# Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2026 – 10:56 am BST

| | | |
|---|---|---|
| PDB ID | : | 2WSF / pdb_00002wsf |
| Title | : | Improved Model of Plant Photosystem I |
| Authors | : | Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N. |
| Deposited on | : | 2009-09-05 |
| Resolution | : | 3.48 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

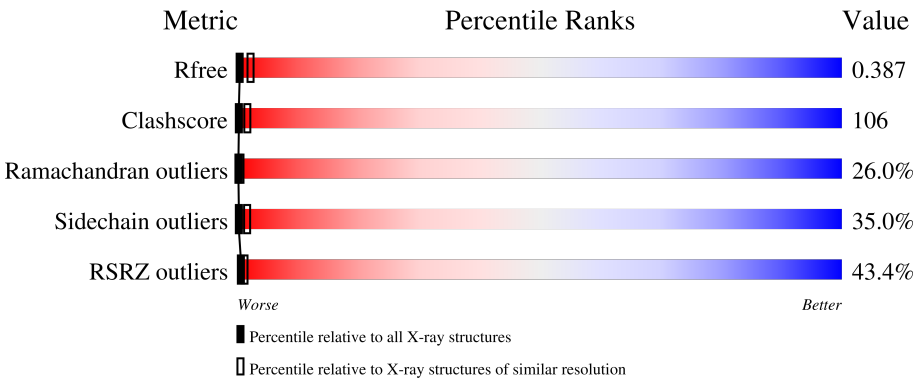
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4 | : | 9.0.015 (Gargrove) |
| Density-Fitness | : | 1.0.12 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.50 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 180053 | 1083 (3.52-3.44) |
| Clashscore | 190562 | 1139 (3.52-3.44) |
| Ramachandran outliers | 187476 | 1111 (3.52-3.44) |
| Sidechain outliers | 187428 | 1112 (3.52-3.44) |
| RSRZ outliers | 180081 | 1082 (3.52-3.44) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1 | 241 | 26%; 26%, 27%, 12%, ·, 32% |
| 2 | 2 | 269 | 19%; 9%, 24%, 22%, 12%, 35% |
| 3 | 3 | 276 | 36%; 15%, 19%, 14%, 7%, 45% |
| 4 | 4 | 251 | 20%; 6%, 20%, 23%, 17%, 34% |
| 5 | A | 758 | 47%; 9%, 44%, 34%, 9%, · |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 6 | B | 734 | 55% 13% 48% 31% 8% |
| 7 | C | 81 | 52% 7% 44% 32% 16% |
| 8 | D | 212 | 25% 9% 26% 25% 5% 35% |
| 9 | E | 143 | 15% 6% 21% 11% 7% 55% |
| 10 | F | 231 | 22% 12% 28% 22% 6% 33% |
| 11 | G | 167 | 20% • 23% 18% 11% 43% |
| 12 | H | 144 | 15% 5% 15% 16% 12% 52% |
| 13 | I | 40 | 18% 8% 45% 18% 5% 25% |
| 14 | J | 44 | 36% 7% 48% 27% 14% 5% |
| 15 | K | 131 | 14% 27% 19% 8% 10% 36% |
| 16 | L | 216 | 25% 13% 32% 23% 7% 25% |
| 17 | N | 170 | 9% • 12% 16% 19% 50% |
| 18 | R | 53 | 30% 43% 26% |
| 19 | M | 2 | 50% 50% |
| 19 | O | 2 | 100% |
| 19 | P | 2 | 100% |
| 19 | Q | 2 | 100% |
| 19 | S | 2 | 50% 50% |
| 19 | T | 2 | 100% |
| 19 | U | 2 | 100% |
| 19 | V | 2 | 100% |
| 19 | W | 2 | 50% 50% |
| 19 | X | 2 | 50% 50% |
| 19 | Y | 2 | 100% |
| 19 | Z | 2 | 50% 50% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 19 | a | 2 | 50% 50% |

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 |
|---|---|---|---|---|---|---|---|
| 19 | FRU | M | 2 | X | - | - | - |
| 19 | GLC | O | 1 | - | - | X | - |
| 19 | FRU | O | 2 | X | - | - | - |
| 19 | GLC | P | 1 | - | - | X | - |
| 19 | FRU | P | 2 | X | - | X | - |
| 19 | FRU | Q | 2 | X | - | X | - |
| 19 | FRU | S | 2 | X | - | - | - |
| 19 | FRU | T | 2 | X | - | - | - |
| 19 | FRU | U | 2 | X | - | - | - |
| 19 | FRU | V | 2 | X | - | - | - |
| 19 | FRU | W | 2 | X | - | - | - |
| 19 | FRU | X | 2 | X | - | - | - |
| 19 | GLC | Y | 1 | - | - | X | - |
| 19 | FRU | Y | 2 | X | - | X | - |
| 19 | FRU | Z | 2 | X | - | X | - |
| 19 | FRU | a | 2 | X | - | - | - |
| 20 | CLA | 1 | 206 | X | - | - | - |
| 20 | CLA | 1 | 207 | X | - | - | - |
| 20 | CLA | 1 | 211 | X | - | - | - |
| 20 | CLA | 1 | 213 | X | - | - | - |
| 20 | CLA | 1 | 215 | X | - | - | - |
| 20 | CLA | 2 | 303 | X | - | X | - |
| 20 | CLA | 2 | 307 | X | - | X | - |
| 20 | CLA | 2 | 312 | X | - | - | - |
| 20 | CLA | 2 | 316 | X | - | - | - |
| 20 | CLA | 3 | 310 | X | - | - | - |
| 20 | CLA | 3 | 311 | X | - | - | - |
| 20 | CLA | 3 | 314 | X | - | - | - |
| 20 | CLA | 4 | 301 | X | - | X | - |
| 20 | CLA | 4 | 303 | X | - | - | - |
| 20 | CLA | 4 | 304 | X | - | X | - |
| 20 | CLA | 4 | 306 | X | - | - | - |
| 20 | CLA | 4 | 310 | - | - | X | - |
| 20 | CLA | A | 801 | X | - | - | - |
| 20 | CLA | A | 804 | X | - | X | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 20 | CLA | A | 806 | X | - | - | - |
| 20 | CLA | A | 807 | - | - | X | - |
| 20 | CLA | A | 808 | X | - | - | - |
| 20 | CLA | A | 809 | - | - | X | - |
| 20 | CLA | A | 811 | X | - | - | - |
| 20 | CLA | A | 818 | X | - | X | - |
| 20 | CLA | A | 819 | X | - | X | - |
| 20 | CLA | A | 823 | X | - | - | - |
| 20 | CLA | A | 824 | X | - | X | - |
| 20 | CLA | A | 825 | X | - | X | - |
| 20 | CLA | A | 826 | X | - | X | - |
| 20 | CLA | A | 827 | X | - | - | - |
| 20 | CLA | A | 828 | X | - | - | - |
| 20 | CLA | A | 830 | X | - | X | - |
| 20 | CLA | A | 831 | X | - | X | - |
| 20 | CLA | A | 835 | X | - | - | - |
| 20 | CLA | A | 838 | X | - | X | - |
| 20 | CLA | A | 839 | X | - | X | - |
| 20 | CLA | A | 840 | X | - | - | - |
| 20 | CLA | A | 849 | X | - | - | - |
| 20 | CLA | A | 850 | X | - | X | - |
| 20 | CLA | A | 851 | X | - | X | - |
| 20 | CLA | B | 803 | X | - | X | - |
| 20 | CLA | B | 806 | X | - | X | - |
| 20 | CLA | B | 808 | X | - | X | - |
| 20 | CLA | B | 809 | X | - | X | - |
| 20 | CLA | B | 810 | X | - | - | - |
| 20 | CLA | B | 812 | X | - | - | - |
| 20 | CLA | B | 813 | X | - | - | - |
| 20 | CLA | B | 814 | X | - | X | - |
| 20 | CLA | B | 815 | X | - | - | - |
| 20 | CLA | B | 816 | X | - | - | - |
| 20 | CLA | B | 820 | X | - | - | - |
| 20 | CLA | B | 823 | X | - | - | - |
| 20 | CLA | B | 824 | X | - | X | - |
| 20 | CLA | B | 825 | - | - | X | - |
| 20 | CLA | B | 826 | X | - | X | - |
| 20 | CLA | B | 827 | X | - | X | - |
| 20 | CLA | B | 828 | X | - | - | - |
| 20 | CLA | B | 829 | X | - | X | - |
| 20 | CLA | B | 830 | X | - | X | - |
| 20 | CLA | B | 832 | X | - | X | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 20 | CLA | B | 834 | - | - | X | - |
| 20 | CLA | B | 835 | - | - | X | - |
| 20 | CLA | B | 837 | X | - | - | - |
| 20 | CLA | B | 838 | X | - | X | - |
| 20 | CLA | B | 839 | - | - | X | - |
| 20 | CLA | B | 840 | X | - | - | - |
| 20 | CLA | B | 841 | X | - | - | - |
| 20 | CLA | B | 850 | X | - | - | - |
| 20 | CLA | F | 201 | - | - | X | - |
| 20 | CLA | F | 207 | X | - | - | - |
| 20 | CLA | H | 101 | X | - | - | - |
| 20 | CLA | H | 102 | X | - | - | - |
| 20 | CLA | H | 108 | X | - | X | - |
| 20 | CLA | H | 109 | X | - | - | - |
| 20 | CLA | I | 102 | X | - | - | - |
| 20 | CLA | J | 103 | X | - | - | - |
| 20 | CLA | K | 102 | - | - | X | - |
| 20 | CLA | K | 104 | X | - | - | - |
| 20 | CLA | L | 201 | X | - | X | - |
| 20 | CLA | L | 202 | X | - | - | - |
| 20 | CLA | L | 203 | X | - | X | - |
| 20 | CLA | L | 204 | X | - | - | - |
| 20 | CLA | L | 207 | - | - | X | - |
| 20 | CLA | L | 208 | X | - | - | - |
| 20 | CLA | R | 107 | X | - | - | - |
| 20 | CLA | R | 108 | X | - | - | - |
| 21 | LMU | 2 | 313 | - | - | X | - |
| 21 | LMU | A | 853 | - | - | X | - |
| 21 | LMU | G | 101 | - | - | X | - |
| 21 | LMU | K | 107 | - | - | X | - |
| 22 | BCR | A | 843 | - | - | X | - |
| 22 | BCR | A | 844 | - | - | X | - |
| 22 | BCR | A | 845 | - | - | X | - |
| 22 | BCR | B | 801 | - | - | X | - |
| 22 | BCR | B | 846 | - | - | X | - |
| 22 | BCR | B | 847 | - | - | X | - |
| 22 | BCR | F | 203 | - | - | X | - |
| 22 | BCR | F | 204 | - | - | X | - |
| 22 | BCR | I | 103 | - | - | X | - |
| 22 | BCR | J | 102 | - | - | X | - |
| 22 | BCR | L | 209 | - | - | X | - |
| 23 | PQN | A | 842 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 23 | PQN | B | 843 | X | - | X | - |
| 24 | SF4 | A | 856 | - | - | X | - |
| 24 | SF4 | C | 102 | - | - | X | - |

# 2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 36033 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 AT3G54890.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | 1 | 165 | 1264 | 822 | 208 | 230 | 4 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 1 | -33 | ILE | LYS | conflict | UNP Q9C5R7 |
| 1 | -1 | ARG | LYS | conflict | UNP Q9C5R7 |

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 2 | 2 | 176 | 1374 | 899 | 226 | 245 | 4 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 2 | 195 | ALA | - | insertion | UNP Q41038 |
| 2 | ? | - | GLY | deletion | UNP Q41038 |

- Molecule 3 is a protein called LHCA3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | 3 | 153 | 1186 | 781 | 193 | 207 | 5 | 0 | 0 | 0 |

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | 4 | 166 | 1319 | 861 | 219 | 236 | 3 | 0 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 4 | ? | - | ALA | deletion | UNP Q9SQL2 |

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | A | 730 | 5745 | 3766 | 974 | 987 | 18 | 0 | 0 | 0 |

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 6 | B | 733 | 5848 | 3843 | 997 | 995 | 13 | 0 | 0 | 0 |

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 7 | C | 81 | 619 | 384 | 108 | 115 | 12 | 0 | 0 | 0 |

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 8 | D | 138 | 1095 | 704 | 189 | 198 | 4 | 0 | 0 | 0 |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | -52 | GLY | ALA | conflict | UNP P12353 |
| D | -50 | PRO | GLN | conflict | UNP P12353 |
| D | -44 | ARG | PRO | conflict | UNP P12353 |
| D | -34 | GLU | ASP | conflict | UNP P12353 |
| D | -11 | LEU | HIS | conflict | UNP P12353 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | -9 | THR | SER | conflict | UNP P12353 |
| D | 12 | THR | PRO | conflict | UNP P12353 |
| D | 14 | ALA | GLY | conflict | UNP P12353 |

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 9 | E | 65 | 520 | 332 | 93 | 95 | 0 | 0 | 0 |

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 10 | F | 154 | 1221 | 794 | 207 | 217 | 3 | 0 | 0 | 0 |

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 11 | G | 95 | 740 | 481 | 120 | 137 | 2 | 0 | 0 | 0 |

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 12 | H | 69 | 529 | 344 | 82 | 103 | 0 | 0 | 0 |

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 13 | I | 30 | 229 | 158 | 34 | 35 | 2 | 0 | 0 | 0 |

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 14 | J | 42 | 338 | 230 | 51 | 56 | 1 | 0 | 0 | 0 |

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 15 | K | 84 | 593 | 374 | 102 | 113 | 4 | 0 | 0 | 0 |

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 16 | L | 162 | 1215 | 800 | 194 | 216 | 5 | 0 | 0 | 0 |

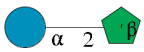
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 17 | N | 85 | 685 | 436 | 113 | 132 | 4 | 0 | 0 | 0 |

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 18 | R | 53 | 265 | 159 | 53 | 53 | 0 | 0 | 0 |

- Molecule 19 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | | |
| 19 | M | 2 | 23 | 12 | 11 | 0 | 0 | 0 |
| 19 | O | 2 | 22 | 12 | 10 | 0 | 0 | 0 |
| 19 | P | 2 | 23 | 12 | 11 | 0 | 0 | 0 |

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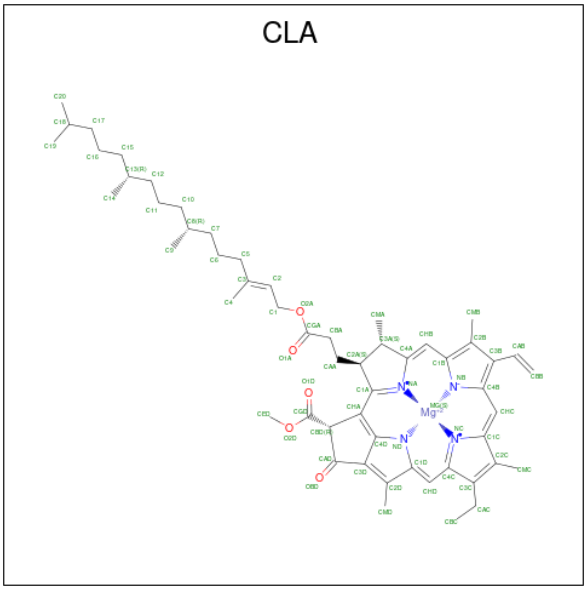
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | | | |
| 19 | Q | 2 | 23 | 12 | 11 | | 0 | 0 | 0 |
| | | | Total | C | O | | | | |
| 19 | S | 2 | 23 | 12 | 11 | | 0 | 0 | 0 |
| | | | Total | C | O | | | | |
| 19 | T | 2 | 23 | 12 | 11 | | 0 | 0 | 0 |
| | | | Total | C | O | | | | |
| 19 | U | 2 | 23 | 12 | 11 | | 0 | 0 | 0 |
| | | | Total | C | O | | | | |
| 19 | V | 2 | 23 | 12 | 11 | | 0 | 0 | 0 |
| | | | Total | C | O | | | | |
| 19 | W | 2 | 23 | 12 | 11 | | 0 | 0 | 0 |
| | | | Total | C | O | | | | |
| 19 | X | 2 | 22 | 12 | 10 | | 0 | 0 | 0 |
| | | | Total | C | O | | | | |
| 19 | Y | 2 | 23 | 12 | 11 | | 0 | 0 | 0 |
| | | | Total | C | O | | | | |
| 19 | Z | 2 | 23 | 12 | 11 | | 0 | 0 | 0 |
| | | | Total | C | O | | | | |
| 19 | a | 2 | 23 | 12 | 11 | | 0 | 0 | 0 |

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Mg | N | O | | |
| 20 | 1 | 1 | 46 | 36 | 1 | 4 | 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 20 | 1 | 1 | Total C Mg N O<br>41 33 1 4 3 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N O<br>47 37 1 4 5 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N O<br>46 36 1 4 5 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N O<br>36 30 1 4 1 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N O<br>61 51 1 4 5 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N O<br>51 41 1 4 5 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N O<br>36 30 1 4 1 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N O<br>51 41 1 4 5 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N O<br>51 41 1 4 5 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 1 | 1 | Total C Mg N O<br>51 41 1 4 5 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N O<br>51 41 1 4 5 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N O<br>58 48 1 4 5 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N O<br>50 40 1 4 5 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N O<br>65 55 1 4 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 20 | 2 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N O<br>50 40 1 4 5 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N O<br>50 40 1 4 5 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N O<br>61 51 1 4 5 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N O<br>50 40 1 4 5 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 2 | 1 | Total C Mg N O<br>65 55 1 4 5 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N O<br>36 30 1 4 1 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N O<br>36 30 1 4 1 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N O<br>42 34 1 4 3 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N O<br>65 55 1 4 5 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N O<br>65 55 1 4 5 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N O<br>50 40 1 4 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 20 | 3 | 1 | Total C Mg N O<br>65 55 1 4 5 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 3 | 1 | Total C Mg N O<br>36 30 1 4 1 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>55 45 1 4 5 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>36 30 1 4 1 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>65 55 1 4 5 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>55 45 1 4 5 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>50 40 1 4 5 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>52 42 1 4 5 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>50 40 1 4 5 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>36 30 1 4 1 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>46 36 1 4 5 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>52 42 1 4 5 | 0 | 0 |
| 20 | 4 | 1 | Total C Mg N O<br>47 37 1 4 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 20 | A | 1 | Total C Mg N O<br>46 36 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>46 36 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>55 45 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>54 44 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>56 46 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>46 36 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>60 50 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>52 42 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>45 35 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>65 55 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>54 44 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>50 40 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N<br>25 20 1 4 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>50 40 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>54 44 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>52 42 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>60 50 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>58 48 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>51 41 1 4 5 | 0 | 0 |
| 20 | A | 1 | Total C Mg N O<br>42 34 1 4 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 58 | 48 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 59 | 49 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 55 | 45 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 45 | 35 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 46 | 36 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 47 | 37 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 51 | 41 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 59 | 49 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 55 | 45 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | | | |
| 20 | A | 1 | 25 | 20 | 1 | 4 | | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 54 | 44 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 45 | 35 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 61 | 51 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 60 | 50 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | | | |
| 20 | B | 1 | 25 | 20 | 1 | 4 | | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 54 | 44 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 55 | 45 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 60 | 50 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 60 | 50 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 46 | 36 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 53 | 43 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 41 | 33 | 1 | 4 | 3 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 61 | 51 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 46 | 36 | 1 | 4 | 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 55 | 45 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 54 | 44 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 58 | 48 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 59 | 49 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 45 | 35 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 45 | 35 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 51 | 41 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 60 | 50 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 47 | 37 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 36 | 30 | 1 | 4 | 1 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | B | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Mg | N | O | | |
| 20 | F | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | F | 1 | 36 | 30 | 1 | 4 | 1 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | F | 1 | 41 | 33 | 1 | 4 | 3 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | F | 1 | 53 | 43 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | G | 1 | 51 | 41 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | H | 1 | 55 | 45 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | H | 1 | 55 | 45 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | H | 1 | 58 | 48 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | H | 1 | 55 | 45 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | H | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | I | 1 | 60 | 50 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | J | 1 | 48 | 38 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | J | 1 | 61 | 51 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | K | 1 | 46 | 36 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | K | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | K | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | K | 1 | 56 | 46 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | L | 1 | 60 | 50 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | L | 1 | 55 | 45 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | L | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | L | 1 | 55 | 45 | 1 | 4 | 5 | 0 | 0 |

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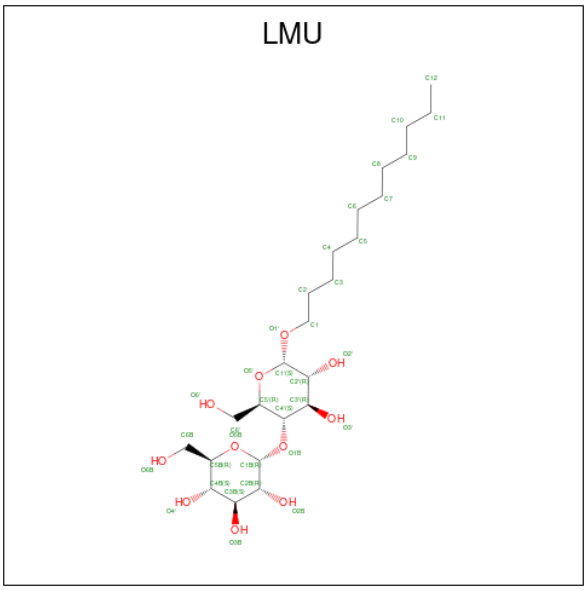
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Mg | N | O | | |
| 20 | L | 1 | 47 | 37 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | L | 1 | 50 | 40 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | R | 1 | 57 | 47 | 1 | 4 | 5 | 0 | 0 |
| | | | Total | C | Mg | N | O | | |
| 20 | R | 1 | 65 | 55 | 1 | 4 | 5 | 0 | 0 |

- Molecule 21 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 21 | 1 | 1 | 35 | 24 | 11 | 0 | 0 |
| | | | Total | C | O | | |
| 21 | 1 | 1 | 35 | 24 | 11 | 0 | 0 |
| | | | Total | C | O | | |
| 21 | 1 | 1 | 35 | 24 | 11 | 0 | 0 |
| | | | Total | C | O | | |
| 21 | 2 | 1 | 35 | 24 | 11 | 0 | 0 |
| | | | Total | C | O | | |
| 21 | 2 | 1 | 35 | 24 | 11 | 0 | 0 |
| | | | Total | C | O | | |
| 21 | 2 | 1 | 35 | 24 | 11 | 0 | 0 |
| | | | Total | C | O | | |
| 21 | 2 | 1 | 35 | 24 | 11 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 21 | 2 | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | 3 | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | 3 | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | 4 | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | 4 | 1 | 34 | 23 | 11 | 0 | 0 |
| 21 | 4 | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | 4 | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | A | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | A | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | A | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | A | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | A | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | A | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | A | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | B | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | B | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | B | 1 | 25 | 14 | 11 | 0 | 0 |
| 21 | C | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | D | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | E | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | F | 1 | 34 | 23 | 11 | 0 | 0 |

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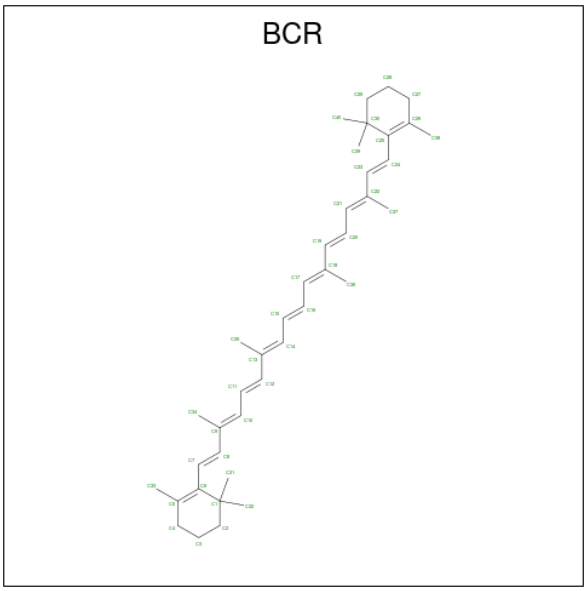
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 21 | G | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | G | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | G | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | H | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | H | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | H | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | H | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | K | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | K | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | K | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | L | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | L | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | L | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | R | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | R | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | R | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | R | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | R | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | R | 1 | 35 | 24 | 11 | 0 | 0 |
| 21 | R | 1 | 35 | 24 | 11 | 0 | 0 |

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).




| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | C | | |
| 22 | 2 | 1 | 40 | 40 | 0 | 0 |
| 22 | A | 1 | 40 | 40 | 0 | 0 |
| 22 | A | 1 | 40 | 40 | 0 | 0 |
| 22 | A | 1 | 40 | 40 | 0 | 0 |
| 22 | B | 1 | 40 | 40 | 0 | 0 |
| 22 | B | 1 | 40 | 40 | 0 | 0 |
| 22 | B | 1 | 40 | 40 | 0 | 0 |
| 22 | B | 1 | 40 | 40 | 0 | 0 |
| 22 | B | 1 | 40 | 40 | 0 | 0 |
| 22 | F | 1 | 40 | 40 | 0 | 0 |
| 22 | F | 1 | 40 | 40 | 0 | 0 |
| 22 | G | 1 | 40 | 40 | 0 | 0 |
| 22 | I | 1 | 39 | 39 | 0 | 0 |
| 22 | I | 1 | 40 | 40 | 0 | 0 |

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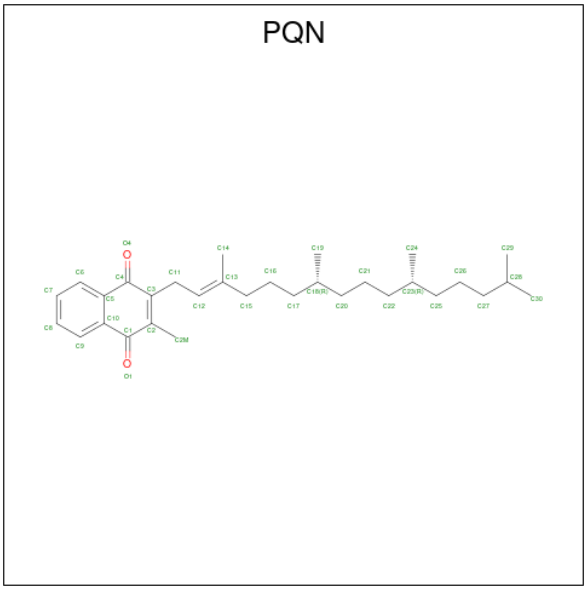
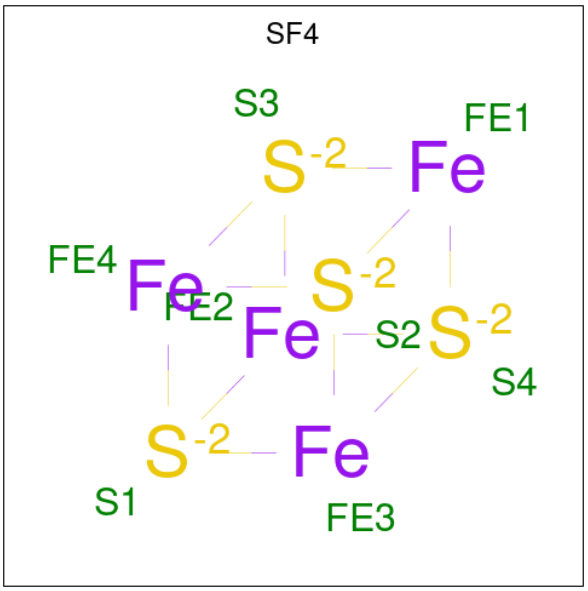
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | C | | |
| 22 | J | 1 | 40 | 40 | 0 | 0 |
| | | | Total | C | | |
| 22 | L | 1 | 40 | 40 | 0 | 0 |

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



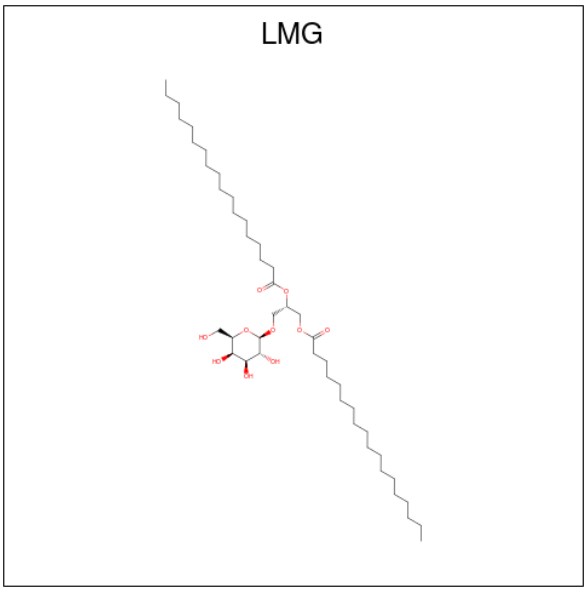

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 23 | A | 1 | 33 | 31 | 2 | 0 | 0 |
| | | | Total | C | O | | |
| 23 | B | 1 | 33 | 31 | 2 | 0 | 0 |

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: $Fe_4S_4$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | Fe | S | | |
| 24 | A | 1 | 8 | 4 | 4 | 0 | 0 |
| | | | Total | Fe | S | | |
| 24 | C | 1 | 8 | 4 | 4 | 0 | 0 |
| | | | Total | Fe | S | | |
| 24 | C | 1 | 8 | 4 | 4 | 0 | 0 |

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 25 | B | 1 | 49 | 39 | 10 | 0 | 0 |

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

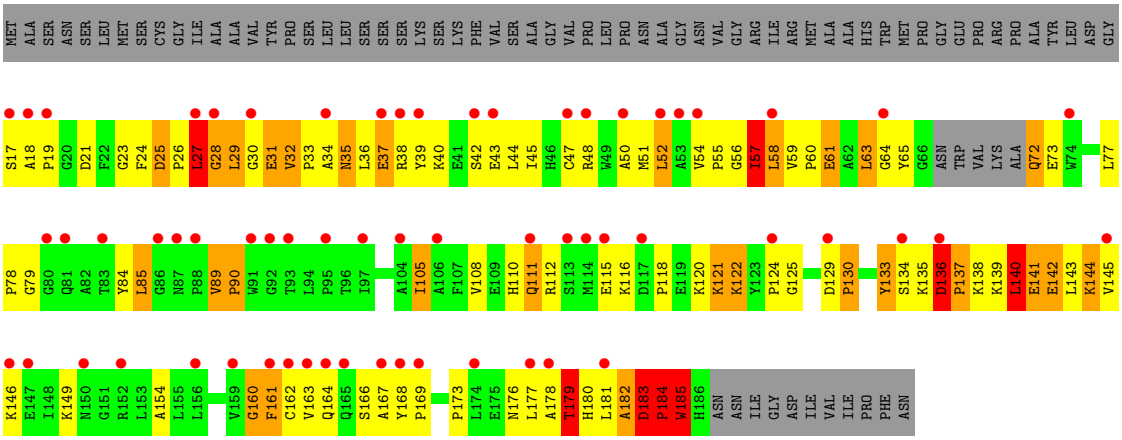
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 26 | H | 1 | 23 | 12 | 11 | 0 | 0 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

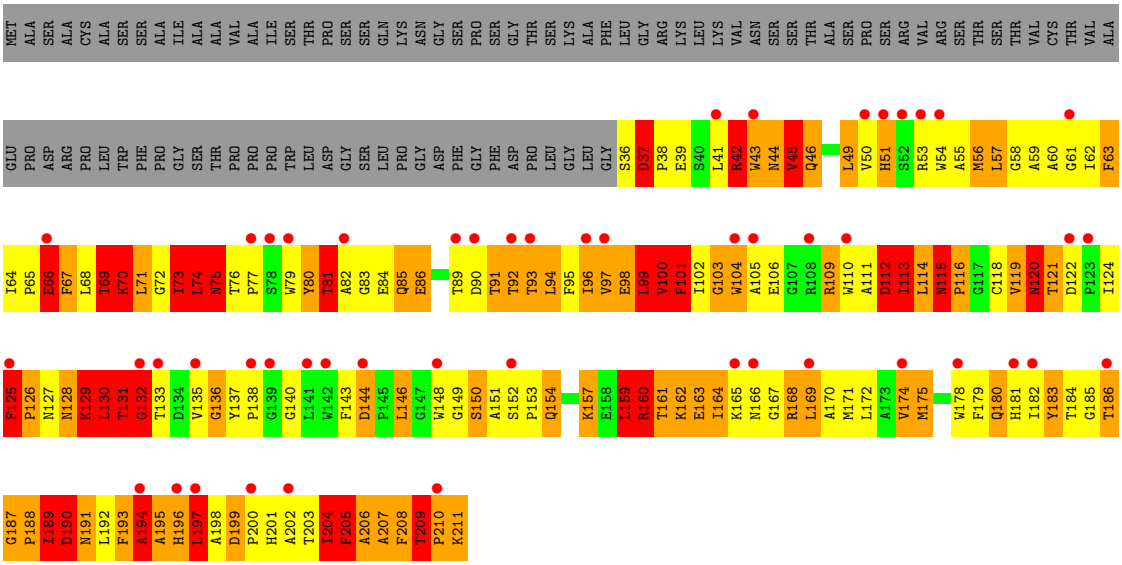
• Molecule 1: AT3G54890

Chain 1:



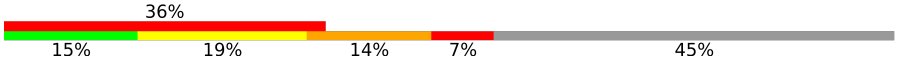
• Molecule 2: TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I

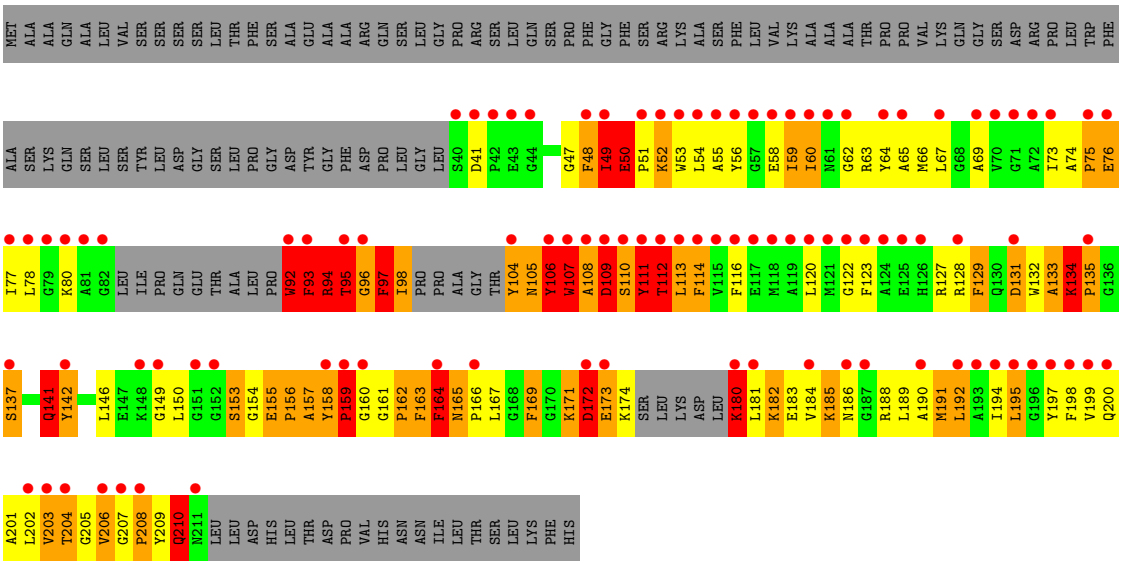
Chain 2:



- Molecule 3: LHCA3

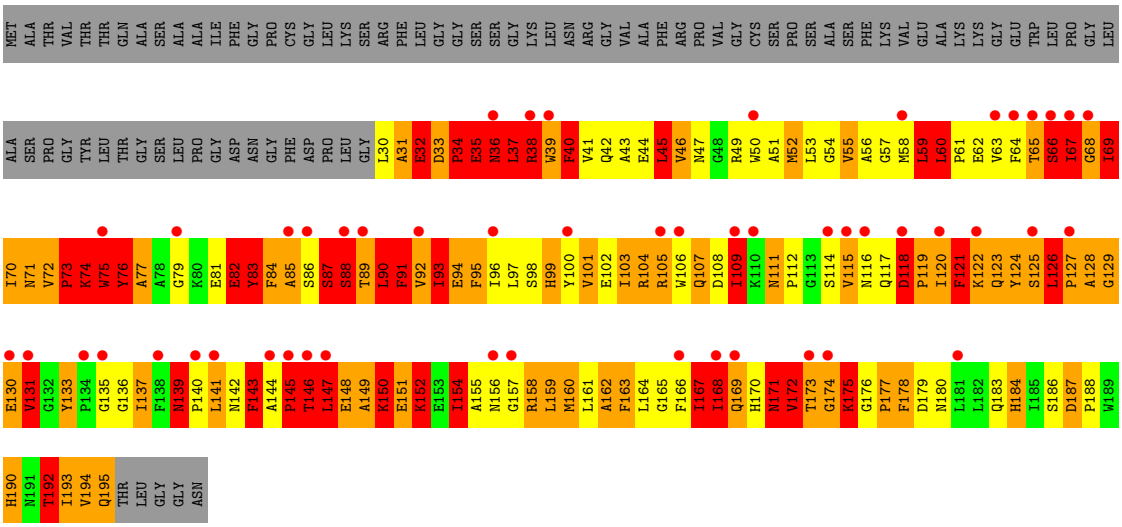
Chain 3:



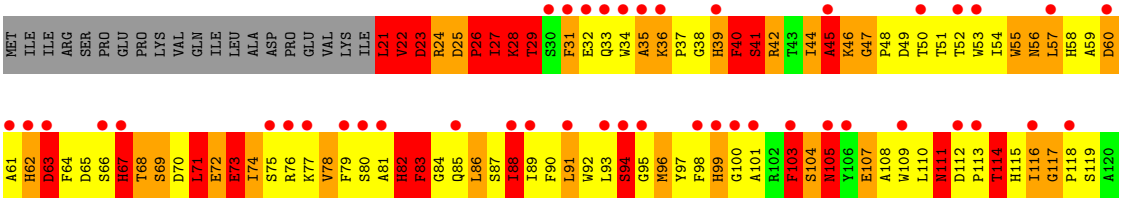

- Molecule 4: CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC

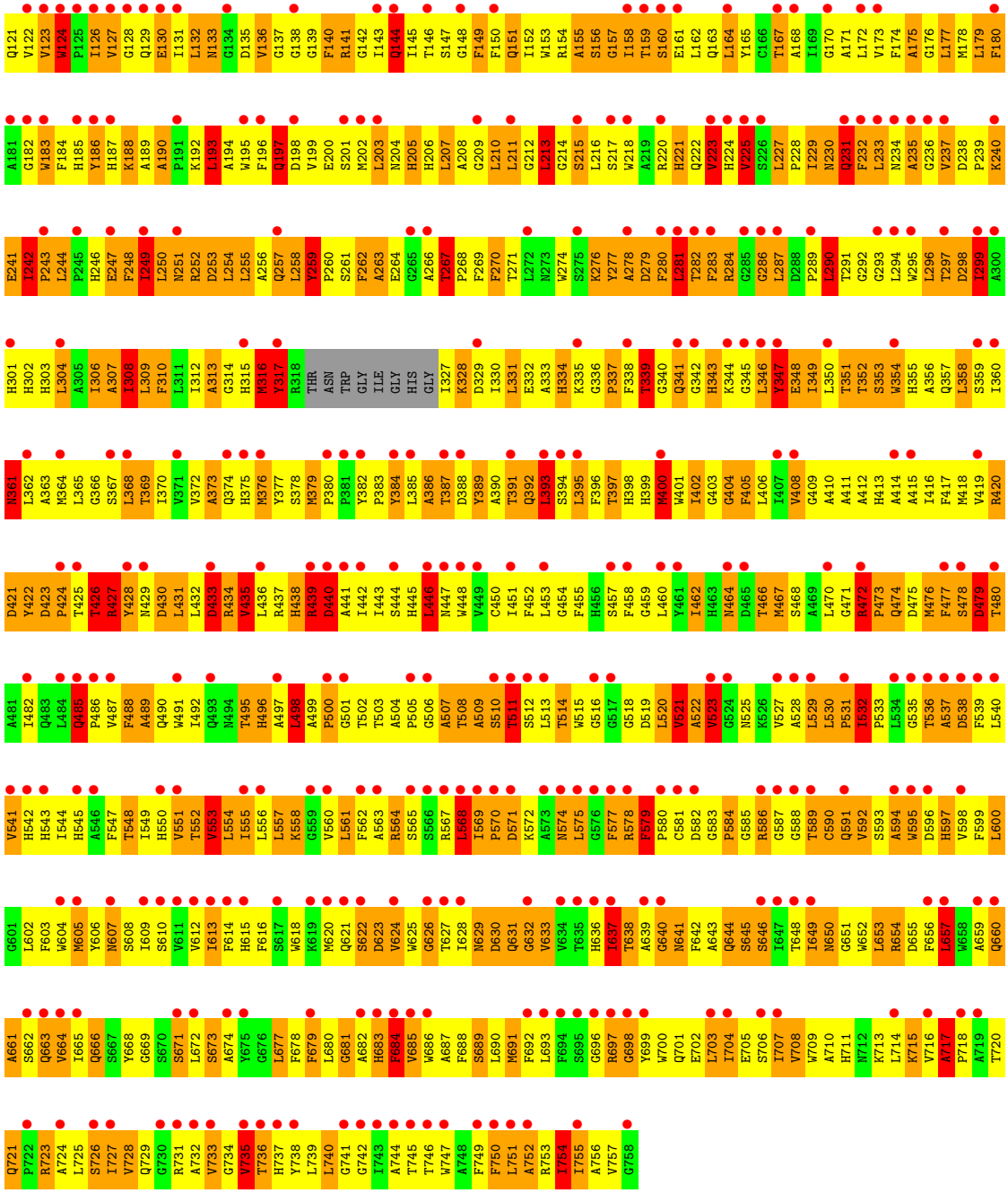
Chain 4:




- Molecule 5: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1

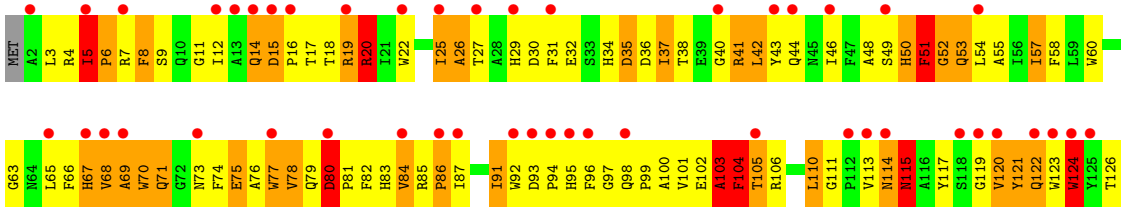
Chain A:

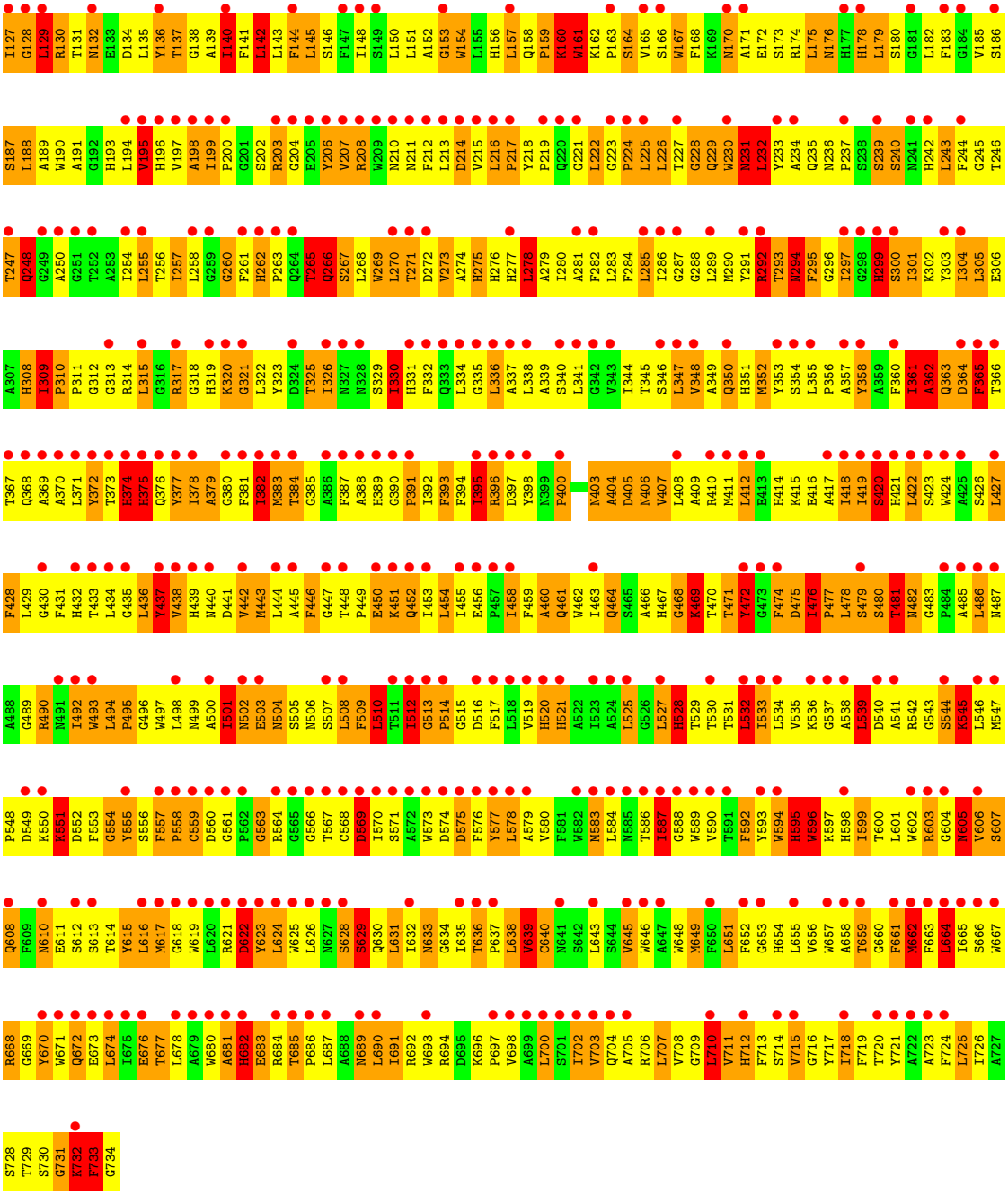





• Molecule 6: PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2

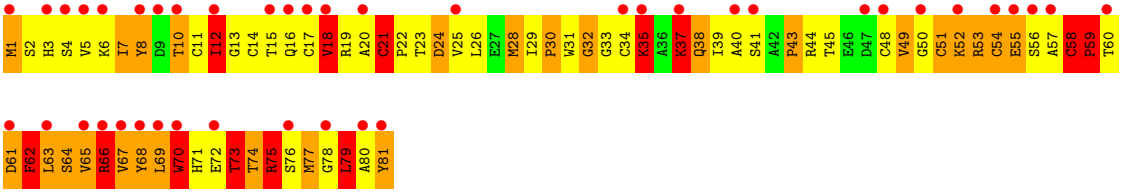
Chain B: 55% 13% 48% 31% 8%





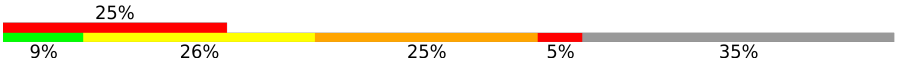

- Molecule 7: PHOTOSYSTEM I IRON-SULFUR CENTER

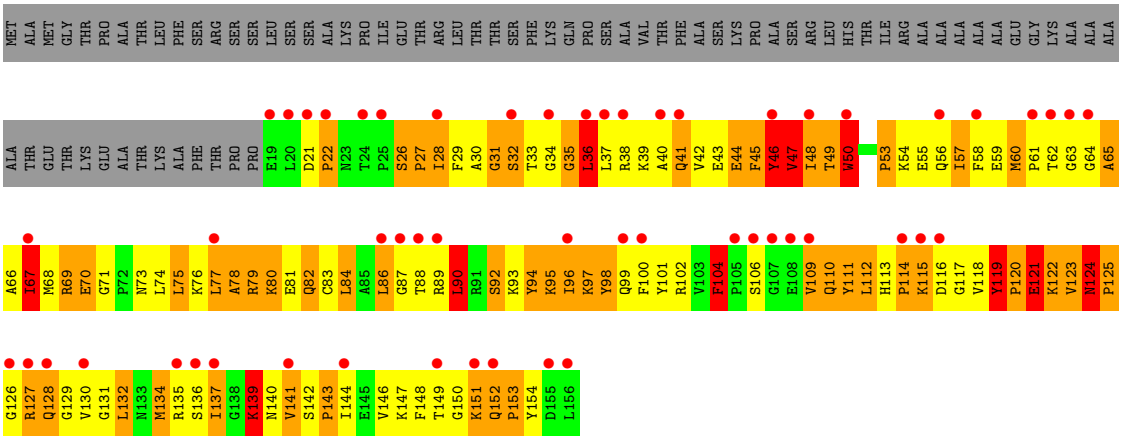
Chain C:




- Molecule 8: PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC

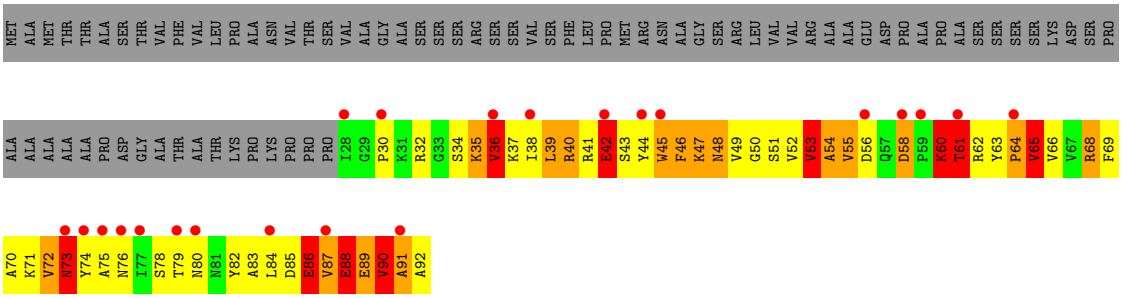
Chain D:



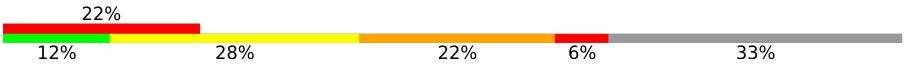

• Molecule 9: PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC

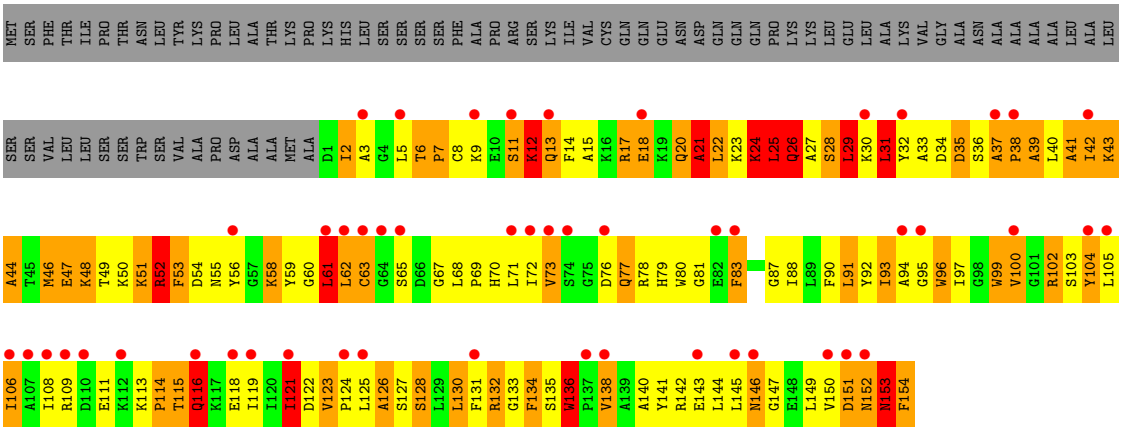
Chain E:




• Molecule 10: PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC

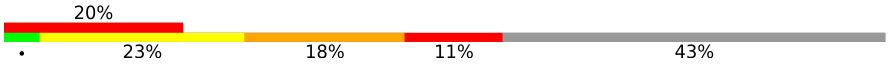
Chain F:

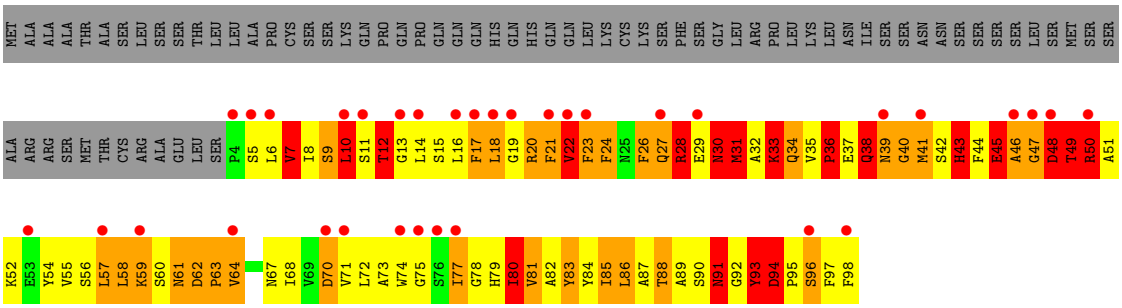



• Molecule 11: PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC

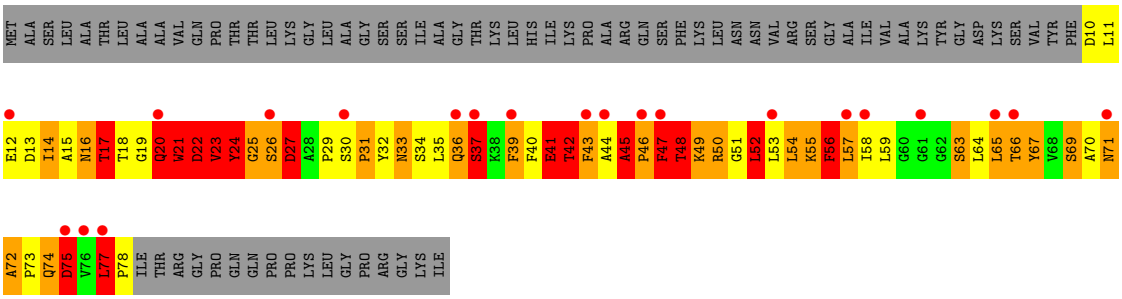
Chain G:





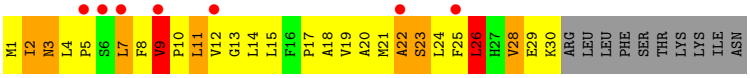

• Molecule 12: PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC

Chain H:




• Molecule 13: PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII

Chain I:

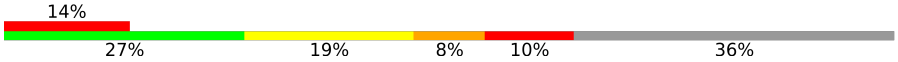


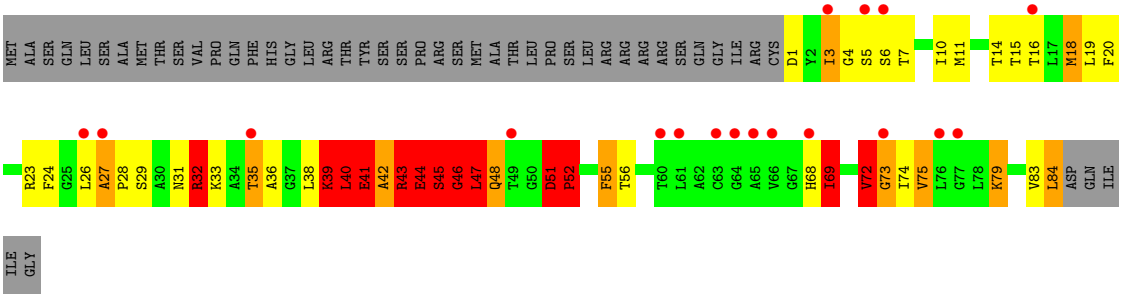

• Molecule 14: PHOTOSYSTEM I REACTION CENTER SUBUNIT IX

Chain J:

• Molecule 15: PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC

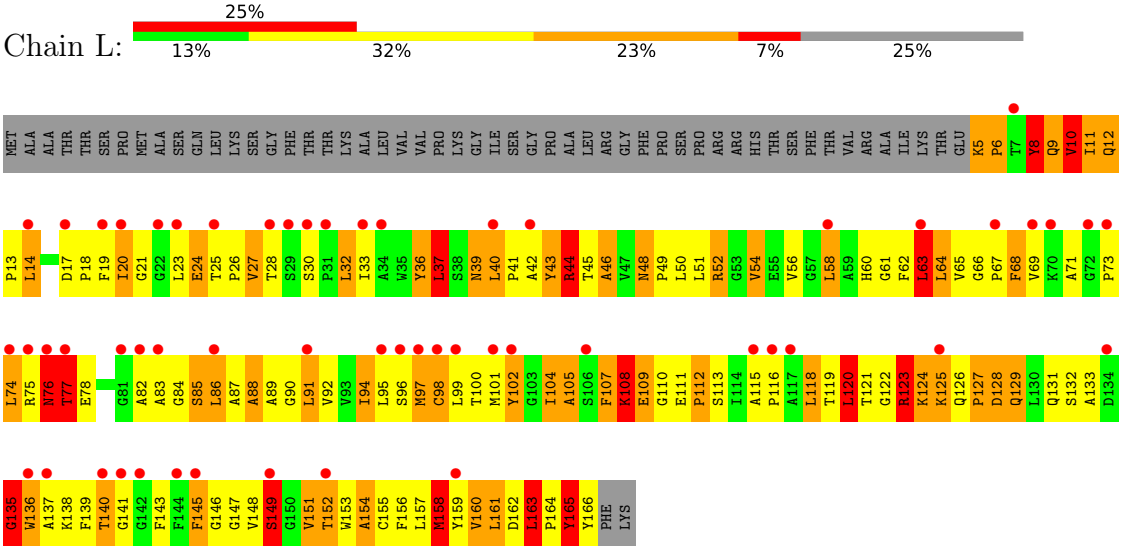
Chain K:



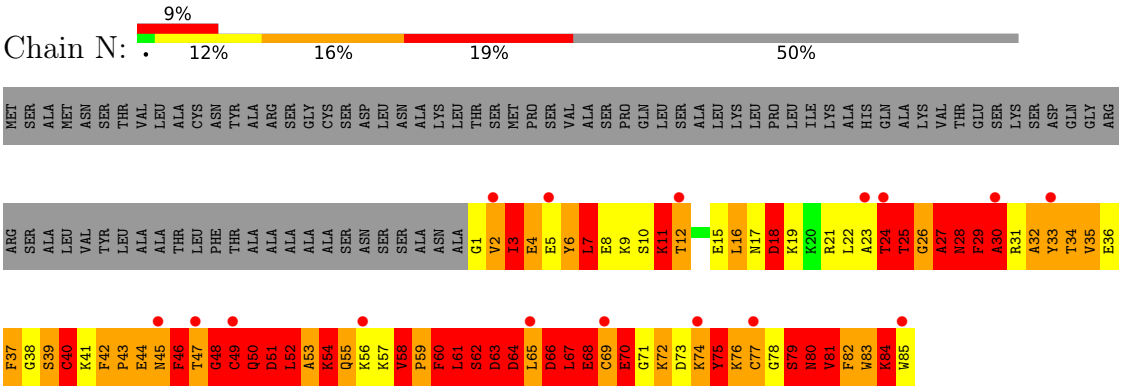
• Molecule 16: PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC

Chain L:



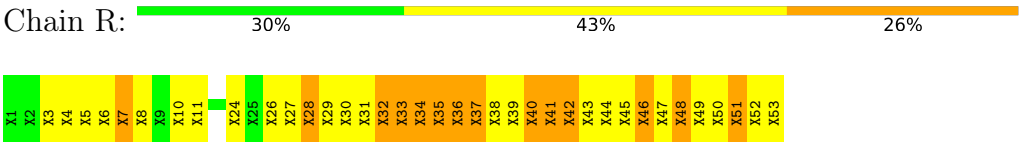

• Molecule 17: PHOTOSYSTEM I-N SUBUNIT

Chain N:




• Molecule 18: PHOTOSYSTEM I-N SUBUNIT

Chain R:

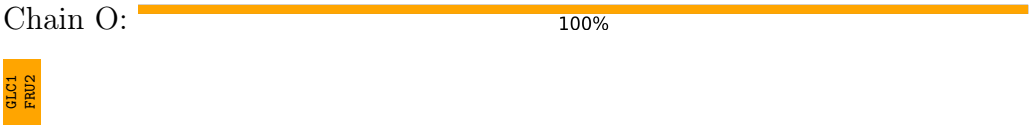



• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M:

• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O:



- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain P: 100%

GLC1 FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Q: 100%

GLC1 FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain S: 50% 50%

GLC1 FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain T: 100%

GLC1 FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain U: 100%

GLC1 FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain V: 100%

GLC1 FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain W: 50% 50%

GLC1 FRU2

- Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain X: 50% 50%

• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Y:


• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Z:


• Molecule 19: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain a:

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 120.20Å 190.20Å 130.30Å<br>90.00° 91.53° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.48<br>50.00 – 3.48 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 96.4 (50.00-3.48)<br>96.6 (50.00-3.48) | Depositor<br>EDS |
| $R_{merge}$ | 0.13 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.61 (at 3.48Å) | Xtriage |
| Refinement program | REFMAC 5.5.0072 | Depositor |
| R, $R_{free}$ | 0.391 , 0.425<br>0.383 , 0.387 | Depositor<br>DCC |
| $R_{free}$ test set | 1456 reflections (1.95%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 81.0 | Xtriage |
| Anisotropy | 0.408 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.10 , 14.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.31$ | Xtriage |
| Estimated twinning fraction | 0.016 for h,-k,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.74 | EDS |
| Total number of atoms | 36033 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 26.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, LMG, CLA, GLC, LMU, BCR, SF4, UNL, FRU

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 | 1 | 0.67 | 0/1303 | 1.07 | 7/1774 (0.4%) |
| 2 | 2 | 0.85 | 0/1420 | 1.50 | 23/1943 (1.2%) |
| 3 | 3 | 0.66 | 0/1221 | 1.38 | 13/1642 (0.8%) |
| 4 | 4 | 1.05 | 5/1359 (0.4%) | 1.59 | 32/1851 (1.7%) |
| 5 | A | 0.79 | 4/5938 (0.1%) | 1.27 | 59/8104 (0.7%) |
| 6 | B | 0.76 | 1/6058 (0.0%) | 1.18 | 44/8278 (0.5%) |
| 7 | C | 0.96 | 0/632 | 1.50 | 9/856 (1.1%) |
| 8 | D | 0.96 | 0/1122 | 1.33 | 17/1514 (1.1%) |
| 9 | E | 0.95 | 0/530 | 1.25 | 3/718 (0.4%) |
| 10 | F | 0.82 | 0/1250 | 1.27 | 9/1687 (0.5%) |
| 11 | G | 1.13 | 7/760 (0.9%) | 1.83 | 19/1031 (1.8%) |
| 12 | H | 0.90 | 0/543 | 1.48 | 11/741 (1.5%) |
| 13 | I | 0.84 | 0/235 | 1.11 | 1/320 (0.3%) |
| 14 | J | 0.81 | 0/349 | 1.40 | 7/475 (1.5%) |
| 15 | K | 0.86 | 1/599 (0.2%) | 1.25 | 6/810 (0.7%) |
| 16 | L | 0.84 | 0/1251 | 1.25 | 12/1709 (0.7%) |
| 17 | N | 1.17 | 5/699 (0.7%) | 1.61 | 18/936 (1.9%) |
| All | All | 0.84 | 23/25269 (0.1%) | 1.32 | 290/34389 (0.8%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | 1 | 0 | 3 |
| 2 | 2 | 0 | 17 |
| 3 | 3 | 0 | 17 |
| 4 | 4 | 0 | 20 |
| 5 | A | 0 | 20 |
| 6 | B | 0 | 12 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 7 | C | 0 | 1 |
| 8 | D | 0 | 1 |
| 9 | E | 0 | 3 |
| 10 | F | 0 | 7 |
| 11 | G | 1 | 13 |
| 12 | H | 0 | 9 |
| 15 | K | 0 | 6 |
| 16 | L | 0 | 2 |
| 17 | N | 0 | 22 |
| 18 | R | 0 | 16 |
| All | All | 1 | 169 |

All (23) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | 4 | 39 | TRP | CA-C | -7.67 | 1.42 | 1.52 |
| 5 | A | 22 | VAL | CA-CB | -7.58 | 1.44 | 1.54 |
| 17 | N | 51 | ASP | N-CA | 7.28 | 1.55 | 1.46 |
| 17 | N | 40 | CYS | C-O | 7.01 | 1.32 | 1.24 |
| 17 | N | 52 | LEU | N-CA | -6.99 | 1.41 | 1.46 |
| 4 | 4 | 74 | LYS | C-O | 6.82 | 1.32 | 1.24 |
| 11 | G | 43 | HIS | CA-C | -6.46 | 1.44 | 1.52 |
| 11 | G | 46 | ALA | C-O | -6.11 | 1.17 | 1.24 |
| 4 | 4 | 40 | PHE | N-CA | -5.79 | 1.39 | 1.46 |
| 6 | B | 639 | VAL | CA-CB | 5.73 | 1.62 | 1.54 |
| 4 | 4 | 154 | ILE | CA-CB | 5.55 | 1.62 | 1.54 |
| 5 | A | 532 | ILE | CA-CB | 5.55 | 1.61 | 1.54 |
| 11 | G | 46 | ALA | N-CA | -5.47 | 1.39 | 1.46 |
| 4 | 4 | 37 | LEU | N-CA | 5.42 | 1.52 | 1.46 |
| 11 | G | 46 | ALA | CA-CB | -5.42 | 1.44 | 1.53 |
| 5 | A | 29 | THR | CA-CB | -5.38 | 1.44 | 1.53 |
| 5 | A | 242 | ILE | CA-CB | 5.30 | 1.61 | 1.54 |
| 17 | N | 84 | LYS | C-O | 5.26 | 1.30 | 1.24 |
| 17 | N | 48 | GLY | C-O | 5.24 | 1.30 | 1.23 |
| 11 | G | 43 | HIS | C-O | -5.22 | 1.17 | 1.23 |
| 15 | K | 43 | ARG | CA-C | 5.11 | 1.59 | 1.52 |
| 11 | G | 22 | VAL | CA-C | 5.03 | 1.59 | 1.52 |
| 11 | G | 49 | THR | N-CA | -5.01 | 1.39 | 1.46 |

All (290) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 11 | G | 46 | ALA | N-CA-C | -25.52 | 83.47 | 111.28 |
| 3 | 3 | 180 | LYS | CA-C-N | -16.91 | 95.85 | 123.91 |
| 3 | 3 | 180 | LYS | C-N-CA | -16.91 | 95.85 | 123.91 |
| 11 | G | 51 | ALA | N-CA-C | 13.21 | 128.32 | 110.35 |
| 11 | G | 45 | GLU | N-CA-C | 13.08 | 125.07 | 111.07 |
| 12 | H | 26 | SER | N-CA-C | -12.98 | 97.74 | 113.19 |
| 17 | N | 31 | ARG | N-CA-C | -12.07 | 98.10 | 111.14 |
| 5 | A | 532 | ILE | CA-C-N | 11.54 | 131.45 | 120.03 |
| 5 | A | 532 | ILE | C-N-CA | 11.54 | 131.45 | 120.03 |
| 17 | N | 33 | TYR | N-CA-C | -11.25 | 92.95 | 109.15 |
| 5 | A | 152 | ILE | N-CA-C | -10.97 | 100.22 | 110.53 |
| 5 | A | 472 | ARG | CA-C-N | 10.74 | 133.26 | 119.84 |
| 5 | A | 472 | ARG | C-N-CA | 10.74 | 133.26 | 119.84 |
| 11 | G | 21 | PHE | N-CA-C | 10.65 | 125.65 | 112.23 |
| 3 | 3 | 50 | GLU | N-CA-C | -10.61 | 98.13 | 112.35 |
| 5 | A | 316 | MET | N-CA-C | -10.60 | 94.07 | 109.96 |
| 7 | C | 58 | CYS | CA-C-N | 10.19 | 132.58 | 119.84 |
| 7 | C | 58 | CYS | C-N-CA | 10.19 | 132.58 | 119.84 |
| 14 | J | 35 | ASP | N-CA-C | 9.92 | 124.22 | 109.24 |
| 5 | A | 65 | ASP | N-CA-C | -9.90 | 99.59 | 114.64 |
| 16 | L | 104 | ILE | N-CA-C | -9.88 | 103.71 | 113.20 |
| 4 | 4 | 37 | LEU | N-CA-C | 9.72 | 126.10 | 111.04 |
| 4 | 4 | 39 | TRP | CA-C-N | -9.63 | 108.12 | 122.86 |
| 4 | 4 | 39 | TRP | C-N-CA | -9.63 | 108.12 | 122.86 |
| 2 | 2 | 121 | THR | N-CA-C | 9.54 | 126.08 | 113.30 |
| 6 | B | 51 | PHE | N-CA-C | -9.37 | 101.98 | 113.41 |
| 2 | 2 | 100 | VAL | N-CA-C | -9.32 | 101.66 | 110.42 |
| 8 | D | 152 | GLN | CA-C-N | 9.27 | 131.43 | 119.84 |
| 8 | D | 152 | GLN | C-N-CA | 9.27 | 131.43 | 119.84 |
| 6 | B | 575 | ASP | N-CA-C | -8.70 | 102.59 | 113.55 |
| 11 | G | 40 | GLY | N-CA-C | -8.65 | 101.41 | 112.65 |
| 12 | H | 45 | ALA | CA-C-N | 8.60 | 130.59 | 119.84 |
| 12 | H | 45 | ALA | C-N-CA | 8.60 | 130.59 | 119.84 |
| 16 | L | 77 | THR | N-CA-C | 8.54 | 122.89 | 110.42 |
| 5 | A | 117 | GLY | CA-C-N | 8.47 | 128.98 | 119.92 |
| 5 | A | 117 | GLY | C-N-CA | 8.47 | 128.98 | 119.92 |
| 10 | F | 24 | LYS | N-CA-C | -8.42 | 102.78 | 113.72 |
| 1 | 1 | 136 | ASP | CA-C-N | 8.38 | 130.32 | 119.84 |
| 1 | 1 | 136 | ASP | C-N-CA | 8.38 | 130.32 | 119.84 |
| 5 | A | 627 | THR | N-CA-C | 8.38 | 121.11 | 108.46 |
| 4 | 4 | 126 | LEU | N-CA-C | 8.28 | 128.10 | 109.81 |
| 4 | 4 | 33 | ASP | CA-C-N | 8.26 | 130.17 | 119.84 |
| 4 | 4 | 33 | ASP | C-N-CA | 8.26 | 130.17 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | B | 731 | GLY | N-CA-C | -8.21 | 93.73 | 113.18 |
| 8 | D | 84 | LEU | N-CA-C | -8.07 | 104.58 | 114.75 |
| 2 | 2 | 74 | LEU | N-CA-C | -8.06 | 93.63 | 110.80 |
| 14 | J | 4 | PHE | N-CA-C | 8.06 | 121.99 | 108.13 |
| 17 | N | 16 | LEU | N-CA-C | -8.03 | 96.88 | 109.72 |
| 6 | B | 52 | GLY | N-CA-C | -7.99 | 103.77 | 113.99 |
| 6 | B | 551 | LYS | N-CA-C | 7.99 | 119.09 | 108.07 |
| 2 | 2 | 101 | PHE | N-CA-C | 7.95 | 119.57 | 111.07 |
| 6 | B | 176 | ASN | N-CA-C | -7.92 | 103.41 | 113.23 |
| 2 | 2 | 101 | PHE | N-CA-CB | 7.91 | 121.47 | 110.01 |
| 5 | A | 259 | TYR | CA-C-N | 7.90 | 129.72 | 119.84 |
| 5 | A | 259 | TYR | C-N-CA | 7.90 | 129.72 | 119.84 |
| 2 | 2 | 93 | THR | N-CA-C | -7.88 | 103.11 | 112.89 |
| 10 | F | 6 | THR | CA-C-N | 7.88 | 129.69 | 119.84 |
| 10 | F | 6 | THR | C-N-CA | 7.88 | 129.69 | 119.84 |
| 11 | G | 50 | ARG | N-CA-C | 7.77 | 127.35 | 110.80 |
| 7 | C | 18 | VAL | N-CA-C | 7.75 | 117.98 | 108.06 |
| 14 | J | 27 | ILE | N-CA-C | -7.73 | 102.74 | 110.62 |
| 3 | 3 | 133 | ALA | N-CA-C | -7.71 | 102.51 | 112.23 |
| 11 | G | 94 | ASP | CA-C-N | 7.70 | 128.84 | 120.13 |
| 11 | G | 94 | ASP | C-N-CA | 7.70 | 128.84 | 120.13 |
| 17 | N | 24 | THR | N-CA-C | -7.69 | 94.42 | 110.80 |
| 7 | C | 51 | CYS | N-CA-C | 7.68 | 121.14 | 111.24 |
| 4 | 4 | 40 | PHE | CB-CA-C | 7.67 | 123.48 | 111.13 |
| 4 | 4 | 67 | ILE | N-CA-C | 7.65 | 119.09 | 107.77 |
| 4 | 4 | 143 | PHE | N-CA-C | 7.65 | 127.09 | 110.80 |
| 6 | B | 336 | LEU | N-CA-C | -7.62 | 104.13 | 113.50 |
| 2 | 2 | 56 | MET | N-CA-C | 7.61 | 122.80 | 112.68 |
| 12 | H | 65 | LEU | N-CA-C | -7.50 | 101.34 | 113.19 |
| 4 | 4 | 76 | TYR | N-CA-C | -7.45 | 104.80 | 114.04 |
| 7 | C | 53 | ARG | N-CA-C | -7.44 | 103.31 | 112.38 |
| 5 | A | 646 | SER | N-CA-C | -7.43 | 104.45 | 113.97 |
| 5 | A | 140 | PHE | N-CA-C | 7.40 | 120.12 | 108.79 |
| 6 | B | 710 | LEU | N-CA-C | -7.40 | 95.03 | 110.80 |
| 4 | 4 | 88 | SER | N-CA-C | 7.37 | 126.50 | 110.80 |
| 2 | 2 | 195 | ALA | N-CA-C | -7.34 | 102.66 | 111.69 |
| 4 | 4 | 66 | SER | N-CA-C | 7.34 | 126.43 | 110.80 |
| 6 | B | 37 | ILE | N-CA-C | 7.33 | 120.14 | 108.85 |
| 2 | 2 | 105 | ALA | N-CA-C | 7.28 | 119.21 | 111.28 |
| 2 | 2 | 131 | THR | N-CA-C | -7.27 | 104.54 | 113.41 |
| 5 | A | 348 | GLU | N-CA-C | -7.25 | 102.17 | 111.02 |
| 2 | 2 | 174 | VAL | N-CA-C | 7.24 | 122.56 | 112.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | A | 485 | GLN | CA-C-N | 7.18 | 128.82 | 119.84 |
| 5 | A | 485 | GLN | C-N-CA | 7.18 | 128.82 | 119.84 |
| 5 | A | 595 | TRP | N-CA-C | -7.18 | 103.46 | 111.28 |
| 5 | A | 650 | ASN | N-CA-C | -7.17 | 104.15 | 113.12 |
| 11 | G | 27 | GLN | N-CA-C | 7.17 | 120.63 | 107.73 |
| 2 | 2 | 125 | PHE | N-CA-C | 7.07 | 125.44 | 109.81 |
| 6 | B | 260 | GLY | N-CA-C | 7.07 | 118.56 | 111.21 |
| 17 | N | 18 | ASP | N-CA-C | 7.07 | 119.59 | 111.11 |
| 4 | 4 | 79 | GLY | N-CA-C | 7.01 | 123.24 | 112.51 |
| 4 | 4 | 111 | ASN | CA-C-N | 6.98 | 128.56 | 119.84 |
| 4 | 4 | 111 | ASN | C-N-CA | 6.98 | 128.56 | 119.84 |
| 17 | N | 27 | ALA | N-CA-C | -6.96 | 95.98 | 110.80 |
| 5 | A | 626 | GLY | N-CA-C | -6.91 | 101.25 | 110.58 |
| 5 | A | 211 | LEU | N-CA-C | -6.91 | 102.82 | 111.11 |
| 12 | H | 39 | PHE | N-CA-C | -6.91 | 104.43 | 112.92 |
| 5 | A | 42 | ARG | N-CA-C | 6.88 | 121.91 | 112.90 |
| 4 | 4 | 75 | TRP | N-CA-C | 6.87 | 120.89 | 112.23 |
| 8 | D | 119 | TYR | CA-C-N | 6.84 | 128.39 | 119.84 |
| 8 | D | 119 | TYR | C-N-CA | 6.84 | 128.39 | 119.84 |
| 17 | N | 60 | PHE | CA-C-N | -6.83 | 108.49 | 121.54 |
| 17 | N | 60 | PHE | C-N-CA | -6.83 | 108.49 | 121.54 |
| 11 | G | 91 | ASN | N-CA-C | 6.82 | 125.33 | 110.80 |
| 4 | 4 | 149 | ALA | N-CA-C | 6.81 | 119.77 | 109.41 |
| 5 | A | 541 | VAL | N-CA-C | -6.80 | 103.89 | 110.42 |
| 10 | F | 121 | ILE | N-CA-C | 6.75 | 117.77 | 107.77 |
| 6 | B | 266 | GLN | N-CA-C | -6.74 | 101.05 | 110.35 |
| 12 | H | 22 | ASP | N-CA-C | 6.74 | 121.03 | 110.32 |
| 6 | B | 104 | PHE | N-CA-C | -6.71 | 96.51 | 110.80 |
| 6 | B | 358 | TYR | N-CA-C | 6.68 | 120.06 | 109.50 |
| 4 | 4 | 124 | TYR | N-CA-C | -6.67 | 96.60 | 110.80 |
| 16 | L | 102 | TYR | N-CA-C | -6.66 | 105.79 | 114.04 |
| 2 | 2 | 67 | PHE | N-CA-C | 6.65 | 119.35 | 111.71 |
| 5 | A | 698 | GLY | N-CA-C | -6.63 | 107.08 | 115.31 |
| 1 | 1 | 182 | ALA | O-C-N | -6.63 | 115.47 | 122.30 |
| 5 | A | 241 | GLU | N-CA-C | -6.61 | 105.52 | 112.93 |
| 8 | D | 92 | SER | N-CA-C | -6.58 | 102.65 | 110.41 |
| 5 | A | 683 | HIS | N-CA-C | -6.54 | 104.87 | 112.92 |
| 15 | K | 40 | LEU | O-C-N | -6.54 | 113.89 | 122.59 |
| 15 | K | 51 | ASP | CA-C-N | 6.52 | 127.99 | 119.84 |
| 15 | K | 51 | ASP | C-N-CA | 6.52 | 127.99 | 119.84 |
| 9 | E | 60 | LYS | N-CA-C | 6.50 | 124.65 | 110.80 |
| 8 | D | 77 | LEU | N-CA-C | 6.49 | 119.03 | 107.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | N | 3 | ILE | N-CA-C | 6.42 | 117.54 | 108.36 |
| 5 | A | 271 | THR | N-CA-C | -6.41 | 97.14 | 110.80 |
| 6 | B | 541 | ALA | N-CA-C | -6.41 | 105.43 | 113.18 |
| 12 | H | 42 | THR | N-CA-C | -6.40 | 105.22 | 113.16 |
| 6 | B | 435 | GLY | N-CA-C | -6.39 | 104.75 | 112.49 |
| 4 | 4 | 39 | TRP | CA-CB-CG | 6.39 | 125.74 | 113.60 |
| 3 | 3 | 122 | GLY | N-CA-C | -6.37 | 106.76 | 114.66 |
| 8 | D | 47 | VAL | N-CA-C | 6.33 | 116.17 | 108.06 |
| 15 | K | 39 | LYS | N-CA-C | 6.32 | 119.56 | 108.56 |
| 5 | A | 579 | PHE | CA-C-N | 6.31 | 127.73 | 119.84 |
| 5 | A | 579 | PHE | C-N-CA | 6.31 | 127.73 | 119.84 |
| 16 | L | 98 | CYS | N-CA-C | -6.30 | 104.51 | 111.82 |
| 4 | 4 | 109 | ILE | N-CA-C | 6.30 | 120.86 | 112.04 |
| 5 | A | 267 | THR | CA-C-N | 6.29 | 127.70 | 119.84 |
| 5 | A | 267 | THR | C-N-CA | 6.29 | 127.70 | 119.84 |
| 5 | A | 183 | TRP | N-CA-C | -6.28 | 104.35 | 111.14 |
| 9 | E | 36 | VAL | N-CA-C | 6.28 | 117.33 | 108.17 |
| 16 | L | 12 | GLN | CA-C-N | 6.25 | 127.65 | 119.84 |
| 16 | L | 12 | GLN | C-N-CA | 6.25 | 127.65 | 119.84 |
| 2 | 2 | 174 | VAL | CA-C-N | -6.22 | 112.71 | 122.73 |
| 2 | 2 | 174 | VAL | C-N-CA | -6.22 | 112.71 | 122.73 |
| 10 | F | 21 | ALA | N-CA-C | -6.21 | 97.58 | 110.80 |
| 11 | G | 17 | PHE | N-CA-C | 6.20 | 119.31 | 111.69 |
| 5 | A | 521 | VAL | N-CA-C | 6.19 | 122.21 | 109.34 |
| 5 | A | 343 | HIS | N-CA-C | -6.18 | 101.23 | 111.37 |
| 3 | 3 | 111 | TYR | N-CA-C | 6.14 | 123.87 | 110.80 |
| 4 | 4 | 145 | PRO | N-CA-C | -6.12 | 99.86 | 112.47 |
| 4 | 4 | 133 | TYR | N-CA-C | -6.11 | 102.36 | 109.93 |
| 2 | 2 | 132 | GLY | N-CA-C | 6.09 | 127.61 | 113.18 |
| 6 | B | 374 | HIS | N-CA-C | -6.08 | 104.93 | 113.20 |
| 6 | B | 93 | ASP | CA-C-N | 6.05 | 127.40 | 119.84 |
| 6 | B | 93 | ASP | C-N-CA | 6.05 | 127.40 | 119.84 |
| 11 | G | 30 | ASN | N-CA-C | 6.04 | 118.12 | 110.33 |
| 2 | 2 | 75 | ASN | N-CA-C | 6.03 | 123.64 | 110.80 |
| 3 | 3 | 182 | LYS | N-CA-C | -6.03 | 106.25 | 113.97 |
| 5 | A | 568 | LEU | N-CA-C | -6.02 | 105.17 | 113.18 |
| 5 | A | 681 | GLY | N-CA-C | -6.01 | 105.72 | 112.33 |
| 2 | 2 | 115 | ASN | N-CA-C | 6.00 | 123.07 | 109.81 |
| 8 | D | 80 | LYS | N-CA-C | 6.00 | 120.20 | 113.01 |
| 17 | N | 64 | ASP | N-CA-C | -5.96 | 98.11 | 110.80 |
| 5 | A | 277 | TYR | N-CA-C | 5.96 | 115.71 | 107.73 |
| 6 | B | 512 | ILE | N-CA-C | 5.92 | 121.66 | 109.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | B | 299 | HIS | N-CA-C | 5.90 | 118.82 | 109.50 |
| 3 | 3 | 76 | GLU | N-CA-C | -5.89 | 104.45 | 111.69 |
| 3 | 3 | 172 | ASP | N-CA-C | -5.88 | 98.27 | 110.80 |
| 5 | A | 597 | HIS | N-CA-C | -5.86 | 105.02 | 111.82 |
| 6 | B | 275 | HIS | N-CA-C | -5.85 | 104.81 | 111.07 |
| 11 | G | 12 | THR | N-CA-C | -5.85 | 103.88 | 111.02 |
| 6 | B | 372 | TYR | N-CA-C | -5.85 | 105.64 | 112.89 |
| 1 | 1 | 184 | PRO | N-CA-C | 5.84 | 124.50 | 112.47 |
| 6 | B | 395 | ILE | N-CA-C | 5.83 | 116.96 | 111.48 |
| 11 | G | 45 | GLU | CA-C-O | -5.78 | 114.75 | 120.82 |
| 8 | D | 123 | VAL | N-CA-C | 5.77 | 116.93 | 107.24 |
| 6 | B | 115 | ASN | N-CA-C | 5.76 | 123.07 | 110.80 |
| 9 | E | 65 | VAL | N-CA-C | 5.75 | 121.30 | 109.34 |
| 1 | 1 | 32 | VAL | N-CA-C | 5.75 | 121.30 | 108.88 |
| 6 | B | 124 | TRP | N-CA-C | -5.73 | 105.12 | 111.71 |
| 17 | N | 50 | GLN | CA-C-N | -5.73 | 110.60 | 121.54 |
| 17 | N | 50 | GLN | C-N-CA | -5.73 | 110.60 | 121.54 |
| 2 | 2 | 51 | HIS | N-CA-C | -5.71 | 106.31 | 113.28 |
| 5 | A | 440 | ASP | N-CA-C | -5.70 | 105.45 | 113.20 |
| 4 | 4 | 147 | LEU | N-CA-C | 5.70 | 122.94 | 110.80 |
| 5 | A | 111 | ASN | N-CA-C | -5.68 | 105.18 | 111.71 |
| 16 | L | 135 | GLY | N-CA-C | -5.67 | 99.75 | 113.18 |
| 7 | C | 21 | CYS | CA-C-N | 5.66 | 126.91 | 119.84 |
| 7 | C | 21 | CYS | C-N-CA | 5.66 | 126.91 | 119.84 |
| 3 | 3 | 112 | THR | O-C-N | 5.63 | 125.00 | 120.83 |
| 6 | B | 365 | PHE | N-CA-C | 5.62 | 122.78 | 110.80 |
| 4 | 4 | 152 | LYS | N-CA-C | -5.61 | 106.47 | 113.15 |
| 3 | 3 | 129 | PHE | N-CA-C | -5.59 | 105.89 | 114.16 |
| 8 | D | 50 | TRP | N-CA-C | 5.58 | 116.61 | 108.14 |
| 6 | B | 532 | LEU | N-CA-C | -5.57 | 105.31 | 111.71 |
| 4 | 4 | 146 | THR | CB-CA-C | 5.56 | 117.44 | 109.71 |
| 14 | J | 39 | PHE | CA-C-N | 5.56 | 125.53 | 120.03 |
| 14 | J | 39 | PHE | C-N-CA | 5.56 | 125.53 | 120.03 |
| 8 | D | 112 | LEU | N-CA-C | 5.56 | 117.14 | 111.14 |
| 16 | L | 39 | ASN | N-CA-C | -5.55 | 106.01 | 112.89 |
| 5 | A | 351 | THR | N-CA-C | -5.50 | 104.82 | 113.02 |
| 4 | 4 | 145 | PRO | CA-C-N | -5.50 | 112.98 | 121.56 |
| 4 | 4 | 145 | PRO | C-N-CA | -5.50 | 112.98 | 121.56 |
| 5 | A | 94 | SER | N-CA-C | -5.49 | 104.94 | 111.03 |
| 17 | N | 63 | ASP | N-CA-C | -5.49 | 99.12 | 110.80 |
| 3 | 3 | 114 | PHE | N-CA-C | -5.48 | 106.52 | 113.43 |
| 11 | G | 7 | VAL | N-CA-C | -5.47 | 105.76 | 110.74 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 2 | 175 | MET | CB-CA-C | 5.47 | 119.96 | 110.94 |
| 10 | F | 32 | TYR | N-CA-C | 5.47 | 122.44 | 110.80 |
| 6 | B | 105 | THR | N-CA-C | -5.46 | 99.17 | 110.80 |
| 5 | A | 380 | PRO | CA-C-N | 5.46 | 127.64 | 121.04 |
| 5 | A | 380 | PRO | C-N-CA | 5.46 | 127.64 | 121.04 |
| 6 | B | 80 | ASP | CA-C-N | 5.45 | 126.65 | 119.84 |
| 6 | B | 80 | ASP | C-N-CA | 5.45 | 126.65 | 119.84 |
| 6 | B | 596 | TRP | N-CA-C | -5.45 | 99.20 | 110.80 |
| 15 | K | 42 | ALA | N-CA-C | 5.44 | 117.96 | 108.76 |
| 16 | L | 109 | GLU | N-CA-C | 5.43 | 117.84 | 107.75 |
| 7 | C | 48 | CYS | N-CA-C | 5.42 | 117.66 | 109.41 |
| 12 | H | 47 | PHE | N-CA-C | -5.42 | 106.67 | 113.72 |
| 5 | A | 552 | THR | N-CA-C | -5.42 | 102.02 | 110.10 |
| 6 | B | 680 | TRP | N-CA-C | -5.42 | 107.04 | 113.97 |
| 4 | 4 | 36 | ASN | N-CA-C | 5.41 | 122.33 | 110.80 |
| 16 | L | 76 | ASN | N-CA-C | 5.39 | 122.29 | 110.80 |
| 11 | G | 10 | LEU | N-CA-C | 5.39 | 120.13 | 113.50 |
| 6 | B | 404 | ALA | N-CA-C | 5.38 | 117.47 | 110.53 |
| 4 | 4 | 146 | THR | N-CA-CB | 5.37 | 117.55 | 109.34 |
| 17 | N | 45 | ASN | N-CA-C | -5.36 | 105.84 | 112.38 |
| 2 | 2 | 100 | VAL | N-CA-CB | 5.36 | 116.70 | 110.65 |
| 6 | B | 114 | ASN | N-CA-C | 5.36 | 121.65 | 113.19 |
| 5 | A | 29 | THR | CB-CA-C | -5.35 | 99.09 | 109.68 |
| 10 | F | 99 | TRP | N-CA-C | -5.34 | 105.45 | 111.28 |
| 14 | J | 11 | ALA | CA-C-N | 5.34 | 126.52 | 119.84 |
| 14 | J | 11 | ALA | C-N-CA | 5.34 | 126.52 | 119.84 |
| 17 | N | 30 | ALA | N-CA-C | -5.34 | 106.53 | 112.57 |
| 5 | A | 717 | ALA | N-CA-C | 5.34 | 121.60 | 109.81 |
| 6 | B | 513 | GLY | CA-C-N | 5.29 | 126.46 | 119.84 |
| 6 | B | 513 | GLY | C-N-CA | 5.29 | 126.46 | 119.84 |
| 12 | H | 52 | LEU | N-CA-C | 5.29 | 122.08 | 110.80 |
| 17 | N | 84 | LYS | CA-C-N | -5.29 | 112.17 | 121.70 |
| 17 | N | 84 | LYS | C-N-CA | -5.29 | 112.17 | 121.70 |
| 15 | K | 46 | GLY | N-CA-C | -5.29 | 100.65 | 113.18 |
| 16 | L | 110 | GLY | N-CA-C | 5.28 | 118.98 | 111.12 |
| 6 | B | 27 | THR | N-CA-C | -5.27 | 106.75 | 114.39 |
| 5 | A | 435 | VAL | N-CA-CB | 5.26 | 116.35 | 110.51 |
| 8 | D | 68 | MET | N-CA-C | 5.25 | 121.99 | 110.80 |
| 12 | H | 63 | SER | N-CA-C | -5.24 | 106.92 | 113.72 |
| 5 | A | 225 | VAL | N-CA-C | 5.23 | 120.22 | 109.34 |
| 4 | 4 | 93 | ILE | N-CA-C | 5.22 | 120.19 | 109.34 |
| 5 | A | 270 | PHE | N-CA-C | 5.21 | 117.30 | 108.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | A | 523 | VAL | N-CA-C | 5.21 | 120.18 | 109.34 |
| 7 | C | 75 | ARG | N-CA-C | -5.21 | 105.57 | 112.34 |
| 6 | B | 195 | VAL | N-CA-C | 5.20 | 115.87 | 110.82 |
| 11 | G | 9 | SER | N-CA-C | -5.20 | 105.50 | 111.07 |
| 8 | D | 141 | VAL | N-CA-C | -5.20 | 104.47 | 111.44 |
| 5 | A | 522 | ALA | N-CA-C | 5.17 | 117.74 | 108.17 |
| 13 | I | 26 | LEU | N-CA-C | -5.17 | 106.82 | 113.23 |
| 5 | A | 47 | GLY | CA-C-N | 5.17 | 126.30 | 119.84 |
| 5 | A | 47 | GLY | C-N-CA | 5.17 | 126.30 | 119.84 |
| 4 | 4 | 171 | ASN | N-CA-C | -5.15 | 99.83 | 110.80 |
| 8 | D | 45 | PHE | N-CA-C | 5.14 | 119.01 | 112.12 |
| 6 | B | 483 | GLY | CA-C-N | -5.13 | 114.51 | 119.90 |
| 6 | B | 483 | GLY | C-N-CA | -5.13 | 114.51 | 119.90 |
| 10 | F | 62 | LEU | N-CA-C | 5.13 | 116.68 | 111.14 |
| 5 | A | 489 | ALA | N-CA-C | 5.12 | 121.70 | 110.80 |
| 12 | H | 75 | ASP | N-CA-C | 5.11 | 121.69 | 110.80 |
| 6 | B | 466 | ALA | N-CA-C | -5.11 | 104.22 | 110.61 |
| 11 | G | 12 | THR | CA-C-N | 5.11 | 125.77 | 119.99 |
| 11 | G | 12 | THR | C-N-CA | 5.11 | 125.77 | 119.99 |
| 2 | 2 | 37 | ASP | N-CA-C | 5.10 | 121.09 | 109.81 |
| 5 | A | 231 | GLN | N-CA-C | -5.10 | 105.42 | 111.69 |
| 3 | 3 | 111 | TYR | CA-CB-CG | 5.09 | 123.06 | 113.90 |
| 6 | B | 628 | SER | N-CA-C | -5.08 | 99.97 | 110.80 |
| 5 | A | 430 | ASP | N-CA-C | 5.07 | 114.73 | 108.19 |
| 8 | D | 98 | TYR | N-CA-C | -5.07 | 100.81 | 108.46 |
| 5 | A | 233 | LEU | N-CA-C | -5.07 | 106.79 | 113.12 |
| 1 | 1 | 183 | ASP | CA-C-N | 5.06 | 126.16 | 119.84 |
| 1 | 1 | 183 | ASP | C-N-CA | 5.06 | 126.16 | 119.84 |
| 6 | B | 476 | ILE | CA-C-N | 5.05 | 126.15 | 119.84 |
| 6 | B | 476 | ILE | C-N-CA | 5.05 | 126.15 | 119.84 |
| 5 | A | 684 | PHE | N-CA-C | -5.05 | 106.26 | 112.72 |
| 8 | D | 56 | GLN | N-CA-C | 5.05 | 117.67 | 109.24 |
| 10 | F | 134 | PHE | N-CA-C | -5.05 | 105.97 | 111.82 |
| 16 | L | 105 | ALA | N-CA-C | -5.04 | 106.81 | 113.17 |
| 17 | N | 62 | SER | N-CA-C | -5.03 | 100.09 | 110.80 |
| 4 | 4 | 174 | GLY | N-CA-C | 5.02 | 116.82 | 110.20 |
| 2 | 2 | 81 | THR | N-CA-C | -5.00 | 100.15 | 110.80 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 11 | G | 21 | PHE | CA |

All (169) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | 1 | 184 | PRO | Peptide |
| 1 | 1 | 185 | TRP | Peptide |
| 1 | 1 | 72 | GLN | Peptide |
| 2 | 2 | 111 | ALA | Peptide |
| 2 | 2 | 112 | ASP | Peptide |
| 2 | 2 | 120 | ASN | Peptide |
| 2 | 2 | 126 | PRO | Peptide |
| 2 | 2 | 131 | THR | Peptide |
| 2 | 2 | 144 | ASP | Peptide |
| 2 | 2 | 194 | ALA | Peptide |
| 2 | 2 | 197 | LEU | Peptide |
| 2 | 2 | 209 | THR | Peptide |
| 2 | 2 | 42 | ARG | Peptide |
| 2 | 2 | 73 | ILE | Peptide |
| 2 | 2 | 74 | LEU | Peptide |
| 2 | 2 | 75 | ASN | Peptide |
| 2 | 2 | 80 | TYR | Peptide |
| 2 | 2 | 84 | GLU | Peptide |
| 2 | 2 | 92 | THR | Peptide |
| 2 | 2 | 99 | LEU | Peptide |
| 3 | 3 | 104 | TYR | Peptide |
| 3 | 3 | 105 | ASN | Peptide |
| 3 | 3 | 106 | TYR | Peptide |
| 3 | 3 | 107 | TRP | Peptide |
| 3 | 3 | 109 | ASP | Peptide |
| 3 | 3 | 111 | TYR | Peptide |
| 3 | 3 | 112 | THR | Peptide |
| 3 | 3 | 155 | GLU | Peptide |
| 3 | 3 | 159 | PRO | Peptide |
| 3 | 3 | 169 | PHE | Peptide |
| 3 | 3 | 172 | ASP | Peptide |
| 3 | 3 | 180 | LYS | Peptide |
| 3 | 3 | 49 | ILE | Peptide |
| 3 | 3 | 92 | TRP | Peptide |
| 3 | 3 | 93 | PHE | Peptide |
| 3 | 3 | 95 | THR | Peptide |
| 3 | 3 | 96 | GLY | Peptide |
| 4 | 4 | 143 | PHE | Peptide |
| 4 | 4 | 146 | THR | Peptide |
| 4 | 4 | 152 | LYS | Peptide |
| 4 | 4 | 190 | HIS | Peptide |
| 4 | 4 | 192 | THR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 4 | 4 | 194 | VAL | Peptide |
| 4 | 4 | 34 | PRO | Peptide |
| 4 | 4 | 35 | GLU | Peptide |
| 4 | 4 | 36 | ASN | Peptide |
| 4 | 4 | 37 | LEU | Peptide |
| 4 | 4 | 38 | ARG | Peptide |
| 4 | 4 | 63 | VAL | Peptide |
| 4 | 4 | 65 | THR | Peptide |
| 4 | 4 | 68 | GLY | Peptide |
| 4 | 4 | 74 | LYS | Peptide |
| 4 | 4 | 83 | TYR | Peptide |
| 4 | 4 | 87 | SER | Peptide |
| 4 | 4 | 88 | SER | Peptide |
| 4 | 4 | 89 | THR | Peptide |
| 4 | 4 | 90 | LEU | Peptide |
| 5 | A | 103 | PHE | Peptide |
| 5 | A | 117 | GLY | Peptide |
| 5 | A | 123 | VAL | Peptide |
| 5 | A | 197 | GLN | Peptide |
| 5 | A | 21 | LEU | Peptide |
| 5 | A | 23 | ASP | Peptide |
| 5 | A | 240 | LYS | Peptide |
| 5 | A | 242 | ILE | Peptide |
| 5 | A | 26 | PRO | Peptide |
| 5 | A | 27 | ILE | Peptide |
| 5 | A | 28 | LYS | Peptide |
| 5 | A | 29 | THR | Peptide |
| 5 | A | 316 | MET | Peptide |
| 5 | A | 347 | TYR | Peptide |
| 5 | A | 393 | LEU | Peptide |
| 5 | A | 41 | SER | Peptide |
| 5 | A | 427 | ARG | Peptide |
| 5 | A | 45 | ALA | Peptide |
| 5 | A | 55 | TRP | Peptide |
| 5 | A | 67 | HIS | Peptide |
| 6 | B | 103 | ALA | Peptide |
| 6 | B | 104 | PHE | Peptide |
| 6 | B | 232 | LEU | Peptide |
| 6 | B | 265 | THR | Peptide |
| 6 | B | 304 | ILE | Peptide |
| 6 | B | 362 | ALA | Peptide |
| 6 | B | 377 | TYR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 6 | B | 481 | THR | Peptide |
| 6 | B | 510 | LEU | Peptide |
| 6 | B | 563 | GLY | Peptide |
| 6 | B | 595 | HIS | Peptide |
| 6 | B | 622 | ASP | Peptide |
| 7 | C | 79 | LEU | Peptide |
| 8 | D | 90 | LEU | Peptide |
| 9 | E | 86 | GLU | Peptide |
| 9 | E | 88 | GLU | Peptide |
| 9 | E | 91 | ALA | Peptide |
| 10 | F | 136 | TRP | Peptide |
| 10 | F | 20 | GLN | Peptide |
| 10 | F | 24 | LYS | Peptide |
| 10 | F | 31 | LEU | Peptide |
| 10 | F | 41 | ALA | Peptide |
| 10 | F | 51 | LYS | Peptide |
| 10 | F | 56 | TYR | Peptide |
| 11 | G | 15 | SER | Peptide |
| 11 | G | 22 | VAL | Peptide |
| 11 | G | 26 | PHE | Peptide |
| 11 | G | 36 | PRO | Peptide |
| 11 | G | 39 | ASN | Peptide |
| 11 | G | 43 | HIS | Peptide |
| 11 | G | 45 | GLU | Mainchain |
| 11 | G | 48 | ASP | Peptide |
| 11 | G | 49 | THR | Peptide |
| 11 | G | 50 | ARG | Peptide |
| 11 | G | 90 | SER | Peptide |
| 11 | G | 93 | TYR | Peptide |
| 11 | G | 94 | ASP | Peptide |
| 12 | H | 12 | GLU | Peptide |
| 12 | H | 20 | GLN | Peptide |
| 12 | H | 21 | TRP | Peptide |
| 12 | H | 22 | ASP | Peptide |
| 12 | H | 24 | TYR | Peptide |
| 12 | H | 25 | GLY | Peptide |
| 12 | H | 27 | ASP | Peptide |
| 12 | H | 43 | PHE | Peptide |
| 12 | H | 48 | THR | Peptide |
| 15 | K | 41 | GLU | Peptide |
| 15 | K | 43 | ARG | Peptide |
| 15 | K | 44 | GLU | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 15 | K | 45 | SER | Peptide |
| 15 | K | 46 | GLY | Peptide |
| 15 | K | 47 | LEU | Peptide |
| 16 | L | 160 | VAL | Peptide |
| 16 | L | 165 | TYR | Peptide |
| 17 | N | 12 | THR | Peptide |
| 17 | N | 15 | GLU | Peptide |
| 17 | N | 23 | ALA | Peptide |
| 17 | N | 26 | GLY | Peptide |
| 17 | N | 28 | ASN | Peptide |
| 17 | N | 29 | PHE | Peptide |
| 17 | N | 30 | ALA | Peptide |
| 17 | N | 32 | ALA | Peptide |
| 17 | N | 44 | GLU | Peptide |
| 17 | N | 46 | PHE | Peptide |
| 17 | N | 48 | GLY | Peptide |
| 17 | N | 50 | GLN | Peptide |
| 17 | N | 52 | LEU | Peptide |
| 17 | N | 54 | LYS | Peptide |
| 17 | N | 60 | PHE | Peptide |
| 17 | N | 63 | ASP | Peptide |
| 17 | N | 67 | LEU | Peptide |
| 17 | N | 7 | LEU | Peptide |
| 17 | N | 70 | GLU | Peptide |
| 17 | N | 75 | TYR | Peptide |
| 17 | N | 79 | SER | Peptide |
| 17 | N | 84 | LYS | Peptide |
| 18 | R | 28 | UNK | Peptide |
| 18 | R | 31 | UNK | Peptide |
| 18 | R | 32 | UNK | Peptide |
| 18 | R | 33 | UNK | Peptide |
| 18 | R | 34 | UNK | Peptide |
| 18 | R | 35 | UNK | Peptide |
| 18 | R | 36 | UNK | Peptide |
| 18 | R | 37 | UNK | Peptide |
| 18 | R | 40 | UNK | Peptide |
| 18 | R | 41 | UNK | Peptide |
| 18 | R | 42 | UNK | Peptide |
| 18 | R | 45 | UNK | Peptide |
| 18 | R | 46 | UNK | Peptide |
| 18 | R | 48 | UNK | Peptide |
| 18 | R | 51 | UNK | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 18 | R | 7 | UNK | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 1 | 1264 | 0 | 1229 | 143 | 3 |
| 2 | 2 | 1374 | 0 | 1331 | 304 | 2 |
| 3 | 3 | 1186 | 0 | 1147 | 303 | 16 |
| 4 | 4 | 1319 | 0 | 1282 | 628 | 5 |
| 5 | A | 5745 | 0 | 5597 | 1401 | 0 |
| 6 | B | 5848 | 0 | 5655 | 1231 | 15 |
| 7 | C | 619 | 0 | 608 | 206 | 0 |
| 8 | D | 1095 | 0 | 1112 | 193 | 0 |
| 9 | E | 520 | 0 | 528 | 129 | 0 |
| 10 | F | 1221 | 0 | 1249 | 214 | 0 |
| 11 | G | 740 | 0 | 708 | 199 | 1 |
| 12 | H | 529 | 0 | 514 | 108 | 0 |
| 13 | I | 229 | 0 | 252 | 56 | 0 |
| 14 | J | 338 | 0 | 340 | 64 | 0 |
| 15 | K | 593 | 0 | 619 | 111 | 0 |
| 16 | L | 1215 | 0 | 1222 | 317 | 5 |
| 17 | N | 685 | 0 | 668 | 330 | 1 |
| 18 | R | 265 | 0 | 68 | 78 | 0 |
| 19 | M | 23 | 0 | 21 | 0 | 0 |
| 19 | O | 22 | 0 | 18 | 10 | 0 |
| 19 | P | 23 | 0 | 21 | 10 | 0 |
| 19 | Q | 23 | 0 | 21 | 6 | 0 |
| 19 | S | 23 | 0 | 21 | 1 | 0 |
| 19 | T | 23 | 0 | 21 | 2 | 0 |
| 19 | U | 23 | 0 | 21 | 1 | 0 |
| 19 | V | 23 | 0 | 21 | 4 | 0 |
| 19 | W | 23 | 0 | 21 | 3 | 0 |
| 19 | X | 22 | 0 | 18 | 3 | 0 |
| 19 | Y | 23 | 0 | 21 | 1 | 28 |
| 19 | Z | 23 | 0 | 21 | 14 | 0 |
| 19 | a | 23 | 0 | 21 | 1 | 0 |
| 20 | 1 | 617 | 0 | 388 | 89 | 1 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 20 | 2 | 650 | 0 | 465 | 142 | 0 |
| 20 | 3 | 620 | 0 | 362 | 70 | 0 |
| 20 | 4 | 694 | 0 | 443 | 168 | 0 |
| 20 | A | 2346 | 0 | 2062 | 697 | 0 |
| 20 | B | 2226 | 0 | 2061 | 666 | 0 |
| 20 | F | 180 | 0 | 123 | 47 | 0 |
| 20 | G | 51 | 0 | 40 | 4 | 0 |
| 20 | H | 273 | 0 | 235 | 58 | 0 |
| 20 | I | 60 | 0 | 58 | 11 | 0 |
| 20 | J | 109 | 0 | 95 | 26 | 0 |
| 20 | K | 202 | 0 | 158 | 51 | 1 |
| 20 | L | 332 | 0 | 297 | 94 | 0 |
| 20 | R | 122 | 0 | 123 | 14 | 0 |
| 21 | 1 | 105 | 0 | 137 | 32 | 0 |
| 21 | 2 | 175 | 0 | 230 | 45 | 0 |
| 21 | 3 | 70 | 0 | 92 | 16 | 0 |
| 21 | 4 | 139 | 0 | 179 | 24 | 3 |
| 21 | A | 245 | 0 | 322 | 53 | 0 |
| 21 | B | 95 | 0 | 115 | 11 | 0 |
| 21 | C | 35 | 0 | 46 | 0 | 0 |
| 21 | D | 35 | 0 | 46 | 3 | 0 |
| 21 | E | 35 | 0 | 46 | 11 | 0 |
| 21 | F | 34 | 0 | 41 | 8 | 0 |
| 21 | G | 105 | 0 | 138 | 27 | 28 |
| 21 | H | 140 | 0 | 184 | 42 | 0 |
| 21 | K | 105 | 0 | 138 | 40 | 0 |
| 21 | L | 105 | 0 | 138 | 2 | 0 |
| 21 | R | 245 | 0 | 322 | 43 | 3 |
| 22 | 2 | 40 | 0 | 54 | 9 | 0 |
| 22 | A | 120 | 0 | 162 | 103 | 0 |
| 22 | B | 200 | 0 | 270 | 117 | 0 |
| 22 | F | 80 | 0 | 108 | 61 | 0 |
| 22 | G | 40 | 0 | 54 | 4 | 0 |
| 22 | I | 79 | 0 | 105 | 44 | 0 |
| 22 | J | 40 | 0 | 54 | 34 | 0 |
| 22 | L | 40 | 0 | 54 | 36 | 0 |
| 23 | A | 33 | 0 | 46 | 7 | 0 |
| 23 | B | 33 | 0 | 46 | 27 | 0 |
| 24 | A | 8 | 0 | 0 | 18 | 0 |
| 24 | C | 16 | 0 | 0 | 5 | 0 |
| 25 | B | 49 | 0 | 71 | 16 | 0 |
| 26 | H | 23 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 36033 | 0 | 34504 | 7467 | 56 |

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 106.

