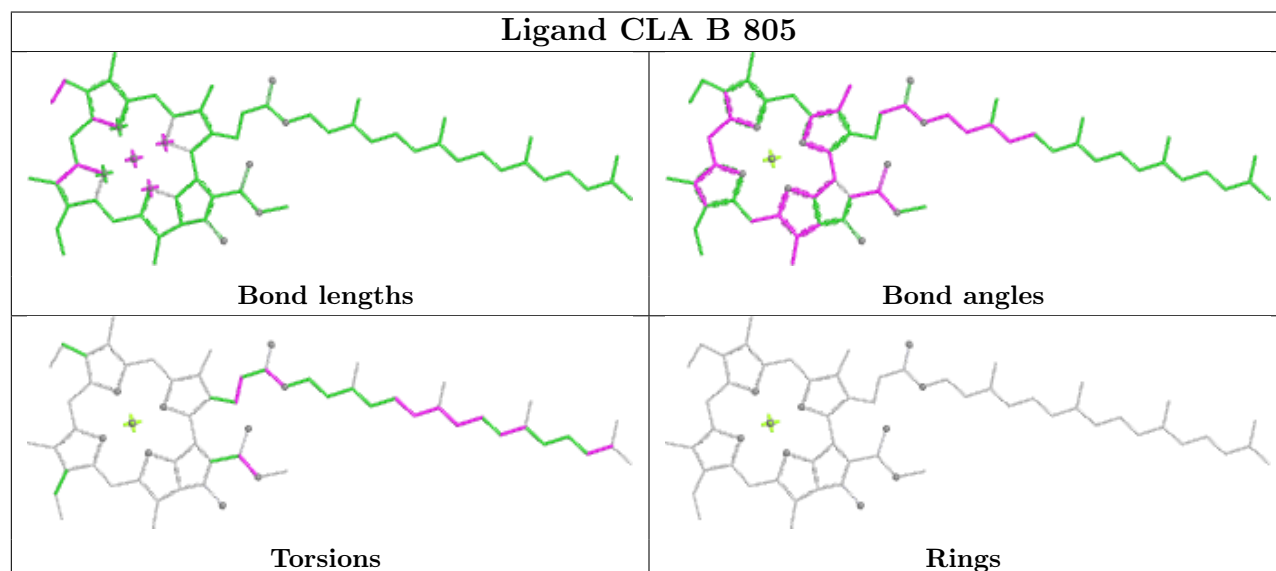
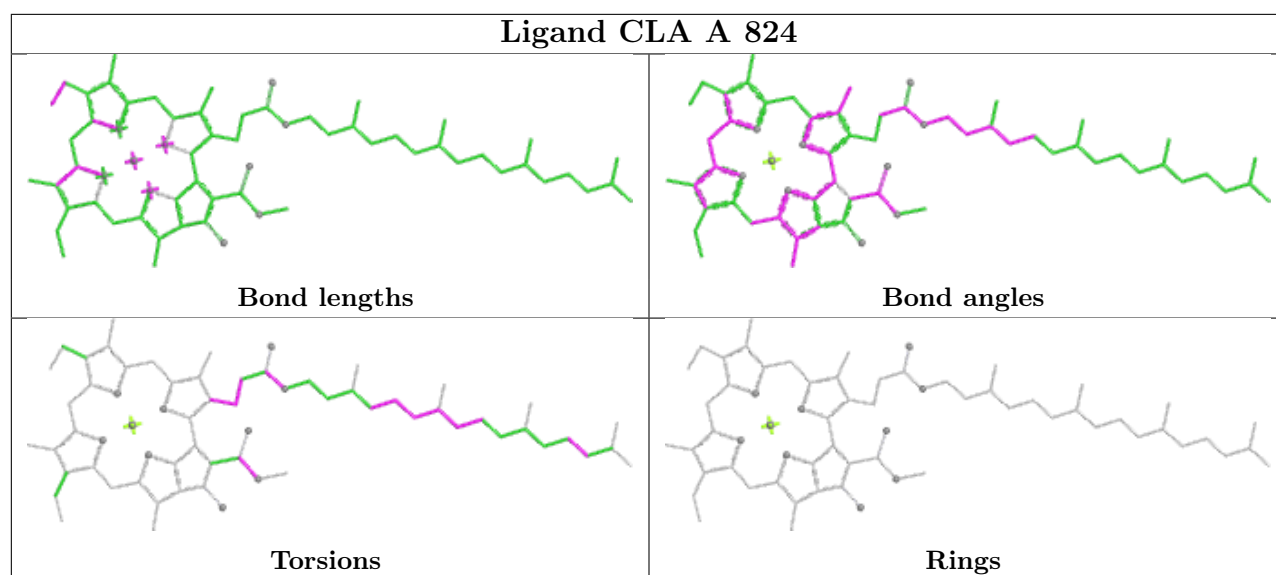


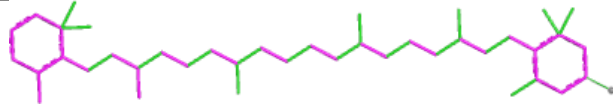
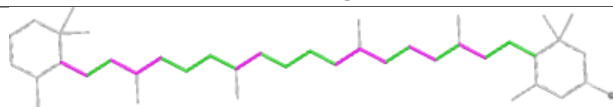
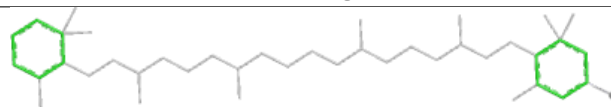
## Ligand CLA 1 309

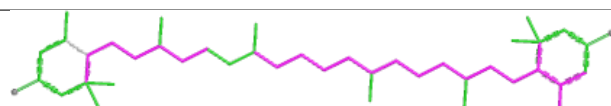
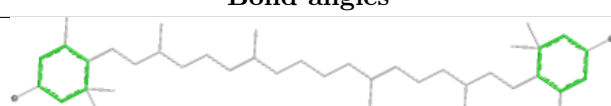


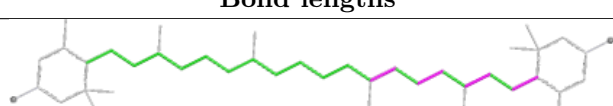
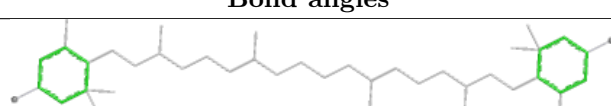
## Ligand CLA A 839



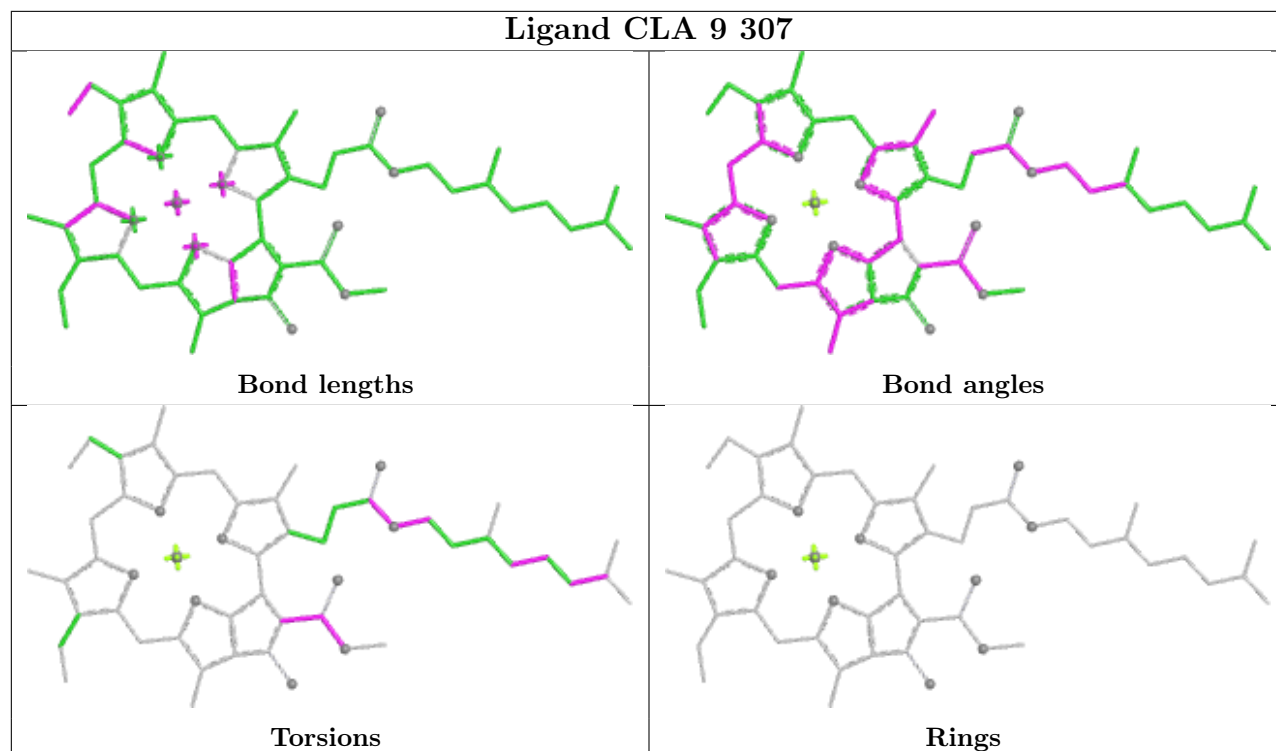


| Ligand RRX F 306                                                                   |              |
|------------------------------------------------------------------------------------|--------------|
|   | Bond lengths |
|  | Bond angles  |
|   | Torsions     |
|  | Rings        |

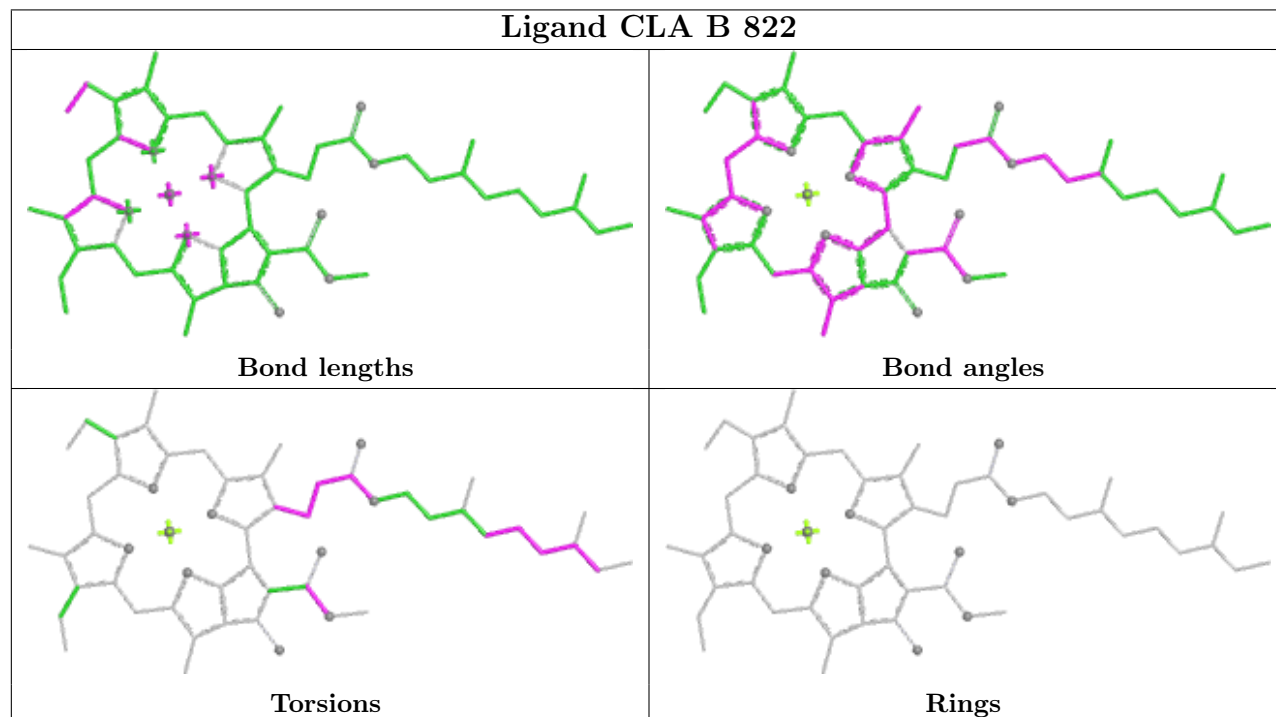
| Ligand LUT 6 304                                                                   |              |
|------------------------------------------------------------------------------------|--------------|
|   | Bond lengths |
|  | Bond angles  |
|   | Torsions     |
|  | Rings        |

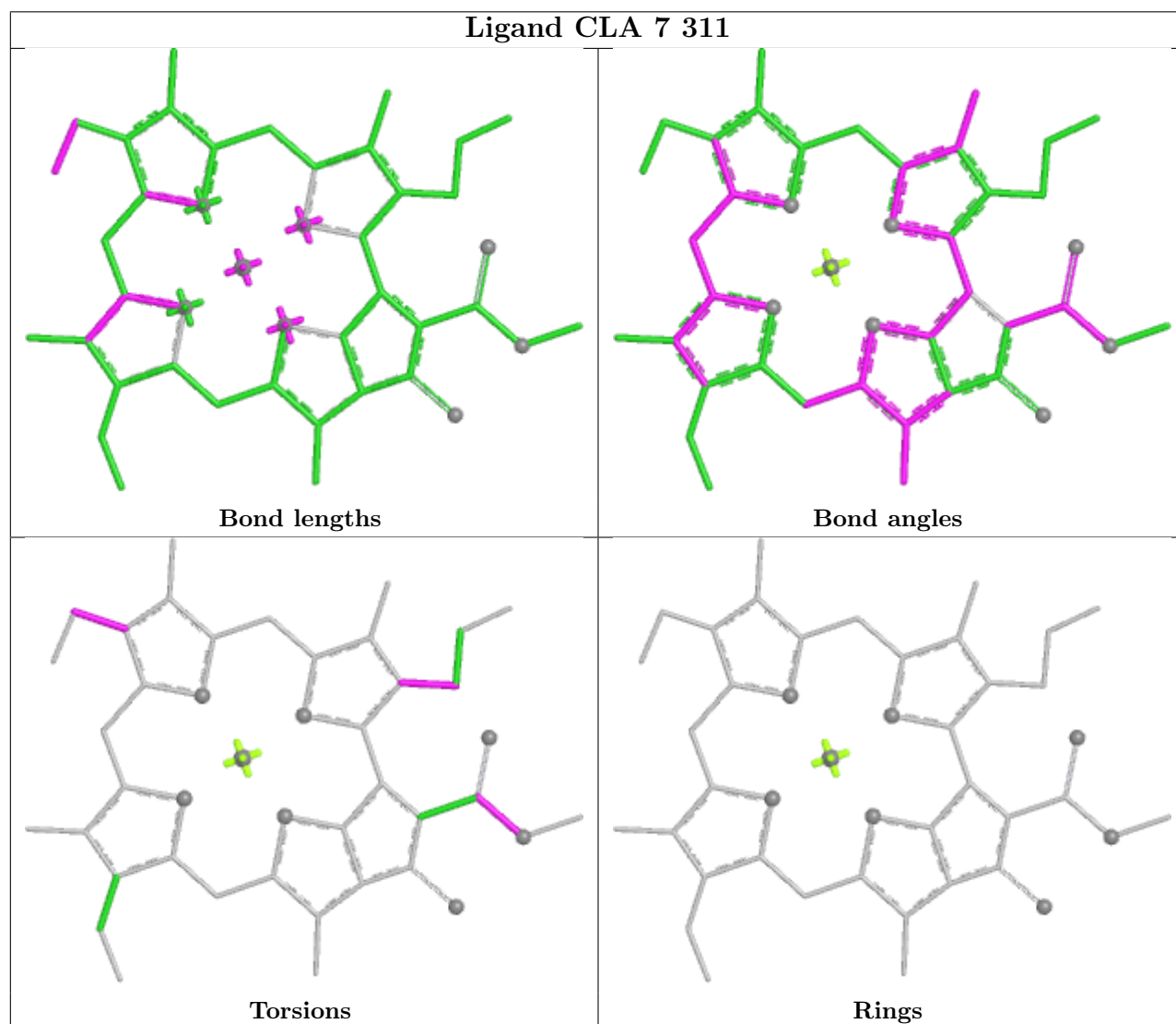
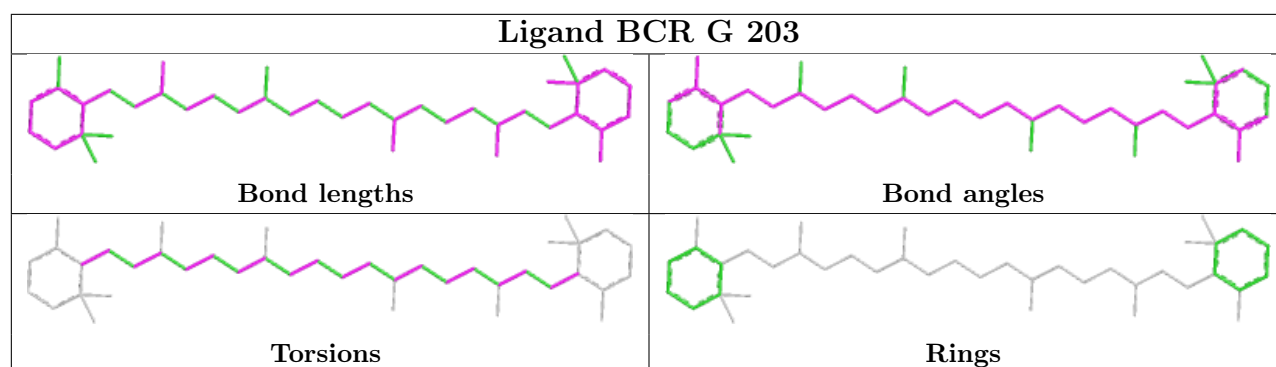
| Ligand LUT 5 303                                                                     |              |
|--------------------------------------------------------------------------------------|--------------|
|    | Bond lengths |
|   | Bond angles  |
|   | Torsions     |
|  | Rings        |

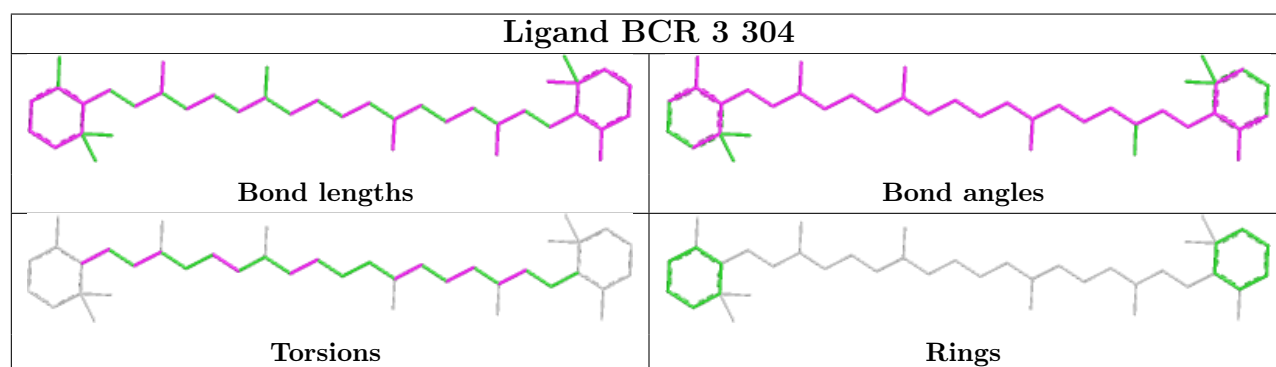
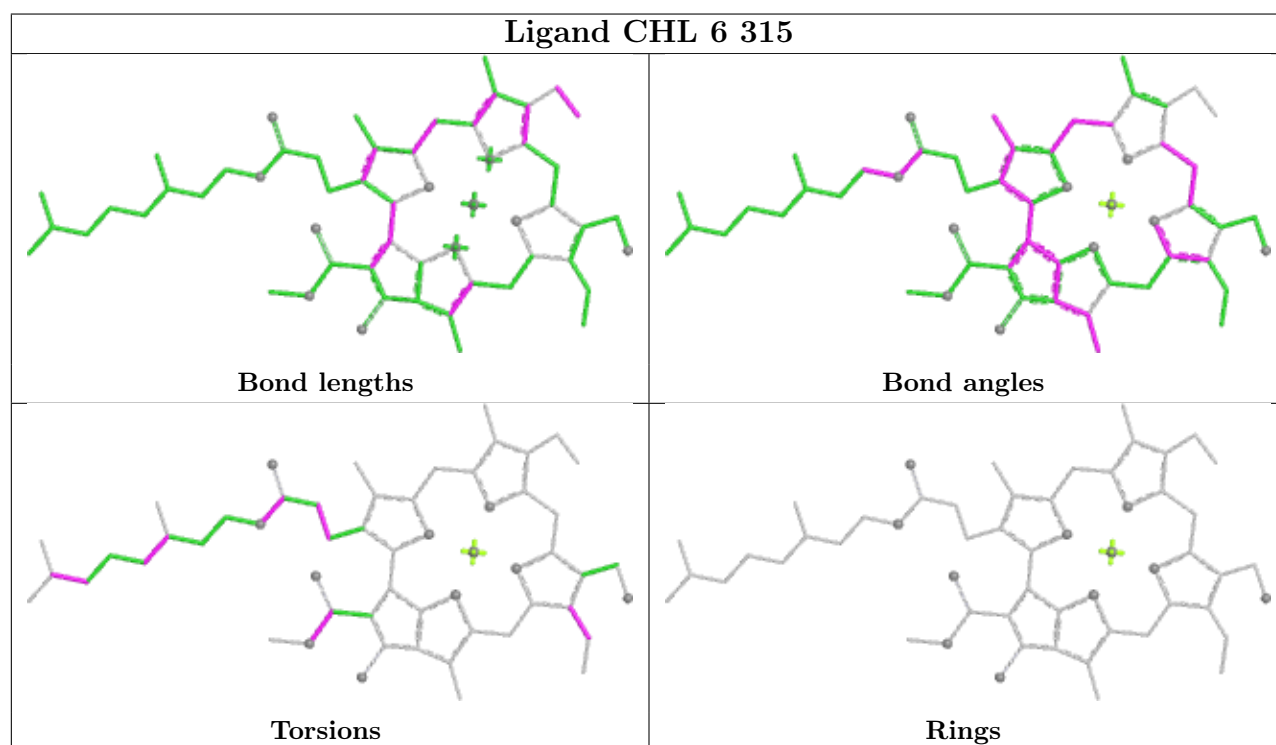
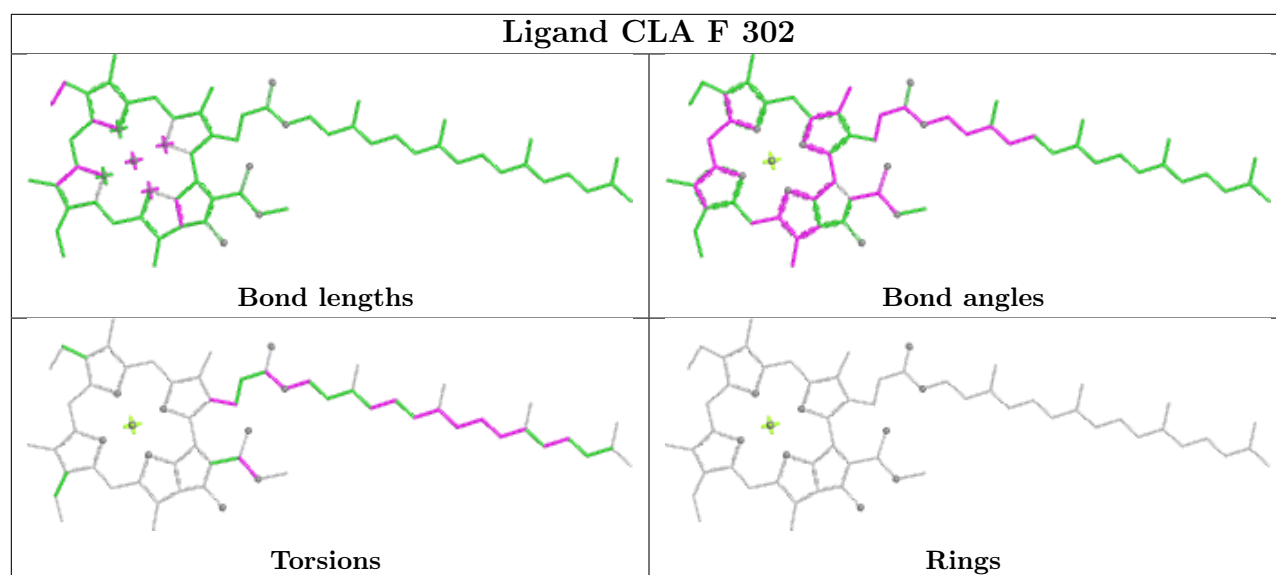
## Ligand CLA 9 307