All (7467) 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) |
|---|---|---|---|
| 4:4:160:MET:CE | 20:4:306:CLA:HBB2 | 1.18 | 1.65 |
| 4:4:69:ILE:HD11 | 4:4:175:LYS:CB | 1.26 | 1.65 |
| 3:3:97:PHE:CD2 | 3:3:98:ILE:HG23 | 1.33 | 1.62 |
| 1:1:185:TRP:CH2 | 20:1:213:CLA:H12 | 1.38 | 1.59 |
| 3:3:132:TRP:CH2 | 3:3:155:GLU:CD | 1.76 | 1.58 |
| 3:3:97:PHE:CE2 | 3:3:98:ILE:HD13 | 1.42 | 1.55 |
| 17:N:41:LYS:CG | 17:N:42:PHE:HB3 | 1.31 | 1.55 |
| 3:3:132:TRP:CZ3 | 3:3:155:GLU:HG2 | 1.37 | 1.55 |
| 17:N:45:ASN:HD22 | 17:N:54:LYS:CG | 1.21 | 1.52 |
| 7:C:5:VAL:CG2 | 7:C:65:VAL:HG13 | 1.35 | 1.51 |
| 17:N:45:ASN:CB | 17:N:57:LYS:NZ | 1.71 | 1.51 |
| 3:3:92:TRP:HA | 3:3:95:THR:CG2 | 1.33 | 1.51 |
| 22:B:801:BCR:C33 | 20:L:207:CLA:C4B | 1.86 | 1.49 |
| 20:A:803:CLA:HBB2 | 20:A:804:CLA:C3C | 1.41 | 1.49 |
| 3:3:132:TRP:CZ3 | 3:3:155:GLU:CG | 1.91 | 1.48 |
| 1:1:185:TRP:CH2 | 20:1:213:CLA:C1 | 1.97 | 1.45 |
| 11:G:37:GLU:CD | 11:G:42:SER:HB3 | 1.39 | 1.45 |
| 7:C:5:VAL:HG21 | 7:C:65:VAL:CG1 | 1.44 | 1.45 |
| 3:3:80:LYS:HZ1 | 3:3:92:TRP:CD1 | 1.36 | 1.44 |
| 17:N:45:ASN:HB3 | 17:N:57:LYS:NZ | 1.18 | 1.43 |
| 22:B:801:BCR:H333 | 20:L:207:CLA:C4B | 1.42 | 1.43 |
| 4:4:160:MET:SD | 20:4:306:CLA:HBB2 | 1.55 | 1.43 |
| 5:A:27:ILE:HG22 | 5:A:28:LYS:CG | 1.50 | 1.42 |
| 17:N:72:LYS:CG | 17:N:74:LYS:HG3 | 1.50 | 1.42 |
| 1:1:183:ASP:CG | 1:1:184:PRO:HD2 | 1.45 | 1.41 |
| 6:B:732:LYS:HB3 | 6:B:733:PHE:CA | 1.47 | 1.41 |
| 4:4:37:LEU:C | 4:4:39:TRP:HB3 | 1.43 | 1.40 |
| 3:3:132:TRP:CH2 | 3:3:155:GLU:OE2 | 1.68 | 1.39 |
| 20:A:803:CLA:HBB2 | 20:A:804:CLA:C2C | 1.49 | 1.39 |
| 11:G:37:GLU:OE2 | 11:G:42:SER:CB | 1.70 | 1.39 |
| 16:L:163:LEU:CG | 16:L:164:PRO:HD3 | 1.51 | 1.39 |
| 4:4:106:TRP:CD1 | 20:4:301:CLA:HED3 | 1.58 | 1.38 |
| 20:A:822:CLA:C4C | 22:A:844:BCR:H19C | 1.52 | 1.38 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:L:164:PRO:HG3 | 16:L:165:TYR:CE1 | 1.57 | 1.37 |
| 1:1:185:TRP:CZ3 | 20:1:213:CLA:H12 | 1.59 | 1.36 |
| 11:G:94:ASP:H | 11:G:95:PRO:CD | 1.34 | 1.36 |
| 4:4:160:MET:CE | 20:4:306:CLA:CBB | 2.01 | 1.35 |
| 6:B:403:ASN:O | 6:B:406:ASN:HB3 | 1.22 | 1.35 |
| 4:4:95:PHE:CE2 | 20:4:314:CLA:C3C | 2.10 | 1.34 |
| 4:4:106:TRP:NE1 | 20:4:301:CLA:HED3 | 1.38 | 1.34 |
| 23:B:843:PQN:H162 | 22:B:847:BCR:C33 | 1.57 | 1.34 |
| 1:1:27:LEU:HD11 | 6:B:314:ARG:CZ | 1.54 | 1.33 |
| 9:E:40:ARG:CZ | 9:E:86:GLU:OE1 | 1.75 | 1.33 |
| 16:L:164:PRO:HA | 16:L:165:TYR:CG | 1.61 | 1.33 |
| 3:3:94:ARG:NH2 | 3:3:98:ILE:HG21 | 1.42 | 1.32 |
| 20:B:813:CLA:HAC2 | 20:B:814:CLA:CBB | 1.60 | 1.32 |
| 7:C:14:CYS:HA | 7:C:17:CYS:SG | 1.68 | 1.31 |
| 11:G:44:PHE:C | 11:G:47:GLY:HA3 | 1.53 | 1.31 |
| 17:N:61:LEU:HD11 | 17:N:63:ASP:O | 1.18 | 1.31 |
| 18:R:39:UNK:HA | 18:R:42:UNK:CB | 1.59 | 1.31 |
| 3:3:132:TRP:CZ3 | 3:3:155:GLU:CD | 2.06 | 1.31 |
| 4:4:122:LYS:HB2 | 4:4:143:PHE:CD2 | 1.65 | 1.31 |
| 15:K:79:LYS:HE3 | 15:K:84:LEU:O | 1.21 | 1.31 |
| 17:N:45:ASN:HD22 | 17:N:54:LYS:CD | 1.42 | 1.31 |
| 11:G:37:GLU:CD | 11:G:42:SER:CB | 2.03 | 1.31 |
| 17:N:72:LYS:CB | 17:N:73:ASP:HA | 1.49 | 1.31 |
| 4:4:102:GLU:OE2 | 20:4:313:CLA:C3B | 1.78 | 1.30 |
| 4:4:95:PHE:HE2 | 20:4:314:CLA:C3C | 1.41 | 1.30 |
| 4:4:106:TRP:CE2 | 20:4:301:CLA:HED3 | 1.65 | 1.30 |
| 4:4:128:ALA:HB2 | 4:4:143:PHE:CE2 | 1.65 | 1.30 |
| 17:N:62:SER:HB3 | 17:N:66:ASP:CB | 1.60 | 1.30 |
| 20:A:825:CLA:HBB2 | 20:A:832:CLA:CMA | 1.60 | 1.30 |
| 3:3:97:PHE:HE2 | 3:3:98:ILE:CD1 | 1.42 | 1.29 |
| 3:3:94:ARG:HG3 | 3:3:97:PHE:CZ | 1.67 | 1.29 |
| 4:4:69:ILE:HD11 | 4:4:175:LYS:CG | 1.61 | 1.29 |
| 4:4:122:LYS:CD | 4:4:150:LYS:HD3 | 1.61 | 1.29 |
| 23:B:843:PQN:C19 | 22:B:847:BCR:H10C | 1.62 | 1.28 |
| 11:G:44:PHE:O | 11:G:47:GLY:HA3 | 1.32 | 1.28 |
| 11:G:94:ASP:N | 11:G:95:PRO:HD3 | 1.48 | 1.28 |
| 16:L:163:LEU:HD12 | 16:L:164:PRO:CD | 1.62 | 1.28 |
| 17:N:58:VAL:HB | 17:N:59:PRO:CD | 1.63 | 1.27 |
| 16:L:164:PRO:HA | 16:L:165:TYR:CB | 1.39 | 1.26 |
| 4:4:36:ASN:O | 4:4:39:TRP:HB2 | 1.25 | 1.26 |
| 5:A:331:LEU:HD21 | 5:A:343:HIS:O | 1.11 | 1.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:80:LYS:NZ | 3:3:92:TRP:CD1 | 2.03 | 1.26 |
| 4:4:160:MET:HE3 | 20:4:306:CLA:CBB | 1.60 | 1.26 |
| 15:K:44:GLU:CG | 15:K:45:SER:HA | 1.64 | 1.26 |
| 17:N:6:TYR:O | 17:N:8:GLU:N | 1.66 | 1.26 |
| 17:N:72:LYS:HB3 | 17:N:73:ASP:CA | 1.65 | 1.26 |
| 3:3:132:TRP:CH2 | 3:3:155:GLU:CG | 2.12 | 1.26 |
| 17:N:72:LYS:HE2 | 17:N:74:LYS:CE | 1.66 | 1.26 |
| 3:3:94:ARG:CA | 3:3:97:PHE:HE1 | 1.49 | 1.25 |
| 5:A:27:ILE:C | 5:A:28:LYS:HG2 | 1.48 | 1.25 |
| 7:C:1:MET:N | 7:C:4:SER:HB3 | 1.50 | 1.25 |
| 4:4:124:TYR:O | 4:4:127:PRO:HD2 | 1.32 | 1.24 |
| 6:B:25:ILE:HG21 | 22:L:209:BCR:C29 | 1.66 | 1.24 |
| 5:A:567:ARG:NH1 | 8:D:35:GLY:HA2 | 1.51 | 1.24 |
| 12:H:69:SER:OG | 20:H:108:CLA:H2 | 1.27 | 1.24 |
| 16:L:164:PRO:HG3 | 16:L:165:TYR:CD1 | 1.71 | 1.24 |
| 20:A:838:CLA:H141 | 22:A:845:BCR:C2 | 1.67 | 1.23 |
| 4:4:36:ASN:HB2 | 4:4:39:TRP:CE3 | 1.71 | 1.23 |
| 17:N:72:LYS:CE | 17:N:74:LYS:HE2 | 1.69 | 1.23 |
| 11:G:45:GLU:O | 11:G:49:THR:HG23 | 1.32 | 1.23 |
| 15:K:44:GLU:HG3 | 15:K:45:SER:CA | 1.67 | 1.23 |
| 3:3:97:PHE:CE2 | 3:3:98:ILE:HG23 | 1.74 | 1.23 |
| 4:4:40:PHE:HB3 | 4:4:43:ALA:CB | 1.69 | 1.23 |
| 16:L:164:PRO:CB | 16:L:165:TYR:HD1 | 1.50 | 1.23 |
| 17:N:45:ASN:ND2 | 17:N:54:LYS:CG | 2.01 | 1.23 |
| 4:4:94:GLU:HG2 | 4:4:95:PHE:CD1 | 1.74 | 1.22 |
| 20:4:310:CLA:HBA2 | 20:4:310:CLA:CGD | 1.68 | 1.22 |
| 5:A:744:ALA:CB | 22:A:845:BCR:H391 | 1.69 | 1.22 |
| 7:C:5:VAL:CB | 7:C:65:VAL:HG13 | 1.69 | 1.22 |
| 4:4:36:ASN:HB2 | 4:4:39:TRP:CZ3 | 1.73 | 1.22 |
| 4:4:174:GLY:O | 4:4:175:LYS:HG3 | 1.37 | 1.22 |
| 17:N:61:LEU:HD11 | 17:N:63:ASP:C | 1.64 | 1.22 |
| 5:A:27:ILE:CG2 | 5:A:28:LYS:HD3 | 1.68 | 1.22 |
| 1:1:112:ARG:HH12 | 20:1:210:CLA:CGD | 1.52 | 1.22 |
| 7:C:5:VAL:CG2 | 7:C:65:VAL:CG1 | 2.04 | 1.22 |
| 22:B:801:BCR:C33 | 20:L:207:CLA:CHC | 2.18 | 1.21 |
| 5:A:24:ARG:NH1 | 5:A:29:THR:HB | 1.54 | 1.21 |
| 20:A:819:CLA:CMD | 20:A:821:CLA:HBB2 | 1.71 | 1.21 |
| 17:N:72:LYS:HE2 | 17:N:74:LYS:CG | 1.68 | 1.21 |
| 3:3:48:PHE:CD2 | 3:3:49:ILE:HG22 | 1.74 | 1.20 |
| 4:4:36:ASN:C | 4:4:39:TRP:HB2 | 1.65 | 1.20 |
| 4:4:39:TRP:C | 4:4:40:PHE:HD1 | 1.48 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:B:835:CLA:CMB | 22:B:846:BCR:H292 | 1.70 | 1.20 |
| 3:3:94:ARG:HD2 | 3:3:97:PHE:CE1 | 1.77 | 1.20 |
| 3:3:132:TRP:HH2 | 3:3:155:GLU:CD | 1.21 | 1.20 |
| 3:3:205:GLY:N | 5:A:252:ARG:HH22 | 1.38 | 1.20 |
| 5:A:331:LEU:CD2 | 5:A:343:HIS:O | 1.90 | 1.20 |
| 20:A:825:CLA:CBB | 20:A:832:CLA:CMA | 2.20 | 1.20 |
| 17:N:45:ASN:CB | 17:N:54:LYS:HG2 | 1.69 | 1.20 |
| 20:2:307:CLA:CBB | 20:2:307:CLA:H71 | 1.71 | 1.19 |
| 3:3:110:SER:C | 3:3:111:TYR:HD2 | 1.49 | 1.19 |
| 20:B:813:CLA:CAC | 20:B:814:CLA:HBB2 | 1.70 | 1.19 |
| 12:H:69:SER:HB2 | 20:H:108:CLA:H61 | 1.25 | 1.19 |
| 4:4:107:GLN:C | 20:4:301:CLA:CMA | 2.16 | 1.19 |
| 4:4:192:THR:CG2 | 4:4:195:GLN:H | 1.55 | 1.19 |
| 1:1:27:LEU:HD11 | 6:B:314:ARG:NH1 | 1.58 | 1.19 |
| 5:A:25:ASP:HB2 | 5:A:26:PRO:CA | 1.71 | 1.19 |
| 3:3:74:ALA:HA | 20:3:306:CLA:C3D | 1.73 | 1.18 |
| 4:4:69:ILE:CD1 | 4:4:175:LYS:CB | 2.21 | 1.18 |
| 4:4:121:PHE:O | 4:4:122:LYS:HD2 | 1.39 | 1.18 |
| 7:C:54:CYS:HB2 | 24:C:102:SF4:S1 | 1.83 | 1.18 |
| 20:A:839:CLA:CMA | 20:A:839:CLA:HBA1 | 1.70 | 1.18 |
| 6:B:732:LYS:HB3 | 6:B:733:PHE:C | 1.68 | 1.18 |
| 20:A:818:CLA:H121 | 20:A:818:CLA:HBB2 | 1.26 | 1.18 |
| 12:H:73:PRO:HD3 | 19:Z:2:FRU:C6 | 1.73 | 1.18 |
| 17:N:72:LYS:HB3 | 17:N:74:LYS:N | 1.59 | 1.18 |
| 2:2:102:ILE:C | 20:2:310:CLA:HBB2 | 1.67 | 1.18 |
| 3:3:94:ARG:HA | 3:3:97:PHE:CE1 | 1.77 | 1.18 |
| 17:N:41:LYS:CD | 17:N:42:PHE:HB3 | 1.74 | 1.18 |
| 20:B:826:CLA:HBB2 | 20:B:839:CLA:CMB | 1.73 | 1.17 |
| 5:A:744:ALA:HB2 | 22:A:845:BCR:C39 | 1.75 | 1.17 |
| 6:B:493:TRP:CE2 | 20:B:835:CLA:O1A | 1.96 | 1.17 |
| 20:B:806:CLA:H191 | 10:F:104:TYR:HB3 | 1.18 | 1.17 |
| 20:2:303:CLA:HBC3 | 20:2:303:CLA:HHD | 1.24 | 1.17 |
| 5:A:25:ASP:HB2 | 5:A:26:PRO:HA | 1.24 | 1.17 |
| 1:1:24:PHE:HB3 | 6:B:314:ARG:NH2 | 1.60 | 1.17 |
| 17:N:45:ASN:ND2 | 17:N:53:ALA:O | 1.78 | 1.16 |
| 3:3:132:TRP:HH2 | 3:3:155:GLU:OE2 | 0.82 | 1.16 |
| 4:4:69:ILE:HD11 | 4:4:175:LYS:HB2 | 1.28 | 1.16 |
| 21:A:853:LMU:H81 | 21:A:853:LMU:C2 | 1.74 | 1.16 |
| 6:B:25:ILE:CG2 | 22:L:209:BCR:H292 | 1.75 | 1.16 |
| 20:B:838:CLA:H93 | 20:B:838:CLA:CBB | 1.74 | 1.16 |
| 16:L:163:LEU:HB3 | 16:L:164:PRO:CD | 1.75 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:122:LYS:HD3 | 4:4:150:LYS:CD | 1.75 | 1.16 |
| 4:4:142:ASN:C | 4:4:150:LYS:NZ | 2.04 | 1.16 |
| 4:4:160:MET:SD | 20:4:306:CLA:CBB | 2.33 | 1.16 |
| 5:A:28:LYS:HB3 | 5:A:28:LYS:NZ | 1.50 | 1.16 |
| 5:A:269:PHE:CE1 | 15:K:14:THR:HG21 | 1.80 | 1.16 |
| 11:G:6:LEU:HB3 | 11:G:9:SER:CB | 1.76 | 1.16 |
| 20:A:825:CLA:CAB | 20:A:832:CLA:HMA3 | 1.73 | 1.16 |
| 20:F:201:CLA:HBC3 | 20:F:201:CLA:HHD | 1.17 | 1.16 |
| 3:3:205:GLY:H | 5:A:252:ARG:NH2 | 1.44 | 1.16 |
| 20:B:838:CLA:HBB2 | 20:B:838:CLA:C9 | 1.76 | 1.16 |
| 2:2:128:ASN:C | 2:2:130:LEU:H | 1.48 | 1.15 |
| 4:4:171:ASN:O | 4:4:173:THR:N | 1.79 | 1.15 |
| 20:A:818:CLA:HBB2 | 20:A:818:CLA:C12 | 1.74 | 1.15 |
| 1:1:144:LYS:NZ | 20:1:201:CLA:HED3 | 1.32 | 1.15 |
| 4:4:69:ILE:HD11 | 4:4:175:LYS:HB3 | 1.27 | 1.15 |
| 3:3:94:ARG:CZ | 3:3:97:PHE:CE2 | 2.29 | 1.15 |
| 5:A:316:MET:HG2 | 5:A:317:TYR:CD1 | 1.82 | 1.15 |
| 10:F:102:ARG:HG2 | 10:F:106:ILE:HD11 | 1.27 | 1.15 |
| 13:I:7:LEU:HD12 | 22:I:103:BCR:H333 | 1.28 | 1.15 |
| 15:K:44:GLU:CD | 15:K:45:SER:HA | 1.71 | 1.15 |
| 16:L:164:PRO:CB | 16:L:165:TYR:CD1 | 2.30 | 1.15 |
| 16:L:164:PRO:CG | 16:L:165:TYR:CD1 | 2.29 | 1.15 |
| 20:1:205:CLA:CAB | 20:1:211:CLA:HBC2 | 1.76 | 1.15 |
| 3:3:94:ARG:CD | 3:3:97:PHE:CZ | 2.30 | 1.15 |
| 20:L:208:CLA:HBC3 | 20:L:208:CLA:HHD | 1.28 | 1.15 |
| 17:N:62:SER:HB3 | 17:N:66:ASP:CA | 1.75 | 1.15 |
| 22:2:317:BCR:H23C | 22:2:317:BCR:H393 | 1.26 | 1.15 |
| 5:A:27:ILE:HG22 | 5:A:28:LYS:CD | 1.74 | 1.15 |
| 20:K:102:CLA:HAC2 | 21:K:105:LMU:O3B | 1.43 | 1.15 |
| 17:N:45:ASN:HB2 | 17:N:57:LYS:NZ | 1.57 | 1.15 |
| 21:R:102:LMU:H5B | 21:R:102:LMU:H6E | 1.20 | 1.15 |
| 21:R:104:LMU:C2' | 21:R:104:LMU:H21 | 1.74 | 1.15 |
| 5:A:51:THR:HG21 | 20:A:837:CLA:HBB2 | 1.22 | 1.14 |
| 16:L:164:PRO:CA | 16:L:165:TYR:CD1 | 2.29 | 1.14 |
| 1:1:24:PHE:CB | 6:B:314:ARG:HH21 | 1.60 | 1.14 |
| 6:B:120:VAL:HA | 6:B:123:TRP:CD1 | 1.81 | 1.14 |
| 3:3:94:ARG:CG | 3:3:97:PHE:CE1 | 2.28 | 1.14 |
| 20:A:824:CLA:HED1 | 20:A:825:CLA:C2D | 1.77 | 1.14 |
| 15:K:44:GLU:O | 15:K:47:LEU:HG | 1.46 | 1.14 |
| 2:2:169:LEU:HD22 | 20:2:305:CLA:CAB | 1.77 | 1.14 |
| 3:3:97:PHE:CD2 | 3:3:98:ILE:CG2 | 2.30 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:122:LYS:CD | 4:4:150:LYS:CD | 2.24 | 1.14 |
| 12:H:20:GLN:CB | 12:H:22:ASP:HB3 | 1.77 | 1.13 |
| 17:N:72:LYS:CE | 17:N:74:LYS:HG2 | 1.77 | 1.13 |
| 3:3:94:ARG:CG | 3:3:97:PHE:CZ | 2.30 | 1.13 |
| 3:3:110:SER:O | 3:3:111:TYR:HD2 | 1.31 | 1.13 |
| 20:3:307:CLA:HAC2 | 20:K:104:CLA:H72 | 1.29 | 1.13 |
| 6:B:323:TYR:HE2 | 11:G:48:ASP:O | 1.27 | 1.13 |
| 20:2:314:CLA:C5 | 20:2:314:CLA:HMA1 | 1.77 | 1.13 |
| 3:3:97:PHE:HD2 | 3:3:97:PHE:C | 1.57 | 1.13 |
| 11:G:6:LEU:CB | 11:G:9:SER:HB3 | 1.76 | 1.13 |
| 12:H:73:PRO:HG3 | 19:Z:2:FRU:H5 | 1.14 | 1.13 |
| 17:N:45:ASN:HB2 | 17:N:54:LYS:HG2 | 1.16 | 1.13 |
| 17:N:57:LYS:O | 17:N:60:PHE:O | 1.64 | 1.13 |
| 1:1:144:LYS:HZ2 | 20:1:201:CLA:CED | 1.62 | 1.13 |
| 20:A:825:CLA:CBB | 20:A:832:CLA:HMA1 | 1.75 | 1.13 |
| 3:3:94:ARG:CD | 3:3:97:PHE:CE1 | 2.30 | 1.13 |
| 11:G:43:HIS:HB2 | 11:G:44:PHE:CD1 | 1.84 | 1.13 |
| 4:4:34:PRO:HA | 4:4:35:GLU:HB2 | 1.31 | 1.12 |
| 4:4:104:ARG:HH11 | 4:4:105:ARG:CB | 1.61 | 1.12 |
| 20:B:835:CLA:HMB1 | 22:B:846:BCR:H292 | 1.24 | 1.12 |
| 20:F:201:CLA:HHD | 20:F:201:CLA:CBC | 1.76 | 1.12 |
| 20:J:101:CLA:HBD | 20:J:101:CLA:HBA2 | 1.12 | 1.12 |
| 16:L:157:LEU:O | 16:L:158:MET:O | 1.67 | 1.12 |
| 17:N:41:LYS:CG | 17:N:42:PHE:CB | 2.26 | 1.12 |
| 20:A:824:CLA:HED1 | 20:A:825:CLA:CMD | 1.79 | 1.12 |
| 20:A:826:CLA:H203 | 22:J:102:BCR:H17C | 1.17 | 1.12 |
| 22:I:103:BCR:HC8 | 22:I:103:BCR:C31 | 1.74 | 1.12 |
| 22:J:102:BCR:H393 | 22:J:102:BCR:H23C | 1.18 | 1.12 |
| 16:L:163:LEU:CD1 | 16:L:164:PRO:HD3 | 1.77 | 1.12 |
| 17:N:72:LYS:HE2 | 17:N:74:LYS:CD | 1.79 | 1.12 |
| 5:A:452:PHE:CE1 | 20:A:835:CLA:HBB2 | 1.84 | 1.12 |
| 20:B:826:CLA:HBC2 | 20:B:826:CLA:HHD | 1.31 | 1.12 |
| 23:B:843:PQN:H162 | 22:B:847:BCR:H333 | 1.12 | 1.12 |
| 7:C:62:PHE:CE2 | 9:E:42:GLU:OE1 | 2.02 | 1.12 |
| 1:1:27:LEU:CD1 | 6:B:314:ARG:NH1 | 2.12 | 1.12 |
| 22:B:801:BCR:H333 | 20:L:207:CLA:CHC | 1.79 | 1.12 |
| 7:C:1:MET:HB3 | 7:C:4:SER:OG | 1.50 | 1.12 |
| 11:G:8:ILE:O | 11:G:12:THR:OG1 | 1.66 | 1.12 |
| 15:K:38:LEU:HG | 15:K:39:LYS:HD3 | 1.17 | 1.12 |
| 3:3:158:TYR:HB3 | 3:3:159:PRO:HD2 | 1.32 | 1.11 |
| 5:A:22:VAL:HG23 | 5:A:23:ASP:N | 1.50 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:402:ILE:HG13 | 20:A:827:CLA:HBB2 | 1.14 | 1.11 |
| 7:C:1:MET:H1 | 7:C:4:SER:CB | 1.60 | 1.11 |
| 17:N:45:ASN:ND2 | 17:N:54:LYS:HD3 | 1.65 | 1.11 |
| 4:4:69:ILE:CD1 | 4:4:175:LYS:HG2 | 1.79 | 1.11 |
| 4:4:107:GLN:C | 20:4:301:CLA:HMA2 | 1.71 | 1.11 |
| 5:A:423:ASP:HB3 | 5:A:424:PRO:HD3 | 1.26 | 1.11 |
| 5:A:588:GLY:CA | 6:B:668:ARG:HD3 | 1.81 | 1.11 |
| 5:A:707:ILE:HG22 | 5:A:711:HIS:NE2 | 1.65 | 1.11 |
| 2:2:51:HIS:HB2 | 20:2:310:CLA:CAD | 1.80 | 1.11 |
| 2:2:169:LEU:CD2 | 20:2:305:CLA:HBB2 | 1.79 | 1.11 |
| 3:3:94:ARG:CA | 3:3:97:PHE:CE1 | 2.29 | 1.11 |
| 3:3:52:LYS:O | 3:3:56:TYR:CD2 | 2.03 | 1.11 |
| 4:4:104:ARG:HD2 | 20:4:312:CLA:C2C | 1.80 | 1.11 |
| 11:G:33:LYS:HA | 11:G:33:LYS:CE | 1.74 | 1.11 |
| 15:K:44:GLU:HG3 | 15:K:45:SER:HA | 1.17 | 1.11 |
| 16:L:163:LEU:CD1 | 16:L:164:PRO:CD | 2.29 | 1.11 |
| 20:1:204:CLA:HED3 | 20:1:204:CLA:HAA1 | 1.16 | 1.11 |
| 20:4:303:CLA:HED3 | 20:4:303:CLA:HAA2 | 1.20 | 1.11 |
| 6:B:732:LYS:HB3 | 6:B:733:PHE:HA | 1.15 | 1.11 |
| 20:B:810:CLA:HBB2 | 20:B:810:CLA:H92 | 1.11 | 1.11 |
| 22:F:204:BCR:H321 | 22:F:204:BCR:C8 | 1.71 | 1.11 |
| 20:K:104:CLA:H41 | 20:K:104:CLA:C8 | 1.81 | 1.11 |
| 20:A:819:CLA:H92 | 22:A:844:BCR:C37 | 1.81 | 1.10 |
| 22:A:843:BCR:H311 | 22:A:843:BCR:HC8 | 1.22 | 1.10 |
| 6:B:421:HIS:NE2 | 20:F:201:CLA:ND | 1.98 | 1.10 |
| 6:B:596:TRP:CH2 | 6:B:612:SER:O | 2.04 | 1.10 |
| 11:G:37:GLU:OE2 | 11:G:42:SER:HB3 | 0.93 | 1.10 |
| 4:4:95:PHE:CE2 | 20:4:314:CLA:C2C | 2.34 | 1.10 |
| 5:A:25:ASP:CB | 5:A:26:PRO:HA | 1.81 | 1.10 |
| 16:L:164:PRO:HA | 16:L:165:TYR:CD1 | 1.86 | 1.10 |
| 4:4:40:PHE:CB | 4:4:43:ALA:HB2 | 1.79 | 1.10 |
| 4:4:93:ILE:HA | 4:4:96:ILE:HD12 | 1.34 | 1.10 |
| 18:R:34:UNK:CB | 18:R:35:UNK:CB | 2.30 | 1.10 |
| 17:N:57:LYS:C | 17:N:60:PHE:O | 1.94 | 1.10 |
| 1:1:24:PHE:CD2 | 6:B:314:ARG:NH2 | 2.20 | 1.10 |
| 22:A:845:BCR:H311 | 22:A:845:BCR:HC8 | 1.31 | 1.10 |
| 15:K:43:ARG:HH11 | 15:K:43:ARG:HG3 | 1.00 | 1.10 |
| 18:R:46:UNK:CB | 18:R:47:UNK:CB | 2.30 | 1.10 |
| 1:1:184:PRO:C | 1:1:185:TRP:CD1 | 2.30 | 1.09 |
| 3:3:92:TRP:HA | 3:3:95:THR:HG23 | 1.10 | 1.09 |
| 5:A:328:LYS:HG2 | 5:A:332:GLU:HB2 | 1.23 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:342:GLY:CA | 5:A:430:ASP:HB2 | 1.80 | 1.09 |
| 20:A:822:CLA:CHD | 22:A:844:BCR:H19C | 1.81 | 1.09 |
| 23:B:843:PQN:H191 | 22:B:847:BCR:H10C | 1.16 | 1.09 |
| 17:N:57:LYS:HG3 | 17:N:58:VAL:N | 1.49 | 1.09 |
| 17:N:72:LYS:CD | 17:N:74:LYS:CG | 2.30 | 1.09 |
| 18:R:39:UNK:C | 18:R:41:UNK:CB | 2.30 | 1.09 |
| 18:R:41:UNK:CB | 18:R:42:UNK:CB | 2.30 | 1.09 |
| 6:B:87:ILE:HA | 6:B:115:ASN:HA | 1.34 | 1.09 |
| 6:B:131:THR:HB | 6:B:134:ASP:HB2 | 1.29 | 1.09 |
| 17:N:45:ASN:ND2 | 17:N:54:LYS:CD | 2.12 | 1.09 |
| 3:3:92:TRP:CA | 3:3:95:THR:CG2 | 2.30 | 1.09 |
| 4:4:52:MET:HG3 | 4:4:160:MET:HG3 | 1.27 | 1.09 |
| 5:A:27:ILE:CG2 | 5:A:28:LYS:CD | 2.29 | 1.09 |
| 5:A:27:ILE:CG2 | 5:A:28:LYS:CG | 2.30 | 1.09 |
| 20:A:818:CLA:O1A | 20:A:827:CLA:H71 | 1.52 | 1.09 |
| 6:B:561:GLY:HA3 | 7:C:52:LYS:HG2 | 1.17 | 1.09 |
| 9:E:40:ARG:NE | 9:E:86:GLU:OE1 | 1.85 | 1.09 |
| 22:F:204:BCR:C32 | 22:F:204:BCR:HC8 | 1.80 | 1.09 |
| 16:L:163:LEU:CB | 16:L:164:PRO:HD3 | 1.83 | 1.09 |
| 6:B:58:PHE:HB2 | 6:B:146:SER:HB3 | 1.31 | 1.09 |
| 20:B:834:CLA:ND | 20:B:835:CLA:HBB2 | 1.65 | 1.09 |
| 17:N:41:LYS:HG3 | 17:N:42:PHE:CB | 1.81 | 1.09 |
| 18:R:52:UNK:CB | 18:R:53:UNK:CB | 2.30 | 1.09 |
| 21:R:103:LMU:H22 | 21:R:103:LMU:H62 | 1.30 | 1.09 |
| 3:3:107:TRP:CD1 | 3:3:108:ALA:N | 2.21 | 1.08 |
| 4:4:94:GLU:HG2 | 4:4:95:PHE:CE1 | 1.87 | 1.08 |
| 4:4:106:TRP:CD1 | 20:4:301:CLA:CED | 2.36 | 1.08 |
| 20:A:839:CLA:H71 | 20:A:839:CLA:H122 | 1.11 | 1.08 |
| 21:A:853:LMU:H22 | 21:A:853:LMU:H61 | 1.32 | 1.08 |
| 11:G:93:TYR:HA | 11:G:94:ASP:CB | 1.81 | 1.08 |
| 17:N:72:LYS:HG3 | 17:N:74:LYS:CG | 1.82 | 1.08 |
| 5:A:394:SER:HB2 | 20:A:826:CLA:HMA3 | 1.34 | 1.08 |
| 5:A:435:VAL:O | 5:A:438:HIS:O | 1.69 | 1.08 |
| 20:A:804:CLA:H12 | 20:A:811:CLA:H61 | 1.30 | 1.08 |
| 6:B:493:TRP:NE1 | 20:B:835:CLA:O1A | 1.85 | 1.08 |
| 22:B:801:BCR:H331 | 20:L:207:CLA:CHC | 1.82 | 1.08 |
| 20:K:104:CLA:H8 | 20:K:104:CLA:C4 | 1.82 | 1.08 |
| 21:R:102:LMU:H6E | 21:R:102:LMU:C5B | 1.82 | 1.08 |
| 1:1:144:LYS:HE3 | 20:1:201:CLA:O2D | 1.48 | 1.08 |
| 3:3:198:PHE:HA | 3:3:201:ALA:HB2 | 1.36 | 1.08 |
| 4:4:122:LYS:HB3 | 4:4:143:PHE:CB | 1.83 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:122:LYS:HB3 | 4:4:143:PHE:HB2 | 1.28 | 1.08 |
| 4:4:149:ALA:HB3 | 4:4:151:GLU:HG2 | 1.35 | 1.08 |
| 20:A:803:CLA:CBB | 20:A:804:CLA:C2C | 2.32 | 1.08 |
| 6:B:382:ILE:HG22 | 6:B:383:MET:H | 1.06 | 1.08 |
| 7:C:1:MET:N | 7:C:4:SER:CB | 2.14 | 1.08 |
| 18:R:39:UNK:CA | 18:R:42:UNK:CB | 2.30 | 1.08 |
| 21:R:103:LMU:H1' | 21:R:103:LMU:H31 | 1.32 | 1.08 |
| 2:2:55:ALA:HB3 | 2:2:56:MET:HE2 | 1.12 | 1.08 |
| 4:4:122:LYS:CB | 4:4:143:PHE:HB2 | 1.83 | 1.08 |
| 16:L:164:PRO:HA | 16:L:165:TYR:HB3 | 1.30 | 1.08 |
| 17:N:72:LYS:CE | 17:N:74:LYS:CG | 2.32 | 1.08 |
| 1:1:24:PHE:HD2 | 6:B:314:ARG:NH2 | 1.49 | 1.07 |
| 20:B:822:CLA:HHD | 20:B:822:CLA:HBC2 | 1.36 | 1.07 |
| 8:D:78:ALA:HB3 | 8:D:82:GLN:HE22 | 1.15 | 1.07 |
| 15:K:84:LEU:H | 15:K:84:LEU:CD2 | 1.66 | 1.07 |
| 17:N:45:ASN:ND2 | 17:N:54:LYS:HG2 | 1.62 | 1.07 |
| 20:2:314:CLA:HBD | 20:2:314:CLA:HBA1 | 1.36 | 1.07 |
| 5:A:342:GLY:HA3 | 5:A:430:ASP:CB | 1.83 | 1.07 |
| 5:A:466:THR:HG22 | 20:B:811:CLA:HHC | 1.13 | 1.07 |
| 16:L:163:LEU:HG | 16:L:164:PRO:HD3 | 1.35 | 1.07 |
| 20:1:211:CLA:O1D | 20:1:211:CLA:HAA2 | 1.53 | 1.07 |
| 20:2:314:CLA:HBD | 20:2:314:CLA:CBA | 1.83 | 1.07 |
| 3:3:180:LYS:O | 3:3:182:LYS:N | 1.87 | 1.07 |
| 4:4:69:ILE:CD1 | 4:4:175:LYS:CG | 2.33 | 1.07 |
| 21:G:102:LMU:H3' | 21:G:102:LMU:H6'2 | 1.33 | 1.07 |
| 17:N:61:LEU:CD1 | 17:N:63:ASP:O | 2.02 | 1.07 |
| 5:A:472:ARG:HH12 | 16:L:74:LEU:HG | 1.10 | 1.07 |
| 6:B:672:GLN:HA | 6:B:672:GLN:HE21 | 1.14 | 1.07 |
| 11:G:12:THR:HG22 | 11:G:72:LEU:HG | 1.07 | 1.07 |
| 11:G:93:TYR:HA | 11:G:94:ASP:HB2 | 1.11 | 1.07 |
| 20:2:303:CLA:H43 | 20:2:303:CLA:ND | 1.67 | 1.07 |
| 4:4:119:PRO:HG3 | 20:4:312:CLA:C2D | 1.85 | 1.07 |
| 5:A:58:HIS:HE1 | 20:A:803:CLA:ND | 1.51 | 1.07 |
| 20:A:814:CLA:HHC | 22:A:843:BCR:H17C | 1.26 | 1.07 |
| 15:K:84:LEU:N | 15:K:84:LEU:HD23 | 1.54 | 1.07 |
| 16:L:163:LEU:CB | 16:L:164:PRO:CD | 2.30 | 1.07 |
| 4:4:104:ARG:HH11 | 4:4:105:ARG:HB2 | 1.20 | 1.06 |
| 16:L:82:ALA:HB2 | 16:L:86:LEU:HD13 | 1.34 | 1.06 |
| 17:N:45:ASN:HD22 | 17:N:54:LYS:HG2 | 1.15 | 1.06 |
| 3:3:92:TRP:CA | 3:3:95:THR:HG23 | 1.85 | 1.06 |
| 5:A:25:ASP:HB2 | 5:A:26:PRO:C | 1.79 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:E:52:VAL:O | 9:E:53:VAL:CG2 | 2.04 | 1.06 |
| 20:2:312:CLA:H41 | 20:2:312:CLA:H8 | 1.38 | 1.06 |
| 4:4:122:LYS:HZ3 | 4:4:150:LYS:HD2 | 1.15 | 1.06 |
| 4:4:147:LEU:HD13 | 4:4:148:GLU:H | 1.12 | 1.06 |
| 6:B:608:GLN:HE21 | 6:B:608:GLN:HA | 1.14 | 1.06 |
| 6:B:663:PHE:O | 6:B:664:LEU:HB2 | 1.55 | 1.06 |
| 17:N:57:LYS:CG | 17:N:58:VAL:H | 1.69 | 1.06 |
| 17:N:63:ASP:H | 17:N:64:ASP:HB3 | 1.17 | 1.06 |
| 4:4:74:LYS:N | 4:4:75:TRP:HA | 1.70 | 1.06 |
| 4:4:160:MET:HE3 | 20:4:306:CLA:HBB2 | 1.06 | 1.06 |
| 5:A:249:ILE:HG12 | 5:A:250:LEU:H | 0.94 | 1.06 |
| 5:A:581:CYS:HB2 | 5:A:590:CYS:HA | 1.34 | 1.06 |
| 20:H:109:CLA:CAC | 22:I:103:BCR:HC31 | 1.86 | 1.06 |
| 15:K:44:GLU:CG | 15:K:45:SER:CA | 2.30 | 1.06 |
| 17:N:6:TYR:C | 17:N:8:GLU:N | 2.09 | 1.06 |
| 1:1:185:TRP:HH2 | 20:1:213:CLA:C2 | 1.68 | 1.05 |
| 20:2:316:CLA:HAA1 | 20:2:316:CLA:H12 | 1.36 | 1.05 |
| 4:4:99:HIS:CE1 | 4:4:103:ILE:CD1 | 2.37 | 1.05 |
| 4:4:101:VAL:HG13 | 4:4:104:ARG:NH2 | 1.71 | 1.05 |
| 20:A:803:CLA:CBB | 20:A:804:CLA:C3C | 2.34 | 1.05 |
| 6:B:558:PRO:HG2 | 6:B:703:VAL:HB | 1.34 | 1.05 |
| 17:N:45:ASN:HB2 | 17:N:54:LYS:CG | 1.83 | 1.05 |
| 17:N:72:LYS:HE2 | 17:N:74:LYS:HG2 | 1.33 | 1.05 |
| 20:A:824:CLA:HED1 | 20:A:825:CLA:C3D | 1.85 | 1.05 |
| 6:B:247:THR:HA | 6:B:250:ALA:HB2 | 1.14 | 1.05 |
| 20:B:838:CLA:HMA2 | 20:B:839:CLA:HED1 | 1.38 | 1.05 |
| 3:3:107:TRP:CG | 3:3:108:ALA:H | 1.72 | 1.05 |
| 20:A:838:CLA:H141 | 22:A:845:BCR:HC22 | 1.33 | 1.05 |
| 10:F:24:LYS:N | 10:F:24:LYS:HE2 | 1.71 | 1.05 |
| 16:L:164:PRO:CA | 16:L:165:TYR:CB | 2.30 | 1.05 |
| 5:A:116:ILE:HG23 | 5:A:137:GLY:HA3 | 1.38 | 1.05 |
| 5:A:466:THR:CG2 | 20:B:811:CLA:HHC | 1.86 | 1.05 |
| 6:B:310:PRO:HG3 | 20:B:824:CLA:HMA3 | 1.36 | 1.05 |
| 12:H:20:GLN:HB3 | 12:H:22:ASP:HB3 | 1.06 | 1.05 |
| 15:K:79:LYS:CE | 15:K:84:LEU:O | 2.05 | 1.05 |
| 21:K:105:LMU:H42 | 21:K:105:LMU:H81 | 1.32 | 1.05 |
| 17:N:40:CYS:H | 17:N:41:LYS:HA | 1.16 | 1.05 |
| 1:1:183:ASP:CG | 1:1:184:PRO:CD | 2.29 | 1.05 |
| 20:2:303:CLA:H43 | 20:2:303:CLA:C1D | 1.86 | 1.05 |
| 4:4:36:ASN:O | 4:4:39:TRP:CB | 2.04 | 1.05 |
| 5:A:331:LEU:HD11 | 5:A:346:LEU:HB3 | 1.33 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:302:LYS:O | 6:B:303:TYR:HB2 | 1.57 | 1.05 |
| 6:B:474:PHE:HE2 | 6:B:476:ILE:HG13 | 1.13 | 1.05 |
| 6:B:493:TRP:O | 6:B:495:PRO:HD3 | 1.57 | 1.05 |
| 12:H:73:PRO:HD3 | 19:Z:2:FRU:H62 | 1.12 | 1.05 |
| 15:K:38:LEU:HG | 15:K:39:LYS:CD | 1.87 | 1.05 |
| 15:K:44:GLU:CD | 15:K:45:SER:CA | 2.30 | 1.05 |
| 4:4:122:LYS:CE | 4:4:150:LYS:HD3 | 1.87 | 1.04 |
| 4:4:128:ALA:CB | 4:4:143:PHE:CE2 | 2.39 | 1.04 |
| 20:B:802:CLA:H93 | 20:B:803:CLA:H91 | 1.34 | 1.04 |
| 11:G:42:SER:OG | 11:G:46:ALA:HB2 | 1.57 | 1.04 |
| 16:L:108:LYS:O | 16:L:132:SER:HB2 | 1.54 | 1.04 |
| 21:1:217:LMU:H91 | 21:G:103:LMU:O3' | 1.56 | 1.04 |
| 5:A:27:ILE:C | 5:A:28:LYS:CG | 2.28 | 1.04 |
| 5:A:370:ILE:HG23 | 5:A:403:GLY:HA3 | 1.39 | 1.04 |
| 6:B:340:SER:HA | 20:B:827:CLA:H51 | 1.39 | 1.04 |
| 22:2:317:BCR:H23C | 22:2:317:BCR:C39 | 1.88 | 1.04 |
| 4:4:36:ASN:OD1 | 4:4:37:LEU:HA | 1.57 | 1.04 |
| 5:A:21:LEU:HD12 | 5:A:21:LEU:N | 1.66 | 1.04 |
| 20:K:102:CLA:CAC | 21:K:105:LMU:O3B | 2.05 | 1.04 |
| 2:2:205:PHE:CD1 | 2:2:206:ALA:N | 2.25 | 1.04 |
| 20:2:312:CLA:O1A | 20:2:312:CLA:H3A | 1.57 | 1.04 |
| 4:4:69:ILE:HG22 | 4:4:70:ILE:H | 0.91 | 1.04 |
| 6:B:323:TYR:CE2 | 11:G:48:ASP:O | 2.10 | 1.04 |
| 7:C:39:ILE:HG12 | 7:C:40:ALA:H | 1.23 | 1.04 |
| 10:F:5:LEU:HG | 10:F:6:THR:H | 0.92 | 1.04 |
| 10:F:23:LYS:O | 10:F:26:GLN:HB2 | 1.57 | 1.04 |
| 2:2:196:HIS:CE1 | 19:O:1:GLC:O3 | 2.11 | 1.04 |
| 20:2:307:CLA:H71 | 20:2:307:CLA:HBB2 | 1.05 | 1.04 |
| 3:3:110:SER:O | 3:3:111:TYR:CD2 | 2.10 | 1.04 |
| 5:A:28:LYS:HB3 | 5:A:28:LYS:HZ3 | 0.99 | 1.04 |
| 20:A:824:CLA:HBC2 | 20:A:824:CLA:HHD | 1.35 | 1.04 |
| 10:F:25:LEU:CD2 | 10:F:46:MET:HB3 | 1.88 | 1.04 |
| 11:G:37:GLU:OE1 | 11:G:42:SER:HB2 | 1.54 | 1.04 |
| 21:R:102:LMU:H5B | 21:R:102:LMU:C6' | 1.86 | 1.04 |
| 20:3:307:CLA:CAC | 20:K:104:CLA:H72 | 1.88 | 1.03 |
| 4:4:122:LYS:HB2 | 4:4:143:PHE:HD2 | 0.88 | 1.03 |
| 5:A:197:GLN:HE21 | 5:A:197:GLN:HA | 0.88 | 1.03 |
| 6:B:422:LEU:HD13 | 6:B:535:VAL:HG11 | 1.39 | 1.03 |
| 6:B:661:PHE:HB2 | 20:B:803:CLA:HMC2 | 1.37 | 1.03 |
| 7:C:74:THR:OG1 | 7:C:80:ALA:HB2 | 1.57 | 1.03 |
| 21:E:101:LMU:H32 | 21:E:101:LMU:H72 | 1.40 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:2:307:CLA:HBB2 | 20:2:307:CLA:C7 | 1.87 | 1.03 |
| 3:3:97:PHE:CD2 | 3:3:97:PHE:C | 2.29 | 1.03 |
| 6:B:293:THR:O | 11:G:38:GLN:OE1 | 1.76 | 1.03 |
| 9:E:86:GLU:HG3 | 9:E:87:VAL:N | 1.68 | 1.03 |
| 21:H:105:LMU:C1B | 21:H:105:LMU:H31 | 1.86 | 1.03 |
| 17:N:72:LYS:CB | 17:N:73:ASP:CA | 2.30 | 1.03 |
| 21:R:101:LMU:H11 | 21:R:101:LMU:H62 | 1.39 | 1.03 |
| 2:2:211:LYS:HG2 | 3:3:113:LEU:HD11 | 1.36 | 1.03 |
| 5:A:316:MET:HB3 | 5:A:317:TYR:HB2 | 1.35 | 1.03 |
| 20:B:838:CLA:H152 | 22:F:204:BCR:C31 | 1.88 | 1.03 |
| 15:K:44:GLU:HG3 | 15:K:45:SER:N | 1.73 | 1.03 |
| 15:K:84:LEU:H | 15:K:84:LEU:HD23 | 0.87 | 1.03 |
| 16:L:27:VAL:HA | 20:L:204:CLA:HMA2 | 1.36 | 1.03 |
| 17:N:67:LEU:HB2 | 17:N:68:GLU:HG2 | 1.37 | 1.03 |
| 1:1:24:PHE:HB3 | 6:B:314:ARG:HH21 | 0.86 | 1.03 |
| 21:3:319:LMU:H81 | 21:3:319:LMU:H32 | 1.05 | 1.03 |
| 5:A:251:ASN:O | 5:A:253:ASP:N | 1.89 | 1.03 |
| 5:A:588:GLY:HA3 | 6:B:668:ARG:HD3 | 1.40 | 1.03 |
| 20:A:839:CLA:CBC | 20:A:839:CLA:HHD | 1.87 | 1.03 |
| 6:B:269:TRP:HB2 | 6:B:497:TRP:HH2 | 1.22 | 1.03 |
| 12:H:44:ALA:HB2 | 16:L:145:PHE:CD1 | 1.93 | 1.03 |
| 13:I:11:LEU:CD1 | 22:I:103:BCR:H10C | 1.87 | 1.03 |
| 21:K:107:LMU:C6' | 21:K:107:LMU:H32 | 1.87 | 1.03 |
| 21:2:313:LMU:H21 | 21:2:313:LMU:H6D | 1.40 | 1.03 |
| 5:A:22:VAL:HG23 | 5:A:23:ASP:CA | 1.88 | 1.03 |
| 21:A:854:LMU:H91 | 21:A:854:LMU:H21 | 1.39 | 1.03 |
| 6:B:58:PHE:CB | 6:B:146:SER:HB3 | 1.87 | 1.03 |
| 4:4:40:PHE:HB3 | 4:4:43:ALA:HB2 | 1.33 | 1.02 |
| 4:4:122:LYS:CE | 4:4:150:LYS:CD | 2.36 | 1.02 |
| 5:A:81:ALA:HB2 | 20:A:804:CLA:CMA | 1.88 | 1.02 |
| 5:A:368:LEU:CD2 | 20:A:818:CLA:H93 | 1.89 | 1.02 |
| 20:A:826:CLA:H203 | 22:J:102:BCR:C17 | 1.88 | 1.02 |
| 21:A:853:LMU:H21 | 21:A:853:LMU:C8 | 1.89 | 1.02 |
| 9:E:86:GLU:HG3 | 9:E:87:VAL:H | 0.90 | 1.02 |
| 4:4:142:ASN:O | 4:4:150:LYS:HE2 | 1.57 | 1.02 |
| 5:A:81:ALA:CB | 20:A:804:CLA:CMA | 2.37 | 1.02 |
| 20:A:819:CLA:HMD1 | 20:A:821:CLA:HBB2 | 1.37 | 1.02 |
| 6:B:594:TRP:O | 6:B:595:HIS:HB3 | 1.54 | 1.02 |
| 7:C:66:ARG:HG2 | 7:C:66:ARG:HH21 | 1.21 | 1.02 |
| 4:4:39:TRP:C | 4:4:40:PHE:CD1 | 2.38 | 1.02 |
| 4:4:39:TRP:CG | 4:4:40:PHE:H | 1.78 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:103:ILE:HG13 | 20:4:302:CLA:HMD3 | 1.41 | 1.02 |
| 20:A:838:CLA:H141 | 22:A:845:BCR:HC21 | 1.36 | 1.02 |
| 7:C:62:PHE:CZ | 9:E:42:GLU:OE1 | 2.12 | 1.02 |
| 10:F:47:GLU:HG3 | 10:F:51:LYS:HE3 | 1.40 | 1.02 |
| 11:G:49:THR:OG1 | 11:G:50:ARG:HG2 | 1.59 | 1.02 |
| 18:R:33:UNK:C | 18:R:36:UNK:CB | 2.37 | 1.02 |
| 20:1:204:CLA:HED3 | 20:1:204:CLA:CAA | 1.89 | 1.02 |
| 5:A:27:ILE:CG2 | 5:A:28:LYS:HG2 | 1.89 | 1.02 |
| 20:B:826:CLA:HBB2 | 20:B:839:CLA:HMB1 | 1.02 | 1.02 |
| 17:N:40:CYS:N | 17:N:41:LYS:HA | 1.71 | 1.02 |
| 2:2:169:LEU:HD22 | 20:2:305:CLA:CBB | 1.90 | 1.02 |
| 3:3:94:ARG:CB | 3:3:97:PHE:HE1 | 1.73 | 1.02 |
| 3:3:97:PHE:CE2 | 3:3:98:ILE:CG2 | 2.42 | 1.02 |
| 4:4:93:ILE:HA | 4:4:96:ILE:CD1 | 1.89 | 1.02 |
| 20:4:301:CLA:HBC2 | 20:4:301:CLA:HHD | 1.38 | 1.02 |
| 22:B:801:BCR:H333 | 20:L:207:CLA:NB | 1.74 | 1.02 |
| 13:I:11:LEU:HD12 | 22:I:103:BCR:H10C | 1.03 | 1.02 |
| 18:R:41:UNK:CB | 18:R:42:UNK:CA | 2.38 | 1.02 |
| 4:4:35:GLU:HB3 | 4:4:36:ASN:HB3 | 1.41 | 1.01 |
| 4:4:91:PHE:CD2 | 20:4:311:CLA:C3C | 2.43 | 1.01 |
| 4:4:193:ILE:HG22 | 4:4:194:VAL:H | 1.25 | 1.01 |
| 5:A:590:CYS:SG | 24:A:856:SF4:S1 | 2.58 | 1.01 |
| 5:A:702:GLU:OE2 | 6:B:550:LYS:NZ | 1.93 | 1.01 |
| 20:A:839:CLA:H71 | 20:A:839:CLA:C12 | 1.89 | 1.01 |
| 10:F:130:LEU:HG | 10:F:131:PHE:H | 1.24 | 1.01 |
| 11:G:28:ARG:HG2 | 11:G:28:ARG:HH21 | 1.23 | 1.01 |
| 11:G:68:ILE:HG23 | 11:G:72:LEU:HD13 | 1.42 | 1.01 |
| 17:N:72:LYS:CE | 17:N:74:LYS:CE | 2.30 | 1.01 |
| 17:N:72:LYS:NZ | 17:N:74:LYS:HE2 | 1.72 | 1.01 |
| 3:3:92:TRP:HA | 3:3:95:THR:HG21 | 1.37 | 1.01 |
| 4:4:34:PRO:HA | 4:4:35:GLU:CB | 1.89 | 1.01 |
| 5:A:269:PHE:HE1 | 15:K:14:THR:HG21 | 1.18 | 1.01 |
| 6:B:438:VAL:HG22 | 20:B:833:CLA:HMC2 | 1.42 | 1.01 |
| 20:B:836:CLA:HHD | 20:B:836:CLA:CBC | 1.91 | 1.01 |
| 20:R:108:CLA:HBA2 | 20:R:108:CLA:HBD | 1.38 | 1.01 |
| 3:3:205:GLY:HA3 | 5:A:252:ARG:HH12 | 1.24 | 1.01 |
| 4:4:106:TRP:NE1 | 20:4:301:CLA:CED | 2.22 | 1.01 |
| 20:4:303:CLA:HAA2 | 20:4:303:CLA:CED | 1.89 | 1.01 |
| 20:4:306:CLA:HBA1 | 20:4:306:CLA:HMA2 | 1.40 | 1.01 |
| 5:A:335:LYS:HG2 | 5:A:336:GLY:H | 1.21 | 1.01 |
| 20:A:814:CLA:C4B | 22:A:843:BCR:H19C | 1.90 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:B:809:CLA:HHB | 20:B:830:CLA:HBB2 | 1.41 | 1.01 |
| 7:C:17:CYS:HB2 | 7:C:58:CYS:SG | 2.01 | 1.01 |
| 16:L:164:PRO:HB3 | 16:L:165:TYR:HD1 | 1.23 | 1.01 |
| 3:3:95:THR:N | 3:3:97:PHE:CE1 | 2.29 | 1.01 |
| 4:4:107:GLN:O | 20:4:301:CLA:HMA2 | 1.59 | 1.01 |
| 5:A:452:PHE:HE1 | 20:A:835:CLA:HBB2 | 1.17 | 1.01 |
| 11:G:44:PHE:C | 11:G:47:GLY:CA | 2.34 | 1.01 |
| 20:H:101:CLA:H2 | 20:H:101:CLA:HMA2 | 1.39 | 1.01 |
| 1:1:112:ARG:NH1 | 20:1:210:CLA:CGD | 2.22 | 1.01 |
| 20:1:205:CLA:CMC | 20:1:208:CLA:HHD | 1.89 | 1.01 |
| 5:A:541:VAL:HG11 | 5:A:615:HIS:CD2 | 1.94 | 1.01 |
| 20:A:833:CLA:CMA | 20:A:839:CLA:HBB1 | 1.90 | 1.01 |
| 22:B:801:BCR:C33 | 20:L:207:CLA:C3B | 2.38 | 1.01 |
| 14:J:11:ALA:HB1 | 14:J:12:PRO:HD2 | 1.42 | 1.01 |
| 15:K:1:ASP:HA | 15:K:5:SER:HB3 | 1.43 | 1.01 |
| 2:2:55:ALA:CB | 2:2:56:MET:HE2 | 1.92 | 1.00 |
| 4:4:106:TRP:CG | 20:4:301:CLA:HED3 | 1.94 | 1.00 |
| 5:A:249:ILE:HG12 | 5:A:250:LEU:N | 1.73 | 1.00 |
| 5:A:454:GLY:H | 5:A:457:SER:HB3 | 1.24 | 1.00 |
| 6:B:202:SER:O | 6:B:245:GLY:HA2 | 1.60 | 1.00 |
| 21:H:105:LMU:H3' | 21:H:105:LMU:O5B | 1.60 | 1.00 |
| 17:N:45:ASN:CG | 17:N:54:LYS:HG2 | 1.86 | 1.00 |
| 17:N:58:VAL:HB | 17:N:59:PRO:HD2 | 1.04 | 1.00 |
| 21:R:104:LMU:H21 | 21:R:104:LMU:H2' | 1.05 | 1.00 |
| 1:1:25:ASP:H | 6:B:314:ARG:HH22 | 1.07 | 1.00 |
| 21:2:313:LMU:H82 | 21:2:313:LMU:H41 | 1.35 | 1.00 |
| 3:3:48:PHE:HD2 | 3:3:49:ILE:HG22 | 0.85 | 1.00 |
| 21:3:319:LMU:H81 | 21:3:319:LMU:C3 | 1.90 | 1.00 |
| 4:4:122:LYS:CG | 4:4:150:LYS:HD3 | 1.91 | 1.00 |
| 4:4:128:ALA:N | 4:4:143:PHE:HZ | 1.58 | 1.00 |
| 5:A:402:ILE:CG1 | 20:A:827:CLA:HBB2 | 1.90 | 1.00 |
| 20:A:851:CLA:HMD3 | 6:B:578:LEU:HD23 | 1.42 | 1.00 |
| 10:F:26:GLN:OE1 | 10:F:26:GLN:HA | 1.55 | 1.00 |
| 17:N:32:ALA:HB1 | 17:N:35:VAL:HG22 | 1.42 | 1.00 |
| 3:3:94:ARG:NH1 | 3:3:97:PHE:CD2 | 2.29 | 1.00 |
| 4:4:142:ASN:C | 4:4:150:LYS:HZ3 | 1.65 | 1.00 |
| 20:B:824:CLA:H151 | 20:B:824:CLA:H102 | 1.37 | 1.00 |
| 8:D:44:GLU:HB2 | 8:D:46:TYR:HE2 | 1.24 | 1.00 |
| 16:L:163:LEU:CG | 16:L:164:PRO:CD | 2.40 | 1.00 |
| 17:N:72:LYS:HB3 | 17:N:73:ASP:HA | 1.05 | 1.00 |
| 20:A:819:CLA:C9 | 22:A:844:BCR:H373 | 1.91 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:697:PRO:O | 7:C:79:LEU:CD1 | 2.09 | 1.00 |
| 1:1:27:LEU:CD1 | 6:B:314:ARG:CZ | 2.39 | 1.00 |
| 1:1:179:THR:CG2 | 4:4:87:SER:HB3 | 1.91 | 1.00 |
| 4:4:170:HIS:O | 4:4:171:ASN:O | 1.79 | 1.00 |
| 6:B:119:GLY:HA3 | 20:B:829:CLA:HED1 | 1.01 | 1.00 |
| 4:4:142:ASN:O | 4:4:150:LYS:CE | 2.10 | 1.00 |
| 3:3:94:ARG:NH1 | 3:3:97:PHE:CE2 | 2.29 | 1.00 |
| 20:A:824:CLA:CED | 20:A:825:CLA:CMD | 2.40 | 1.00 |
| 8:D:117:GLY:O | 8:D:118:VAL:HG23 | 1.60 | 1.00 |
| 20:K:102:CLA:O1A | 20:K:102:CLA:H3A | 1.62 | 1.00 |
| 16:L:163:LEU:HB3 | 16:L:164:PRO:HD2 | 1.44 | 1.00 |
| 4:4:34:PRO:CA | 4:4:35:GLU:HB2 | 1.91 | 0.99 |
| 6:B:103:ALA:O | 6:B:104:PHE:HB2 | 1.58 | 0.99 |
| 6:B:732:LYS:CB | 6:B:733:PHE:CA | 2.35 | 0.99 |
| 20:B:810:CLA:HBB2 | 20:B:810:CLA:C9 | 1.92 | 0.99 |
| 22:B:846:BCR:H382 | 22:B:846:BCR:H23C | 1.41 | 0.99 |
| 17:N:41:LYS:HB2 | 17:N:42:PHE:HA | 1.43 | 0.99 |
| 5:A:27:ILE:CA | 5:A:28:LYS:HG2 | 1.91 | 0.99 |
| 5:A:197:GLN:HA | 5:A:197:GLN:NE2 | 1.69 | 0.99 |
| 5:A:645:SER:HB3 | 6:B:637:PRO:HG3 | 1.42 | 0.99 |
| 20:A:826:CLA:C20 | 22:J:102:BCR:H17C | 1.92 | 0.99 |
| 6:B:119:GLY:CA | 20:B:829:CLA:HED1 | 1.92 | 0.99 |
| 16:L:163:LEU:HD12 | 16:L:164:PRO:N | 1.75 | 0.99 |
| 17:N:72:LYS:CD | 17:N:74:LYS:HG3 | 1.89 | 0.99 |
| 3:3:110:SER:C | 3:3:111:TYR:CD2 | 2.40 | 0.99 |
| 5:A:25:ASP:CB | 5:A:26:PRO:CA | 2.29 | 0.99 |
| 20:L:202:CLA:H12 | 20:L:202:CLA:O1D | 1.62 | 0.99 |
| 17:N:72:LYS:HB3 | 17:N:73:ASP:C | 1.85 | 0.99 |
| 21:F:202:LMU:H71 | 21:F:202:LMU:H31 | 1.41 | 0.99 |
| 3:3:74:ALA:HB3 | 3:3:75:PRO:HD3 | 1.45 | 0.99 |
| 20:H:101:CLA:H61 | 20:H:101:CLA:CMA | 1.93 | 0.99 |
| 21:H:106:LMU:H102 | 21:H:106:LMU:H62 | 1.44 | 0.99 |
| 4:4:121:PHE:CE2 | 4:4:122:LYS:O | 2.16 | 0.99 |
| 11:G:33:LYS:HA | 11:G:33:LYS:HE3 | 1.41 | 0.99 |
| 16:L:122:GLY:C | 16:L:124:LYS:H | 1.67 | 0.99 |
| 16:L:164:PRO:CA | 16:L:165:TYR:CG | 2.46 | 0.99 |
| 20:3:311:CLA:H102 | 20:3:311:CLA:H142 | 1.45 | 0.99 |
| 4:4:69:ILE:CG2 | 4:4:70:ILE:H | 1.76 | 0.99 |
| 5:A:208:ALA:HA | 5:A:310:PHE:O | 1.60 | 0.99 |
| 20:B:823:CLA:H72 | 20:B:823:CLA:HBB2 | 1.43 | 0.99 |
| 17:N:67:LEU:C | 17:N:68:GLU:HG3 | 1.87 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:N:72:LYS:HB2 | 17:N:73:ASP:HA | 1.43 | 0.99 |
| 3:3:94:ARG:NE | 3:3:97:PHE:CZ | 2.29 | 0.98 |
| 4:4:37:LEU:O | 4:4:39:TRP:HB3 | 1.61 | 0.98 |
| 8:D:32:SER:O | 16:L:21:GLY:HA2 | 1.62 | 0.98 |
| 5:A:27:ILE:HG22 | 5:A:28:LYS:HG2 | 1.42 | 0.98 |
| 20:A:824:CLA:H72 | 20:A:825:CLA:CED | 1.91 | 0.98 |
| 6:B:247:THR:CA | 6:B:250:ALA:HB2 | 1.92 | 0.98 |
| 22:B:847:BCR:H23C | 22:B:847:BCR:H382 | 1.45 | 0.98 |
| 11:G:42:SER:O | 11:G:46:ALA:HB3 | 1.61 | 0.98 |
| 12:H:44:ALA:CB | 16:L:145:PHE:HD1 | 1.75 | 0.98 |
| 2:2:70:LYS:HG3 | 2:2:73:ILE:CG1 | 1.92 | 0.98 |
| 3:3:98:ILE:O | 17:N:63:ASP:O | 1.81 | 0.98 |
| 4:4:106:TRP:CD2 | 20:4:301:CLA:HED3 | 1.96 | 0.98 |
| 5:A:267:THR:O | 5:A:269:PHE:HD2 | 1.45 | 0.98 |
| 20:A:807:CLA:HMB2 | 22:J:102:BCR:HC7 | 1.44 | 0.98 |
| 16:L:56:VAL:HA | 20:L:207:CLA:HED2 | 1.45 | 0.98 |
| 20:4:306:CLA:CGD | 20:4:306:CLA:HAA2 | 1.93 | 0.98 |
| 10:F:153:ASN:C | 10:F:153:ASN:HD22 | 1.69 | 0.98 |
| 1:1:144:LYS:NZ | 20:1:201:CLA:CED | 2.15 | 0.98 |
| 4:4:95:PHE:CE2 | 20:4:314:CLA:C4C | 2.46 | 0.98 |
| 2:2:70:LYS:HG3 | 2:2:73:ILE:HG13 | 1.42 | 0.98 |
| 4:4:69:ILE:HD12 | 4:4:175:LYS:HG2 | 1.45 | 0.98 |
| 22:I:103:BCR:HC8 | 22:I:103:BCR:H313 | 1.02 | 0.98 |
| 16:L:88:ALA:C | 16:L:90:GLY:H | 1.67 | 0.98 |
| 5:A:24:ARG:H | 5:A:24:ARG:CD | 1.76 | 0.98 |
| 10:F:5:LEU:HG | 10:F:6:THR:N | 1.74 | 0.98 |
| 20:2:316:CLA:H151 | 20:2:316:CLA:C19 | 1.94 | 0.98 |
| 4:4:37:LEU:C | 4:4:39:TRP:CB | 2.36 | 0.98 |
| 4:4:192:THR:HG22 | 4:4:193:ILE:C | 1.88 | 0.98 |
| 6:B:732:LYS:CB | 6:B:733:PHE:C | 2.37 | 0.98 |
| 10:F:42:ILE:HG13 | 10:F:43:LYS:H | 1.27 | 0.98 |
| 15:K:46:GLY:O | 15:K:47:LEU:HD12 | 1.64 | 0.98 |
| 17:N:63:ASP:H | 17:N:64:ASP:CB | 1.77 | 0.98 |
| 2:2:174:VAL:O | 2:2:178:TRP:CD1 | 2.16 | 0.98 |
| 3:3:173:GLU:HG2 | 3:3:174:LYS:H | 1.29 | 0.98 |
| 4:4:128:ALA:HB2 | 4:4:143:PHE:CZ | 1.99 | 0.98 |
| 5:A:401:TRP:CD1 | 20:A:826:CLA:HHC | 1.98 | 0.98 |
| 9:E:39:LEU:H | 9:E:40:ARG:NH1 | 1.61 | 0.98 |
| 16:L:64:LEU:HB3 | 16:L:68:PHE:HE1 | 1.28 | 0.98 |
| 5:A:316:MET:CG | 5:A:317:TYR:CD1 | 2.47 | 0.97 |
| 5:A:715:LYS:HD2 | 10:F:153:ASN:OD1 | 1.64 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:A:818:CLA:C12 | 20:A:818:CLA:CBB | 2.42 | 0.97 |
| 20:B:838:CLA:HBC1 | 10:F:83:PHE:CZ | 2.00 | 0.97 |
| 7:C:14:CYS:HA | 7:C:17:CYS:HG | 1.27 | 0.97 |
| 11:G:12:THR:HG22 | 11:G:72:LEU:CG | 1.94 | 0.97 |
| 17:N:72:LYS:CB | 17:N:74:LYS:H | 1.77 | 0.97 |
| 17:N:72:LYS:CD | 17:N:74:LYS:HG2 | 1.89 | 0.97 |
| 20:3:311:CLA:H142 | 20:3:311:CLA:C10 | 1.94 | 0.97 |
| 20:B:826:CLA:CBB | 20:B:839:CLA:HMB1 | 1.94 | 0.97 |
| 4:4:69:ILE:HG22 | 4:4:70:ILE:N | 1.73 | 0.97 |
| 4:4:118:ASP:OD1 | 4:4:123:GLN:HB2 | 1.63 | 0.97 |
| 13:I:11:LEU:HD12 | 22:I:103:BCR:C10 | 1.93 | 0.97 |
| 17:N:79:SER:HA | 17:N:80:ASN:O | 1.63 | 0.97 |
| 6:B:58:PHE:HB2 | 6:B:146:SER:CB | 1.92 | 0.97 |
| 20:1:215:CLA:HAA2 | 20:1:215:CLA:O1D | 1.61 | 0.97 |
| 4:4:106:TRP:CE2 | 20:4:301:CLA:CED | 2.46 | 0.97 |
| 6:B:517:PHE:CD2 | 6:B:517:PHE:O | 2.18 | 0.97 |
| 17:N:41:LYS:HG3 | 17:N:42:PHE:HB3 | 0.99 | 0.97 |
| 3:3:107:TRP:CD1 | 3:3:108:ALA:H | 1.79 | 0.97 |
| 20:4:304:CLA:HMC1 | 20:4:304:CLA:HBC3 | 1.46 | 0.97 |
| 7:C:7:ILE:HG22 | 7:C:65:VAL:CG2 | 1.94 | 0.97 |
| 5:A:304:LEU:HD22 | 20:A:816:CLA:CBB | 1.95 | 0.97 |
| 6:B:596:TRP:HH2 | 6:B:612:SER:O | 1.40 | 0.97 |
| 13:I:8:PHE:HB2 | 20:I:102:CLA:OBD | 1.64 | 0.97 |
| 22:I:103:BCR:H313 | 22:I:103:BCR:C8 | 1.93 | 0.97 |
| 5:A:365:LEU:HD23 | 20:A:805:CLA:HED3 | 1.45 | 0.97 |
| 20:B:824:CLA:H43 | 20:B:824:CLA:HAA1 | 1.46 | 0.97 |
| 10:F:22:LEU:H | 10:F:22:LEU:HD12 | 1.30 | 0.97 |
| 17:N:47:THR:HG21 | 17:N:54:LYS:NZ | 1.77 | 0.97 |
| 7:C:74:THR:OG1 | 7:C:80:ALA:CB | 2.12 | 0.97 |
| 15:K:40:LEU:O | 15:K:41:GLU:HB2 | 1.63 | 0.97 |
| 20:2:312:CLA:H8 | 20:2:312:CLA:C4 | 1.94 | 0.96 |
| 7:C:7:ILE:HG22 | 7:C:65:VAL:HG21 | 1.46 | 0.96 |
| 3:3:158:TYR:OH | 20:3:304:CLA:C3B | 2.13 | 0.96 |
| 5:A:599:PHE:CE2 | 5:A:735:VAL:HG21 | 2.00 | 0.96 |
| 20:A:839:CLA:HBA1 | 20:A:839:CLA:HMA3 | 1.45 | 0.96 |
| 17:N:6:TYR:C | 17:N:8:GLU:H | 1.70 | 0.96 |
| 2:2:169:LEU:CD2 | 20:2:305:CLA:CBB | 2.43 | 0.96 |
| 4:4:147:LEU:CD1 | 4:4:148:GLU:H | 1.78 | 0.96 |
| 6:B:551:LYS:NZ | 8:D:140:ASN:O | 1.98 | 0.96 |
| 20:B:824:CLA:HMD1 | 20:B:825:CLA:HBB2 | 1.43 | 0.96 |
| 21:E:101:LMU:H51 | 21:E:101:LMU:H12 | 1.47 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:G:12:THR:CG2 | 11:G:72:LEU:HG | 1.95 | 0.96 |
| 5:A:462:ILE:HD11 | 20:B:802:CLA:H51 | 1.46 | 0.96 |
| 7:C:1:MET:H1 | 7:C:4:SER:CA | 1.79 | 0.96 |
| 2:2:55:ALA:HB3 | 2:2:56:MET:CE | 1.95 | 0.96 |
| 4:4:142:ASN:CA | 4:4:150:LYS:HZ3 | 1.79 | 0.96 |
| 4:4:151:GLU:C | 4:4:154:ILE:H | 1.71 | 0.96 |
| 5:A:22:VAL:CB | 5:A:23:ASP:CA | 2.41 | 0.96 |
| 5:A:316:MET:CB | 5:A:317:TYR:CD1 | 2.49 | 0.96 |
| 4:4:192:THR:HG22 | 4:4:195:GLN:H | 1.27 | 0.96 |
| 20:4:315:CLA:HBD | 20:4:315:CLA:HBA1 | 1.47 | 0.96 |
| 5:A:78:VAL:HG11 | 20:A:805:CLA:HBC3 | 1.48 | 0.96 |
| 6:B:5:ILE:HB | 6:B:6:PRO:HD2 | 1.48 | 0.96 |
| 6:B:697:PRO:O | 7:C:79:LEU:HD13 | 1.65 | 0.96 |
| 18:R:40:UNK:N | 18:R:41:UNK:CB | 2.29 | 0.96 |
| 3:3:94:ARG:HG3 | 3:3:97:PHE:CE1 | 1.95 | 0.96 |
| 7:C:44:ARG:HH21 | 8:D:127:ARG:HB3 | 1.25 | 0.96 |
| 12:H:73:PRO:CG | 19:Z:2:FRU:H5 | 1.96 | 0.96 |
| 22:A:845:BCR:C31 | 20:A:851:CLA:H143 | 1.96 | 0.96 |
| 20:B:826:CLA:H11 | 20:B:839:CLA:HED3 | 1.46 | 0.96 |
| 20:H:109:CLA:HAC2 | 22:I:103:BCR:HC31 | 1.46 | 0.96 |
| 5:A:365:LEU:CD2 | 20:A:805:CLA:HED3 | 1.96 | 0.95 |
| 4:4:94:GLU:CG | 4:4:95:PHE:CD1 | 2.49 | 0.95 |
| 5:A:22:VAL:CA | 5:A:23:ASP:C | 2.38 | 0.95 |
| 6:B:269:TRP:HB2 | 6:B:497:TRP:CH2 | 2.02 | 0.95 |
| 6:B:732:LYS:HD2 | 6:B:734:GLY:N | 1.80 | 0.95 |
| 18:R:34:UNK:N | 18:R:36:UNK:CB | 2.29 | 0.95 |
| 5:A:58:HIS:CE1 | 20:A:803:CLA:ND | 2.34 | 0.95 |
| 5:A:606:TYR:O | 5:A:610:SER:HB2 | 1.66 | 0.95 |
| 20:A:801:CLA:O1D | 20:A:801:CLA:HAA1 | 1.66 | 0.95 |
| 20:A:819:CLA:H92 | 22:A:844:BCR:H373 | 0.97 | 0.95 |
| 20:B:824:CLA:H71 | 20:B:824:CLA:C2 | 1.95 | 0.95 |
| 22:F:204:BCR:H321 | 22:F:204:BCR:HC8 | 0.98 | 0.95 |
| 17:N:61:LEU:C | 17:N:61:LEU:HD12 | 1.88 | 0.95 |
| 4:4:91:PHE:CG | 20:4:311:CLA:C3C | 2.49 | 0.95 |
| 5:A:27:ILE:O | 5:A:27:ILE:HG23 | 1.66 | 0.95 |
| 20:A:819:CLA:HMD2 | 20:A:821:CLA:HBB2 | 1.49 | 0.95 |
| 10:F:23:LYS:HD3 | 10:F:23:LYS:N | 1.78 | 0.95 |
| 3:3:94:ARG:HH22 | 3:3:98:ILE:CG2 | 1.78 | 0.95 |
| 22:A:844:BCR:H23C | 22:A:844:BCR:H382 | 1.48 | 0.95 |
| 6:B:403:ASN:O | 6:B:406:ASN:CB | 2.14 | 0.95 |
| 20:B:824:CLA:H43 | 20:B:824:CLA:C1A | 1.96 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:H:44:ALA:HB2 | 16:L:145:PHE:HD1 | 1.26 | 0.95 |
| 20:J:101:CLA:HBA2 | 20:J:101:CLA:CBD | 1.95 | 0.95 |
| 3:3:92:TRP:N | 3:3:93:PHE:CB | 2.30 | 0.95 |
| 4:4:36:ASN:CB | 4:4:39:TRP:CE3 | 2.49 | 0.95 |
| 5:A:217:SER:OG | 22:A:843:BCR:C17 | 2.15 | 0.95 |
| 20:A:839:CLA:HBA1 | 20:A:839:CLA:HMA2 | 1.45 | 0.95 |
| 6:B:266:GLN:O | 6:B:267:SER:HB3 | 1.65 | 0.95 |
| 5:A:453:LEU:HB3 | 5:A:547:PHE:HB2 | 1.48 | 0.95 |
| 20:B:806:CLA:C19 | 10:F:104:TYR:HB3 | 1.96 | 0.95 |
| 17:N:75:TYR:O | 17:N:76:LYS:O | 1.84 | 0.95 |
| 18:R:34:UNK:CB | 18:R:36:UNK:N | 2.29 | 0.95 |
| 4:4:95:PHE:CZ | 20:4:314:CLA:C4C | 2.50 | 0.95 |
| 9:E:86:GLU:CG | 9:E:87:VAL:H | 1.72 | 0.95 |
| 17:N:41:LYS:HD2 | 17:N:42:PHE:CB | 1.97 | 0.95 |
| 22:A:845:BCR:H313 | 20:A:851:CLA:H143 | 1.46 | 0.95 |
| 2:2:118:CYS:O | 2:2:119:VAL:HG13 | 1.67 | 0.95 |
| 6:B:561:GLY:HA3 | 7:C:52:LYS:CG | 1.97 | 0.95 |
| 20:B:835:CLA:HMB1 | 22:B:846:BCR:C29 | 1.96 | 0.95 |
| 7:C:78:GLY:O | 7:C:81:TYR:HE1 | 1.50 | 0.95 |
| 3:3:94:ARG:CZ | 3:3:97:PHE:CZ | 2.49 | 0.94 |
| 20:3:310:CLA:HHD | 20:3:310:CLA:HBC3 | 1.49 | 0.94 |
| 5:A:24:ARG:NH1 | 5:A:29:THR:CB | 2.29 | 0.94 |
| 17:N:41:LYS:CD | 17:N:42:PHE:CB | 2.45 | 0.94 |
| 2:2:73:ILE:O | 2:2:74:LEU:HG | 1.67 | 0.94 |
| 2:2:169:LEU:HD23 | 20:2:305:CLA:HBB2 | 1.46 | 0.94 |
| 4:4:40:PHE:CG | 4:4:43:ALA:HB2 | 2.00 | 0.94 |
| 20:A:818:CLA:CBB | 20:A:818:CLA:H122 | 1.97 | 0.94 |
| 11:G:28:ARG:HG2 | 11:G:29:GLU:N | 1.78 | 0.94 |
| 16:L:56:VAL:HA | 20:L:207:CLA:CED | 1.97 | 0.94 |
| 17:N:57:LYS:HG3 | 17:N:58:VAL:H | 0.78 | 0.94 |
| 21:K:107:LMU:H32 | 21:K:107:LMU:H6D | 1.47 | 0.94 |
| 17:N:72:LYS:HE2 | 17:N:74:LYS:HE2 | 1.25 | 0.94 |
| 5:A:79:PHE:CE2 | 5:A:185:HIS:CD2 | 2.55 | 0.94 |
| 5:A:362:LEU:HD11 | 20:A:828:CLA:HBB2 | 1.48 | 0.94 |
| 20:A:839:CLA:H122 | 20:A:839:CLA:C7 | 1.92 | 0.94 |
| 23:B:843:PQN:C16 | 22:B:847:BCR:C33 | 2.44 | 0.94 |
| 26:H:107:UNL:O6 | 26:H:107:UNL:O4' | 1.85 | 0.94 |
| 17:N:72:LYS:NZ | 17:N:74:LYS:CE | 2.30 | 0.94 |
| 1:1:163:VAL:HA | 1:1:166:SER:HB3 | 1.47 | 0.94 |
| 4:4:94:GLU:HB3 | 4:4:95:PHE:CE1 | 2.03 | 0.94 |
| 4:4:122:LYS:NZ | 4:4:150:LYS:HD2 | 1.82 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:147:LEU:CD2 | 4:4:148:GLU:HG3 | 1.97 | 0.94 |
| 4:4:194:VAL:HB | 4:4:195:GLN:C | 1.93 | 0.94 |
| 5:A:76:ARG:CZ | 5:A:192:LYS:HG2 | 1.98 | 0.94 |
| 6:B:25:ILE:CG2 | 22:L:209:BCR:H282 | 1.97 | 0.94 |
| 2:2:54:TRP:CZ2 | 2:2:109:ARG:HD2 | 2.02 | 0.94 |
| 6:B:119:GLY:HA3 | 20:B:829:CLA:CED | 1.94 | 0.94 |
| 4:4:75:TRP:CE3 | 4:4:76:TYR:N | 2.35 | 0.94 |
| 4:4:122:LYS:CB | 4:4:143:PHE:CD2 | 2.50 | 0.94 |
| 5:A:328:LYS:CG | 5:A:332:GLU:HB2 | 1.95 | 0.94 |
| 12:H:20:GLN:HB3 | 12:H:22:ASP:CB | 1.98 | 0.94 |
| 4:4:38:ARG:HG3 | 4:4:39:TRP:N | 1.82 | 0.94 |
| 4:4:147:LEU:HD21 | 4:4:148:GLU:HG3 | 1.48 | 0.94 |
| 5:A:160:SER:O | 5:A:163:GLN:HG2 | 1.66 | 0.94 |
| 6:B:708:VAL:O | 6:B:712:HIS:HB2 | 1.65 | 0.94 |
| 22:B:801:BCR:H332 | 20:L:207:CLA:C3B | 1.97 | 0.94 |
| 7:C:14:CYS:CA | 7:C:17:CYS:SG | 2.55 | 0.94 |
| 7:C:20:ALA:O | 7:C:21:CYS:HB2 | 1.64 | 0.94 |
| 9:E:52:VAL:O | 9:E:53:VAL:HG23 | 1.65 | 0.94 |
| 16:L:163:LEU:HD12 | 16:L:164:PRO:CG | 1.98 | 0.94 |
| 2:2:178:TRP:O | 2:2:182:ILE:HG13 | 1.66 | 0.94 |
| 20:2:307:CLA:H41 | 20:2:307:CLA:H93 | 1.50 | 0.94 |
| 20:A:814:CLA:CHC | 22:A:843:BCR:H17C | 1.98 | 0.94 |
| 20:B:803:CLA:HHB | 20:B:803:CLA:H43 | 1.50 | 0.94 |
| 7:C:54:CYS:CB | 24:C:102:SF4:S1 | 2.55 | 0.94 |
| 16:L:161:LEU:CD1 | 16:L:162:ASP:O | 2.15 | 0.94 |
| 1:1:184:PRO:C | 1:1:185:TRP:CG | 2.44 | 0.94 |
| 3:3:92:TRP:HA | 3:3:95:THR:CB | 1.98 | 0.94 |
| 4:4:122:LYS:CB | 4:4:143:PHE:HD2 | 1.80 | 0.94 |
| 4:4:169:GLN:NE2 | 20:4:304:CLA:HHD | 1.83 | 0.94 |
| 5:A:368:LEU:HD21 | 20:A:818:CLA:H93 | 1.48 | 0.94 |
| 5:A:511:THR:HG23 | 20:A:817:CLA:O1A | 1.68 | 0.94 |
| 20:A:818:CLA:H71 | 20:A:818:CLA:CAB | 1.97 | 0.94 |
| 6:B:5:ILE:HB | 6:B:6:PRO:CD | 1.98 | 0.94 |
| 6:B:661:PHE:HB2 | 20:B:803:CLA:CMC | 1.97 | 0.94 |
| 20:B:810:CLA:H92 | 20:B:810:CLA:CBB | 1.98 | 0.94 |
| 7:C:1:MET:H3 | 7:C:4:SER:HB3 | 1.10 | 0.94 |
| 21:F:202:LMU:H22 | 21:F:202:LMU:H82 | 1.50 | 0.94 |
| 3:3:92:TRP:N | 3:3:93:PHE:CD1 | 2.36 | 0.93 |
| 5:A:22:VAL:CG2 | 5:A:23:ASP:CA | 2.45 | 0.93 |
| 4:4:149:ALA:CB | 4:4:151:GLU:HG2 | 1.98 | 0.93 |
| 4:4:154:ILE:HG13 | 4:4:155:ALA:H | 1.34 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:192:THR:HG21 | 4:4:195:GLN:H | 1.31 | 0.93 |
| 6:B:432:HIS:HE1 | 20:B:832:CLA:NB | 1.65 | 0.93 |
| 16:L:161:LEU:HD12 | 16:L:162:ASP:O | 1.68 | 0.93 |
| 2:2:50:VAL:O | 2:2:54:TRP:HD1 | 1.51 | 0.93 |
| 3:3:74:ALA:HA | 20:3:306:CLA:C4D | 1.96 | 0.93 |
| 2:2:102:ILE:C | 20:2:310:CLA:CBB | 2.40 | 0.93 |
| 2:2:211:LYS:HE2 | 2:2:211:LYS:HA | 1.50 | 0.93 |
| 3:3:94:ARG:HG3 | 3:3:97:PHE:HZ | 1.14 | 0.93 |
| 6:B:25:ILE:HG21 | 22:L:209:BCR:H292 | 0.94 | 0.93 |
| 7:C:59:PRO:O | 24:C:103:SF4:S3 | 2.26 | 0.93 |
| 20:3:314:CLA:CGA | 20:3:314:CLA:H3A | 1.98 | 0.93 |
| 24:A:856:SF4:S1 | 24:A:856:SF4:S2 | 2.66 | 0.93 |
| 6:B:294:ASN:HB3 | 11:G:36:PRO:HD2 | 1.50 | 0.93 |
| 4:4:118:ASP:HA | 4:4:122:LYS:C | 1.94 | 0.93 |
| 20:A:824:CLA:CED | 20:A:825:CLA:HMD2 | 1.97 | 0.93 |
| 20:A:825:CLA:O1D | 20:A:825:CLA:HBA1 | 1.68 | 0.93 |
| 17:N:62:SER:HB3 | 17:N:66:ASP:HB3 | 1.47 | 0.93 |
| 2:2:110:TRP:O | 2:2:113:ILE:HG12 | 1.69 | 0.93 |
| 6:B:474:PHE:CE2 | 6:B:476:ILE:HG13 | 2.03 | 0.93 |
| 9:E:68:ARG:HE | 9:E:68:ARG:C | 1.76 | 0.93 |
| 16:L:37:LEU:O | 16:L:42:ALA:HB3 | 1.68 | 0.93 |
| 2:2:110:TRP:HD1 | 2:2:113:ILE:HG21 | 1.33 | 0.93 |
| 5:A:242:ILE:HG12 | 5:A:243:PRO:HD3 | 1.50 | 0.93 |
| 3:3:92:TRP:N | 3:3:93:PHE:HB2 | 1.84 | 0.93 |
| 5:A:27:ILE:HG22 | 5:A:28:LYS:HG3 | 1.48 | 0.93 |
| 6:B:310:PRO:HG2 | 6:B:311:PRO:HD2 | 1.51 | 0.93 |
| 20:H:108:CLA:O1A | 20:H:108:CLA:H43 | 1.67 | 0.93 |
| 17:N:66:ASP:O | 17:N:67:LEU:HG | 1.69 | 0.93 |
| 6:B:732:LYS:CB | 6:B:733:PHE:HA | 1.97 | 0.93 |
| 7:C:1:MET:H1 | 7:C:4:SER:N | 1.66 | 0.93 |
| 11:G:49:THR:OG1 | 11:G:50:ARG:CG | 2.13 | 0.93 |
| 20:A:850:CLA:H11 | 6:B:616:LEU:HG | 1.51 | 0.92 |
| 6:B:127:ILE:HD13 | 6:B:198:ALA:HB2 | 1.51 | 0.92 |
| 6:B:612:SER:HA | 6:B:615:TYR:HE1 | 1.33 | 0.92 |
| 22:B:801:BCR:H332 | 20:L:207:CLA:C4B | 1.97 | 0.92 |
| 9:E:51:SER:HB3 | 9:E:68:ARG:CZ | 1.99 | 0.92 |
| 18:R:35:UNK:C | 18:R:38:UNK:CB | 2.46 | 0.92 |
| 9:E:72:VAL:O | 9:E:73:ASN:HB3 | 1.68 | 0.92 |
| 2:2:129:LYS:O | 2:2:132:GLY:N | 2.01 | 0.92 |
| 5:A:370:ILE:HG22 | 5:A:400:MET:HA | 1.51 | 0.92 |
| 5:A:390:ALA:HB2 | 5:A:754:ILE:HB | 1.52 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:A:845:BCR:H313 | 20:A:851:CLA:C14 | 1.99 | 0.92 |
| 24:A:856:SF4:S2 | 24:A:856:SF4:S4 | 2.67 | 0.92 |
| 12:H:27:ASP:O | 12:H:29:PRO:HD3 | 1.68 | 0.92 |
| 3:3:94:ARG:NH2 | 3:3:98:ILE:CG2 | 2.30 | 0.92 |
| 4:4:124:TYR:O | 4:4:127:PRO:CD | 2.17 | 0.92 |
| 4:4:160:MET:HE2 | 4:4:163:PHE:HD2 | 1.34 | 0.92 |
| 22:A:845:BCR:H393 | 22:A:845:BCR:H23C | 1.49 | 0.92 |
| 9:E:56:ASP:HB2 | 9:E:64:PRO:HB3 | 1.49 | 0.92 |
| 2:2:94:LEU:O | 2:2:98:GLU:HB3 | 1.69 | 0.92 |
| 5:A:669:GLY:H | 6:B:445:ALA:HA | 1.31 | 0.92 |
| 5:A:705:GLU:HB3 | 6:B:545:LYS:HZ1 | 1.33 | 0.92 |
| 6:B:493:TRP:CZ2 | 20:B:835:CLA:HBA1 | 2.05 | 0.92 |
| 10:F:5:LEU:CG | 10:F:6:THR:H | 1.81 | 0.92 |
| 4:4:142:ASN:CA | 4:4:150:LYS:NZ | 2.33 | 0.92 |
| 20:A:831:CLA:C4 | 16:L:64:LEU:HD23 | 1.99 | 0.92 |
| 20:B:823:CLA:HBC2 | 20:B:824:CLA:HBA1 | 1.51 | 0.92 |
| 20:B:824:CLA:H2A | 20:B:824:CLA:O2D | 1.70 | 0.92 |
| 20:B:829:CLA:H142 | 22:B:845:BCR:H10C | 1.49 | 0.92 |
| 20:K:104:CLA:HBC3 | 20:K:104:CLA:HHD | 1.51 | 0.92 |
| 17:N:72:LYS:CG | 17:N:74:LYS:CG | 2.41 | 0.92 |
| 2:2:128:ASN:C | 2:2:130:LEU:N | 2.16 | 0.92 |
| 20:A:831:CLA:H51 | 16:L:67:PRO:HB3 | 1.51 | 0.92 |
| 21:A:853:LMU:H22 | 21:A:853:LMU:C6 | 1.89 | 0.92 |
| 7:C:14:CYS:SG | 7:C:18:VAL:O | 2.28 | 0.92 |
| 16:L:163:LEU:CD1 | 16:L:164:PRO:N | 2.31 | 0.92 |
| 5:A:472:ARG:NH1 | 16:L:74:LEU:HG | 1.84 | 0.92 |
| 13:I:11:LEU:HG | 22:I:103:BCR:C7 | 2.00 | 0.92 |
| 17:N:76:LYS:HG3 | 17:N:77:CYS:H | 1.34 | 0.92 |
| 2:2:64:ILE:O | 2:2:68:LEU:HB2 | 1.69 | 0.91 |
| 6:B:361:ILE:HG23 | 6:B:368:GLN:OE1 | 1.69 | 0.91 |
| 6:B:442:VAL:HG21 | 20:B:833:CLA:HAC2 | 1.52 | 0.91 |
| 7:C:74:THR:CB | 7:C:80:ALA:HB2 | 2.00 | 0.91 |
| 13:I:26:LEU:HA | 13:I:29:GLU:O | 1.70 | 0.91 |
| 5:A:25:ASP:CG | 5:A:26:PRO:HA | 1.96 | 0.91 |
| 5:A:316:MET:HB3 | 5:A:317:TYR:CB | 2.00 | 0.91 |
| 20:A:818:CLA:O1A | 20:A:827:CLA:HMD3 | 1.70 | 0.91 |
| 10:F:22:LEU:O | 10:F:25:LEU:HB2 | 1.70 | 0.91 |
| 18:R:34:UNK:H | 18:R:36:UNK:C | 1.82 | 0.91 |
| 5:A:22:VAL:CG2 | 5:A:23:ASP:N | 2.29 | 0.91 |
| 11:G:60:SER:HA | 11:G:63:PRO:HD2 | 1.53 | 0.91 |
| 1:1:179:THR:HG21 | 4:4:87:SER:HB3 | 1.49 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:A:808:CLA:CHC | 20:A:809:CLA:HMD2 | 2.01 | 0.91 |
| 2:2:96:ILE:HG13 | 2:2:97:VAL:H | 1.35 | 0.91 |
| 3:3:74:ALA:HA | 20:3:306:CLA:C2D | 2.01 | 0.91 |
| 5:A:51:THR:CG2 | 20:A:837:CLA:HBB2 | 1.99 | 0.91 |
| 5:A:340:GLY:O | 5:A:343:HIS:HB2 | 1.70 | 0.91 |
| 4:4:74:LYS:H | 4:4:75:TRP:HA | 1.36 | 0.91 |
| 5:A:302:HIS:O | 5:A:306:ILE:HG12 | 1.70 | 0.91 |
| 5:A:316:MET:HG2 | 5:A:317:TYR:CE1 | 2.05 | 0.91 |
| 6:B:382:ILE:CG2 | 6:B:383:MET:H | 1.83 | 0.91 |
| 21:G:101:LMU:H22 | 21:G:101:LMU:C6' | 2.00 | 0.91 |
| 4:4:107:GLN:CA | 20:4:301:CLA:HMA2 | 2.01 | 0.91 |
| 6:B:247:THR:HA | 6:B:250:ALA:CB | 2.00 | 0.91 |
| 12:H:69:SER:HG | 20:H:108:CLA:H2 | 1.26 | 0.91 |
| 5:A:197:GLN:HE21 | 5:A:197:GLN:CA | 1.80 | 0.91 |
| 1:1:185:TRP:HH2 | 20:1:213:CLA:C1 | 1.57 | 0.91 |
| 5:A:648:THR:HG23 | 5:A:651:GLY:H | 1.36 | 0.91 |
| 7:C:1:MET:N | 7:C:3:HIS:C | 2.29 | 0.91 |
| 11:G:26:PHE:HB2 | 11:G:27:GLN:HE21 | 1.35 | 0.91 |
| 20:4:306:CLA:HBA1 | 20:4:306:CLA:CMA | 1.94 | 0.90 |
| 5:A:342:GLY:HA3 | 5:A:430:ASP:HB2 | 0.93 | 0.90 |
| 1:1:37:GLU:HA | 1:1:40:LYS:HB2 | 1.50 | 0.90 |
| 5:A:22:VAL:HB | 5:A:23:ASP:CA | 2.01 | 0.90 |
| 20:B:817:CLA:HBC2 | 20:B:817:CLA:HHD | 1.53 | 0.90 |
| 1:1:185:TRP:CH2 | 20:1:213:CLA:C2 | 2.49 | 0.90 |
| 2:2:171:MET:HE1 | 2:2:175:MET:HB2 | 1.54 | 0.90 |
| 4:4:102:GLU:OE2 | 20:4:313:CLA:C4B | 2.18 | 0.90 |
| 4:4:145:PRO:O | 4:4:147:LEU:HA | 1.70 | 0.90 |
| 5:A:40:PHE:HE1 | 5:A:53:TRP:CD1 | 1.89 | 0.90 |
| 20:A:824:CLA:HBA2 | 20:A:836:CLA:HED1 | 1.53 | 0.90 |
| 12:H:69:SER:HB2 | 20:H:108:CLA:C6 | 2.02 | 0.90 |
| 20:H:109:CLA:C4C | 22:I:103:BCR:HC22 | 2.01 | 0.90 |
| 18:R:52:UNK:CA | 18:R:53:UNK:CB | 2.48 | 0.90 |
| 1:1:89:VAL:HB | 1:1:90:PRO:HD3 | 1.50 | 0.90 |
| 20:A:806:CLA:H43 | 20:A:828:CLA:H11 | 1.50 | 0.90 |
| 21:A:853:LMU:H1' | 21:A:853:LMU:H31 | 1.53 | 0.90 |
| 7:C:73:THR:OG1 | 7:C:76:SER:HB3 | 1.70 | 0.90 |
| 11:G:37:GLU:CD | 11:G:42:SER:HB2 | 1.91 | 0.90 |
| 19:W:1:GLC:C1 | 19:W:2:FRU:H5 | 2.02 | 0.90 |
| 4:4:142:ASN:C | 4:4:150:LYS:CE | 2.44 | 0.90 |
| 4:4:106:TRP:C | 4:4:108:ASP:H | 1.77 | 0.90 |
| 17:N:58:VAL:CB | 17:N:59:PRO:CD | 2.48 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:2:302:CLA:HBC2 | 20:2:302:CLA:HHD | 1.54 | 0.90 |
| 20:2:303:CLA:C4 | 20:2:303:CLA:C4C | 2.50 | 0.90 |
| 3:3:66:MET:HE1 | 3:3:69:ALA:HB3 | 1.51 | 0.90 |
| 3:3:80:LYS:HZ1 | 3:3:92:TRP:CG | 1.89 | 0.90 |
| 5:A:114:THR:HG22 | 5:A:115:HIS:CE1 | 2.05 | 0.90 |
| 6:B:666:SER:HB3 | 6:B:671:TRP:HE1 | 1.34 | 0.90 |
| 11:G:68:ILE:CG2 | 11:G:72:LEU:HD13 | 2.02 | 0.90 |
| 15:K:83:VAL:O | 15:K:84:LEU:O | 1.88 | 0.90 |
| 3:3:92:TRP:N | 3:3:93:PHE:CG | 2.40 | 0.90 |
| 20:3:314:CLA:H3A | 20:3:314:CLA:O1A | 1.72 | 0.90 |
| 5:A:27:ILE:HG23 | 5:A:28:LYS:HD3 | 1.52 | 0.90 |
| 5:A:73:GLU:O | 5:A:76:ARG:N | 2.05 | 0.90 |
| 5:A:451:ILE:HD12 | 20:A:830:CLA:HED3 | 1.53 | 0.90 |
| 20:B:808:CLA:C9 | 20:B:825:CLA:O1D | 2.19 | 0.90 |
| 9:E:45:TRP:CH2 | 9:E:78:SER:OG | 2.24 | 0.90 |
| 21:E:101:LMU:H12 | 21:E:101:LMU:C5 | 2.01 | 0.90 |
| 20:K:104:CLA:H41 | 20:K:104:CLA:H8 | 0.92 | 0.90 |
| 5:A:466:THR:HG22 | 20:B:811:CLA:CHC | 2.01 | 0.90 |
| 8:D:113:HIS:H | 8:D:114:PRO:HD2 | 1.34 | 0.90 |
| 2:2:127:ASN:HB3 | 14:J:1:MET:O | 1.70 | 0.90 |
| 5:A:162:LEU:O | 5:A:165:TYR:HB3 | 1.72 | 0.90 |
| 20:A:833:CLA:H3A | 20:A:839:CLA:CBB | 2.02 | 0.90 |
| 23:B:843:PQN:H162 | 22:B:847:BCR:H331 | 1.53 | 0.90 |
| 21:H:104:LMU:H4' | 21:H:104:LMU:O2B | 1.71 | 0.90 |
| 22:J:102:BCR:H23C | 22:J:102:BCR:C39 | 2.02 | 0.90 |
| 16:L:163:LEU:HD11 | 16:L:165:TYR:CZ | 2.06 | 0.90 |
| 1:1:144:LYS:CE | 20:1:201:CLA:O2D | 2.16 | 0.89 |
| 4:4:107:GLN:C | 20:4:301:CLA:HMA1 | 1.95 | 0.89 |
| 5:A:626:GLY:HA3 | 5:A:636:HIS:HA | 1.54 | 0.89 |
| 20:A:814:CLA:C3B | 22:A:843:BCR:H19C | 2.01 | 0.89 |
| 9:E:42:GLU:HG2 | 9:E:43:SER:N | 1.87 | 0.89 |
| 8:D:124:ASN:HB3 | 8:D:125:PRO:HD3 | 1.54 | 0.89 |
| 9:E:83:ALA:O | 9:E:86:GLU:HG2 | 1.72 | 0.89 |
| 4:4:40:PHE:CB | 4:4:43:ALA:CB | 2.45 | 0.89 |
| 18:R:41:UNK:CB | 18:R:42:UNK:HA | 2.02 | 0.89 |
| 21:2:313:LMU:H12 | 21:2:313:LMU:H62 | 1.53 | 0.89 |
| 5:A:28:LYS:NZ | 5:A:28:LYS:CB | 2.30 | 0.89 |
| 5:A:586:ARG:HG3 | 7:C:49:VAL:HG21 | 1.54 | 0.89 |
| 20:B:838:CLA:H161 | 22:F:204:BCR:H313 | 1.54 | 0.89 |
| 7:C:5:VAL:HG21 | 7:C:65:VAL:HG11 | 1.50 | 0.89 |
| 15:K:42:ALA:O | 15:K:43:ARG:HD3 | 1.71 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:N:62:SER:CB | 17:N:66:ASP:CB | 2.47 | 0.89 |
| 20:B:806:CLA:H191 | 10:F:104:TYR:CB | 2.01 | 0.89 |
| 11:G:13:GLY:HA2 | 11:G:16:LEU:HG | 1.54 | 0.89 |
| 18:R:34:UNK:CA | 18:R:36:UNK:N | 2.36 | 0.89 |
| 2:2:59:ALA:HB3 | 2:2:172:LEU:HD13 | 1.54 | 0.89 |
| 21:A:854:LMU:H91 | 21:A:854:LMU:C2 | 2.02 | 0.89 |
| 6:B:25:ILE:CG2 | 22:L:209:BCR:C29 | 2.41 | 0.89 |
| 20:B:838:CLA:H152 | 22:F:204:BCR:H312 | 1.51 | 0.89 |
| 13:I:12:VAL:O | 13:I:17:PRO:HD3 | 1.73 | 0.89 |
| 2:2:116:PRO:O | 2:2:131:THR:HB | 1.72 | 0.89 |
| 4:4:94:GLU:CG | 4:4:95:PHE:CE1 | 2.55 | 0.89 |
| 4:4:118:ASP:HA | 4:4:123:GLN:N | 1.87 | 0.89 |
| 4:4:128:ALA:CB | 4:4:143:PHE:HE2 | 1.85 | 0.89 |
| 4:4:149:ALA:HB3 | 4:4:151:GLU:CG | 2.02 | 0.89 |
| 6:B:292:ARG:NE | 6:B:292:ARG:HA | 1.87 | 0.89 |
| 16:L:148:VAL:O | 16:L:149:SER:HB3 | 1.72 | 0.89 |
| 17:N:41:LYS:CB | 17:N:42:PHE:HB3 | 2.03 | 0.89 |
| 3:3:180:LYS:O | 3:3:181:LEU:C | 2.06 | 0.89 |
| 6:B:574:ASP:HA | 6:B:577:TYR:HB3 | 1.52 | 0.89 |
| 6:B:608:GLN:HA | 6:B:608:GLN:NE2 | 1.88 | 0.89 |
| 20:1:205:CLA:HMC2 | 20:1:208:CLA:HHD | 1.53 | 0.89 |
| 5:A:79:PHE:CE2 | 5:A:185:HIS:NE2 | 2.41 | 0.89 |
| 20:A:824:CLA:CED | 20:A:825:CLA:CAD | 2.50 | 0.89 |
| 20:F:201:CLA:CBC | 20:F:201:CLA:CHD | 2.51 | 0.89 |
| 11:G:16:LEU:HD23 | 11:G:68:ILE:HG23 | 1.54 | 0.89 |
| 5:A:368:LEU:CD2 | 20:A:818:CLA:C9 | 2.50 | 0.89 |
| 21:A:853:LMU:H81 | 21:A:853:LMU:H21 | 0.93 | 0.89 |
| 22:B:801:BCR:H331 | 20:L:207:CLA:C4B | 2.00 | 0.89 |
| 23:B:843:PQN:H192 | 22:B:847:BCR:H10C | 1.52 | 0.89 |
| 11:G:93:TYR:CA | 11:G:94:ASP:HB2 | 2.01 | 0.89 |
| 20:A:813:CLA:HBA1 | 20:A:823:CLA:H41 | 1.54 | 0.88 |
| 6:B:504:ASN:HD22 | 6:B:504:ASN:H | 1.15 | 0.88 |
| 18:R:38:UNK:O | 18:R:42:UNK:HA | 1.73 | 0.88 |
| 2:2:102:ILE:O | 20:2:310:CLA:HBB2 | 1.71 | 0.88 |
| 5:A:131:ILE:HG21 | 6:B:446:PHE:HA | 1.55 | 0.88 |
| 5:A:672:LEU:O | 5:A:674:ALA:N | 2.05 | 0.88 |
| 21:A:852:LMU:H3' | 21:A:852:LMU:O2B | 1.72 | 0.88 |
| 6:B:561:GLY:CA | 7:C:52:LYS:HG2 | 2.02 | 0.88 |
| 10:F:23:LYS:C | 10:F:24:LYS:HE2 | 1.98 | 0.88 |
| 22:I:103:BCR:C31 | 22:I:103:BCR:C8 | 2.42 | 0.88 |
| 16:L:164:PRO:CA | 16:L:165:TYR:HB3 | 1.91 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:205:GLY:CA | 5:A:252:ARG:HH12 | 1.86 | 0.88 |
| 20:2:314:CLA:CGD | 20:2:314:CLA:HBA2 | 2.04 | 0.88 |
| 22:2:317:BCR:H393 | 22:2:317:BCR:C23 | 2.01 | 0.88 |
| 5:A:22:VAL:CG2 | 5:A:23:ASP:HA | 2.01 | 0.88 |
| 5:A:328:LYS:HE3 | 5:A:332:GLU:HG3 | 1.52 | 0.88 |
| 24:A:856:SF4:S1 | 24:A:856:SF4:S4 | 2.71 | 0.88 |
| 6:B:190:TRP:HA | 20:B:815:CLA:HBB2 | 1.55 | 0.88 |
| 17:N:67:LEU:C | 17:N:68:GLU:CG | 2.45 | 0.88 |
| 17:N:18:ASP:HB2 | 17:N:22:LEU:HG | 1.53 | 0.88 |
| 17:N:47:THR:OG1 | 17:N:54:LYS:HD3 | 1.72 | 0.88 |
| 21:1:217:LMU:C9 | 21:G:103:LMU:O3' | 2.20 | 0.88 |
| 4:4:118:ASP:CG | 4:4:123:GLN:HB2 | 1.97 | 0.88 |
| 6:B:382:ILE:HG22 | 6:B:383:MET:N | 1.88 | 0.88 |
| 6:B:492:ILE:H | 6:B:492:ILE:HD13 | 1.39 | 0.88 |
| 6:B:556:SER:C | 6:B:558:PRO:HD2 | 1.99 | 0.88 |
| 16:L:163:LEU:HD12 | 16:L:165:TYR:CD1 | 2.09 | 0.88 |
| 5:A:81:ALA:CB | 20:A:804:CLA:HMA3 | 2.04 | 0.88 |
| 6:B:212:PHE:HE1 | 20:B:815:CLA:HHD | 1.37 | 0.88 |
| 17:N:72:LYS:HB3 | 17:N:74:LYS:H | 1.14 | 0.88 |
| 21:2:313:LMU:C1 | 21:2:313:LMU:H72 | 2.03 | 0.88 |
| 4:4:60:LEU:HG | 4:4:61:PRO:HD3 | 1.56 | 0.88 |
| 5:A:301:HIS:NE2 | 20:A:816:CLA:O1D | 2.07 | 0.88 |
| 5:A:425:THR:HG21 | 8:D:59:GLU:OE2 | 1.72 | 0.88 |
| 6:B:230:TRP:CH2 | 11:G:11:SER:HB2 | 2.09 | 0.88 |
| 15:K:43:ARG:HG3 | 15:K:43:ARG:NH1 | 1.71 | 0.88 |
| 5:A:100:GLY:HA3 | 5:A:153:TRP:CH2 | 2.09 | 0.88 |
| 5:A:316:MET:CB | 5:A:317:TYR:HD1 | 1.86 | 0.88 |
| 21:G:101:LMU:H22 | 21:G:101:LMU:H6D | 1.54 | 0.88 |
| 21:K:107:LMU:O2B | 21:K:107:LMU:H5' | 1.74 | 0.88 |
| 16:L:161:LEU:HD12 | 16:L:162:ASP:N | 1.88 | 0.88 |
| 2:2:110:TRP:HA | 2:2:113:ILE:HG23 | 1.56 | 0.88 |
| 6:B:86:PRO:O | 6:B:87:ILE:HG13 | 1.74 | 0.88 |
| 20:B:808:CLA:H93 | 20:B:825:CLA:O1D | 1.74 | 0.88 |
| 10:F:40:LEU:HA | 10:F:42:ILE:HG12 | 1.56 | 0.88 |
| 12:H:25:GLY:HA3 | 12:H:27:ASP:H | 1.38 | 0.88 |
| 4:4:89:THR:O | 4:4:92:VAL:HB | 1.74 | 0.87 |
| 20:A:831:CLA:H41 | 16:L:64:LEU:HD23 | 1.54 | 0.87 |
| 21:R:103:LMU:H31 | 21:R:103:LMU:C1' | 2.02 | 0.87 |
| 2:2:168:ARG:O | 2:2:172:LEU:HD12 | 1.74 | 0.87 |
| 4:4:151:GLU:HA | 4:4:154:ILE:HG23 | 1.56 | 0.87 |
| 5:A:141:ARG:HG3 | 5:A:141:ARG:HH21 | 1.38 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:328:LYS:CE | 5:A:332:GLU:HG3 | 2.04 | 0.87 |
| 6:B:174:ARG:HB2 | 20:B:814:CLA:CBC | 2.03 | 0.87 |
| 5:A:239:PRO:HA | 5:A:242:ILE:CD1 | 2.05 | 0.87 |
| 20:B:826:CLA:HED1 | 20:B:827:CLA:HMD2 | 1.53 | 0.87 |
| 23:B:843:PQN:H191 | 22:B:847:BCR:C10 | 2.04 | 0.87 |
| 10:F:93:ILE:O | 10:F:96:TRP:HD1 | 1.56 | 0.87 |
| 3:3:93:PHE:HB2 | 3:3:95:THR:HG23 | 1.52 | 0.87 |
| 4:4:192:THR:CG2 | 4:4:195:GLN:N | 2.37 | 0.87 |
| 5:A:114:THR:OG1 | 5:A:525:ASN:HB2 | 1.74 | 0.87 |
| 5:A:331:LEU:HD11 | 5:A:346:LEU:CB | 2.03 | 0.87 |
| 20:A:825:CLA:CAB | 20:A:832:CLA:CMA | 2.45 | 0.87 |
| 20:A:830:CLA:H161 | 22:L:209:BCR:C36 | 2.04 | 0.87 |
| 20:A:833:CLA:C3A | 20:A:839:CLA:HBB1 | 2.05 | 0.87 |
| 22:A:845:BCR:C31 | 20:A:851:CLA:C14 | 2.51 | 0.87 |
| 19:W:1:GLC:C1 | 19:W:2:FRU:C5 | 2.52 | 0.87 |
| 20:2:303:CLA:HBC3 | 20:2:303:CLA:CHD | 2.04 | 0.87 |
| 3:3:94:ARG:HA | 3:3:97:PHE:CD1 | 2.09 | 0.87 |
| 5:A:217:SER:OG | 22:A:843:BCR:H17C | 1.71 | 0.87 |
| 17:N:70:GLU:C | 17:N:72:LYS:H | 1.81 | 0.87 |
| 20:A:816:CLA:H2 | 20:A:816:CLA:HBA2 | 1.55 | 0.87 |
| 24:A:856:SF4:S4 | 24:A:856:SF4:S3 | 2.72 | 0.87 |
| 20:L:208:CLA:HAA1 | 20:L:208:CLA:CGD | 2.04 | 0.87 |
| 17:N:70:GLU:O | 17:N:72:LYS:HD3 | 1.74 | 0.87 |
| 20:2:312:CLA:HBA1 | 20:2:312:CLA:C4A | 2.03 | 0.87 |
| 3:3:157:ALA:C | 3:3:158:TYR:HD2 | 1.83 | 0.87 |
| 4:4:33:ASP:HB3 | 4:4:34:PRO:CD | 2.03 | 0.87 |
| 4:4:104:ARG:HH11 | 4:4:105:ARG:HB3 | 1.39 | 0.87 |
| 16:L:157:LEU:C | 16:L:158:MET:O | 2.17 | 0.87 |
| 2:2:66:GLU:O | 2:2:69:THR:N | 2.07 | 0.87 |
| 5:A:412:ALA:HB2 | 5:A:598:VAL:HG11 | 1.55 | 0.87 |
| 6:B:461:GLN:O | 6:B:464:GLN:HG2 | 1.74 | 0.87 |
| 5:A:204:ASN:O | 5:A:205:HIS:HB2 | 1.73 | 0.87 |
| 5:A:249:ILE:CG1 | 5:A:250:LEU:H | 1.85 | 0.87 |
| 3:3:112:THR:OG1 | 3:3:113:LEU:N | 2.04 | 0.86 |
| 5:A:382:TYR:OH | 20:A:827:CLA:H42 | 1.73 | 0.86 |
| 6:B:87:ILE:CA | 6:B:115:ASN:HA | 2.04 | 0.86 |
| 6:B:180:SER:HB2 | 6:B:288:GLY:HA3 | 1.57 | 0.86 |
| 9:E:52:VAL:HG12 | 9:E:53:VAL:H | 1.35 | 0.86 |
| 20:L:208:CLA:HHD | 20:L:208:CLA:CBC | 2.04 | 0.86 |
| 18:R:34:UNK:N | 18:R:36:UNK:CA | 2.37 | 0.86 |
| 4:4:107:GLN:CA | 20:4:301:CLA:CMA | 2.53 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:81:ALA:HB1 | 20:A:804:CLA:HMA2 | 1.56 | 0.86 |
| 5:A:368:LEU:HD21 | 20:A:818:CLA:C9 | 2.04 | 0.86 |
| 20:A:803:CLA:HBB2 | 20:A:804:CLA:C4C | 2.04 | 0.86 |
| 20:A:839:CLA:HHD | 20:A:839:CLA:HBC2 | 1.56 | 0.86 |
| 9:E:58:ASP:OD2 | 9:E:60:LYS:HG2 | 1.75 | 0.86 |
| 13:I:24:LEU:C | 13:I:26:LEU:H | 1.78 | 0.86 |
| 4:4:75:TRP:HB2 | 20:4:310:CLA:HMD2 | 1.57 | 0.86 |
| 6:B:391:PRO:HB3 | 6:B:538:ALA:HA | 1.55 | 0.86 |
| 1:1:144:LYS:HZ2 | 20:1:201:CLA:HED3 | 0.78 | 0.86 |
| 3:3:94:ARG:HH22 | 3:3:98:ILE:HG21 | 1.05 | 0.86 |
| 4:4:122:LYS:HD3 | 4:4:150:LYS:HD2 | 1.54 | 0.86 |
| 5:A:470:LEU:CD1 | 6:B:95:HIS:HB3 | 2.06 | 0.86 |
| 9:E:40:ARG:NH2 | 9:E:86:GLU:OE1 | 2.07 | 0.86 |
| 11:G:94:ASP:H | 11:G:95:PRO:HD3 | 0.71 | 0.86 |
| 16:L:27:VAL:HA | 20:L:204:CLA:CMA | 2.05 | 0.86 |
| 1:1:184:PRO:O | 1:1:185:TRP:CD1 | 2.28 | 0.86 |
| 21:1:217:LMU:H51 | 21:G:103:LMU:H12 | 1.57 | 0.86 |
| 4:4:68:GLY:O | 4:4:71:ASN:HB2 | 1.74 | 0.86 |
| 5:A:316:MET:HB3 | 5:A:317:TYR:CD1 | 2.10 | 0.86 |
| 5:A:328:LYS:HG2 | 5:A:332:GLU:CB | 2.05 | 0.86 |
| 6:B:398:TYR:O | 8:D:143:PRO:HG2 | 1.74 | 0.86 |
| 11:G:94:ASP:N | 11:G:95:PRO:CD | 2.14 | 0.86 |
| 3:3:132:TRP:HZ3 | 3:3:155:GLU:HG2 | 1.07 | 0.86 |
| 20:3:310:CLA:HBC3 | 20:3:310:CLA:CHD | 2.06 | 0.86 |
| 21:3:319:LMU:H32 | 21:3:319:LMU:C8 | 2.00 | 0.86 |
| 7:C:44:ARG:NH2 | 8:D:127:ARG:HB3 | 1.88 | 0.86 |
| 17:N:72:LYS:HG3 | 17:N:74:LYS:HG3 | 0.86 | 0.86 |
| 6:B:374:HIS:HB2 | 20:B:828:CLA:C1B | 2.06 | 0.86 |
| 7:C:5:VAL:CG2 | 7:C:65:VAL:HG11 | 2.05 | 0.86 |
| 17:N:67:LEU:O | 17:N:68:GLU:HG3 | 1.75 | 0.86 |
| 20:2:312:CLA:HBA1 | 20:2:312:CLA:NA | 1.88 | 0.86 |
| 4:4:124:TYR:HB3 | 4:4:143:PHE:CD1 | 2.11 | 0.86 |
| 20:A:824:CLA:HED2 | 20:A:825:CLA:CAD | 2.05 | 0.86 |
| 6:B:588:GLY:O | 6:B:592:PHE:HB2 | 1.76 | 0.86 |
| 20:B:802:CLA:HBB2 | 20:B:803:CLA:C1B | 2.06 | 0.86 |
| 8:D:39:LYS:HD2 | 8:D:42:VAL:CG1 | 2.05 | 0.86 |
| 14:J:2:ARG:HH12 | 14:J:8:LEU:HD13 | 1.41 | 0.86 |
| 2:2:103:GLY:N | 20:2:310:CLA:HBB2 | 1.89 | 0.86 |
| 4:4:147:LEU:HD13 | 4:4:148:GLU:N | 1.89 | 0.86 |
| 5:A:599:PHE:CE2 | 5:A:731:ARG:HB3 | 2.11 | 0.86 |
| 20:A:807:CLA:C3B | 22:J:102:BCR:H331 | 2.05 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:25:ILE:HG21 | 22:L:209:BCR:C28 | 2.05 | 0.86 |
| 20:B:808:CLA:OBD | 20:B:808:CLA:H122 | 1.74 | 0.86 |
| 8:D:32:SER:H | 16:L:23:LEU:HG | 1.38 | 0.86 |
| 3:3:132:TRP:CH2 | 3:3:155:GLU:HG3 | 2.08 | 0.85 |
| 5:A:452:PHE:HE1 | 20:A:835:CLA:CBB | 1.88 | 0.85 |
| 16:L:165:TYR:HA | 16:L:166:TYR:O | 1.76 | 0.85 |
| 3:3:63:ARG:HH22 | 3:3:189:LEU:HD23 | 1.40 | 0.85 |
| 4:4:95:PHE:N | 4:4:95:PHE:HD1 | 1.73 | 0.85 |
| 5:A:114:THR:HG22 | 5:A:115:HIS:ND1 | 1.90 | 0.85 |
| 5:A:259:TYR:HB3 | 5:A:260:PRO:HD2 | 1.58 | 0.85 |
| 7:C:5:VAL:C | 7:C:65:VAL:HG22 | 2.00 | 0.85 |
| 20:F:201:CLA:HBC3 | 20:F:201:CLA:CHD | 2.05 | 0.85 |
| 16:L:165:TYR:CD1 | 16:L:165:TYR:O | 2.29 | 0.85 |
| 3:3:80:LYS:HD3 | 3:3:105:ASN:HB2 | 1.58 | 0.85 |
| 4:4:145:PRO:O | 4:4:146:THR:C | 2.16 | 0.85 |
| 4:4:169:GLN:NE2 | 4:4:169:GLN:HA | 1.90 | 0.85 |
| 4:4:169:GLN:CD | 20:4:304:CLA:HHD | 2.01 | 0.85 |
| 20:A:804:CLA:HBB2 | 20:A:806:CLA:C3D | 2.06 | 0.85 |
| 20:A:825:CLA:HBB2 | 20:A:832:CLA:HMA1 | 0.86 | 0.85 |
| 6:B:571:SER:OG | 6:B:574:ASP:OD1 | 1.94 | 0.85 |
| 21:B:805:LMU:O3' | 21:B:805:LMU:H1B | 1.74 | 0.85 |
| 10:F:42:ILE:HG13 | 10:F:43:LYS:N | 1.87 | 0.85 |
| 2:2:91:THR:O | 2:2:94:LEU:HB3 | 1.75 | 0.85 |
| 6:B:421:HIS:NE2 | 20:F:201:CLA:C4D | 2.40 | 0.85 |
| 6:B:545:LYS:HG2 | 9:E:74:TYR:CE2 | 2.11 | 0.85 |
| 21:1:218:LMU:C6B | 21:1:218:LMU:H3' | 2.07 | 0.85 |
| 2:2:54:TRP:CE2 | 2:2:109:ARG:HD2 | 2.12 | 0.85 |
| 4:4:169:GLN:CG | 20:4:304:CLA:HAC2 | 2.06 | 0.85 |
| 5:A:87:SER:HB2 | 5:A:178:MET:O | 1.75 | 0.85 |
| 6:B:295:PHE:H | 6:B:295:PHE:HD2 | 1.19 | 0.85 |
| 16:L:66:GLY:HA3 | 20:L:208:CLA:CHC | 2.07 | 0.85 |
| 5:A:24:ARG:H | 5:A:24:ARG:HD2 | 1.40 | 0.85 |
| 5:A:462:ILE:HG21 | 20:A:831:CLA:HMC1 | 1.57 | 0.85 |
| 5:A:684:PHE:C | 5:A:684:PHE:CD2 | 2.55 | 0.85 |
| 20:A:818:CLA:O1A | 20:A:827:CLA:CMD | 2.23 | 0.85 |
| 20:A:839:CLA:HHD | 20:A:839:CLA:HBC3 | 1.58 | 0.85 |
| 20:B:806:CLA:CMD | 22:F:203:BCR:HC41 | 2.07 | 0.85 |
| 8:D:102:ARG:HE | 8:D:110:GLN:HB2 | 1.40 | 0.85 |
| 20:1:205:CLA:HMC3 | 20:1:208:CLA:HHD | 1.56 | 0.85 |
| 3:3:97:PHE:CD2 | 3:3:97:PHE:O | 2.29 | 0.85 |
| 20:3:310:CLA:H193 | 20:3:310:CLA:H152 | 1.59 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:74:LYS:H | 4:4:75:TRP:CA | 1.90 | 0.85 |
| 5:A:22:VAL:HB | 5:A:23:ASP:C | 2.01 | 0.85 |
| 5:A:723:ARG:CG | 5:A:723:ARG:HH11 | 1.88 | 0.85 |
| 6:B:715:VAL:HG23 | 6:B:719:PHE:CD2 | 2.12 | 0.85 |
| 20:R:107:CLA:HED3 | 20:R:107:CLA:CHA | 2.05 | 0.85 |
| 6:B:521:HIS:HE1 | 20:B:838:CLA:NA | 1.74 | 0.85 |
| 6:B:531:THR:HG22 | 20:B:826:CLA:HMC2 | 1.59 | 0.85 |
| 20:B:806:CLA:HED3 | 20:B:806:CLA:H2A | 1.56 | 0.85 |
| 5:A:27:ILE:O | 5:A:28:LYS:HG2 | 1.76 | 0.85 |
| 5:A:246:HIS:O | 5:A:248:PHE:N | 2.10 | 0.85 |
| 5:A:599:PHE:CE2 | 5:A:735:VAL:CG2 | 2.60 | 0.85 |
| 6:B:174:ARG:HB2 | 20:B:814:CLA:HBC2 | 1.57 | 0.85 |
| 6:B:282:PHE:HZ | 20:B:817:CLA:C1 | 1.90 | 0.85 |
| 20:2:314:CLA:HBA2 | 20:2:314:CLA:CBD | 2.07 | 0.85 |
| 4:4:107:GLN:HA | 20:4:301:CLA:CMA | 2.05 | 0.85 |
| 9:E:52:VAL:O | 9:E:53:VAL:HG22 | 1.74 | 0.85 |
| 20:H:108:CLA:HBB2 | 13:I:13:GLY:O | 1.77 | 0.85 |
| 20:B:826:CLA:HHD | 20:B:826:CLA:CBC | 2.06 | 0.84 |
| 4:4:124:TYR:CB | 4:4:143:PHE:CD1 | 2.60 | 0.84 |
| 6:B:388:ALA:C | 6:B:391:PRO:HD2 | 2.00 | 0.84 |
| 7:C:5:VAL:HG21 | 7:C:65:VAL:HG13 | 0.93 | 0.84 |
| 15:K:44:GLU:O | 15:K:46:GLY:HA2 | 1.77 | 0.84 |
| 3:3:158:TYR:HB3 | 3:3:159:PRO:CD | 2.06 | 0.84 |
| 4:4:91:PHE:CD2 | 4:4:91:PHE:C | 2.54 | 0.84 |
| 20:A:822:CLA:C4C | 22:A:844:BCR:C19 | 2.49 | 0.84 |
| 6:B:419:ILE:O | 6:B:420:SER:OG | 1.94 | 0.84 |
| 16:L:14:LEU:HA | 16:L:24:GLU:HG3 | 1.59 | 0.84 |
| 4:4:128:ALA:HB2 | 4:4:143:PHE:HE2 | 1.40 | 0.84 |
| 20:A:850:CLA:C3B | 6:B:589:TRP:HH2 | 1.91 | 0.84 |
| 20:B:824:CLA:H151 | 20:B:824:CLA:C10 | 2.04 | 0.84 |
| 10:F:151:ASP:O | 10:F:154:PHE:HB3 | 1.76 | 0.84 |
| 17:N:63:ASP:N | 17:N:64:ASP:HB3 | 1.91 | 0.84 |
| 3:3:95:THR:N | 3:3:97:PHE:CD1 | 2.42 | 0.84 |
| 5:A:567:ARG:HH11 | 8:D:35:GLY:HA2 | 1.37 | 0.84 |
| 20:A:826:CLA:HBA1 | 20:A:826:CLA:H43 | 1.60 | 0.84 |
| 6:B:353:TYR:CG | 6:B:594:TRP:HZ3 | 1.94 | 0.84 |
| 11:G:43:HIS:CE1 | 11:G:45:GLU:HG2 | 2.13 | 0.84 |
| 20:H:109:CLA:HAC1 | 22:I:103:BCR:HC31 | 1.60 | 0.84 |
| 4:4:160:MET:HE2 | 4:4:163:PHE:CD2 | 2.13 | 0.84 |
| 21:4:321:LMU:O2' | 21:4:321:LMU:H22 | 1.77 | 0.84 |
| 20:A:822:CLA:CHD | 22:A:844:BCR:C19 | 2.54 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:120:VAL:HA | 6:B:123:TRP:NE1 | 1.92 | 0.84 |
| 20:B:826:CLA:C1 | 20:B:839:CLA:HED3 | 2.06 | 0.84 |
| 20:B:836:CLA:HHD | 20:B:836:CLA:HBC2 | 1.59 | 0.84 |
| 1:1:184:PRO:O | 1:1:185:TRP:CG | 2.30 | 0.84 |
| 20:2:305:CLA:H2 | 20:2:307:CLA:HMD2 | 1.59 | 0.84 |
| 20:3:311:CLA:H102 | 20:3:311:CLA:C14 | 2.07 | 0.84 |
| 6:B:22:TRP:HE1 | 20:B:840:CLA:CBB | 1.90 | 0.84 |
| 6:B:608:GLN:HE21 | 6:B:608:GLN:CA | 1.91 | 0.84 |
| 7:C:63:LEU:HG | 7:C:64:SER:N | 1.92 | 0.84 |
| 16:L:123:ARG:CZ | 16:L:123:ARG:HA | 2.07 | 0.84 |
| 17:N:41:LYS:HB2 | 17:N:42:PHE:CA | 2.06 | 0.84 |
| 21:R:104:LMU:H2' | 21:R:104:LMU:C2 | 2.01 | 0.84 |
| 19:a:1:GLC:O2 | 19:a:2:FRU:H3 | 1.78 | 0.84 |
| 1:1:183:ASP:CB | 1:1:184:PRO:HD2 | 2.05 | 0.84 |
| 5:A:110:LEU:HD11 | 5:A:239:PRO:HG2 | 1.60 | 0.84 |
| 6:B:142:LEU:HD22 | 22:B:845:BCR:H333 | 1.60 | 0.84 |
| 6:B:732:LYS:HD2 | 6:B:733:PHE:C | 2.01 | 0.84 |
| 20:H:101:CLA:HMA2 | 20:H:101:CLA:C2 | 2.07 | 0.84 |
| 17:N:62:SER:CB | 17:N:66:ASP:HB3 | 2.08 | 0.84 |
| 20:2:314:CLA:C5 | 20:2:314:CLA:CMA | 2.55 | 0.84 |
| 6:B:140:ILE:HD13 | 6:B:140:ILE:H | 1.41 | 0.84 |
| 6:B:393:PHE:HD2 | 6:B:397:ASP:OD1 | 1.61 | 0.84 |
| 15:K:44:GLU:CD | 15:K:45:SER:C | 2.46 | 0.84 |
| 5:A:131:ILE:O | 5:A:671:SER:HA | 1.77 | 0.84 |
| 5:A:711:HIS:HB3 | 5:A:717:ALA:HB2 | 1.58 | 0.84 |
| 22:A:845:BCR:H311 | 22:A:845:BCR:C8 | 2.07 | 0.84 |
| 6:B:293:THR:C | 11:G:38:GLN:OE1 | 2.21 | 0.84 |
| 22:F:204:BCR:C8 | 22:F:204:BCR:C32 | 2.47 | 0.84 |
| 1:1:39:TYR:CB | 20:1:210:CLA:OBD | 2.25 | 0.83 |
| 2:2:196:HIS:NE2 | 19:O:1:GLC:O3 | 2.10 | 0.83 |
| 22:A:845:BCR:C39 | 22:A:845:BCR:H23C | 2.08 | 0.83 |
| 5:A:547:PHE:O | 5:A:551:VAL:HG13 | 1.78 | 0.83 |
| 5:A:711:HIS:CD2 | 20:A:837:CLA:HBC1 | 2.13 | 0.83 |
| 11:G:17:PHE:O | 11:G:20:ARG:HB2 | 1.76 | 0.83 |
| 20:2:303:CLA:C4 | 20:2:303:CLA:CHD | 2.56 | 0.83 |
| 20:2:314:CLA:HBD | 20:2:314:CLA:HBA2 | 1.60 | 0.83 |
| 3:3:132:TRP:HZ3 | 3:3:155:GLU:CG | 1.60 | 0.83 |
| 4:4:154:ILE:HG13 | 4:4:155:ALA:N | 1.92 | 0.83 |
| 4:4:174:GLY:O | 4:4:175:LYS:CG | 2.23 | 0.83 |
| 5:A:335:LYS:HG2 | 5:A:336:GLY:N | 1.88 | 0.83 |
| 17:N:72:LYS:HD2 | 17:N:74:LYS:HG2 | 1.60 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:189:ALA:CB | 20:B:829:CLA:H203 | 2.07 | 0.83 |
| 8:D:124:ASN:CB | 8:D:125:PRO:HD3 | 2.08 | 0.83 |
| 20:4:304:CLA:HAA1 | 20:F:207:CLA:H42 | 1.59 | 0.83 |
| 6:B:233:TYR:CD2 | 20:B:817:CLA:HED1 | 2.13 | 0.83 |
| 6:B:374:HIS:HB2 | 20:B:828:CLA:NB | 1.92 | 0.83 |
| 6:B:560:ASP:OD1 | 6:B:561:GLY:N | 2.12 | 0.83 |
| 2:2:178:TRP:C | 2:2:182:ILE:HG13 | 2.03 | 0.83 |
| 3:3:64:TYR:HB3 | 20:3:310:CLA:H42 | 1.58 | 0.83 |
| 21:A:853:LMU:C7 | 21:A:853:LMU:H112 | 2.08 | 0.83 |
| 6:B:382:ILE:O | 6:B:384:THR:N | 2.11 | 0.83 |
| 15:K:40:LEU:O | 15:K:41:GLU:CB | 2.22 | 0.83 |
| 2:2:167:GLY:O | 2:2:170:ALA:N | 2.12 | 0.83 |
| 3:3:80:LYS:HD3 | 3:3:105:ASN:CB | 2.07 | 0.83 |
| 3:3:92:TRP:C | 3:3:94:ARG:C | 2.47 | 0.83 |
| 8:D:113:HIS:NE2 | 8:D:118:VAL:HG11 | 1.94 | 0.83 |
| 12:H:25:GLY:CA | 12:H:27:ASP:H | 1.91 | 0.83 |
| 15:K:74:ILE:HG22 | 15:K:75:VAL:HG22 | 1.61 | 0.83 |
| 21:K:107:LMU:H2B | 21:K:107:LMU:H3' | 1.61 | 0.83 |
| 16:L:152:THR:O | 16:L:156:PHE:N | 2.09 | 0.83 |
| 5:A:248:PHE:H | 5:A:248:PHE:HD2 | 1.25 | 0.83 |
| 6:B:304:ILE:HD11 | 20:B:820:CLA:CED | 2.08 | 0.83 |
| 25:B:848:LMG:O3 | 7:C:70:TRP:NE1 | 2.12 | 0.83 |
| 12:H:73:PRO:CD | 19:Z:2:FRU:C6 | 2.57 | 0.83 |
| 21:K:105:LMU:H81 | 21:K:105:LMU:C4 | 1.97 | 0.83 |
| 20:1:203:CLA:HBD | 20:1:203:CLA:CBA | 2.08 | 0.83 |
| 20:3:310:CLA:H2A | 20:3:310:CLA:O1D | 1.79 | 0.83 |
| 4:4:95:PHE:CD1 | 4:4:95:PHE:N | 2.44 | 0.83 |
| 5:A:555:ILE:HG22 | 6:B:670:TYR:CE2 | 2.14 | 0.83 |
| 20:B:836:CLA:HHD | 20:B:836:CLA:HBC3 | 1.60 | 0.83 |
| 17:N:67:LEU:CB | 17:N:68:GLU:HG2 | 2.08 | 0.83 |
| 11:G:19:GLY:C | 11:G:21:PHE:N | 2.33 | 0.83 |
| 17:N:41:LYS:HD2 | 17:N:42:PHE:HB2 | 1.58 | 0.83 |
| 4:4:39:TRP:CG | 4:4:40:PHE:N | 2.37 | 0.82 |
| 4:4:117:GLN:O | 4:4:121:PHE:CE2 | 2.30 | 0.82 |
| 4:4:171:ASN:O | 4:4:172:VAL:C | 2.21 | 0.82 |
| 20:4:318:CLA:HMC3 | 20:4:318:CLA:HBC2 | 1.61 | 0.82 |
| 5:A:217:SER:OG | 22:A:843:BCR:C15 | 2.27 | 0.82 |
| 5:A:746:THR:HA | 5:A:749:PHE:HB3 | 1.59 | 0.82 |
| 20:A:838:CLA:C14 | 22:A:845:BCR:HC21 | 2.09 | 0.82 |
| 6:B:310:PRO:HG3 | 20:B:824:CLA:CMA | 2.09 | 0.82 |
| 17:N:4:GLU:OE2 | 17:N:5:GLU:HB2 | 1.78 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:25:ILE:CG2 | 22:L:209:BCR:C28 | 2.56 | 0.82 |
| 6:B:203:ARG:HG2 | 6:B:204:GLY:N | 1.94 | 0.82 |
| 17:N:62:SER:HB3 | 17:N:66:ASP:CG | 2.04 | 0.82 |
| 4:4:122:LYS:CB | 4:4:143:PHE:CB | 2.50 | 0.82 |
| 20:A:824:CLA:O1A | 20:A:825:CLA:HED3 | 1.79 | 0.82 |
| 20:A:830:CLA:H161 | 22:L:209:BCR:H361 | 1.58 | 0.82 |
| 20:H:109:CLA:C3C | 22:I:103:BCR:C2 | 2.57 | 0.82 |
| 21:R:106:LMU:O5B | 21:R:106:LMU:H6D | 1.77 | 0.82 |
| 4:4:124:TYR:CB | 4:4:143:PHE:HD1 | 1.93 | 0.82 |
| 10:F:93:ILE:HG21 | 22:F:203:BCR:H371 | 1.61 | 0.82 |
| 18:R:34:UNK:CB | 18:R:35:UNK:CA | 2.53 | 0.82 |
| 17:N:57:LYS:CA | 17:N:60:PHE:O | 2.27 | 0.82 |
| 20:2:316:CLA:HAA1 | 20:2:316:CLA:C1 | 2.08 | 0.82 |
| 4:4:36:ASN:CG | 4:4:39:TRP:CD2 | 2.58 | 0.82 |
| 4:4:121:PHE:O | 4:4:122:LYS:CD | 2.26 | 0.82 |
| 20:A:807:CLA:CBA | 20:A:809:CLA:H12 | 2.10 | 0.82 |
| 20:A:830:CLA:H52 | 22:B:847:BCR:H343 | 1.62 | 0.82 |
| 20:B:838:CLA:H93 | 20:B:838:CLA:HBB2 | 0.86 | 0.82 |
| 16:L:163:LEU:HD11 | 16:L:165:TYR:CE2 | 2.14 | 0.82 |
| 21:2:313:LMU:O2B | 21:2:313:LMU:H6E | 1.79 | 0.82 |
| 4:4:142:ASN:C | 4:4:150:LYS:HE2 | 2.05 | 0.82 |
| 5:A:24:ARG:CD | 5:A:24:ARG:N | 2.36 | 0.82 |
| 20:A:826:CLA:H171 | 22:J:102:BCR:H15C | 1.60 | 0.82 |
| 21:1:218:LMU:H3' | 21:1:218:LMU:H6'2 | 1.62 | 0.82 |
| 20:3:307:CLA:CAC | 20:K:104:CLA:C7 | 2.58 | 0.82 |
| 4:4:151:GLU:O | 4:4:154:ILE:N | 2.03 | 0.82 |
| 5:A:668:TYR:OH | 6:B:441:ASP:OD1 | 1.95 | 0.82 |
| 6:B:545:LYS:HG2 | 9:E:74:TYR:HE2 | 1.43 | 0.82 |
| 7:C:54:CYS:SG | 24:C:102:SF4:S1 | 2.78 | 0.82 |
| 20:1:206:CLA:HHD | 20:1:206:CLA:CBC | 2.09 | 0.82 |
| 4:4:40:PHE:HB3 | 4:4:43:ALA:HB3 | 1.60 | 0.82 |
| 8:D:104:PHE:HB3 | 8:D:106:SER:H | 1.43 | 0.82 |
| 14:J:31:ARG:HH22 | 20:J:103:CLA:C4B | 1.92 | 0.82 |
| 20:K:102:CLA:H3A | 20:K:102:CLA:CGA | 2.09 | 0.82 |
| 16:L:118:LEU:HD12 | 16:L:119:THR:H | 1.45 | 0.82 |
| 20:1:213:CLA:HBC2 | 20:1:213:CLA:HMC1 | 1.62 | 0.81 |
| 5:A:25:ASP:CB | 5:A:26:PRO:C | 2.51 | 0.81 |
| 5:A:308:ILE:CD1 | 20:A:816:CLA:H91 | 2.10 | 0.81 |
| 20:A:807:CLA:C3B | 22:J:102:BCR:C33 | 2.58 | 0.81 |
| 20:3:307:CLA:HBD | 20:3:307:CLA:CBA | 2.09 | 0.81 |
| 20:A:824:CLA:O1A | 20:A:824:CLA:H2 | 1.80 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:137:THR:HA | 6:B:140:ILE:HG13 | 1.63 | 0.81 |
| 9:E:68:ARG:HH21 | 9:E:69:PHE:HA | 1.43 | 0.81 |
| 20:F:206:CLA:C3B | 20:F:207:CLA:CAC | 2.55 | 0.81 |
| 15:K:6:SER:O | 15:K:10:ILE:HD13 | 1.78 | 0.81 |
| 15:K:47:LEU:O | 15:K:48:GLN:HG3 | 1.79 | 0.81 |
| 2:2:54:TRP:CZ2 | 2:2:109:ARG:CD | 2.62 | 0.81 |
| 3:3:93:PHE:CB | 3:3:94:ARG:O | 2.28 | 0.81 |
| 3:3:203:VAL:O | 5:A:252:ARG:NH2 | 2.14 | 0.81 |
| 4:4:96:ILE:O | 4:4:99:HIS:HB3 | 1.79 | 0.81 |
| 4:4:122:LYS:HG2 | 4:4:150:LYS:HD3 | 1.59 | 0.81 |
| 4:4:169:GLN:HG2 | 20:4:304:CLA:HAC2 | 1.61 | 0.81 |
| 5:A:217:SER:HA | 22:A:843:BCR:H351 | 1.62 | 0.81 |
| 5:A:316:MET:HB3 | 5:A:317:TYR:CG | 2.15 | 0.81 |
| 5:A:356:ALA:HB2 | 5:A:417:PHE:CD2 | 2.15 | 0.81 |
| 5:A:723:ARG:HH11 | 5:A:723:ARG:HG2 | 1.45 | 0.81 |
| 20:A:824:CLA:H72 | 20:A:825:CLA:HED1 | 1.61 | 0.81 |
| 20:A:833:CLA:C3A | 20:A:839:CLA:CBB | 2.59 | 0.81 |
| 6:B:594:TRP:O | 6:B:595:HIS:CB | 2.28 | 0.81 |
| 10:F:102:ARG:CG | 10:F:106:ILE:HD11 | 2.08 | 0.81 |
| 15:K:27:ALA:HB3 | 15:K:28:PRO:HD3 | 1.60 | 0.81 |
| 17:N:1:GLY:O | 17:N:2:VAL:HG13 | 1.80 | 0.81 |
| 2:2:102:ILE:HG13 | 20:2:311:CLA:HMD2 | 1.62 | 0.81 |
| 21:H:105:LMU:H31 | 21:H:105:LMU:C2B | 2.10 | 0.81 |
| 17:N:67:LEU:HB2 | 17:N:68:GLU:CG | 2.11 | 0.81 |
| 17:N:79:SER:HA | 17:N:80:ASN:C | 2.05 | 0.81 |
| 1:1:39:TYR:HB3 | 20:1:210:CLA:OBD | 1.81 | 0.81 |
| 3:3:52:LYS:O | 3:3:56:TYR:HD2 | 1.63 | 0.81 |
| 20:3:307:CLA:CMC | 20:3:307:CLA:HBC3 | 2.10 | 0.81 |
| 4:4:99:HIS:CE1 | 4:4:103:ILE:HD11 | 2.16 | 0.81 |
| 20:4:318:CLA:CBB | 21:4:321:LMU:O3B | 2.29 | 0.81 |
| 18:R:38:UNK:C | 18:R:42:UNK:O | 2.29 | 0.81 |
| 5:A:22:VAL:CB | 5:A:23:ASP:C | 2.53 | 0.81 |
| 5:A:27:ILE:O | 5:A:28:LYS:CD | 2.29 | 0.81 |
| 6:B:493:TRP:CZ2 | 20:B:835:CLA:O1A | 2.32 | 0.81 |
| 9:E:61:THR:HG22 | 9:E:62:ARG:H | 1.46 | 0.81 |
| 15:K:46:GLY:O | 15:K:47:LEU:CG | 2.29 | 0.81 |
| 17:N:18:ASP:CB | 17:N:22:LEU:HG | 2.09 | 0.81 |
| 17:N:40:CYS:H | 17:N:41:LYS:CA | 1.88 | 0.81 |
| 1:1:185:TRP:CH2 | 20:1:213:CLA:O2A | 2.33 | 0.81 |
| 3:3:80:LYS:NZ | 3:3:92:TRP:HD1 | 1.73 | 0.81 |
| 3:3:92:TRP:CB | 3:3:95:THR:OG1 | 2.29 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:37:LEU:CA | 4:4:39:TRP:HB3 | 2.10 | 0.81 |
| 21:A:853:LMU:C2 | 21:A:853:LMU:H61 | 2.08 | 0.81 |
| 7:C:1:MET:H2 | 7:C:3:HIS:C | 1.89 | 0.81 |
| 21:H:106:LMU:H62 | 21:H:106:LMU:C10 | 2.11 | 0.81 |
| 16:L:122:GLY:C | 16:L:124:LYS:N | 2.36 | 0.81 |
| 17:N:72:LYS:HZ1 | 17:N:74:LYS:HE2 | 1.45 | 0.81 |
| 19:Q:1:GLC:H5 | 19:Q:2:FRU:O5 | 1.79 | 0.81 |
| 5:A:21:LEU:CA | 5:A:22:VAL:O | 2.29 | 0.81 |
| 5:A:331:LEU:HD23 | 5:A:331:LEU:O | 1.81 | 0.81 |
| 20:A:823:CLA:H112 | 20:A:823:CLA:OBD | 1.80 | 0.81 |
| 22:B:801:BCR:H331 | 22:B:801:BCR:C8 | 2.09 | 0.81 |
| 11:G:42:SER:OG | 11:G:46:ALA:CB | 2.28 | 0.81 |
| 11:G:68:ILE:O | 11:G:72:LEU:HB3 | 1.80 | 0.81 |
| 18:R:7:UNK:O | 18:R:11:UNK:N | 2.14 | 0.81 |
| 20:2:314:CLA:CBA | 20:2:314:CLA:CBD | 2.58 | 0.81 |
| 20:A:814:CLA:C4B | 22:A:843:BCR:C19 | 2.59 | 0.81 |
| 6:B:70:TRP:CD1 | 6:B:71:GLN:OE1 | 2.34 | 0.81 |
| 22:B:801:BCR:H331 | 22:B:801:BCR:HC8 | 1.62 | 0.81 |
| 8:D:134:MET:N | 8:D:134:MET:SD | 2.54 | 0.81 |
| 4:4:165:GLY:O | 4:4:169:GLN:HG2 | 1.81 | 0.81 |
| 5:A:40:PHE:HE1 | 5:A:53:TRP:HD1 | 1.29 | 0.81 |
| 20:A:807:CLA:HMB3 | 20:A:808:CLA:HHB | 1.63 | 0.81 |
| 6:B:199:ILE:HG23 | 6:B:270:LEU:HD22 | 1.63 | 0.81 |
| 6:B:732:LYS:CB | 6:B:733:PHE:O | 2.29 | 0.81 |
| 21:1:217:LMU:O6B | 21:1:217:LMU:H1B | 1.79 | 0.80 |
| 21:2:313:LMU:H12 | 21:2:313:LMU:C7 | 2.12 | 0.80 |
| 4:4:74:LYS:N | 4:4:75:TRP:CA | 2.44 | 0.80 |
| 5:A:187:HIS:CD2 | 20:A:811:CLA:NC | 2.38 | 0.80 |
| 20:B:834:CLA:HBB2 | 22:B:846:BCR:H381 | 1.63 | 0.80 |
| 17:N:45:ASN:O | 17:N:46:PHE:O | 1.98 | 0.80 |
| 21:R:103:LMU:H1' | 21:R:103:LMU:C3 | 2.08 | 0.80 |
| 3:3:107:TRP:CG | 3:3:108:ALA:N | 2.38 | 0.80 |
| 4:4:37:LEU:N | 4:4:39:TRP:HB2 | 1.95 | 0.80 |
| 4:4:107:GLN:O | 20:4:301:CLA:CMA | 2.23 | 0.80 |
| 6:B:275:HIS:O | 6:B:279:ALA:N | 2.11 | 0.80 |
| 6:B:732:LYS:HD2 | 6:B:734:GLY:CA | 2.10 | 0.80 |
| 15:K:84:LEU:CD2 | 15:K:84:LEU:N | 2.30 | 0.80 |
| 17:N:40:CYS:N | 17:N:41:LYS:CA | 2.44 | 0.80 |
| 18:R:33:UNK:O | 18:R:36:UNK:CB | 2.29 | 0.80 |
| 2:2:103:GLY:N | 20:2:310:CLA:CBB | 2.44 | 0.80 |
| 5:A:472:ARG:HE | 5:A:474:GLN:HG3 | 1.45 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:A:839:CLA:HMA3 | 20:A:839:CLA:CBA | 2.11 | 0.80 |
| 20:B:838:CLA:C15 | 22:F:204:BCR:C31 | 2.58 | 0.80 |
| 11:G:42:SER:O | 11:G:46:ALA:CB | 2.29 | 0.80 |
| 20:H:109:CLA:CAC | 22:I:103:BCR:C3 | 2.59 | 0.80 |
| 20:A:822:CLA:CBB | 22:A:844:BCR:H351 | 2.11 | 0.80 |
| 6:B:110:LEU:HD12 | 6:B:111:GLY:H | 1.46 | 0.80 |
| 15:K:46:GLY:O | 15:K:47:LEU:CD1 | 2.29 | 0.80 |
| 2:2:162:LYS:NZ | 20:2:305:CLA:OBD | 2.14 | 0.80 |
| 20:2:314:CLA:H2 | 20:2:314:CLA:HAA1 | 1.62 | 0.80 |
| 3:3:92:TRP:CA | 3:3:95:THR:OG1 | 2.30 | 0.80 |
| 4:4:150:LYS:CG | 4:4:150:LYS:O | 2.23 | 0.80 |
| 5:A:27:ILE:O | 5:A:28:LYS:CG | 2.30 | 0.80 |
| 5:A:246:HIS:HE1 | 20:A:840:CLA:HMA2 | 1.46 | 0.80 |
| 5:A:488:PHE:CE2 | 5:A:533:PRO:HB3 | 2.16 | 0.80 |
| 5:A:497:ALA:HB2 | 5:A:515:TRP:HB2 | 1.62 | 0.80 |
| 6:B:732:LYS:CG | 6:B:733:PHE:O | 2.30 | 0.80 |
| 20:B:835:CLA:HBB1 | 22:B:846:BCR:H281 | 1.63 | 0.80 |
| 7:C:5:VAL:HB | 7:C:65:VAL:HG13 | 1.64 | 0.80 |
| 16:L:165:TYR:CA | 16:L:166:TYR:O | 2.30 | 0.80 |
| 17:N:45:ASN:HB3 | 17:N:57:LYS:HZ1 | 1.46 | 0.80 |
| 17:N:74:LYS:O | 17:N:76:LYS:N | 2.13 | 0.80 |
| 18:R:38:UNK:CB | 18:R:42:UNK:O | 2.30 | 0.80 |
| 20:1:204:CLA:HED2 | 20:1:204:CLA:H2A | 1.62 | 0.80 |
| 5:A:22:VAL:CA | 5:A:23:ASP:O | 2.30 | 0.80 |
| 5:A:25:ASP:OD2 | 5:A:26:PRO:CD | 2.30 | 0.80 |
| 5:A:100:GLY:HA3 | 5:A:153:TRP:HH2 | 1.45 | 0.80 |
| 20:A:819:CLA:HMD3 | 20:A:820:CLA:HHD | 1.63 | 0.80 |
| 24:A:856:SF4:S1 | 24:A:856:SF4:S3 | 2.78 | 0.80 |
| 16:L:115:ALA:H | 16:L:116:PRO:HD2 | 1.44 | 0.80 |
| 18:R:34:UNK:N | 18:R:36:UNK:N | 2.29 | 0.80 |
| 20:1:204:CLA:HMC3 | 20:1:204:CLA:HBC2 | 1.63 | 0.80 |
| 5:A:22:VAL:HA | 5:A:23:ASP:C | 2.05 | 0.80 |
| 5:A:599:PHE:HD1 | 5:A:600:LEU:HD23 | 1.44 | 0.80 |
| 5:A:705:GLU:HB3 | 6:B:545:LYS:NZ | 1.96 | 0.80 |
| 20:A:801:CLA:HAA1 | 20:A:801:CLA:CGD | 2.12 | 0.80 |
| 20:B:808:CLA:O1A | 20:B:814:CLA:CGA | 2.30 | 0.80 |
| 22:B:846:BCR:H23C | 22:B:846:BCR:C38 | 2.09 | 0.80 |
| 15:K:42:ALA:O | 15:K:43:ARG:CG | 2.30 | 0.80 |
| 15:K:44:GLU:O | 15:K:46:GLY:CA | 2.29 | 0.80 |
| 15:K:47:LEU:O | 15:K:48:GLN:CG | 2.29 | 0.80 |
| 4:4:99:HIS:CE1 | 4:4:103:ILE:HD12 | 2.14 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:A:831:CLA:H51 | 16:L:67:PRO:CB | 2.11 | 0.80 |
| 6:B:549:ASP:OD1 | 7:C:63:LEU:HB3 | 1.82 | 0.80 |
| 3:3:104:TYR:HB2 | 3:3:106:TYR:N | 1.96 | 0.80 |
| 5:A:360:ILE:HD13 | 22:A:844:BCR:H371 | 1.64 | 0.80 |
| 5:A:714:LEU:HD13 | 22:F:204:BCR:C39 | 2.12 | 0.80 |
| 6:B:172:GLU:O | 6:B:176:ASN:HB2 | 1.81 | 0.80 |
| 6:B:696:LYS:HG2 | 7:C:80:ALA:HA | 1.64 | 0.80 |
| 20:B:808:CLA:HMC1 | 20:B:830:CLA:HMA2 | 1.63 | 0.80 |
| 20:B:818:CLA:CAD | 20:B:827:CLA:HBB2 | 2.12 | 0.80 |
| 15:K:44:GLU:O | 15:K:47:LEU:CG | 2.30 | 0.80 |
| 20:K:101:CLA:CMD | 20:K:102:CLA:NA | 2.45 | 0.80 |
| 20:2:312:CLA:HBC3 | 20:2:312:CLA:HHD | 1.63 | 0.80 |
| 5:A:22:VAL:CB | 5:A:23:ASP:HA | 2.10 | 0.80 |
| 5:A:22:VAL:HB | 5:A:23:ASP:HA | 1.63 | 0.80 |
| 5:A:368:LEU:HD11 | 20:A:825:CLA:H61 | 1.64 | 0.80 |
| 20:A:822:CLA:NC | 22:A:844:BCR:H19C | 1.97 | 0.80 |
| 22:A:843:BCR:HC8 | 22:A:843:BCR:C31 | 2.04 | 0.80 |
| 18:R:38:UNK:O | 18:R:42:UNK:CA | 2.28 | 0.80 |
| 20:1:204:CLA:HBC2 | 20:1:204:CLA:CMC | 2.12 | 0.79 |
| 20:2:316:CLA:H151 | 20:2:316:CLA:H192 | 1.64 | 0.79 |
| 4:4:166:PHE:O | 4:4:169:GLN:HB2 | 1.81 | 0.79 |
| 5:A:24:ARG:HD2 | 5:A:24:ARG:N | 1.96 | 0.79 |
| 6:B:160:LYS:HZ2 | 6:B:160:LYS:HB2 | 1.46 | 0.79 |
| 6:B:558:PRO:CG | 6:B:703:VAL:HB | 2.12 | 0.79 |
| 12:H:69:SER:OG | 20:H:108:CLA:C2 | 2.22 | 0.79 |
| 15:K:42:ALA:O | 15:K:43:ARG:CD | 2.30 | 0.79 |
| 1:1:183:ASP:OD2 | 1:1:184:PRO:CD | 2.30 | 0.79 |
| 3:3:92:TRP:CA | 3:3:93:PHE:HB2 | 2.12 | 0.79 |
| 4:4:36:ASN:C | 4:4:39:TRP:CB | 2.52 | 0.79 |
| 4:4:124:TYR:HB2 | 4:4:143:PHE:HD1 | 1.48 | 0.79 |
| 5:A:151:GLN:NE2 | 5:A:384:TYR:O | 2.15 | 0.79 |
| 20:A:824:CLA:HED3 | 20:A:825:CLA:HMD2 | 1.65 | 0.79 |
| 20:B:806:CLA:HMD1 | 22:F:203:BCR:HC41 | 1.64 | 0.79 |
| 11:G:37:GLU:OE2 | 11:G:42:SER:CA | 2.29 | 0.79 |
| 19:T:1:GLC:H5 | 19:T:2:FRU:O1 | 1.82 | 0.79 |
| 20:2:303:CLA:C1D | 20:2:303:CLA:C4 | 2.59 | 0.79 |
| 20:2:316:CLA:H151 | 20:2:316:CLA:H193 | 1.61 | 0.79 |
| 5:A:81:ALA:HB1 | 20:A:805:CLA:HBB2 | 1.62 | 0.79 |
| 5:A:402:ILE:HG13 | 20:A:827:CLA:CBB | 2.07 | 0.79 |
| 5:A:618:TRP:O | 5:A:622:SER:HB3 | 1.82 | 0.79 |
| 20:A:818:CLA:H121 | 20:A:818:CLA:CBB | 2.07 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:516:ASP:O | 6:B:520:HIS:HB2 | 1.82 | 0.79 |
| 6:B:621:ARG:O | 6:B:625:TRP:HB3 | 1.81 | 0.79 |
| 16:L:164:PRO:HG3 | 16:L:165:TYR:HE1 | 1.44 | 0.79 |
| 5:A:25:ASP:OD2 | 5:A:26:PRO:CA | 2.30 | 0.79 |
| 25:B:848:LMG:O3 | 7:C:70:TRP:CE2 | 2.35 | 0.79 |
| 14:J:9:SER:O | 14:J:10:VAL:HB | 1.83 | 0.79 |
| 21:2:313:LMU:H12 | 21:2:313:LMU:C6 | 2.12 | 0.79 |
| 4:4:36:ASN:CG | 4:4:39:TRP:CE2 | 2.61 | 0.79 |
| 6:B:128:GLY:HA2 | 6:B:130:ARG:HE | 1.47 | 0.79 |
| 6:B:469:LYS:HG2 | 6:B:471:THR:OG1 | 1.83 | 0.79 |
| 6:B:664:LEU:C | 6:B:667:TRP:HZ3 | 1.89 | 0.79 |
| 20:B:839:CLA:HMC1 | 20:B:839:CLA:HBC3 | 1.65 | 0.79 |
| 11:G:16:LEU:HD23 | 11:G:68:ILE:CG2 | 2.12 | 0.79 |
| 18:R:38:UNK:O | 18:R:41:UNK:CB | 2.30 | 0.79 |
| 4:4:37:LEU:CA | 4:4:39:TRP:CB | 2.60 | 0.79 |
| 5:A:22:VAL:HA | 5:A:23:ASP:O | 1.82 | 0.79 |
| 20:A:839:CLA:CBC | 20:A:839:CLA:CHD | 2.61 | 0.79 |
| 20:B:836:CLA:H2A | 20:B:836:CLA:O1D | 1.80 | 0.79 |
| 23:B:843:PQN:C16 | 22:B:847:BCR:H331 | 2.09 | 0.79 |
| 3:3:94:ARG:CZ | 3:3:98:ILE:HG21 | 2.12 | 0.79 |
| 4:4:123:GLN:O | 4:4:143:PHE:CD1 | 2.35 | 0.79 |
| 5:A:21:LEU:O | 5:A:21:LEU:CD1 | 2.30 | 0.79 |
| 20:A:835:CLA:H203 | 20:L:201:CLA:HBB2 | 1.64 | 0.79 |
| 18:R:32:UNK:CB | 18:R:33:UNK:CB | 2.59 | 0.79 |
| 18:R:35:UNK:O | 18:R:38:UNK:CB | 2.30 | 0.79 |
| 20:1:203:CLA:HBD | 20:1:203:CLA:HBA2 | 1.62 | 0.79 |
| 5:A:92:TRP:CD1 | 20:A:807:CLA:HBB1 | 2.17 | 0.79 |
| 20:A:833:CLA:HMA1 | 20:A:839:CLA:HBB1 | 1.63 | 0.79 |
| 20:B:830:CLA:HMC3 | 20:B:830:CLA:HBC2 | 1.62 | 0.79 |
| 8:D:30:ALA:O | 16:L:18:PRO:HB2 | 1.82 | 0.79 |
| 12:H:73:PRO:CD | 19:Z:2:FRU:H62 | 2.06 | 0.79 |
| 17:N:39:SER:OG | 17:N:41:LYS:HA | 1.83 | 0.79 |
| 1:1:185:TRP:CZ3 | 20:1:213:CLA:C1 | 2.47 | 0.79 |
| 20:3:314:CLA:CGA | 20:3:314:CLA:C3A | 2.61 | 0.79 |
| 5:A:588:GLY:N | 6:B:668:ARG:HD3 | 1.97 | 0.79 |
| 14:J:10:VAL:HG13 | 14:J:14:LEU:HG | 1.64 | 0.79 |
| 3:3:97:PHE:HD2 | 3:3:98:ILE:HG23 | 0.98 | 0.79 |
| 5:A:239:PRO:HA | 5:A:242:ILE:HD11 | 1.64 | 0.79 |
| 20:B:835:CLA:HMB2 | 22:B:846:BCR:H292 | 1.64 | 0.79 |
| 12:H:21:TRP:H | 12:H:22:ASP:CA | 1.95 | 0.79 |
| 3:3:158:TYR:O | 3:3:160:GLY:N | 2.16 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:121:PHE:HD1 | 4:4:128:ALA:HB3 | 1.48 | 0.78 |
| 5:A:207:LEU:CB | 20:A:819:CLA:HBB2 | 2.13 | 0.78 |
| 5:A:726:SER:O | 5:A:728:VAL:N | 2.16 | 0.78 |
| 21:A:853:LMU:C2 | 21:A:853:LMU:C6 | 2.60 | 0.78 |
| 6:B:661:PHE:CB | 20:B:803:CLA:HMC2 | 2.12 | 0.78 |
| 8:D:78:ALA:O | 8:D:79:ARG:HD3 | 1.83 | 0.78 |
| 16:L:27:VAL:O | 20:L:201:CLA:O2A | 2.00 | 0.78 |
| 17:N:70:GLU:HB3 | 17:N:72:LYS:H | 1.48 | 0.78 |
| 4:4:75:TRP:HE3 | 4:4:76:TYR:H | 1.25 | 0.78 |
| 4:4:126:LEU:HD23 | 4:4:127:PRO:HD3 | 1.65 | 0.78 |
| 5:A:53:TRP:HA | 5:A:56:ASN:HB2 | 1.66 | 0.78 |
| 21:A:853:LMU:H112 | 21:A:853:LMU:H71 | 1.64 | 0.78 |
| 6:B:362:ALA:HB2 | 6:B:368:GLN:HG2 | 1.64 | 0.78 |
| 6:B:438:VAL:HG23 | 20:B:833:CLA:HAC1 | 1.65 | 0.78 |
| 20:B:802:CLA:HBB2 | 20:B:803:CLA:CHB | 2.13 | 0.78 |
| 25:B:848:LMG:HC61 | 7:C:70:TRP:CH2 | 2.18 | 0.78 |
| 9:E:39:LEU:N | 9:E:40:ARG:NH1 | 2.31 | 0.78 |
| 1:1:27:LEU:CD1 | 1:1:28:GLY:H | 1.95 | 0.78 |
| 4:4:128:ALA:N | 4:4:143:PHE:CZ | 2.48 | 0.78 |
| 6:B:65:LEU:HD22 | 6:B:124:TRP:HE3 | 1.47 | 0.78 |
| 6:B:325:THR:O | 6:B:329:SER:HB2 | 1.83 | 0.78 |
| 23:B:843:PQN:C19 | 22:B:847:BCR:C10 | 2.55 | 0.78 |
| 1:1:183:ASP:OD2 | 1:1:184:PRO:HD2 | 1.84 | 0.78 |
| 2:2:127:ASN:HD21 | 14:J:7:TYR:HA | 1.49 | 0.78 |
| 4:4:94:GLU:CB | 4:4:95:PHE:CE1 | 2.67 | 0.78 |
| 4:4:100:TYR:HA | 4:4:103:ILE:CG1 | 2.14 | 0.78 |
| 5:A:397:THR:HB | 5:A:613:ILE:CG1 | 2.13 | 0.78 |
| 5:A:475:ASP:OD2 | 16:L:74:LEU:HA | 1.82 | 0.78 |
| 20:A:826:CLA:H102 | 22:A:845:BCR:H372 | 1.64 | 0.78 |
| 9:E:60:LYS:HG3 | 9:E:61:THR:H | 1.46 | 0.78 |
| 12:H:25:GLY:HA3 | 12:H:27:ASP:CB | 2.12 | 0.78 |
| 17:N:44:GLU:O | 17:N:46:PHE:N | 2.16 | 0.78 |
| 21:2:313:LMU:H82 | 21:2:313:LMU:C4 | 2.13 | 0.78 |
| 5:A:242:ILE:HG12 | 5:A:243:PRO:CD | 2.13 | 0.78 |
| 5:A:349:ILE:HG23 | 5:A:352:THR:O | 1.82 | 0.78 |
| 20:A:833:CLA:CMA | 20:A:839:CLA:CBB | 2.61 | 0.78 |
| 6:B:189:ALA:HB2 | 20:B:829:CLA:H203 | 1.63 | 0.78 |
| 7:C:8:TYR:O | 7:C:60:THR:HA | 1.83 | 0.78 |
| 8:D:28:ILE:HG12 | 8:D:67:ILE:HG13 | 1.66 | 0.78 |
| 21:E:101:LMU:H32 | 21:E:101:LMU:C7 | 2.10 | 0.78 |
| 21:2:319:LMU:H12 | 21:2:319:LMU:O2' | 1.82 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:69:ILE:CD1 | 4:4:175:LYS:HB3 | 1.95 | 0.78 |
| 20:B:810:CLA:HBA1 | 20:B:828:CLA:OBD | 1.84 | 0.78 |
| 20:B:838:CLA:HMA2 | 20:B:839:CLA:CED | 2.13 | 0.78 |
| 20:B:839:CLA:HMC1 | 20:B:839:CLA:CBC | 2.14 | 0.78 |
| 20:J:103:CLA:H143 | 20:J:103:CLA:O1A | 1.83 | 0.78 |
| 17:N:72:LYS:HD2 | 17:N:74:LYS:CG | 2.12 | 0.78 |
| 3:3:112:THR:O | 3:3:114:PHE:N | 2.17 | 0.78 |
| 5:A:170:GLY:O | 5:A:173:VAL:HG22 | 1.83 | 0.78 |
| 6:B:317:ARG:NH1 | 6:B:405:ASP:O | 2.16 | 0.78 |
| 10:F:153:ASN:C | 10:F:153:ASN:ND2 | 2.41 | 0.78 |
| 5:A:691:MET:HE3 | 23:A:842:PQN:H2M2 | 1.65 | 0.78 |
| 10:F:20:GLN:CD | 10:F:21:ALA:H | 1.92 | 0.78 |
| 16:L:48:ASN:HB3 | 16:L:49:PRO:HD2 | 1.66 | 0.78 |
| 2:2:188:PRO:O | 2:2:190:ASP:N | 2.17 | 0.78 |
| 4:4:104:ARG:NH1 | 4:4:105:ARG:CB | 2.45 | 0.78 |
| 4:4:142:ASN:N | 4:4:150:LYS:HZ3 | 1.81 | 0.78 |
| 5:A:345:GLY:O | 5:A:347:TYR:N | 2.17 | 0.78 |
| 6:B:11:GLY:HA3 | 7:C:71:HIS:HD2 | 1.49 | 0.78 |
| 6:B:317:ARG:NE | 6:B:317:ARG:HA | 1.98 | 0.78 |
| 6:B:353:TYR:CG | 6:B:594:TRP:CZ3 | 2.71 | 0.78 |
| 7:C:52:LYS:O | 7:C:52:LYS:HG3 | 1.84 | 0.78 |
| 8:D:113:HIS:N | 8:D:114:PRO:HD2 | 1.99 | 0.78 |
| 13:I:9:VAL:HG12 | 13:I:10:PRO:HD3 | 1.65 | 0.78 |
| 17:N:45:ASN:HD22 | 17:N:54:LYS:CB | 1.97 | 0.78 |
| 1:1:179:THR:HG21 | 4:4:87:SER:CB | 2.14 | 0.78 |
| 4:4:128:ALA:CB | 4:4:143:PHE:CZ | 2.63 | 0.78 |
| 20:B:824:CLA:C4A | 20:B:824:CLA:H42 | 2.14 | 0.78 |
| 20:B:826:CLA:H11 | 20:B:839:CLA:CED | 2.14 | 0.78 |
| 10:F:100:VAL:HA | 10:F:103:SER:OG | 1.84 | 0.78 |
| 16:L:36:TYR:CG | 16:L:36:TYR:O | 2.36 | 0.78 |
| 16:L:128:ASP:CG | 16:L:129:GLN:H | 1.91 | 0.78 |
| 2:2:205:PHE:HD1 | 2:2:206:ALA:N | 1.80 | 0.77 |
| 4:4:58:MET:O | 4:4:61:PRO:HD2 | 1.84 | 0.77 |
| 22:A:845:BCR:C32 | 22:J:102:BCR:H391 | 2.14 | 0.77 |
| 6:B:91:ILE:HD12 | 6:B:104:PHE:HE2 | 1.48 | 0.77 |
| 6:B:404:ALA:C | 6:B:406:ASN:H | 1.92 | 0.77 |
| 12:H:50:ARG:HH12 | 12:H:53:LEU:C | 1.92 | 0.77 |
| 15:K:27:ALA:CB | 15:K:28:PRO:HD3 | 2.14 | 0.77 |
| 5:A:567:ARG:NH1 | 8:D:35:GLY:CA | 2.42 | 0.77 |
| 6:B:124:TRP:NE1 | 6:B:129:LEU:HD22 | 2.00 | 0.77 |
| 7:C:26:LEU:H | 7:C:43:PRO:HG3 | 1.50 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:F:96:TRP:HZ3 | 10:F:134:PHE:HB2 | 1.48 | 0.77 |
| 15:K:69:ILE:HA | 15:K:72:VAL:HG12 | 1.66 | 0.77 |
| 16:L:95:LEU:HD13 | 22:L:209:BCR:C31 | 2.14 | 0.77 |
| 3:3:93:PHE:CA | 3:3:94:ARG:O | 2.31 | 0.77 |
| 24:A:856:SF4:S1 | 24:A:856:SF4:FE3 | 1.77 | 0.77 |
| 6:B:310:PRO:CG | 6:B:311:PRO:HD2 | 2.13 | 0.77 |
| 6:B:349:ALA:HB2 | 6:B:375:HIS:HB3 | 1.67 | 0.77 |
| 20:B:827:CLA:H122 | 22:B:846:BCR:C14 | 2.15 | 0.77 |
| 20:B:836:CLA:CBC | 20:B:836:CLA:CHD | 2.62 | 0.77 |
| 22:F:204:BCR:H403 | 22:F:204:BCR:H271 | 1.63 | 0.77 |
| 16:L:124:LYS:C | 16:L:126:GLN:H | 1.92 | 0.77 |
| 21:R:104:LMU:C2' | 21:R:104:LMU:C2 | 2.55 | 0.77 |
| 20:A:809:CLA:HBB2 | 20:B:833:CLA:HMD3 | 1.63 | 0.77 |
| 6:B:216:LEU:HD21 | 6:B:221:GLY:HA2 | 1.67 | 0.77 |
| 5:A:21:LEU:HD12 | 5:A:21:LEU:O | 1.84 | 0.77 |
| 5:A:51:THR:HG21 | 20:A:837:CLA:CBB | 2.11 | 0.77 |
| 20:A:803:CLA:CBB | 20:A:804:CLA:C1C | 2.62 | 0.77 |
| 11:G:92:GLY:O | 11:G:93:TYR:O | 2.03 | 0.77 |
| 21:H:105:LMU:H31 | 21:H:105:LMU:O5B | 1.83 | 0.77 |
| 18:R:49:UNK:O | 18:R:50:UNK:C | 2.30 | 0.77 |
| 4:4:192:THR:HG22 | 4:4:195:GLN:N | 1.96 | 0.77 |
| 5:A:25:ASP:OD2 | 5:A:26:PRO:HA | 1.84 | 0.77 |
| 5:A:451:ILE:CD1 | 20:A:830:CLA:CED | 2.62 | 0.77 |
| 5:A:542:HIS:HA | 5:A:545:HIS:HD2 | 1.50 | 0.77 |
| 5:A:700:TRP:O | 5:A:704:ILE:HB | 1.83 | 0.77 |
| 20:A:824:CLA:CED | 20:A:825:CLA:C3D | 2.63 | 0.77 |
| 20:B:809:CLA:H2A | 20:B:809:CLA:O1D | 1.83 | 0.77 |
| 10:F:130:LEU:HG | 10:F:131:PHE:N | 2.00 | 0.77 |
| 20:L:201:CLA:H52 | 20:L:204:CLA:HHB | 1.66 | 0.77 |
| 20:3:307:CLA:HHD | 20:K:104:CLA:H92 | 1.66 | 0.77 |
| 20:B:824:CLA:C4A | 20:B:824:CLA:C4 | 2.57 | 0.77 |
| 9:E:40:ARG:HB2 | 9:E:42:GLU:OE2 | 1.85 | 0.77 |
| 20:K:102:CLA:CBC | 21:K:105:LMU:O3B | 2.32 | 0.77 |
| 20:1:204:CLA:H2A | 20:1:204:CLA:CED | 2.14 | 0.77 |
| 2:2:85:GLN:OE1 | 2:2:85:GLN:HA | 1.83 | 0.77 |
| 5:A:22:VAL:CB | 5:A:24:ARG:HA | 2.14 | 0.77 |
| 20:A:803:CLA:HBB2 | 20:A:804:CLA:C1C | 2.12 | 0.77 |
| 20:B:803:CLA:H3A | 20:B:803:CLA:CGA | 2.15 | 0.77 |
| 2:2:42:ARG:O | 2:2:44:ASN:N | 2.18 | 0.77 |
| 3:3:48:PHE:HD2 | 3:3:49:ILE:CG2 | 1.82 | 0.77 |
| 20:4:303:CLA:H151 | 20:4:303:CLA:H203 | 1.66 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:22:VAL:HB | 5:A:24:ARG:HA | 1.66 | 0.77 |
| 5:A:76:ARG:NH1 | 5:A:192:LYS:HG2 | 1.99 | 0.77 |
| 5:A:246:HIS:O | 5:A:248:PHE:HD2 | 1.67 | 0.77 |
| 5:A:355:HIS:CE1 | 5:A:416:ILE:HG21 | 2.18 | 0.77 |
| 20:A:839:CLA:CMA | 20:A:839:CLA:CBA | 2.55 | 0.77 |
| 6:B:8:PHE:O | 6:B:35:ASP:HB2 | 1.84 | 0.77 |
| 20:B:803:CLA:H3A | 20:B:803:CLA:O2A | 1.84 | 0.77 |
| 20:B:826:CLA:H72 | 20:B:839:CLA:C2D | 2.15 | 0.77 |
| 20:B:838:CLA:H121 | 22:F:204:BCR:C31 | 2.15 | 0.77 |
| 15:K:51:ASP:HB3 | 15:K:52:PRO:CD | 2.14 | 0.77 |
| 5:A:244:LEU:HD22 | 5:A:247:GLU:OE2 | 1.85 | 0.77 |
| 20:B:826:CLA:CBB | 20:B:839:CLA:CMB | 2.58 | 0.77 |
| 13:I:8:PHE:CB | 20:I:102:CLA:OBD | 2.32 | 0.77 |
| 17:N:59:PRO:HB3 | 17:N:75:TYR:HE1 | 1.48 | 0.77 |
| 5:A:146:THR:HG21 | 5:A:751:LEU:HD22 | 1.66 | 0.76 |
| 5:A:713:LYS:NZ | 20:F:201:CLA:C4 | 2.48 | 0.76 |
| 20:B:839:CLA:CBC | 20:F:201:CLA:HMC1 | 2.14 | 0.76 |
| 11:G:68:ILE:O | 11:G:72:LEU:CB | 2.32 | 0.76 |
| 20:K:101:CLA:HMD2 | 20:K:102:CLA:NA | 2.00 | 0.76 |
| 16:L:63:LEU:HD22 | 16:L:64:LEU:H | 1.50 | 0.76 |
| 2:2:126:PRO:CD | 2:2:129:LYS:HB2 | 2.16 | 0.76 |
| 5:A:27:ILE:CG2 | 5:A:27:ILE:O | 2.30 | 0.76 |
| 5:A:81:ALA:HB1 | 20:A:804:CLA:CMA | 2.13 | 0.76 |
| 6:B:586:THR:C | 6:B:588:GLY:H | 1.91 | 0.76 |
| 22:B:845:BCR:H331 | 22:B:845:BCR:C8 | 2.13 | 0.76 |
| 4:4:129:GLY:C | 4:4:131:VAL:H | 1.93 | 0.76 |
| 20:K:101:CLA:HED2 | 20:K:102:CLA:HMB3 | 1.68 | 0.76 |
| 5:A:217:SER:OG | 22:A:843:BCR:H15C | 1.83 | 0.76 |
| 20:B:838:CLA:CMA | 20:B:839:CLA:HED1 | 2.15 | 0.76 |
| 3:3:92:TRP:C | 3:3:94:ARG:O | 2.29 | 0.76 |
| 5:A:194:ALA:O | 5:A:198:ASP:N | 2.16 | 0.76 |
| 6:B:122:GLN:HG3 | 6:B:361:ILE:HG12 | 1.67 | 0.76 |
| 8:D:44:GLU:HB2 | 8:D:46:TYR:CE2 | 2.16 | 0.76 |
| 2:2:168:ARG:NH2 | 2:2:171:MET:HB2 | 2.00 | 0.76 |
| 4:4:122:LYS:HE2 | 4:4:150:LYS:HD3 | 1.66 | 0.76 |
| 5:A:25:ASP:CA | 5:A:26:PRO:C | 2.58 | 0.76 |
| 5:A:207:LEU:O | 5:A:310:PHE:HB3 | 1.85 | 0.76 |
| 5:A:581:CYS:HB2 | 5:A:590:CYS:CA | 2.13 | 0.76 |
| 20:A:814:CLA:CHC | 22:A:843:BCR:C19 | 2.64 | 0.76 |
| 7:C:7:ILE:O | 7:C:8:TYR:O | 2.03 | 0.76 |
| 11:G:28:ARG:HH21 | 11:G:29:GLU:H | 1.34 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:H:25:GLY:C | 12:H:27:ASP:H | 1.93 | 0.76 |
| 17:N:59:PRO:HB3 | 17:N:75:TYR:CE1 | 2.20 | 0.76 |
| 2:2:116:PRO:HB2 | 2:2:136:GLY:HA2 | 1.67 | 0.76 |
| 4:4:192:THR:HG22 | 4:4:193:ILE:O | 1.86 | 0.76 |
| 20:4:305:CLA:CMC | 20:4:305:CLA:HBC2 | 2.15 | 0.76 |
| 6:B:586:THR:O | 6:B:588:GLY:N | 2.19 | 0.76 |
| 21:B:804:LMU:H4' | 21:B:804:LMU:O2B | 1.85 | 0.76 |
| 9:E:43:SER:HB2 | 9:E:82:TYR:HE1 | 1.49 | 0.76 |
| 16:L:88:ALA:C | 16:L:90:GLY:N | 2.40 | 0.76 |
| 2:2:189:ILE:HD13 | 2:2:189:ILE:H | 1.48 | 0.76 |
| 4:4:39:TRP:O | 4:4:40:PHE:CD1 | 2.38 | 0.76 |
| 4:4:103:ILE:O | 4:4:106:TRP:HB3 | 1.85 | 0.76 |
| 4:4:128:ALA:O | 4:4:130:GLU:N | 2.18 | 0.76 |
| 5:A:393:LEU:O | 5:A:397:THR:HG23 | 1.85 | 0.76 |
| 5:A:680:LEU:HB3 | 20:A:850:CLA:O2A | 1.86 | 0.76 |
| 5:A:684:PHE:C | 5:A:684:PHE:HD2 | 1.93 | 0.76 |
| 20:A:824:CLA:C7 | 20:A:825:CLA:HED1 | 2.15 | 0.76 |
| 6:B:693:TRP:HD1 | 20:B:840:CLA:C2D | 1.99 | 0.76 |
| 2:2:73:ILE:H | 2:2:73:ILE:HD12 | 1.51 | 0.76 |
| 20:4:310:CLA:CGD | 20:4:310:CLA:CBA | 2.59 | 0.76 |
| 5:A:691:MET:HE3 | 23:A:842:PQN:C2M | 2.15 | 0.76 |
| 22:A:845:BCR:HC8 | 22:A:845:BCR:C31 | 2.13 | 0.76 |
| 6:B:398:TYR:HD1 | 6:B:542:ARG:HH21 | 1.32 | 0.76 |
| 20:B:826:CLA:HED1 | 20:B:827:CLA:CMD | 2.15 | 0.76 |
| 7:C:5:VAL:CB | 7:C:65:VAL:CG1 | 2.55 | 0.76 |
| 8:D:111:TYR:HD2 | 8:D:114:PRO:HB3 | 1.50 | 0.76 |
| 4:4:91:PHE:CD2 | 4:4:92:VAL:N | 2.54 | 0.76 |
| 4:4:94:GLU:CB | 4:4:95:PHE:CD1 | 2.68 | 0.76 |
| 4:4:104:ARG:HA | 4:4:107:GLN:HB2 | 1.68 | 0.76 |
| 20:B:838:CLA:C20 | 22:F:204:BCR:HC41 | 2.16 | 0.76 |
| 2:2:196:HIS:O | 2:2:197:LEU:HB2 | 1.85 | 0.75 |
| 20:2:303:CLA:O1D | 20:2:303:CLA:H2A | 1.85 | 0.75 |
| 3:3:173:GLU:CG | 3:3:174:LYS:H | 1.98 | 0.75 |
| 4:4:93:ILE:CA | 4:4:96:ILE:HD12 | 2.13 | 0.75 |
| 5:A:362:LEU:HB3 | 5:A:410:ALA:HB2 | 1.67 | 0.75 |
| 5:A:692:PHE:CE2 | 20:A:838:CLA:HBC3 | 2.20 | 0.75 |
| 24:A:856:SF4:S1 | 24:A:856:SF4:FE4 | 1.77 | 0.75 |
| 6:B:334:LEU:HB2 | 20:B:808:CLA:HMD3 | 1.68 | 0.75 |
| 14:J:23:ALA:O | 14:J:26:LEU:HB3 | 1.87 | 0.75 |
| 1:1:43:GLU:OE2 | 20:1:204:CLA:HBC3 | 1.85 | 0.75 |
| 2:2:110:TRP:CD1 | 2:2:113:ILE:HG21 | 2.20 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:116:PRO:O | 2:2:131:THR:CB | 2.34 | 0.75 |
| 2:2:128:ASN:O | 2:2:130:LEU:HD13 | 1.86 | 0.75 |
| 4:4:171:ASN:C | 4:4:173:THR:N | 2.43 | 0.75 |
| 5:A:629:ASN:HD21 | 5:A:633:VAL:HG23 | 1.52 | 0.75 |
| 24:A:856:SF4:S4 | 24:A:856:SF4:FE1 | 1.78 | 0.75 |
| 6:B:98:GLN:C | 6:B:100:ALA:H | 1.93 | 0.75 |
| 20:B:826:CLA:H52 | 20:B:839:CLA:CAD | 2.15 | 0.75 |
| 9:E:55:VAL:HG23 | 9:E:65:VAL:HB | 1.68 | 0.75 |
| 15:K:44:GLU:OE1 | 15:K:45:SER:C | 2.29 | 0.75 |
| 17:N:56:LYS:O | 17:N:60:PHE:HD1 | 1.68 | 0.75 |
| 3:3:97:PHE:O | 3:3:98:ILE:CG2 | 2.35 | 0.75 |
| 4:4:69:ILE:O | 4:4:70:ILE:C | 2.29 | 0.75 |
| 4:4:142:ASN:O | 4:4:150:LYS:NZ | 2.14 | 0.75 |
| 5:A:423:ASP:CB | 5:A:424:PRO:HD3 | 2.14 | 0.75 |
| 6:B:732:LYS:CD | 6:B:734:GLY:CA | 2.64 | 0.75 |
| 20:B:818:CLA:CBD | 20:B:827:CLA:HBB2 | 2.16 | 0.75 |
| 13:I:8:PHE:CE1 | 20:I:102:CLA:H43 | 2.22 | 0.75 |
| 2:2:72:GLY:O | 2:2:74:LEU:N | 2.18 | 0.75 |
| 2:2:124:ILE:HB | 2:2:129:LYS:HB3 | 1.67 | 0.75 |
| 5:A:24:ARG:O | 5:A:25:ASP:CG | 2.30 | 0.75 |
| 5:A:62:HIS:O | 20:A:828:CLA:HAA2 | 1.85 | 0.75 |
| 5:A:356:ALA:HB2 | 5:A:417:PHE:HD2 | 1.51 | 0.75 |
| 20:A:814:CLA:CHC | 22:A:843:BCR:C17 | 2.64 | 0.75 |
| 6:B:174:ARG:NH1 | 20:B:825:CLA:CMD | 2.48 | 0.75 |
| 6:B:351:HIS:HB3 | 20:B:818:CLA:HED1 | 1.68 | 0.75 |
| 20:B:834:CLA:CBB | 22:B:846:BCR:H381 | 2.16 | 0.75 |
| 11:G:28:ARG:HG2 | 11:G:28:ARG:NH2 | 2.00 | 0.75 |
| 1:1:25:ASP:H | 6:B:314:ARG:NH2 | 1.83 | 0.75 |
| 20:4:318:CLA:HMC3 | 20:4:318:CLA:CBC | 2.16 | 0.75 |
| 5:A:578:ARG:HB2 | 5:A:578:ARG:CZ | 2.15 | 0.75 |
| 20:A:801:CLA:O1D | 20:A:801:CLA:CAA | 2.34 | 0.75 |
| 20:A:834:CLA:HBD | 20:A:834:CLA:HBA2 | 1.68 | 0.75 |
| 17:N:47:THR:HG21 | 17:N:54:LYS:HZ1 | 1.50 | 0.75 |
| 3:3:92:TRP:O | 3:3:94:ARG:C | 2.29 | 0.75 |
| 4:4:121:PHE:CD1 | 4:4:143:PHE:CE2 | 2.75 | 0.75 |
| 4:4:126:LEU:HD23 | 4:4:127:PRO:CD | 2.17 | 0.75 |
| 5:A:316:MET:CB | 5:A:317:TYR:HB2 | 2.14 | 0.75 |
| 6:B:53:GLN:C | 6:B:55:ALA:H | 1.95 | 0.75 |
| 6:B:278:LEU:HD12 | 20:B:817:CLA:HMA3 | 1.68 | 0.75 |
| 12:H:45:ALA:O | 12:H:48:THR:N | 2.18 | 0.75 |
| 17:N:54:LYS:HB3 | 17:N:57:LYS:HE2 | 1.69 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:N:62:SER:HB3 | 17:N:66:ASP:HA | 1.68 | 0.75 |
| 3:3:183:GLU:HG3 | 20:3:307:CLA:OBD | 1.87 | 0.75 |
| 3:3:205:GLY:HA3 | 5:A:252:ARG:NH1 | 2.01 | 0.75 |
| 4:4:75:TRP:CB | 20:4:310:CLA:HMD2 | 2.16 | 0.75 |
| 5:A:27:ILE:HG23 | 5:A:28:LYS:CD | 2.10 | 0.75 |
| 5:A:248:PHE:N | 5:A:248:PHE:CD2 | 2.55 | 0.75 |
| 21:A:854:LMU:H6'1 | 21:A:854:LMU:O3B | 1.87 | 0.75 |
| 24:A:856:SF4:S2 | 24:A:856:SF4:FE4 | 1.77 | 0.75 |
| 6:B:29:HIS:CG | 20:B:808:CLA:HBB2 | 2.21 | 0.75 |
| 6:B:85:ARG:O | 6:B:86:PRO:O | 2.05 | 0.75 |
| 6:B:292:ARG:NH1 | 6:B:296:GLY:H | 1.85 | 0.75 |
| 10:F:103:SER:C | 10:F:105:LEU:H | 1.95 | 0.75 |
| 16:L:95:LEU:HA | 16:L:98:CYS:HB2 | 1.68 | 0.75 |
| 16:L:165:TYR:C | 16:L:166:TYR:O | 2.30 | 0.75 |
| 3:3:157:ALA:C | 3:3:158:TYR:CD2 | 2.64 | 0.75 |
| 4:4:104:ARG:NH1 | 4:4:105:ARG:HB2 | 1.98 | 0.75 |
| 24:A:856:SF4:S2 | 24:A:856:SF4:FE1 | 1.77 | 0.75 |
| 7:C:63:LEU:HG | 7:C:64:SER:H | 1.49 | 0.75 |
| 21:G:101:LMU:H22 | 21:G:101:LMU:O6' | 1.87 | 0.75 |
| 20:H:108:CLA:CHD | 22:I:101:BCR:H342 | 2.17 | 0.75 |
| 4:4:95:PHE:CZ | 20:4:314:CLA:NC | 2.55 | 0.75 |
| 4:4:128:ALA:HB1 | 4:4:141:LEU:HD23 | 1.68 | 0.75 |
| 5:A:103:PHE:CE1 | 20:A:807:CLA:O1D | 2.40 | 0.75 |
| 5:A:334:HIS:HB3 | 20:A:820:CLA:HMA1 | 1.68 | 0.75 |
| 20:A:818:CLA:HBB2 | 20:A:818:CLA:C8 | 2.16 | 0.75 |
| 20:A:825:CLA:HBC2 | 20:A:825:CLA:HMC1 | 1.69 | 0.75 |
| 20:A:850:CLA:HED2 | 20:A:850:CLA:CAD | 2.16 | 0.75 |
| 20:B:826:CLA:HBC2 | 20:B:826:CLA:CHD | 2.15 | 0.75 |
| 22:B:847:BCR:HC31 | 20:L:203:CLA:CMD | 2.17 | 0.75 |
| 10:F:24:LYS:HE2 | 10:F:24:LYS:CA | 2.08 | 0.75 |
| 10:F:28:SER:O | 10:F:29:LEU:C | 2.29 | 0.75 |
| 10:F:62:LEU:HG | 10:F:72:ILE:HD13 | 1.68 | 0.75 |
| 12:H:10:ASP:HB3 | 12:H:13:ASP:HB2 | 1.67 | 0.75 |
| 13:I:1:MET:O | 13:I:2:ILE:HG22 | 1.85 | 0.75 |
| 17:N:72:LYS:CG | 17:N:74:LYS:H | 2.00 | 0.75 |
| 20:1:213:CLA:HBA2 | 20:1:213:CLA:CMA | 2.16 | 0.74 |
| 3:3:93:PHE:C | 3:3:94:ARG:O | 2.29 | 0.74 |
| 3:3:112:THR:OG1 | 3:3:113:LEU:HG | 1.87 | 0.74 |
| 4:4:33:ASP:HB3 | 4:4:34:PRO:HD2 | 1.69 | 0.74 |
| 4:4:36:ASN:OD1 | 4:4:37:LEU:CA | 2.35 | 0.74 |
| 5:A:28:LYS:HZ3 | 5:A:28:LYS:CB | 1.90 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:530:LEU:HB2 | 5:A:531:PRO:HD2 | 1.66 | 0.74 |
| 20:A:803:CLA:CBB | 20:A:804:CLA:C4C | 2.64 | 0.74 |
| 22:A:843:BCR:H23C | 22:A:843:BCR:H402 | 1.69 | 0.74 |
| 6:B:120:VAL:HA | 6:B:123:TRP:HD1 | 1.46 | 0.74 |
| 6:B:557:PHE:N | 6:B:558:PRO:CD | 2.49 | 0.74 |
| 6:B:732:LYS:CD | 6:B:734:GLY:HA3 | 2.17 | 0.74 |
| 4:4:100:TYR:HA | 4:4:103:ILE:HG12 | 1.67 | 0.74 |
| 5:A:331:LEU:HD23 | 5:A:331:LEU:C | 2.12 | 0.74 |
| 22:A:843:BCR:H402 | 22:A:843:BCR:C23 | 2.16 | 0.74 |
| 6:B:167:TRP:CD1 | 11:G:41:MET:HE3 | 2.22 | 0.74 |
| 20:J:101:CLA:HBD | 20:J:101:CLA:CBA | 2.06 | 0.74 |
| 17:N:47:THR:HG21 | 17:N:54:LYS:HZ3 | 1.51 | 0.74 |
| 1:1:39:TYR:CD2 | 20:1:210:CLA:OBD | 2.40 | 0.74 |
| 4:4:121:PHE:CZ | 4:4:122:LYS:O | 2.41 | 0.74 |
| 20:A:839:CLA:O2D | 20:A:839:CLA:HAA2 | 1.87 | 0.74 |
| 6:B:87:ILE:HA | 6:B:115:ASN:CA | 2.13 | 0.74 |
| 6:B:369:ALA:O | 6:B:725:LEU:HD11 | 1.86 | 0.74 |
| 20:B:826:CLA:C1 | 20:B:839:CLA:CED | 2.65 | 0.74 |
| 5:A:208:ALA:HB2 | 5:A:314:GLY:HA3 | 1.68 | 0.74 |
| 7:C:31:TRP:HB2 | 7:C:39:ILE:HG21 | 1.69 | 0.74 |
| 11:G:73:ALA:O | 11:G:75:GLY:N | 2.20 | 0.74 |
| 20:H:109:CLA:HAC1 | 22:I:103:BCR:C3 | 2.17 | 0.74 |
| 17:N:58:VAL:HG23 | 17:N:60:PHE:CE1 | 2.22 | 0.74 |
| 5:A:25:ASP:HB2 | 5:A:26:PRO:O | 1.86 | 0.74 |
| 5:A:567:ARG:HH12 | 8:D:35:GLY:HA2 | 1.46 | 0.74 |
| 2:2:128:ASN:O | 2:2:130:LEU:N | 2.19 | 0.74 |
| 5:A:21:LEU:CB | 5:A:22:VAL:O | 2.36 | 0.74 |
| 5:A:197:GLN:HE22 | 5:A:351:THR:HB | 1.53 | 0.74 |
| 5:A:496:HIS:HB3 | 5:A:515:TRP:CE3 | 2.23 | 0.74 |
| 6:B:11:GLY:HA3 | 7:C:71:HIS:CD2 | 2.22 | 0.74 |
| 6:B:395:ILE:HD12 | 6:B:396:ARG:HG2 | 1.69 | 0.74 |
| 20:B:812:CLA:H62 | 20:B:812:CLA:CAD | 2.17 | 0.74 |
| 20:2:303:CLA:HHD | 20:2:303:CLA:CBC | 2.11 | 0.74 |
| 4:4:94:GLU:HB3 | 4:4:95:PHE:HE1 | 1.45 | 0.74 |
| 5:A:24:ARG:HH12 | 5:A:29:THR:CA | 2.00 | 0.74 |
| 24:A:856:SF4:S1 | 24:A:856:SF4:FE2 | 1.79 | 0.74 |
| 6:B:411:MET:HE1 | 20:B:831:CLA:CHD | 2.18 | 0.74 |
| 7:C:5:VAL:HB | 7:C:65:VAL:HA | 1.69 | 0.74 |
| 15:K:44:GLU:OE1 | 15:K:44:GLU:CA | 2.33 | 0.74 |
| 18:R:38:UNK:CA | 18:R:42:UNK:O | 2.35 | 0.74 |
| 2:2:96:ILE:HG13 | 2:2:97:VAL:N | 2.02 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:126:PRO:HD2 | 2:2:129:LYS:HB2 | 1.69 | 0.74 |
| 2:2:129:LYS:C | 2:2:131:THR:H | 1.96 | 0.74 |
| 2:2:205:PHE:CD1 | 2:2:205:PHE:C | 2.66 | 0.74 |
| 4:4:38:ARG:CG | 4:4:39:TRP:N | 2.48 | 0.74 |
| 20:4:303:CLA:H151 | 20:4:303:CLA:C20 | 2.18 | 0.74 |
| 5:A:401:TRP:CD1 | 20:A:826:CLA:CHC | 2.69 | 0.74 |
| 6:B:230:TRP:HB3 | 20:B:817:CLA:HED3 | 1.68 | 0.74 |
| 6:B:649:MET:HE3 | 6:B:723:ALA:HB2 | 1.69 | 0.74 |
| 20:B:802:CLA:C9 | 20:B:803:CLA:H91 | 2.16 | 0.74 |
| 21:H:105:LMU:H3' | 21:H:105:LMU:C5B | 2.17 | 0.74 |
| 1:1:183:ASP:CB | 1:1:184:PRO:CD | 2.61 | 0.74 |
| 5:A:267:THR:O | 5:A:269:PHE:CD2 | 2.35 | 0.74 |
| 5:A:665:ILE:HD13 | 6:B:621:ARG:HG3 | 1.70 | 0.74 |
| 6:B:16:PRO:HG3 | 7:C:74:THR:CG2 | 2.17 | 0.74 |
| 6:B:685:THR:OG1 | 20:L:201:CLA:H3A | 1.88 | 0.74 |
| 20:B:803:CLA:H41 | 20:B:803:CLA:HMB3 | 1.69 | 0.74 |
| 21:F:202:LMU:H31 | 21:F:202:LMU:C7 | 2.15 | 0.74 |
| 20:F:206:CLA:C3B | 20:F:207:CLA:HAC2 | 2.16 | 0.74 |
| 2:2:44:ASN:C | 2:2:46:GLN:H | 1.93 | 0.74 |
| 5:A:331:LEU:HD21 | 5:A:343:HIS:C | 2.12 | 0.74 |
| 6:B:378:ILE:O | 6:B:380:GLY:N | 2.20 | 0.74 |
| 6:B:464:GLN:CD | 6:B:469:LYS:HD3 | 2.13 | 0.74 |
| 20:B:839:CLA:HBC1 | 20:F:201:CLA:CMC | 2.18 | 0.74 |
| 7:C:39:ILE:CG1 | 7:C:40:ALA:H | 1.97 | 0.74 |
| 8:D:94:TYR:O | 8:D:95:LYS:HG2 | 1.88 | 0.74 |
| 17:N:54:LYS:O | 17:N:57:LYS:N | 2.21 | 0.74 |
| 4:4:106:TRP:C | 4:4:108:ASP:N | 2.45 | 0.73 |
| 4:4:118:ASP:C | 4:4:122:LYS:HA | 2.12 | 0.73 |
| 20:A:824:CLA:H2 | 20:A:825:CLA:HED3 | 1.70 | 0.73 |
| 6:B:211:ASN:HB2 | 6:B:214:ASP:HB3 | 1.70 | 0.73 |
| 6:B:373:THR:HA | 6:B:376:GLN:HB2 | 1.68 | 0.73 |
| 6:B:469:LYS:HE2 | 6:B:471:THR:OG1 | 1.87 | 0.73 |
| 20:B:822:CLA:HBC2 | 20:B:822:CLA:CHD | 2.15 | 0.73 |
| 10:F:63:CYS:HA | 10:F:69:PRO:HA | 1.70 | 0.73 |
| 15:K:44:GLU:OE1 | 15:K:44:GLU:HA | 1.87 | 0.73 |
| 16:L:99:LEU:HD11 | 22:L:209:BCR:HC7 | 1.69 | 0.73 |
| 2:2:51:HIS:HB2 | 20:2:310:CLA:OBD | 1.87 | 0.73 |
| 2:2:120:ASN:HB3 | 2:2:121:THR:HB | 1.69 | 0.73 |
| 3:3:94:ARG:C | 3:3:97:PHE:CE1 | 2.65 | 0.73 |
| 5:A:107:GLU:CD | 5:A:161:GLU:HG3 | 2.13 | 0.73 |
| 5:A:470:LEU:HD13 | 6:B:95:HIS:HB3 | 1.68 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:591:GLN:HA | 5:A:591:GLN:HE21 | 1.52 | 0.73 |
| 20:B:809:CLA:H91 | 20:B:809:CLA:H193 | 1.69 | 0.73 |
| 20:B:838:CLA:H152 | 22:F:204:BCR:H313 | 1.69 | 0.73 |
| 7:C:29:ILE:HG23 | 8:D:126:GLY:HA2 | 1.69 | 0.73 |
| 15:K:24:PHE:HB3 | 15:K:52:PRO:HG2 | 1.69 | 0.73 |
| 15:K:46:GLY:O | 15:K:47:LEU:CB | 2.36 | 0.73 |
| 17:N:54:LYS:O | 17:N:56:LYS:N | 2.20 | 0.73 |
| 4:4:34:PRO:HA | 4:4:35:GLU:CG | 2.19 | 0.73 |
| 8:D:78:ALA:HB3 | 8:D:82:GLN:NE2 | 1.97 | 0.73 |
| 11:G:45:GLU:O | 11:G:46:ALA:C | 2.29 | 0.73 |
| 21:2:313:LMU:C6 | 21:2:313:LMU:C2 | 2.66 | 0.73 |
| 5:A:79:PHE:CZ | 5:A:185:HIS:NE2 | 2.54 | 0.73 |
| 6:B:374:HIS:CG | 6:B:374:HIS:O | 2.41 | 0.73 |
| 6:B:427:LEU:HD23 | 6:B:431:PHE:CZ | 2.24 | 0.73 |
| 6:B:507:SER:O | 6:B:508:LEU:HB2 | 1.86 | 0.73 |
| 17:N:11:LYS:HD2 | 17:N:12:THR:O | 1.89 | 0.73 |
| 17:N:47:THR:O | 17:N:48:GLY:O | 2.07 | 0.73 |
| 5:A:81:ALA:CB | 20:A:804:CLA:HMA2 | 2.12 | 0.73 |
| 6:B:174:ARG:O | 6:B:175:LEU:HB3 | 1.88 | 0.73 |
| 6:B:431:PHE:CD2 | 20:B:832:CLA:HMA1 | 2.24 | 0.73 |
| 6:B:594:TRP:CD1 | 6:B:594:TRP:C | 2.67 | 0.73 |
| 7:C:5:VAL:HB | 7:C:65:VAL:CB | 2.18 | 0.73 |
| 11:G:8:ILE:O | 11:G:8:ILE:HG13 | 1.88 | 0.73 |
| 17:N:29:PHE:CD1 | 17:N:32:ALA:HB3 | 2.24 | 0.73 |
| 1:1:57:ILE:HG23 | 1:1:58:LEU:H | 1.53 | 0.73 |
| 1:1:57:ILE:O | 1:1:59:VAL:N | 2.22 | 0.73 |
| 3:3:208:PRO:HB3 | 3:3:210:GLN:OE1 | 1.89 | 0.73 |
| 5:A:108:ALA:HB1 | 5:A:138:GLY:HA3 | 1.70 | 0.73 |
| 5:A:596:ASP:HA | 5:A:599:PHE:HB3 | 1.70 | 0.73 |
| 6:B:612:SER:HA | 6:B:615:TYR:CE1 | 2.22 | 0.73 |
| 6:B:709:GLY:O | 6:B:710:LEU:HB2 | 1.88 | 0.73 |
| 20:B:813:CLA:HAC2 | 20:B:814:CLA:HBB2 | 0.80 | 0.73 |
| 20:H:108:CLA:CMA | 20:H:108:CLA:CGA | 2.66 | 0.73 |
| 16:L:36:TYR:O | 16:L:36:TYR:CD1 | 2.40 | 0.73 |
| 3:3:52:LYS:C | 3:3:56:TYR:CD2 | 2.65 | 0.73 |
| 4:4:144:ALA:HB3 | 4:4:147:LEU:O | 1.89 | 0.73 |
| 20:A:838:CLA:C14 | 22:A:845:BCR:C2 | 2.59 | 0.73 |
| 6:B:362:ALA:O | 6:B:363:GLN:HG3 | 1.87 | 0.73 |
| 20:B:817:CLA:HHD | 20:B:817:CLA:CBC | 2.19 | 0.73 |
| 21:E:101:LMU:C5 | 21:E:101:LMU:C1 | 2.67 | 0.73 |
| 10:F:7:PRO:HA | 10:F:61:LEU:O | 1.89 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:F:147:GLY:CA | 10:F:150:VAL:HB | 2.19 | 0.73 |
| 16:L:49:PRO:HB2 | 16:L:139:PHE:HB2 | 1.71 | 0.73 |
| 2:2:168:ARG:HH21 | 2:2:171:MET:HB2 | 1.51 | 0.73 |
| 21:2:313:LMU:H6E | 21:2:313:LMU:C2B | 2.18 | 0.73 |
| 3:3:50:GLU:N | 3:3:51:PRO:CD | 2.52 | 0.73 |
| 4:4:193:ILE:HG22 | 4:4:194:VAL:N | 2.02 | 0.73 |
| 5:A:289:PRO:O | 5:A:290:LEU:HB2 | 1.89 | 0.73 |
| 20:A:807:CLA:HBA2 | 20:A:809:CLA:H12 | 1.71 | 0.73 |
| 6:B:255:LEU:HD13 | 6:B:275:HIS:HB2 | 1.69 | 0.73 |
| 20:B:808:CLA:O1A | 20:B:814:CLA:HBA1 | 1.87 | 0.73 |
| 11:G:28:ARG:NH2 | 11:G:29:GLU:H | 1.86 | 0.73 |
| 5:A:331:LEU:CD1 | 5:A:346:LEU:HB3 | 2.15 | 0.73 |
| 20:A:830:CLA:HMB1 | 20:A:831:CLA:CHB | 2.19 | 0.73 |
| 6:B:394:PHE:O | 6:B:542:ARG:NE | 2.19 | 0.73 |
| 9:E:87:VAL:C | 9:E:89:GLU:H | 1.97 | 0.73 |
| 16:L:123:ARG:HA | 16:L:123:ARG:NE | 2.03 | 0.73 |
| 5:A:423:ASP:HB3 | 5:A:424:PRO:CD | 2.12 | 0.73 |
| 5:A:626:GLY:CA | 5:A:636:HIS:HA | 2.19 | 0.73 |
| 22:A:845:BCR:H393 | 22:A:845:BCR:C23 | 2.13 | 0.73 |
| 24:A:856:SF4:S4 | 24:A:856:SF4:FE2 | 1.81 | 0.73 |
| 6:B:50:HIS:CD2 | 20:B:808:CLA:HAA2 | 2.23 | 0.73 |
| 20:B:827:CLA:H8 | 22:B:846:BCR:H12C | 1.70 | 0.73 |
| 10:F:83:PHE:O | 10:F:87:GLY:HA3 | 1.89 | 0.73 |
| 12:H:50:ARG:HG2 | 16:L:137:ALA:HB1 | 1.71 | 0.73 |
| 4:4:57:GLY:O | 4:4:60:LEU:HD23 | 1.88 | 0.72 |
| 4:4:70:ILE:C | 4:4:72:VAL:N | 2.44 | 0.72 |
| 5:A:24:ARG:H | 5:A:24:ARG:HD3 | 1.51 | 0.72 |
| 5:A:355:HIS:ND1 | 5:A:416:ILE:HG21 | 2.04 | 0.72 |
| 20:A:837:CLA:C1C | 20:B:806:CLA:HBC2 | 2.19 | 0.72 |
| 20:B:830:CLA:H72 | 25:B:848:LMG:H311 | 1.70 | 0.72 |
| 20:B:839:CLA:O1D | 20:B:839:CLA:H2A | 1.89 | 0.72 |
| 21:G:102:LMU:H3' | 21:G:102:LMU:C6B | 2.17 | 0.72 |
| 2:2:70:LYS:HG3 | 2:2:73:ILE:HG12 | 1.70 | 0.72 |
| 4:4:160:MET:HE1 | 20:4:306:CLA:CBB | 2.17 | 0.72 |
| 20:A:850:CLA:HMB3 | 20:B:850:CLA:H18 | 1.71 | 0.72 |
| 6:B:48:ALA:CB | 6:B:157:LEU:HD22 | 2.19 | 0.72 |
| 6:B:50:HIS:HD2 | 20:B:808:CLA:HAA2 | 1.54 | 0.72 |
| 6:B:53:GLN:NE2 | 20:B:807:CLA:HBB1 | 2.03 | 0.72 |
| 6:B:635:ILE:O | 6:B:636:THR:O | 2.07 | 0.72 |
| 19:P:1:GLC:H3 | 19:P:2:FRU:O5 | 1.88 | 0.72 |
| 20:4:304:CLA:HBC3 | 20:4:304:CLA:CMC | 2.18 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:451:ILE:CD1 | 20:A:830:CLA:HED3 | 2.20 | 0.72 |
| 20:A:818:CLA:CAB | 20:A:818:CLA:C7 | 2.67 | 0.72 |
| 21:A:854:LMU:H32 | 21:A:854:LMU:H82 | 1.71 | 0.72 |
| 6:B:697:PRO:HB3 | 20:B:840:CLA:HBC3 | 1.70 | 0.72 |
| 9:E:87:VAL:O | 9:E:89:GLU:N | 2.19 | 0.72 |
| 20:K:101:CLA:CED | 20:K:102:CLA:CMB | 2.67 | 0.72 |
| 18:R:52:UNK:HA | 18:R:53:UNK:CB | 2.19 | 0.72 |
| 20:2:312:CLA:HED3 | 20:2:312:CLA:OBD | 1.89 | 0.72 |
| 21:2:313:LMU:H62 | 21:2:313:LMU:C1 | 2.19 | 0.72 |
| 3:3:106:TYR:CD2 | 3:3:107:TRP:CD1 | 2.78 | 0.72 |
| 4:4:100:TYR:HA | 4:4:103:ILE:HD11 | 1.72 | 0.72 |
| 4:4:192:THR:HG21 | 4:4:195:GLN:N | 2.00 | 0.72 |
| 5:A:21:LEU:C | 5:A:22:VAL:O | 2.30 | 0.72 |
| 5:A:96:MET:HE2 | 20:A:807:CLA:HBB2 | 1.70 | 0.72 |
| 5:A:654:ARG:HA | 6:B:632:ILE:HD13 | 1.71 | 0.72 |
| 6:B:75:GLU:HB2 | 6:B:132:ASN:HB3 | 1.69 | 0.72 |
| 6:B:547:MET:HE2 | 6:B:550:LYS:HA | 1.71 | 0.72 |
| 6:B:583:MET:HE2 | 6:B:583:MET:O | 1.90 | 0.72 |
| 7:C:78:GLY:O | 7:C:81:TYR:CE1 | 2.38 | 0.72 |
| 1:1:39:TYR:CG | 20:1:210:CLA:OBD | 2.41 | 0.72 |
| 20:1:206:CLA:HHD | 20:1:206:CLA:HBC2 | 1.70 | 0.72 |
| 5:A:368:LEU:HD22 | 20:A:818:CLA:C9 | 2.19 | 0.72 |
| 24:A:856:SF4:S2 | 24:A:856:SF4:FE3 | 1.80 | 0.72 |
| 6:B:315:LEU:O | 6:B:315:LEU:HD13 | 1.90 | 0.72 |
| 6:B:663:PHE:O | 6:B:664:LEU:CB | 2.37 | 0.72 |
| 20:B:838:CLA:H202 | 22:F:204:BCR:HC41 | 1.72 | 0.72 |
| 7:C:17:CYS:C | 7:C:58:CYS:HB2 | 2.14 | 0.72 |
| 20:H:108:CLA:CGA | 20:H:108:CLA:HMA1 | 2.19 | 0.72 |
| 20:2:302:CLA:HBC2 | 20:2:302:CLA:CHD | 2.19 | 0.72 |
| 20:2:305:CLA:C2 | 20:2:307:CLA:HMD2 | 2.19 | 0.72 |
| 3:3:52:LYS:HA | 3:3:55:ALA:HB3 | 1.70 | 0.72 |
| 5:A:309:LEU:HD21 | 20:A:819:CLA:CMC | 2.20 | 0.72 |
| 5:A:349:ILE:O | 5:A:349:ILE:HG22 | 1.87 | 0.72 |
| 5:A:684:PHE:HD2 | 5:A:685:VAL:N | 1.88 | 0.72 |
| 5:A:697:ARG:NH2 | 6:B:566:GLY:O | 2.21 | 0.72 |
| 6:B:142:LEU:CD2 | 22:B:845:BCR:H333 | 2.19 | 0.72 |
| 12:H:69:SER:CB | 20:H:108:CLA:H2 | 2.19 | 0.72 |
| 2:2:73:ILE:O | 2:2:74:LEU:CG | 2.36 | 0.72 |
| 5:A:207:LEU:HD12 | 5:A:310:PHE:HD1 | 1.53 | 0.72 |
| 5:A:558:LYS:NZ | 6:B:674:LEU:HB3 | 2.05 | 0.72 |
| 20:A:801:CLA:HMC3 | 20:A:801:CLA:HBC2 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:F:61:LEU:HD23 | 10:F:69:PRO:CB | 2.20 | 0.72 |
| 11:G:40:GLY:O | 11:G:41:MET:SD | 2.48 | 0.72 |
| 12:H:23:VAL:O | 12:H:23:VAL:HG12 | 1.88 | 0.72 |
| 20:A:824:CLA:HED1 | 20:A:825:CLA:HMD2 | 1.59 | 0.72 |
| 6:B:493:TRP:HE1 | 20:B:817:CLA:HAC2 | 1.55 | 0.72 |
| 20:R:108:CLA:HBA2 | 20:R:108:CLA:CBD | 2.20 | 0.72 |
| 2:2:98:GLU:HG3 | 2:2:99:LEU:HG | 1.70 | 0.72 |
| 5:A:224:HIS:O | 5:A:225:VAL:HG22 | 1.90 | 0.72 |
| 5:A:497:ALA:HB2 | 5:A:515:TRP:CB | 2.20 | 0.72 |
| 21:A:853:LMU:O6' | 21:A:853:LMU:H51 | 1.89 | 0.72 |
| 6:B:542:ARG:NH2 | 8:D:141:VAL:O | 2.21 | 0.72 |
| 10:F:93:ILE:CG2 | 22:F:203:BCR:H371 | 2.19 | 0.72 |
| 11:G:43:HIS:O | 11:G:45:GLU:HG3 | 1.89 | 0.72 |
| 12:H:25:GLY:HA3 | 12:H:27:ASP:HB2 | 1.71 | 0.72 |
| 21:H:104:LMU:H21 | 21:H:104:LMU:O5' | 1.86 | 0.72 |
| 20:L:202:CLA:H12 | 20:L:202:CLA:CGD | 2.17 | 0.72 |
| 4:4:106:TRP:O | 4:4:108:ASP:N | 2.22 | 0.72 |
| 5:A:454:GLY:H | 5:A:457:SER:CB | 2.02 | 0.72 |
| 5:A:470:LEU:HD11 | 6:B:95:HIS:HB3 | 1.70 | 0.72 |
| 5:A:705:GLU:CB | 6:B:545:LYS:NZ | 2.53 | 0.72 |
| 20:A:808:CLA:H142 | 22:J:102:BCR:C14 | 2.20 | 0.72 |
| 6:B:334:LEU:HG | 6:B:334:LEU:O | 1.90 | 0.72 |
| 10:F:93:ILE:HG21 | 22:F:203:BCR:C37 | 2.19 | 0.72 |
| 11:G:7:VAL:HG22 | 11:G:8:ILE:H | 1.55 | 0.72 |
| 16:L:64:LEU:HB3 | 16:L:68:PHE:CE1 | 2.19 | 0.72 |
| 17:N:50:GLN:CA | 17:N:51:ASP:O | 2.38 | 0.72 |
| 20:3:307:CLA:HAC2 | 20:K:104:CLA:C7 | 2.15 | 0.71 |
| 4:4:44:GLU:O | 4:4:47:ASN:N | 2.22 | 0.71 |
| 20:4:310:CLA:HBA2 | 20:4:310:CLA:O1D | 1.90 | 0.71 |
| 5:A:400:MET:HE3 | 5:A:612:VAL:HG11 | 1.72 | 0.71 |
| 5:A:545:HIS:O | 5:A:549:ILE:HG13 | 1.90 | 0.71 |
| 6:B:167:TRP:HD1 | 11:G:41:MET:HE3 | 1.54 | 0.71 |
| 6:B:347:LEU:HD22 | 6:B:351:HIS:CE1 | 2.25 | 0.71 |
| 10:F:93:ILE:CG2 | 22:F:203:BCR:C37 | 2.68 | 0.71 |
| 17:N:63:ASP:CA | 17:N:64:ASP:C | 2.63 | 0.71 |
| 17:N:77:CYS:O | 17:N:79:SER:N | 2.23 | 0.71 |
| 1:1:27:LEU:HD21 | 6:B:314:ARG:HG2 | 1.73 | 0.71 |
| 4:4:114:SER:OG | 4:4:120:ILE:HD11 | 1.90 | 0.71 |
| 20:4:310:CLA:HBA2 | 20:4:310:CLA:CBD | 2.20 | 0.71 |
| 5:A:28:LYS:HB3 | 5:A:28:LYS:HZ2 | 1.50 | 0.71 |
| 5:A:690:LEU:HD21 | 6:B:661:PHE:HE1 | 1.55 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:A:851:CLA:CMD | 6:B:578:LEU:HD23 | 2.19 | 0.71 |
| 6:B:174:ARG:CB | 20:B:814:CLA:HBC2 | 2.20 | 0.71 |
| 6:B:504:ASN:H | 6:B:504:ASN:ND2 | 1.87 | 0.71 |
| 6:B:557:PHE:HE2 | 7:C:66:ARG:HE | 1.35 | 0.71 |
| 20:B:808:CLA:O1A | 20:B:814:CLA:CBA | 2.38 | 0.71 |
| 11:G:46:ALA:O | 11:G:47:GLY:C | 2.30 | 0.71 |
| 11:G:93:TYR:CA | 11:G:94:ASP:CB | 2.64 | 0.71 |
| 4:4:37:LEU:O | 4:4:39:TRP:CD1 | 2.43 | 0.71 |
| 5:A:284:ARG:HA | 5:A:284:ARG:CZ | 2.19 | 0.71 |
| 20:A:822:CLA:CBB | 22:A:844:BCR:C35 | 2.68 | 0.71 |
| 6:B:349:ALA:CB | 6:B:375:HIS:HB3 | 2.21 | 0.71 |
| 6:B:732:LYS:C | 6:B:733:PHE:O | 2.29 | 0.71 |
| 7:C:12:ILE:HB | 7:C:39:ILE:HA | 1.71 | 0.71 |
| 10:F:25:LEU:HD22 | 10:F:46:MET:HB3 | 1.70 | 0.71 |
| 16:L:64:LEU:HA | 16:L:67:PRO:HG2 | 1.72 | 0.71 |
| 21:L:205:LMU:O3' | 21:L:205:LMU:H1B | 1.91 | 0.71 |
| 1:1:45:ILE:HG22 | 1:1:48:ARG:HD2 | 1.73 | 0.71 |
| 4:4:70:ILE:HG13 | 4:4:71:ASN:N | 2.05 | 0.71 |
| 4:4:98:SER:CB | 4:4:102:GLU:OE1 | 2.38 | 0.71 |
| 5:A:25:ASP:OD2 | 5:A:26:PRO:HD3 | 1.91 | 0.71 |
| 5:A:62:HIS:HB2 | 20:A:828:CLA:HBA1 | 1.72 | 0.71 |
| 5:A:316:MET:HA | 5:A:317:TYR:HD1 | 1.54 | 0.71 |
| 5:A:370:ILE:CG2 | 5:A:400:MET:HA | 2.21 | 0.71 |
| 5:A:393:LEU:HD11 | 5:A:750:PHE:CE1 | 2.25 | 0.71 |
| 20:B:812:CLA:HAA2 | 20:B:812:CLA:H12 | 1.70 | 0.71 |
| 20:B:840:CLA:H11 | 20:L:203:CLA:HMC2 | 1.71 | 0.71 |
| 9:E:39:LEU:C | 9:E:40:ARG:HD3 | 2.15 | 0.71 |
| 16:L:161:LEU:HD11 | 16:L:162:ASP:O | 1.91 | 0.71 |
| 17:N:42:PHE:CD1 | 17:N:43:PRO:N | 2.59 | 0.71 |
| 3:3:94:ARG:CG | 3:3:97:PHE:HZ | 1.85 | 0.71 |
| 3:3:97:PHE:HD2 | 3:3:98:ILE:N | 1.88 | 0.71 |
| 4:4:101:VAL:HG13 | 4:4:104:ARG:HH22 | 1.55 | 0.71 |
| 5:A:220:ARG:O | 5:A:221:HIS:HB2 | 1.91 | 0.71 |
| 6:B:387:PHE:O | 6:B:391:PRO:HD3 | 1.91 | 0.71 |
| 7:C:1:MET:HE1 | 8:D:154:TYR:OH | 1.91 | 0.71 |
| 9:E:60:LYS:HG3 | 9:E:61:THR:N | 2.04 | 0.71 |
| 9:E:85:ASP:O | 9:E:86:GLU:HB3 | 1.90 | 0.71 |
| 10:F:140:ALA:O | 10:F:144:LEU:HB3 | 1.90 | 0.71 |
| 20:3:311:CLA:HMC1 | 20:3:311:CLA:HBC3 | 1.73 | 0.71 |
| 4:4:100:TYR:HA | 4:4:103:ILE:CD1 | 2.20 | 0.71 |
| 4:4:122:LYS:NZ | 4:4:150:LYS:CD | 2.52 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:4:315:CLA:HBA1 | 20:4:315:CLA:CBD | 2.21 | 0.71 |
| 5:A:545:HIS:CG | 20:A:834:CLA:HBB2 | 2.25 | 0.71 |
| 5:A:680:LEU:HD21 | 6:B:617:MET:HE3 | 1.73 | 0.71 |
| 20:A:818:CLA:HBB2 | 20:A:818:CLA:C10 | 2.21 | 0.71 |
| 24:A:856:SF4:S3 | 24:A:856:SF4:FE1 | 1.82 | 0.71 |
| 7:C:31:TRP:O | 7:C:33:GLY:N | 2.23 | 0.71 |
| 21:G:102:LMU:H6'2 | 21:G:102:LMU:C3' | 2.17 | 0.71 |
| 15:K:51:ASP:HB3 | 15:K:52:PRO:HD3 | 1.70 | 0.71 |
| 16:L:164:PRO:CA | 16:L:165:TYR:HD1 | 1.86 | 0.71 |
| 1:1:27:LEU:HD13 | 1:1:28:GLY:H | 1.55 | 0.71 |
| 2:2:169:LEU:CD2 | 20:2:305:CLA:CAB | 2.63 | 0.71 |
| 3:3:52:LYS:O | 3:3:56:TYR:N | 2.21 | 0.71 |
| 5:A:27:ILE:CB | 5:A:28:LYS:HG2 | 2.21 | 0.71 |
| 5:A:218:TRP:O | 5:A:222:GLN:HB2 | 1.90 | 0.71 |
| 6:B:530:THR:HG21 | 20:B:826:CLA:HAC1 | 1.72 | 0.71 |
| 6:B:697:PRO:O | 7:C:79:LEU:HD11 | 1.88 | 0.71 |
| 21:B:805:LMU:O3' | 21:B:805:LMU:C1B | 2.38 | 0.71 |
| 20:B:815:CLA:HMB1 | 22:B:845:BCR:C8 | 2.21 | 0.71 |
| 9:E:88:GLU:O | 9:E:90:VAL:CA | 2.39 | 0.71 |
| 10:F:151:ASP:OD2 | 10:F:154:PHE:CD1 | 2.44 | 0.71 |
| 12:H:42:THR:HG22 | 12:H:45:ALA:HB2 | 1.72 | 0.71 |
| 15:K:79:LYS:HE3 | 15:K:84:LEU:C | 2.13 | 0.71 |
| 16:L:164:PRO:CG | 16:L:165:TYR:CE1 | 2.51 | 0.71 |
| 17:N:61:LEU:HD11 | 17:N:63:ASP:CA | 2.21 | 0.71 |
| 5:A:464:ASN:HD22 | 5:A:464:ASN:N | 1.86 | 0.71 |
| 5:A:714:LEU:HA | 10:F:149:LEU:HD11 | 1.73 | 0.71 |
| 6:B:172:GLU:O | 6:B:176:ASN:CB | 2.39 | 0.71 |
| 6:B:692:ARG:HH22 | 6:B:694:ARG:HG2 | 1.54 | 0.71 |
| 20:B:820:CLA:OBD | 20:B:823:CLA:HBC3 | 1.89 | 0.71 |
| 20:B:830:CLA:H62 | 25:B:848:LMG:H182 | 1.73 | 0.71 |
| 7:C:26:LEU:N | 7:C:43:PRO:HG3 | 2.05 | 0.71 |
| 10:F:53:PHE:C | 10:F:55:ASN:H | 1.97 | 0.71 |
| 17:N:41:LYS:CB | 17:N:42:PHE:CB | 2.65 | 0.71 |
| 21:1:217:LMU:H91 | 21:G:103:LMU:C3' | 2.21 | 0.71 |
| 4:4:70:ILE:O | 4:4:73:PRO:HD3 | 1.91 | 0.71 |
| 5:A:349:ILE:O | 5:A:349:ILE:CG2 | 2.39 | 0.71 |
| 20:A:822:CLA:HBB2 | 22:A:844:BCR:C35 | 2.21 | 0.71 |
| 6:B:310:PRO:HB2 | 6:B:311:PRO:CD | 2.21 | 0.71 |
| 8:D:113:HIS:NE2 | 8:D:118:VAL:CG1 | 2.54 | 0.71 |
| 10:F:95:GLY:O | 10:F:99:TRP:HB2 | 1.91 | 0.71 |
| 13:I:12:VAL:O | 13:I:17:PRO:CD | 2.37 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:N:41:LYS:HB2 | 17:N:42:PHE:CB | 2.21 | 0.71 |
| 4:4:58:MET:O | 4:4:61:PRO:CD | 2.39 | 0.70 |
| 5:A:81:ALA:HB2 | 20:A:804:CLA:HMA3 | 1.68 | 0.70 |
| 5:A:214:GLY:O | 5:A:215:SER:HB3 | 1.91 | 0.70 |
| 5:A:723:ARG:HG2 | 5:A:723:ARG:NH1 | 2.04 | 0.70 |
| 7:C:63:LEU:CG | 7:C:64:SER:H | 2.04 | 0.70 |
| 20:H:109:CLA:C3C | 22:I:103:BCR:HC22 | 2.17 | 0.70 |
| 17:N:63:ASP:N | 17:N:64:ASP:CB | 2.51 | 0.70 |
| 18:R:30:UNK:O | 18:R:32:UNK:O | 2.08 | 0.70 |
| 3:3:80:LYS:HZ3 | 3:3:92:TRP:CD1 | 2.09 | 0.70 |
| 4:4:144:ALA:C | 4:4:145:PRO:O | 2.29 | 0.70 |
| 5:A:168:ALA:O | 5:A:171:ALA:HB3 | 1.90 | 0.70 |
| 20:A:818:CLA:HBB2 | 20:A:818:CLA:H8 | 1.72 | 0.70 |
| 20:A:824:CLA:H43 | 20:A:835:CLA:HBA1 | 1.73 | 0.70 |
| 21:A:853:LMU:C2 | 21:A:853:LMU:C8 | 2.61 | 0.70 |
| 6:B:123:TRP:CZ3 | 20:B:814:CLA:H191 | 2.25 | 0.70 |
| 6:B:687:LEU:HD12 | 22:B:801:BCR:HC31 | 1.72 | 0.70 |
| 6:B:732:LYS:HD3 | 6:B:734:GLY:HA3 | 1.73 | 0.70 |
| 7:C:1:MET:CB | 7:C:4:SER:OG | 2.36 | 0.70 |
| 22:I:103:BCR:H391 | 22:L:209:BCR:H401 | 1.73 | 0.70 |
| 1:1:24:PHE:CG | 6:B:314:ARG:NH2 | 2.59 | 0.70 |
| 1:1:25:ASP:HB3 | 1:1:26:PRO:CD | 2.20 | 0.70 |
| 21:2:318:LMU:O5B | 21:2:318:LMU:H5' | 1.88 | 0.70 |
| 4:4:106:TRP:HD1 | 20:4:301:CLA:O1D | 1.75 | 0.70 |
| 6:B:137:THR:HA | 6:B:140:ILE:CG1 | 2.20 | 0.70 |
| 6:B:167:TRP:HB2 | 11:G:41:MET:CE | 2.21 | 0.70 |
| 6:B:463:ILE:O | 6:B:464:GLN:HB3 | 1.91 | 0.70 |
| 6:B:545:LYS:HD3 | 6:B:546:LEU:H | 1.56 | 0.70 |
| 10:F:22:LEU:O | 10:F:25:LEU:N | 2.23 | 0.70 |
| 19:X:1:GLC:C6 | 19:X:2:FRU:H3 | 2.22 | 0.70 |
| 2:2:110:TRP:HD1 | 2:2:113:ILE:CG2 | 2.04 | 0.70 |
| 3:3:97:PHE:HD2 | 3:3:98:ILE:CG2 | 1.85 | 0.70 |
| 3:3:106:TYR:O | 3:3:108:ALA:HB2 | 1.91 | 0.70 |
| 5:A:22:VAL:C | 5:A:23:ASP:O | 2.29 | 0.70 |
| 5:A:187:HIS:CE1 | 20:A:811:CLA:C4D | 2.73 | 0.70 |
| 5:A:217:SER:HG | 22:A:843:BCR:H17C | 1.56 | 0.70 |
| 5:A:605:MET:HA | 5:A:608:SER:OG | 1.92 | 0.70 |
| 5:A:661:ALA:O | 5:A:664:VAL:HG22 | 1.92 | 0.70 |
| 20:A:804:CLA:HBA2 | 20:A:811:CLA:H62 | 1.74 | 0.70 |
| 22:B:847:BCR:H23C | 22:B:847:BCR:C38 | 2.21 | 0.70 |
| 9:E:42:GLU:HG2 | 9:E:43:SER:H | 1.53 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:F:12:LYS:HG2 | 10:F:13:GLN:N | 2.07 | 0.70 |
| 12:H:45:ALA:O | 12:H:47:PHE:N | 2.25 | 0.70 |
| 16:L:163:LEU:HD12 | 16:L:164:PRO:HG3 | 1.74 | 0.70 |
| 18:R:34:UNK:H | 18:R:36:UNK:CA | 2.00 | 0.70 |
| 20:R:107:CLA:CHA | 20:R:107:CLA:CED | 2.69 | 0.70 |
| 3:3:64:TYR:HB3 | 20:3:310:CLA:C4 | 2.21 | 0.70 |
| 4:4:149:ALA:HB3 | 4:4:151:GLU:OE1 | 1.91 | 0.70 |
| 20:A:804:CLA:C1 | 20:A:811:CLA:H61 | 2.16 | 0.70 |
| 6:B:202:SER:HB3 | 6:B:270:LEU:HD11 | 1.74 | 0.70 |
| 6:B:323:TYR:CE1 | 20:B:825:CLA:HBC1 | 2.26 | 0.70 |
| 6:B:471:THR:HG23 | 6:B:502:ASN:ND2 | 2.07 | 0.70 |
| 20:B:838:CLA:H121 | 22:F:204:BCR:H312 | 1.73 | 0.70 |
| 15:K:4:GLY:HA2 | 15:K:7:THR:HB | 1.72 | 0.70 |
| 15:K:43:ARG:HH11 | 15:K:43:ARG:CG | 1.86 | 0.70 |
| 21:K:107:LMU:O3' | 21:K:107:LMU:H1B | 1.89 | 0.70 |
| 21:2:313:LMU:C1 | 21:2:313:LMU:C7 | 2.69 | 0.70 |
| 4:4:52:MET:HE3 | 4:4:156:ASN:HB2 | 1.73 | 0.70 |
| 4:4:69:ILE:CD1 | 4:4:175:LYS:HB2 | 2.08 | 0.70 |
| 4:4:117:GLN:O | 4:4:121:PHE:HE2 | 1.73 | 0.70 |
| 4:4:149:ALA:HB3 | 4:4:151:GLU:CD | 2.17 | 0.70 |
| 4:4:150:LYS:O | 4:4:150:LYS:HG3 | 1.90 | 0.70 |
| 6:B:131:THR:O | 6:B:135:LEU:N | 2.24 | 0.70 |
| 6:B:317:ARG:HA | 6:B:317:ARG:HE | 1.54 | 0.70 |
| 6:B:438:VAL:HG22 | 20:B:833:CLA:CMC | 2.18 | 0.70 |
| 11:G:27:GLN:O | 11:G:28:ARG:HB3 | 1.90 | 0.70 |
| 15:K:16:THR:O | 15:K:20:PHE:HB3 | 1.92 | 0.70 |
| 21:R:103:LMU:H22 | 21:R:103:LMU:C6 | 2.14 | 0.70 |
| 5:A:567:ARG:HH11 | 8:D:35:GLY:CA | 2.04 | 0.70 |
| 20:A:850:CLA:C3B | 6:B:589:TRP:CH2 | 2.74 | 0.70 |
| 21:A:854:LMU:H41 | 21:A:854:LMU:C9 | 2.22 | 0.70 |
| 6:B:732:LYS:HG2 | 6:B:733:PHE:O | 1.91 | 0.70 |
| 10:F:116:GLN:C | 10:F:118:GLU:H | 2.00 | 0.70 |
| 17:N:45:ASN:ND2 | 17:N:54:LYS:CB | 2.54 | 0.70 |
| 17:N:72:LYS:NZ | 17:N:74:LYS:HE3 | 2.07 | 0.70 |
| 2:2:113:ILE:HG13 | 2:2:114:LEU:H | 1.57 | 0.70 |
| 3:3:163:PHE:O | 3:3:164:PHE:HB2 | 1.91 | 0.70 |
| 4:4:91:PHE:C | 4:4:91:PHE:HD2 | 1.99 | 0.70 |
| 4:4:124:TYR:HB3 | 4:4:143:PHE:CE1 | 2.26 | 0.70 |
| 4:4:124:TYR:HB2 | 4:4:143:PHE:CD1 | 2.25 | 0.70 |
| 5:A:187:HIS:CE1 | 20:A:811:CLA:C1A | 2.61 | 0.70 |
| 6:B:124:TRP:O | 6:B:129:LEU:HB3 | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:C:5:VAL:HG23 | 7:C:65:VAL:CG1 | 2.19 | 0.70 |
| 8:D:102:ARG:HE | 8:D:110:GLN:CB | 2.03 | 0.70 |
| 12:H:58:ILE:HD11 | 16:L:97:MET:SD | 2.31 | 0.70 |
| 14:J:31:ARG:HA | 14:J:34:PRO:HA | 1.72 | 0.70 |
| 17:N:41:LYS:CB | 17:N:42:PHE:CA | 2.68 | 0.70 |
| 21:1:217:LMU:H91 | 21:G:103:LMU:C4' | 2.21 | 0.70 |
| 2:2:166:ASN:OD1 | 2:2:169:LEU:HD12 | 1.91 | 0.70 |
| 5:A:246:HIS:CE1 | 20:A:840:CLA:HMA2 | 2.26 | 0.70 |
| 5:A:422:TYR:N | 5:A:422:TYR:CD1 | 2.57 | 0.70 |
| 22:A:845:BCR:C31 | 22:A:845:BCR:C8 | 2.69 | 0.70 |
| 6:B:58:PHE:HB3 | 6:B:146:SER:HB3 | 1.72 | 0.70 |
| 6:B:396:ARG:HH11 | 20:B:830:CLA:HED2 | 1.57 | 0.70 |
| 6:B:596:TRP:CD1 | 6:B:623:TYR:HB2 | 2.26 | 0.70 |
| 6:B:672:GLN:HA | 6:B:672:GLN:NE2 | 1.97 | 0.70 |
| 20:B:838:CLA:C16 | 22:F:204:BCR:H313 | 2.20 | 0.70 |
| 7:C:7:ILE:CG2 | 7:C:65:VAL:HG21 | 2.21 | 0.70 |
| 9:E:45:TRP:HH2 | 9:E:78:SER:OG | 1.73 | 0.70 |
| 21:G:101:LMU:H6D | 21:G:101:LMU:C2 | 2.22 | 0.70 |
| 4:4:106:TRP:CD1 | 20:4:301:CLA:O1D | 2.44 | 0.70 |
| 5:A:685:VAL:HG12 | 5:A:741:GLY:HA2 | 1.74 | 0.70 |
| 20:A:824:CLA:H72 | 20:A:825:CLA:HED2 | 1.72 | 0.70 |
| 6:B:293:THR:C | 6:B:294:ASN:ND2 | 2.50 | 0.70 |
| 6:B:654:HIS:CE1 | 20:B:850:CLA:NB | 2.60 | 0.70 |
| 20:B:839:CLA:HBA1 | 20:B:839:CLA:CHA | 2.20 | 0.70 |
| 7:C:55:GLU:C | 7:C:57:ALA:H | 2.00 | 0.70 |
| 10:F:151:ASP:HA | 10:F:154:PHE:HB3 | 1.73 | 0.70 |
| 20:J:101:CLA:H2 | 20:J:101:CLA:HMA3 | 1.73 | 0.70 |
| 21:2:313:LMU:O5' | 21:2:313:LMU:C3 | 2.39 | 0.69 |
| 3:3:163:PHE:HD1 | 3:3:163:PHE:C | 1.99 | 0.69 |
| 5:A:27:ILE:HG22 | 5:A:28:LYS:HD3 | 1.44 | 0.69 |
| 5:A:56:ASN:O | 5:A:57:LEU:HB3 | 1.91 | 0.69 |
| 6:B:16:PRO:HG3 | 7:C:74:THR:HB | 1.74 | 0.69 |
| 6:B:190:TRP:CZ2 | 20:B:819:CLA:HMD1 | 2.27 | 0.69 |
| 6:B:424:TRP:CZ2 | 20:F:201:CLA:HAC1 | 2.26 | 0.69 |
| 20:B:824:CLA:C1A | 20:B:824:CLA:C4 | 2.60 | 0.69 |
| 10:F:90:PHE:HA | 22:F:203:BCR:C39 | 2.22 | 0.69 |
| 10:F:93:ILE:O | 10:F:96:TRP:CD1 | 2.41 | 0.69 |
| 11:G:28:ARG:CG | 11:G:29:GLU:N | 2.54 | 0.69 |
| 20:H:108:CLA:O1A | 20:H:108:CLA:C4 | 2.39 | 0.69 |
| 5:A:131:ILE:HD13 | 6:B:447:GLY:HA3 | 1.71 | 0.69 |
| 5:A:705:GLU:HA | 5:A:708:VAL:HB | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:292:ARG:HA | 6:B:292:ARG:CZ | 2.21 | 0.69 |
| 6:B:295:PHE:HD2 | 6:B:295:PHE:N | 1.90 | 0.69 |
| 6:B:295:PHE:CD2 | 6:B:295:PHE:N | 2.60 | 0.69 |
| 6:B:421:HIS:CE1 | 20:F:201:CLA:C4D | 2.74 | 0.69 |
| 21:F:202:LMU:H82 | 21:F:202:LMU:C2 | 2.21 | 0.69 |
| 13:I:7:LEU:CD1 | 22:I:103:BCR:H333 | 2.15 | 0.69 |
| 2:2:44:ASN:ND2 | 14:J:1:MET:HB2 | 2.08 | 0.69 |
| 2:2:102:ILE:CG1 | 20:2:311:CLA:HMD2 | 2.22 | 0.69 |
| 20:2:316:CLA:H12 | 20:2:316:CLA:CAA | 2.20 | 0.69 |
| 4:4:106:TRP:CD2 | 20:4:301:CLA:CED | 2.72 | 0.69 |
| 4:4:147:LEU:CG | 4:4:148:GLU:H | 2.05 | 0.69 |
| 5:A:27:ILE:O | 5:A:28:LYS:HD2 | 1.92 | 0.69 |
| 5:A:281:LEU:HA | 5:A:297:THR:O | 1.92 | 0.69 |
| 20:A:819:CLA:HMD2 | 20:A:821:CLA:CBB | 2.22 | 0.69 |
| 21:A:854:LMU:H2B | 21:A:854:LMU:C6B | 2.22 | 0.69 |
| 6:B:120:VAL:CA | 6:B:123:TRP:CD1 | 2.71 | 0.69 |
| 7:C:74:THR:C | 7:C:76:SER:N | 2.47 | 0.69 |
| 11:G:28:ARG:HG2 | 11:G:29:GLU:H | 1.55 | 0.69 |
| 14:J:11:ALA:HB1 | 14:J:12:PRO:CD | 2.20 | 0.69 |
| 15:K:44:GLU:CD | 15:K:45:SER:O | 2.35 | 0.69 |
| 4:4:147:LEU:HD22 | 4:4:148:GLU:HG3 | 1.75 | 0.69 |
| 5:A:603:PHE:HZ | 5:A:693:LEU:HD21 | 1.56 | 0.69 |
| 20:A:824:CLA:H52 | 20:A:825:CLA:HED1 | 1.73 | 0.69 |
| 6:B:437:TYR:HB3 | 6:B:616:LEU:CD2 | 2.22 | 0.69 |
| 20:B:834:CLA:C1D | 20:B:835:CLA:HBB2 | 2.21 | 0.69 |
| 20:B:838:CLA:HBC1 | 10:F:83:PHE:HZ | 1.53 | 0.69 |
| 9:E:68:ARG:NE | 9:E:68:ARG:O | 2.24 | 0.69 |
| 21:K:107:LMU:H6D | 21:K:107:LMU:C3 | 2.20 | 0.69 |
| 16:L:36:TYR:CE1 | 20:L:201:CLA:H93 | 2.27 | 0.69 |
| 2:2:164:ILE:O | 2:2:167:GLY:HA3 | 1.92 | 0.69 |
| 4:4:89:THR:N | 4:4:90:LEU:HD22 | 2.08 | 0.69 |
| 4:4:163:PHE:O | 4:4:166:PHE:HB3 | 1.91 | 0.69 |
| 20:A:824:CLA:C5 | 20:A:825:CLA:HED1 | 2.22 | 0.69 |
| 6:B:224:PRO:HB3 | 6:B:227:THR:HB | 1.74 | 0.69 |
| 6:B:672:GLN:HE21 | 6:B:672:GLN:CA | 1.92 | 0.69 |
| 21:H:104:LMU:O2B | 21:H:104:LMU:C4' | 2.40 | 0.69 |
| 5:A:259:TYR:CB | 5:A:260:PRO:HD2 | 2.21 | 0.69 |
| 5:A:393:LEU:CD1 | 5:A:750:PHE:CE1 | 2.76 | 0.69 |
| 6:B:438:VAL:CG2 | 20:B:833:CLA:HAC1 | 2.22 | 0.69 |
| 6:B:531:THR:O | 6:B:535:VAL:HG12 | 1.93 | 0.69 |
| 1:1:179:THR:HG23 | 4:4:87:SER:HB3 | 1.72 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:472:ARG:HH22 | 16:L:74:LEU:HD21 | 1.58 | 0.69 |
| 20:A:824:CLA:HBC2 | 20:A:824:CLA:CHD | 2.19 | 0.69 |
| 20:B:827:CLA:C8 | 22:B:846:BCR:H14C | 2.23 | 0.69 |
| 20:B:829:CLA:H43 | 22:B:844:BCR:HC7 | 1.75 | 0.69 |
| 12:H:25:GLY:HA3 | 12:H:27:ASP:N | 2.08 | 0.69 |
| 20:L:208:CLA:HBC3 | 20:L:208:CLA:CHD | 2.14 | 0.69 |
| 1:1:27:LEU:HD21 | 6:B:314:ARG:CG | 2.22 | 0.69 |
| 2:2:129:LYS:O | 2:2:132:GLY:CA | 2.41 | 0.69 |
| 20:2:314:CLA:HAA1 | 20:2:314:CLA:C2 | 2.22 | 0.69 |
| 3:3:96:GLY:O | 3:3:97:PHE:HB3 | 1.92 | 0.69 |
| 5:A:669:GLY:N | 6:B:445:ALA:HA | 2.07 | 0.69 |
| 20:A:850:CLA:H11 | 6:B:616:LEU:CG | 2.22 | 0.69 |
| 21:A:853:LMU:H31 | 21:A:853:LMU:C1' | 2.23 | 0.69 |
| 6:B:20:ARG:HB3 | 6:B:20:ARG:HH11 | 1.57 | 0.69 |
| 6:B:76:ALA:O | 6:B:78:VAL:N | 2.25 | 0.69 |
| 6:B:279:ALA:O | 20:B:817:CLA:HMB3 | 1.92 | 0.69 |
| 6:B:305:LEU:HD22 | 20:B:824:CLA:O1D | 1.91 | 0.69 |
| 6:B:427:LEU:HD23 | 6:B:431:PHE:HZ | 1.56 | 0.69 |
| 20:B:832:CLA:HBB2 | 22:F:203:BCR:H272 | 1.74 | 0.69 |
| 10:F:61:LEU:HD23 | 10:F:69:PRO:HB2 | 1.73 | 0.69 |
| 4:4:42:GLN:OE1 | 4:4:120:ILE:HA | 1.92 | 0.69 |
| 4:4:118:ASP:O | 4:4:122:LYS:HA | 1.93 | 0.69 |
| 4:4:194:VAL:HG12 | 4:4:195:GLN:CB | 2.23 | 0.69 |
| 5:A:304:LEU:HD22 | 20:A:816:CLA:HBB2 | 1.75 | 0.69 |
| 5:A:747:TRP:CD2 | 22:A:845:BCR:H401 | 2.28 | 0.69 |
| 6:B:167:TRP:HD1 | 11:G:41:MET:CE | 2.06 | 0.69 |
| 6:B:666:SER:HB3 | 6:B:671:TRP:NE1 | 2.08 | 0.69 |
| 8:D:86:LEU:HD13 | 8:D:90:LEU:HG | 1.75 | 0.69 |
| 11:G:28:ARG:HD2 | 11:G:33:LYS:HE2 | 1.75 | 0.69 |
| 21:K:107:LMU:H22 | 21:K:107:LMU:H71 | 1.73 | 0.69 |
| 20:2:303:CLA:C4C | 20:2:303:CLA:H42 | 2.21 | 0.69 |
| 20:3:314:CLA:HHD | 20:3:314:CLA:HBC2 | 1.75 | 0.69 |
| 5:A:21:LEU:N | 5:A:21:LEU:CD1 | 2.30 | 0.69 |
| 5:A:41:SER:O | 5:A:44:ILE:HA | 1.92 | 0.69 |
| 5:A:103:PHE:CD2 | 5:A:103:PHE:N | 2.60 | 0.69 |
| 5:A:353:SER:O | 5:A:354:TRP:HB2 | 1.93 | 0.69 |
| 5:A:527:VAL:CG1 | 5:A:528:ALA:N | 2.55 | 0.69 |
| 20:A:832:CLA:CBC | 20:A:832:CLA:HMC1 | 2.23 | 0.69 |
| 20:A:837:CLA:OBD | 10:F:105:LEU:HD11 | 1.93 | 0.69 |
| 16:L:77:THR:HG21 | 16:L:82:ALA:HB1 | 1.75 | 0.69 |
| 17:N:61:LEU:CD1 | 17:N:63:ASP:C | 2.56 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:R:30:UNK:O | 18:R:32:UNK:N | 2.26 | 0.69 |
| 4:4:128:ALA:HB1 | 4:4:141:LEU:CD2 | 2.23 | 0.68 |
| 5:A:244:LEU:HB2 | 5:A:247:GLU:HB2 | 1.75 | 0.68 |
| 5:A:308:ILE:HG22 | 5:A:309:LEU:N | 2.07 | 0.68 |
| 5:A:358:LEU:HD11 | 5:A:413:HIS:CG | 2.28 | 0.68 |
| 20:A:818:CLA:H2A | 20:A:818:CLA:O1D | 1.92 | 0.68 |
| 6:B:174:ARG:HH11 | 20:B:825:CLA:HMD1 | 1.58 | 0.68 |
| 6:B:493:TRP:CZ2 | 20:B:835:CLA:CBA | 2.76 | 0.68 |
| 6:B:525:LEU:O | 6:B:525:LEU:HD22 | 1.92 | 0.68 |
| 8:D:126:GLY:C | 8:D:127:ARG:HG2 | 2.17 | 0.68 |
| 11:G:13:GLY:O | 11:G:16:LEU:HG | 1.93 | 0.68 |
| 2:2:137:TYR:CD1 | 2:2:138:PRO:HD2 | 2.28 | 0.68 |
| 20:2:305:CLA:H2 | 20:2:307:CLA:CMD | 2.23 | 0.68 |
| 21:2:320:LMU:H1B | 21:2:320:LMU:O6' | 1.93 | 0.68 |
| 6:B:278:LEU:HD12 | 20:B:817:CLA:CMA | 2.23 | 0.68 |
| 6:B:304:ILE:HD11 | 20:B:820:CLA:HED3 | 1.73 | 0.68 |
| 6:B:409:ALA:C | 6:B:411:MET:H | 2.01 | 0.68 |
| 3:3:92:TRP:O | 3:3:97:PHE:HD1 | 1.75 | 0.68 |
| 5:A:195:TRP:CZ2 | 20:A:810:CLA:CMA | 2.76 | 0.68 |
| 5:A:581:CYS:CB | 5:A:590:CYS:HA | 2.16 | 0.68 |
| 5:A:737:HIS:HA | 5:A:740:LEU:CD2 | 2.23 | 0.68 |
| 20:A:831:CLA:HBC3 | 20:A:831:CLA:CMC | 2.23 | 0.68 |
| 7:C:28:MET:HG2 | 7:C:38:GLN:HE21 | 1.58 | 0.68 |
| 8:D:69:ARG:O | 8:D:70:GLU:HB2 | 1.94 | 0.68 |
| 1:1:24:PHE:CB | 6:B:314:ARG:NH2 | 2.35 | 0.68 |
| 2:2:44:ASN:C | 2:2:46:GLN:N | 2.51 | 0.68 |
| 2:2:59:ALA:HB1 | 2:2:172:LEU:HD22 | 1.74 | 0.68 |
| 4:4:70:ILE:C | 4:4:72:VAL:H | 2.00 | 0.68 |
| 5:A:663:GLN:HB3 | 5:A:752:ALA:O | 1.93 | 0.68 |
| 20:A:824:CLA:HHD | 20:A:824:CLA:CBC | 2.16 | 0.68 |
| 20:A:831:CLA:H43 | 16:L:64:LEU:HD23 | 1.73 | 0.68 |
| 20:A:849:CLA:HAA1 | 20:B:850:CLA:HBB2 | 1.75 | 0.68 |
| 6:B:347:LEU:CD2 | 6:B:351:HIS:CE1 | 2.77 | 0.68 |
| 6:B:468:GLY:O | 6:B:470:THR:N | 2.26 | 0.68 |
| 20:B:824:CLA:HAA2 | 20:B:824:CLA:HBD | 1.75 | 0.68 |
| 7:C:6:LYS:HB3 | 7:C:63:LEU:HD21 | 1.75 | 0.68 |
| 17:N:49:CYS:O | 17:N:50:GLN:O | 2.10 | 0.68 |
| 21:R:109:LMU:O6B | 21:R:109:LMU:H1B | 1.93 | 0.68 |
| 2:2:161:THR:HB | 2:2:165:LYS:HD2 | 1.75 | 0.68 |
| 2:2:168:ARG:HG2 | 2:2:168:ARG:HH11 | 1.59 | 0.68 |
| 2:2:187:GLY:O | 2:2:189:ILE:HG12 | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:163:PHE:C | 3:3:163:PHE:CD1 | 2.72 | 0.68 |
| 4:4:99:HIS:ND1 | 4:4:103:ILE:CD1 | 2.56 | 0.68 |
| 5:A:96:MET:CE | 20:A:807:CLA:HBB2 | 2.23 | 0.68 |
| 5:A:438:HIS:CE1 | 5:A:442:ILE:HD11 | 2.29 | 0.68 |
| 5:A:555:ILE:HG22 | 6:B:670:TYR:HE2 | 1.56 | 0.68 |
| 20:A:807:CLA:C2B | 22:J:102:BCR:H331 | 2.23 | 0.68 |
| 6:B:623:TYR:O | 6:B:624:LEU:HB2 | 1.91 | 0.68 |
| 20:B:832:CLA:HBB2 | 22:F:203:BCR:C26 | 2.23 | 0.68 |
| 7:C:49:VAL:HG22 | 7:C:50:GLY:H | 1.59 | 0.68 |
| 20:2:312:CLA:H8 | 20:2:312:CLA:C3 | 2.19 | 0.68 |
| 4:4:121:PHE:CD1 | 4:4:128:ALA:HB3 | 2.29 | 0.68 |
| 4:4:170:HIS:C | 4:4:171:ASN:O | 2.37 | 0.68 |
| 5:A:22:VAL:HB | 5:A:24:ARG:CA | 2.22 | 0.68 |
| 5:A:24:ARG:CZ | 5:A:29:THR:HB | 2.21 | 0.68 |
| 5:A:690:LEU:CD2 | 6:B:661:PHE:HE1 | 2.06 | 0.68 |
| 6:B:404:ALA:C | 6:B:406:ASN:N | 2.51 | 0.68 |
| 6:B:560:ASP:HB2 | 7:C:66:ARG:NE | 2.08 | 0.68 |
| 11:G:30:ASN:O | 11:G:33:LYS:NZ | 2.26 | 0.68 |
| 12:H:49:LYS:O | 12:H:51:GLY:N | 2.26 | 0.68 |
| 4:4:147:LEU:HD22 | 4:4:148:GLU:CG | 2.24 | 0.68 |
| 4:4:192:THR:C | 4:4:193:ILE:O | 2.34 | 0.68 |
| 20:A:839:CLA:H51 | 20:A:839:CLA:H102 | 1.76 | 0.68 |
| 6:B:212:PHE:HZ | 20:B:815:CLA:HAC1 | 1.59 | 0.68 |
| 6:B:560:ASP:OD1 | 7:C:52:LYS:NZ | 2.26 | 0.68 |
| 20:B:826:CLA:CBB | 20:B:839:CLA:HHB | 2.24 | 0.68 |
| 20:B:838:CLA:H161 | 22:F:204:BCR:C31 | 2.22 | 0.68 |
| 21:H:105:LMU:H12 | 21:H:105:LMU:O2' | 1.94 | 0.68 |
| 16:L:48:ASN:HD22 | 16:L:115:ALA:HB2 | 1.58 | 0.68 |
| 20:R:107:CLA:HED3 | 20:R:107:CLA:C4D | 2.23 | 0.68 |
| 3:3:63:ARG:CZ | 3:3:185:LYS:HG2 | 2.24 | 0.68 |
| 4:4:47:ASN:HB3 | 4:4:161:LEU:HD23 | 1.76 | 0.68 |
| 4:4:163:PHE:O | 4:4:167:ILE:N | 2.26 | 0.68 |
| 5:A:376:MET:HE1 | 20:A:827:CLA:OBD | 1.93 | 0.68 |
| 6:B:269:TRP:HE3 | 6:B:270:LEU:H | 1.40 | 0.68 |
| 7:C:20:ALA:O | 7:C:21:CYS:CB | 2.39 | 0.68 |
| 8:D:31:GLY:HA2 | 16:L:13:PRO:HB3 | 1.74 | 0.68 |
| 12:H:53:LEU:HG | 12:H:54:LEU:H | 1.57 | 0.68 |
| 16:L:13:PRO:O | 16:L:14:LEU:HB2 | 1.94 | 0.68 |
| 17:N:47:THR:HB | 17:N:52:LEU:O | 1.93 | 0.68 |
| 17:N:62:SER:CB | 17:N:66:ASP:CG | 2.67 | 0.68 |
| 21:R:103:LMU:H41 | 21:R:103:LMU:H6D | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:165:LYS:O | 2:2:168:ARG:N | 2.27 | 0.68 |
| 3:3:50:GLU:O | 3:3:53:TRP:N | 2.27 | 0.68 |
| 5:A:207:LEU:HA | 5:A:211:LEU:HG | 1.75 | 0.68 |
| 5:A:207:LEU:HD21 | 5:A:314:GLY:HA2 | 1.75 | 0.68 |
| 5:A:665:ILE:O | 6:B:621:ARG:HD3 | 1.93 | 0.68 |
| 6:B:598:HIS:HB3 | 6:B:602:TRP:CZ3 | 2.29 | 0.68 |
| 10:F:20:GLN:CD | 10:F:21:ALA:N | 2.51 | 0.68 |
| 11:G:7:VAL:CG2 | 11:G:8:ILE:H | 2.07 | 0.68 |
| 11:G:13:GLY:O | 11:G:16:LEU:CB | 2.42 | 0.68 |
| 11:G:23:PHE:CD2 | 11:G:24:PHE:HB2 | 2.29 | 0.68 |
| 15:K:38:LEU:CG | 15:K:39:LYS:HD3 | 2.10 | 0.68 |
| 17:N:82:PHE:O | 17:N:84:LYS:N | 2.26 | 0.68 |
| 1:1:25:ASP:HB3 | 1:1:26:PRO:HD2 | 1.75 | 0.68 |
| 1:1:45:ILE:HA | 1:1:48:ARG:HB2 | 1.76 | 0.68 |
| 22:2:317:BCR:H311 | 22:2:317:BCR:C8 | 2.23 | 0.68 |
| 20:3:311:CLA:H142 | 20:3:311:CLA:H101 | 1.75 | 0.68 |
| 4:4:171:ASN:C | 4:4:173:THR:H | 2.01 | 0.68 |
| 5:A:85:GLN:O | 5:A:89:ILE:HG13 | 1.93 | 0.68 |
| 20:A:804:CLA:O2D | 20:A:804:CLA:H2A | 1.93 | 0.68 |
| 6:B:533:ILE:HD11 | 6:B:575:ASP:O | 1.93 | 0.68 |
| 7:C:5:VAL:HB | 7:C:65:VAL:CG1 | 2.23 | 0.68 |
| 7:C:7:ILE:HG22 | 7:C:65:VAL:HG23 | 1.73 | 0.68 |
| 12:H:25:GLY:C | 12:H:27:ASP:N | 2.49 | 0.68 |
| 21:H:105:LMU:C1B | 21:H:105:LMU:C3 | 2.71 | 0.68 |
| 16:L:163:LEU:HD12 | 16:L:165:TYR:CE1 | 2.28 | 0.68 |
| 17:N:57:LYS:CG | 17:N:58:VAL:N | 2.35 | 0.68 |
| 4:4:84:PHE:O | 4:4:85:ALA:HB3 | 1.93 | 0.67 |
| 7:C:74:THR:OG1 | 7:C:80:ALA:HB3 | 1.93 | 0.67 |
| 15:K:27:ALA:HB3 | 15:K:28:PRO:CD | 2.24 | 0.67 |
| 2:2:43:TRP:C | 2:2:45:VAL:H | 2.01 | 0.67 |
| 5:A:107:GLU:OE1 | 5:A:161:GLU:HG3 | 1.94 | 0.67 |
| 6:B:212:PHE:CZ | 20:B:815:CLA:HAC1 | 2.28 | 0.67 |
| 6:B:615:TYR:HD1 | 6:B:615:TYR:H | 1.42 | 0.67 |
| 10:F:90:PHE:HA | 22:F:203:BCR:H392 | 1.75 | 0.67 |
| 11:G:33:LYS:HA | 11:G:33:LYS:NZ | 2.09 | 0.67 |
| 16:L:13:PRO:HG2 | 16:L:18:PRO:HB3 | 1.75 | 0.67 |
| 17:N:60:PHE:C | 17:N:61:LEU:O | 2.37 | 0.67 |
| 20:R:107:CLA:HED3 | 20:R:107:CLA:C1A | 2.24 | 0.67 |
| 2:2:98:GLU:CG | 2:2:99:LEU:CD1 | 2.73 | 0.67 |
| 2:2:127:ASN:OD1 | 14:J:2:ARG:HA | 1.94 | 0.67 |
| 20:2:314:CLA:CHD | 20:2:314:CLA:HBC2 | 2.24 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:144:ALA:HB3 | 4:4:148:GLU:O | 1.93 | 0.67 |
| 20:A:824:CLA:HED2 | 20:A:824:CLA:HAA1 | 1.74 | 0.67 |
| 6:B:546:LEU:HD11 | 6:B:567:THR:HG22 | 1.77 | 0.67 |
| 6:B:732:LYS:CD | 6:B:733:PHE:C | 2.67 | 0.67 |
| 20:B:802:CLA:H93 | 20:B:803:CLA:C9 | 2.17 | 0.67 |
| 11:G:7:VAL:CG2 | 11:G:8:ILE:N | 2.57 | 0.67 |
| 18:R:37:UNK:C | 18:R:42:UNK:O | 2.42 | 0.67 |
| 2:2:189:ILE:O | 2:2:190:ASP:HB3 | 1.93 | 0.67 |
| 20:2:312:CLA:H3A | 20:2:312:CLA:CGA | 2.23 | 0.67 |
| 21:2:313:LMU:H72 | 21:2:313:LMU:O1' | 1.94 | 0.67 |
| 4:4:52:MET:HE3 | 4:4:156:ASN:CB | 2.25 | 0.67 |
| 4:4:70:ILE:HG13 | 4:4:71:ASN:H | 1.60 | 0.67 |
| 5:A:713:LYS:HZ2 | 20:F:201:CLA:C4 | 2.08 | 0.67 |
| 20:A:807:CLA:CMB | 22:J:102:BCR:HC7 | 2.23 | 0.67 |
| 20:A:838:CLA:NC | 20:A:838:CLA:H43 | 2.09 | 0.67 |
| 6:B:432:HIS:CE1 | 20:B:832:CLA:NB | 2.55 | 0.67 |
| 7:C:44:ARG:HH22 | 8:D:127:ARG:NE | 1.92 | 0.67 |
| 7:C:70:TRP:O | 7:C:72:GLU:HB2 | 1.94 | 0.67 |
| 21:E:101:LMU:H51 | 21:E:101:LMU:C1 | 2.23 | 0.67 |
| 13:I:23:SER:O | 13:I:26:LEU:HD23 | 1.95 | 0.67 |
| 14:J:31:ARG:NH2 | 20:J:103:CLA:C4B | 2.56 | 0.67 |
| 5:A:365:LEU:HD23 | 20:A:805:CLA:CED | 2.22 | 0.67 |
| 5:A:387:THR:CG2 | 5:A:523:VAL:HG11 | 2.25 | 0.67 |
| 5:A:387:THR:HG23 | 5:A:523:VAL:HG11 | 1.75 | 0.67 |
| 5:A:615:HIS:CE1 | 20:A:834:CLA:HBC3 | 2.30 | 0.67 |
| 5:A:636:HIS:C | 5:A:638:THR:N | 2.51 | 0.67 |
| 20:A:824:CLA:C6 | 20:A:825:CLA:HED1 | 2.25 | 0.67 |
| 24:A:856:SF4:S2 | 24:A:856:SF4:S3 | 2.92 | 0.67 |
| 6:B:454:LEU:HD11 | 10:F:69:PRO:O | 1.93 | 0.67 |
| 6:B:492:ILE:H | 6:B:492:ILE:CD1 | 2.05 | 0.67 |
| 6:B:661:PHE:HB3 | 20:B:803:CLA:HBC3 | 1.76 | 0.67 |
| 20:B:839:CLA:HBC1 | 20:F:201:CLA:HMC1 | 1.74 | 0.67 |
| 13:I:24:LEU:HD21 | 22:L:209:BCR:H271 | 1.75 | 0.67 |
| 21:K:107:LMU:H22 | 21:K:107:LMU:C7 | 2.25 | 0.67 |
| 17:N:33:TYR:O | 17:N:34:THR:HG22 | 1.95 | 0.67 |
| 2:2:113:ILE:HG13 | 2:2:114:LEU:N | 2.10 | 0.67 |
| 4:4:37:LEU:HA | 4:4:39:TRP:CG | 2.29 | 0.67 |
| 4:4:106:TRP:CZ3 | 20:4:303:CLA:HBC1 | 2.30 | 0.67 |
| 20:4:306:CLA:CMA | 20:4:306:CLA:CBA | 2.70 | 0.67 |
| 5:A:301:HIS:CD2 | 20:A:816:CLA:O1D | 2.47 | 0.67 |
| 5:A:308:ILE:HD11 | 20:A:816:CLA:H91 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:396:PHE:CE2 | 5:A:616:PHE:CG | 2.83 | 0.67 |
| 6:B:178:HIS:C | 6:B:180:SER:H | 2.00 | 0.67 |
| 11:G:13:GLY:O | 11:G:16:LEU:CG | 2.43 | 0.67 |
| 2:2:61:GLY:O | 2:2:65:PRO:HG2 | 1.95 | 0.67 |
| 3:3:97:PHE:HD2 | 3:3:97:PHE:O | 1.70 | 0.67 |
| 3:3:107:TRP:CD1 | 3:3:108:ALA:CA | 2.77 | 0.67 |
| 4:4:122:LYS:HE2 | 4:4:150:LYS:CD | 2.21 | 0.67 |
| 5:A:259:TYR:CE2 | 5:A:280:PHE:HA | 2.30 | 0.67 |
| 5:A:308:ILE:O | 5:A:312:ILE:N | 2.24 | 0.67 |
| 6:B:160:LYS:HG3 | 6:B:161:TRP:H | 1.59 | 0.67 |
| 6:B:648:TRP:CZ3 | 22:B:847:BCR:H392 | 2.29 | 0.67 |
| 20:B:806:CLA:HMD2 | 22:F:203:BCR:HC41 | 1.77 | 0.67 |
| 8:D:102:ARG:NH1 | 8:D:104:PHE:CE1 | 2.63 | 0.67 |
| 10:F:24:LYS:C | 10:F:26:GLN:N | 2.49 | 0.67 |
| 21:K:106:LMU:O6' | 21:K:106:LMU:H1B | 1.94 | 0.67 |
| 1:1:183:ASP:OD2 | 1:1:184:PRO:HD3 | 1.94 | 0.67 |
| 2:2:103:GLY:CA | 20:2:310:CLA:HBB2 | 2.24 | 0.67 |
| 3:3:173:GLU:CG | 3:3:174:LYS:N | 2.57 | 0.67 |
| 4:4:122:LYS:CE | 4:4:150:LYS:HD2 | 2.14 | 0.67 |
| 4:4:158:ARG:HA | 4:4:161:LEU:HD12 | 1.77 | 0.67 |
| 20:4:318:CLA:CAB | 21:4:321:LMU:O3B | 2.42 | 0.67 |
| 21:4:319:LMU:H22 | 21:4:319:LMU:O2' | 1.94 | 0.67 |
| 5:A:286:GLY:C | 5:A:287:LEU:HD22 | 2.19 | 0.67 |
| 5:A:370:ILE:HG23 | 5:A:403:GLY:CA | 2.19 | 0.67 |
| 6:B:456:GLU:HG2 | 10:F:70:HIS:HB3 | 1.77 | 0.67 |
| 10:F:42:ILE:C | 10:F:43:LYS:HE3 | 2.20 | 0.67 |
| 21:H:104:LMU:H3B | 21:H:104:LMU:O3' | 1.95 | 0.67 |
| 13:I:12:VAL:HG23 | 13:I:13:GLY:H | 1.58 | 0.67 |
| 20:J:103:CLA:O1A | 20:J:103:CLA:H152 | 1.95 | 0.67 |
| 20:2:307:CLA:CBB | 20:2:307:CLA:C7 | 2.58 | 0.67 |
| 20:2:312:CLA:C4A | 20:2:312:CLA:CBA | 2.73 | 0.67 |
| 3:3:94:ARG:CB | 3:3:97:PHE:CE1 | 2.61 | 0.67 |
| 20:A:831:CLA:C4 | 16:L:64:LEU:CD2 | 2.71 | 0.67 |
| 20:A:838:CLA:H161 | 22:A:845:BCR:HC22 | 1.76 | 0.67 |
| 7:C:12:ILE:HB | 7:C:38:GLN:O | 1.95 | 0.67 |
| 7:C:55:GLU:O | 7:C:57:ALA:N | 2.20 | 0.67 |
| 9:E:53:VAL:HG12 | 9:E:54:ALA:H | 1.60 | 0.67 |
| 10:F:96:TRP:CZ3 | 10:F:134:PHE:HB2 | 2.28 | 0.67 |
| 16:L:58:LEU:HD21 | 16:L:153:TRP:CZ2 | 2.30 | 0.67 |
| 2:2:168:ARG:HH21 | 2:2:171:MET:CB | 2.08 | 0.67 |
| 5:A:119:SER:HB2 | 5:A:136:VAL:HG21 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:204:ASN:O | 5:A:205:HIS:CB | 2.42 | 0.67 |
| 5:A:708:VAL:HA | 5:A:711:HIS:HD2 | 1.59 | 0.67 |
| 20:A:830:CLA:C16 | 22:L:209:BCR:C36 | 2.72 | 0.67 |
| 21:A:848:LMU:H52 | 21:A:848:LMU:O1' | 1.95 | 0.67 |
| 20:A:849:CLA:HMB2 | 20:A:850:CLA:CAD | 2.25 | 0.67 |
| 6:B:187:SER:O | 6:B:189:ALA:N | 2.28 | 0.67 |
| 6:B:374:HIS:HB2 | 20:B:828:CLA:C4B | 2.23 | 0.67 |
| 20:B:808:CLA:HBA2 | 20:B:808:CLA:HBD | 1.77 | 0.67 |
| 9:E:39:LEU:H | 9:E:40:ARG:CZ | 2.08 | 0.67 |
| 13:I:7:LEU:HD12 | 22:I:103:BCR:C33 | 2.17 | 0.67 |
| 14:J:4:PHE:O | 14:J:5:LYS:HB2 | 1.93 | 0.67 |
| 16:L:30:SER:OG | 16:L:32:LEU:HB2 | 1.94 | 0.67 |
| 20:L:208:CLA:CBC | 20:L:208:CLA:CHD | 2.73 | 0.67 |
| 17:N:49:CYS:C | 17:N:51:ASP:O | 2.38 | 0.67 |
| 17:N:62:SER:CB | 17:N:66:ASP:CA | 2.66 | 0.67 |
| 3:3:63:ARG:NH1 | 3:3:185:LYS:O | 2.28 | 0.66 |
| 4:4:94:GLU:HB3 | 4:4:95:PHE:CD1 | 2.27 | 0.66 |
| 6:B:174:ARG:NH1 | 20:B:825:CLA:HMD2 | 2.10 | 0.66 |
| 6:B:429:LEU:HD11 | 20:B:838:CLA:HMB2 | 1.75 | 0.66 |
| 20:B:810:CLA:CMC | 22:B:847:BCR:H281 | 2.25 | 0.66 |
| 15:K:7:THR:HA | 15:K:10:ILE:HB | 1.78 | 0.66 |
| 20:K:101:CLA:CED | 20:K:102:CLA:HMB1 | 2.25 | 0.66 |
| 16:L:8:TYR:HE1 | 16:L:11:ILE:HG23 | 1.59 | 0.66 |
| 17:N:46:PHE:O | 17:N:47:THR:HG23 | 1.95 | 0.66 |
| 21:3:319:LMU:C4 | 21:3:319:LMU:O1' | 2.43 | 0.66 |
| 20:4:304:CLA:O2A | 20:4:304:CLA:H2A | 1.94 | 0.66 |
| 20:4:310:CLA:HED2 | 20:4:310:CLA:CHA | 2.24 | 0.66 |
| 5:A:707:ILE:C | 5:A:711:HIS:CD2 | 2.73 | 0.66 |
| 20:A:806:CLA:HED2 | 20:A:806:CLA:H12 | 1.77 | 0.66 |
| 6:B:194:LEU:O | 6:B:199:ILE:HG13 | 1.96 | 0.66 |
| 6:B:266:GLN:O | 6:B:267:SER:CB | 2.41 | 0.66 |
| 20:B:808:CLA:OBD | 20:B:808:CLA:C12 | 2.43 | 0.66 |
| 11:G:43:HIS:O | 11:G:43:HIS:ND1 | 2.28 | 0.66 |
| 20:H:101:CLA:H61 | 20:H:101:CLA:HMA1 | 1.75 | 0.66 |
| 20:L:208:CLA:HAA1 | 20:L:208:CLA:O1D | 1.96 | 0.66 |
| 17:N:50:GLN:HA | 17:N:51:ASP:O | 1.96 | 0.66 |
| 2:2:205:PHE:HD1 | 2:2:206:ALA:H | 1.42 | 0.66 |
| 3:3:47:GLY:O | 3:3:49:ILE:N | 2.27 | 0.66 |
| 3:3:94:ARG:CZ | 3:3:98:ILE:CG2 | 2.73 | 0.66 |
| 3:3:106:TYR:CG | 3:3:107:TRP:CD1 | 2.84 | 0.66 |
| 4:4:95:PHE:CE2 | 20:4:314:CLA:C1C | 2.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:122:LYS:HB2 | 4:4:143:PHE:CG | 2.27 | 0.66 |
| 5:A:443:ILE:HD11 | 5:A:557:LEU:HG | 1.77 | 0.66 |
| 5:A:451:ILE:CD1 | 20:A:830:CLA:HED1 | 2.25 | 0.66 |
| 5:A:713:LYS:NZ | 20:F:201:CLA:H41 | 2.10 | 0.66 |
| 20:A:808:CLA:H111 | 22:J:102:BCR:C11 | 2.25 | 0.66 |
| 6:B:350:GLN:OE1 | 20:B:837:CLA:HBB2 | 1.95 | 0.66 |
| 16:L:66:GLY:N | 16:L:67:PRO:HD2 | 2.10 | 0.66 |
| 16:L:118:LEU:CD1 | 16:L:119:THR:H | 2.07 | 0.66 |
| 16:L:163:LEU:CD1 | 16:L:165:TYR:CE1 | 2.78 | 0.66 |
| 20:2:312:CLA:HED2 | 20:J:101:CLA:HMA3 | 1.77 | 0.66 |
| 5:A:398:HIS:CD2 | 20:A:826:CLA:ND | 2.64 | 0.66 |
| 5:A:462:ILE:CG2 | 20:A:831:CLA:HMC1 | 2.25 | 0.66 |
| 5:A:527:VAL:CG1 | 5:A:528:ALA:H | 2.08 | 0.66 |
| 5:A:700:TRP:CZ3 | 20:A:851:CLA:O1D | 2.48 | 0.66 |
| 20:A:826:CLA:C10 | 22:A:845:BCR:H372 | 2.25 | 0.66 |
| 6:B:167:TRP:CD1 | 11:G:41:MET:CE | 2.78 | 0.66 |
| 6:B:596:TRP:NE1 | 6:B:623:TYR:HB2 | 2.10 | 0.66 |
| 6:B:707:LEU:O | 6:B:710:LEU:HB3 | 1.94 | 0.66 |
| 11:G:21:PHE:CD1 | 22:G:104:BCR:H343 | 2.30 | 0.66 |
| 20:K:101:CLA:HED2 | 20:K:102:CLA:CMB | 2.26 | 0.66 |
| 18:R:38:UNK:C | 18:R:39:UNK:O | 2.42 | 0.66 |
| 2:2:72:GLY:C | 2:2:74:LEU:H | 2.04 | 0.66 |
| 4:4:75:TRP:CD1 | 20:4:310:CLA:CHD | 2.78 | 0.66 |
| 20:4:301:CLA:HHD | 20:4:301:CLA:CBC | 2.21 | 0.66 |
| 5:A:210:LEU:HD13 | 20:A:813:CLA:HHB | 1.77 | 0.66 |
| 5:A:604:TRP:HE1 | 20:B:803:CLA:C1D | 2.07 | 0.66 |
| 6:B:300:SER:HB3 | 11:G:52:LYS:CB | 2.26 | 0.66 |
| 9:E:88:GLU:O | 9:E:90:VAL:N | 2.28 | 0.66 |
| 22:F:204:BCR:H403 | 22:F:204:BCR:C27 | 2.20 | 0.66 |
| 16:L:43:TYR:O | 16:L:44:ARG:HB2 | 1.94 | 0.66 |
| 16:L:95:LEU:HD22 | 20:L:203:CLA:H141 | 1.76 | 0.66 |
| 16:L:126:GLN:N | 16:L:127:PRO:HD2 | 2.11 | 0.66 |
| 2:2:98:GLU:HG3 | 2:2:99:LEU:CD1 | 2.25 | 0.66 |
| 4:4:35:GLU:HB3 | 4:4:36:ASN:CB | 2.24 | 0.66 |
| 5:A:401:TRP:O | 5:A:405:PHE:HB2 | 1.95 | 0.66 |
| 5:A:519:ASP:C | 5:A:520:LEU:HG | 2.19 | 0.66 |
| 5:A:621:GLN:HG2 | 5:A:637:ILE:HD12 | 1.77 | 0.66 |
| 6:B:331:HIS:CE1 | 6:B:392:ILE:HG21 | 2.30 | 0.66 |
| 6:B:689:ASN:OD1 | 6:B:689:ASN:N | 2.29 | 0.66 |
| 6:B:729:THR:O | 6:B:729:THR:HG22 | 1.96 | 0.66 |
| 20:B:810:CLA:HMC1 | 22:B:847:BCR:H281 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:I:24:LEU:C | 13:I:26:LEU:N | 2.50 | 0.66 |
| 16:L:9:GLN:C | 16:L:11:ILE:H | 2.03 | 0.66 |
| 4:4:142:ASN:C | 4:4:150:LYS:HZ1 | 2.01 | 0.66 |
| 4:4:172:VAL:O | 4:4:173:THR:HG22 | 1.95 | 0.66 |
| 5:A:744:ALA:HB2 | 22:A:845:BCR:H391 | 0.79 | 0.66 |
| 24:A:856:SF4:S3 | 6:B:560:ASP:O | 2.53 | 0.66 |
| 6:B:167:TRP:HB2 | 11:G:41:MET:HE2 | 1.78 | 0.66 |
| 6:B:424:TRP:HZ3 | 20:B:839:CLA:HBC3 | 1.61 | 0.66 |
| 25:B:848:LMG:O3 | 7:C:70:TRP:CZ2 | 2.43 | 0.66 |
| 7:C:1:MET:H1 | 7:C:3:HIS:C | 1.96 | 0.66 |
| 11:G:13:GLY:CA | 11:G:16:LEU:HG | 2.25 | 0.66 |
| 21:H:105:LMU:H31 | 21:H:105:LMU:H1B | 1.77 | 0.66 |
| 17:N:63:ASP:H | 17:N:64:ASP:CA | 2.08 | 0.66 |
| 20:3:307:CLA:HAC1 | 20:K:104:CLA:C7 | 2.25 | 0.66 |
| 21:3:319:LMU:O2' | 21:3:319:LMU:H11 | 1.95 | 0.66 |
| 4:4:121:PHE:C | 4:4:122:LYS:HD2 | 2.20 | 0.66 |
| 5:A:25:ASP:OD2 | 5:A:26:PRO:N | 2.29 | 0.66 |
| 5:A:133:ASN:ND2 | 5:A:142:GLY:HA2 | 2.11 | 0.66 |
| 20:B:808:CLA:H151 | 20:B:814:CLA:OBD | 1.96 | 0.66 |
| 20:B:808:CLA:H43 | 22:B:844:BCR:H331 | 1.78 | 0.66 |
| 20:B:835:CLA:CBB | 22:B:846:BCR:H281 | 2.26 | 0.66 |
| 10:F:94:ALA:HA | 10:F:97:ILE:HG12 | 1.76 | 0.66 |
| 21:H:105:LMU:H31 | 21:H:105:LMU:H2B | 1.77 | 0.66 |
| 16:L:27:VAL:HB | 20:L:201:CLA:OBD | 1.96 | 0.66 |
| 17:N:83:TRP:O | 17:N:83:TRP:HE3 | 1.77 | 0.66 |
| 21:1:217:LMU:H51 | 21:G:103:LMU:C1 | 2.25 | 0.66 |
| 4:4:75:TRP:CG | 20:4:310:CLA:HMD2 | 2.31 | 0.66 |
| 5:A:24:ARG:NH1 | 5:A:28:LYS:O | 2.29 | 0.66 |
| 5:A:201:SER:O | 5:A:204:ASN:HB2 | 1.95 | 0.66 |
| 5:A:443:ILE:HG21 | 5:A:558:LYS:HB2 | 1.77 | 0.66 |
| 5:A:747:TRP:CE3 | 22:A:845:BCR:H401 | 2.31 | 0.66 |
| 20:A:801:CLA:HBC2 | 20:A:801:CLA:CMC | 2.26 | 0.66 |
| 6:B:175:LEU:HD11 | 20:B:820:CLA:HMA2 | 1.76 | 0.66 |
| 6:B:375:HIS:HE1 | 20:B:829:CLA:NC | 1.94 | 0.66 |
| 6:B:656:VAL:HG22 | 20:B:841:CLA:HMB3 | 1.77 | 0.66 |
| 9:E:44:TYR:CG | 9:E:73:ASN:HB2 | 2.31 | 0.66 |
| 17:N:57:LYS:O | 17:N:60:PHE:C | 2.39 | 0.66 |
| 4:4:75:TRP:HD1 | 20:4:310:CLA:CHD | 2.09 | 0.66 |
| 5:A:78:VAL:O | 5:A:82:HIS:HB2 | 1.96 | 0.66 |
| 5:A:103:PHE:HE1 | 20:A:807:CLA:O1D | 1.79 | 0.66 |
| 5:A:239:PRO:HA | 5:A:242:ILE:HD13 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:375:HIS:CE1 | 20:A:825:CLA:NC | 2.64 | 0.66 |
| 20:A:809:CLA:HBB2 | 20:B:833:CLA:CMD | 2.25 | 0.66 |
| 21:A:854:LMU:H2B | 21:A:854:LMU:H6'2 | 1.78 | 0.66 |
| 6:B:292:ARG:O | 6:B:293:THR:OG1 | 2.14 | 0.66 |
| 12:H:44:ALA:HB2 | 16:L:145:PHE:CE1 | 2.30 | 0.66 |
| 13:I:12:VAL:HG21 | 20:I:102:CLA:O1A | 1.96 | 0.66 |
| 17:N:59:PRO:HA | 17:N:66:ASP:OD1 | 1.96 | 0.66 |
| 3:3:52:LYS:O | 3:3:56:TYR:CG | 2.49 | 0.65 |
| 4:4:58:MET:O | 4:4:59:LEU:C | 2.39 | 0.65 |
| 4:4:154:ILE:CG1 | 4:4:155:ALA:H | 2.08 | 0.65 |
| 4:4:160:MET:CE | 20:4:306:CLA:CAB | 2.72 | 0.65 |
| 5:A:399:HIS:O | 5:A:400:MET:HB2 | 1.94 | 0.65 |
| 5:A:545:HIS:ND1 | 20:A:834:CLA:HBB2 | 2.10 | 0.65 |
| 20:A:807:CLA:HAA2 | 20:A:809:CLA:CED | 2.25 | 0.65 |
| 20:A:850:CLA:C1 | 6:B:616:LEU:HG | 2.25 | 0.65 |
| 6:B:38:THR:OG1 | 6:B:41:ARG:HB2 | 1.95 | 0.65 |
| 6:B:353:TYR:CD2 | 6:B:594:TRP:CZ3 | 2.83 | 0.65 |
| 9:E:44:TYR:CD1 | 9:E:73:ASN:HB2 | 2.31 | 0.65 |
| 17:N:11:LYS:HG2 | 17:N:12:THR:H | 1.61 | 0.65 |
| 17:N:68:GLU:O | 17:N:69:CYS:HB2 | 1.96 | 0.65 |
| 3:3:92:TRP:O | 3:3:95:THR:N | 2.29 | 0.65 |
| 4:4:73:PRO:O | 4:4:74:LYS:CB | 2.44 | 0.65 |
| 4:4:75:TRP:CZ3 | 4:4:76:TYR:HB3 | 2.30 | 0.65 |
| 4:4:99:HIS:HE1 | 4:4:103:ILE:HD12 | 1.59 | 0.65 |
| 4:4:121:PHE:HZ | 4:4:125:SER:O | 1.79 | 0.65 |
| 6:B:267:SER:HA | 6:B:356:PRO:O | 1.96 | 0.65 |
| 20:B:806:CLA:CBC | 22:F:203:BCR:H332 | 2.26 | 0.65 |
| 7:C:1:MET:CE | 8:D:154:TYR:OH | 2.43 | 0.65 |
| 7:C:2:SER:O | 7:C:69:LEU:HB2 | 1.96 | 0.65 |
| 8:D:49:THR:HG22 | 8:D:99:GLN:HB3 | 1.78 | 0.65 |
| 20:L:201:CLA:H52 | 20:L:204:CLA:CHB | 2.25 | 0.65 |
| 20:1:201:CLA:HBC3 | 20:1:201:CLA:CMC | 2.25 | 0.65 |
| 20:2:303:CLA:CHD | 20:2:303:CLA:H41 | 2.25 | 0.65 |
| 21:2:320:LMU:O2' | 21:2:320:LMU:H11 | 1.91 | 0.65 |
| 4:4:71:ASN:O | 4:4:72:VAL:C | 2.39 | 0.65 |
| 5:A:98:PHE:CZ | 20:A:807:CLA:HMD3 | 2.32 | 0.65 |
| 5:A:217:SER:OG | 22:A:843:BCR:C16 | 2.44 | 0.65 |
| 5:A:328:LYS:HE2 | 5:A:332:GLU:CG | 2.26 | 0.65 |
| 6:B:91:ILE:HD12 | 6:B:104:PHE:CE2 | 2.31 | 0.65 |
| 6:B:174:ARG:HH12 | 20:B:825:CLA:HMD2 | 1.62 | 0.65 |
| 22:B:847:BCR:HC31 | 20:L:203:CLA:HMD2 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:D:31:GLY:HA3 | 16:L:23:LEU:HD21 | 1.77 | 0.65 |
| 20:J:103:CLA:CHA | 20:J:103:CLA:HED3 | 2.26 | 0.65 |
| 17:N:57:LYS:O | 17:N:60:PHE:CD1 | 2.49 | 0.65 |
| 17:N:80:ASN:C | 17:N:82:PHE:H | 2.03 | 0.65 |
| 21:R:109:LMU:O6' | 21:R:109:LMU:H1' | 1.96 | 0.65 |
| 1:1:179:THR:CG2 | 4:4:87:SER:CB | 2.71 | 0.65 |
| 20:1:204:CLA:CED | 20:1:204:CLA:C2A | 2.73 | 0.65 |
| 21:1:217:LMU:H91 | 21:G:103:LMU:H4' | 1.78 | 0.65 |
| 2:2:171:MET:SD | 2:2:172:LEU:HG | 2.36 | 0.65 |
| 3:3:107:TRP:CD1 | 3:3:108:ALA:HA | 2.32 | 0.65 |
| 4:4:106:TRP:CG | 20:4:301:CLA:CED | 2.68 | 0.65 |
| 5:A:259:TYR:CD2 | 5:A:280:PHE:HA | 2.32 | 0.65 |
| 5:A:599:PHE:CD2 | 5:A:735:VAL:HG21 | 2.31 | 0.65 |
| 20:A:826:CLA:C17 | 22:J:102:BCR:H15C | 2.24 | 0.65 |
| 6:B:686:PRO:HG2 | 20:L:201:CLA:H12 | 1.77 | 0.65 |
| 9:E:83:ALA:O | 9:E:86:GLU:CG | 2.44 | 0.65 |
| 21:E:101:LMU:H72 | 21:E:101:LMU:C3 | 2.11 | 0.65 |
| 11:G:42:SER:OG | 11:G:46:ALA:N | 2.30 | 0.65 |
| 11:G:43:HIS:O | 11:G:45:GLU:N | 2.29 | 0.65 |
| 21:K:106:LMU:H6'2 | 21:K:107:LMU:H21 | 1.79 | 0.65 |
| 16:L:163:LEU:CD1 | 16:L:165:TYR:CD1 | 2.79 | 0.65 |
| 20:4:310:CLA:H2A | 20:4:310:CLA:HED3 | 1.79 | 0.65 |
| 5:A:203:LEU:H | 5:A:203:LEU:HD12 | 1.60 | 0.65 |
| 5:A:452:PHE:CE1 | 20:A:835:CLA:CBB | 2.67 | 0.65 |
| 5:A:628:ILE:HG13 | 5:A:632:GLY:HA2 | 1.77 | 0.65 |
| 20:A:830:CLA:O1A | 20:L:203:CLA:H11 | 1.96 | 0.65 |
| 6:B:65:LEU:HD22 | 6:B:124:TRP:CE3 | 2.31 | 0.65 |
| 6:B:415:LYS:HE3 | 6:B:539:LEU:O | 1.96 | 0.65 |
| 6:B:489:GLY:O | 6:B:490:ARG:HG2 | 1.95 | 0.65 |
| 6:B:556:SER:C | 6:B:558:PRO:CD | 2.69 | 0.65 |
| 10:F:2:ILE:HG22 | 10:F:3:ALA:N | 2.11 | 0.65 |
| 20:J:103:CLA:HED3 | 20:J:103:CLA:C1A | 2.27 | 0.65 |
| 16:L:36:TYR:OH | 20:L:207:CLA:HBA2 | 1.97 | 0.65 |
| 17:N:63:ASP:H | 17:N:65:LEU:N | 1.93 | 0.65 |
| 18:R:34:UNK:C | 18:R:36:UNK:O | 2.45 | 0.65 |
| 5:A:80:SER:O | 5:A:83:PHE:HB2 | 1.96 | 0.65 |
| 5:A:205:HIS:CE1 | 20:A:813:CLA:HMC2 | 2.32 | 0.65 |
| 5:A:737:HIS:HA | 5:A:740:LEU:HD23 | 1.78 | 0.65 |
| 6:B:81:PRO:HG2 | 6:B:360:PHE:CD1 | 2.32 | 0.65 |
| 20:B:838:CLA:H61 | 22:F:204:BCR:H323 | 1.79 | 0.65 |
| 8:D:102:ARG:NH1 | 8:D:104:PHE:CD1 | 2.64 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:F:15:ALA:O | 10:F:18:GLU:HB2 | 1.97 | 0.65 |
| 18:R:49:UNK:O | 18:R:51:UNK:N | 2.30 | 0.65 |
| 21:2:313:LMU:C1 | 21:2:313:LMU:C6 | 2.75 | 0.65 |
| 3:3:94:ARG:NH1 | 3:3:97:PHE:CZ | 2.63 | 0.65 |
| 3:3:198:PHE:HA | 3:3:201:ALA:CB | 2.18 | 0.65 |
| 5:A:370:ILE:HD12 | 20:A:824:CLA:O1D | 1.96 | 0.65 |
| 5:A:393:LEU:HG | 5:A:394:SER:H | 1.62 | 0.65 |
| 5:A:432:LEU:HA | 5:A:435:VAL:HG13 | 1.79 | 0.65 |
| 5:A:709:TRP:CH2 | 6:B:417:ALA:HB2 | 2.31 | 0.65 |
| 6:B:602:TRP:O | 6:B:604:GLY:N | 2.24 | 0.65 |
| 20:B:823:CLA:O1A | 11:G:54:TYR:OH | 2.13 | 0.65 |
| 20:L:201:CLA:H2 | 20:L:204:CLA:HMB3 | 1.77 | 0.65 |
| 17:N:65:LEU:C | 17:N:65:LEU:HD23 | 2.22 | 0.65 |
| 17:N:80:ASN:OD1 | 17:N:82:PHE:HA | 1.96 | 0.65 |
| 5:A:29:THR:HG23 | 5:A:29:THR:O | 1.95 | 0.65 |
| 20:A:830:CLA:H161 | 22:L:209:BCR:H362 | 1.78 | 0.65 |
| 21:A:846:LMU:O6' | 21:A:848:LMU:O3B | 2.10 | 0.65 |
| 6:B:143:LEU:C | 6:B:145:LEU:H | 2.04 | 0.65 |
| 17:N:32:ALA:HB1 | 17:N:35:VAL:CG2 | 2.21 | 0.65 |
| 20:2:303:CLA:H43 | 20:2:303:CLA:CHD | 2.23 | 0.65 |
| 5:A:747:TRP:CD2 | 22:A:845:BCR:C40 | 2.80 | 0.65 |
| 22:A:845:BCR:HC31 | 22:F:203:BCR:H17C | 1.78 | 0.65 |
| 6:B:697:PRO:CB | 20:B:840:CLA:HBC3 | 2.27 | 0.65 |
| 20:B:821:CLA:NB | 20:B:821:CLA:H2 | 2.12 | 0.65 |
| 12:H:32:TYR:OH | 16:L:44:ARG:NE | 2.25 | 0.65 |
| 17:N:60:PHE:CA | 17:N:61:LEU:O | 2.44 | 0.65 |
| 17:N:70:GLU:HB3 | 17:N:72:LYS:N | 2.12 | 0.65 |
| 20:1:211:CLA:HAA2 | 20:1:211:CLA:CGD | 2.26 | 0.65 |
| 2:2:162:LYS:HD3 | 2:2:162:LYS:C | 2.22 | 0.65 |
| 4:4:37:LEU:O | 4:4:39:TRP:CB | 2.42 | 0.65 |
| 5:A:129:GLN:O | 5:A:130:GLU:HB2 | 1.94 | 0.65 |
| 5:A:691:MET:HB2 | 20:A:851:CLA:C1C | 2.27 | 0.65 |
| 5:A:693:LEU:HD21 | 5:A:735:VAL:H | 1.62 | 0.65 |
| 20:A:837:CLA:H43 | 10:F:121:ILE:HG21 | 1.79 | 0.65 |
| 6:B:454:LEU:CD1 | 10:F:69:PRO:O | 2.45 | 0.65 |
| 21:B:804:LMU:C6 | 21:B:804:LMU:H101 | 2.26 | 0.65 |
| 22:B:846:BCR:H382 | 22:B:846:BCR:C23 | 2.24 | 0.65 |
| 10:F:2:ILE:HG22 | 10:F:3:ALA:H | 1.62 | 0.65 |
| 12:H:53:LEU:CG | 12:H:54:LEU:H | 2.09 | 0.65 |
| 20:K:102:CLA:HBC1 | 21:K:105:LMU:C3B | 2.27 | 0.65 |
| 16:L:64:LEU:HD21 | 20:L:203:CLA:H201 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:355:HIS:ND1 | 5:A:416:ILE:CG2 | 2.60 | 0.64 |
| 20:A:816:CLA:HBA2 | 20:A:816:CLA:C2 | 2.25 | 0.64 |
| 20:A:832:CLA:OBD | 20:A:833:CLA:HAC1 | 1.97 | 0.64 |
| 20:B:826:CLA:CBC | 20:B:826:CLA:CHD | 2.73 | 0.64 |
| 8:D:78:ALA:CB | 8:D:82:GLN:HE22 | 2.02 | 0.64 |
| 18:R:34:UNK:N | 18:R:36:UNK:C | 2.57 | 0.64 |
| 2:2:125:PHE:O | 2:2:126:PRO:C | 2.40 | 0.64 |
| 2:2:171:MET:SD | 2:2:171:MET:C | 2.80 | 0.64 |
| 4:4:169:GLN:CD | 20:4:304:CLA:HAC2 | 2.22 | 0.64 |
| 5:A:221:HIS:CE1 | 20:A:814:CLA:C4A | 2.81 | 0.64 |
| 5:A:426:THR:HA | 5:A:428:TYR:CE2 | 2.32 | 0.64 |
| 20:A:831:CLA:H41 | 16:L:64:LEU:CD2 | 2.25 | 0.64 |
| 6:B:273:VAL:O | 6:B:277:HIS:HD2 | 1.80 | 0.64 |
| 12:H:25:GLY:HA3 | 12:H:27:ASP:OD2 | 1.97 | 0.64 |
| 16:L:99:LEU:CD1 | 22:L:209:BCR:HC7 | 2.27 | 0.64 |
| 16:L:164:PRO:HB3 | 16:L:165:TYR:CD1 | 2.15 | 0.64 |
| 3:3:94:ARG:NH1 | 3:3:97:PHE:CG | 2.65 | 0.64 |
| 4:4:40:PHE:O | 4:4:43:ALA:HB3 | 1.98 | 0.64 |
| 20:4:310:CLA:CHA | 20:4:310:CLA:CED | 2.75 | 0.64 |
| 5:A:396:PHE:HE2 | 5:A:616:PHE:CB | 2.10 | 0.64 |
| 6:B:16:PRO:CG | 7:C:74:THR:HB | 2.28 | 0.64 |
| 6:B:154:TRP:HD1 | 6:B:158:GLN:HG2 | 1.61 | 0.64 |
| 6:B:398:TYR:HD1 | 6:B:542:ARG:NH2 | 1.94 | 0.64 |
| 12:H:19:GLY:O | 12:H:20:GLN:HB2 | 1.98 | 0.64 |
| 20:J:103:CLA:O1A | 20:J:103:CLA:C15 | 2.45 | 0.64 |
| 16:L:10:VAL:HG22 | 16:L:10:VAL:O | 1.97 | 0.64 |
| 16:L:115:ALA:N | 16:L:116:PRO:HD2 | 2.12 | 0.64 |
| 17:N:63:ASP:N | 17:N:65:LEU:N | 2.46 | 0.64 |
| 5:A:54:ILE:O | 5:A:58:HIS:CD2 | 2.50 | 0.64 |
| 5:A:90:PHE:CE1 | 20:A:805:CLA:H91 | 2.32 | 0.64 |
| 5:A:98:PHE:O | 5:A:99:HIS:HB2 | 1.96 | 0.64 |
| 5:A:207:LEU:HB2 | 20:A:819:CLA:HBB2 | 1.79 | 0.64 |
| 5:A:553:VAL:H | 5:A:556:LEU:HD12 | 1.62 | 0.64 |
| 20:B:817:CLA:HBA2 | 20:B:817:CLA:HED2 | 1.79 | 0.64 |
| 19:V:1:GLC:O2 | 19:V:2:FRU:H11 | 1.97 | 0.64 |
| 5:A:113:PRO:C | 5:A:115:HIS:H | 2.04 | 0.64 |
| 5:A:373:ALA:HB1 | 5:A:396:PHE:CD1 | 2.31 | 0.64 |
| 5:A:479:ASP:HA | 5:A:536:THR:HG23 | 1.80 | 0.64 |
| 22:A:845:BCR:H322 | 22:J:102:BCR:H391 | 1.79 | 0.64 |
| 6:B:127:ILE:CD1 | 6:B:198:ALA:HB2 | 2.26 | 0.64 |
| 6:B:190:TRP:HE3 | 20:B:815:CLA:HBB2 | 1.61 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:521:HIS:CE1 | 20:B:838:CLA:NA | 2.63 | 0.64 |
| 8:D:102:ARG:NE | 8:D:110:GLN:HB2 | 2.10 | 0.64 |
| 9:E:39:LEU:O | 9:E:40:ARG:HD3 | 1.97 | 0.64 |
| 10:F:26:GLN:OE1 | 10:F:26:GLN:CA | 2.39 | 0.64 |
| 11:G:13:GLY:O | 11:G:16:LEU:HB2 | 1.96 | 0.64 |
| 17:N:63:ASP:H | 17:N:64:ASP:C | 2.05 | 0.64 |
| 2:2:44:ASN:ND2 | 14:J:1:MET:SD | 2.71 | 0.64 |
| 2:2:95:PHE:HA | 2:2:98:GLU:HG2 | 1.80 | 0.64 |
| 5:A:269:PHE:CD1 | 15:K:14:THR:HG21 | 2.32 | 0.64 |
| 5:A:547:PHE:HE2 | 20:B:803:CLA:O1A | 1.81 | 0.64 |
| 5:A:631:GLN:HG3 | 5:A:631:GLN:O | 1.96 | 0.64 |
| 20:A:814:CLA:HHC | 22:A:843:BCR:C17 | 2.13 | 0.64 |
| 22:A:844:BCR:H23C | 22:A:844:BCR:C38 | 2.25 | 0.64 |
| 6:B:98:GLN:C | 6:B:100:ALA:N | 2.56 | 0.64 |
| 20:B:816:CLA:O2D | 20:B:816:CLA:OBD | 2.12 | 0.64 |
| 17:N:72:LYS:HZ3 | 17:N:74:LYS:HE3 | 1.61 | 0.64 |
| 2:2:43:TRP:C | 2:2:45:VAL:N | 2.56 | 0.64 |
| 21:2:320:LMU:H6E | 21:2:320:LMU:O2B | 1.97 | 0.64 |
| 5:A:466:THR:O | 5:A:470:LEU:HG | 1.97 | 0.64 |
| 6:B:160:LYS:HE3 | 6:B:161:TRP:CD2 | 2.33 | 0.64 |
| 20:B:838:CLA:C16 | 22:F:204:BCR:C31 | 2.76 | 0.64 |
| 7:C:5:VAL:HB | 7:C:65:VAL:CA | 2.27 | 0.64 |
| 12:H:14:ILE:HG13 | 12:H:17:THR:OG1 | 1.97 | 0.64 |
| 13:I:10:PRO:HA | 13:I:14:LEU:HB2 | 1.79 | 0.64 |
| 15:K:44:GLU:O | 15:K:46:GLY:C | 2.40 | 0.64 |
| 4:4:38:ARG:HG3 | 4:4:39:TRP:H | 1.63 | 0.64 |
| 5:A:298:ASP:OD2 | 5:A:298:ASP:N | 2.31 | 0.64 |
| 5:A:618:TRP:CZ2 | 5:A:655:ASP:HB2 | 2.32 | 0.64 |
| 20:A:826:CLA:H43 | 20:A:826:CLA:CBA | 2.27 | 0.64 |
| 6:B:5:ILE:CB | 6:B:6:PRO:HD2 | 2.23 | 0.64 |
| 6:B:422:LEU:CD1 | 6:B:535:VAL:HG11 | 2.22 | 0.64 |
| 6:B:693:TRP:CD1 | 20:B:840:CLA:C2D | 2.80 | 0.64 |
| 6:B:732:LYS:CG | 6:B:733:PHE:C | 2.69 | 0.64 |
| 22:B:801:BCR:H333 | 20:L:207:CLA:C1C | 2.28 | 0.64 |
| 22:B:846:BCR:H321 | 22:B:846:BCR:HC8 | 1.80 | 0.64 |
| 10:F:23:LYS:HB2 | 10:F:24:LYS:NZ | 2.13 | 0.64 |
| 10:F:83:PHE:O | 10:F:87:GLY:CA | 2.45 | 0.64 |
| 10:F:147:GLY:HA2 | 10:F:150:VAL:HB | 1.80 | 0.64 |
| 15:K:83:VAL:O | 15:K:84:LEU:C | 2.39 | 0.64 |
| 20:K:101:CLA:CED | 20:K:102:CLA:HMB3 | 2.28 | 0.64 |
| 16:L:64:LEU:HD22 | 16:L:91:LEU:HD22 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:L:202:CLA:O1A | 20:L:202:CLA:C2 | 2.45 | 0.64 |
| 18:R:34:UNK:N | 18:R:36:UNK:O | 2.30 | 0.64 |
| 1:1:44:LEU:HD22 | 1:1:154:ALA:HB3 | 1.79 | 0.64 |
| 2:2:196:HIS:HE1 | 19:O:1:GLC:O3 | 1.74 | 0.64 |
| 5:A:103:PHE:N | 5:A:103:PHE:HD2 | 1.95 | 0.64 |
| 5:A:316:MET:CG | 5:A:317:TYR:HD1 | 1.99 | 0.64 |
| 20:A:826:CLA:H172 | 22:J:102:BCR:H17C | 1.79 | 0.64 |
| 20:A:839:CLA:HAA2 | 20:A:839:CLA:CGD | 2.28 | 0.64 |
| 6:B:127:ILE:HG12 | 6:B:193:HIS:HE1 | 1.63 | 0.64 |
| 10:F:151:ASP:C | 10:F:154:PHE:HB3 | 2.23 | 0.64 |
| 1:1:184:PRO:CA | 1:1:185:TRP:CD1 | 2.81 | 0.64 |
| 2:2:79:TRP:CD1 | 2:2:81:THR:HG21 | 2.32 | 0.64 |
| 4:4:122:LYS:CD | 4:4:150:LYS:HD2 | 2.14 | 0.64 |
| 6:B:661:PHE:CB | 20:B:803:CLA:CMC | 2.74 | 0.64 |
| 20:H:109:CLA:C3C | 22:I:103:BCR:HC21 | 2.27 | 0.64 |
| 16:L:66:GLY:HA3 | 20:L:208:CLA:HHC | 1.78 | 0.64 |
| 17:N:61:LEU:CD1 | 17:N:63:ASP:HB2 | 2.28 | 0.64 |
| 20:3:307:CLA:HBC3 | 20:3:307:CLA:HMC1 | 1.79 | 0.63 |
| 4:4:75:TRP:CD1 | 20:4:310:CLA:C1D | 2.80 | 0.63 |
| 4:4:95:PHE:CD2 | 20:4:314:CLA:C2C | 2.79 | 0.63 |
| 5:A:328:LYS:O | 5:A:330:ILE:N | 2.31 | 0.63 |
| 5:A:361:ASN:HD22 | 5:A:362:LEU:N | 1.96 | 0.63 |
| 20:A:828:CLA:H152 | 20:A:828:CLA:H101 | 1.80 | 0.63 |
| 6:B:341:LEU:O | 6:B:345:THR:OG1 | 2.10 | 0.63 |
| 20:B:807:CLA:HBC3 | 20:B:830:CLA:H51 | 1.80 | 0.63 |
| 7:C:52:LYS:CG | 7:C:52:LYS:O | 2.46 | 0.63 |
| 11:G:16:LEU:HA | 11:G:68:ILE:HG13 | 1.79 | 0.63 |
| 21:K:107:LMU:H32 | 21:K:107:LMU:C5' | 2.28 | 0.63 |
| 16:L:32:LEU:HD13 | 20:L:204:CLA:HED1 | 1.78 | 0.63 |
| 16:L:64:LEU:HD21 | 20:L:203:CLA:C20 | 2.27 | 0.63 |
| 20:1:204:CLA:HMC2 | 20:1:210:CLA:CAC | 2.29 | 0.63 |
| 3:3:106:TYR:HB3 | 3:3:107:TRP:CD1 | 2.32 | 0.63 |
| 4:4:121:PHE:O | 4:4:143:PHE:HD2 | 1.81 | 0.63 |
| 5:A:123:VAL:O | 5:A:124:TRP:HB2 | 1.98 | 0.63 |
| 5:A:374:GLN:O | 5:A:377:TYR:HD2 | 1.81 | 0.63 |
| 5:A:485:GLN:O | 5:A:487:VAL:N | 2.31 | 0.63 |
| 5:A:606:TYR:O | 5:A:610:SER:CB | 2.46 | 0.63 |
| 20:A:822:CLA:CAB | 22:A:844:BCR:H351 | 2.28 | 0.63 |
| 20:A:830:CLA:C16 | 22:L:209:BCR:H362 | 2.28 | 0.63 |
| 20:A:832:CLA:HMC1 | 20:A:832:CLA:HBC3 | 1.80 | 0.63 |
| 6:B:304:ILE:HG22 | 20:B:823:CLA:CGD | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:97:VAL:HA | 2:2:100:VAL:HG13 | 1.79 | 0.63 |
| 20:2:305:CLA:H42 | 20:2:307:CLA:HMD3 | 1.79 | 0.63 |
| 20:2:312:CLA:HBC3 | 20:2:312:CLA:CHD | 2.28 | 0.63 |
| 5:A:25:ASP:CG | 5:A:26:PRO:CA | 2.64 | 0.63 |
| 5:A:346:LEU:HD11 | 20:A:822:CLA:CHD | 2.29 | 0.63 |
| 6:B:456:GLU:OE1 | 10:F:70:HIS:ND1 | 2.30 | 0.63 |
| 7:C:62:PHE:HE2 | 9:E:42:GLU:OE1 | 1.78 | 0.63 |
| 2:2:56:MET:SD | 2:2:169:LEU:HA | 2.38 | 0.63 |
| 4:4:75:TRP:CD1 | 20:4:310:CLA:C2D | 2.82 | 0.63 |
| 5:A:401:TRP:HB3 | 20:A:826:CLA:HMC2 | 1.79 | 0.63 |
| 5:A:582:ASP:HB3 | 5:A:589:THR:HG22 | 1.80 | 0.63 |
| 6:B:269:TRP:CB | 6:B:497:TRP:HH2 | 2.03 | 0.63 |
| 6:B:426:SER:O | 6:B:430:GLY:N | 2.31 | 0.63 |
| 8:D:31:GLY:HA2 | 16:L:13:PRO:CB | 2.28 | 0.63 |
| 20:H:101:CLA:H2 | 20:H:101:CLA:CMA | 2.24 | 0.63 |
| 20:K:103:CLA:HMD3 | 21:K:105:LMU:H52 | 1.80 | 0.63 |
| 20:2:307:CLA:H2A | 20:2:307:CLA:O1D | 1.99 | 0.63 |
| 3:3:50:GLU:N | 3:3:51:PRO:HD3 | 2.13 | 0.63 |
| 3:3:97:PHE:O | 3:3:98:ILE:HG22 | 1.97 | 0.63 |
| 5:A:257:GLN:O | 5:A:258:LEU:HB2 | 1.98 | 0.63 |
| 5:A:680:LEU:CD2 | 6:B:617:MET:HB2 | 2.29 | 0.63 |
| 20:A:819:CLA:HAA2 | 20:A:823:CLA:HBB2 | 1.78 | 0.63 |
| 6:B:510:LEU:HD22 | 6:B:510:LEU:H | 1.62 | 0.63 |
| 7:C:31:TRP:CB | 7:C:39:ILE:HG21 | 2.27 | 0.63 |
| 8:D:111:TYR:HD2 | 8:D:114:PRO:CB | 2.10 | 0.63 |
| 10:F:125:LEU:O | 10:F:126:ALA:CB | 2.46 | 0.63 |
| 16:L:163:LEU:CD1 | 16:L:165:TYR:CD2 | 2.82 | 0.63 |
| 16:L:163:LEU:CD1 | 16:L:165:TYR:CZ | 2.80 | 0.63 |
| 21:2:313:LMU:C6 | 21:2:313:LMU:H22 | 2.20 | 0.63 |
| 3:3:180:LYS:HB2 | 3:3:181:LEU:HB2 | 1.81 | 0.63 |
| 21:4:321:LMU:C2B | 21:4:321:LMU:H5' | 2.18 | 0.63 |
| 5:A:42:ARG:C | 5:A:44:ILE:H | 2.06 | 0.63 |
| 5:A:361:ASN:HD21 | 20:A:805:CLA:CED | 2.11 | 0.63 |
| 5:A:706:SER:HB3 | 6:B:419:ILE:O | 1.98 | 0.63 |
| 6:B:130:ARG:O | 6:B:135:LEU:HD23 | 1.98 | 0.63 |
| 20:B:818:CLA:H52 | 20:B:827:CLA:HMB1 | 1.81 | 0.63 |
| 7:C:1:MET:N | 7:C:3:HIS:O | 2.30 | 0.63 |
| 8:D:47:VAL:HB | 8:D:76:LYS:HA | 1.81 | 0.63 |
| 11:G:34:GLN:O | 11:G:35:VAL:C | 2.42 | 0.63 |
| 20:H:108:CLA:CGA | 20:H:108:CLA:C3A | 2.76 | 0.63 |
| 20:L:203:CLA:H92 | 22:L:209:BCR:H321 | 1.78 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:128:ASN:CG | 2:2:130:LEU:HB2 | 2.24 | 0.63 |
| 20:2:303:CLA:O1A | 20:2:303:CLA:C4A | 2.47 | 0.63 |
| 20:2:314:CLA:HBC2 | 20:2:314:CLA:HHD | 1.81 | 0.63 |
| 4:4:36:ASN:CB | 4:4:39:TRP:CD2 | 2.81 | 0.63 |
| 5:A:221:HIS:CE1 | 20:A:814:CLA:NA | 2.66 | 0.63 |
| 5:A:328:LYS:HE2 | 5:A:332:GLU:HG3 | 1.80 | 0.63 |
| 5:A:544:ILE:HD11 | 20:A:849:CLA:H193 | 1.80 | 0.63 |
| 6:B:353:TYR:O | 6:B:354:SER:OG | 2.15 | 0.63 |
| 6:B:545:LYS:CG | 9:E:74:TYR:HE2 | 2.12 | 0.63 |
| 7:C:62:PHE:CE2 | 8:D:137:ILE:HB | 2.34 | 0.63 |
| 8:D:79:ARG:O | 8:D:82:GLN:HB2 | 1.97 | 0.63 |
| 15:K:42:ALA:C | 15:K:43:ARG:HD3 | 2.23 | 0.63 |
| 21:K:107:LMU:H32 | 21:K:107:LMU:O5' | 1.99 | 0.63 |
| 1:1:179:THR:HG21 | 4:4:87:SER:CA | 2.27 | 0.63 |
| 4:4:122:LYS:HD3 | 4:4:150:LYS:CE | 2.29 | 0.63 |
| 5:A:316:MET:CA | 5:A:317:TYR:HD1 | 2.11 | 0.63 |
| 5:A:464:ASN:HD22 | 5:A:464:ASN:H | 1.45 | 0.63 |
| 20:A:808:CLA:HBB2 | 20:A:809:CLA:C4D | 2.29 | 0.63 |
| 20:A:824:CLA:H2 | 20:A:825:CLA:CED | 2.28 | 0.63 |
| 6:B:14:GLN:HE21 | 6:B:14:GLN:H | 1.47 | 0.63 |
| 6:B:141:PHE:HA | 6:B:144:PHE:CD1 | 2.34 | 0.63 |
| 6:B:247:THR:C | 6:B:250:ALA:HB2 | 2.24 | 0.63 |
| 6:B:337:ALA:HA | 20:B:825:CLA:HAA1 | 1.81 | 0.63 |
| 10:F:76:ASP:O | 10:F:78:ARG:N | 2.32 | 0.63 |
| 11:G:48:ASP:H | 11:G:49:THR:HG22 | 1.64 | 0.63 |
| 17:N:56:LYS:O | 17:N:60:PHE:CD1 | 2.50 | 0.63 |
| 21:R:102:LMU:C5B | 21:R:102:LMU:C6' | 2.61 | 0.63 |
| 21:1:217:LMU:H5B | 21:G:103:LMU:H3B | 1.81 | 0.63 |
| 21:1:218:LMU:H3' | 21:1:218:LMU:O5B | 1.98 | 0.63 |
| 2:2:103:GLY:HA2 | 20:2:310:CLA:CBB | 2.29 | 0.63 |
| 3:3:92:TRP:HB2 | 3:3:95:THR:OG1 | 1.98 | 0.63 |
| 4:4:39:TRP:O | 4:4:40:PHE:HD1 | 1.72 | 0.63 |
| 5:A:24:ARG:HH12 | 5:A:29:THR:CB | 2.12 | 0.63 |
| 5:A:39:HIS:O | 5:A:40:PHE:HB3 | 1.98 | 0.63 |
| 5:A:368:LEU:CD1 | 20:A:825:CLA:H61 | 2.28 | 0.63 |
| 5:A:514:THR:O | 5:A:531:PRO:O | 2.16 | 0.63 |
| 20:A:820:CLA:H2A | 20:A:820:CLA:O1D | 1.99 | 0.63 |
| 6:B:174:ARG:HB2 | 20:B:814:CLA:HBC3 | 1.81 | 0.63 |
| 6:B:302:LYS:O | 6:B:303:TYR:CB | 2.41 | 0.63 |
| 20:B:824:CLA:H102 | 20:B:824:CLA:C15 | 2.22 | 0.63 |
| 11:G:92:GLY:O | 11:G:93:TYR:C | 2.41 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:54:TRP:CE2 | 20:2:310:CLA:O1D | 2.52 | 0.62 |
| 3:3:194:ILE:HG13 | 20:3:303:CLA:HMC2 | 1.81 | 0.62 |
| 4:4:101:VAL:HG13 | 4:4:104:ARG:HH21 | 1.60 | 0.62 |
| 4:4:174:GLY:C | 4:4:175:LYS:HG3 | 2.23 | 0.62 |
| 20:4:301:CLA:OBD | 20:4:301:CLA:O2D | 2.14 | 0.62 |
| 5:A:434:ARG:O | 5:A:437:ARG:HB2 | 1.99 | 0.62 |
| 5:A:520:LEU:O | 5:A:522:ALA:N | 2.28 | 0.62 |
| 5:A:661:ALA:HA | 5:A:664:VAL:HG13 | 1.81 | 0.62 |
| 20:A:825:CLA:HMC1 | 20:A:825:CLA:CBC | 2.28 | 0.62 |
| 6:B:711:VAL:O | 6:B:711:VAL:HG12 | 1.96 | 0.62 |
| 6:B:711:VAL:HG22 | 25:B:848:LMG:H391 | 1.80 | 0.62 |
| 6:B:733:PHE:CD1 | 6:B:733:PHE:N | 2.58 | 0.62 |
| 20:B:824:CLA:O2D | 20:B:824:CLA:C2A | 2.47 | 0.62 |
| 23:B:843:PQN:H291 | 25:B:848:LMG:H201 | 1.80 | 0.62 |
| 7:C:74:THR:HB | 7:C:80:ALA:HB2 | 1.77 | 0.62 |
| 8:D:84:LEU:HD12 | 8:D:100:PHE:HZ | 1.64 | 0.62 |
| 8:D:111:TYR:CD2 | 8:D:114:PRO:HB3 | 2.33 | 0.62 |
| 10:F:123:VAL:HB | 10:F:126:ALA:C | 2.24 | 0.62 |
| 16:L:78:GLU:HG3 | 16:L:78:GLU:O | 1.99 | 0.62 |
| 16:L:95:LEU:HD11 | 16:L:143:PHE:CZ | 2.34 | 0.62 |
| 17:N:65:LEU:O | 17:N:67:LEU:N | 2.32 | 0.62 |
| 3:3:59:ILE:O | 3:3:63:ARG:HG3 | 1.99 | 0.62 |
| 4:4:81:GLU:O | 4:4:82:GLU:CB | 2.47 | 0.62 |
| 5:A:95:GLY:H | 20:A:807:CLA:HMC2 | 1.63 | 0.62 |
| 5:A:207:LEU:HD13 | 20:A:819:CLA:HBB2 | 1.79 | 0.62 |
| 5:A:281:LEU:O | 5:A:282:THR:C | 2.42 | 0.62 |
| 5:A:527:VAL:HG12 | 5:A:528:ALA:N | 2.14 | 0.62 |
| 6:B:593:TYR:O | 6:B:596:TRP:O | 2.17 | 0.62 |
| 20:B:830:CLA:HMC3 | 20:B:830:CLA:CBC | 2.29 | 0.62 |
| 10:F:21:ALA:O | 10:F:22:LEU:C | 2.42 | 0.62 |
| 10:F:81:GLY:O | 14:J:38:THR:HG23 | 1.98 | 0.62 |
| 12:H:73:PRO:HG3 | 19:Z:2:FRU:C5 | 2.09 | 0.62 |
| 21:K:107:LMU:H71 | 21:K:107:LMU:C2 | 2.28 | 0.62 |
| 16:L:45:THR:HA | 16:L:52:ARG:HH12 | 1.63 | 0.62 |
| 16:L:64:LEU:HA | 16:L:67:PRO:CG | 2.29 | 0.62 |
| 2:2:211:LYS:HA | 2:2:211:LYS:CE | 2.28 | 0.62 |
| 4:4:107:GLN:HA | 20:4:301:CLA:HMA2 | 1.74 | 0.62 |
| 20:4:315:CLA:HHD | 20:4:315:CLA:HBC3 | 1.81 | 0.62 |
| 5:A:680:LEU:HD21 | 6:B:617:MET:HB2 | 1.81 | 0.62 |
| 5:A:708:VAL:HA | 5:A:711:HIS:CD2 | 2.34 | 0.62 |
| 20:A:809:CLA:CBB | 20:B:833:CLA:CMD | 2.77 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:G:40:GLY:C | 11:G:41:MET:SD | 2.83 | 0.62 |
| 17:N:70:GLU:C | 17:N:72:LYS:N | 2.46 | 0.62 |
| 20:1:211:CLA:HED2 | 20:1:211:CLA:CAD | 2.30 | 0.62 |
| 4:4:118:ASP:OD1 | 4:4:118:ASP:N | 2.31 | 0.62 |
| 5:A:173:VAL:HG23 | 5:A:174:PHE:HD1 | 1.64 | 0.62 |
| 5:A:385:LEU:O | 5:A:386:ALA:CB | 2.47 | 0.62 |
| 6:B:427:LEU:HB3 | 20:B:832:CLA:HED1 | 1.81 | 0.62 |
| 6:B:493:TRP:CZ2 | 20:B:835:CLA:CGA | 2.82 | 0.62 |
| 20:B:841:CLA:H102 | 13:I:21:MET:SD | 2.40 | 0.62 |
| 7:C:29:ILE:CG2 | 8:D:126:GLY:HA2 | 2.29 | 0.62 |
| 11:G:44:PHE:CA | 11:G:47:GLY:HA3 | 2.29 | 0.62 |
| 12:H:65:LEU:HD23 | 20:H:108:CLA:H52 | 1.82 | 0.62 |
| 12:H:67:TYR:C | 12:H:67:TYR:HD1 | 2.08 | 0.62 |
| 2:2:210:PRO:O | 2:2:211:LYS:HB2 | 1.99 | 0.62 |
| 3:3:94:ARG:O | 3:3:95:THR:HG23 | 1.99 | 0.62 |
| 21:3:319:LMU:O1' | 21:3:319:LMU:H41 | 1.99 | 0.62 |
| 5:A:229:ILE:O | 5:A:229:ILE:HG22 | 1.98 | 0.62 |
| 5:A:237:VAL:HG21 | 5:A:242:ILE:HD12 | 1.81 | 0.62 |
| 5:A:453:LEU:HD13 | 5:A:547:PHE:HA | 1.80 | 0.62 |
| 20:A:813:CLA:HBA1 | 20:A:823:CLA:C4 | 2.28 | 0.62 |
| 6:B:152:ALA:O | 6:B:153:GLY:C | 2.42 | 0.62 |
| 6:B:178:HIS:O | 6:B:180:SER:N | 2.32 | 0.62 |
| 6:B:293:THR:HG22 | 6:B:294:ASN:ND2 | 2.14 | 0.62 |
| 6:B:336:LEU:CD2 | 20:B:825:CLA:HBB1 | 2.30 | 0.62 |
| 6:B:390:GLY:O | 22:B:846:BCR:HC42 | 2.00 | 0.62 |
| 20:B:836:CLA:H3A | 20:B:836:CLA:O2A | 2.00 | 0.62 |
| 12:H:73:PRO:HD3 | 19:Z:2:FRU:C5 | 2.28 | 0.62 |
| 16:L:95:LEU:HD13 | 22:L:209:BCR:H312 | 1.81 | 0.62 |
| 20:1:204:CLA:CAA | 20:1:204:CLA:CED | 2.73 | 0.62 |
| 20:1:207:CLA:CGD | 20:1:207:CLA:HAA2 | 2.30 | 0.62 |
| 3:3:93:PHE:HB2 | 3:3:94:ARG:O | 2.00 | 0.62 |
| 4:4:36:ASN:O | 4:4:39:TRP:CE3 | 2.52 | 0.62 |
| 4:4:99:HIS:ND1 | 4:4:103:ILE:HD11 | 2.15 | 0.62 |
| 20:A:822:CLA:C1D | 22:A:844:BCR:C19 | 2.77 | 0.62 |
| 6:B:203:ARG:HG2 | 6:B:204:GLY:H | 1.65 | 0.62 |
| 6:B:269:TRP:CD1 | 6:B:497:TRP:CH2 | 2.87 | 0.62 |
| 6:B:503:GLU:HB3 | 6:B:507:SER:CB | 2.30 | 0.62 |
| 6:B:594:TRP:C | 6:B:594:TRP:HD1 | 2.08 | 0.62 |
| 6:B:689:ASN:O | 6:B:691:ILE:N | 2.31 | 0.62 |
| 6:B:715:VAL:O | 6:B:719:PHE:N | 2.31 | 0.62 |
| 20:B:824:CLA:CMD | 20:B:825:CLA:HBB2 | 2.24 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:G:60:SER:OG | 11:G:63:PRO:HB2 | 1.99 | 0.62 |
| 12:H:23:VAL:O | 12:H:23:VAL:CG1 | 2.47 | 0.62 |
| 22:I:103:BCR:C29 | 22:L:209:BCR:H281 | 2.30 | 0.62 |
| 17:N:62:SER:HA | 17:N:64:ASP:HB3 | 1.82 | 0.62 |
| 17:N:84:LYS:C | 17:N:85:TRP:HD1 | 2.08 | 0.62 |
| 20:3:307:CLA:HAC1 | 20:K:104:CLA:H71 | 1.80 | 0.62 |
| 5:A:193:LEU:HA | 5:A:196:PHE:CE2 | 2.34 | 0.62 |
| 5:A:457:SER:O | 5:A:544:ILE:HD13 | 1.99 | 0.62 |
| 6:B:44:GLN:OE1 | 6:B:163:PRO:HB2 | 1.99 | 0.62 |
| 6:B:58:PHE:HB2 | 6:B:146:SER:HB2 | 1.81 | 0.62 |
| 6:B:82:PHE:O | 6:B:84:VAL:N | 2.32 | 0.62 |
| 20:B:839:CLA:CBC | 20:B:839:CLA:CMC | 2.77 | 0.62 |
| 7:C:73:THR:HG1 | 7:C:76:SER:HB3 | 1.63 | 0.62 |
| 10:F:25:LEU:HD23 | 10:F:46:MET:HB3 | 1.78 | 0.62 |
| 17:N:74:LYS:O | 17:N:75:TYR:C | 2.41 | 0.62 |
| 21:R:101:LMU:H62 | 21:R:101:LMU:C1 | 2.24 | 0.62 |
| 2:2:98:GLU:HG3 | 2:2:99:LEU:CG | 2.29 | 0.62 |
| 20:3:310:CLA:H152 | 20:3:310:CLA:C19 | 2.29 | 0.62 |
| 4:4:142:ASN:CA | 4:4:150:LYS:HZ1 | 2.13 | 0.62 |
| 5:A:58:HIS:CE1 | 20:A:803:CLA:C4D | 2.82 | 0.62 |
| 5:A:131:ILE:HG12 | 6:B:445:ALA:O | 1.99 | 0.62 |
| 5:A:340:GLY:O | 5:A:343:HIS:N | 2.32 | 0.62 |
| 20:A:807:CLA:C3B | 22:J:102:BCR:H333 | 2.29 | 0.62 |
| 20:A:814:CLA:CHC | 22:A:843:BCR:H19C | 2.26 | 0.62 |
| 6:B:73:ASN:HB3 | 6:B:76:ALA:HB3 | 1.79 | 0.62 |
| 20:B:813:CLA:H11 | 20:B:813:CLA:H61 | 1.82 | 0.62 |
| 20:B:814:CLA:H151 | 20:B:829:CLA:HMD1 | 1.82 | 0.62 |
| 7:C:55:GLU:C | 7:C:57:ALA:N | 2.53 | 0.62 |
| 20:J:101:CLA:CGA | 20:J:101:CLA:CGD | 2.77 | 0.62 |
| 17:N:72:LYS:HD3 | 17:N:72:LYS:N | 2.13 | 0.62 |
| 18:R:34:UNK:CB | 18:R:35:UNK:C | 2.77 | 0.62 |
| 21:2:313:LMU:H21 | 21:2:313:LMU:C6' | 2.24 | 0.62 |
| 3:3:97:PHE:O | 3:3:98:ILE:HG23 | 2.00 | 0.62 |
| 4:4:72:VAL:O | 4:4:73:PRO:O | 2.17 | 0.62 |
| 20:4:304:CLA:HED1 | 20:4:304:CLA:H2 | 1.82 | 0.62 |
| 20:B:809:CLA:C4 | 25:B:848:LMG:H321 | 2.30 | 0.62 |
| 11:G:67:ASN:HA | 11:G:70:ASP:OD2 | 1.99 | 0.62 |
| 15:K:31:ASN:H | 15:K:32:ARG:HH11 | 1.48 | 0.62 |
| 20:L:207:CLA:HAC1 | 22:L:209:BCR:H322 | 1.80 | 0.62 |
| 17:N:34:THR:C | 17:N:36:GLU:H | 2.07 | 0.62 |
| 20:1:206:CLA:H122 | 20:1:206:CLA:H61 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:1:213:CLA:HMC2 | 20:4:303:CLA:HMB2 | 1.82 | 0.62 |
| 2:2:187:GLY:O | 2:2:188:PRO:C | 2.42 | 0.62 |
| 3:3:62:GLY:HA2 | 3:3:65:ALA:HB3 | 1.82 | 0.62 |
| 3:3:74:ALA:CA | 20:3:306:CLA:C2D | 2.75 | 0.62 |
| 3:3:94:ARG:NH1 | 3:3:98:ILE:CG2 | 2.63 | 0.62 |
| 4:4:93:ILE:O | 4:4:94:GLU:C | 2.42 | 0.62 |
| 4:4:145:PRO:O | 4:4:147:LEU:CA | 2.47 | 0.62 |
| 5:A:64:PHE:HZ | 5:A:77:LYS:CE | 2.12 | 0.62 |
| 5:A:217:SER:CA | 22:A:843:BCR:H351 | 2.28 | 0.62 |
| 5:A:369:THR:CG2 | 20:A:827:CLA:HMC2 | 2.30 | 0.62 |
| 5:A:370:ILE:CD1 | 20:A:824:CLA:O1D | 2.48 | 0.62 |
| 5:A:490:GLN:HG2 | 16:L:166:TYR:CE1 | 2.35 | 0.62 |
| 5:A:710:ALA:CB | 20:B:806:CLA:HED2 | 2.30 | 0.62 |
| 6:B:464:GLN:OE1 | 6:B:469:LYS:HD3 | 1.99 | 0.62 |
| 6:B:694:ARG:HE | 16:L:105:ALA:HA | 1.64 | 0.62 |
| 20:B:834:CLA:O2A | 20:B:835:CLA:HMB3 | 2.00 | 0.62 |
| 9:E:35:LYS:NZ | 9:E:89:GLU:OE2 | 2.33 | 0.62 |
| 22:F:204:BCR:H333 | 20:F:206:CLA:HHB | 1.81 | 0.62 |
| 22:I:103:BCR:C4 | 22:I:103:BCR:H322 | 2.30 | 0.62 |
| 16:L:163:LEU:CD1 | 16:L:165:TYR:CG | 2.83 | 0.62 |
| 17:N:34:THR:OG1 | 17:N:36:GLU:HB3 | 1.99 | 0.62 |
| 1:1:140:LEU:HD23 | 1:1:140:LEU:H | 1.65 | 0.61 |
| 2:2:50:VAL:O | 2:2:54:TRP:CD1 | 2.43 | 0.61 |
| 2:2:93:THR:O | 2:2:97:VAL:HG22 | 1.99 | 0.61 |
| 20:3:310:CLA:O1D | 20:3:310:CLA:C2A | 2.47 | 0.61 |
| 4:4:98:SER:HB2 | 4:4:102:GLU:OE1 | 1.99 | 0.61 |
| 5:A:131:ILE:HD13 | 6:B:447:GLY:CA | 2.30 | 0.61 |
| 5:A:340:GLY:O | 5:A:343:HIS:CB | 2.47 | 0.61 |
| 5:A:454:GLY:N | 5:A:457:SER:HB3 | 2.07 | 0.61 |
| 20:A:823:CLA:OBD | 20:A:823:CLA:H92 | 2.00 | 0.61 |
| 21:A:854:LMU:H41 | 21:A:854:LMU:H92 | 1.82 | 0.61 |
| 6:B:130:ARG:HG2 | 6:B:130:ARG:HH11 | 1.64 | 0.61 |
| 6:B:282:PHE:O | 6:B:286:ILE:HG13 | 1.99 | 0.61 |
| 6:B:310:PRO:CB | 6:B:311:PRO:CD | 2.78 | 0.61 |
| 20:B:839:CLA:CBC | 20:F:201:CLA:CMC | 2.77 | 0.61 |
| 8:D:48:ILE:HB | 8:D:100:PHE:HB3 | 1.82 | 0.61 |
| 15:K:46:GLY:C | 15:K:47:LEU:CG | 2.74 | 0.61 |
| 16:L:113:SER:O | 16:L:116:PRO:HD2 | 2.00 | 0.61 |
| 21:1:216:LMU:O6' | 21:1:216:LMU:H11 | 1.99 | 0.61 |
| 3:3:52:LYS:CA | 3:3:55:ALA:HB3 | 2.30 | 0.61 |
| 3:3:104:TYR:HB2 | 3:3:106:TYR:H | 1.64 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:95:GLY:HA3 | 20:A:807:CLA:C1C | 2.30 | 0.61 |
| 20:A:818:CLA:CGA | 20:A:827:CLA:CMD | 2.77 | 0.61 |
| 20:A:824:CLA:HED2 | 20:A:824:CLA:CAA | 2.30 | 0.61 |
| 8:D:113:HIS:CD2 | 8:D:118:VAL:HG21 | 2.36 | 0.61 |
| 2:2:63:PHE:HD2 | 2:2:172:LEU:HD21 | 1.64 | 0.61 |
| 2:2:203:THR:C | 2:2:204:ILE:HG12 | 2.25 | 0.61 |
| 21:2:313:LMU:C2B | 21:2:313:LMU:C6' | 2.78 | 0.61 |
| 4:4:38:ARG:CG | 4:4:39:TRP:H | 2.10 | 0.61 |
| 5:A:91:LEU:O | 20:A:807:CLA:CMC | 2.48 | 0.61 |
| 5:A:195:TRP:CZ2 | 20:A:810:CLA:HMA2 | 2.35 | 0.61 |
| 5:A:197:GLN:NE2 | 5:A:351:THR:HB | 2.15 | 0.61 |
| 5:A:467:MET:HA | 5:A:470:LEU:HB2 | 1.83 | 0.61 |
| 6:B:190:TRP:HE3 | 20:B:815:CLA:CBB | 2.12 | 0.61 |
| 6:B:221:GLY:C | 6:B:223:GLY:H | 2.08 | 0.61 |
| 6:B:294:ASN:CB | 11:G:36:PRO:HD2 | 2.27 | 0.61 |
| 6:B:560:ASP:CG | 7:C:52:LYS:HZ3 | 2.08 | 0.61 |
| 8:D:45:PHE:C | 8:D:46:TYR:HD2 | 2.08 | 0.61 |
| 11:G:16:LEU:HD12 | 11:G:17:PHE:CE2 | 2.36 | 0.61 |
| 11:G:68:ILE:HD12 | 11:G:68:ILE:H | 1.66 | 0.61 |
| 17:N:32:ALA:CB | 17:N:35:VAL:HG22 | 2.23 | 0.61 |
| 17:N:61:LEU:CG | 17:N:62:SER:N | 2.61 | 0.61 |
| 17:N:63:ASP:N | 17:N:64:ASP:C | 2.59 | 0.61 |
| 20:2:302:CLA:H42 | 20:2:302:CLA:CGA | 2.31 | 0.61 |
| 21:2:318:LMU:H22 | 21:2:318:LMU:C2' | 2.31 | 0.61 |
| 4:4:30:LEU:CB | 21:4:316:LMU:H121 | 2.30 | 0.61 |
| 4:4:33:ASP:HB3 | 4:4:34:PRO:HD3 | 1.82 | 0.61 |
| 4:4:193:ILE:H | 4:4:193:ILE:HD12 | 1.66 | 0.61 |
| 5:A:88:ILE:HG22 | 5:A:89:ILE:N | 2.16 | 0.61 |
| 5:A:445:HIS:O | 5:A:446:LEU:CB | 2.48 | 0.61 |
| 6:B:175:LEU:O | 6:B:179:LEU:HG | 2.00 | 0.61 |
| 6:B:290:MET:HA | 20:B:822:CLA:CAC | 2.30 | 0.61 |
| 6:B:437:TYR:HB3 | 6:B:616:LEU:HD23 | 1.81 | 0.61 |
| 20:B:822:CLA:HHD | 20:B:822:CLA:CBC | 2.20 | 0.61 |
| 8:D:86:LEU:C | 8:D:90:LEU:HB3 | 2.26 | 0.61 |
| 12:H:21:TRP:H | 12:H:22:ASP:CB | 2.13 | 0.61 |
| 21:H:103:LMU:H2B | 21:H:103:LMU:H6'2 | 1.82 | 0.61 |
| 17:N:42:PHE:O | 17:N:43:PRO:C | 2.43 | 0.61 |
| 1:1:27:LEU:CG | 6:B:314:ARG:NH1 | 2.63 | 0.61 |
| 20:1:207:CLA:HMA3 | 20:1:207:CLA:HBA2 | 1.80 | 0.61 |
| 3:3:173:GLU:HG2 | 3:3:174:LYS:N | 2.08 | 0.61 |
| 4:4:76:TYR:CD1 | 4:4:76:TYR:O | 2.54 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:95:PHE:HZ | 20:4:314:CLA:C4C | 2.10 | 0.61 |
| 4:4:122:LYS:HZ3 | 4:4:150:LYS:CD | 2.01 | 0.61 |
| 20:4:304:CLA:CMC | 20:4:304:CLA:CBC | 2.78 | 0.61 |
| 5:A:720:THR:O | 5:A:720:THR:HG22 | 2.01 | 0.61 |
| 20:A:809:CLA:HBD | 20:A:809:CLA:HBA2 | 1.81 | 0.61 |
| 20:A:819:CLA:C3C | 20:A:825:CLA:H172 | 2.31 | 0.61 |
| 6:B:8:PHE:O | 6:B:35:ASP:CB | 2.49 | 0.61 |
| 6:B:247:THR:HG23 | 6:B:250:ALA:HB3 | 1.83 | 0.61 |
| 9:E:68:ARG:NH2 | 9:E:69:PHE:HA | 2.15 | 0.61 |
| 10:F:22:LEU:H | 10:F:22:LEU:CD1 | 2.09 | 0.61 |
| 10:F:22:LEU:O | 10:F:25:LEU:CB | 2.47 | 0.61 |
| 20:1:203:CLA:HBA2 | 20:1:203:CLA:CBD | 2.29 | 0.61 |
| 2:2:203:THR:O | 2:2:204:ILE:HG23 | 1.99 | 0.61 |
| 20:2:312:CLA:H41 | 20:2:312:CLA:C8 | 2.23 | 0.61 |
| 4:4:128:ALA:C | 4:4:130:GLU:H | 2.08 | 0.61 |
| 20:4:301:CLA:HBC2 | 20:4:301:CLA:CHD | 2.21 | 0.61 |
| 5:A:223:VAL:HG23 | 5:A:227:LEU:HD13 | 1.83 | 0.61 |
| 5:A:281:LEU:HG | 5:A:282:THR:H | 1.65 | 0.61 |
| 5:A:452:PHE:CD1 | 20:A:835:CLA:HBB2 | 2.32 | 0.61 |
| 6:B:29:HIS:CG | 20:B:808:CLA:CBB | 2.83 | 0.61 |
| 6:B:632:ILE:C | 6:B:634:GLY:H | 2.08 | 0.61 |
| 7:C:39:ILE:HG12 | 7:C:40:ALA:N | 2.06 | 0.61 |
| 9:E:69:PHE:CD2 | 9:E:71:LYS:HG2 | 2.35 | 0.61 |
| 9:E:72:VAL:O | 9:E:73:ASN:CB | 2.48 | 0.61 |
| 10:F:42:ILE:CG1 | 10:F:43:LYS:H | 2.06 | 0.61 |
| 17:N:18:ASP:HB2 | 17:N:22:LEU:CG | 2.27 | 0.61 |
| 17:N:47:THR:CB | 17:N:52:LEU:O | 2.49 | 0.61 |
| 21:R:109:LMU:O5B | 21:R:109:LMU:H6D | 2.00 | 0.61 |
| 2:2:70:LYS:CG | 2:2:73:ILE:HG13 | 2.26 | 0.61 |
| 20:2:311:CLA:HMC1 | 20:2:311:CLA:HBC3 | 1.83 | 0.61 |
| 4:4:101:VAL:O | 4:4:104:ARG:CZ | 2.49 | 0.61 |
| 4:4:122:LYS:HB3 | 4:4:143:PHE:HB3 | 1.77 | 0.61 |
| 5:A:154:ARG:HG3 | 5:A:383:PRO:HB2 | 1.83 | 0.61 |
| 5:A:527:VAL:HG13 | 5:A:528:ALA:H | 1.65 | 0.61 |
| 5:A:545:HIS:CE1 | 5:A:612:VAL:HG22 | 2.36 | 0.61 |
| 5:A:631:GLN:O | 21:A:846:LMU:H6E | 2.01 | 0.61 |
| 5:A:668:TYR:CE2 | 6:B:617:MET:SD | 2.94 | 0.61 |
| 20:A:838:CLA:H62 | 20:A:851:CLA:H193 | 1.83 | 0.61 |
| 6:B:16:PRO:HG3 | 7:C:74:THR:CB | 2.30 | 0.61 |
| 20:B:829:CLA:O1D | 20:B:829:CLA:OBD | 2.12 | 0.61 |
| 20:B:832:CLA:HBB2 | 22:F:203:BCR:C27 | 2.31 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:F:24:LYS:O | 10:F:27:ALA:HB2 | 2.01 | 0.61 |
| 20:K:101:CLA:CMD | 20:K:102:CLA:C1A | 2.79 | 0.61 |
| 16:L:161:LEU:HD12 | 16:L:161:LEU:C | 2.26 | 0.61 |
| 5:A:412:ALA:HA | 5:A:598:VAL:HG21 | 1.83 | 0.61 |
| 5:A:478:SER:HB3 | 5:A:644:GLN:OE1 | 2.01 | 0.61 |
| 5:A:701:GLN:OE1 | 9:E:74:TYR:CE1 | 2.54 | 0.61 |
| 20:A:804:CLA:HBB2 | 20:A:806:CLA:C4D | 2.30 | 0.61 |
| 20:A:807:CLA:CGA | 20:A:809:CLA:H12 | 2.31 | 0.61 |
| 20:A:826:CLA:C20 | 22:J:102:BCR:C17 | 2.68 | 0.61 |
| 21:A:854:LMU:C6B | 21:A:854:LMU:C2B | 2.75 | 0.61 |
| 6:B:710:LEU:C | 6:B:712:HIS:N | 2.58 | 0.61 |
| 20:B:806:CLA:H122 | 20:B:806:CLA:HBB2 | 1.83 | 0.61 |
| 20:B:824:CLA:HAA2 | 20:B:824:CLA:CBD | 2.30 | 0.61 |
| 7:C:7:ILE:O | 7:C:8:TYR:C | 2.42 | 0.61 |
| 8:D:39:LYS:HD2 | 8:D:42:VAL:HG13 | 1.81 | 0.61 |
| 17:N:49:CYS:O | 17:N:50:GLN:C | 2.44 | 0.61 |
| 17:N:72:LYS:CB | 17:N:74:LYS:N | 2.43 | 0.61 |
| 3:3:106:TYR:CD1 | 3:3:107:TRP:N | 2.68 | 0.61 |
| 5:A:40:PHE:CE1 | 5:A:53:TRP:CD1 | 2.82 | 0.61 |
| 5:A:150:PHE:H | 5:A:153:TRP:HE3 | 1.49 | 0.61 |
| 5:A:455:PHE:HD1 | 20:A:830:CLA:HMA3 | 1.65 | 0.61 |
| 5:A:588:GLY:H | 6:B:668:ARG:NH1 | 1.97 | 0.61 |
| 5:A:701:GLN:OE1 | 9:E:74:TYR:HE1 | 1.83 | 0.61 |
| 20:A:824:CLA:C7 | 20:A:825:CLA:CED | 2.70 | 0.61 |
| 20:A:850:CLA:CED | 20:B:850:CLA:H2 | 2.30 | 0.61 |
| 6:B:317:ARG:NE | 6:B:317:ARG:CA | 2.60 | 0.61 |
| 6:B:517:PHE:O | 6:B:517:PHE:HD2 | 1.82 | 0.61 |
| 6:B:557:PHE:CD1 | 6:B:571:SER:HB3 | 2.35 | 0.61 |
| 15:K:44:GLU:C | 15:K:46:GLY:HA2 | 2.25 | 0.61 |
| 20:K:103:CLA:H2A | 20:K:103:CLA:O1A | 1.99 | 0.61 |
| 20:R:107:CLA:H2A | 20:R:107:CLA:O1A | 2.00 | 0.61 |
| 2:2:60:ALA:HA | 2:2:63:PHE:CE2 | 2.35 | 0.61 |
| 5:A:229:ILE:O | 5:A:229:ILE:CG2 | 2.49 | 0.61 |
| 5:A:360:ILE:O | 5:A:361:ASN:CB | 2.48 | 0.61 |
| 20:A:830:CLA:HAA1 | 22:B:801:BCR:C13 | 2.31 | 0.61 |
| 20:A:838:CLA:H192 | 14:J:19:PHE:CD2 | 2.36 | 0.61 |
| 6:B:280:ILE:HD13 | 20:B:819:CLA:HBB2 | 1.83 | 0.61 |
| 6:B:409:ALA:O | 6:B:411:MET:N | 2.26 | 0.61 |
| 6:B:510:LEU:HD21 | 20:B:837:CLA:HHD | 1.82 | 0.61 |
| 7:C:5:VAL:HB | 7:C:65:VAL:HG22 | 1.82 | 0.61 |
| 14:J:10:VAL:CG1 | 14:J:11:ALA:N | 2.64 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:K:101:CLA:HMD3 | 20:K:102:CLA:C1A | 2.31 | 0.61 |
| 16:L:158:MET:CG | 16:L:159:TYR:H | 2.14 | 0.61 |
| 2:2:36:SER:O | 2:2:37:ASP:HB2 | 2.01 | 0.60 |
| 3:3:97:PHE:CE2 | 3:3:98:ILE:CD1 | 2.33 | 0.60 |
| 4:4:36:ASN:OD1 | 4:4:39:TRP:CG | 2.54 | 0.60 |
| 5:A:309:LEU:O | 5:A:310:PHE:HB2 | 2.01 | 0.60 |
| 5:A:402:ILE:C | 5:A:404:GLY:H | 2.08 | 0.60 |
| 5:A:604:TRP:O | 5:A:607:ASN:N | 2.32 | 0.60 |
| 5:A:678:PHE:O | 5:A:680:LEU:N | 2.33 | 0.60 |
| 20:A:804:CLA:CBA | 20:A:811:CLA:H62 | 2.31 | 0.60 |
| 6:B:196:HIS:CE1 | 20:B:816:CLA:HED2 | 2.36 | 0.60 |
| 6:B:388:ALA:C | 6:B:391:PRO:CD | 2.73 | 0.60 |
| 20:B:838:CLA:C15 | 22:F:204:BCR:H313 | 2.28 | 0.60 |
| 8:D:46:TYR:HE1 | 8:D:80:LYS:HE2 | 1.64 | 0.60 |
| 17:N:4:GLU:OE2 | 17:N:5:GLU:CB | 2.47 | 0.60 |
| 19:P:1:GLC:C3 | 19:P:2:FRU:O5 | 2.49 | 0.60 |
| 4:4:194:VAL:HG12 | 4:4:195:GLN:HB2 | 1.83 | 0.60 |
| 20:4:304:CLA:HMC1 | 20:4:304:CLA:CBC | 2.27 | 0.60 |
| 5:A:396:PHE:HE2 | 5:A:616:PHE:CG | 2.18 | 0.60 |
| 5:A:472:ARG:O | 5:A:474:GLN:N | 2.34 | 0.60 |
| 5:A:492:ILE:HD11 | 20:A:834:CLA:O1D | 2.00 | 0.60 |
| 20:A:830:CLA:H11 | 20:L:203:CLA:H43 | 1.83 | 0.60 |
| 6:B:551:LYS:CG | 6:B:552:ASP:H | 2.14 | 0.60 |
| 7:C:1:MET:N | 7:C:4:SER:CA | 2.54 | 0.60 |
| 10:F:46:MET:O | 10:F:49:THR:N | 2.34 | 0.60 |
| 22:F:204:BCR:HC32 | 20:F:206:CLA:CMA | 2.31 | 0.60 |
| 11:G:44:PHE:CA | 11:G:47:GLY:CA | 2.78 | 0.60 |
| 12:H:47:PHE:CD2 | 16:L:141:GLY:HA2 | 2.35 | 0.60 |
| 12:H:72:ALA:HA | 19:Z:2:FRU:H62 | 1.82 | 0.60 |
| 13:I:22:ALA:O | 13:I:23:SER:C | 2.43 | 0.60 |
| 14:J:22:LEU:O | 14:J:25:LEU:N | 2.34 | 0.60 |
| 20:K:101:CLA:HMD3 | 20:K:102:CLA:NA | 2.15 | 0.60 |
| 20:K:102:CLA:CAC | 21:K:105:LMU:C3B | 2.79 | 0.60 |
| 21:R:103:LMU:H41 | 21:R:103:LMU:C6' | 2.31 | 0.60 |
| 21:1:217:LMU:H3O2 | 21:G:103:LMU:H6' | 1.48 | 0.60 |
| 5:A:353:SER:HB2 | 5:A:356:ALA:HB3 | 1.82 | 0.60 |
| 5:A:364:MET:O | 5:A:368:LEU:N | 2.33 | 0.60 |
| 20:A:832:CLA:C3D | 20:A:833:CLA:HAC1 | 2.31 | 0.60 |
| 6:B:406:ASN:C | 6:B:406:ASN:HD22 | 2.09 | 0.60 |
| 20:B:818:CLA:H52 | 20:B:827:CLA:CMB | 2.31 | 0.60 |
| 20:B:838:CLA:H121 | 22:F:204:BCR:H311 | 1.81 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:F:7:PRO:HB3 | 10:F:60:GLY:O | 2.00 | 0.60 |
| 12:H:67:TYR:C | 12:H:67:TYR:CD1 | 2.80 | 0.60 |
| 18:R:34:UNK:H | 18:R:36:UNK:CB | 2.10 | 0.60 |
| 1:1:144:LYS:NZ | 20:1:201:CLA:OBD | 2.25 | 0.60 |
| 5:A:442:ILE:HG23 | 20:A:829:CLA:HMC3 | 1.82 | 0.60 |
| 5:A:478:SER:C | 5:A:480:THR:H | 2.10 | 0.60 |
| 5:A:581:CYS:SG | 24:A:856:SF4:S2 | 3.00 | 0.60 |
| 5:A:668:TYR:HH | 6:B:441:ASP:CG | 2.05 | 0.60 |
| 6:B:282:PHE:CZ | 20:B:817:CLA:C1 | 2.79 | 0.60 |
| 6:B:288:GLY:O | 6:B:289:LEU:HB2 | 2.01 | 0.60 |
| 6:B:305:LEU:O | 6:B:306:GLU:C | 2.44 | 0.60 |
| 6:B:347:LEU:HD21 | 6:B:351:HIS:HE1 | 1.66 | 0.60 |
| 6:B:732:LYS:CA | 6:B:733:PHE:O | 2.49 | 0.60 |
| 7:C:12:ILE:CB | 7:C:39:ILE:HA | 2.31 | 0.60 |
| 9:E:88:GLU:O | 9:E:90:VAL:CB | 2.49 | 0.60 |
| 15:K:79:LYS:CD | 15:K:84:LEU:O | 2.48 | 0.60 |
| 21:R:106:LMU:H41 | 21:R:106:LMU:O2' | 2.01 | 0.60 |
| 21:1:217:LMU:O3' | 21:G:103:LMU:O6' | 2.19 | 0.60 |
| 4:4:99:HIS:HE1 | 4:4:103:ILE:CD1 | 2.10 | 0.60 |
| 4:4:121:PHE:CD2 | 4:4:122:LYS:O | 2.54 | 0.60 |
| 5:A:618:TRP:CZ2 | 5:A:655:ASP:CB | 2.84 | 0.60 |
| 5:A:707:ILE:O | 5:A:711:HIS:CD2 | 2.55 | 0.60 |
| 6:B:450:GLU:O | 6:B:452:GLN:N | 2.27 | 0.60 |
| 10:F:23:LYS:HB2 | 10:F:24:LYS:HZ1 | 1.65 | 0.60 |
| 21:H:106:LMU:H102 | 21:H:106:LMU:C6 | 2.27 | 0.60 |
| 16:L:160:VAL:O | 16:L:160:VAL:HG22 | 2.00 | 0.60 |
| 17:N:29:PHE:CE1 | 17:N:32:ALA:HB3 | 2.36 | 0.60 |
| 3:3:201:ALA:C | 3:3:202:LEU:HD22 | 2.27 | 0.60 |
| 4:4:104:ARG:NH1 | 4:4:105:ARG:HB3 | 2.10 | 0.60 |
| 4:4:169:GLN:NE2 | 20:4:304:CLA:CHD | 2.61 | 0.60 |
| 5:A:94:SER:HB3 | 20:A:807:CLA:HMC2 | 1.83 | 0.60 |
| 5:A:187:HIS:CD2 | 20:A:811:CLA:C4C | 2.85 | 0.60 |
| 5:A:249:ILE:C | 5:A:251:ASN:H | 2.09 | 0.60 |
| 5:A:467:MET:HE1 | 5:A:475:ASP:O | 2.02 | 0.60 |
| 5:A:500:PRO:HB3 | 5:A:506:GLY:HA2 | 1.84 | 0.60 |
| 5:A:660:GLN:O | 5:A:661:ALA:CB | 2.48 | 0.60 |
| 20:A:851:CLA:H93 | 6:B:431:PHE:HD1 | 1.66 | 0.60 |
| 6:B:51:PHE:CD1 | 20:B:814:CLA:HED1 | 2.37 | 0.60 |
| 6:B:144:PHE:CD2 | 6:B:144:PHE:O | 2.54 | 0.60 |
| 6:B:276:HIS:HB2 | 20:B:818:CLA:C1B | 2.31 | 0.60 |
| 6:B:696:LYS:HG2 | 7:C:80:ALA:CA | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:732:LYS:HB2 | 6:B:732:LYS:HZ3 | 1.66 | 0.60 |
| 8:D:28:ILE:HG12 | 8:D:67:ILE:CG1 | 2.31 | 0.60 |
| 10:F:22:LEU:C | 10:F:24:LYS:H | 2.09 | 0.60 |
| 12:H:45:ALA:HB3 | 12:H:46:PRO:CD | 2.31 | 0.60 |
| 12:H:67:TYR:O | 12:H:70:ALA:O | 2.20 | 0.60 |
| 13:I:8:PHE:CD1 | 20:I:102:CLA:H12 | 2.36 | 0.60 |
| 16:L:128:ASP:CG | 16:L:129:GLN:N | 2.59 | 0.60 |
| 16:L:163:LEU:CD1 | 16:L:165:TYR:CE2 | 2.84 | 0.60 |
| 21:2:313:LMU:H62 | 21:2:313:LMU:C2 | 2.32 | 0.60 |
| 5:A:42:ARG:C | 5:A:44:ILE:N | 2.59 | 0.60 |
| 5:A:281:LEU:CD1 | 20:A:816:CLA:H2A | 2.32 | 0.60 |
| 5:A:679:PHE:CE2 | 5:A:683:HIS:HD2 | 2.19 | 0.60 |
| 5:A:697:ARG:HD3 | 6:B:566:GLY:O | 1.99 | 0.60 |
| 5:A:713:LYS:NZ | 20:F:201:CLA:H43 | 2.15 | 0.60 |
| 20:A:835:CLA:H192 | 20:L:201:CLA:HBB2 | 1.83 | 0.60 |
| 20:A:851:CLA:H93 | 6:B:431:PHE:CD1 | 2.37 | 0.60 |
| 6:B:467:HIS:NE2 | 20:B:834:CLA:C1A | 2.65 | 0.60 |
| 6:B:531:THR:HG22 | 20:B:826:CLA:CMC | 2.30 | 0.60 |
| 6:B:670:TYR:C | 6:B:670:TYR:CD1 | 2.80 | 0.60 |
| 10:F:102:ARG:HG2 | 10:F:106:ILE:CD1 | 2.19 | 0.60 |
| 17:N:55:GLN:O | 17:N:56:LYS:HG3 | 2.00 | 0.60 |
| 1:1:23:GLY:HA3 | 20:1:212:CLA:C3C | 2.32 | 0.60 |
| 2:2:103:GLY:CA | 20:2:310:CLA:CBB | 2.79 | 0.60 |
| 20:2:303:CLA:H43 | 20:2:303:CLA:C4C | 2.30 | 0.60 |
| 20:2:316:CLA:C19 | 20:2:316:CLA:C15 | 2.66 | 0.60 |
| 20:2:316:CLA:C1 | 20:2:316:CLA:CAA | 2.80 | 0.60 |
| 3:3:141:GLN:HG2 | 3:3:142:TYR:N | 2.16 | 0.60 |
| 4:4:34:PRO:HG3 | 4:4:35:GLU:OE1 | 2.01 | 0.60 |
| 4:4:121:PHE:CZ | 4:4:125:SER:O | 2.53 | 0.60 |
| 5:A:76:ARG:O | 5:A:186:TYR:HD2 | 1.84 | 0.60 |
| 5:A:370:ILE:HG22 | 5:A:400:MET:CA | 2.29 | 0.60 |
| 5:A:586:ARG:H | 7:C:49:VAL:HG22 | 1.66 | 0.60 |
| 5:A:620:MET:HG3 | 5:A:625:TRP:CE2 | 2.37 | 0.60 |
| 5:A:705:GLU:CB | 6:B:545:LYS:HZ2 | 2.14 | 0.60 |
| 20:A:817:CLA:H52 | 20:A:832:CLA:HBA1 | 1.83 | 0.60 |
| 6:B:98:GLN:O | 6:B:100:ALA:N | 2.35 | 0.60 |
| 6:B:396:ARG:NH1 | 20:B:830:CLA:HED2 | 2.17 | 0.60 |
| 6:B:724:PHE:CG | 20:B:850:CLA:HMD1 | 2.37 | 0.60 |
| 8:D:94:TYR:O | 8:D:95:LYS:CG | 2.49 | 0.60 |
| 9:E:40:ARG:NE | 9:E:86:GLU:CD | 2.60 | 0.60 |
| 9:E:44:TYR:HB3 | 9:E:45:TRP:CE3 | 2.36 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:E:51:SER:HB3 | 9:E:68:ARG:NH1 | 2.16 | 0.60 |
| 9:E:73:ASN:HD22 | 9:E:73:ASN:C | 2.08 | 0.60 |
| 9:E:87:VAL:C | 9:E:89:GLU:N | 2.57 | 0.60 |
| 14:J:10:VAL:HG13 | 14:J:11:ALA:H | 1.66 | 0.60 |
| 15:K:27:ALA:CB | 15:K:28:PRO:CD | 2.79 | 0.60 |
| 17:N:11:LYS:HG2 | 17:N:12:THR:N | 2.17 | 0.60 |
| 1:1:61:GLU:HG2 | 1:1:61:GLU:O | 2.02 | 0.60 |
| 21:2:313:LMU:H62 | 21:2:313:LMU:H22 | 1.83 | 0.60 |
| 3:3:181:LEU:HD13 | 3:3:184:VAL:HG21 | 1.82 | 0.60 |
| 4:4:121:PHE:O | 4:4:122:LYS:HB2 | 2.01 | 0.60 |
| 5:A:227:LEU:HD23 | 5:A:231:GLN:HE22 | 1.66 | 0.60 |
| 5:A:249:ILE:O | 5:A:251:ASN:N | 2.34 | 0.60 |
| 5:A:284:ARG:HH22 | 5:A:507:ALA:C | 2.10 | 0.60 |
| 6:B:280:ILE:HA | 6:B:283:LEU:HD12 | 1.84 | 0.60 |
| 20:B:809:CLA:HBB2 | 20:B:829:CLA:HHC | 1.82 | 0.60 |
| 20:B:818:CLA:HBD | 20:B:827:CLA:CBB | 2.32 | 0.60 |
| 7:C:73:THR:OG1 | 7:C:76:SER:CB | 2.46 | 0.60 |
| 9:E:40:ARG:CB | 9:E:42:GLU:OE2 | 2.50 | 0.60 |
| 11:G:28:ARG:HH21 | 11:G:29:GLU:N | 1.98 | 0.60 |
| 21:K:106:LMU:H5' | 21:K:106:LMU:O2' | 2.01 | 0.60 |
| 16:L:158:MET:SD | 16:L:159:TYR:N | 2.75 | 0.60 |
| 4:4:71:ASN:C | 4:4:73:PRO:HD3 | 2.27 | 0.60 |
| 5:A:81:ALA:CB | 20:A:805:CLA:HBB2 | 2.29 | 0.60 |
| 5:A:301:HIS:HE2 | 20:A:816:CLA:CHA | 2.15 | 0.60 |
| 5:A:578:ARG:HA | 5:A:595:TRP:HB2 | 1.83 | 0.60 |
| 5:A:585:GLY:O | 5:A:589:THR:OG1 | 2.20 | 0.60 |
| 5:A:669:GLY:H | 6:B:445:ALA:CA | 2.08 | 0.60 |
| 6:B:124:TRP:CD1 | 6:B:124:TRP:C | 2.79 | 0.60 |
| 6:B:390:GLY:N | 6:B:391:PRO:CD | 2.65 | 0.60 |
| 6:B:438:VAL:CG2 | 20:B:833:CLA:HMC2 | 2.24 | 0.60 |
| 20:B:824:CLA:HBC3 | 20:B:824:CLA:CMC | 2.32 | 0.60 |
| 7:C:35:LYS:C | 7:C:37:LYS:H | 2.08 | 0.60 |
| 10:F:17:ARG:HA | 10:F:17:ARG:HE | 1.66 | 0.60 |
| 10:F:90:PHE:CD1 | 22:F:203:BCR:H23C | 2.36 | 0.60 |
| 10:F:126:ALA:O | 10:F:128:SER:N | 2.35 | 0.60 |
| 11:G:62:ASP:HB2 | 11:G:63:PRO:HD3 | 1.84 | 0.60 |
| 12:H:44:ALA:CB | 16:L:145:PHE:CD1 | 2.62 | 0.60 |
| 1:1:183:ASP:OD1 | 1:1:184:PRO:HD2 | 1.98 | 0.59 |
| 20:2:312:CLA:HED2 | 20:J:101:CLA:CMA | 2.32 | 0.59 |
| 20:3:310:CLA:H193 | 20:3:310:CLA:C15 | 2.31 | 0.59 |
| 4:4:37:LEU:O | 4:4:39:TRP:HD1 | 1.82 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:73:PRO:O | 4:4:74:LYS:HB2 | 2.02 | 0.59 |
| 5:A:707:ILE:C | 5:A:711:HIS:HD2 | 2.10 | 0.59 |
| 20:A:829:CLA:HMB2 | 20:L:201:CLA:C1D | 2.32 | 0.59 |
| 6:B:409:ALA:C | 6:B:411:MET:N | 2.60 | 0.59 |
| 17:N:65:LEU:O | 17:N:66:ASP:C | 2.44 | 0.59 |
| 17:N:79:SER:CA | 17:N:80:ASN:O | 2.45 | 0.59 |
| 2:2:182:ILE:O | 2:2:204:ILE:O | 2.19 | 0.59 |
| 2:2:191:ASN:HB3 | 19:O:1:GLC:C6 | 2.33 | 0.59 |
| 4:4:34:PRO:CB | 4:4:35:GLU:HB2 | 2.32 | 0.59 |
| 5:A:735:VAL:O | 5:A:739:LEU:HG | 2.01 | 0.59 |
| 22:A:845:BCR:C31 | 20:A:851:CLA:H142 | 2.28 | 0.59 |
| 6:B:131:THR:HB | 6:B:134:ASP:CB | 2.19 | 0.59 |
| 6:B:154:TRP:CD1 | 6:B:158:GLN:HG2 | 2.37 | 0.59 |
| 6:B:290:MET:HA | 20:B:822:CLA:HAC2 | 1.84 | 0.59 |
| 22:B:801:BCR:H352 | 20:L:203:CLA:H152 | 1.83 | 0.59 |
| 20:B:823:CLA:H72 | 20:B:823:CLA:CBB | 2.25 | 0.59 |
| 20:B:826:CLA:H12 | 20:B:839:CLA:CED | 2.32 | 0.59 |
| 20:B:827:CLA:H41 | 20:B:827:CLA:H72 | 1.84 | 0.59 |
| 8:D:75:LEU:HD21 | 16:L:19:PHE:CE2 | 2.37 | 0.59 |
| 10:F:24:LYS:O | 10:F:27:ALA:CB | 2.50 | 0.59 |
| 11:G:93:TYR:HA | 11:G:94:ASP:CG | 2.26 | 0.59 |
| 16:L:161:LEU:HD12 | 16:L:162:ASP:C | 2.26 | 0.59 |
| 20:L:201:CLA:HAC2 | 20:L:204:CLA:HMC3 | 1.83 | 0.59 |
| 20:L:203:CLA:H203 | 20:L:207:CLA:HBB2 | 1.84 | 0.59 |
| 19:P:1:GLC:O2 | 19:P:2:FRU:H12 | 2.02 | 0.59 |
| 19:V:1:GLC:O2 | 19:V:2:FRU:C1 | 2.50 | 0.59 |
| 1:1:167:ALA:C | 1:1:169:PRO:HD3 | 2.27 | 0.59 |
| 2:2:143:PHE:HD1 | 2:2:144:ASP:N | 2.00 | 0.59 |
| 2:2:182:ILE:HG23 | 2:2:205:PHE:HB2 | 1.83 | 0.59 |
| 20:2:303:CLA:C4 | 20:2:303:CLA:NC | 2.65 | 0.59 |
| 4:4:122:LYS:CB | 4:4:143:PHE:CG | 2.85 | 0.59 |
| 5:A:47:GLY:O | 10:F:115:THR:HB | 2.02 | 0.59 |
| 5:A:141:ARG:HH21 | 5:A:141:ARG:CG | 2.11 | 0.59 |
| 5:A:218:TRP:HD1 | 5:A:303:HIS:HD1 | 1.49 | 0.59 |
| 5:A:370:ILE:CG2 | 5:A:403:GLY:HA3 | 2.26 | 0.59 |
| 5:A:679:PHE:O | 5:A:683:HIS:HB2 | 2.03 | 0.59 |
| 20:A:803:CLA:CGA | 20:A:838:CLA:H2 | 2.33 | 0.59 |
| 21:A:847:LMU:O5B | 21:A:847:LMU:H5' | 2.01 | 0.59 |
| 6:B:310:PRO:CB | 6:B:311:PRO:HD2 | 2.31 | 0.59 |
| 11:G:68:ILE:HG23 | 11:G:72:LEU:CD1 | 2.26 | 0.59 |
| 13:I:26:LEU:HD13 | 13:I:30:LYS:HB3 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:K:103:CLA:O1A | 20:K:103:CLA:C2A | 2.49 | 0.59 |
| 1:1:24:PHE:HD2 | 6:B:314:ARG:CZ | 2.13 | 0.59 |
| 2:2:208:PHE:CG | 2:2:209:THR:N | 2.70 | 0.59 |
| 5:A:451:ILE:HD12 | 20:A:830:CLA:CED | 2.24 | 0.59 |
| 20:A:824:CLA:HMA3 | 20:A:825:CLA:O1A | 2.01 | 0.59 |
| 6:B:187:SER:O | 6:B:188:LEU:C | 2.43 | 0.59 |
| 6:B:622:ASP:HA | 6:B:626:LEU:HB3 | 1.82 | 0.59 |
| 16:L:40:LEU:HB3 | 16:L:41:PRO:CD | 2.33 | 0.59 |
| 20:1:213:CLA:CMC | 20:4:303:CLA:HMB2 | 2.31 | 0.59 |
| 2:2:129:LYS:C | 2:2:131:THR:N | 2.60 | 0.59 |
| 20:2:303:CLA:H42 | 20:2:303:CLA:NC | 2.18 | 0.59 |
| 21:2:313:LMU:H2B | 21:2:313:LMU:O6' | 2.03 | 0.59 |
| 4:4:33:ASP:CB | 4:4:34:PRO:CD | 2.75 | 0.59 |
| 4:4:99:HIS:ND1 | 4:4:99:HIS:C | 2.59 | 0.59 |
| 4:4:160:MET:HA | 4:4:163:PHE:HB2 | 1.83 | 0.59 |
| 20:4:310:CLA:CED | 20:4:310:CLA:C1A | 2.81 | 0.59 |
| 5:A:217:SER:HG | 22:A:843:BCR:H15C | 1.67 | 0.59 |
| 5:A:681:GLY:HA2 | 5:A:684:PHE:HB3 | 1.84 | 0.59 |
| 22:A:845:BCR:H313 | 20:A:851:CLA:H142 | 1.84 | 0.59 |
| 6:B:464:GLN:HA | 6:B:467:HIS:HB2 | 1.83 | 0.59 |
| 20:B:812:CLA:HAA2 | 20:B:812:CLA:H43 | 1.85 | 0.59 |
| 20:B:826:CLA:HBB2 | 20:B:839:CLA:HHB | 1.84 | 0.59 |
| 22:B:847:BCR:C33 | 22:B:847:BCR:HC8 | 2.32 | 0.59 |
| 7:C:66:ARG:HG2 | 7:C:66:ARG:NH2 | 1.99 | 0.59 |
| 8:D:125:PRO:HG2 | 8:D:127:ARG:HD3 | 1.83 | 0.59 |
| 9:E:52:VAL:C | 9:E:53:VAL:HG23 | 2.26 | 0.59 |
| 11:G:43:HIS:HB2 | 11:G:44:PHE:HD1 | 1.59 | 0.59 |
| 17:N:70:GLU:O | 17:N:72:LYS:CD | 2.48 | 0.59 |
| 3:3:98:ILE:C | 17:N:63:ASP:O | 2.45 | 0.59 |
| 3:3:134:LYS:O | 3:3:135:PRO:C | 2.45 | 0.59 |
| 4:4:73:PRO:HB2 | 4:4:75:TRP:HB2 | 1.83 | 0.59 |
| 5:A:544:ILE:O | 5:A:548:THR:OG1 | 2.14 | 0.59 |
| 5:A:603:PHE:CE2 | 6:B:665:ILE:HG21 | 2.37 | 0.59 |
| 6:B:188:LEU:O | 6:B:191:ALA:N | 2.35 | 0.59 |
| 6:B:190:TRP:CA | 20:B:815:CLA:HBB2 | 2.31 | 0.59 |
| 6:B:212:PHE:CE1 | 20:B:815:CLA:HHD | 2.29 | 0.59 |
| 6:B:292:ARG:NH2 | 6:B:297:ILE:HG13 | 2.18 | 0.59 |
| 6:B:529:THR:HA | 6:B:532:LEU:HD23 | 1.84 | 0.59 |
| 6:B:651:LEU:HB3 | 20:B:802:CLA:O2A | 2.03 | 0.59 |
| 20:B:824:CLA:HMD1 | 20:B:825:CLA:CBB | 2.25 | 0.59 |
| 22:B:847:BCR:HC31 | 20:L:203:CLA:HMD1 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:D:86:LEU:CD1 | 8:D:90:LEU:HG | 2.33 | 0.59 |
| 11:G:68:ILE:O | 11:G:72:LEU:HB2 | 2.03 | 0.59 |
| 13:I:12:VAL:HG21 | 20:I:102:CLA:HBA1 | 1.85 | 0.59 |
| 2:2:124:ILE:CB | 2:2:129:LYS:HB3 | 2.32 | 0.59 |
| 20:2:312:CLA:C4 | 20:2:312:CLA:C8 | 2.78 | 0.59 |
| 20:2:312:CLA:OBD | 20:2:312:CLA:CED | 2.51 | 0.59 |
| 3:3:180:LYS:CB | 3:3:181:LEU:HB2 | 2.33 | 0.59 |
| 5:A:472:ARG:N | 5:A:473:PRO:CD | 2.64 | 0.59 |
| 20:A:804:CLA:H12 | 20:A:811:CLA:H92 | 1.84 | 0.59 |
| 20:A:838:CLA:H71 | 20:A:851:CLA:H171 | 1.84 | 0.59 |
| 6:B:141:PHE:HD2 | 6:B:144:PHE:CE1 | 2.21 | 0.59 |
| 6:B:193:HIS:HB2 | 20:B:815:CLA:CHC | 2.33 | 0.59 |
| 6:B:403:ASN:C | 6:B:406:ASN:HB3 | 2.19 | 0.59 |
| 9:E:36:VAL:C | 9:E:49:VAL:HG13 | 2.28 | 0.59 |
| 13:I:20:ALA:O | 13:I:24:LEU:HB3 | 2.03 | 0.59 |
| 14:J:10:VAL:HG13 | 14:J:11:ALA:N | 2.17 | 0.59 |
| 1:1:184:PRO:HB2 | 20:1:213:CLA:O1D | 2.02 | 0.59 |
| 2:2:195:ALA:HB1 | 2:2:197:LEU:HG | 1.84 | 0.59 |
| 3:3:156:PRO:O | 3:3:157:ALA:C | 2.46 | 0.59 |
| 3:3:199:VAL:HG22 | 20:3:305:CLA:C4C | 2.32 | 0.59 |
| 4:4:123:GLN:O | 4:4:143:PHE:CG | 2.55 | 0.59 |
| 20:A:850:CLA:CAD | 20:A:850:CLA:CED | 2.80 | 0.59 |
| 6:B:224:PRO:CB | 6:B:227:THR:HB | 2.32 | 0.59 |
| 6:B:378:ILE:HG22 | 6:B:379:ALA:H | 1.67 | 0.59 |
| 6:B:595:HIS:HD2 | 6:B:623:TYR:OH | 1.86 | 0.59 |
| 20:B:827:CLA:H8 | 22:B:846:BCR:H14C | 1.84 | 0.59 |
| 16:L:99:LEU:O | 16:L:102:TYR:N | 2.34 | 0.59 |
| 3:3:194:ILE:HG23 | 3:3:197:TYR:OH | 2.02 | 0.59 |
| 4:4:101:VAL:O | 4:4:104:ARG:HB3 | 2.02 | 0.59 |
| 5:A:361:ASN:HD22 | 5:A:361:ASN:C | 2.11 | 0.59 |
| 20:A:819:CLA:CMD | 20:A:821:CLA:CBB | 2.64 | 0.59 |
| 22:A:845:BCR:H353 | 20:A:850:CLA:H41 | 1.85 | 0.59 |
| 6:B:438:VAL:CG2 | 20:B:833:CLA:CMC | 2.81 | 0.59 |
| 6:B:568:CYS:O | 6:B:570:ILE:N | 2.35 | 0.59 |
| 2:2:163:GLU:HG2 | 20:2:307:CLA:C2C | 2.33 | 0.59 |
| 2:2:203:THR:C | 2:2:204:ILE:CG1 | 2.76 | 0.59 |
| 5:A:207:LEU:HA | 5:A:211:LEU:HB2 | 1.85 | 0.59 |
| 5:A:361:ASN:O | 5:A:365:LEU:N | 2.35 | 0.59 |
| 5:A:665:ILE:HB | 6:B:621:ARG:HB2 | 1.83 | 0.59 |
| 20:A:839:CLA:C12 | 20:A:839:CLA:C7 | 2.66 | 0.59 |
| 6:B:79:GLN:O | 6:B:80:ASP:HB3 | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:E:34:SER:O | 9:E:35:LYS:HB3 | 2.02 | 0.59 |
| 17:N:49:CYS:O | 17:N:51:ASP:O | 2.21 | 0.59 |
| 19:P:1:GLC:C2 | 19:P:2:FRU:O5 | 2.50 | 0.59 |
| 1:1:25:ASP:CB | 1:1:26:PRO:CD | 2.81 | 0.58 |
| 20:2:303:CLA:CHD | 20:2:303:CLA:CBC | 2.73 | 0.58 |
| 5:A:158:ILE:O | 5:A:243:PRO:HG2 | 2.02 | 0.58 |
| 5:A:373:ALA:HB1 | 5:A:396:PHE:HD1 | 1.68 | 0.58 |
| 5:A:645:SER:HB3 | 6:B:637:PRO:CG | 2.27 | 0.58 |
| 5:A:679:PHE:HE1 | 5:A:749:PHE:HB2 | 1.68 | 0.58 |
| 5:A:713:LYS:HZ1 | 20:F:201:CLA:H41 | 1.68 | 0.58 |
| 20:A:838:CLA:NC | 20:A:838:CLA:C4 | 2.66 | 0.58 |
| 6:B:424:TRP:CZ3 | 20:B:839:CLA:HBC3 | 2.38 | 0.58 |
| 6:B:692:ARG:NH2 | 6:B:694:ARG:HG2 | 2.18 | 0.58 |
| 21:B:804:LMU:C6 | 21:B:804:LMU:C10 | 2.80 | 0.58 |
| 20:B:806:CLA:H52 | 20:B:806:CLA:NC | 2.18 | 0.58 |
| 20:1:204:CLA:HED3 | 20:1:204:CLA:C2A | 2.32 | 0.58 |
| 4:4:36:ASN:ND2 | 4:4:39:TRP:CE2 | 2.72 | 0.58 |
| 4:4:62:GLU:C | 4:4:65:THR:HG22 | 2.28 | 0.58 |
| 4:4:123:GLN:HG2 | 4:4:124:TYR:N | 2.18 | 0.58 |
| 20:4:305:CLA:HBC2 | 20:4:305:CLA:HMC3 | 1.84 | 0.58 |
| 5:A:232:PHE:CZ | 5:A:242:ILE:HG22 | 2.38 | 0.58 |
| 5:A:555:ILE:HG23 | 20:B:803:CLA:OBD | 2.03 | 0.58 |
| 6:B:15:ASP:O | 6:B:20:ARG:HG2 | 2.04 | 0.58 |
| 6:B:370:ALA:O | 20:B:828:CLA:HMA3 | 2.03 | 0.58 |
| 6:B:444:LEU:O | 6:B:445:ALA:HB3 | 2.02 | 0.58 |
| 6:B:586:THR:C | 6:B:588:GLY:N | 2.61 | 0.58 |
| 20:B:812:CLA:H12 | 20:B:812:CLA:CAA | 2.29 | 0.58 |
| 8:D:118:VAL:CG1 | 8:D:119:TYR:N | 2.66 | 0.58 |
| 9:E:65:VAL:HG13 | 9:E:82:TYR:O | 2.02 | 0.58 |
| 11:G:30:ASN:C | 11:G:30:ASN:HD22 | 2.10 | 0.58 |
| 12:H:41:GLU:OE2 | 12:H:42:THR:OG1 | 2.20 | 0.58 |
| 20:H:101:CLA:HMA2 | 20:H:101:CLA:H61 | 1.84 | 0.58 |
| 15:K:42:ALA:O | 15:K:43:ARG:CB | 2.50 | 0.58 |
| 18:R:39:UNK:N | 18:R:42:UNK:CB | 2.65 | 0.58 |
| 2:2:60:ALA:HA | 2:2:63:PHE:CD2 | 2.39 | 0.58 |
| 3:3:157:ALA:O | 3:3:158:TYR:HB2 | 2.02 | 0.58 |
| 4:4:104:ARG:HE | 4:4:105:ARG:N | 2.00 | 0.58 |
| 5:A:195:TRP:CE2 | 20:A:810:CLA:HMA2 | 2.38 | 0.58 |
| 5:A:459:GLY:O | 5:A:462:ILE:HG22 | 2.03 | 0.58 |
| 20:A:818:CLA:O2A | 20:A:818:CLA:H42 | 2.03 | 0.58 |
| 20:A:826:CLA:C7 | 22:A:845:BCR:C37 | 2.81 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:67:HIS:O | 6:B:68:VAL:HG23 | 2.02 | 0.58 |
| 6:B:160:LYS:HE3 | 6:B:161:TRP:CE2 | 2.39 | 0.58 |
| 20:B:824:CLA:H43 | 20:B:824:CLA:CAA | 2.29 | 0.58 |
| 7:C:12:ILE:N | 7:C:12:ILE:HD12 | 2.18 | 0.58 |
| 8:D:31:GLY:CA | 16:L:13:PRO:HB3 | 2.33 | 0.58 |
| 20:K:101:CLA:HED1 | 20:K:102:CLA:HMB1 | 1.84 | 0.58 |
| 16:L:122:GLY:O | 16:L:124:LYS:N | 2.36 | 0.58 |
| 20:1:203:CLA:CAD | 20:1:203:CLA:CED | 2.81 | 0.58 |
| 5:A:281:LEU:HD13 | 20:A:816:CLA:H2A | 1.85 | 0.58 |
| 5:A:373:ALA:O | 5:A:396:PHE:CD1 | 2.57 | 0.58 |
| 5:A:692:PHE:CZ | 20:A:838:CLA:HBC3 | 2.38 | 0.58 |
| 5:A:708:VAL:CA | 5:A:711:HIS:HD2 | 2.17 | 0.58 |
| 20:B:834:CLA:HMD1 | 20:B:835:CLA:C2C | 2.32 | 0.58 |
| 10:F:22:LEU:O | 10:F:24:LYS:N | 2.36 | 0.58 |
| 11:G:42:SER:OG | 11:G:46:ALA:CA | 2.50 | 0.58 |
| 16:L:58:LEU:HD11 | 16:L:153:TRP:HZ2 | 1.68 | 0.58 |
| 16:L:107:PHE:HB2 | 16:L:109:GLU:OE1 | 2.02 | 0.58 |
| 20:L:203:CLA:H112 | 20:L:203:CLA:C6 | 2.32 | 0.58 |
| 2:2:74:LEU:O | 2:2:75:ASN:ND2 | 2.36 | 0.58 |
| 3:3:52:LYS:N | 3:3:55:ALA:HB3 | 2.19 | 0.58 |
| 3:3:208:PRO:HB3 | 3:3:210:GLN:CD | 2.29 | 0.58 |
| 4:4:47:ASN:HB3 | 4:4:161:LEU:CD2 | 2.34 | 0.58 |
| 4:4:61:PRO:HB3 | 4:4:67:ILE:O | 2.04 | 0.58 |
| 4:4:72:VAL:O | 4:4:72:VAL:HG13 | 2.03 | 0.58 |
| 4:4:88:SER:O | 4:4:90:LEU:HA | 2.03 | 0.58 |
| 5:A:74:ILE:O | 5:A:78:VAL:HG13 | 2.04 | 0.58 |
| 5:A:114:THR:CG2 | 5:A:115:HIS:CE1 | 2.84 | 0.58 |
| 5:A:229:ILE:CG1 | 5:A:243:PRO:HB3 | 2.33 | 0.58 |
| 5:A:389:TYR:HE1 | 5:A:625:TRP:CD1 | 2.22 | 0.58 |
| 5:A:432:LEU:C | 5:A:434:ARG:N | 2.59 | 0.58 |
| 5:A:558:LYS:HZ1 | 6:B:674:LEU:HB3 | 1.68 | 0.58 |
| 20:A:819:CLA:CBA | 20:A:823:CLA:HBB2 | 2.34 | 0.58 |
| 20:A:831:CLA:CMD | 6:B:95:HIS:HD2 | 2.17 | 0.58 |
| 9:E:85:ASP:O | 9:E:86:GLU:CB | 2.52 | 0.58 |
| 11:G:88:THR:OG1 | 11:G:92:GLY:HA3 | 2.04 | 0.58 |
| 12:H:16:ASN:HD22 | 12:H:19:GLY:HA2 | 1.68 | 0.58 |
| 21:H:105:LMU:H22 | 21:H:105:LMU:H6'2 | 1.85 | 0.58 |
| 16:L:40:LEU:HB3 | 16:L:41:PRO:HD3 | 1.84 | 0.58 |
| 16:L:56:VAL:HA | 20:L:207:CLA:HED1 | 1.80 | 0.58 |
| 1:1:27:LEU:HD12 | 6:B:314:ARG:NH1 | 2.16 | 0.58 |
| 1:1:184:PRO:O | 1:1:185:TRP:CD2 | 2.56 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:618:TRP:CH2 | 5:A:655:ASP:HB2 | 2.39 | 0.58 |
| 20:A:818:CLA:CBB | 20:A:818:CLA:H71 | 2.33 | 0.58 |
| 6:B:203:ARG:H | 6:B:270:LEU:HD11 | 1.68 | 0.58 |
| 6:B:284:PHE:CE1 | 20:B:820:CLA:HHC | 2.39 | 0.58 |
| 6:B:569:ASP:HB3 | 6:B:574:ASP:HB3 | 1.86 | 0.58 |
| 6:B:633:ASN:ND2 | 6:B:636:THR:HB | 2.19 | 0.58 |
| 6:B:664:LEU:C | 6:B:667:TRP:CZ3 | 2.77 | 0.58 |
| 8:D:60:MET:SD | 8:D:61:PRO:HD2 | 2.43 | 0.58 |
| 8:D:111:TYR:CD2 | 8:D:114:PRO:CB | 2.86 | 0.58 |
| 15:K:46:GLY:C | 15:K:47:LEU:HG | 2.28 | 0.58 |
| 16:L:163:LEU:CD1 | 16:L:163:LEU:C | 2.75 | 0.58 |
| 17:N:24:THR:O | 17:N:26:GLY:N | 2.36 | 0.58 |
| 20:4:303:CLA:CGD | 20:4:303:CLA:C2A | 2.81 | 0.58 |
| 5:A:81:ALA:HB2 | 20:A:804:CLA:HMA1 | 1.82 | 0.58 |
| 5:A:255:LEU:CD1 | 5:A:280:PHE:HZ | 2.15 | 0.58 |
| 5:A:607:ASN:HD21 | 20:A:849:CLA:H42 | 1.68 | 0.58 |
| 22:A:843:BCR:C12 | 22:A:843:BCR:H341 | 2.32 | 0.58 |
| 6:B:44:GLN:CD | 6:B:163:PRO:HB2 | 2.29 | 0.58 |
| 6:B:269:TRP:HD1 | 6:B:497:TRP:CH2 | 2.22 | 0.58 |
| 6:B:406:ASN:C | 6:B:406:ASN:ND2 | 2.62 | 0.58 |
| 20:B:803:CLA:HHB | 20:B:803:CLA:C4 | 2.29 | 0.58 |
| 20:H:110:CLA:HED2 | 20:H:110:CLA:HAA2 | 1.86 | 0.58 |
| 17:N:75:TYR:C | 17:N:76:LYS:O | 2.44 | 0.58 |
| 18:R:3:UNK:O | 18:R:4:UNK:CB | 2.51 | 0.58 |
| 4:4:106:TRP:CH2 | 20:4:303:CLA:HBC1 | 2.38 | 0.58 |
| 4:4:107:GLN:CA | 20:4:301:CLA:HMA1 | 2.29 | 0.58 |
| 5:A:21:LEU:O | 5:A:21:LEU:HD13 | 2.03 | 0.58 |
| 5:A:21:LEU:HB2 | 5:A:22:VAL:O | 2.04 | 0.58 |
| 5:A:91:LEU:O | 20:A:807:CLA:HMC1 | 2.03 | 0.58 |
| 5:A:122:VAL:HA | 5:A:133:ASN:HD21 | 1.68 | 0.58 |
| 5:A:513:LEU:HB3 | 5:A:529:LEU:HD13 | 1.85 | 0.58 |
| 5:A:708:VAL:O | 5:A:711:HIS:HB2 | 2.04 | 0.58 |
| 5:A:733:VAL:HG11 | 20:A:838:CLA:C1D | 2.33 | 0.58 |
| 6:B:127:ILE:CD1 | 6:B:193:HIS:CE1 | 2.87 | 0.58 |
| 6:B:351:HIS:NE2 | 20:B:827:CLA:NC | 2.52 | 0.58 |
| 6:B:493:TRP:CH2 | 20:B:835:CLA:HBA1 | 2.38 | 0.58 |
| 6:B:577:TYR:HE2 | 6:B:578:LEU:HD12 | 1.68 | 0.58 |
| 6:B:648:TRP:CZ2 | 20:B:802:CLA:H62 | 2.39 | 0.58 |
| 7:C:74:THR:C | 7:C:76:SER:H | 2.11 | 0.58 |
| 12:H:72:ALA:HA | 19:Z:2:FRU:C6 | 2.33 | 0.58 |
| 20:K:103:CLA:O1A | 20:K:103:CLA:CMA | 2.52 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:L:10:VAL:O | 16:L:10:VAL:CG2 | 2.52 | 0.58 |
| 2:2:79:TRP:CG | 2:2:79:TRP:O | 2.57 | 0.58 |
| 4:4:90:LEU:HD22 | 4:4:90:LEU:N | 2.17 | 0.58 |
| 21:A:853:LMU:H81 | 21:A:853:LMU:C3 | 2.34 | 0.58 |
| 21:A:853:LMU:C9 | 21:A:853:LMU:H32 | 2.34 | 0.58 |
| 6:B:266:GLN:HE21 | 6:B:363:GLN:HG2 | 1.69 | 0.58 |
| 9:E:48:ASN:ND2 | 9:E:71:LYS:NZ | 2.51 | 0.58 |
| 20:F:201:CLA:HHD | 20:F:201:CLA:HBC2 | 1.80 | 0.58 |
| 20:1:206:CLA:CBC | 20:1:206:CLA:CHD | 2.82 | 0.58 |
| 20:2:303:CLA:O1A | 20:2:303:CLA:H2 | 2.04 | 0.58 |
| 4:4:90:LEU:H | 4:4:90:LEU:CD2 | 2.16 | 0.58 |
| 5:A:141:ARG:HG3 | 5:A:141:ARG:NH2 | 2.10 | 0.58 |
| 5:A:413:HIS:ND1 | 5:A:416:ILE:HD12 | 2.19 | 0.58 |
| 5:A:415:ALA:HB2 | 5:A:560:VAL:HG12 | 1.85 | 0.58 |
| 23:A:842:PQN:H142 | 22:F:203:BCR:HC22 | 1.84 | 0.58 |
| 6:B:156:HIS:O | 6:B:163:PRO:HB3 | 2.04 | 0.58 |
| 20:B:826:CLA:H11 | 20:B:839:CLA:CAD | 2.33 | 0.58 |
| 20:B:834:CLA:HBB2 | 22:B:846:BCR:C38 | 2.34 | 0.58 |
| 20:B:838:CLA:HHB | 20:B:839:CLA:OBD | 2.04 | 0.58 |
| 9:E:39:LEU:HA | 9:E:46:PHE:CE1 | 2.38 | 0.58 |
| 10:F:46:MET:O | 10:F:48:LYS:N | 2.37 | 0.58 |
| 20:H:101:CLA:CMA | 20:H:101:CLA:C2 | 2.81 | 0.58 |
| 16:L:25:THR:HB | 16:L:26:PRO:CD | 2.34 | 0.58 |
| 17:N:65:LEU:HD23 | 17:N:66:ASP:O | 2.03 | 0.58 |
| 19:Q:1:GLC:C5 | 19:Q:2:FRU:O5 | 2.51 | 0.58 |
| 2:2:54:TRP:HZ2 | 2:2:109:ARG:HB3 | 1.69 | 0.57 |
| 4:4:147:LEU:CD2 | 4:4:148:GLU:CG | 2.76 | 0.57 |
| 4:4:158:ARG:O | 4:4:159:LEU:C | 2.46 | 0.57 |
| 5:A:397:THR:HB | 5:A:613:ILE:HG12 | 1.85 | 0.57 |
| 5:A:431:LEU:O | 5:A:435:VAL:HG12 | 2.04 | 0.57 |
| 20:A:826:CLA:C7 | 22:A:845:BCR:H372 | 2.33 | 0.57 |
| 22:A:843:BCR:C23 | 22:A:843:BCR:C40 | 2.82 | 0.57 |
| 6:B:122:GLN:O | 6:B:126:THR:OG1 | 2.13 | 0.57 |
| 6:B:510:LEU:H | 6:B:510:LEU:CD2 | 2.16 | 0.57 |
| 20:B:835:CLA:HBC2 | 20:B:835:CLA:HHD | 1.85 | 0.57 |
| 10:F:33:ALA:HA | 10:F:36:SER:HB2 | 1.85 | 0.57 |
| 20:H:108:CLA:HHD | 20:H:108:CLA:HBC2 | 1.86 | 0.57 |
| 16:L:63:LEU:HD22 | 16:L:64:LEU:N | 2.17 | 0.57 |
| 16:L:135:GLY:HA2 | 16:L:138:LYS:HE2 | 1.86 | 0.57 |
| 2:2:211:LYS:HG2 | 3:3:113:LEU:CD1 | 2.23 | 0.57 |
| 3:3:162:PRO:HG2 | 3:3:164:PHE:CD1 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:3:319:LMU:O1' | 21:3:319:LMU:C5 | 2.51 | 0.57 |
| 4:4:36:ASN:ND2 | 4:4:39:TRP:CZ2 | 2.72 | 0.57 |
| 5:A:365:LEU:HD22 | 20:A:805:CLA:HED3 | 1.83 | 0.57 |
| 6:B:29:HIS:HB2 | 20:B:830:CLA:HBA1 | 1.86 | 0.57 |
| 6:B:277:HIS:HE1 | 20:B:819:CLA:NC | 2.02 | 0.57 |
| 6:B:382:ILE:CG2 | 6:B:383:MET:N | 2.51 | 0.57 |
| 6:B:556:SER:HG | 6:B:573:TRP:CG | 2.22 | 0.57 |
| 20:B:808:CLA:HMC1 | 20:B:830:CLA:CMA | 2.33 | 0.57 |
| 20:B:839:CLA:O1D | 20:B:839:CLA:C2A | 2.52 | 0.57 |
| 22:I:103:BCR:H291 | 22:L:209:BCR:H281 | 1.86 | 0.57 |
| 15:K:55:PHE:N | 15:K:55:PHE:CD1 | 2.72 | 0.57 |
| 20:L:203:CLA:HMB2 | 20:L:207:CLA:HBC1 | 1.86 | 0.57 |
| 3:3:92:TRP:HA | 3:3:95:THR:OG1 | 1.98 | 0.57 |
| 4:4:97:LEU:O | 4:4:98:SER:C | 2.47 | 0.57 |
| 4:4:164:LEU:O | 4:4:165:GLY:C | 2.46 | 0.57 |
| 5:A:25:ASP:HA | 5:A:26:PRO:C | 2.29 | 0.57 |
| 5:A:229:ILE:HG12 | 5:A:243:PRO:HB3 | 1.85 | 0.57 |
| 5:A:508:THR:O | 5:A:509:ALA:CB | 2.53 | 0.57 |
| 6:B:172:GLU:HG3 | 6:B:301:ILE:HG13 | 1.85 | 0.57 |
| 6:B:665:ILE:HD12 | 20:B:803:CLA:HBC1 | 1.86 | 0.57 |
| 21:H:105:LMU:C3 | 21:H:105:LMU:H1B | 2.32 | 0.57 |
| 2:2:98:GLU:HG2 | 2:2:99:LEU:CD1 | 2.34 | 0.57 |
| 3:3:205:GLY:N | 5:A:252:ARG:NH2 | 2.22 | 0.57 |
| 5:A:697:ARG:C | 5:A:699:TYR:H | 2.13 | 0.57 |
| 20:A:822:CLA:C1D | 22:A:844:BCR:H19C | 2.33 | 0.57 |
| 20:A:824:CLA:CHD | 20:A:824:CLA:CBC | 2.81 | 0.57 |
| 6:B:76:ALA:O | 6:B:79:GLN:N | 2.38 | 0.57 |
| 6:B:183:PHE:HE1 | 20:B:814:CLA:H71 | 1.69 | 0.57 |
| 6:B:693:TRP:HD1 | 20:B:840:CLA:C1D | 2.17 | 0.57 |
| 20:B:834:CLA:O2A | 20:B:835:CLA:CMB | 2.51 | 0.57 |
| 10:F:93:ILE:HG22 | 22:F:203:BCR:C37 | 2.35 | 0.57 |
| 10:F:147:GLY:C | 10:F:150:VAL:HB | 2.30 | 0.57 |
| 11:G:26:PHE:HB2 | 11:G:27:GLN:NE2 | 2.14 | 0.57 |
| 13:I:11:LEU:CD1 | 22:I:103:BCR:C10 | 2.67 | 0.57 |
| 17:N:61:LEU:HD12 | 17:N:62:SER:N | 2.19 | 0.57 |
| 17:N:76:LYS:O | 17:N:77:CYS:O | 2.21 | 0.57 |
| 4:4:58:MET:O | 4:4:60:LEU:N | 2.37 | 0.57 |
| 4:4:75:TRP:HB2 | 20:4:310:CLA:CMD | 2.33 | 0.57 |
| 4:4:116:ASN:O | 4:4:123:GLN:HG3 | 2.04 | 0.57 |
| 5:A:53:TRP:HA | 5:A:56:ASN:CB | 2.34 | 0.57 |
| 5:A:68:THR:C | 5:A:70:ASP:H | 2.13 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:109:TRP:HA | 5:A:116:ILE:HG13 | 1.86 | 0.57 |
| 20:A:806:CLA:HBA2 | 20:A:806:CLA:CED | 2.34 | 0.57 |
| 20:A:851:CLA:CGA | 20:A:851:CLA:H3A | 2.34 | 0.57 |
| 6:B:329:SER:O | 6:B:330:ILE:HG22 | 2.03 | 0.57 |
| 6:B:418:ILE:O | 6:B:422:LEU:HD12 | 2.04 | 0.57 |
| 6:B:576:PHE:CE2 | 20:B:830:CLA:HAC1 | 2.39 | 0.57 |
| 20:B:841:CLA:C19 | 13:I:21:MET:HB3 | 2.34 | 0.57 |
| 8:D:102:ARG:HH21 | 8:D:110:GLN:HB2 | 1.70 | 0.57 |
| 9:E:86:GLU:CG | 9:E:87:VAL:N | 2.42 | 0.57 |
| 10:F:53:PHE:C | 10:F:55:ASN:N | 2.62 | 0.57 |
| 20:K:103:CLA:O1A | 20:K:103:CLA:HMA2 | 2.04 | 0.57 |
| 20:R:107:CLA:HBA2 | 20:R:107:CLA:HBD | 1.87 | 0.57 |
| 2:2:128:ASN:ND2 | 14:J:3:ASP:HB3 | 2.19 | 0.57 |
| 21:2:313:LMU:C6' | 21:2:313:LMU:H2B | 2.35 | 0.57 |
| 21:2:319:LMU:O2' | 21:2:319:LMU:C1 | 2.51 | 0.57 |
| 5:A:54:ILE:O | 5:A:58:HIS:HD2 | 1.87 | 0.57 |
| 5:A:382:TYR:CE2 | 20:A:827:CLA:HED3 | 2.39 | 0.57 |
| 5:A:547:PHE:CE2 | 20:B:803:CLA:O1A | 2.56 | 0.57 |
| 5:A:690:LEU:HD21 | 5:A:738:TYR:HE1 | 1.69 | 0.57 |
| 5:A:733:VAL:HG11 | 20:A:838:CLA:C2D | 2.34 | 0.57 |
| 6:B:120:VAL:CA | 6:B:123:TRP:HD1 | 2.14 | 0.57 |
| 6:B:132:ASN:C | 6:B:132:ASN:OD1 | 2.48 | 0.57 |
| 20:B:809:CLA:H71 | 25:B:848:LMG:H381 | 1.85 | 0.57 |
| 12:H:20:GLN:CB | 12:H:22:ASP:CB | 2.68 | 0.57 |
| 15:K:44:GLU:OE1 | 15:K:44:GLU:C | 2.47 | 0.57 |
| 18:R:43:UNK:O | 18:R:44:UNK:C | 2.50 | 0.57 |
| 2:2:126:PRO:HG2 | 2:2:129:LYS:H | 1.70 | 0.57 |
| 21:2:313:LMU:H72 | 21:2:313:LMU:H31 | 1.86 | 0.57 |
| 4:4:70:ILE:O | 4:4:72:VAL:N | 2.37 | 0.57 |
| 4:4:122:LYS:HD3 | 4:4:142:ASN:O | 2.04 | 0.57 |
| 5:A:109:TRP:CH2 | 5:A:154:ARG:HD3 | 2.39 | 0.57 |
| 5:A:725:LEU:HD21 | 20:A:838:CLA:HMD3 | 1.87 | 0.57 |
| 20:A:804:CLA:H12 | 20:A:811:CLA:C6 | 2.20 | 0.57 |
| 6:B:77:TRP:CZ2 | 6:B:122:GLN:NE2 | 2.73 | 0.57 |
| 6:B:347:LEU:CD2 | 6:B:351:HIS:HE1 | 2.16 | 0.57 |
| 20:B:841:CLA:H2 | 23:B:843:PQN:H251 | 1.86 | 0.57 |
| 12:H:27:ASP:C | 12:H:29:PRO:HD3 | 2.28 | 0.57 |
| 12:H:75:ASP:CG | 12:H:77:LEU:HG | 2.29 | 0.57 |
| 13:I:14:LEU:C | 13:I:17:PRO:HD2 | 2.29 | 0.57 |
| 20:L:203:CLA:H112 | 20:L:203:CLA:H61 | 1.86 | 0.57 |
| 17:N:61:LEU:HD12 | 17:N:62:SER:C | 2.30 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:N:66:ASP:C | 17:N:67:LEU:HD12 | 2.29 | 0.57 |
| 17:N:70:GLU:CD | 17:N:72:LYS:O | 2.48 | 0.57 |
| 2:2:127:ASN:O | 2:2:128:ASN:HB2 | 2.03 | 0.57 |
| 4:4:106:TRP:CD1 | 20:4:301:CLA:CGD | 2.88 | 0.57 |
| 5:A:112:ASP:O | 5:A:116:ILE:HG12 | 2.05 | 0.57 |
| 5:A:426:THR:HA | 5:A:428:TYR:CZ | 2.40 | 0.57 |
| 6:B:299:HIS:CE1 | 20:B:823:CLA:HMD1 | 2.40 | 0.57 |
| 6:B:408:LEU:O | 6:B:411:MET:HB3 | 2.04 | 0.57 |
| 10:F:151:ASP:CA | 10:F:154:PHE:HB3 | 2.34 | 0.57 |
| 11:G:64:VAL:O | 11:G:64:VAL:HG12 | 2.04 | 0.57 |
| 16:L:63:LEU:O | 16:L:64:LEU:C | 2.47 | 0.57 |
| 1:1:28:GLY:HA2 | 20:1:212:CLA:C3C | 2.35 | 0.57 |
| 1:1:105:ILE:O | 1:1:108:VAL:HG12 | 2.05 | 0.57 |
| 2:2:54:TRP:HZ2 | 2:2:109:ARG:CD | 2.13 | 0.57 |
| 21:2:313:LMU:H12 | 21:2:313:LMU:H72 | 1.76 | 0.57 |
| 4:4:91:PHE:CG | 4:4:92:VAL:N | 2.73 | 0.57 |
| 5:A:25:ASP:OD2 | 5:A:25:ASP:C | 2.46 | 0.57 |
| 5:A:101:ALA:O | 5:A:104:SER:HA | 2.05 | 0.57 |
| 5:A:105:ASN:HB2 | 5:A:140:PHE:HZ | 1.70 | 0.57 |
| 5:A:699:TYR:HD1 | 5:A:700:TRP:CD1 | 2.23 | 0.57 |
| 20:A:804:CLA:HBB2 | 20:A:806:CLA:CAD | 2.34 | 0.57 |
| 20:A:831:CLA:CGD | 16:L:73:PRO:HA | 2.35 | 0.57 |
| 6:B:197:VAL:O | 6:B:197:VAL:HG12 | 2.03 | 0.57 |
| 20:B:818:CLA:HBD | 20:B:827:CLA:HBB2 | 1.87 | 0.57 |
| 15:K:42:ALA:O | 15:K:43:ARG:HG2 | 2.05 | 0.57 |
| 17:N:70:GLU:OE2 | 17:N:72:LYS:O | 2.23 | 0.57 |
| 18:R:27:UNK:O | 18:R:29:UNK:N | 2.31 | 0.57 |
| 2:2:100:VAL:CG2 | 2:2:101:PHE:N | 2.67 | 0.57 |
| 20:3:307:CLA:CBA | 20:3:307:CLA:CBD | 2.83 | 0.57 |
| 4:4:93:ILE:HG22 | 4:4:94:GLU:N | 2.19 | 0.57 |
| 4:4:121:PHE:O | 4:4:143:PHE:CD2 | 2.58 | 0.57 |
| 4:4:128:ALA:HB3 | 4:4:143:PHE:HE2 | 1.65 | 0.57 |
| 5:A:210:LEU:HB2 | 20:A:813:CLA:HMB2 | 1.85 | 0.57 |
| 6:B:20:ARG:HH11 | 6:B:20:ARG:CB | 2.17 | 0.57 |
| 6:B:347:LEU:HD13 | 6:B:351:HIS:HD1 | 1.70 | 0.57 |
| 6:B:414:HIS:O | 6:B:414:HIS:CG | 2.58 | 0.57 |
| 6:B:693:TRP:CD1 | 20:B:840:CLA:C1D | 2.88 | 0.57 |
| 7:C:77:MET:O | 7:C:79:LEU:N | 2.34 | 0.57 |
| 8:D:75:LEU:HD21 | 16:L:19:PHE:CD2 | 2.39 | 0.57 |
| 9:E:80:ASN:HB3 | 9:E:82:TYR:CE2 | 2.40 | 0.57 |
| 15:K:55:PHE:N | 15:K:55:PHE:HD1 | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:K:69:ILE:HA | 15:K:72:VAL:CG1 | 2.33 | 0.57 |
| 16:L:25:THR:HB | 16:L:26:PRO:HD2 | 1.87 | 0.57 |
| 17:N:42:PHE:H | 17:N:43:PRO:CD | 2.18 | 0.57 |
| 17:N:80:ASN:C | 17:N:82:PHE:N | 2.63 | 0.57 |
| 2:2:116:PRO:HB2 | 2:2:136:GLY:CA | 2.35 | 0.56 |
| 4:4:169:GLN:CG | 20:4:304:CLA:CAC | 2.82 | 0.56 |
| 5:A:132:LEU:HD11 | 5:A:674:ALA:HB2 | 1.86 | 0.56 |
| 5:A:137:GLY:C | 5:A:139:GLY:H | 2.12 | 0.56 |
| 5:A:364:MET:O | 5:A:368:LEU:HB2 | 2.04 | 0.56 |
| 5:A:439:ARG:NH1 | 5:A:565:SER:O | 2.37 | 0.56 |
| 6:B:127:ILE:CD1 | 6:B:193:HIS:HE1 | 2.18 | 0.56 |
| 6:B:143:LEU:C | 6:B:145:LEU:N | 2.61 | 0.56 |
| 6:B:284:PHE:O | 6:B:288:GLY:N | 2.31 | 0.56 |
| 6:B:576:PHE:HE2 | 20:B:830:CLA:HAC1 | 1.70 | 0.56 |
| 6:B:686:PRO:HD3 | 20:L:201:CLA:O1A | 2.05 | 0.56 |
| 20:B:828:CLA:O1D | 20:B:829:CLA:CMA | 2.53 | 0.56 |
| 11:G:44:PHE:N | 11:G:47:GLY:H | 2.02 | 0.56 |
| 22:2:317:BCR:H321 | 22:2:317:BCR:HC8 | 1.87 | 0.56 |
| 3:3:47:GLY:C | 3:3:49:ILE:H | 2.10 | 0.56 |
| 3:3:97:PHE:C | 3:3:98:ILE:HG23 | 2.30 | 0.56 |
| 4:4:73:PRO:CB | 4:4:75:TRP:HB2 | 2.34 | 0.56 |
| 4:4:102:GLU:OE2 | 20:4:313:CLA:CHC | 2.53 | 0.56 |
| 4:4:104:ARG:HA | 4:4:107:GLN:HE21 | 1.69 | 0.56 |
| 5:A:40:PHE:CZ | 5:A:56:ASN:HB3 | 2.41 | 0.56 |
| 5:A:207:LEU:HD12 | 5:A:310:PHE:CD1 | 2.38 | 0.56 |
| 5:A:307:ALA:O | 5:A:308:ILE:C | 2.49 | 0.56 |
| 5:A:389:TYR:CE1 | 5:A:625:TRP:CD1 | 2.93 | 0.56 |
| 5:A:402:ILE:CD1 | 20:A:827:CLA:HBB2 | 2.35 | 0.56 |
| 5:A:700:TRP:HZ3 | 20:A:851:CLA:O1D | 1.87 | 0.56 |
| 5:A:711:HIS:HB3 | 5:A:717:ALA:CB | 2.32 | 0.56 |
| 6:B:196:HIS:CE1 | 20:B:816:CLA:ND | 2.73 | 0.56 |
| 6:B:674:LEU:C | 6:B:674:LEU:HD12 | 2.30 | 0.56 |
| 7:C:60:THR:CG2 | 7:C:63:LEU:O | 2.53 | 0.56 |
| 10:F:37:ALA:N | 10:F:38:PRO:HD3 | 2.20 | 0.56 |
| 10:F:91:LEU:O | 10:F:94:ALA:O | 2.23 | 0.56 |
| 14:J:18:TRP:CH2 | 14:J:22:LEU:HD22 | 2.40 | 0.56 |
| 20:J:103:CLA:O1A | 20:J:103:CLA:C14 | 2.52 | 0.56 |
| 16:L:124:LYS:O | 16:L:126:GLN:N | 2.35 | 0.56 |
| 2:2:164:ILE:O | 2:2:167:GLY:CA | 2.53 | 0.56 |
| 20:3:311:CLA:O2D | 20:3:311:CLA:H2A | 2.05 | 0.56 |
| 20:3:314:CLA:HBC2 | 20:3:314:CLA:CHD | 2.35 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:71:ASN:O | 4:4:73:PRO:N | 2.38 | 0.56 |
| 4:4:93:ILE:O | 4:4:95:PHE:N | 2.39 | 0.56 |
| 4:4:104:ARG:NE | 4:4:105:ARG:N | 2.53 | 0.56 |
| 4:4:140:PRO:O | 4:4:141:LEU:HB2 | 2.04 | 0.56 |
| 5:A:44:ILE:O | 5:A:45:ALA:C | 2.48 | 0.56 |
| 5:A:177:LEU:C | 5:A:179:LEU:H | 2.13 | 0.56 |
| 5:A:553:VAL:O | 5:A:557:LEU:HB2 | 2.05 | 0.56 |
| 5:A:625:TRP:HB3 | 5:A:637:ILE:HD11 | 1.87 | 0.56 |
| 20:A:826:CLA:H111 | 22:J:102:BCR:H353 | 1.87 | 0.56 |
| 6:B:34:HIS:O | 6:B:36:ASP:N | 2.37 | 0.56 |
| 6:B:70:TRP:HB3 | 6:B:136:TYR:OH | 2.03 | 0.56 |
| 6:B:482:ASN:OD1 | 6:B:485:ALA:HB2 | 2.04 | 0.56 |
| 20:B:826:CLA:H72 | 20:B:839:CLA:C3D | 2.35 | 0.56 |
| 20:B:836:CLA:HBC3 | 20:B:836:CLA:CHD | 2.33 | 0.56 |
| 7:C:14:CYS:C | 7:C:17:CYS:SG | 2.87 | 0.56 |
| 9:E:44:TYR:CE1 | 9:E:73:ASN:HA | 2.40 | 0.56 |
| 9:E:90:VAL:C | 9:E:92:ALA:N | 2.61 | 0.56 |
| 10:F:52:ARG:NH1 | 10:F:55:ASN:OD1 | 2.36 | 0.56 |
| 12:H:14:ILE:O | 12:H:16:ASN:N | 2.37 | 0.56 |
| 15:K:46:GLY:O | 15:K:47:LEU:HB2 | 2.03 | 0.56 |
| 21:K:105:LMU:H42 | 21:K:105:LMU:C8 | 2.21 | 0.56 |
| 16:L:9:GLN:HG3 | 16:L:10:VAL:H | 1.71 | 0.56 |
| 16:L:124:LYS:HB2 | 16:L:124:LYS:NZ | 2.19 | 0.56 |
| 16:L:163:LEU:HB3 | 16:L:164:PRO:HD3 | 1.57 | 0.56 |
| 1:1:48:ARG:O | 1:1:52:LEU:HB2 | 2.05 | 0.56 |
| 2:2:90:ASP:HB3 | 2:2:94:LEU:HB2 | 1.87 | 0.56 |
| 3:3:74:ALA:CA | 20:3:306:CLA:C3D | 2.67 | 0.56 |
| 5:A:66:SER:O | 5:A:67:HIS:HB2 | 2.05 | 0.56 |
| 5:A:105:ASN:HB2 | 5:A:140:PHE:CZ | 2.41 | 0.56 |
| 5:A:174:PHE:O | 5:A:175:ALA:HB2 | 2.04 | 0.56 |
| 5:A:392:GLN:HA | 5:A:395:LEU:HD23 | 1.88 | 0.56 |
| 20:B:828:CLA:O1D | 20:B:829:CLA:HMA1 | 2.06 | 0.56 |
| 20:B:831:CLA:CMA | 20:F:201:CLA:O1A | 2.54 | 0.56 |
| 20:B:831:CLA:HMA2 | 20:F:201:CLA:O1A | 2.05 | 0.56 |
| 10:F:20:GLN:O | 10:F:21:ALA:CB | 2.54 | 0.56 |
| 15:K:1:ASP:CA | 15:K:5:SER:HB3 | 2.27 | 0.56 |
| 17:N:57:LYS:N | 17:N:60:PHE:O | 2.38 | 0.56 |
| 1:1:111:GLN:HA | 1:1:111:GLN:HE21 | 1.71 | 0.56 |
| 1:1:115:GLU:HG3 | 1:1:116:LYS:H | 1.71 | 0.56 |
| 4:4:35:GLU:CB | 4:4:36:ASN:HB3 | 2.28 | 0.56 |
| 4:4:81:GLU:O | 4:4:82:GLU:HG2 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:58:HIS:CE1 | 20:A:803:CLA:C1D | 2.89 | 0.56 |
| 5:A:79:PHE:HE2 | 5:A:185:HIS:CE1 | 2.24 | 0.56 |
| 5:A:109:TRP:HH2 | 5:A:154:ARG:HD3 | 1.70 | 0.56 |
| 5:A:699:TYR:O | 6:B:536:LYS:NZ | 2.38 | 0.56 |
| 20:A:826:CLA:H71 | 22:A:845:BCR:H372 | 1.87 | 0.56 |
| 20:A:835:CLA:C20 | 20:L:201:CLA:HBB2 | 2.35 | 0.56 |
| 20:A:851:CLA:H11 | 6:B:431:PHE:CE1 | 2.41 | 0.56 |
| 6:B:74:PHE:C | 6:B:76:ALA:H | 2.13 | 0.56 |
| 6:B:154:TRP:CD1 | 6:B:158:GLN:CG | 2.89 | 0.56 |
| 6:B:222:LEU:HA | 20:B:816:CLA:HMD2 | 1.85 | 0.56 |
| 20:B:810:CLA:H102 | 20:B:810:CLA:H142 | 1.86 | 0.56 |
| 8:D:44:GLU:CB | 8:D:46:TYR:HE2 | 2.08 | 0.56 |
| 8:D:58:PHE:HD2 | 8:D:59:GLU:H | 1.52 | 0.56 |
| 15:K:72:VAL:HG13 | 15:K:73:GLY:N | 2.20 | 0.56 |
| 16:L:124:LYS:C | 16:L:126:GLN:N | 2.61 | 0.56 |
| 3:3:194:ILE:HA | 3:3:197:TYR:CE1 | 2.40 | 0.56 |
| 5:A:302:HIS:HB2 | 20:A:817:CLA:CHB | 2.35 | 0.56 |
| 5:A:680:LEU:HB3 | 20:A:850:CLA:C2 | 2.36 | 0.56 |
| 20:A:806:CLA:HED2 | 20:A:806:CLA:HBA2 | 1.86 | 0.56 |
| 6:B:278:LEU:O | 6:B:281:ALA:N | 2.38 | 0.56 |
| 6:B:577:TYR:CE2 | 6:B:578:LEU:HD12 | 2.41 | 0.56 |
| 20:B:803:CLA:CBC | 20:B:803:CLA:HMC3 | 2.35 | 0.56 |
| 20:B:817:CLA:HED2 | 20:B:817:CLA:CBA | 2.36 | 0.56 |
| 7:C:28:MET:HB3 | 8:D:122:LYS:O | 2.06 | 0.56 |
| 20:H:101:CLA:HMC1 | 20:H:101:CLA:HBC3 | 1.87 | 0.56 |
| 16:L:48:ASN:HB2 | 16:L:50:LEU:HD22 | 1.88 | 0.56 |
| 21:R:106:LMU:H6D | 21:R:106:LMU:O6B | 2.06 | 0.56 |
| 20:2:307:CLA:H41 | 20:2:307:CLA:C9 | 2.29 | 0.56 |
| 5:A:377:TYR:CD1 | 5:A:616:PHE:HE1 | 2.24 | 0.56 |
| 5:A:711:HIS:CE1 | 20:A:837:CLA:HAC1 | 2.40 | 0.56 |
| 20:A:809:CLA:CBB | 20:B:833:CLA:HMD1 | 2.36 | 0.56 |
| 6:B:496:GLY:O | 6:B:499:ASN:HB2 | 2.06 | 0.56 |
| 20:B:820:CLA:OBD | 20:B:823:CLA:CBC | 2.52 | 0.56 |
| 9:E:36:VAL:CG2 | 9:E:52:VAL:HG22 | 2.35 | 0.56 |
| 9:E:44:TYR:CZ | 9:E:73:ASN:HA | 2.41 | 0.56 |
| 15:K:44:GLU:C | 15:K:47:LEU:HG | 2.27 | 0.56 |
| 21:R:104:LMU:O2' | 21:R:104:LMU:H1B | 2.05 | 0.56 |
| 1:1:182:ALA:O | 1:1:183:ASP:C | 2.48 | 0.56 |
| 2:2:191:ASN:CB | 19:O:1:GLC:C6 | 2.84 | 0.56 |
| 5:A:310:PHE:H | 5:A:313:ALA:HB3 | 1.71 | 0.56 |
| 5:A:491:TRP:CD1 | 5:A:492:ILE:HG23 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:698:GLY:CA | 6:B:570:ILE:HG21 | 2.36 | 0.56 |
| 21:A:848:LMU:H52 | 21:A:848:LMU:C1 | 2.36 | 0.56 |
| 6:B:120:VAL:HA | 6:B:123:TRP:HE1 | 1.71 | 0.56 |
| 6:B:558:PRO:HG2 | 6:B:703:VAL:CB | 2.21 | 0.56 |
| 20:B:827:CLA:H71 | 22:B:846:BCR:H14C | 1.87 | 0.56 |
| 8:D:75:LEU:HD21 | 16:L:19:PHE:CZ | 2.41 | 0.56 |
| 11:G:24:PHE:CE1 | 11:G:27:GLN:O | 2.59 | 0.56 |
| 13:I:2:ILE:HG12 | 13:I:3:ASN:CG | 2.31 | 0.56 |
| 17:N:38:GLY:HA3 | 17:N:46:PHE:CD1 | 2.41 | 0.56 |
| 17:N:63:ASP:HA | 17:N:64:ASP:C | 2.29 | 0.56 |
| 18:R:38:UNK:O | 18:R:42:UNK:CB | 2.53 | 0.56 |
| 1:1:149:LYS:HB3 | 20:1:206:CLA:CMC | 2.35 | 0.56 |
| 2:2:129:LYS:HA | 2:2:131:THR:HG23 | 1.86 | 0.56 |
| 5:A:401:TRP:HD1 | 20:A:826:CLA:CHC | 2.18 | 0.56 |
| 5:A:448:TRP:CD1 | 20:A:830:CLA:CED | 2.89 | 0.56 |
| 5:A:455:PHE:HD1 | 20:A:830:CLA:CMA | 2.19 | 0.56 |
| 5:A:641:ASN:HD22 | 5:A:641:ASN:H | 1.54 | 0.56 |
| 20:A:825:CLA:H143 | 20:A:825:CLA:H101 | 1.88 | 0.56 |
| 6:B:49:SER:O | 6:B:52:GLY:N | 2.39 | 0.56 |
| 6:B:213:LEU:HD12 | 6:B:214:ASP:N | 2.21 | 0.56 |
| 6:B:293:THR:C | 6:B:294:ASN:CG | 2.74 | 0.56 |
| 6:B:475:ASP:HA | 6:B:480:SER:HA | 1.88 | 0.56 |
| 20:B:803:CLA:HMC3 | 20:B:803:CLA:HBC2 | 1.88 | 0.56 |
| 7:C:5:VAL:HB | 7:C:65:VAL:CG2 | 2.36 | 0.56 |
| 8:D:48:ILE:HG22 | 8:D:83:CYS:HB2 | 1.86 | 0.56 |
| 8:D:79:ARG:H | 8:D:82:GLN:NE2 | 2.04 | 0.56 |
| 10:F:17:ARG:HA | 10:F:17:ARG:NE | 2.20 | 0.56 |
| 11:G:28:ARG:NH2 | 11:G:29:GLU:O | 2.39 | 0.56 |
| 20:K:102:CLA:HBC1 | 21:K:105:LMU:O3B | 2.04 | 0.56 |
| 16:L:48:ASN:HB3 | 16:L:49:PRO:CD | 2.36 | 0.56 |
| 17:N:25:THR:CG2 | 17:N:26:GLY:N | 2.69 | 0.56 |
| 17:N:61:LEU:O | 17:N:62:SER:HB2 | 2.05 | 0.56 |
| 17:N:76:LYS:HG3 | 17:N:77:CYS:N | 2.12 | 0.56 |
| 17:N:79:SER:CA | 17:N:80:ASN:C | 2.74 | 0.56 |
| 18:R:38:UNK:C | 18:R:42:UNK:CB | 2.83 | 0.56 |
| 19:Q:2:FRU:H62 | 19:Q:2:FRU:H11 | 1.88 | 0.56 |
| 22:2:317:BCR:H311 | 22:2:317:BCR:HC8 | 1.87 | 0.56 |
| 3:3:49:ILE:HA | 3:3:51:PRO:HD2 | 1.88 | 0.56 |
| 3:3:97:PHE:CE2 | 3:3:98:ILE:HG21 | 2.35 | 0.56 |
| 4:4:34:PRO:HA | 4:4:35:GLU:CD | 2.31 | 0.56 |
| 4:4:84:PHE:O | 4:4:85:ALA:CB | 2.54 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:124:TRP:HD1 | 20:A:809:CLA:HED2 | 1.71 | 0.56 |
| 5:A:672:LEU:HD23 | 5:A:672:LEU:H | 1.71 | 0.56 |
| 6:B:731:GLY:O | 6:B:732:LYS:HB2 | 2.04 | 0.56 |
| 20:B:838:CLA:CGA | 20:B:838:CLA:C1A | 2.84 | 0.56 |
| 7:C:52:LYS:C | 7:C:54:CYS:N | 2.62 | 0.56 |
| 9:E:63:TYR:HA | 9:E:83:ALA:HB2 | 1.88 | 0.56 |
| 22:I:103:BCR:C8 | 22:I:103:BCR:H311 | 2.35 | 0.56 |
| 3:3:48:PHE:CD2 | 3:3:49:ILE:CG2 | 2.69 | 0.55 |
| 4:4:36:ASN:OD1 | 4:4:39:TRP:CD2 | 2.59 | 0.55 |
| 5:A:578:ARG:O | 5:A:579:PHE:CD1 | 2.59 | 0.55 |
| 20:A:820:CLA:C1C | 20:A:820:CLA:H52 | 2.36 | 0.55 |
| 20:A:831:CLA:O1D | 16:L:73:PRO:HA | 2.04 | 0.55 |
| 6:B:55:ALA:HB1 | 6:B:150:LEU:CD1 | 2.37 | 0.55 |
| 6:B:649:MET:O | 6:B:653:GLY:N | 2.38 | 0.55 |
| 6:B:681:ALA:O | 6:B:684:ARG:N | 2.30 | 0.55 |
| 22:B:801:BCR:C33 | 20:L:207:CLA:NB | 2.44 | 0.55 |
| 8:D:113:HIS:N | 8:D:114:PRO:CD | 2.69 | 0.55 |
| 9:E:73:ASN:C | 9:E:73:ASN:ND2 | 2.64 | 0.55 |
| 12:H:63:SER:O | 12:H:67:TYR:CB | 2.54 | 0.55 |
| 13:I:11:LEU:HG | 22:I:103:BCR:HC7 | 1.85 | 0.55 |
| 17:N:1:GLY:O | 17:N:2:VAL:CG1 | 2.53 | 0.55 |
| 5:A:123:VAL:HG22 | 5:A:133:ASN:OD1 | 2.06 | 0.55 |
| 5:A:214:GLY:O | 5:A:215:SER:CB | 2.53 | 0.55 |
| 5:A:436:LEU:O | 5:A:439:ARG:HB3 | 2.05 | 0.55 |
| 6:B:353:TYR:C | 6:B:355:LEU:H | 2.13 | 0.55 |
| 6:B:645:VAL:HG11 | 20:B:810:CLA:HAC1 | 1.88 | 0.55 |
| 6:B:646:TRP:O | 6:B:649:MET:HB2 | 2.06 | 0.55 |
| 6:B:666:SER:CB | 6:B:671:TRP:HE1 | 2.14 | 0.55 |
| 6:B:710:LEU:C | 6:B:712:HIS:H | 2.13 | 0.55 |
| 20:B:838:CLA:C6 | 22:F:204:BCR:H323 | 2.36 | 0.55 |
| 8:D:48:ILE:CG2 | 8:D:83:CYS:HB2 | 2.37 | 0.55 |
| 8:D:75:LEU:HD22 | 8:D:76:LYS:H | 1.70 | 0.55 |
| 10:F:23:LYS:C | 10:F:24:LYS:CE | 2.77 | 0.55 |
| 13:I:2:ILE:HG12 | 13:I:3:ASN:ND2 | 2.21 | 0.55 |
| 22:I:103:BCR:C39 | 22:L:209:BCR:H401 | 2.35 | 0.55 |
| 20:L:203:CLA:C9 | 22:L:209:BCR:H321 | 2.36 | 0.55 |
| 1:1:185:TRP:CH2 | 20:1:213:CLA:H2 | 2.41 | 0.55 |
| 3:3:94:ARG:C | 3:3:97:PHE:HE1 | 2.03 | 0.55 |
| 5:A:144:GLN:CG | 5:A:145:ILE:H | 2.19 | 0.55 |
| 5:A:230:ASN:HA | 5:A:233:LEU:HB2 | 1.88 | 0.55 |
| 5:A:472:ARG:HG2 | 6:B:97:GLY:HA3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:709:TRP:CZ3 | 6:B:417:ALA:HA | 2.42 | 0.55 |
| 20:A:826:CLA:H72 | 22:A:845:BCR:H371 | 1.87 | 0.55 |
| 20:A:832:CLA:H2A | 20:A:832:CLA:O1D | 2.05 | 0.55 |
| 6:B:559:CYS:HB2 | 6:B:702:ILE:HD12 | 1.87 | 0.55 |
| 20:B:822:CLA:CHD | 20:B:822:CLA:CBC | 2.83 | 0.55 |
| 10:F:92:TYR:C | 10:F:92:TYR:CD2 | 2.84 | 0.55 |
| 21:F:202:LMU:H11 | 21:F:202:LMU:H92 | 1.87 | 0.55 |
| 20:K:101:CLA:OBD | 20:K:102:CLA:CHB | 2.55 | 0.55 |
| 2:2:170:ALA:O | 2:2:171:MET:C | 2.48 | 0.55 |
| 4:4:73:PRO:O | 4:4:74:LYS:CG | 2.54 | 0.55 |
| 5:A:88:ILE:HG22 | 5:A:89:ILE:H | 1.72 | 0.55 |
| 5:A:103:PHE:HE1 | 20:A:807:CLA:CGD | 2.19 | 0.55 |
| 5:A:255:LEU:HD11 | 5:A:280:PHE:HZ | 1.71 | 0.55 |
| 5:A:479:ASP:OD2 | 5:A:536:THR:HG23 | 2.05 | 0.55 |
| 5:A:514:THR:HB | 5:A:532:ILE:CG2 | 2.37 | 0.55 |
| 5:A:586:ARG:H | 7:C:49:VAL:CG2 | 2.18 | 0.55 |
| 20:A:830:CLA:H101 | 20:A:830:CLA:C14 | 2.36 | 0.55 |
| 6:B:17:THR:HA | 6:B:696:LYS:H | 1.71 | 0.55 |
| 6:B:167:TRP:CZ2 | 20:B:814:CLA:HAC2 | 2.41 | 0.55 |
| 6:B:195:VAL:HA | 6:B:199:ILE:HG13 | 1.89 | 0.55 |
| 9:E:69:PHE:HD2 | 9:E:71:LYS:HG2 | 1.72 | 0.55 |
| 10:F:103:SER:C | 10:F:105:LEU:N | 2.60 | 0.55 |
| 16:L:102:TYR:C | 16:L:104:ILE:H | 2.14 | 0.55 |
| 16:L:165:TYR:CG | 16:L:165:TYR:O | 2.58 | 0.55 |
| 18:R:26:UNK:O | 18:R:27:UNK:C | 2.55 | 0.55 |
| 21:2:313:LMU:C2 | 21:2:313:LMU:O5' | 2.53 | 0.55 |
| 3:3:50:GLU:H | 3:3:51:PRO:HD3 | 1.71 | 0.55 |
| 21:4:321:LMU:O2B | 21:4:321:LMU:H6D | 2.06 | 0.55 |
| 5:A:132:LEU:HD23 | 6:B:446:PHE:HE1 | 1.72 | 0.55 |
| 5:A:269:PHE:HE1 | 15:K:14:THR:CG2 | 2.06 | 0.55 |
| 20:A:808:CLA:HBB2 | 20:A:809:CLA:C3D | 2.36 | 0.55 |
| 20:A:808:CLA:CMB | 20:A:809:CLA:H11 | 2.37 | 0.55 |
| 6:B:50:HIS:HA | 6:B:53:GLN:HB2 | 1.89 | 0.55 |
| 6:B:529:THR:O | 6:B:533:ILE:HG22 | 2.07 | 0.55 |
| 6:B:573:TRP:O | 6:B:577:TYR:N | 2.31 | 0.55 |
| 7:C:62:PHE:CE1 | 9:E:42:GLU:HB2 | 2.41 | 0.55 |
| 10:F:131:PHE:O | 10:F:133:GLY:N | 2.40 | 0.55 |
| 12:H:21:TRP:H | 12:H:22:ASP:HB3 | 1.72 | 0.55 |
| 12:H:36:GLN:HG2 | 12:H:36:GLN:O | 2.05 | 0.55 |
| 20:K:103:CLA:HBC2 | 20:K:103:CLA:CMC | 2.37 | 0.55 |
| 17:N:50:GLN:HA | 17:N:51:ASP:C | 2.31 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:R:8:UNK:CB | 20:R:107:CLA:CED | 2.84 | 0.55 |
| 2:2:44:ASN:HD21 | 14:J:1:MET:HB2 | 1.70 | 0.55 |
| 2:2:59:ALA:CB | 2:2:172:LEU:HD22 | 2.36 | 0.55 |
| 3:3:202:LEU:HB3 | 3:3:204:THR:HG23 | 1.87 | 0.55 |
| 20:3:310:CLA:CHD | 20:3:310:CLA:CBC | 2.77 | 0.55 |
| 20:4:318:CLA:CBC | 20:4:318:CLA:CMC | 2.79 | 0.55 |
| 5:A:393:LEU:HG | 5:A:394:SER:N | 2.21 | 0.55 |
| 5:A:396:PHE:CG | 5:A:396:PHE:O | 2.58 | 0.55 |
| 5:A:464:ASN:O | 5:A:468:SER:N | 2.39 | 0.55 |
| 5:A:478:SER:HB3 | 5:A:644:GLN:CD | 2.31 | 0.55 |
| 20:A:831:CLA:HBC2 | 20:H:108:CLA:HBC1 | 1.88 | 0.55 |
| 6:B:197:VAL:O | 6:B:198:ALA:HB2 | 2.06 | 0.55 |
| 6:B:203:ARG:HB3 | 6:B:270:LEU:HD12 | 1.87 | 0.55 |
| 20:B:815:CLA:HMA3 | 22:B:845:BCR:H313 | 1.87 | 0.55 |
| 7:C:55:GLU:HG3 | 7:C:60:THR:HG22 | 1.88 | 0.55 |
| 17:N:4:GLU:HG3 | 17:N:4:GLU:O | 2.06 | 0.55 |
| 17:N:73:ASP:O | 17:N:75:TYR:N | 2.39 | 0.55 |
| 21:R:102:LMU:H5B | 21:R:102:LMU:O6' | 2.06 | 0.55 |
| 2:2:188:PRO:HB2 | 2:2:189:ILE:HD13 | 1.88 | 0.55 |
| 4:4:95:PHE:HD1 | 4:4:95:PHE:H | 1.51 | 0.55 |
| 4:4:105:ARG:HG3 | 4:4:105:ARG:O | 2.05 | 0.55 |
| 6:B:132:ASN:HA | 6:B:135:LEU:HG | 1.88 | 0.55 |
| 6:B:166:SER:C | 6:B:168:PHE:H | 2.14 | 0.55 |
| 6:B:174:ARG:CB | 20:B:814:CLA:CBC | 2.79 | 0.55 |
| 6:B:424:TRP:CE2 | 20:F:201:CLA:HAC1 | 2.42 | 0.55 |
| 6:B:544:SER:O | 6:B:546:LEU:N | 2.39 | 0.55 |
| 20:B:838:CLA:CMA | 20:B:839:CLA:CED | 2.80 | 0.55 |
| 14:J:9:SER:O | 14:J:10:VAL:CB | 2.54 | 0.55 |
| 20:K:104:CLA:HBC3 | 20:K:104:CLA:CHD | 2.31 | 0.55 |
| 16:L:163:LEU:C | 16:L:163:LEU:HD13 | 2.31 | 0.55 |
| 17:N:54:LYS:HB3 | 17:N:57:LYS:CE | 2.37 | 0.55 |
| 21:2:313:LMU:O5' | 21:2:313:LMU:H32 | 2.07 | 0.55 |
| 3:3:199:VAL:HG22 | 20:3:305:CLA:C3C | 2.36 | 0.55 |
| 4:4:76:TYR:CD1 | 4:4:76:TYR:C | 2.83 | 0.55 |
| 5:A:25:ASP:HA | 5:A:27:ILE:N | 2.22 | 0.55 |
| 6:B:292:ARG:NH2 | 6:B:297:ILE:H | 2.04 | 0.55 |
| 20:B:826:CLA:HBA1 | 20:B:827:CLA:HED3 | 1.88 | 0.55 |
| 20:H:101:CLA:C3A | 20:H:101:CLA:CGA | 2.85 | 0.55 |
| 17:N:67:LEU:HB2 | 17:N:68:GLU:CB | 2.37 | 0.55 |
| 18:R:27:UNK:C | 18:R:29:UNK:H | 2.14 | 0.55 |
| 1:1:182:ALA:O | 1:1:183:ASP:O | 2.24 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:1:211:CLA:HED2 | 20:1:211:CLA:OBD | 2.07 | 0.55 |
| 20:1:211:CLA:CAD | 20:1:211:CLA:CED | 2.84 | 0.55 |
| 4:4:121:PHE:HB2 | 4:4:128:ALA:HB3 | 1.89 | 0.55 |
| 5:A:98:PHE:O | 5:A:99:HIS:CB | 2.54 | 0.55 |
| 5:A:225:VAL:O | 5:A:229:ILE:HB | 2.07 | 0.55 |
| 5:A:372:VAL:HG22 | 20:A:818:CLA:C4 | 2.37 | 0.55 |
| 5:A:425:THR:O | 5:A:428:TYR:CE1 | 2.60 | 0.55 |
| 6:B:31:PHE:O | 6:B:37:ILE:HG21 | 2.06 | 0.55 |
| 6:B:304:ILE:HD11 | 20:B:820:CLA:HED2 | 1.87 | 0.55 |
| 6:B:535:VAL:HG22 | 6:B:539:LEU:HD23 | 1.89 | 0.55 |
| 20:B:802:CLA:CBB | 20:B:803:CLA:CHB | 2.84 | 0.55 |
| 20:B:829:CLA:H101 | 22:B:845:BCR:H343 | 1.89 | 0.55 |
| 22:B:845:BCR:H331 | 22:B:845:BCR:HC8 | 1.87 | 0.55 |
| 7:C:11:CYS:SG | 7:C:12:ILE:N | 2.79 | 0.55 |
| 8:D:41:GLN:HG3 | 16:L:125:LYS:HZ2 | 1.71 | 0.55 |
| 8:D:60:MET:HG3 | 8:D:61:PRO:O | 2.07 | 0.55 |
| 8:D:64:GLY:O | 8:D:65:ALA:CB | 2.55 | 0.55 |
| 8:D:122:LYS:NZ | 8:D:124:ASN:OD1 | 2.40 | 0.55 |
| 11:G:83:TYR:O | 11:G:83:TYR:CG | 2.59 | 0.55 |
| 20:K:104:CLA:H2A | 20:K:104:CLA:O2D | 2.06 | 0.55 |
| 18:R:8:UNK:CB | 20:R:107:CLA:O2D | 2.55 | 0.55 |
| 18:R:38:UNK:C | 18:R:42:UNK:C | 2.85 | 0.55 |
| 4:4:97:LEU:C | 4:4:99:HIS:N | 2.60 | 0.55 |
| 4:4:101:VAL:O | 4:4:104:ARG:NH2 | 2.40 | 0.55 |
| 5:A:251:ASN:C | 5:A:253:ASP:N | 2.65 | 0.55 |
| 5:A:281:LEU:O | 5:A:283:PHE:N | 2.39 | 0.55 |
| 5:A:284:ARG:HA | 5:A:284:ARG:NH1 | 2.21 | 0.55 |
| 5:A:418:MET:O | 5:A:564:ARG:HD2 | 2.06 | 0.55 |
| 5:A:584:PRO:HG3 | 6:B:559:CYS:SG | 2.46 | 0.55 |
| 20:A:808:CLA:HAA2 | 20:A:826:CLA:HED3 | 1.89 | 0.55 |
| 21:A:854:LMU:H1' | 21:A:854:LMU:O6' | 2.07 | 0.55 |
| 6:B:261:PHE:CZ | 6:B:500:ALA:HB2 | 2.42 | 0.55 |
| 6:B:291:TYR:CE1 | 20:B:820:CLA:HED1 | 2.42 | 0.55 |
| 6:B:646:TRP:CH2 | 6:B:726:ILE:HG21 | 2.42 | 0.55 |
| 20:B:810:CLA:CGA | 20:B:810:CLA:C1A | 2.85 | 0.55 |
| 20:B:820:CLA:HBB2 | 20:B:825:CLA:H41 | 1.88 | 0.55 |
| 10:F:58:LYS:O | 10:F:60:GLY:N | 2.40 | 0.55 |
| 11:G:43:HIS:CB | 11:G:44:PHE:CD1 | 2.76 | 0.55 |
| 11:G:78:GLY:O | 11:G:79:HIS:ND1 | 2.40 | 0.55 |
| 21:H:105:LMU:H1B | 21:H:105:LMU:O1' | 2.07 | 0.55 |
| 17:N:33:TYR:O | 17:N:34:THR:CG2 | 2.55 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:158:TYR:OH | 20:3:304:CLA:C2B | 2.54 | 0.54 |
| 4:4:52:MET:CE | 4:4:156:ASN:HB2 | 2.37 | 0.54 |
| 4:4:158:ARG:HA | 4:4:161:LEU:CD1 | 2.36 | 0.54 |
| 5:A:79:PHE:CE2 | 5:A:185:HIS:CE1 | 2.95 | 0.54 |
| 5:A:209:GLY:C | 5:A:213:LEU:HB2 | 2.32 | 0.54 |
| 5:A:362:LEU:CB | 5:A:410:ALA:HB2 | 2.35 | 0.54 |
| 6:B:29:HIS:CD2 | 20:B:808:CLA:CBB | 2.90 | 0.54 |
| 6:B:232:LEU:HD21 | 6:B:235:GLN:OE1 | 2.08 | 0.54 |
| 20:B:821:CLA:HBB2 | 11:G:18:LEU:HD13 | 1.88 | 0.54 |
| 10:F:116:GLN:C | 10:F:118:GLU:N | 2.64 | 0.54 |
| 15:K:39:LYS:N | 15:K:39:LYS:HD2 | 2.21 | 0.54 |
| 2:2:79:TRP:CD1 | 2:2:81:THR:CG2 | 2.91 | 0.54 |
| 21:2:313:LMU:H72 | 21:2:313:LMU:C3 | 2.37 | 0.54 |
| 3:3:56:TYR:HD1 | 3:3:185:LYS:HZ1 | 1.52 | 0.54 |
| 20:3:311:CLA:HBC3 | 20:3:311:CLA:CMC | 2.37 | 0.54 |
| 4:4:81:GLU:O | 4:4:82:GLU:CG | 2.55 | 0.54 |
| 4:4:147:LEU:HD22 | 4:4:148:GLU:N | 2.22 | 0.54 |
| 20:4:318:CLA:HBA1 | 20:4:318:CLA:CED | 2.37 | 0.54 |
| 5:A:195:TRP:CZ2 | 20:A:810:CLA:HMA1 | 2.42 | 0.54 |
| 5:A:462:ILE:CD1 | 20:B:802:CLA:H72 | 2.37 | 0.54 |
| 6:B:124:TRP:CG | 6:B:129:LEU:HD13 | 2.42 | 0.54 |
| 6:B:292:ARG:HH22 | 6:B:297:ILE:HG13 | 1.72 | 0.54 |
| 6:B:681:ALA:O | 6:B:682:HIS:C | 2.50 | 0.54 |
| 12:H:21:TRP:H | 12:H:22:ASP:HA | 1.68 | 0.54 |
| 12:H:37:SER:C | 12:H:39:PHE:H | 2.15 | 0.54 |
| 16:L:36:TYR:O | 16:L:37:LEU:HB3 | 2.06 | 0.54 |
| 17:N:62:SER:HB2 | 17:N:66:ASP:OD1 | 2.07 | 0.54 |
| 19:Z:1:GLC:O2 | 19:Z:1:GLC:H5 | 2.06 | 0.54 |
| 2:2:41:LEU:O | 2:2:43:TRP:N | 2.41 | 0.54 |
| 2:2:103:GLY:O | 2:2:104:TRP:C | 2.49 | 0.54 |
| 4:4:103:ILE:HG13 | 20:4:302:CLA:CMD | 2.28 | 0.54 |
| 4:4:160:MET:CE | 4:4:163:PHE:CD2 | 2.89 | 0.54 |
| 5:A:581:CYS:HB2 | 5:A:590:CYS:O | 2.07 | 0.54 |
| 20:A:809:CLA:H51 | 22:J:102:BCR:H10C | 1.90 | 0.54 |
| 21:A:852:LMU:O3' | 21:A:852:LMU:H1B | 2.08 | 0.54 |
| 6:B:292:ARG:HH22 | 20:B:821:CLA:HED1 | 1.72 | 0.54 |
| 6:B:393:PHE:CD2 | 6:B:397:ASP:OD1 | 2.53 | 0.54 |
| 6:B:561:GLY:HA3 | 7:C:52:LYS:CB | 2.38 | 0.54 |
| 7:C:44:ARG:HH21 | 8:D:127:ARG:CB | 2.09 | 0.54 |
| 16:L:60:HIS:HD1 | 20:L:203:CLA:C19 | 2.19 | 0.54 |
| 17:N:61:LEU:HG | 17:N:64:ASP:HB2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:N:84:LYS:C | 17:N:85:TRP:CD1 | 2.85 | 0.54 |
| 2:2:128:ASN:CG | 14:J:3:ASP:HB3 | 2.31 | 0.54 |
| 20:2:312:CLA:CGA | 20:2:312:CLA:C3A | 2.86 | 0.54 |
| 3:3:66:MET:HG2 | 3:3:195:LEU:HD11 | 1.88 | 0.54 |
| 20:3:310:CLA:HHC | 20:3:310:CLA:HBB1 | 1.88 | 0.54 |
| 4:4:36:ASN:C | 4:4:39:TRP:CG | 2.86 | 0.54 |
| 5:A:157:GLY:O | 5:A:158:ILE:HB | 2.07 | 0.54 |
| 5:A:176:GLY:O | 5:A:180:PHE:HB2 | 2.08 | 0.54 |
| 5:A:612:VAL:O | 5:A:615:HIS:HB3 | 2.07 | 0.54 |
| 5:A:714:LEU:HD13 | 22:F:204:BCR:H393 | 1.89 | 0.54 |
| 5:A:747:TRP:CE3 | 22:A:845:BCR:C40 | 2.90 | 0.54 |
| 20:A:807:CLA:HBA2 | 20:A:809:CLA:C1 | 2.36 | 0.54 |
| 6:B:178:HIS:HE1 | 20:B:814:CLA:NC | 2.05 | 0.54 |
| 6:B:228:GLY:HA3 | 11:G:8:ILE:HB | 1.88 | 0.54 |
| 6:B:282:PHE:HE2 | 20:B:817:CLA:H3A | 1.72 | 0.54 |
| 20:B:803:CLA:HBA2 | 20:B:803:CLA:HED3 | 1.89 | 0.54 |
| 9:E:41:ARG:HG3 | 9:E:46:PHE:CZ | 2.42 | 0.54 |
| 12:H:25:GLY:HA3 | 12:H:27:ASP:CG | 2.32 | 0.54 |
| 19:U:1:GLC:O5 | 19:U:2:FRU:H12 | 2.07 | 0.54 |
| 1:1:29:LEU:O | 1:1:31:GLU:N | 2.41 | 0.54 |
| 2:2:37:ASP:OD2 | 3:3:41:ASP:CG | 2.50 | 0.54 |
| 2:2:85:GLN:OE1 | 2:2:86:GLU:N | 2.41 | 0.54 |
| 2:2:143:PHE:CD1 | 2:2:144:ASP:N | 2.76 | 0.54 |
| 20:2:312:CLA:O1A | 20:2:312:CLA:C3A | 2.44 | 0.54 |
| 3:3:94:ARG:HH12 | 3:3:98:ILE:CG2 | 2.19 | 0.54 |
| 4:4:81:GLU:O | 4:4:82:GLU:HB3 | 2.06 | 0.54 |
| 5:A:22:VAL:HB | 5:A:24:ARG:N | 2.22 | 0.54 |
| 5:A:158:ILE:HG23 | 5:A:163:GLN:NE2 | 2.23 | 0.54 |
| 5:A:378:SER:HG | 5:A:512:SER:HG | 1.54 | 0.54 |
| 5:A:678:PHE:O | 5:A:681:GLY:O | 2.25 | 0.54 |
| 6:B:124:TRP:CZ2 | 6:B:135:LEU:HD22 | 2.43 | 0.54 |
| 6:B:412:LEU:O | 6:B:415:LYS:HB3 | 2.07 | 0.54 |
| 6:B:555:TYR:O | 6:B:571:SER:HB2 | 2.07 | 0.54 |
| 20:B:836:CLA:HBC2 | 20:B:836:CLA:CHD | 2.32 | 0.54 |
| 10:F:40:LEU:HA | 10:F:42:ILE:CG1 | 2.34 | 0.54 |
| 20:K:101:CLA:HED1 | 20:K:102:CLA:CMB | 2.37 | 0.54 |
| 16:L:123:ARG:HB3 | 16:L:126:GLN:CG | 2.37 | 0.54 |
| 17:N:38:GLY:HA3 | 17:N:46:PHE:HD1 | 1.72 | 0.54 |
| 17:N:48:GLY:CA | 17:N:49:CYS:SG | 2.96 | 0.54 |
| 4:4:93:ILE:O | 4:4:96:ILE:HD12 | 2.08 | 0.54 |
| 4:4:107:GLN:HA | 20:4:301:CLA:H2A | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:213:LEU:O | 5:A:217:SER:HB2 | 2.07 | 0.54 |
| 5:A:308:ILE:CG2 | 5:A:309:LEU:N | 2.70 | 0.54 |
| 5:A:664:VAL:HG11 | 5:A:749:PHE:HA | 1.88 | 0.54 |
| 5:A:697:ARG:NH1 | 5:A:724:ALA:HB3 | 2.22 | 0.54 |
| 20:A:824:CLA:O1A | 20:A:824:CLA:C2 | 2.52 | 0.54 |
| 6:B:421:HIS:NE2 | 20:F:201:CLA:C1D | 2.69 | 0.54 |
| 6:B:732:LYS:HD3 | 6:B:734:GLY:CA | 2.33 | 0.54 |
| 20:B:838:CLA:CBC | 10:F:83:PHE:HZ | 2.20 | 0.54 |
| 10:F:78:ARG:O | 10:F:80:TRP:HD1 | 1.90 | 0.54 |
| 3:3:53:TRP:HA | 3:3:56:TYR:HD2 | 1.73 | 0.54 |
| 4:4:39:TRP:CA | 4:4:40:PHE:HD1 | 2.19 | 0.54 |
| 4:4:117:GLN:O | 4:4:122:LYS:O | 2.24 | 0.54 |
| 5:A:207:LEU:HB3 | 20:A:819:CLA:HBB2 | 1.89 | 0.54 |
| 5:A:295:TRP:HB2 | 5:A:298:ASP:OD2 | 2.08 | 0.54 |
| 5:A:425:THR:OG1 | 5:A:428:TYR:HE1 | 1.91 | 0.54 |
| 5:A:472:ARG:HH22 | 16:L:74:LEU:CD2 | 2.21 | 0.54 |
| 20:A:824:CLA:HBA2 | 20:A:836:CLA:CED | 2.32 | 0.54 |
| 6:B:231:ASN:OD1 | 11:G:5:SER:HB2 | 2.08 | 0.54 |
| 6:B:519:VAL:HG11 | 6:B:593:TYR:HB2 | 1.89 | 0.54 |
| 7:C:1:MET:HA | 7:C:2:SER:C | 2.33 | 0.54 |
| 7:C:6:LYS:HE2 | 8:D:137:ILE:HG12 | 1.90 | 0.54 |
| 8:D:102:ARG:NH2 | 8:D:109:VAL:O | 2.40 | 0.54 |
| 21:D:201:LMU:H42 | 21:D:201:LMU:O1' | 2.08 | 0.54 |
| 9:E:53:VAL:O | 9:E:55:VAL:N | 2.40 | 0.54 |
| 10:F:42:ILE:CG1 | 10:F:43:LYS:N | 2.66 | 0.54 |
| 11:G:48:ASP:N | 11:G:48:ASP:OD2 | 2.41 | 0.54 |
| 17:N:62:SER:CA | 17:N:66:ASP:H | 2.21 | 0.54 |
| 17:N:66:ASP:O | 17:N:67:LEU:CG | 2.50 | 0.54 |
| 4:4:33:ASP:CB | 4:4:34:PRO:HD3 | 2.37 | 0.54 |
| 5:A:170:GLY:C | 5:A:173:VAL:HG22 | 2.33 | 0.54 |
| 5:A:405:PHE:CD1 | 5:A:605:MET:HE1 | 2.43 | 0.54 |
| 6:B:289:LEU:O | 20:B:822:CLA:HAC1 | 2.08 | 0.54 |
| 6:B:707:LEU:HD11 | 6:B:711:VAL:HG21 | 1.90 | 0.54 |
| 10:F:144:LEU:CD1 | 10:F:149:LEU:HD13 | 2.37 | 0.54 |
| 11:G:43:HIS:HE1 | 11:G:45:GLU:HG2 | 1.72 | 0.54 |
| 20:H:109:CLA:CAC | 22:I:103:BCR:C2 | 2.86 | 0.54 |
| 21:K:107:LMU:H5' | 21:K:107:LMU:C2B | 2.37 | 0.54 |
| 3:3:106:TYR:HB3 | 3:3:107:TRP:HD1 | 1.71 | 0.54 |
| 5:A:88:ILE:CG2 | 5:A:89:ILE:N | 2.70 | 0.54 |
| 5:A:393:LEU:HD11 | 5:A:750:PHE:CD1 | 2.42 | 0.54 |
| 20:A:818:CLA:CGA | 20:A:827:CLA:HMD3 | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:171:ALA:O | 6:B:172:GLU:HB2 | 2.08 | 0.54 |
| 6:B:463:ILE:O | 6:B:464:GLN:CB | 2.54 | 0.54 |
| 6:B:654:HIS:HE1 | 20:B:850:CLA:NB | 2.05 | 0.54 |
| 20:B:809:CLA:C19 | 20:B:828:CLA:H141 | 2.38 | 0.54 |
| 9:E:36:VAL:HG22 | 9:E:52:VAL:CG2 | 2.38 | 0.54 |
| 10:F:104:TYR:O | 10:F:104:TYR:CD2 | 2.60 | 0.54 |
| 16:L:52:ARG:O | 16:L:56:VAL:HG23 | 2.08 | 0.54 |
| 16:L:96:SER:OG | 16:L:143:PHE:HD2 | 1.91 | 0.54 |
| 2:2:174:VAL:O | 2:2:178:TRP:HD1 | 1.85 | 0.54 |
| 2:2:188:PRO:O | 2:2:189:ILE:C | 2.50 | 0.54 |
| 4:4:90:LEU:N | 4:4:90:LEU:CD2 | 2.71 | 0.54 |
| 4:4:106:TRP:CE3 | 20:4:313:CLA:HMA2 | 2.43 | 0.54 |
| 20:4:318:CLA:CBA | 20:4:318:CLA:O2D | 2.56 | 0.54 |
| 5:A:24:ARG:C | 5:A:25:ASP:CG | 2.76 | 0.54 |
| 5:A:114:THR:O | 5:A:525:ASN:ND2 | 2.41 | 0.54 |
| 5:A:263:ALA:O | 5:A:264:GLU:HG3 | 2.08 | 0.54 |
| 5:A:327:ILE:O | 5:A:328:LYS:C | 2.50 | 0.54 |
| 5:A:425:THR:O | 5:A:427:ARG:NE | 2.40 | 0.54 |
| 5:A:439:ARG:HG2 | 5:A:562:PHE:CE2 | 2.42 | 0.54 |
| 5:A:491:TRP:HE1 | 20:A:834:CLA:C1 | 2.21 | 0.54 |
| 20:A:824:CLA:HAA2 | 20:A:825:CLA:CAD | 2.38 | 0.54 |
| 6:B:294:ASN:OD1 | 11:G:38:GLN:N | 2.41 | 0.54 |
| 20:B:824:CLA:HBC3 | 20:B:824:CLA:HMC1 | 1.88 | 0.54 |
| 8:D:27:PRO:O | 16:L:19:PHE:HZ | 1.91 | 0.54 |
| 11:G:45:GLU:C | 11:G:47:GLY:N | 2.54 | 0.54 |
| 14:J:26:LEU:C | 14:J:26:LEU:HD23 | 2.33 | 0.54 |
| 20:J:103:CLA:H143 | 20:J:103:CLA:HAA1 | 1.90 | 0.54 |
| 16:L:54:VAL:O | 16:L:58:LEU:HB2 | 2.07 | 0.54 |
| 20:L:202:CLA:O2D | 20:L:202:CLA:H2A | 2.06 | 0.54 |
| 21:R:102:LMU:O6' | 21:R:102:LMU:H3B | 2.08 | 0.54 |
| 3:3:49:ILE:HG13 | 3:3:52:LYS:HB2 | 1.90 | 0.53 |
| 4:4:95:PHE:CZ | 20:4:314:CLA:C1C | 2.91 | 0.53 |
| 21:4:319:LMU:H3' | 21:4:319:LMU:O5B | 2.07 | 0.53 |
| 5:A:158:ILE:HG23 | 5:A:163:GLN:HE22 | 1.73 | 0.53 |
| 5:A:193:LEU:O | 5:A:194:ALA:C | 2.50 | 0.53 |
| 5:A:653:LEU:HD23 | 20:B:850:CLA:HBC2 | 1.89 | 0.53 |
| 20:A:824:CLA:O2A | 20:A:836:CLA:O2D | 2.26 | 0.53 |
| 23:A:842:PQN:C13 | 22:F:203:BCR:H322 | 2.38 | 0.53 |
| 6:B:458:ILE:HG13 | 6:B:459:PHE:N | 2.22 | 0.53 |
| 20:B:803:CLA:H142 | 22:I:101:BCR:C4 | 2.37 | 0.53 |
| 22:B:844:BCR:H331 | 22:B:844:BCR:HC8 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:44:GLU:O | 4:4:46:VAL:N | 2.41 | 0.53 |
| 4:4:119:PRO:CG | 20:4:312:CLA:C2D | 2.73 | 0.53 |
| 5:A:233:LEU:O | 5:A:235:ALA:N | 2.36 | 0.53 |
| 5:A:466:THR:CG2 | 20:B:811:CLA:CHC | 2.74 | 0.53 |
| 5:A:558:LYS:NZ | 6:B:674:LEU:HD23 | 2.22 | 0.53 |
| 5:A:704:ILE:HA | 5:A:707:ILE:HG13 | 1.89 | 0.53 |
| 20:A:825:CLA:HBA1 | 20:A:825:CLA:CGD | 2.38 | 0.53 |
| 20:A:831:CLA:H171 | 20:A:835:CLA:C20 | 2.38 | 0.53 |
| 21:A:854:LMU:H82 | 21:A:854:LMU:C3 | 2.36 | 0.53 |
| 6:B:70:TRP:NE1 | 6:B:71:GLN:OE1 | 2.41 | 0.53 |
| 6:B:560:ASP:HB2 | 7:C:66:ARG:HE | 1.71 | 0.53 |
| 8:D:46:TYR:N | 8:D:46:TYR:CD2 | 2.76 | 0.53 |
| 9:E:37:LYS:HB2 | 9:E:49:VAL:HG22 | 1.90 | 0.53 |
| 15:K:43:ARG:NH1 | 15:K:43:ARG:CG | 2.52 | 0.53 |
| 20:K:102:CLA:CGA | 20:K:102:CLA:C3A | 2.84 | 0.53 |
| 16:L:14:LEU:CD2 | 16:L:21:GLY:O | 2.57 | 0.53 |
| 17:N:27:ALA:O | 17:N:28:ASN:C | 2.51 | 0.53 |
| 21:R:103:LMU:H62 | 21:R:103:LMU:C2 | 2.21 | 0.53 |
| 1:1:136:ASP:HB2 | 1:1:140:LEU:HB3 | 1.89 | 0.53 |
| 21:1:218:LMU:H3' | 21:1:218:LMU:C5B | 2.37 | 0.53 |
| 2:2:98:GLU:OE2 | 20:2:311:CLA:ND | 2.40 | 0.53 |
| 4:4:115:VAL:HG13 | 4:4:116:ASN:H | 1.72 | 0.53 |
| 4:4:147:LEU:CG | 4:4:148:GLU:N | 2.70 | 0.53 |
| 20:4:306:CLA:O1A | 20:4:306:CLA:C2 | 2.54 | 0.53 |
| 5:A:79:PHE:HE2 | 5:A:185:HIS:CD2 | 2.22 | 0.53 |
| 5:A:207:LEU:HA | 5:A:211:LEU:CG | 2.38 | 0.53 |
| 5:A:216:LEU:HD12 | 22:A:843:BCR:C35 | 2.38 | 0.53 |
| 5:A:246:HIS:O | 5:A:248:PHE:CD2 | 2.56 | 0.53 |
| 5:A:331:LEU:CD2 | 5:A:331:LEU:C | 2.80 | 0.53 |
| 5:A:497:ALA:HA | 5:A:510:SER:OG | 2.08 | 0.53 |
| 20:A:809:CLA:HBA2 | 20:A:809:CLA:CBD | 2.38 | 0.53 |
| 20:A:815:CLA:CBB | 22:A:843:BCR:H352 | 2.38 | 0.53 |
| 20:A:830:CLA:H52 | 22:B:847:BCR:C34 | 2.36 | 0.53 |
| 20:A:849:CLA:HBB2 | 20:A:850:CLA:HED1 | 1.91 | 0.53 |
| 6:B:400:PRO:HG2 | 8:D:141:VAL:C | 2.34 | 0.53 |
| 6:B:475:ASP:CA | 6:B:480:SER:HA | 2.38 | 0.53 |
| 20:B:836:CLA:O1D | 20:B:836:CLA:C2A | 2.53 | 0.53 |
| 8:D:28:ILE:CG2 | 8:D:67:ILE:HG13 | 2.37 | 0.53 |
| 9:E:44:TYR:CD2 | 9:E:45:TRP:HE3 | 2.25 | 0.53 |
| 10:F:153:ASN:ND2 | 10:F:153:ASN:O | 2.41 | 0.53 |
| 21:R:106:LMU:O6B | 21:R:106:LMU:C6' | 2.57 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:128:ASN:ND2 | 14:J:4:PHE:H | 2.06 | 0.53 |
| 5:A:698:GLY:HA3 | 6:B:570:ILE:HG21 | 1.91 | 0.53 |
| 21:A:854:LMU:C9 | 21:A:854:LMU:C4 | 2.86 | 0.53 |
| 6:B:574:ASP:OD2 | 6:B:706:ARG:NE | 2.42 | 0.53 |
| 20:B:832:CLA:H51 | 22:F:204:BCR:C40 | 2.38 | 0.53 |
| 20:H:109:CLA:CHD | 22:I:103:BCR:HC22 | 2.38 | 0.53 |
| 22:I:101:BCR:H272 | 22:I:103:BCR:H352 | 1.89 | 0.53 |
| 16:L:41:PRO:HG3 | 16:L:52:ARG:HD3 | 1.91 | 0.53 |
| 17:N:58:VAL:C | 17:N:60:PHE:H | 2.16 | 0.53 |
| 17:N:59:PRO:CA | 17:N:66:ASP:OD1 | 2.57 | 0.53 |
| 17:N:80:ASN:O | 17:N:82:PHE:HD2 | 1.92 | 0.53 |
| 2:2:68:LEU:O | 2:2:70:LYS:N | 2.42 | 0.53 |
| 4:4:150:LYS:O | 4:4:150:LYS:HG2 | 2.05 | 0.53 |
| 5:A:123:VAL:HB | 5:A:129:GLN:OE1 | 2.09 | 0.53 |
| 5:A:472:ARG:O | 5:A:474:GLN:HG3 | 2.09 | 0.53 |
| 20:A:818:CLA:O1A | 20:A:827:CLA:HMD1 | 2.08 | 0.53 |
| 20:A:830:CLA:HAA1 | 22:B:801:BCR:C14 | 2.39 | 0.53 |
| 6:B:20:ARG:HH11 | 6:B:20:ARG:CG | 2.21 | 0.53 |
| 6:B:102:GLU:O | 6:B:103:ALA:C | 2.51 | 0.53 |
| 6:B:117:TYR:O | 6:B:367:THR:HG23 | 2.09 | 0.53 |
| 6:B:696:LYS:HD2 | 7:C:81:TYR:HA | 1.90 | 0.53 |
| 20:B:810:CLA:HMC3 | 22:B:847:BCR:C28 | 2.38 | 0.53 |
| 20:B:827:CLA:H122 | 22:B:846:BCR:H14C | 1.91 | 0.53 |
| 7:C:5:VAL:CB | 7:C:65:VAL:HG22 | 2.37 | 0.53 |
| 7:C:12:ILE:HG21 | 7:C:39:ILE:C | 2.34 | 0.53 |
| 9:E:87:VAL:O | 9:E:87:VAL:HG12 | 2.07 | 0.53 |
| 10:F:22:LEU:HB3 | 10:F:23:LYS:NZ | 2.24 | 0.53 |
| 18:R:30:UNK:C | 18:R:32:UNK:N | 2.72 | 0.53 |
| 1:1:27:LEU:HD12 | 1:1:28:GLY:H | 1.72 | 0.53 |
| 21:1:218:LMU:H6'2 | 21:1:218:LMU:O2' | 2.09 | 0.53 |
| 21:1:218:LMU:O5B | 21:1:218:LMU:C3' | 2.56 | 0.53 |
| 3:3:56:TYR:O | 3:3:60:ILE:HD12 | 2.07 | 0.53 |
| 4:4:168:ILE:O | 4:4:168:ILE:HG13 | 2.09 | 0.53 |
| 20:4:304:CLA:H2 | 20:4:304:CLA:CED | 2.39 | 0.53 |
| 5:A:281:LEU:CD1 | 20:A:816:CLA:HED2 | 2.39 | 0.53 |
| 5:A:578:ARG:HB2 | 5:A:578:ARG:NH1 | 2.23 | 0.53 |
| 5:A:581:CYS:CB | 5:A:590:CYS:O | 2.56 | 0.53 |
| 20:A:808:CLA:HMB2 | 20:A:809:CLA:H11 | 1.89 | 0.53 |
| 20:A:809:CLA:HBA2 | 20:A:809:CLA:CHA | 2.37 | 0.53 |
| 6:B:189:ALA:HB1 | 20:B:829:CLA:H203 | 1.90 | 0.53 |
| 6:B:536:LYS:O | 6:B:537:GLY:C | 2.51 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:615:TYR:HD1 | 6:B:615:TYR:N | 2.06 | 0.53 |
| 20:B:835:CLA:CMB | 22:B:846:BCR:H391 | 2.38 | 0.53 |
| 7:C:11:CYS:C | 7:C:13:GLY:H | 2.17 | 0.53 |
| 8:D:94:TYR:O | 8:D:95:LYS:CB | 2.57 | 0.53 |
| 8:D:124:ASN:CB | 8:D:125:PRO:CD | 2.85 | 0.53 |
| 11:G:18:LEU:C | 11:G:21:PHE:H | 2.17 | 0.53 |
| 11:G:44:PHE:C | 11:G:47:GLY:N | 2.65 | 0.53 |
| 2:2:51:HIS:HA | 2:2:54:TRP:HB2 | 1.91 | 0.53 |
| 5:A:118:PRO:HB3 | 5:A:150:PHE:CE2 | 2.43 | 0.53 |
| 5:A:648:THR:CG2 | 5:A:651:GLY:H | 2.16 | 0.53 |
| 20:A:832:CLA:CAD | 20:A:833:CLA:HAC1 | 2.37 | 0.53 |
| 6:B:25:ILE:HG22 | 22:L:209:BCR:H282 | 1.89 | 0.53 |
| 6:B:224:PRO:O | 6:B:226:LEU:N | 2.42 | 0.53 |
| 6:B:293:THR:O | 6:B:294:ASN:ND2 | 2.41 | 0.53 |
| 6:B:310:PRO:HB2 | 6:B:311:PRO:HD2 | 1.91 | 0.53 |
| 21:B:804:LMU:C10 | 21:B:804:LMU:H62 | 2.38 | 0.53 |
| 21:B:805:LMU:C1B | 21:B:805:LMU:H3O2 | 2.22 | 0.53 |
| 20:B:838:CLA:CBC | 10:F:83:PHE:CZ | 2.83 | 0.53 |
| 7:C:59:PRO:HB3 | 7:C:61:ASP:OD1 | 2.08 | 0.53 |
| 8:D:31:GLY:HA3 | 16:L:23:LEU:CD2 | 2.39 | 0.53 |
| 11:G:60:SER:HG | 11:G:63:PRO:HB2 | 1.71 | 0.53 |
| 11:G:60:SER:CA | 11:G:63:PRO:HD2 | 2.31 | 0.53 |
| 12:H:63:SER:O | 12:H:67:TYR:HB2 | 2.08 | 0.53 |
| 13:I:19:VAL:O | 13:I:23:SER:N | 2.42 | 0.53 |
| 2:2:51:HIS:C | 2:2:54:TRP:HB2 | 2.34 | 0.53 |
| 2:2:203:THR:O | 2:2:204:ILE:HG12 | 2.09 | 0.53 |
| 3:3:92:TRP:CA | 3:3:95:THR:HG21 | 2.20 | 0.53 |
| 4:4:40:PHE:CD2 | 4:4:43:ALA:HB2 | 2.43 | 0.53 |
| 4:4:98:SER:O | 4:4:102:GLU:HG3 | 2.09 | 0.53 |
| 4:4:169:GLN:HE22 | 20:4:304:CLA:HHD | 1.69 | 0.53 |
| 20:4:317:CLA:HHD | 20:4:317:CLA:HBC2 | 1.90 | 0.53 |
| 5:A:26:PRO:HB2 | 5:A:27:ILE:HB | 1.90 | 0.53 |
| 5:A:124:TRP:HA | 5:A:124:TRP:CE3 | 2.44 | 0.53 |
| 5:A:392:GLN:CG | 5:A:392:GLN:O | 2.57 | 0.53 |
| 5:A:397:THR:HB | 5:A:613:ILE:HD11 | 1.91 | 0.53 |
| 20:A:804:CLA:HBA2 | 20:A:811:CLA:C6 | 2.38 | 0.53 |
| 20:A:819:CLA:C2C | 20:A:825:CLA:C17 | 2.86 | 0.53 |
| 20:B:835:CLA:CMB | 22:B:846:BCR:C29 | 2.61 | 0.53 |
| 8:D:124:ASN:HB3 | 8:D:125:PRO:CD | 2.33 | 0.53 |
| 17:N:70:GLU:CB | 17:N:72:LYS:H | 2.18 | 0.53 |
| 3:3:64:TYR:CB | 20:3:310:CLA:H42 | 2.36 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:80:LYS:HB2 | 20:3:305:CLA:C3D | 2.39 | 0.53 |
| 5:A:46:LYS:HG3 | 5:A:48:PRO:HB2 | 1.91 | 0.53 |
| 5:A:174:PHE:O | 5:A:175:ALA:CB | 2.56 | 0.53 |
| 5:A:185:HIS:O | 5:A:188:LYS:N | 2.42 | 0.53 |
| 5:A:309:LEU:HD23 | 5:A:309:LEU:C | 2.34 | 0.53 |
| 5:A:368:LEU:HD21 | 20:A:818:CLA:H91 | 1.90 | 0.53 |
| 5:A:435:VAL:HA | 5:A:438:HIS:CE1 | 2.44 | 0.53 |
| 6:B:154:TRP:CD1 | 6:B:154:TRP:C | 2.86 | 0.53 |
| 6:B:167:TRP:HB2 | 11:G:41:MET:HE3 | 1.89 | 0.53 |
| 6:B:708:VAL:O | 6:B:710:LEU:O | 2.27 | 0.53 |
| 6:B:715:VAL:O | 6:B:719:PHE:HB2 | 2.09 | 0.53 |
| 23:B:843:PQN:H192 | 22:B:847:BCR:C10 | 2.33 | 0.53 |
| 7:C:17:CYS:SG | 7:C:18:VAL:N | 2.81 | 0.53 |
| 9:E:35:LYS:CE | 9:E:89:GLU:OE2 | 2.57 | 0.53 |
| 11:G:33:LYS:HE3 | 11:G:33:LYS:CA | 2.27 | 0.53 |
| 21:G:102:LMU:C6B | 21:G:102:LMU:C3' | 2.84 | 0.53 |
| 21:H:104:LMU:O5' | 21:H:104:LMU:C2 | 2.55 | 0.53 |
| 15:K:42:ALA:C | 15:K:43:ARG:CD | 2.80 | 0.53 |
| 18:R:5:UNK:O | 18:R:6:UNK:CB | 2.57 | 0.53 |
| 2:2:110:TRP:CD2 | 20:2:310:CLA:HED1 | 2.44 | 0.53 |
| 2:2:163:GLU:HG2 | 20:2:307:CLA:C3C | 2.38 | 0.53 |
| 20:2:302:CLA:H2A | 20:2:302:CLA:CGD | 2.39 | 0.53 |
| 20:3:307:CLA:CMC | 20:3:307:CLA:CBC | 2.85 | 0.53 |
| 4:4:194:VAL:CB | 4:4:195:GLN:C | 2.77 | 0.53 |
| 5:A:87:SER:O | 5:A:88:ILE:HB | 2.08 | 0.53 |
| 5:A:114:THR:HG1 | 5:A:525:ASN:HB2 | 1.74 | 0.53 |
| 5:A:448:TRP:CD1 | 20:A:830:CLA:HED2 | 2.43 | 0.53 |
| 5:A:703:LEU:O | 5:A:707:ILE:HG12 | 2.09 | 0.53 |
| 5:A:713:LYS:HZ1 | 20:F:201:CLA:C4 | 2.21 | 0.53 |
| 20:B:822:CLA:HBA2 | 20:B:823:CLA:O1A | 2.09 | 0.53 |
| 20:B:830:CLA:CBC | 20:B:830:CLA:CMC | 2.86 | 0.53 |
| 20:J:103:CLA:H2 | 20:J:103:CLA:C16 | 2.39 | 0.53 |
| 17:N:50:GLN:C | 17:N:51:ASP:O | 2.52 | 0.53 |
| 18:R:26:UNK:O | 18:R:28:UNK:CB | 2.57 | 0.53 |
| 20:2:314:CLA:CAD | 20:2:314:CLA:HED3 | 2.38 | 0.52 |
| 21:2:318:LMU:H22 | 21:2:318:LMU:H2' | 1.91 | 0.52 |
| 3:3:132:TRP:CZ3 | 3:3:155:GLU:OE1 | 2.57 | 0.52 |
| 4:4:37:LEU:HA | 4:4:39:TRP:CD1 | 2.44 | 0.52 |
| 5:A:132:LEU:HD11 | 5:A:674:ALA:CB | 2.39 | 0.52 |
| 5:A:316:MET:HA | 5:A:317:TYR:CD1 | 2.39 | 0.52 |
| 5:A:710:ALA:HB1 | 20:B:806:CLA:HED2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:141:PHE:O | 6:B:143:LEU:N | 2.42 | 0.52 |
| 6:B:664:LEU:O | 6:B:667:TRP:CZ3 | 2.61 | 0.52 |
| 20:B:807:CLA:C4C | 22:I:103:BCR:H401 | 2.39 | 0.52 |
| 20:B:834:CLA:CGA | 20:B:835:CLA:HMB3 | 2.39 | 0.52 |
| 8:D:37:LEU:O | 8:D:39:LYS:N | 2.42 | 0.52 |
| 11:G:19:GLY:C | 11:G:21:PHE:H | 2.15 | 0.52 |
| 12:H:25:GLY:CA | 12:H:27:ASP:N | 2.66 | 0.52 |
| 16:L:62:PHE:HB2 | 16:L:154:ALA:HB2 | 1.90 | 0.52 |
| 19:W:1:GLC:C1 | 19:W:2:FRU:C4 | 2.86 | 0.52 |
| 1:1:27:LEU:HD11 | 6:B:314:ARG:NE | 2.17 | 0.52 |
| 20:1:205:CLA:CAB | 20:1:211:CLA:CHD | 2.88 | 0.52 |
| 20:1:206:CLA:HHD | 20:1:206:CLA:HBC3 | 1.88 | 0.52 |
| 2:2:54:TRP:NE1 | 20:2:310:CLA:O1D | 2.42 | 0.52 |
| 2:2:68:LEU:O | 2:2:69:THR:C | 2.52 | 0.52 |
| 3:3:92:TRP:O | 3:3:97:PHE:CD1 | 2.59 | 0.52 |
| 4:4:127:PRO:O | 4:4:129:GLY:N | 2.35 | 0.52 |
| 4:4:142:ASN:HA | 4:4:150:LYS:HZ1 | 1.72 | 0.52 |
| 5:A:338:PHE:O | 5:A:339:THR:O | 2.27 | 0.52 |
| 5:A:408:VAL:HG21 | 5:A:602:LEU:HG | 1.90 | 0.52 |
| 5:A:651:GLY:O | 5:A:655:ASP:N | 2.42 | 0.52 |
| 5:A:696:GLY:HA3 | 6:B:569:ASP:HB2 | 1.92 | 0.52 |
| 20:A:819:CLA:CAA | 20:A:823:CLA:HBB2 | 2.39 | 0.52 |
| 6:B:140:ILE:HD13 | 6:B:140:ILE:N | 2.18 | 0.52 |
| 6:B:247:THR:CG2 | 6:B:250:ALA:HB3 | 2.39 | 0.52 |
| 23:B:843:PQN:C16 | 22:B:847:BCR:H333 | 2.08 | 0.52 |
| 8:D:39:LYS:NZ | 8:D:43:GLU:OE2 | 2.41 | 0.52 |
| 4:4:183:GLN:HG2 | 4:4:183:GLN:O | 2.09 | 0.52 |
| 5:A:309:LEU:O | 5:A:310:PHE:CB | 2.56 | 0.52 |
| 5:A:443:ILE:HG12 | 5:A:558:LYS:HB2 | 1.91 | 0.52 |
| 5:A:555:ILE:HG21 | 20:B:803:CLA:CMD | 2.39 | 0.52 |
| 5:A:571:ASP:OD2 | 8:D:88:THR:HG21 | 2.09 | 0.52 |
| 5:A:662:SER:HA | 5:A:665:ILE:HD11 | 1.92 | 0.52 |
| 6:B:50:HIS:HB3 | 20:B:808:CLA:CHB | 2.39 | 0.52 |
| 6:B:87:ILE:O | 6:B:121:TYR:HE2 | 1.91 | 0.52 |
| 6:B:628:SER:O | 6:B:631:LEU:HD23 | 2.10 | 0.52 |
| 20:B:809:CLA:H41 | 25:B:848:LMG:H321 | 1.90 | 0.52 |
| 11:G:96:SER:C | 11:G:98:PHE:H | 2.16 | 0.52 |
| 12:H:25:GLY:CA | 12:H:27:ASP:OD2 | 2.56 | 0.52 |
| 17:N:42:PHE:H | 17:N:43:PRO:HD2 | 1.74 | 0.52 |
| 20:1:207:CLA:HBA2 | 20:1:207:CLA:CMA | 2.40 | 0.52 |
| 3:3:74:ALA:HA | 20:3:306:CLA:C1D | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:4:303:CLA:H2A | 20:4:303:CLA:O1D | 2.09 | 0.52 |
| 20:4:310:CLA:CBA | 20:4:310:CLA:CBD | 2.85 | 0.52 |
| 20:4:310:CLA:HED3 | 20:4:310:CLA:C2A | 2.38 | 0.52 |
| 5:A:331:LEU:CD2 | 5:A:343:HIS:C | 2.77 | 0.52 |
| 5:A:661:ALA:O | 5:A:665:ILE:HG13 | 2.08 | 0.52 |
| 5:A:680:LEU:HD21 | 6:B:617:MET:CE | 2.40 | 0.52 |
| 6:B:475:ASP:HA | 6:B:480:SER:O | 2.09 | 0.52 |
| 20:B:834:CLA:C1D | 20:B:835:CLA:CBB | 2.87 | 0.52 |
| 8:D:101:TYR:CD1 | 8:D:114:PRO:HD3 | 2.44 | 0.52 |
| 9:E:61:THR:HG22 | 9:E:62:ARG:N | 2.20 | 0.52 |
| 11:G:19:GLY:O | 11:G:22:VAL:N | 2.43 | 0.52 |
| 16:L:30:SER:C | 16:L:32:LEU:N | 2.68 | 0.52 |
| 16:L:46:ALA:HB2 | 16:L:52:ARG:NH2 | 2.24 | 0.52 |
| 21:1:217:LMU:H92 | 21:G:103:LMU:O3' | 2.08 | 0.52 |
| 2:2:168:ARG:HA | 2:2:168:ARG:NE | 2.24 | 0.52 |
| 3:3:60:ILE:HA | 3:3:63:ARG:HD2 | 1.92 | 0.52 |
| 4:4:104:ARG:HA | 4:4:107:GLN:CB | 2.38 | 0.52 |
| 4:4:118:ASP:HA | 4:4:122:LYS:CA | 2.39 | 0.52 |
| 4:4:136:GLY:O | 4:4:137:ILE:HB | 2.09 | 0.52 |
| 4:4:161:LEU:O | 4:4:162:ALA:CB | 2.57 | 0.52 |
| 5:A:182:GLY:C | 20:A:811:CLA:HAC1 | 2.35 | 0.52 |
| 5:A:312:ILE:O | 5:A:313:ALA:CB | 2.57 | 0.52 |
| 5:A:701:GLN:O | 5:A:704:ILE:N | 2.42 | 0.52 |
| 20:A:826:CLA:C1A | 20:A:826:CLA:CGA | 2.88 | 0.52 |
| 6:B:289:LEU:O | 20:B:822:CLA:HMC1 | 2.09 | 0.52 |
| 6:B:398:TYR:CD1 | 6:B:542:ARG:NH2 | 2.77 | 0.52 |
| 20:B:820:CLA:HBD | 20:B:820:CLA:HBA1 | 1.92 | 0.52 |
| 20:B:837:CLA:O2D | 20:B:837:CLA:OBD | 2.27 | 0.52 |
| 20:B:841:CLA:H151 | 16:L:98:CYS:SG | 2.49 | 0.52 |
| 18:R:41:UNK:CA | 18:R:42:UNK:CB | 2.88 | 0.52 |
| 2:2:50:VAL:O | 2:2:50:VAL:CG1 | 2.58 | 0.52 |
| 3:3:49:ILE:CG1 | 3:3:52:LYS:HB2 | 2.39 | 0.52 |
| 5:A:361:ASN:C | 5:A:361:ASN:ND2 | 2.67 | 0.52 |
| 5:A:425:THR:HG1 | 5:A:428:TYR:HE1 | 1.56 | 0.52 |
| 20:A:814:CLA:C2D | 20:A:840:CLA:HBC3 | 2.40 | 0.52 |
| 20:A:832:CLA:CBC | 20:A:832:CLA:CMC | 2.88 | 0.52 |
| 6:B:186:SER:C | 6:B:187:SER:O | 2.52 | 0.52 |
| 6:B:437:TYR:CG | 6:B:616:LEU:HD22 | 2.44 | 0.52 |
| 6:B:630:GLN:HE21 | 6:B:731:GLY:HA3 | 1.75 | 0.52 |
| 20:B:803:CLA:H142 | 22:I:101:BCR:HC42 | 1.92 | 0.52 |
| 20:B:825:CLA:C8 | 20:B:827:CLA:H43 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:D:28:ILE:HG21 | 8:D:67:ILE:HG13 | 1.91 | 0.52 |
| 8:D:69:ARG:O | 8:D:70:GLU:CB | 2.57 | 0.52 |
| 21:K:107:LMU:H71 | 21:K:107:LMU:C1 | 2.40 | 0.52 |
| 16:L:95:LEU:HA | 16:L:98:CYS:CB | 2.39 | 0.52 |
| 20:2:302:CLA:O1A | 20:2:302:CLA:NA | 2.43 | 0.52 |
| 20:3:310:CLA:CHC | 20:3:310:CLA:CBB | 2.82 | 0.52 |
| 4:4:160:MET:HE1 | 20:4:306:CLA:CAB | 2.37 | 0.52 |
| 20:4:310:CLA:HED3 | 20:4:310:CLA:C1A | 2.39 | 0.52 |
| 5:A:42:ARG:HA | 5:A:44:ILE:HG12 | 1.92 | 0.52 |
| 5:A:81:ALA:CA | 20:A:804:CLA:HMA3 | 2.39 | 0.52 |
| 20:A:819:CLA:C1C | 20:A:825:CLA:H171 | 2.40 | 0.52 |
| 6:B:124:TRP:CD1 | 6:B:129:LEU:HD13 | 2.45 | 0.52 |
| 6:B:175:LEU:HA | 6:B:178:HIS:HB2 | 1.91 | 0.52 |
| 6:B:419:ILE:C | 6:B:420:SER:OG | 2.53 | 0.52 |
| 20:B:817:CLA:CBC | 20:B:817:CLA:CHD | 2.88 | 0.52 |
| 20:B:839:CLA:HBC2 | 20:F:201:CLA:HMC1 | 1.91 | 0.52 |
| 8:D:32:SER:N | 16:L:23:LEU:HG | 2.19 | 0.52 |
| 8:D:96:ILE:O | 8:D:97:LYS:HB2 | 2.08 | 0.52 |
| 12:H:65:LEU:HD11 | 16:L:90:GLY:HA2 | 1.92 | 0.52 |
| 19:O:1:GLC:C2 | 19:O:2:FRU:O5 | 2.57 | 0.52 |
| 4:4:36:ASN:O | 4:4:39:TRP:CG | 2.62 | 0.52 |
| 4:4:104:ARG:CA | 4:4:107:GLN:HB2 | 2.39 | 0.52 |
| 5:A:157:GLY:HA2 | 5:A:229:ILE:HG21 | 1.91 | 0.52 |
| 5:A:205:HIS:ND1 | 20:A:813:CLA:HMC2 | 2.25 | 0.52 |
| 5:A:302:HIS:HE1 | 20:A:818:CLA:CHB | 2.23 | 0.52 |
| 5:A:368:LEU:CD2 | 20:A:818:CLA:H91 | 2.36 | 0.52 |
| 5:A:750:PHE:O | 5:A:752:ALA:N | 2.42 | 0.52 |
| 20:A:849:CLA:H192 | 20:B:802:CLA:C2B | 2.40 | 0.52 |
| 6:B:272:ASP:C | 6:B:274:ALA:H | 2.18 | 0.52 |
| 6:B:557:PHE:HE2 | 7:C:66:ARG:NE | 2.05 | 0.52 |
| 6:B:595:HIS:CE1 | 6:B:599:ILE:HD11 | 2.45 | 0.52 |
| 6:B:625:TRP:HE3 | 6:B:626:LEU:N | 2.08 | 0.52 |
| 6:B:633:ASN:ND2 | 6:B:636:THR:CB | 2.72 | 0.52 |
| 6:B:707:LEU:CD1 | 6:B:711:VAL:HG21 | 2.40 | 0.52 |
| 20:B:829:CLA:H62 | 22:B:845:BCR:H321 | 1.91 | 0.52 |
| 9:E:39:LEU:H | 9:E:40:ARG:HH11 | 1.54 | 0.52 |
| 17:N:51:ASP:C | 17:N:52:LEU:HD22 | 2.34 | 0.52 |
| 1:1:179:THR:HG21 | 4:4:87:SER:O | 2.10 | 0.52 |
| 20:1:204:CLA:CMC | 20:1:204:CLA:CBC | 2.84 | 0.52 |
| 20:3:307:CLA:HBC3 | 20:3:307:CLA:HMC2 | 1.92 | 0.52 |
| 20:4:310:CLA:CBA | 20:4:310:CLA:O1D | 2.53 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:162:LEU:C | 5:A:165:TYR:HB3 | 2.35 | 0.52 |
| 5:A:223:VAL:O | 5:A:228:PRO:HD3 | 2.09 | 0.52 |
| 5:A:261:SER:O | 5:A:262:PHE:CD2 | 2.63 | 0.52 |
| 5:A:360:ILE:HD11 | 20:A:823:CLA:HMB2 | 1.91 | 0.52 |
| 5:A:370:ILE:HD13 | 20:A:824:CLA:CAD | 2.40 | 0.52 |
| 20:A:837:CLA:H41 | 20:B:806:CLA:H202 | 1.92 | 0.52 |
| 6:B:194:LEU:O | 6:B:198:ALA:HB3 | 2.10 | 0.52 |
| 6:B:199:ILE:HG22 | 6:B:203:ARG:CZ | 2.40 | 0.52 |
| 6:B:322:LEU:O | 6:B:326:ILE:HG22 | 2.10 | 0.52 |
| 6:B:442:VAL:HG21 | 20:B:833:CLA:CAC | 2.33 | 0.52 |
| 6:B:724:PHE:CD1 | 20:B:850:CLA:HMD1 | 2.45 | 0.52 |
| 20:B:808:CLA:H43 | 22:B:844:BCR:C33 | 2.39 | 0.52 |
| 14:J:26:LEU:HA | 14:J:29:ILE:HG22 | 1.91 | 0.52 |
| 20:L:201:CLA:H92 | 20:L:204:CLA:H2 | 1.92 | 0.52 |
| 2:2:54:TRP:CZ2 | 2:2:109:ARG:CG | 2.93 | 0.52 |
| 3:3:52:LYS:C | 3:3:56:TYR:HD2 | 2.10 | 0.52 |
| 3:3:92:TRP:O | 3:3:95:THR:OG1 | 2.28 | 0.52 |
| 3:3:104:TYR:CB | 3:3:106:TYR:H | 2.22 | 0.52 |
| 4:4:122:LYS:HB2 | 4:4:143:PHE:HB2 | 1.81 | 0.52 |
| 21:4:321:LMU:O2' | 21:4:321:LMU:C2 | 2.55 | 0.52 |
| 21:4:321:LMU:O2B | 21:4:321:LMU:C5' | 2.58 | 0.52 |
| 5:A:370:ILE:CD1 | 20:A:824:CLA:CAD | 2.88 | 0.52 |
| 5:A:539:PHE:HD2 | 5:A:539:PHE:O | 1.93 | 0.52 |
| 5:A:591:GLN:OE1 | 5:A:600:LEU:HD21 | 2.10 | 0.52 |
| 5:A:684:PHE:HB2 | 20:A:850:CLA:HAA1 | 1.91 | 0.52 |
| 20:A:831:CLA:OBD | 20:H:108:CLA:HMD3 | 2.09 | 0.52 |
| 20:A:850:CLA:HED1 | 20:B:850:CLA:H61 | 1.92 | 0.52 |
| 6:B:135:LEU:O | 6:B:135:LEU:HD12 | 2.10 | 0.52 |
| 6:B:295:PHE:O | 11:G:33:LYS:HB2 | 2.09 | 0.52 |
| 6:B:369:ALA:O | 6:B:725:LEU:CD1 | 2.57 | 0.52 |
| 6:B:391:PRO:HB3 | 6:B:538:ALA:CA | 2.32 | 0.52 |
| 6:B:696:LYS:HG2 | 7:C:80:ALA:C | 2.35 | 0.52 |
| 21:B:804:LMU:C6' | 21:B:804:LMU:H1B | 2.40 | 0.52 |
| 20:B:829:CLA:C14 | 22:B:845:BCR:H10C | 2.32 | 0.52 |
| 9:E:69:PHE:HD2 | 9:E:71:LYS:H | 1.54 | 0.52 |
| 10:F:73:VAL:HG11 | 10:F:83:PHE:HB2 | 1.90 | 0.52 |
| 14:J:2:ARG:HH12 | 14:J:8:LEU:CD1 | 2.17 | 0.52 |
| 20:J:103:CLA:O2D | 20:J:103:CLA:H2A | 2.10 | 0.52 |
| 16:L:8:TYR:CE1 | 16:L:11:ILE:HG23 | 2.42 | 0.52 |
| 3:3:153:SER:OG | 3:3:154:GLY:N | 2.43 | 0.51 |
| 3:3:189:LEU:C | 3:3:191:MET:H | 2.18 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:194:ILE:CG1 | 20:3:303:CLA:HMC2 | 2.39 | 0.51 |
| 21:3:318:LMU:H3B | 19:S:2:FRU:O4 | 2.10 | 0.51 |
| 4:4:30:LEU:O | 4:4:32:GLU:N | 2.43 | 0.51 |
| 5:A:92:TRP:O | 5:A:93:LEU:HB2 | 2.10 | 0.51 |
| 5:A:281:LEU:HB2 | 5:A:301:HIS:HD2 | 1.74 | 0.51 |
| 5:A:374:GLN:O | 5:A:377:TYR:CD2 | 2.63 | 0.51 |
| 5:A:475:ASP:HB3 | 20:A:831:CLA:HED3 | 1.91 | 0.51 |
| 5:A:629:ASN:HD21 | 5:A:633:VAL:CG2 | 2.22 | 0.51 |
| 6:B:528:HIS:HE1 | 20:B:839:CLA:NB | 2.07 | 0.51 |
| 6:B:597:LYS:O | 6:B:598:HIS:HB2 | 2.09 | 0.51 |
| 6:B:615:TYR:N | 6:B:615:TYR:CD1 | 2.77 | 0.51 |
| 20:B:803:CLA:H111 | 22:B:847:BCR:C35 | 2.40 | 0.51 |
| 20:B:806:CLA:H52 | 20:B:806:CLA:C4C | 2.40 | 0.51 |
| 14:J:22:LEU:O | 14:J:23:ALA:C | 2.53 | 0.51 |
| 17:N:61:LEU:HD21 | 17:N:63:ASP:O | 2.09 | 0.51 |
| 4:4:103:ILE:O | 4:4:107:GLN:HB2 | 2.10 | 0.51 |
| 5:A:28:LYS:CB | 5:A:28:LYS:HZ2 | 2.10 | 0.51 |
| 5:A:165:TYR:CD2 | 5:A:165:TYR:O | 2.63 | 0.51 |
| 5:A:464:ASN:H | 5:A:464:ASN:ND2 | 2.08 | 0.51 |
| 5:A:681:GLY:C | 5:A:683:HIS:H | 2.16 | 0.51 |
| 5:A:697:ARG:C | 5:A:699:TYR:N | 2.67 | 0.51 |
| 20:A:806:CLA:H51 | 20:A:828:CLA:C4C | 2.40 | 0.51 |
| 6:B:124:TRP:C | 6:B:124:TRP:HD1 | 2.18 | 0.51 |
| 6:B:130:ARG:HH11 | 6:B:130:ARG:CG | 2.22 | 0.51 |
| 6:B:427:LEU:C | 20:B:832:CLA:HED2 | 2.36 | 0.51 |
| 6:B:451:LYS:HD2 | 20:B:833:CLA:O2D | 2.10 | 0.51 |
| 6:B:542:ARG:HH12 | 8:D:141:VAL:HA | 1.75 | 0.51 |
| 6:B:587:ILE:O | 6:B:587:ILE:CG2 | 2.58 | 0.51 |
| 6:B:652:PHE:O | 6:B:656:VAL:HG23 | 2.09 | 0.51 |
| 20:B:803:CLA:H111 | 22:B:847:BCR:H351 | 1.92 | 0.51 |
| 8:D:117:GLY:O | 8:D:118:VAL:CG2 | 2.48 | 0.51 |
| 16:L:163:LEU:O | 16:L:165:TYR:HB3 | 2.09 | 0.51 |
| 17:N:58:VAL:C | 17:N:60:PHE:N | 2.67 | 0.51 |
| 1:1:29:LEU:O | 1:1:33:PRO:HD3 | 2.10 | 0.51 |
| 3:3:106:TYR:CB | 3:3:107:TRP:CD1 | 2.92 | 0.51 |
| 5:A:164:LEU:HA | 5:A:167:THR:HG23 | 1.91 | 0.51 |
| 5:A:328:LYS:HE2 | 5:A:332:GLU:CD | 2.35 | 0.51 |
| 5:A:492:ILE:HA | 5:A:495:THR:HG23 | 1.91 | 0.51 |
| 5:A:536:THR:HA | 5:A:539:PHE:CB | 2.40 | 0.51 |
| 5:A:701:GLN:NE2 | 5:A:724:ALA:H | 2.08 | 0.51 |
| 22:A:843:BCR:H311 | 22:A:843:BCR:C8 | 2.12 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:479:SER:C | 6:B:481:THR:H | 2.19 | 0.51 |
| 20:B:809:CLA:CBB | 20:B:829:CLA:HHC | 2.40 | 0.51 |
| 20:B:813:CLA:CAC | 20:B:814:CLA:CBB | 2.52 | 0.51 |
| 10:F:72:ILE:HG22 | 10:F:73:VAL:N | 2.25 | 0.51 |
| 10:F:104:TYR:CD2 | 10:F:104:TYR:C | 2.89 | 0.51 |
| 10:F:104:TYR:C | 10:F:104:TYR:HD2 | 2.18 | 0.51 |
| 20:H:109:CLA:H2A | 20:H:109:CLA:O1D | 2.09 | 0.51 |
| 15:K:47:LEU:HB3 | 15:K:48:GLN:HB2 | 1.91 | 0.51 |
| 17:N:62:SER:HB3 | 17:N:66:ASP:N | 2.23 | 0.51 |
| 5:A:397:THR:HB | 5:A:613:ILE:CD1 | 2.41 | 0.51 |
| 5:A:588:GLY:HA3 | 6:B:668:ARG:HB3 | 1.92 | 0.51 |
| 5:A:708:VAL:N | 5:A:711:HIS:HD2 | 2.09 | 0.51 |
| 20:A:833:CLA:H3A | 20:A:833:CLA:O1A | 2.11 | 0.51 |
| 20:A:833:CLA:HMA3 | 20:A:839:CLA:CBB | 2.38 | 0.51 |
| 6:B:429:LEU:HB3 | 6:B:525:LEU:HB2 | 1.91 | 0.51 |
| 6:B:438:VAL:O | 6:B:441:ASP:N | 2.42 | 0.51 |
| 6:B:538:ALA:O | 6:B:540:ASP:N | 2.43 | 0.51 |
| 6:B:551:LYS:O | 6:B:553:PHE:CD2 | 2.64 | 0.51 |
| 6:B:694:ARG:HE | 16:L:105:ALA:CB | 2.23 | 0.51 |
| 6:B:715:VAL:HA | 6:B:718:ILE:HG22 | 1.92 | 0.51 |
| 20:B:822:CLA:HMA2 | 20:B:823:CLA:C3D | 2.40 | 0.51 |
| 9:E:88:GLU:O | 9:E:89:GLU:C | 2.53 | 0.51 |
| 12:H:45:ALA:C | 12:H:48:THR:H | 2.12 | 0.51 |
| 22:I:101:BCR:H392 | 20:I:102:CLA:H142 | 1.93 | 0.51 |
| 18:R:4:UNK:O | 18:R:5:UNK:CB | 2.59 | 0.51 |
| 1:1:89:VAL:HB | 1:1:90:PRO:CD | 2.32 | 0.51 |
| 20:2:302:CLA:O1A | 20:2:302:CLA:C4A | 2.58 | 0.51 |
| 3:3:127:ARG:C | 3:3:129:PHE:H | 2.18 | 0.51 |
| 3:3:157:ALA:O | 3:3:158:TYR:CD2 | 2.63 | 0.51 |
| 3:3:164:PHE:O | 3:3:165:ASN:C | 2.53 | 0.51 |
| 5:A:144:GLN:HG3 | 5:A:145:ILE:H | 1.75 | 0.51 |
| 5:A:385:LEU:O | 5:A:386:ALA:HB3 | 2.10 | 0.51 |
| 5:A:462:ILE:HD11 | 20:B:802:CLA:C5 | 2.29 | 0.51 |
| 5:A:555:ILE:HG22 | 6:B:670:TYR:CZ | 2.45 | 0.51 |
| 20:A:850:CLA:H152 | 20:A:850:CLA:H101 | 1.92 | 0.51 |
| 6:B:580:VAL:CG1 | 6:B:710:LEU:HD21 | 2.41 | 0.51 |
| 20:B:826:CLA:O1A | 20:B:839:CLA:HED2 | 2.10 | 0.51 |
| 7:C:12:ILE:HD13 | 7:C:39:ILE:HG13 | 1.93 | 0.51 |
| 7:C:30:PRO:HB3 | 7:C:37:LYS:O | 2.10 | 0.51 |
| 20:H:101:CLA:CGA | 20:H:101:CLA:H3A | 2.34 | 0.51 |
| 14:J:2:ARG:NH1 | 14:J:8:LEU:HB2 | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:L:69:VAL:HG11 | 16:L:84:GLY:N | 2.25 | 0.51 |
| 17:N:62:SER:O | 17:N:63:ASP:CB | 2.58 | 0.51 |
| 2:2:124:ILE:CG2 | 2:2:129:LYS:HB3 | 2.40 | 0.51 |
| 3:3:116:PHE:O | 3:3:120:LEU:HB2 | 2.10 | 0.51 |
| 3:3:180:LYS:C | 3:3:182:LYS:H | 2.18 | 0.51 |
| 4:4:121:PHE:O | 4:4:122:LYS:CB | 2.58 | 0.51 |
| 4:4:164:LEU:O | 4:4:167:ILE:N | 2.44 | 0.51 |
| 21:4:319:LMU:H5' | 21:4:319:LMU:O2B | 2.10 | 0.51 |
| 5:A:121:GLN:NE2 | 20:A:809:CLA:HMD1 | 2.25 | 0.51 |
| 5:A:472:ARG:N | 5:A:473:PRO:HD2 | 2.24 | 0.51 |
| 20:A:807:CLA:HAA2 | 20:A:809:CLA:HED1 | 1.93 | 0.51 |
| 20:A:808:CLA:HMC3 | 20:A:809:CLA:HHD | 1.93 | 0.51 |
| 20:A:824:CLA:CED | 20:A:825:CLA:HMD1 | 2.35 | 0.51 |
| 20:A:837:CLA:HED1 | 20:B:806:CLA:H18 | 1.93 | 0.51 |
| 6:B:40:GLY:HA2 | 6:B:165:VAL:HG23 | 1.91 | 0.51 |
| 6:B:228:GLY:HA3 | 11:G:8:ILE:HD13 | 1.93 | 0.51 |
| 6:B:388:ALA:O | 6:B:391:PRO:HD2 | 2.10 | 0.51 |
| 6:B:479:SER:O | 6:B:481:THR:N | 2.38 | 0.51 |
| 6:B:555:TYR:CD2 | 6:B:573:TRP:HB2 | 2.44 | 0.51 |
| 6:B:592:PHE:HA | 6:B:721:TYR:OH | 2.11 | 0.51 |
| 15:K:32:ARG:NE | 15:K:32:ARG:HA | 2.25 | 0.51 |
| 15:K:44:GLU:CG | 15:K:45:SER:N | 2.30 | 0.51 |
| 17:N:45:ASN:C | 17:N:46:PHE:O | 2.52 | 0.51 |
| 2:2:81:THR:O | 2:2:83:GLY:N | 2.44 | 0.51 |
| 3:3:63:ARG:NH2 | 3:3:189:LEU:HD23 | 2.19 | 0.51 |
| 3:3:97:PHE:C | 3:3:98:ILE:CG2 | 2.83 | 0.51 |
| 5:A:114:THR:CG2 | 5:A:115:HIS:ND1 | 2.71 | 0.51 |
| 5:A:302:HIS:HB2 | 20:A:817:CLA:C1B | 2.41 | 0.51 |
| 5:A:438:HIS:HB2 | 5:A:441:ALA:HB3 | 1.91 | 0.51 |
| 6:B:378:ILE:CA | 6:B:381:PHE:HB2 | 2.41 | 0.51 |
| 6:B:724:PHE:CD2 | 20:B:850:CLA:HMD1 | 2.45 | 0.51 |
| 20:B:832:CLA:H51 | 22:F:204:BCR:H401 | 1.93 | 0.51 |
| 20:B:837:CLA:HBC3 | 20:B:837:CLA:CMC | 2.40 | 0.51 |
| 7:C:70:TRP:O | 7:C:72:GLU:CB | 2.59 | 0.51 |
| 7:C:79:LEU:CD2 | 7:C:81:TYR:C | 2.83 | 0.51 |
| 8:D:36:LEU:HB2 | 16:L:19:PHE:O | 2.10 | 0.51 |
| 8:D:78:ALA:O | 8:D:79:ARG:NH1 | 2.37 | 0.51 |
| 9:E:45:TRP:CZ3 | 9:E:78:SER:OG | 2.61 | 0.51 |
| 11:G:17:PHE:O | 11:G:20:ARG:CB | 2.54 | 0.51 |
| 12:H:74:GLN:OE1 | 12:H:74:GLN:O | 2.29 | 0.51 |
| 22:I:103:BCR:H292 | 22:L:209:BCR:H281 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:141:GLU:O | 1:1:143:LEU:O | 2.29 | 0.51 |
| 21:3:319:LMU:O2B | 21:3:319:LMU:H5B | 2.10 | 0.51 |
| 4:4:32:GLU:HA | 4:4:32:GLU:OE2 | 2.10 | 0.51 |
| 21:4:321:LMU:O2B | 21:4:321:LMU:C4' | 2.59 | 0.51 |
| 5:A:122:VAL:HG22 | 5:A:142:GLY:HA2 | 1.92 | 0.51 |
| 5:A:243:PRO:O | 5:A:244:LEU:O | 2.28 | 0.51 |
| 5:A:462:ILE:CG2 | 20:A:831:CLA:CMC | 2.89 | 0.51 |
| 5:A:520:LEU:HD22 | 21:A:846:LMU:O1' | 2.10 | 0.51 |
| 5:A:624:VAL:O | 5:A:636:HIS:CD2 | 2.64 | 0.51 |
| 5:A:732:ALA:HB1 | 20:A:838:CLA:HED2 | 1.93 | 0.51 |
| 20:A:830:CLA:HED1 | 20:L:203:CLA:O1A | 2.11 | 0.51 |
| 6:B:63:GLY:HA2 | 6:B:66:PHE:HB3 | 1.93 | 0.51 |
| 6:B:124:TRP:O | 6:B:124:TRP:HD1 | 1.94 | 0.51 |
| 6:B:127:ILE:O | 6:B:128:GLY:C | 2.53 | 0.51 |
| 6:B:400:PRO:HD2 | 8:D:143:PRO:HD3 | 1.92 | 0.51 |
| 6:B:655:LEU:CD2 | 20:B:841:CLA:CBB | 2.89 | 0.51 |
| 8:D:75:LEU:HD21 | 16:L:19:PHE:CG | 2.45 | 0.51 |
| 10:F:46:MET:C | 10:F:50:LYS:HB2 | 2.36 | 0.51 |
| 10:F:50:LYS:C | 10:F:52:ARG:N | 2.65 | 0.51 |
| 21:H:106:LMU:C11 | 21:H:106:LMU:H71 | 2.41 | 0.51 |
| 13:I:10:PRO:O | 13:I:15:LEU:N | 2.35 | 0.51 |
| 17:N:81:VAL:O | 17:N:82:PHE:C | 2.53 | 0.51 |
| 3:3:182:LYS:O | 3:3:185:LYS:HB3 | 2.11 | 0.51 |
| 20:4:310:CLA:CBA | 20:4:310:CLA:HBD | 2.41 | 0.51 |
| 5:A:86:LEU:HD22 | 5:A:86:LEU:H | 1.76 | 0.51 |
| 5:A:258:LEU:O | 5:A:280:PHE:CE1 | 2.64 | 0.51 |
| 5:A:327:ILE:O | 5:A:328:LYS:O | 2.29 | 0.51 |
| 5:A:445:HIS:CE1 | 20:A:829:CLA:HMB1 | 2.46 | 0.51 |
| 5:A:713:LYS:CE | 20:F:201:CLA:H43 | 2.41 | 0.51 |
| 20:A:808:CLA:H43 | 22:A:845:BCR:H383 | 1.93 | 0.51 |
| 20:A:816:CLA:H2 | 20:A:816:CLA:CBA | 2.33 | 0.51 |
| 20:A:825:CLA:HBC2 | 20:A:825:CLA:CMC | 2.41 | 0.51 |
| 23:A:842:PQN:H241 | 23:A:842:PQN:H272 | 1.93 | 0.51 |
| 20:A:851:CLA:HMD3 | 6:B:578:LEU:CD2 | 2.30 | 0.51 |
| 6:B:362:ALA:C | 6:B:364:ASP:H | 2.19 | 0.51 |
| 6:B:503:GLU:HB3 | 6:B:507:SER:HB2 | 1.92 | 0.51 |
| 20:B:810:CLA:HMC3 | 22:B:847:BCR:H282 | 1.93 | 0.51 |
| 10:F:44:ALA:C | 10:F:46:MET:N | 2.69 | 0.51 |
| 12:H:65:LEU:HD23 | 20:H:108:CLA:C5 | 2.41 | 0.51 |
| 13:I:12:VAL:CG2 | 20:I:102:CLA:O1A | 2.59 | 0.51 |
| 16:L:5:LYS:HA | 16:L:5:LYS:HE2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:L:33:ILE:HD11 | 16:L:36:TYR:HD1 | 1.75 | 0.51 |
| 17:N:50:GLN:OE1 | 17:N:51:ASP:HA | 2.10 | 0.51 |
| 17:N:80:ASN:O | 17:N:82:PHE:N | 2.32 | 0.51 |
| 1:1:42:SER:HA | 1:1:45:ILE:HG12 | 1.92 | 0.51 |
| 20:2:302:CLA:H42 | 20:2:302:CLA:O2A | 2.10 | 0.51 |
| 3:3:132:TRP:HZ3 | 3:3:155:GLU:CD | 1.82 | 0.51 |
| 4:4:144:ALA:HB3 | 4:4:147:LEU:C | 2.36 | 0.51 |
| 5:A:458:PHE:CD2 | 20:B:802:CLA:HMB3 | 2.46 | 0.51 |
| 5:A:598:VAL:O | 5:A:598:VAL:HG12 | 2.11 | 0.51 |
| 20:A:804:CLA:HMC3 | 20:A:806:CLA:O2D | 2.10 | 0.51 |
| 20:A:824:CLA:HAA2 | 20:A:825:CLA:OBD | 2.12 | 0.51 |
| 20:A:839:CLA:HBC2 | 20:A:839:CLA:CHD | 2.31 | 0.51 |
| 6:B:320:LYS:O | 6:B:322:LEU:N | 2.44 | 0.51 |
| 6:B:354:SER:O | 6:B:355:LEU:HD13 | 2.11 | 0.51 |
| 6:B:378:ILE:HA | 6:B:381:PHE:HB2 | 1.92 | 0.51 |
| 6:B:464:GLN:HG3 | 6:B:469:LYS:HD3 | 1.93 | 0.51 |
| 20:B:802:CLA:C9 | 20:B:803:CLA:C9 | 2.86 | 0.51 |
| 20:B:806:CLA:HBC3 | 22:F:203:BCR:H332 | 1.92 | 0.51 |
| 7:C:69:LEU:HD23 | 7:C:70:TRP:N | 2.26 | 0.51 |
| 8:D:46:TYR:HD1 | 8:D:80:LYS:HB3 | 1.75 | 0.51 |
| 8:D:93:LYS:NZ | 8:D:93:LYS:HB3 | 2.26 | 0.51 |
| 21:1:217:LMU:O6B | 21:1:217:LMU:C1B | 2.54 | 0.50 |
| 2:2:50:VAL:O | 2:2:50:VAL:HG12 | 2.10 | 0.50 |
| 5:A:141:ARG:HD3 | 10:F:39:ALA:HA | 1.92 | 0.50 |
| 5:A:160:SER:HB2 | 5:A:163:GLN:OE1 | 2.11 | 0.50 |
| 5:A:210:LEU:N | 5:A:213:LEU:H | 2.09 | 0.50 |
| 5:A:309:LEU:HA | 5:A:312:ILE:O | 2.11 | 0.50 |
| 5:A:446:LEU:CD1 | 5:A:554:LEU:HA | 2.42 | 0.50 |
| 5:A:514:THR:HB | 5:A:532:ILE:HG23 | 1.93 | 0.50 |
| 5:A:555:ILE:HG21 | 20:B:803:CLA:HMD1 | 1.92 | 0.50 |
| 5:A:711:HIS:CB | 5:A:717:ALA:HB2 | 2.35 | 0.50 |
| 6:B:77:TRP:CE2 | 6:B:81:PRO:HB3 | 2.45 | 0.50 |
| 6:B:551:LYS:HG2 | 6:B:552:ASP:H | 1.76 | 0.50 |
| 6:B:696:LYS:NZ | 8:D:39:LYS:HE3 | 2.25 | 0.50 |
| 20:B:838:CLA:C6 | 22:F:204:BCR:C32 | 2.89 | 0.50 |
| 8:D:36:LEU:HD21 | 8:D:45:PHE:CZ | 2.45 | 0.50 |
| 9:E:32:ARG:HH22 | 9:E:53:VAL:HA | 1.76 | 0.50 |
| 17:N:61:LEU:HD11 | 17:N:63:ASP:CB | 2.40 | 0.50 |
| 20:1:207:CLA:H43 | 20:1:207:CLA:CGA | 2.41 | 0.50 |
| 2:2:128:ASN:HD21 | 14:J:4:PHE:H | 1.58 | 0.50 |
| 20:2:303:CLA:O2D | 20:2:303:CLA:OBD | 2.30 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:157:ALA:O | 3:3:158:TYR:CB | 2.59 | 0.50 |
| 20:4:304:CLA:HAA1 | 20:F:207:CLA:C4 | 2.36 | 0.50 |
| 5:A:149:PHE:O | 5:A:150:PHE:HB2 | 2.10 | 0.50 |
| 5:A:262:PHE:O | 5:A:264:GLU:N | 2.44 | 0.50 |
| 5:A:552:THR:O | 5:A:553:VAL:HB | 2.11 | 0.50 |
| 5:A:746:THR:HG1 | 20:A:849:CLA:CGD | 2.24 | 0.50 |
| 20:A:820:CLA:HBC3 | 20:A:822:CLA:HED1 | 1.92 | 0.50 |
| 20:A:831:CLA:H171 | 20:A:835:CLA:H202 | 1.93 | 0.50 |
| 6:B:55:ALA:HB1 | 6:B:150:LEU:HD12 | 1.93 | 0.50 |
| 6:B:92:TRP:O | 6:B:92:TRP:CD1 | 2.64 | 0.50 |
| 7:C:7:ILE:O | 7:C:60:THR:HA | 2.11 | 0.50 |
| 10:F:125:LEU:HD11 | 14:J:18:TRP:CZ3 | 2.45 | 0.50 |
| 11:G:28:ARG:HA | 20:G:105:CLA:HMA2 | 1.94 | 0.50 |
| 14:J:15:SER:HA | 14:J:18:TRP:HB3 | 1.93 | 0.50 |
| 22:J:102:BCR:C39 | 22:J:102:BCR:C23 | 2.77 | 0.50 |
| 16:L:33:ILE:CD1 | 16:L:36:TYR:HD1 | 2.25 | 0.50 |
| 16:L:128:ASP:OD2 | 16:L:129:GLN:N | 2.41 | 0.50 |
| 17:N:51:ASP:O | 17:N:52:LEU:HD22 | 2.11 | 0.50 |
| 18:R:49:UNK:O | 18:R:51:UNK:CB | 2.58 | 0.50 |
| 2:2:57:LEU:HD23 | 2:2:58:GLY:N | 2.26 | 0.50 |
| 2:2:154:GLN:HA | 2:2:154:GLN:OE1 | 2.11 | 0.50 |
| 4:4:93:ILE:C | 4:4:96:ILE:HD12 | 2.35 | 0.50 |
| 4:4:142:ASN:C | 4:4:143:PHE:CG | 2.89 | 0.50 |
| 5:A:98:PHE:CZ | 20:A:807:CLA:CMD | 2.95 | 0.50 |
| 5:A:149:PHE:C | 5:A:151:GLN:N | 2.67 | 0.50 |
| 5:A:157:GLY:HA2 | 5:A:229:ILE:CG2 | 2.41 | 0.50 |
| 20:A:817:CLA:C4A | 20:A:817:CLA:H12 | 2.42 | 0.50 |
| 20:A:830:CLA:H191 | 23:B:843:PQN:H303 | 1.93 | 0.50 |
| 22:A:845:BCR:C3 | 22:F:203:BCR:H17C | 2.41 | 0.50 |
| 21:A:853:LMU:C8 | 21:A:853:LMU:C3 | 2.89 | 0.50 |
| 6:B:75:GLU:HB2 | 6:B:132:ASN:HD22 | 1.76 | 0.50 |
| 6:B:398:TYR:C | 8:D:143:PRO:HG2 | 2.37 | 0.50 |
| 6:B:527:LEU:HD12 | 20:B:826:CLA:C1D | 2.42 | 0.50 |
| 6:B:694:ARG:HE | 16:L:105:ALA:CA | 2.24 | 0.50 |
| 21:H:103:LMU:H2B | 21:H:103:LMU:C6B | 2.41 | 0.50 |
| 14:J:2:ARG:HB3 | 14:J:7:TYR:CZ | 2.45 | 0.50 |
| 15:K:4:GLY:HA2 | 15:K:7:THR:CB | 2.41 | 0.50 |
| 17:N:45:ASN:ND2 | 17:N:54:LYS:HB2 | 2.26 | 0.50 |
| 17:N:48:GLY:HA3 | 17:N:49:CYS:SG | 2.51 | 0.50 |
| 17:N:61:LEU:HD12 | 17:N:63:ASP:HB2 | 1.93 | 0.50 |
| 18:R:47:UNK:O | 18:R:48:UNK:O | 2.30 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:165:LYS:C | 2:2:167:GLY:N | 2.67 | 0.50 |
| 3:3:109:ASP:O | 3:3:110:SER:O | 2.28 | 0.50 |
| 3:3:182:LYS:O | 3:3:182:LYS:HG2 | 2.12 | 0.50 |
| 4:4:46:VAL:HG21 | 4:4:105:ARG:NH1 | 2.26 | 0.50 |
| 4:4:98:SER:C | 4:4:102:GLU:OE1 | 2.54 | 0.50 |
| 4:4:114:SER:O | 4:4:117:GLN:N | 2.44 | 0.50 |
| 21:4:319:LMU:C4B | 21:4:319:LMU:O1B | 2.56 | 0.50 |
| 5:A:44:ILE:O | 5:A:46:LYS:HA | 2.11 | 0.50 |
| 5:A:188:LYS:O | 5:A:190:ALA:N | 2.45 | 0.50 |
| 5:A:360:ILE:O | 5:A:361:ASN:HB3 | 2.11 | 0.50 |
| 5:A:390:ALA:HB1 | 5:A:754:ILE:HD13 | 1.93 | 0.50 |
| 5:A:475:ASP:HB3 | 20:A:831:CLA:CED | 2.41 | 0.50 |
| 5:A:592:VAL:O | 5:A:597:HIS:CD2 | 2.65 | 0.50 |
| 20:A:826:CLA:C17 | 22:J:102:BCR:H17C | 2.40 | 0.50 |
| 6:B:74:PHE:C | 6:B:76:ALA:N | 2.69 | 0.50 |
| 6:B:127:ILE:CG1 | 6:B:193:HIS:HE1 | 2.24 | 0.50 |
| 6:B:558:PRO:O | 6:B:559:CYS:HB3 | 2.12 | 0.50 |
| 6:B:560:ASP:CG | 6:B:561:GLY:N | 2.69 | 0.50 |
| 20:B:829:CLA:H62 | 22:B:845:BCR:C32 | 2.42 | 0.50 |
| 8:D:29:PHE:O | 8:D:30:ALA:HB3 | 2.12 | 0.50 |
| 10:F:22:LEU:HD12 | 10:F:22:LEU:N | 2.10 | 0.50 |
| 10:F:26:GLN:O | 10:F:28:SER:N | 2.44 | 0.50 |
| 21:F:202:LMU:C7 | 21:F:202:LMU:C3 | 2.85 | 0.50 |
| 11:G:68:ILE:HG22 | 11:G:72:LEU:HD13 | 1.91 | 0.50 |
| 21:H:106:LMU:C11 | 21:H:106:LMU:C7 | 2.88 | 0.50 |
| 15:K:44:GLU:OE2 | 15:K:45:SER:O | 2.29 | 0.50 |
| 18:R:34:UNK:C | 18:R:36:UNK:N | 2.75 | 0.50 |
| 20:1:203:CLA:HBD | 20:1:203:CLA:CAA | 2.41 | 0.50 |
| 20:1:213:CLA:HMC2 | 20:4:303:CLA:CMB | 2.41 | 0.50 |
| 2:2:98:GLU:CG | 2:2:99:LEU:HD12 | 2.41 | 0.50 |
| 2:2:163:GLU:HA | 2:2:163:GLU:OE1 | 2.10 | 0.50 |
| 20:2:307:CLA:H93 | 20:2:307:CLA:C4 | 2.32 | 0.50 |
| 5:A:58:HIS:HE1 | 20:A:803:CLA:C4D | 2.20 | 0.50 |
| 5:A:445:HIS:O | 5:A:446:LEU:HB2 | 2.11 | 0.50 |
| 5:A:583:GLY:O | 5:A:589:THR:HB | 2.11 | 0.50 |
| 20:A:825:CLA:CBB | 20:A:832:CLA:C3A | 2.90 | 0.50 |
| 20:A:838:CLA:C19 | 14:J:19:PHE:CD2 | 2.94 | 0.50 |
| 6:B:338:LEU:O | 6:B:339:ALA:HB3 | 2.11 | 0.50 |
| 6:B:440:ASN:ND2 | 6:B:453:ILE:O | 2.45 | 0.50 |
| 6:B:558:PRO:HB3 | 6:B:706:ARG:HH21 | 1.75 | 0.50 |
| 6:B:594:TRP:HD1 | 6:B:595:HIS:HB2 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:B:809:CLA:H43 | 25:B:848:LMG:H321 | 1.93 | 0.50 |
| 20:B:812:CLA:HED2 | 20:B:812:CLA:O2A | 2.11 | 0.50 |
| 20:B:827:CLA:C7 | 22:B:846:BCR:H14C | 2.42 | 0.50 |
| 23:B:843:PQN:H192 | 22:B:847:BCR:C8 | 2.41 | 0.50 |
| 7:C:60:THR:HG23 | 7:C:63:LEU:O | 2.11 | 0.50 |
| 8:D:116:ASP:HB3 | 8:D:127:ARG:HH12 | 1.76 | 0.50 |
| 9:E:88:GLU:O | 9:E:90:VAL:HB | 2.11 | 0.50 |
| 11:G:37:GLU:OE2 | 11:G:42:SER:N | 2.44 | 0.50 |
| 12:H:45:ALA:HB3 | 12:H:46:PRO:HD3 | 1.92 | 0.50 |
| 14:J:36:ALA:O | 14:J:37:LEU:HB2 | 2.11 | 0.50 |
| 15:K:47:LEU:O | 15:K:48:GLN:OE1 | 2.30 | 0.50 |
| 20:K:104:CLA:O2D | 20:K:104:CLA:HBA1 | 2.11 | 0.50 |
| 16:L:17:ASP:OD1 | 16:L:17:ASP:O | 2.29 | 0.50 |
| 18:R:34:UNK:O | 18:R:36:UNK:O | 2.29 | 0.50 |
| 2:2:162:LYS:HD3 | 2:2:162:LYS:O | 2.12 | 0.50 |
| 2:2:203:THR:CG2 | 2:2:204:ILE:N | 2.73 | 0.50 |
| 3:3:106:TYR:O | 3:3:107:TRP:C | 2.54 | 0.50 |
| 4:4:69:ILE:O | 4:4:71:ASN:N | 2.45 | 0.50 |
| 4:4:103:ILE:CG1 | 20:4:302:CLA:HMD3 | 2.27 | 0.50 |
| 4:4:114:SER:O | 4:4:117:GLN:HG3 | 2.12 | 0.50 |
| 20:4:303:CLA:CED | 20:4:303:CLA:CAA | 2.78 | 0.50 |
| 5:A:223:VAL:HA | 5:A:227:LEU:HB2 | 1.94 | 0.50 |
| 5:A:707:ILE:HG22 | 5:A:711:HIS:CD2 | 2.45 | 0.50 |
| 20:A:826:CLA:C11 | 22:J:102:BCR:H353 | 2.40 | 0.50 |
| 20:A:828:CLA:H152 | 20:A:828:CLA:C10 | 2.41 | 0.50 |
| 20:A:850:CLA:HED1 | 20:B:850:CLA:H2 | 1.93 | 0.50 |
| 6:B:30:ASP:O | 6:B:34:HIS:HD2 | 1.95 | 0.50 |
| 6:B:54:LEU:HD11 | 20:B:814:CLA:HBA2 | 1.94 | 0.50 |
| 6:B:75:GLU:CB | 6:B:132:ASN:HD22 | 2.24 | 0.50 |
| 6:B:439:HIS:CD2 | 6:B:453:ILE:HG22 | 2.47 | 0.50 |
| 20:B:810:CLA:H42 | 20:B:810:CLA:C4C | 2.42 | 0.50 |
| 20:B:839:CLA:CMC | 20:B:839:CLA:HBC2 | 2.42 | 0.50 |
| 10:F:80:TRP:HB3 | 20:F:207:CLA:HHC | 1.93 | 0.50 |
| 16:L:63:LEU:CD2 | 16:L:64:LEU:H | 2.22 | 0.50 |
| 20:L:201:CLA:H141 | 20:L:204:CLA:H93 | 1.93 | 0.50 |
| 20:L:202:CLA:CGD | 20:L:202:CLA:C1 | 2.88 | 0.50 |
| 17:N:83:TRP:O | 17:N:83:TRP:CE3 | 2.63 | 0.50 |
| 18:R:38:UNK:O | 18:R:39:UNK:O | 2.29 | 0.50 |
| 2:2:56:MET:O | 2:2:57:LEU:C | 2.55 | 0.50 |
| 21:2:318:LMU:H3' | 21:2:318:LMU:C5B | 2.42 | 0.50 |
| 3:3:112:THR:C | 3:3:114:PHE:N | 2.69 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:30:LEU:O | 4:4:32:GLU:CD | 2.55 | 0.50 |
| 4:4:40:PHE:HA | 4:4:43:ALA:H | 1.75 | 0.50 |
| 4:4:192:THR:CG2 | 4:4:193:ILE:N | 2.75 | 0.50 |
| 5:A:131:ILE:CG2 | 6:B:446:PHE:HA | 2.36 | 0.50 |
| 5:A:555:ILE:CG2 | 20:B:803:CLA:OBD | 2.60 | 0.50 |
| 20:A:803:CLA:HBA2 | 20:A:838:CLA:H2 | 1.93 | 0.50 |
| 20:A:836:CLA:HBC3 | 20:A:836:CLA:CMC | 2.42 | 0.50 |
| 6:B:91:ILE:CD1 | 6:B:104:PHE:CE2 | 2.95 | 0.50 |
| 6:B:353:TYR:CD1 | 6:B:594:TRP:HZ3 | 2.30 | 0.50 |
| 11:G:28:ARG:HG3 | 11:G:29:GLU:CG | 2.41 | 0.50 |
| 15:K:35:THR:HG23 | 15:K:36:ALA:H | 1.77 | 0.50 |
| 17:N:54:LYS:HB3 | 17:N:57:LYS:HB2 | 1.94 | 0.50 |
| 17:N:80:ASN:OD1 | 17:N:82:PHE:CA | 2.60 | 0.50 |
| 17:N:80:ASN:OD1 | 17:N:82:PHE:N | 2.45 | 0.50 |
| 18:R:43:UNK:O | 18:R:44:UNK:O | 2.29 | 0.50 |
| 2:2:97:VAL:CA | 2:2:100:VAL:HG13 | 2.41 | 0.50 |
| 22:2:317:BCR:H361 | 20:A:840:CLA:H92 | 1.94 | 0.50 |
| 4:4:68:GLY:C | 4:4:71:ASN:HB2 | 2.35 | 0.50 |
| 4:4:142:ASN:N | 4:4:150:LYS:NZ | 2.56 | 0.50 |
| 20:4:301:CLA:O1D | 20:4:301:CLA:H2A | 2.12 | 0.50 |
| 5:A:24:ARG:O | 5:A:25:ASP:OD1 | 2.30 | 0.50 |
| 5:A:49:ASP:HB2 | 5:A:720:THR:HA | 1.94 | 0.50 |
| 5:A:59:ALA:O | 5:A:61:ALA:N | 2.44 | 0.50 |
| 6:B:119:GLY:O | 6:B:121:TYR:N | 2.45 | 0.50 |
| 6:B:193:HIS:CD2 | 20:B:815:CLA:NB | 2.80 | 0.50 |
| 6:B:196:HIS:NE2 | 20:B:816:CLA:ND | 2.60 | 0.50 |
| 6:B:492:ILE:HD13 | 6:B:492:ILE:N | 2.17 | 0.50 |
| 6:B:594:TRP:CD2 | 6:B:598:HIS:CE1 | 3.00 | 0.50 |
| 20:B:809:CLA:H191 | 20:B:828:CLA:H141 | 1.93 | 0.50 |
| 8:D:58:PHE:CD2 | 8:D:59:GLU:N | 2.80 | 0.50 |
| 20:H:101:CLA:HMA1 | 20:H:101:CLA:C6 | 2.41 | 0.50 |
| 16:L:148:VAL:O | 16:L:149:SER:CB | 2.54 | 0.50 |
| 1:1:27:LEU:HG | 6:B:314:ARG:NH1 | 2.26 | 0.50 |
| 3:3:106:TYR:CD2 | 3:3:107:TRP:CG | 2.99 | 0.50 |
| 4:4:92:VAL:HG12 | 4:4:93:ILE:N | 2.27 | 0.50 |
| 4:4:119:PRO:C | 4:4:121:PHE:H | 2.18 | 0.50 |
| 4:4:127:PRO:HB2 | 4:4:143:PHE:CE1 | 2.47 | 0.50 |
| 5:A:638:THR:OG1 | 5:A:641:ASN:ND2 | 2.44 | 0.50 |
| 20:A:819:CLA:HMC3 | 20:A:819:CLA:HBC2 | 1.93 | 0.50 |
| 20:A:822:CLA:CAB | 22:A:844:BCR:C35 | 2.90 | 0.50 |
| 6:B:124:TRP:O | 6:B:124:TRP:CD1 | 2.64 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:174:ARG:HH11 | 20:B:825:CLA:CMD | 2.16 | 0.50 |
| 6:B:202:SER:CB | 6:B:270:LEU:HD21 | 2.42 | 0.50 |
| 6:B:385:GLY:N | 20:B:830:CLA:HBC3 | 2.27 | 0.50 |
| 16:L:65:VAL:C | 16:L:67:PRO:HD2 | 2.37 | 0.50 |
| 16:L:135:GLY:O | 16:L:138:LYS:HG2 | 2.12 | 0.50 |
| 16:L:163:LEU:HD11 | 16:L:165:TYR:CE1 | 2.45 | 0.50 |
| 2:2:98:GLU:HG2 | 2:2:99:LEU:HD12 | 1.93 | 0.49 |
| 3:3:158:TYR:CB | 3:3:159:PRO:HD2 | 2.22 | 0.49 |
| 5:A:44:ILE:O | 5:A:46:LYS:CA | 2.60 | 0.49 |
| 5:A:98:PHE:HD1 | 5:A:99:HIS:HD2 | 1.58 | 0.49 |
| 5:A:335:LYS:HE3 | 5:A:341:GLN:HB2 | 1.93 | 0.49 |
| 5:A:464:ASN:N | 5:A:464:ASN:ND2 | 2.57 | 0.49 |
| 5:A:599:PHE:CD1 | 5:A:600:LEU:HD23 | 2.35 | 0.49 |
| 5:A:618:TRP:O | 5:A:618:TRP:CD1 | 2.64 | 0.49 |
| 5:A:651:GLY:O | 5:A:655:ASP:HB2 | 2.12 | 0.49 |
| 5:A:683:HIS:O | 20:A:850:CLA:HAA2 | 2.11 | 0.49 |
| 5:A:711:HIS:NE2 | 20:A:837:CLA:CAC | 2.74 | 0.49 |
| 20:A:830:CLA:H152 | 22:L:209:BCR:C36 | 2.42 | 0.49 |
| 20:A:831:CLA:HBC3 | 20:A:831:CLA:HMC2 | 1.94 | 0.49 |
| 6:B:152:ALA:HB2 | 20:B:812:CLA:HMC2 | 1.94 | 0.49 |
| 6:B:299:HIS:NE2 | 6:B:304:ILE:HG21 | 2.27 | 0.49 |
| 6:B:321:GLY:O | 6:B:325:THR:HG22 | 2.11 | 0.49 |
| 6:B:438:VAL:O | 6:B:442:VAL:N | 2.44 | 0.49 |
| 6:B:454:LEU:HD12 | 6:B:454:LEU:N | 2.27 | 0.49 |
| 6:B:475:ASP:O | 6:B:479:SER:OG | 2.30 | 0.49 |
| 6:B:595:HIS:CD2 | 6:B:623:TYR:OH | 2.65 | 0.49 |
| 20:B:828:CLA:CGA | 20:B:828:CLA:H3A | 2.38 | 0.49 |
| 7:C:7:ILE:C | 7:C:8:TYR:O | 2.54 | 0.49 |
| 10:F:123:VAL:HB | 10:F:126:ALA:O | 2.12 | 0.49 |
| 10:F:124:PRO:C | 10:F:126:ALA:H | 2.20 | 0.49 |
| 20:F:206:CLA:H2A | 20:F:206:CLA:O1D | 2.12 | 0.49 |
| 16:L:48:ASN:CB | 16:L:49:PRO:HD2 | 2.39 | 0.49 |
| 21:2:320:LMU:O2B | 21:2:320:LMU:H4' | 2.12 | 0.49 |
| 21:3:319:LMU:H81 | 21:3:319:LMU:C4 | 2.42 | 0.49 |
| 4:4:36:ASN:C | 4:4:36:ASN:OD1 | 2.55 | 0.49 |
| 4:4:82:GLU:O | 4:4:83:TYR:HD1 | 1.95 | 0.49 |
| 5:A:308:ILE:HG13 | 20:A:816:CLA:CBB | 2.43 | 0.49 |
| 5:A:690:LEU:HD23 | 5:A:693:LEU:HD12 | 1.93 | 0.49 |
| 5:A:736:THR:HG21 | 20:A:828:CLA:H91 | 1.94 | 0.49 |
| 6:B:242:HIS:O | 6:B:243:LEU:HG | 2.12 | 0.49 |
| 6:B:553:PHE:O | 6:B:554:GLY:C | 2.54 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:583:MET:HA | 20:B:826:CLA:HBC1 | 1.93 | 0.49 |
| 20:B:834:CLA:CMD | 20:B:835:CLA:C1C | 2.90 | 0.49 |
| 20:B:835:CLA:HBB1 | 22:B:846:BCR:C28 | 2.39 | 0.49 |
| 7:C:65:VAL:HG12 | 7:C:66:ARG:N | 2.26 | 0.49 |
| 8:D:36:LEU:HD12 | 8:D:78:ALA:H | 1.77 | 0.49 |
| 15:K:44:GLU:O | 15:K:46:GLY:O | 2.30 | 0.49 |
| 17:N:47:THR:O | 17:N:48:GLY:C | 2.56 | 0.49 |
| 18:R:37:UNK:O | 18:R:42:UNK:O | 2.30 | 0.49 |
| 20:2:302:CLA:O2A | 20:2:302:CLA:C4 | 2.60 | 0.49 |
| 5:A:182:GLY:HA3 | 20:A:811:CLA:HAC1 | 1.94 | 0.49 |
| 5:A:207:LEU:CD1 | 20:A:819:CLA:HBB2 | 2.42 | 0.49 |
| 5:A:398:HIS:HD2 | 20:A:826:CLA:ND | 2.10 | 0.49 |
| 5:A:582:ASP:HB3 | 5:A:589:THR:CG2 | 2.41 | 0.49 |
| 20:A:835:CLA:ND | 20:A:835:CLA:H11 | 2.26 | 0.49 |
| 6:B:31:PHE:O | 6:B:32:GLU:C | 2.55 | 0.49 |
| 6:B:292:ARG:NE | 6:B:297:ILE:O | 2.45 | 0.49 |
| 6:B:305:LEU:O | 6:B:308:HIS:N | 2.28 | 0.49 |
| 6:B:309:ILE:HG22 | 6:B:319:HIS:CD2 | 2.48 | 0.49 |
| 6:B:357:ALA:O | 6:B:358:TYR:CD1 | 2.65 | 0.49 |
| 6:B:382:ILE:O | 6:B:385:GLY:N | 2.43 | 0.49 |
| 6:B:459:PHE:O | 6:B:463:ILE:HD13 | 2.12 | 0.49 |
| 6:B:542:ARG:NH2 | 8:D:143:PRO:HG3 | 2.27 | 0.49 |
| 6:B:607:SER:HA | 6:B:610:ASN:ND2 | 2.27 | 0.49 |
| 20:B:806:CLA:H61 | 22:F:203:BCR:H12C | 1.94 | 0.49 |
| 7:C:62:PHE:CE2 | 9:E:42:GLU:CD | 2.87 | 0.49 |
| 8:D:50:TRP:N | 8:D:50:TRP:CD1 | 2.80 | 0.49 |
| 20:K:103:CLA:HBC2 | 20:K:103:CLA:HMC3 | 1.92 | 0.49 |
| 17:N:62:SER:C | 17:N:66:ASP:H | 2.20 | 0.49 |
| 20:2:305:CLA:H42 | 20:2:307:CLA:CMD | 2.42 | 0.49 |
| 4:4:98:SER:OG | 4:4:102:GLU:OE1 | 2.28 | 0.49 |
| 4:4:175:LYS:O | 4:4:175:LYS:HD2 | 2.12 | 0.49 |
| 5:A:56:ASN:O | 5:A:57:LEU:CB | 2.56 | 0.49 |
| 5:A:63:ASP:HA | 20:A:828:CLA:HED2 | 1.94 | 0.49 |
| 5:A:258:LEU:O | 5:A:259:TYR:HB2 | 2.11 | 0.49 |
| 5:A:312:ILE:O | 5:A:313:ALA:HB2 | 2.12 | 0.49 |
| 5:A:435:VAL:HA | 5:A:438:HIS:HE1 | 1.77 | 0.49 |
| 5:A:443:ILE:HD13 | 5:A:561:LEU:HD12 | 1.95 | 0.49 |
| 5:A:625:TRP:CB | 5:A:637:ILE:HD11 | 2.43 | 0.49 |
| 20:A:838:CLA:C4A | 20:A:838:CLA:HBA2 | 2.35 | 0.49 |
| 6:B:53:GLN:OE1 | 6:B:53:GLN:HA | 2.04 | 0.49 |
| 6:B:325:THR:HG21 | 6:B:403:ASN:HD21 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:376:GLN:OE1 | 6:B:376:GLN:HA | 2.12 | 0.49 |
| 6:B:450:GLU:C | 6:B:452:GLN:H | 2.16 | 0.49 |
| 6:B:535:VAL:HG13 | 6:B:536:LYS:N | 2.28 | 0.49 |
| 6:B:596:TRP:O | 6:B:597:LYS:CB | 2.60 | 0.49 |
| 6:B:616:LEU:O | 6:B:619:TRP:HB2 | 2.12 | 0.49 |
| 20:B:841:CLA:HMC3 | 20:B:841:CLA:HBC2 | 1.94 | 0.49 |
| 7:C:1:MET:HB3 | 7:C:4:SER:CB | 2.37 | 0.49 |
| 10:F:50:LYS:O | 10:F:52:ARG:C | 2.56 | 0.49 |
| 10:F:125:LEU:O | 10:F:126:ALA:HB2 | 2.12 | 0.49 |
| 20:F:207:CLA:CAD | 20:F:207:CLA:HED2 | 2.41 | 0.49 |
| 12:H:37:SER:HB3 | 16:L:51:LEU:HG | 1.94 | 0.49 |
| 20:J:101:CLA:CBD | 20:J:101:CLA:CBA | 2.78 | 0.49 |
| 17:N:59:PRO:C | 17:N:66:ASP:OD1 | 2.55 | 0.49 |
| 18:R:27:UNK:C | 18:R:29:UNK:N | 2.73 | 0.49 |
| 1:1:136:ASP:O | 1:1:138:LYS:N | 2.46 | 0.49 |
| 1:1:142:GLU:OE1 | 20:1:201:CLA:C2D | 2.60 | 0.49 |
| 2:2:57:LEU:O | 2:2:60:ALA:CB | 2.61 | 0.49 |
| 2:2:167:GLY:O | 2:2:168:ARG:C | 2.55 | 0.49 |
| 2:2:192:LEU:HG | 2:2:193:PHE:N | 2.27 | 0.49 |
| 3:3:133:ALA:O | 3:3:134:LYS:HB2 | 2.12 | 0.49 |
| 3:3:158:TYR:C | 3:3:160:GLY:N | 2.70 | 0.49 |
| 5:A:113:PRO:C | 5:A:115:HIS:N | 2.71 | 0.49 |
| 5:A:636:HIS:O | 5:A:638:THR:N | 2.45 | 0.49 |
| 5:A:746:THR:O | 5:A:750:PHE:N | 2.40 | 0.49 |
| 20:A:818:CLA:O2A | 20:A:818:CLA:C4 | 2.58 | 0.49 |
| 22:A:845:BCR:H323 | 22:J:102:BCR:H391 | 1.93 | 0.49 |
| 6:B:175:LEU:HD11 | 20:B:820:CLA:CMA | 2.41 | 0.49 |
| 6:B:376:GLN:HB3 | 6:B:587:ILE:HD12 | 1.94 | 0.49 |
| 6:B:527:LEU:HD13 | 6:B:586:THR:HG21 | 1.94 | 0.49 |
| 6:B:602:TRP:C | 6:B:604:GLY:H | 2.17 | 0.49 |
| 6:B:646:TRP:CZ2 | 6:B:726:ILE:HG21 | 2.47 | 0.49 |
| 20:B:822:CLA:HMA2 | 20:B:823:CLA:C4D | 2.42 | 0.49 |
| 20:B:826:CLA:C1 | 20:B:839:CLA:HED2 | 2.43 | 0.49 |
| 9:E:58:ASP:OD1 | 9:E:58:ASP:N | 2.39 | 0.49 |
| 10:F:24:LYS:C | 10:F:26:GLN:H | 2.20 | 0.49 |
| 20:G:105:CLA:H2A | 20:G:105:CLA:O1D | 2.12 | 0.49 |
| 20:K:104:CLA:HHD | 20:K:104:CLA:CBC | 2.34 | 0.49 |
| 18:R:6:UNK:CB | 18:R:10:UNK:CB | 2.90 | 0.49 |
| 21:R:102:LMU:H6E | 21:R:102:LMU:C6B | 2.42 | 0.49 |
| 1:1:144:LYS:HE3 | 20:1:201:CLA:CGD | 2.41 | 0.49 |
| 2:2:128:ASN:CG | 14:J:3:ASP:CB | 2.85 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:24:ARG:O | 5:A:25:ASP:O | 2.30 | 0.49 |
| 5:A:83:PHE:HA | 5:A:86:LEU:HD23 | 1.94 | 0.49 |
| 5:A:369:THR:HG21 | 5:A:402:ILE:CG2 | 2.43 | 0.49 |
| 5:A:369:THR:HG21 | 20:A:827:CLA:HMC2 | 1.93 | 0.49 |
| 5:A:679:PHE:O | 5:A:683:HIS:CB | 2.60 | 0.49 |
| 20:A:821:CLA:HAA1 | 15:K:32:ARG:CZ | 2.43 | 0.49 |
| 20:A:826:CLA:H171 | 22:J:102:BCR:H351 | 1.94 | 0.49 |
| 6:B:247:THR:HB | 6:B:248:GLN:OE1 | 2.12 | 0.49 |
| 6:B:436:LEU:O | 6:B:437:TYR:HB2 | 2.13 | 0.49 |
| 20:B:814:CLA:H192 | 20:B:819:CLA:OBD | 2.13 | 0.49 |
| 20:B:838:CLA:C12 | 22:F:204:BCR:H311 | 2.43 | 0.49 |
| 8:D:75:LEU:HD21 | 16:L:19:PHE:CE1 | 2.47 | 0.49 |
| 10:F:83:PHE:O | 10:F:87:GLY:N | 2.46 | 0.49 |
| 14:J:20:GLY:O | 14:J:21:SER:HB2 | 2.11 | 0.49 |
| 14:J:26:LEU:H | 14:J:28:GLU:H | 1.60 | 0.49 |
| 15:K:38:LEU:HG | 15:K:39:LYS:HD2 | 1.87 | 0.49 |
| 17:N:5:GLU:OE1 | 17:N:5:GLU:O | 2.30 | 0.49 |
| 17:N:27:ALA:O | 17:N:28:ASN:O | 2.30 | 0.49 |
| 17:N:34:THR:C | 17:N:36:GLU:N | 2.71 | 0.49 |
| 18:R:36:UNK:C | 18:R:38:UNK:CB | 2.90 | 0.49 |
| 3:3:74:ALA:CB | 3:3:75:PRO:HD3 | 2.26 | 0.49 |
| 3:3:129:PHE:O | 3:3:129:PHE:CD1 | 2.66 | 0.49 |
| 5:A:225:VAL:HG12 | 5:A:248:PHE:CD1 | 2.48 | 0.49 |
| 5:A:281:LEU:HD12 | 20:A:816:CLA:HED2 | 1.95 | 0.49 |
| 5:A:382:TYR:HB2 | 5:A:385:LEU:HD11 | 1.94 | 0.49 |
| 5:A:636:HIS:C | 5:A:638:THR:H | 2.19 | 0.49 |
| 20:A:807:CLA:HBA2 | 20:A:807:CLA:H3A | 1.50 | 0.49 |
| 20:A:810:CLA:HBB2 | 20:A:813:CLA:HMA2 | 1.94 | 0.49 |
| 6:B:190:TRP:CH2 | 20:B:819:CLA:HMD1 | 2.48 | 0.49 |
| 6:B:221:GLY:C | 6:B:223:GLY:N | 2.71 | 0.49 |
| 6:B:363:GLN:HA | 6:B:365:PHE:CE1 | 2.47 | 0.49 |
| 20:B:826:CLA:HBB2 | 20:B:839:CLA:HMB2 | 1.85 | 0.49 |
| 20:B:826:CLA:CED | 20:B:827:CLA:CMD | 2.87 | 0.49 |
| 20:B:826:CLA:C2B | 22:B:846:BCR:H352 | 2.42 | 0.49 |
| 7:C:8:TYR:HB2 | 7:C:41:SER:OG | 2.13 | 0.49 |
| 10:F:131:PHE:C | 10:F:133:GLY:N | 2.69 | 0.49 |
| 21:H:106:LMU:H71 | 21:H:106:LMU:H112 | 1.93 | 0.49 |
| 13:I:28:VAL:O | 13:I:29:GLU:CD | 2.56 | 0.49 |
| 17:N:39:SER:OG | 17:N:41:LYS:CA | 2.58 | 0.49 |
| 17:N:62:SER:CA | 17:N:64:ASP:HB3 | 2.42 | 0.49 |
| 20:R:108:CLA:H92 | 21:R:109:LMU:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:184:PRO:O | 1:1:185:TRP:CE2 | 2.66 | 0.49 |
| 2:2:57:LEU:HD23 | 2:2:57:LEU:C | 2.37 | 0.49 |
| 2:2:120:ASN:CG | 14:J:5:LYS:HD2 | 2.38 | 0.49 |
| 20:3:310:CLA:HHC | 20:3:310:CLA:CBB | 2.43 | 0.49 |
| 20:4:303:CLA:O1A | 20:4:303:CLA:C2 | 2.59 | 0.49 |
| 5:A:22:VAL:CG1 | 5:A:24:ARG:HA | 2.42 | 0.49 |
| 5:A:78:VAL:O | 5:A:82:HIS:CD2 | 2.65 | 0.49 |
| 5:A:83:PHE:CE2 | 5:A:185:HIS:CD2 | 3.01 | 0.49 |
| 5:A:207:LEU:HB3 | 20:A:819:CLA:CBB | 2.43 | 0.49 |
| 5:A:536:THR:HA | 5:A:539:PHE:HB3 | 1.95 | 0.49 |
| 20:A:819:CLA:HMC3 | 20:A:819:CLA:CBC | 2.43 | 0.49 |
| 6:B:172:GLU:C | 6:B:176:ASN:HB2 | 2.37 | 0.49 |
| 6:B:256:THR:HG22 | 6:B:271:THR:OG1 | 2.12 | 0.49 |
| 7:C:1:MET:CB | 7:C:4:SER:CB | 2.91 | 0.49 |
| 9:E:89:GLU:O | 9:E:90:VAL:HB | 2.13 | 0.49 |
| 10:F:130:LEU:CG | 10:F:131:PHE:H | 2.09 | 0.49 |
| 20:F:207:CLA:HED2 | 20:F:207:CLA:OBD | 2.12 | 0.49 |
| 11:G:13:GLY:C | 11:G:16:LEU:HG | 2.37 | 0.49 |
| 13:I:8:PHE:CZ | 20:I:102:CLA:H43 | 2.48 | 0.49 |
| 16:L:97:MET:HA | 16:L:100:THR:HG23 | 1.95 | 0.49 |
| 17:N:45:ASN:HB2 | 17:N:54:LYS:CB | 2.42 | 0.49 |
| 17:N:70:GLU:O | 17:N:72:LYS:CE | 2.61 | 0.49 |
| 4:4:107:GLN:HA | 20:4:301:CLA:C2A | 2.42 | 0.49 |
| 5:A:96:MET:N | 5:A:98:PHE:O | 2.46 | 0.49 |
| 5:A:146:THR:HA | 5:A:391:THR:HG23 | 1.95 | 0.49 |
| 5:A:230:ASN:C | 5:A:230:ASN:HD22 | 2.21 | 0.49 |
| 5:A:536:THR:O | 5:A:537:ALA:HB3 | 2.13 | 0.49 |
| 5:A:549:ILE:O | 5:A:552:THR:O | 2.31 | 0.49 |
| 5:A:713:LYS:HE3 | 20:F:201:CLA:H43 | 1.94 | 0.49 |
| 20:A:815:CLA:CED | 20:A:815:CLA:HAA1 | 2.43 | 0.49 |
| 20:A:818:CLA:CBB | 20:A:818:CLA:C10 | 2.90 | 0.49 |
| 6:B:53:GLN:C | 6:B:55:ALA:N | 2.63 | 0.49 |
| 6:B:60:TRP:CD1 | 20:B:809:CLA:HBC1 | 2.48 | 0.49 |
| 6:B:304:ILE:CD1 | 20:B:820:CLA:HED3 | 2.41 | 0.49 |
| 6:B:340:SER:O | 6:B:344:ILE:HG13 | 2.13 | 0.49 |
| 6:B:352:MET:HE2 | 6:B:352:MET:HB3 | 1.72 | 0.49 |
| 6:B:354:SER:OG | 20:B:827:CLA:HBC3 | 2.13 | 0.49 |
| 6:B:481:THR:O | 6:B:482:ASN:HB2 | 2.13 | 0.49 |
| 20:B:834:CLA:HMD1 | 20:B:835:CLA:C1C | 2.43 | 0.49 |
| 20:B:841:CLA:HED1 | 25:B:848:LMG:C21 | 2.43 | 0.49 |
| 9:E:69:PHE:CD2 | 9:E:70:ALA:N | 2.80 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:F:33:ALA:C | 10:F:35:ASP:H | 2.20 | 0.49 |
| 16:L:50:LEU:HG | 16:L:51:LEU:HD23 | 1.95 | 0.49 |
| 16:L:64:LEU:CD2 | 20:L:203:CLA:H201 | 2.41 | 0.49 |
| 1:1:184:PRO:N | 1:1:185:TRP:CD1 | 2.81 | 0.49 |
| 20:1:207:CLA:HAA2 | 20:1:207:CLA:CBD | 2.43 | 0.49 |
| 2:2:120:ASN:OD1 | 2:2:120:ASN:N | 2.45 | 0.49 |
| 2:2:127:ASN:OD1 | 14:J:7:TYR:CD2 | 2.65 | 0.49 |
| 2:2:166:ASN:OD1 | 2:2:169:LEU:CD1 | 2.58 | 0.49 |
| 20:4:315:CLA:HBC3 | 20:4:315:CLA:CHD | 2.42 | 0.49 |
| 5:A:59:ALA:C | 5:A:61:ALA:H | 2.21 | 0.49 |
| 5:A:73:GLU:O | 5:A:74:ILE:C | 2.56 | 0.49 |
| 5:A:100:GLY:HA3 | 5:A:153:TRP:CZ3 | 2.48 | 0.49 |
| 6:B:255:LEU:HA | 6:B:271:THR:HB | 1.95 | 0.49 |
| 6:B:361:ILE:C | 6:B:362:ALA:O | 2.56 | 0.49 |
| 20:B:814:CLA:H41 | 20:B:819:CLA:CBC | 2.43 | 0.49 |
| 7:C:52:LYS:NZ | 7:C:64:SER:OG | 2.33 | 0.49 |
| 8:D:31:GLY:O | 8:D:32:SER:CB | 2.61 | 0.49 |
| 21:D:201:LMU:O1' | 21:D:201:LMU:C4 | 2.58 | 0.49 |
| 20:L:202:CLA:HHD | 20:L:202:CLA:HBC3 | 1.95 | 0.49 |
| 19:P:1:GLC:O6 | 19:P:1:GLC:C1 | 2.60 | 0.49 |
| 2:2:98:GLU:CG | 2:2:99:LEU:HD11 | 2.42 | 0.48 |
| 4:4:104:ARG:HA | 4:4:107:GLN:NE2 | 2.28 | 0.48 |
| 4:4:116:ASN:HB3 | 4:4:118:ASP:OD1 | 2.13 | 0.48 |
| 20:4:318:CLA:HBB2 | 21:4:321:LMU:O3B | 2.08 | 0.48 |
| 5:A:107:GLU:OE1 | 5:A:161:GLU:CG | 2.59 | 0.48 |
| 5:A:221:HIS:NE2 | 20:A:814:CLA:NA | 2.61 | 0.48 |
| 5:A:711:HIS:O | 5:A:716:VAL:HG22 | 2.14 | 0.48 |
| 6:B:291:TYR:HE1 | 20:B:820:CLA:HED1 | 1.78 | 0.48 |
| 6:B:336:LEU:HD21 | 20:B:825:CLA:HBB1 | 1.94 | 0.48 |
| 6:B:715:VAL:O | 6:B:716:GLY:C | 2.56 | 0.48 |
| 20:B:831:CLA:HBA2 | 20:B:831:CLA:H3A | 1.48 | 0.48 |
| 8:D:40:ALA:HA | 8:D:44:GLU:O | 2.13 | 0.48 |
| 8:D:75:LEU:HD21 | 16:L:19:PHE:CD1 | 2.48 | 0.48 |
| 8:D:152:GLN:HA | 8:D:153:PRO:HD2 | 1.69 | 0.48 |
| 12:H:50:ARG:NH1 | 12:H:53:LEU:C | 2.67 | 0.48 |
| 15:K:44:GLU:OE1 | 15:K:45:SER:O | 2.29 | 0.48 |
| 16:L:101:MET:SD | 16:L:104:ILE:HG12 | 2.53 | 0.48 |
| 17:N:4:GLU:OE2 | 17:N:4:GLU:C | 2.56 | 0.48 |
| 17:N:35:VAL:HG12 | 17:N:37:PHE:CE1 | 2.48 | 0.48 |
| 17:N:45:ASN:HD21 | 17:N:54:LYS:HD3 | 1.68 | 0.48 |
| 2:2:191:ASN:HD21 | 2:2:194:ALA:HA | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:2:320:LMU:O2B | 21:2:320:LMU:C6' | 2.61 | 0.48 |
| 4:4:69:ILE:CG2 | 4:4:70:ILE:N | 2.47 | 0.48 |
| 5:A:212:GLY:C | 5:A:214:GLY:H | 2.20 | 0.48 |
| 20:A:804:CLA:H2A | 20:A:804:CLA:CED | 2.43 | 0.48 |
| 20:A:819:CLA:HMB2 | 20:A:823:CLA:HED2 | 1.96 | 0.48 |
| 20:A:830:CLA:H101 | 20:A:830:CLA:H143 | 1.93 | 0.48 |
| 6:B:68:VAL:O | 6:B:69:ALA:CB | 2.60 | 0.48 |
| 6:B:145:LEU:HA | 6:B:148:ILE:HD12 | 1.95 | 0.48 |
| 6:B:216:LEU:HD22 | 6:B:218:TYR:H | 1.77 | 0.48 |
| 6:B:356:PRO:HB2 | 6:B:361:ILE:CG2 | 2.44 | 0.48 |
| 6:B:462:TRP:HZ3 | 20:B:834:CLA:CBC | 2.26 | 0.48 |
| 6:B:664:LEU:O | 6:B:667:TRP:HZ3 | 1.96 | 0.48 |
| 10:F:123:VAL:O | 10:F:126:ALA:N | 2.46 | 0.48 |
| 11:G:33:LYS:O | 11:G:34:GLN:O | 2.31 | 0.48 |
| 20:H:108:CLA:HBB2 | 13:I:13:GLY:C | 2.37 | 0.48 |
| 13:I:9:VAL:H | 13:I:10:PRO:CD | 2.26 | 0.48 |
| 20:1:203:CLA:O1A | 20:1:203:CLA:C2 | 2.61 | 0.48 |
| 2:2:168:ARG:HG2 | 2:2:168:ARG:NH1 | 2.28 | 0.48 |
| 5:A:40:PHE:CE1 | 5:A:53:TRP:HD1 | 2.19 | 0.48 |
| 5:A:83:PHE:HE2 | 5:A:185:HIS:CD2 | 2.31 | 0.48 |
| 5:A:148:GLY:C | 5:A:149:PHE:O | 2.54 | 0.48 |
| 5:A:350:LEU:HA | 5:A:350:LEU:HD23 | 1.66 | 0.48 |
| 5:A:583:GLY:O | 5:A:585:GLY:N | 2.47 | 0.48 |
| 20:A:819:CLA:C2C | 20:A:825:CLA:H171 | 2.43 | 0.48 |
| 20:A:824:CLA:HAA1 | 20:A:824:CLA:HBD | 1.94 | 0.48 |
| 6:B:336:LEU:HD22 | 20:B:825:CLA:HBB1 | 1.95 | 0.48 |
| 6:B:550:LYS:CG | 6:B:550:LYS:O | 2.60 | 0.48 |
| 9:E:41:ARG:HG3 | 9:E:46:PHE:CE1 | 2.48 | 0.48 |
| 10:F:47:GLU:CG | 10:F:51:LYS:HE3 | 2.28 | 0.48 |
| 10:F:151:ASP:O | 10:F:154:PHE:CB | 2.56 | 0.48 |
| 11:G:13:GLY:HA2 | 11:G:16:LEU:CG | 2.35 | 0.48 |
| 11:G:32:ALA:O | 11:G:33:LYS:C | 2.56 | 0.48 |
| 11:G:58:LEU:HD12 | 11:G:59:LYS:HE3 | 1.95 | 0.48 |
| 16:L:32:LEU:CD1 | 20:L:204:CLA:HED1 | 2.43 | 0.48 |
| 16:L:95:LEU:O | 16:L:99:LEU:HD13 | 2.13 | 0.48 |
| 16:L:163:LEU:HD12 | 16:L:165:TYR:CG | 2.46 | 0.48 |
| 17:N:62:SER:CB | 17:N:66:ASP:HA | 2.37 | 0.48 |
| 1:1:25:ASP:O | 1:1:26:PRO:C | 2.55 | 0.48 |
| 1:1:179:THR:OG1 | 4:4:87:SER:OG | 2.16 | 0.48 |
| 2:2:167:GLY:O | 2:2:169:LEU:N | 2.47 | 0.48 |
| 2:2:178:TRP:O | 2:2:182:ILE:N | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:2:302:CLA:CGD | 20:2:302:CLA:C2A | 2.91 | 0.48 |
| 4:4:36:ASN:OD1 | 4:4:39:TRP:CD1 | 2.67 | 0.48 |
| 5:A:648:THR:C | 5:A:650:ASN:H | 2.21 | 0.48 |
| 5:A:755:ILE:O | 5:A:756:ALA:HB3 | 2.12 | 0.48 |
| 20:A:818:CLA:OBD | 20:A:827:CLA:H43 | 2.13 | 0.48 |
| 6:B:166:SER:O | 6:B:168:PHE:N | 2.44 | 0.48 |
| 6:B:464:GLN:CG | 6:B:469:LYS:HD3 | 2.42 | 0.48 |
| 6:B:528:HIS:CE1 | 20:B:839:CLA:NB | 2.81 | 0.48 |
| 20:B:837:CLA:HBC3 | 20:B:837:CLA:HMC1 | 1.94 | 0.48 |
| 9:E:52:VAL:HG12 | 9:E:53:VAL:N | 2.16 | 0.48 |
| 9:E:58:ASP:OD2 | 9:E:60:LYS:NZ | 2.38 | 0.48 |
| 11:G:21:PHE:CE1 | 22:G:104:BCR:H343 | 2.48 | 0.48 |
| 11:G:33:LYS:HA | 11:G:33:LYS:HZ2 | 1.76 | 0.48 |
| 11:G:57:LEU:O | 11:G:61:ASN:OD1 | 2.31 | 0.48 |
| 20:H:108:CLA:CMA | 20:H:108:CLA:O2A | 2.61 | 0.48 |
| 18:R:38:UNK:O | 18:R:39:UNK:C | 2.61 | 0.48 |
| 1:1:179:THR:HG21 | 4:4:87:SER:C | 2.39 | 0.48 |
| 2:2:54:TRP:NE1 | 2:2:109:ARG:HD2 | 2.29 | 0.48 |
| 3:3:157:ALA:O | 3:3:158:TYR:HD2 | 1.94 | 0.48 |
| 4:4:195:GLN:OE1 | 4:4:195:GLN:HA | 2.13 | 0.48 |
| 5:A:24:ARG:NH1 | 5:A:29:THR:CA | 2.64 | 0.48 |
| 5:A:341:GLN:HB3 | 5:A:434:ARG:NH1 | 2.28 | 0.48 |
| 5:A:430:ASP:H | 5:A:433:ASP:CG | 2.21 | 0.48 |
| 5:A:468:SER:HB2 | 5:A:476:MET:SD | 2.54 | 0.48 |
| 5:A:723:ARG:NH2 | 9:E:73:ASN:O | 2.45 | 0.48 |
| 6:B:48:ALA:HB3 | 6:B:157:LEU:HD22 | 1.93 | 0.48 |
| 6:B:172:GLU:O | 6:B:173:SER:C | 2.56 | 0.48 |
| 6:B:428:PHE:HA | 20:B:832:CLA:O1D | 2.14 | 0.48 |
| 20:B:802:CLA:NB | 20:B:803:CLA:HBB2 | 2.29 | 0.48 |
| 20:B:812:CLA:HAA2 | 20:B:812:CLA:C1 | 2.42 | 0.48 |
| 20:B:839:CLA:HBC1 | 20:F:201:CLA:HMC3 | 1.94 | 0.48 |
| 8:D:61:PRO:HD3 | 8:D:86:LEU:HD21 | 1.96 | 0.48 |
| 8:D:87:GLY:N | 8:D:90:LEU:HB3 | 2.29 | 0.48 |
| 21:E:101:LMU:H61 | 21:E:101:LMU:H11 | 1.96 | 0.48 |
| 11:G:7:VAL:HG23 | 11:G:8:ILE:N | 2.28 | 0.48 |
| 16:L:5:LYS:N | 16:L:6:PRO:HD3 | 2.28 | 0.48 |
| 1:1:89:VAL:HG12 | 11:G:77:ILE:HG21 | 1.96 | 0.48 |
| 2:2:97:VAL:HG23 | 2:2:98:GLU:H | 1.79 | 0.48 |
| 4:4:193:ILE:HG21 | 14:J:42:PHE:HD1 | 1.79 | 0.48 |
| 20:4:317:CLA:C6 | 20:4:317:CLA:C1 | 2.91 | 0.48 |
| 5:A:151:GLN:HA | 5:A:154:ARG:HG2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:281:LEU:CD2 | 20:A:816:CLA:HMA1 | 2.43 | 0.48 |
| 5:A:359:SER:OG | 5:A:414:ALA:HB2 | 2.14 | 0.48 |
| 5:A:458:PHE:CD2 | 20:B:802:CLA:CMB | 2.96 | 0.48 |
| 5:A:462:ILE:HG21 | 20:A:831:CLA:CMC | 2.36 | 0.48 |
| 5:A:603:PHE:CZ | 5:A:735:VAL:HG22 | 2.49 | 0.48 |
| 5:A:631:GLN:O | 5:A:632:GLY:C | 2.56 | 0.48 |
| 6:B:715:VAL:HG23 | 6:B:719:PHE:HD2 | 1.75 | 0.48 |
| 20:B:807:CLA:H3A | 20:B:807:CLA:HBA2 | 1.61 | 0.48 |
| 7:C:81:TYR:N | 7:C:81:TYR:CD1 | 2.82 | 0.48 |
| 21:K:106:LMU:H82 | 21:K:106:LMU:H111 | 1.76 | 0.48 |
| 4:4:36:ASN:O | 4:4:39:TRP:HE3 | 1.93 | 0.48 |
| 4:4:128:ALA:O | 4:4:130:GLU:HG2 | 2.14 | 0.48 |
| 21:4:321:LMU:C2B | 21:4:321:LMU:C5' | 2.87 | 0.48 |
| 5:A:132:LEU:HD13 | 5:A:671:SER:O | 2.14 | 0.48 |
| 5:A:257:GLN:O | 5:A:258:LEU:CB | 2.62 | 0.48 |
| 5:A:370:ILE:HD11 | 20:A:824:CLA:C3D | 2.43 | 0.48 |
| 5:A:567:ARG:NH2 | 8:D:82:GLN:OE1 | 2.44 | 0.48 |
| 5:A:685:VAL:HG12 | 5:A:741:GLY:CA | 2.42 | 0.48 |
| 6:B:625:TRP:CE3 | 6:B:625:TRP:C | 2.92 | 0.48 |
| 20:B:807:CLA:HBC3 | 20:B:830:CLA:H41 | 1.94 | 0.48 |
| 10:F:2:ILE:HD11 | 10:F:76:ASP:OD2 | 2.13 | 0.48 |
| 10:F:123:VAL:HG13 | 14:J:7:TYR:H | 1.77 | 0.48 |
| 21:H:106:LMU:C10 | 21:H:106:LMU:C6 | 2.80 | 0.48 |
| 15:K:47:LEU:O | 15:K:48:GLN:CB | 2.59 | 0.48 |
| 17:N:18:ASP:HB2 | 17:N:22:LEU:CD1 | 2.44 | 0.48 |
| 21:3:319:LMU:O2' | 21:3:319:LMU:C1 | 2.61 | 0.48 |
| 5:A:40:PHE:HZ | 5:A:56:ASN:HB3 | 1.77 | 0.48 |
| 5:A:88:ILE:C | 5:A:90:PHE:N | 2.70 | 0.48 |
| 5:A:216:LEU:HD12 | 22:A:843:BCR:H353 | 1.93 | 0.48 |
| 20:A:803:CLA:CBA | 20:A:838:CLA:H2 | 2.43 | 0.48 |
| 20:A:824:CLA:HED3 | 20:A:825:CLA:CMD | 2.28 | 0.48 |
| 6:B:433:THR:O | 6:B:436:LEU:O | 2.31 | 0.48 |
| 6:B:517:PHE:CD2 | 6:B:517:PHE:C | 2.92 | 0.48 |
| 20:B:820:CLA:H41 | 20:B:820:CLA:H61 | 1.63 | 0.48 |
| 20:B:831:CLA:HAA1 | 20:B:831:CLA:HED2 | 1.96 | 0.48 |
| 20:B:841:CLA:HBC2 | 20:B:841:CLA:CMC | 2.44 | 0.48 |
| 20:B:841:CLA:H51 | 23:B:843:PQN:H251 | 1.95 | 0.48 |
| 8:D:139:LYS:NZ | 9:E:41:ARG:NH1 | 2.62 | 0.48 |
| 12:H:36:GLN:HE22 | 20:H:110:CLA:CAD | 2.26 | 0.48 |
| 12:H:53:LEU:O | 12:H:54:LEU:HB3 | 2.13 | 0.48 |
| 1:1:149:LYS:HB3 | 20:1:206:CLA:HMC1 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:96:ILE:O | 2:2:100:VAL:HG13 | 2.14 | 0.48 |
| 5:A:154:ARG:HH21 | 5:A:233:LEU:HD13 | 1.78 | 0.48 |
| 5:A:202:MET:HG3 | 20:A:813:CLA:HBC2 | 1.95 | 0.48 |
| 5:A:622:SER:OG | 5:A:642:PHE:HB2 | 2.14 | 0.48 |
| 20:A:822:CLA:HBC1 | 22:A:844:BCR:C39 | 2.44 | 0.48 |
| 23:A:842:PQN:H243 | 23:A:842:PQN:H212 | 1.77 | 0.48 |
| 6:B:170:ASN:O | 6:B:323:TYR:OH | 2.29 | 0.48 |
| 6:B:420:SER:O | 6:B:424:TRP:N | 2.36 | 0.48 |
| 20:B:806:CLA:H191 | 10:F:104:TYR:CG | 2.48 | 0.48 |
| 20:B:823:CLA:HBA2 | 20:B:823:CLA:H3A | 1.48 | 0.48 |
| 8:D:75:LEU:HD11 | 16:L:19:PHE:CD1 | 2.49 | 0.48 |
| 21:E:101:LMU:H1B | 21:E:101:LMU:H4B | 1.47 | 0.48 |
| 10:F:62:LEU:CG | 10:F:72:ILE:HD13 | 2.41 | 0.48 |
| 11:G:60:SER:C | 11:G:62:ASP:N | 2.71 | 0.48 |
| 21:H:105:LMU:H81 | 21:H:105:LMU:H52 | 1.51 | 0.48 |
| 16:L:68:PHE:H | 16:L:68:PHE:HD1 | 1.60 | 0.48 |
| 16:L:99:LEU:O | 16:L:136:TRP:HZ3 | 1.96 | 0.48 |
| 2:2:73:ILE:H | 2:2:73:ILE:CD1 | 2.18 | 0.48 |
| 2:2:159:LEU:O | 2:2:160:ARG:C | 2.56 | 0.48 |
| 21:2:319:LMU:H2B | 21:2:319:LMU:C6B | 2.44 | 0.48 |
| 3:3:181:LEU:HD13 | 3:3:184:VAL:CG2 | 2.44 | 0.48 |
| 4:4:144:ALA:CB | 4:4:148:GLU:O | 2.61 | 0.48 |
| 5:A:22:VAL:HG23 | 5:A:23:ASP:HA | 1.70 | 0.48 |
| 5:A:24:ARG:O | 5:A:25:ASP:C | 2.55 | 0.48 |
| 5:A:38:GLY:O | 5:A:39:HIS:HB3 | 2.14 | 0.48 |
| 5:A:172:LEU:O | 5:A:175:ALA:O | 2.32 | 0.48 |
| 5:A:185:HIS:O | 5:A:186:TYR:C | 2.57 | 0.48 |
| 5:A:431:LEU:O | 5:A:435:VAL:CG1 | 2.62 | 0.48 |
| 5:A:660:GLN:HE21 | 5:A:660:GLN:H | 1.61 | 0.48 |
| 5:A:746:THR:OG1 | 20:A:849:CLA:O1D | 2.32 | 0.48 |
| 6:B:697:PRO:HB3 | 20:B:840:CLA:CBC | 2.41 | 0.48 |
| 22:B:801:BCR:H332 | 20:L:207:CLA:C2B | 2.42 | 0.48 |
| 20:B:809:CLA:H91 | 20:B:809:CLA:H161 | 1.95 | 0.48 |
| 20:B:826:CLA:CBB | 20:B:839:CLA:HMB2 | 2.43 | 0.48 |
| 9:E:73:ASN:ND2 | 9:E:78:SER:HB2 | 2.29 | 0.48 |
| 21:K:106:LMU:O2' | 21:K:106:LMU:C5' | 2.61 | 0.48 |
| 20:1:204:CLA:CMC | 20:1:210:CLA:CAC | 2.91 | 0.47 |
| 2:2:102:ILE:HG22 | 2:2:106:GLU:HG3 | 1.96 | 0.47 |
| 2:2:148:TRP:O | 2:2:150:SER:N | 2.47 | 0.47 |
| 3:3:93:PHE:N | 3:3:94:ARG:O | 2.46 | 0.47 |
| 4:4:53:LEU:O | 4:4:54:GLY:C | 2.57 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:192:THR:HG21 | 4:4:195:GLN:CA | 2.44 | 0.47 |
| 21:4:321:LMU:H5' | 21:4:321:LMU:H1B | 1.31 | 0.47 |
| 5:A:240:LYS:H | 5:A:243:PRO:HD3 | 1.78 | 0.47 |
| 5:A:309:LEU:HD21 | 20:A:819:CLA:HMC1 | 1.95 | 0.47 |
| 5:A:369:THR:O | 5:A:372:VAL:HG23 | 2.14 | 0.47 |
| 5:A:379:MET:SD | 5:A:511:THR:O | 2.71 | 0.47 |
| 5:A:506:GLY:O | 5:A:507:ALA:HB3 | 2.14 | 0.47 |
| 5:A:723:ARG:HH11 | 5:A:723:ARG:HG3 | 1.75 | 0.47 |
| 5:A:734:GLY:O | 5:A:736:THR:N | 2.47 | 0.47 |
| 20:A:818:CLA:CAB | 20:A:818:CLA:H101 | 2.44 | 0.47 |
| 20:A:831:CLA:HAA2 | 16:L:71:ALA:O | 2.14 | 0.47 |
| 6:B:30:ASP:OD2 | 6:B:396:ARG:NH1 | 2.38 | 0.47 |
| 6:B:42:LEU:O | 6:B:43:TYR:C | 2.57 | 0.47 |
| 6:B:185:VAL:HG22 | 6:B:188:LEU:HD23 | 1.96 | 0.47 |
| 6:B:628:SER:O | 6:B:629:SER:C | 2.56 | 0.47 |
| 8:D:113:HIS:HD2 | 8:D:118:VAL:HG21 | 1.77 | 0.47 |
| 16:L:125:LYS:C | 16:L:127:PRO:HD2 | 2.39 | 0.47 |
| 17:N:7:LEU:O | 17:N:8:GLU:HB2 | 2.14 | 0.47 |
| 17:N:25:THR:HG22 | 17:N:26:GLY:H | 1.79 | 0.47 |
| 1:1:34:ALA:O | 1:1:35:ASN:C | 2.57 | 0.47 |
| 4:4:142:ASN:O | 4:4:143:PHE:CD2 | 2.66 | 0.47 |
| 20:4:303:CLA:HAA2 | 20:4:303:CLA:O2D | 2.11 | 0.47 |
| 5:A:569:ILE:HB | 5:A:572:LYS:HG3 | 1.96 | 0.47 |
| 5:A:684:PHE:CD2 | 5:A:685:VAL:N | 2.74 | 0.47 |
| 20:A:818:CLA:CBB | 20:A:818:CLA:H101 | 2.44 | 0.47 |
| 20:A:826:CLA:H172 | 22:J:102:BCR:C17 | 2.43 | 0.47 |
| 20:A:831:CLA:H18 | 20:L:207:CLA:CMB | 2.43 | 0.47 |
| 6:B:373:THR:O | 6:B:377:TYR:N | 2.36 | 0.47 |
| 6:B:442:VAL:O | 6:B:446:PHE:HB2 | 2.14 | 0.47 |
| 6:B:498:LEU:HD12 | 6:B:498:LEU:O | 2.14 | 0.47 |
| 20:B:827:CLA:H41 | 20:B:827:CLA:C7 | 2.44 | 0.47 |
| 20:B:841:CLA:H192 | 13:I:21:MET:HB3 | 1.96 | 0.47 |
| 8:D:118:VAL:HG12 | 8:D:119:TYR:N | 2.29 | 0.47 |
| 9:E:50:GLY:HA3 | 9:E:69:PHE:HB2 | 1.96 | 0.47 |
| 10:F:95:GLY:O | 10:F:99:TRP:CB | 2.62 | 0.47 |
| 12:H:14:ILE:O | 12:H:14:ILE:HD13 | 2.14 | 0.47 |
| 21:H:105:LMU:H3' | 21:H:105:LMU:H5B | 1.96 | 0.47 |
| 15:K:44:GLU:O | 15:K:47:LEU:CD1 | 2.62 | 0.47 |
| 16:L:112:PRO:O | 16:L:113:SER:HB3 | 2.14 | 0.47 |
| 18:R:38:UNK:O | 18:R:42:UNK:O | 2.32 | 0.47 |
| 2:2:51:HIS:O | 2:2:54:TRP:HB2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:154:ILE:O | 4:4:157:GLY:HA3 | 2.14 | 0.47 |
| 5:A:211:LEU:O | 5:A:214:GLY:O | 2.33 | 0.47 |
| 5:A:369:THR:HG21 | 5:A:402:ILE:HG22 | 1.95 | 0.47 |
| 20:A:831:CLA:H91 | 20:A:831:CLA:H111 | 1.58 | 0.47 |
| 20:A:840:CLA:H52 | 20:A:840:CLA:H11 | 1.64 | 0.47 |
| 6:B:334:LEU:O | 6:B:334:LEU:CG | 2.60 | 0.47 |
| 6:B:420:SER:H | 6:B:422:LEU:H | 1.62 | 0.47 |
| 6:B:509:PHE:CD2 | 6:B:509:PHE:N | 2.80 | 0.47 |
| 6:B:708:VAL:C | 6:B:710:LEU:O | 2.57 | 0.47 |
| 20:B:813:CLA:C3C | 20:B:814:CLA:HBB2 | 2.41 | 0.47 |
| 12:H:66:THR:HA | 12:H:69:SER:OG | 2.13 | 0.47 |
| 17:N:41:LYS:HG3 | 17:N:42:PHE:CD2 | 2.49 | 0.47 |
| 17:N:61:LEU:CD1 | 17:N:63:ASP:CB | 2.92 | 0.47 |
| 19:Y:2:FRU:C6 | 19:Y:2:FRU:H12 | 2.44 | 0.47 |
| 1:1:18:ALA:N | 1:1:19:PRO:HD2 | 2.28 | 0.47 |
| 1:1:121:LYS:HG3 | 1:1:122:LYS:HG2 | 1.96 | 0.47 |
| 1:1:184:PRO:O | 1:1:185:TRP:NE1 | 2.48 | 0.47 |
| 21:2:318:LMU:O5B | 21:2:318:LMU:C5' | 2.58 | 0.47 |
| 3:3:192:LEU:C | 3:3:194:ILE:H | 2.23 | 0.47 |
| 3:3:195:LEU:HA | 3:3:198:PHE:HB2 | 1.96 | 0.47 |
| 4:4:126:LEU:HD23 | 4:4:127:PRO:CG | 2.44 | 0.47 |
| 21:4:321:LMU:O2B | 21:4:321:LMU:C6' | 2.61 | 0.47 |
| 5:A:227:LEU:O | 5:A:231:GLN:HB2 | 2.14 | 0.47 |
| 5:A:281:LEU:C | 5:A:283:PHE:N | 2.72 | 0.47 |
| 5:A:328:LYS:CE | 5:A:332:GLU:CG | 2.80 | 0.47 |
| 5:A:362:LEU:HD11 | 20:A:828:CLA:CBB | 2.33 | 0.47 |
| 5:A:396:PHE:CE2 | 5:A:616:PHE:CB | 2.96 | 0.47 |
| 5:A:417:PHE:CD1 | 5:A:417:PHE:C | 2.92 | 0.47 |
| 20:A:811:CLA:H141 | 20:A:811:CLA:H171 | 1.96 | 0.47 |
| 22:A:845:BCR:H312 | 20:A:851:CLA:H143 | 1.90 | 0.47 |
| 6:B:86:PRO:C | 6:B:115:ASN:HB3 | 2.40 | 0.47 |
| 6:B:309:ILE:HD12 | 6:B:312:GLY:HA3 | 1.96 | 0.47 |
| 9:E:48:ASN:ND2 | 9:E:71:LYS:HZ1 | 2.11 | 0.47 |
| 16:L:36:TYR:HE1 | 20:L:201:CLA:H93 | 1.78 | 0.47 |
| 1:1:85:LEU:HD13 | 1:1:85:LEU:H | 1.78 | 0.47 |
| 1:1:115:GLU:O | 1:1:116:LYS:HB2 | 2.14 | 0.47 |
| 2:2:205:PHE:O | 2:2:206:ALA:CB | 2.62 | 0.47 |
| 20:3:314:CLA:CGA | 20:3:314:CLA:CMA | 2.91 | 0.47 |
| 20:4:306:CLA:CGD | 20:4:306:CLA:CAA | 2.81 | 0.47 |
| 5:A:42:ARG:O | 5:A:44:ILE:HG13 | 2.15 | 0.47 |
| 5:A:99:HIS:C | 5:A:101:ALA:H | 2.21 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:103:PHE:HD2 | 5:A:103:PHE:H | 1.59 | 0.47 |
| 5:A:693:LEU:HD11 | 5:A:738:TYR:CD1 | 2.50 | 0.47 |
| 20:A:809:CLA:H51 | 22:J:102:BCR:C10 | 2.43 | 0.47 |
| 20:A:826:CLA:H18 | 20:A:826:CLA:H122 | 1.96 | 0.47 |
| 20:A:826:CLA:H2A | 20:A:826:CLA:O1D | 2.14 | 0.47 |
| 20:A:831:CLA:H141 | 20:A:831:CLA:H161 | 1.71 | 0.47 |
| 6:B:230:TRP:O | 6:B:231:ASN:C | 2.56 | 0.47 |
| 6:B:427:LEU:HB3 | 20:B:832:CLA:CED | 2.44 | 0.47 |
| 6:B:462:TRP:CZ3 | 20:B:834:CLA:CBC | 2.98 | 0.47 |
| 7:C:19:ARG:NE | 8:D:121:GLU:OE2 | 2.48 | 0.47 |
| 9:E:40:ARG:N | 9:E:46:PHE:HE1 | 2.12 | 0.47 |
| 10:F:12:LYS:HG2 | 10:F:13:GLN:H | 1.76 | 0.47 |
| 11:G:30:ASN:ND2 | 11:G:34:GLN:H | 2.13 | 0.47 |
| 16:L:33:ILE:O | 16:L:36:TYR:N | 2.47 | 0.47 |
| 17:N:47:THR:OG1 | 17:N:52:LEU:O | 2.29 | 0.47 |
| 17:N:54:LYS:CB | 17:N:57:LYS:NZ | 2.77 | 0.47 |
| 2:2:70:LYS:O | 2:2:71:LEU:C | 2.57 | 0.47 |
| 2:2:128:ASN:O | 2:2:130:LEU:CD1 | 2.60 | 0.47 |
| 4:4:75:TRP:CD1 | 20:4:310:CLA:CMD | 2.98 | 0.47 |
| 4:4:159:LEU:O | 4:4:163:PHE:HB2 | 2.15 | 0.47 |
| 5:A:53:TRP:HA | 5:A:56:ASN:CG | 2.39 | 0.47 |
| 5:A:87:SER:OG | 5:A:179:LEU:HB2 | 2.14 | 0.47 |
| 5:A:207:LEU:CB | 20:A:819:CLA:CBB | 2.90 | 0.47 |
| 5:A:237:VAL:CG2 | 5:A:242:ILE:HD12 | 2.44 | 0.47 |
| 20:A:804:CLA:HBC3 | 20:A:804:CLA:HHD | 1.95 | 0.47 |
| 6:B:387:PHE:HE2 | 20:B:826:CLA:HHC | 1.79 | 0.47 |
| 6:B:492:ILE:O | 6:B:493:TRP:HB2 | 2.14 | 0.47 |
| 6:B:668:ARG:NH2 | 6:B:672:GLN:OE1 | 2.48 | 0.47 |
| 6:B:711:VAL:O | 6:B:711:VAL:CG1 | 2.62 | 0.47 |
| 20:B:827:CLA:H8 | 22:B:846:BCR:C12 | 2.41 | 0.47 |
| 22:B:845:BCR:H382 | 22:B:845:BCR:H23C | 1.97 | 0.47 |
| 10:F:124:PRO:O | 10:F:125:LEU:HB2 | 2.14 | 0.47 |
| 21:F:202:LMU:C6' | 21:F:202:LMU:O5B | 2.62 | 0.47 |
| 11:G:41:MET:O | 11:G:42:SER:C | 2.55 | 0.47 |
| 16:L:14:LEU:HD22 | 16:L:21:GLY:O | 2.14 | 0.47 |
| 16:L:124:LYS:HB2 | 16:L:124:LYS:HZ2 | 1.80 | 0.47 |
| 20:L:204:CLA:H62 | 20:L:204:CLA:H41 | 1.56 | 0.47 |
| 20:1:206:CLA:HBC3 | 20:1:206:CLA:H121 | 1.96 | 0.47 |
| 2:2:63:PHE:CD1 | 2:2:64:ILE:N | 2.83 | 0.47 |
| 2:2:161:THR:HB | 2:2:165:LYS:HB2 | 1.97 | 0.47 |
| 20:2:316:CLA:ND | 20:2:316:CLA:H18 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:3:59:ILE:HB | 3:3:63:ARG:HH21 | 1.79 | 0.47 |
| 3:3:141:GLN:O | 3:3:142:TYR:HB2 | 2.14 | 0.47 |
| 4:4:60:LEU:HG | 4:4:61:PRO:CD | 2.36 | 0.47 |
| 4:4:99:HIS:CE1 | 4:4:103:ILE:HD13 | 2.44 | 0.47 |
| 4:4:124:TYR:HD1 | 4:4:127:PRO:HG2 | 1.80 | 0.47 |
| 4:4:126:LEU:HD23 | 4:4:127:PRO:HG3 | 1.96 | 0.47 |
| 4:4:128:ALA:HB3 | 4:4:143:PHE:CE2 | 2.38 | 0.47 |
| 4:4:169:GLN:OE1 | 20:4:304:CLA:HHD | 2.15 | 0.47 |
| 5:A:128:GLY:HA3 | 6:B:446:PHE:CD2 | 2.49 | 0.47 |
| 5:A:157:GLY:O | 5:A:248:PHE:CE1 | 2.68 | 0.47 |
| 5:A:337:PRO:HG2 | 20:A:841:CLA:C3B | 2.44 | 0.47 |
| 5:A:365:LEU:O | 5:A:369:THR:HG23 | 2.15 | 0.47 |
| 5:A:409:GLY:C | 5:A:411:ALA:N | 2.72 | 0.47 |
| 5:A:502:THR:C | 5:A:504:ALA:N | 2.67 | 0.47 |
| 5:A:744:ALA:HA | 5:A:747:TRP:HB3 | 1.95 | 0.47 |
| 20:A:818:CLA:H121 | 20:A:818:CLA:H8 | 1.74 | 0.47 |
| 20:A:826:CLA:H43 | 20:A:826:CLA:CGA | 2.44 | 0.47 |
| 22:A:845:BCR:H17C | 20:A:850:CLA:H172 | 1.96 | 0.47 |
| 20:A:851:CLA:CMA | 20:A:851:CLA:H2 | 2.44 | 0.47 |
| 6:B:80:ASP:HA | 6:B:81:PRO:HD3 | 1.55 | 0.47 |
| 6:B:124:TRP:HE1 | 6:B:129:LEU:HD22 | 1.73 | 0.47 |
| 6:B:203:ARG:HB3 | 6:B:270:LEU:CD1 | 2.44 | 0.47 |
| 6:B:460:ALA:O | 6:B:461:GLN:C | 2.57 | 0.47 |
| 6:B:596:TRP:O | 6:B:597:LYS:HB3 | 2.13 | 0.47 |
| 6:B:608:GLN:O | 6:B:612:SER:HB3 | 2.15 | 0.47 |
| 6:B:694:ARG:HH11 | 16:L:105:ALA:C | 2.23 | 0.47 |
| 6:B:714:SER:O | 6:B:718:ILE:HG22 | 2.15 | 0.47 |
| 20:B:813:CLA:H61 | 20:B:813:CLA:C1 | 2.43 | 0.47 |
| 20:B:826:CLA:CED | 20:B:827:CLA:OBD | 2.63 | 0.47 |
| 20:B:827:CLA:HMA1 | 22:B:846:BCR:H393 | 1.97 | 0.47 |
| 20:B:829:CLA:H142 | 22:B:845:BCR:C10 | 2.33 | 0.47 |
| 20:B:835:CLA:HBC2 | 20:B:835:CLA:CHD | 2.45 | 0.47 |
| 8:D:46:TYR:HE1 | 8:D:80:LYS:CE | 2.28 | 0.47 |
| 11:G:16:LEU:CA | 11:G:68:ILE:HG13 | 2.45 | 0.47 |
| 12:H:73:PRO:CD | 19:Z:2:FRU:H5 | 2.43 | 0.47 |
| 20:H:102:CLA:C10 | 20:H:102:CLA:H41 | 2.45 | 0.47 |
| 21:K:107:LMU:H52 | 21:K:107:LMU:H81 | 1.48 | 0.47 |
| 16:L:5:LYS:N | 16:L:6:PRO:CD | 2.78 | 0.47 |
| 16:L:66:GLY:N | 16:L:67:PRO:CD | 2.78 | 0.47 |
| 20:L:201:CLA:C9 | 20:L:204:CLA:H2 | 2.44 | 0.47 |
| 17:N:41:LYS:HG3 | 17:N:42:PHE:CG | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:P:1:GLC:HO2 | 19:P:2:FRU:H12 | 1.78 | 0.47 |
| 19:V:1:GLC:O2 | 19:V:2:FRU:C2 | 2.63 | 0.47 |
| 2:2:64:ILE:CG2 | 2:2:65:PRO:HD3 | 2.44 | 0.47 |
| 2:2:86:GLU:OE2 | 2:2:86:GLU:HA | 2.15 | 0.47 |
| 3:3:94:ARG:CA | 3:3:97:PHE:CD1 | 2.80 | 0.47 |
| 20:4:303:CLA:CGD | 20:4:303:CLA:H2A | 2.45 | 0.47 |
| 5:A:127:VAL:CG1 | 14:J:30:ASN:ND2 | 2.78 | 0.47 |
| 5:A:347:TYR:HE1 | 5:A:417:PHE:HZ | 1.61 | 0.47 |
| 5:A:362:LEU:HB3 | 5:A:406:LEU:O | 2.14 | 0.47 |
| 5:A:393:LEU:HD21 | 5:A:754:ILE:HG12 | 1.95 | 0.47 |
| 5:A:401:TRP:CZ3 | 5:A:609:ILE:HB | 2.49 | 0.47 |
| 5:A:466:THR:O | 5:A:470:LEU:CG | 2.62 | 0.47 |
| 5:A:473:PRO:C | 5:A:475:ASP:N | 2.71 | 0.47 |
| 5:A:592:VAL:HG23 | 5:A:593:SER:N | 2.30 | 0.47 |
| 5:A:630:ASP:C | 5:A:632:GLY:N | 2.70 | 0.47 |
| 20:A:819:CLA:C4C | 20:A:825:CLA:H172 | 2.44 | 0.47 |
| 20:A:822:CLA:HBB2 | 22:A:844:BCR:H353 | 1.96 | 0.47 |
| 20:A:831:CLA:HMD3 | 6:B:95:HIS:HD2 | 1.78 | 0.47 |
| 20:A:835:CLA:H171 | 20:L:204:CLA:CBB | 2.45 | 0.47 |
| 6:B:421:HIS:CE1 | 20:F:201:CLA:CHA | 2.98 | 0.47 |
| 6:B:493:TRP:NE1 | 20:B:817:CLA:HAC2 | 2.27 | 0.47 |
| 6:B:575:ASP:O | 6:B:579:ALA:N | 2.44 | 0.47 |
| 20:B:803:CLA:H41 | 20:B:803:CLA:CMB | 2.41 | 0.47 |
| 9:E:85:ASP:O | 9:E:85:ASP:OD1 | 2.32 | 0.47 |
| 13:I:12:VAL:HG21 | 20:I:102:CLA:CGA | 2.43 | 0.47 |
| 14:J:2:ARG:NH1 | 14:J:8:LEU:HD13 | 2.21 | 0.47 |
| 17:N:5:GLU:HA | 17:N:6:TYR:CD2 | 2.50 | 0.47 |
| 2:2:49:LEU:CB | 20:2:305:CLA:HAC2 | 2.45 | 0.47 |
| 3:3:63:ARG:NH1 | 3:3:189:LEU:H | 2.13 | 0.47 |
| 3:3:97:PHE:CE2 | 3:3:98:ILE:CG1 | 2.97 | 0.47 |
| 3:3:171:LYS:HE3 | 3:3:171:LYS:N | 2.29 | 0.47 |
| 4:4:62:GLU:O | 4:4:65:THR:HG22 | 2.14 | 0.47 |
| 4:4:69:ILE:C | 4:4:71:ASN:N | 2.70 | 0.47 |
| 5:A:98:PHE:CD1 | 5:A:98:PHE:C | 2.93 | 0.47 |
| 5:A:183:TRP:C | 5:A:185:HIS:H | 2.23 | 0.47 |
| 5:A:211:LEU:HB3 | 5:A:310:PHE:CD2 | 2.50 | 0.47 |
| 5:A:390:ALA:HA | 5:A:393:LEU:HD23 | 1.97 | 0.47 |
| 5:A:567:ARG:NH2 | 5:A:567:ARG:HB3 | 2.30 | 0.47 |
| 5:A:705:GLU:O | 5:A:706:SER:C | 2.58 | 0.47 |
| 5:A:711:HIS:NE2 | 20:A:837:CLA:HAC1 | 2.30 | 0.47 |
| 20:A:806:CLA:HMA1 | 20:A:806:CLA:H2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:A:839:CLA:O2D | 20:A:839:CLA:CAA | 2.58 | 0.47 |
| 6:B:53:GLN:HE21 | 20:B:807:CLA:HBB1 | 1.78 | 0.47 |
| 6:B:216:LEU:O | 6:B:218:TYR:N | 2.48 | 0.47 |
| 6:B:224:PRO:HB3 | 6:B:227:THR:CB | 2.43 | 0.47 |
| 6:B:486:LEU:HB2 | 6:B:489:GLY:O | 2.14 | 0.47 |
| 6:B:599:ILE:O | 6:B:734:GLY:C | 2.58 | 0.47 |
| 20:B:821:CLA:HMA2 | 11:G:21:PHE:CE2 | 2.50 | 0.47 |
| 8:D:39:LYS:HG3 | 8:D:43:GLU:HG2 | 1.96 | 0.47 |
| 8:D:99:GLN:OE1 | 8:D:101:TYR:OH | 2.33 | 0.47 |
| 20:H:101:CLA:HBC3 | 20:H:101:CLA:CMC | 2.45 | 0.47 |
| 20:J:101:CLA:H12 | 20:J:101:CLA:O1D | 2.15 | 0.47 |
| 16:L:40:LEU:CB | 16:L:41:PRO:CD | 2.90 | 0.47 |
| 17:N:46:PHE:O | 17:N:47:THR:OG1 | 2.33 | 0.47 |
| 21:2:313:LMU:C7 | 21:2:313:LMU:C3 | 2.91 | 0.47 |
| 3:3:80:LYS:HD3 | 3:3:105:ASN:HB3 | 1.91 | 0.47 |
| 4:4:36:ASN:C | 4:4:39:TRP:CE3 | 2.93 | 0.47 |
| 4:4:88:SER:HB3 | 4:4:89:THR:HG22 | 1.96 | 0.47 |
| 5:A:457:SER:OG | 5:A:544:ILE:HA | 2.15 | 0.47 |
| 5:A:508:THR:O | 5:A:509:ALA:HB3 | 2.15 | 0.47 |
| 5:A:697:ARG:CD | 6:B:566:GLY:O | 2.63 | 0.47 |
| 20:A:808:CLA:H2A | 20:A:808:CLA:O2D | 2.15 | 0.47 |
| 6:B:29:HIS:CD2 | 20:B:808:CLA:HBB1 | 2.50 | 0.47 |
| 6:B:29:HIS:CE1 | 20:B:830:CLA:H43 | 2.49 | 0.47 |
| 6:B:211:ASN:CB | 6:B:214:ASP:HB3 | 2.42 | 0.47 |
| 6:B:546:LEU:HD12 | 6:B:570:ILE:HD13 | 1.97 | 0.47 |
| 20:B:807:CLA:CHD | 22:I:103:BCR:H401 | 2.44 | 0.47 |
| 20:B:818:CLA:CBD | 20:B:827:CLA:CBB | 2.89 | 0.47 |
| 20:B:841:CLA:CHD | 23:B:843:PQN:H18 | 2.44 | 0.47 |
| 8:D:70:GLU:HB3 | 8:D:71:GLY:H | 1.48 | 0.47 |
| 9:E:69:PHE:CG | 9:E:70:ALA:N | 2.82 | 0.47 |
| 10:F:123:VAL:HG13 | 14:J:7:TYR:HB2 | 1.96 | 0.47 |
| 20:L:203:CLA:C1A | 20:L:203:CLA:CGA | 2.93 | 0.47 |
| 17:N:28:ASN:HA | 17:N:30:ALA:H | 1.79 | 0.47 |
| 20:2:302:CLA:H3A | 20:2:302:CLA:HBA2 | 1.62 | 0.46 |
| 4:4:75:TRP:CD1 | 20:4:310:CLA:HMD2 | 2.50 | 0.46 |
| 20:4:306:CLA:HAA2 | 20:4:306:CLA:O1D | 2.14 | 0.46 |
| 5:A:127:VAL:CG2 | 20:A:809:CLA:CBB | 2.94 | 0.46 |
| 5:A:539:PHE:C | 5:A:539:PHE:CD2 | 2.93 | 0.46 |
| 20:A:818:CLA:C4D | 20:A:827:CLA:H72 | 2.45 | 0.46 |
| 20:A:839:CLA:H62 | 20:A:839:CLA:H41 | 1.55 | 0.46 |
| 6:B:605:ASN:C | 6:B:605:ASN:HD22 | 2.23 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:662:MET:HE3 | 6:B:671:TRP:CH2 | 2.51 | 0.46 |
| 6:B:670:TYR:OH | 20:B:803:CLA:CAD | 2.63 | 0.46 |
| 20:B:839:CLA:CHA | 20:B:839:CLA:CBA | 2.91 | 0.46 |
| 7:C:28:MET:HA | 7:C:38:GLN:HB2 | 1.97 | 0.46 |
| 9:E:52:VAL:CG1 | 9:E:53:VAL:H | 2.15 | 0.46 |
| 12:H:14:ILE:HD11 | 12:H:17:THR:H | 1.80 | 0.46 |
| 20:H:108:CLA:CHD | 20:H:108:CLA:HBC2 | 2.45 | 0.46 |
| 22:I:103:BCR:H322 | 22:I:103:BCR:HC42 | 1.96 | 0.46 |
| 17:N:18:ASP:HB3 | 17:N:22:LEU:HG | 1.93 | 0.46 |
| 17:N:61:LEU:HG | 17:N:62:SER:N | 2.29 | 0.46 |
| 1:1:160:GLY:CA | 20:1:203:CLA:HBB2 | 2.44 | 0.46 |
| 2:2:209:THR:HG23 | 2:2:209:THR:O | 2.14 | 0.46 |
| 20:3:310:CLA:HBD | 20:3:310:CLA:HAA1 | 1.97 | 0.46 |
| 5:A:76:ARG:C | 5:A:186:TYR:HD2 | 2.23 | 0.46 |
| 5:A:159:THR:O | 5:A:160:SER:CB | 2.64 | 0.46 |
| 5:A:206:HIS:O | 5:A:211:LEU:HD23 | 2.14 | 0.46 |
| 5:A:254:LEU:C | 5:A:256:ALA:N | 2.73 | 0.46 |
| 5:A:389:TYR:CD1 | 5:A:625:TRP:CG | 3.03 | 0.46 |
| 5:A:568:LEU:O | 5:A:586:ARG:HD3 | 2.15 | 0.46 |
| 5:A:595:TRP:HE3 | 5:A:596:ASP:OD2 | 1.98 | 0.46 |
| 5:A:729:GLN:HE21 | 20:A:838:CLA:HMD1 | 1.80 | 0.46 |
| 6:B:50:HIS:CA | 6:B:53:GLN:HB2 | 2.44 | 0.46 |
| 6:B:478:LEU:O | 6:B:479:SER:HB3 | 2.13 | 0.46 |
| 6:B:658:ALA:O | 6:B:661:PHE:HD2 | 1.98 | 0.46 |
| 6:B:732:LYS:HZ2 | 6:B:732:LYS:HG3 | 1.50 | 0.46 |
| 16:L:25:THR:O | 16:L:28:THR:HB | 2.15 | 0.46 |
| 17:N:62:SER:O | 17:N:66:ASP:CG | 2.59 | 0.46 |
| 1:1:50:ALA:O | 1:1:54:VAL:HG23 | 2.15 | 0.46 |
| 1:1:54:VAL:C | 1:1:56:GLY:H | 2.23 | 0.46 |
| 2:2:183:TYR:O | 2:2:184:THR:C | 2.58 | 0.46 |
| 20:2:302:CLA:O1A | 20:2:302:CLA:C1A | 2.63 | 0.46 |
| 3:3:56:TYR:HD1 | 3:3:185:LYS:CE | 2.29 | 0.46 |
| 4:4:73:PRO:O | 4:4:74:LYS:HG3 | 2.14 | 0.46 |
| 4:4:109:ILE:HG22 | 4:4:120:ILE:HG23 | 1.96 | 0.46 |
| 4:4:128:ALA:CA | 4:4:143:PHE:CZ | 2.98 | 0.46 |
| 20:4:303:CLA:H3A | 20:4:303:CLA:HBA2 | 1.09 | 0.46 |
| 20:4:305:CLA:HED3 | 20:4:315:CLA:C1 | 2.45 | 0.46 |
| 5:A:75:SER:HB3 | 5:A:354:TRP:CZ2 | 2.50 | 0.46 |
| 5:A:156:SER:O | 5:A:158:ILE:N | 2.49 | 0.46 |
| 5:A:253:ASP:O | 5:A:256:ALA:HB3 | 2.14 | 0.46 |
| 5:A:358:LEU:O | 5:A:361:ASN:HB3 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:574:ASN:OD1 | 5:A:574:ASN:N | 2.48 | 0.46 |
| 20:A:809:CLA:CHA | 20:A:809:CLA:CBA | 2.92 | 0.46 |
| 20:A:837:CLA:H3A | 20:A:837:CLA:HBA1 | 1.64 | 0.46 |
| 6:B:436:LEU:O | 6:B:437:TYR:CB | 2.63 | 0.46 |
| 6:B:471:THR:CG2 | 6:B:502:ASN:ND2 | 2.78 | 0.46 |
| 20:B:810:CLA:H141 | 20:B:828:CLA:H91 | 1.97 | 0.46 |
| 7:C:81:TYR:N | 7:C:81:TYR:HD1 | 2.14 | 0.46 |
| 9:E:56:ASP:HB2 | 9:E:64:PRO:CB | 2.32 | 0.46 |
| 12:H:57:LEU:O | 12:H:57:LEU:HD13 | 2.14 | 0.46 |
| 20:H:101:CLA:H3A | 20:H:101:CLA:HBA1 | 1.79 | 0.46 |
| 14:J:21:SER:O | 14:J:22:LEU:C | 2.58 | 0.46 |
| 1:1:34:ALA:O | 1:1:38:ARG:N | 2.39 | 0.46 |
| 2:2:91:THR:C | 2:2:94:LEU:HB3 | 2.41 | 0.46 |
| 20:2:307:CLA:HBA1 | 21:3:318:LMU:H51 | 1.97 | 0.46 |
| 3:3:207:GLY:O | 3:3:208:PRO:C | 2.58 | 0.46 |
| 20:3:311:CLA:CMA | 20:3:311:CLA:O1A | 2.63 | 0.46 |
| 4:4:192:THR:HG21 | 4:4:195:GLN:HA | 1.98 | 0.46 |
| 5:A:81:ALA:HA | 20:A:804:CLA:HMA3 | 1.96 | 0.46 |
| 5:A:127:VAL:HG12 | 14:J:30:ASN:ND2 | 2.30 | 0.46 |
| 5:A:163:GLN:C | 5:A:165:TYR:N | 2.72 | 0.46 |
| 5:A:467:MET:HE1 | 5:A:475:ASP:C | 2.41 | 0.46 |
| 5:A:614:PHE:HE1 | 20:A:849:CLA:H62 | 1.80 | 0.46 |
| 6:B:15:ASP:O | 6:B:20:ARG:CG | 2.63 | 0.46 |
| 6:B:130:ARG:CG | 6:B:130:ARG:NH1 | 2.78 | 0.46 |
| 6:B:247:THR:O | 6:B:248:GLN:C | 2.58 | 0.46 |
| 6:B:439:HIS:HB2 | 20:B:833:CLA:C1C | 2.45 | 0.46 |
| 6:B:545:LYS:HG2 | 6:B:546:LEU:N | 2.30 | 0.46 |
| 6:B:553:PHE:O | 6:B:555:TYR:N | 2.49 | 0.46 |
| 6:B:606:VAL:C | 6:B:608:GLN:N | 2.72 | 0.46 |
| 21:B:804:LMU:H101 | 21:B:804:LMU:H61 | 1.97 | 0.46 |
| 20:B:827:CLA:C10 | 22:B:846:BCR:H14C | 2.45 | 0.46 |
| 22:B:847:BCR:H331 | 22:B:847:BCR:C8 | 2.46 | 0.46 |
| 8:D:49:THR:C | 8:D:50:TRP:HD1 | 2.23 | 0.46 |
| 10:F:40:LEU:HD12 | 10:F:42:ILE:HD11 | 1.97 | 0.46 |
| 21:K:107:LMU:O2B | 21:K:107:LMU:C5' | 2.55 | 0.46 |
| 16:L:30:SER:C | 16:L:32:LEU:H | 2.22 | 0.46 |
| 16:L:46:ALA:CB | 16:L:52:ARG:NH2 | 2.78 | 0.46 |
| 16:L:68:PHE:CD1 | 16:L:68:PHE:N | 2.84 | 0.46 |
| 19:V:2:FRU:O3 | 19:V:2:FRU:O1 | 2.33 | 0.46 |
| 2:2:72:GLY:C | 2:2:74:LEU:N | 2.69 | 0.46 |
| 2:2:112:ASP:C | 2:2:114:LEU:N | 2.72 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:2:316:CLA:H193 | 20:2:316:CLA:C15 | 2.35 | 0.46 |
| 5:A:208:ALA:HA | 5:A:310:PHE:C | 2.38 | 0.46 |
| 5:A:313:ALA:C | 5:A:315:HIS:H | 2.24 | 0.46 |
| 5:A:378:SER:OG | 20:A:825:CLA:HBC2 | 2.16 | 0.46 |
| 20:A:811:CLA:C4A | 20:A:811:CLA:CBA | 2.93 | 0.46 |
| 20:A:819:CLA:H43 | 20:A:822:CLA:H2 | 1.96 | 0.46 |
| 20:A:849:CLA:C1A | 20:B:850:CLA:HBB2 | 2.46 | 0.46 |
| 6:B:197:VAL:O | 6:B:198:ALA:CB | 2.63 | 0.46 |
| 6:B:308:HIS:HD1 | 6:B:309:ILE:N | 2.12 | 0.46 |
| 6:B:395:ILE:HD13 | 6:B:555:TYR:H | 1.80 | 0.46 |
| 20:B:808:CLA:CAB | 20:B:809:CLA:HBA2 | 2.46 | 0.46 |
| 7:C:14:CYS:SG | 7:C:14:CYS:O | 2.73 | 0.46 |
| 7:C:31:TRP:CD1 | 7:C:31:TRP:C | 2.93 | 0.46 |
| 9:E:44:TYR:HD2 | 9:E:45:TRP:HE3 | 1.62 | 0.46 |
| 9:E:90:VAL:O | 9:E:91:ALA:C | 2.58 | 0.46 |
| 12:H:23:VAL:O | 12:H:24:TYR:C | 2.59 | 0.46 |
| 2:2:73:ILE:HD12 | 2:2:73:ILE:N | 2.24 | 0.46 |
| 3:3:56:TYR:HD1 | 3:3:185:LYS:NZ | 2.12 | 0.46 |
| 4:4:125:SER:HB3 | 4:4:126:LEU:H | 1.43 | 0.46 |
| 20:4:304:CLA:HAA1 | 20:F:207:CLA:H12 | 1.97 | 0.46 |
| 5:A:72:GLU:HB2 | 5:A:73:GLU:H | 1.57 | 0.46 |
| 5:A:187:HIS:CE1 | 20:A:811:CLA:CHA | 2.95 | 0.46 |
| 5:A:356:ALA:O | 5:A:360:ILE:HG22 | 2.15 | 0.46 |
| 5:A:370:ILE:CD1 | 20:A:824:CLA:C3D | 2.94 | 0.46 |
| 5:A:374:GLN:C | 5:A:376:MET:H | 2.24 | 0.46 |
| 5:A:374:GLN:C | 5:A:376:MET:N | 2.73 | 0.46 |
| 5:A:662:SER:O | 5:A:666:GLN:HB2 | 2.15 | 0.46 |
| 6:B:54:LEU:HD11 | 20:B:814:CLA:CBA | 2.46 | 0.46 |
| 6:B:180:SER:CB | 6:B:288:GLY:HA3 | 2.38 | 0.46 |
| 6:B:231:ASN:O | 6:B:233:TYR:N | 2.48 | 0.46 |
| 6:B:233:TYR:HB3 | 6:B:254:ILE:O | 2.16 | 0.46 |
| 6:B:309:ILE:HD11 | 6:B:313:GLY:H | 1.80 | 0.46 |
| 6:B:311:PRO:HD3 | 20:B:842:CLA:C3C | 2.46 | 0.46 |
| 6:B:350:GLN:HG3 | 6:B:372:TYR:HE1 | 1.80 | 0.46 |
| 6:B:377:TYR:O | 6:B:378:ILE:HB | 2.16 | 0.46 |
| 7:C:62:PHE:CD1 | 9:E:42:GLU:HB2 | 2.51 | 0.46 |
| 20:F:207:CLA:HBD | 20:F:207:CLA:HAA2 | 1.97 | 0.46 |
| 16:L:118:LEU:HD12 | 16:L:119:THR:N | 2.21 | 0.46 |
| 18:R:38:UNK:O | 18:R:42:UNK:C | 2.64 | 0.46 |
| 21:R:106:LMU:H62 | 21:R:106:LMU:H92 | 1.62 | 0.46 |
| 3:3:165:ASN:HD22 | 3:3:165:ASN:HA | 1.59 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:33:ASP:O | 4:4:34:PRO:O | 2.32 | 0.46 |
| 4:4:142:ASN:O | 4:4:143:PHE:CB | 2.63 | 0.46 |
| 5:A:293:GLY:O | 5:A:294:LEU:HB3 | 2.15 | 0.46 |
| 5:A:392:GLN:O | 5:A:392:GLN:HG2 | 2.14 | 0.46 |
| 5:A:686:TRP:O | 5:A:689:SER:OG | 2.28 | 0.46 |
| 20:A:801:CLA:O1D | 20:A:801:CLA:CBA | 2.64 | 0.46 |
| 6:B:48:ALA:HB1 | 6:B:157:LEU:HD22 | 1.95 | 0.46 |
| 6:B:50:HIS:HB2 | 6:B:53:GLN:HB2 | 1.98 | 0.46 |
| 6:B:138:GLY:H | 6:B:140:ILE:HG12 | 1.79 | 0.46 |
| 6:B:183:PHE:HB3 | 6:B:284:PHE:HD2 | 1.81 | 0.46 |
| 6:B:350:GLN:CD | 20:B:837:CLA:HBB2 | 2.41 | 0.46 |
| 6:B:594:TRP:CD1 | 6:B:595:HIS:N | 2.84 | 0.46 |
| 6:B:625:TRP:CE3 | 6:B:626:LEU:N | 2.83 | 0.46 |
| 6:B:672:GLN:HE22 | 6:B:698:VAL:HA | 1.81 | 0.46 |
| 6:B:721:TYR:HA | 6:B:724:PHE:HB3 | 1.97 | 0.46 |
| 22:B:801:BCR:HC8 | 20:L:207:CLA:HHC | 1.97 | 0.46 |
| 20:B:824:CLA:C9 | 20:B:824:CLA:HBB2 | 2.46 | 0.46 |
| 20:B:826:CLA:CGA | 20:B:839:CLA:HAA1 | 2.46 | 0.46 |
| 9:E:53:VAL:HG12 | 9:E:54:ALA:N | 2.30 | 0.46 |
| 10:F:96:TRP:CZ2 | 20:F:205:CLA:C3B | 2.99 | 0.46 |
| 16:L:26:PRO:C | 16:L:28:THR:H | 2.22 | 0.46 |
| 17:N:46:PHE:O | 17:N:47:THR:CG2 | 2.63 | 0.46 |
| 17:N:59:PRO:CB | 17:N:75:TYR:CE1 | 2.96 | 0.46 |
| 21:R:109:LMU:O5B | 21:R:109:LMU:C5' | 2.60 | 0.46 |
| 2:2:54:TRP:CB | 20:2:310:CLA:OBD | 2.64 | 0.46 |
| 2:2:129:LYS:O | 2:2:132:GLY:HA3 | 2.14 | 0.46 |
| 22:2:317:BCR:H11C | 22:2:317:BCR:H341 | 1.64 | 0.46 |
| 3:3:97:PHE:HE2 | 3:3:98:ILE:HD13 | 0.49 | 0.46 |
| 3:3:153:SER:C | 3:3:161:GLY:HA2 | 2.40 | 0.46 |
| 20:3:310:CLA:HBB1 | 20:3:310:CLA:CHC | 2.45 | 0.46 |
| 4:4:75:TRP:CD2 | 4:4:76:TYR:N | 2.84 | 0.46 |
| 4:4:165:GLY:O | 4:4:169:GLN:CG | 2.59 | 0.46 |
| 21:4:319:LMU:H1B | 21:4:319:LMU:O1' | 2.16 | 0.46 |
| 5:A:118:PRO:HB3 | 5:A:150:PHE:CD2 | 2.50 | 0.46 |
| 5:A:246:HIS:CE1 | 20:A:840:CLA:CMA | 2.98 | 0.46 |
| 5:A:656:PHE:O | 5:A:659:ALA:N | 2.48 | 0.46 |
| 5:A:680:LEU:HB3 | 20:A:850:CLA:C1 | 2.45 | 0.46 |
| 20:A:818:CLA:HBA2 | 20:A:818:CLA:H3A | 1.34 | 0.46 |
| 20:A:850:CLA:HED2 | 20:A:850:CLA:C3D | 2.46 | 0.46 |
| 6:B:17:THR:HA | 6:B:696:LYS:N | 2.31 | 0.46 |
| 6:B:348:VAL:HG12 | 6:B:349:ALA:N | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:B:820:CLA:HMD3 | 20:B:823:CLA:HAC1 | 1.98 | 0.46 |
| 8:D:48:ILE:CB | 8:D:100:PHE:HB3 | 2.45 | 0.46 |
| 8:D:90:LEU:O | 8:D:90:LEU:HD13 | 2.16 | 0.46 |
| 11:G:44:PHE:O | 11:G:47:GLY:CA | 2.28 | 0.46 |
| 12:H:40:PHE:O | 12:H:41:GLU:C | 2.59 | 0.46 |
| 12:H:65:LEU:O | 20:H:108:CLA:H52 | 2.16 | 0.46 |
| 21:H:104:LMU:H21 | 21:H:104:LMU:C6' | 2.45 | 0.46 |
| 15:K:24:PHE:HB3 | 15:K:52:PRO:CG | 2.43 | 0.46 |
| 15:K:31:ASN:H | 15:K:32:ARG:NH1 | 2.12 | 0.46 |
| 16:L:64:LEU:CA | 16:L:67:PRO:HG2 | 2.45 | 0.46 |
| 2:2:49:LEU:HB3 | 20:2:305:CLA:HAC2 | 1.98 | 0.46 |
| 2:2:196:HIS:CE1 | 19:O:1:GLC:HO3 | 2.27 | 0.46 |
| 3:3:162:PRO:HG2 | 3:3:164:PHE:CG | 2.51 | 0.46 |
| 4:4:38:ARG:CG | 4:4:38:ARG:HH11 | 2.28 | 0.46 |
| 4:4:101:VAL:O | 4:4:104:ARG:HD3 | 2.15 | 0.46 |
| 5:A:207:LEU:O | 5:A:310:PHE:CB | 2.58 | 0.46 |
| 5:A:242:ILE:HG12 | 5:A:243:PRO:CG | 2.45 | 0.46 |
| 5:A:389:TYR:CE1 | 5:A:625:TRP:CG | 3.03 | 0.46 |
| 5:A:581:CYS:HB2 | 5:A:590:CYS:C | 2.40 | 0.46 |
| 5:A:690:LEU:HB2 | 20:A:851:CLA:HMC2 | 1.98 | 0.46 |
| 22:A:845:BCR:H11C | 22:A:845:BCR:H341 | 1.69 | 0.46 |
| 21:A:853:LMU:O6' | 21:A:853:LMU:C4 | 2.64 | 0.46 |
| 6:B:271:THR:OG1 | 6:B:272:ASP:N | 2.49 | 0.46 |
| 6:B:378:ILE:HG22 | 6:B:379:ALA:N | 2.31 | 0.46 |
| 20:B:834:CLA:O1A | 20:B:835:CLA:HMB3 | 2.16 | 0.46 |
| 7:C:77:MET:C | 7:C:79:LEU:H | 2.19 | 0.46 |
| 8:D:36:LEU:HB3 | 16:L:20:ILE:HG13 | 1.97 | 0.46 |
| 11:G:85:ILE:O | 11:G:86:LEU:HB2 | 2.14 | 0.46 |
| 21:H:105:LMU:O5B | 21:H:105:LMU:C3 | 2.59 | 0.46 |
| 1:1:44:LEU:O | 1:1:48:ARG:HG3 | 2.16 | 0.46 |
| 2:2:93:THR:HA | 2:2:96:ILE:HG12 | 1.99 | 0.46 |
| 2:2:205:PHE:CD1 | 2:2:206:ALA:CA | 2.99 | 0.46 |
| 20:2:303:CLA:HBA2 | 20:2:303:CLA:H3A | 1.34 | 0.46 |
| 3:3:97:PHE:CD2 | 3:3:98:ILE:N | 2.73 | 0.46 |
| 3:3:188:ARG:HA | 3:3:191:MET:HB2 | 1.97 | 0.46 |
| 4:4:36:ASN:O | 4:4:38:ARG:NH1 | 2.49 | 0.46 |
| 4:4:37:LEU:O | 4:4:38:ARG:C | 2.59 | 0.46 |
| 4:4:128:ALA:C | 4:4:130:GLU:N | 2.72 | 0.46 |
| 4:4:142:ASN:O | 4:4:143:PHE:CG | 2.68 | 0.46 |
| 4:4:163:PHE:O | 4:4:164:LEU:C | 2.58 | 0.46 |
| 5:A:207:LEU:CD2 | 5:A:314:GLY:HA2 | 2.43 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:567:ARG:HH11 | 8:D:35:GLY:N | 2.13 | 0.46 |
| 5:A:594:ALA:O | 5:A:598:VAL:HG23 | 2.16 | 0.46 |
| 5:A:654:ARG:HH21 | 6:B:637:PRO:HD2 | 1.80 | 0.46 |
| 20:A:838:CLA:H192 | 14:J:19:PHE:HD2 | 1.78 | 0.46 |
| 6:B:29:HIS:CB | 20:B:830:CLA:HBA1 | 2.46 | 0.46 |
| 6:B:545:LYS:CD | 6:B:546:LEU:H | 2.26 | 0.46 |
| 20:B:826:CLA:CAD | 20:B:837:CLA:CBB | 2.94 | 0.46 |
| 20:B:839:CLA:HMC1 | 20:B:839:CLA:HBC2 | 1.96 | 0.46 |
| 7:C:66:ARG:NH2 | 7:C:66:ARG:CG | 2.74 | 0.46 |
| 8:D:102:ARG:NH2 | 8:D:110:GLN:HB2 | 2.29 | 0.46 |
| 10:F:11:SER:OG | 10:F:14:PHE:HB3 | 2.16 | 0.46 |
| 10:F:24:LYS:CA | 10:F:26:GLN:H | 2.29 | 0.46 |
| 22:J:102:BCR:H393 | 22:J:102:BCR:C23 | 2.08 | 0.46 |
| 21:K:107:LMU:H61 | 21:K:107:LMU:H31 | 1.39 | 0.46 |
| 1:1:144:LYS:NZ | 20:1:201:CLA:CGD | 2.79 | 0.45 |
| 20:1:205:CLA:HMC3 | 20:1:208:CLA:CHD | 2.37 | 0.45 |
| 2:2:97:VAL:HA | 2:2:100:VAL:CG1 | 2.46 | 0.45 |
| 20:3:311:CLA:H61 | 20:3:311:CLA:H41 | 1.61 | 0.45 |
| 4:4:42:GLN:NE2 | 4:4:119:PRO:HB2 | 2.31 | 0.45 |
| 5:A:132:LEU:HD23 | 6:B:446:PHE:CE1 | 2.51 | 0.45 |
| 5:A:145:ILE:HG22 | 5:A:147:SER:H | 1.80 | 0.45 |
| 5:A:210:LEU:CD1 | 20:A:813:CLA:CMB | 2.94 | 0.45 |
| 5:A:291:THR:O | 5:A:293:GLY:N | 2.42 | 0.45 |
| 5:A:353:SER:O | 5:A:354:TRP:CB | 2.64 | 0.45 |
| 5:A:374:GLN:O | 5:A:376:MET:N | 2.49 | 0.45 |
| 5:A:409:GLY:C | 5:A:411:ALA:H | 2.23 | 0.45 |
| 5:A:458:PHE:CD1 | 5:A:458:PHE:C | 2.94 | 0.45 |
| 5:A:538:ASP:O | 5:A:542:HIS:HB2 | 2.16 | 0.45 |
| 5:A:603:PHE:HZ | 5:A:693:LEU:CD2 | 2.25 | 0.45 |
| 20:A:839:CLA:HBC3 | 20:A:839:CLA:CHD | 2.32 | 0.45 |
| 20:A:849:CLA:CBB | 20:A:850:CLA:HED1 | 2.46 | 0.45 |
| 6:B:122:GLN:HG3 | 6:B:361:ILE:CG1 | 2.43 | 0.45 |
| 6:B:292:ARG:NH2 | 20:B:821:CLA:HED1 | 2.31 | 0.45 |
| 22:B:801:BCR:C23 | 22:B:801:BCR:C38 | 2.93 | 0.45 |
| 20:B:817:CLA:HBC2 | 20:B:817:CLA:CHD | 2.37 | 0.45 |
| 8:D:139:LYS:HZ3 | 9:E:41:ARG:NH1 | 2.14 | 0.45 |
| 11:G:24:PHE:C | 11:G:26:PHE:N | 2.71 | 0.45 |
| 21:G:102:LMU:H82 | 21:G:102:LMU:H112 | 1.53 | 0.45 |
| 12:H:73:PRO:CD | 19:Z:2:FRU:C5 | 2.93 | 0.45 |
| 20:L:207:CLA:HBA1 | 20:L:207:CLA:CHA | 2.47 | 0.45 |
| 2:2:168:ARG:HH21 | 2:2:171:MET:CG | 2.29 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:189:ILE:HD13 | 2:2:189:ILE:N | 2.22 | 0.45 |
| 2:2:205:PHE:CE1 | 2:2:206:ALA:HA | 2.51 | 0.45 |
| 3:3:58:GLU:HG2 | 20:3:309:CLA:C1D | 2.46 | 0.45 |
| 5:A:95:GLY:N | 20:A:807:CLA:HMC2 | 2.28 | 0.45 |
| 5:A:284:ARG:HH12 | 5:A:507:ALA:HB1 | 1.81 | 0.45 |
| 5:A:308:ILE:HD13 | 20:A:816:CLA:H91 | 1.94 | 0.45 |
| 5:A:347:TYR:CE1 | 5:A:417:PHE:HZ | 2.33 | 0.45 |
| 5:A:458:PHE:C | 5:A:460:LEU:N | 2.73 | 0.45 |
| 5:A:520:LEU:HD13 | 21:A:846:LMU:O2' | 2.16 | 0.45 |
| 5:A:618:TRP:HB2 | 5:A:656:PHE:CE1 | 2.51 | 0.45 |
| 20:A:807:CLA:C4B | 22:J:102:BCR:H333 | 2.46 | 0.45 |
| 6:B:120:VAL:HG22 | 6:B:123:TRP:HE1 | 1.82 | 0.45 |
| 6:B:353:TYR:HB2 | 6:B:594:TRP:HH2 | 1.81 | 0.45 |
| 6:B:543:GLY:HA3 | 6:B:548:PRO:O | 2.16 | 0.45 |
| 6:B:592:PHE:CZ | 20:B:850:CLA:H62 | 2.52 | 0.45 |
| 6:B:606:VAL:C | 6:B:608:GLN:H | 2.24 | 0.45 |
| 6:B:621:ARG:HE | 6:B:621:ARG:HB3 | 1.60 | 0.45 |
| 20:B:810:CLA:H42 | 20:B:810:CLA:CHD | 2.46 | 0.45 |
| 20:B:832:CLA:HBA1 | 20:B:832:CLA:HBD | 1.98 | 0.45 |
| 20:B:832:CLA:HBC1 | 20:B:838:CLA:H151 | 1.97 | 0.45 |
| 7:C:60:THR:HG21 | 7:C:64:SER:HB3 | 1.97 | 0.45 |
| 7:C:75:ARG:HH22 | 8:D:110:GLN:CD | 2.24 | 0.45 |
| 8:D:21:ASP:HB3 | 8:D:22:PRO:HD3 | 1.98 | 0.45 |
| 22:F:204:BCR:H371 | 22:F:204:BCR:H24C | 1.72 | 0.45 |
| 11:G:31:MET:O | 11:G:34:GLN:N | 2.38 | 0.45 |
| 16:L:21:GLY:C | 16:L:23:LEU:H | 2.24 | 0.45 |
| 18:R:39:UNK:C | 18:R:42:UNK:CB | 2.92 | 0.45 |
| 2:2:79:TRP:O | 2:2:79:TRP:CD2 | 2.69 | 0.45 |
| 3:3:112:THR:HG1 | 3:3:113:LEU:H | 1.56 | 0.45 |
| 3:3:190:ALA:HB1 | 20:3:303:CLA:HMC1 | 1.98 | 0.45 |
| 20:4:318:CLA:O2D | 20:4:318:CLA:O1A | 2.33 | 0.45 |
| 20:4:318:CLA:O2D | 20:4:318:CLA:HAA2 | 2.17 | 0.45 |
| 5:A:185:HIS:O | 5:A:187:HIS:N | 2.49 | 0.45 |
| 5:A:354:TRP:O | 5:A:358:LEU:N | 2.49 | 0.45 |
| 5:A:672:LEU:C | 5:A:674:ALA:H | 2.23 | 0.45 |
| 20:A:830:CLA:C16 | 22:L:209:BCR:H361 | 2.37 | 0.45 |
| 20:A:850:CLA:CMB | 20:B:850:CLA:H18 | 2.45 | 0.45 |
| 6:B:58:PHE:CE2 | 6:B:145:LEU:HD12 | 2.51 | 0.45 |
| 6:B:247:THR:HG23 | 6:B:250:ALA:CB | 2.46 | 0.45 |
| 6:B:294:ASN:HB2 | 11:G:38:GLN:NE2 | 2.17 | 0.45 |
| 6:B:346:SER:O | 6:B:350:GLN:N | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:459:PHE:CD2 | 20:B:838:CLA:C2D | 3.00 | 0.45 |
| 6:B:471:THR:O | 6:B:472:TYR:C | 2.58 | 0.45 |
| 6:B:551:LYS:O | 6:B:553:PHE:CE2 | 2.69 | 0.45 |
| 6:B:662:MET:HG2 | 23:B:843:PQN:O1 | 2.17 | 0.45 |
| 7:C:73:THR:HB | 7:C:74:THR:H | 1.37 | 0.45 |
| 8:D:41:GLN:HG3 | 16:L:125:LYS:NZ | 2.31 | 0.45 |
| 10:F:44:ALA:HB1 | 10:F:48:LYS:HB3 | 1.97 | 0.45 |
| 12:H:37:SER:C | 12:H:39:PHE:N | 2.73 | 0.45 |
| 15:K:44:GLU:C | 15:K:46:GLY:CA | 2.88 | 0.45 |
| 21:K:107:LMU:C3 | 21:K:107:LMU:O5' | 2.63 | 0.45 |
| 17:N:61:LEU:HG | 17:N:62:SER:H | 1.81 | 0.45 |
| 21:R:102:LMU:O2' | 21:R:102:LMU:H5' | 2.16 | 0.45 |
| 1:1:183:ASP:HB3 | 1:1:185:TRP:HE1 | 1.81 | 0.45 |
| 20:1:213:CLA:HMC1 | 20:1:213:CLA:CBC | 2.40 | 0.45 |
| 4:4:58:MET:O | 4:4:61:PRO:HD3 | 2.13 | 0.45 |
| 5:A:21:LEU:HA | 5:A:22:VAL:O | 2.15 | 0.45 |
| 5:A:95:GLY:HA3 | 20:A:807:CLA:CHC | 2.46 | 0.45 |
| 5:A:126:ILE:O | 5:A:129:GLN:HB2 | 2.15 | 0.45 |
| 5:A:206:HIS:C | 5:A:211:LEU:HD23 | 2.42 | 0.45 |
| 5:A:665:ILE:C | 5:A:665:ILE:HD12 | 2.41 | 0.45 |
| 6:B:8:PHE:O | 6:B:35:ASP:CG | 2.60 | 0.45 |
| 6:B:323:TYR:HE1 | 20:B:825:CLA:HBC1 | 1.78 | 0.45 |
| 6:B:667:TRP:O | 6:B:669:GLY:N | 2.49 | 0.45 |
| 6:B:726:ILE:C | 6:B:728:SER:H | 2.23 | 0.45 |
| 10:F:131:PHE:O | 10:F:132:ARG:C | 2.58 | 0.45 |
| 20:H:109:CLA:C2C | 22:I:103:BCR:HC21 | 2.47 | 0.45 |
| 14:J:19:PHE:CD2 | 14:J:19:PHE:C | 2.93 | 0.45 |
| 19:P:1:GLC:O2 | 19:P:2:FRU:C2 | 2.63 | 0.45 |
| 2:2:126:PRO:HG2 | 2:2:129:LYS:N | 2.31 | 0.45 |
| 3:3:92:TRP:C | 3:3:95:THR:OG1 | 2.59 | 0.45 |
| 4:4:38:ARG:HG3 | 4:4:39:TRP:CA | 2.43 | 0.45 |
| 5:A:258:LEU:HG | 5:A:280:PHE:CD1 | 2.51 | 0.45 |
| 5:A:497:ALA:O | 5:A:498:LEU:HB2 | 2.17 | 0.45 |
| 5:A:618:TRP:CZ2 | 5:A:655:ASP:HB3 | 2.52 | 0.45 |
| 5:A:655:ASP:O | 5:A:660:GLN:NE2 | 2.49 | 0.45 |
| 20:A:831:CLA:C3 | 16:L:67:PRO:HB2 | 2.46 | 0.45 |
| 21:A:852:LMU:H22 | 21:A:852:LMU:H51 | 1.67 | 0.45 |
| 21:A:853:LMU:H32 | 21:A:853:LMU:H91 | 1.98 | 0.45 |
| 6:B:375:HIS:CE1 | 20:B:829:CLA:NC | 2.82 | 0.45 |
| 6:B:568:CYS:C | 6:B:570:ILE:HG23 | 2.42 | 0.45 |
| 6:B:598:HIS:O | 6:B:599:ILE:C | 2.59 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:B:801:BCR:C35 | 20:L:203:CLA:H152 | 2.47 | 0.45 |
| 20:B:824:CLA:HAA1 | 20:B:824:CLA:H12 | 1.99 | 0.45 |
| 20:B:826:CLA:H11 | 20:B:839:CLA:CBD | 2.45 | 0.45 |
| 20:B:834:CLA:H3A | 20:B:834:CLA:HBA2 | 1.40 | 0.45 |
| 20:B:834:CLA:NC | 20:B:835:CLA:CBB | 2.79 | 0.45 |
| 20:B:838:CLA:C12 | 22:F:204:BCR:C31 | 2.92 | 0.45 |
| 20:B:839:CLA:O1A | 20:B:839:CLA:C4A | 2.64 | 0.45 |
| 8:D:87:GLY:H | 8:D:90:LEU:H | 1.64 | 0.45 |
| 9:E:43:SER:CB | 9:E:82:TYR:HE1 | 2.26 | 0.45 |
| 10:F:63:CYS:CA | 10:F:69:PRO:HA | 2.43 | 0.45 |
| 11:G:19:GLY:N | 11:G:21:PHE:H | 2.15 | 0.45 |
| 16:L:65:VAL:HG11 | 16:L:154:ALA:HB1 | 1.98 | 0.45 |
| 16:L:108:LYS:O | 16:L:132:SER:CB | 2.45 | 0.45 |
| 20:L:202:CLA:O2D | 20:L:202:CLA:H2 | 2.16 | 0.45 |
| 2:2:205:PHE:O | 2:2:206:ALA:HB2 | 2.15 | 0.45 |
| 22:2:317:BCR:C8 | 22:2:317:BCR:C31 | 2.92 | 0.45 |
| 4:4:36:ASN:C | 4:4:39:TRP:CD2 | 2.95 | 0.45 |
| 20:4:305:CLA:HBC2 | 20:4:305:CLA:HMC2 | 1.95 | 0.45 |
| 5:A:64:PHE:CZ | 5:A:77:LYS:HE2 | 2.50 | 0.45 |
| 5:A:97:TYR:HA | 5:A:153:TRP:HZ2 | 1.82 | 0.45 |
| 5:A:155:ALA:O | 5:A:156:SER:C | 2.59 | 0.45 |
| 5:A:170:GLY:O | 5:A:173:VAL:CG2 | 2.59 | 0.45 |
| 5:A:471:GLY:O | 5:A:472:ARG:HG2 | 2.16 | 0.45 |
| 5:A:499:ALA:N | 5:A:500:PRO:CD | 2.79 | 0.45 |
| 20:A:808:CLA:ND | 20:A:826:CLA:H42 | 2.32 | 0.45 |
| 21:A:853:LMU:O6' | 21:A:853:LMU:C3 | 2.65 | 0.45 |
| 6:B:216:LEU:HD21 | 6:B:221:GLY:CA | 2.41 | 0.45 |
| 6:B:224:PRO:HA | 6:B:227:THR:OG1 | 2.16 | 0.45 |
| 6:B:262:HIS:O | 6:B:265:THR:O | 2.35 | 0.45 |
| 6:B:557:PHE:CE2 | 7:C:66:ARG:NE | 2.85 | 0.45 |
| 20:B:826:CLA:H3A | 20:B:826:CLA:HBA2 | 1.59 | 0.45 |
| 8:D:34:GLY:HA3 | 8:D:62:THR:HB | 1.97 | 0.45 |
| 9:E:73:ASN:ND2 | 9:E:75:ALA:H | 2.15 | 0.45 |
| 10:F:20:GLN:CD | 10:F:20:GLN:C | 2.83 | 0.45 |
| 10:F:22:LEU:C | 10:F:24:LYS:N | 2.74 | 0.45 |
| 10:F:62:LEU:HG | 10:F:72:ILE:CD1 | 2.42 | 0.45 |
| 21:H:103:LMU:C1B | 21:H:103:LMU:O6B | 2.64 | 0.45 |
| 21:1:217:LMU:H112 | 21:G:103:LMU:O5B | 2.17 | 0.45 |
| 2:2:51:HIS:CB | 20:2:310:CLA:OBD | 2.63 | 0.45 |
| 2:2:110:TRP:CD2 | 20:2:310:CLA:CED | 3.00 | 0.45 |
| 4:4:36:ASN:HB2 | 4:4:39:TRP:CH2 | 2.42 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:37:LEU:O | 4:4:39:TRP:CG | 2.70 | 0.45 |
| 4:4:76:TYR:HB2 | 20:4:310:CLA:O2D | 2.17 | 0.45 |
| 20:4:318:CLA:HBA1 | 20:4:318:CLA:HED1 | 1.99 | 0.45 |
| 20:4:318:CLA:HAA2 | 20:4:318:CLA:CGD | 2.47 | 0.45 |
| 5:A:25:ASP:CA | 5:A:27:ILE:N | 2.78 | 0.45 |
| 5:A:358:LEU:HD11 | 5:A:413:HIS:CB | 2.47 | 0.45 |
| 5:A:388:ASP:O | 5:A:390:ALA:N | 2.50 | 0.45 |
| 5:A:490:GLN:HG2 | 16:L:166:TYR:HE1 | 1.76 | 0.45 |
| 5:A:539:PHE:HE2 | 5:A:543:HIS:CE1 | 2.34 | 0.45 |
| 5:A:733:VAL:HG12 | 5:A:737:HIS:CE1 | 2.51 | 0.45 |
| 20:A:821:CLA:HAA1 | 15:K:32:ARG:NE | 2.32 | 0.45 |
| 6:B:232:LEU:HD22 | 6:B:232:LEU:HA | 1.69 | 0.45 |
| 6:B:287:GLY:O | 6:B:290:MET:HB2 | 2.16 | 0.45 |
| 6:B:411:MET:HE3 | 20:B:824:CLA:HMC2 | 1.98 | 0.45 |
| 6:B:535:VAL:CG2 | 6:B:539:LEU:HD23 | 2.47 | 0.45 |
| 6:B:570:ILE:O | 6:B:570:ILE:HG13 | 2.17 | 0.45 |
| 6:B:587:ILE:HD13 | 6:B:587:ILE:HA | 1.76 | 0.45 |
| 6:B:655:LEU:HD21 | 20:B:841:CLA:HBB1 | 1.99 | 0.45 |
| 20:B:808:CLA:NC | 20:B:830:CLA:HMB1 | 2.31 | 0.45 |
| 20:B:818:CLA:C3D | 20:B:827:CLA:HBB2 | 2.47 | 0.45 |
| 12:H:39:PHE:O | 12:H:40:PHE:CD1 | 2.69 | 0.45 |
| 21:H:105:LMU:C3 | 21:H:105:LMU:H2B | 2.46 | 0.45 |
| 1:1:51:MET:SD | 1:1:54:VAL:HB | 2.57 | 0.45 |
| 2:2:118:CYS:O | 2:2:119:VAL:CG1 | 2.52 | 0.45 |
| 20:2:303:CLA:O1A | 20:2:303:CLA:C2 | 2.64 | 0.45 |
| 3:3:94:ARG:NH1 | 3:3:98:ILE:HG23 | 2.30 | 0.45 |
| 3:3:111:TYR:HB2 | 3:3:112:THR:H | 1.68 | 0.45 |
| 4:4:100:TYR:CA | 4:4:103:ILE:HG12 | 2.42 | 0.45 |
| 21:4:320:LMU:H32 | 21:4:320:LMU:O2' | 2.16 | 0.45 |
| 5:A:34:TRP:O | 5:A:35:ALA:CB | 2.65 | 0.45 |
| 5:A:230:ASN:C | 5:A:230:ASN:ND2 | 2.75 | 0.45 |
| 5:A:284:ARG:NH1 | 5:A:507:ALA:HB1 | 2.30 | 0.45 |
| 5:A:358:LEU:C | 5:A:358:LEU:HD12 | 2.42 | 0.45 |
| 5:A:363:ALA:O | 5:A:367:SER:CB | 2.65 | 0.45 |
| 5:A:398:HIS:HD2 | 20:A:826:CLA:NC | 2.15 | 0.45 |
| 20:A:806:CLA:H51 | 20:A:828:CLA:NC | 2.32 | 0.45 |
| 6:B:29:HIS:O | 20:B:830:CLA:HAA2 | 2.16 | 0.45 |
| 6:B:278:LEU:O | 6:B:279:ALA:C | 2.59 | 0.45 |
| 6:B:323:TYR:CD1 | 20:B:825:CLA:HBC1 | 2.51 | 0.45 |
| 6:B:655:LEU:HD21 | 20:B:841:CLA:CBB | 2.46 | 0.45 |
| 6:B:704:GLN:HG3 | 25:B:848:LMG:H132 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:B:827:CLA:H122 | 22:B:846:BCR:C13 | 2.46 | 0.45 |
| 8:D:45:PHE:C | 8:D:46:TYR:CD2 | 2.92 | 0.45 |
| 21:H:105:LMU:O5B | 21:H:105:LMU:C3' | 2.49 | 0.45 |
| 17:N:48:GLY:HA3 | 17:N:49:CYS:CB | 2.47 | 0.45 |
| 17:N:61:LEU:CG | 17:N:62:SER:H | 2.29 | 0.45 |
| 19:O:1:GLC:H2 | 19:O:2:FRU:O5 | 2.17 | 0.45 |
| 1:1:34:ALA:HB3 | 1:1:137:PRO:CB | 2.47 | 0.45 |
| 21:1:217:LMU:H3O2 | 21:1:217:LMU:C1B | 2.30 | 0.45 |
| 2:2:181:HIS:CE1 | 20:2:304:CLA:ND | 2.85 | 0.45 |
| 20:2:316:CLA:HAA2 | 20:2:316:CLA:HBD | 1.99 | 0.45 |
| 4:4:94:GLU:CB | 4:4:95:PHE:HD1 | 2.26 | 0.45 |
| 4:4:108:ASP:N | 20:4:301:CLA:HMA1 | 2.32 | 0.45 |
| 4:4:123:GLN:CG | 4:4:124:TYR:N | 2.80 | 0.45 |
| 21:4:319:LMU:H1B | 21:4:319:LMU:C1' | 2.47 | 0.45 |
| 5:A:207:LEU:HA | 5:A:211:LEU:CB | 2.45 | 0.45 |
| 5:A:388:ASP:OD1 | 5:A:391:THR:HB | 2.17 | 0.45 |
| 5:A:428:TYR:CD1 | 8:D:57:ILE:HG12 | 2.52 | 0.45 |
| 5:A:654:ARG:HA | 6:B:632:ILE:CD1 | 2.44 | 0.45 |
| 5:A:731:ARG:O | 5:A:735:VAL:HG23 | 2.15 | 0.45 |
| 20:A:808:CLA:ND | 20:A:826:CLA:C4 | 2.80 | 0.45 |
| 20:A:816:CLA:HBC3 | 20:A:816:CLA:CMC | 2.47 | 0.45 |
| 20:A:830:CLA:O1A | 20:L:203:CLA:C1 | 2.62 | 0.45 |
| 6:B:190:TRP:CE3 | 20:B:815:CLA:HBB2 | 2.47 | 0.45 |
| 6:B:558:PRO:CB | 6:B:703:VAL:HB | 2.47 | 0.45 |
| 6:B:618:GLY:HA2 | 6:B:621:ARG:HB3 | 1.98 | 0.45 |
| 6:B:655:LEU:HD22 | 20:B:841:CLA:CBB | 2.46 | 0.45 |
| 6:B:673:GLU:O | 6:B:676:GLU:HB2 | 2.17 | 0.45 |
| 22:B:801:BCR:C33 | 22:B:801:BCR:C8 | 2.86 | 0.45 |
| 20:B:824:CLA:HAA1 | 20:B:824:CLA:C4 | 2.31 | 0.45 |
| 20:B:826:CLA:CED | 20:B:827:CLA:HMD1 | 2.47 | 0.45 |
| 20:B:838:CLA:C9 | 20:B:839:CLA:HAC1 | 2.47 | 0.45 |
| 9:E:36:VAL:HG22 | 9:E:52:VAL:HG22 | 1.98 | 0.45 |
| 10:F:20:GLN:HG2 | 10:F:24:LYS:HD2 | 1.99 | 0.45 |
| 10:F:96:TRP:CE3 | 10:F:134:PHE:N | 2.85 | 0.45 |
| 10:F:113:LYS:HA | 10:F:114:PRO:HD3 | 1.68 | 0.45 |
| 11:G:58:LEU:O | 11:G:60:SER:N | 2.48 | 0.45 |
| 13:I:7:LEU:HB2 | 22:I:103:BCR:H333 | 1.98 | 0.45 |
| 20:K:102:CLA:CBC | 21:K:105:LMU:C3B | 2.93 | 0.45 |
| 16:L:108:LYS:C | 16:L:108:LYS:HE2 | 2.42 | 0.45 |
| 18:R:24:UNK:O | 18:R:27:UNK:CB | 2.65 | 0.45 |
| 21:1:217:LMU:O5' | 21:1:217:LMU:H22 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:43:TRP:O | 2:2:45:VAL:N | 2.50 | 0.45 |
| 2:2:101:PHE:O | 2:2:102:ILE:C | 2.60 | 0.45 |
| 21:2:319:LMU:H31 | 21:2:319:LMU:H62 | 1.53 | 0.45 |
| 3:3:49:ILE:CG1 | 3:3:52:LYS:CB | 2.94 | 0.45 |
| 4:4:42:GLN:O | 4:4:43:ALA:C | 2.60 | 0.45 |
| 4:4:193:ILE:O | 4:4:194:VAL:C | 2.59 | 0.45 |
| 20:4:303:CLA:CGD | 20:4:303:CLA:CAA | 2.94 | 0.45 |
| 20:4:317:CLA:HBC2 | 20:4:317:CLA:CHD | 2.47 | 0.45 |
| 5:A:435:VAL:O | 5:A:438:HIS:ND1 | 2.44 | 0.45 |
| 5:A:440:ASP:HA | 6:B:677:THR:HB | 1.98 | 0.45 |
| 5:A:607:ASN:HD22 | 5:A:607:ASN:HA | 1.65 | 0.45 |
| 20:A:831:CLA:H43 | 16:L:64:LEU:CD2 | 2.42 | 0.45 |
| 6:B:29:HIS:HB3 | 20:B:808:CLA:HBB2 | 1.98 | 0.45 |
| 6:B:36:ASP:O | 6:B:41:ARG:NE | 2.50 | 0.45 |
| 6:B:594:TRP:HD1 | 6:B:595:HIS:N | 2.15 | 0.45 |
| 20:B:841:CLA:C19 | 13:I:21:MET:CB | 2.94 | 0.45 |
| 7:C:5:VAL:CG1 | 7:C:65:VAL:HG13 | 2.41 | 0.45 |
| 7:C:52:LYS:C | 7:C:54:CYS:H | 2.24 | 0.45 |
| 8:D:132:LEU:HD12 | 8:D:136:SER:OG | 2.17 | 0.45 |
| 8:D:140:ASN:HA | 8:D:142:SER:OG | 2.16 | 0.45 |
| 17:N:2:VAL:HG23 | 17:N:2:VAL:O | 2.17 | 0.45 |
| 17:N:57:LYS:HE2 | 17:N:57:LYS:HB2 | 1.44 | 0.45 |
| 18:R:38:UNK:C | 18:R:42:UNK:CA | 2.94 | 0.45 |
| 1:1:27:LEU:O | 1:1:31:GLU:HB2 | 2.16 | 0.44 |
| 21:1:218:LMU:H5' | 21:1:218:LMU:H1B | 1.59 | 0.44 |
| 2:2:51:HIS:CA | 2:2:54:TRP:HB2 | 2.47 | 0.44 |
| 2:2:163:GLU:CD | 20:2:307:CLA:CAC | 2.89 | 0.44 |
| 3:3:189:LEU:C | 3:3:191:MET:N | 2.74 | 0.44 |
| 4:4:58:MET:SD | 4:4:59:LEU:HA | 2.56 | 0.44 |
| 4:4:184:HIS:ND1 | 4:4:184:HIS:C | 2.75 | 0.44 |
| 20:4:305:CLA:CMC | 20:4:305:CLA:CBC | 2.89 | 0.44 |
| 5:A:143:ILE:HG12 | 20:A:808:CLA:HBC2 | 1.99 | 0.44 |
| 5:A:360:ILE:HD13 | 22:A:844:BCR:C37 | 2.43 | 0.44 |
| 5:A:648:THR:O | 5:A:649:ILE:HG22 | 2.16 | 0.44 |
| 5:A:733:VAL:HG13 | 20:A:838:CLA:C3D | 2.47 | 0.44 |
| 20:A:809:CLA:HBB1 | 6:B:446:PHE:HE2 | 1.82 | 0.44 |
| 20:A:832:CLA:O1A | 20:A:833:CLA:HBC3 | 2.17 | 0.44 |
| 21:A:847:LMU:O1' | 21:A:847:LMU:O6B | 2.29 | 0.44 |
| 6:B:217:PRO:HB2 | 6:B:218:TYR:HD1 | 1.82 | 0.44 |
| 6:B:389:HIS:HE1 | 20:B:830:CLA:NC | 2.15 | 0.44 |
| 6:B:444:LEU:O | 6:B:445:ALA:CB | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:458:ILE:HG13 | 6:B:459:PHE:CD1 | 2.53 | 0.44 |
| 6:B:732:LYS:CB | 6:B:732:LYS:HZ3 | 2.16 | 0.44 |
| 20:B:816:CLA:O1D | 20:B:816:CLA:H2A | 2.17 | 0.44 |
| 20:B:832:CLA:NB | 10:F:90:PHE:CE1 | 2.85 | 0.44 |
| 8:D:131:GLY:O | 8:D:132:LEU:HB2 | 2.15 | 0.44 |
| 9:E:38:ILE:HB | 9:E:46:PHE:O | 2.18 | 0.44 |
| 10:F:144:LEU:HD12 | 10:F:149:LEU:HD13 | 1.99 | 0.44 |
| 11:G:16:LEU:CD2 | 11:G:68:ILE:HG21 | 2.47 | 0.44 |
| 11:G:32:ALA:C | 11:G:34:GLN:N | 2.75 | 0.44 |
| 11:G:79:HIS:NE2 | 11:G:82:ALA:HB2 | 2.33 | 0.44 |
| 12:H:19:GLY:O | 12:H:20:GLN:CB | 2.63 | 0.44 |
| 20:H:108:CLA:H41 | 16:L:87:ALA:HB2 | 1.98 | 0.44 |
| 17:N:57:LYS:O | 17:N:60:PHE:N | 2.49 | 0.44 |
| 1:1:29:LEU:C | 1:1:33:PRO:HD3 | 2.43 | 0.44 |
| 2:2:63:PHE:HE2 | 2:2:168:ARG:CD | 2.30 | 0.44 |
| 2:2:102:ILE:HD13 | 2:2:102:ILE:N | 2.32 | 0.44 |
| 2:2:185:GLY:O | 2:2:186:THR:C | 2.60 | 0.44 |
| 21:2:313:LMU:H4' | 21:2:313:LMU:H1' | 1.46 | 0.44 |
| 3:3:74:ALA:N | 20:3:306:CLA:C2D | 2.80 | 0.44 |
| 21:3:319:LMU:H22 | 21:3:319:LMU:H51 | 1.85 | 0.44 |
| 4:4:73:PRO:HG2 | 20:4:310:CLA:HMD1 | 1.99 | 0.44 |
| 4:4:144:ALA:O | 4:4:147:LEU:O | 2.35 | 0.44 |
| 20:4:304:CLA:CAA | 20:F:207:CLA:H42 | 2.40 | 0.44 |
| 5:A:157:GLY:O | 5:A:248:PHE:HE1 | 2.00 | 0.44 |
| 5:A:209:GLY:HA3 | 5:A:213:LEU:HD12 | 1.99 | 0.44 |
| 5:A:258:LEU:HG | 5:A:280:PHE:CE1 | 2.52 | 0.44 |
| 5:A:345:GLY:C | 5:A:347:TYR:N | 2.76 | 0.44 |
| 5:A:362:LEU:CD1 | 20:A:828:CLA:HBB2 | 2.34 | 0.44 |
| 5:A:570:PRO:C | 5:A:572:LYS:H | 2.24 | 0.44 |
| 5:A:723:ARG:O | 20:A:837:CLA:CBB | 2.66 | 0.44 |
| 20:A:826:CLA:HBD | 20:A:826:CLA:HAA1 | 1.98 | 0.44 |
| 20:B:827:CLA:H71 | 22:B:846:BCR:C14 | 2.47 | 0.44 |
| 7:C:29:ILE:CG2 | 8:D:126:GLY:CA | 2.95 | 0.44 |
| 12:H:55:LYS:O | 12:H:56:PHE:HB2 | 2.18 | 0.44 |
| 16:L:23:LEU:O | 16:L:25:THR:N | 2.50 | 0.44 |
| 16:L:67:PRO:O | 16:L:71:ALA:HB3 | 2.18 | 0.44 |
| 16:L:123:ARG:HB3 | 16:L:126:GLN:HG3 | 1.97 | 0.44 |
| 16:L:163:LEU:HD12 | 16:L:164:PRO:CA | 2.44 | 0.44 |
| 17:N:4:GLU:O | 17:N:4:GLU:CG | 2.64 | 0.44 |
| 1:1:168:TYR:N | 1:1:169:PRO:HD3 | 2.32 | 0.44 |
| 1:1:179:THR:HB | 1:1:180:HIS:H | 1.49 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:2:314:CLA:C2 | 20:2:314:CLA:CAA | 2.94 | 0.44 |
| 4:4:139:ASN:HD22 | 4:4:139:ASN:HA | 1.62 | 0.44 |
| 5:A:126:ILE:O | 5:A:126:ILE:HD12 | 2.17 | 0.44 |
| 5:A:558:LYS:HZ2 | 6:B:674:LEU:HB3 | 1.80 | 0.44 |
| 5:A:567:ARG:HH11 | 8:D:34:GLY:C | 2.26 | 0.44 |
| 20:A:818:CLA:ND | 20:A:827:CLA:H72 | 2.32 | 0.44 |
| 20:A:826:CLA:H191 | 20:A:850:CLA:H13 | 1.98 | 0.44 |
| 21:A:846:LMU:H22 | 21:A:846:LMU:H51 | 1.77 | 0.44 |
| 6:B:174:ARG:C | 6:B:176:ASN:H | 2.25 | 0.44 |
| 6:B:290:MET:O | 6:B:290:MET:HG2 | 2.16 | 0.44 |
| 6:B:362:ALA:O | 6:B:363:GLN:CG | 2.61 | 0.44 |
| 6:B:390:GLY:HA3 | 22:B:846:BCR:HC22 | 1.98 | 0.44 |
| 6:B:454:LEU:HD13 | 10:F:69:PRO:O | 2.18 | 0.44 |
| 6:B:467:HIS:NE2 | 20:B:834:CLA:CHA | 2.80 | 0.44 |
| 7:C:39:ILE:HG23 | 7:C:40:ALA:N | 2.31 | 0.44 |
| 8:D:28:ILE:O | 8:D:66:ALA:HB3 | 2.18 | 0.44 |
| 8:D:28:ILE:HG13 | 8:D:66:ALA:HB1 | 1.98 | 0.44 |
| 8:D:33:THR:HG23 | 16:L:23:LEU:HD12 | 1.98 | 0.44 |
| 10:F:23:LYS:C | 10:F:26:GLN:H | 2.25 | 0.44 |
| 15:K:3:ILE:HD13 | 15:K:3:ILE:O | 2.17 | 0.44 |
| 16:L:65:VAL:O | 16:L:69:VAL:N | 2.51 | 0.44 |
| 1:1:56:GLY:HA3 | 20:1:205:CLA:C4D | 2.48 | 0.44 |
| 1:1:149:LYS:HB3 | 20:1:206:CLA:HMC3 | 2.00 | 0.44 |
| 21:2:318:LMU:H3' | 21:2:318:LMU:H5B | 1.99 | 0.44 |
| 3:3:50:GLU:OE1 | 3:3:54:LEU:HB2 | 2.17 | 0.44 |
| 5:A:22:VAL:CA | 5:A:24:ARG:HA | 2.48 | 0.44 |
| 5:A:22:VAL:HG12 | 5:A:24:ARG:HA | 1.99 | 0.44 |
| 5:A:349:ILE:HD13 | 5:A:422:TYR:HB3 | 1.99 | 0.44 |
| 5:A:639:ALA:O | 5:A:640:GLY:C | 2.61 | 0.44 |
| 20:A:851:CLA:H2 | 20:A:851:CLA:HMA2 | 1.98 | 0.44 |
| 6:B:260:GLY:H | 6:B:269:TRP:NE1 | 2.16 | 0.44 |
| 6:B:356:PRO:HB2 | 6:B:361:ILE:HG22 | 2.00 | 0.44 |
| 6:B:431:PHE:CD2 | 20:B:832:CLA:CMA | 2.98 | 0.44 |
| 6:B:447:GLY:O | 6:B:449:PRO:HD3 | 2.18 | 0.44 |
| 20:B:803:CLA:O2A | 20:B:803:CLA:C3A | 2.61 | 0.44 |
| 20:B:803:CLA:HED3 | 20:B:803:CLA:CBA | 2.48 | 0.44 |
| 20:B:840:CLA:HMD1 | 20:L:203:CLA:HBB2 | 1.99 | 0.44 |
| 8:D:30:ALA:O | 16:L:18:PRO:CB | 2.59 | 0.44 |
| 10:F:22:LEU:HA | 10:F:25:LEU:HD13 | 1.99 | 0.44 |
| 10:F:116:GLN:HE21 | 10:F:116:GLN:HB2 | 1.60 | 0.44 |
| 11:G:10:LEU:HD23 | 11:G:13:GLY:HA3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:G:92:GLY:C | 11:G:94:ASP:OD1 | 2.61 | 0.44 |
| 15:K:43:ARG:HA | 15:K:43:ARG:HD2 | 1.48 | 0.44 |
| 16:L:65:VAL:HG23 | 16:L:66:GLY:H | 1.82 | 0.44 |
| 1:1:144:LYS:C | 1:1:146:LYS:H | 2.26 | 0.44 |
| 3:3:164:PHE:HD1 | 3:3:164:PHE:HA | 1.71 | 0.44 |
| 4:4:32:GLU:O | 4:4:33:ASP:OD1 | 2.35 | 0.44 |
| 4:4:36:ASN:CA | 4:4:39:TRP:CE3 | 3.01 | 0.44 |
| 4:4:75:TRP:HD1 | 20:4:310:CLA:HHD | 1.80 | 0.44 |
| 5:A:183:TRP:C | 5:A:185:HIS:N | 2.76 | 0.44 |
| 5:A:260:PRO:HG3 | 5:A:277:TYR:CZ | 2.52 | 0.44 |
| 5:A:277:TYR:HD2 | 5:A:279:ASP:H | 1.64 | 0.44 |
| 5:A:420:ARG:HG2 | 5:A:421:ASP:N | 2.31 | 0.44 |
| 5:A:473:PRO:O | 5:A:474:GLN:C | 2.61 | 0.44 |
| 5:A:631:GLN:HG2 | 5:A:633:VAL:HG13 | 1.98 | 0.44 |
| 20:A:820:CLA:H3A | 20:A:820:CLA:HBA2 | 1.75 | 0.44 |
| 20:A:826:CLA:H72 | 22:A:845:BCR:C37 | 2.45 | 0.44 |
| 20:A:831:CLA:H92 | 20:A:831:CLA:H62 | 1.73 | 0.44 |
| 21:A:853:LMU:O6' | 21:A:853:LMU:C5 | 2.60 | 0.44 |
| 6:B:188:LEU:HG | 6:B:189:ALA:N | 2.32 | 0.44 |
| 6:B:202:SER:O | 6:B:245:GLY:CA | 2.50 | 0.44 |
| 6:B:202:SER:HB3 | 6:B:270:LEU:HD21 | 1.99 | 0.44 |
| 6:B:257:ILE:HA | 6:B:272:ASP:OD2 | 2.17 | 0.44 |
| 6:B:395:ILE:HG22 | 6:B:551:LYS:HG3 | 2.00 | 0.44 |
| 6:B:545:LYS:CG | 6:B:546:LEU:N | 2.79 | 0.44 |
| 6:B:568:CYS:HB3 | 6:B:569:ASP:H | 1.65 | 0.44 |
| 6:B:573:TRP:O | 6:B:576:PHE:HB3 | 2.18 | 0.44 |
| 20:B:821:CLA:HMA2 | 11:G:21:PHE:CD2 | 2.53 | 0.44 |
| 22:B:844:BCR:H24C | 22:B:844:BCR:H371 | 1.58 | 0.44 |
| 22:B:847:BCR:C33 | 22:B:847:BCR:C8 | 2.93 | 0.44 |
| 7:C:28:MET:HB2 | 8:D:121:GLU:HA | 1.98 | 0.44 |
| 12:H:77:LEU:HB3 | 12:H:78:PRO:CD | 2.47 | 0.44 |
| 21:H:104:LMU:H61 | 21:H:104:LMU:H31 | 1.52 | 0.44 |
| 20:K:101:CLA:HAA2 | 20:K:101:CLA:HBD | 1.99 | 0.44 |
| 20:L:202:CLA:CED | 20:L:202:CLA:H72 | 2.47 | 0.44 |
| 17:N:58:VAL:O | 17:N:60:PHE:N | 2.51 | 0.44 |
| 17:N:67:LEU:CA | 17:N:68:GLU:HG2 | 2.47 | 0.44 |
| 20:2:302:CLA:CHD | 20:2:302:CLA:CBC | 2.88 | 0.44 |
| 3:3:173:GLU:CD | 3:3:174:LYS:N | 2.74 | 0.44 |
| 4:4:115:VAL:HG13 | 4:4:116:ASN:N | 2.32 | 0.44 |
| 5:A:222:GLN:O | 5:A:227:LEU:HD12 | 2.18 | 0.44 |
| 5:A:335:LYS:CG | 5:A:336:GLY:N | 2.67 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:419:VAL:HG21 | 5:A:577:PHE:HB2 | 2.00 | 0.44 |
| 23:A:842:PQN:H293 | 23:A:842:PQN:H261 | 1.87 | 0.44 |
| 6:B:22:TRP:HE1 | 20:B:840:CLA:HBB2 | 1.75 | 0.44 |
| 6:B:53:GLN:O | 6:B:54:LEU:HB2 | 2.16 | 0.44 |
| 6:B:190:TRP:CE2 | 20:B:819:CLA:HMD1 | 2.52 | 0.44 |
| 6:B:326:ILE:O | 6:B:326:ILE:HG12 | 2.17 | 0.44 |
| 6:B:365:PHE:HB3 | 6:B:602:TRP:CZ2 | 2.53 | 0.44 |
| 6:B:517:PHE:O | 6:B:517:PHE:CG | 2.69 | 0.44 |
| 6:B:700:LEU:N | 23:B:843:PQN:O4 | 2.34 | 0.44 |
| 20:B:803:CLA:H202 | 20:B:803:CLA:H162 | 1.72 | 0.44 |
| 20:B:829:CLA:H3A | 20:B:829:CLA:HBA2 | 1.52 | 0.44 |
| 8:D:83:CYS:O | 8:D:83:CYS:SG | 2.75 | 0.44 |
| 9:E:86:GLU:O | 9:E:87:VAL:C | 2.61 | 0.44 |
| 20:J:101:CLA:O1D | 20:J:101:CLA:H2A | 2.18 | 0.44 |
| 16:L:68:PHE:HD1 | 16:L:68:PHE:N | 2.14 | 0.44 |
| 21:L:210:LMU:H52 | 21:L:210:LMU:H82 | 1.81 | 0.44 |
| 17:N:54:LYS:HA | 17:N:54:LYS:HD2 | 1.32 | 0.44 |
| 21:R:106:LMU:O2' | 21:R:106:LMU:H21 | 2.18 | 0.44 |
| 2:2:164:ILE:O | 2:2:168:ARG:NH1 | 2.50 | 0.44 |
| 20:2:307:CLA:H142 | 20:2:307:CLA:H112 | 1.67 | 0.44 |
| 3:3:94:ARG:C | 3:3:97:PHE:CD1 | 2.91 | 0.44 |
| 20:3:314:CLA:H112 | 20:3:314:CLA:H72 | 1.28 | 0.44 |
| 4:4:88:SER:C | 4:4:89:THR:HG22 | 2.43 | 0.44 |
| 4:4:142:ASN:HA | 4:4:150:LYS:NZ | 2.21 | 0.44 |
| 4:4:143:PHE:N | 4:4:150:LYS:HE2 | 2.33 | 0.44 |
| 20:4:301:CLA:CBC | 20:4:301:CLA:CHD | 2.85 | 0.44 |
| 5:A:34:TRP:O | 5:A:35:ALA:HB3 | 2.18 | 0.44 |
| 5:A:64:PHE:HZ | 5:A:77:LYS:HE2 | 1.79 | 0.44 |
| 5:A:254:LEU:C | 5:A:256:ALA:H | 2.25 | 0.44 |
| 5:A:509:ALA:O | 5:A:510:SER:OG | 2.25 | 0.44 |
| 20:A:819:CLA:HMD1 | 20:A:821:CLA:CBB | 2.27 | 0.44 |
| 21:A:854:LMU:O6' | 21:A:854:LMU:C1' | 2.65 | 0.44 |
| 6:B:190:TRP:CZ3 | 20:B:815:CLA:HMB2 | 2.52 | 0.44 |
| 6:B:230:TRP:CE3 | 20:B:817:CLA:HAA2 | 2.52 | 0.44 |
| 6:B:387:PHE:O | 6:B:391:PRO:HG3 | 2.17 | 0.44 |
| 7:C:73:THR:N | 7:C:76:SER:OG | 2.50 | 0.44 |
| 8:D:41:GLN:CD | 8:D:41:GLN:C | 2.86 | 0.44 |
| 22:G:104:BCR:H15C | 22:G:104:BCR:H351 | 1.86 | 0.44 |
| 20:K:104:CLA:H41 | 20:K:104:CLA:C9 | 2.44 | 0.44 |
| 2:2:100:VAL:HG22 | 2:2:101:PHE:N | 2.32 | 0.44 |
| 2:2:137:TYR:CD1 | 2:2:138:PRO:CD | 3.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:4:69:ILE:CG1 | 4:4:175:LYS:HB2 | 2.48 | 0.44 |
| 4:4:86:SER:O | 4:4:88:SER:N | 2.49 | 0.44 |
| 4:4:108:ASP:OD2 | 4:4:108:ASP:C | 2.58 | 0.44 |
| 5:A:239:PRO:CA | 5:A:242:ILE:HD11 | 2.43 | 0.44 |
| 5:A:274:TRP:NE1 | 5:A:277:TYR:CE2 | 2.86 | 0.44 |
| 20:A:831:CLA:HBA1 | 20:A:831:CLA:H3A | 1.45 | 0.44 |
| 22:A:843:BCR:C31 | 22:A:843:BCR:C8 | 2.80 | 0.44 |
| 20:A:849:CLA:HBB1 | 6:B:624:LEU:HD11 | 2.00 | 0.44 |
| 6:B:244:PHE:C | 6:B:244:PHE:CD2 | 2.95 | 0.44 |
| 6:B:597:LYS:HG2 | 20:B:837:CLA:HBC1 | 2.00 | 0.44 |
| 10:F:22:LEU:C | 10:F:23:LYS:HD3 | 2.42 | 0.44 |
| 11:G:12:THR:HG22 | 11:G:72:LEU:CD1 | 2.46 | 0.44 |
| 11:G:60:SER:O | 11:G:61:ASN:C | 2.61 | 0.44 |
| 20:G:105:CLA:H12 | 20:G:105:CLA:H52 | 1.75 | 0.44 |
| 20:J:103:CLA:CHA | 20:J:103:CLA:CED | 2.94 | 0.44 |
| 20:J:103:CLA:HBA2 | 20:J:103:CLA:H3A | 1.25 | 0.44 |
| 16:L:64:LEU:HD21 | 20:L:203:CLA:H202 | 2.00 | 0.44 |
| 16:L:64:LEU:CG | 20:L:203:CLA:H201 | 2.48 | 0.44 |
| 17:N:62:SER:CB | 17:N:66:ASP:OD1 | 2.65 | 0.44 |
| 17:N:62:SER:O | 17:N:63:ASP:CG | 2.61 | 0.44 |
| 17:N:62:SER:O | 17:N:63:ASP:HB2 | 2.17 | 0.44 |
| 1:1:161:PHE:HB2 | 1:1:164:GLN:CD | 2.42 | 0.44 |
| 2:2:206:ALA:O | 2:2:207:ALA:CB | 2.66 | 0.44 |
| 3:3:50:GLU:OE2 | 3:3:54:LEU:HD13 | 2.17 | 0.44 |
| 4:4:104:ARG:HE | 4:4:105:ARG:CA | 2.31 | 0.44 |
| 5:A:41:SER:O | 5:A:44:ILE:CA | 2.61 | 0.44 |
| 5:A:308:ILE:HD12 | 20:A:816:CLA:HHC | 2.00 | 0.44 |
| 5:A:430:ASP:O | 5:A:432:LEU:N | 2.51 | 0.44 |
| 5:A:472:ARG:HG3 | 6:B:97:GLY:HA2 | 1.99 | 0.44 |
| 5:A:672:LEU:C | 5:A:674:ALA:N | 2.75 | 0.44 |
| 5:A:701:GLN:NE2 | 5:A:701:GLN:HA | 2.33 | 0.44 |
| 20:A:822:CLA:CHD | 22:A:844:BCR:C20 | 2.95 | 0.44 |
| 6:B:144:PHE:O | 6:B:144:PHE:HD2 | 1.98 | 0.44 |
| 6:B:160:LYS:CG | 6:B:161:TRP:H | 2.30 | 0.44 |
| 6:B:193:HIS:HD2 | 20:B:815:CLA:NC | 2.16 | 0.44 |
| 6:B:513:GLY:O | 6:B:515:GLY:N | 2.51 | 0.44 |
| 22:B:801:BCR:H23C | 22:B:801:BCR:H383 | 1.99 | 0.44 |
| 20:B:808:CLA:H71 | 20:B:825:CLA:O1A | 2.17 | 0.44 |
| 8:D:139:LYS:HG2 | 8:D:141:VAL:HG22 | 2.00 | 0.44 |
| 9:E:43:SER:HB2 | 9:E:82:TYR:CE1 | 2.39 | 0.44 |
| 10:F:96:TRP:HE3 | 10:F:133:GLY:C | 2.25 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:G:8:ILE:O | 11:G:8:ILE:CG1 | 2.63 | 0.44 |
| 21:H:103:LMU:O6B | 21:H:103:LMU:H1B | 2.17 | 0.44 |
| 20:H:108:CLA:HBA1 | 20:H:108:CLA:H3A | 1.59 | 0.44 |
| 20:J:101:CLA:H2A | 20:J:101:CLA:O2A | 2.18 | 0.44 |
| 15:K:14:THR:O | 15:K:18:MET:HG2 | 2.17 | 0.44 |
| 16:L:33:ILE:HG12 | 20:L:201:CLA:H42 | 2.00 | 0.44 |
| 16:L:69:VAL:HG11 | 16:L:84:GLY:H | 1.83 | 0.44 |
| 17:N:37:PHE:CD2 | 17:N:37:PHE:N | 2.84 | 0.44 |
| 2:2:62:ILE:HG13 | 2:2:66:GLU:OE2 | 2.18 | 0.43 |
| 20:2:303:CLA:H43 | 20:2:303:CLA:NC | 2.32 | 0.43 |
| 3:3:111:TYR:HB2 | 3:3:112:THR:HG22 | 2.00 | 0.43 |
| 4:4:108:ASP:O | 4:4:111:ASN:C | 2.61 | 0.43 |
| 4:4:179:ASP:H | 4:4:184:HIS:CD2 | 2.36 | 0.43 |
| 5:A:24:ARG:HH12 | 5:A:29:THR:HA | 1.77 | 0.43 |
| 5:A:84:GLY:C | 5:A:87:SER:O | 2.61 | 0.43 |
| 5:A:299:ILE:HD11 | 20:A:818:CLA:HMA1 | 2.00 | 0.43 |
| 5:A:346:LEU:O | 5:A:347:TYR:HB2 | 2.17 | 0.43 |
| 5:A:365:LEU:O | 5:A:369:THR:CG2 | 2.66 | 0.43 |
| 5:A:411:ALA:O | 5:A:412:ALA:C | 2.61 | 0.43 |
| 5:A:584:PRO:CB | 7:C:67:VAL:HB | 2.48 | 0.43 |
| 5:A:660:GLN:O | 5:A:661:ALA:HB3 | 2.17 | 0.43 |
| 20:A:803:CLA:CBB | 20:A:804:CLA:NC | 2.81 | 0.43 |
| 20:A:826:CLA:H193 | 20:A:826:CLA:H162 | 1.83 | 0.43 |
| 6:B:25:ILE:H | 6:B:25:ILE:HG13 | 1.57 | 0.43 |
| 6:B:297:ILE:HG21 | 11:G:21:PHE:HZ | 1.82 | 0.43 |
| 6:B:615:TYR:OH | 6:B:621:ARG:NH2 | 2.50 | 0.43 |
| 20:B:818:CLA:C1A | 20:B:818:CLA:H12 | 2.48 | 0.43 |
| 20:B:838:CLA:HBB2 | 20:B:838:CLA:C8 | 2.45 | 0.43 |
| 7:C:51:CYS:N | 24:C:102:SF4:S4 | 2.86 | 0.43 |
| 8:D:96:ILE:O | 8:D:97:LYS:CB | 2.66 | 0.43 |
| 11:G:43:HIS:N | 11:G:43:HIS:HD1 | 2.16 | 0.43 |
| 20:H:101:CLA:H2 | 20:H:101:CLA:H61 | 1.84 | 0.43 |
| 13:I:15:LEU:HD12 | 13:I:18:ALA:HB3 | 2.00 | 0.43 |
| 15:K:51:ASP:CB | 15:K:52:PRO:CD | 2.92 | 0.43 |
| 21:K:106:LMU:O6' | 21:K:106:LMU:C1B | 2.64 | 0.43 |
| 17:N:5:GLU:CD | 17:N:5:GLU:C | 2.86 | 0.43 |
| 17:N:35:VAL:HG12 | 17:N:37:PHE:CZ | 2.53 | 0.43 |
| 17:N:82:PHE:H | 17:N:82:PHE:HD2 | 1.66 | 0.43 |
| 20:1:204:CLA:CHA | 20:1:204:CLA:HBA1 | 2.39 | 0.43 |
| 2:2:114:LEU:O | 2:2:116:PRO:HD3 | 2.19 | 0.43 |
| 2:2:208:PHE:O | 2:2:209:THR:HB | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:2:211:LYS:O | 20:2:308:CLA:C3B | 2.66 | 0.43 |
| 21:3:319:LMU:O2B | 21:3:319:LMU:C5B | 2.66 | 0.43 |
| 4:4:123:GLN:CG | 4:4:124:TYR:H | 2.32 | 0.43 |
| 4:4:129:GLY:C | 4:4:131:VAL:N | 2.61 | 0.43 |
| 4:4:147:LEU:O | 4:4:148:GLU:O | 2.36 | 0.43 |
| 5:A:70:ASP:O | 5:A:71:LEU:C | 2.61 | 0.43 |
| 5:A:131:ILE:CG2 | 5:A:132:LEU:N | 2.81 | 0.43 |
| 5:A:210:LEU:CD1 | 20:A:813:CLA:HMB3 | 2.49 | 0.43 |
| 5:A:473:PRO:C | 5:A:475:ASP:H | 2.26 | 0.43 |
| 5:A:499:ALA:C | 5:A:501:GLY:H | 2.25 | 0.43 |
| 5:A:571:ASP:O | 5:A:574:ASN:ND2 | 2.51 | 0.43 |
| 5:A:578:ARG:HG2 | 5:A:595:TRP:CD1 | 2.53 | 0.43 |
| 5:A:679:PHE:O | 5:A:679:PHE:CD2 | 2.70 | 0.43 |
| 20:A:803:CLA:HBB1 | 20:A:804:CLA:C1C | 2.47 | 0.43 |
| 20:A:827:CLA:CMD | 20:A:827:CLA:H52 | 2.48 | 0.43 |
| 6:B:29:HIS:CB | 20:B:808:CLA:HBB2 | 2.48 | 0.43 |
| 6:B:50:HIS:HA | 6:B:53:GLN:H | 1.84 | 0.43 |
| 6:B:274:ALA:O | 6:B:278:LEU:HB2 | 2.18 | 0.43 |
| 6:B:275:HIS:HD1 | 20:B:818:CLA:HMB3 | 1.82 | 0.43 |
| 6:B:353:TYR:C | 6:B:355:LEU:N | 2.76 | 0.43 |
| 6:B:710:LEU:HA | 6:B:713:PHE:HB3 | 2.00 | 0.43 |
| 20:B:810:CLA:HMD2 | 20:B:828:CLA:HBA1 | 2.00 | 0.43 |
| 20:B:822:CLA:CBA | 20:B:823:CLA:O1A | 2.66 | 0.43 |
| 20:B:825:CLA:H61 | 20:B:825:CLA:CMA | 2.48 | 0.43 |
| 20:B:832:CLA:HBB2 | 22:F:203:BCR:C25 | 2.48 | 0.43 |
| 20:B:832:CLA:CBB | 22:F:203:BCR:C23 | 2.96 | 0.43 |
| 20:B:832:CLA:CBB | 22:F:203:BCR:H23C | 2.48 | 0.43 |
| 11:G:43:HIS:CE1 | 11:G:45:GLU:CG | 2.96 | 0.43 |
| 21:H:104:LMU:H41 | 21:H:104:LMU:O6' | 2.18 | 0.43 |
| 13:I:4:LEU:HG | 13:I:4:LEU:O | 2.18 | 0.43 |
| 13:I:10:PRO:O | 13:I:11:LEU:C | 2.60 | 0.43 |
| 17:N:63:ASP:HA | 17:N:64:ASP:O | 2.17 | 0.43 |
| 17:N:66:ASP:C | 17:N:67:LEU:CG | 2.91 | 0.43 |
| 2:2:96:ILE:O | 2:2:100:VAL:CG1 | 2.66 | 0.43 |
| 3:3:114:PHE:CD1 | 20:3:308:CLA:CHA | 3.01 | 0.43 |
| 20:3:313:CLA:HAA2 | 20:3:313:CLA:HBD | 2.00 | 0.43 |
| 4:4:98:SER:O | 4:4:102:GLU:CG | 2.66 | 0.43 |
| 5:A:73:GLU:HA | 5:A:76:ARG:HD2 | 1.99 | 0.43 |
| 20:A:805:CLA:HBA1 | 20:A:805:CLA:H3A | 1.68 | 0.43 |
| 20:A:824:CLA:C6 | 20:A:825:CLA:CED | 2.93 | 0.43 |
| 6:B:564:ARG:CZ | 7:C:64:SER:OG | 2.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:B:815:CLA:H71 | 20:B:815:CLA:H111 | 1.50 | 0.43 |
| 10:F:80:TRP:HZ3 | 20:F:206:CLA:HMC1 | 1.83 | 0.43 |
| 21:F:202:LMU:H82 | 21:F:202:LMU:C3 | 2.46 | 0.43 |
| 11:G:16:LEU:CD2 | 11:G:68:ILE:CG2 | 2.89 | 0.43 |
| 14:J:38:THR:O | 14:J:39:PHE:CB | 2.66 | 0.43 |
| 16:L:58:LEU:CD2 | 16:L:153:TRP:CZ2 | 3.01 | 0.43 |
| 16:L:115:ALA:N | 16:L:116:PRO:CD | 2.77 | 0.43 |
| 17:N:70:GLU:O | 17:N:72:LYS:NZ | 2.51 | 0.43 |
| 2:2:54:TRP:O | 2:2:55:ALA:C | 2.62 | 0.43 |
| 3:3:47:GLY:C | 3:3:49:ILE:N | 2.76 | 0.43 |
| 4:4:34:PRO:HB3 | 4:4:35:GLU:HB2 | 1.99 | 0.43 |
| 4:4:70:ILE:CG1 | 4:4:71:ASN:N | 2.80 | 0.43 |
| 4:4:89:THR:O | 4:4:92:VAL:CB | 2.59 | 0.43 |
| 4:4:118:ASP:HA | 4:4:122:LYS:HA | 1.99 | 0.43 |
| 4:4:139:ASN:HA | 4:4:140:PRO:HD3 | 1.85 | 0.43 |
| 4:4:193:ILE:CG2 | 4:4:194:VAL:N | 2.74 | 0.43 |
| 5:A:84:GLY:O | 5:A:87:SER:O | 2.36 | 0.43 |
| 5:A:216:LEU:CD1 | 22:A:843:BCR:H352 | 2.48 | 0.43 |
| 5:A:555:ILE:H | 5:A:555:ILE:HG12 | 1.55 | 0.43 |
| 5:A:582:ASP:OD1 | 7:C:53:ARG:NH2 | 2.52 | 0.43 |
| 5:A:650:ASN:C | 5:A:652:TRP:N | 2.75 | 0.43 |
| 20:A:825:CLA:H111 | 20:A:825:CLA:H151 | 1.52 | 0.43 |
| 6:B:91:ILE:CD1 | 6:B:104:PHE:HE2 | 2.24 | 0.43 |
| 6:B:183:PHE:HB3 | 6:B:284:PHE:CD2 | 2.52 | 0.43 |
| 6:B:285:LEU:HD11 | 20:B:821:CLA:HBC2 | 1.98 | 0.43 |
| 6:B:416:GLU:O | 6:B:420:SER:OG | 2.36 | 0.43 |
| 6:B:440:ASN:CG | 6:B:614:THR:O | 2.61 | 0.43 |
| 6:B:590:VAL:O | 6:B:593:TYR:HB3 | 2.18 | 0.43 |
| 20:B:806:CLA:HBC1 | 22:F:203:BCR:C33 | 2.49 | 0.43 |
| 20:B:810:CLA:CMC | 22:B:847:BCR:C28 | 2.92 | 0.43 |
| 20:B:833:CLA:H3A | 20:B:833:CLA:HBA1 | 1.63 | 0.43 |
| 10:F:23:LYS:CB | 10:F:24:LYS:NZ | 2.80 | 0.43 |
| 11:G:59:LYS:HD3 | 11:G:59:LYS:HA | 1.83 | 0.43 |
| 13:I:11:LEU:HD13 | 13:I:11:LEU:O | 2.19 | 0.43 |
| 20:J:103:CLA:O1A | 20:J:103:CLA:C16 | 2.66 | 0.43 |
| 17:N:61:LEU:O | 17:N:62:SER:O | 2.36 | 0.43 |
| 17:N:72:LYS:HZ1 | 17:N:74:LYS:CE | 2.13 | 0.43 |
| 21:R:109:LMU:O5B | 21:R:109:LMU:C6' | 2.66 | 0.43 |
| 21:1:216:LMU:O6' | 21:1:216:LMU:H1' | 2.18 | 0.43 |
| 21:1:217:LMU:H4' | 21:G:103:LMU:O6' | 2.19 | 0.43 |
| 3:3:94:ARG:NH2 | 3:3:97:PHE:CE2 | 2.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:78:VAL:O | 5:A:82:HIS:CB | 2.65 | 0.43 |
| 5:A:85:GLN:O | 5:A:88:ILE:HG22 | 2.18 | 0.43 |
| 5:A:113:PRO:O | 5:A:115:HIS:CD2 | 2.72 | 0.43 |
| 5:A:149:PHE:C | 5:A:151:GLN:H | 2.26 | 0.43 |
| 5:A:210:LEU:HD13 | 20:A:813:CLA:CMB | 2.48 | 0.43 |
| 5:A:223:VAL:CG1 | 5:A:224:HIS:N | 2.80 | 0.43 |
| 5:A:249:ILE:C | 5:A:251:ASN:N | 2.71 | 0.43 |
| 5:A:250:LEU:C | 5:A:252:ARG:H | 2.27 | 0.43 |
| 5:A:250:LEU:O | 5:A:252:ARG:HG2 | 2.19 | 0.43 |
| 5:A:347:TYR:HE1 | 5:A:417:PHE:CZ | 2.36 | 0.43 |
| 5:A:530:LEU:HB2 | 5:A:531:PRO:CD | 2.43 | 0.43 |
| 5:A:541:VAL:O | 5:A:544:ILE:HG22 | 2.17 | 0.43 |
| 5:A:679:PHE:CE2 | 5:A:683:HIS:CD2 | 3.03 | 0.43 |
| 6:B:317:ARG:HD3 | 6:B:410:ARG:HG2 | 2.00 | 0.43 |
| 6:B:438:VAL:O | 6:B:442:VAL:HG23 | 2.17 | 0.43 |
| 6:B:475:ASP:HA | 6:B:480:SER:C | 2.44 | 0.43 |
| 6:B:707:LEU:HD11 | 20:B:830:CLA:C9 | 2.49 | 0.43 |
| 22:B:846:BCR:C8 | 22:B:846:BCR:H311 | 2.48 | 0.43 |
| 7:C:64:SER:O | 7:C:65:VAL:HB | 2.19 | 0.43 |
| 11:G:48:ASP:N | 11:G:49:THR:HG22 | 2.31 | 0.43 |
| 12:H:42:THR:O | 12:H:45:ALA:N | 2.52 | 0.43 |
| 14:J:32:PHE:HE2 | 14:J:33:PHE:CZ | 2.36 | 0.43 |
| 17:N:47:THR:O | 17:N:52:LEU:O | 2.36 | 0.43 |
| 21:R:106:LMU:O2' | 21:R:106:LMU:C4 | 2.67 | 0.43 |
| 4:4:39:TRP:CD1 | 4:4:41:VAL:H | 2.36 | 0.43 |
| 4:4:40:PHE:CD1 | 4:4:40:PHE:N | 2.77 | 0.43 |
| 5:A:87:SER:HA | 5:A:90:PHE:HB2 | 1.99 | 0.43 |
| 5:A:91:LEU:O | 20:A:807:CLA:HMC2 | 2.17 | 0.43 |
| 5:A:338:PHE:C | 5:A:338:PHE:CD2 | 2.96 | 0.43 |
| 5:A:570:PRO:C | 5:A:572:LYS:N | 2.77 | 0.43 |
| 5:A:685:VAL:CG1 | 5:A:741:GLY:HA2 | 2.44 | 0.43 |
| 6:B:81:PRO:HG2 | 6:B:360:PHE:CE1 | 2.52 | 0.43 |
| 21:B:804:LMU:H1B | 21:B:804:LMU:O6' | 2.18 | 0.43 |
| 8:D:48:ILE:HA | 8:D:100:PHE:HB3 | 1.99 | 0.43 |
| 9:E:46:PHE:CD2 | 9:E:47:LYS:N | 2.86 | 0.43 |
| 10:F:20:GLN:NE2 | 10:F:21:ALA:N | 2.67 | 0.43 |
| 16:L:9:GLN:C | 16:L:11:ILE:N | 2.72 | 0.43 |
| 16:L:136:TRP:O | 16:L:140:THR:HG23 | 2.19 | 0.43 |
| 17:N:50:GLN:N | 17:N:51:ASP:O | 2.51 | 0.43 |
| 17:N:82:PHE:N | 17:N:82:PHE:CD2 | 2.86 | 0.43 |
| 20:R:107:CLA:CED | 20:R:107:CLA:C1A | 2.96 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:Q:2:FRU:H62 | 19:Q:2:FRU:C1 | 2.48 | 0.43 |
| 21:1:217:LMU:H42 | 21:1:217:LMU:H11 | 1.67 | 0.43 |
| 2:2:64:ILE:HG22 | 2:2:65:PRO:HD3 | 2.01 | 0.43 |
| 21:3:319:LMU:H42 | 21:3:319:LMU:H72 | 1.48 | 0.43 |
| 20:4:303:CLA:H122 | 20:4:303:CLA:H161 | 1.41 | 0.43 |
| 20:4:304:CLA:H92 | 20:4:304:CLA:H61 | 1.88 | 0.43 |
| 5:A:57:LEU:O | 5:A:61:ALA:HB2 | 2.18 | 0.43 |
| 5:A:96:MET:HE1 | 20:A:807:CLA:HBB2 | 2.00 | 0.43 |
| 5:A:147:SER:OG | 20:A:826:CLA:HED2 | 2.19 | 0.43 |
| 5:A:287:LEU:N | 5:A:295:TRP:HE1 | 2.16 | 0.43 |
| 5:A:342:GLY:O | 5:A:343:HIS:C | 2.61 | 0.43 |
| 5:A:462:ILE:O | 5:A:466:THR:OG1 | 2.34 | 0.43 |
| 5:A:709:TRP:CE3 | 5:A:710:ALA:N | 2.87 | 0.43 |
| 20:A:831:CLA:H111 | 20:A:831:CLA:H142 | 1.58 | 0.43 |
| 6:B:31:PHE:HB2 | 6:B:42:LEU:CD1 | 2.49 | 0.43 |
| 6:B:334:LEU:HD22 | 20:B:808:CLA:CHD | 2.49 | 0.43 |
| 6:B:555:TYR:CE2 | 6:B:573:TRP:HA | 2.54 | 0.43 |
| 20:B:810:CLA:H2 | 20:B:810:CLA:H71 | 2.00 | 0.43 |
| 20:B:814:CLA:C19 | 20:B:819:CLA:OBD | 2.66 | 0.43 |
| 20:B:835:CLA:CBB | 22:B:846:BCR:C28 | 2.95 | 0.43 |
| 21:E:101:LMU:C6' | 21:E:101:LMU:O3' | 2.67 | 0.43 |
| 11:G:28:ARG:NH2 | 11:G:28:ARG:CG | 2.74 | 0.43 |
| 20:H:108:CLA:O1D | 20:H:108:CLA:OBD | 2.32 | 0.43 |
| 13:I:12:VAL:HG21 | 20:I:102:CLA:CBA | 2.49 | 0.43 |
| 13:I:26:LEU:HD22 | 13:I:30:LYS:HA | 2.01 | 0.43 |
| 16:L:51:LEU:O | 16:L:52:ARG:C | 2.62 | 0.43 |
| 21:R:101:LMU:H1B | 21:R:101:LMU:H3' | 1.25 | 0.43 |
| 1:1:143:LEU:HD23 | 1:1:143:LEU:HA | 1.89 | 0.43 |
| 21:1:217:LMU:H4' | 21:G:103:LMU:C6' | 2.49 | 0.43 |
| 2:2:54:TRP:CD1 | 20:2:310:CLA:O1D | 2.72 | 0.43 |
| 2:2:100:VAL:HG22 | 2:2:101:PHE:H | 1.84 | 0.43 |
| 21:2:319:LMU:H11 | 21:2:319:LMU:H42 | 1.85 | 0.43 |
| 3:3:96:GLY:C | 3:3:97:PHE:CG | 2.95 | 0.43 |
| 3:3:158:TYR:C | 3:3:160:GLY:H | 2.25 | 0.43 |
| 4:4:99:HIS:C | 4:4:99:HIS:HD1 | 2.25 | 0.43 |
| 5:A:58:HIS:HB3 | 20:A:804:CLA:HBC1 | 2.00 | 0.43 |
| 5:A:246:HIS:HE1 | 20:A:840:CLA:CMA | 2.24 | 0.43 |
| 5:A:495:THR:O | 5:A:495:THR:OG1 | 2.37 | 0.43 |
| 6:B:439:HIS:CD2 | 6:B:439:HIS:C | 2.96 | 0.43 |
| 6:B:486:LEU:O | 6:B:487:ASN:HB3 | 2.19 | 0.43 |
| 6:B:556:SER:O | 25:B:848:LMG:HC2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:B:835:CLA:HMB1 | 22:B:846:BCR:C28 | 2.48 | 0.43 |
| 8:D:80:LYS:HD3 | 8:D:112:LEU:HD21 | 2.01 | 0.43 |
| 9:E:32:ARG:NH2 | 9:E:53:VAL:HA | 2.33 | 0.43 |
| 10:F:115:THR:O | 10:F:116:GLN:CB | 2.67 | 0.43 |
| 11:G:58:LEU:HB2 | 11:G:59:LYS:H | 1.40 | 0.43 |
| 16:L:88:ALA:O | 16:L:90:GLY:N | 2.45 | 0.43 |
| 16:L:164:PRO:N | 16:L:165:TYR:CD1 | 2.86 | 0.43 |
| 1:1:63:LEU:HD22 | 1:1:63:LEU:H | 1.84 | 0.43 |
| 1:1:160:GLY:C | 1:1:162:CYS:H | 2.27 | 0.43 |
| 20:1:213:CLA:HBA2 | 20:1:213:CLA:HMA3 | 1.99 | 0.43 |
| 2:2:85:GLN:OE1 | 2:2:85:GLN:CA | 2.61 | 0.43 |
| 20:2:311:CLA:HBC3 | 20:2:311:CLA:CMC | 2.47 | 0.43 |
| 4:4:86:SER:C | 4:4:88:SER:N | 2.76 | 0.43 |
| 5:A:348:GLU:O | 5:A:350:LEU:N | 2.51 | 0.43 |
| 5:A:397:THR:HB | 5:A:613:ILE:HG13 | 1.98 | 0.43 |
| 5:A:447:ASN:ND2 | 6:B:678:LEU:HD21 | 2.34 | 0.43 |
| 5:A:450:CYS:HB3 | 20:B:803:CLA:HBA1 | 2.00 | 0.43 |
| 5:A:654:ARG:HG3 | 5:A:655:ASP:N | 2.34 | 0.43 |
| 20:A:826:CLA:H18 | 20:A:850:CLA:H18 | 2.00 | 0.43 |
| 20:A:849:CLA:CAA | 20:B:850:CLA:HBB2 | 2.45 | 0.43 |
| 6:B:60:TRP:HH2 | 20:B:829:CLA:CHB | 2.32 | 0.43 |
| 6:B:288:GLY:O | 6:B:289:LEU:CB | 2.66 | 0.43 |
| 6:B:449:PRO:C | 6:B:450:GLU:O | 2.61 | 0.43 |
| 6:B:674:LEU:C | 6:B:674:LEU:CD1 | 2.92 | 0.43 |
| 20:B:832:CLA:C4B | 10:F:90:PHE:CE1 | 3.02 | 0.43 |
| 7:C:77:MET:C | 7:C:79:LEU:N | 2.76 | 0.43 |
| 8:D:84:LEU:HD12 | 8:D:100:PHE:CZ | 2.49 | 0.43 |
| 10:F:24:LYS:O | 10:F:27:ALA:HB3 | 2.18 | 0.43 |
| 10:F:26:GLN:C | 10:F:28:SER:H | 2.27 | 0.43 |
| 12:H:24:TYR:HB3 | 12:H:25:GLY:H | 1.59 | 0.43 |
| 21:H:103:LMU:C6B | 21:H:103:LMU:C2B | 2.95 | 0.43 |
| 20:H:110:CLA:H3A | 20:H:110:CLA:HBA2 | 1.55 | 0.43 |
| 22:I:101:BCR:H371 | 22:I:101:BCR:H24C | 1.57 | 0.43 |
| 16:L:65:VAL:C | 16:L:69:VAL:HG22 | 2.43 | 0.43 |
| 17:N:65:LEU:C | 17:N:65:LEU:CD2 | 2.91 | 0.43 |
| 19:P:1:GLC:O2 | 19:P:2:FRU:C1 | 2.66 | 0.43 |
| 2:2:54:TRP:HZ2 | 2:2:109:ARG:CB | 2.32 | 0.43 |
| 2:2:181:HIS:CE1 | 20:2:304:CLA:C4D | 3.01 | 0.43 |
| 3:3:94:ARG:NH2 | 3:3:98:ILE:CD1 | 2.82 | 0.43 |
| 4:4:127:PRO:C | 4:4:143:PHE:HZ | 2.20 | 0.43 |
| 4:4:151:GLU:CA | 4:4:154:ILE:HG23 | 2.40 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:4:301:CLA:HBD | 20:4:301:CLA:HAA1 | 2.00 | 0.43 |
| 5:A:110:LEU:O | 5:A:113:PRO:HD3 | 2.19 | 0.43 |
| 5:A:119:SER:CB | 5:A:136:VAL:HG21 | 2.48 | 0.43 |
| 5:A:128:GLY:HA3 | 6:B:446:PHE:HD2 | 1.83 | 0.43 |
| 5:A:132:LEU:HD21 | 5:A:674:ALA:HB2 | 2.00 | 0.43 |
| 5:A:229:ILE:HG13 | 5:A:243:PRO:HB3 | 2.00 | 0.43 |
| 5:A:567:ARG:HH22 | 8:D:82:GLN:CD | 2.27 | 0.43 |
| 5:A:588:GLY:HA3 | 6:B:668:ARG:CD | 2.28 | 0.43 |
| 5:A:701:GLN:O | 5:A:702:GLU:C | 2.62 | 0.43 |
| 20:A:826:CLA:C18 | 22:J:102:BCR:H17C | 2.46 | 0.43 |
| 20:A:831:CLA:H2A | 20:A:831:CLA:O2D | 2.18 | 0.43 |
| 6:B:193:HIS:O | 6:B:194:LEU:C | 2.62 | 0.43 |
| 21:B:849:LMU:H3' | 21:B:849:LMU:H1B | 1.47 | 0.43 |
| 7:C:44:ARG:NH2 | 8:D:127:ARG:NE | 2.65 | 0.43 |
| 21:E:101:LMU:C6' | 21:E:101:LMU:H3O2 | 2.32 | 0.43 |
| 17:N:39:SER:OG | 17:N:40:CYS:N | 2.52 | 0.43 |
| 21:R:106:LMU:O5B | 21:R:106:LMU:C6' | 2.57 | 0.43 |
| 1:1:34:ALA:HB3 | 1:1:137:PRO:HB3 | 2.01 | 0.42 |
| 2:2:73:ILE:O | 2:2:73:ILE:HG22 | 2.19 | 0.42 |
| 3:3:132:TRP:CE3 | 3:3:155:GLU:HG2 | 2.26 | 0.42 |
| 20:3:314:CLA:H143 | 20:3:314:CLA:H162 | 1.85 | 0.42 |
| 4:4:101:VAL:O | 4:4:104:ARG:CD | 2.67 | 0.42 |
| 20:4:318:CLA:O2D | 20:4:318:CLA:CAA | 2.67 | 0.42 |
| 5:A:182:GLY:CA | 20:A:811:CLA:HAC1 | 2.49 | 0.42 |
| 5:A:197:GLN:HE22 | 5:A:351:THR:CB | 2.26 | 0.42 |
| 5:A:210:LEU:HD12 | 20:A:813:CLA:HMB3 | 2.01 | 0.42 |
| 5:A:346:LEU:HD11 | 20:A:822:CLA:HHD | 2.01 | 0.42 |
| 5:A:412:ALA:O | 5:A:415:ALA:HB3 | 2.18 | 0.42 |
| 5:A:434:ARG:O | 5:A:435:VAL:C | 2.61 | 0.42 |
| 5:A:606:TYR:HB2 | 5:A:739:LEU:CD2 | 2.49 | 0.42 |
| 20:A:801:CLA:O1D | 20:A:801:CLA:HBA2 | 2.19 | 0.42 |
| 6:B:127:ILE:HD13 | 6:B:193:HIS:CE1 | 2.53 | 0.42 |
| 6:B:290:MET:HG3 | 20:B:822:CLA:C2C | 2.49 | 0.42 |
| 6:B:378:ILE:H | 6:B:381:PHE:HD1 | 1.67 | 0.42 |
| 6:B:649:MET:HG2 | 22:B:847:BCR:H381 | 2.01 | 0.42 |
| 6:B:683:GLU:CD | 6:B:683:GLU:H | 2.27 | 0.42 |
| 20:B:809:CLA:HHB | 20:B:830:CLA:CBB | 2.30 | 0.42 |
| 23:B:843:PQN:H161 | 22:B:847:BCR:H331 | 1.95 | 0.42 |
| 22:B:845:BCR:H15C | 22:B:845:BCR:H351 | 1.85 | 0.42 |
| 14:J:13:VAL:CG1 | 14:J:15:SER:HB2 | 2.48 | 0.42 |
| 14:J:25:LEU:HA | 14:J:28:GLU:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:K:47:LEU:O | 15:K:48:GLN:CD | 2.62 | 0.42 |
| 16:L:126:GLN:O | 16:L:127:PRO:O | 2.37 | 0.42 |
| 22:L:209:BCR:H341 | 22:L:209:BCR:H11C | 1.81 | 0.42 |
| 17:N:61:LEU:CD1 | 17:N:62:SER:N | 2.80 | 0.42 |
| 2:2:56:MET:SD | 2:2:169:LEU:HD23 | 2.59 | 0.42 |
| 2:2:196:HIS:HB3 | 2:2:197:LEU:H | 1.54 | 0.42 |
| 20:2:307:CLA:HBD | 20:2:307:CLA:HAA1 | 2.01 | 0.42 |
| 3:3:109:ASP:O | 3:3:109:ASP:CG | 2.62 | 0.42 |
| 3:3:204:THR:C | 3:3:206:VAL:H | 2.27 | 0.42 |
| 4:4:104:ARG:HD2 | 20:4:312:CLA:C3C | 2.42 | 0.42 |
| 4:4:194:VAL:HG12 | 4:4:195:GLN:HB3 | 1.98 | 0.42 |
| 5:A:259:TYR:HB3 | 5:A:260:PRO:CD | 2.38 | 0.42 |
| 5:A:361:ASN:ND2 | 20:A:805:CLA:CED | 2.81 | 0.42 |
| 5:A:478:SER:C | 5:A:480:THR:N | 2.76 | 0.42 |
| 20:A:803:CLA:C1 | 20:A:838:CLA:H61 | 2.49 | 0.42 |
| 6:B:123:TRP:CZ3 | 20:B:814:CLA:C19 | 2.98 | 0.42 |
| 6:B:198:ALA:H | 6:B:200:PRO:HG2 | 1.83 | 0.42 |
| 6:B:366:THR:C | 6:B:368:GLN:N | 2.77 | 0.42 |
| 6:B:377:TYR:OH | 6:B:717:TYR:HE1 | 2.02 | 0.42 |
| 6:B:387:PHE:O | 6:B:391:PRO:CD | 2.65 | 0.42 |
| 6:B:439:HIS:NE2 | 6:B:443:MET:SD | 2.92 | 0.42 |
| 6:B:503:GLU:O | 6:B:507:SER:HB2 | 2.18 | 0.42 |
| 7:C:44:ARG:NH2 | 8:D:127:ARG:CB | 2.71 | 0.42 |
| 21:G:103:LMU:H82 | 21:G:103:LMU:H112 | 1.80 | 0.42 |
| 20:J:101:CLA:HBC2 | 20:J:101:CLA:CMC | 2.50 | 0.42 |
| 16:L:66:GLY:HA2 | 16:L:69:VAL:HG22 | 2.01 | 0.42 |
| 21:1:218:LMU:C6B | 21:1:218:LMU:C3' | 2.89 | 0.42 |
| 2:2:103:GLY:HA2 | 20:2:310:CLA:HBB2 | 1.94 | 0.42 |
| 2:2:127:ASN:OD1 | 14:J:2:ARG:CG | 2.67 | 0.42 |
| 2:2:168:ARG:HH21 | 2:2:171:MET:HG3 | 1.84 | 0.42 |
| 3:3:49:ILE:O | 3:3:49:ILE:HG23 | 2.18 | 0.42 |
| 3:3:182:LYS:O | 3:3:186:ASN:N | 2.33 | 0.42 |
| 4:4:31:ALA:O | 4:4:32:GLU:C | 2.62 | 0.42 |
| 4:4:32:GLU:OE2 | 4:4:32:GLU:CA | 2.68 | 0.42 |
| 4:4:99:HIS:ND1 | 4:4:103:ILE:HD13 | 2.34 | 0.42 |
| 4:4:169:GLN:NE2 | 4:4:169:GLN:CA | 2.70 | 0.42 |
| 20:4:303:CLA:CAA | 20:4:303:CLA:O2D | 2.67 | 0.42 |
| 5:A:22:VAL:H | 5:A:22:VAL:HG13 | 1.45 | 0.42 |
| 5:A:76:ARG:NH1 | 5:A:192:LYS:CG | 2.77 | 0.42 |
| 5:A:127:VAL:HG21 | 20:A:809:CLA:CBB | 2.49 | 0.42 |
| 5:A:210:LEU:HD11 | 20:A:813:CLA:H42 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:277:TYR:CD2 | 5:A:278:ALA:N | 2.87 | 0.42 |
| 5:A:338:PHE:HB2 | 20:A:829:CLA:HBD | 2.01 | 0.42 |
| 5:A:400:MET:O | 5:A:609:ILE:HD12 | 2.19 | 0.42 |
| 5:A:472:ARG:O | 5:A:474:GLN:CG | 2.67 | 0.42 |
| 5:A:685:VAL:O | 5:A:688:PHE:HB3 | 2.19 | 0.42 |
| 20:A:812:CLA:HBD | 20:A:812:CLA:HAA1 | 1.99 | 0.42 |
| 22:A:845:BCR:H17C | 20:A:850:CLA:C17 | 2.50 | 0.42 |
| 6:B:124:TRP:HZ2 | 6:B:135:LEU:HB2 | 1.83 | 0.42 |
| 6:B:301:ILE:O | 6:B:301:ILE:CG2 | 2.67 | 0.42 |
| 6:B:549:ASP:CG | 7:C:63:LEU:HB3 | 2.41 | 0.42 |
| 6:B:550:LYS:O | 6:B:550:LYS:HG2 | 2.18 | 0.42 |
| 6:B:704:GLN:O | 6:B:707:LEU:HB3 | 2.19 | 0.42 |
| 7:C:35:LYS:C | 7:C:37:LYS:N | 2.76 | 0.42 |
| 10:F:30:LYS:O | 10:F:31:LEU:CB | 2.68 | 0.42 |
| 11:G:80:ILE:O | 11:G:81:VAL:C | 2.63 | 0.42 |
| 15:K:14:THR:HG23 | 15:K:15:THR:N | 2.35 | 0.42 |
| 16:L:50:LEU:HG | 16:L:51:LEU:CD2 | 2.49 | 0.42 |
| 16:L:107:PHE:HA | 16:L:133:ALA:HB2 | 2.01 | 0.42 |
| 17:N:48:GLY:C | 17:N:49:CYS:O | 2.62 | 0.42 |
| 20:1:203:CLA:CBA | 20:1:203:CLA:CBD | 2.90 | 0.42 |
| 3:3:106:TYR:CB | 3:3:107:TRP:HD1 | 2.31 | 0.42 |
| 5:A:137:GLY:C | 5:A:139:GLY:N | 2.77 | 0.42 |
| 5:A:210:LEU:CD1 | 20:A:813:CLA:HHB | 2.46 | 0.42 |
| 5:A:347:TYR:CE1 | 5:A:417:PHE:CZ | 3.07 | 0.42 |
| 5:A:682:ALA:HA | 5:A:685:VAL:HG12 | 2.01 | 0.42 |
| 5:A:688:PHE:HD1 | 20:A:851:CLA:CMB | 2.33 | 0.42 |
| 20:A:804:CLA:C4A | 20:A:811:CLA:H71 | 2.49 | 0.42 |
| 20:A:835:CLA:H71 | 20:A:835:CLA:H112 | 1.46 | 0.42 |
| 21:A:854:LMU:H91 | 21:A:854:LMU:H41 | 1.99 | 0.42 |
| 6:B:235:GLN:O | 6:B:236:ASN:C | 2.63 | 0.42 |
| 6:B:441:ASP:OD1 | 6:B:617:MET:HB3 | 2.19 | 0.42 |
| 6:B:674:LEU:O | 6:B:678:LEU:HB2 | 2.19 | 0.42 |
| 20:B:834:CLA:CMC | 20:B:837:CLA:H2 | 2.49 | 0.42 |
| 20:B:840:CLA:H171 | 16:L:94:ILE:HG12 | 2.00 | 0.42 |
| 7:C:58:CYS:HA | 7:C:59:PRO:HD2 | 1.60 | 0.42 |
| 8:D:27:PRO:HG2 | 8:D:75:LEU:HD23 | 2.00 | 0.42 |
| 21:H:103:LMU:O2' | 21:H:103:LMU:H21 | 2.18 | 0.42 |
| 21:H:104:LMU:O6' | 21:H:104:LMU:C4 | 2.67 | 0.42 |
| 20:H:108:CLA:O2A | 20:H:108:CLA:HMA3 | 2.19 | 0.42 |
| 15:K:5:SER:C | 15:K:7:THR:N | 2.78 | 0.42 |
| 16:L:84:GLY:HA3 | 16:L:155:CYS:CB | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:L:99:LEU:HB3 | 16:L:140:THR:HG21 | 2.02 | 0.42 |
| 16:L:119:THR:O | 16:L:120:LEU:C | 2.62 | 0.42 |
| 19:O:1:GLC:O2 | 19:O:2:FRU:H5 | 2.19 | 0.42 |
| 21:1:217:LMU:C4' | 21:G:103:LMU:O6' | 2.68 | 0.42 |
| 2:2:164:ILE:O | 2:2:168:ARG:N | 2.52 | 0.42 |
| 4:4:36:ASN:CB | 4:4:39:TRP:CZ3 | 2.69 | 0.42 |
| 4:4:37:LEU:CA | 4:4:39:TRP:CG | 2.98 | 0.42 |
| 4:4:51:ALA:O | 4:4:55:VAL:HG13 | 2.19 | 0.42 |
| 4:4:122:LYS:HE2 | 4:4:150:LYS:CG | 2.49 | 0.42 |
| 20:4:301:CLA:H41 | 20:4:301:CLA:H62 | 1.84 | 0.42 |
| 5:A:361:ASN:OD1 | 20:A:805:CLA:OBD | 2.38 | 0.42 |
| 5:A:430:ASP:HA | 5:A:434:ARG:HH21 | 1.84 | 0.42 |
| 5:A:603:PHE:CZ | 5:A:693:LEU:CD2 | 3.02 | 0.42 |
| 5:A:652:TRP:O | 5:A:656:PHE:HB3 | 2.19 | 0.42 |
| 20:A:801:CLA:HAA1 | 20:A:801:CLA:CBD | 2.49 | 0.42 |
| 21:A:847:LMU:H12 | 21:A:847:LMU:H41 | 1.79 | 0.42 |
| 21:A:848:LMU:C1 | 21:A:848:LMU:C5 | 2.96 | 0.42 |
| 21:A:854:LMU:H4O1 | 21:A:854:LMU:C1B | 2.33 | 0.42 |
| 6:B:29:HIS:C | 20:B:830:CLA:HAA2 | 2.45 | 0.42 |
| 6:B:37:ILE:HD12 | 6:B:37:ILE:C | 2.45 | 0.42 |
| 6:B:633:ASN:HD22 | 6:B:636:THR:HB | 1.85 | 0.42 |
| 20:B:824:CLA:CMD | 20:B:825:CLA:CBB | 2.91 | 0.42 |
| 22:B:844:BCR:H11C | 22:B:844:BCR:H341 | 1.77 | 0.42 |
| 7:C:12:ILE:O | 7:C:38:GLN:HG2 | 2.18 | 0.42 |
| 7:C:25:VAL:HA | 7:C:43:PRO:CD | 2.50 | 0.42 |
| 7:C:34:CYS:SG | 7:C:39:ILE:HD12 | 2.59 | 0.42 |
| 8:D:137:ILE:H | 8:D:137:ILE:HG13 | 1.55 | 0.42 |
| 11:G:30:ASN:ND2 | 11:G:31:MET:O | 2.52 | 0.42 |
| 12:H:32:TYR:HB3 | 12:H:33:ASN:H | 1.62 | 0.42 |
| 12:H:47:PHE:HD2 | 16:L:141:GLY:CA | 2.32 | 0.42 |
| 14:J:9:SER:HB2 | 14:J:10:VAL:H | 1.67 | 0.42 |
| 20:K:102:CLA:C4 | 20:K:102:CLA:O2A | 2.67 | 0.42 |
| 16:L:49:PRO:HG3 | 16:L:131:GLN:NE2 | 2.35 | 0.42 |
| 17:N:72:LYS:HG3 | 17:N:74:LYS:H | 1.82 | 0.42 |
| 1:1:108:VAL:HG23 | 20:1:209:CLA:NA | 2.35 | 0.42 |
| 2:2:198:ALA:O | 2:2:199:ASP:CB | 2.67 | 0.42 |
| 20:2:307:CLA:H3A | 20:2:307:CLA:HBA2 | 1.68 | 0.42 |
| 5:A:76:ARG:NE | 5:A:192:LYS:HA | 2.34 | 0.42 |
| 5:A:363:ALA:O | 5:A:367:SER:HB3 | 2.19 | 0.42 |
| 5:A:703:LEU:HD13 | 5:A:707:ILE:HD11 | 2.01 | 0.42 |
| 5:A:733:VAL:CG1 | 20:A:838:CLA:C3D | 2.97 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:A:808:CLA:H142 | 22:J:102:BCR:H14C | 1.99 | 0.42 |
| 20:A:817:CLA:HBA2 | 20:A:817:CLA:H3A | 1.21 | 0.42 |
| 20:A:834:CLA:HBA2 | 20:A:834:CLA:CBD | 2.44 | 0.42 |
| 6:B:225:LEU:HD22 | 6:B:230:TRP:CD1 | 2.54 | 0.42 |
| 6:B:365:PHE:HB3 | 6:B:602:TRP:CH2 | 2.54 | 0.42 |
| 6:B:592:PHE:CE2 | 20:B:850:CLA:H62 | 2.54 | 0.42 |
| 6:B:710:LEU:H | 6:B:713:PHE:H | 1.67 | 0.42 |
| 8:D:58:PHE:HE2 | 8:D:60:MET:HA | 1.85 | 0.42 |
| 8:D:79:ARG:H | 8:D:82:GLN:HE21 | 1.65 | 0.42 |
| 15:K:11:MET:O | 15:K:15:THR:OG1 | 2.33 | 0.42 |
| 15:K:38:LEU:C | 15:K:39:LYS:HD2 | 2.44 | 0.42 |
| 20:K:104:CLA:CHD | 20:K:104:CLA:CBC | 2.95 | 0.42 |
| 19:Q:2:FRU:C1 | 19:Q:2:FRU:C6 | 2.97 | 0.42 |
| 1:1:54:VAL:O | 1:1:56:GLY:N | 2.53 | 0.42 |
| 3:3:127:ARG:HG2 | 3:3:131:ASP:OD1 | 2.18 | 0.42 |
| 4:4:142:ASN:O | 4:4:143:PHE:HB2 | 2.20 | 0.42 |
| 4:4:143:PHE:HB2 | 4:4:150:LYS:HE2 | 2.02 | 0.42 |
| 4:4:177:PRO:HB2 | 4:4:178:PHE:CD1 | 2.54 | 0.42 |
| 5:A:35:ALA:O | 5:A:36:LYS:HB2 | 2.20 | 0.42 |
| 5:A:241:GLU:O | 5:A:242:ILE:HG23 | 2.20 | 0.42 |
| 5:A:499:ALA:O | 5:A:501:GLY:N | 2.42 | 0.42 |
| 5:A:620:MET:C | 5:A:623:ASP:O | 2.63 | 0.42 |
| 5:A:629:ASN:CG | 5:A:630:ASP:N | 2.77 | 0.42 |
| 20:A:806:CLA:H2 | 20:A:806:CLA:C7 | 2.49 | 0.42 |
| 20:A:814:CLA:CHC | 22:A:843:BCR:C18 | 2.97 | 0.42 |
| 20:A:819:CLA:H102 | 22:A:844:BCR:C21 | 2.50 | 0.42 |
| 21:A:853:LMU:H1' | 21:A:853:LMU:H6D | 1.72 | 0.42 |
| 6:B:136:TYR:O | 6:B:140:ILE:HD11 | 2.20 | 0.42 |
| 6:B:153:GLY:O | 6:B:157:LEU:HB2 | 2.19 | 0.42 |
| 6:B:684:ARG:HD3 | 6:B:684:ARG:HA | 1.80 | 0.42 |
| 6:B:685:THR:HA | 6:B:686:PRO:HD3 | 1.92 | 0.42 |
| 6:B:705:ALA:CB | 23:B:843:PQN:C8 | 2.97 | 0.42 |
| 20:B:809:CLA:H193 | 20:B:809:CLA:H161 | 1.79 | 0.42 |
| 20:B:814:CLA:H42 | 22:B:844:BCR:H10C | 2.00 | 0.42 |
| 8:D:114:PRO:HB2 | 8:D:115:LYS:H | 1.68 | 0.42 |
| 8:D:118:VAL:HG13 | 8:D:119:TYR:H | 1.84 | 0.42 |
| 10:F:47:GLU:N | 10:F:50:LYS:HB2 | 2.34 | 0.42 |
| 10:F:144:LEU:O | 10:F:149:LEU:O | 2.38 | 0.42 |
| 10:F:151:ASP:HA | 10:F:154:PHE:CB | 2.47 | 0.42 |
| 13:I:12:VAL:CG1 | 22:I:101:BCR:H271 | 2.49 | 0.42 |
| 16:L:43:TYR:O | 16:L:44:ARG:CB | 2.65 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:L:126:GLN:C | 16:L:127:PRO:O | 2.62 | 0.42 |
| 17:N:25:THR:HG22 | 17:N:26:GLY:N | 2.35 | 0.42 |
| 17:N:39:SER:O | 17:N:40:CYS:HB2 | 2.19 | 0.42 |
| 17:N:83:TRP:O | 17:N:84:LYS:HG2 | 2.19 | 0.42 |
| 21:1:216:LMU:O6' | 21:1:216:LMU:C1' | 2.67 | 0.42 |
| 3:3:52:LYS:O | 3:3:56:TYR:CB | 2.68 | 0.42 |
| 4:4:193:ILE:C | 4:4:195:GLN:N | 2.75 | 0.42 |
| 5:A:199:VAL:O | 5:A:201:SER:N | 2.53 | 0.42 |
| 5:A:270:PHE:CZ | 20:A:839:CLA:O2A | 2.73 | 0.42 |
| 5:A:441:ALA:HA | 5:A:444:SER:HB3 | 2.02 | 0.42 |
| 5:A:535:GLY:O | 5:A:539:PHE:HB2 | 2.20 | 0.42 |
| 5:A:684:PHE:HD2 | 5:A:685:VAL:CA | 2.32 | 0.42 |
| 20:A:807:CLA:HAA2 | 20:A:809:CLA:O2D | 2.20 | 0.42 |
| 20:A:826:CLA:C7 | 22:A:845:BCR:H371 | 2.47 | 0.42 |
| 20:A:832:CLA:HMC1 | 20:A:832:CLA:HBC2 | 2.00 | 0.42 |
| 20:A:849:CLA:H111 | 20:A:849:CLA:H71 | 1.75 | 0.42 |
| 20:A:850:CLA:H11 | 6:B:616:LEU:CB | 2.50 | 0.42 |
| 6:B:25:ILE:O | 6:B:26:ALA:HB2 | 2.20 | 0.42 |
| 6:B:273:VAL:O | 6:B:277:HIS:CD2 | 2.66 | 0.42 |
| 6:B:339:ALA:O | 6:B:340:SER:CB | 2.68 | 0.42 |
| 6:B:470:THR:H | 6:B:501:ILE:HG23 | 1.84 | 0.42 |
| 6:B:589:TRP:CD1 | 20:B:850:CLA:H152 | 2.54 | 0.42 |
| 6:B:596:TRP:CZ3 | 6:B:613:SER:HB3 | 2.55 | 0.42 |
| 6:B:639:VAL:HG22 | 6:B:640:CYS:N | 2.35 | 0.42 |
| 20:B:808:CLA:H102 | 20:B:808:CLA:H62 | 1.59 | 0.42 |
| 20:B:815:CLA:H3A | 20:B:815:CLA:HBA2 | 1.57 | 0.42 |
| 20:B:835:CLA:HMB1 | 22:B:846:BCR:C39 | 2.50 | 0.42 |
| 20:B:837:CLA:H71 | 20:B:837:CLA:H112 | 1.78 | 0.42 |
| 10:F:134:PHE:C | 10:F:136:TRP:H | 2.28 | 0.42 |
| 11:G:27:GLN:HG2 | 20:G:105:CLA:C4D | 2.49 | 0.42 |
| 11:G:88:THR:HG23 | 11:G:91:ASN:O | 2.19 | 0.42 |
| 12:H:42:THR:HG22 | 12:H:45:ALA:CB | 2.46 | 0.42 |
| 12:H:63:SER:O | 12:H:67:TYR:HB3 | 2.19 | 0.42 |
| 15:K:52:PRO:O | 15:K:56:THR:HG22 | 2.19 | 0.42 |
| 19:P:2:FRU:C1 | 19:P:2:FRU:H62 | 2.50 | 0.42 |
| 20:2:312:CLA:H111 | 20:2:312:CLA:H152 | 1.14 | 0.42 |
| 3:3:114:PHE:HE1 | 20:3:308:CLA:C3D | 2.33 | 0.42 |
| 20:3:314:CLA:C1 | 20:3:314:CLA:HMA1 | 2.50 | 0.42 |
| 21:4:319:LMU:H102 | 21:4:319:LMU:H71 | 1.38 | 0.42 |
| 21:4:321:LMU:O6' | 21:4:321:LMU:H1' | 2.19 | 0.42 |
| 5:A:90:PHE:HB3 | 5:A:175:ALA:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:126:ILE:HG12 | 20:A:809:CLA:HMA3 | 2.02 | 0.42 |
| 5:A:242:ILE:HG12 | 5:A:243:PRO:HG3 | 2.01 | 0.42 |
| 5:A:390:ALA:CB | 5:A:754:ILE:HD13 | 2.50 | 0.42 |
| 20:A:838:CLA:HBA2 | 20:A:838:CLA:H3A | 1.60 | 0.42 |
| 6:B:51:PHE:C | 6:B:53:GLN:N | 2.76 | 0.42 |
| 6:B:67:HIS:CD2 | 6:B:71:GLN:HE22 | 2.37 | 0.42 |
| 6:B:120:VAL:C | 6:B:123:TRP:HD1 | 2.27 | 0.42 |
| 6:B:255:LEU:HD12 | 20:B:817:CLA:O2D | 2.20 | 0.42 |
| 6:B:500:ALA:C | 6:B:501:ILE:HG12 | 2.44 | 0.42 |
| 6:B:503:GLU:HB3 | 6:B:507:SER:CA | 2.50 | 0.42 |
| 6:B:607:SER:HA | 6:B:610:ASN:HD22 | 1.85 | 0.42 |
| 6:B:720:THR:O | 6:B:724:PHE:N | 2.48 | 0.42 |
| 20:B:809:CLA:HBA1 | 20:B:809:CLA:H3A | 1.78 | 0.42 |
| 20:B:810:CLA:H13 | 20:B:828:CLA:C12 | 2.49 | 0.42 |
| 20:B:824:CLA:O1D | 20:B:824:CLA:OBD | 2.37 | 0.42 |
| 20:B:838:CLA:H41 | 22:F:204:BCR:H323 | 2.02 | 0.42 |
| 7:C:31:TRP:HD1 | 7:C:32:GLY:N | 2.18 | 0.42 |
| 10:F:41:ALA:O | 10:F:44:ALA:O | 2.38 | 0.42 |
| 10:F:73:VAL:HG21 | 10:F:83:PHE:HB2 | 2.01 | 0.42 |
| 10:F:123:VAL:HG13 | 14:J:7:TYR:N | 2.34 | 0.42 |
| 11:G:35:VAL:HG13 | 11:G:38:GLN:HB2 | 2.02 | 0.42 |
| 11:G:42:SER:CB | 11:G:46:ALA:HB2 | 2.46 | 0.42 |
| 12:H:73:PRO:CD | 19:Z:2:FRU:O6 | 2.68 | 0.42 |
| 21:H:106:LMU:H62 | 21:H:106:LMU:C11 | 2.49 | 0.42 |
| 15:K:74:ILE:CG2 | 15:K:75:VAL:HG22 | 2.41 | 0.42 |
| 21:K:107:LMU:H71 | 21:K:107:LMU:H11 | 2.01 | 0.42 |
| 1:1:135:LYS:HB3 | 1:1:136:ASP:H | 1.54 | 0.42 |
| 4:4:36:ASN:O | 4:4:39:TRP:CD2 | 2.73 | 0.42 |
| 4:4:123:GLN:HG2 | 4:4:124:TYR:H | 1.84 | 0.42 |
| 4:4:127:PRO:HB2 | 4:4:143:PHE:HE1 | 1.83 | 0.42 |
| 4:4:179:ASP:N | 4:4:184:HIS:HD2 | 2.17 | 0.42 |
| 5:A:131:ILE:HG21 | 6:B:446:PHE:HD1 | 1.84 | 0.42 |
| 5:A:185:HIS:O | 5:A:188:LYS:HG3 | 2.20 | 0.42 |
| 5:A:430:ASP:C | 5:A:432:LEU:H | 2.28 | 0.42 |
| 5:A:502:THR:H | 5:A:504:ALA:HB3 | 1.84 | 0.42 |
| 5:A:553:VAL:O | 5:A:557:LEU:CB | 2.67 | 0.42 |
| 5:A:604:TRP:O | 5:A:605:MET:C | 2.62 | 0.42 |
| 5:A:607:ASN:O | 5:A:608:SER:C | 2.63 | 0.42 |
| 20:A:808:CLA:H111 | 22:J:102:BCR:C10 | 2.50 | 0.42 |
| 20:A:832:CLA:HBA2 | 20:A:832:CLA:H3A | 1.56 | 0.42 |
| 6:B:239:SER:C | 6:B:240:SER:HG | 2.28 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:255:LEU:N | 6:B:255:LEU:HD23 | 2.34 | 0.42 |
| 6:B:291:TYR:HE1 | 20:B:820:CLA:CED | 2.32 | 0.42 |
| 6:B:304:ILE:HG22 | 20:B:823:CLA:O1D | 2.20 | 0.42 |
| 6:B:352:MET:SD | 20:B:829:CLA:OBD | 2.78 | 0.42 |
| 6:B:476:ILE:HA | 6:B:477:PRO:HD2 | 1.83 | 0.42 |
| 6:B:509:PHE:N | 6:B:509:PHE:HD2 | 2.18 | 0.42 |
| 6:B:681:ALA:O | 6:B:683:GLU:N | 2.53 | 0.42 |
| 6:B:693:TRP:CZ2 | 6:B:697:PRO:HG3 | 2.54 | 0.42 |
| 20:B:839:CLA:O1D | 20:B:839:CLA:C1A | 2.62 | 0.42 |
| 7:C:11:CYS:C | 7:C:13:GLY:N | 2.76 | 0.42 |
| 8:D:120:PRO:O | 8:D:121:GLU:HB3 | 2.19 | 0.42 |
| 20:K:103:CLA:O1A | 20:K:103:CLA:C3A | 2.68 | 0.42 |
| 16:L:58:LEU:HA | 16:L:146:GLY:O | 2.20 | 0.42 |
| 20:R:108:CLA:H141 | 20:R:108:CLA:H161 | 1.88 | 0.42 |
| 21:1:218:LMU:H31 | 21:1:218:LMU:H61 | 1.72 | 0.41 |
| 2:2:102:ILE:HG22 | 20:2:310:CLA:CBB | 2.50 | 0.41 |
| 2:2:162:LYS:CE | 20:2:305:CLA:OBD | 2.68 | 0.41 |
| 2:2:178:TRP:CD1 | 2:2:178:TRP:N | 2.88 | 0.41 |
| 20:2:310:CLA:HHD | 20:2:310:CLA:HAC1 | 1.87 | 0.41 |
| 4:4:70:ILE:O | 4:4:73:PRO:CD | 2.66 | 0.41 |
| 4:4:118:ASP:CA | 4:4:122:LYS:HA | 2.49 | 0.41 |
| 5:A:59:ALA:C | 5:A:61:ALA:N | 2.78 | 0.41 |
| 5:A:123:VAL:O | 20:A:809:CLA:O1D | 2.38 | 0.41 |
| 5:A:358:LEU:HD11 | 5:A:413:HIS:CD2 | 2.54 | 0.41 |
| 5:A:364:MET:CE | 20:A:825:CLA:H2 | 2.49 | 0.41 |
| 5:A:372:VAL:HG22 | 20:A:818:CLA:H43 | 2.02 | 0.41 |
| 5:A:582:ASP:OD1 | 5:A:586:ARG:NH1 | 2.24 | 0.41 |
| 20:A:832:CLA:C3D | 20:A:833:CLA:CAC | 2.97 | 0.41 |
| 6:B:70:TRP:HD1 | 6:B:70:TRP:H | 1.66 | 0.41 |
| 6:B:160:LYS:HG3 | 6:B:161:TRP:N | 2.30 | 0.41 |
| 20:B:808:CLA:H62 | 20:B:808:CLA:H2 | 1.86 | 0.41 |
| 20:B:824:CLA:HHD | 20:B:824:CLA:HAC2 | 1.83 | 0.41 |
| 20:B:841:CLA:C2 | 23:B:843:PQN:H251 | 2.50 | 0.41 |
| 8:D:101:TYR:CE1 | 8:D:114:PRO:HD3 | 2.55 | 0.41 |
| 10:F:65:SER:C | 10:F:67:GLY:H | 2.28 | 0.41 |
| 11:G:16:LEU:HD12 | 11:G:17:PHE:CZ | 2.55 | 0.41 |
| 11:G:28:ARG:NH2 | 11:G:29:GLU:C | 2.78 | 0.41 |
| 11:G:43:HIS:ND1 | 11:G:43:HIS:N | 2.68 | 0.41 |
| 12:H:34:SER:OG | 12:H:36:GLN:NE2 | 2.53 | 0.41 |
| 13:I:24:LEU:HD23 | 22:L:209:BCR:H23C | 2.01 | 0.41 |
| 22:I:103:BCR:C39 | 22:L:209:BCR:C40 | 2.97 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:L:65:VAL:H | 16:L:67:PRO:HD2 | 1.85 | 0.41 |
| 17:N:65:LEU:C | 17:N:66:ASP:OD2 | 2.63 | 0.41 |
| 2:2:77:PRO:O | 17:N:3:ILE:CD1 | 2.68 | 0.41 |
| 2:2:191:ASN:O | 2:2:191:ASN:CG | 2.61 | 0.41 |
| 3:3:111:TYR:HB2 | 3:3:112:THR:CG2 | 2.51 | 0.41 |
| 3:3:206:VAL:HB | 3:3:207:GLY:H | 1.69 | 0.41 |
| 20:3:311:CLA:O1A | 20:3:311:CLA:HMA1 | 2.20 | 0.41 |
| 4:4:58:MET:SD | 4:4:58:MET:C | 3.03 | 0.41 |
| 4:4:121:PHE:CD1 | 4:4:143:PHE:HE2 | 2.32 | 0.41 |
| 5:A:131:ILE:HD11 | 5:A:669:GLY:C | 2.46 | 0.41 |
| 5:A:306:ILE:O | 5:A:309:LEU:N | 2.52 | 0.41 |
| 5:A:341:GLN:O | 5:A:344:LYS:HB2 | 2.19 | 0.41 |
| 5:A:402:ILE:C | 5:A:404:GLY:N | 2.77 | 0.41 |
| 20:A:828:CLA:HAA1 | 20:A:828:CLA:HBD | 2.03 | 0.41 |
| 20:A:829:CLA:H2A | 16:L:25:THR:HG21 | 2.02 | 0.41 |
| 20:A:830:CLA:C15 | 22:L:209:BCR:C36 | 2.98 | 0.41 |
| 20:A:849:CLA:H122 | 20:A:849:CLA:H162 | 1.58 | 0.41 |
| 6:B:222:LEU:HD21 | 6:B:226:LEU:HD12 | 2.01 | 0.41 |
| 6:B:233:TYR:HD1 | 6:B:254:ILE:HG13 | 1.85 | 0.41 |
| 6:B:292:ARG:NH1 | 6:B:293:THR:H | 2.18 | 0.41 |
| 6:B:416:GLU:CD | 6:B:416:GLU:H | 2.27 | 0.41 |
| 6:B:563:GLY:C | 6:B:564:ARG:O | 2.61 | 0.41 |
| 6:B:580:VAL:HG13 | 6:B:710:LEU:HD21 | 2.01 | 0.41 |
| 6:B:646:TRP:CH2 | 6:B:726:ILE:HD13 | 2.55 | 0.41 |
| 6:B:660:GLY:O | 6:B:663:PHE:O | 2.39 | 0.41 |
| 8:D:49:THR:C | 8:D:50:TRP:CD1 | 2.98 | 0.41 |
| 10:F:130:LEU:CD1 | 10:F:131:PHE:HD1 | 2.33 | 0.41 |
| 11:G:14:LEU:O | 11:G:14:LEU:HG | 2.19 | 0.41 |
| 12:H:26:SER:C | 12:H:27:ASP:O | 2.61 | 0.41 |
| 12:H:70:ALA:O | 12:H:71:ASN:CB | 2.68 | 0.41 |
| 16:L:96:SER:OG | 16:L:143:PHE:CD2 | 2.73 | 0.41 |
| 16:L:126:GLN:N | 16:L:127:PRO:CD | 2.82 | 0.41 |
| 17:N:38:GLY:C | 17:N:39:SER:O | 2.62 | 0.41 |
| 17:N:51:ASP:C | 17:N:52:LEU:CD2 | 2.94 | 0.41 |
| 17:N:72:LYS:CE | 17:N:74:LYS:HE3 | 2.38 | 0.41 |
| 1:1:179:THR:OG1 | 4:4:87:SER:CB | 2.69 | 0.41 |
| 20:2:302:CLA:O1A | 20:2:302:CLA:C2 | 2.67 | 0.41 |
| 4:4:53:LEU:O | 4:4:56:ALA:N | 2.53 | 0.41 |
| 4:4:75:TRP:CE3 | 4:4:76:TYR:HB3 | 2.55 | 0.41 |
| 4:4:163:PHE:O | 4:4:166:PHE:CB | 2.66 | 0.41 |
| 5:A:40:PHE:N | 5:A:44:ILE:HG21 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:145:ILE:HG23 | 20:A:808:CLA:OBD | 2.20 | 0.41 |
| 5:A:372:VAL:HG22 | 20:A:818:CLA:H41 | 2.00 | 0.41 |
| 5:A:553:VAL:H | 5:A:556:LEU:CD1 | 2.31 | 0.41 |
| 5:A:585:GLY:C | 5:A:587:GLY:H | 2.28 | 0.41 |
| 5:A:586:ARG:CG | 7:C:49:VAL:HG21 | 2.38 | 0.41 |
| 5:A:650:ASN:O | 5:A:653:LEU:HD13 | 2.19 | 0.41 |
| 5:A:677:LEU:HD11 | 6:B:442:VAL:HG13 | 2.02 | 0.41 |
| 20:A:818:CLA:CBB | 20:A:818:CLA:C8 | 2.93 | 0.41 |
| 6:B:141:PHE:O | 6:B:142:LEU:C | 2.63 | 0.41 |
| 6:B:199:ILE:N | 6:B:200:PRO:HD2 | 2.35 | 0.41 |
| 6:B:260:GLY:H | 6:B:269:TRP:HE1 | 1.68 | 0.41 |
| 6:B:309:ILE:HA | 6:B:310:PRO:HD3 | 1.77 | 0.41 |
| 6:B:407:VAL:HG23 | 20:B:831:CLA:CMD | 2.49 | 0.41 |
| 6:B:456:GLU:HA | 6:B:514:PRO:HD3 | 2.03 | 0.41 |
| 6:B:569:ASP:OD2 | 6:B:569:ASP:N | 2.54 | 0.41 |
| 20:B:822:CLA:HBC3 | 22:G:104:BCR:HC7 | 2.03 | 0.41 |
| 20:B:824:CLA:C2A | 20:B:824:CLA:CGD | 2.98 | 0.41 |
| 20:B:828:CLA:HMC1 | 20:B:828:CLA:HBC3 | 2.02 | 0.41 |
| 8:D:30:ALA:HA | 16:L:13:PRO:HG3 | 2.01 | 0.41 |
| 10:F:62:LEU:CD2 | 10:F:72:ILE:HD13 | 2.50 | 0.41 |
| 20:F:201:CLA:CHD | 20:F:201:CLA:HBC2 | 2.44 | 0.41 |
| 12:H:30:SER:O | 12:H:31:PRO:O | 2.37 | 0.41 |
| 14:J:21:SER:O | 14:J:23:ALA:N | 2.52 | 0.41 |
| 15:K:46:GLY:O | 15:K:47:LEU:HG | 2.12 | 0.41 |
| 21:K:106:LMU:H4' | 21:K:106:LMU:H2B | 1.70 | 0.41 |
| 16:L:12:GLN:HA | 16:L:13:PRO:HD3 | 1.85 | 0.41 |
| 17:N:9:LYS:HB3 | 17:N:9:LYS:HE2 | 1.78 | 0.41 |
| 17:N:60:PHE:HA | 17:N:61:LEU:O | 2.20 | 0.41 |
| 17:N:82:PHE:N | 17:N:82:PHE:HD2 | 2.17 | 0.41 |
| 18:R:26:UNK:C | 18:R:28:UNK:N | 2.81 | 0.41 |
| 20:2:303:CLA:O1D | 20:2:303:CLA:C2A | 2.63 | 0.41 |
| 3:3:56:TYR:CD1 | 3:3:185:LYS:NZ | 2.84 | 0.41 |
| 20:3:314:CLA:H18 | 20:3:314:CLA:H151 | 1.36 | 0.41 |
| 4:4:61:PRO:HA | 4:4:65:THR:O | 2.20 | 0.41 |
| 4:4:193:ILE:HG22 | 4:4:195:GLN:O | 2.20 | 0.41 |
| 21:4:320:LMU:H72 | 21:4:320:LMU:H101 | 1.69 | 0.41 |
| 5:A:98:PHE:HD1 | 5:A:99:HIS:CD2 | 2.37 | 0.41 |
| 5:A:183:TRP:O | 5:A:185:HIS:N | 2.54 | 0.41 |
| 5:A:585:GLY:C | 5:A:587:GLY:N | 2.76 | 0.41 |
| 5:A:656:PHE:O | 5:A:657:LEU:C | 2.64 | 0.41 |
| 5:A:672:LEU:H | 5:A:672:LEU:CD2 | 2.32 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:A:801:CLA:CMC | 20:A:801:CLA:CBC | 2.94 | 0.41 |
| 6:B:262:HIS:HA | 6:B:263:PRO:HD2 | 1.93 | 0.41 |
| 6:B:290:MET:HA | 20:B:822:CLA:C3C | 2.49 | 0.41 |
| 6:B:293:THR:O | 6:B:295:PHE:CD2 | 2.73 | 0.41 |
| 6:B:373:THR:C | 6:B:376:GLN:H | 2.29 | 0.41 |
| 6:B:431:PHE:HE2 | 20:B:832:CLA:HED3 | 1.85 | 0.41 |
| 6:B:564:ARG:NE | 7:C:64:SER:OG | 2.52 | 0.41 |
| 6:B:662:MET:HE2 | 23:B:843:PQN:H2M3 | 2.02 | 0.41 |
| 20:B:840:CLA:HMD2 | 20:L:203:CLA:CAB | 2.51 | 0.41 |
| 9:E:62:ARG:O | 9:E:83:ALA:CB | 2.69 | 0.41 |
| 10:F:29:LEU:HB3 | 10:F:30:LYS:H | 1.74 | 0.41 |
| 10:F:123:VAL:CG1 | 14:J:7:TYR:HB2 | 2.50 | 0.41 |
| 11:G:34:GLN:O | 11:G:36:PRO:N | 2.53 | 0.41 |
| 15:K:24:PHE:CB | 15:K:52:PRO:HG2 | 2.46 | 0.41 |
| 21:K:105:LMU:H42 | 21:K:105:LMU:H102 | 2.01 | 0.41 |
| 21:K:106:LMU:H1B | 21:K:106:LMU:H4B | 1.67 | 0.41 |
| 16:L:10:VAL:HG13 | 16:L:12:GLN:HE22 | 1.85 | 0.41 |
| 16:L:50:LEU:HD23 | 16:L:51:LEU:H | 1.85 | 0.41 |
| 20:L:202:CLA:O1D | 20:L:202:CLA:OBD | 2.35 | 0.41 |
| 17:N:63:ASP:N | 17:N:64:ASP:CA | 2.76 | 0.41 |
| 19:X:1:GLC:O5 | 19:X:2:FRU:C5 | 2.68 | 0.41 |
| 1:1:58:LEU:O | 1:1:60:PRO:HD3 | 2.21 | 0.41 |
| 3:3:94:ARG:NH2 | 3:3:98:ILE:HD13 | 2.36 | 0.41 |
| 4:4:105:ARG:O | 4:4:108:ASP:HB3 | 2.20 | 0.41 |
| 5:A:53:TRP:CA | 5:A:56:ASN:HB2 | 2.44 | 0.41 |
| 5:A:97:TYR:HA | 5:A:153:TRP:CZ2 | 2.55 | 0.41 |
| 5:A:366:GLY:O | 5:A:403:GLY:HA2 | 2.19 | 0.41 |
| 5:A:382:TYR:HE2 | 20:A:827:CLA:HED3 | 1.84 | 0.41 |
| 5:A:560:VAL:O | 5:A:563:ALA:HB2 | 2.21 | 0.41 |
| 5:A:638:THR:O | 5:A:639:ALA:C | 2.63 | 0.41 |
| 5:A:639:ALA:O | 5:A:641:ASN:N | 2.54 | 0.41 |
| 20:A:818:CLA:CBB | 20:A:818:CLA:C7 | 2.97 | 0.41 |
| 20:A:826:CLA:H71 | 22:A:845:BCR:C37 | 2.48 | 0.41 |
| 20:A:830:CLA:C2D | 20:A:831:CLA:H121 | 2.51 | 0.41 |
| 6:B:289:LEU:HD21 | 20:B:821:CLA:NA | 2.35 | 0.41 |
| 6:B:317:ARG:HH12 | 6:B:407:VAL:N | 2.18 | 0.41 |
| 6:B:694:ARG:NH1 | 16:L:105:ALA:O | 2.50 | 0.41 |
| 20:B:809:CLA:HED1 | 20:B:830:CLA:H52 | 2.01 | 0.41 |
| 20:B:834:CLA:NC | 20:B:835:CLA:HBB2 | 2.34 | 0.41 |
| 20:B:834:CLA:C4C | 20:B:835:CLA:CBB | 2.98 | 0.41 |
| 23:B:843:PQN:H2M1 | 23:B:843:PQN:H111 | 1.90 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:D:28:ILE:O | 8:D:66:ALA:CB | 2.69 | 0.41 |
| 9:E:55:VAL:CG2 | 9:E:65:VAL:HB | 2.44 | 0.41 |
| 10:F:104:TYR:O | 10:F:104:TYR:HD2 | 2.01 | 0.41 |
| 11:G:43:HIS:C | 11:G:47:GLY:H | 2.27 | 0.41 |
| 11:G:60:SER:O | 11:G:62:ASP:N | 2.53 | 0.41 |
| 13:I:17:PRO:O | 13:I:18:ALA:C | 2.63 | 0.41 |
| 16:L:149:SER:C | 16:L:151:VAL:N | 2.78 | 0.41 |
| 18:R:8:UNK:CB | 20:R:107:CLA:HED1 | 2.51 | 0.41 |
| 21:R:109:LMU:H71 | 21:R:109:LMU:H102 | 1.55 | 0.41 |
| 2:2:152:SER:C | 2:2:154:GLN:H | 2.29 | 0.41 |
| 2:2:179:PHE:O | 2:2:183:TYR:CD2 | 2.73 | 0.41 |
| 3:3:158:TYR:CB | 3:3:159:PRO:CD | 2.82 | 0.41 |
| 4:4:30:LEU:O | 4:4:32:GLU:OE1 | 2.38 | 0.41 |
| 4:4:83:TYR:HB3 | 4:4:84:PHE:H | 1.53 | 0.41 |
| 4:4:119:PRO:O | 4:4:121:PHE:N | 2.54 | 0.41 |
| 5:A:25:ASP:HA | 5:A:27:ILE:H | 1.85 | 0.41 |
| 5:A:82:HIS:O | 5:A:84:GLY:N | 2.54 | 0.41 |
| 5:A:453:LEU:CB | 5:A:547:PHE:HB2 | 2.35 | 0.41 |
| 5:A:605:MET:C | 5:A:605:MET:SD | 3.03 | 0.41 |
| 5:A:702:GLU:HA | 6:B:545:LYS:HE2 | 2.02 | 0.41 |
| 20:A:818:CLA:H93 | 20:A:818:CLA:H62 | 1.30 | 0.41 |
| 6:B:18:THR:O | 6:B:19:ARG:C | 2.64 | 0.41 |
| 6:B:50:HIS:C | 6:B:53:GLN:H | 2.29 | 0.41 |
| 6:B:87:ILE:C | 6:B:115:ASN:HA | 2.43 | 0.41 |
| 6:B:462:TRP:HZ3 | 20:B:834:CLA:HBC1 | 1.86 | 0.41 |
| 6:B:471:THR:HB | 6:B:472:TYR:CE1 | 2.56 | 0.41 |
| 6:B:510:LEU:HG | 6:B:597:LYS:NZ | 2.36 | 0.41 |
| 6:B:668:ARG:HH12 | 6:B:672:GLN:HG2 | 1.85 | 0.41 |
| 20:B:820:CLA:C3 | 20:B:825:CLA:H92 | 2.51 | 0.41 |
| 10:F:44:ALA:O | 10:F:46:MET:N | 2.53 | 0.41 |
| 15:K:38:LEU:CG | 15:K:39:LYS:CD | 2.78 | 0.41 |
| 16:L:14:LEU:CA | 16:L:24:GLU:HG3 | 2.40 | 0.41 |
| 16:L:160:VAL:O | 16:L:160:VAL:CG2 | 2.66 | 0.41 |
| 20:L:207:CLA:HAC2 | 22:L:209:BCR:HC42 | 2.02 | 0.41 |
| 17:N:81:VAL:C | 17:N:83:TRP:N | 2.79 | 0.41 |
| 2:2:70:LYS:HB3 | 2:2:70:LYS:HE3 | 1.62 | 0.41 |
| 2:2:171:MET:SD | 2:2:172:LEU:HA | 2.60 | 0.41 |
| 20:3:314:CLA:H92 | 20:3:314:CLA:H142 | 2.03 | 0.41 |
| 21:3:319:LMU:H1B | 21:3:319:LMU:H3' | 1.30 | 0.41 |
| 4:4:38:ARG:O | 4:4:39:TRP:O | 2.39 | 0.41 |
| 4:4:152:LYS:HA | 4:4:152:LYS:HD2 | 1.73 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:131:ILE:HD13 | 6:B:446:PHE:C | 2.46 | 0.41 |
| 5:A:249:ILE:CG1 | 5:A:250:LEU:N | 2.55 | 0.41 |
| 5:A:298:ASP:O | 5:A:301:HIS:N | 2.54 | 0.41 |
| 5:A:532:ILE:N | 5:A:533:PRO:HD3 | 2.34 | 0.41 |
| 20:A:808:CLA:H3A | 20:A:808:CLA:HBA2 | 1.39 | 0.41 |
| 20:A:816:CLA:HHD | 20:A:816:CLA:HAC2 | 1.93 | 0.41 |
| 20:A:837:CLA:NC | 20:B:806:CLA:HBC2 | 2.35 | 0.41 |
| 6:B:189:ALA:HA | 20:B:816:CLA:HBB1 | 2.03 | 0.41 |
| 6:B:353:TYR:CB | 6:B:594:TRP:CH2 | 3.03 | 0.41 |
| 6:B:434:LEU:O | 6:B:438:VAL:HG13 | 2.21 | 0.41 |
| 20:B:806:CLA:H52 | 20:B:806:CLA:C1C | 2.51 | 0.41 |
| 20:B:806:CLA:H201 | 10:F:104:TYR:CD1 | 2.56 | 0.41 |
| 20:B:829:CLA:H62 | 22:B:845:BCR:HC7 | 2.02 | 0.41 |
| 7:C:29:ILE:HG23 | 8:D:126:GLY:CA | 2.44 | 0.41 |
| 8:D:53:PRO:HB2 | 8:D:54:LYS:H | 1.66 | 0.41 |
| 8:D:102:ARG:CZ | 8:D:110:GLN:HB2 | 2.51 | 0.41 |
| 8:D:126:GLY:C | 8:D:127:ARG:CG | 2.89 | 0.41 |
| 10:F:21:ALA:O | 10:F:23:LYS:N | 2.54 | 0.41 |
| 10:F:44:ALA:HA | 10:F:47:GLU:HB3 | 2.03 | 0.41 |
| 10:F:104:TYR:OH | 10:F:122:ASP:N | 2.42 | 0.41 |
| 20:H:102:CLA:HBD | 20:H:102:CLA:HAA2 | 2.02 | 0.41 |
| 21:K:107:LMU:C7 | 21:K:107:LMU:C2 | 2.92 | 0.41 |
| 16:L:163:LEU:HD13 | 16:L:164:PRO:N | 2.28 | 0.41 |
| 20:L:203:CLA:H91 | 22:L:209:BCR:H10C | 2.03 | 0.41 |
| 20:1:201:CLA:HBC3 | 20:1:201:CLA:HMC1 | 2.00 | 0.41 |
| 2:2:42:ARG:C | 2:2:44:ASN:N | 2.79 | 0.41 |
| 2:2:171:MET:HE1 | 2:2:175:MET:CB | 2.36 | 0.41 |
| 3:3:120:LEU:O | 3:3:123:PHE:HB3 | 2.21 | 0.41 |
| 4:4:93:ILE:C | 4:4:95:PHE:N | 2.74 | 0.41 |
| 5:A:131:ILE:HG21 | 6:B:446:PHE:CD1 | 2.55 | 0.41 |
| 5:A:177:LEU:C | 5:A:179:LEU:N | 2.79 | 0.41 |
| 5:A:236:GLY:O | 5:A:237:VAL:HG22 | 2.20 | 0.41 |
| 5:A:490:GLN:HE21 | 5:A:490:GLN:C | 2.29 | 0.41 |
| 5:A:538:ASP:O | 5:A:542:HIS:CD2 | 2.73 | 0.41 |
| 5:A:586:ARG:HB2 | 5:A:589:THR:OG1 | 2.21 | 0.41 |
| 5:A:747:TRP:HB2 | 20:A:826:CLA:CBB | 2.51 | 0.41 |
| 20:A:828:CLA:H122 | 20:A:838:CLA:HMA2 | 2.01 | 0.41 |
| 20:A:832:CLA:CMC | 20:A:832:CLA:HBC2 | 2.51 | 0.41 |
| 6:B:5:ILE:HG13 | 6:B:20:ARG:HH21 | 1.85 | 0.41 |
| 6:B:414:HIS:O | 6:B:414:HIS:CD2 | 2.74 | 0.41 |
| 6:B:549:ASP:OD1 | 7:C:63:LEU:HD22 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:557:PHE:N | 6:B:558:PRO:HD3 | 2.34 | 0.41 |
| 21:D:201:LMU:C1 | 21:D:201:LMU:H52 | 2.48 | 0.41 |
| 9:E:60:LYS:HG3 | 9:E:61:THR:OG1 | 2.21 | 0.41 |
| 10:F:51:LYS:C | 10:F:53:PHE:N | 2.78 | 0.41 |
| 10:F:90:PHE:N | 22:F:203:BCR:H391 | 2.36 | 0.41 |
| 21:G:102:LMU:H4B | 21:G:102:LMU:H1B | 1.53 | 0.41 |
| 22:J:102:BCR:H341 | 22:J:102:BCR:H11C | 1.80 | 0.41 |
| 17:N:79:SER:OG | 17:N:80:ASN:N | 2.53 | 0.41 |
| 2:2:37:ASP:HA | 2:2:38:PRO:HD3 | 1.81 | 0.41 |
| 2:2:102:ILE:CG2 | 2:2:106:GLU:HG3 | 2.50 | 0.41 |
| 2:2:191:ASN:HB2 | 19:O:1:GLC:C6 | 2.51 | 0.41 |
| 2:2:206:ALA:O | 2:2:207:ALA:HB3 | 2.21 | 0.41 |
| 20:2:314:CLA:HHD | 20:2:314:CLA:CBC | 2.47 | 0.41 |
| 3:3:47:GLY:O | 3:3:48:PHE:CD2 | 2.74 | 0.41 |
| 3:3:49:ILE:CA | 3:3:51:PRO:HD2 | 2.51 | 0.41 |
| 3:3:94:ARG:HD2 | 3:3:94:ARG:HA | 1.76 | 0.41 |
| 3:3:205:GLY:CA | 5:A:252:ARG:NH1 | 2.67 | 0.41 |
| 4:4:40:PHE:CA | 4:4:43:ALA:CB | 2.97 | 0.41 |
| 4:4:44:GLU:O | 4:4:45:LEU:C | 2.64 | 0.41 |
| 4:4:58:MET:SD | 4:4:59:LEU:N | 2.94 | 0.41 |
| 4:4:94:GLU:O | 4:4:97:LEU:HB3 | 2.20 | 0.41 |
| 4:4:98:SER:O | 4:4:102:GLU:CD | 2.64 | 0.41 |
| 4:4:107:GLN:HA | 20:4:301:CLA:C3A | 2.50 | 0.41 |
| 4:4:128:ALA:CA | 4:4:143:PHE:HZ | 2.31 | 0.41 |
| 4:4:149:ALA:HB1 | 4:4:150:LYS:HE3 | 2.03 | 0.41 |
| 4:4:154:ILE:CG1 | 4:4:155:ALA:N | 2.62 | 0.41 |
| 5:A:40:PHE:CD1 | 5:A:40:PHE:O | 2.74 | 0.41 |
| 5:A:55:TRP:CD2 | 5:A:729:GLN:NE2 | 2.89 | 0.41 |
| 5:A:420:ARG:CZ | 5:A:420:ARG:HB3 | 2.51 | 0.41 |
| 5:A:553:VAL:O | 5:A:557:LEU:N | 2.37 | 0.41 |
| 5:A:628:ILE:HG13 | 5:A:632:GLY:CA | 2.48 | 0.41 |
| 5:A:656:PHE:HB3 | 5:A:657:LEU:H | 1.71 | 0.41 |
| 5:A:668:TYR:CD1 | 6:B:445:ALA:HB2 | 2.55 | 0.41 |
| 5:A:685:VAL:CG1 | 5:A:741:GLY:CA | 2.99 | 0.41 |
| 20:A:815:CLA:HAA1 | 20:A:815:CLA:HED2 | 2.03 | 0.41 |
| 20:A:819:CLA:HBA1 | 20:A:823:CLA:HBB2 | 2.00 | 0.41 |
| 20:A:831:CLA:H161 | 20:A:831:CLA:H202 | 1.80 | 0.41 |
| 20:A:835:CLA:H192 | 20:L:201:CLA:CBB | 2.51 | 0.41 |
| 20:A:840:CLA:HBA1 | 20:A:840:CLA:H3A | 1.13 | 0.41 |
| 21:A:852:LMU:O2B | 21:A:852:LMU:C3' | 2.56 | 0.41 |
| 6:B:96:PHE:HZ | 6:B:104:PHE:CE2 | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:104:PHE:CZ | 6:B:645:VAL:HG22 | 2.55 | 0.41 |
| 6:B:145:LEU:HD22 | 6:B:148:ILE:HD12 | 2.02 | 0.41 |
| 6:B:279:ALA:O | 20:B:817:CLA:CMB | 2.67 | 0.41 |
| 6:B:529:THR:O | 6:B:533:ILE:CG2 | 2.68 | 0.41 |
| 6:B:534:LEU:HD21 | 6:B:579:ALA:CB | 2.51 | 0.41 |
| 6:B:535:VAL:CG1 | 6:B:536:LYS:N | 2.84 | 0.41 |
| 6:B:553:PHE:CD1 | 6:B:553:PHE:C | 2.98 | 0.41 |
| 6:B:598:HIS:HB3 | 6:B:602:TRP:CH2 | 2.56 | 0.41 |
| 6:B:600:THR:O | 6:B:605:ASN:O | 2.38 | 0.41 |
| 20:B:809:CLA:CBC | 20:B:828:CLA:CMD | 2.99 | 0.41 |
| 20:B:820:CLA:HBA1 | 20:B:820:CLA:CHA | 2.51 | 0.41 |
| 20:B:831:CLA:HMA1 | 20:F:201:CLA:O1A | 2.21 | 0.41 |
| 20:B:832:CLA:H71 | 22:F:204:BCR:H402 | 2.03 | 0.41 |
| 23:B:843:PQN:H161 | 23:B:843:PQN:H141 | 1.60 | 0.41 |
| 7:C:65:VAL:HG12 | 7:C:66:ARG:H | 1.85 | 0.41 |
| 12:H:77:LEU:HB3 | 12:H:78:PRO:HD2 | 2.03 | 0.41 |
| 16:L:64:LEU:CD2 | 16:L:91:LEU:HD22 | 2.51 | 0.41 |
| 16:L:90:GLY:O | 16:L:94:ILE:N | 2.49 | 0.41 |
| 16:L:104:ILE:C | 16:L:104:ILE:HD12 | 2.46 | 0.41 |
| 16:L:160:VAL:O | 16:L:161:LEU:O | 2.38 | 0.41 |
| 20:L:201:CLA:H72 | 20:L:204:CLA:HBA1 | 2.03 | 0.41 |
| 20:L:202:CLA:H93 | 20:L:202:CLA:H62 | 1.85 | 0.41 |
| 17:N:42:PHE:N | 17:N:43:PRO:CD | 2.83 | 0.41 |
| 17:N:46:PHE:O | 17:N:47:THR:CB | 2.68 | 0.41 |
| 18:R:35:UNK:CA | 18:R:38:UNK:CB | 2.97 | 0.41 |
| 21:R:109:LMU:H62 | 21:R:109:LMU:H32 | 1.85 | 0.41 |
| 19:T:1:GLC:H5 | 19:T:2:FRU:C1 | 2.51 | 0.41 |
| 2:2:150:SER:HB3 | 2:2:151:ALA:H | 1.51 | 0.41 |
| 20:2:307:CLA:H41 | 20:2:307:CLA:H62 | 1.47 | 0.41 |
| 3:3:94:ARG:CZ | 3:3:98:ILE:HD13 | 2.50 | 0.41 |
| 5:A:48:PRO:HB3 | 9:E:72:VAL:HG22 | 2.02 | 0.41 |
| 5:A:205:HIS:CE1 | 20:A:813:CLA:CMC | 3.02 | 0.41 |
| 5:A:220:ARG:O | 5:A:221:HIS:CB | 2.65 | 0.41 |
| 5:A:378:SER:O | 5:A:379:MET:HG3 | 2.21 | 0.41 |
| 5:A:587:GLY:HA3 | 6:B:668:ARG:CZ | 2.51 | 0.41 |
| 5:A:650:ASN:HA | 5:A:653:LEU:HD13 | 2.03 | 0.41 |
| 5:A:664:VAL:HG23 | 5:A:665:ILE:HG23 | 2.02 | 0.41 |
| 20:A:838:CLA:C10 | 20:A:851:CLA:H152 | 2.51 | 0.41 |
| 21:A:854:LMU:H91 | 21:A:854:LMU:C3 | 2.50 | 0.41 |
| 6:B:139:ALA:O | 6:B:140:ILE:C | 2.64 | 0.41 |
| 6:B:140:ILE:O | 6:B:144:PHE:HD1 | 2.04 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:183:PHE:CE1 | 20:B:814:CLA:H71 | 2.54 | 0.41 |
| 6:B:551:LYS:HE2 | 8:D:143:PRO:HA | 2.03 | 0.41 |
| 6:B:631:LEU:HG | 6:B:632:ILE:HG23 | 2.03 | 0.41 |
| 20:B:809:CLA:H62 | 25:B:848:LMG:H351 | 2.02 | 0.41 |
| 20:B:839:CLA:HBA2 | 20:B:839:CLA:H11 | 1.86 | 0.41 |
| 22:B:847:BCR:H331 | 22:B:847:BCR:HC8 | 2.01 | 0.41 |
| 8:D:75:LEU:HD22 | 8:D:76:LYS:N | 2.35 | 0.41 |
| 20:F:207:CLA:CAD | 20:F:207:CLA:CED | 2.99 | 0.41 |
| 11:G:60:SER:C | 11:G:63:PRO:HD2 | 2.46 | 0.41 |
| 12:H:25:GLY:HA3 | 12:H:27:ASP:CA | 2.51 | 0.41 |
| 21:R:103:LMU:H41 | 21:R:103:LMU:O6' | 2.20 | 0.41 |
| 21:R:109:LMU:O6B | 21:R:109:LMU:C1B | 2.67 | 0.41 |
| 20:1:206:CLA:H41 | 20:1:206:CLA:H62 | 1.78 | 0.40 |
| 2:2:197:LEU:HD23 | 2:2:197:LEU:HA | 1.85 | 0.40 |
| 4:4:91:PHE:CE2 | 20:4:311:CLA:C3C | 3.01 | 0.40 |
| 4:4:120:ILE:H | 4:4:120:ILE:HD12 | 1.85 | 0.40 |
| 21:4:319:LMU:H82 | 21:4:319:LMU:H52 | 1.61 | 0.40 |
| 5:A:197:GLN:NE2 | 5:A:351:THR:O | 2.53 | 0.40 |
| 5:A:227:LEU:HB3 | 5:A:258:LEU:HD21 | 2.03 | 0.40 |
| 5:A:229:ILE:HG12 | 5:A:243:PRO:CB | 2.50 | 0.40 |
| 5:A:343:HIS:O | 5:A:346:LEU:HB2 | 2.20 | 0.40 |
| 20:A:805:CLA:H41 | 20:A:805:CLA:H61 | 1.70 | 0.40 |
| 20:A:819:CLA:HBA1 | 20:A:823:CLA:CBB | 2.51 | 0.40 |
| 21:A:847:LMU:H1' | 21:A:847:LMU:H21 | 1.61 | 0.40 |
| 6:B:292:ARG:CZ | 6:B:297:ILE:H | 2.34 | 0.40 |
| 6:B:459:PHE:CD2 | 20:B:838:CLA:C3D | 3.04 | 0.40 |
| 6:B:460:ALA:O | 6:B:463:ILE:N | 2.55 | 0.40 |
| 6:B:492:ILE:CD1 | 6:B:492:ILE:N | 2.80 | 0.40 |
| 6:B:659:THR:OG1 | 20:B:803:CLA:C3B | 2.69 | 0.40 |
| 6:B:721:TYR:N | 20:B:850:CLA:O1D | 2.53 | 0.40 |
| 20:B:818:CLA:CAD | 20:B:827:CLA:CBB | 2.92 | 0.40 |
| 20:B:818:CLA:HBA2 | 20:B:818:CLA:H3A | 1.30 | 0.40 |
| 7:C:28:MET:CG | 7:C:38:GLN:HE21 | 2.32 | 0.40 |
| 10:F:93:ILE:HG22 | 22:F:203:BCR:H372 | 2.03 | 0.40 |
| 11:G:23:PHE:CE2 | 11:G:24:PHE:HB2 | 2.56 | 0.40 |
| 11:G:45:GLU:O | 11:G:46:ALA:O | 2.38 | 0.40 |
| 12:H:57:LEU:HD13 | 12:H:57:LEU:C | 2.46 | 0.40 |
| 21:H:105:LMU:C1B | 21:H:105:LMU:O1' | 2.69 | 0.40 |
| 16:L:92:VAL:O | 16:L:96:SER:CB | 2.69 | 0.40 |
| 17:N:65:LEU:O | 17:N:67:LEU:CA | 2.70 | 0.40 |
| 21:R:106:LMU:O2' | 21:R:106:LMU:C2 | 2.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:36:LEU:O | 1:1:40:LYS:N | 2.54 | 0.40 |
| 2:2:128:ASN:O | 2:2:129:LYS:C | 2.63 | 0.40 |
| 2:2:183:TYR:CD2 | 2:2:184:THR:N | 2.89 | 0.40 |
| 20:2:314:CLA:CAD | 20:2:314:CLA:CED | 2.99 | 0.40 |
| 3:3:50:GLU:HG3 | 3:3:51:PRO:N | 2.35 | 0.40 |
| 4:4:52:MET:HE3 | 4:4:156:ASN:HB3 | 2.01 | 0.40 |
| 4:4:58:MET:SD | 4:4:59:LEU:CA | 3.09 | 0.40 |
| 4:4:76:TYR:O | 4:4:77:ALA:HB3 | 2.22 | 0.40 |
| 4:4:193:ILE:HG21 | 14:J:42:PHE:CD1 | 2.56 | 0.40 |
| 5:A:64:PHE:HZ | 5:A:77:LYS:HE3 | 1.84 | 0.40 |
| 5:A:90:PHE:HE2 | 5:A:178:MET:SD | 2.44 | 0.40 |
| 5:A:173:VAL:HG23 | 5:A:174:PHE:N | 2.36 | 0.40 |
| 5:A:308:ILE:HG22 | 5:A:309:LEU:H | 1.81 | 0.40 |
| 5:A:400:MET:HE3 | 5:A:612:VAL:CG1 | 2.46 | 0.40 |
| 5:A:652:TRP:CE2 | 20:A:849:CLA:H142 | 2.56 | 0.40 |
| 5:A:687:ALA:O | 20:A:851:CLA:CBB | 2.70 | 0.40 |
| 5:A:690:LEU:CD2 | 6:B:661:PHE:CE1 | 2.95 | 0.40 |
| 5:A:692:PHE:HE2 | 20:A:838:CLA:HBC3 | 1.78 | 0.40 |
| 6:B:14:GLN:HE21 | 6:B:14:GLN:N | 2.14 | 0.40 |
| 6:B:22:TRP:HA | 6:B:25:ILE:HD11 | 2.03 | 0.40 |
| 6:B:185:VAL:HA | 6:B:188:LEU:HB3 | 2.04 | 0.40 |
| 6:B:273:VAL:HG21 | 20:B:819:CLA:HED2 | 2.02 | 0.40 |
| 6:B:428:PHE:C | 6:B:428:PHE:CD2 | 2.99 | 0.40 |
| 6:B:633:ASN:HD22 | 6:B:633:ASN:HA | 1.67 | 0.40 |
| 6:B:636:THR:C | 6:B:638:LEU:N | 2.79 | 0.40 |
| 20:B:803:CLA:CMC | 20:B:803:CLA:CBC | 2.98 | 0.40 |
| 20:B:831:CLA:HED2 | 20:B:831:CLA:CAA | 2.51 | 0.40 |
| 7:C:79:LEU:HD22 | 7:C:81:TYR:O | 2.21 | 0.40 |
| 8:D:31:GLY:HA2 | 16:L:13:PRO:HB2 | 2.00 | 0.40 |
| 10:F:23:LYS:HD2 | 10:F:23:LYS:HA | 1.82 | 0.40 |
| 10:F:145:LEU:C | 10:F:146:ASN:ND2 | 2.80 | 0.40 |
| 14:J:2:ARG:HB3 | 14:J:7:TYR:CE1 | 2.57 | 0.40 |
| 14:J:41:PHE:CD1 | 14:J:41:PHE:N | 2.89 | 0.40 |
| 21:K:107:LMU:H32 | 21:K:107:LMU:O6' | 2.19 | 0.40 |
| 16:L:9:GLN:O | 16:L:11:ILE:N | 2.54 | 0.40 |
| 16:L:82:ALA:O | 16:L:83:ALA:HB3 | 2.21 | 0.40 |
| 17:N:83:TRP:CE3 | 17:N:83:TRP:C | 3.00 | 0.40 |
| 19:Q:1:GLC:O6 | 19:Q:2:FRU:H5 | 2.21 | 0.40 |
| 2:2:57:LEU:O | 2:2:60:ALA:HB3 | 2.21 | 0.40 |
| 2:2:126:PRO:HG3 | 2:2:129:LYS:HD2 | 2.03 | 0.40 |
| 2:2:153:PRO:HB2 | 2:2:157:LYS:NZ | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:2:314:CLA:CBA | 20:2:314:CLA:CHA | 2.99 | 0.40 |
| 4:4:72:VAL:O | 4:4:72:VAL:HG22 | 2.21 | 0.40 |
| 4:4:107:GLN:HA | 20:4:301:CLA:HMA1 | 1.92 | 0.40 |
| 4:4:114:SER:HG | 4:4:120:ILE:HD11 | 1.81 | 0.40 |
| 5:A:55:TRP:C | 5:A:56:ASN:O | 2.64 | 0.40 |
| 5:A:154:ARG:O | 5:A:155:ALA:C | 2.63 | 0.40 |
| 5:A:216:LEU:HD12 | 22:A:843:BCR:H352 | 2.03 | 0.40 |
| 5:A:274:TRP:CZ2 | 5:A:278:ALA:HA | 2.56 | 0.40 |
| 5:A:277:TYR:HD2 | 5:A:278:ALA:N | 2.20 | 0.40 |
| 5:A:296:LEU:C | 5:A:298:ASP:N | 2.75 | 0.40 |
| 5:A:335:LYS:HG3 | 5:A:341:GLN:HA | 2.02 | 0.40 |
| 5:A:506:GLY:O | 5:A:507:ALA:CB | 2.69 | 0.40 |
| 5:A:550:HIS:O | 5:A:552:THR:O | 2.39 | 0.40 |
| 5:A:575:LEU:H | 5:A:575:LEU:HD12 | 1.85 | 0.40 |
| 5:A:578:ARG:O | 5:A:593:SER:OG | 2.26 | 0.40 |
| 20:A:811:CLA:H152 | 20:A:811:CLA:H202 | 2.03 | 0.40 |
| 20:A:812:CLA:CGD | 20:A:813:CLA:HMC1 | 2.51 | 0.40 |
| 20:A:818:CLA:O1D | 20:A:818:CLA:C2A | 2.68 | 0.40 |
| 22:A:845:BCR:C39 | 22:A:845:BCR:C23 | 2.76 | 0.40 |
| 6:B:211:ASN:ND2 | 6:B:214:ASP:OD1 | 2.55 | 0.40 |
| 20:B:807:CLA:HBB2 | 20:B:809:CLA:CHA | 2.51 | 0.40 |
| 20:B:824:CLA:HMD3 | 20:B:825:CLA:CAB | 2.52 | 0.40 |
| 7:C:12:ILE:O | 7:C:12:ILE:HG22 | 2.21 | 0.40 |
| 7:C:62:PHE:HB3 | 7:C:63:LEU:H | 1.59 | 0.40 |
| 8:D:77:LEU:HD23 | 8:D:77:LEU:HA | 1.81 | 0.40 |
| 9:E:40:ARG:N | 9:E:46:PHE:CE1 | 2.85 | 0.40 |
| 9:E:90:VAL:O | 9:E:90:VAL:HG12 | 2.21 | 0.40 |
| 10:F:80:TRP:HE3 | 20:F:207:CLA:HMC2 | 1.86 | 0.40 |
| 13:I:29:GLU:HA | 13:I:29:GLU:OE2 | 2.20 | 0.40 |
| 16:L:26:PRO:C | 16:L:28:THR:N | 2.80 | 0.40 |
| 16:L:63:LEU:O | 16:L:65:VAL:N | 2.54 | 0.40 |
| 16:L:99:LEU:HD11 | 22:L:209:BCR:C7 | 2.44 | 0.40 |
| 1:1:136:ASP:CG | 1:1:140:LEU:HD13 | 2.46 | 0.40 |
| 2:2:204:ILE:O | 2:2:205:PHE:HB3 | 2.21 | 0.40 |
| 4:4:86:SER:C | 4:4:88:SER:H | 2.28 | 0.40 |
| 4:4:176:GLY:HA2 | 4:4:177:PRO:HD3 | 1.92 | 0.40 |
| 20:4:306:CLA:O2A | 20:4:306:CLA:HMA3 | 2.21 | 0.40 |
| 5:A:32:GLU:HG3 | 5:A:33:GLN:N | 2.37 | 0.40 |
| 5:A:111:ASN:C | 5:A:111:ASN:HD22 | 2.30 | 0.40 |
| 5:A:146:THR:O | 20:A:826:CLA:CMA | 2.70 | 0.40 |
| 5:A:249:ILE:N | 5:A:251:ASN:OD1 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:A:393:LEU:O | 5:A:394:SER:C | 2.63 | 0.40 |
| 5:A:636:HIS:O | 5:A:637:ILE:C | 2.64 | 0.40 |
| 5:A:681:GLY:C | 5:A:683:HIS:N | 2.79 | 0.40 |
| 5:A:720:THR:O | 5:A:721:GLN:C | 2.65 | 0.40 |
| 20:A:826:CLA:H102 | 22:A:845:BCR:C37 | 2.44 | 0.40 |
| 20:A:851:CLA:O2A | 6:B:430:GLY:HA3 | 2.22 | 0.40 |
| 6:B:57:ILE:HG22 | 6:B:58:PHE:CD1 | 2.55 | 0.40 |
| 6:B:86:PRO:O | 6:B:115:ASN:HB3 | 2.22 | 0.40 |
| 6:B:98:GLN:HE21 | 6:B:101:VAL:HG13 | 1.87 | 0.40 |
| 6:B:216:LEU:O | 6:B:217:PRO:C | 2.62 | 0.40 |
| 6:B:390:GLY:CA | 22:B:846:BCR:HC22 | 2.52 | 0.40 |
| 6:B:424:TRP:HD1 | 20:B:806:CLA:O1A | 2.05 | 0.40 |
| 6:B:525:LEU:HD22 | 6:B:529:THR:OG1 | 2.21 | 0.40 |
| 20:B:818:CLA:H12 | 20:B:818:CLA:NA | 2.36 | 0.40 |
| 8:D:113:HIS:CD2 | 8:D:113:HIS:O | 2.74 | 0.40 |
| 10:F:53:PHE:HB2 | 10:F:55:ASN:HD22 | 1.87 | 0.40 |
| 10:F:131:PHE:C | 10:F:133:GLY:H | 2.29 | 0.40 |
| 11:G:20:ARG:NH1 | 11:G:64:VAL:C | 2.80 | 0.40 |
| 16:L:99:LEU:HD23 | 16:L:140:THR:HG22 | 2.04 | 0.40 |
| 17:N:61:LEU:CD1 | 17:N:63:ASP:CA | 2.96 | 0.40 |
| 19:P:2:FRU:C1 | 19:P:2:FRU:C6 | 2.99 | 0.40 |
| 19:X:1:GLC:O5 | 19:X:2:FRU:H5 | 2.21 | 0.40 |
| 1:1:160:GLY:O | 1:1:162:CYS:N | 2.54 | 0.40 |
| 1:1:185:TRP:CZ2 | 20:1:213:CLA:O2A | 2.71 | 0.40 |
| 2:2:62:ILE:O | 2:2:66:GLU:HB2 | 2.22 | 0.40 |
| 4:4:141:LEU:HB3 | 4:4:142:ASN:H | 1.79 | 0.40 |
| 5:A:44:ILE:H | 5:A:44:ILE:HG13 | 1.58 | 0.40 |
| 5:A:53:TRP:HA | 5:A:56:ASN:ND2 | 2.37 | 0.40 |
| 5:A:417:PHE:O | 5:A:418:MET:C | 2.64 | 0.40 |
| 5:A:439:ARG:C | 5:A:441:ALA:H | 2.29 | 0.40 |
| 5:A:588:GLY:N | 6:B:668:ARG:NH1 | 2.67 | 0.40 |
| 5:A:591:GLN:HA | 5:A:591:GLN:NE2 | 2.28 | 0.40 |
| 5:A:593:SER:OG | 5:A:594:ALA:N | 2.53 | 0.40 |
| 5:A:714:LEU:HB2 | 5:A:716:VAL:HG13 | 2.03 | 0.40 |
| 5:A:723:ARG:O | 20:A:837:CLA:HBB1 | 2.21 | 0.40 |
| 5:A:746:THR:OG1 | 20:A:849:CLA:CGD | 2.69 | 0.40 |
| 6:B:159:PRO:O | 6:B:163:PRO:HD3 | 2.21 | 0.40 |
| 6:B:310:PRO:O | 20:B:842:CLA:CHD | 2.69 | 0.40 |
| 6:B:334:LEU:CB | 20:B:808:CLA:HMD3 | 2.46 | 0.40 |
| 6:B:377:TYR:O | 6:B:378:ILE:CB | 2.69 | 0.40 |
| 6:B:429:LEU:HD23 | 6:B:429:LEU:HA | 1.90 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:559:CYS:SG | 6:B:560:ASP:N | 2.94 | 0.40 |
| 6:B:580:VAL:HG11 | 6:B:710:LEU:HD11 | 2.03 | 0.40 |
| 20:B:808:CLA:HBD | 20:B:808:CLA:CBA | 2.48 | 0.40 |
| 20:B:829:CLA:C6 | 22:B:845:BCR:H322 | 2.52 | 0.40 |
| 20:B:838:CLA:H62 | 20:B:838:CLA:H101 | 1.88 | 0.40 |
| 23:B:843:PQN:H302 | 22:L:209:BCR:H24C | 2.04 | 0.40 |
| 7:C:17:CYS:O | 7:C:58:CYS:HB2 | 2.21 | 0.40 |
| 9:E:44:TYR:HB3 | 9:E:45:TRP:CZ3 | 2.57 | 0.40 |
| 10:F:26:GLN:C | 10:F:28:SER:N | 2.79 | 0.40 |
| 10:F:77:GLN:C | 10:F:77:GLN:CD | 2.89 | 0.40 |
| 21:G:102:LMU:H92 | 21:G:102:LMU:H61 | 1.99 | 0.40 |
| 21:H:106:LMU:H3' | 21:H:106:LMU:H1B | 1.72 | 0.40 |
| 20:K:101:CLA:OBD | 20:K:102:CLA:C1B | 2.70 | 0.40 |