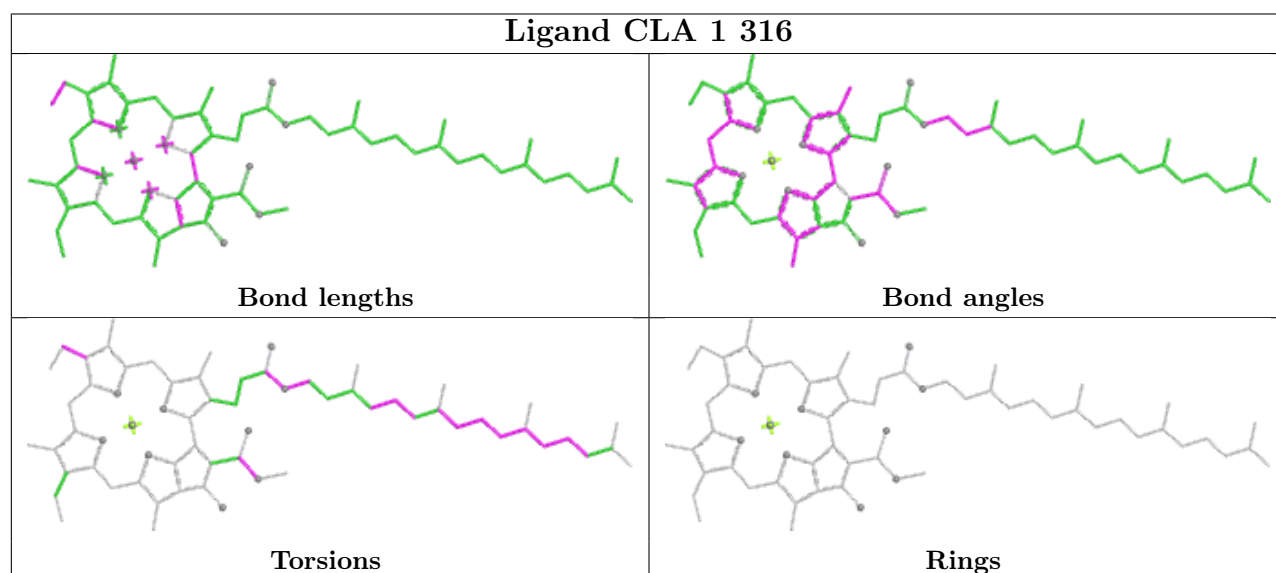
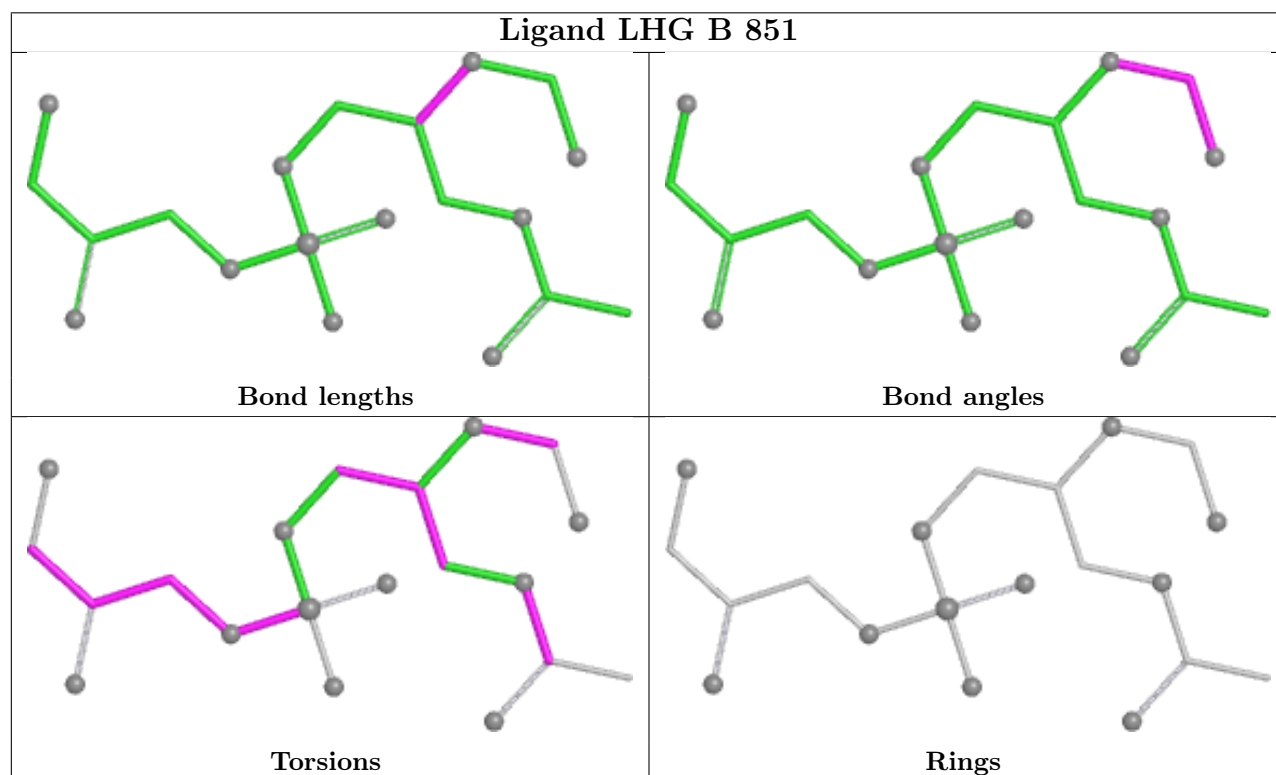
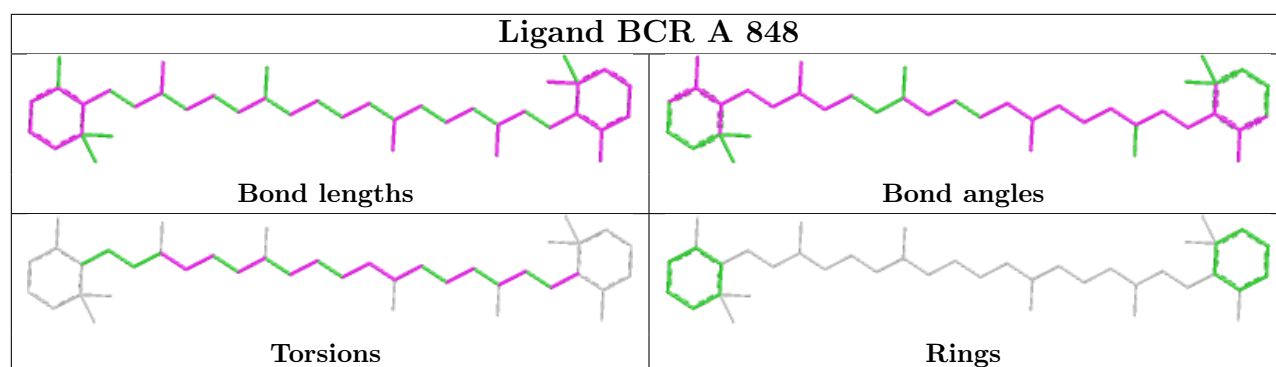


## Ligand CLA B 822

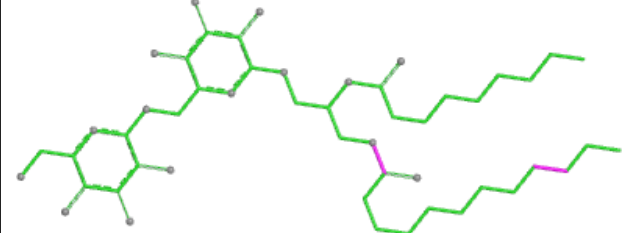
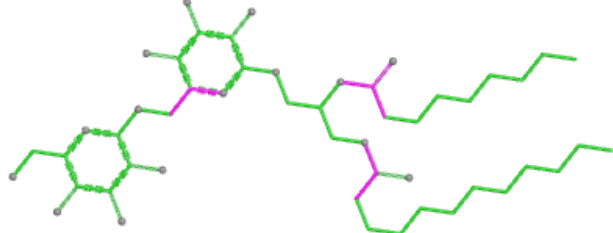
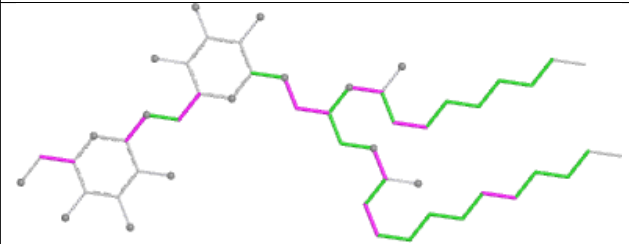
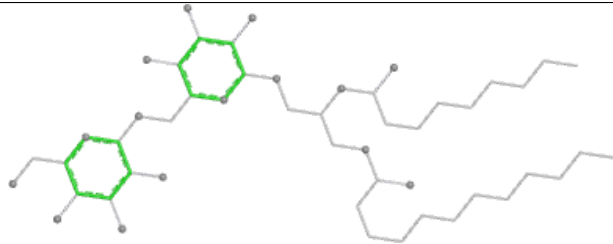
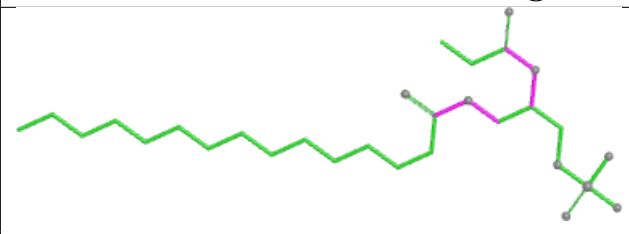
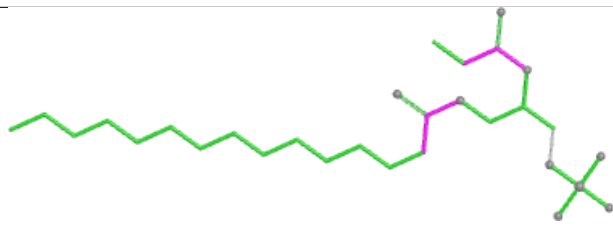
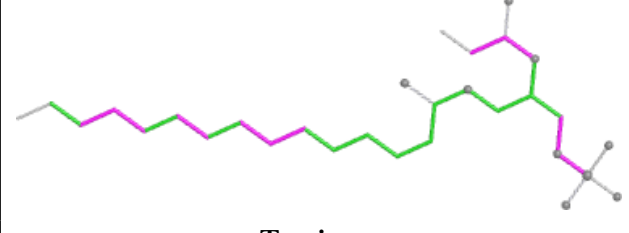
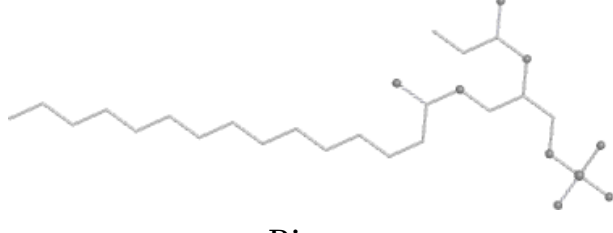
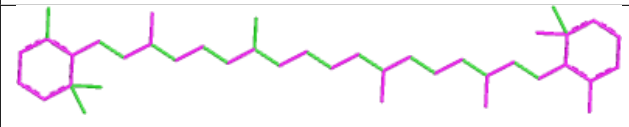
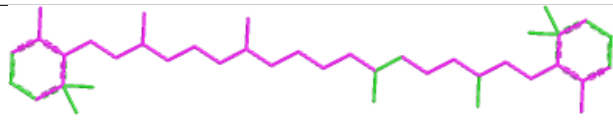
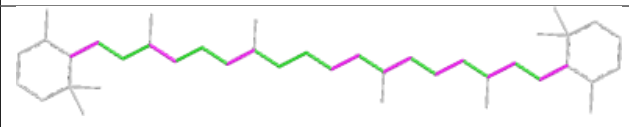
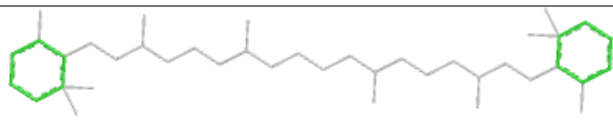


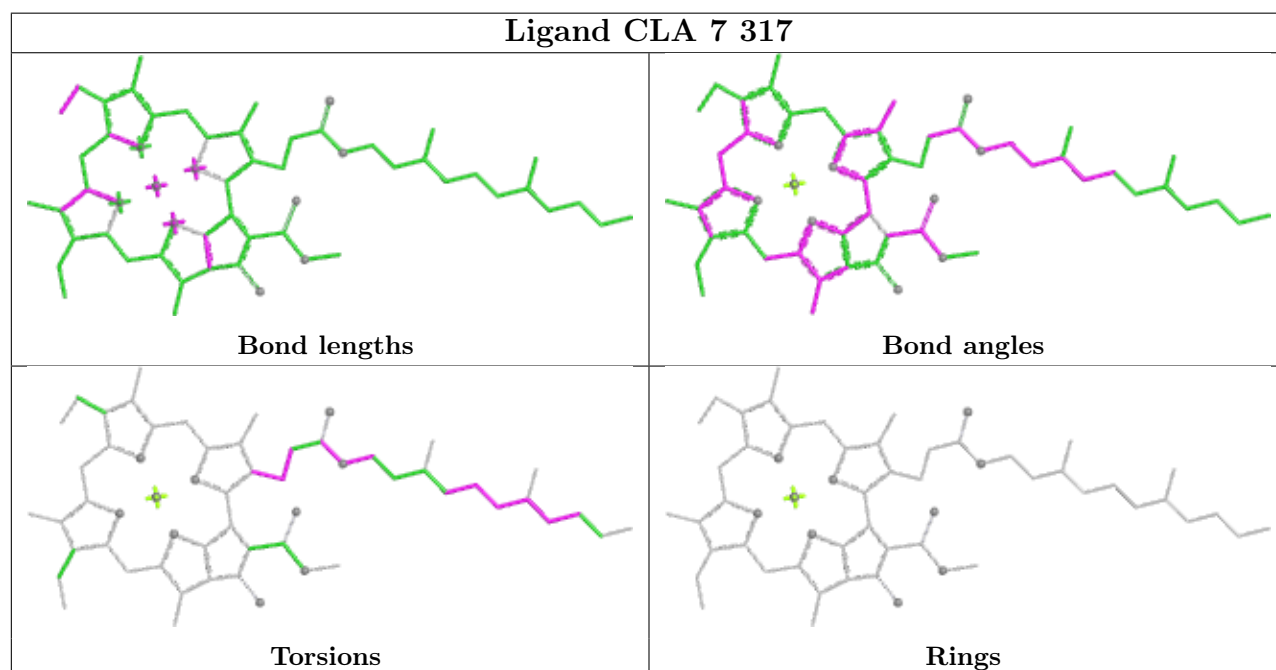
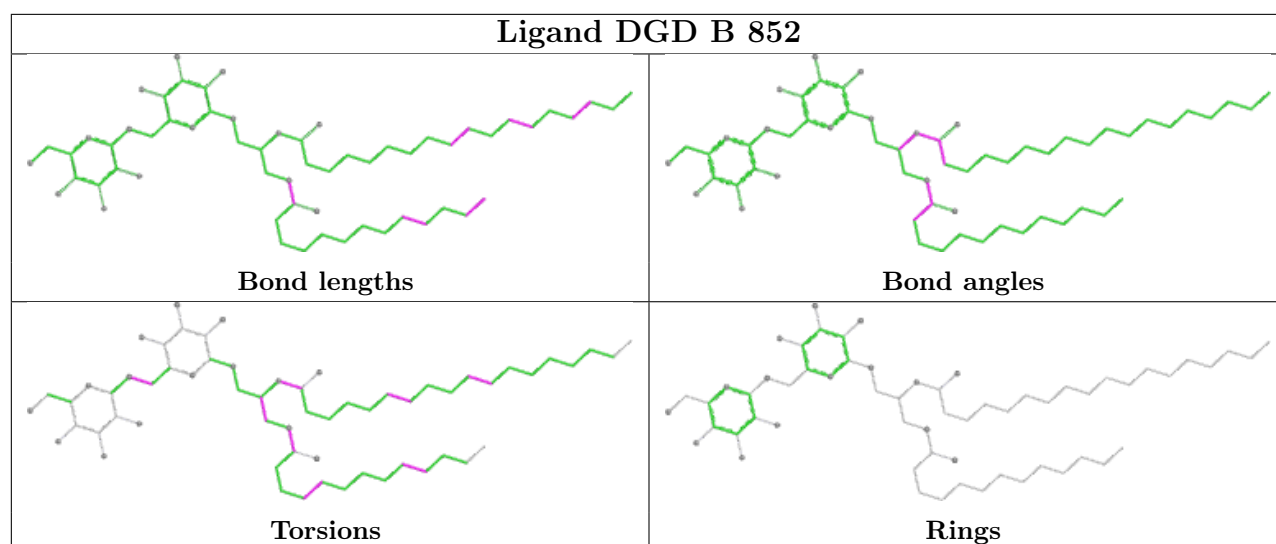


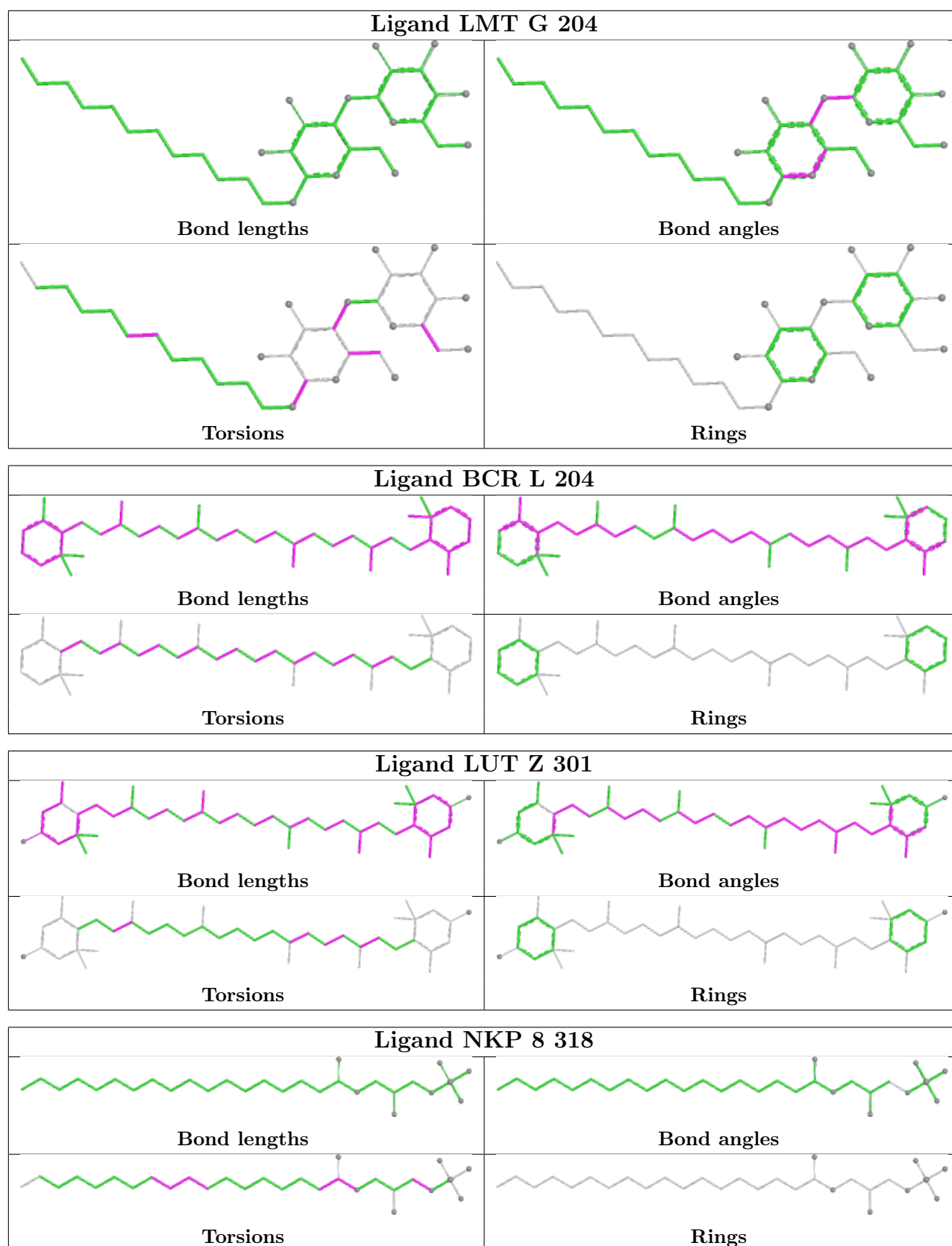




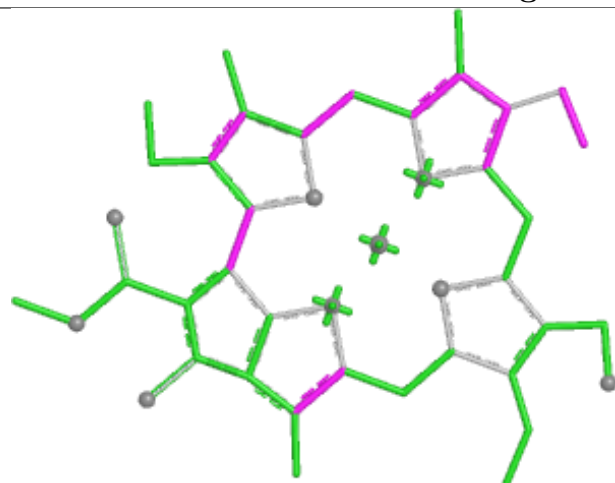


| Ligand DGD 1 319                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand 3PH 8 320                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>  |  <p>Bond angles</p>  |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand BCR A 844                                                                                        |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

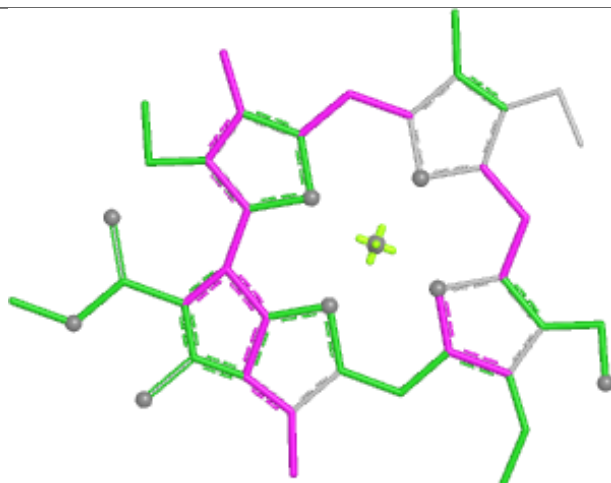




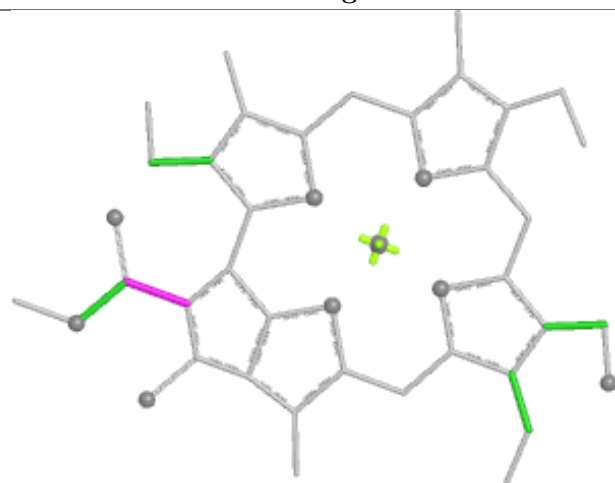
## Ligand CHL 6 320



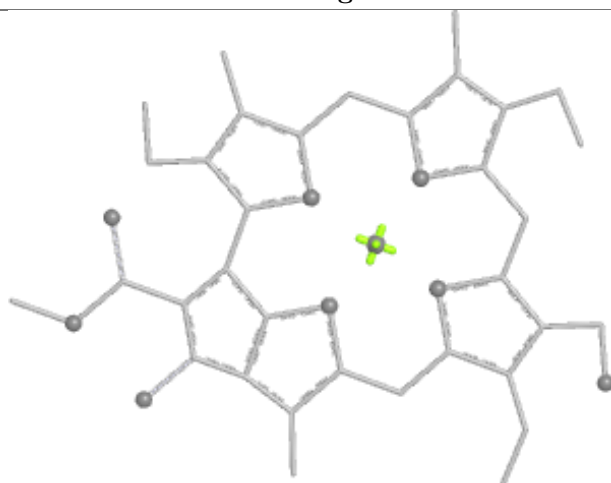
Bond lengths



Bond angles

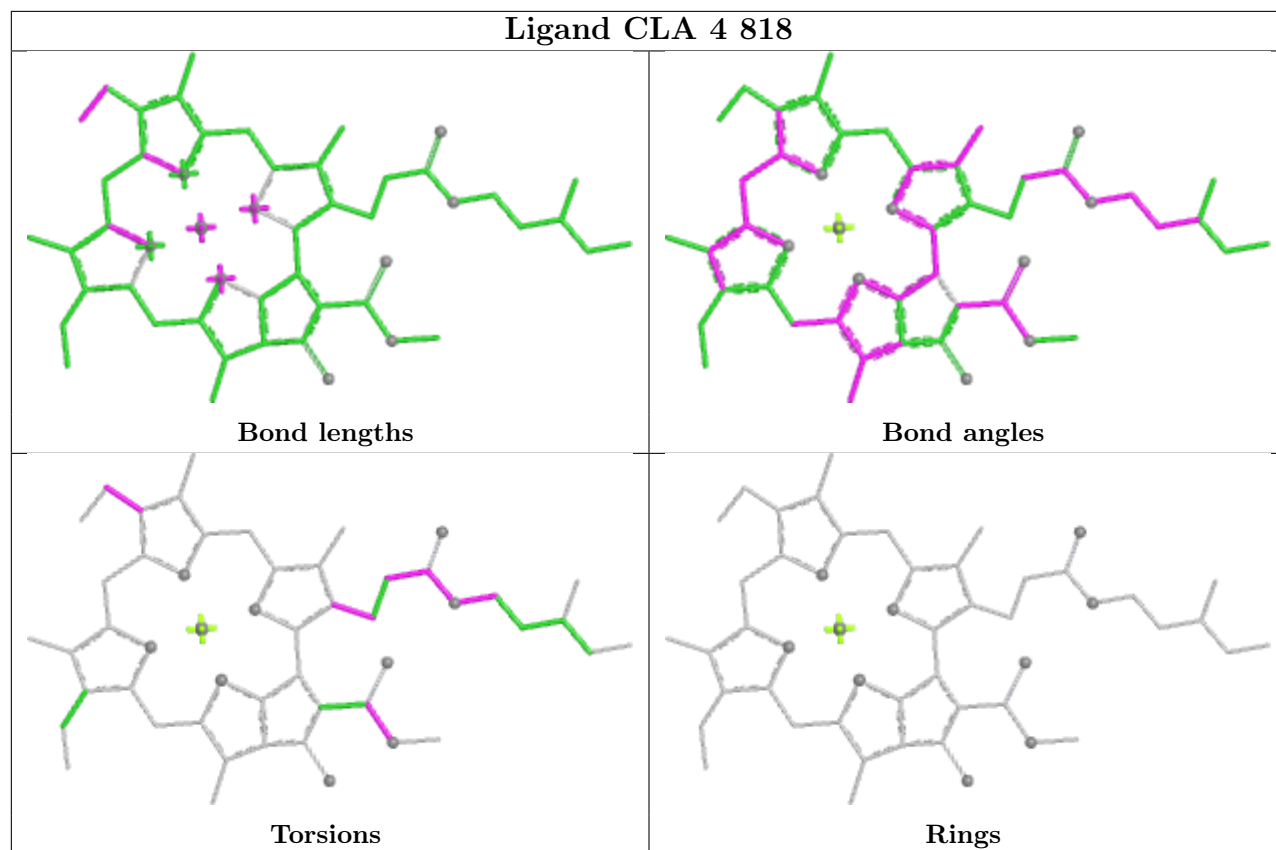


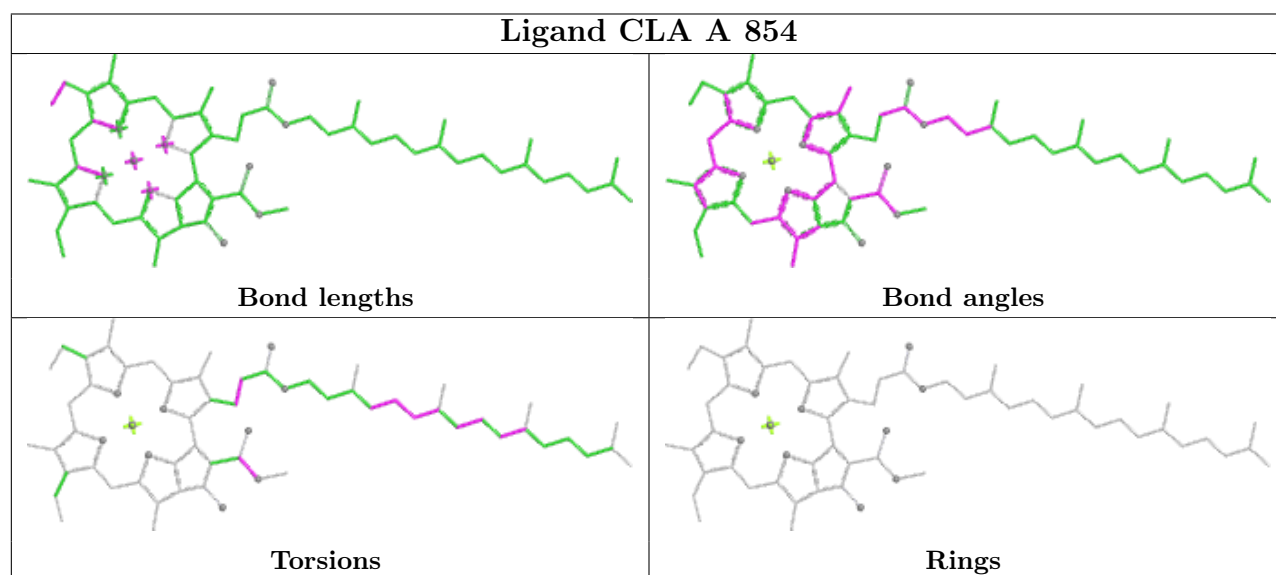
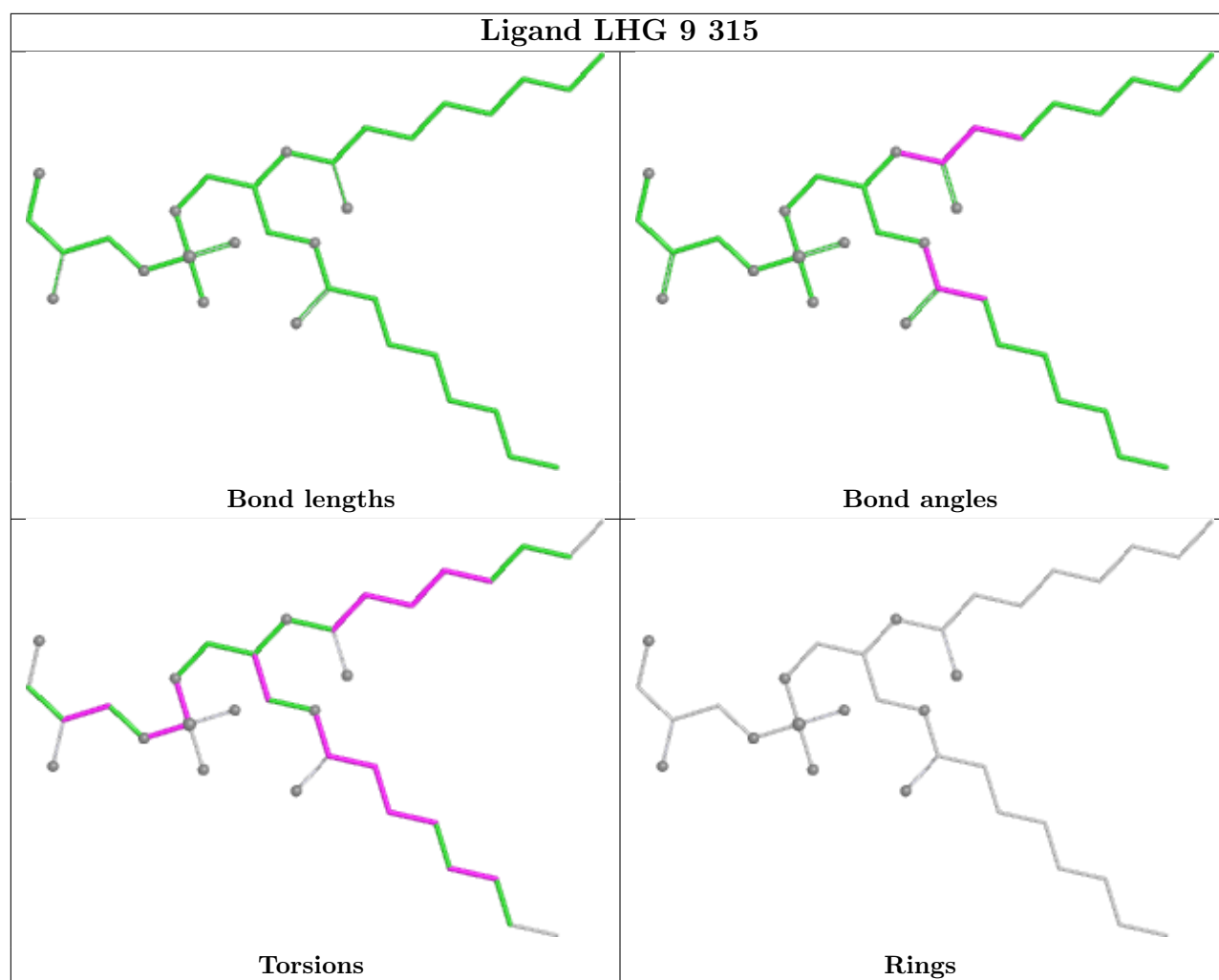
Torsions

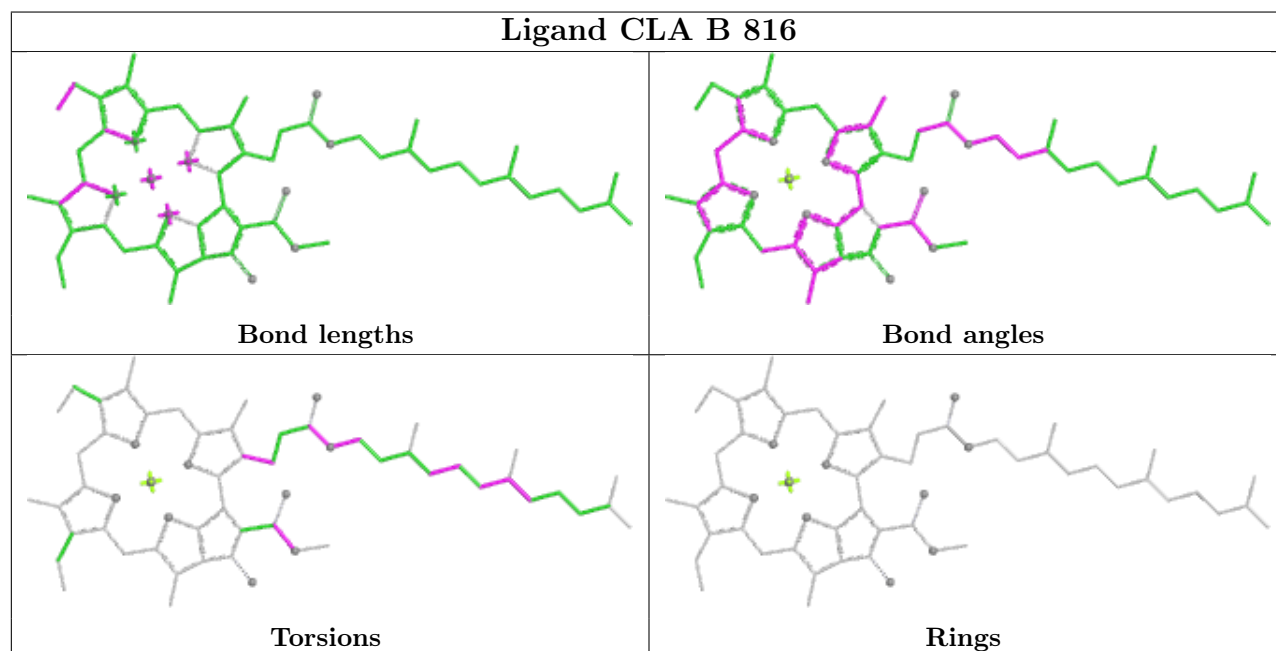
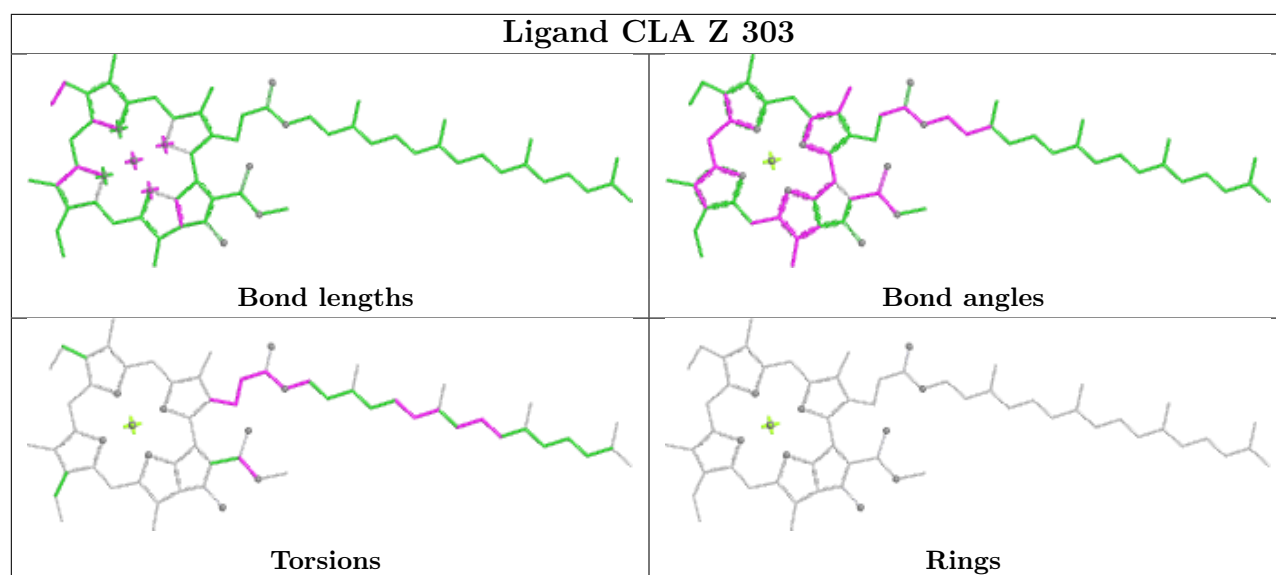