All (56) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:Y:2:FRU:O2 | 21:G:101:LMU:C5B[1_456] | 0.08 | 2.12 |
| 3:3:180:LYS:CD | 6:B:490:ARG:CZ[1_556] | 0.31 | 1.89 |
| 3:3:180:LYS:NZ | 6:B:490:ARG:CD[1_556] | 0.56 | 1.64 |
| 19:Y:1:GLC:O2 | 21:G:101:LMU:O4'[1_456] | 1.01 | 1.19 |
| 3:3:180:LYS:CG | 6:B:490:ARG:NE[1_556] | 1.05 | 1.15 |
| 19:Y:1:GLC:O5 | 21:G:101:LMU:C3B[1_456] | 1.06 | 1.14 |
| 3:3:180:LYS:CD | 6:B:490:ARG:NH1[1_556] | 1.09 | 1.11 |
| 3:3:180:LYS:CG | 6:B:490:ARG:CZ[1_556] | 1.22 | 0.98 |
| 4:4:130:GLU:C | 16:L:159:TYR:OH[1_655] | 1.34 | 0.86 |
| 19:Y:1:GLC:O3 | 21:G:101:LMU:O3B[1_456] | 1.37 | 0.83 |
| 3:3:180:LYS:CD | 6:B:490:ARG:NE[1_556] | 1.47 | 0.73 |
| 3:3:180:LYS:CD | 6:B:490:ARG:NH2[1_556] | 1.48 | 0.72 |
| 4:4:130:GLU:O | 16:L:159:TYR:OH[1_655] | 1.49 | 0.71 |
| 3:3:180:LYS:CE | 6:B:490:ARG:NH1[1_556] | 1.50 | 0.70 |
| 19:Y:2:FRU:O2 | 21:G:101:LMU:O5B[1_456] | 1.53 | 0.67 |
| 19:Y:2:FRU:O2 | 21:G:101:LMU:C6B[1_456] | 1.55 | 0.65 |
| 3:3:180:LYS:NZ | 6:B:490:ARG:NE[1_556] | 1.60 | 0.60 |
| 19:Y:2:FRU:O4 | 21:G:101:LMU:C3'[1_456] | 1.60 | 0.60 |
| 19:Y:2:FRU:O3 | 21:G:101:LMU:O2B[1_456] | 1.60 | 0.60 |
| 21:4:319:LMU:O6B | 21:R:109:LMU:C9[1_654] | 1.61 | 0.59 |
| 19:Y:1:GLC:C2 | 21:G:101:LMU:O4'[1_456] | 1.61 | 0.59 |
| 19:Y:2:FRU:O2 | 21:G:101:LMU:C4B[1_456] | 1.61 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:Y:2:FRU:C3 | 21:G:101:LMU:O5B[1_456] | 1.62 | 0.58 |
| 3:3:180:LYS:CE | 6:B:490:ARG:CZ[1_556] | 1.67 | 0.53 |
| 3:3:180:LYS:CE | 6:B:490:ARG:CD[1_556] | 1.67 | 0.53 |
| 3:3:180:LYS:CE | 6:B:490:ARG:CG[1_556] | 1.68 | 0.52 |
| 3:3:180:LYS:NZ | 6:B:490:ARG:CG[1_556] | 1.68 | 0.52 |
| 19:Y:1:GLC:C2 | 21:G:101:LMU:C4B[1_456] | 1.69 | 0.51 |
| 3:3:180:LYS:CE | 6:B:490:ARG:NE[1_556] | 1.70 | 0.50 |
| 19:Y:2:FRU:O5 | 21:G:101:LMU:O6B[1_456] | 1.73 | 0.47 |
| 3:3:180:LYS:CG | 6:B:490:ARG:NH2[1_556] | 1.78 | 0.42 |
| 19:Y:1:GLC:C3 | 21:G:101:LMU:C3B[1_456] | 1.78 | 0.42 |
| 21:4:319:LMU:C6B | 21:R:109:LMU:C10[1_654] | 1.80 | 0.40 |
| 19:Y:2:FRU:O1 | 21:G:101:LMU:O6B[1_456] | 1.80 | 0.40 |
| 4:4:130:GLU:CA | 16:L:159:TYR:OH[1_655] | 1.83 | 0.37 |
| 19:Y:2:FRU:C5 | 21:G:101:LMU:O3'[1_456] | 1.84 | 0.36 |
| 19:Y:2:FRU:O4 | 21:G:101:LMU:C4'[1_456] | 1.86 | 0.34 |
| 19:Y:2:FRU:O5 | 21:G:101:LMU:O5B[1_456] | 1.89 | 0.31 |
| 19:Y:2:FRU:O4 | 21:G:101:LMU:C1'[1_456] | 1.90 | 0.30 |
| 19:Y:1:GLC:O5 | 21:G:101:LMU:O3B[1_456] | 1.92 | 0.28 |
| 4:4:126:LEU:O | 16:L:78:GLU:N[1_655] | 1.93 | 0.27 |
| 19:Y:1:GLC:C1 | 21:G:101:LMU:C2B[1_456] | 1.96 | 0.24 |
| 21:4:319:LMU:O6B | 21:R:109:LMU:C10[1_654] | 1.98 | 0.22 |
| 19:Y:1:GLC:C5 | 21:G:101:LMU:C3B[1_456] | 2.01 | 0.19 |
| 19:Y:1:GLC:O3 | 21:G:101:LMU:C3B[1_456] | 2.03 | 0.17 |
| 1:1:130:PRO:O | 2:2:72:GLY:O[2_545] | 2.04 | 0.16 |
| 20:1:207:CLA:O2D | 20:K:101:CLA:C1[1_654] | 2.04 | 0.16 |
| 11:G:31:MET:SD | 17:N:85:TRP:CE2[2_445] | 2.08 | 0.12 |
| 19:Y:2:FRU:O6 | 21:G:101:LMU:O6B[1_456] | 2.08 | 0.12 |
| 19:Y:2:FRU:C2 | 21:G:101:LMU:O6B[1_456] | 2.11 | 0.09 |
| 4:4:133:TYR:OH | 16:L:156:PHE:O[1_655] | 2.12 | 0.08 |
| 19:Y:1:GLC:C5 | 21:G:101:LMU:O3B[1_456] | 2.12 | 0.08 |
| 1:1:176:ASN:ND2 | 3:3:149:GLY:O[1_554] | 2.13 | 0.07 |
| 19:Y:2:FRU:C2 | 21:G:101:LMU:C6B[1_456] | 2.13 | 0.07 |
| 19:Y:1:GLC:O5 | 21:G:101:LMU:O5B[1_456] | 2.16 | 0.04 |
| 1:1:130:PRO:CA | 2:2:72:GLY:O[2_545] | 2.18 | 0.02 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