Rings

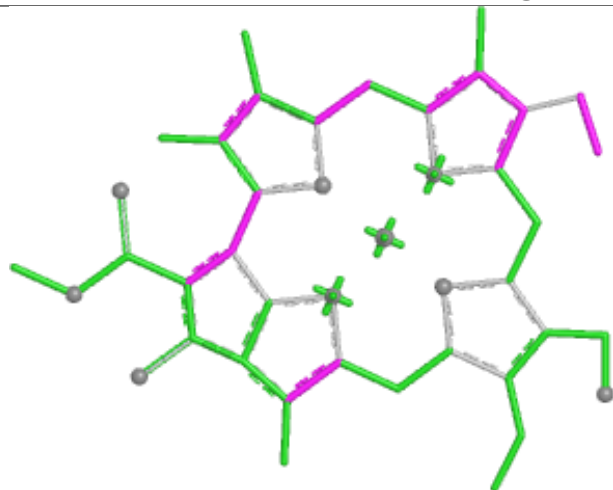
## Ligand CLA 4 818



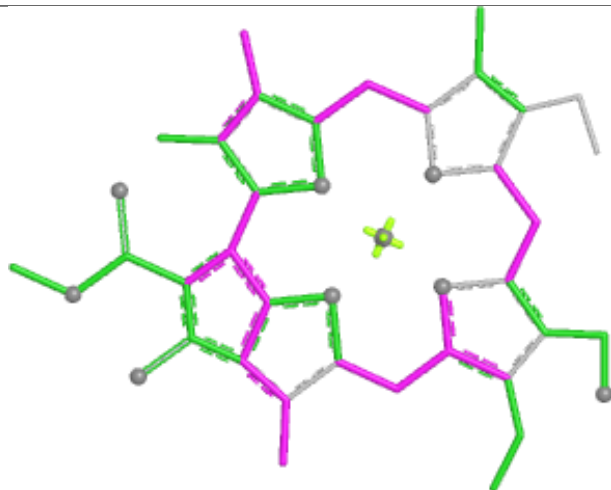




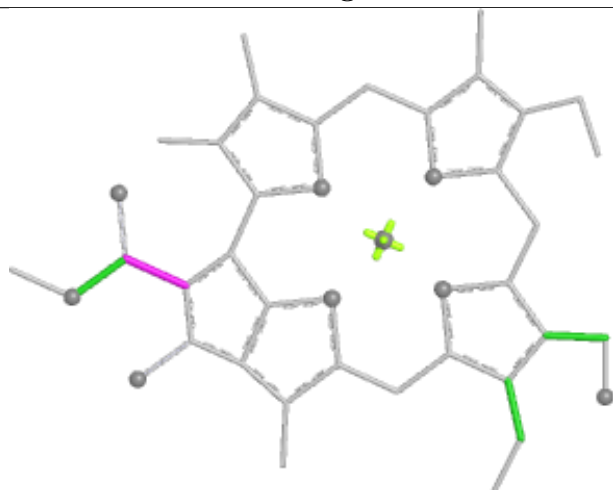
## Ligand CHL 9 314



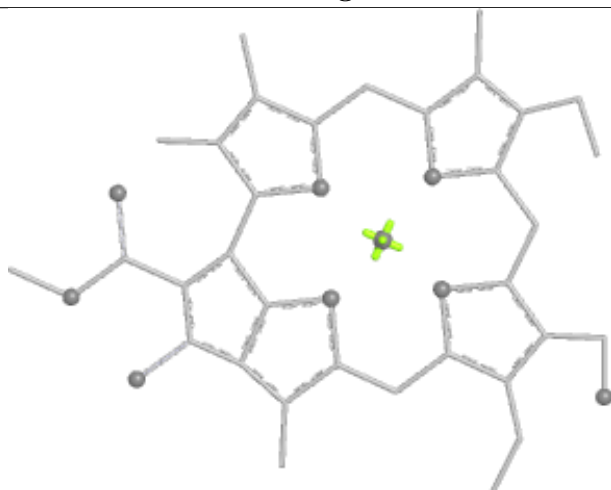
Bond lengths



Bond angles

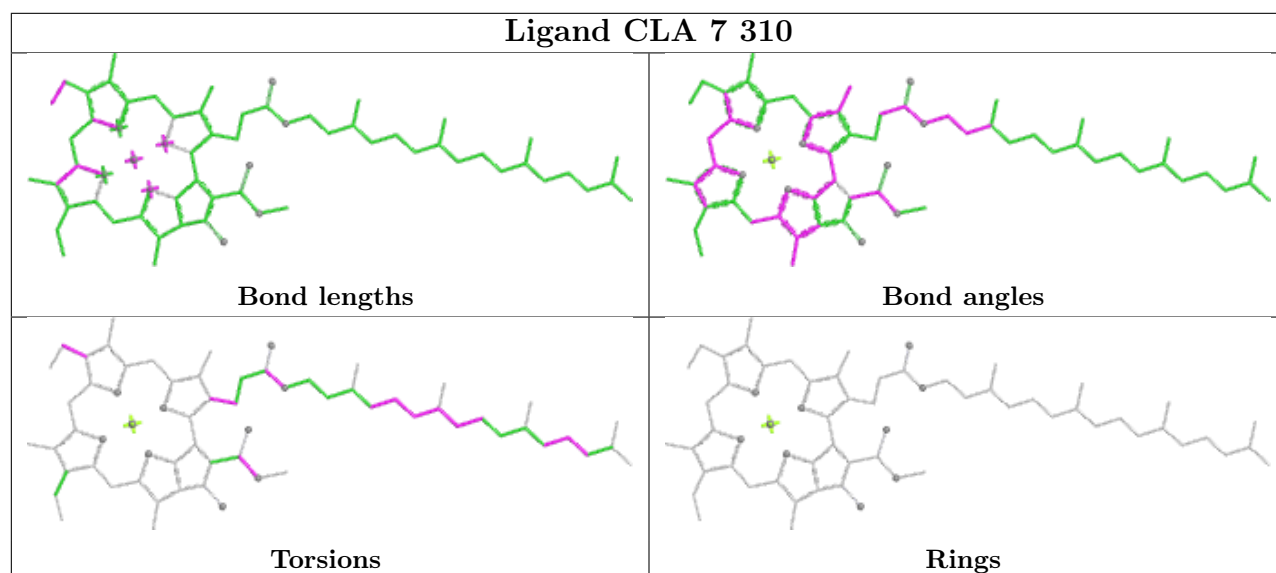
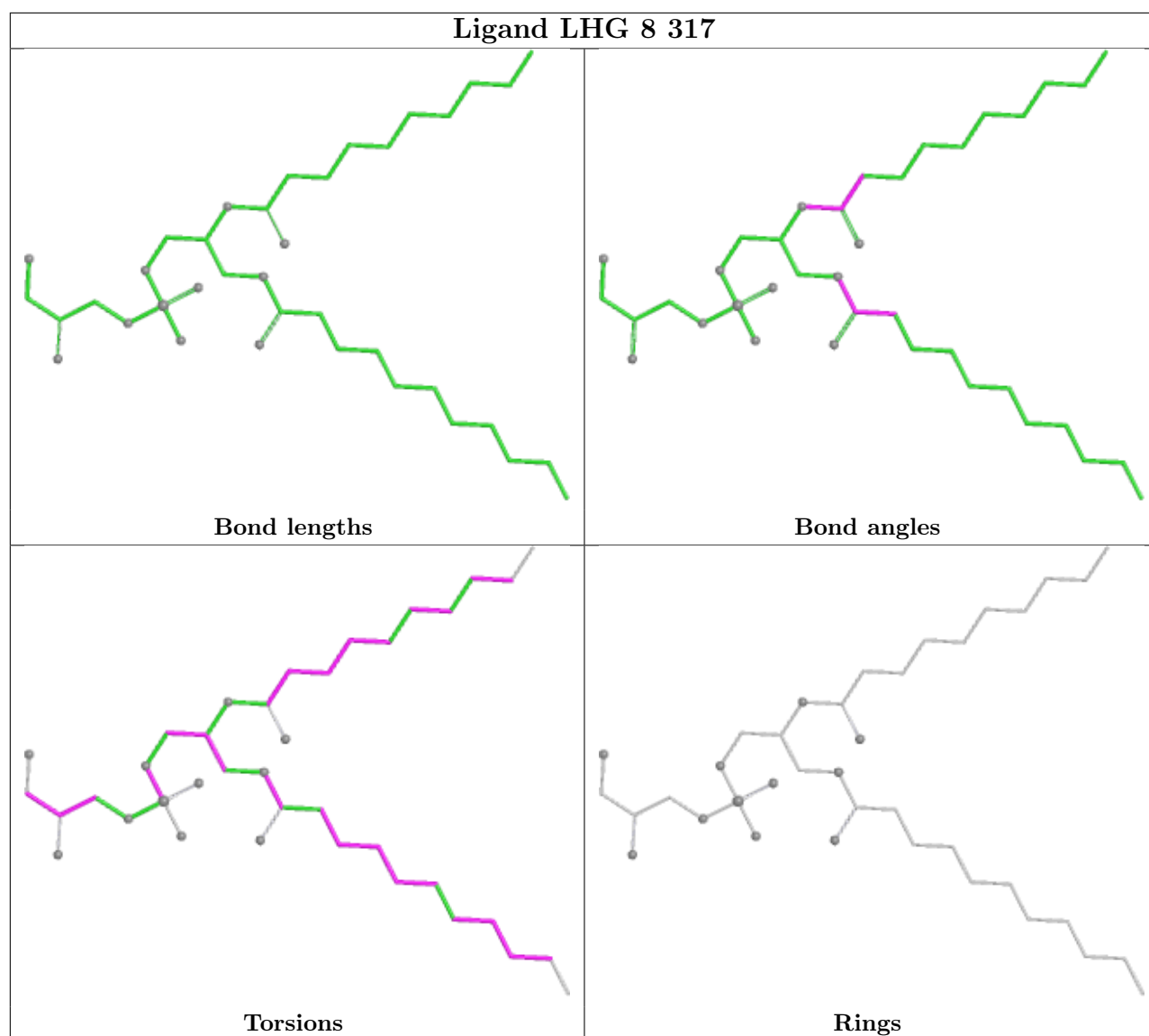


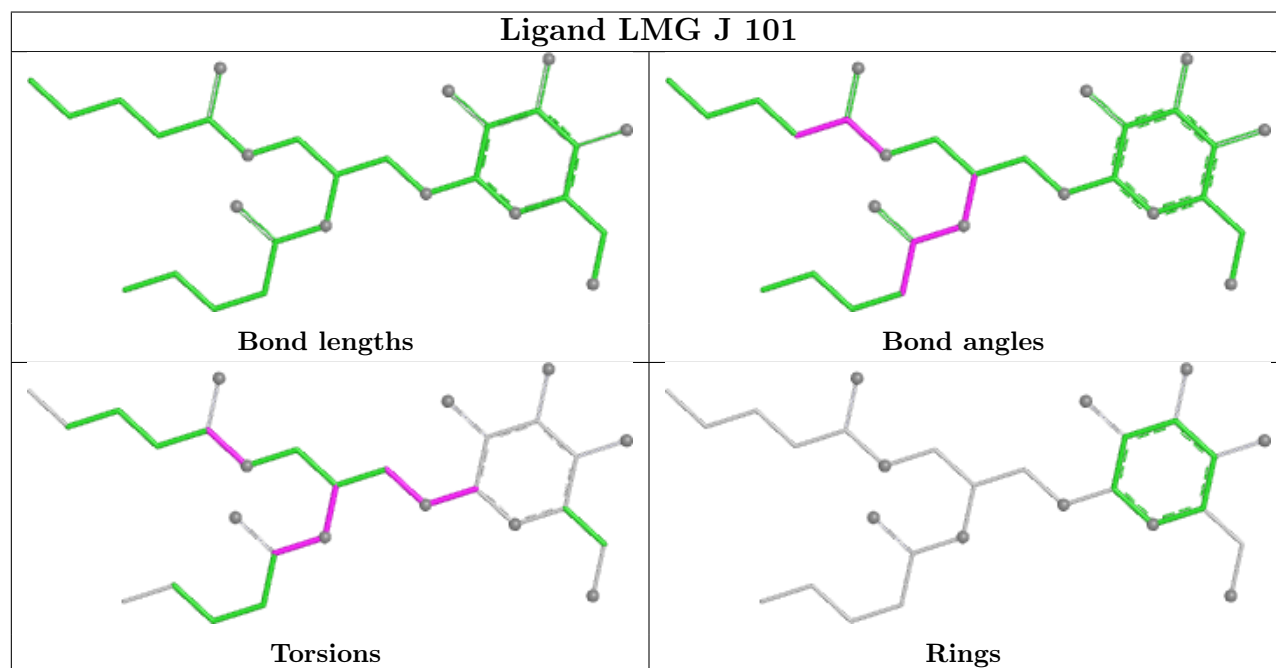
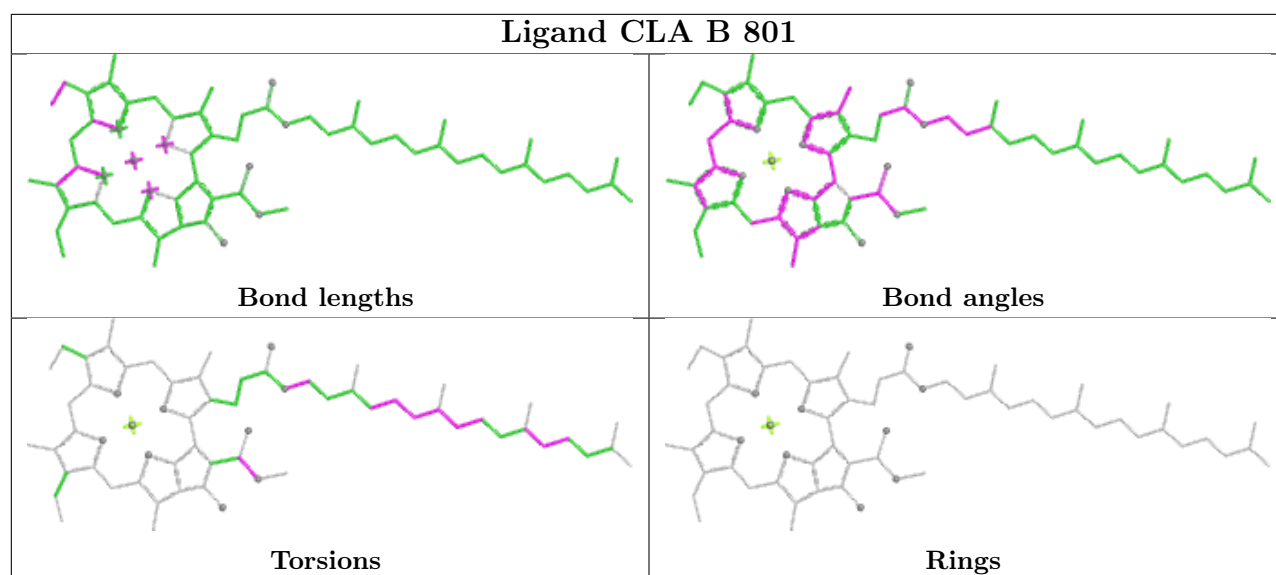
Torsions

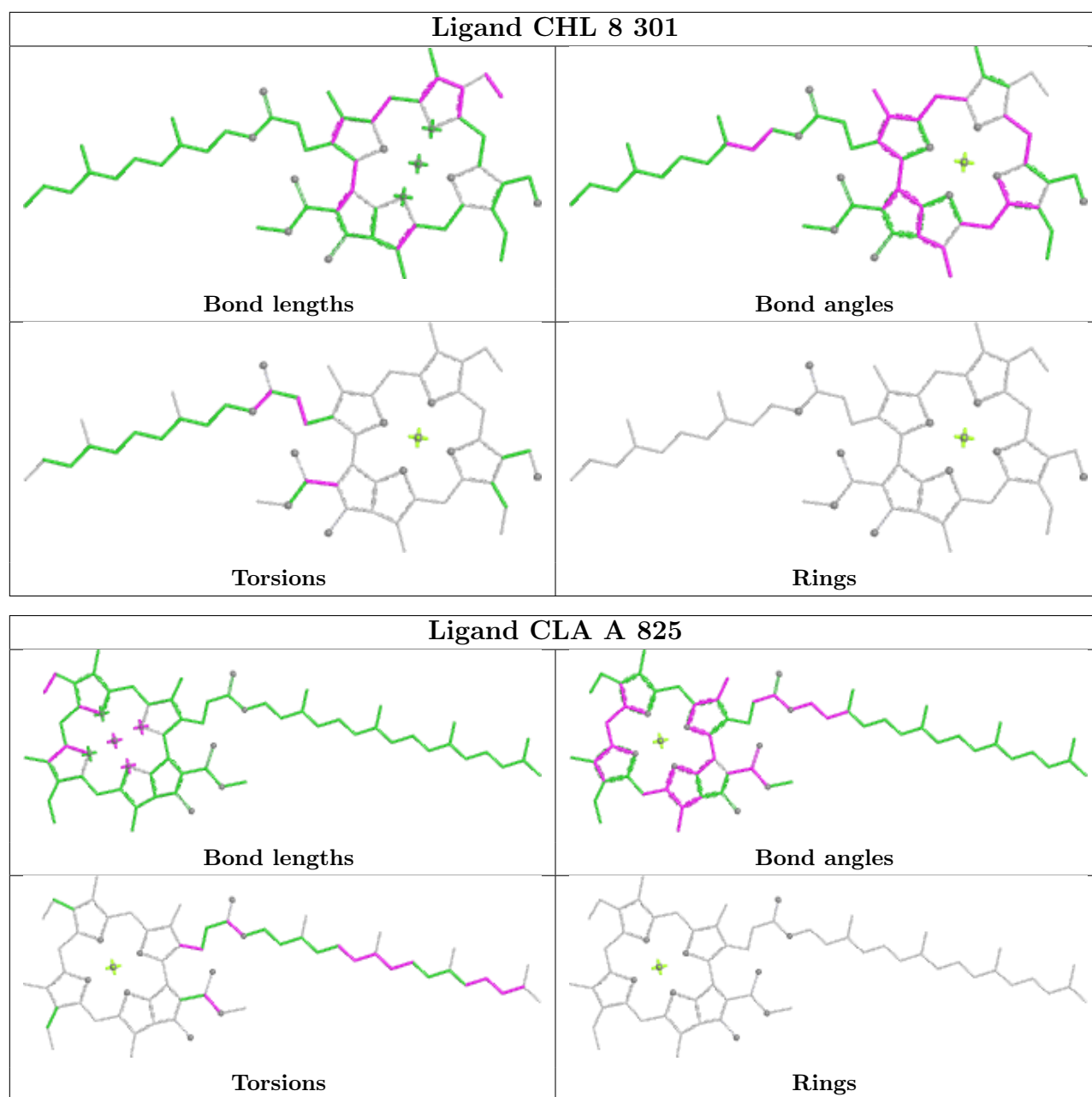


Rings

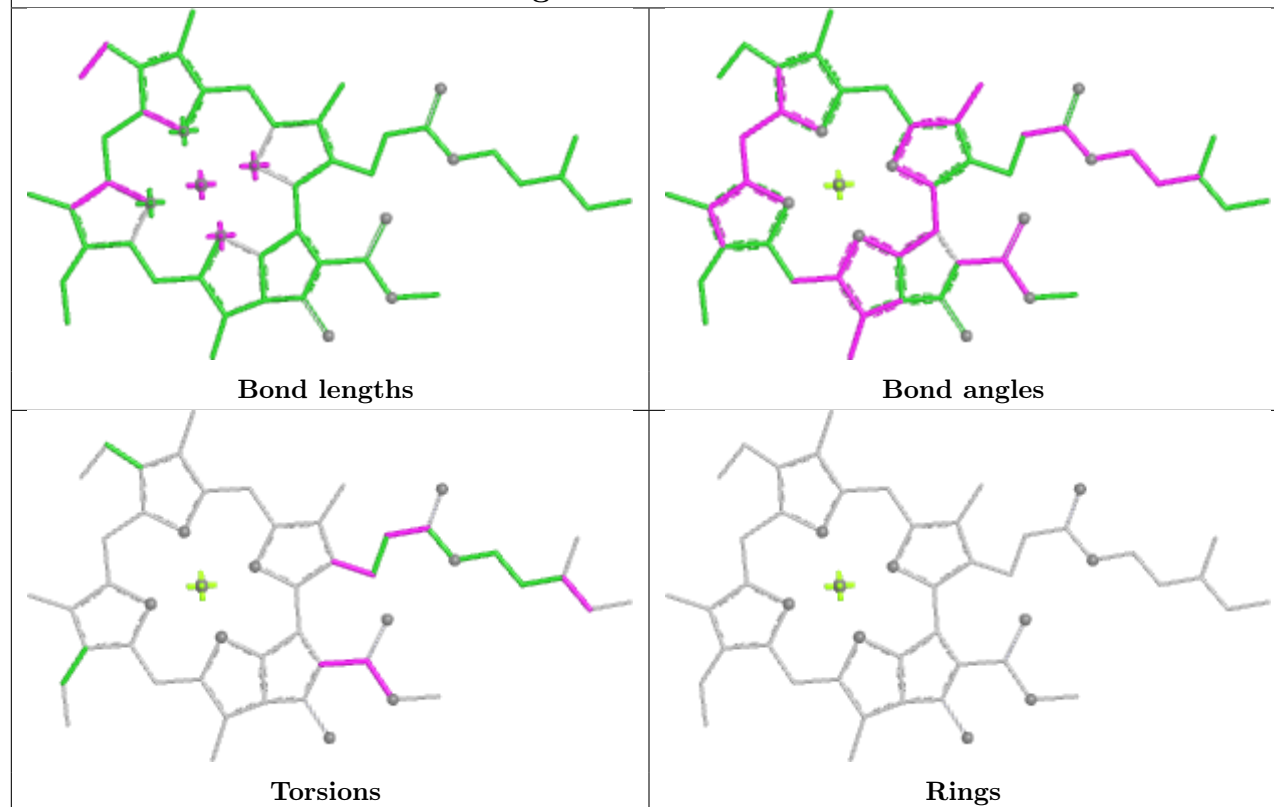




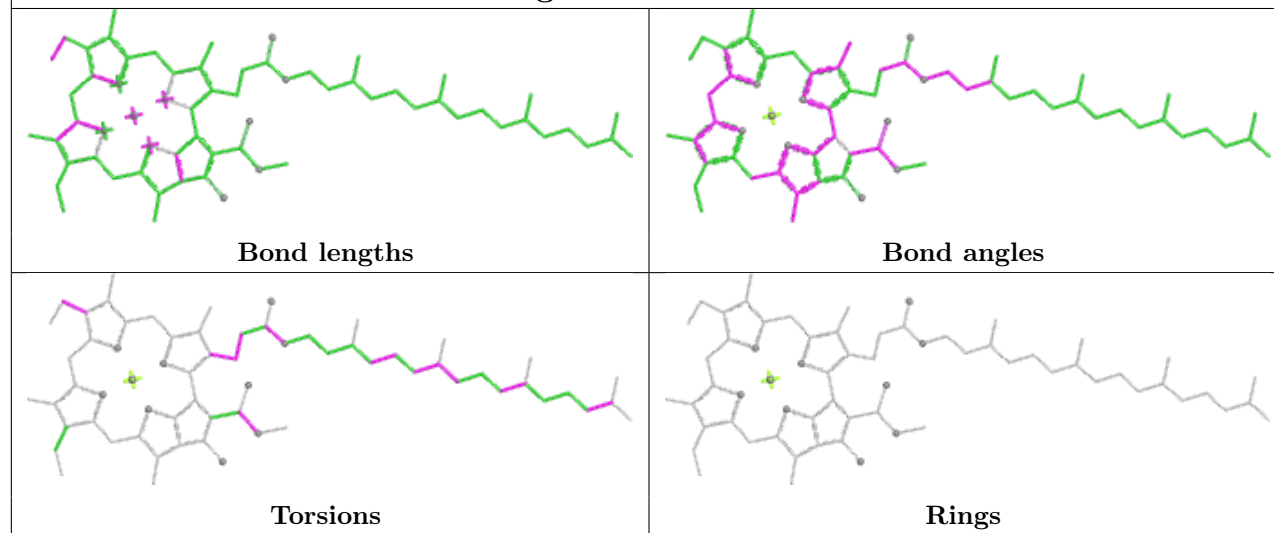




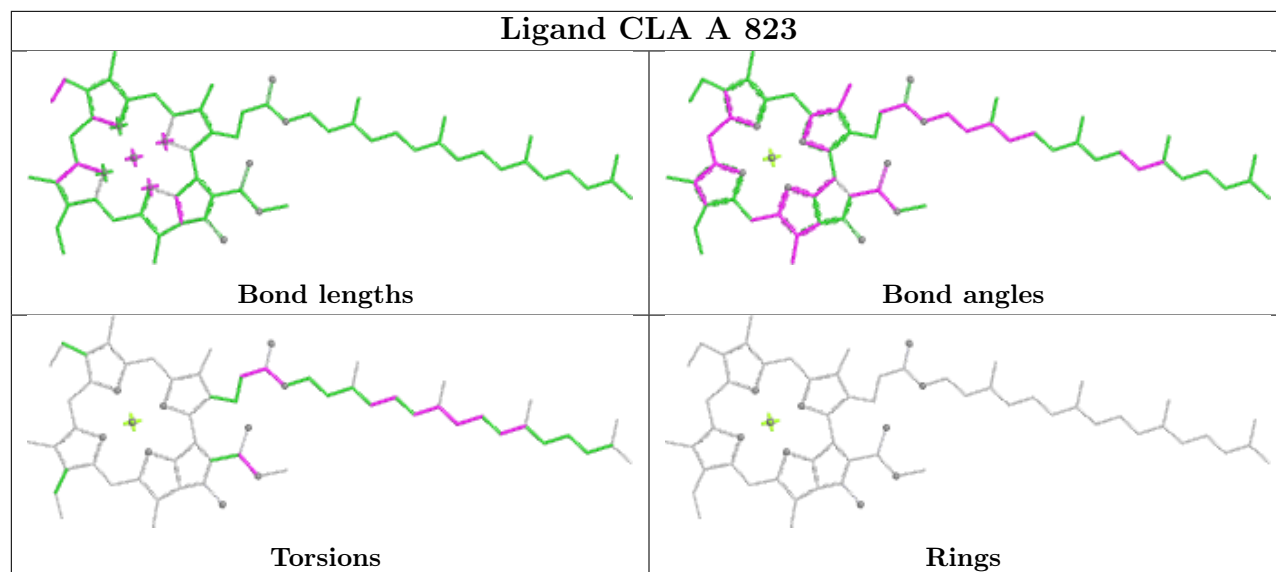
## Ligand CLA B 837



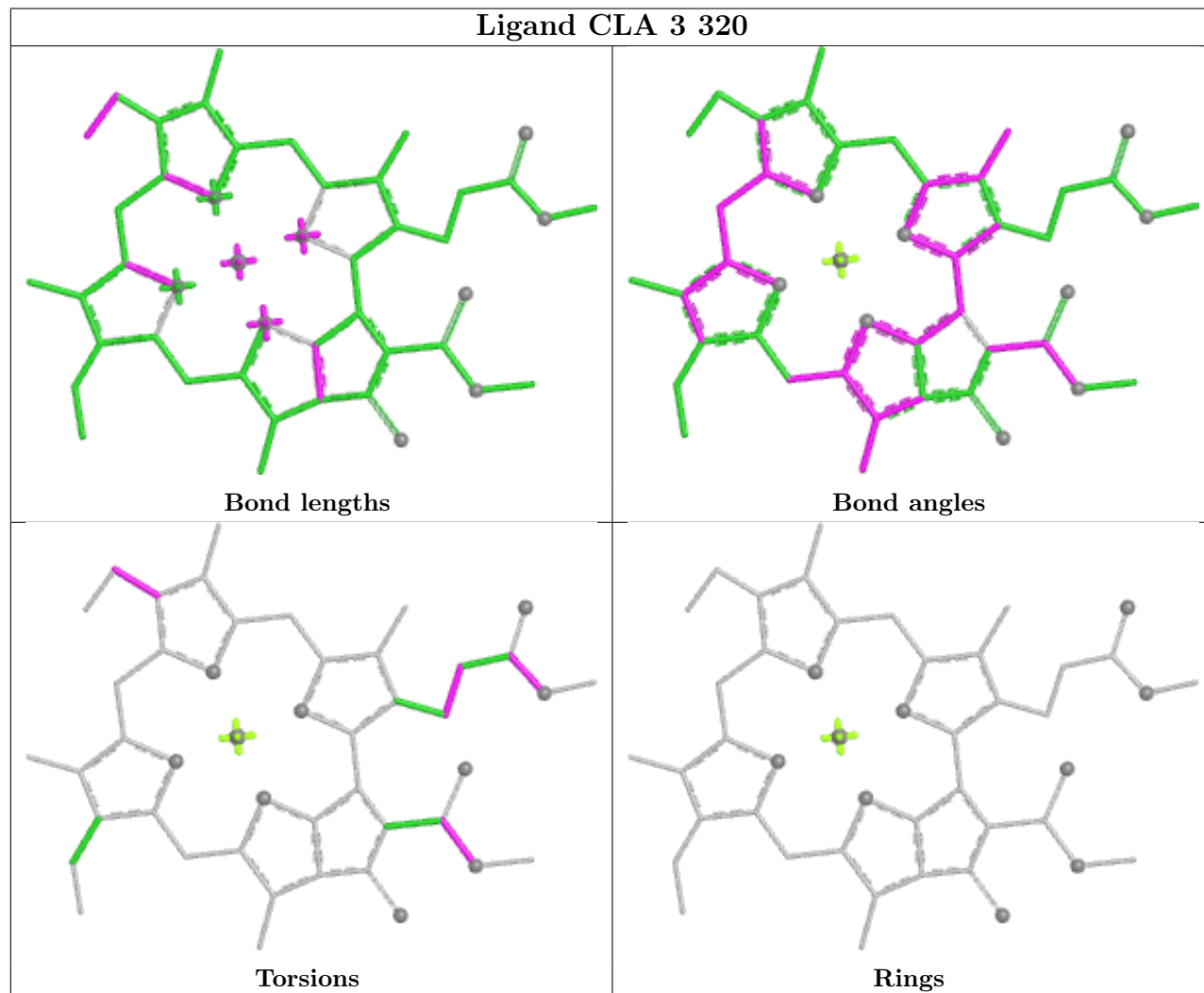
## Ligand CLA 6 310

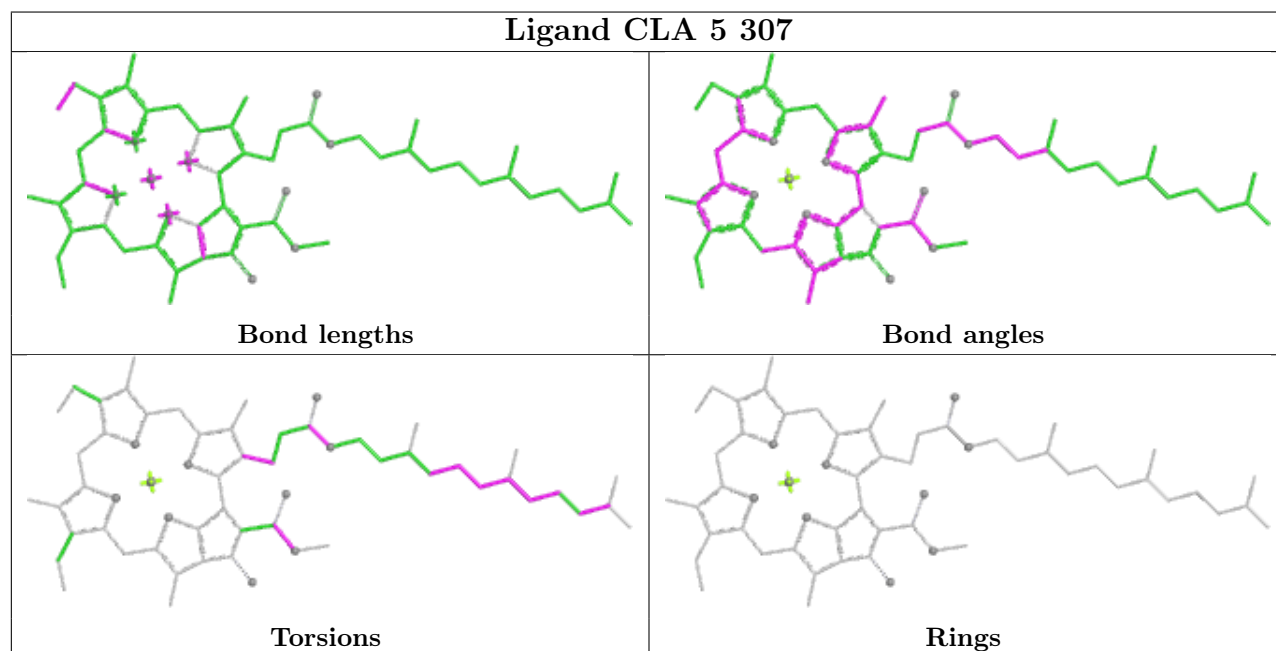
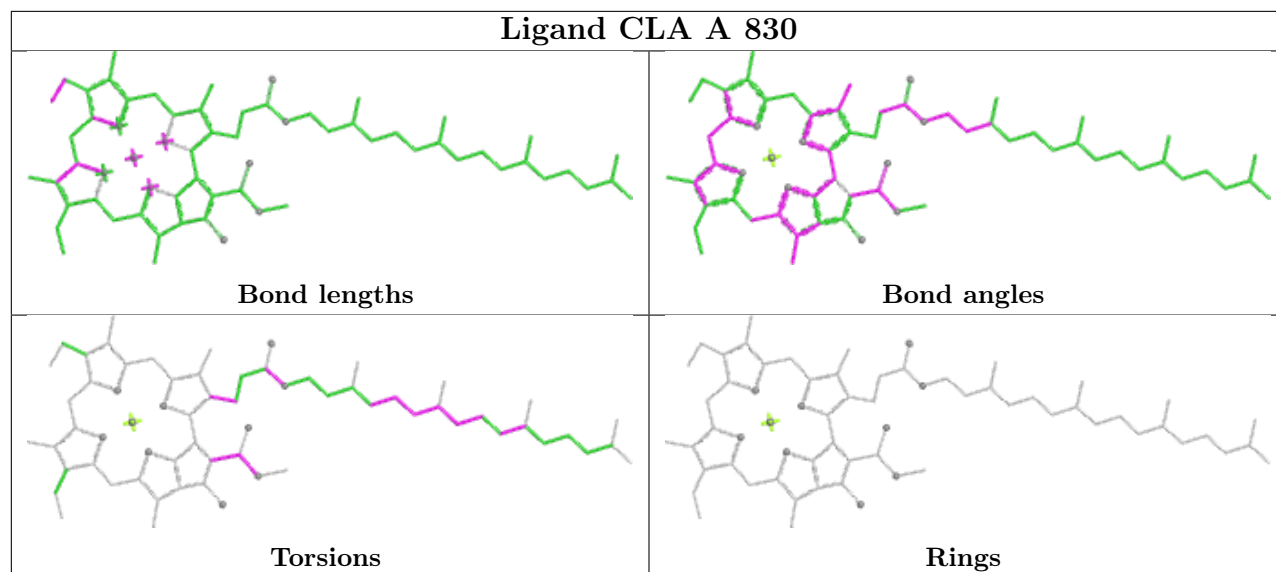