of similar resolution.

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 | 1 | 161/241 (67%) | 84 (52%) | 39 (24%) | 38 (24%) | 0 | 0 |
| 2 | 2 | 174/269 (65%) | 67 (38%) | 51 (29%) | 56 (32%) | 0 | 0 |
| 3 | 3 | 145/276 (52%) | 76 (52%) | 36 (25%) | 33 (23%) | 0 | 1 |
| 4 | 4 | 164/251 (65%) | 57 (35%) | 44 (27%) | 63 (38%) | 0 | 0 |
| 5 | A | 726/758 (96%) | 366 (50%) | 187 (26%) | 173 (24%) | 0 | 0 |
| 6 | B | 731/734 (100%) | 379 (52%) | 204 (28%) | 148 (20%) | 0 | 1 |
| 7 | C | 79/81 (98%) | 23 (29%) | 31 (39%) | 25 (32%) | 0 | 0 |
| 8 | D | 136/212 (64%) | 47 (35%) | 48 (35%) | 41 (30%) | 0 | 0 |
| 9 | E | 63/143 (44%) | 30 (48%) | 15 (24%) | 18 (29%) | 0 | 0 |
| 10 | F | 152/231 (66%) | 71 (47%) | 40 (26%) | 41 (27%) | 0 | 0 |
| 11 | G | 93/167 (56%) | 38 (41%) | 27 (29%) | 28 (30%) | 0 | 0 |
| 12 | H | 67/144 (46%) | 30 (45%) | 16 (24%) | 21 (31%) | 0 | 0 |
| 13 | I | 28/40 (70%) | 11 (39%) | 10 (36%) | 7 (25%) | 0 | 0 |
| 14 | J | 40/44 (91%) | 19 (48%) | 11 (28%) | 10 (25%) | 0 | 0 |
| 15 | K | 82/131 (63%) | 50 (61%) | 13 (16%) | 19 (23%) | 0 | 0 |
| 16 | L | 160/216 (74%) | 72 (45%) | 49 (31%) | 39 (24%) | 0 | 0 |
| 17 | N | 83/170 (49%) | 21 (25%) | 19 (23%) | 43 (52%) | 0 | 0 |
| All | All | 3084/4108 (75%) | 1441 (47%) | 840 (27%) | 803 (26%) | 0 | 0 |