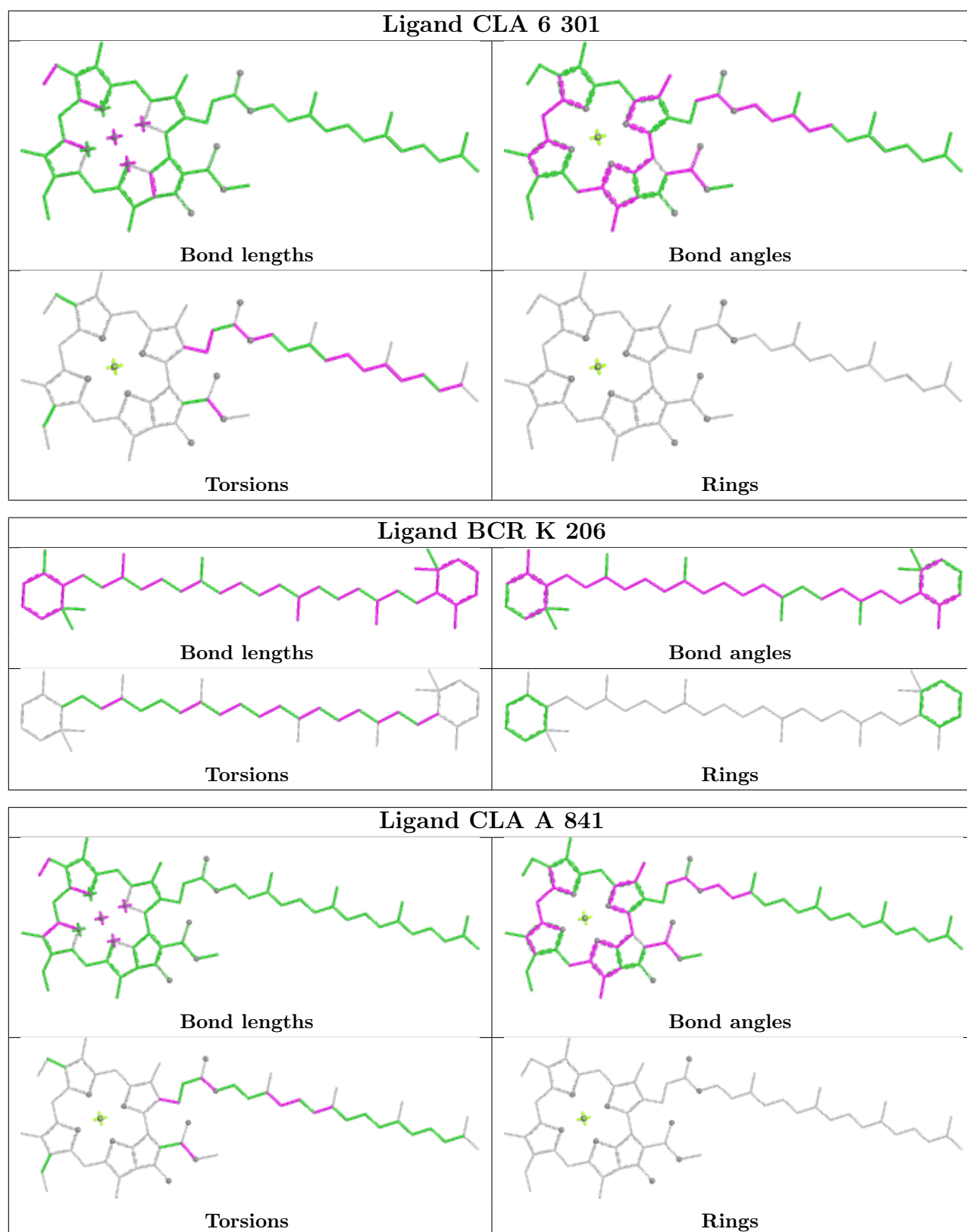
## Ligand CLA A 823

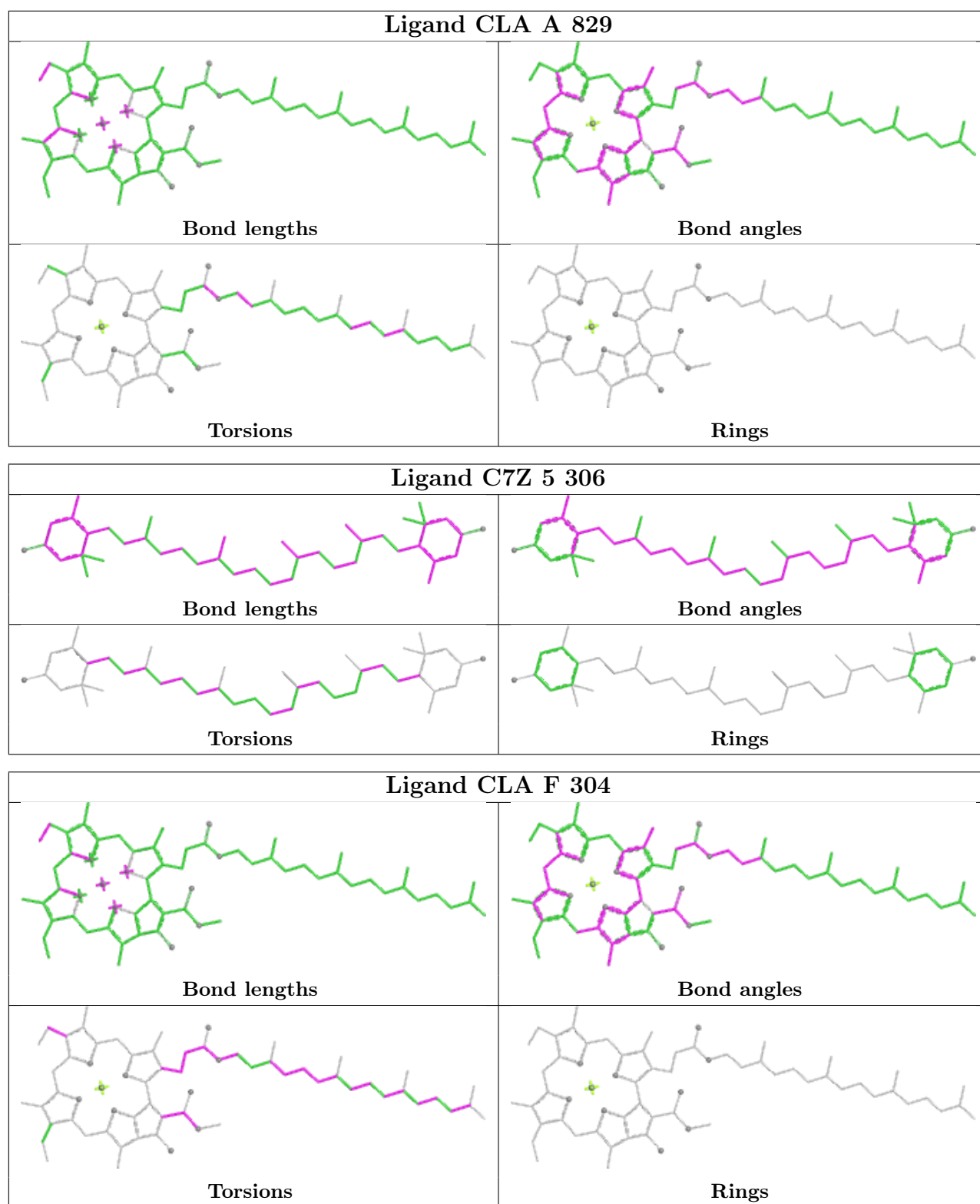


## Ligand CLA 3 320



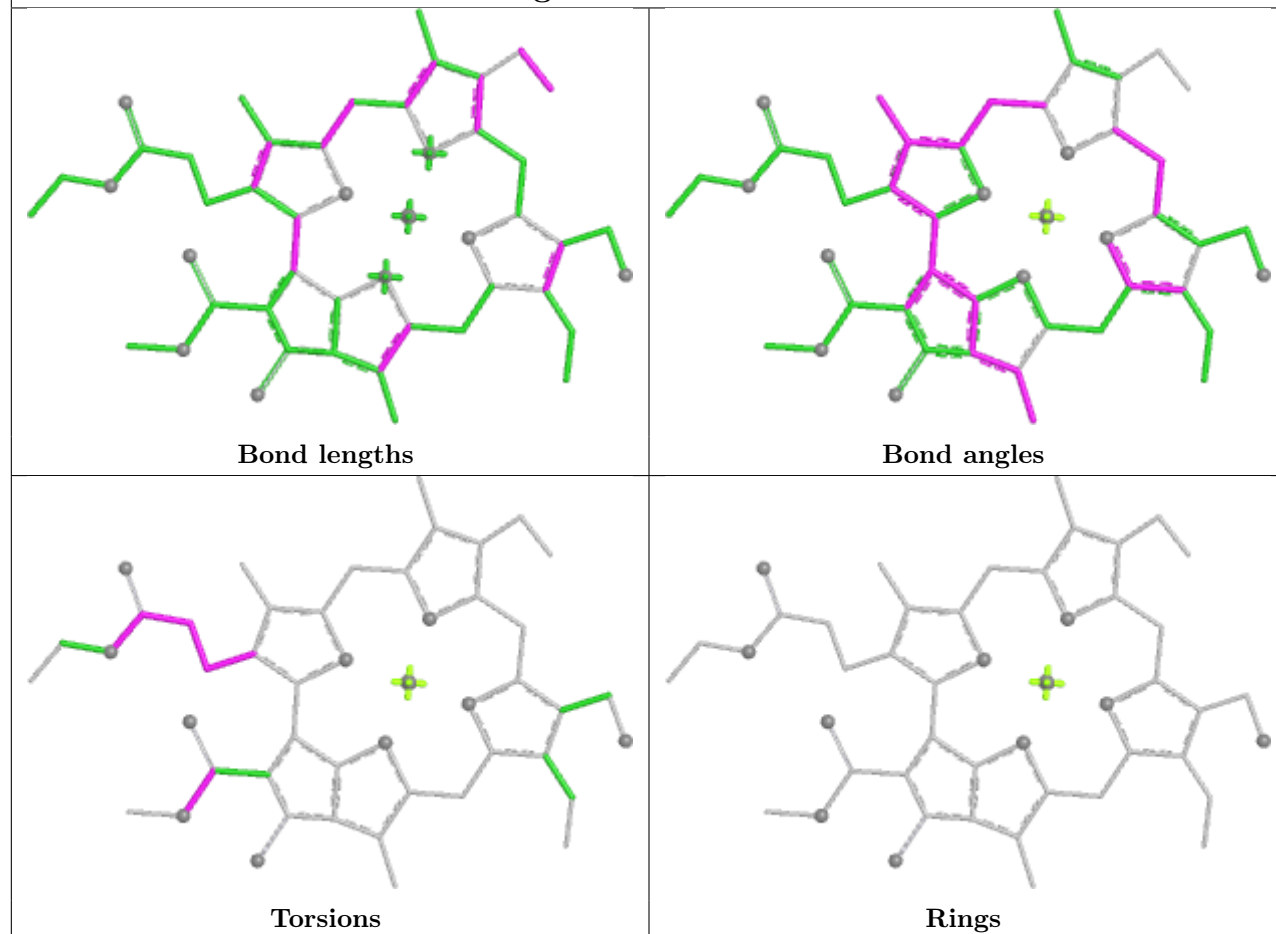




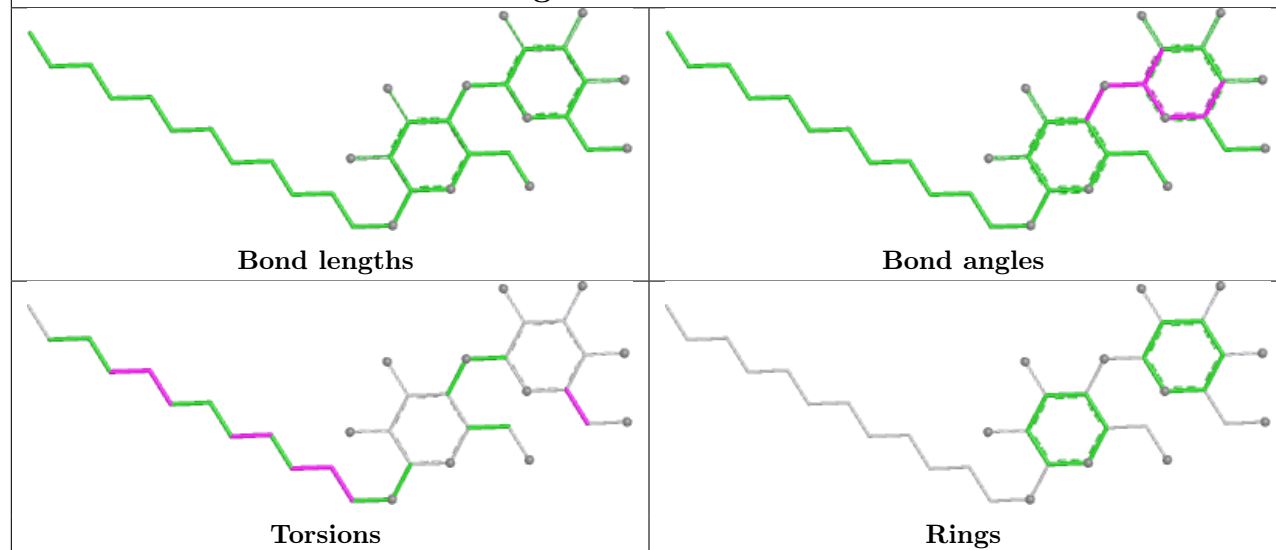


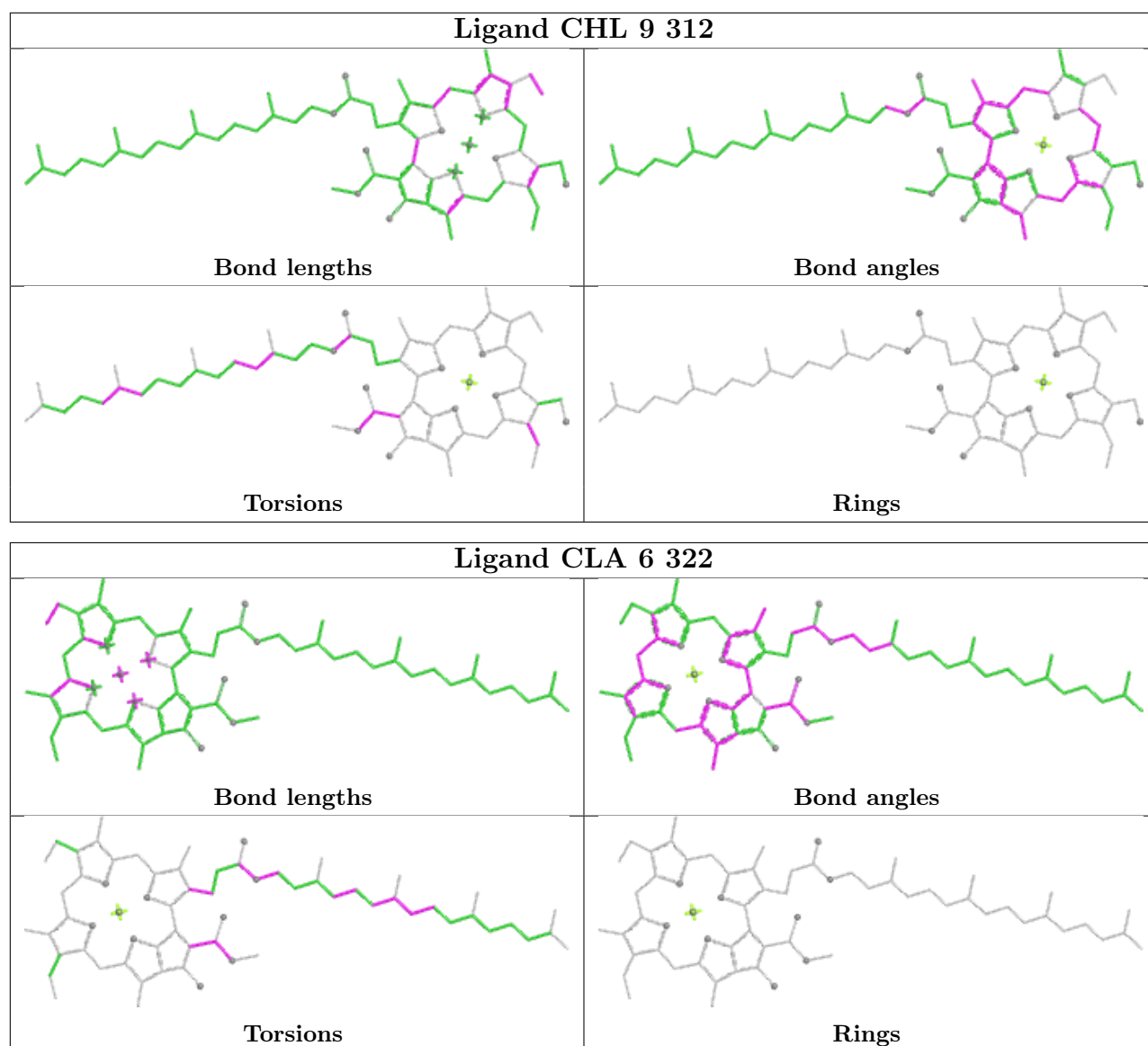


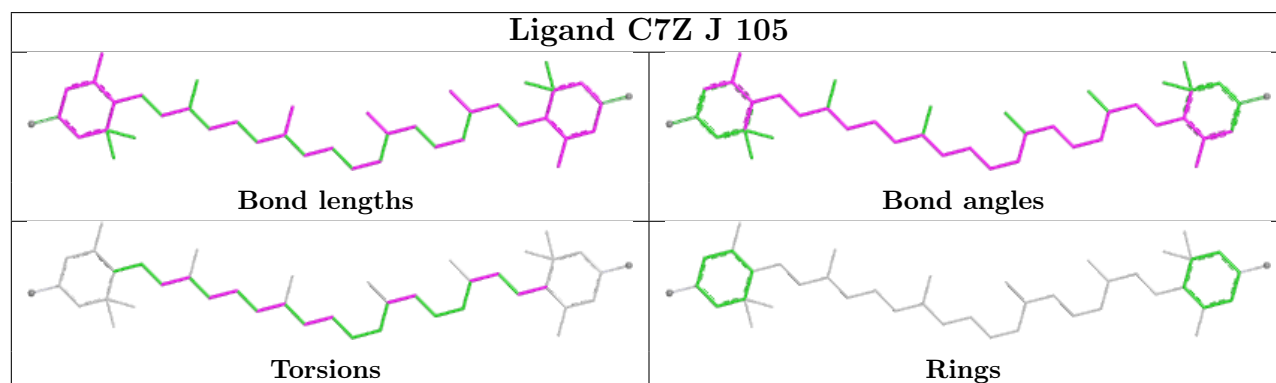
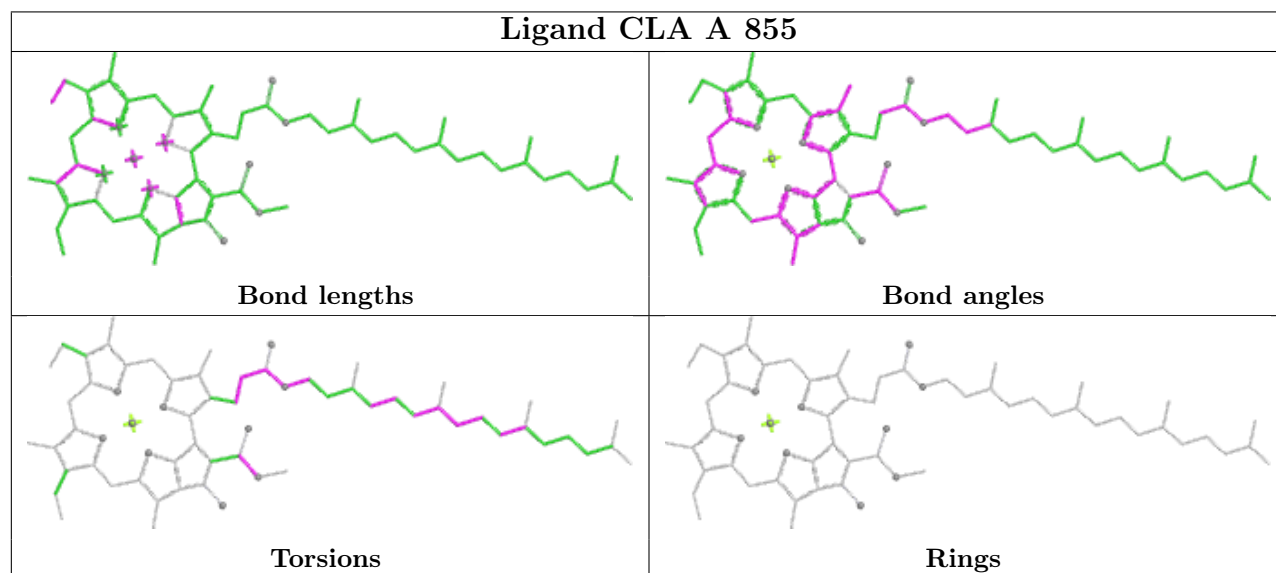
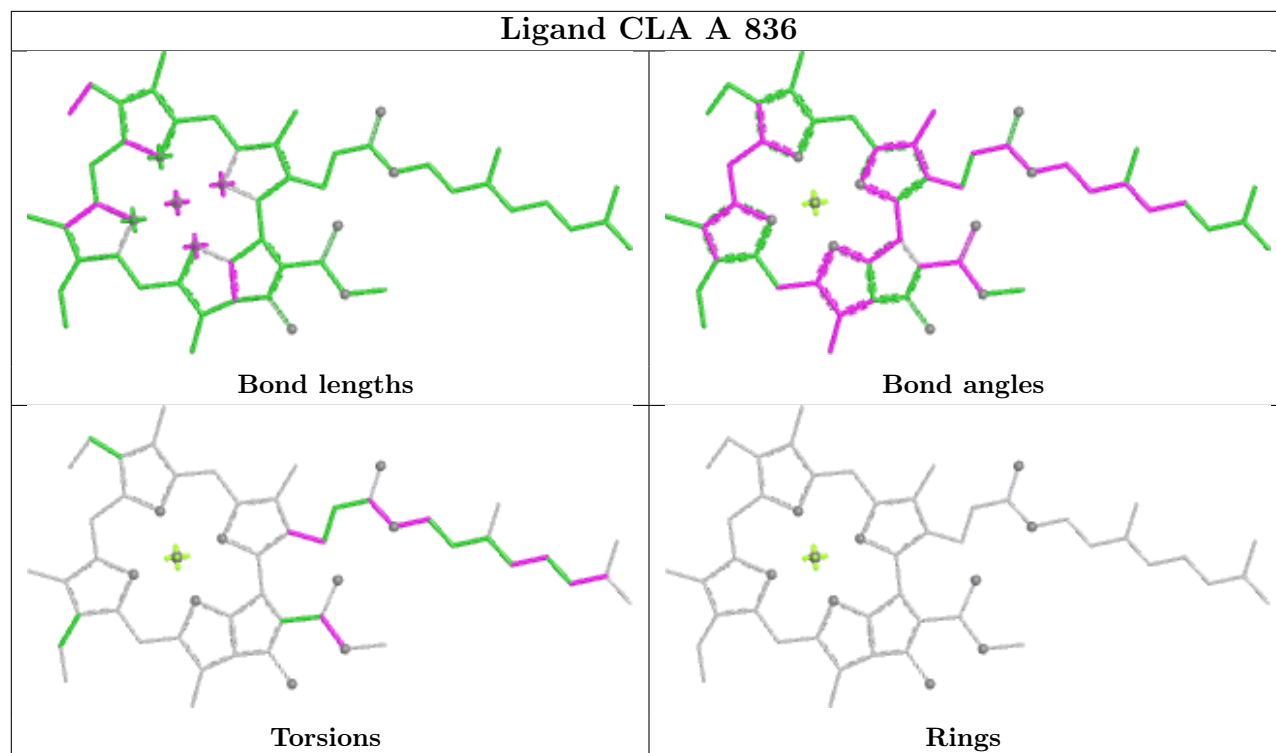
## Ligand CHL Z 312