All (803) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 25 | ASP |
| 1 | 1 | 30 | GLY |
| 1 | 1 | 35 | ASN |
| 1 | 1 | 58 | LEU |
| 1 | 1 | 73 | GLU |
| 1 | 1 | 90 | PRO |
| 1 | 1 | 130 | PRO |
| 1 | 1 | 137 | PRO |
| 1 | 1 | 183 | ASP |
| 2 | 2 | 37 | ASP |
| 2 | 2 | 42 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 2 | 43 | TRP |
| 2 | 2 | 44 | ASN |
| 2 | 2 | 66 | GLU |
| 2 | 2 | 70 | LYS |
| 2 | 2 | 73 | ILE |
| 2 | 2 | 74 | LEU |
| 2 | 2 | 75 | ASN |
| 2 | 2 | 125 | PHE |
| 2 | 2 | 128 | ASN |
| 2 | 2 | 129 | LYS |
| 2 | 2 | 149 | GLY |
| 2 | 2 | 154 | GLN |
| 2 | 2 | 159 | LEU |
| 2 | 2 | 160 | ARG |
| 2 | 2 | 163 | GLU |
| 2 | 2 | 188 | PRO |
| 2 | 2 | 189 | ILE |
| 2 | 2 | 190 | ASP |
| 2 | 2 | 197 | LEU |
| 2 | 2 | 200 | PRO |
| 2 | 2 | 204 | ILE |
| 2 | 2 | 206 | ALA |
| 2 | 2 | 207 | ALA |
| 2 | 2 | 209 | THR |
| 2 | 2 | 210 | PRO |
| 3 | 3 | 48 | PHE |
| 3 | 3 | 49 | ILE |
| 3 | 3 | 94 | ARG |
| 3 | 3 | 97 | PHE |
| 3 | 3 | 107 | TRP |
| 3 | 3 | 108 | ALA |
| 3 | 3 | 110 | SER |
| 3 | 3 | 111 | TYR |
| 3 | 3 | 113 | LEU |
| 3 | 3 | 134 | LYS |
| 3 | 3 | 135 | PRO |
| 3 | 3 | 142 | TYR |
| 3 | 3 | 158 | TYR |
| 3 | 3 | 159 | PRO |
| 3 | 3 | 164 | PHE |
| 3 | 3 | 166 | PRO |
| 3 | 3 | 167 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 3 | 172 | ASP |
| 3 | 3 | 206 | VAL |
| 3 | 3 | 210 | GLN |
| 4 | 4 | 31 | ALA |
| 4 | 4 | 32 | GLU |
| 4 | 4 | 34 | PRO |
| 4 | 4 | 38 | ARG |
| 4 | 4 | 66 | SER |
| 4 | 4 | 69 | ILE |
| 4 | 4 | 73 | PRO |
| 4 | 4 | 74 | LYS |
| 4 | 4 | 82 | GLU |
| 4 | 4 | 84 | PHE |
| 4 | 4 | 87 | SER |
| 4 | 4 | 88 | SER |
| 4 | 4 | 91 | PHE |
| 4 | 4 | 107 | GLN |
| 4 | 4 | 115 | VAL |
| 4 | 4 | 121 | PHE |
| 4 | 4 | 122 | LYS |
| 4 | 4 | 125 | SER |
| 4 | 4 | 128 | ALA |
| 4 | 4 | 141 | LEU |
| 4 | 4 | 143 | PHE |
| 4 | 4 | 148 | GLU |
| 4 | 4 | 150 | LYS |
| 4 | 4 | 171 | ASN |
| 4 | 4 | 172 | VAL |
| 4 | 4 | 173 | THR |
| 4 | 4 | 175 | LYS |
| 4 | 4 | 193 | ILE |
| 5 | A | 22 | VAL |
| 5 | A | 28 | LYS |
| 5 | A | 35 | ALA |
| 5 | A | 36 | LYS |
| 5 | A | 40 | PHE |
| 5 | A | 67 | HIS |
| 5 | A | 71 | LEU |
| 5 | A | 82 | HIS |
| 5 | A | 83 | PHE |
| 5 | A | 88 | ILE |
| 5 | A | 99 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 104 | SER |
| 5 | A | 156 | SER |
| 5 | A | 158 | ILE |
| 5 | A | 159 | THR |
| 5 | A | 160 | SER |
| 5 | A | 175 | ALA |
| 5 | A | 189 | ALA |
| 5 | A | 193 | LEU |
| 5 | A | 205 | HIS |
| 5 | A | 215 | SER |
| 5 | A | 221 | HIS |
| 5 | A | 237 | VAL |
| 5 | A | 244 | LEU |
| 5 | A | 247 | GLU |
| 5 | A | 250 | LEU |
| 5 | A | 252 | ARG |
| 5 | A | 258 | LEU |
| 5 | A | 268 | PRO |
| 5 | A | 279 | ASP |
| 5 | A | 280 | PHE |
| 5 | A | 281 | LEU |
| 5 | A | 283 | PHE |
| 5 | A | 286 | GLY |
| 5 | A | 307 | ALA |
| 5 | A | 310 | PHE |
| 5 | A | 317 | TYR |
| 5 | A | 329 | ASP |
| 5 | A | 339 | THR |
| 5 | A | 349 | ILE |
| 5 | A | 361 | ASN |
| 5 | A | 386 | ALA |
| 5 | A | 389 | TYR |
| 5 | A | 473 | PRO |
| 5 | A | 474 | GLN |
| 5 | A | 476 | MET |
| 5 | A | 477 | PHE |
| 5 | A | 486 | PRO |
| 5 | A | 489 | ALA |
| 5 | A | 498 | LEU |
| 5 | A | 507 | ALA |
| 5 | A | 508 | THR |
| 5 | A | 509 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 510 | SER |
| 5 | A | 521 | VAL |
| 5 | A | 523 | VAL |
| 5 | A | 553 | VAL |
| 5 | A | 578 | ARG |
| 5 | A | 579 | PHE |
| 5 | A | 643 | ALA |
| 5 | A | 649 | ILE |
| 5 | A | 657 | LEU |
| 5 | A | 673 | SER |
| 5 | A | 679 | PHE |
| 5 | A | 727 | ILE |
| 5 | A | 735 | VAL |
| 5 | A | 750 | PHE |
| 5 | A | 751 | LEU |
| 5 | A | 752 | ALA |
| 5 | A | 757 | VAL |
| 6 | B | 5 | ILE |
| 6 | B | 6 | PRO |
| 6 | B | 26 | ALA |
| 6 | B | 35 | ASP |
| 6 | B | 68 | VAL |
| 6 | B | 69 | ALA |
| 6 | B | 77 | TRP |
| 6 | B | 80 | ASP |
| 6 | B | 83 | HIS |
| 6 | B | 86 | PRO |
| 6 | B | 104 | PHE |
| 6 | B | 115 | ASN |
| 6 | B | 120 | VAL |
| 6 | B | 129 | LEU |
| 6 | B | 140 | ILE |
| 6 | B | 142 | LEU |
| 6 | B | 159 | PRO |
| 6 | B | 160 | LYS |
| 6 | B | 167 | TRP |
| 6 | B | 182 | LEU |
| 6 | B | 187 | SER |
| 6 | B | 188 | LEU |
| 6 | B | 198 | ALA |
| 6 | B | 208 | ARG |
| 6 | B | 248 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | B | 267 | SER |
| 6 | B | 293 | THR |
| 6 | B | 308 | HIS |
| 6 | B | 310 | PRO |
| 6 | B | 320 | LYS |
| 6 | B | 321 | GLY |
| 6 | B | 362 | ALA |
| 6 | B | 375 | HIS |
| 6 | B | 378 | ILE |
| 6 | B | 382 | ILE |
| 6 | B | 383 | MET |
| 6 | B | 405 | ASP |
| 6 | B | 420 | SER |
| 6 | B | 450 | GLU |
| 6 | B | 469 | LYS |
| 6 | B | 479 | SER |
| 6 | B | 490 | ARG |
| 6 | B | 494 | LEU |
| 6 | B | 495 | PRO |
| 6 | B | 506 | ASN |
| 6 | B | 512 | ILE |
| 6 | B | 528 | HIS |
| 6 | B | 545 | LYS |
| 6 | B | 555 | TYR |
| 6 | B | 569 | ASP |
| 6 | B | 587 | ILE |
| 6 | B | 603 | ARG |
| 6 | B | 610 | ASN |
| 6 | B | 629 | SER |
| 6 | B | 636 | THR |
| 6 | B | 639 | VAL |
| 6 | B | 661 | PHE |
| 6 | B | 662 | MET |
| 6 | B | 668 | ARG |
| 6 | B | 681 | ALA |
| 6 | B | 682 | HIS |
| 6 | B | 691 | ILE |
| 6 | B | 710 | LEU |
| 6 | B | 732 | LYS |
| 6 | B | 733 | PHE |
| 7 | C | 8 | TYR |
| 7 | C | 21 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | C | 32 | GLY |
| 7 | C | 49 | VAL |
| 7 | C | 56 | SER |
| 7 | C | 59 | PRO |
| 7 | C | 62 | PHE |
| 7 | C | 65 | VAL |
| 7 | C | 66 | ARG |
| 7 | C | 70 | TRP |
| 8 | D | 32 | SER |
| 8 | D | 36 | LEU |
| 8 | D | 38 | ARG |
| 8 | D | 65 | ALA |
| 8 | D | 70 | GLU |
| 8 | D | 78 | ALA |
| 8 | D | 94 | TYR |
| 8 | D | 95 | LYS |
| 8 | D | 97 | LYS |
| 8 | D | 110 | GLN |
| 8 | D | 114 | PRO |
| 8 | D | 115 | LYS |
| 8 | D | 119 | TYR |
| 8 | D | 120 | PRO |
| 8 | D | 121 | GLU |
| 8 | D | 124 | ASN |
| 8 | D | 139 | LYS |
| 8 | D | 151 | LYS |
| 8 | D | 153 | PRO |
| 9 | E | 46 | PHE |
| 9 | E | 54 | ALA |
| 9 | E | 60 | LYS |
| 9 | E | 65 | VAL |
| 9 | E | 72 | VAL |
| 9 | E | 73 | ASN |
| 9 | E | 86 | GLU |
| 9 | E | 87 | VAL |
| 9 | E | 89 | GLU |
| 10 | F | 2 | ILE |
| 10 | F | 7 | PRO |
| 10 | F | 12 | LYS |
| 10 | F | 21 | ALA |
| 10 | F | 25 | LEU |
| 10 | F | 26 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | F | 31 | LEU |
| 10 | F | 35 | ASP |
| 10 | F | 38 | PRO |
| 10 | F | 42 | ILE |
| 10 | F | 47 | GLU |
| 10 | F | 52 | ARG |
| 10 | F | 54 | ASP |
| 10 | F | 58 | LYS |
| 10 | F | 59 | TYR |
| 10 | F | 77 | GLN |
| 10 | F | 109 | ARG |
| 10 | F | 116 | GLN |
| 10 | F | 127 | SER |
| 10 | F | 130 | LEU |
| 11 | G | 28 | ARG |
| 11 | G | 31 | MET |
| 11 | G | 34 | GLN |
| 11 | G | 38 | GLN |
| 11 | G | 47 | GLY |
| 11 | G | 50 | ARG |
| 11 | G | 59 | LYS |
| 11 | G | 61 | ASN |
| 11 | G | 70 | ASP |
| 11 | G | 74 | TRP |
| 11 | G | 81 | VAL |
| 11 | G | 86 | LEU |
| 11 | G | 93 | TYR |
| 11 | G | 94 | ASP |
| 12 | H | 15 | ALA |
| 12 | H | 20 | GLN |
| 12 | H | 21 | TRP |
| 12 | H | 23 | VAL |
| 12 | H | 24 | TYR |
| 12 | H | 31 | PRO |
| 12 | H | 41 | GLU |
| 12 | H | 46 | PRO |
| 12 | H | 50 | ARG |
| 12 | H | 52 | LEU |
| 12 | H | 56 | PHE |
| 12 | H | 71 | ASN |
| 12 | H | 77 | LEU |
| 13 | I | 22 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | I | 23 | SER |
| 14 | J | 5 | LYS |
| 14 | J | 6 | THR |
| 14 | J | 10 | VAL |
| 14 | J | 22 | LEU |
| 14 | J | 26 | LEU |
| 15 | K | 41 | GLU |
| 15 | K | 43 | ARG |
| 15 | K | 47 | LEU |
| 15 | K | 48 | GLN |
| 15 | K | 51 | ASP |
| 15 | K | 52 | PRO |
| 15 | K | 75 | VAL |
| 16 | L | 8 | TYR |
| 16 | L | 10 | VAL |
| 16 | L | 37 | LEU |
| 16 | L | 43 | TYR |
| 16 | L | 44 | ARG |
| 16 | L | 46 | ALA |
| 16 | L | 76 | ASN |
| 16 | L | 88 | ALA |
| 16 | L | 97 | MET |
| 16 | L | 121 | THR |
| 16 | L | 123 | ARG |
| 16 | L | 127 | PRO |
| 16 | L | 129 | GLN |
| 16 | L | 149 | SER |
| 16 | L | 158 | MET |
| 16 | L | 161 | LEU |
| 16 | L | 163 | LEU |
| 16 | L | 165 | TYR |
| 17 | N | 7 | LEU |
| 17 | N | 24 | THR |
| 17 | N | 27 | ALA |
| 17 | N | 28 | ASN |
| 17 | N | 40 | CYS |
| 17 | N | 46 | PHE |
| 17 | N | 48 | GLY |
| 17 | N | 49 | CYS |
| 17 | N | 50 | GLN |
| 17 | N | 51 | ASP |
| 17 | N | 58 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | N | 61 | LEU |
| 17 | N | 63 | ASP |
| 17 | N | 69 | CYS |
| 17 | N | 74 | LYS |
| 17 | N | 75 | TYR |
| 17 | N | 76 | LYS |
| 17 | N | 77 | CYS |
| 17 | N | 78 | GLY |
| 17 | N | 80 | ASN |
| 1 | 1 | 21 | ASP |
| 1 | 1 | 28 | GLY |
| 1 | 1 | 29 | LEU |
| 1 | 1 | 161 | PHE |
| 1 | 1 | 178 | ALA |
| 1 | 1 | 185 | TRP |
| 2 | 2 | 69 | THR |
| 2 | 2 | 71 | LEU |
| 2 | 2 | 81 | THR |
| 2 | 2 | 82 | ALA |
| 2 | 2 | 103 | GLY |
| 2 | 2 | 104 | TRP |
| 2 | 2 | 130 | LEU |
| 2 | 2 | 132 | GLY |
| 2 | 2 | 136 | GLY |
| 2 | 2 | 208 | PHE |
| 3 | 3 | 52 | LYS |
| 3 | 3 | 77 | ILE |
| 3 | 3 | 106 | TYR |
| 3 | 3 | 137 | SER |
| 3 | 3 | 162 | PRO |
| 3 | 3 | 208 | PRO |
| 4 | 4 | 45 | LEU |
| 4 | 4 | 59 | LEU |
| 4 | 4 | 70 | ILE |
| 4 | 4 | 71 | ASN |
| 4 | 4 | 127 | PRO |
| 4 | 4 | 129 | GLY |
| 4 | 4 | 145 | PRO |
| 4 | 4 | 162 | ALA |
| 4 | 4 | 178 | PHE |
| 4 | 4 | 186 | SER |
| 4 | 4 | 188 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 25 | ASP |
| 5 | A | 39 | HIS |
| 5 | A | 60 | ASP |
| 5 | A | 69 | SER |
| 5 | A | 74 | ILE |
| 5 | A | 96 | MET |
| 5 | A | 130 | GLU |
| 5 | A | 157 | GLY |
| 5 | A | 200 | GLU |
| 5 | A | 210 | LEU |
| 5 | A | 242 | ILE |
| 5 | A | 243 | PRO |
| 5 | A | 266 | ALA |
| 5 | A | 278 | ALA |
| 5 | A | 282 | THR |
| 5 | A | 290 | LEU |
| 5 | A | 299 | ILE |
| 5 | A | 313 | ALA |
| 5 | A | 328 | LYS |
| 5 | A | 333 | ALA |
| 5 | A | 337 | PRO |
| 5 | A | 346 | LEU |
| 5 | A | 400 | MET |
| 5 | A | 404 | GLY |
| 5 | A | 421 | ASP |
| 5 | A | 424 | PRO |
| 5 | A | 427 | ARG |
| 5 | A | 428 | TYR |
| 5 | A | 429 | ASN |
| 5 | A | 431 | LEU |
| 5 | A | 433 | ASP |
| 5 | A | 439 | ARG |
| 5 | A | 511 | THR |
| 5 | A | 516 | GLY |
| 5 | A | 518 | GLY |
| 5 | A | 538 | ASP |
| 5 | A | 574 | ASN |
| 5 | A | 592 | VAL |
| 5 | A | 594 | ALA |
| 5 | A | 624 | VAL |
| 5 | A | 640 | GLY |
| 5 | A | 661 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 717 | ALA |
| 6 | B | 99 | PRO |
| 6 | B | 105 | THR |
| 6 | B | 128 | GLY |
| 6 | B | 136 | TYR |
| 6 | B | 164 | SER |
| 6 | B | 179 | LEU |
| 6 | B | 224 | PRO |
| 6 | B | 225 | LEU |
| 6 | B | 231 | ASN |
| 6 | B | 237 | PRO |
| 6 | B | 247 | THR |
| 6 | B | 265 | THR |
| 6 | B | 292 | ARG |
| 6 | B | 309 | ILE |
| 6 | B | 330 | ILE |
| 6 | B | 437 | TYR |
| 6 | B | 464 | GLN |
| 6 | B | 474 | PHE |
| 6 | B | 480 | SER |
| 6 | B | 503 | GLU |
| 6 | B | 505 | SER |
| 6 | B | 539 | LEU |
| 6 | B | 554 | GLY |
| 6 | B | 599 | ILE |
| 6 | B | 657 | TRP |
| 6 | B | 664 | LEU |
| 6 | B | 690 | LEU |
| 7 | C | 10 | THR |
| 7 | C | 43 | PRO |
| 7 | C | 61 | ASP |
| 7 | C | 64 | SER |
| 8 | D | 26 | SER |
| 8 | D | 31 | GLY |
| 8 | D | 53 | PRO |
| 8 | D | 109 | VAL |
| 8 | D | 129 | GLY |
| 8 | D | 130 | VAL |
| 8 | D | 132 | LEU |
| 8 | D | 146 | VAL |
| 9 | E | 30 | PRO |
| 9 | E | 35 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | E | 42 | GLU |
| 9 | E | 53 | VAL |
| 9 | E | 64 | PRO |
| 9 | E | 90 | VAL |
| 10 | F | 114 | PRO |
| 10 | F | 126 | ALA |
| 10 | F | 132 | ARG |
| 11 | G | 33 | LYS |
| 11 | G | 63 | PRO |
| 11 | G | 80 | ILE |
| 11 | G | 84 | TYR |
| 11 | G | 85 | ILE |
| 11 | G | 87 | ALA |
| 12 | H | 17 | THR |
| 12 | H | 27 | ASP |
| 12 | H | 45 | ALA |
| 12 | H | 75 | ASP |
| 13 | I | 25 | PHE |
| 14 | J | 9 | SER |
| 14 | J | 37 | LEU |
| 14 | J | 39 | PHE |
| 15 | K | 27 | ALA |
| 15 | K | 35 | THR |
| 15 | K | 45 | SER |
| 15 | K | 73 | GLY |
| 15 | K | 79 | LYS |
| 16 | L | 24 | GLU |
| 16 | L | 27 | VAL |
| 16 | L | 63 | LEU |
| 16 | L | 89 | ALA |
| 16 | L | 108 | LYS |
| 16 | L | 120 | LEU |
| 16 | L | 125 | LYS |
| 16 | L | 128 | ASP |
| 16 | L | 147 | GLY |
| 17 | N | 2 | VAL |
| 17 | N | 11 | LYS |
| 17 | N | 35 | VAL |
| 17 | N | 47 | THR |
| 17 | N | 54 | LYS |
| 17 | N | 64 | ASP |
| 17 | N | 66 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | N | 68 | GLU |
| 17 | N | 81 | VAL |
| 17 | N | 82 | PHE |
| 17 | N | 83 | TRP |
| 1 | 1 | 78 | PRO |
| 1 | 1 | 79 | GLY |
| 1 | 1 | 118 | PRO |
| 2 | 2 | 91 | THR |
| 2 | 2 | 114 | LEU |
| 2 | 2 | 194 | ALA |
| 2 | 2 | 205 | PHE |
| 3 | 3 | 153 | SER |
| 3 | 3 | 157 | ALA |
| 4 | 4 | 35 | GLU |
| 4 | 4 | 119 | PRO |
| 4 | 4 | 139 | ASN |
| 5 | A | 23 | ASP |
| 5 | A | 31 | PHE |
| 5 | A | 45 | ALA |
| 5 | A | 57 | LEU |
| 5 | A | 105 | ASN |
| 5 | A | 124 | TRP |
| 5 | A | 144 | GLN |
| 5 | A | 155 | ALA |
| 5 | A | 184 | PHE |
| 5 | A | 213 | LEU |
| 5 | A | 263 | ALA |
| 5 | A | 276 | LYS |
| 5 | A | 354 | TRP |
| 5 | A | 373 | ALA |
| 5 | A | 426 | THR |
| 5 | A | 446 | LEU |
| 5 | A | 479 | ASP |
| 5 | A | 485 | GLN |
| 5 | A | 505 | PRO |
| 5 | A | 514 | THR |
| 5 | A | 671 | SER |
| 6 | B | 103 | ALA |
| 6 | B | 153 | GLY |
| 6 | B | 161 | TRP |
| 6 | B | 230 | TRP |
| 6 | B | 294 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | B | 335 | GLY |
| 6 | B | 371 | LEU |
| 6 | B | 379 | ALA |
| 6 | B | 451 | LYS |
| 6 | B | 468 | GLY |
| 6 | B | 481 | THR |
| 6 | B | 493 | TRP |
| 6 | B | 501 | ILE |
| 6 | B | 514 | PRO |
| 6 | B | 558 | PRO |
| 6 | B | 595 | HIS |
| 6 | B | 605 | ASN |
| 6 | B | 623 | TYR |
| 6 | B | 707 | LEU |
| 7 | C | 22 | PRO |
| 7 | C | 68 | TYR |
| 7 | C | 73 | THR |
| 8 | D | 55 | GLU |
| 8 | D | 63 | GLY |
| 8 | D | 128 | GLN |
| 8 | D | 150 | GLY |
| 9 | E | 88 | GLU |
| 10 | F | 11 | SER |
| 10 | F | 22 | LEU |
| 10 | F | 29 | LEU |
| 10 | F | 46 | MET |
| 10 | F | 53 | PHE |
| 10 | F | 63 | CYS |
| 10 | F | 138 | VAL |
| 10 | F | 153 | ASN |
| 11 | G | 96 | SER |
| 12 | H | 16 | ASN |
| 12 | H | 18 | THR |
| 12 | H | 37 | SER |
| 14 | J | 38 | THR |
| 15 | K | 32 | ARG |
| 15 | K | 44 | GLU |
| 15 | K | 46 | GLY |
| 16 | L | 6 | PRO |
| 16 | L | 11 | ILE |
| 16 | L | 64 | LEU |
| 16 | L | 75 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | N | 25 | THR |
| 17 | N | 42 | PHE |
| 17 | N | 43 | PRO |
| 17 | N | 53 | ALA |
| 17 | N | 62 | SER |
| 17 | N | 71 | GLY |
| 17 | N | 72 | LYS |
| 1 | 1 | 27 | LEU |
| 1 | 1 | 55 | PRO |
| 1 | 1 | 65 | TYR |
| 1 | 1 | 122 | LYS |
| 1 | 1 | 124 | PRO |
| 1 | 1 | 133 | TYR |
| 1 | 1 | 145 | VAL |
| 1 | 1 | 177 | LEU |
| 1 | 1 | 184 | PRO |
| 2 | 2 | 94 | LEU |
| 2 | 2 | 113 | ILE |
| 2 | 2 | 180 | GLN |
| 2 | 2 | 186 | THR |
| 2 | 2 | 202 | ALA |
| 3 | 3 | 75 | PRO |
| 3 | 3 | 93 | PHE |
| 3 | 3 | 141 | GLN |
| 3 | 3 | 156 | PRO |
| 3 | 3 | 169 | PHE |
| 4 | 4 | 60 | LEU |
| 4 | 4 | 77 | ALA |
| 4 | 4 | 123 | GLN |
| 4 | 4 | 126 | LEU |
| 4 | 4 | 131 | VAL |
| 4 | 4 | 177 | PRO |
| 4 | 4 | 187 | ASP |
| 4 | 4 | 192 | THR |
| 5 | A | 37 | PRO |
| 5 | A | 41 | SER |
| 5 | A | 63 | ASP |
| 5 | A | 116 | ILE |
| 5 | A | 127 | VAL |
| 5 | A | 186 | TYR |
| 5 | A | 225 | VAL |
| 5 | A | 234 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 235 | ALA |
| 5 | A | 292 | GLY |
| 5 | A | 306 | ILE |
| 5 | A | 308 | ILE |
| 5 | A | 347 | TYR |
| 5 | A | 423 | ASP |
| 6 | B | 8 | PHE |
| 6 | B | 20 | ARG |
| 6 | B | 42 | LEU |
| 6 | B | 71 | GLN |
| 6 | B | 170 | ASN |
| 6 | B | 178 | HIS |
| 6 | B | 206 | TYR |
| 6 | B | 207 | VAL |
| 6 | B | 229 | GLN |
| 6 | B | 234 | ALA |
| 6 | B | 239 | SER |
| 6 | B | 240 | SER |
| 6 | B | 273 | VAL |
| 6 | B | 460 | ALA |
| 6 | B | 472 | TYR |
| 6 | B | 476 | ILE |
| 6 | B | 482 | ASN |
| 7 | C | 12 | ILE |
| 7 | C | 55 | GLU |
| 7 | C | 58 | CYS |
| 7 | C | 75 | ARG |
| 8 | D | 35 | GLY |
| 8 | D | 46 | TYR |
| 8 | D | 104 | PHE |
| 8 | D | 125 | PRO |
| 8 | D | 143 | PRO |
| 8 | D | 148 | PHE |
| 9 | E | 61 | THR |
| 10 | F | 34 | ASP |
| 10 | F | 44 | ALA |
| 10 | F | 128 | SER |
| 10 | F | 151 | ASP |
| 10 | F | 152 | ASN |
| 11 | G | 20 | ARG |
| 11 | G | 56 | SER |
| 11 | G | 89 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | G | 91 | ASN |
| 13 | I | 2 | ILE |
| 13 | I | 5 | PRO |
| 13 | I | 9 | VAL |
| 14 | J | 23 | ALA |
| 16 | L | 36 | TYR |
| 16 | L | 85 | SER |
| 16 | L | 86 | LEU |
| 16 | L | 112 | PRO |
| 16 | L | 154 | ALA |
| 17 | N | 21 | ARG |
| 17 | N | 34 | THR |
| 1 | 1 | 84 | TYR |
| 1 | 1 | 140 | LEU |
| 1 | 1 | 179 | THR |
| 2 | 2 | 45 | VAL |
| 2 | 2 | 120 | ASN |
| 2 | 2 | 140 | GLY |
| 2 | 2 | 168 | ARG |
| 4 | 4 | 72 | VAL |
| 4 | 4 | 83 | TYR |
| 4 | 4 | 85 | ALA |
| 4 | 4 | 90 | LEU |
| 4 | 4 | 112 | PRO |
| 4 | 4 | 130 | GLU |
| 5 | A | 73 | GLU |
| 5 | A | 114 | THR |
| 5 | A | 149 | PHE |
| 5 | A | 259 | TYR |
| 5 | A | 472 | ARG |
| 5 | A | 537 | ALA |
| 5 | A | 570 | PRO |
| 5 | A | 571 | ASP |
| 5 | A | 580 | PRO |
| 6 | B | 228 | GLY |
| 6 | B | 232 | LEU |
| 6 | B | 278 | LEU |
| 6 | B | 361 | ILE |
| 6 | B | 475 | ASP |
| 6 | B | 477 | PRO |
| 6 | B | 559 | CYS |
| 6 | B | 592 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | B | 730 | SER |
| 8 | D | 22 | PRO |
| 8 | D | 60 | MET |
| 9 | E | 84 | LEU |
| 10 | F | 39 | ALA |
| 10 | F | 61 | LEU |
| 10 | F | 73 | VAL |
| 10 | F | 83 | PHE |
| 11 | G | 23 | PHE |
| 11 | G | 36 | PRO |
| 15 | K | 29 | SER |
| 15 | K | 72 | VAL |
| 16 | L | 48 | ASN |
| 16 | L | 135 | GLY |
| 17 | N | 17 | ASN |
| 17 | N | 70 | GLU |
| 1 | 1 | 32 | VAL |
| 1 | 1 | 160 | GLY |
| 2 | 2 | 96 | ILE |
| 2 | 2 | 115 | ASN |
| 2 | 2 | 116 | PRO |
| 2 | 2 | 146 | LEU |
| 4 | 4 | 36 | ASN |
| 4 | 4 | 118 | ASP |
| 5 | A | 478 | SER |
| 5 | A | 584 | PRO |
| 5 | A | 586 | ARG |
| 5 | A | 718 | PRO |
| 5 | A | 754 | ILE |
| 6 | B | 219 | PRO |
| 6 | B | 222 | LEU |
| 6 | B | 318 | GLY |
| 6 | B | 391 | PRO |
| 6 | B | 596 | TRP |
| 6 | B | 711 | VAL |
| 7 | C | 24 | ASP |
| 7 | C | 30 | PRO |
| 7 | C | 35 | LYS |
| 7 | C | 37 | LYS |
| 13 | I | 28 | VAL |
| 15 | K | 40 | LEU |
| 16 | L | 61 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 57 | ILE |
| 1 | 1 | 125 | GLY |
| 4 | 4 | 167 | ILE |
| 4 | 4 | 168 | ILE |
| 5 | A | 267 | THR |
| 5 | A | 531 | PRO |
| 5 | A | 637 | ILE |
| 5 | A | 721 | GLN |
| 5 | A | 742 | GLY |
| 6 | B | 400 | PRO |
| 6 | B | 557 | PHE |
| 8 | D | 27 | PRO |
| 10 | F | 37 | ALA |
| 2 | 2 | 187 | GLY |
| 4 | 4 | 135 | GLY |
| 4 | 4 | 154 | ILE |
| 5 | A | 229 | ILE |
| 5 | A | 500 | PRO |
| 6 | B | 217 | PRO |
| 11 | G | 64 | VAL |
| 1 | 1 | 64 | GLY |
| 1 | 1 | 77 | LEU |
| 1 | 1 | 89 | VAL |
| 1 | 1 | 173 | PRO |
| 12 | H | 72 | ALA |
| 2 | 2 | 135 | VAL |
| 5 | A | 190 | ALA |
| 5 | A | 223 | VAL |
| 5 | A | 632 | GLY |
| 8 | D | 67 | ILE |
| 15 | K | 69 | ILE |
| 17 | N | 59 | PRO |
| 4 | 4 | 137 | ILE |
| 5 | A | 249 | ILE |
| 6 | B | 94 | PRO |
| 6 | B | 162 | LYS |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 | 1 | 127/190 (67%) | 100 (79%) | 27 (21%) | 1 | 6 |
| 2 | 2 | 140/216 (65%) | 83 (59%) | 57 (41%) | 0 | 0 |
| 3 | 3 | 112/215 (52%) | 73 (65%) | 39 (35%) | 0 | 2 |
| 4 | 4 | 138/201 (69%) | 79 (57%) | 59 (43%) | 0 | 0 |
| 5 | A | 592/618 (96%) | 387 (65%) | 205 (35%) | 0 | 2 |
| 6 | B | 598/600 (100%) | 392 (66%) | 206 (34%) | 0 | 2 |
| 7 | C | 70/70 (100%) | 41 (59%) | 29 (41%) | 0 | 0 |
| 8 | D | 118/173 (68%) | 77 (65%) | 41 (35%) | 0 | 2 |
| 9 | E | 56/114 (49%) | 39 (70%) | 17 (30%) | 0 | 2 |
| 10 | F | 127/190 (67%) | 83 (65%) | 44 (35%) | 0 | 2 |
| 11 | G | 79/144 (55%) | 50 (63%) | 29 (37%) | 0 | 1 |
| 12 | H | 57/115 (50%) | 28 (49%) | 29 (51%) | 0 | 0 |
| 13 | I | 26/36 (72%) | 21 (81%) | 5 (19%) | 1 | 8 |
| 14 | J | 36/39 (92%) | 23 (64%) | 13 (36%) | 0 | 1 |
| 15 | K | 61/102 (60%) | 43 (70%) | 18 (30%) | 0 | 2 |
| 16 | L | 125/169 (74%) | 87 (70%) | 38 (30%) | 0 | 2 |
| 17 | N | 74/139 (53%) | 43 (58%) | 31 (42%) | 0 | 0 |
| All | All | 2536/3331 (76%) | 1649 (65%) | 887 (35%) | 0 | 1 |