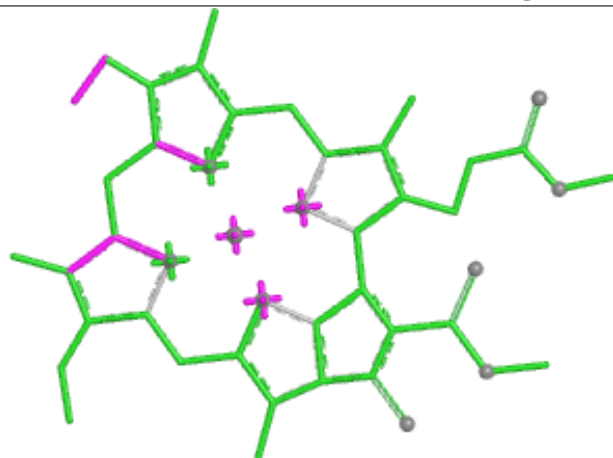
## Ligand LMT 4 822



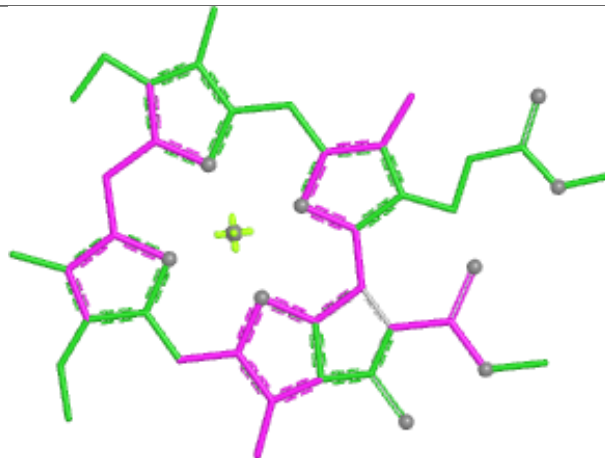




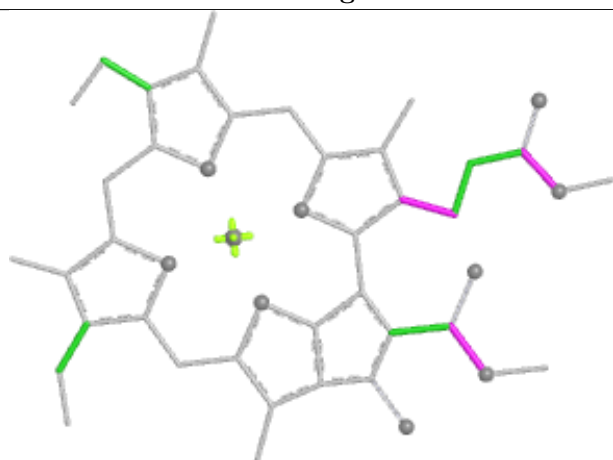
## Ligand CLA 9 311



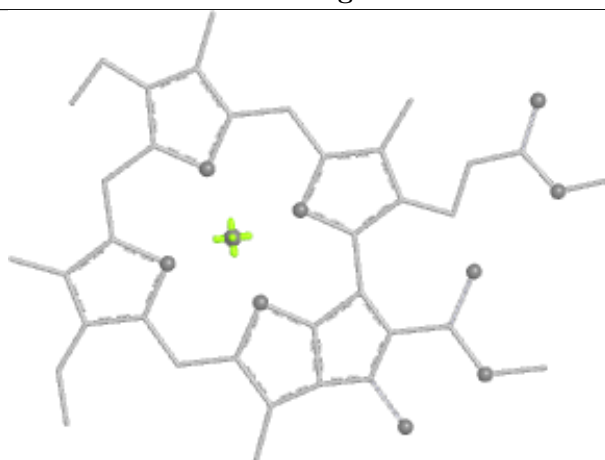
Bond lengths



Bond angles

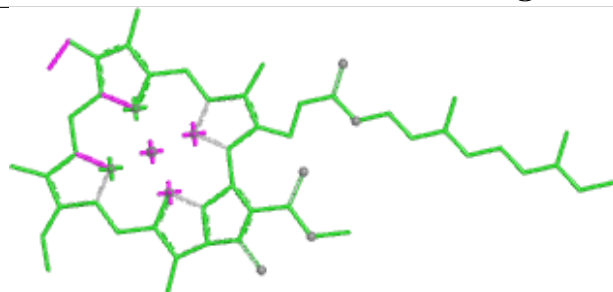


Torsions

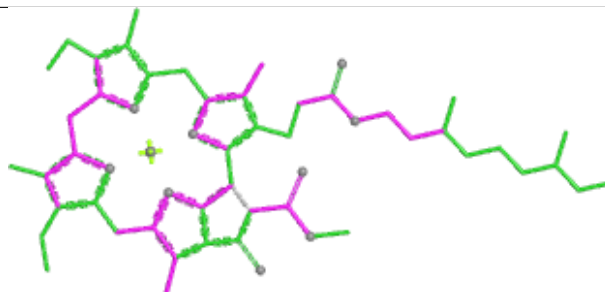


Rings

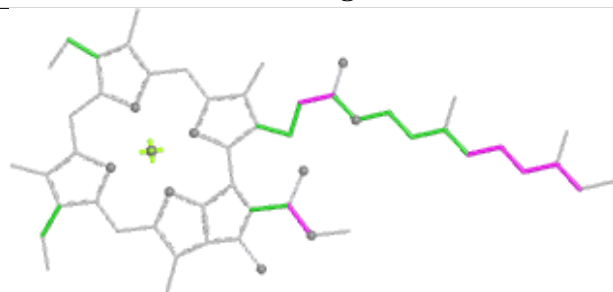
## Ligand CLA Z 305



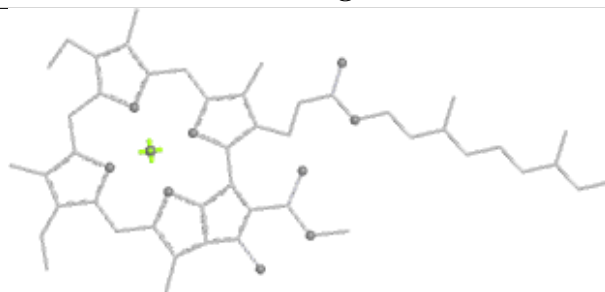
Bond lengths



Bond angles

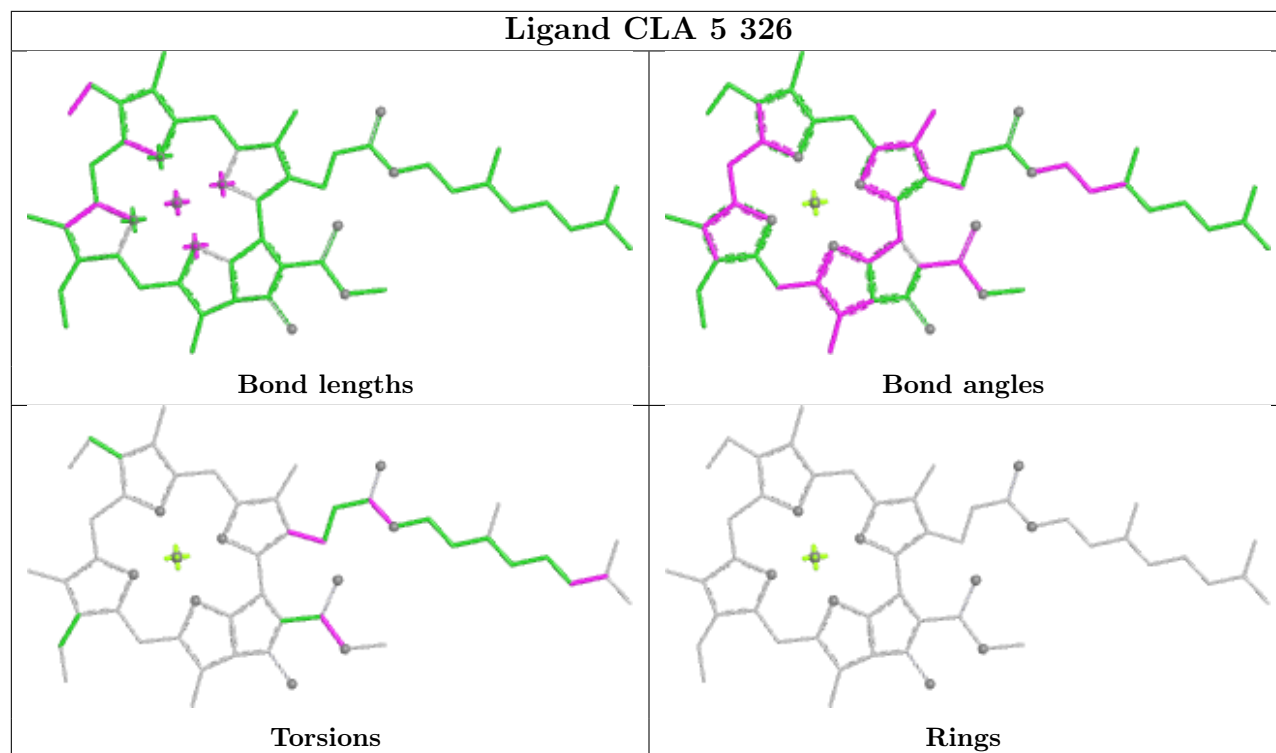


Torsions

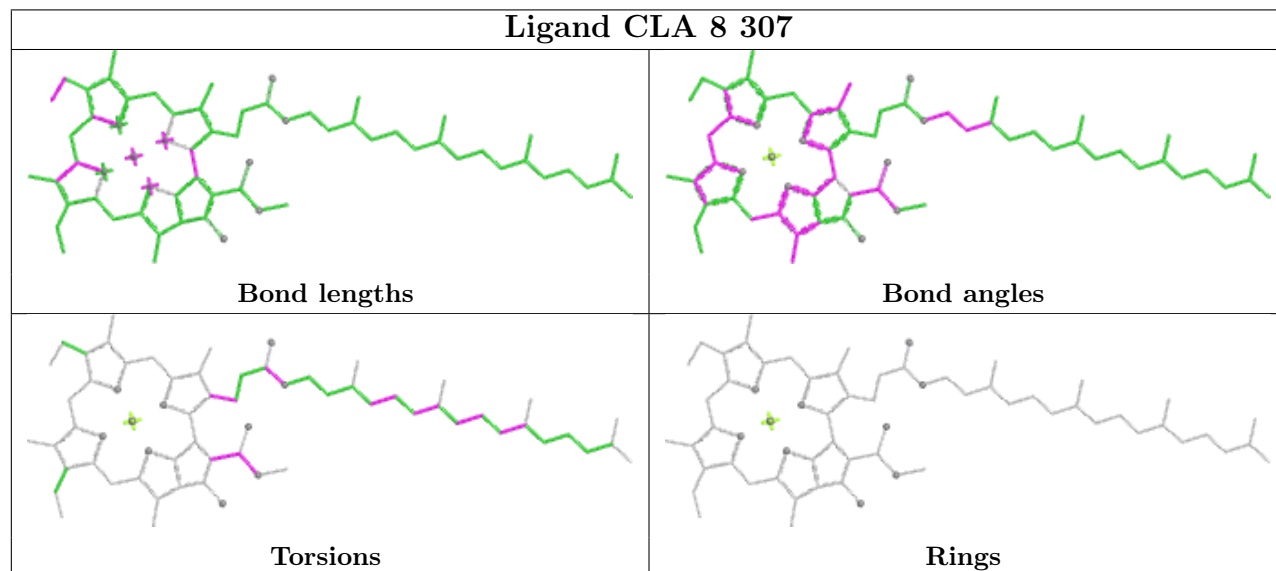


Rings

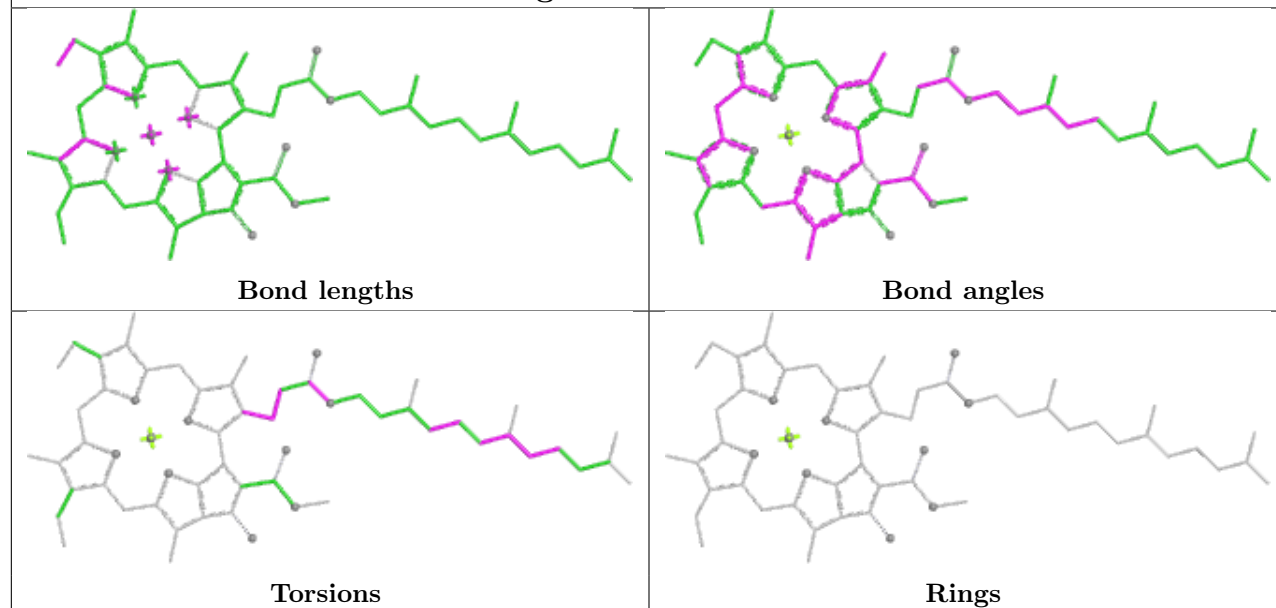
## Ligand CLA 5 326



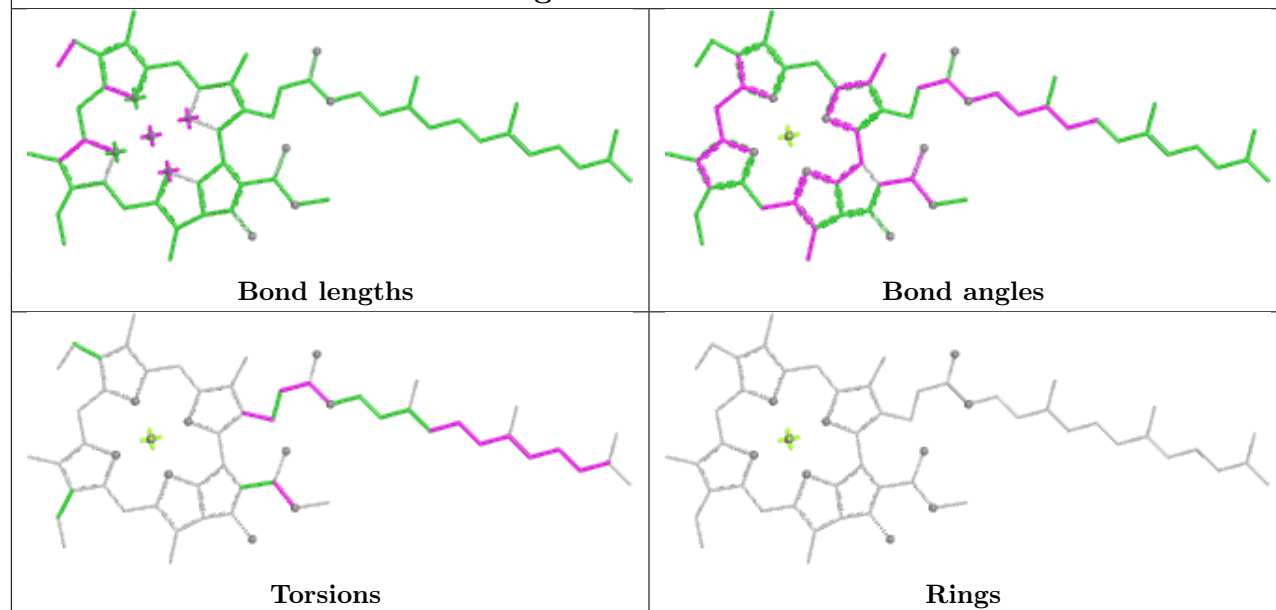
## Ligand CLA 8 307

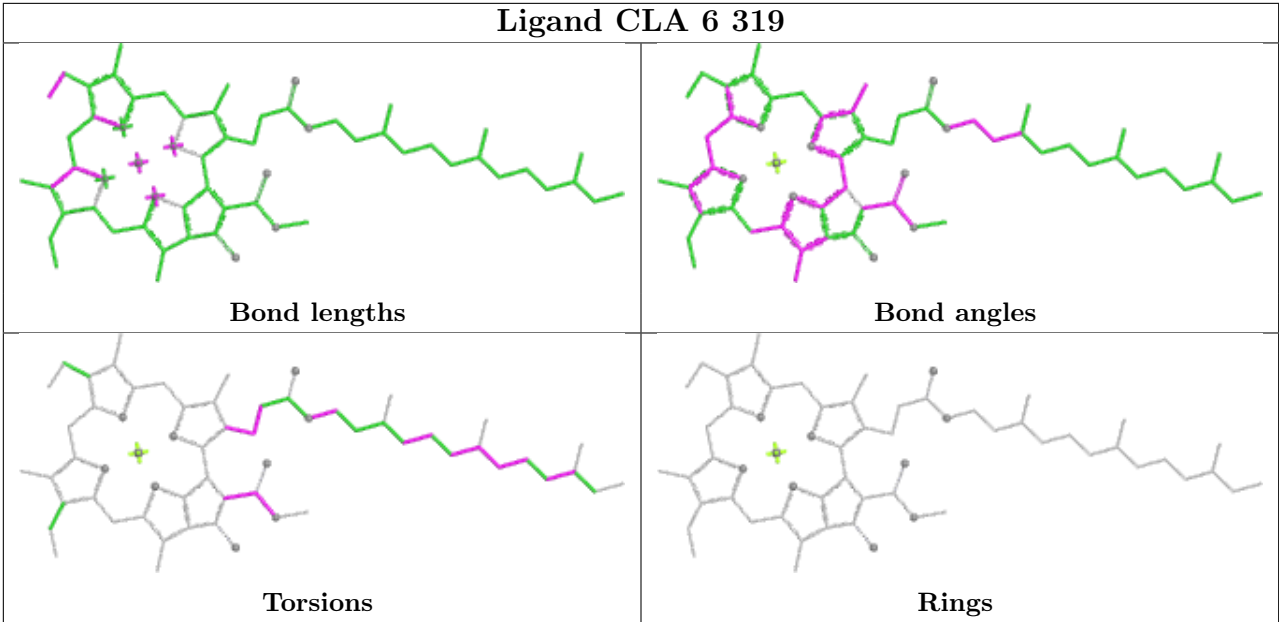


## Ligand CLA 3 311



## Ligand CLA Z 309





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 11  | L     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | L     | 144:PRO   | C      | 158:ARG   | N      | 6.44         |

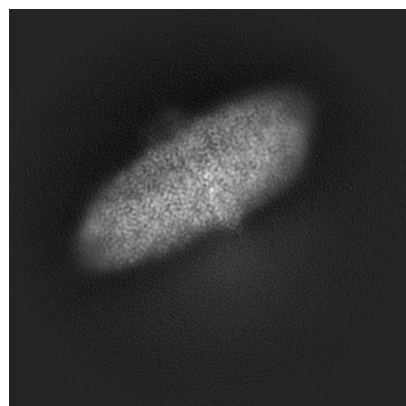
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16732. These allow visual inspection of the internal detail of the map and identification of artifacts.

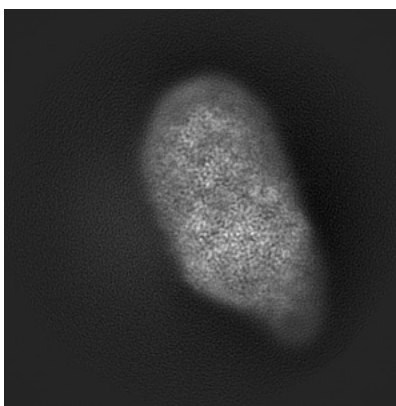
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

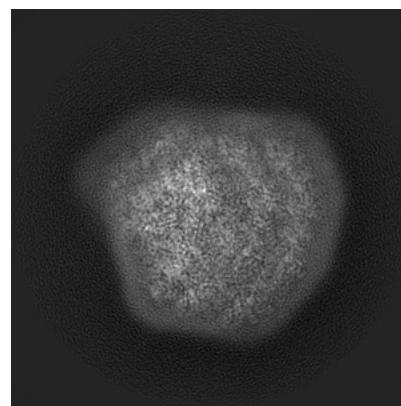
#### 6.1.1 Primary map



X

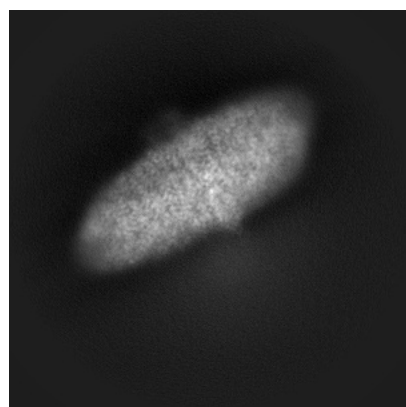


Y

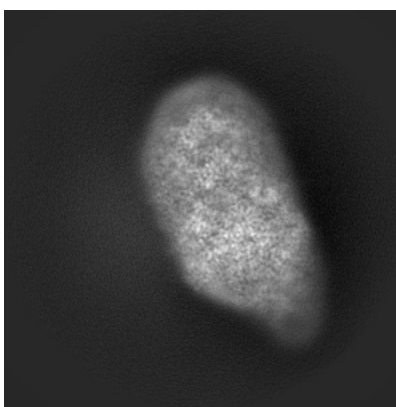


Z

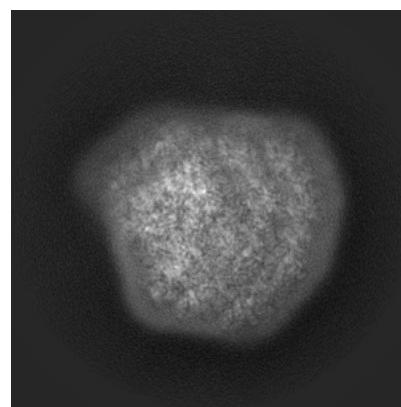
#### 6.1.2 Raw map



X



Y



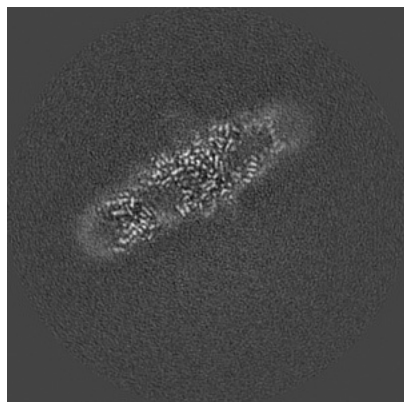
Z

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

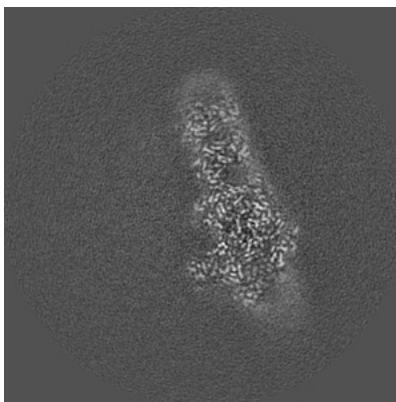


## 6.2 Central slices [i](#)

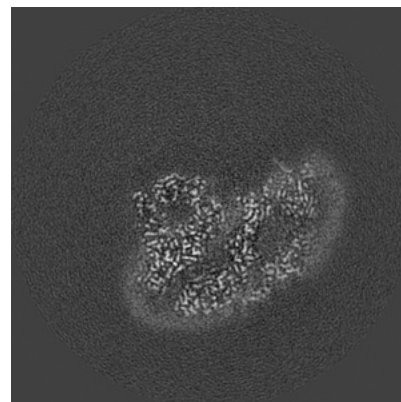
### 6.2.1 Primary map



X Index: 250

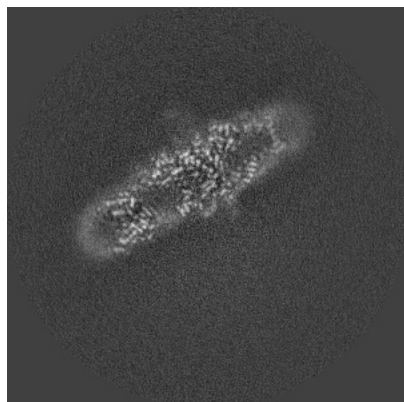


Y Index: 250

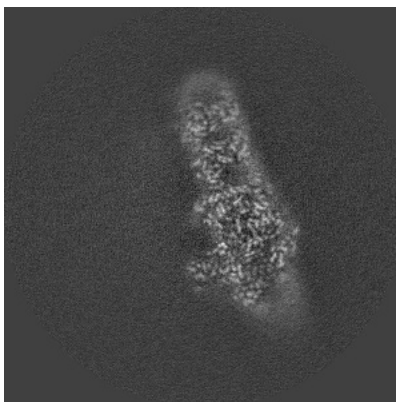


Z Index: 250

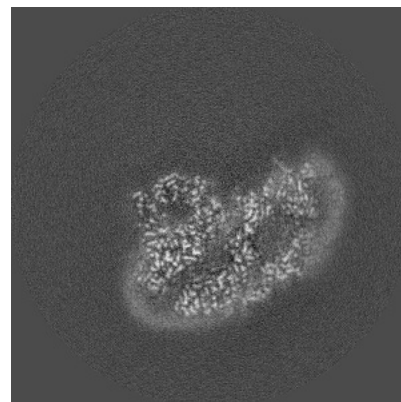
### 6.2.2 Raw map



X Index: 250



Y Index: 250

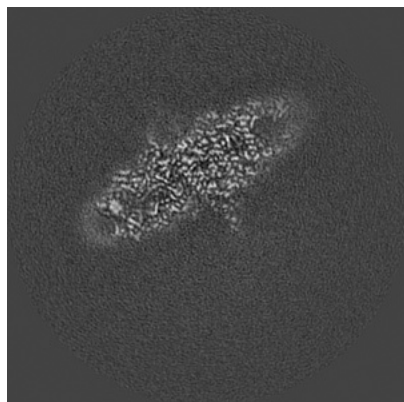


Z Index: 250

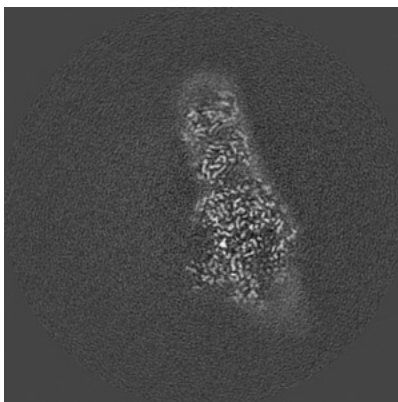
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

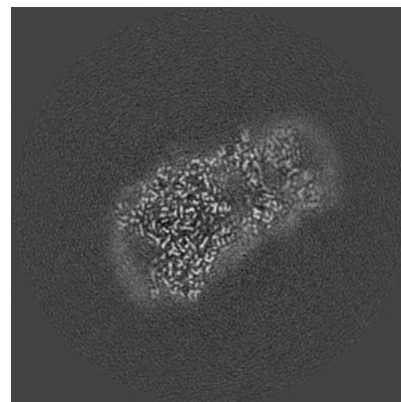
### 6.3.1 Primary map



X Index: 218

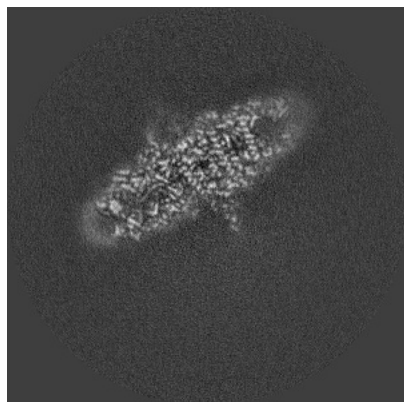


Y Index: 252

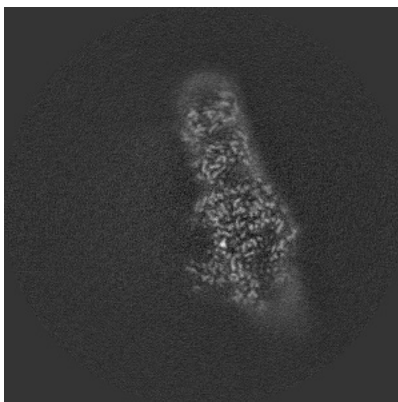


Z Index: 289

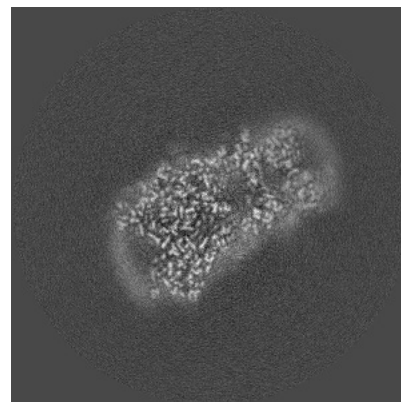
### 6.3.2 Raw map



X Index: 218



Y Index: 252

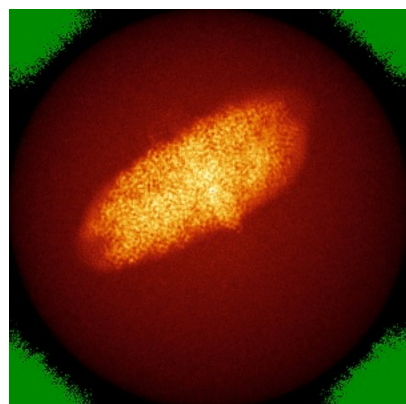


Z Index: 289

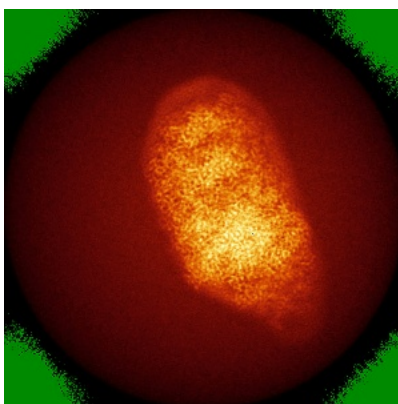
The images above show the largest variance slices of the map in three orthogonal directions.

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

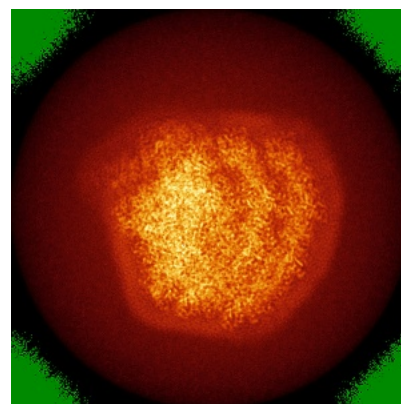
### 6.4.1 Primary map



X

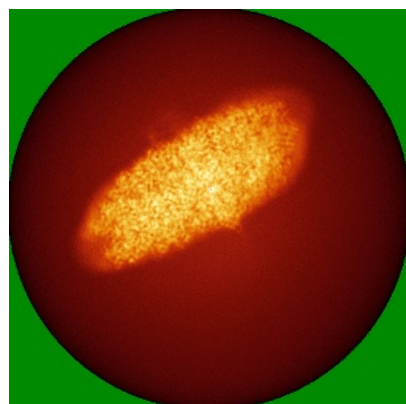


Y

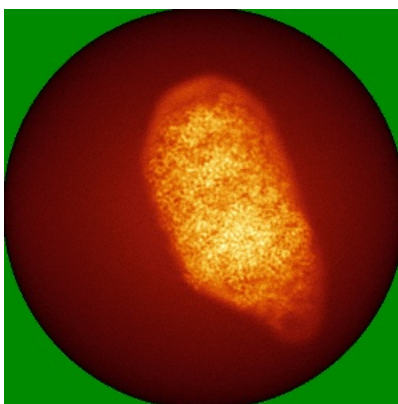


Z

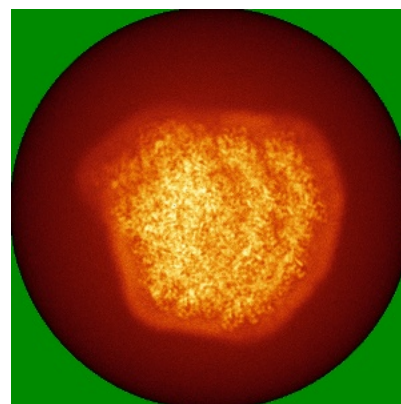
### 6.4.2 Raw map



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.

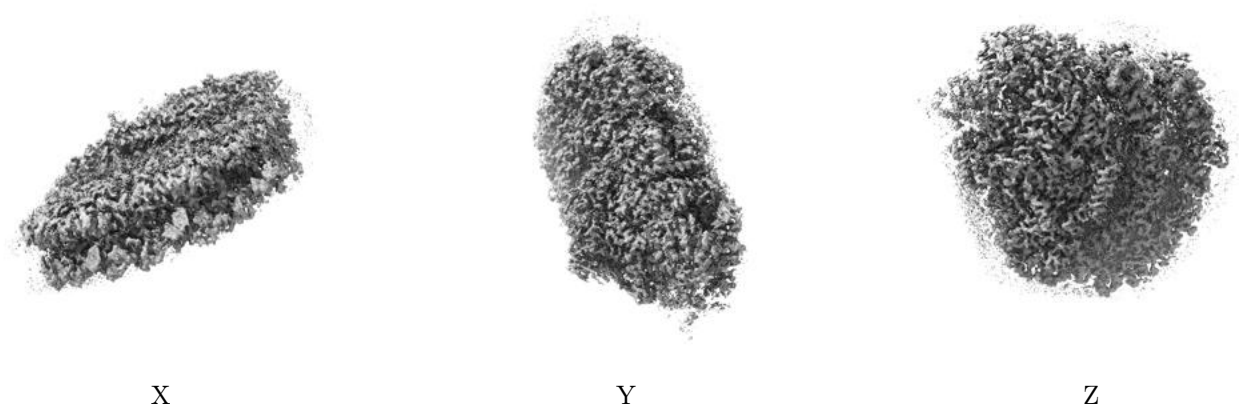
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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



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](#)

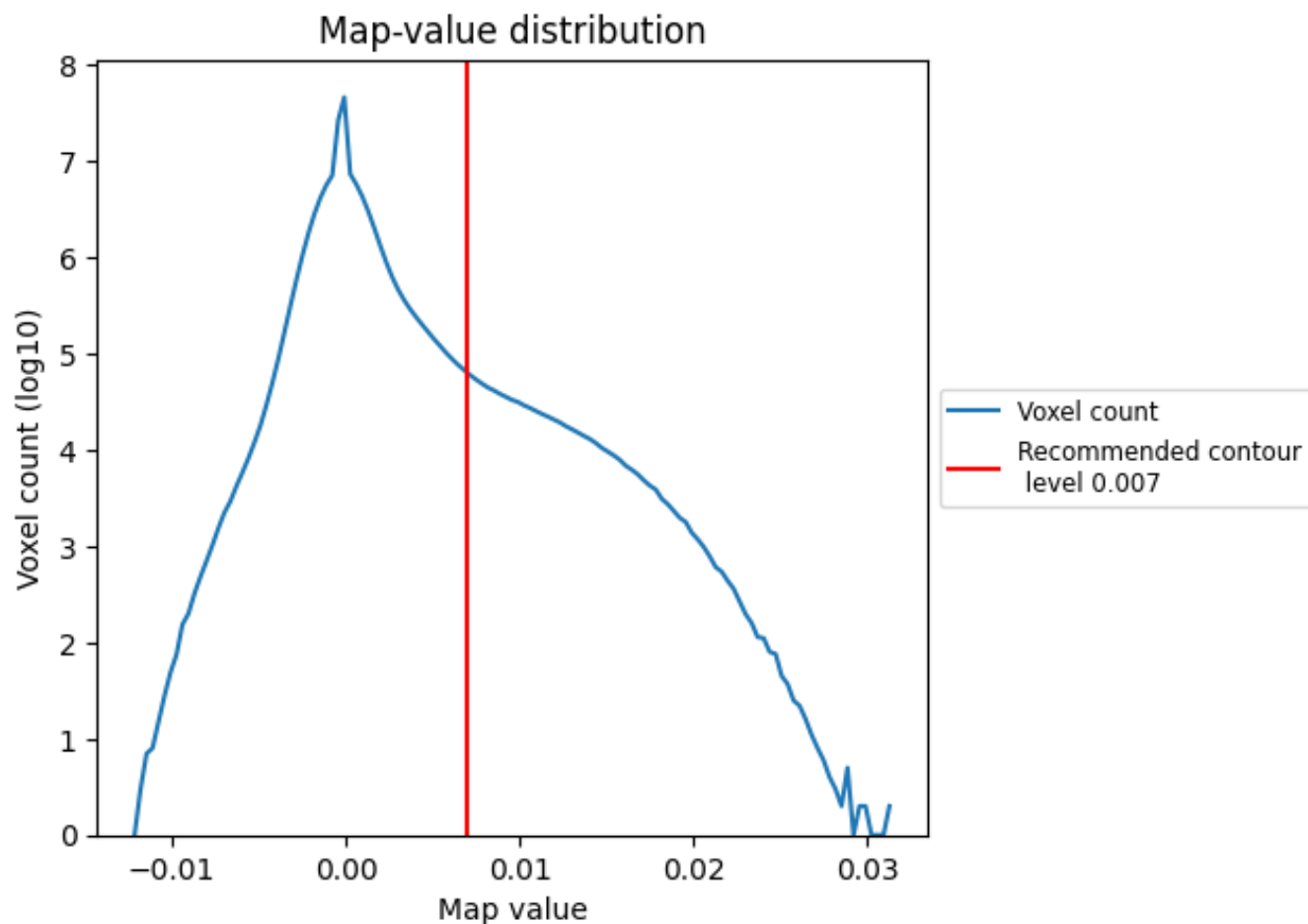
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

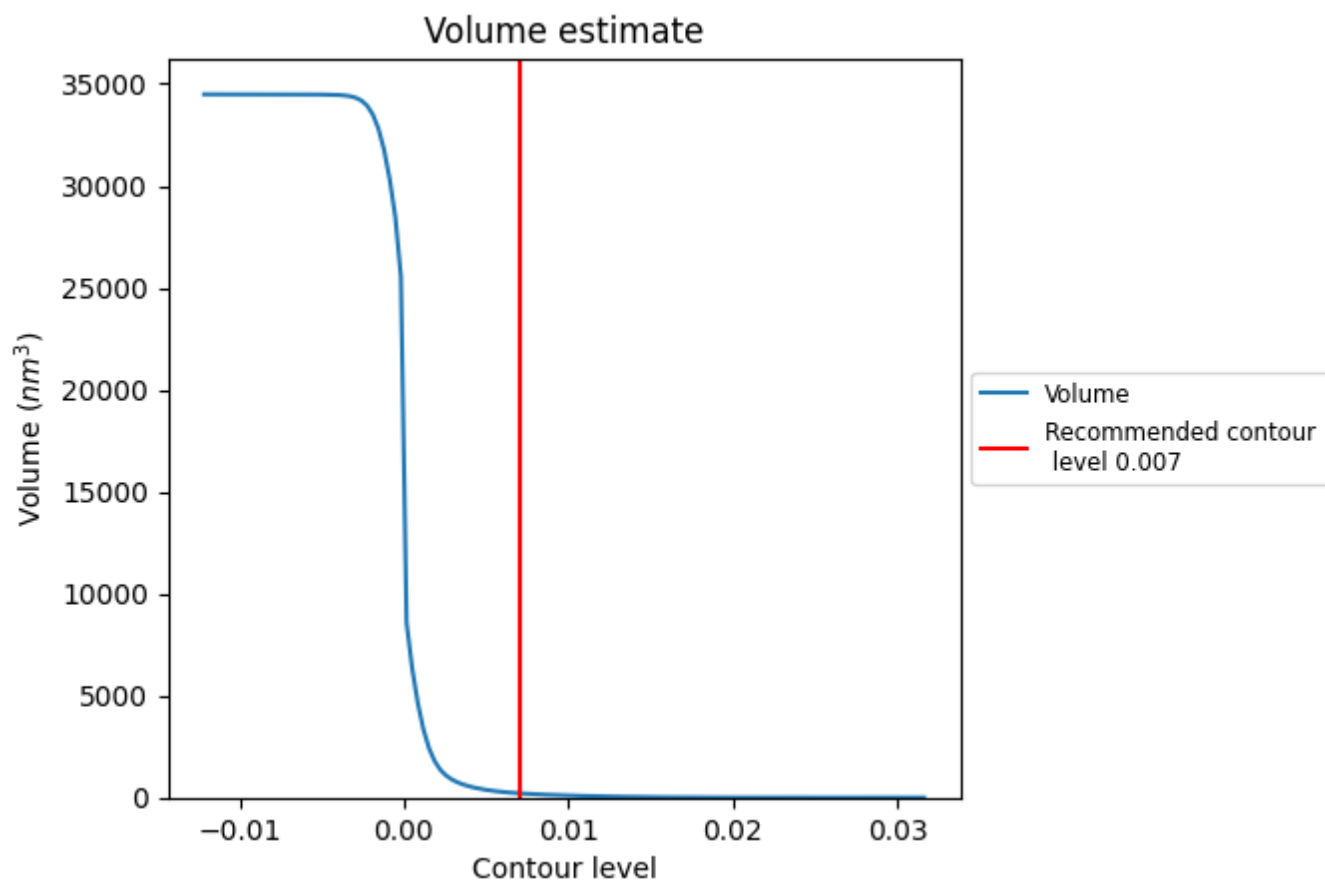
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

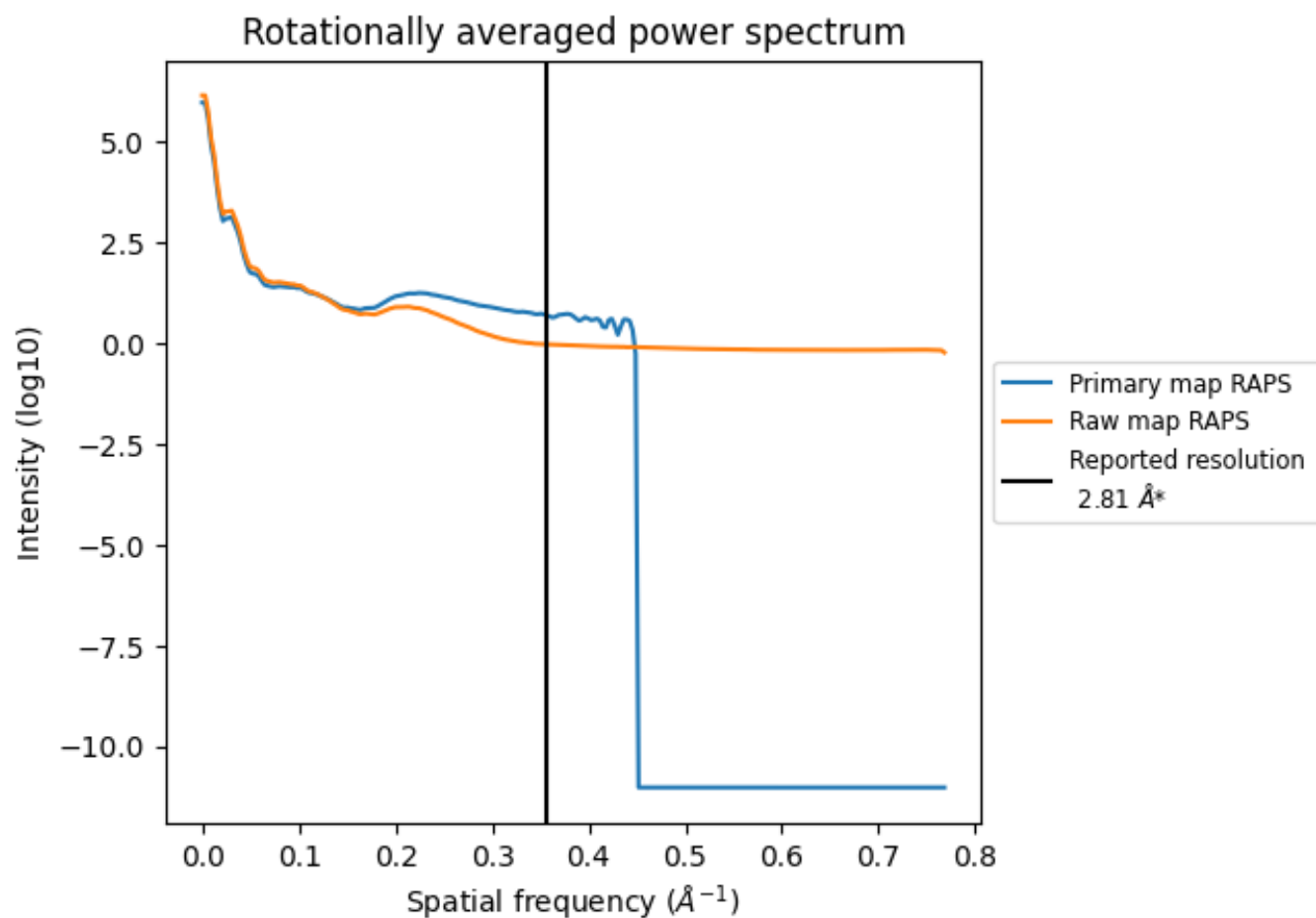
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $210 \text{ nm}^3$ ; this corresponds to an approximate mass of 190 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 ⓘ

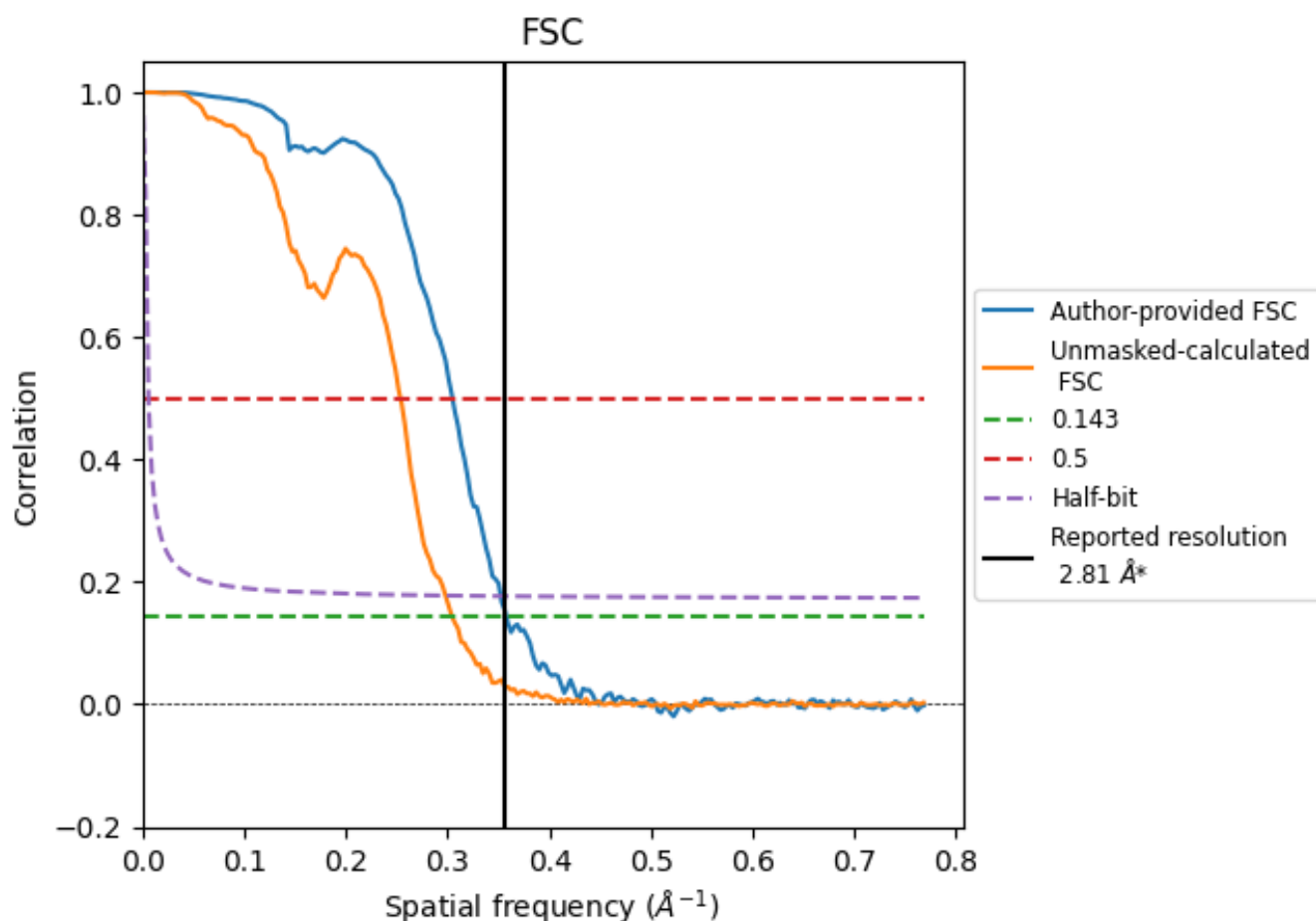


\*Reported resolution corresponds to spatial frequency of 0.356 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.356  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

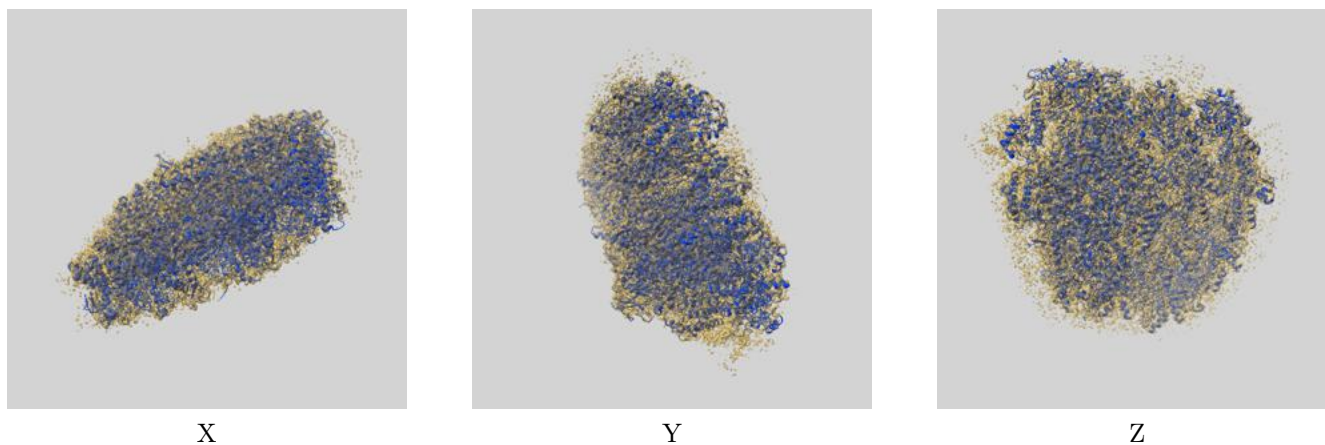
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.81                               | -    | -        |
| Author-provided FSC curve | 2.79                               | 3.28 | 2.84     |
| Unmasked-calculated*      | 3.28                               | 3.94 | 3.36     |

\*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 3.28 differs from the reported value 2.81 by more than 10 %

## 9 Map-model fit [i](#)

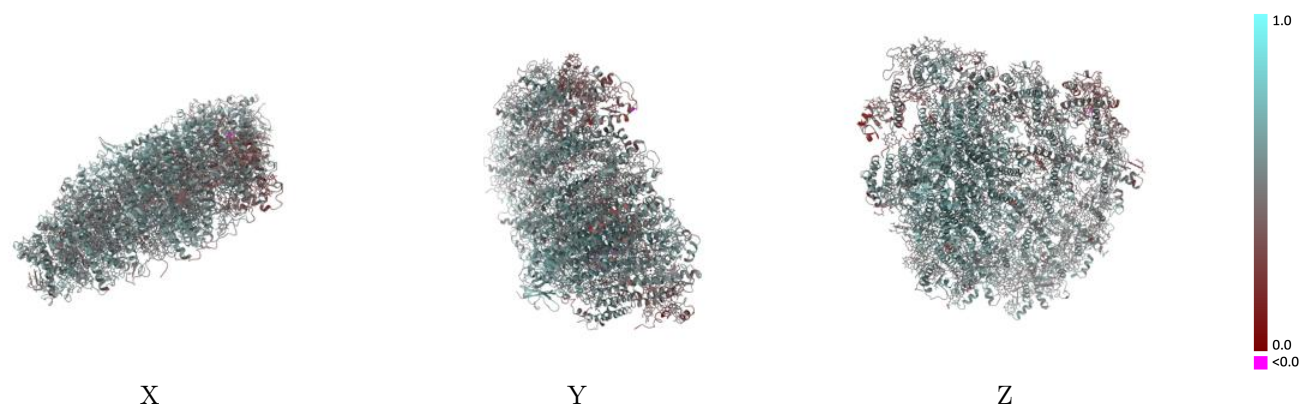
This section contains information regarding the fit between EMDB map EMD-16732 and PDB model 8CMO. Per-residue inclusion information can be found in section [3](#) on page [41](#).

### 9.1 Map-model overlay [i](#)



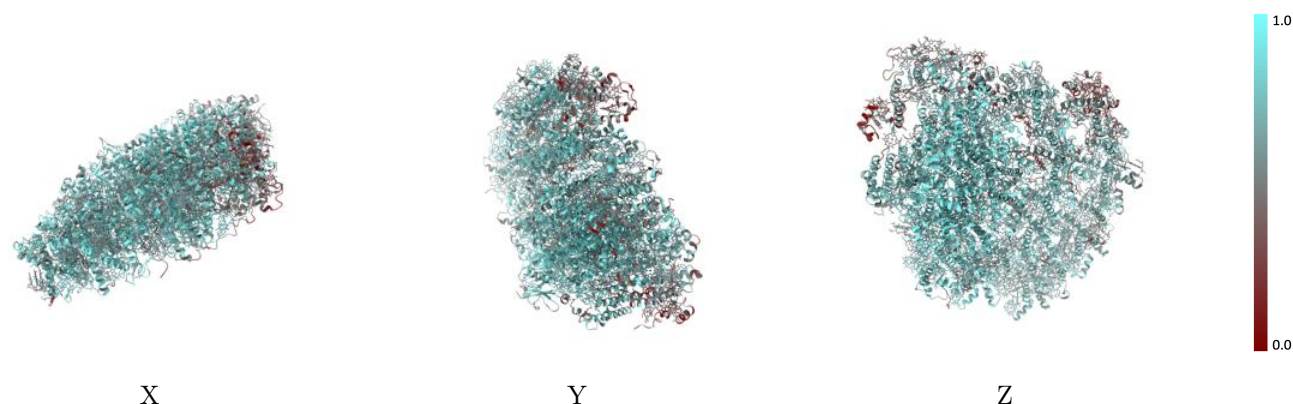
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



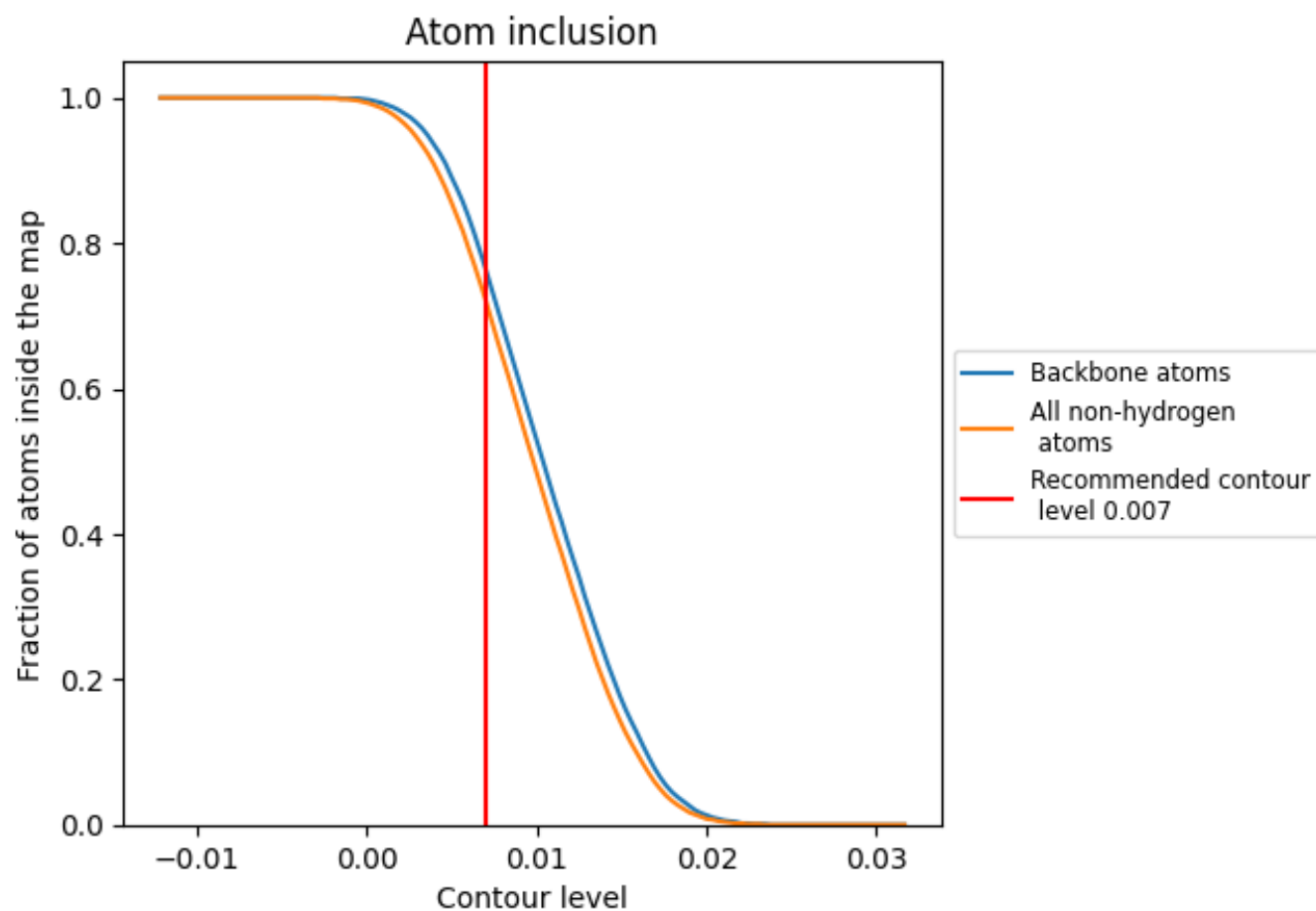
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.007) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7200 | <div></div> 0.5370 |
| 1     | <div></div> 0.6350 | <div></div> 0.4980 |
| 2     | <div></div> 0.3310 | <div></div> 0.3380 |
| 3     | <div></div> 0.7710 | <div></div> 0.5610 |
| 4     | <div></div> 0.6470 | <div></div> 0.5050 |
| 5     | <div></div> 0.6780 | <div></div> 0.5150 |
| 6     | <div></div> 0.6810 | <div></div> 0.5140 |
| 7     | <div></div> 0.7840 | <div></div> 0.5510 |
| 8     | <div></div> 0.7410 | <div></div> 0.5310 |
| 9     | <div></div> 0.5380 | <div></div> 0.4770 |
| A     | <div></div> 0.8270 | <div></div> 0.5920 |
| B     | <div></div> 0.8210 | <div></div> 0.5830 |
| C     | <div></div> 0.7720 | <div></div> 0.6020 |
| D     | <div></div> 0.6520 | <div></div> 0.5660 |
| E     | <div></div> 0.6830 | <div></div> 0.5660 |
| F     | <div></div> 0.6980 | <div></div> 0.5310 |
| G     | <div></div> 0.4660 | <div></div> 0.4150 |
| I     | <div></div> 0.6720 | <div></div> 0.5270 |
| J     | <div></div> 0.7000 | <div></div> 0.5310 |
| K     | <div></div> 0.7110 | <div></div> 0.5230 |
| L     | <div></div> 0.6550 | <div></div> 0.5030 |
| Z     | <div></div> 0.4730 | <div></div> 0.4100 |

1.0

0.0

<0.0