All (887) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 17 | SER |
| 1 | 1 | 27 | LEU |
| 1 | 1 | 31 | GLU |
| 1 | 1 | 37 | GLU |
| 1 | 1 | 47 | CYS |
| 1 | 1 | 52 | LEU |
| 1 | 1 | 57 | ILE |
| 1 | 1 | 61 | GLU |
| 1 | 1 | 63 | LEU |
| 1 | 1 | 72 | GLN |
| 1 | 1 | 85 | LEU |
| 1 | 1 | 105 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 110 | HIS |
| 1 | 1 | 111 | GLN |
| 1 | 1 | 120 | LYS |
| 1 | 1 | 121 | LYS |
| 1 | 1 | 129 | ASP |
| 1 | 1 | 133 | TYR |
| 1 | 1 | 134 | SER |
| 1 | 1 | 136 | ASP |
| 1 | 1 | 139 | LYS |
| 1 | 1 | 140 | LEU |
| 1 | 1 | 141 | GLU |
| 1 | 1 | 142 | GLU |
| 1 | 1 | 144 | LYS |
| 1 | 1 | 179 | THR |
| 1 | 1 | 181 | LEU |
| 2 | 2 | 37 | ASP |
| 2 | 2 | 39 | GLU |
| 2 | 2 | 45 | VAL |
| 2 | 2 | 46 | GLN |
| 2 | 2 | 49 | LEU |
| 2 | 2 | 53 | ARG |
| 2 | 2 | 57 | LEU |
| 2 | 2 | 63 | PHE |
| 2 | 2 | 66 | GLU |
| 2 | 2 | 67 | PHE |
| 2 | 2 | 69 | THR |
| 2 | 2 | 70 | LYS |
| 2 | 2 | 73 | ILE |
| 2 | 2 | 75 | ASN |
| 2 | 2 | 76 | THR |
| 2 | 2 | 80 | TYR |
| 2 | 2 | 85 | GLN |
| 2 | 2 | 86 | GLU |
| 2 | 2 | 89 | THR |
| 2 | 2 | 92 | THR |
| 2 | 2 | 97 | VAL |
| 2 | 2 | 98 | GLU |
| 2 | 2 | 99 | LEU |
| 2 | 2 | 100 | VAL |
| 2 | 2 | 101 | PHE |
| 2 | 2 | 109 | ARG |
| 2 | 2 | 112 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 2 | 113 | ILE |
| 2 | 2 | 115 | ASN |
| 2 | 2 | 119 | VAL |
| 2 | 2 | 120 | ASN |
| 2 | 2 | 122 | ASP |
| 2 | 2 | 129 | LYS |
| 2 | 2 | 130 | LEU |
| 2 | 2 | 131 | THR |
| 2 | 2 | 133 | THR |
| 2 | 2 | 146 | LEU |
| 2 | 2 | 150 | SER |
| 2 | 2 | 157 | LYS |
| 2 | 2 | 159 | LEU |
| 2 | 2 | 160 | ARG |
| 2 | 2 | 161 | THR |
| 2 | 2 | 162 | LYS |
| 2 | 2 | 164 | ILE |
| 2 | 2 | 169 | LEU |
| 2 | 2 | 180 | GLN |
| 2 | 2 | 183 | TYR |
| 2 | 2 | 189 | ILE |
| 2 | 2 | 190 | ASP |
| 2 | 2 | 191 | ASN |
| 2 | 2 | 193 | PHE |
| 2 | 2 | 196 | HIS |
| 2 | 2 | 199 | ASP |
| 2 | 2 | 201 | HIS |
| 2 | 2 | 204 | ILE |
| 2 | 2 | 205 | PHE |
| 2 | 2 | 211 | LYS |
| 3 | 3 | 49 | ILE |
| 3 | 3 | 50 | GLU |
| 3 | 3 | 59 | ILE |
| 3 | 3 | 60 | ILE |
| 3 | 3 | 67 | LEU |
| 3 | 3 | 73 | ILE |
| 3 | 3 | 76 | GLU |
| 3 | 3 | 78 | LEU |
| 3 | 3 | 92 | TRP |
| 3 | 3 | 93 | PHE |
| 3 | 3 | 94 | ARG |
| 3 | 3 | 95 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 3 | 97 | PHE |
| 3 | 3 | 98 | ILE |
| 3 | 3 | 109 | ASP |
| 3 | 3 | 111 | TYR |
| 3 | 3 | 112 | THR |
| 3 | 3 | 128 | ARG |
| 3 | 3 | 131 | ASP |
| 3 | 3 | 134 | LYS |
| 3 | 3 | 137 | SER |
| 3 | 3 | 141 | GLN |
| 3 | 3 | 146 | LEU |
| 3 | 3 | 150 | LEU |
| 3 | 3 | 163 | PHE |
| 3 | 3 | 164 | PHE |
| 3 | 3 | 165 | ASN |
| 3 | 3 | 171 | LYS |
| 3 | 3 | 173 | GLU |
| 3 | 3 | 180 | LYS |
| 3 | 3 | 185 | LYS |
| 3 | 3 | 191 | MET |
| 3 | 3 | 192 | LEU |
| 3 | 3 | 195 | LEU |
| 3 | 3 | 200 | GLN |
| 3 | 3 | 203 | VAL |
| 3 | 3 | 204 | THR |
| 3 | 3 | 209 | TYR |
| 3 | 3 | 210 | GLN |
| 4 | 4 | 32 | GLU |
| 4 | 4 | 35 | GLU |
| 4 | 4 | 36 | ASN |
| 4 | 4 | 38 | ARG |
| 4 | 4 | 40 | PHE |
| 4 | 4 | 45 | LEU |
| 4 | 4 | 46 | VAL |
| 4 | 4 | 49 | ARG |
| 4 | 4 | 50 | TRP |
| 4 | 4 | 52 | MET |
| 4 | 4 | 55 | VAL |
| 4 | 4 | 59 | LEU |
| 4 | 4 | 60 | LEU |
| 4 | 4 | 64 | PHE |
| 4 | 4 | 66 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 4 | 67 | ILE |
| 4 | 4 | 69 | ILE |
| 4 | 4 | 73 | PRO |
| 4 | 4 | 75 | TRP |
| 4 | 4 | 76 | TYR |
| 4 | 4 | 82 | GLU |
| 4 | 4 | 83 | TYR |
| 4 | 4 | 90 | LEU |
| 4 | 4 | 91 | PHE |
| 4 | 4 | 92 | VAL |
| 4 | 4 | 93 | ILE |
| 4 | 4 | 94 | GLU |
| 4 | 4 | 95 | PHE |
| 4 | 4 | 99 | HIS |
| 4 | 4 | 101 | VAL |
| 4 | 4 | 103 | ILE |
| 4 | 4 | 104 | ARG |
| 4 | 4 | 105 | ARG |
| 4 | 4 | 109 | ILE |
| 4 | 4 | 118 | ASP |
| 4 | 4 | 120 | ILE |
| 4 | 4 | 121 | PHE |
| 4 | 4 | 126 | LEU |
| 4 | 4 | 131 | VAL |
| 4 | 4 | 139 | ASN |
| 4 | 4 | 146 | THR |
| 4 | 4 | 147 | LEU |
| 4 | 4 | 150 | LYS |
| 4 | 4 | 151 | GLU |
| 4 | 4 | 158 | ARG |
| 4 | 4 | 159 | LEU |
| 4 | 4 | 160 | MET |
| 4 | 4 | 163 | PHE |
| 4 | 4 | 167 | ILE |
| 4 | 4 | 168 | ILE |
| 4 | 4 | 169 | GLN |
| 4 | 4 | 172 | VAL |
| 4 | 4 | 175 | LYS |
| 4 | 4 | 180 | ASN |
| 4 | 4 | 184 | HIS |
| 4 | 4 | 187 | ASP |
| 4 | 4 | 190 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 4 | 192 | THR |
| 4 | 4 | 195 | GLN |
| 5 | A | 21 | LEU |
| 5 | A | 22 | VAL |
| 5 | A | 24 | ARG |
| 5 | A | 26 | PRO |
| 5 | A | 27 | ILE |
| 5 | A | 28 | LYS |
| 5 | A | 29 | THR |
| 5 | A | 31 | PHE |
| 5 | A | 40 | PHE |
| 5 | A | 44 | ILE |
| 5 | A | 46 | LYS |
| 5 | A | 50 | THR |
| 5 | A | 52 | THR |
| 5 | A | 56 | ASN |
| 5 | A | 60 | ASP |
| 5 | A | 62 | HIS |
| 5 | A | 63 | ASP |
| 5 | A | 67 | HIS |
| 5 | A | 68 | THR |
| 5 | A | 69 | SER |
| 5 | A | 71 | LEU |
| 5 | A | 72 | GLU |
| 5 | A | 73 | GLU |
| 5 | A | 78 | VAL |
| 5 | A | 82 | HIS |
| 5 | A | 83 | PHE |
| 5 | A | 86 | LEU |
| 5 | A | 88 | ILE |
| 5 | A | 91 | LEU |
| 5 | A | 94 | SER |
| 5 | A | 103 | PHE |
| 5 | A | 105 | ASN |
| 5 | A | 107 | GLU |
| 5 | A | 111 | ASN |
| 5 | A | 114 | THR |
| 5 | A | 124 | TRP |
| 5 | A | 126 | ILE |
| 5 | A | 132 | LEU |
| 5 | A | 133 | ASN |
| 5 | A | 135 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 136 | VAL |
| 5 | A | 141 | ARG |
| 5 | A | 144 | GLN |
| 5 | A | 151 | GLN |
| 5 | A | 164 | LEU |
| 5 | A | 167 | THR |
| 5 | A | 177 | LEU |
| 5 | A | 179 | LEU |
| 5 | A | 180 | PHE |
| 5 | A | 188 | LYS |
| 5 | A | 193 | LEU |
| 5 | A | 197 | GLN |
| 5 | A | 203 | LEU |
| 5 | A | 207 | LEU |
| 5 | A | 213 | LEU |
| 5 | A | 223 | VAL |
| 5 | A | 225 | VAL |
| 5 | A | 227 | LEU |
| 5 | A | 230 | ASN |
| 5 | A | 231 | GLN |
| 5 | A | 232 | PHE |
| 5 | A | 238 | ASP |
| 5 | A | 242 | ILE |
| 5 | A | 248 | PHE |
| 5 | A | 249 | ILE |
| 5 | A | 251 | ASN |
| 5 | A | 253 | ASP |
| 5 | A | 254 | LEU |
| 5 | A | 255 | LEU |
| 5 | A | 257 | GLN |
| 5 | A | 262 | PHE |
| 5 | A | 276 | LYS |
| 5 | A | 281 | LEU |
| 5 | A | 284 | ARG |
| 5 | A | 287 | LEU |
| 5 | A | 290 | LEU |
| 5 | A | 296 | LEU |
| 5 | A | 297 | THR |
| 5 | A | 298 | ASP |
| 5 | A | 299 | ILE |
| 5 | A | 304 | LEU |
| 5 | A | 308 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 309 | LEU |
| 5 | A | 316 | MET |
| 5 | A | 317 | TYR |
| 5 | A | 331 | LEU |
| 5 | A | 334 | HIS |
| 5 | A | 339 | THR |
| 5 | A | 341 | GLN |
| 5 | A | 352 | THR |
| 5 | A | 353 | SER |
| 5 | A | 357 | GLN |
| 5 | A | 358 | LEU |
| 5 | A | 361 | ASN |
| 5 | A | 368 | LEU |
| 5 | A | 369 | THR |
| 5 | A | 376 | MET |
| 5 | A | 379 | MET |
| 5 | A | 384 | TYR |
| 5 | A | 387 | THR |
| 5 | A | 391 | THR |
| 5 | A | 392 | GLN |
| 5 | A | 393 | LEU |
| 5 | A | 395 | LEU |
| 5 | A | 397 | THR |
| 5 | A | 400 | MET |
| 5 | A | 402 | ILE |
| 5 | A | 405 | PHE |
| 5 | A | 408 | VAL |
| 5 | A | 420 | ARG |
| 5 | A | 422 | TYR |
| 5 | A | 426 | THR |
| 5 | A | 427 | ARG |
| 5 | A | 433 | ASP |
| 5 | A | 434 | ARG |
| 5 | A | 435 | VAL |
| 5 | A | 438 | HIS |
| 5 | A | 439 | ARG |
| 5 | A | 440 | ASP |
| 5 | A | 446 | LEU |
| 5 | A | 462 | ILE |
| 5 | A | 464 | ASN |
| 5 | A | 466 | THR |
| 5 | A | 467 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 477 | PHE |
| 5 | A | 479 | ASP |
| 5 | A | 480 | THR |
| 5 | A | 482 | ILE |
| 5 | A | 488 | PHE |
| 5 | A | 495 | THR |
| 5 | A | 496 | HIS |
| 5 | A | 498 | LEU |
| 5 | A | 503 | THR |
| 5 | A | 511 | THR |
| 5 | A | 520 | LEU |
| 5 | A | 521 | VAL |
| 5 | A | 523 | VAL |
| 5 | A | 529 | LEU |
| 5 | A | 530 | LEU |
| 5 | A | 532 | ILE |
| 5 | A | 536 | THR |
| 5 | A | 540 | LEU |
| 5 | A | 548 | THR |
| 5 | A | 551 | VAL |
| 5 | A | 553 | VAL |
| 5 | A | 554 | LEU |
| 5 | A | 555 | ILE |
| 5 | A | 557 | LEU |
| 5 | A | 558 | LYS |
| 5 | A | 561 | LEU |
| 5 | A | 564 | ARG |
| 5 | A | 568 | LEU |
| 5 | A | 569 | ILE |
| 5 | A | 575 | LEU |
| 5 | A | 577 | PHE |
| 5 | A | 589 | THR |
| 5 | A | 590 | CYS |
| 5 | A | 591 | GLN |
| 5 | A | 600 | LEU |
| 5 | A | 605 | MET |
| 5 | A | 607 | ASN |
| 5 | A | 613 | ILE |
| 5 | A | 622 | SER |
| 5 | A | 623 | ASP |
| 5 | A | 629 | ASN |
| 5 | A | 630 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 631 | GLN |
| 5 | A | 633 | VAL |
| 5 | A | 637 | ILE |
| 5 | A | 638 | THR |
| 5 | A | 641 | ASN |
| 5 | A | 644 | GLN |
| 5 | A | 645 | SER |
| 5 | A | 646 | SER |
| 5 | A | 653 | LEU |
| 5 | A | 654 | ARG |
| 5 | A | 657 | LEU |
| 5 | A | 660 | GLN |
| 5 | A | 663 | GLN |
| 5 | A | 664 | VAL |
| 5 | A | 666 | GLN |
| 5 | A | 673 | SER |
| 5 | A | 677 | LEU |
| 5 | A | 684 | PHE |
| 5 | A | 685 | VAL |
| 5 | A | 689 | SER |
| 5 | A | 691 | MET |
| 5 | A | 697 | ARG |
| 5 | A | 703 | LEU |
| 5 | A | 704 | ILE |
| 5 | A | 707 | ILE |
| 5 | A | 708 | VAL |
| 5 | A | 715 | LYS |
| 5 | A | 723 | ARG |
| 5 | A | 726 | SER |
| 5 | A | 727 | ILE |
| 5 | A | 728 | VAL |
| 5 | A | 733 | VAL |
| 5 | A | 735 | VAL |
| 5 | A | 736 | THR |
| 5 | A | 740 | LEU |
| 5 | A | 745 | THR |
| 5 | A | 753 | ARG |
| 5 | A | 754 | ILE |
| 5 | A | 755 | ILE |
| 6 | B | 3 | LEU |
| 6 | B | 4 | ARG |
| 6 | B | 5 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | B | 7 | ARG |
| 6 | B | 9 | SER |
| 6 | B | 12 | ILE |
| 6 | B | 14 | GLN |
| 6 | B | 15 | ASP |
| 6 | B | 19 | ARG |
| 6 | B | 20 | ARG |
| 6 | B | 25 | ILE |
| 6 | B | 41 | ARG |
| 6 | B | 46 | ILE |
| 6 | B | 50 | HIS |
| 6 | B | 51 | PHE |
| 6 | B | 53 | GLN |
| 6 | B | 57 | ILE |
| 6 | B | 67 | HIS |
| 6 | B | 70 | TRP |
| 6 | B | 75 | GLU |
| 6 | B | 78 | VAL |
| 6 | B | 84 | VAL |
| 6 | B | 91 | ILE |
| 6 | B | 106 | ARG |
| 6 | B | 110 | LEU |
| 6 | B | 113 | VAL |
| 6 | B | 114 | ASN |
| 6 | B | 121 | TYR |
| 6 | B | 122 | GLN |
| 6 | B | 124 | TRP |
| 6 | B | 127 | ILE |
| 6 | B | 129 | LEU |
| 6 | B | 130 | ARG |
| 6 | B | 132 | ASN |
| 6 | B | 137 | THR |
| 6 | B | 140 | ILE |
| 6 | B | 142 | LEU |
| 6 | B | 144 | PHE |
| 6 | B | 145 | LEU |
| 6 | B | 151 | LEU |
| 6 | B | 154 | TRP |
| 6 | B | 157 | LEU |
| 6 | B | 160 | LYS |
| 6 | B | 161 | TRP |
| 6 | B | 164 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | B | 175 | LEU |
| 6 | B | 195 | VAL |
| 6 | B | 199 | ILE |
| 6 | B | 203 | ARG |
| 6 | B | 206 | TYR |
| 6 | B | 207 | VAL |
| 6 | B | 208 | ARG |
| 6 | B | 210 | ASN |
| 6 | B | 214 | ASP |
| 6 | B | 215 | VAL |
| 6 | B | 216 | LEU |
| 6 | B | 226 | LEU |
| 6 | B | 229 | GLN |
| 6 | B | 231 | ASN |
| 6 | B | 232 | LEU |
| 6 | B | 243 | LEU |
| 6 | B | 246 | THR |
| 6 | B | 248 | GLN |
| 6 | B | 255 | LEU |
| 6 | B | 257 | ILE |
| 6 | B | 258 | LEU |
| 6 | B | 262 | HIS |
| 6 | B | 265 | THR |
| 6 | B | 266 | GLN |
| 6 | B | 268 | LEU |
| 6 | B | 269 | TRP |
| 6 | B | 270 | LEU |
| 6 | B | 271 | THR |
| 6 | B | 278 | LEU |
| 6 | B | 285 | LEU |
| 6 | B | 292 | ARG |
| 6 | B | 294 | ASN |
| 6 | B | 295 | PHE |
| 6 | B | 297 | ILE |
| 6 | B | 299 | HIS |
| 6 | B | 300 | SER |
| 6 | B | 301 | ILE |
| 6 | B | 305 | LEU |
| 6 | B | 309 | ILE |
| 6 | B | 315 | LEU |
| 6 | B | 317 | ARG |
| 6 | B | 325 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | B | 326 | ILE |
| 6 | B | 330 | ILE |
| 6 | B | 332 | PHE |
| 6 | B | 347 | LEU |
| 6 | B | 348 | VAL |
| 6 | B | 350 | GLN |
| 6 | B | 352 | MET |
| 6 | B | 361 | ILE |
| 6 | B | 363 | GLN |
| 6 | B | 364 | ASP |
| 6 | B | 365 | PHE |
| 6 | B | 374 | HIS |
| 6 | B | 375 | HIS |
| 6 | B | 382 | ILE |
| 6 | B | 384 | THR |
| 6 | B | 393 | PHE |
| 6 | B | 395 | ILE |
| 6 | B | 396 | ARG |
| 6 | B | 403 | ASN |
| 6 | B | 406 | ASN |
| 6 | B | 407 | VAL |
| 6 | B | 412 | LEU |
| 6 | B | 418 | ILE |
| 6 | B | 419 | ILE |
| 6 | B | 420 | SER |
| 6 | B | 422 | LEU |
| 6 | B | 423 | SER |
| 6 | B | 427 | LEU |
| 6 | B | 428 | PHE |
| 6 | B | 436 | LEU |
| 6 | B | 437 | TYR |
| 6 | B | 438 | VAL |
| 6 | B | 442 | VAL |
| 6 | B | 443 | MET |
| 6 | B | 446 | PHE |
| 6 | B | 448 | THR |
| 6 | B | 452 | GLN |
| 6 | B | 454 | LEU |
| 6 | B | 455 | ILE |
| 6 | B | 458 | ILE |
| 6 | B | 461 | GLN |
| 6 | B | 469 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | B | 471 | THR |
| 6 | B | 472 | TYR |
| 6 | B | 478 | LEU |
| 6 | B | 481 | THR |
| 6 | B | 486 | LEU |
| 6 | B | 492 | ILE |
| 6 | B | 494 | LEU |
| 6 | B | 501 | ILE |
| 6 | B | 502 | ASN |
| 6 | B | 504 | ASN |
| 6 | B | 508 | LEU |
| 6 | B | 509 | PHE |
| 6 | B | 510 | LEU |
| 6 | B | 512 | ILE |
| 6 | B | 520 | HIS |
| 6 | B | 521 | HIS |
| 6 | B | 525 | LEU |
| 6 | B | 527 | LEU |
| 6 | B | 528 | HIS |
| 6 | B | 532 | LEU |
| 6 | B | 533 | ILE |
| 6 | B | 539 | LEU |
| 6 | B | 544 | SER |
| 6 | B | 545 | LYS |
| 6 | B | 551 | LYS |
| 6 | B | 569 | ASP |
| 6 | B | 577 | TYR |
| 6 | B | 578 | LEU |
| 6 | B | 583 | MET |
| 6 | B | 584 | LEU |
| 6 | B | 587 | ILE |
| 6 | B | 594 | TRP |
| 6 | B | 596 | TRP |
| 6 | B | 601 | LEU |
| 6 | B | 603 | ARG |
| 6 | B | 605 | ASN |
| 6 | B | 606 | VAL |
| 6 | B | 607 | SER |
| 6 | B | 608 | GLN |
| 6 | B | 611 | GLU |
| 6 | B | 615 | TYR |
| 6 | B | 616 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | B | 617 | MET |
| 6 | B | 622 | ASP |
| 6 | B | 624 | LEU |
| 6 | B | 629 | SER |
| 6 | B | 631 | LEU |
| 6 | B | 633 | ASN |
| 6 | B | 638 | LEU |
| 6 | B | 640 | CYS |
| 6 | B | 643 | LEU |
| 6 | B | 645 | VAL |
| 6 | B | 649 | MET |
| 6 | B | 651 | LEU |
| 6 | B | 659 | THR |
| 6 | B | 662 | MET |
| 6 | B | 664 | LEU |
| 6 | B | 670 | TYR |
| 6 | B | 672 | GLN |
| 6 | B | 674 | LEU |
| 6 | B | 676 | GLU |
| 6 | B | 677 | THR |
| 6 | B | 682 | HIS |
| 6 | B | 683 | GLU |
| 6 | B | 685 | THR |
| 6 | B | 689 | ASN |
| 6 | B | 690 | LEU |
| 6 | B | 700 | LEU |
| 6 | B | 702 | ILE |
| 6 | B | 703 | VAL |
| 6 | B | 710 | LEU |
| 6 | B | 712 | HIS |
| 6 | B | 715 | VAL |
| 6 | B | 718 | ILE |
| 6 | B | 725 | LEU |
| 6 | B | 732 | LYS |
| 6 | B | 733 | PHE |
| 7 | C | 1 | MET |
| 7 | C | 7 | ILE |
| 7 | C | 10 | THR |
| 7 | C | 12 | ILE |
| 7 | C | 15 | THR |
| 7 | C | 16 | GLN |
| 7 | C | 18 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | C | 23 | THR |
| 7 | C | 24 | ASP |
| 7 | C | 28 | MET |
| 7 | C | 35 | LYS |
| 7 | C | 37 | LYS |
| 7 | C | 38 | GLN |
| 7 | C | 45 | THR |
| 7 | C | 52 | LYS |
| 7 | C | 54 | CYS |
| 7 | C | 59 | PRO |
| 7 | C | 62 | PHE |
| 7 | C | 63 | LEU |
| 7 | C | 66 | ARG |
| 7 | C | 67 | VAL |
| 7 | C | 68 | TYR |
| 7 | C | 69 | LEU |
| 7 | C | 70 | TRP |
| 7 | C | 73 | THR |
| 7 | C | 74 | THR |
| 7 | C | 77 | MET |
| 7 | C | 79 | LEU |
| 7 | C | 81 | TYR |
| 8 | D | 26 | SER |
| 8 | D | 28 | ILE |
| 8 | D | 36 | LEU |
| 8 | D | 41 | GLN |
| 8 | D | 44 | GLU |
| 8 | D | 46 | TYR |
| 8 | D | 47 | VAL |
| 8 | D | 48 | ILE |
| 8 | D | 49 | THR |
| 8 | D | 50 | TRP |
| 8 | D | 57 | ILE |
| 8 | D | 67 | ILE |
| 8 | D | 69 | ARG |
| 8 | D | 73 | ASN |
| 8 | D | 74 | LEU |
| 8 | D | 75 | LEU |
| 8 | D | 79 | ARG |
| 8 | D | 81 | GLU |
| 8 | D | 82 | GLN |
| 8 | D | 86 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | D | 89 | ARG |
| 8 | D | 90 | LEU |
| 8 | D | 92 | SER |
| 8 | D | 96 | ILE |
| 8 | D | 98 | TYR |
| 8 | D | 104 | PHE |
| 8 | D | 111 | TYR |
| 8 | D | 121 | GLU |
| 8 | D | 122 | LYS |
| 8 | D | 123 | VAL |
| 8 | D | 124 | ASN |
| 8 | D | 127 | ARG |
| 8 | D | 128 | GLN |
| 8 | D | 134 | MET |
| 8 | D | 135 | ARG |
| 8 | D | 137 | ILE |
| 8 | D | 139 | LYS |
| 8 | D | 144 | ILE |
| 8 | D | 147 | LYS |
| 8 | D | 149 | THR |
| 8 | D | 151 | LYS |
| 9 | E | 36 | VAL |
| 9 | E | 39 | LEU |
| 9 | E | 40 | ARG |
| 9 | E | 42 | GLU |
| 9 | E | 45 | TRP |
| 9 | E | 47 | LYS |
| 9 | E | 48 | ASN |
| 9 | E | 53 | VAL |
| 9 | E | 55 | VAL |
| 9 | E | 58 | ASP |
| 9 | E | 61 | THR |
| 9 | E | 66 | VAL |
| 9 | E | 68 | ARG |
| 9 | E | 73 | ASN |
| 9 | E | 76 | ASN |
| 9 | E | 79 | THR |
| 9 | E | 90 | VAL |
| 10 | F | 8 | CYS |
| 10 | F | 9 | LYS |
| 10 | F | 12 | LYS |
| 10 | F | 13 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | F | 17 | ARG |
| 10 | F | 18 | GLU |
| 10 | F | 24 | LYS |
| 10 | F | 25 | LEU |
| 10 | F | 26 | GLN |
| 10 | F | 28 | SER |
| 10 | F | 29 | LEU |
| 10 | F | 31 | LEU |
| 10 | F | 43 | LYS |
| 10 | F | 48 | LYS |
| 10 | F | 52 | ARG |
| 10 | F | 61 | LEU |
| 10 | F | 68 | LEU |
| 10 | F | 71 | LEU |
| 10 | F | 79 | HIS |
| 10 | F | 88 | ILE |
| 10 | F | 91 | LEU |
| 10 | F | 93 | ILE |
| 10 | F | 96 | TRP |
| 10 | F | 100 | VAL |
| 10 | F | 102 | ARG |
| 10 | F | 104 | TYR |
| 10 | F | 106 | ILE |
| 10 | F | 108 | ILE |
| 10 | F | 111 | GLU |
| 10 | F | 115 | THR |
| 10 | F | 116 | GLN |
| 10 | F | 119 | ILE |
| 10 | F | 121 | ILE |
| 10 | F | 123 | VAL |
| 10 | F | 135 | SER |
| 10 | F | 136 | TRP |
| 10 | F | 138 | VAL |
| 10 | F | 141 | TYR |
| 10 | F | 142 | ARG |
| 10 | F | 143 | GLU |
| 10 | F | 146 | ASN |
| 10 | F | 152 | ASN |
| 10 | F | 153 | ASN |
| 10 | F | 154 | PHE |
| 11 | G | 7 | VAL |
| 11 | G | 10 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | G | 12 | THR |
| 11 | G | 18 | LEU |
| 11 | G | 22 | VAL |
| 11 | G | 24 | PHE |
| 11 | G | 28 | ARG |
| 11 | G | 30 | ASN |
| 11 | G | 31 | MET |
| 11 | G | 33 | LYS |
| 11 | G | 38 | GLN |
| 11 | G | 39 | ASN |
| 11 | G | 41 | MET |
| 11 | G | 43 | HIS |
| 11 | G | 45 | GLU |
| 11 | G | 48 | ASP |
| 11 | G | 49 | THR |
| 11 | G | 50 | ARG |
| 11 | G | 55 | VAL |
| 11 | G | 57 | LEU |
| 11 | G | 58 | LEU |
| 11 | G | 62 | ASP |
| 11 | G | 71 | VAL |
| 11 | G | 77 | ILE |
| 11 | G | 80 | ILE |
| 11 | G | 83 | TYR |
| 11 | G | 88 | THR |
| 11 | G | 91 | ASN |
| 11 | G | 97 | PHE |
| 12 | H | 11 | LEU |
| 12 | H | 14 | ILE |
| 12 | H | 17 | THR |
| 12 | H | 20 | GLN |
| 12 | H | 21 | TRP |
| 12 | H | 23 | VAL |
| 12 | H | 33 | ASN |
| 12 | H | 35 | LEU |
| 12 | H | 36 | GLN |
| 12 | H | 37 | SER |
| 12 | H | 41 | GLU |
| 12 | H | 42 | THR |
| 12 | H | 43 | PHE |
| 12 | H | 47 | PHE |
| 12 | H | 48 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | H | 49 | LYS |
| 12 | H | 52 | LEU |
| 12 | H | 54 | LEU |
| 12 | H | 55 | LYS |
| 12 | H | 56 | PHE |
| 12 | H | 57 | LEU |
| 12 | H | 59 | LEU |
| 12 | H | 64 | LEU |
| 12 | H | 66 | THR |
| 12 | H | 67 | TYR |
| 12 | H | 69 | SER |
| 12 | H | 74 | GLN |
| 12 | H | 75 | ASP |
| 12 | H | 77 | LEU |
| 13 | I | 3 | ASN |
| 13 | I | 7 | LEU |
| 13 | I | 9 | VAL |
| 13 | I | 11 | LEU |
| 13 | I | 26 | LEU |
| 14 | J | 2 | ARG |
| 14 | J | 3 | ASP |
| 14 | J | 4 | PHE |
| 14 | J | 9 | SER |
| 14 | J | 10 | VAL |
| 14 | J | 13 | VAL |
| 14 | J | 14 | LEU |
| 14 | J | 16 | THR |
| 14 | J | 19 | PHE |
| 14 | J | 22 | LEU |
| 14 | J | 35 | ASP |
| 14 | J | 37 | LEU |
| 14 | J | 41 | PHE |
| 15 | K | 3 | ILE |
| 15 | K | 18 | MET |
| 15 | K | 19 | LEU |
| 15 | K | 23 | ARG |
| 15 | K | 26 | LEU |
| 15 | K | 32 | ARG |
| 15 | K | 33 | LYS |
| 15 | K | 39 | LYS |
| 15 | K | 40 | LEU |
| 15 | K | 43 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | K | 44 | GLU |
| 15 | K | 47 | LEU |
| 15 | K | 52 | PRO |
| 15 | K | 55 | PHE |
| 15 | K | 68 | HIS |
| 15 | K | 69 | ILE |
| 15 | K | 72 | VAL |
| 15 | K | 84 | LEU |
| 16 | L | 5 | LYS |
| 16 | L | 8 | TYR |
| 16 | L | 9 | GLN |
| 16 | L | 10 | VAL |
| 16 | L | 14 | LEU |
| 16 | L | 20 | ILE |
| 16 | L | 32 | LEU |
| 16 | L | 37 | LEU |
| 16 | L | 39 | ASN |
| 16 | L | 40 | LEU |
| 16 | L | 44 | ARG |
| 16 | L | 52 | ARG |
| 16 | L | 54 | VAL |
| 16 | L | 58 | LEU |
| 16 | L | 63 | LEU |
| 16 | L | 68 | PHE |
| 16 | L | 74 | LEU |
| 16 | L | 76 | ASN |
| 16 | L | 77 | THR |
| 16 | L | 85 | SER |
| 16 | L | 91 | LEU |
| 16 | L | 94 | ILE |
| 16 | L | 107 | PHE |
| 16 | L | 108 | LYS |
| 16 | L | 111 | GLU |
| 16 | L | 118 | LEU |
| 16 | L | 120 | LEU |
| 16 | L | 123 | ARG |
| 16 | L | 124 | LYS |
| 16 | L | 136 | TRP |
| 16 | L | 140 | THR |
| 16 | L | 145 | PHE |
| 16 | L | 149 | SER |
| 16 | L | 151 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | L | 152 | THR |
| 16 | L | 158 | MET |
| 16 | L | 163 | LEU |
| 16 | L | 165 | TYR |
| 17 | N | 3 | ILE |
| 17 | N | 4 | GLU |
| 17 | N | 6 | TYR |
| 17 | N | 10 | SER |
| 17 | N | 11 | LYS |
| 17 | N | 16 | LEU |
| 17 | N | 18 | ASP |
| 17 | N | 19 | LYS |
| 17 | N | 25 | THR |
| 17 | N | 28 | ASN |
| 17 | N | 29 | PHE |
| 17 | N | 37 | PHE |
| 17 | N | 39 | SER |
| 17 | N | 46 | PHE |
| 17 | N | 49 | CYS |
| 17 | N | 50 | GLN |
| 17 | N | 52 | LEU |
| 17 | N | 54 | LYS |
| 17 | N | 55 | GLN |
| 17 | N | 58 | VAL |
| 17 | N | 60 | PHE |
| 17 | N | 61 | LEU |
| 17 | N | 65 | LEU |
| 17 | N | 66 | ASP |
| 17 | N | 67 | LEU |
| 17 | N | 68 | GLU |
| 17 | N | 75 | TYR |
| 17 | N | 79 | SER |
| 17 | N | 80 | ASN |
| 17 | N | 81 | VAL |
| 17 | N | 84 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 111 | GLN |
| 1 | 1 | 150 | ASN |
| 2 | 2 | 44 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 2 | 128 | ASN |
| 2 | 2 | 191 | ASN |
| 3 | 3 | 61 | ASN |
| 3 | 3 | 126 | HIS |
| 3 | 3 | 130 | GLN |
| 3 | 3 | 165 | ASN |
| 3 | 3 | 200 | GLN |
| 4 | 4 | 47 | ASN |
| 4 | 4 | 71 | ASN |
| 4 | 4 | 139 | ASN |
| 4 | 4 | 169 | GLN |
| 5 | A | 33 | GLN |
| 5 | A | 58 | HIS |
| 5 | A | 121 | GLN |
| 5 | A | 129 | GLN |
| 5 | A | 151 | GLN |
| 5 | A | 187 | HIS |
| 5 | A | 197 | GLN |
| 5 | A | 224 | HIS |
| 5 | A | 230 | ASN |
| 5 | A | 231 | GLN |
| 5 | A | 246 | HIS |
| 5 | A | 315 | HIS |
| 5 | A | 341 | GLN |
| 5 | A | 343 | HIS |
| 5 | A | 361 | ASN |
| 5 | A | 447 | ASN |
| 5 | A | 464 | ASN |
| 5 | A | 490 | GLN |
| 5 | A | 494 | ASN |
| 5 | A | 542 | HIS |
| 5 | A | 543 | HIS |
| 5 | A | 545 | HIS |
| 5 | A | 591 | GLN |
| 5 | A | 607 | ASN |
| 5 | A | 629 | ASN |
| 5 | A | 631 | GLN |
| 5 | A | 636 | HIS |
| 5 | A | 641 | ASN |
| 5 | A | 644 | GLN |
| 5 | A | 660 | GLN |
| 5 | A | 683 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | A | 701 | GLN |
| 5 | A | 711 | HIS |
| 5 | A | 729 | GLN |
| 6 | B | 14 | GLN |
| 6 | B | 34 | HIS |
| 6 | B | 67 | HIS |
| 6 | B | 79 | GLN |
| 6 | B | 95 | HIS |
| 6 | B | 98 | GLN |
| 6 | B | 115 | ASN |
| 6 | B | 122 | GLN |
| 6 | B | 158 | GLN |
| 6 | B | 177 | HIS |
| 6 | B | 178 | HIS |
| 6 | B | 193 | HIS |
| 6 | B | 220 | GLN |
| 6 | B | 266 | GLN |
| 6 | B | 276 | HIS |
| 6 | B | 277 | HIS |
| 6 | B | 333 | GLN |
| 6 | B | 375 | HIS |
| 6 | B | 403 | ASN |
| 6 | B | 439 | HIS |
| 6 | B | 461 | GLN |
| 6 | B | 491 | ASN |
| 6 | B | 502 | ASN |
| 6 | B | 504 | ASN |
| 6 | B | 506 | ASN |
| 6 | B | 520 | HIS |
| 6 | B | 521 | HIS |
| 6 | B | 528 | HIS |
| 6 | B | 595 | HIS |
| 6 | B | 605 | ASN |
| 6 | B | 608 | GLN |
| 6 | B | 610 | ASN |
| 6 | B | 630 | GLN |
| 6 | B | 633 | ASN |
| 6 | B | 641 | ASN |
| 6 | B | 672 | GLN |
| 6 | B | 712 | HIS |
| 7 | C | 38 | GLN |
| 7 | C | 71 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | D | 23 | ASN |
| 8 | D | 41 | GLN |
| 8 | D | 56 | GLN |
| 8 | D | 73 | ASN |
| 8 | D | 82 | GLN |
| 8 | D | 128 | GLN |
| 8 | D | 133 | ASN |
| 8 | D | 140 | ASN |
| 9 | E | 48 | ASN |
| 9 | E | 73 | ASN |
| 10 | F | 116 | GLN |
| 10 | F | 146 | ASN |
| 10 | F | 152 | ASN |
| 10 | F | 153 | ASN |
| 11 | G | 61 | ASN |
| 11 | G | 67 | ASN |
| 12 | H | 16 | ASN |
| 12 | H | 36 | GLN |
| 15 | K | 31 | ASN |
| 16 | L | 12 | GLN |
| 16 | L | 39 | ASN |
| 16 | L | 48 | ASN |
| 16 | L | 129 | GLN |
| 17 | N | 45 | ASN |
| 17 | N | 55 | GLN |

### 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)

26 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 19 | GLC | M | 1 | 19 | 11,11,12 | 0.54 | 0 | 15,15,17 | 2.23 | 2 (13%) |
| 19 | FRU | M | 2 | 19 | 11,12,12 | 0.71 | 0 | 10,18,18 | 0.74 | 0 |
| 19 | GLC | O | 1 | 19 | 10,10,12 | 0.91 | 0 | 14,14,17 | 2.46 | 4 (28%) |
| 19 | FRU | O | 2 | 19 | 11,12,12 | 0.62 | 0 | 10,18,18 | 1.15 | 1 (10%) |
| 19 | GLC | P | 1 | 19 | 11,11,12 | 0.52 | 0 | 15,15,17 | 1.77 | 4 (26%) |
| 19 | FRU | P | 2 | 19 | 11,12,12 | 0.70 | 0 | 10,18,18 | 1.23 | 2 (20%) |
| 19 | GLC | Q | 1 | 19 | 11,11,12 | 0.60 | 0 | 15,15,17 | 2.44 | 5 (33%) |
| 19 | FRU | Q | 2 | 19 | 11,12,12 | 0.78 | 0 | 10,18,18 | 1.18 | 1 (10%) |
| 19 | GLC | S | 1 | 19 | 11,11,12 | 0.63 | 0 | 15,15,17 | 1.10 | 1 (6%) |
| 19 | FRU | S | 2 | 19 | 11,12,12 | 0.79 | 0 | 10,18,18 | 1.56 | 2 (20%) |
| 19 | GLC | T | 1 | 19 | 11,11,12 | 0.51 | 0 | 15,15,17 | 0.79 | 1 (6%) |
| 19 | FRU | T | 2 | 19 | 11,12,12 | 0.64 | 0 | 10,18,18 | 1.26 | 1 (10%) |
| 19 | GLC | U | 1 | 19 | 11,11,12 | 0.64 | 0 | 15,15,17 | 2.64 | 4 (26%) |
| 19 | FRU | U | 2 | 19 | 11,12,12 | 0.65 | 0 | 10,18,18 | 1.39 | 3 (30%) |
| 19 | GLC | V | 1 | 19 | 11,11,12 | 0.57 | 0 | 15,15,17 | 1.97 | 4 (26%) |
| 19 | FRU | V | 2 | 19 | 11,12,12 | 0.76 | 0 | 10,18,18 | 1.22 | 1 (10%) |
| 19 | GLC | W | 1 | 19 | 11,11,12 | 0.59 | 0 | 15,15,17 | 1.01 | 2 (13%) |
| 19 | FRU | W | 2 | 19 | 11,12,12 | 0.55 | 0 | 10,18,18 | 1.18 | 0 |
| 19 | GLC | X | 1 | 19 | 10,10,12 | 0.91 | 0 | 14,14,17 | 2.11 | 5 (35%) |
| 19 | FRU | X | 2 | 19 | 11,12,12 | 0.57 | 0 | 10,18,18 | 0.64 | 0 |
| 19 | GLC | Y | 1 | 21,19 | 11,11,12 | 1.69 | 3 (27%) | 15,15,17 | 2.66 | 6 (40%) |
| 19 | FRU | Y | 2 | 21,19 | 11,12,12 | 1.41 | 1 (9%) | 10,18,18 | 1.43 | 2 (20%) |
| 19 | GLC | Z | 1 | 19 | 11,11,12 | 0.43 | 0 | 15,15,17 | 1.12 | 2 (13%) |
| 19 | FRU | Z | 2 | 19 | 11,12,12 | 0.68 | 0 | 10,18,18 | 1.12 | 0 |
| 19 | GLC | a | 1 | 19 | 11,11,12 | 0.78 | 0 | 15,15,17 | 1.58 | 2 (13%) |
| 19 | FRU | a | 2 | 19 | 11,12,12 | 0.42 | 0 | 10,18,18 | 1.12 | 0 |

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 |
|---|---|---|---|---|---|---|---|
| 19 | GLC | M | 1 | 19 | - | 2/2/19/22 | 0/1/1/1 |
| 19 | FRU | M | 2 | 19 | 1/1/4/4 | 1/5/24/24 | 0/1/1/1 |
| 19 | GLC | O | 1 | 19 | - | - | 0/1/1/1 |
| 19 | FRU | O | 2 | 19 | 1/1/4/4 | 0/5/24/24 | 0/1/1/1 |
| 19 | GLC | P | 1 | 19 | - | 0/2/19/22 | 0/1/1/1 |
| 19 | FRU | P | 2 | 19 | 1/1/4/4 | 3/5/24/24 | 0/1/1/1 |
| 19 | GLC | Q | 1 | 19 | - | 2/2/19/22 | 0/1/1/1 |
| 19 | FRU | Q | 2 | 19 | 1/1/4/4 | 5/5/24/24 | 0/1/1/1 |
| 19 | GLC | S | 1 | 19 | - | 2/2/19/22 | 0/1/1/1 |
| 19 | FRU | S | 2 | 19 | 1/1/4/4 | 0/5/24/24 | 0/1/1/1 |
| 19 | GLC | T | 1 | 19 | - | 2/2/19/22 | 0/1/1/1 |
| 19 | FRU | T | 2 | 19 | 1/1/4/4 | 2/5/24/24 | 0/1/1/1 |
| 19 | GLC | U | 1 | 19 | - | 1/2/19/22 | 0/1/1/1 |
| 19 | FRU | U | 2 | 19 | 1/1/4/4 | 0/5/24/24 | 0/1/1/1 |
| 19 | GLC | V | 1 | 19 | - | 2/2/19/22 | 0/1/1/1 |
| 19 | FRU | V | 2 | 19 | 1/1/4/4 | 3/5/24/24 | 0/1/1/1 |
| 19 | GLC | W | 1 | 19 | - | 2/2/19/22 | 0/1/1/1 |
| 19 | FRU | W | 2 | 19 | 1/1/4/4 | 3/5/24/24 | 0/1/1/1 |
| 19 | GLC | X | 1 | 19 | - | - | 0/1/1/1 |
| 19 | FRU | X | 2 | 19 | 1/1/4/4 | 5/5/24/24 | 0/1/1/1 |
| 19 | GLC | Y | 1 | 21,19 | - | 0/2/19/22 | 0/1/1/1 |
| 19 | FRU | Y | 2 | 21,19 | 1/1/4/4 | 3/5/24/24 | 0/1/1/1 |
| 19 | GLC | Z | 1 | 19 | - | 1/2/19/22 | 0/1/1/1 |
| 19 | FRU | Z | 2 | 19 | 1/1/4/4 | 0/5/24/24 | 0/1/1/1 |
| 19 | GLC | a | 1 | 19 | - | 0/2/19/22 | 0/1/1/1 |
| 19 | FRU | a | 2 | 19 | 1/1/4/4 | 4/5/24/24 | 0/1/1/1 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | Y | 2 | FRU | O2-C2 | 4.27 | 1.48 | 1.40 |
| 19 | Y | 1 | GLC | C1-C2 | 3.36 | 1.59 | 1.52 |
| 19 | Y | 1 | GLC | C2-C3 | 2.99 | 1.56 | 1.52 |
| 19 | Y | 1 | GLC | O2-C2 | 2.25 | 1.48 | 1.43 |

All (55) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | M | 1 | GLC | C1-O5-C5 | 7.84 | 122.82 | 112.19 |
| 19 | U | 1 | GLC | C1-O5-C5 | 7.72 | 122.65 | 112.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | O | 1 | GLC | C1-C2-C3 | 7.09 | 118.38 | 109.67 |
| 19 | Y | 1 | GLC | C6-C5-C4 | 5.98 | 127.01 | 113.00 |
| 19 | V | 1 | GLC | C1-O5-C5 | 4.74 | 118.61 | 112.19 |
| 19 | Q | 1 | GLC | C1-O5-C5 | 4.64 | 118.48 | 112.19 |
| 19 | X | 1 | GLC | C1-C2-C3 | -4.61 | 104.00 | 109.67 |
| 19 | Q | 1 | GLC | C3-C4-C5 | -4.43 | 102.34 | 110.24 |
| 19 | a | 1 | GLC | C1-C2-C3 | -4.42 | 104.23 | 109.67 |
| 19 | U | 1 | GLC | O5-C5-C6 | 4.04 | 113.54 | 107.20 |
| 19 | V | 1 | GLC | O5-C5-C6 | 4.00 | 113.47 | 107.20 |
| 19 | Y | 1 | GLC | O5-C1-C2 | -3.98 | 104.63 | 110.77 |
| 19 | Y | 1 | GLC | O5-C5-C6 | 3.78 | 113.12 | 107.20 |
| 19 | Q | 1 | GLC | C2-C3-C4 | -3.66 | 104.57 | 110.89 |
| 19 | Q | 1 | GLC | O3-C3-C2 | 3.64 | 116.97 | 109.99 |
| 19 | X | 1 | GLC | O5-C1-C2 | -3.51 | 105.35 | 110.77 |
| 19 | S | 2 | FRU | O1-C1-C2 | -3.42 | 104.60 | 111.86 |
| 19 | Q | 1 | GLC | O5-C1-C2 | 3.39 | 116.01 | 110.77 |
| 19 | U | 1 | GLC | C2-C3-C4 | -3.36 | 105.09 | 110.89 |
| 19 | X | 1 | GLC | C3-C4-C5 | 3.31 | 114.93 | 109.77 |
| 19 | Y | 1 | GLC | O5-C5-C4 | -3.26 | 102.89 | 110.83 |
| 19 | P | 1 | GLC | C2-C3-C4 | -3.19 | 105.37 | 110.89 |
| 19 | Y | 1 | GLC | O2-C2-C1 | 3.04 | 115.37 | 109.15 |
| 19 | Y | 1 | GLC | C1-O5-C5 | -2.97 | 108.16 | 112.19 |
| 19 | O | 1 | GLC | O2-C2-C3 | -2.92 | 104.28 | 110.14 |
| 19 | Y | 2 | FRU | C6-C5-C4 | -2.85 | 108.23 | 115.09 |
| 19 | P | 1 | GLC | C1-C2-C3 | -2.84 | 106.18 | 109.67 |
| 19 | O | 2 | FRU | O4-C4-C3 | -2.80 | 103.75 | 112.15 |
| 19 | U | 1 | GLC | C3-C4-C5 | -2.79 | 105.27 | 110.24 |
| 19 | a | 1 | GLC | O5-C5-C6 | 2.72 | 111.47 | 107.20 |
| 19 | Z | 1 | GLC | O5-C5-C6 | 2.69 | 111.42 | 107.20 |
| 19 | P | 1 | GLC | O3-C3-C4 | 2.66 | 116.49 | 110.35 |
| 19 | S | 2 | FRU | O2-C2-O5 | -2.63 | 104.43 | 109.50 |
| 19 | Y | 2 | FRU | O2-C2-O5 | 2.57 | 114.47 | 109.50 |
| 19 | T | 2 | FRU | C6-C5-C4 | -2.56 | 108.91 | 115.09 |
| 19 | P | 2 | FRU | O1-C1-C2 | -2.56 | 106.42 | 111.86 |
| 19 | X | 1 | GLC | C6-C5-C4 | -2.54 | 108.38 | 113.07 |
| 19 | V | 1 | GLC | C1-C2-C3 | 2.52 | 112.77 | 109.67 |
| 19 | V | 1 | GLC | C6-C5-C4 | -2.52 | 107.10 | 113.00 |
| 19 | U | 2 | FRU | O5-C5-C6 | 2.47 | 115.73 | 108.85 |
| 19 | O | 1 | GLC | O5-C5-C4 | -2.47 | 105.09 | 109.52 |
| 19 | X | 1 | GLC | C1-O5-C5 | -2.45 | 107.23 | 112.78 |
| 19 | O | 1 | GLC | O5-C1-C2 | 2.39 | 114.45 | 110.77 |
| 19 | Q | 2 | FRU | O2-C2-O5 | 2.38 | 114.09 | 109.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | Z | 1 | GLC | C1-O5-C5 | 2.36 | 115.39 | 112.19 |
| 19 | U | 2 | FRU | O3-C3-C4 | -2.31 | 105.34 | 113.32 |
| 19 | S | 1 | GLC | C1-C2-C3 | 2.29 | 112.48 | 109.67 |
| 19 | M | 1 | GLC | O5-C5-C4 | 2.23 | 116.24 | 110.83 |
| 19 | V | 2 | FRU | O4-C4-C5 | -2.15 | 104.84 | 111.05 |
| 19 | U | 2 | FRU | O1-C1-C2 | -2.10 | 107.40 | 111.86 |
| 19 | T | 1 | GLC | C1-O5-C5 | 2.08 | 115.01 | 112.19 |
| 19 | W | 1 | GLC | C6-C5-C4 | -2.03 | 108.26 | 113.00 |
| 19 | P | 1 | GLC | O2-C2-C1 | 2.01 | 113.27 | 109.15 |
| 19 | W | 1 | GLC | C2-C3-C4 | -2.01 | 107.41 | 110.89 |
| 19 | P | 2 | FRU | O2-C2-O5 | 2.01 | 113.39 | 109.50 |

All (13) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 19 | M | 2 | FRU | C2 |
| 19 | O | 2 | FRU | C2 |
| 19 | P | 2 | FRU | C2 |
| 19 | Q | 2 | FRU | C2 |
| 19 | S | 2 | FRU | C2 |
| 19 | T | 2 | FRU | C2 |
| 19 | U | 2 | FRU | C2 |
| 19 | V | 2 | FRU | C2 |
| 19 | W | 2 | FRU | C2 |
| 19 | X | 2 | FRU | C2 |
| 19 | Y | 2 | FRU | C2 |
| 19 | Z | 2 | FRU | C2 |
| 19 | a | 2 | FRU | C2 |

All (43) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 19 | P | 2 | FRU | C4-C5-C6-O6 |
| 19 | P | 2 | FRU | O5-C5-C6-O6 |
| 19 | Q | 2 | FRU | O1-C1-C2-C3 |
| 19 | Q | 2 | FRU | O1-C1-C2-O2 |
| 19 | V | 2 | FRU | O1-C1-C2-C3 |
| 19 | V | 2 | FRU | O1-C1-C2-O2 |
| 19 | V | 2 | FRU | O1-C1-C2-O5 |
| 19 | W | 2 | FRU | O1-C1-C2-C3 |
| 19 | W | 2 | FRU | O1-C1-C2-O2 |
| 19 | W | 2 | FRU | O1-C1-C2-O5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 19 | X | 2 | FRU | O1-C1-C2-C3 |
| 19 | X | 2 | FRU | O1-C1-C2-O2 |
| 19 | X | 2 | FRU | O1-C1-C2-O5 |
| 19 | Y | 2 | FRU | C4-C5-C6-O6 |
| 19 | Q | 2 | FRU | O5-C5-C6-O6 |
| 19 | V | 1 | GLC | C4-C5-C6-O6 |
| 19 | Q | 2 | FRU | C4-C5-C6-O6 |
| 19 | X | 2 | FRU | C4-C5-C6-O6 |
| 19 | W | 1 | GLC | C4-C5-C6-O6 |
| 19 | Y | 2 | FRU | O5-C5-C6-O6 |
| 19 | X | 2 | FRU | O5-C5-C6-O6 |
| 19 | S | 1 | GLC | O5-C5-C6-O6 |
| 19 | V | 1 | GLC | O5-C5-C6-O6 |
| 19 | W | 1 | GLC | O5-C5-C6-O6 |
| 19 | Q | 1 | GLC | C4-C5-C6-O6 |
| 19 | S | 1 | GLC | C4-C5-C6-O6 |
| 19 | Q | 2 | FRU | O1-C1-C2-O5 |
| 19 | T | 1 | GLC | C4-C5-C6-O6 |
| 19 | T | 1 | GLC | O5-C5-C6-O6 |
| 19 | Q | 1 | GLC | O5-C5-C6-O6 |
| 19 | a | 2 | FRU | O1-C1-C2-O5 |
| 19 | U | 1 | GLC | O5-C5-C6-O6 |
| 19 | Z | 1 | GLC | O5-C5-C6-O6 |
| 19 | T | 2 | FRU | O1-C1-C2-O5 |
| 19 | M | 1 | GLC | O5-C5-C6-O6 |
| 19 | M | 2 | FRU | O5-C5-C6-O6 |
| 19 | a | 2 | FRU | O1-C1-C2-O2 |
| 19 | a | 2 | FRU | O1-C1-C2-C3 |
| 19 | a | 2 | FRU | O5-C5-C6-O6 |
| 19 | P | 2 | FRU | O1-C1-C2-O2 |
| 19 | T | 2 | FRU | O1-C1-C2-O2 |
| 19 | Y | 2 | FRU | O1-C1-C2-C3 |
| 19 | M | 1 | GLC | C4-C5-C6-O6 |

There are no ring outliers.

23 monomers are involved in 84 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 19 | T | 2 | FRU | 2 | 0 |
| 19 | W | 2 | FRU | 3 | 0 |
| 19 | a | 2 | FRU | 1 | 0 |
| 19 | U | 2 | FRU | 1 | 0 |

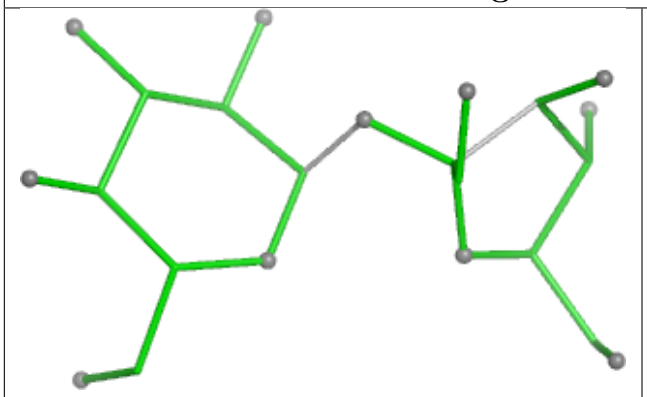
*Continued on next page...*

*Continued from previous page...*

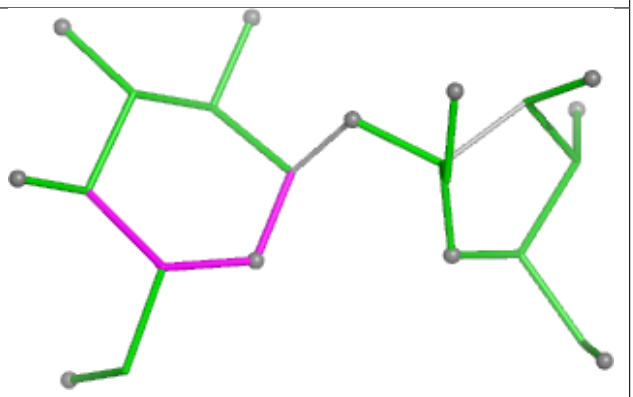
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 19 | T | 1 | GLC | 2 | 0 |
| 19 | W | 1 | GLC | 3 | 0 |
| 19 | Y | 2 | FRU | 1 | 16 |
| 19 | Z | 1 | GLC | 1 | 0 |
| 19 | U | 1 | GLC | 1 | 0 |
| 19 | V | 1 | GLC | 3 | 0 |
| 19 | Y | 1 | GLC | 0 | 12 |
| 19 | P | 1 | GLC | 8 | 0 |
| 19 | X | 2 | FRU | 3 | 0 |
| 19 | Q | 2 | FRU | 6 | 0 |
| 19 | S | 2 | FRU | 1 | 0 |
| 19 | Z | 2 | FRU | 13 | 0 |
| 19 | V | 2 | FRU | 4 | 0 |
| 19 | X | 1 | GLC | 3 | 0 |
| 19 | O | 2 | FRU | 3 | 0 |
| 19 | O | 1 | GLC | 10 | 0 |
| 19 | Q | 1 | GLC | 3 | 0 |
| 19 | a | 1 | GLC | 1 | 0 |
| 19 | P | 2 | FRU | 9 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

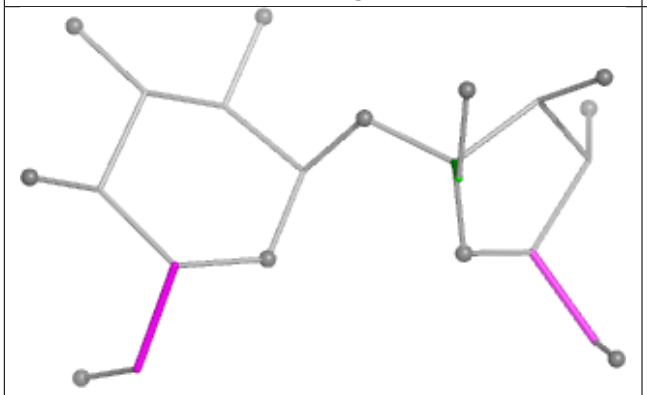
**Oligosaccharide Chain M**



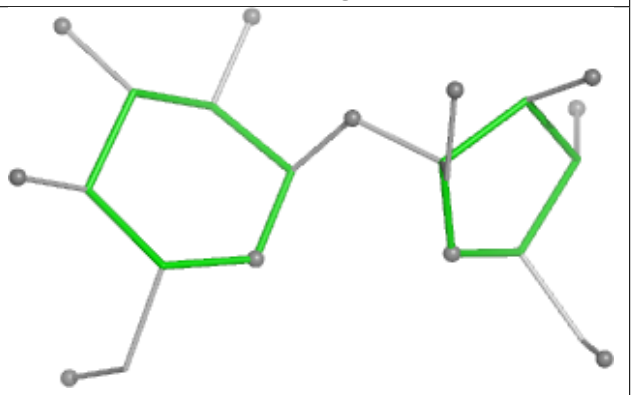
**Bond lengths**



**Bond angles**

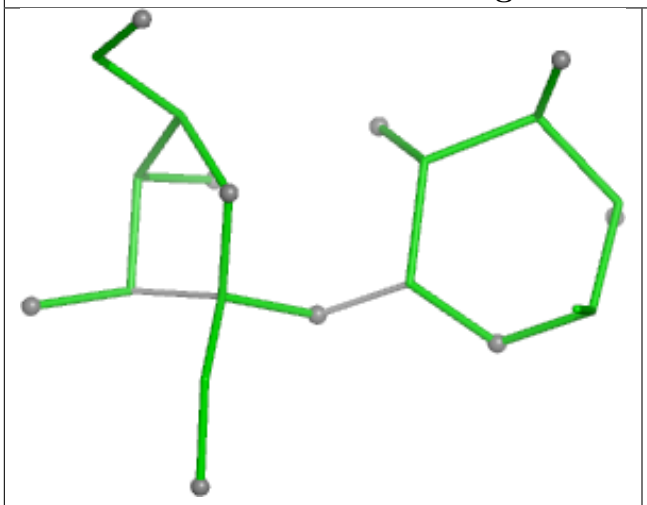


**Torsions**

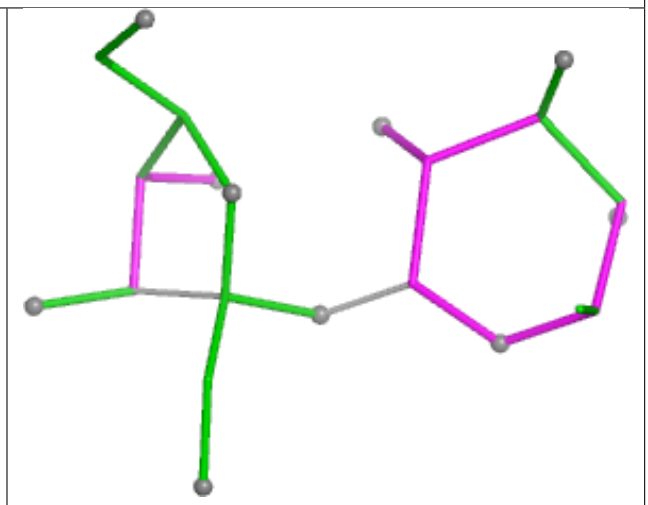


**Rings**

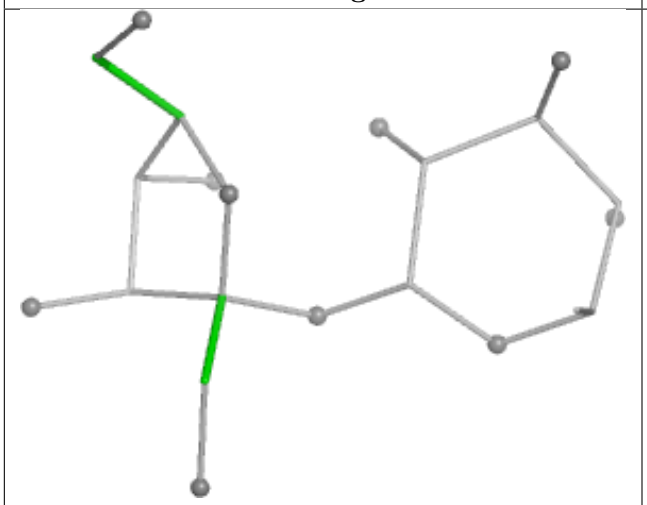
**Oligosaccharide Chain O**



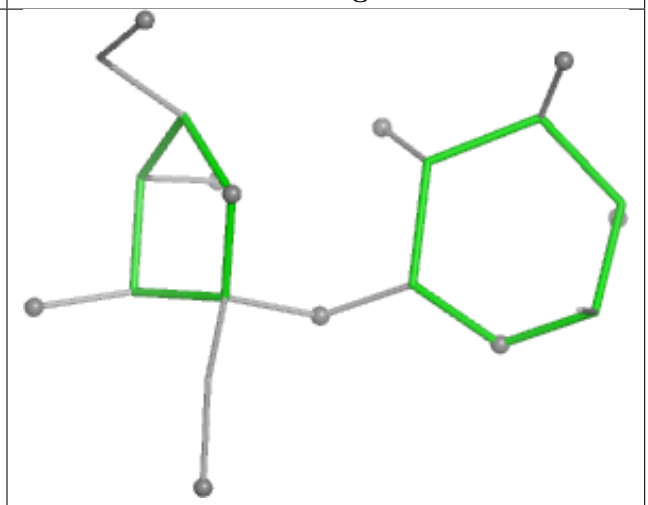
**Bond lengths**



**Bond angles**

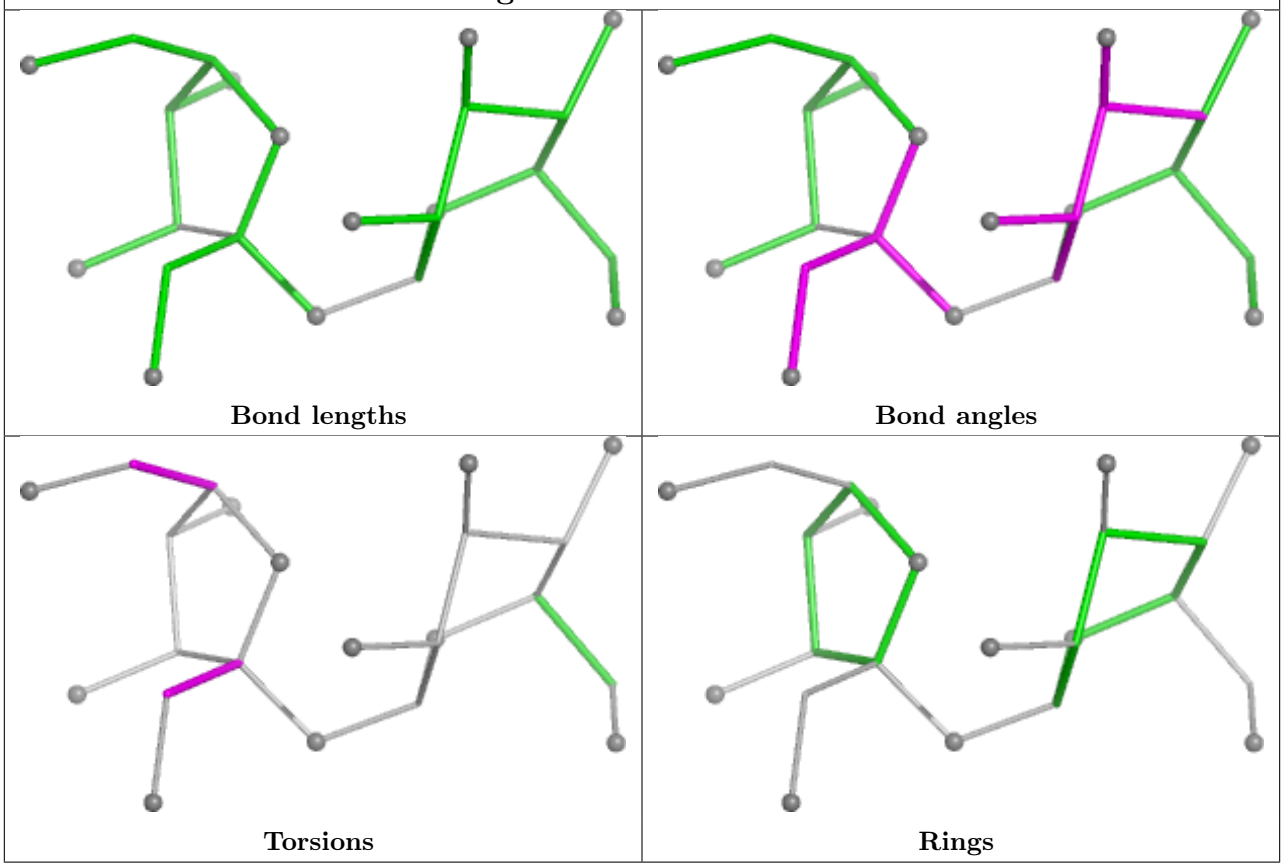


**Torsions**

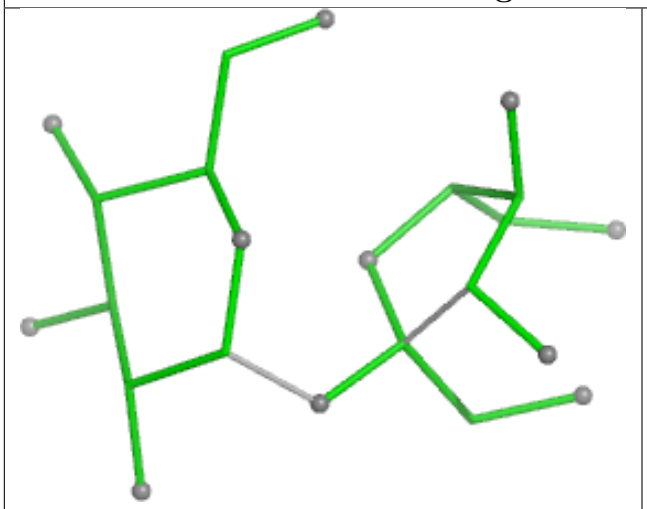


**Rings**

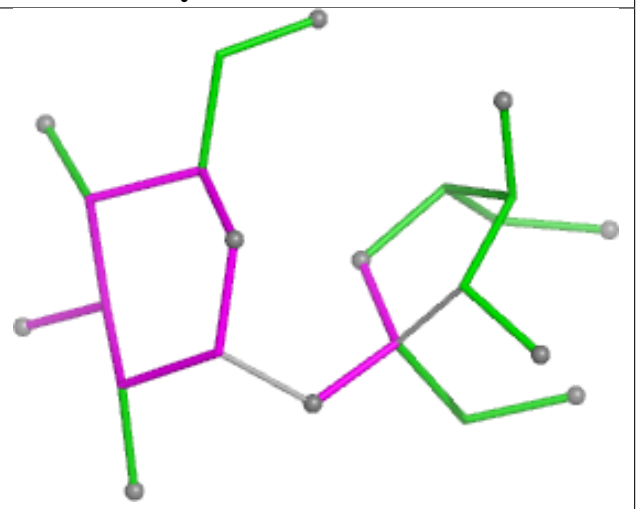
**Oligosaccharide Chain P**



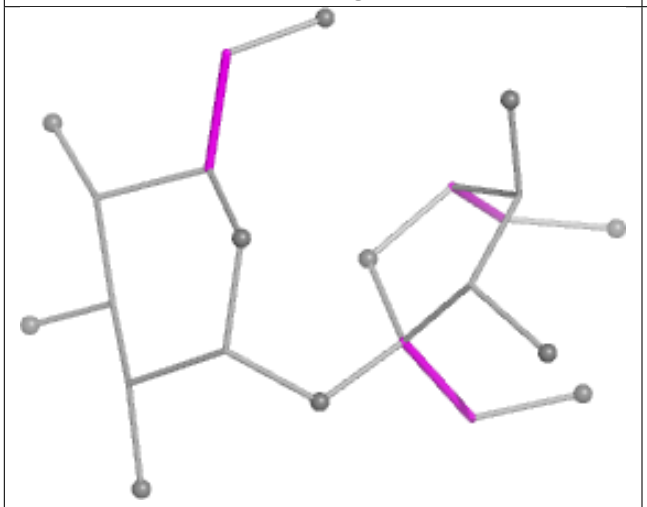
**Oligosaccharide Chain Q**



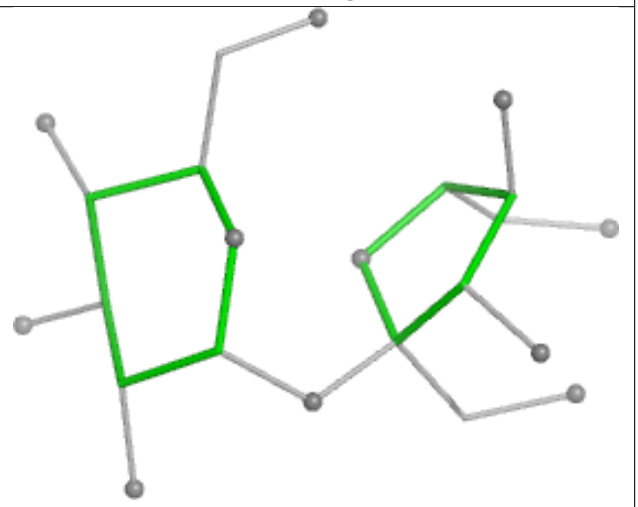
**Bond lengths**



**Bond angles**

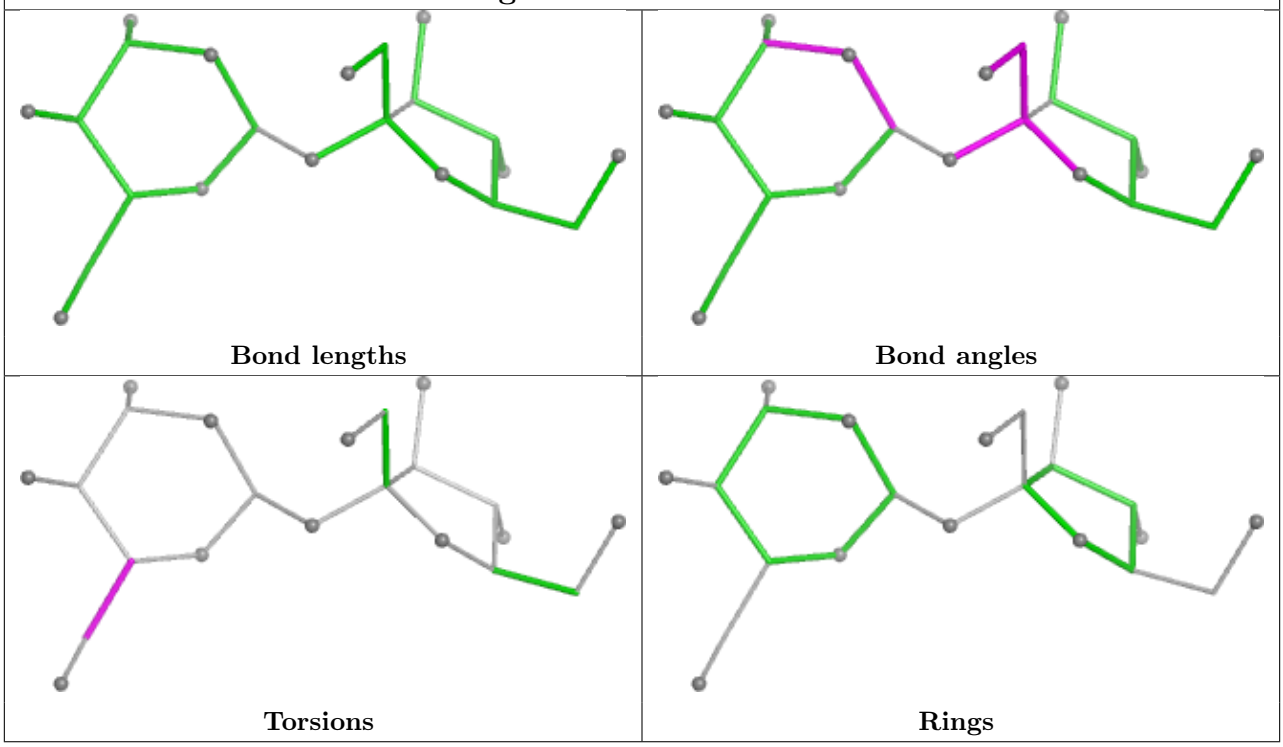


**Torsions**

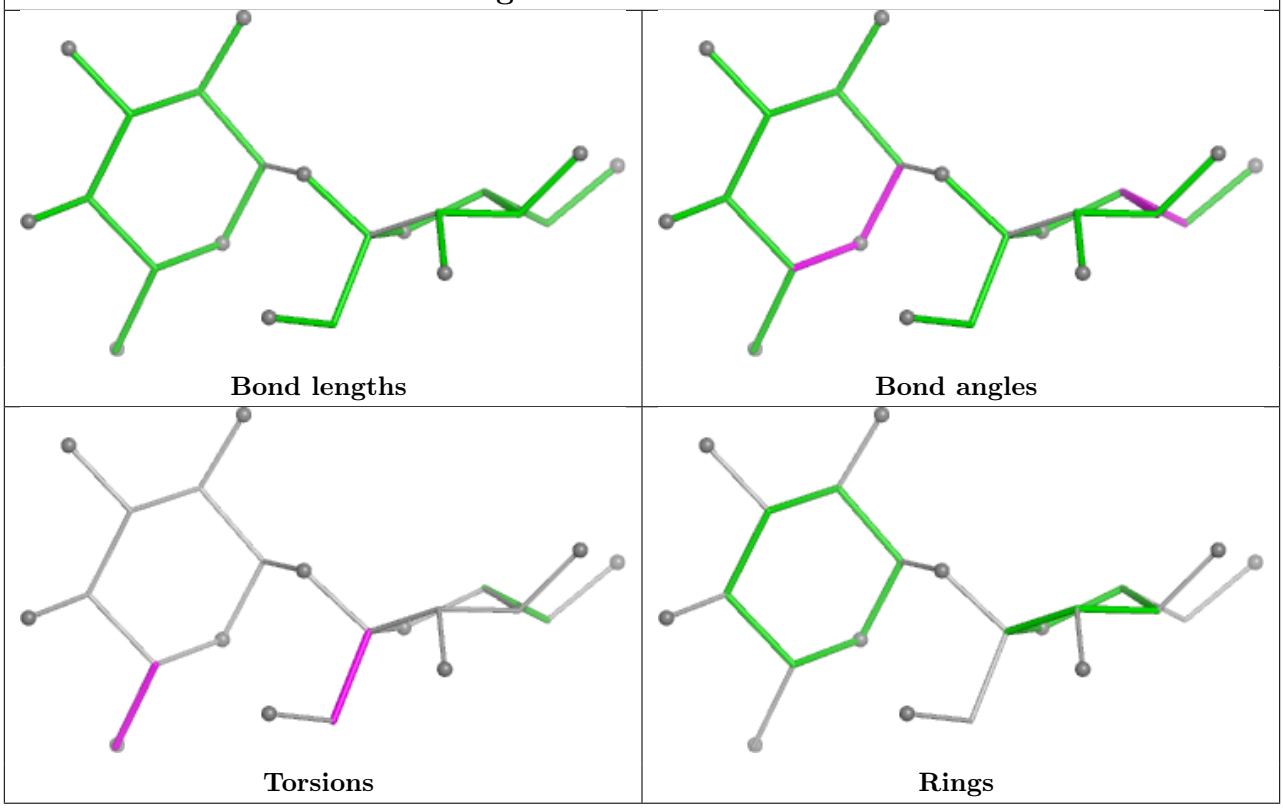


**Rings**

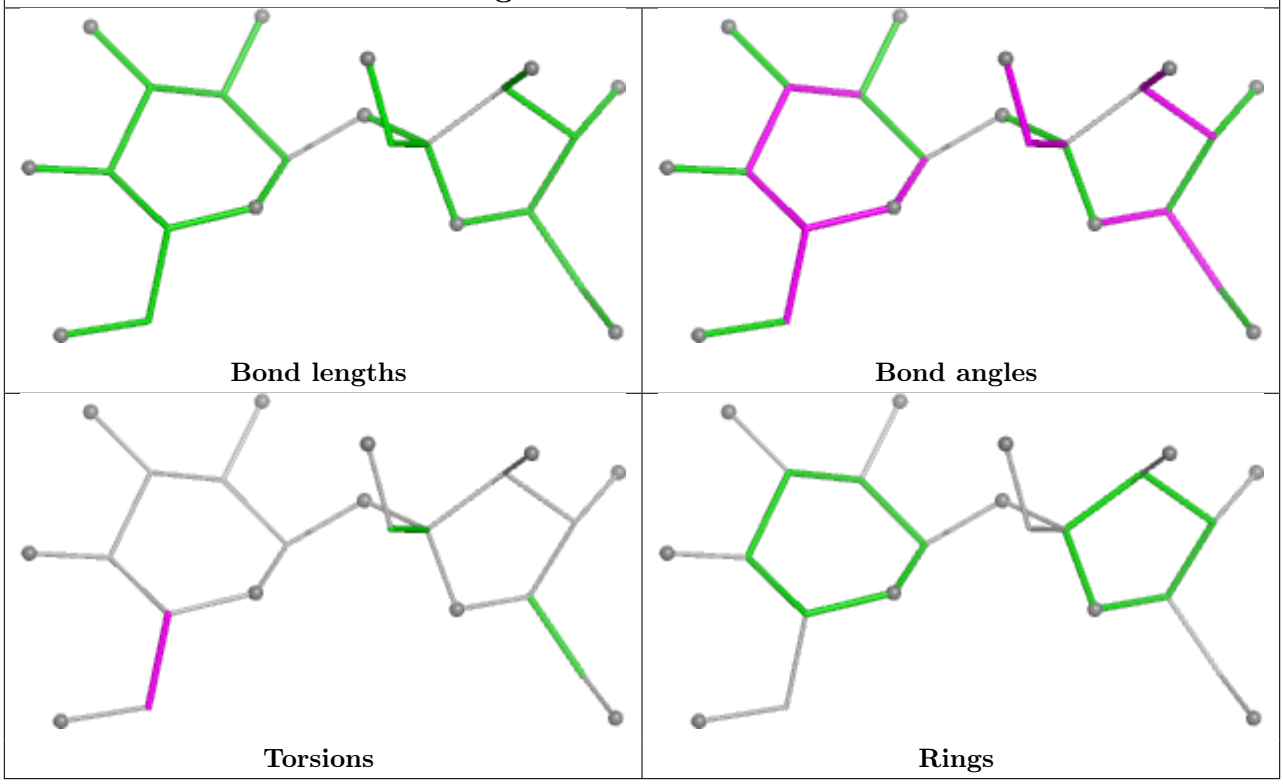
## Oligosaccharide Chain S



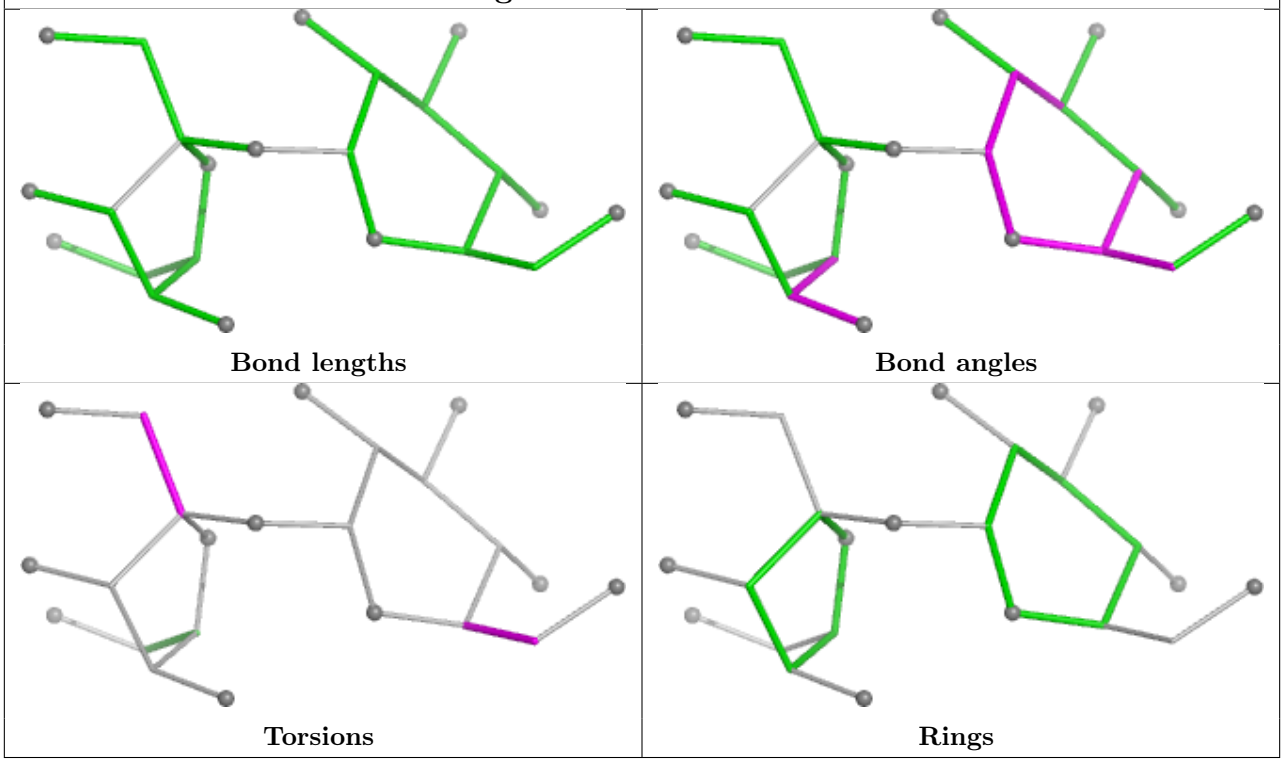

## Oligosaccharide Chain T



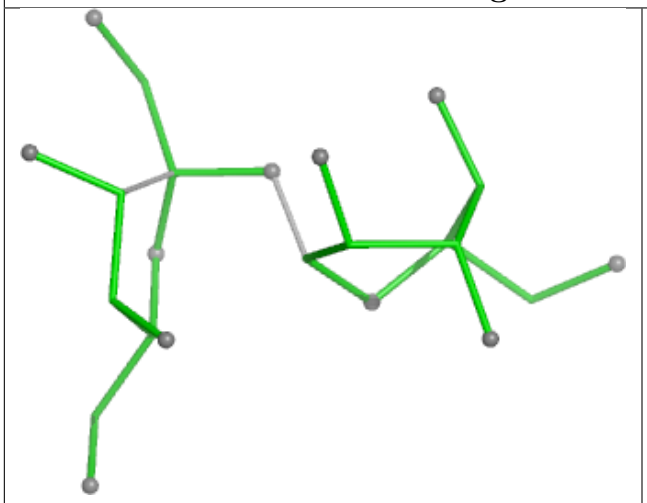
**Oligosaccharide Chain U**



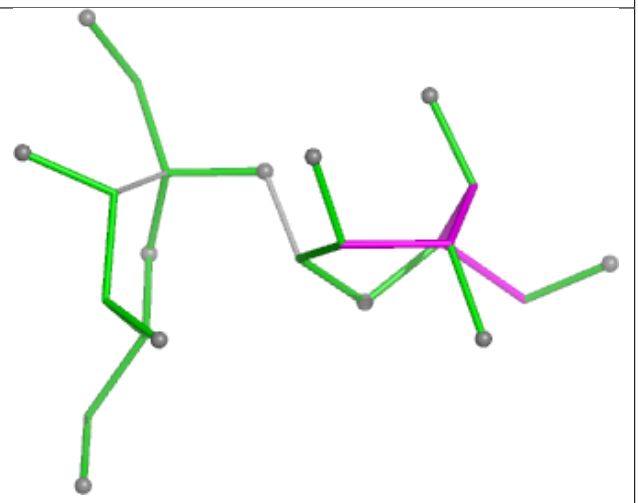

**Oligosaccharide Chain V**



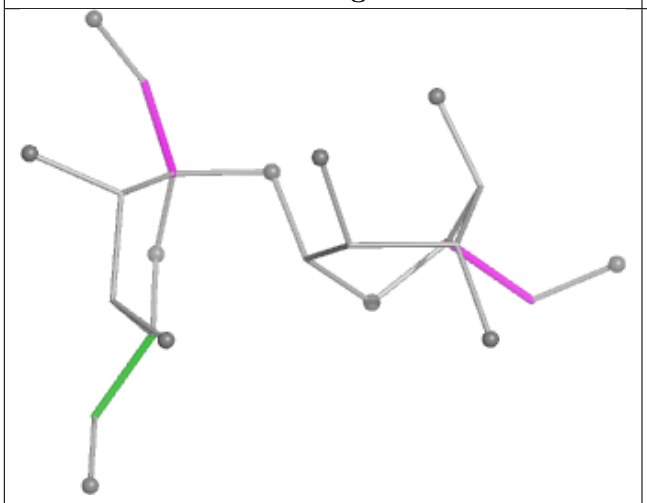
**Oligosaccharide Chain W**



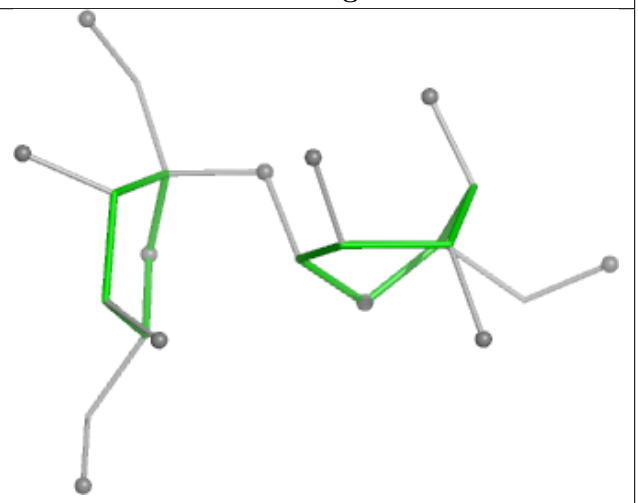
**Bond lengths**



**Bond angles**

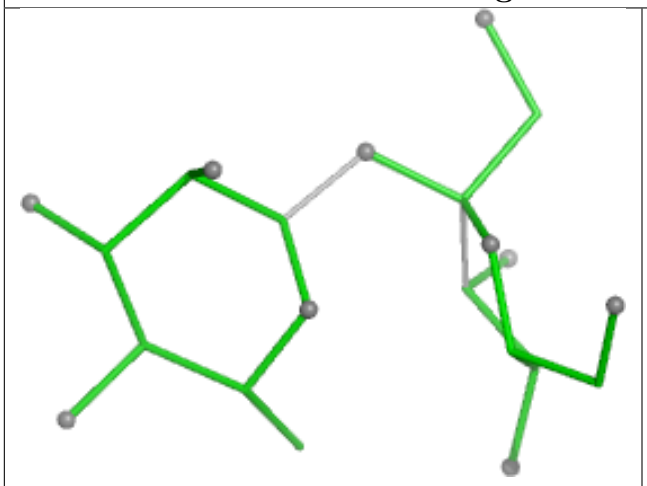


**Torsions**

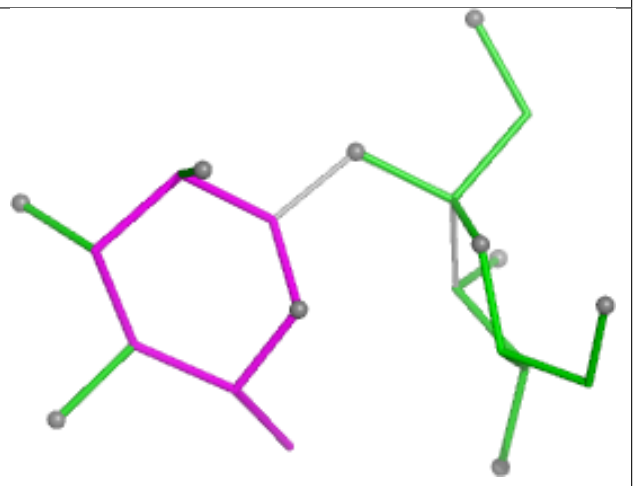


**Rings**

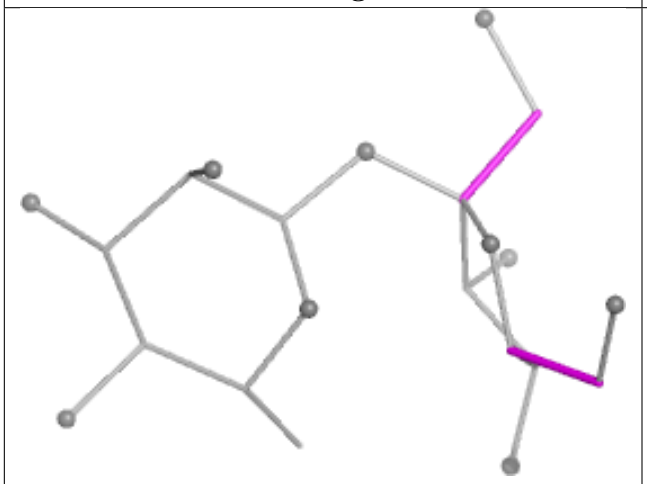
**Oligosaccharide Chain X**



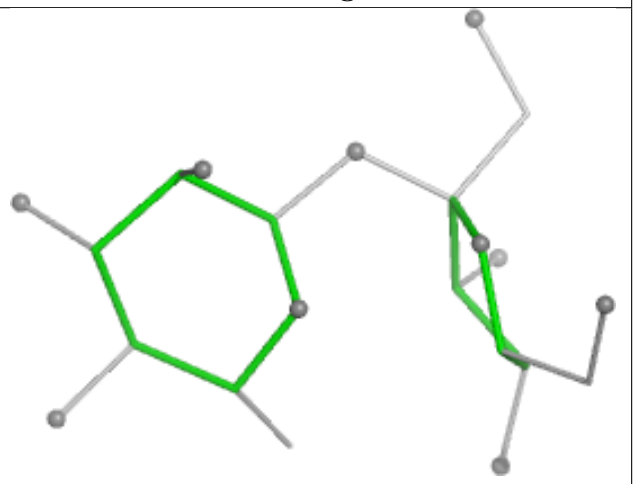
**Bond lengths**



**Bond angles**

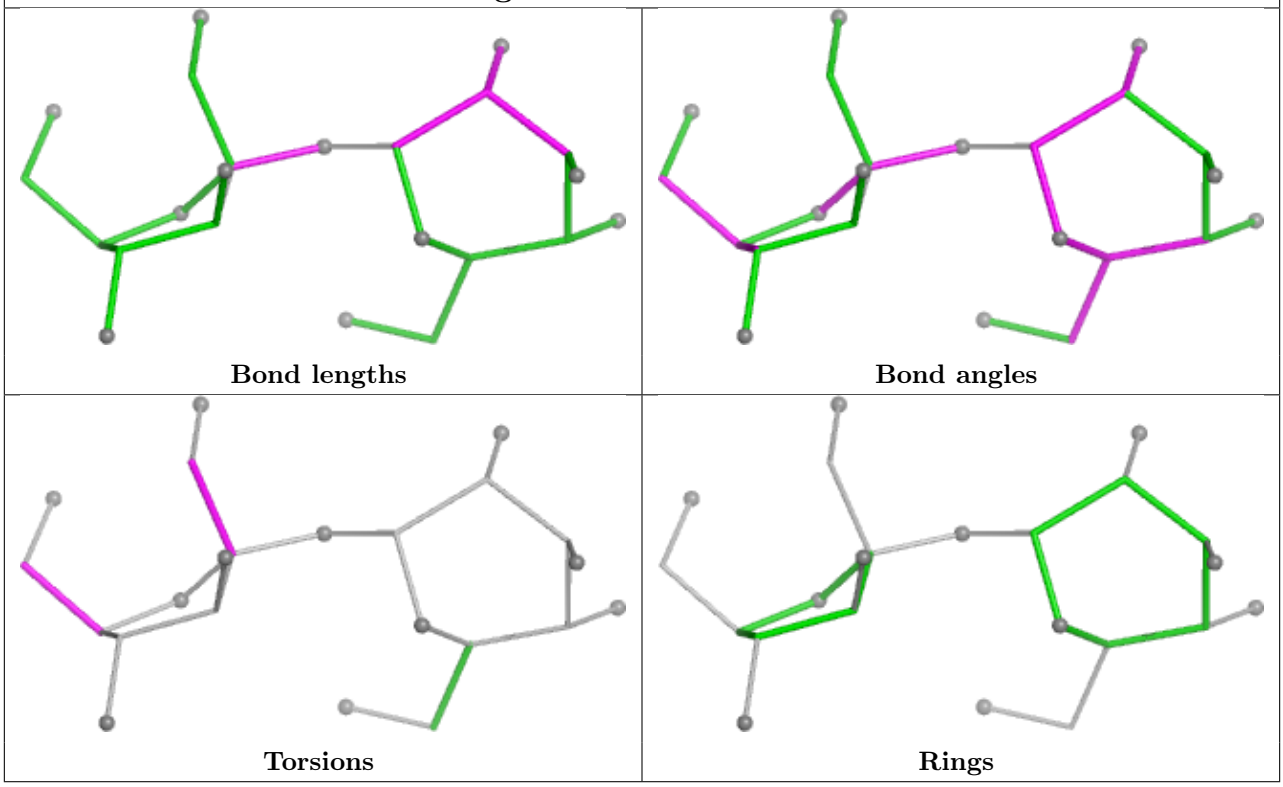


**Torsions**

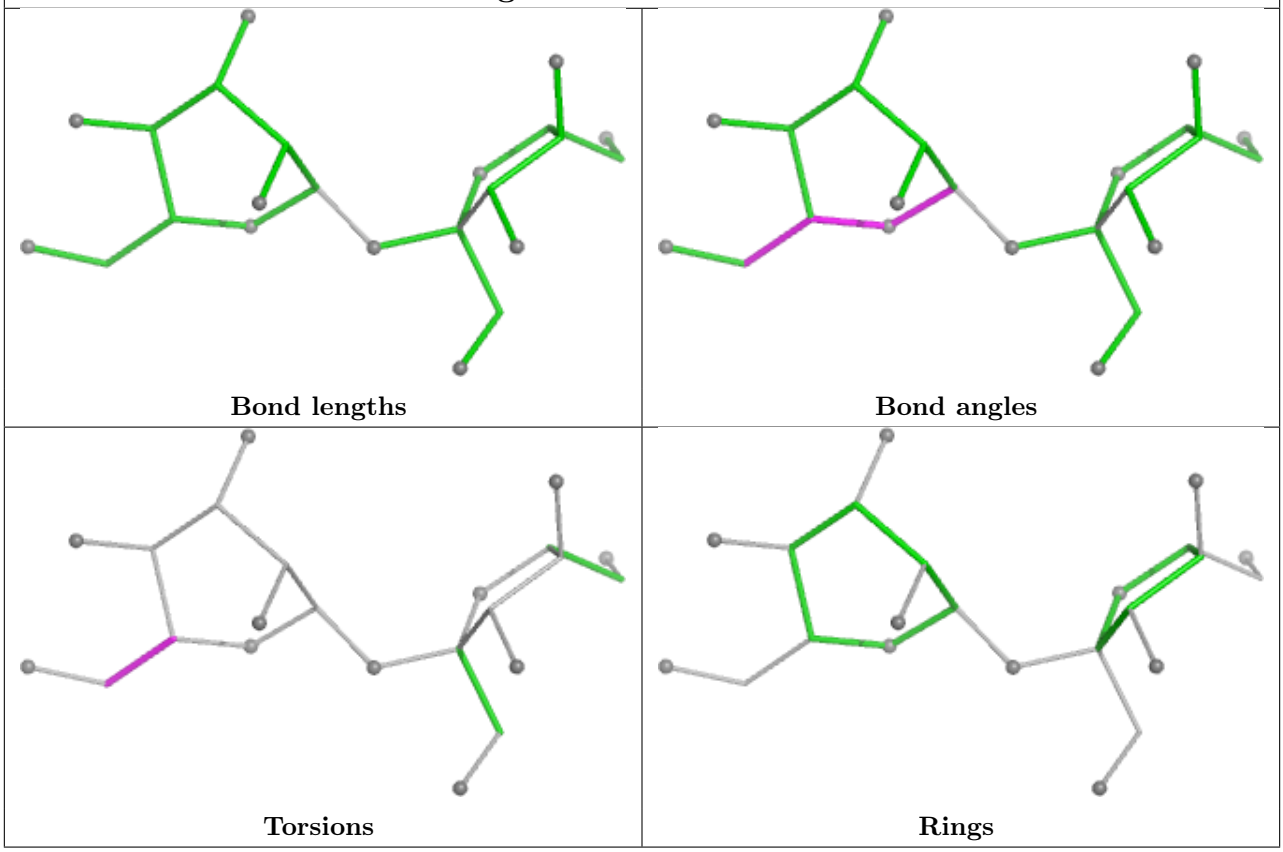


**Rings**

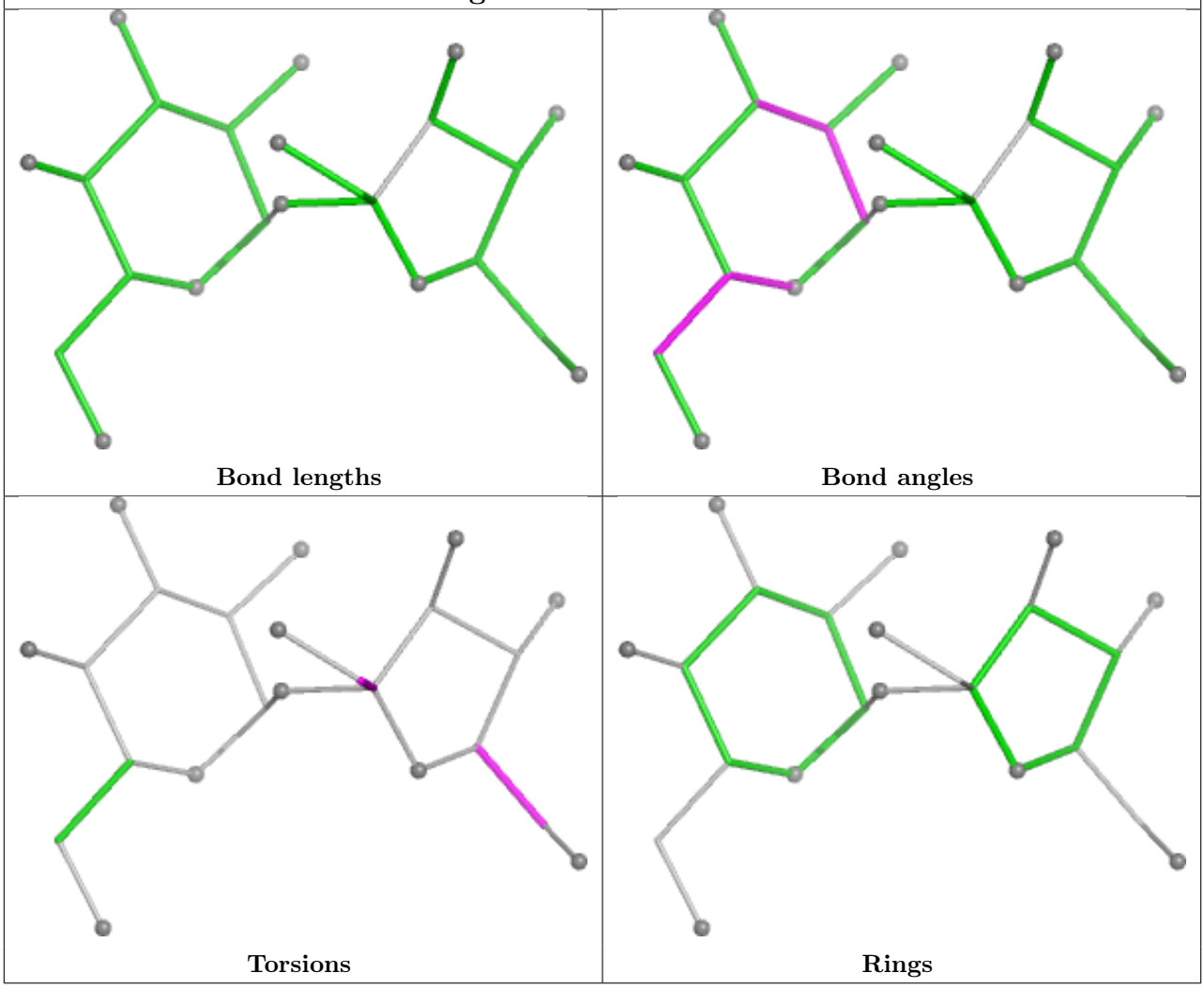
## Oligosaccharide Chain Y




## Oligosaccharide Chain Z



**Oligosaccharide Chain a**




## 5.6 Ligand geometry (i)

Of 244 ligands modelled in this entry, 1 is unknown - leaving 243 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 | $\#\|Z\| > 2$ |
| 20 | CLA | A | 822 | 5 | 54,58,73 | 2.45 | 16 (29%) | 65,95,113 | 2.86 | 24 (36%) |
| 20 | CLA | A | 851 | - | 69,73,73 | 2.23 | 15 (21%) | 83,113,113 | 2.77 | 29 (34%) |
| 20 | CLA | A | 808 | 5 | 64,68,73 | 2.29 | 17 (26%) | 77,107,113 | 2.82 | 29 (37%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 21 | LMU | D | 201 | - | 36,36,36 | 0.47 | 0 | 47,47,47 | 1.44 | 6 (12%) |
| 21 | LMU | 4 | 321 | - | 36,36,36 | 0.46 | 0 | 47,47,47 | 1.46 | 7 (14%) |
| 21 | LMU | L | 210 | - | 36,36,36 | 0.71 | 1 (2%) | 47,47,47 | 1.29 | 4 (8%) |
| 21 | LMU | R | 106 | - | 36,36,36 | 0.52 | 0 | 47,47,47 | 1.23 | 4 (8%) |
| 20 | CLA | 3 | 301 | - | 39,44,73 | 2.76 | 13 (33%) | 52,78,113 | 3.38 | 22 (42%) |
| 21 | LMU | R | 101 | - | 36,36,36 | 0.86 | 2 (5%) | 47,47,47 | 2.08 | 11 (23%) |
| 21 | LMU | B | 849 | - | 26,26,36 | 0.77 | 1 (3%) | 37,37,47 | 1.28 | 6 (16%) |
| 20 | CLA | K | 103 | - | 54,58,73 | 2.58 | 19 (35%) | 65,95,113 | 3.04 | 26 (40%) |
| 20 | CLA | 1 | 214 | - | 26,32,73 | 2.36 | 8 (30%) | 34,54,113 | 3.17 | 21 (61%) |
| 20 | CLA | A | 821 | 5 | 46,50,73 | 2.52 | 12 (26%) | 55,85,113 | 3.34 | 22 (40%) |
| 20 | CLA | B | 831 | 6 | 54,58,73 | 2.51 | 16 (29%) | 65,95,113 | 2.83 | 26 (40%) |
| 20 | CLA | 1 | 206 | - | 65,69,73 | 2.21 | 15 (23%) | 78,108,113 | 2.71 | 30 (38%) |
| 20 | CLA | B | 802 | - | 58,62,73 | 2.32 | 15 (25%) | 69,99,113 | 2.99 | 27 (39%) |
| 20 | CLA | J | 101 | - | 52,56,73 | 2.48 | 16 (30%) | 62,92,113 | 2.96 | 22 (35%) |
| 20 | CLA | B | 818 | - | 57,61,73 | 2.39 | 14 (24%) | 68,98,113 | 2.74 | 22 (32%) |
| 20 | CLA | L | 204 | - | 59,63,73 | 2.35 | 14 (23%) | 71,101,113 | 2.77 | 29 (40%) |
| 20 | CLA | B | 842 | - | 39,44,73 | 2.82 | 13 (33%) | 52,78,113 | 3.33 | 26 (50%) |
| 20 | CLA | 3 | 307 | - | 46,50,73 | 2.69 | 15 (32%) | 55,85,113 | 3.39 | 27 (49%) |
| 20 | CLA | 2 | 314 | - | 54,58,73 | 2.52 | 19 (35%) | 65,95,113 | 3.34 | 24 (36%) |
| 20 | CLA | 4 | 308 | - | 26,32,73 | 2.38 | 10 (38%) | 34,54,113 | 3.06 | 21 (61%) |
| 20 | CLA | A | 817 | - | 56,60,73 | 2.41 | 16 (28%) | 67,97,113 | 2.97 | 25 (37%) |
| 20 | CLA | 4 | 301 | - | 59,63,73 | 2.36 | 16 (27%) | 71,101,113 | 2.86 | 25 (35%) |
| 20 | CLA | B | 806 | - | 69,73,73 | 2.16 | 16 (23%) | 83,113,113 | 2.70 | 27 (32%) |
| 20 | CLA | K | 104 | - | 60,64,73 | 2.40 | 19 (31%) | 72,102,113 | 3.01 | 27 (37%) |
| 20 | CLA | B | 810 | - | 64,68,73 | 2.29 | 16 (25%) | 77,107,113 | 2.83 | 27 (35%) |
| 21 | LMU | 2 | 313 | - | 36,36,36 | 0.52 | 0 | 47,47,47 | 1.60 | 6 (12%) |
| 21 | LMU | 4 | 319 | - | 35,35,36 | 0.80 | 2 (5%) | 46,46,47 | 1.81 | 11 (23%) |
| 20 | CLA | A | 801 | - | 50,54,73 | 2.68 | 15 (30%) | 63,90,113 | 3.62 | 31 (49%) |
| 24 | SF4 | C | 103 | 7 | 0,12,12 | - | - | - | | |
| 20 | CLA | 3 | 312 | - | 26,32,73 | 2.39 | 9 (34%) | 34,54,113 | 3.00 | 21 (61%) |
| 21 | LMU | A | 847 | - | 36,36,36 | 0.68 | 1 (2%) | 47,47,47 | 1.42 | 7 (14%) |
| 20 | CLA | 2 | 304 | - | 26,32,73 | 2.35 | 11 (42%) | 34,54,113 | 3.05 | 21 (61%) |
| 21 | LMU | B | 805 | - | 36,36,36 | 0.67 | 1 (2%) | 47,47,47 | 1.66 | 12 (25%) |
| 20 | CLA | L | 202 | - | 59,63,73 | 2.36 | 16 (27%) | 71,101,113 | 2.85 | 26 (36%) |
| 20 | CLA | A | 841 | - | 26,32,73 | 2.41 | 9 (34%) | 34,54,113 | 3.11 | 23 (67%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 20 | CLA | B | 809 | - | 69,73,73 | 2.18 | 15 (21%) | 83,113,113 | 2.95 | 30 (36%) |
| 20 | CLA | A | 816 | - | 58,62,73 | 2.44 | 21 (36%) | 69,99,113 | 2.96 | 26 (37%) |
| 21 | LMU | H | 104 | - | 36,36,36 | 0.60 | 0 | 47,47,47 | 1.63 | 7 (14%) |
| 20 | CLA | B | 832 | 6 | 63,67,73 | 2.32 | 16 (25%) | 75,105,113 | 2.92 | 26 (34%) |
| 21 | LMU | 4 | 320 | - | 36,36,36 | 0.77 | 1 (2%) | 47,47,47 | 1.28 | 7 (14%) |
| 21 | LMU | R | 103 | - | 36,36,36 | 0.70 | 1 (2%) | 47,47,47 | 1.46 | 6 (12%) |
| 20 | CLA | B | 836 | - | 55,59,73 | 2.48 | 21 (38%) | 66,96,113 | 3.16 | 24 (36%) |
| 20 | CLA | 4 | 314 | 4 | 26,32,73 | 2.36 | 8 (30%) | 34,54,113 | 2.94 | 20 (58%) |
| 20 | CLA | B | 825 | - | 58,62,73 | 2.39 | 18 (31%) | 69,99,113 | 2.85 | 26 (37%) |
| 22 | BCR | B | 845 | - | 41,41,41 | 1.76 | 3 (7%) | 56,56,56 | 4.78 | 19 (33%) |
| 21 | LMU | A | 852 | - | 36,36,36 | 0.55 | 1 (2%) | 47,47,47 | 0.85 | 1 (2%) |
| 21 | LMU | K | 105 | - | 36,36,36 | 0.68 | 1 (2%) | 47,47,47 | 1.54 | 8 (17%) |
| 21 | LMU | E | 101 | - | 36,36,36 | 0.61 | 0 | 47,47,47 | 1.88 | 13 (27%) |
| 20 | CLA | B | 835 | 20 | 49,53,73 | 2.60 | 16 (32%) | 59,89,113 | 2.92 | 19 (32%) |
| 20 | CLA | H | 109 | - | 59,63,73 | 2.34 | 14 (23%) | 71,101,113 | 2.73 | 25 (35%) |
| 20 | CLA | A | 807 | 5 | 50,54,73 | 2.51 | 16 (32%) | 60,90,113 | 2.96 | 25 (41%) |
| 21 | LMU | 2 | 321 | - | 36,36,36 | 0.82 | 1 (2%) | 47,47,47 | 1.18 | 4 (8%) |
| 21 | LMU | K | 106 | - | 36,36,36 | 0.37 | 0 | 47,47,47 | 1.06 | 4 (8%) |
| 21 | LMU | R | 104 | - | 36,36,36 | 0.57 | 0 | 47,47,47 | 1.29 | 5 (10%) |
| 20 | CLA | B | 814 | - | 69,73,73 | 2.17 | 15 (21%) | 83,113,113 | 2.52 | 27 (32%) |
| 20 | CLA | B | 807 | 6 | 49,53,73 | 2.61 | 16 (32%) | 59,89,113 | 3.14 | 22 (37%) |
| 20 | CLA | A | 805 | 5 | 58,62,73 | 2.29 | 13 (22%) | 69,99,113 | 2.90 | 25 (36%) |
| 20 | CLA | 4 | 304 | - | 59,63,73 | 2.32 | 14 (23%) | 71,101,113 | 2.87 | 25 (35%) |
| 21 | LMU | 3 | 318 | - | 36,36,36 | 0.49 | 0 | 47,47,47 | 0.72 | 1 (2%) |
| 20 | CLA | A | 830 | 5 | 69,73,73 | 2.17 | 15 (21%) | 83,113,113 | 2.61 | 21 (25%) |
| 21 | LMU | H | 103 | - | 36,36,36 | 0.86 | 1 (2%) | 47,47,47 | 2.09 | 12 (25%) |
| 21 | LMU | G | 102 | - | 36,36,36 | 0.61 | 0 | 47,47,47 | 1.59 | 8 (17%) |
| 21 | LMU | R | 109 | - | 36,36,36 | 0.49 | 0 | 47,47,47 | 0.82 | 1 (2%) |
| 20 | CLA | L | 208 | - | 54,58,73 | 2.48 | 18 (33%) | 65,95,113 | 3.13 | 24 (36%) |
| 22 | BCR | B | 801 | - | 41,41,41 | 2.52 | 6 (14%) | 56,56,56 | 6.08 | 21 (37%) |
| 22 | BCR | B | 847 | - | 41,41,41 | 1.95 | 3 (7%) | 56,56,56 | 5.45 | 17 (30%) |
| 21 | LMU | C | 101 | - | 36,36,36 | 0.70 | 1 (2%) | 47,47,47 | 1.26 | 4 (8%) |
| 20 | CLA | A | 836 | - | 51,55,73 | 2.51 | 14 (27%) | 61,91,113 | 2.85 | 22 (36%) |
| 21 | LMU | F | 202 | - | 35,35,36 | 0.57 | 0 | 46,46,47 | 1.36 | 5 (10%) |
| 20 | CLA | 4 | 311 | - | 26,32,73 | 2.33 | 11 (42%) | 34,54,113 | 3.13 | 21 (61%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 20 | CLA | A | 828 | 5 | 69,73,73 | 2.14 | 14 (20%) | 83,113,113 | 2.57 | 28 (33%) |
| 20 | CLA | 3 | 305 | - | 26,32,73 | 2.30 | 8 (30%) | 34,54,113 | 2.98 | 19 (55%) |
| 20 | CLA | A | 835 | 5 | 69,73,73 | 2.22 | 17 (24%) | 83,113,113 | 2.79 | 31 (37%) |
| 20 | CLA | 1 | 215 | - | 55,59,73 | 2.50 | 23 (41%) | 66,96,113 | 3.10 | 26 (39%) |
| 20 | CLA | 2 | 316 | - | 69,73,73 | 2.33 | 23 (33%) | 83,113,113 | 2.80 | 26 (31%) |
| 20 | CLA | A | 806 | - | 60,64,73 | 2.29 | 14 (23%) | 72,102,113 | 2.95 | 27 (37%) |
| 20 | CLA | K | 101 | - | 50,54,73 | 2.58 | 18 (36%) | 60,90,113 | 3.02 | 23 (38%) |
| 20 | CLA | B | 824 | - | 69,73,73 | 2.43 | 23 (33%) | 83,113,113 | 2.73 | 26 (31%) |
| 20 | CLA | 3 | 317 | - | 39,44,73 | 2.79 | 13 (33%) | 52,78,113 | 3.30 | 25 (48%) |
| 20 | CLA | A | 814 | 5 | 26,32,73 | 2.38 | 10 (38%) | 34,54,113 | 3.14 | 19 (55%) |
| 20 | CLA | H | 102 | - | 59,63,73 | 2.31 | 13 (22%) | 71,101,113 | 2.90 | 26 (36%) |
| 20 | CLA | B | 833 | 6 | 54,58,73 | 2.45 | 17 (31%) | 65,95,113 | 3.06 | 25 (38%) |
| 20 | CLA | 1 | 204 | - | 50,54,73 | 2.73 | 21 (42%) | 60,90,113 | 3.45 | 28 (46%) |
| 21 | LMU | A | 846 | - | 36,36,36 | 0.70 | 0 | 47,47,47 | 1.27 | 7 (14%) |
| 22 | BCR | I | 101 | - | 39,40,41 | 1.67 | 3 (7%) | 52,53,56 | 4.25 | 19 (36%) |
| 20 | CLA | G | 105 | - | 55,59,73 | 2.49 | 19 (34%) | 66,96,113 | 3.00 | 24 (36%) |
| 20 | CLA | 3 | 304 | - | 26,32,73 | 2.34 | 10 (38%) | 34,54,113 | 3.22 | 21 (61%) |
| 21 | LMU | 1 | 216 | - | 36,36,36 | 0.45 | 0 | 47,47,47 | 1.38 | 6 (12%) |
| 20 | CLA | H | 101 | - | 59,63,73 | 2.39 | 15 (25%) | 71,101,113 | 2.92 | 27 (38%) |
| 20 | CLA | 4 | 318 | - | 51,55,73 | 2.54 | 19 (37%) | 61,91,113 | 3.23 | 29 (47%) |
| 20 | CLA | B | 829 | - | 69,73,73 | 2.11 | 15 (21%) | 83,113,113 | 2.75 | 28 (33%) |
| 20 | CLA | A | 834 | - | 50,54,73 | 2.53 | 15 (30%) | 60,90,113 | 3.03 | 25 (41%) |
| 22 | BCR | B | 844 | - | 41,41,41 | 1.86 | 3 (7%) | 56,56,56 | 5.19 | 24 (42%) |
| 20 | CLA | 4 | 305 | - | 54,58,73 | 2.53 | 19 (35%) | 65,95,113 | 2.97 | 27 (41%) |
| 20 | CLA | 4 | 312 | - | 26,32,73 | 2.44 | 8 (30%) | 34,54,113 | 3.12 | 21 (61%) |
| 20 | CLA | 3 | 314 | - | 69,73,73 | 2.30 | 24 (34%) | 83,113,113 | 2.90 | 28 (33%) |
| 20 | CLA | B | 823 | 6 | 59,63,73 | 2.38 | 17 (28%) | 71,101,113 | 2.74 | 27 (38%) |
| 20 | CLA | H | 110 | 16 | 54,58,73 | 2.45 | 13 (24%) | 65,95,113 | 2.87 | 26 (40%) |
| 20 | CLA | A | 824 | - | 63,67,73 | 2.25 | 16 (25%) | 75,105,113 | 2.77 | 28 (37%) |
| 20 | CLA | A | 826 | - | 69,73,73 | 2.15 | 17 (24%) | 83,113,113 | 2.69 | 27 (32%) |
| 22 | BCR | G | 104 | - | 41,41,41 | 1.87 | 3 (7%) | 56,56,56 | 5.73 | 17 (30%) |
| 20 | CLA | 2 | 303 | - | 62,66,73 | 2.42 | 21 (33%) | 74,104,113 | 3.13 | 29 (39%) |
| 20 | CLA | 3 | 311 | - | 69,73,73 | 2.18 | 16 (23%) | 83,113,113 | 2.70 | 24 (28%) |
| 20 | CLA | K | 102 | - | 54,58,73 | 2.46 | 16 (29%) | 65,95,113 | 2.99 | 24 (36%) |
| 20 | CLA | B | 811 | 6 | 26,32,73 | 2.40 | 11 (42%) | 34,54,113 | 2.87 | 20 (58%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 25 | LMG | B | 848 | - | 49,49,55 | 0.99 | 2 (4%) | 57,57,63 | 1.08 | 3 (5%) |
| 20 | CLA | I | 102 | - | 64,68,73 | 2.24 | 14 (21%) | 77,107,113 | 2.70 | 23 (29%) |
| 20 | CLA | 2 | 312 | - | 65,69,73 | 2.29 | 20 (30%) | 78,108,113 | 2.95 | 32 (41%) |
| 20 | CLA | B | 821 | - | 54,58,73 | 2.40 | 14 (25%) | 65,95,113 | 2.99 | 26 (40%) |
| 22 | BCR | F | 203 | - | 41,41,41 | 2.01 | 3 (7%) | 56,56,56 | 5.47 | 19 (33%) |
| 20 | CLA | A | 804 | 20 | 59,63,73 | 2.37 | 15 (25%) | 71,101,113 | 2.96 | 27 (38%) |
| 20 | CLA | 1 | 211 | - | 55,59,73 | 2.57 | 22 (40%) | 66,96,113 | 3.42 | 29 (43%) |
| 20 | CLA | B | 819 | 6 | 45,49,73 | 2.93 | 23 (51%) | 54,84,113 | 3.52 | 25 (46%) |
| 21 | LMU | H | 105 | - | 36,36,36 | 0.72 | 1 (2%) | 47,47,47 | 1.66 | 9 (19%) |
| 20 | CLA | B | 834 | 20 | 49,53,73 | 2.61 | 15 (30%) | 59,89,113 | 3.00 | 20 (33%) |
| 20 | CLA | B | 822 | - | 50,54,73 | 2.48 | 15 (30%) | 60,90,113 | 3.14 | 20 (33%) |
| 20 | CLA | 2 | 306 | - | 26,32,73 | 2.26 | 9 (34%) | 34,54,113 | 3.03 | 21 (61%) |
| 24 | SF4 | A | 856 | 6,5 | 0,12,12 | - | - | - | | |
| 20 | CLA | B | 850 | 6 | 69,73,73 | 2.14 | 16 (23%) | 83,113,113 | 2.76 | 32 (38%) |
| 20 | CLA | R | 107 | - | 61,65,73 | 2.31 | 13 (21%) | 73,103,113 | 2.85 | 28 (38%) |
| 20 | CLA | R | 108 | - | 69,73,73 | 2.17 | 13 (18%) | 83,113,113 | 2.62 | 28 (33%) |
| 21 | LMU | R | 102 | - | 36,36,36 | 0.57 | 0 | 47,47,47 | 1.51 | 9 (19%) |
| 24 | SF4 | C | 102 | 7 | 0,12,12 | - | - | - | | |
| 20 | CLA | B | 841 | - | 69,73,73 | 2.09 | 16 (23%) | 83,113,113 | 2.68 | 25 (30%) |
| 20 | CLA | 1 | 209 | - | 26,32,73 | 2.40 | 8 (30%) | 34,54,113 | 3.07 | 23 (67%) |
| 21 | LMU | R | 105 | - | 36,36,36 | 0.75 | 1 (2%) | 47,47,47 | 1.39 | 8 (17%) |
| 20 | CLA | F | 201 | 6,10 | 54,58,73 | 2.53 | 23 (42%) | 65,95,113 | 3.18 | 26 (40%) |
| 20 | CLA | F | 205 | - | 39,44,73 | 2.75 | 15 (38%) | 52,78,113 | 3.20 | 25 (48%) |
| 20 | CLA | 3 | 310 | - | 69,73,73 | 2.26 | 21 (30%) | 83,113,113 | 2.81 | 32 (38%) |
| 20 | CLA | L | 201 | 5 | 64,68,73 | 2.28 | 15 (23%) | 77,107,113 | 2.65 | 25 (32%) |
| 20 | CLA | 4 | 309 | - | 26,32,73 | 2.37 | 8 (30%) | 34,54,113 | 3.10 | 19 (55%) |
| 20 | CLA | 3 | 316 | - | 26,32,73 | 2.39 | 11 (42%) | 34,54,113 | 3.14 | 20 (58%) |
| 20 | CLA | 4 | 315 | - | 50,54,73 | 2.52 | 18 (36%) | 60,90,113 | 3.01 | 23 (38%) |
| 20 | CLA | A | 818 | - | 64,68,73 | 2.41 | 22 (34%) | 77,107,113 | 2.96 | 32 (41%) |
| 22 | BCR | A | 845 | - | 41,41,41 | 2.01 | 4 (9%) | 56,56,56 | 5.71 | 26 (46%) |
| 23 | PQN | A | 842 | - | 34,34,34 | 1.69 | 2 (5%) | 42,45,45 | 1.21 | 5 (11%) |
| 20 | CLA | F | 206 | 20 | 45,49,73 | 2.68 | 16 (35%) | 54,84,113 | 3.16 | 23 (42%) |
| 20 | CLA | B | 827 | 6 | 69,73,73 | 2.15 | 16 (23%) | 83,113,113 | 2.57 | 25 (30%) |
| 20 | CLA | A | 837 | - | 55,59,73 | 2.42 | 16 (29%) | 66,96,113 | 3.15 | 25 (37%) |
| 21 | LMU | L | 206 | - | 36,36,36 | 0.51 | 0 | 47,47,47 | 1.00 | 3 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 20 | CLA | L | 203 | - | 69,73,73 | 2.09 | 13 (18%) | 83,113,113 | 2.71 | 29 (34%) |
| 20 | CLA | A | 819 | - | 62,66,73 | 2.31 | 17 (27%) | 74,104,113 | 2.80 | 25 (33%) |
| 20 | CLA | 2 | 310 | 2 | 54,58,73 | 2.61 | 18 (33%) | 65,95,113 | 3.06 | 26 (40%) |
| 20 | CLA | 3 | 313 | - | 54,58,73 | 2.46 | 13 (24%) | 65,95,113 | 2.80 | 25 (38%) |
| 20 | CLA | A | 850 | - | 69,73,73 | 2.19 | 16 (23%) | 83,113,113 | 2.69 | 26 (31%) |
| 21 | LMU | 4 | 316 | - | 36,36,36 | 0.72 | 1 (2%) | 47,47,47 | 1.08 | 3 (6%) |
| 20 | CLA | 1 | 212 | - | 26,32,73 | 2.36 | 8 (30%) | 34,54,113 | 3.02 | 21 (61%) |
| 22 | BCR | A | 844 | - | 41,41,41 | 2.02 | 3 (7%) | 56,56,56 | 5.57 | 21 (37%) |
| 20 | CLA | B | 840 | - | 69,73,73 | 2.15 | 15 (21%) | 83,113,113 | 2.63 | 27 (32%) |
| 20 | CLA | F | 207 | 20 | 57,61,73 | 2.69 | 25 (43%) | 68,98,113 | 3.05 | 30 (44%) |
| 20 | CLA | A | 838 | 5 | 69,73,73 | 2.17 | 16 (23%) | 83,113,113 | 2.67 | 31 (37%) |
| 20 | CLA | A | 823 | - | 62,66,73 | 2.23 | 14 (22%) | 74,104,113 | 2.68 | 25 (33%) |
| 20 | CLA | A | 815 | 5 | 54,58,73 | 2.48 | 13 (24%) | 65,95,113 | 2.91 | 28 (43%) |
| 20 | CLA | L | 207 | 16 | 51,55,73 | 2.50 | 13 (25%) | 61,91,113 | 3.19 | 26 (42%) |
| 21 | LMU | B | 804 | - | 36,36,36 | 0.70 | 0 | 47,47,47 | 1.75 | 12 (25%) |
| 21 | LMU | 2 | 320 | - | 36,36,36 | 0.46 | 0 | 47,47,47 | 1.27 | 3 (6%) |
| 20 | CLA | B | 826 | - | 62,66,73 | 2.29 | 16 (25%) | 74,104,113 | 2.73 | 24 (32%) |
| 20 | CLA | A | 827 | 5 | 59,63,73 | 2.31 | 16 (27%) | 71,101,113 | 2.85 | 27 (38%) |
| 20 | CLA | 3 | 303 | - | 39,44,73 | 2.84 | 11 (28%) | 52,78,113 | 3.20 | 23 (44%) |
| 20 | CLA | 3 | 308 | - | 26,32,73 | 2.33 | 8 (30%) | 34,54,113 | 3.15 | 20 (58%) |
| 21 | LMU | 1 | 217 | - | 36,36,36 | 0.57 | 0 | 47,47,47 | 0.98 | 1 (2%) |
| 20 | CLA | A | 810 | - | 49,53,73 | 2.62 | 14 (28%) | 59,89,113 | 3.21 | 26 (44%) |
| 21 | LMU | 2 | 318 | - | 36,36,36 | 0.56 | 0 | 47,47,47 | 0.68 | 0 |
| 21 | LMU | G | 101 | 19 | 36,36,36 | 1.11 | 4 (11%) | 47,47,47 | 2.03 | 11 (23%) |
| 22 | BCR | A | 843 | - | 41,41,41 | 1.95 | 3 (7%) | 56,56,56 | 5.48 | 21 (37%) |
| 20 | CLA | 2 | 305 | 2 | 54,58,73 | 2.43 | 13 (24%) | 65,95,113 | 2.77 | 25 (38%) |
| 20 | CLA | 1 | 202 | 1 | 45,49,73 | 2.66 | 14 (31%) | 54,84,113 | 3.09 | 21 (38%) |
| 20 | CLA | 3 | 315 | - | 26,32,73 | 2.43 | 10 (38%) | 34,54,113 | 3.20 | 23 (67%) |
| 20 | CLA | 4 | 317 | - | 56,60,73 | 2.44 | 16 (28%) | 67,97,113 | 3.20 | 30 (44%) |
| 20 | CLA | J | 103 | - | 65,69,73 | 2.27 | 20 (30%) | 78,108,113 | 2.62 | 24 (30%) |
| 20 | CLA | 4 | 310 | - | 54,58,73 | 2.50 | 19 (35%) | 65,95,113 | 3.10 | 25 (38%) |
| 21 | LMU | 3 | 319 | - | 36,36,36 | 0.44 | 0 | 47,47,47 | 1.12 | 4 (8%) |
| 22 | BCR | J | 102 | - | 41,41,41 | 1.92 | 3 (7%) | 56,56,56 | 5.54 | 18 (32%) |
| 20 | CLA | 2 | 311 | - | 54,58,73 | 2.46 | 15 (27%) | 65,95,113 | 3.00 | 30 (46%) |
| 20 | CLA | B | 838 | 6 | 69,73,73 | 2.10 | 14 (20%) | 83,113,113 | 2.60 | 26 (31%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 20 | CLA | A | 849 | - | 69,73,73 | 2.11 | 17 (24%) | 83,113,113 | 2.78 | 27 (32%) |
| 20 | CLA | A | 812 | 5 | 58,62,73 | 2.32 | 16 (27%) | 69,99,113 | 2.70 | 21 (30%) |
| 20 | CLA | 2 | 308 | - | 26,32,73 | 2.37 | 12 (46%) | 34,54,113 | 3.24 | 21 (61%) |
| 20 | CLA | A | 832 | 5 | 54,58,73 | 2.44 | 15 (27%) | 65,95,113 | 2.89 | 25 (38%) |
| 20 | CLA | A | 840 | - | 59,63,73 | 2.29 | 14 (23%) | 71,101,113 | 2.93 | 24 (33%) |
| 23 | PQN | B | 843 | - | 34,34,34 | 1.66 | 2 (5%) | 42,45,45 | 1.35 | 6 (14%) |
| 20 | CLA | 4 | 303 | - | 69,73,73 | 2.28 | 22 (31%) | 83,113,113 | 2.99 | 32 (38%) |
| 20 | CLA | 2 | 301 | - | 26,32,73 | 2.33 | 8 (30%) | 34,54,113 | 3.07 | 23 (67%) |
| 22 | BCR | L | 209 | - | 41,41,41 | 2.00 | 4 (9%) | 56,56,56 | 5.64 | 17 (30%) |
| 21 | LMU | 2 | 319 | - | 36,36,36 | 0.82 | 1 (2%) | 47,47,47 | 1.56 | 11 (23%) |
| 21 | LMU | A | 855 | - | 36,36,36 | 0.66 | 1 (2%) | 47,47,47 | 1.38 | 7 (14%) |
| 20 | CLA | 2 | 309 | - | 26,32,73 | 2.34 | 10 (38%) | 34,54,113 | 3.07 | 21 (61%) |
| 20 | CLA | 2 | 315 | - | 26,32,73 | 2.36 | 10 (38%) | 34,54,113 | 3.03 | 19 (55%) |
| 20 | CLA | A | 825 | 5 | 69,73,73 | 2.15 | 16 (23%) | 83,113,113 | 2.45 | 22 (26%) |
| 20 | CLA | 4 | 306 | 4 | 56,60,73 | 2.66 | 21 (37%) | 67,97,113 | 3.25 | 35 (52%) |
| 20 | CLA | B | 813 | 6 | 59,63,73 | 2.28 | 15 (25%) | 71,101,113 | 2.80 | 24 (33%) |
| 20 | CLA | 3 | 302 | 6 | 26,32,73 | 2.37 | 8 (30%) | 34,54,113 | 2.99 | 19 (55%) |
| 20 | CLA | B | 828 | - | 69,73,73 | 2.23 | 15 (21%) | 83,113,113 | 2.74 | 27 (32%) |
| 20 | CLA | 1 | 201 | 1 | 50,54,73 | 2.53 | 19 (38%) | 60,90,113 | 3.54 | 31 (51%) |
| 20 | CLA | 1 | 205 | - | 39,44,73 | 2.89 | 13 (33%) | 52,78,113 | 3.14 | 22 (42%) |
| 20 | CLA | A | 839 | 20 | 63,67,73 | 2.47 | 21 (33%) | 75,105,113 | 3.02 | 31 (41%) |
| 20 | CLA | 4 | 302 | - | 39,44,73 | 2.98 | 16 (41%) | 52,78,113 | 3.37 | 24 (46%) |
| 21 | LMU | K | 107 | - | 36,36,36 | 0.52 | 0 | 47,47,47 | 1.31 | 6 (12%) |
| 21 | LMU | H | 106 | - | 36,36,36 | 0.60 | 1 (2%) | 47,47,47 | 1.58 | 11 (23%) |
| 20 | CLA | A | 829 | 5 | 54,58,73 | 2.46 | 13 (24%) | 65,95,113 | 2.95 | 25 (38%) |
| 20 | CLA | 2 | 302 | - | 55,59,73 | 2.62 | 21 (38%) | 66,96,113 | 3.11 | 26 (39%) |
| 20 | CLA | B | 803 | - | 69,73,73 | 2.18 | 15 (21%) | 83,113,113 | 2.69 | 27 (32%) |
| 20 | CLA | 1 | 203 | - | 51,55,73 | 2.61 | 18 (35%) | 61,91,113 | 3.42 | 30 (49%) |
| 20 | CLA | B | 812 | 6 | 58,62,73 | 2.71 | 24 (41%) | 73,100,113 | 3.20 | 28 (38%) |
| 21 | LMU | L | 205 | - | 36,36,36 | 0.65 | 0 | 47,47,47 | 1.92 | 13 (27%) |
| 20 | CLA | 1 | 210 | 1 | 39,44,73 | 2.78 | 12 (30%) | 52,78,113 | 3.22 | 22 (42%) |
| 20 | CLA | 2 | 307 | - | 69,73,73 | 2.17 | 17 (24%) | 83,113,113 | 2.76 | 30 (36%) |
| 20 | CLA | A | 820 | - | 55,59,73 | 2.44 | 14 (25%) | 66,96,113 | 2.96 | 22 (33%) |
| 20 | CLA | B | 808 | - | 65,69,73 | 2.25 | 20 (30%) | 78,108,113 | 2.75 | 29 (37%) |
| 22 | BCR | B | 846 | - | 41,41,41 | 1.98 | 4 (9%) | 56,56,56 | 5.56 | 21 (37%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 20 | CLA | 4 | 313 | - | 39,44,73 | 2.75 | 14 (35%) | 52,78,113 | 3.41 | 25 (48%) |
| 20 | CLA | A | 813 | 5 | 54,58,73 | 2.39 | 15 (27%) | 65,95,113 | 2.93 | 27 (41%) |
| 21 | LMU | 1 | 218 | - | 36,36,36 | 0.70 | 0 | 47,47,47 | 1.65 | 8 (17%) |
| 22 | BCR | I | 103 | - | 41,41,41 | 2.13 | 5 (12%) | 56,56,56 | 6.16 | 28 (50%) |
| 20 | CLA | 1 | 207 | - | 55,59,73 | 2.48 | 17 (30%) | 66,96,113 | 3.36 | 26 (39%) |
| 20 | CLA | 3 | 306 | - | 26,32,73 | 2.33 | 10 (38%) | 34,54,113 | 3.06 | 20 (58%) |
| 20 | CLA | B | 816 | 6 | 64,68,73 | 2.20 | 12 (18%) | 77,107,113 | 2.61 | 26 (33%) |
| 21 | LMU | A | 854 | - | 36,36,36 | 0.51 | 0 | 47,47,47 | 1.28 | 7 (14%) |
| 20 | CLA | 3 | 309 | - | 26,32,73 | 2.33 | 9 (34%) | 34,54,113 | 3.19 | 21 (61%) |
| 20 | CLA | A | 833 | 20,5 | 49,53,73 | 2.61 | 15 (30%) | 59,89,113 | 3.21 | 27 (45%) |
| 22 | BCR | F | 204 | - | 41,41,41 | 2.16 | 5 (12%) | 56,56,56 | 5.75 | 24 (42%) |
| 20 | CLA | A | 811 | 20,5 | 69,73,73 | 2.16 | 13 (18%) | 83,113,113 | 2.82 | 29 (34%) |
| 20 | CLA | B | 815 | - | 64,68,73 | 2.24 | 13 (20%) | 77,107,113 | 2.66 | 25 (32%) |
| 20 | CLA | A | 831 | 5 | 69,73,73 | 2.33 | 25 (36%) | 83,113,113 | 3.17 | 31 (37%) |
| 20 | CLA | B | 820 | - | 65,69,73 | 2.15 | 15 (23%) | 78,108,113 | 2.77 | 25 (32%) |
| 20 | CLA | B | 839 | - | 51,55,73 | 2.73 | 23 (45%) | 61,91,113 | 3.55 | 27 (44%) |
| 21 | LMU | G | 103 | - | 36,36,36 | 0.50 | 0 | 47,47,47 | 0.93 | 1 (2%) |
| 20 | CLA | B | 837 | 6 | 64,68,73 | 2.20 | 14 (21%) | 77,107,113 | 2.75 | 22 (28%) |
| 20 | CLA | A | 809 | 5 | 56,60,73 | 2.37 | 14 (25%) | 67,97,113 | 2.93 | 32 (47%) |
| 20 | CLA | A | 802 | - | 26,32,73 | 2.41 | 8 (30%) | 34,54,113 | 3.13 | 22 (64%) |
| 20 | CLA | 1 | 208 | - | 26,32,73 | 2.31 | 8 (30%) | 34,54,113 | 2.94 | 21 (61%) |
| 20 | CLA | B | 830 | 6 | 69,73,73 | 2.16 | 16 (23%) | 83,113,113 | 2.77 | 28 (33%) |
| 20 | CLA | H | 108 | - | 62,66,73 | 2.52 | 22 (35%) | 74,104,113 | 3.06 | 31 (41%) |
| 20 | CLA | 4 | 307 | - | 26,32,73 | 2.38 | 9 (34%) | 34,54,113 | 3.03 | 21 (61%) |
| 20 | CLA | A | 803 | - | 50,54,73 | 2.64 | 21 (42%) | 60,90,113 | 3.36 | 24 (40%) |
| 21 | LMU | A | 848 | - | 36,36,36 | 0.49 | 0 | 47,47,47 | 0.86 | 3 (6%) |
| 21 | LMU | A | 853 | - | 36,36,36 | 0.50 | 0 | 47,47,47 | 1.42 | 6 (12%) |
| 20 | CLA | B | 817 | - | 50,54,73 | 2.45 | 13 (26%) | 60,90,113 | 2.97 | 27 (45%) |
| 22 | BCR | 2 | 317 | - | 41,41,41 | 1.96 | 3 (7%) | 56,56,56 | 5.70 | 19 (33%) |
| 20 | CLA | 1 | 213 | - | 55,59,73 | 2.73 | 26 (47%) | 66,96,113 | 3.22 | 29 (43%) |

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 |
|---|---|---|---|---|---|---|---|
| 20 | CLA | A | 822 | 5 | - | 6/21/97/115 | - |
| 20 | CLA | A | 851 | - | 1/1/15/20 | 25/39/115/115 | - |
| 20 | CLA | A | 808 | 5 | 1/1/14/20 | 16/33/109/115 | - |
| 21 | LMU | D | 201 | - | - | 9/21/61/61 | 0/2/2/2 |
| 21 | LMU | 4 | 321 | - | - | 15/21/61/61 | 0/2/2/2 |
| 21 | LMU | L | 210 | - | - | 16/21/61/61 | 0/2/2/2 |
| 21 | LMU | R | 106 | - | - | 12/21/61/61 | 0/2/2/2 |
| 21 | LMU | R | 101 | - | - | 13/21/61/61 | 0/2/2/2 |
| 21 | LMU | B | 849 | - | - | 5/11/51/61 | 0/2/2/2 |
| 20 | CLA | K | 103 | - | - | 12/21/97/115 | - |
| 20 | CLA | A | 821 | 5 | - | 3/12/88/115 | - |
| 20 | CLA | B | 831 | 6 | - | 11/21/97/115 | - |
| 20 | CLA | 1 | 206 | - | 1/1/14/20 | 21/35/111/115 | - |
| 20 | CLA | B | 802 | - | - | 11/26/102/115 | - |
| 20 | CLA | J | 101 | - | - | 10/19/95/115 | - |
| 20 | CLA | B | 818 | - | - | 9/25/101/115 | - |
| 20 | CLA | L | 204 | - | 1/1/13/20 | 8/27/103/115 | - |
| 20 | CLA | 3 | 307 | - | - | 9/12/88/115 | - |
| 20 | CLA | 2 | 314 | - | - | 9/21/97/115 | - |
| 20 | CLA | B | 806 | - | 1/1/15/20 | 21/39/115/115 | - |
| 20 | CLA | A | 817 | - | - | 15/24/100/115 | - |
| 20 | CLA | 4 | 301 | - | 1/1/13/20 | 14/27/103/115 | - |
| 20 | CLA | K | 104 | - | 1/1/13/20 | 11/29/105/115 | - |
| 21 | LMU | 2 | 313 | - | - | 16/21/61/61 | 0/2/2/2 |
| 20 | CLA | B | 810 | - | 1/1/14/20 | 11/33/109/115 | - |
| 21 | LMU | 4 | 319 | - | - | 13/20/60/61 | 0/2/2/2 |
| 20 | CLA | A | 801 | - | 2/2/11/20 | 11/16/92/115 | - |
| 24 | SF4 | C | 103 | 7 | - | - | 0/6/5/5 |
| 21 | LMU | A | 847 | - | - | 13/21/61/61 | 0/2/2/2 |
| 21 | LMU | B | 805 | - | - | 13/21/61/61 | 0/2/2/2 |
| 20 | CLA | L | 202 | - | 1/1/13/20 | 14/27/103/115 | - |
| 20 | CLA | B | 809 | - | 1/1/15/20 | 18/39/115/115 | - |
| 20 | CLA | A | 816 | - | - | 11/26/102/115 | - |
| 21 | LMU | H | 104 | - | - | 12/21/61/61 | 0/2/2/2 |
| 20 | CLA | B | 832 | 6 | 1/1/13/20 | 17/32/108/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | LMU | 4 | 320 | - | - | 16/21/61/61 | 0/2/2/2 |
| 21 | LMU | R | 103 | - | - | 11/21/61/61 | 0/2/2/2 |
| 20 | CLA | B | 836 | - | - | 11/23/99/115 | - |
| 20 | CLA | B | 825 | - | - | 10/26/102/115 | - |
| 22 | BCR | B | 845 | - | - | 9/29/63/63 | 0/2/2/2 |
| 21 | LMU | A | 852 | - | - | 20/21/61/61 | 0/2/2/2 |
| 21 | LMU | K | 105 | - | - | 12/21/61/61 | 0/2/2/2 |
| 21 | LMU | E | 101 | - | - | 14/21/61/61 | 0/2/2/2 |
| 20 | CLA | B | 835 | 20 | - | 8/15/91/115 | - |
| 20 | CLA | H | 109 | - | 1/1/13/20 | 9/27/103/115 | - |
| 20 | CLA | A | 807 | 5 | - | 9/17/93/115 | - |
| 21 | LMU | 2 | 321 | - | - | 8/21/61/61 | 0/2/2/2 |
| 21 | LMU | K | 106 | - | - | 13/21/61/61 | 0/2/2/2 |
| 21 | LMU | R | 104 | - | - | 14/21/61/61 | 0/2/2/2 |
| 20 | CLA | B | 814 | - | 1/1/15/20 | 23/39/115/115 | - |
| 20 | CLA | B | 807 | 6 | - | 6/15/91/115 | - |
| 20 | CLA | A | 805 | 5 | - | 14/26/102/115 | - |
| 20 | CLA | 4 | 304 | - | 1/1/13/20 | 13/27/103/115 | - |
| 21 | LMU | 3 | 318 | - | - | 12/21/61/61 | 0/2/2/2 |
| 20 | CLA | A | 830 | 5 | 1/1/15/20 | 20/39/115/115 | - |
| 21 | LMU | H | 103 | - | - | 14/21/61/61 | 0/2/2/2 |
| 21 | LMU | G | 102 | - | - | 14/21/61/61 | 0/2/2/2 |
| 21 | LMU | R | 109 | - | - | 14/21/61/61 | 0/2/2/2 |
| 20 | CLA | L | 208 | - | 1/1/12/20 | 11/21/97/115 | - |
| 22 | BCR | B | 801 | - | - | 13/29/63/63 | 0/2/2/2 |
| 22 | BCR | B | 847 | - | - | 12/29/63/63 | 0/2/2/2 |
| 21 | LMU | C | 101 | - | - | 14/21/61/61 | 0/2/2/2 |
| 20 | CLA | A | 836 | - | - | 8/18/94/115 | - |
| 21 | LMU | F | 202 | - | - | 13/20/60/61 | 0/2/2/2 |
| 20 | CLA | A | 828 | 5 | 1/1/15/20 | 21/39/115/115 | - |
| 20 | CLA | A | 835 | 5 | 1/1/15/20 | 16/39/115/115 | - |
| 20 | CLA | 1 | 215 | - | 1/1/12/20 | 9/23/99/115 | - |
| 20 | CLA | 2 | 316 | - | 1/1/15/20 | 16/39/115/115 | - |
| 20 | CLA | A | 806 | - | 1/1/13/20 | 7/29/105/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 20 | CLA | K | 101 | - | - | 7/17/93/115 | - |
| 20 | CLA | B | 824 | - | 1/1/15/20 | 21/39/115/115 | - |
| 20 | CLA | H | 102 | - | 1/1/13/20 | 15/27/103/115 | - |
| 20 | CLA | B | 833 | 6 | - | 8/21/97/115 | - |
| 20 | CLA | 1 | 204 | - | - | 11/17/93/115 | - |
| 21 | LMU | A | 846 | - | - | 17/21/61/61 | 0/2/2/2 |
| 22 | BCR | I | 101 | - | - | 10/29/60/63 | 0/2/2/2 |
| 20 | CLA | G | 105 | - | - | 11/23/99/115 | - |
| 21 | LMU | 1 | 216 | - | - | 11/21/61/61 | 0/2/2/2 |
| 20 | CLA | H | 101 | - | 2/2/13/20 | 11/27/103/115 | - |
| 20 | CLA | 4 | 318 | - | - | 13/18/94/115 | - |
| 20 | CLA | B | 829 | - | 1/1/15/20 | 20/39/115/115 | - |
| 20 | CLA | A | 834 | - | - | 9/17/93/115 | - |
| 22 | BCR | B | 844 | - | - | 7/29/63/63 | 0/2/2/2 |
| 20 | CLA | 4 | 305 | - | - | 11/21/97/115 | - |
| 20 | CLA | 3 | 314 | - | 1/1/15/20 | 18/39/115/115 | - |
| 20 | CLA | B | 823 | 6 | 1/1/13/20 | 11/27/103/115 | - |
| 20 | CLA | H | 110 | 16 | - | 9/21/97/115 | - |
| 20 | CLA | A | 824 | - | 1/1/13/20 | 15/32/108/115 | - |
| 20 | CLA | A | 826 | - | 1/1/15/20 | 15/39/115/115 | - |
| 22 | BCR | G | 104 | - | - | 14/29/63/63 | 0/2/2/2 |
| 20 | CLA | 2 | 303 | - | 1/1/13/20 | 16/31/107/115 | - |
| 20 | CLA | 3 | 311 | - | 1/1/15/20 | 22/39/115/115 | - |
| 20 | CLA | K | 102 | - | - | 5/21/97/115 | - |
| 25 | LMG | B | 848 | - | - | 27/44/64/70 | 0/1/1/1 |
| 20 | CLA | I | 102 | - | 1/1/14/20 | 14/33/109/115 | - |
| 20 | CLA | 2 | 312 | - | 1/1/14/20 | 23/35/111/115 | - |
| 20 | CLA | B | 821 | - | - | 7/21/97/115 | - |
| 22 | BCR | F | 203 | - | - | 13/29/63/63 | 0/2/2/2 |
| 20 | CLA | A | 804 | 20 | 1/1/13/20 | 12/27/103/115 | - |
| 20 | CLA | 1 | 211 | - | 1/1/12/20 | 9/23/99/115 | - |
| 20 | CLA | B | 819 | 6 | - | 2/10/86/115 | - |
| 21 | LMU | H | 105 | - | - | 17/21/61/61 | 0/2/2/2 |
| 20 | CLA | B | 834 | 20 | - | 11/15/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 20 | CLA | B | 822 | - | - | 13/17/93/115 | - |
| 24 | SF4 | A | 856 | 6,5 | - | - | 0/6/5/5 |
| 20 | CLA | B | 850 | 6 | 1/1/15/20 | 23/39/115/115 | - |
| 20 | CLA | R | 107 | - | 1/1/13/20 | 15/30/106/115 | - |
| 20 | CLA | R | 108 | - | 1/1/15/20 | 21/39/115/115 | - |
| 21 | LMU | R | 102 | - | - | 11/21/61/61 | 0/2/2/2 |
| 24 | SF4 | C | 102 | 7 | - | - | 0/6/5/5 |
| 20 | CLA | B | 841 | - | 1/1/15/20 | 19/39/115/115 | - |
| 21 | LMU | R | 105 | - | - | 14/21/61/61 | 0/2/2/2 |
| 20 | CLA | F | 201 | 6,10 | - | 11/21/97/115 | - |
| 20 | CLA | 3 | 310 | - | 1/1/15/20 | 18/39/115/115 | - |
| 20 | CLA | L | 201 | 5 | 1/1/14/20 | 14/33/109/115 | - |
| 20 | CLA | 4 | 315 | - | - | 10/17/93/115 | - |
| 23 | PQN | A | 842 | - | 1/1/8/9 | 11/23/43/43 | 0/2/2/2 |
| 20 | CLA | A | 818 | - | 1/1/14/20 | 15/33/109/115 | - |
| 22 | BCR | A | 845 | - | - | 10/29/63/63 | 0/2/2/2 |
| 20 | CLA | F | 206 | 20 | - | 5/10/86/115 | - |
| 20 | CLA | B | 827 | 6 | 1/1/15/20 | 22/39/115/115 | - |
| 20 | CLA | A | 837 | - | - | 15/23/99/115 | - |
| 21 | LMU | L | 206 | - | - | 14/21/61/61 | 0/2/2/2 |
| 20 | CLA | L | 203 | - | 1/1/15/20 | 17/39/115/115 | - |
| 20 | CLA | A | 819 | - | 1/1/13/20 | 11/31/107/115 | - |
| 20 | CLA | 2 | 310 | 2 | - | 6/21/97/115 | - |
| 20 | CLA | A | 850 | - | 1/1/15/20 | 18/39/115/115 | - |
| 20 | CLA | 3 | 313 | - | - | 10/21/97/115 | - |
| 21 | LMU | 4 | 316 | - | - | 13/21/61/61 | 0/2/2/2 |
| 22 | BCR | A | 844 | - | - | 14/29/63/63 | 0/2/2/2 |
| 20 | CLA | B | 840 | - | 1/1/15/20 | 18/39/115/115 | - |
| 20 | CLA | F | 207 | 20 | 3/3/12/20 | 12/25/101/115 | - |
| 20 | CLA | A | 838 | 5 | 1/1/15/20 | 19/39/115/115 | - |
| 20 | CLA | A | 823 | - | 1/1/13/20 | 13/31/107/115 | - |
| 20 | CLA | A | 815 | 5 | - | 11/21/97/115 | - |
| 20 | CLA | L | 207 | 16 | - | 11/18/94/115 | - |
| 21 | LMU | B | 804 | - | - | 16/21/61/61 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | LMU | 2 | 320 | - | - | 18/21/61/61 | 0/2/2/2 |
| 20 | CLA | B | 826 | - | 1/1/13/20 | 19/31/107/115 | - |
| 20 | CLA | A | 827 | 5 | 1/1/13/20 | 10/27/103/115 | - |
| 21 | LMU | 1 | 217 | - | - | 9/21/61/61 | 0/2/2/2 |
| 21 | LMU | 2 | 318 | - | - | 13/21/61/61 | 0/2/2/2 |
| 20 | CLA | A | 810 | - | - | 5/15/91/115 | - |
| 21 | LMU | G | 101 | 19 | - | 13/21/61/61 | 0/2/2/2 |
| 22 | BCR | A | 843 | - | - | 14/29/63/63 | 0/2/2/2 |
| 22 | BCR | J | 102 | - | - | 11/29/63/63 | 0/2/2/2 |
| 20 | CLA | 2 | 305 | 2 | - | 7/21/97/115 | - |
| 20 | CLA | 1 | 202 | 1 | - | 5/10/86/115 | - |
| 20 | CLA | J | 103 | - | 1/1/14/20 | 21/35/111/115 | - |
| 20 | CLA | 4 | 317 | - | - | 12/24/100/115 | - |
| 21 | LMU | 3 | 319 | - | - | 11/21/61/61 | 0/2/2/2 |
| 20 | CLA | 4 | 310 | - | - | 11/21/97/115 | - |
| 20 | CLA | B | 838 | 6 | 1/1/15/20 | 13/39/115/115 | - |
| 20 | CLA | 2 | 311 | - | - | 12/21/97/115 | - |
| 20 | CLA | A | 849 | - | 1/1/15/20 | 26/39/115/115 | - |
| 20 | CLA | A | 840 | - | 1/1/13/20 | 8/27/103/115 | - |
| 20 | CLA | A | 812 | 5 | - | 14/26/102/115 | - |
| 20 | CLA | A | 832 | 5 | - | 12/21/97/115 | - |
| 23 | PQN | B | 843 | - | 1/1/8/9 | 10/23/43/43 | 0/2/2/2 |
| 20 | CLA | 4 | 303 | - | 2/2/15/20 | 23/39/115/115 | - |
| 22 | BCR | L | 209 | - | - | 10/29/63/63 | 0/2/2/2 |
| 21 | LMU | 2 | 319 | - | - | 11/21/61/61 | 0/2/2/2 |
| 21 | LMU | A | 855 | - | - | 13/21/61/61 | 0/2/2/2 |
| 20 | CLA | A | 825 | 5 | 1/1/15/20 | 25/39/115/115 | - |
| 20 | CLA | 4 | 306 | 4 | 1/1/12/20 | 8/24/100/115 | - |
| 20 | CLA | B | 813 | 6 | 1/1/13/20 | 13/27/103/115 | - |
| 20 | CLA | B | 828 | - | 1/1/15/20 | 17/39/115/115 | - |
| 20 | CLA | 1 | 201 | 1 | - | 12/17/93/115 | - |
| 20 | CLA | A | 839 | 20 | 1/1/13/20 | 15/31/107/115 | - |
| 21 | LMU | K | 107 | - | - | 17/21/61/61 | 0/2/2/2 |
| 21 | LMU | H | 106 | - | - | 9/21/61/61 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 20 | CLA | A | 829 | 5 | - | 6/21/97/115 | - |
| 20 | CLA | 2 | 302 | - | - | 13/23/99/115 | - |
| 20 | CLA | B | 803 | - | 1/1/15/20 | 20/39/115/115 | - |
| 20 | CLA | 1 | 203 | - | - | 10/18/94/115 | - |
| 20 | CLA | B | 812 | 6 | 1/1/13/20 | 8/25/101/115 | - |
| 21 | LMU | L | 205 | - | - | 13/21/61/61 | 0/2/2/2 |
| 20 | CLA | 2 | 307 | - | 1/1/15/20 | 22/39/115/115 | - |
| 20 | CLA | B | 808 | - | 1/1/14/20 | 20/35/111/115 | - |
| 20 | CLA | A | 820 | - | - | 9/23/99/115 | - |
| 22 | BCR | B | 846 | - | - | 14/29/63/63 | 0/2/2/2 |
| 20 | CLA | A | 813 | 5 | - | 10/21/97/115 | - |
| 21 | LMU | 1 | 218 | - | - | 13/21/61/61 | 0/2/2/2 |
| 22 | BCR | I | 103 | - | - | 15/29/63/63 | 0/2/2/2 |
| 20 | CLA | 1 | 207 | - | 1/1/12/20 | 10/23/99/115 | - |
| 20 | CLA | B | 816 | 6 | 1/1/14/20 | 16/33/109/115 | - |
| 21 | LMU | A | 854 | - | - | 16/21/61/61 | 0/2/2/2 |
| 20 | CLA | A | 833 | 20,5 | - | 7/15/91/115 | - |
| 22 | BCR | F | 204 | - | - | 9/29/63/63 | 0/2/2/2 |
| 20 | CLA | A | 811 | 20,5 | 1/1/15/20 | 25/39/115/115 | - |
| 20 | CLA | B | 815 | - | 1/1/14/20 | 19/33/109/115 | - |
| 20 | CLA | A | 831 | 5 | 1/1/15/20 | 20/39/115/115 | - |
| 20 | CLA | B | 820 | - | 1/1/14/20 | 15/35/111/115 | - |
| 20 | CLA | B | 839 | - | - | 11/18/94/115 | - |
| 21 | LMU | G | 103 | - | - | 14/21/61/61 | 0/2/2/2 |
| 20 | CLA | B | 837 | 6 | 1/1/14/20 | 15/33/109/115 | - |
| 20 | CLA | A | 809 | 5 | - | 11/24/100/115 | - |
| 20 | CLA | H | 108 | - | 1/1/13/20 | 20/31/107/115 | - |
| 20 | CLA | B | 830 | 6 | 1/1/15/20 | 27/39/115/115 | - |
| 21 | LMU | A | 848 | - | - | 12/21/61/61 | 0/2/2/2 |
| 20 | CLA | A | 803 | - | - | 5/17/93/115 | - |
| 21 | LMU | A | 853 | - | - | 11/21/61/61 | 0/2/2/2 |
| 20 | CLA | B | 817 | - | - | 13/17/93/115 | - |
| 22 | BCR | 2 | 317 | - | - | 15/29/63/63 | 0/2/2/2 |
| 20 | CLA | 1 | 213 | - | 2/2/12/20 | 11/23/99/115 | - |

All (2740) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | B | 801 | BCR | C21-C22 | -9.91 | 1.22 | 1.35 |
| 22 | B | 801 | BCR | C20-C21 | -9.21 | 1.14 | 1.43 |
| 22 | F | 204 | BCR | C21-C22 | -8.47 | 1.24 | 1.35 |
| 22 | A | 843 | BCR | C20-C21 | -8.38 | 1.17 | 1.43 |
| 22 | A | 844 | BCR | C20-C21 | -8.34 | 1.17 | 1.43 |
| 22 | F | 203 | BCR | C20-C21 | -8.31 | 1.17 | 1.43 |
| 22 | L | 209 | BCR | C20-C21 | -8.31 | 1.17 | 1.43 |
| 22 | F | 204 | BCR | C20-C21 | -8.29 | 1.17 | 1.43 |
| 22 | A | 845 | BCR | C20-C21 | -8.27 | 1.17 | 1.43 |
| 20 | 1 | 205 | CLA | CAB-C3B | -8.26 | 1.33 | 1.50 |
| 22 | 2 | 317 | BCR | C20-C21 | -8.25 | 1.17 | 1.43 |
| 22 | A | 844 | BCR | C21-C22 | -8.19 | 1.24 | 1.35 |
| 22 | B | 847 | BCR | C20-C21 | -8.19 | 1.18 | 1.43 |
| 20 | B | 812 | CLA | CAB-C3B | -8.17 | 1.33 | 1.50 |
| 22 | B | 846 | BCR | C20-C21 | -8.15 | 1.18 | 1.43 |
| 22 | J | 102 | BCR | C20-C21 | -8.14 | 1.18 | 1.43 |
| 22 | I | 103 | BCR | C21-C22 | -8.02 | 1.25 | 1.35 |
| 22 | I | 103 | BCR | C20-C21 | -8.02 | 1.18 | 1.43 |
| 22 | G | 104 | BCR | C20-C21 | -8.01 | 1.18 | 1.43 |
| 22 | F | 203 | BCR | C21-C22 | -8.01 | 1.25 | 1.35 |
| 23 | B | 843 | PQN | C3-C2 | 7.95 | 1.49 | 1.35 |
| 20 | 4 | 302 | CLA | CAB-C3B | -7.94 | 1.34 | 1.50 |
| 22 | B | 846 | BCR | C21-C22 | -7.91 | 1.25 | 1.35 |
| 22 | A | 845 | BCR | C21-C22 | -7.91 | 1.25 | 1.35 |
| 23 | A | 842 | PQN | C3-C2 | 7.89 | 1.49 | 1.35 |
| 22 | A | 843 | BCR | C21-C22 | -7.81 | 1.25 | 1.35 |
| 22 | 2 | 317 | BCR | C21-C22 | -7.78 | 1.25 | 1.35 |
| 22 | L | 209 | BCR | C21-C22 | -7.70 | 1.25 | 1.35 |
| 20 | B | 842 | CLA | CAB-C3B | -7.70 | 1.34 | 1.50 |
| 22 | J | 102 | BCR | C21-C22 | -7.68 | 1.25 | 1.35 |
| 22 | B | 847 | BCR | C21-C22 | -7.63 | 1.25 | 1.35 |
| 20 | 1 | 210 | CLA | CAB-C3B | -7.62 | 1.34 | 1.50 |
| 22 | B | 844 | BCR | C20-C21 | -7.62 | 1.19 | 1.43 |
| 20 | 3 | 303 | CLA | CHC-C1C | 7.60 | 1.53 | 1.38 |
| 20 | 3 | 317 | CLA | CAB-C3B | -7.57 | 1.34 | 1.50 |
| 20 | 3 | 301 | CLA | CAB-C3B | -7.55 | 1.34 | 1.50 |
| 20 | A | 801 | CLA | CAB-C3B | -7.48 | 1.35 | 1.50 |
| 20 | 4 | 313 | CLA | CAB-C3B | -7.44 | 1.35 | 1.50 |
| 20 | 3 | 303 | CLA | CAB-C3B | -7.42 | 1.35 | 1.50 |
| 22 | B | 845 | BCR | C20-C21 | -7.34 | 1.20 | 1.43 |
| 22 | G | 104 | BCR | C21-C22 | -7.17 | 1.26 | 1.35 |
| 22 | I | 101 | BCR | C21-C22 | -7.16 | 1.26 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 809 | CLA | CHD-C1D | 6.81 | 1.51 | 1.38 |
| 20 | A | 815 | CLA | CHD-C1D | 6.72 | 1.51 | 1.38 |
| 20 | B | 819 | CLA | C3A-C2A | -6.72 | 1.48 | 1.54 |
| 20 | 3 | 313 | CLA | CHC-C1C | 6.70 | 1.52 | 1.38 |
| 20 | 2 | 305 | CLA | CHC-C1C | 6.68 | 1.52 | 1.38 |
| 20 | A | 810 | CLA | CHC-C1C | 6.62 | 1.52 | 1.38 |
| 20 | B | 807 | CLA | CHC-C1C | 6.62 | 1.52 | 1.38 |
| 20 | B | 831 | CLA | CHD-C1D | 6.60 | 1.51 | 1.38 |
| 20 | B | 814 | CLA | CHC-C1C | 6.58 | 1.51 | 1.38 |
| 20 | A | 811 | CLA | CHD-C1D | 6.57 | 1.51 | 1.38 |
| 22 | B | 844 | BCR | C21-C22 | -6.55 | 1.27 | 1.35 |
| 20 | 4 | 304 | CLA | CHD-C1D | 6.55 | 1.51 | 1.38 |
| 20 | H | 110 | CLA | CHC-C1C | 6.52 | 1.51 | 1.38 |
| 20 | A | 851 | CLA | CHD-C1D | 6.52 | 1.51 | 1.38 |
| 20 | 3 | 313 | CLA | CHD-C1D | 6.51 | 1.51 | 1.38 |
| 20 | H | 101 | CLA | CHD-C1D | 6.50 | 1.51 | 1.38 |
| 20 | A | 819 | CLA | CHC-C1C | 6.50 | 1.51 | 1.38 |
| 20 | A | 801 | CLA | CHD-C1D | 6.49 | 1.51 | 1.38 |
| 20 | A | 820 | CLA | CHC-C1C | 6.47 | 1.51 | 1.38 |
| 20 | B | 816 | CLA | CHC-C1C | 6.44 | 1.51 | 1.38 |
| 20 | A | 830 | CLA | CHD-C1D | 6.43 | 1.50 | 1.38 |
| 20 | B | 806 | CLA | CHC-C1C | 6.42 | 1.51 | 1.38 |
| 20 | B | 832 | CLA | CHC-C1C | 6.41 | 1.51 | 1.38 |
| 20 | 1 | 203 | CLA | CHC-C1C | 6.41 | 1.51 | 1.38 |
| 20 | A | 804 | CLA | CHC-C1C | 6.41 | 1.51 | 1.38 |
| 20 | B | 828 | CLA | CHC-C1C | 6.40 | 1.51 | 1.38 |
| 20 | A | 810 | CLA | CHD-C1D | 6.40 | 1.50 | 1.38 |
| 20 | 1 | 210 | CLA | CHC-C1C | 6.39 | 1.51 | 1.38 |
| 20 | 4 | 312 | CLA | CHC-C1C | 6.39 | 1.51 | 1.38 |
| 20 | 1 | 207 | CLA | CHC-C1C | 6.39 | 1.51 | 1.38 |
| 20 | I | 102 | CLA | CHC-C1C | 6.39 | 1.51 | 1.38 |
| 20 | H | 109 | CLA | CHD-C1D | 6.38 | 1.50 | 1.38 |
| 20 | A | 808 | CLA | CHC-C1C | 6.38 | 1.51 | 1.38 |
| 20 | 2 | 305 | CLA | CHD-C1D | 6.37 | 1.50 | 1.38 |
| 22 | B | 845 | BCR | C21-C22 | -6.37 | 1.27 | 1.35 |
| 20 | 3 | 312 | CLA | CHC-C1C | 6.37 | 1.51 | 1.38 |
| 20 | A | 829 | CLA | CHD-C1D | 6.36 | 1.50 | 1.38 |
| 20 | G | 105 | CLA | CHC-C1C | 6.36 | 1.51 | 1.38 |
| 20 | 4 | 318 | CLA | CHD-C1D | 6.35 | 1.50 | 1.38 |
| 20 | B | 831 | CLA | CHC-C1C | 6.35 | 1.51 | 1.38 |
| 20 | B | 807 | CLA | CHD-C1D | 6.33 | 1.50 | 1.38 |
| 20 | A | 821 | CLA | CHD-C1D | 6.32 | 1.50 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 810 | CLA | CHD-C1D | 6.32 | 1.50 | 1.38 |
| 20 | A | 838 | CLA | CHC-C1C | 6.32 | 1.51 | 1.38 |
| 20 | A | 822 | CLA | CHD-C1D | 6.31 | 1.50 | 1.38 |
| 20 | 1 | 205 | CLA | CHD-C1D | 6.31 | 1.50 | 1.38 |
| 20 | B | 840 | CLA | CHC-C1C | 6.30 | 1.51 | 1.38 |
| 20 | A | 819 | CLA | CHD-C1D | 6.30 | 1.50 | 1.38 |
| 20 | B | 823 | CLA | CHD-C1D | 6.30 | 1.50 | 1.38 |
| 20 | L | 204 | CLA | CHC-C1C | 6.29 | 1.51 | 1.38 |
| 20 | H | 109 | CLA | CHC-C1C | 6.29 | 1.51 | 1.38 |
| 20 | 4 | 314 | CLA | CHC-C1C | 6.28 | 1.51 | 1.38 |
| 20 | B | 803 | CLA | CHD-C1D | 6.28 | 1.50 | 1.38 |
| 20 | A | 835 | CLA | CHC-C1C | 6.27 | 1.51 | 1.38 |
| 20 | B | 818 | CLA | CHC-C1C | 6.26 | 1.51 | 1.38 |
| 20 | 4 | 302 | CLA | CHC-C1C | 6.26 | 1.51 | 1.38 |
| 20 | A | 813 | CLA | CHC-C1C | 6.26 | 1.51 | 1.38 |
| 20 | 3 | 302 | CLA | CHC-C1C | 6.26 | 1.51 | 1.38 |
| 20 | 3 | 307 | CLA | CHD-C1D | 6.25 | 1.50 | 1.38 |
| 20 | B | 819 | CLA | C3D-C4D | -6.25 | 1.30 | 1.44 |
| 20 | B | 821 | CLA | CHC-C1C | 6.25 | 1.51 | 1.38 |
| 20 | 1 | 215 | CLA | CHC-C1C | 6.24 | 1.51 | 1.38 |
| 20 | L | 201 | CLA | CHC-C1C | 6.24 | 1.51 | 1.38 |
| 20 | A | 840 | CLA | CHC-C1C | 6.23 | 1.51 | 1.38 |
| 20 | A | 836 | CLA | CHC-C1C | 6.22 | 1.51 | 1.38 |
| 20 | 3 | 316 | CLA | CHC-C1C | 6.22 | 1.50 | 1.38 |
| 20 | A | 815 | CLA | CHC-C1C | 6.22 | 1.51 | 1.38 |
| 20 | F | 205 | CLA | CHC-C1C | 6.22 | 1.51 | 1.38 |
| 20 | A | 832 | CLA | CHD-C1D | 6.21 | 1.50 | 1.38 |
| 20 | A | 820 | CLA | CHD-C1D | 6.21 | 1.50 | 1.38 |
| 20 | B | 835 | CLA | CHC-C1C | 6.21 | 1.51 | 1.38 |
| 20 | A | 807 | CLA | CHD-C1D | 6.21 | 1.50 | 1.38 |
| 20 | 1 | 202 | CLA | CHD-C1D | 6.20 | 1.50 | 1.38 |
| 20 | B | 828 | CLA | CHD-C1D | 6.20 | 1.50 | 1.38 |
| 20 | A | 824 | CLA | CHC-C1C | 6.20 | 1.51 | 1.38 |
| 20 | 1 | 210 | CLA | CHD-C1D | 6.19 | 1.50 | 1.38 |
| 20 | K | 101 | CLA | CHC-C1C | 6.19 | 1.51 | 1.38 |
| 20 | H | 102 | CLA | CHD-C1D | 6.19 | 1.50 | 1.38 |
| 20 | A | 823 | CLA | CHC-C1C | 6.19 | 1.51 | 1.38 |
| 20 | 1 | 202 | CLA | O2D-CGD | 6.18 | 1.48 | 1.33 |
| 20 | B | 803 | CLA | CHC-C1C | 6.17 | 1.51 | 1.38 |
| 20 | 4 | 301 | CLA | CHC-C1C | 6.17 | 1.51 | 1.38 |
| 20 | B | 815 | CLA | CHC-C1C | 6.16 | 1.51 | 1.38 |
| 20 | L | 202 | CLA | CHC-C1C | 6.16 | 1.51 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | R | 108 | CLA | CHC-C1C | 6.16 | 1.51 | 1.38 |
| 20 | A | 829 | CLA | CHC-C1C | 6.16 | 1.51 | 1.38 |
| 20 | B | 839 | CLA | C3D-C4D | -6.16 | 1.30 | 1.44 |
| 20 | L | 207 | CLA | CHD-C1D | 6.16 | 1.50 | 1.38 |
| 20 | 2 | 310 | CLA | CHD-C1D | 6.16 | 1.50 | 1.38 |
| 20 | A | 827 | CLA | CHC-C1C | 6.16 | 1.51 | 1.38 |
| 20 | B | 809 | CLA | CHD-C1D | 6.15 | 1.50 | 1.38 |
| 20 | 4 | 317 | CLA | CHD-C1D | 6.15 | 1.50 | 1.38 |
| 20 | L | 208 | CLA | CHC-C1C | 6.15 | 1.51 | 1.38 |
| 20 | L | 201 | CLA | CHD-C1D | 6.15 | 1.50 | 1.38 |
| 20 | B | 812 | CLA | C3D-C4D | -6.15 | 1.30 | 1.44 |
| 20 | A | 815 | CLA | CHD-C4C | 6.14 | 1.53 | 1.39 |
| 20 | B | 802 | CLA | CHC-C1C | 6.14 | 1.51 | 1.38 |
| 20 | A | 817 | CLA | CHD-C1D | 6.13 | 1.50 | 1.38 |
| 20 | B | 839 | CLA | CHC-C1C | 6.13 | 1.51 | 1.38 |
| 20 | H | 102 | CLA | CHC-C1C | 6.13 | 1.51 | 1.38 |
| 20 | H | 101 | CLA | CHC-C1C | 6.13 | 1.51 | 1.38 |
| 20 | A | 811 | CLA | CHD-C4C | 6.13 | 1.53 | 1.39 |
| 20 | B | 836 | CLA | CHC-C1C | 6.12 | 1.51 | 1.38 |
| 20 | B | 817 | CLA | CHC-C1C | 6.12 | 1.50 | 1.38 |
| 20 | B | 815 | CLA | CHD-C1D | 6.12 | 1.50 | 1.38 |
| 20 | B | 822 | CLA | CHC-C1C | 6.11 | 1.50 | 1.38 |
| 20 | A | 851 | CLA | CHD-C4C | 6.11 | 1.53 | 1.39 |
| 20 | 3 | 317 | CLA | CHC-C1C | 6.11 | 1.50 | 1.38 |
| 20 | 3 | 301 | CLA | CHC-C1C | 6.11 | 1.50 | 1.38 |
| 20 | A | 831 | CLA | C3D-C4D | -6.11 | 1.30 | 1.44 |
| 20 | 2 | 315 | CLA | CHC-C1C | 6.11 | 1.50 | 1.38 |
| 20 | 3 | 301 | CLA | CHD-C1D | 6.11 | 1.50 | 1.38 |
| 20 | R | 108 | CLA | CHD-C1D | 6.11 | 1.50 | 1.38 |
| 20 | 3 | 317 | CLA | CHD-C1D | 6.10 | 1.50 | 1.38 |
| 20 | 1 | 208 | CLA | CHC-C1C | 6.10 | 1.50 | 1.38 |
| 20 | B | 834 | CLA | CHC-C1C | 6.10 | 1.50 | 1.38 |
| 20 | A | 810 | CLA | CHD-C4C | 6.10 | 1.53 | 1.39 |
| 20 | 2 | 302 | CLA | CHC-C1C | 6.10 | 1.50 | 1.38 |
| 20 | L | 207 | CLA | CHC-C1C | 6.10 | 1.50 | 1.38 |
| 20 | A | 832 | CLA | CHC-C1C | 6.09 | 1.50 | 1.38 |
| 20 | K | 103 | CLA | CHD-C1D | 6.09 | 1.50 | 1.38 |
| 20 | A | 826 | CLA | CHD-C1D | 6.08 | 1.50 | 1.38 |
| 20 | 1 | 212 | CLA | CHC-C1C | 6.08 | 1.50 | 1.38 |
| 20 | 1 | 206 | CLA | CHC-C1C | 6.08 | 1.50 | 1.38 |
| 20 | A | 828 | CLA | CHC-C1C | 6.08 | 1.50 | 1.38 |
| 20 | A | 835 | CLA | CHD-C1D | 6.07 | 1.50 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | R | 107 | CLA | CHC-C1C | 6.07 | 1.50 | 1.38 |
| 20 | B | 840 | CLA | CHD-C1D | 6.07 | 1.50 | 1.38 |
| 20 | 3 | 311 | CLA | CHC-C1C | 6.07 | 1.50 | 1.38 |
| 20 | 2 | 312 | CLA | CHC-C1C | 6.06 | 1.50 | 1.38 |
| 20 | A | 840 | CLA | CHD-C1D | 6.06 | 1.50 | 1.38 |
| 20 | B | 818 | CLA | CHD-C1D | 6.06 | 1.50 | 1.38 |
| 20 | 1 | 214 | CLA | CHC-C1C | 6.06 | 1.50 | 1.38 |
| 20 | H | 109 | CLA | CHD-C4C | 6.06 | 1.53 | 1.39 |
| 20 | A | 836 | CLA | CHD-C1D | 6.06 | 1.50 | 1.38 |
| 20 | B | 838 | CLA | CHD-C1D | 6.05 | 1.50 | 1.38 |
| 20 | H | 108 | CLA | C3D-C4D | -6.05 | 1.30 | 1.44 |
| 20 | A | 817 | CLA | CHC-C1C | 6.05 | 1.50 | 1.38 |
| 20 | B | 827 | CLA | CHC-C1C | 6.05 | 1.50 | 1.38 |
| 20 | B | 842 | CLA | CHC-C1C | 6.05 | 1.50 | 1.38 |
| 20 | A | 834 | CLA | CHC-C1C | 6.04 | 1.50 | 1.38 |
| 20 | 2 | 316 | CLA | C3D-C4D | -6.04 | 1.30 | 1.44 |
| 20 | K | 104 | CLA | CHD-C1D | 6.04 | 1.50 | 1.38 |
| 20 | K | 102 | CLA | CHD-C1D | 6.04 | 1.50 | 1.38 |
| 20 | A | 823 | CLA | CHD-C1D | 6.03 | 1.50 | 1.38 |
| 20 | 4 | 315 | CLA | CHC-C1C | 6.03 | 1.50 | 1.38 |
| 20 | A | 827 | CLA | CHD-C1D | 6.03 | 1.50 | 1.38 |
| 20 | B | 850 | CLA | CHC-C1C | 6.03 | 1.50 | 1.38 |
| 20 | F | 205 | CLA | CAB-C3B | -6.03 | 1.38 | 1.50 |
| 20 | B | 832 | CLA | CHD-C1D | 6.02 | 1.50 | 1.38 |
| 20 | 3 | 308 | CLA | CHC-C1C | 6.02 | 1.50 | 1.38 |
| 20 | A | 825 | CLA | CHC-C1C | 6.02 | 1.50 | 1.38 |
| 20 | 2 | 311 | CLA | CHC-C1C | 6.02 | 1.50 | 1.38 |
| 20 | 1 | 209 | CLA | CHC-C1C | 6.02 | 1.50 | 1.38 |
| 20 | F | 205 | CLA | CHD-C1D | 6.02 | 1.50 | 1.38 |
| 20 | A | 806 | CLA | CHD-C1D | 6.01 | 1.50 | 1.38 |
| 20 | 3 | 311 | CLA | CHD-C1D | 6.01 | 1.50 | 1.38 |
| 20 | 4 | 309 | CLA | CHC-C1C | 6.01 | 1.50 | 1.38 |
| 20 | 1 | 207 | CLA | CHD-C1D | 6.00 | 1.50 | 1.38 |
| 20 | A | 806 | CLA | CHC-C1C | 6.00 | 1.50 | 1.38 |
| 20 | 1 | 205 | CLA | CHC-C1C | 6.00 | 1.50 | 1.38 |
| 20 | A | 821 | CLA | CHD-C4C | 5.99 | 1.52 | 1.39 |
| 20 | B | 834 | CLA | CHD-C1D | 5.99 | 1.50 | 1.38 |
| 20 | A | 812 | CLA | CHC-C1C | 5.99 | 1.50 | 1.38 |
| 20 | 3 | 306 | CLA | CHC-C1C | 5.99 | 1.50 | 1.38 |
| 20 | B | 824 | CLA | C3D-C4D | -5.99 | 1.30 | 1.44 |
| 20 | A | 816 | CLA | CHC-C1C | 5.98 | 1.50 | 1.38 |
| 20 | 2 | 304 | CLA | CHC-C1C | 5.98 | 1.50 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | H | 101 | CLA | O2D-CGD | 5.98 | 1.47 | 1.33 |
| 20 | 4 | 313 | CLA | CHC-C1C | 5.98 | 1.50 | 1.38 |
| 20 | 4 | 306 | CLA | CHC-C1C | 5.98 | 1.50 | 1.38 |
| 20 | A | 849 | CLA | CHC-C1C | 5.98 | 1.50 | 1.38 |
| 20 | L | 203 | CLA | CHC-C1C | 5.98 | 1.50 | 1.38 |
| 20 | L | 201 | CLA | CHD-C4C | 5.97 | 1.52 | 1.39 |
| 20 | A | 801 | CLA | CHC-C1C | 5.97 | 1.50 | 1.38 |
| 20 | B | 837 | CLA | CHD-C1D | 5.97 | 1.50 | 1.38 |
| 20 | 3 | 307 | CLA | CHD-C4C | 5.96 | 1.52 | 1.39 |
| 20 | B | 831 | CLA | CHD-C4C | 5.96 | 1.52 | 1.39 |
| 20 | B | 828 | CLA | CHD-C4C | 5.96 | 1.52 | 1.39 |
| 20 | A | 830 | CLA | CHC-C1C | 5.96 | 1.50 | 1.38 |
| 20 | A | 850 | CLA | CHC-C1C | 5.96 | 1.50 | 1.38 |
| 20 | B | 826 | CLA | CHC-C1C | 5.96 | 1.50 | 1.38 |
| 20 | B | 802 | CLA | CHD-C1D | 5.96 | 1.50 | 1.38 |
| 20 | 3 | 303 | CLA | CHD-C1D | 5.96 | 1.50 | 1.38 |
| 20 | A | 826 | CLA | CHC-C1C | 5.95 | 1.50 | 1.38 |
| 20 | A | 833 | CLA | CHD-C1D | 5.94 | 1.49 | 1.38 |
| 20 | B | 812 | CLA | CHC-C1C | 5.94 | 1.50 | 1.38 |
| 20 | A | 807 | CLA | CHC-C1C | 5.94 | 1.50 | 1.38 |
| 20 | A | 808 | CLA | CHD-C1D | 5.94 | 1.49 | 1.38 |
| 20 | 3 | 313 | CLA | CHD-C4C | 5.93 | 1.52 | 1.39 |
| 20 | B | 810 | CLA | CHC-C1C | 5.93 | 1.50 | 1.38 |
| 20 | A | 805 | CLA | CHD-C1D | 5.93 | 1.49 | 1.38 |
| 20 | F | 205 | CLA | CHD-C4C | 5.93 | 1.52 | 1.39 |
| 20 | A | 812 | CLA | CHD-C1D | 5.93 | 1.49 | 1.38 |
| 20 | J | 101 | CLA | CHC-C1C | 5.92 | 1.50 | 1.38 |
| 20 | A | 829 | CLA | CHD-C4C | 5.92 | 1.52 | 1.39 |
| 20 | J | 101 | CLA | CHD-C1D | 5.92 | 1.49 | 1.38 |
| 20 | B | 823 | CLA | CHC-C1C | 5.92 | 1.50 | 1.38 |
| 20 | I | 102 | CLA | CHD-C1D | 5.92 | 1.49 | 1.38 |
| 20 | 4 | 305 | CLA | CHC-C1C | 5.92 | 1.50 | 1.38 |
| 20 | A | 802 | CLA | CHD-C1D | 5.91 | 1.51 | 1.38 |
| 20 | A | 832 | CLA | CHD-C4C | 5.91 | 1.52 | 1.39 |
| 20 | B | 842 | CLA | CHD-C1D | 5.90 | 1.49 | 1.38 |
| 20 | B | 841 | CLA | CHD-C1D | 5.90 | 1.49 | 1.38 |
| 20 | A | 826 | CLA | CHD-C4C | 5.90 | 1.52 | 1.39 |
| 20 | B | 837 | CLA | CHC-C1C | 5.90 | 1.50 | 1.38 |
| 20 | 3 | 313 | CLA | O2D-CGD | 5.90 | 1.47 | 1.33 |
| 20 | A | 833 | CLA | CHC-C1C | 5.89 | 1.50 | 1.38 |
| 20 | A | 811 | CLA | CHC-C1C | 5.89 | 1.50 | 1.38 |
| 20 | A | 801 | CLA | CHD-C4C | 5.89 | 1.52 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 831 | CLA | O2D-CGD | 5.89 | 1.47 | 1.33 |
| 20 | A | 822 | CLA | CHC-C1C | 5.89 | 1.50 | 1.38 |
| 20 | B | 806 | CLA | CHD-C4C | 5.89 | 1.52 | 1.39 |
| 20 | A | 841 | CLA | CHD-C1D | 5.89 | 1.51 | 1.38 |
| 20 | B | 850 | CLA | CHD-C1D | 5.88 | 1.49 | 1.38 |
| 20 | A | 818 | CLA | CAB-C3B | -5.88 | 1.31 | 1.47 |
| 20 | B | 820 | CLA | CHC-C1C | 5.88 | 1.50 | 1.38 |
| 20 | 2 | 311 | CLA | CHD-C1D | 5.87 | 1.49 | 1.38 |
| 20 | A | 813 | CLA | CHD-C1D | 5.87 | 1.49 | 1.38 |
| 20 | R | 107 | CLA | CHD-C1D | 5.87 | 1.49 | 1.38 |
| 20 | A | 802 | CLA | CHC-C1C | 5.86 | 1.50 | 1.38 |
| 20 | K | 101 | CLA | CHD-C1D | 5.86 | 1.49 | 1.38 |
| 20 | B | 816 | CLA | CHD-C1D | 5.86 | 1.49 | 1.38 |
| 20 | B | 818 | CLA | CHD-C4C | 5.86 | 1.52 | 1.39 |
| 20 | 1 | 202 | CLA | CHC-C1C | 5.86 | 1.50 | 1.38 |
| 20 | A | 822 | CLA | CHD-C4C | 5.86 | 1.52 | 1.39 |
| 20 | A | 837 | CLA | CHC-C1C | 5.86 | 1.50 | 1.38 |
| 20 | K | 104 | CLA | CHC-C1C | 5.86 | 1.50 | 1.38 |
| 20 | A | 825 | CLA | CHD-C1D | 5.86 | 1.49 | 1.38 |
| 20 | H | 101 | CLA | CHD-C4C | 5.85 | 1.52 | 1.39 |
| 20 | L | 207 | CLA | CHD-C4C | 5.85 | 1.52 | 1.39 |
| 20 | B | 810 | CLA | CHD-C4C | 5.85 | 1.52 | 1.39 |
| 20 | A | 834 | CLA | CHD-C1D | 5.85 | 1.49 | 1.38 |
| 20 | 3 | 314 | CLA | C3D-C4D | -5.84 | 1.31 | 1.44 |
| 20 | A | 820 | CLA | CHD-C4C | 5.84 | 1.52 | 1.39 |
| 20 | A | 804 | CLA | CHD-C4C | 5.83 | 1.52 | 1.39 |
| 20 | B | 829 | CLA | CHC-C1C | 5.83 | 1.50 | 1.38 |
| 20 | B | 815 | CLA | CHD-C4C | 5.83 | 1.52 | 1.39 |
| 20 | B | 830 | CLA | CHC-C1C | 5.83 | 1.50 | 1.38 |
| 20 | A | 803 | CLA | CAB-C3B | -5.82 | 1.31 | 1.47 |
| 20 | 4 | 303 | CLA | CHD-C4C | 5.82 | 1.52 | 1.39 |
| 20 | B | 827 | CLA | CHD-C1D | 5.82 | 1.49 | 1.38 |
| 20 | B | 823 | CLA | CHD-C4C | 5.81 | 1.52 | 1.39 |
| 20 | 4 | 308 | CLA | CHC-C1C | 5.81 | 1.50 | 1.38 |
| 20 | A | 833 | CLA | O2A-CGA | 5.81 | 1.50 | 1.30 |
| 20 | B | 813 | CLA | CHD-C1D | 5.80 | 1.49 | 1.38 |
| 20 | 4 | 307 | CLA | CHC-C1C | 5.80 | 1.50 | 1.38 |
| 20 | B | 838 | CLA | CHD-C4C | 5.80 | 1.52 | 1.39 |
| 20 | B | 821 | CLA | CHD-C1D | 5.80 | 1.49 | 1.38 |
| 20 | B | 811 | CLA | CHD-C1D | 5.80 | 1.51 | 1.38 |
| 20 | 2 | 310 | CLA | CHD-C4C | 5.79 | 1.52 | 1.39 |
| 20 | A | 805 | CLA | CHD-C4C | 5.79 | 1.52 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | F | 206 | CLA | CHC-C1C | 5.79 | 1.50 | 1.38 |
| 20 | A | 804 | CLA | CHD-C1D | 5.78 | 1.49 | 1.38 |
| 20 | 4 | 302 | CLA | CHD-C1D | 5.78 | 1.49 | 1.38 |
| 20 | B | 835 | CLA | CHD-C1D | 5.78 | 1.49 | 1.38 |
| 20 | B | 807 | CLA | CHD-C4C | 5.78 | 1.52 | 1.39 |
| 20 | B | 809 | CLA | CHC-C1C | 5.78 | 1.50 | 1.38 |
| 20 | B | 813 | CLA | CHC-C1C | 5.78 | 1.50 | 1.38 |
| 20 | B | 830 | CLA | CHD-C1D | 5.77 | 1.49 | 1.38 |
| 20 | A | 839 | CLA | O2D-CGD | 5.77 | 1.47 | 1.33 |
| 20 | A | 801 | CLA | O2D-CGD | 5.77 | 1.47 | 1.33 |
| 20 | 4 | 318 | CLA | CHD-C4C | 5.77 | 1.52 | 1.39 |
| 20 | A | 833 | CLA | CHD-C4C | 5.77 | 1.52 | 1.39 |
| 20 | B | 826 | CLA | CHD-C1D | 5.76 | 1.49 | 1.38 |
| 20 | A | 851 | CLA | CHC-C1C | 5.76 | 1.50 | 1.38 |
| 20 | R | 107 | CLA | O2D-CGD | 5.76 | 1.47 | 1.33 |
| 20 | 4 | 311 | CLA | CHC-C1C | 5.76 | 1.50 | 1.38 |
| 20 | A | 809 | CLA | CHD-C4C | 5.76 | 1.52 | 1.39 |
| 20 | B | 838 | CLA | CHC-C1C | 5.76 | 1.50 | 1.38 |
| 20 | A | 815 | CLA | O2D-CGD | 5.76 | 1.47 | 1.33 |
| 20 | H | 110 | CLA | CHD-C1D | 5.75 | 1.49 | 1.38 |
| 20 | 1 | 205 | CLA | CHD-C4C | 5.75 | 1.52 | 1.39 |
| 20 | 3 | 305 | CLA | CHC-C1C | 5.75 | 1.50 | 1.38 |
| 20 | A | 806 | CLA | CHD-C4C | 5.75 | 1.52 | 1.39 |
| 20 | 4 | 318 | CLA | CHC-C1C | 5.75 | 1.50 | 1.38 |
| 20 | L | 202 | CLA | CHD-C1D | 5.75 | 1.49 | 1.38 |
| 20 | A | 807 | CLA | CHD-C4C | 5.74 | 1.52 | 1.39 |
| 20 | 1 | 206 | CLA | O2D-CGD | 5.74 | 1.47 | 1.33 |
| 20 | 2 | 310 | CLA | CHC-C1C | 5.74 | 1.50 | 1.38 |
| 20 | K | 104 | CLA | C3D-C4D | -5.74 | 1.31 | 1.44 |
| 20 | 2 | 305 | CLA | O2D-CGD | 5.74 | 1.47 | 1.33 |
| 20 | A | 823 | CLA | CHD-C4C | 5.73 | 1.52 | 1.39 |
| 20 | A | 837 | CLA | CHD-C1D | 5.73 | 1.49 | 1.38 |
| 20 | A | 830 | CLA | CHD-C4C | 5.73 | 1.52 | 1.39 |
| 20 | B | 825 | CLA | CHC-C1C | 5.73 | 1.50 | 1.38 |
| 20 | K | 102 | CLA | CHC-C1C | 5.73 | 1.50 | 1.38 |
| 20 | A | 850 | CLA | CHD-C1D | 5.73 | 1.49 | 1.38 |
| 20 | A | 805 | CLA | CHC-C1C | 5.73 | 1.50 | 1.38 |
| 20 | B | 814 | CLA | CHD-C1D | 5.73 | 1.49 | 1.38 |
| 20 | B | 833 | CLA | CHD-C1D | 5.73 | 1.49 | 1.38 |
| 20 | B | 809 | CLA | CHD-C4C | 5.73 | 1.52 | 1.39 |
| 20 | 2 | 314 | CLA | CHC-C1C | 5.73 | 1.50 | 1.38 |
| 20 | F | 206 | CLA | CHD-C1D | 5.73 | 1.49 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 313 | CLA | CHD-C1D | 5.72 | 1.49 | 1.38 |
| 20 | 4 | 312 | CLA | CHD-C1D | 5.72 | 1.51 | 1.38 |
| 20 | 2 | 305 | CLA | CHD-C4C | 5.72 | 1.52 | 1.39 |
| 20 | H | 102 | CLA | O2D-CGD | 5.71 | 1.47 | 1.33 |
| 20 | A | 840 | CLA | CHD-C4C | 5.71 | 1.52 | 1.39 |
| 20 | A | 810 | CLA | O2D-CGD | 5.70 | 1.47 | 1.33 |
| 20 | 1 | 203 | CLA | C3D-C4D | -5.70 | 1.31 | 1.44 |
| 20 | A | 821 | CLA | CHC-C1C | 5.70 | 1.50 | 1.38 |
| 20 | A | 814 | CLA | CHC-C1C | 5.69 | 1.49 | 1.38 |
| 20 | K | 103 | CLA | O2D-CGD | 5.68 | 1.47 | 1.33 |
| 20 | H | 110 | CLA | O2D-CGD | 5.67 | 1.47 | 1.33 |
| 20 | A | 819 | CLA | CHD-C4C | 5.67 | 1.52 | 1.39 |
| 20 | 4 | 301 | CLA | O2D-CGD | 5.67 | 1.47 | 1.33 |
| 20 | A | 824 | CLA | CHD-C1D | 5.67 | 1.49 | 1.38 |
| 20 | 3 | 315 | CLA | CHC-C1C | 5.67 | 1.49 | 1.38 |
| 20 | 4 | 304 | CLA | CHC-C1C | 5.67 | 1.50 | 1.38 |
| 20 | F | 207 | CLA | CHD-C1D | 5.66 | 1.49 | 1.38 |
| 20 | 4 | 303 | CLA | O2D-CGD | 5.66 | 1.47 | 1.33 |
| 20 | 4 | 303 | CLA | CHC-C1C | 5.66 | 1.50 | 1.38 |
| 20 | A | 839 | CLA | CAB-C3B | -5.66 | 1.32 | 1.47 |
| 20 | A | 838 | CLA | CHD-C1D | 5.66 | 1.49 | 1.38 |
| 20 | R | 107 | CLA | CHD-C4C | 5.65 | 1.52 | 1.39 |
| 20 | B | 817 | CLA | CHD-C1D | 5.65 | 1.49 | 1.38 |
| 20 | B | 802 | CLA | CHD-C4C | 5.65 | 1.52 | 1.39 |
| 20 | R | 108 | CLA | O2D-CGD | 5.65 | 1.47 | 1.33 |
| 20 | B | 803 | CLA | CHD-C4C | 5.65 | 1.52 | 1.39 |
| 20 | A | 828 | CLA | CHD-C1D | 5.65 | 1.49 | 1.38 |
| 20 | 4 | 304 | CLA | CHD-C4C | 5.65 | 1.52 | 1.39 |
| 20 | B | 806 | CLA | CHD-C1D | 5.65 | 1.49 | 1.38 |
| 20 | A | 828 | CLA | CHD-C4C | 5.64 | 1.52 | 1.39 |
| 20 | F | 207 | CLA | C3D-C4D | -5.64 | 1.31 | 1.44 |
| 20 | K | 103 | CLA | C3D-C4D | -5.64 | 1.31 | 1.44 |
| 20 | A | 818 | CLA | CHC-C1C | 5.63 | 1.50 | 1.38 |
| 20 | 2 | 301 | CLA | CHC-C1C | 5.63 | 1.49 | 1.38 |
| 20 | A | 827 | CLA | CHD-C4C | 5.63 | 1.52 | 1.39 |
| 20 | B | 816 | CLA | O2D-CGD | 5.63 | 1.46 | 1.33 |
| 20 | A | 835 | CLA | CHD-C4C | 5.63 | 1.52 | 1.39 |
| 20 | L | 203 | CLA | CHD-C1D | 5.63 | 1.49 | 1.38 |
| 20 | 2 | 311 | CLA | O2D-CGD | 5.63 | 1.46 | 1.33 |
| 20 | B | 815 | CLA | O2D-CGD | 5.63 | 1.46 | 1.33 |
| 20 | A | 818 | CLA | C3D-C4D | -5.63 | 1.31 | 1.44 |
| 20 | 4 | 317 | CLA | CHC-C1C | 5.63 | 1.49 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 215 | CLA | O2D-CGD | 5.62 | 1.46 | 1.33 |
| 20 | A | 812 | CLA | CHD-C4C | 5.62 | 1.52 | 1.39 |
| 20 | 1 | 204 | CLA | O2D-CGD | 5.62 | 1.46 | 1.33 |
| 20 | A | 831 | CLA | CHC-C1C | 5.62 | 1.49 | 1.38 |
| 20 | B | 840 | CLA | CHD-C4C | 5.61 | 1.52 | 1.39 |
| 20 | K | 103 | CLA | CHC-C1C | 5.61 | 1.49 | 1.38 |
| 20 | B | 837 | CLA | CHD-C4C | 5.61 | 1.52 | 1.39 |
| 20 | H | 102 | CLA | CHD-C4C | 5.61 | 1.52 | 1.39 |
| 20 | A | 808 | CLA | CHD-C4C | 5.61 | 1.52 | 1.39 |
| 20 | A | 836 | CLA | CHD-C4C | 5.61 | 1.52 | 1.39 |
| 20 | J | 103 | CLA | CHC-C1C | 5.61 | 1.49 | 1.38 |
| 22 | I | 101 | BCR | C20-C21 | -5.61 | 1.26 | 1.43 |
| 20 | L | 208 | CLA | O2D-CGD | 5.61 | 1.46 | 1.33 |
| 20 | B | 825 | CLA | CHD-C1D | 5.61 | 1.49 | 1.38 |
| 20 | 1 | 203 | CLA | CHD-C1D | 5.60 | 1.49 | 1.38 |
| 20 | 1 | 213 | CLA | C3D-C4D | -5.60 | 1.31 | 1.44 |
| 20 | B | 834 | CLA | CHD-C4C | 5.60 | 1.52 | 1.39 |
| 20 | H | 109 | CLA | O2D-CGD | 5.59 | 1.46 | 1.33 |
| 20 | B | 824 | CLA | CHC-C1C | 5.59 | 1.49 | 1.38 |
| 20 | 1 | 201 | CLA | CHD-C1D | 5.59 | 1.49 | 1.38 |
| 20 | A | 840 | CLA | O2D-CGD | 5.59 | 1.46 | 1.33 |
| 20 | 2 | 307 | CLA | CHD-C1D | 5.59 | 1.49 | 1.38 |
| 20 | A | 805 | CLA | O2D-CGD | 5.59 | 1.46 | 1.33 |
| 20 | 2 | 309 | CLA | CHC-C1C | 5.58 | 1.49 | 1.38 |
| 20 | 3 | 317 | CLA | CHD-C4C | 5.58 | 1.52 | 1.39 |
| 20 | 4 | 306 | CLA | C3D-C4D | -5.58 | 1.31 | 1.44 |
| 20 | B | 823 | CLA | O2D-CGD | 5.58 | 1.46 | 1.33 |
| 20 | 2 | 310 | CLA | CAB-C3B | -5.58 | 1.32 | 1.47 |
| 20 | L | 204 | CLA | CHD-C1D | 5.58 | 1.49 | 1.38 |
| 20 | A | 819 | CLA | O2D-CGD | 5.58 | 1.46 | 1.33 |
| 20 | 1 | 204 | CLA | CHD-C1D | 5.57 | 1.49 | 1.38 |
| 20 | G | 105 | CLA | CHD-C1D | 5.57 | 1.49 | 1.38 |
| 20 | B | 850 | CLA | CHD-C4C | 5.57 | 1.52 | 1.39 |
| 20 | A | 841 | CLA | CHC-C1C | 5.57 | 1.49 | 1.38 |
| 20 | L | 204 | CLA | O2D-CGD | 5.57 | 1.46 | 1.33 |
| 20 | 4 | 309 | CLA | CHD-C1D | 5.56 | 1.50 | 1.38 |
| 20 | B | 836 | CLA | C3D-C4D | -5.56 | 1.31 | 1.44 |
| 20 | B | 841 | CLA | CHC-C1C | 5.56 | 1.49 | 1.38 |
| 20 | 4 | 307 | CLA | CHD-C1D | 5.56 | 1.50 | 1.38 |
| 20 | A | 813 | CLA | CHD-C4C | 5.56 | 1.51 | 1.39 |
| 20 | 1 | 211 | CLA | CHC-C1C | 5.56 | 1.49 | 1.38 |
| 20 | 3 | 311 | CLA | CHD-C4C | 5.55 | 1.51 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 817 | CLA | CHD-C4C | 5.55 | 1.51 | 1.39 |
| 20 | B | 817 | CLA | CHD-C4C | 5.55 | 1.51 | 1.39 |
| 20 | 2 | 307 | CLA | CHD-C4C | 5.54 | 1.51 | 1.39 |
| 20 | B | 806 | CLA | O2D-CGD | 5.54 | 1.46 | 1.33 |
| 20 | B | 821 | CLA | CHD-C4C | 5.54 | 1.51 | 1.39 |
| 20 | 4 | 310 | CLA | CHC-C1C | 5.54 | 1.49 | 1.38 |
| 20 | B | 829 | CLA | CHD-C1D | 5.54 | 1.49 | 1.38 |
| 20 | 4 | 306 | CLA | CHD-C1D | 5.54 | 1.49 | 1.38 |
| 20 | A | 816 | CLA | C3D-C4D | -5.54 | 1.31 | 1.44 |
| 20 | R | 108 | CLA | CHD-C4C | 5.53 | 1.51 | 1.39 |
| 20 | 1 | 210 | CLA | CHD-C4C | 5.53 | 1.51 | 1.39 |
| 20 | B | 827 | CLA | CHD-C4C | 5.53 | 1.51 | 1.39 |
| 20 | B | 808 | CLA | CHC-C1C | 5.53 | 1.49 | 1.38 |
| 20 | 3 | 307 | CLA | C3D-C4D | -5.53 | 1.31 | 1.44 |
| 20 | L | 208 | CLA | CHD-C4C | 5.52 | 1.51 | 1.39 |
| 20 | 4 | 317 | CLA | CHD-C4C | 5.52 | 1.51 | 1.39 |
| 20 | B | 828 | CLA | C3D-C4D | -5.52 | 1.31 | 1.44 |
| 20 | 2 | 303 | CLA | CHD-C1D | 5.52 | 1.49 | 1.38 |
| 20 | B | 819 | CLA | CHC-C1C | 5.52 | 1.49 | 1.38 |
| 20 | L | 202 | CLA | CHD-C4C | 5.51 | 1.51 | 1.39 |
| 20 | B | 825 | CLA | CHD-C4C | 5.51 | 1.51 | 1.39 |
| 20 | 1 | 202 | CLA | CHD-C4C | 5.51 | 1.51 | 1.39 |
| 20 | 1 | 207 | CLA | CHD-C4C | 5.51 | 1.51 | 1.39 |
| 20 | K | 103 | CLA | CHD-C4C | 5.51 | 1.51 | 1.39 |
| 20 | B | 816 | CLA | CHD-C4C | 5.51 | 1.51 | 1.39 |
| 20 | A | 803 | CLA | C3D-C4D | -5.51 | 1.31 | 1.44 |
| 20 | 4 | 317 | CLA | O2D-CGD | 5.51 | 1.46 | 1.33 |
| 20 | B | 809 | CLA | CAB-C3B | -5.51 | 1.32 | 1.47 |
| 20 | A | 832 | CLA | O2D-CGD | 5.51 | 1.46 | 1.33 |
| 20 | B | 822 | CLA | CHD-C4C | 5.51 | 1.51 | 1.39 |
| 20 | 2 | 303 | CLA | C3D-C4D | -5.50 | 1.31 | 1.44 |
| 20 | A | 822 | CLA | O2D-CGD | 5.50 | 1.46 | 1.33 |
| 20 | 3 | 301 | CLA | CHD-C4C | 5.50 | 1.51 | 1.39 |
| 20 | 4 | 301 | CLA | CHD-C1D | 5.50 | 1.49 | 1.38 |
| 20 | 2 | 306 | CLA | CHC-C1C | 5.50 | 1.49 | 1.38 |
| 20 | 3 | 304 | CLA | CHC-C1C | 5.50 | 1.49 | 1.38 |
| 20 | A | 820 | CLA | O2D-CGD | 5.49 | 1.46 | 1.33 |
| 20 | A | 834 | CLA | CHD-C4C | 5.49 | 1.51 | 1.39 |
| 20 | I | 102 | CLA | CHD-C4C | 5.49 | 1.51 | 1.39 |
| 20 | B | 822 | CLA | O2D-CGD | 5.49 | 1.46 | 1.33 |
| 20 | K | 104 | CLA | CHD-C4C | 5.49 | 1.51 | 1.39 |
| 20 | F | 206 | CLA | CHC-C4B | 5.49 | 1.51 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 824 | CLA | CHD-C4C | 5.49 | 1.51 | 1.39 |
| 20 | H | 110 | CLA | CHD-C4C | 5.49 | 1.51 | 1.39 |
| 20 | B | 835 | CLA | CHD-C4C | 5.49 | 1.51 | 1.39 |
| 20 | A | 833 | CLA | O2D-CGD | 5.48 | 1.46 | 1.33 |
| 20 | 4 | 310 | CLA | C3D-C4D | -5.48 | 1.31 | 1.44 |
| 20 | 3 | 307 | CLA | O2D-CGD | 5.47 | 1.46 | 1.33 |
| 20 | 3 | 303 | CLA | CHD-C4C | 5.47 | 1.51 | 1.39 |
| 20 | B | 833 | CLA | CHC-C1C | 5.47 | 1.49 | 1.38 |
| 20 | A | 806 | CLA | O2D-CGD | 5.47 | 1.46 | 1.33 |
| 20 | 4 | 310 | CLA | O2D-CGD | 5.47 | 1.46 | 1.33 |
| 20 | J | 101 | CLA | CHD-C4C | 5.47 | 1.51 | 1.39 |
| 20 | A | 812 | CLA | O2D-CGD | 5.47 | 1.46 | 1.33 |
| 20 | B | 826 | CLA | CHD-C4C | 5.47 | 1.51 | 1.39 |
| 20 | L | 203 | CLA | CHD-C4C | 5.46 | 1.51 | 1.39 |
| 20 | A | 838 | CLA | O2D-CGD | 5.46 | 1.46 | 1.33 |
| 20 | K | 101 | CLA | CHD-C4C | 5.45 | 1.51 | 1.39 |
| 20 | B | 839 | CLA | C4C-C3C | -5.45 | 1.35 | 1.45 |
| 20 | K | 102 | CLA | CHD-C4C | 5.45 | 1.51 | 1.39 |
| 20 | B | 834 | CLA | O2D-CGD | 5.45 | 1.46 | 1.33 |
| 20 | L | 207 | CLA | O2D-CGD | 5.45 | 1.46 | 1.33 |
| 20 | A | 838 | CLA | CHD-C4C | 5.44 | 1.51 | 1.39 |
| 20 | A | 835 | CLA | CAB-C3B | -5.44 | 1.32 | 1.47 |
| 20 | B | 818 | CLA | O2D-CGD | 5.44 | 1.46 | 1.33 |
| 20 | A | 839 | CLA | CHC-C1C | 5.44 | 1.49 | 1.38 |
| 20 | L | 201 | CLA | O2D-CGD | 5.44 | 1.46 | 1.33 |
| 20 | 2 | 316 | CLA | CHC-C1C | 5.44 | 1.49 | 1.38 |
| 20 | 3 | 310 | CLA | C3D-C4D | -5.44 | 1.31 | 1.44 |
| 20 | A | 821 | CLA | O2D-CGD | 5.44 | 1.46 | 1.33 |
| 20 | 2 | 303 | CLA | CHC-C1C | 5.44 | 1.49 | 1.38 |
| 20 | 4 | 306 | CLA | CHD-C4C | 5.44 | 1.51 | 1.39 |
| 20 | 1 | 204 | CLA | C3D-C4D | -5.43 | 1.31 | 1.44 |
| 20 | 2 | 314 | CLA | O2D-CGD | 5.43 | 1.46 | 1.33 |
| 20 | 3 | 306 | CLA | CHD-C1D | 5.43 | 1.50 | 1.38 |
| 20 | A | 837 | CLA | CHD-C4C | 5.43 | 1.51 | 1.39 |
| 20 | B | 814 | CLA | CHD-C4C | 5.43 | 1.51 | 1.39 |
| 20 | B | 813 | CLA | CHD-C4C | 5.42 | 1.51 | 1.39 |
| 20 | 1 | 212 | CLA | CHD-C1D | 5.42 | 1.50 | 1.38 |
| 20 | 3 | 309 | CLA | CHD-C1D | 5.42 | 1.50 | 1.38 |
| 20 | 3 | 302 | CLA | CHD-C1D | 5.41 | 1.50 | 1.38 |
| 20 | 1 | 209 | CLA | CHD-C1D | 5.41 | 1.50 | 1.38 |
| 20 | B | 832 | CLA | CHD-C4C | 5.41 | 1.51 | 1.39 |
| 20 | 3 | 311 | CLA | O2D-CGD | 5.41 | 1.46 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 840 | CLA | O2D-CGD | 5.41 | 1.46 | 1.33 |
| 20 | 1 | 204 | CLA | CHD-C4C | 5.40 | 1.51 | 1.39 |
| 20 | A | 850 | CLA | CHD-C4C | 5.40 | 1.51 | 1.39 |
| 20 | 4 | 306 | CLA | C1B-NB | -5.40 | 1.31 | 1.37 |
| 20 | G | 105 | CLA | CHD-C4C | 5.40 | 1.51 | 1.39 |
| 20 | H | 108 | CLA | CHC-C1C | 5.40 | 1.49 | 1.38 |
| 20 | A | 825 | CLA | CHD-C4C | 5.40 | 1.51 | 1.39 |
| 20 | J | 101 | CLA | O2D-CGD | 5.39 | 1.46 | 1.33 |
| 20 | B | 814 | CLA | CHC-C4B | 5.39 | 1.51 | 1.39 |
| 20 | A | 807 | CLA | O2D-CGD | 5.39 | 1.46 | 1.33 |
| 20 | B | 810 | CLA | O2D-CGD | 5.38 | 1.46 | 1.33 |
| 20 | B | 842 | CLA | CHD-C4C | 5.38 | 1.51 | 1.39 |
| 20 | 2 | 307 | CLA | O2D-CGD | 5.38 | 1.46 | 1.33 |
| 20 | F | 207 | CLA | O2D-CGD | 5.38 | 1.46 | 1.33 |
| 20 | F | 206 | CLA | CHD-C4C | 5.38 | 1.51 | 1.39 |
| 20 | B | 817 | CLA | O2D-CGD | 5.38 | 1.46 | 1.33 |
| 20 | B | 835 | CLA | O2D-CGD | 5.38 | 1.46 | 1.33 |
| 20 | 2 | 310 | CLA | C3D-C4D | -5.38 | 1.32 | 1.44 |
| 20 | A | 849 | CLA | O2D-CGD | 5.38 | 1.46 | 1.33 |
| 20 | K | 102 | CLA | O2D-CGD | 5.38 | 1.46 | 1.33 |
| 20 | 3 | 313 | CLA | CHC-C4B | 5.38 | 1.51 | 1.39 |
| 20 | G | 105 | CLA | O2D-CGD | 5.38 | 1.46 | 1.33 |
| 20 | A | 817 | CLA | O2D-CGD | 5.37 | 1.46 | 1.33 |
| 20 | B | 824 | CLA | CAB-C3B | -5.37 | 1.32 | 1.47 |
| 20 | B | 803 | CLA | O2D-CGD | 5.37 | 1.46 | 1.33 |
| 20 | A | 803 | CLA | CHC-C1C | 5.37 | 1.49 | 1.38 |
| 20 | 4 | 308 | CLA | CHD-C1D | 5.37 | 1.50 | 1.38 |
| 20 | F | 207 | CLA | CHC-C1C | 5.36 | 1.49 | 1.38 |
| 20 | B | 830 | CLA | O2D-CGD | 5.36 | 1.46 | 1.33 |
| 20 | B | 825 | CLA | O2D-CGD | 5.36 | 1.46 | 1.33 |
| 20 | B | 808 | CLA | C3D-C4D | -5.36 | 1.32 | 1.44 |
| 20 | 1 | 211 | CLA | O2D-CGD | 5.35 | 1.46 | 1.33 |
| 20 | L | 204 | CLA | CHD-C4C | 5.35 | 1.51 | 1.39 |
| 20 | 4 | 306 | CLA | O2D-CGD | 5.34 | 1.46 | 1.33 |
| 20 | 3 | 315 | CLA | CHD-C1D | 5.34 | 1.50 | 1.38 |
| 20 | A | 834 | CLA | O2D-CGD | 5.34 | 1.46 | 1.33 |
| 20 | B | 832 | CLA | CHC-C4B | 5.34 | 1.51 | 1.39 |
| 20 | 1 | 213 | CLA | CHD-C4C | 5.34 | 1.51 | 1.39 |
| 20 | 4 | 301 | CLA | CHD-C4C | 5.34 | 1.51 | 1.39 |
| 20 | L | 208 | CLA | CHD-C1D | 5.34 | 1.48 | 1.38 |
| 20 | 4 | 304 | CLA | O2D-CGD | 5.33 | 1.46 | 1.33 |
| 20 | 1 | 204 | CLA | CHC-C1C | 5.33 | 1.49 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 3 | 312 | CLA | CHD-C1D | 5.33 | 1.50 | 1.38 |
| 20 | B | 833 | CLA | O2D-CGD | 5.33 | 1.46 | 1.33 |
| 20 | A | 816 | CLA | CHD-C1D | 5.33 | 1.48 | 1.38 |
| 20 | 3 | 309 | CLA | CHC-C1C | 5.33 | 1.49 | 1.38 |
| 20 | 2 | 312 | CLA | C3D-C4D | -5.33 | 1.32 | 1.44 |
| 20 | B | 813 | CLA | O2D-CGD | 5.33 | 1.46 | 1.33 |
| 20 | 2 | 302 | CLA | C3D-C4D | -5.33 | 1.32 | 1.44 |
| 20 | 4 | 302 | CLA | C3D-C4D | -5.33 | 1.32 | 1.44 |
| 20 | B | 835 | CLA | CAB-C3B | -5.33 | 1.32 | 1.47 |
| 20 | K | 101 | CLA | C3D-C4D | -5.33 | 1.32 | 1.44 |
| 20 | B | 824 | CLA | CHD-C1D | 5.32 | 1.48 | 1.38 |
| 20 | A | 851 | CLA | CAB-C3B | -5.32 | 1.32 | 1.47 |
| 20 | K | 102 | CLA | C3D-C4D | -5.32 | 1.32 | 1.44 |
| 20 | A | 834 | CLA | C3D-C4D | -5.32 | 1.32 | 1.44 |
| 20 | 1 | 213 | CLA | CHD-C1D | 5.31 | 1.48 | 1.38 |
| 20 | A | 811 | CLA | O2D-CGD | 5.31 | 1.46 | 1.33 |
| 20 | 1 | 210 | CLA | CHC-C4B | 5.31 | 1.51 | 1.39 |
| 20 | H | 110 | CLA | CHC-C4B | 5.31 | 1.51 | 1.39 |
| 20 | B | 826 | CLA | C3D-C4D | -5.30 | 1.32 | 1.44 |
| 20 | 1 | 201 | CLA | C3D-C4D | -5.30 | 1.32 | 1.44 |
| 20 | B | 807 | CLA | O2D-CGD | 5.30 | 1.46 | 1.33 |
| 20 | 4 | 305 | CLA | C3D-C4D | -5.30 | 1.32 | 1.44 |
| 20 | J | 103 | CLA | C3D-C4D | -5.29 | 1.32 | 1.44 |
| 20 | L | 203 | CLA | O2D-CGD | 5.29 | 1.46 | 1.33 |
| 20 | L | 207 | CLA | CHC-C4B | 5.29 | 1.51 | 1.39 |
| 20 | 3 | 304 | CLA | CHD-C1D | 5.29 | 1.50 | 1.38 |
| 20 | I | 102 | CLA | O2D-CGD | 5.29 | 1.46 | 1.33 |
| 20 | B | 825 | CLA | CAB-C3B | -5.28 | 1.33 | 1.47 |
| 20 | B | 832 | CLA | CAB-C3B | -5.28 | 1.33 | 1.47 |
| 20 | L | 202 | CLA | O2D-CGD | 5.28 | 1.46 | 1.33 |
| 20 | 3 | 308 | CLA | CHD-C1D | 5.28 | 1.50 | 1.38 |
| 20 | B | 833 | CLA | CHD-C4C | 5.28 | 1.51 | 1.39 |
| 20 | 3 | 307 | CLA | CHC-C1C | 5.28 | 1.49 | 1.38 |
| 20 | B | 820 | CLA | CHD-C1D | 5.28 | 1.48 | 1.38 |
| 20 | A | 828 | CLA | O2D-CGD | 5.28 | 1.46 | 1.33 |
| 20 | 4 | 313 | CLA | CHC-C4B | 5.27 | 1.51 | 1.39 |
| 20 | 4 | 313 | CLA | CHD-C4C | 5.27 | 1.51 | 1.39 |
| 20 | A | 814 | CLA | CHD-C1D | 5.27 | 1.50 | 1.38 |
| 20 | B | 802 | CLA | O2D-CGD | 5.26 | 1.46 | 1.33 |
| 20 | A | 849 | CLA | CHC-C4B | 5.26 | 1.51 | 1.39 |
| 20 | G | 105 | CLA | C3D-C4D | -5.26 | 1.32 | 1.44 |
| 20 | 2 | 310 | CLA | O2D-CGD | 5.26 | 1.46 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 213 | CLA | CHC-C1C | 5.25 | 1.49 | 1.38 |
| 20 | 2 | 301 | CLA | CHD-C1D | 5.25 | 1.50 | 1.38 |
| 20 | 2 | 311 | CLA | CHD-C4C | 5.25 | 1.51 | 1.39 |
| 20 | 3 | 314 | CLA | CHD-C1D | 5.25 | 1.48 | 1.38 |
| 20 | A | 825 | CLA | C3D-C4D | -5.25 | 1.32 | 1.44 |
| 20 | 3 | 314 | CLA | CHD-C4C | 5.25 | 1.51 | 1.39 |
| 20 | 4 | 302 | CLA | CHD-C4C | 5.25 | 1.51 | 1.39 |
| 20 | A | 804 | CLA | O2A-CGA | 5.25 | 1.48 | 1.33 |
| 20 | B | 819 | CLA | CHD-C1D | 5.25 | 1.48 | 1.38 |
| 20 | B | 828 | CLA | O2D-CGD | 5.24 | 1.46 | 1.33 |
| 20 | B | 814 | CLA | CAB-C3B | -5.24 | 1.33 | 1.47 |
| 20 | 2 | 307 | CLA | C3D-C4D | -5.24 | 1.32 | 1.44 |
| 20 | A | 810 | CLA | C3D-C4D | -5.24 | 1.32 | 1.44 |
| 20 | 3 | 310 | CLA | O2D-CGD | 5.24 | 1.46 | 1.33 |
| 20 | A | 808 | CLA | C3D-C4D | -5.24 | 1.32 | 1.44 |
| 20 | A | 839 | CLA | CHD-C1D | 5.24 | 1.48 | 1.38 |
| 20 | J | 103 | CLA | CAB-C3B | -5.24 | 1.33 | 1.47 |
| 20 | I | 102 | CLA | CHC-C4B | 5.23 | 1.51 | 1.39 |
| 20 | A | 836 | CLA | O2D-CGD | 5.23 | 1.46 | 1.33 |
| 20 | 1 | 213 | CLA | O2D-CGD | 5.23 | 1.46 | 1.33 |
| 20 | F | 207 | CLA | CHD-C4C | 5.23 | 1.51 | 1.39 |
| 20 | 1 | 208 | CLA | CHD-C1D | 5.23 | 1.50 | 1.38 |
| 20 | A | 850 | CLA | O2D-CGD | 5.23 | 1.46 | 1.33 |
| 20 | B | 834 | CLA | C3D-C4D | -5.22 | 1.32 | 1.44 |
| 20 | A | 819 | CLA | CHC-C4B | 5.22 | 1.51 | 1.39 |
| 20 | L | 208 | CLA | CHC-C4B | 5.22 | 1.51 | 1.39 |
| 20 | A | 803 | CLA | CHD-C1D | 5.22 | 1.48 | 1.38 |
| 20 | A | 829 | CLA | O2D-CGD | 5.22 | 1.45 | 1.33 |
| 20 | 2 | 312 | CLA | O2D-CGD | 5.22 | 1.45 | 1.33 |
| 20 | B | 824 | CLA | C4C-C3C | -5.21 | 1.36 | 1.45 |
| 20 | F | 206 | CLA | O2D-CGD | 5.21 | 1.45 | 1.33 |
| 20 | 2 | 314 | CLA | C3D-C4D | -5.21 | 1.32 | 1.44 |
| 20 | B | 831 | CLA | C3D-C4D | -5.21 | 1.32 | 1.44 |
| 20 | A | 820 | CLA | CHC-C4B | 5.21 | 1.51 | 1.39 |
| 20 | A | 816 | CLA | O2D-CGD | 5.21 | 1.45 | 1.33 |
| 20 | B | 829 | CLA | CHD-C4C | 5.21 | 1.51 | 1.39 |
| 20 | A | 827 | CLA | O2D-CGD | 5.21 | 1.45 | 1.33 |
| 20 | B | 826 | CLA | CAB-C3B | -5.20 | 1.33 | 1.47 |
| 20 | 1 | 211 | CLA | C3D-C4D | -5.20 | 1.32 | 1.44 |
| 20 | A | 837 | CLA | CAB-C3B | -5.20 | 1.33 | 1.47 |
| 20 | 1 | 203 | CLA | O2D-CGD | 5.20 | 1.45 | 1.33 |
| 20 | B | 823 | CLA | CAB-C3B | -5.20 | 1.33 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 841 | CLA | CHD-C4C | 5.20 | 1.51 | 1.39 |
| 20 | 2 | 308 | CLA | CHC-C1C | 5.20 | 1.48 | 1.38 |
| 20 | 1 | 204 | CLA | CAB-C3B | -5.20 | 1.33 | 1.47 |
| 20 | B | 821 | CLA | O2D-CGD | 5.20 | 1.45 | 1.33 |
| 20 | 1 | 211 | CLA | CAB-C3B | -5.20 | 1.33 | 1.47 |
| 20 | 3 | 310 | CLA | C4C-C3C | -5.20 | 1.36 | 1.45 |
| 20 | A | 808 | CLA | CAB-C3B | -5.20 | 1.33 | 1.47 |
| 20 | 3 | 314 | CLA | O2D-CGD | 5.19 | 1.45 | 1.33 |
| 20 | B | 808 | CLA | CHD-C1D | 5.19 | 1.48 | 1.38 |
| 20 | B | 830 | CLA | C3D-C4D | -5.19 | 1.32 | 1.44 |
| 20 | A | 824 | CLA | CAB-C3B | -5.19 | 1.33 | 1.47 |
| 20 | 4 | 318 | CLA | CAB-C3B | -5.19 | 1.33 | 1.47 |
| 20 | 3 | 303 | CLA | CHC-C4B | 5.18 | 1.51 | 1.39 |
| 20 | 4 | 314 | CLA | CHD-C1D | 5.18 | 1.49 | 1.38 |
| 20 | A | 839 | CLA | O2A-CGA | 5.18 | 1.48 | 1.33 |
| 20 | B | 833 | CLA | C3D-C4D | -5.18 | 1.32 | 1.44 |
| 20 | A | 851 | CLA | O2D-CGD | 5.18 | 1.45 | 1.33 |
| 20 | A | 849 | CLA | CHD-C4C | 5.18 | 1.51 | 1.39 |
| 20 | B | 806 | CLA | CAB-C3B | -5.17 | 1.33 | 1.47 |
| 20 | B | 822 | CLA | CHD-C1D | 5.17 | 1.48 | 1.38 |
| 20 | L | 202 | CLA | C3D-C4D | -5.17 | 1.32 | 1.44 |
| 20 | A | 824 | CLA | C3D-C4D | -5.17 | 1.32 | 1.44 |
| 20 | 1 | 206 | CLA | CHD-C4C | 5.16 | 1.51 | 1.39 |
| 20 | B | 810 | CLA | CAB-C3B | -5.16 | 1.33 | 1.47 |
| 20 | A | 808 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 20 | B | 828 | CLA | CHC-C4B | 5.16 | 1.51 | 1.39 |
| 20 | A | 838 | CLA | CHC-C4B | 5.16 | 1.51 | 1.39 |
| 20 | H | 108 | CLA | CAB-C3B | -5.16 | 1.33 | 1.47 |
| 20 | B | 820 | CLA | CHD-C4C | 5.16 | 1.51 | 1.39 |
| 20 | B | 830 | CLA | CHD-C4C | 5.16 | 1.51 | 1.39 |
| 20 | H | 101 | CLA | O2A-CGA | 5.16 | 1.48 | 1.33 |
| 20 | B | 816 | CLA | CHC-C4B | 5.16 | 1.51 | 1.39 |
| 20 | 2 | 311 | CLA | C3D-C4D | -5.15 | 1.32 | 1.44 |
| 20 | A | 833 | CLA | C3D-C4D | -5.15 | 1.32 | 1.44 |
| 20 | 1 | 214 | CLA | CHD-C1D | 5.15 | 1.49 | 1.38 |
| 20 | B | 809 | CLA | O2D-CGD | 5.15 | 1.45 | 1.33 |
| 20 | H | 108 | CLA | C1B-NB | -5.15 | 1.31 | 1.37 |
| 20 | 1 | 207 | CLA | CHC-C4B | 5.15 | 1.51 | 1.39 |
| 20 | 1 | 203 | CLA | CHD-C4C | 5.15 | 1.51 | 1.39 |
| 20 | 2 | 302 | CLA | CHC-C4B | 5.15 | 1.50 | 1.39 |
| 20 | K | 101 | CLA | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 20 | A | 810 | CLA | CHC-C4B | 5.14 | 1.50 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 302 | CLA | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 20 | 2 | 303 | CLA | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 20 | F | 201 | CLA | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 20 | A | 837 | CLA | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 20 | A | 805 | CLA | O2A-CGA | 5.14 | 1.48 | 1.33 |
| 20 | A | 803 | CLA | CHD-C4C | 5.14 | 1.51 | 1.39 |
| 20 | 3 | 305 | CLA | CHD-C1D | 5.14 | 1.49 | 1.38 |
| 20 | A | 812 | CLA | CHC-C4B | 5.14 | 1.50 | 1.39 |
| 20 | 4 | 318 | CLA | C3D-C4D | -5.14 | 1.32 | 1.44 |
| 20 | 4 | 303 | CLA | CHD-C1D | 5.14 | 1.48 | 1.38 |
| 20 | F | 201 | CLA | C3D-C4D | -5.13 | 1.32 | 1.44 |
| 20 | A | 829 | CLA | C3D-C4D | -5.13 | 1.32 | 1.44 |
| 20 | B | 809 | CLA | C3D-C4D | -5.13 | 1.32 | 1.44 |
| 20 | B | 836 | CLA | CHD-C4C | 5.13 | 1.50 | 1.39 |
| 20 | A | 849 | CLA | CHD-C1D | 5.13 | 1.48 | 1.38 |
| 20 | 3 | 311 | CLA | C3D-C4D | -5.13 | 1.32 | 1.44 |
| 20 | 2 | 303 | CLA | CHD-C4C | 5.12 | 1.50 | 1.39 |
| 20 | 1 | 201 | CLA | CHD-C4C | 5.12 | 1.50 | 1.39 |
| 20 | B | 842 | CLA | CHC-C4B | 5.12 | 1.50 | 1.39 |
| 20 | 3 | 310 | CLA | CHC-C1C | 5.11 | 1.48 | 1.38 |
| 20 | A | 835 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 20 | 3 | 301 | CLA | CHC-C4B | 5.11 | 1.50 | 1.39 |
| 20 | B | 817 | CLA | CHC-C4B | 5.11 | 1.50 | 1.39 |
| 20 | A | 827 | CLA | CAB-C3B | -5.11 | 1.33 | 1.47 |
| 20 | 4 | 305 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 20 | A | 839 | CLA | C3D-C4D | -5.10 | 1.32 | 1.44 |
| 20 | F | 201 | CLA | C4C-C3C | -5.10 | 1.36 | 1.45 |
| 20 | 1 | 206 | CLA | CHD-C1D | 5.10 | 1.48 | 1.38 |
| 20 | A | 826 | CLA | CAB-C3B | -5.10 | 1.33 | 1.47 |
| 20 | B | 808 | CLA | CHD-C4C | 5.10 | 1.50 | 1.39 |
| 20 | B | 814 | CLA | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 20 | B | 829 | CLA | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 20 | J | 103 | CLA | CHD-C1D | 5.09 | 1.48 | 1.38 |
| 20 | 2 | 310 | CLA | C1B-NB | -5.09 | 1.31 | 1.37 |
| 20 | 1 | 203 | CLA | CAB-C3B | -5.09 | 1.33 | 1.47 |
| 20 | B | 836 | CLA | CAB-C3B | -5.09 | 1.33 | 1.47 |
| 20 | 2 | 314 | CLA | C4C-C3C | -5.09 | 1.36 | 1.45 |
| 20 | H | 109 | CLA | CHC-C4B | 5.09 | 1.50 | 1.39 |
| 20 | B | 840 | CLA | CHC-C4B | 5.08 | 1.50 | 1.39 |
| 20 | B | 802 | CLA | CAB-C3B | -5.08 | 1.33 | 1.47 |
| 20 | 1 | 206 | CLA | CHC-C4B | 5.08 | 1.50 | 1.39 |
| 20 | B | 827 | CLA | CAB-C3B | -5.08 | 1.33 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 838 | CLA | C3D-C4D | -5.08 | 1.32 | 1.44 |
| 20 | F | 206 | CLA | C3D-C4D | -5.07 | 1.32 | 1.44 |
| 20 | J | 101 | CLA | C3D-C4D | -5.07 | 1.32 | 1.44 |
| 20 | 4 | 317 | CLA | CAB-C3B | -5.07 | 1.33 | 1.47 |
| 20 | I | 102 | CLA | C3D-C4D | -5.07 | 1.32 | 1.44 |
| 20 | L | 203 | CLA | C3D-C4D | -5.07 | 1.32 | 1.44 |
| 20 | B | 837 | CLA | CAB-C3B | -5.07 | 1.33 | 1.47 |
| 20 | B | 837 | CLA | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 20 | B | 841 | CLA | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 20 | B | 819 | CLA | CHD-C4C | 5.06 | 1.50 | 1.39 |
| 23 | A | 842 | PQN | C10-C5 | 5.06 | 1.49 | 1.40 |
| 20 | 1 | 205 | CLA | CHC-C4B | 5.06 | 1.50 | 1.39 |
| 20 | B | 836 | CLA | CHD-C1D | 5.06 | 1.48 | 1.38 |
| 20 | R | 108 | CLA | CHC-C4B | 5.06 | 1.50 | 1.39 |
| 20 | 2 | 316 | CLA | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 20 | 2 | 312 | CLA | CHD-C4C | 5.05 | 1.50 | 1.39 |
| 20 | B | 829 | CLA | CAB-C3B | -5.05 | 1.33 | 1.47 |
| 20 | A | 835 | CLA | C3D-C4D | -5.05 | 1.32 | 1.44 |
| 20 | 3 | 310 | CLA | CAB-C3B | -5.05 | 1.33 | 1.47 |
| 20 | B | 835 | CLA | C3D-C4D | -5.05 | 1.32 | 1.44 |
| 20 | 1 | 207 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 20 | B | 807 | CLA | CHC-C4B | 5.05 | 1.50 | 1.39 |
| 20 | B | 820 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 20 | 3 | 317 | CLA | CHC-C4B | 5.05 | 1.50 | 1.39 |
| 20 | A | 836 | CLA | C3D-C4D | -5.05 | 1.32 | 1.44 |
| 20 | B | 832 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 20 | A | 834 | CLA | CAB-C3B | -5.04 | 1.33 | 1.47 |
| 20 | F | 205 | CLA | C3D-C4D | -5.04 | 1.32 | 1.44 |
| 20 | B | 812 | CLA | CHC-C4B | 5.04 | 1.50 | 1.39 |
| 20 | 4 | 306 | CLA | C4C-C3C | -5.04 | 1.36 | 1.45 |
| 20 | F | 207 | CLA | C3A-C2A | -5.04 | 1.40 | 1.54 |
| 20 | 2 | 312 | CLA | CHC-C4B | 5.04 | 1.50 | 1.39 |
| 20 | B | 834 | CLA | CAB-C3B | -5.04 | 1.33 | 1.47 |
| 20 | K | 104 | CLA | CAB-C3B | -5.04 | 1.33 | 1.47 |
| 20 | A | 823 | CLA | C3D-C4D | -5.04 | 1.32 | 1.44 |
| 20 | 2 | 305 | CLA | CHC-C4B | 5.04 | 1.50 | 1.39 |
| 20 | B | 815 | CLA | CAB-C3B | -5.04 | 1.33 | 1.47 |
| 20 | A | 823 | CLA | CHC-C4B | 5.04 | 1.50 | 1.39 |
| 20 | 4 | 311 | CLA | CHD-C1D | 5.03 | 1.49 | 1.38 |
| 20 | B | 823 | CLA | C3D-C4D | -5.03 | 1.32 | 1.44 |
| 20 | 2 | 311 | CLA | O2A-CGA | 5.03 | 1.48 | 1.33 |
| 20 | A | 829 | CLA | O2A-CGA | 5.03 | 1.48 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | K | 101 | CLA | CHC-C4B | 5.03 | 1.50 | 1.39 |
| 20 | A | 823 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 20 | 1 | 203 | CLA | CHC-C4B | 5.03 | 1.50 | 1.39 |
| 20 | L | 204 | CLA | CHC-C4B | 5.02 | 1.50 | 1.39 |
| 20 | A | 809 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 20 | B | 827 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 20 | A | 816 | CLA | CHD-C4C | 5.02 | 1.50 | 1.39 |
| 20 | B | 822 | CLA | CHC-C4B | 5.02 | 1.50 | 1.39 |
| 20 | A | 851 | CLA | C3D-C4D | -5.02 | 1.32 | 1.44 |
| 20 | A | 831 | CLA | C4C-C3C | -5.01 | 1.36 | 1.45 |
| 20 | 4 | 306 | CLA | CAB-C3B | -5.01 | 1.33 | 1.47 |
| 20 | A | 804 | CLA | CHC-C4B | 5.01 | 1.50 | 1.39 |
| 20 | B | 838 | CLA | CAB-C3B | -5.01 | 1.33 | 1.47 |
| 20 | B | 811 | CLA | CHC-C1C | 5.01 | 1.48 | 1.38 |
| 20 | H | 102 | CLA | CHC-C4B | 5.01 | 1.50 | 1.39 |
| 20 | B | 812 | CLA | CHD-C4C | 5.01 | 1.50 | 1.39 |
| 20 | 2 | 316 | CLA | CHD-C4C | 5.00 | 1.50 | 1.39 |
| 20 | 1 | 213 | CLA | C3A-C2A | -5.00 | 1.40 | 1.54 |
| 20 | A | 820 | CLA | C3D-C4D | -5.00 | 1.32 | 1.44 |
| 20 | A | 834 | CLA | CHC-C4B | 5.00 | 1.50 | 1.39 |
| 20 | 2 | 314 | CLA | CAB-C3B | -5.00 | 1.33 | 1.47 |
| 20 | A | 804 | CLA | CAB-C3B | -4.99 | 1.33 | 1.47 |
| 20 | B | 824 | CLA | C1B-NB | -4.99 | 1.31 | 1.37 |
| 20 | A | 815 | CLA | CHC-C4B | 4.99 | 1.50 | 1.39 |
| 20 | A | 813 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 20 | 4 | 301 | CLA | C3D-C4D | -4.99 | 1.32 | 1.44 |
| 20 | B | 806 | CLA | CHC-C4B | 4.99 | 1.50 | 1.39 |
| 20 | B | 808 | CLA | CAB-C3B | -4.99 | 1.33 | 1.47 |
| 20 | 4 | 305 | CLA | CHD-C1D | 4.98 | 1.48 | 1.38 |
| 20 | A | 832 | CLA | C3D-C4D | -4.98 | 1.32 | 1.44 |
| 20 | B | 821 | CLA | CHC-C4B | 4.98 | 1.50 | 1.39 |
| 20 | 2 | 303 | CLA | CAB-C3B | -4.98 | 1.33 | 1.47 |
| 20 | L | 202 | CLA | CHC-C4B | 4.98 | 1.50 | 1.39 |
| 20 | A | 850 | CLA | O2A-CGA | 4.98 | 1.47 | 1.33 |
| 20 | A | 839 | CLA | CHD-C4C | 4.98 | 1.50 | 1.39 |
| 20 | B | 818 | CLA | CHC-C4B | 4.97 | 1.50 | 1.39 |
| 20 | B | 850 | CLA | C3D-C4D | -4.97 | 1.33 | 1.44 |
| 20 | J | 103 | CLA | CHD-C4C | 4.97 | 1.50 | 1.39 |
| 20 | 1 | 201 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 20 | B | 827 | CLA | C3D-C4D | -4.97 | 1.33 | 1.44 |
| 20 | A | 809 | CLA | CHC-C1C | 4.97 | 1.48 | 1.38 |
| 20 | L | 201 | CLA | CHC-C4B | 4.97 | 1.50 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 312 | CLA | CHD-C1D | 4.96 | 1.48 | 1.38 |
| 20 | A | 850 | CLA | CAB-C3B | -4.96 | 1.33 | 1.47 |
| 20 | B | 831 | CLA | CHC-C4B | 4.96 | 1.50 | 1.39 |
| 20 | 2 | 302 | CLA | CAB-C3B | -4.96 | 1.33 | 1.47 |
| 20 | A | 817 | CLA | CHC-C4B | 4.96 | 1.50 | 1.39 |
| 20 | A | 807 | CLA | C3D-C4D | -4.96 | 1.33 | 1.44 |
| 20 | B | 838 | CLA | C3D-C4D | -4.96 | 1.33 | 1.44 |
| 20 | B | 803 | CLA | CAB-C3B | -4.96 | 1.33 | 1.47 |
| 20 | A | 826 | CLA | CHC-C4B | 4.96 | 1.50 | 1.39 |
| 20 | B | 834 | CLA | CHC-C4B | 4.95 | 1.50 | 1.39 |
| 20 | 1 | 215 | CLA | CHC-C4B | 4.95 | 1.50 | 1.39 |
| 20 | A | 824 | CLA | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 20 | 4 | 315 | CLA | CHC-C4B | 4.95 | 1.50 | 1.39 |
| 20 | R | 108 | CLA | O2A-CGA | 4.94 | 1.47 | 1.33 |
| 20 | K | 104 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 20 | G | 105 | CLA | CHC-C4B | 4.94 | 1.50 | 1.39 |
| 20 | 3 | 301 | CLA | C3D-C4D | -4.94 | 1.33 | 1.44 |
| 20 | 3 | 311 | CLA | CHC-C4B | 4.94 | 1.50 | 1.39 |
| 20 | B | 840 | CLA | C3D-C4D | -4.94 | 1.33 | 1.44 |
| 20 | R | 107 | CLA | CHC-C4B | 4.94 | 1.50 | 1.39 |
| 20 | L | 204 | CLA | OBD-CAD | 4.93 | 1.31 | 1.22 |
| 20 | 2 | 312 | CLA | CAB-C3B | -4.93 | 1.34 | 1.47 |
| 20 | B | 820 | CLA | CHC-C4B | 4.93 | 1.50 | 1.39 |
| 20 | F | 205 | CLA | CHC-C4B | 4.93 | 1.50 | 1.39 |
| 20 | F | 201 | CLA | CAB-C3B | -4.93 | 1.34 | 1.47 |
| 20 | B | 850 | CLA | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 20 | 2 | 314 | CLA | CHD-C4C | 4.93 | 1.50 | 1.39 |
| 20 | 2 | 316 | CLA | CHD-C1D | 4.93 | 1.48 | 1.38 |
| 20 | 2 | 316 | CLA | CAB-C3B | -4.93 | 1.34 | 1.47 |
| 20 | 4 | 303 | CLA | CAB-C3B | -4.93 | 1.34 | 1.47 |
| 20 | B | 802 | CLA | C3D-C4D | -4.92 | 1.33 | 1.44 |
| 20 | A | 836 | CLA | CAB-C3B | -4.92 | 1.34 | 1.47 |
| 20 | A | 851 | CLA | CHC-C4B | 4.92 | 1.50 | 1.39 |
| 20 | B | 819 | CLA | CAB-C3B | -4.92 | 1.34 | 1.47 |
| 20 | B | 836 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 20 | A | 804 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 20 | A | 818 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 20 | 4 | 302 | CLA | CHC-C4B | 4.92 | 1.50 | 1.39 |
| 20 | 4 | 310 | CLA | CHD-C4C | 4.92 | 1.50 | 1.39 |
| 20 | A | 804 | CLA | C3D-C4D | -4.91 | 1.33 | 1.44 |
| 20 | B | 832 | CLA | C3D-C4D | -4.91 | 1.33 | 1.44 |
| 20 | A | 808 | CLA | CHC-C4B | 4.91 | 1.50 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 301 | CLA | CAB-C3B | -4.91 | 1.34 | 1.47 |
| 20 | B | 829 | CLA | C3D-C4D | -4.91 | 1.33 | 1.44 |
| 20 | B | 838 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 20 | H | 110 | CLA | C3D-C4D | -4.91 | 1.33 | 1.44 |
| 20 | A | 828 | CLA | C3D-C4D | -4.91 | 1.33 | 1.44 |
| 20 | A | 818 | CLA | C4C-C3C | -4.91 | 1.36 | 1.45 |
| 20 | B | 826 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 20 | B | 827 | CLA | CHC-C4B | 4.90 | 1.50 | 1.39 |
| 20 | 2 | 302 | CLA | CHD-C1D | 4.90 | 1.47 | 1.38 |
| 20 | B | 812 | CLA | CHD-C1D | 4.90 | 1.47 | 1.38 |
| 20 | B | 815 | CLA | CHC-C4B | 4.90 | 1.50 | 1.39 |
| 20 | 4 | 315 | CLA | CAB-C3B | -4.90 | 1.34 | 1.47 |
| 20 | B | 824 | CLA | CHD-C4C | 4.90 | 1.50 | 1.39 |
| 20 | 3 | 317 | CLA | C3D-C4D | -4.90 | 1.33 | 1.44 |
| 20 | A | 803 | CLA | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 20 | 4 | 302 | CLA | C3A-C2A | -4.90 | 1.49 | 1.54 |
| 20 | R | 107 | CLA | O2A-CGA | 4.90 | 1.47 | 1.33 |
| 20 | 2 | 307 | CLA | CHC-C1C | 4.90 | 1.48 | 1.38 |
| 20 | B | 807 | CLA | C3D-C4D | -4.89 | 1.33 | 1.44 |
| 20 | A | 824 | CLA | CHC-C4B | 4.89 | 1.50 | 1.39 |
| 20 | 2 | 302 | CLA | CHD-C4C | 4.89 | 1.50 | 1.39 |
| 20 | 1 | 215 | CLA | C4C-C3C | -4.89 | 1.36 | 1.45 |
| 20 | A | 818 | CLA | CHD-C4C | 4.89 | 1.50 | 1.39 |
| 20 | 3 | 307 | CLA | CAB-C3B | -4.88 | 1.34 | 1.47 |
| 20 | A | 826 | CLA | C3D-C4D | -4.88 | 1.33 | 1.44 |
| 20 | B | 820 | CLA | C3D-C4D | -4.88 | 1.33 | 1.44 |
| 20 | A | 825 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 20 | A | 817 | CLA | C3D-C4D | -4.88 | 1.33 | 1.44 |
| 20 | L | 207 | CLA | CAB-C3B | -4.88 | 1.34 | 1.47 |
| 20 | A | 822 | CLA | O2A-CGA | 4.88 | 1.47 | 1.33 |
| 20 | I | 102 | CLA | O2A-CGA | 4.87 | 1.47 | 1.33 |
| 20 | 4 | 315 | CLA | CHD-C1D | 4.87 | 1.47 | 1.38 |
| 20 | B | 835 | CLA | CHC-C4B | 4.87 | 1.50 | 1.39 |
| 20 | A | 811 | CLA | CAB-C3B | -4.87 | 1.34 | 1.47 |
| 20 | A | 805 | CLA | C3D-C4D | -4.87 | 1.33 | 1.44 |
| 20 | A | 806 | CLA | C3D-C4D | -4.87 | 1.33 | 1.44 |
| 20 | A | 809 | CLA | C3D-C4D | -4.86 | 1.33 | 1.44 |
| 20 | A | 822 | CLA | CHC-C4B | 4.86 | 1.50 | 1.39 |
| 20 | A | 827 | CLA | O2A-CGA | 4.86 | 1.47 | 1.33 |
| 20 | 4 | 301 | CLA | CHC-C4B | 4.86 | 1.50 | 1.39 |
| 20 | A | 812 | CLA | C3D-C4D | -4.85 | 1.33 | 1.44 |
| 20 | H | 108 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 850 | CLA | CHC-C4B | 4.85 | 1.50 | 1.39 |
| 20 | B | 828 | CLA | CAB-C3B | -4.85 | 1.34 | 1.47 |
| 20 | B | 837 | CLA | C3D-C4D | -4.85 | 1.33 | 1.44 |
| 20 | A | 830 | CLA | C3D-C4D | -4.85 | 1.33 | 1.44 |
| 20 | A | 840 | CLA | CHC-C4B | 4.85 | 1.50 | 1.39 |
| 20 | B | 841 | CLA | CAB-C3B | -4.85 | 1.34 | 1.47 |
| 20 | 4 | 317 | CLA | C3D-C4D | -4.84 | 1.33 | 1.44 |
| 20 | B | 802 | CLA | CHC-C4B | 4.84 | 1.50 | 1.39 |
| 20 | B | 818 | CLA | O2A-CGA | 4.84 | 1.47 | 1.33 |
| 20 | 4 | 305 | CLA | CAB-C3B | -4.84 | 1.34 | 1.47 |
| 20 | J | 101 | CLA | CAB-C3B | -4.84 | 1.34 | 1.47 |
| 20 | G | 105 | CLA | CAB-C3B | -4.84 | 1.34 | 1.47 |
| 20 | I | 102 | CLA | CAB-C3B | -4.84 | 1.34 | 1.47 |
| 20 | 2 | 307 | CLA | CAB-C3B | -4.84 | 1.34 | 1.47 |
| 20 | 1 | 205 | CLA | C3D-C4D | -4.84 | 1.33 | 1.44 |
| 20 | L | 204 | CLA | C3D-C4D | -4.84 | 1.33 | 1.44 |
| 20 | A | 850 | CLA | CHC-C4B | 4.84 | 1.50 | 1.39 |
| 20 | B | 829 | CLA | CHC-C4B | 4.84 | 1.50 | 1.39 |
| 20 | J | 101 | CLA | CHC-C4B | 4.84 | 1.50 | 1.39 |
| 20 | 4 | 315 | CLA | C3D-C4D | -4.83 | 1.33 | 1.44 |
| 20 | A | 806 | CLA | CHC-C4B | 4.83 | 1.50 | 1.39 |
| 20 | B | 839 | CLA | CAB-C3B | -4.83 | 1.34 | 1.47 |
| 20 | 2 | 309 | CLA | CHD-C1D | 4.83 | 1.49 | 1.38 |
| 20 | B | 833 | CLA | CAB-C3B | -4.83 | 1.34 | 1.47 |
| 20 | B | 836 | CLA | CHC-C4B | 4.83 | 1.50 | 1.39 |
| 20 | 3 | 310 | CLA | CHD-C1D | 4.83 | 1.47 | 1.38 |
| 20 | L | 203 | CLA | CAB-C3B | -4.82 | 1.34 | 1.47 |
| 20 | A | 809 | CLA | CAB-C3B | -4.82 | 1.34 | 1.47 |
| 20 | A | 811 | CLA | CHC-C4B | 4.82 | 1.50 | 1.39 |
| 20 | B | 825 | CLA | C3D-C4D | -4.82 | 1.33 | 1.44 |
| 20 | A | 807 | CLA | CHC-C4B | 4.82 | 1.50 | 1.39 |
| 20 | L | 202 | CLA | CAB-C3B | -4.82 | 1.34 | 1.47 |
| 20 | A | 815 | CLA | C3D-C4D | -4.82 | 1.33 | 1.44 |
| 20 | 1 | 210 | CLA | C3D-C4D | -4.81 | 1.33 | 1.44 |
| 20 | B | 841 | CLA | C3D-C4D | -4.81 | 1.33 | 1.44 |
| 20 | 1 | 213 | CLA | CAB-C3B | -4.81 | 1.34 | 1.47 |
| 20 | B | 806 | CLA | C3D-C4D | -4.81 | 1.33 | 1.44 |
| 20 | 2 | 311 | CLA | CHC-C4B | 4.81 | 1.50 | 1.39 |
| 20 | F | 206 | CLA | C3A-C2A | -4.81 | 1.50 | 1.54 |
| 20 | R | 107 | CLA | C3D-C4D | -4.81 | 1.33 | 1.44 |
| 20 | A | 807 | CLA | CAB-C3B | -4.81 | 1.34 | 1.47 |
| 20 | A | 823 | CLA | CAB-C3B | -4.81 | 1.34 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 817 | CLA | CAB-C3B | -4.81 | 1.34 | 1.47 |
| 20 | 1 | 215 | CLA | C3D-C4D | -4.81 | 1.33 | 1.44 |
| 20 | L | 204 | CLA | CAB-C3B | -4.80 | 1.34 | 1.47 |
| 20 | L | 208 | CLA | CAB-C3B | -4.80 | 1.34 | 1.47 |
| 20 | 4 | 315 | CLA | CHD-C4C | 4.80 | 1.50 | 1.39 |
| 20 | A | 826 | CLA | O2D-CGD | 4.80 | 1.44 | 1.33 |
| 20 | A | 816 | CLA | CHC-C4B | 4.80 | 1.50 | 1.39 |
| 20 | A | 801 | CLA | O2A-CGA | 4.80 | 1.47 | 1.33 |
| 20 | 2 | 314 | CLA | CHD-C1D | 4.79 | 1.47 | 1.38 |
| 20 | 3 | 311 | CLA | CAB-C3B | -4.79 | 1.34 | 1.47 |
| 20 | A | 828 | CLA | CHC-C4B | 4.79 | 1.50 | 1.39 |
| 20 | 3 | 303 | CLA | C3D-C4D | -4.79 | 1.33 | 1.44 |
| 20 | 4 | 315 | CLA | O2D-CGD | 4.79 | 1.44 | 1.33 |
| 20 | B | 822 | CLA | C3D-C4D | -4.79 | 1.33 | 1.44 |
| 20 | 1 | 211 | CLA | CHD-C4C | 4.79 | 1.50 | 1.39 |
| 20 | 1 | 211 | CLA | O2A-CGA | 4.79 | 1.47 | 1.33 |
| 20 | H | 109 | CLA | C3D-C4D | -4.79 | 1.33 | 1.44 |
| 20 | A | 827 | CLA | CHC-C4B | 4.79 | 1.50 | 1.39 |
| 20 | F | 201 | CLA | CHC-C1C | 4.79 | 1.48 | 1.38 |
| 20 | 4 | 303 | CLA | C3D-C4D | -4.78 | 1.33 | 1.44 |
| 23 | B | 843 | PQN | C10-C5 | 4.78 | 1.48 | 1.40 |
| 20 | K | 103 | CLA | CAB-C3B | -4.78 | 1.34 | 1.47 |
| 20 | A | 813 | CLA | C3D-C4D | -4.78 | 1.33 | 1.44 |
| 20 | B | 839 | CLA | CHD-C4C | 4.78 | 1.50 | 1.39 |
| 20 | A | 811 | CLA | O2A-CGA | 4.78 | 1.47 | 1.33 |
| 20 | A | 819 | CLA | C3D-C4D | -4.77 | 1.33 | 1.44 |
| 20 | L | 201 | CLA | CAB-C3B | -4.77 | 1.34 | 1.47 |
| 20 | H | 101 | CLA | CHC-C4B | 4.77 | 1.50 | 1.39 |
| 20 | A | 835 | CLA | CHC-C4B | 4.77 | 1.50 | 1.39 |
| 20 | B | 826 | CLA | CHC-C4B | 4.77 | 1.50 | 1.39 |
| 20 | B | 813 | CLA | C3D-C4D | -4.77 | 1.33 | 1.44 |
| 20 | K | 101 | CLA | CAB-C3B | -4.77 | 1.34 | 1.47 |
| 20 | B | 831 | CLA | CAB-C3B | -4.77 | 1.34 | 1.47 |
| 20 | 1 | 207 | CLA | C3D-C4D | -4.77 | 1.33 | 1.44 |
| 20 | B | 815 | CLA | C3D-C4D | -4.77 | 1.33 | 1.44 |
| 20 | B | 816 | CLA | C3D-C4D | -4.77 | 1.33 | 1.44 |
| 20 | A | 808 | CLA | O2A-CGA | 4.77 | 1.47 | 1.33 |
| 20 | A | 811 | CLA | C3D-C4D | -4.76 | 1.33 | 1.44 |
| 20 | B | 850 | CLA | CAB-C3B | -4.76 | 1.34 | 1.47 |
| 20 | L | 207 | CLA | C3D-C4D | -4.76 | 1.33 | 1.44 |
| 20 | 1 | 207 | CLA | O2A-CGA | 4.76 | 1.47 | 1.33 |
| 20 | A | 821 | CLA | CAB-C3B | -4.76 | 1.34 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 815 | CLA | O2A-CGA | 4.76 | 1.47 | 1.33 |
| 20 | A | 812 | CLA | O2A-CGA | 4.76 | 1.47 | 1.33 |
| 20 | B | 814 | CLA | C3D-C4D | -4.76 | 1.33 | 1.44 |
| 20 | 1 | 201 | CLA | CHC-C1C | 4.76 | 1.48 | 1.38 |
| 20 | B | 820 | CLA | CAB-C3B | -4.75 | 1.34 | 1.47 |
| 20 | J | 103 | CLA | O2D-CGD | 4.75 | 1.44 | 1.33 |
| 20 | A | 829 | CLA | CHC-C4B | 4.75 | 1.50 | 1.39 |
| 20 | B | 837 | CLA | O2A-CGA | 4.75 | 1.47 | 1.33 |
| 20 | A | 838 | CLA | CAB-C3B | -4.75 | 1.34 | 1.47 |
| 20 | B | 810 | CLA | O2A-CGA | 4.75 | 1.47 | 1.33 |
| 20 | 3 | 313 | CLA | C3D-C4D | -4.75 | 1.33 | 1.44 |
| 20 | B | 818 | CLA | C3D-C4D | -4.75 | 1.33 | 1.44 |
| 20 | 1 | 213 | CLA | OBD-CAD | 4.75 | 1.30 | 1.22 |
| 20 | B | 824 | CLA | CHC-C4B | 4.74 | 1.50 | 1.39 |
| 20 | 1 | 206 | CLA | C3D-C4D | -4.74 | 1.33 | 1.44 |
| 20 | A | 849 | CLA | CAB-C3B | -4.74 | 1.34 | 1.47 |
| 20 | A | 830 | CLA | CHC-C4B | 4.74 | 1.50 | 1.39 |
| 20 | 2 | 302 | CLA | C4C-C3C | -4.74 | 1.36 | 1.45 |
| 20 | F | 206 | CLA | CAB-C3B | -4.74 | 1.34 | 1.47 |
| 20 | H | 102 | CLA | C3D-C4D | -4.74 | 1.33 | 1.44 |
| 20 | 2 | 306 | CLA | CHD-C1D | 4.73 | 1.48 | 1.38 |
| 20 | A | 830 | CLA | CAB-C3B | -4.73 | 1.34 | 1.47 |
| 20 | A | 825 | CLA | CHC-C4B | 4.73 | 1.50 | 1.39 |
| 20 | 4 | 304 | CLA | O2A-CGA | 4.73 | 1.47 | 1.33 |
| 20 | K | 102 | CLA | CHC-C4B | 4.73 | 1.50 | 1.39 |
| 20 | B | 821 | CLA | CAB-C3B | -4.73 | 1.34 | 1.47 |
| 20 | A | 833 | CLA | CHC-C4B | 4.73 | 1.50 | 1.39 |
| 20 | B | 842 | CLA | C3D-C4D | -4.72 | 1.33 | 1.44 |
| 20 | B | 825 | CLA | CHC-C4B | 4.72 | 1.50 | 1.39 |
| 20 | 2 | 307 | CLA | O2A-CGA | 4.72 | 1.47 | 1.33 |
| 20 | L | 204 | CLA | O2A-CGA | 4.72 | 1.47 | 1.33 |
| 20 | 4 | 305 | CLA | CHD-C4C | 4.72 | 1.50 | 1.39 |
| 20 | 4 | 310 | CLA | CHD-C1D | 4.72 | 1.47 | 1.38 |
| 20 | A | 840 | CLA | CAB-C3B | -4.72 | 1.34 | 1.47 |
| 20 | L | 203 | CLA | CHC-C4B | 4.71 | 1.50 | 1.39 |
| 20 | A | 813 | CLA | CHC-C4B | 4.71 | 1.50 | 1.39 |
| 20 | 4 | 304 | CLA | CAB-C3B | -4.71 | 1.34 | 1.47 |
| 20 | B | 840 | CLA | O2A-CGA | 4.71 | 1.47 | 1.33 |
| 20 | 4 | 314 | CLA | CHC-C4B | 4.71 | 1.51 | 1.40 |
| 20 | 1 | 202 | CLA | C3D-C4D | -4.71 | 1.33 | 1.44 |
| 20 | A | 822 | CLA | C3D-C4D | -4.71 | 1.33 | 1.44 |
| 20 | 1 | 211 | CLA | CHD-C1D | 4.71 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 825 | CLA | OBD-CAD | 4.71 | 1.30 | 1.22 |
| 20 | 1 | 207 | CLA | CAB-C3B | -4.70 | 1.34 | 1.47 |
| 20 | 2 | 315 | CLA | CHD-C1D | 4.70 | 1.48 | 1.38 |
| 20 | 3 | 316 | CLA | CHD-C1D | 4.70 | 1.48 | 1.38 |
| 20 | B | 823 | CLA | CHC-C4B | 4.70 | 1.50 | 1.39 |
| 20 | B | 820 | CLA | O2A-CGA | 4.70 | 1.47 | 1.33 |
| 20 | A | 816 | CLA | CAB-C3B | -4.70 | 1.34 | 1.47 |
| 20 | K | 102 | CLA | CAB-C3B | -4.70 | 1.34 | 1.47 |
| 20 | B | 839 | CLA | O2D-CGD | 4.70 | 1.44 | 1.33 |
| 20 | H | 108 | CLA | CHD-C1D | 4.69 | 1.47 | 1.38 |
| 20 | B | 807 | CLA | O2A-CGA | 4.69 | 1.46 | 1.30 |
| 20 | A | 831 | CLA | CHD-C1D | 4.69 | 1.47 | 1.38 |
| 20 | K | 104 | CLA | CHC-C4B | 4.69 | 1.49 | 1.39 |
| 20 | A | 821 | CLA | C3D-C4D | -4.69 | 1.33 | 1.44 |
| 20 | 1 | 206 | CLA | CAB-C3B | -4.68 | 1.34 | 1.47 |
| 20 | L | 201 | CLA | O2A-CGA | 4.68 | 1.47 | 1.33 |
| 20 | L | 201 | CLA | C3D-C4D | -4.68 | 1.33 | 1.44 |
| 20 | A | 829 | CLA | CAB-C3B | -4.68 | 1.34 | 1.47 |
| 20 | A | 832 | CLA | CHC-C4B | 4.68 | 1.49 | 1.39 |
| 20 | A | 837 | CLA | C3D-C4D | -4.68 | 1.33 | 1.44 |
| 20 | 4 | 304 | CLA | C3D-C4D | -4.67 | 1.33 | 1.44 |
| 20 | B | 819 | CLA | CHC-C4B | 4.67 | 1.49 | 1.39 |
| 20 | B | 807 | CLA | CAB-C3B | -4.67 | 1.34 | 1.47 |
| 20 | 2 | 305 | CLA | C3D-C4D | -4.67 | 1.33 | 1.44 |
| 22 | B | 801 | BCR | C20-C19 | -4.67 | 1.22 | 1.34 |
| 20 | A | 817 | CLA | O2A-CGA | 4.67 | 1.47 | 1.33 |
| 20 | F | 207 | CLA | CAB-C3B | -4.67 | 1.34 | 1.47 |
| 20 | B | 819 | CLA | O2D-CGD | 4.67 | 1.44 | 1.33 |
| 20 | B | 837 | CLA | CHC-C4B | 4.67 | 1.49 | 1.39 |
| 20 | B | 817 | CLA | C3D-C4D | -4.67 | 1.33 | 1.44 |
| 20 | A | 830 | CLA | O2D-CGD | 4.66 | 1.44 | 1.33 |
| 20 | B | 821 | CLA | C3D-C4D | -4.66 | 1.33 | 1.44 |
| 20 | 2 | 305 | CLA | CAB-C3B | -4.66 | 1.34 | 1.47 |
| 20 | B | 832 | CLA | O2A-CGA | 4.66 | 1.47 | 1.33 |
| 20 | A | 850 | CLA | C3D-C4D | -4.66 | 1.33 | 1.44 |
| 20 | A | 810 | CLA | O2A-CGA | 4.66 | 1.46 | 1.30 |
| 20 | 1 | 206 | CLA | OBD-CAD | 4.65 | 1.30 | 1.22 |
| 20 | B | 831 | CLA | O2A-CGA | 4.65 | 1.46 | 1.33 |
| 20 | B | 810 | CLA | CHC-C4B | 4.65 | 1.49 | 1.39 |
| 20 | B | 813 | CLA | CHC-C4B | 4.64 | 1.49 | 1.39 |
| 20 | A | 836 | CLA | CHC-C4B | 4.64 | 1.49 | 1.39 |
| 20 | 2 | 303 | CLA | O2A-CGA | 4.64 | 1.46 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 839 | CLA | CHC-C4B | 4.64 | 1.49 | 1.39 |
| 20 | 3 | 310 | CLA | CHD-C4C | 4.64 | 1.49 | 1.39 |
| 20 | 4 | 318 | CLA | O2D-CGD | 4.64 | 1.44 | 1.33 |
| 20 | 1 | 211 | CLA | C4C-C3C | -4.64 | 1.37 | 1.45 |
| 20 | 1 | 201 | CLA | CAB-C3B | -4.64 | 1.34 | 1.47 |
| 20 | H | 109 | CLA | O2A-CGA | 4.63 | 1.46 | 1.33 |
| 20 | 2 | 304 | CLA | CHD-C1D | 4.63 | 1.48 | 1.38 |
| 20 | A | 820 | CLA | O2A-CGA | 4.62 | 1.46 | 1.33 |
| 20 | 4 | 313 | CLA | C3D-C4D | -4.62 | 1.33 | 1.44 |
| 20 | H | 108 | CLA | CHD-C4C | 4.62 | 1.49 | 1.39 |
| 20 | A | 809 | CLA | O2A-CGA | 4.62 | 1.46 | 1.33 |
| 20 | 2 | 305 | CLA | O2A-CGA | 4.62 | 1.46 | 1.33 |
| 20 | B | 822 | CLA | O2A-CGA | 4.62 | 1.47 | 1.33 |
| 20 | B | 821 | CLA | O2A-CGA | 4.62 | 1.46 | 1.33 |
| 20 | B | 802 | CLA | O2A-CGA | 4.62 | 1.46 | 1.33 |
| 20 | B | 803 | CLA | CHC-C4B | 4.61 | 1.49 | 1.39 |
| 20 | 1 | 213 | CLA | C1B-NB | -4.61 | 1.32 | 1.37 |
| 20 | H | 101 | CLA | CAB-C3B | -4.61 | 1.34 | 1.47 |
| 20 | R | 108 | CLA | C3D-C4D | -4.61 | 1.33 | 1.44 |
| 20 | R | 108 | CLA | CAB-C3B | -4.61 | 1.34 | 1.47 |
| 20 | H | 110 | CLA | O2A-CGA | 4.60 | 1.46 | 1.33 |
| 20 | A | 831 | CLA | O2D-CGD | 4.60 | 1.44 | 1.33 |
| 20 | A | 836 | CLA | OBD-CAD | 4.60 | 1.30 | 1.22 |
| 20 | H | 109 | CLA | CAB-C3B | -4.60 | 1.34 | 1.47 |
| 20 | L | 207 | CLA | O2A-CGA | 4.60 | 1.46 | 1.33 |
| 20 | H | 102 | CLA | O2A-CGA | 4.60 | 1.46 | 1.33 |
| 20 | A | 822 | CLA | CAB-C3B | -4.60 | 1.34 | 1.47 |
| 20 | B | 818 | CLA | CAB-C3B | -4.59 | 1.34 | 1.47 |
| 20 | A | 825 | CLA | O2A-CGA | 4.59 | 1.46 | 1.33 |
| 20 | 3 | 307 | CLA | C1C-C2C | -4.59 | 1.35 | 1.44 |
| 20 | A | 815 | CLA | O2A-CGA | 4.58 | 1.46 | 1.33 |
| 20 | 1 | 206 | CLA | O2A-CGA | 4.58 | 1.46 | 1.33 |
| 20 | B | 816 | CLA | O2A-CGA | 4.58 | 1.46 | 1.33 |
| 20 | A | 821 | CLA | CHC-C4B | 4.58 | 1.49 | 1.39 |
| 20 | K | 103 | CLA | CHC-C4B | 4.58 | 1.49 | 1.39 |
| 20 | A | 819 | CLA | CAB-C3B | -4.57 | 1.35 | 1.47 |
| 20 | A | 832 | CLA | O2A-CGA | 4.57 | 1.46 | 1.33 |
| 20 | B | 841 | CLA | O2A-CGA | 4.57 | 1.46 | 1.33 |
| 20 | B | 825 | CLA | O2A-CGA | 4.57 | 1.46 | 1.33 |
| 20 | A | 835 | CLA | O2A-CGA | 4.57 | 1.46 | 1.33 |
| 20 | A | 832 | CLA | CAB-C3B | -4.57 | 1.35 | 1.47 |
| 20 | J | 103 | CLA | CHC-C4B | 4.57 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | H | 102 | CLA | CAB-C3B | -4.56 | 1.35 | 1.47 |
| 20 | 4 | 310 | CLA | CAB-C3B | -4.56 | 1.35 | 1.47 |
| 20 | B | 813 | CLA | O2A-CGA | 4.56 | 1.46 | 1.33 |
| 20 | B | 833 | CLA | CHC-C4B | 4.56 | 1.49 | 1.39 |
| 20 | L | 208 | CLA | O2A-CGA | 4.55 | 1.46 | 1.33 |
| 20 | 1 | 211 | CLA | CHC-C4B | 4.55 | 1.49 | 1.39 |
| 20 | 4 | 305 | CLA | C4C-C3C | -4.55 | 1.37 | 1.45 |
| 20 | 4 | 310 | CLA | C4C-C3C | -4.55 | 1.37 | 1.45 |
| 20 | A | 828 | CLA | O2A-CGA | 4.55 | 1.46 | 1.33 |
| 20 | B | 810 | CLA | C3D-C4D | -4.55 | 1.33 | 1.44 |
| 20 | A | 810 | CLA | CAB-C3B | -4.55 | 1.35 | 1.47 |
| 20 | L | 208 | CLA | C3D-C4D | -4.55 | 1.33 | 1.44 |
| 20 | A | 827 | CLA | C3D-C4D | -4.54 | 1.33 | 1.44 |
| 20 | B | 839 | CLA | CHD-C1D | 4.54 | 1.47 | 1.38 |
| 20 | A | 813 | CLA | CAB-C3B | -4.53 | 1.35 | 1.47 |
| 20 | 1 | 204 | CLA | C1B-NB | -4.53 | 1.32 | 1.37 |
| 20 | K | 103 | CLA | C1B-NB | -4.53 | 1.32 | 1.37 |
| 20 | B | 841 | CLA | CHC-C4B | 4.53 | 1.49 | 1.39 |
| 20 | 1 | 202 | CLA | CAB-C3B | -4.53 | 1.35 | 1.47 |
| 20 | A | 801 | CLA | CHC-C4B | 4.53 | 1.49 | 1.39 |
| 20 | F | 201 | CLA | CHD-C4C | 4.53 | 1.49 | 1.39 |
| 20 | B | 814 | CLA | O2A-CGA | 4.52 | 1.46 | 1.33 |
| 20 | A | 815 | CLA | CAB-C3B | -4.51 | 1.35 | 1.47 |
| 20 | F | 207 | CLA | CHC-C4B | 4.51 | 1.49 | 1.39 |
| 20 | B | 808 | CLA | CHC-C4B | 4.51 | 1.49 | 1.39 |
| 20 | L | 202 | CLA | O2A-CGA | 4.51 | 1.46 | 1.33 |
| 20 | 2 | 303 | CLA | C4C-C3C | -4.51 | 1.37 | 1.45 |
| 20 | A | 819 | CLA | O2A-CGA | 4.50 | 1.46 | 1.33 |
| 20 | B | 816 | CLA | CAB-C3B | -4.50 | 1.35 | 1.47 |
| 20 | 3 | 313 | CLA | O2A-CGA | 4.50 | 1.46 | 1.33 |
| 20 | B | 803 | CLA | O2A-CGA | 4.50 | 1.46 | 1.33 |
| 20 | 4 | 305 | CLA | CHC-C4B | 4.50 | 1.49 | 1.39 |
| 20 | B | 834 | CLA | O2A-CGA | 4.50 | 1.45 | 1.30 |
| 20 | B | 803 | CLA | C3D-C4D | -4.49 | 1.34 | 1.44 |
| 20 | A | 833 | CLA | CAB-C3B | -4.49 | 1.35 | 1.47 |
| 20 | A | 805 | CLA | CAB-C3B | -4.49 | 1.35 | 1.47 |
| 20 | 1 | 215 | CLA | O2A-CGA | 4.49 | 1.46 | 1.33 |
| 20 | B | 824 | CLA | O2D-CGD | 4.49 | 1.44 | 1.33 |
| 20 | 3 | 314 | CLA | C1C-C2C | -4.49 | 1.35 | 1.44 |
| 20 | B | 817 | CLA | CAB-C3B | -4.47 | 1.35 | 1.47 |
| 20 | A | 838 | CLA | O2A-CGA | 4.47 | 1.46 | 1.33 |
| 20 | B | 835 | CLA | O2A-CGA | 4.47 | 1.45 | 1.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 840 | CLA | C3D-C4D | -4.47 | 1.34 | 1.44 |
| 20 | 1 | 202 | CLA | CHC-C4B | 4.47 | 1.49 | 1.39 |
| 20 | B | 839 | CLA | O2A-CGA | 4.47 | 1.46 | 1.33 |
| 20 | A | 830 | CLA | O2A-CGA | 4.46 | 1.46 | 1.33 |
| 20 | 3 | 314 | CLA | CHC-C1C | 4.46 | 1.47 | 1.38 |
| 20 | A | 813 | CLA | O2A-CGA | 4.46 | 1.46 | 1.33 |
| 20 | H | 108 | CLA | O2A-CGA | 4.46 | 1.46 | 1.33 |
| 20 | A | 825 | CLA | CAB-C3B | -4.46 | 1.35 | 1.47 |
| 20 | B | 830 | CLA | CAB-C3B | -4.46 | 1.35 | 1.47 |
| 20 | 2 | 311 | CLA | CAB-C3B | -4.45 | 1.35 | 1.47 |
| 20 | B | 830 | CLA | CHC-C4B | 4.45 | 1.49 | 1.39 |
| 20 | A | 805 | CLA | CHC-C4B | 4.45 | 1.49 | 1.39 |
| 20 | 4 | 302 | CLA | OBD-CAD | 4.44 | 1.30 | 1.22 |
| 20 | K | 104 | CLA | O2A-CGA | 4.44 | 1.46 | 1.33 |
| 20 | B | 819 | CLA | C4C-C3C | -4.44 | 1.37 | 1.45 |
| 20 | 1 | 205 | CLA | OBD-CAD | 4.44 | 1.30 | 1.22 |
| 20 | H | 110 | CLA | CAB-C3B | -4.44 | 1.35 | 1.47 |
| 20 | R | 107 | CLA | CAB-C3B | -4.43 | 1.35 | 1.47 |
| 20 | A | 820 | CLA | CAB-C3B | -4.42 | 1.35 | 1.47 |
| 20 | 1 | 213 | CLA | O2A-CGA | 4.42 | 1.46 | 1.33 |
| 20 | B | 809 | CLA | CHC-C4B | 4.42 | 1.49 | 1.39 |
| 20 | R | 108 | CLA | OBD-CAD | 4.42 | 1.30 | 1.22 |
| 20 | 3 | 310 | CLA | CHC-C4B | 4.41 | 1.49 | 1.39 |
| 20 | A | 837 | CLA | CHC-C4B | 4.41 | 1.49 | 1.39 |
| 20 | J | 101 | CLA | O2A-CGA | 4.41 | 1.46 | 1.33 |
| 20 | 1 | 215 | CLA | CHD-C1D | 4.41 | 1.46 | 1.38 |
| 20 | B | 828 | CLA | O2A-CGA | 4.41 | 1.46 | 1.33 |
| 20 | B | 826 | CLA | O2A-CGA | 4.40 | 1.46 | 1.33 |
| 20 | 1 | 202 | CLA | OBD-CAD | 4.40 | 1.30 | 1.22 |
| 22 | B | 801 | BCR | C17-C18 | -4.40 | 1.30 | 1.35 |
| 20 | A | 828 | CLA | CAB-C3B | -4.40 | 1.35 | 1.47 |
| 20 | 3 | 313 | CLA | CAB-C3B | -4.39 | 1.35 | 1.47 |
| 20 | 1 | 203 | CLA | C4C-C3C | -4.39 | 1.37 | 1.45 |
| 20 | A | 839 | CLA | CHC-C4B | 4.38 | 1.49 | 1.39 |
| 20 | 3 | 312 | CLA | CHC-C4B | 4.38 | 1.51 | 1.40 |
| 20 | 3 | 310 | CLA | O2A-CGA | 4.38 | 1.46 | 1.33 |
| 20 | 2 | 303 | CLA | CHC-C4B | 4.38 | 1.49 | 1.39 |
| 20 | A | 804 | CLA | OBD-CAD | 4.38 | 1.30 | 1.22 |
| 20 | 2 | 314 | CLA | CHC-C4B | 4.37 | 1.49 | 1.39 |
| 20 | A | 851 | CLA | OBD-CAD | 4.37 | 1.30 | 1.22 |
| 20 | 1 | 215 | CLA | CAB-C3B | -4.37 | 1.35 | 1.47 |
| 20 | 4 | 304 | CLA | CHC-C4B | 4.37 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 308 | CLA | CHD-C1D | 4.37 | 1.48 | 1.38 |
| 20 | 3 | 311 | CLA | O2A-CGA | 4.37 | 1.46 | 1.33 |
| 20 | F | 201 | CLA | C1B-NB | -4.36 | 1.32 | 1.37 |
| 20 | A | 806 | CLA | OBD-CAD | 4.36 | 1.30 | 1.22 |
| 20 | A | 839 | CLA | C1B-NB | -4.36 | 1.32 | 1.37 |
| 20 | 2 | 316 | CLA | C1B-NB | -4.35 | 1.32 | 1.37 |
| 20 | A | 840 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 25 | B | 848 | LMG | O8-C28 | 4.35 | 1.46 | 1.33 |
| 20 | L | 208 | CLA | OBD-CAD | 4.35 | 1.30 | 1.22 |
| 20 | 4 | 306 | CLA | CHC-C4B | 4.35 | 1.49 | 1.39 |
| 20 | 4 | 304 | CLA | OBD-CAD | 4.35 | 1.30 | 1.22 |
| 20 | 4 | 318 | CLA | CHC-C4B | 4.35 | 1.49 | 1.39 |
| 20 | 2 | 316 | CLA | CHC-C4B | 4.35 | 1.49 | 1.39 |
| 20 | B | 838 | CLA | CHC-C4B | 4.34 | 1.49 | 1.39 |
| 20 | H | 109 | CLA | OBD-CAD | 4.34 | 1.30 | 1.22 |
| 20 | A | 818 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 20 | 2 | 308 | CLA | MG-NA | -4.34 | 1.96 | 2.06 |
| 20 | A | 831 | CLA | CHD-C4C | 4.34 | 1.49 | 1.39 |
| 20 | A | 818 | CLA | CHC-C4B | 4.34 | 1.49 | 1.39 |
| 20 | A | 821 | CLA | OBD-CAD | 4.33 | 1.29 | 1.22 |
| 20 | G | 105 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 20 | B | 827 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 20 | B | 840 | CLA | CAB-C3B | -4.33 | 1.35 | 1.47 |
| 20 | A | 806 | CLA | CAB-C3B | -4.33 | 1.35 | 1.47 |
| 20 | A | 837 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 20 | 4 | 318 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 20 | B | 806 | CLA | O2A-CGA | 4.32 | 1.46 | 1.33 |
| 20 | 4 | 301 | CLA | O2A-CGA | 4.32 | 1.46 | 1.33 |
| 20 | B | 842 | CLA | OBD-CAD | 4.32 | 1.29 | 1.22 |
| 20 | B | 838 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 20 | 4 | 303 | CLA | C1B-NB | -4.31 | 1.32 | 1.37 |
| 20 | 4 | 305 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 20 | 1 | 201 | CLA | C1B-NB | -4.31 | 1.32 | 1.37 |
| 20 | 4 | 317 | CLA | CHC-C4B | 4.30 | 1.49 | 1.39 |
| 20 | B | 815 | CLA | OBD-CAD | 4.30 | 1.29 | 1.22 |
| 20 | 1 | 215 | CLA | CHD-C4C | 4.30 | 1.49 | 1.39 |
| 20 | J | 103 | CLA | C1B-NB | -4.29 | 1.32 | 1.37 |
| 20 | 2 | 316 | CLA | C4B-NB | -4.29 | 1.32 | 1.37 |
| 20 | B | 808 | CLA | C4C-C3C | -4.29 | 1.37 | 1.45 |
| 20 | 1 | 209 | CLA | CHC-C4B | 4.29 | 1.50 | 1.40 |
| 20 | H | 108 | CLA | C4C-C3C | -4.28 | 1.37 | 1.45 |
| 25 | B | 848 | LMG | O7-C10 | 4.28 | 1.46 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 822 | CLA | OBD-CAD | 4.28 | 1.29 | 1.22 |
| 20 | 2 | 310 | CLA | CHC-C4B | 4.28 | 1.49 | 1.39 |
| 20 | B | 822 | CLA | CAB-C3B | -4.28 | 1.35 | 1.47 |
| 20 | 3 | 317 | CLA | OBD-CAD | 4.27 | 1.29 | 1.22 |
| 20 | B | 812 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 20 | 4 | 306 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 20 | 3 | 302 | CLA | CHC-C4B | 4.27 | 1.50 | 1.40 |
| 20 | A | 806 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 20 | B | 833 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 20 | 3 | 303 | CLA | OBD-CAD | 4.26 | 1.29 | 1.22 |
| 20 | A | 836 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 20 | A | 823 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 20 | 2 | 314 | CLA | C1B-NB | -4.25 | 1.32 | 1.37 |
| 20 | B | 824 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 20 | 2 | 302 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 20 | B | 808 | CLA | O2D-CGD | 4.24 | 1.43 | 1.33 |
| 20 | B | 823 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 20 | A | 801 | CLA | C3D-C4D | -4.24 | 1.34 | 1.44 |
| 20 | B | 817 | CLA | OBD-CAD | 4.24 | 1.29 | 1.22 |
| 20 | A | 849 | CLA | C3D-C4D | -4.24 | 1.34 | 1.44 |
| 20 | B | 812 | CLA | O2D-CGD | 4.23 | 1.43 | 1.33 |
| 20 | H | 101 | CLA | C3D-C4D | -4.23 | 1.34 | 1.44 |
| 20 | A | 834 | CLA | O2A-CGA | 4.22 | 1.46 | 1.33 |
| 20 | 2 | 316 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 20 | A | 809 | CLA | CHC-C4B | 4.22 | 1.48 | 1.39 |
| 20 | B | 812 | CLA | C4C-C3C | -4.22 | 1.37 | 1.45 |
| 20 | A | 807 | CLA | O2A-CGA | 4.20 | 1.46 | 1.33 |
| 20 | A | 831 | CLA | C1B-NB | -4.20 | 1.32 | 1.37 |
| 20 | R | 108 | CLA | CHB-C1B | 4.20 | 1.48 | 1.39 |
| 20 | B | 830 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 20 | H | 108 | CLA | CHC-C4B | 4.19 | 1.48 | 1.39 |
| 20 | A | 803 | CLA | C1B-NB | -4.19 | 1.32 | 1.37 |
| 20 | B | 829 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 20 | F | 201 | CLA | CHD-C1D | 4.19 | 1.46 | 1.38 |
| 20 | 4 | 310 | CLA | CHC-C4B | 4.19 | 1.48 | 1.39 |
| 20 | 3 | 314 | CLA | C1B-NB | -4.18 | 1.32 | 1.37 |
| 20 | 4 | 317 | CLA | C1B-NB | -4.18 | 1.32 | 1.37 |
| 20 | A | 824 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 20 | 3 | 315 | CLA | MG-NA | -4.18 | 1.96 | 2.06 |
| 20 | B | 807 | CLA | OBD-CAD | 4.17 | 1.29 | 1.22 |
| 20 | 1 | 211 | CLA | OBD-CAD | 4.17 | 1.29 | 1.22 |
| 20 | L | 203 | CLA | CHB-C1B | 4.17 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 816 | CLA | C4C-C3C | -4.17 | 1.37 | 1.45 |
| 20 | 4 | 303 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 20 | 4 | 303 | CLA | CHC-C4B | 4.16 | 1.48 | 1.39 |
| 20 | K | 102 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 20 | 2 | 302 | CLA | C1B-NB | -4.15 | 1.32 | 1.37 |
| 20 | 2 | 314 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 20 | 1 | 213 | CLA | CHC-C4B | 4.15 | 1.48 | 1.39 |
| 20 | 1 | 208 | CLA | CHC-C4B | 4.15 | 1.50 | 1.40 |
| 20 | A | 818 | CLA | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 20 | 4 | 309 | CLA | CHC-C4B | 4.14 | 1.50 | 1.40 |
| 20 | 1 | 211 | CLA | C1B-NB | -4.14 | 1.32 | 1.37 |
| 20 | A | 803 | CLA | O2A-CGA | 4.13 | 1.46 | 1.33 |
| 20 | A | 812 | CLA | CAB-C3B | -4.13 | 1.36 | 1.47 |
| 20 | 1 | 201 | CLA | O2A-CGA | 4.13 | 1.46 | 1.33 |
| 20 | A | 815 | CLA | OBD-CAD | 4.12 | 1.29 | 1.22 |
| 20 | A | 849 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 20 | F | 207 | CLA | C4C-C3C | -4.12 | 1.37 | 1.45 |
| 20 | A | 826 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 20 | A | 831 | CLA | C1C-C2C | -4.12 | 1.36 | 1.44 |
| 20 | 2 | 307 | CLA | CHB-C1B | 4.12 | 1.48 | 1.39 |
| 20 | 1 | 212 | CLA | CHC-C4B | 4.11 | 1.50 | 1.40 |
| 20 | F | 201 | CLA | CHC-C4B | 4.11 | 1.48 | 1.39 |
| 20 | 4 | 310 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 20 | A | 834 | CLA | OBD-CAD | 4.11 | 1.29 | 1.22 |
| 20 | A | 814 | CLA | CHC-C4B | 4.10 | 1.50 | 1.40 |
| 20 | 1 | 202 | CLA | C1B-NB | -4.10 | 1.32 | 1.37 |
| 20 | 2 | 316 | CLA | C4C-C3C | -4.10 | 1.38 | 1.45 |
| 20 | 2 | 311 | CLA | OBD-CAD | 4.10 | 1.29 | 1.22 |
| 20 | J | 103 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 20 | 4 | 312 | CLA | CHC-C4B | 4.10 | 1.50 | 1.40 |
| 20 | R | 107 | CLA | OBD-CAD | 4.10 | 1.29 | 1.22 |
| 20 | 3 | 307 | CLA | C1B-NB | -4.10 | 1.32 | 1.37 |
| 20 | A | 851 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 20 | A | 803 | CLA | C4C-C3C | -4.10 | 1.38 | 1.45 |
| 20 | 1 | 206 | CLA | CHB-C1B | 4.09 | 1.48 | 1.39 |
| 20 | 4 | 313 | CLA | C3A-C2A | -4.08 | 1.50 | 1.54 |
| 20 | B | 818 | CLA | OBD-CAD | 4.08 | 1.29 | 1.22 |
| 20 | 3 | 313 | CLA | OBD-CAD | 4.08 | 1.29 | 1.22 |
| 20 | 1 | 201 | CLA | OBD-CAD | 4.08 | 1.29 | 1.22 |
| 20 | F | 207 | CLA | OBD-CAD | 4.08 | 1.29 | 1.22 |
| 20 | F | 201 | CLA | O2A-CGA | 4.07 | 1.45 | 1.33 |
| 20 | L | 201 | CLA | OBD-CAD | 4.07 | 1.29 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 310 | CLA | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 20 | 1 | 215 | CLA | C1B-NB | -4.06 | 1.32 | 1.37 |
| 20 | 3 | 314 | CLA | CAB-C3B | -4.06 | 1.36 | 1.47 |
| 20 | A | 816 | CLA | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 20 | B | 808 | CLA | O2A-CGA | 4.06 | 1.45 | 1.33 |
| 20 | A | 816 | CLA | C1B-NB | -4.06 | 1.32 | 1.37 |
| 20 | B | 829 | CLA | CHB-C1B | 4.05 | 1.48 | 1.39 |
| 20 | A | 803 | CLA | CHC-C4B | 4.05 | 1.48 | 1.39 |
| 20 | A | 835 | CLA | OBD-CAD | 4.05 | 1.29 | 1.22 |
| 20 | 3 | 311 | CLA | OBD-CAD | 4.05 | 1.29 | 1.22 |
| 20 | 3 | 306 | CLA | CHC-C4B | 4.05 | 1.50 | 1.40 |
| 20 | 1 | 204 | CLA | MG-NA | -4.04 | 1.96 | 2.06 |
| 20 | B | 809 | CLA | O2A-CGA | 4.04 | 1.45 | 1.33 |
| 20 | B | 842 | CLA | C3A-C2A | -4.04 | 1.50 | 1.54 |
| 20 | A | 810 | CLA | OBD-CAD | 4.04 | 1.29 | 1.22 |
| 20 | 4 | 318 | CLA | C1B-NB | -4.03 | 1.32 | 1.37 |
| 20 | 4 | 315 | CLA | O2A-CGA | 4.03 | 1.45 | 1.33 |
| 20 | L | 202 | CLA | OBD-CAD | 4.03 | 1.29 | 1.22 |
| 20 | A | 831 | CLA | CHC-C4B | 4.02 | 1.48 | 1.39 |
| 20 | 2 | 307 | CLA | CHC-C4B | 4.02 | 1.48 | 1.39 |
| 20 | B | 812 | CLA | C1B-NB | -4.02 | 1.32 | 1.37 |
| 20 | B | 850 | CLA | O2A-CGA | 4.02 | 1.45 | 1.33 |
| 20 | A | 840 | CLA | OBD-CAD | 4.01 | 1.29 | 1.22 |
| 20 | A | 801 | CLA | CHB-C1B | 4.01 | 1.48 | 1.39 |
| 20 | 3 | 314 | CLA | C4B-NB | -4.01 | 1.32 | 1.37 |
| 20 | H | 110 | CLA | OBD-CAD | 4.01 | 1.29 | 1.22 |
| 20 | 1 | 207 | CLA | OBD-CAD | 4.00 | 1.29 | 1.22 |
| 20 | K | 103 | CLA | O2A-CGA | 4.00 | 1.45 | 1.33 |
| 20 | B | 813 | CLA | CAB-C3B | -4.00 | 1.36 | 1.47 |
| 20 | A | 821 | CLA | CHB-C1B | 4.00 | 1.48 | 1.39 |
| 20 | F | 201 | CLA | C1C-C2C | -4.00 | 1.36 | 1.44 |
| 20 | 1 | 204 | CLA | CHC-C4B | 3.99 | 1.48 | 1.39 |
| 20 | 3 | 305 | CLA | CHC-C4B | 3.99 | 1.50 | 1.40 |
| 20 | 4 | 303 | CLA | OBD-CAD | 3.99 | 1.29 | 1.22 |
| 20 | F | 206 | CLA | OBD-CAD | 3.99 | 1.29 | 1.22 |
| 20 | A | 828 | CLA | OBD-CAD | 3.99 | 1.29 | 1.22 |
| 20 | F | 205 | CLA | OBD-CAD | 3.99 | 1.29 | 1.22 |
| 20 | B | 817 | CLA | O2A-CGA | 3.99 | 1.45 | 1.33 |
| 20 | B | 813 | CLA | OBD-CAD | 3.99 | 1.29 | 1.22 |
| 20 | 3 | 308 | CLA | CHC-C4B | 3.98 | 1.50 | 1.40 |
| 20 | 3 | 314 | CLA | C4C-C3C | -3.98 | 1.38 | 1.45 |
| 20 | 3 | 309 | CLA | MG-NA | -3.97 | 1.96 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 823 | CLA | OBD-CAD | 3.97 | 1.29 | 1.22 |
| 20 | G | 105 | CLA | C4C-C3C | -3.97 | 1.38 | 1.45 |
| 20 | A | 830 | CLA | OBD-CAD | 3.97 | 1.29 | 1.22 |
| 20 | 3 | 310 | CLA | C4B-NB | -3.97 | 1.32 | 1.37 |
| 20 | B | 840 | CLA | OBD-CAD | 3.97 | 1.29 | 1.22 |
| 20 | L | 207 | CLA | OBD-CAD | 3.96 | 1.29 | 1.22 |
| 20 | B | 806 | CLA | OBD-CAD | 3.96 | 1.29 | 1.22 |
| 20 | L | 204 | CLA | CHB-C1B | 3.96 | 1.48 | 1.39 |
| 20 | 1 | 211 | CLA | CHB-C1B | 3.96 | 1.48 | 1.39 |
| 20 | 4 | 311 | CLA | CHC-C4B | 3.96 | 1.50 | 1.40 |
| 20 | 4 | 315 | CLA | C4C-C3C | -3.96 | 1.38 | 1.45 |
| 20 | 2 | 303 | CLA | C1B-NB | -3.96 | 1.32 | 1.37 |
| 20 | A | 831 | CLA | O2A-CGA | 3.96 | 1.44 | 1.33 |
| 20 | B | 820 | CLA | CHB-C1B | 3.96 | 1.48 | 1.39 |
| 20 | 4 | 306 | CLA | C1C-C2C | -3.95 | 1.36 | 1.44 |
| 20 | K | 102 | CLA | OBD-CAD | 3.94 | 1.29 | 1.22 |
| 20 | A | 833 | CLA | OBD-CAD | 3.94 | 1.29 | 1.22 |
| 20 | B | 838 | CLA | CHB-C1B | 3.93 | 1.48 | 1.39 |
| 20 | A | 812 | CLA | OBD-CAD | 3.93 | 1.29 | 1.22 |
| 20 | A | 807 | CLA | OBD-CAD | 3.92 | 1.29 | 1.22 |
| 20 | 3 | 307 | CLA | CHC-C4B | 3.92 | 1.48 | 1.39 |
| 20 | 4 | 303 | CLA | C1C-C2C | -3.91 | 1.37 | 1.44 |
| 20 | L | 203 | CLA | OBD-CAD | 3.91 | 1.29 | 1.22 |
| 20 | 3 | 315 | CLA | CHC-C4B | 3.90 | 1.49 | 1.40 |
| 20 | A | 814 | CLA | MG-NA | -3.90 | 1.97 | 2.06 |
| 20 | 1 | 214 | CLA | CHC-C4B | 3.90 | 1.49 | 1.40 |
| 20 | 4 | 301 | CLA | OBD-CAD | 3.90 | 1.29 | 1.22 |
| 20 | B | 830 | CLA | OBD-CAD | 3.89 | 1.29 | 1.22 |
| 20 | H | 102 | CLA | OBD-CAD | 3.89 | 1.29 | 1.22 |
| 20 | F | 207 | CLA | O2A-CGA | 3.89 | 1.44 | 1.33 |
| 20 | B | 824 | CLA | C1D-ND | -3.89 | 1.33 | 1.37 |
| 20 | 4 | 305 | CLA | OBD-CAD | 3.89 | 1.29 | 1.22 |
| 20 | K | 101 | CLA | O2A-CGA | 3.88 | 1.45 | 1.33 |
| 20 | B | 836 | CLA | O2A-CGA | 3.88 | 1.44 | 1.33 |
| 20 | 3 | 316 | CLA | MG-NA | -3.88 | 1.97 | 2.06 |
| 20 | 4 | 307 | CLA | CHC-C4B | 3.88 | 1.49 | 1.40 |
| 20 | H | 110 | CLA | CHB-C1B | 3.88 | 1.48 | 1.39 |
| 20 | A | 849 | CLA | C4C-C3C | -3.87 | 1.38 | 1.45 |
| 20 | K | 104 | CLA | C1B-NB | -3.87 | 1.33 | 1.37 |
| 20 | 2 | 304 | CLA | CHC-C4B | 3.87 | 1.49 | 1.40 |
| 20 | B | 812 | CLA | C4D-ND | -3.87 | 1.32 | 1.37 |
| 20 | A | 837 | CLA | C4C-C3C | -3.87 | 1.38 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 814 | CLA | C4C-C3C | -3.87 | 1.38 | 1.45 |
| 20 | 2 | 315 | CLA | CHC-C4B | 3.87 | 1.49 | 1.40 |
| 20 | A | 839 | CLA | OBD-CAD | 3.87 | 1.29 | 1.22 |
| 20 | L | 203 | CLA | O2A-CGA | 3.86 | 1.44 | 1.33 |
| 20 | 3 | 316 | CLA | CHC-C4B | 3.86 | 1.49 | 1.40 |
| 20 | H | 101 | CLA | OBD-CAD | 3.86 | 1.29 | 1.22 |
| 20 | K | 103 | CLA | C1C-C2C | -3.85 | 1.37 | 1.44 |
| 20 | A | 820 | CLA | OBD-CAD | 3.85 | 1.29 | 1.22 |
| 20 | 1 | 204 | CLA | C4C-C3C | -3.85 | 1.38 | 1.45 |
| 20 | 4 | 313 | CLA | OBD-CAD | 3.85 | 1.29 | 1.22 |
| 20 | 2 | 307 | CLA | OBD-CAD | 3.85 | 1.29 | 1.22 |
| 20 | A | 809 | CLA | C1C-C2C | -3.85 | 1.37 | 1.44 |
| 20 | 3 | 304 | CLA | MG-NA | -3.85 | 1.97 | 2.06 |
| 20 | B | 835 | CLA | OBD-CAD | 3.85 | 1.29 | 1.22 |
| 20 | B | 841 | CLA | CHB-C1B | 3.84 | 1.48 | 1.39 |
| 20 | A | 802 | CLA | CHC-C4B | 3.84 | 1.49 | 1.40 |
| 20 | A | 838 | CLA | OBD-CAD | 3.84 | 1.29 | 1.22 |
| 20 | B | 837 | CLA | CHB-C1B | 3.84 | 1.48 | 1.39 |
| 20 | A | 822 | CLA | OBD-CAD | 3.84 | 1.29 | 1.22 |
| 20 | A | 841 | CLA | CHC-C4B | 3.84 | 1.49 | 1.40 |
| 20 | G | 105 | CLA | OBD-CAD | 3.83 | 1.29 | 1.22 |
| 20 | A | 809 | CLA | CHB-C1B | 3.83 | 1.48 | 1.39 |
| 20 | 4 | 305 | CLA | CHB-C1B | 3.83 | 1.48 | 1.39 |
| 20 | 1 | 204 | CLA | O2A-CGA | 3.83 | 1.45 | 1.33 |
| 20 | B | 834 | CLA | OBD-CAD | 3.83 | 1.29 | 1.22 |
| 20 | 1 | 213 | CLA | C1C-C2C | -3.82 | 1.37 | 1.44 |
| 20 | A | 801 | CLA | OBD-CAD | 3.82 | 1.29 | 1.22 |
| 20 | 1 | 214 | CLA | MG-NA | -3.81 | 1.97 | 2.06 |
| 20 | H | 108 | CLA | C1C-C2C | -3.81 | 1.37 | 1.44 |
| 20 | 3 | 307 | CLA | OBD-CAD | 3.81 | 1.29 | 1.22 |
| 20 | 3 | 301 | CLA | CHB-C1B | 3.81 | 1.48 | 1.39 |
| 20 | A | 839 | CLA | C1C-C2C | -3.80 | 1.37 | 1.44 |
| 20 | 2 | 302 | CLA | OBD-CAD | 3.80 | 1.29 | 1.22 |
| 20 | J | 103 | CLA | C1C-C2C | -3.79 | 1.37 | 1.44 |
| 22 | A | 844 | BCR | C20-C19 | -3.79 | 1.24 | 1.34 |
| 20 | B | 810 | CLA | OBD-CAD | 3.79 | 1.29 | 1.22 |
| 20 | A | 850 | CLA | OBD-CAD | 3.79 | 1.29 | 1.22 |
| 20 | F | 207 | CLA | C1B-NB | -3.79 | 1.33 | 1.37 |
| 20 | 3 | 314 | CLA | O2A-CGA | 3.78 | 1.44 | 1.33 |
| 20 | 1 | 203 | CLA | OBD-CAD | 3.78 | 1.29 | 1.22 |
| 20 | A | 826 | CLA | OBD-CAD | 3.78 | 1.29 | 1.22 |
| 20 | A | 817 | CLA | OBD-CAD | 3.77 | 1.29 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 802 | CLA | OBD-CAD | 3.77 | 1.29 | 1.22 |
| 20 | J | 103 | CLA | OBD-CAD | 3.77 | 1.29 | 1.22 |
| 20 | 1 | 213 | CLA | C4C-C3C | -3.77 | 1.38 | 1.45 |
| 20 | B | 816 | CLA | OBD-CAD | 3.77 | 1.29 | 1.22 |
| 20 | 1 | 204 | CLA | C1C-C2C | -3.77 | 1.37 | 1.44 |
| 20 | 4 | 305 | CLA | C1B-NB | -3.76 | 1.33 | 1.37 |
| 20 | B | 826 | CLA | OBD-CAD | 3.76 | 1.29 | 1.22 |
| 20 | G | 105 | CLA | C1B-NB | -3.76 | 1.33 | 1.37 |
| 20 | A | 819 | CLA | OBD-CAD | 3.76 | 1.29 | 1.22 |
| 20 | A | 805 | CLA | CHB-C1B | 3.76 | 1.47 | 1.39 |
| 20 | H | 102 | CLA | CHB-C1B | 3.75 | 1.47 | 1.39 |
| 20 | A | 831 | CLA | OBD-CAD | 3.75 | 1.28 | 1.22 |
| 20 | B | 850 | CLA | OBD-CAD | 3.75 | 1.28 | 1.22 |
| 20 | B | 835 | CLA | C1B-NB | -3.75 | 1.33 | 1.37 |
| 20 | B | 830 | CLA | CHB-C1B | 3.75 | 1.47 | 1.39 |
| 20 | A | 837 | CLA | OBD-CAD | 3.75 | 1.28 | 1.22 |
| 20 | 3 | 314 | CLA | OBD-CAD | 3.74 | 1.28 | 1.22 |
| 22 | I | 103 | BCR | C30-C25 | -3.74 | 1.48 | 1.53 |
| 20 | A | 850 | CLA | C1B-NB | -3.74 | 1.33 | 1.37 |
| 20 | B | 819 | CLA | C1C-C2C | -3.74 | 1.37 | 1.44 |
| 20 | 4 | 303 | CLA | C4C-C3C | -3.73 | 1.38 | 1.45 |
| 20 | A | 838 | CLA | C4C-C3C | -3.73 | 1.38 | 1.45 |
| 20 | 4 | 317 | CLA | C4C-C3C | -3.72 | 1.38 | 1.45 |
| 20 | B | 832 | CLA | OBD-CAD | 3.72 | 1.28 | 1.22 |
| 20 | B | 811 | CLA | CHC-C4B | 3.72 | 1.49 | 1.40 |
| 20 | 4 | 317 | CLA | O2A-CGA | 3.72 | 1.44 | 1.33 |
| 20 | B | 821 | CLA | CHB-C1B | 3.72 | 1.47 | 1.39 |
| 20 | A | 829 | CLA | OBD-CAD | 3.71 | 1.28 | 1.22 |
| 20 | B | 842 | CLA | CHB-C1B | 3.71 | 1.47 | 1.39 |
| 20 | A | 802 | CLA | MG-NA | -3.71 | 1.97 | 2.06 |
| 20 | B | 817 | CLA | CHB-C1B | 3.71 | 1.47 | 1.39 |
| 20 | 3 | 301 | CLA | OBD-CAD | 3.71 | 1.28 | 1.22 |
| 20 | 3 | 309 | CLA | CHC-C4B | 3.70 | 1.49 | 1.40 |
| 20 | A | 839 | CLA | C4C-C3C | -3.70 | 1.38 | 1.45 |
| 20 | 2 | 309 | CLA | CHC-C4B | 3.70 | 1.49 | 1.40 |
| 20 | B | 829 | CLA | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 20 | 2 | 312 | CLA | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 20 | B | 833 | CLA | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 20 | 1 | 210 | CLA | CHB-C1B | 3.69 | 1.47 | 1.39 |
| 20 | 2 | 310 | CLA | C4C-C3C | -3.69 | 1.38 | 1.45 |
| 20 | 1 | 201 | CLA | CHC-C4B | 3.69 | 1.47 | 1.39 |
| 20 | A | 831 | CLA | C1D-ND | -3.69 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | J | 101 | CLA | OBD-CAD | 3.69 | 1.28 | 1.22 |
| 20 | A | 807 | CLA | CHB-C1B | 3.69 | 1.47 | 1.39 |
| 20 | A | 829 | CLA | CHB-C1B | 3.69 | 1.47 | 1.39 |
| 20 | R | 107 | CLA | CHB-C1B | 3.69 | 1.47 | 1.39 |
| 20 | 3 | 307 | CLA | CHB-C1B | 3.68 | 1.47 | 1.39 |
| 20 | B | 831 | CLA | OBD-CAD | 3.68 | 1.28 | 1.22 |
| 20 | 4 | 308 | CLA | MG-NA | -3.68 | 1.97 | 2.06 |
| 20 | A | 809 | CLA | OBD-CAD | 3.68 | 1.28 | 1.22 |
| 22 | F | 203 | BCR | C20-C19 | -3.68 | 1.25 | 1.34 |
| 20 | 2 | 312 | CLA | O2A-CGA | 3.67 | 1.44 | 1.33 |
| 20 | L | 204 | CLA | C4C-C3C | -3.67 | 1.38 | 1.45 |
| 20 | 1 | 215 | CLA | OBD-CAD | 3.67 | 1.28 | 1.22 |
| 22 | L | 209 | BCR | C20-C19 | -3.67 | 1.25 | 1.34 |
| 20 | 2 | 302 | CLA | MG-NA | -3.67 | 1.97 | 2.06 |
| 20 | A | 813 | CLA | OBD-CAD | 3.67 | 1.28 | 1.22 |
| 20 | B | 818 | CLA | C1B-NB | -3.66 | 1.33 | 1.37 |
| 20 | F | 205 | CLA | C3A-C2A | -3.66 | 1.51 | 1.54 |
| 20 | 3 | 314 | CLA | CHC-C4B | 3.66 | 1.47 | 1.39 |
| 20 | B | 836 | CLA | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 20 | B | 839 | CLA | C1B-NB | -3.66 | 1.33 | 1.37 |
| 20 | K | 102 | CLA | C4C-C3C | -3.66 | 1.38 | 1.45 |
| 20 | 4 | 310 | CLA | C1C-C2C | -3.66 | 1.37 | 1.44 |
| 20 | 3 | 317 | CLA | CHB-C1B | 3.65 | 1.47 | 1.39 |
| 20 | A | 841 | CLA | MG-NA | -3.65 | 1.97 | 2.06 |
| 20 | 2 | 303 | CLA | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 20 | A | 834 | CLA | CHB-C1B | 3.64 | 1.47 | 1.39 |
| 20 | H | 108 | CLA | C1D-ND | -3.64 | 1.33 | 1.37 |
| 20 | 2 | 307 | CLA | C1C-C2C | -3.64 | 1.37 | 1.44 |
| 20 | 3 | 310 | CLA | C1B-NB | -3.63 | 1.33 | 1.37 |
| 20 | B | 824 | CLA | C9-C8 | 3.63 | 1.64 | 1.52 |
| 20 | A | 832 | CLA | OBD-CAD | 3.63 | 1.28 | 1.22 |
| 20 | 4 | 310 | CLA | CHB-C1B | 3.63 | 1.47 | 1.39 |
| 20 | 1 | 205 | CLA | CHB-C1B | 3.63 | 1.47 | 1.39 |
| 20 | B | 834 | CLA | C4C-C3C | -3.63 | 1.38 | 1.45 |
| 20 | A | 802 | CLA | CHD-C4C | 3.63 | 1.52 | 1.40 |
| 20 | A | 825 | CLA | CHB-C1B | 3.62 | 1.47 | 1.39 |
| 20 | 1 | 201 | CLA | C1C-C2C | -3.61 | 1.37 | 1.44 |
| 20 | B | 813 | CLA | CHB-C1B | 3.61 | 1.47 | 1.39 |
| 20 | 2 | 308 | CLA | CHC-C4B | 3.61 | 1.49 | 1.40 |
| 20 | B | 830 | CLA | C4C-C3C | -3.61 | 1.38 | 1.45 |
| 20 | A | 831 | CLA | C4B-NB | -3.61 | 1.33 | 1.37 |
| 20 | B | 819 | CLA | C1B-NB | -3.60 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 815 | CLA | CHB-C1B | 3.60 | 1.47 | 1.39 |
| 20 | B | 814 | CLA | C1B-NB | -3.60 | 1.33 | 1.37 |
| 20 | A | 828 | CLA | CHB-C1B | 3.60 | 1.47 | 1.39 |
| 20 | 4 | 310 | CLA | C1B-NB | -3.60 | 1.33 | 1.37 |
| 20 | A | 841 | CLA | CHD-C4C | 3.60 | 1.52 | 1.40 |
| 20 | 2 | 306 | CLA | CHC-C4B | 3.60 | 1.49 | 1.40 |
| 20 | 2 | 312 | CLA | C4C-C3C | -3.59 | 1.38 | 1.45 |
| 20 | B | 816 | CLA | CHB-C1B | 3.59 | 1.47 | 1.39 |
| 20 | A | 827 | CLA | OBD-CAD | 3.59 | 1.28 | 1.22 |
| 20 | K | 103 | CLA | OBD-CAD | 3.59 | 1.28 | 1.22 |
| 20 | B | 826 | CLA | CHB-C1B | 3.58 | 1.47 | 1.39 |
| 20 | B | 825 | CLA | C1B-NB | -3.58 | 1.33 | 1.37 |
| 20 | F | 201 | CLA | CHB-C1B | 3.58 | 1.47 | 1.39 |
| 20 | A | 803 | CLA | C1C-C2C | -3.58 | 1.37 | 1.44 |
| 20 | 2 | 304 | CLA | MG-NA | -3.58 | 1.97 | 2.06 |
| 20 | A | 820 | CLA | CHB-C1B | 3.58 | 1.47 | 1.39 |
| 20 | B | 837 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 20 | A | 818 | CLA | C1C-C2C | -3.57 | 1.37 | 1.44 |
| 20 | H | 108 | CLA | MG-NA | -3.57 | 1.97 | 2.06 |
| 20 | A | 817 | CLA | CHB-C1B | 3.57 | 1.47 | 1.39 |
| 20 | A | 803 | CLA | CHB-C1B | 3.57 | 1.47 | 1.39 |
| 20 | 2 | 311 | CLA | C1B-NB | -3.57 | 1.33 | 1.37 |
| 20 | 2 | 307 | CLA | C4C-C3C | -3.57 | 1.38 | 1.45 |
| 20 | 4 | 318 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 20 | B | 811 | CLA | C3D-C4D | -3.57 | 1.36 | 1.44 |
| 20 | B | 839 | CLA | C1C-C2C | -3.56 | 1.37 | 1.44 |
| 20 | 2 | 302 | CLA | C1C-C2C | -3.56 | 1.37 | 1.44 |
| 22 | F | 204 | BCR | C20-C19 | -3.56 | 1.25 | 1.34 |
| 20 | K | 102 | CLA | C1B-NB | -3.55 | 1.33 | 1.37 |
| 20 | 3 | 310 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 20 | 2 | 309 | CLA | MG-NA | -3.54 | 1.97 | 2.06 |
| 20 | 1 | 204 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 20 | 2 | 305 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 22 | 2 | 317 | BCR | C20-C19 | -3.54 | 1.25 | 1.34 |
| 20 | B | 833 | CLA | CHB-C1B | 3.54 | 1.47 | 1.39 |
| 20 | 1 | 207 | CLA | CHB-C1B | 3.54 | 1.47 | 1.39 |
| 20 | B | 822 | CLA | C4C-C3C | -3.54 | 1.38 | 1.45 |
| 20 | 2 | 301 | CLA | CHC-C4B | 3.53 | 1.48 | 1.40 |
| 20 | A | 818 | CLA | C1B-NB | -3.53 | 1.33 | 1.37 |
| 20 | A | 831 | CLA | CAB-C3B | -3.53 | 1.37 | 1.47 |
| 20 | A | 830 | CLA | C1B-NB | -3.52 | 1.33 | 1.37 |
| 20 | K | 104 | CLA | C1C-C2C | -3.52 | 1.37 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 314 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 20 | 2 | 303 | CLA | MG-NA | -3.52 | 1.97 | 2.06 |
| 20 | A | 833 | CLA | CHB-C1B | 3.51 | 1.47 | 1.39 |
| 20 | B | 827 | CLA | C1B-NB | -3.51 | 1.33 | 1.37 |
| 20 | 3 | 310 | CLA | CHB-C1B | 3.51 | 1.47 | 1.39 |
| 20 | B | 821 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 20 | 2 | 305 | CLA | CHB-C1B | 3.50 | 1.47 | 1.39 |
| 20 | B | 823 | CLA | C1B-NB | -3.50 | 1.33 | 1.37 |
| 22 | A | 843 | BCR | C20-C19 | -3.50 | 1.25 | 1.34 |
| 20 | B | 836 | CLA | C4C-C3C | -3.50 | 1.39 | 1.45 |
| 20 | 4 | 315 | CLA | CHB-C1B | 3.50 | 1.47 | 1.39 |
| 20 | 1 | 213 | CLA | C4B-NB | -3.50 | 1.33 | 1.37 |
| 20 | B | 836 | CLA | C1B-NB | -3.50 | 1.33 | 1.37 |
| 20 | K | 102 | CLA | CHB-C1B | 3.49 | 1.47 | 1.39 |
| 20 | B | 833 | CLA | C1C-C2C | -3.49 | 1.37 | 1.44 |
| 22 | A | 845 | BCR | C20-C19 | -3.49 | 1.25 | 1.34 |
| 20 | B | 827 | CLA | C4C-C3C | -3.49 | 1.39 | 1.45 |
| 20 | K | 101 | CLA | O2A-C1 | 3.49 | 1.53 | 1.45 |
| 20 | 4 | 307 | CLA | MG-NA | -3.48 | 1.98 | 2.06 |
| 20 | 3 | 313 | CLA | CHB-C1B | 3.48 | 1.47 | 1.39 |
| 20 | B | 803 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 20 | B | 808 | CLA | C1B-NB | -3.48 | 1.33 | 1.37 |
| 20 | A | 818 | CLA | MG-NA | -3.48 | 1.98 | 2.06 |
| 20 | 1 | 202 | CLA | C3A-C2A | -3.48 | 1.51 | 1.54 |
| 20 | B | 809 | CLA | C1C-C2C | -3.47 | 1.37 | 1.44 |
| 20 | A | 838 | CLA | CHB-C1B | 3.47 | 1.47 | 1.39 |
| 20 | 2 | 303 | CLA | C4B-NB | -3.47 | 1.33 | 1.37 |
| 20 | 3 | 311 | CLA | C1B-NB | -3.47 | 1.33 | 1.37 |
| 20 | B | 806 | CLA | CHB-C1B | 3.47 | 1.47 | 1.39 |
| 20 | A | 808 | CLA | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 20 | B | 841 | CLA | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 20 | 4 | 315 | CLA | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 20 | K | 101 | CLA | CHB-C1B | 3.46 | 1.47 | 1.39 |
| 20 | 4 | 315 | CLA | C1B-NB | -3.46 | 1.33 | 1.37 |
| 20 | 4 | 308 | CLA | CHC-C4B | 3.46 | 1.48 | 1.40 |
| 20 | 3 | 303 | CLA | CHB-C1B | 3.46 | 1.47 | 1.39 |
| 20 | B | 810 | CLA | C1B-NB | -3.45 | 1.33 | 1.37 |
| 20 | 2 | 314 | CLA | C1C-C2C | -3.45 | 1.37 | 1.44 |
| 20 | A | 825 | CLA | C4C-C3C | -3.45 | 1.39 | 1.45 |
| 20 | A | 811 | CLA | OBD-CAD | 3.45 | 1.28 | 1.22 |
| 20 | B | 829 | CLA | C4C-C3C | -3.45 | 1.39 | 1.45 |
| 20 | 2 | 310 | CLA | C1C-C2C | -3.45 | 1.37 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | B | 847 | BCR | C20-C19 | -3.45 | 1.25 | 1.34 |
| 22 | B | 846 | BCR | C20-C19 | -3.44 | 1.25 | 1.34 |
| 20 | J | 103 | CLA | C4C-C3C | -3.44 | 1.39 | 1.45 |
| 20 | F | 207 | CLA | CAA-C2A | -3.44 | 1.47 | 1.54 |
| 20 | B | 813 | CLA | C1B-NB | -3.44 | 1.33 | 1.37 |
| 20 | 4 | 306 | CLA | MG-NA | -3.44 | 1.98 | 2.06 |
| 20 | A | 810 | CLA | CHB-C1B | 3.43 | 1.47 | 1.39 |
| 20 | 3 | 308 | CLA | MG-NA | -3.43 | 1.98 | 2.06 |
| 20 | B | 834 | CLA | C1B-NB | -3.43 | 1.33 | 1.37 |
| 20 | 1 | 209 | CLA | MG-NA | -3.43 | 1.98 | 2.06 |
| 20 | 4 | 304 | CLA | C1B-NB | -3.43 | 1.33 | 1.37 |
| 20 | 2 | 303 | CLA | C1C-C2C | -3.43 | 1.37 | 1.44 |
| 20 | K | 103 | CLA | C4C-C3C | -3.43 | 1.39 | 1.45 |
| 20 | 3 | 314 | CLA | C4D-ND | -3.42 | 1.33 | 1.37 |
| 20 | 4 | 317 | CLA | C1C-C2C | -3.42 | 1.37 | 1.44 |
| 20 | B | 812 | CLA | OBD-CAD | 3.42 | 1.28 | 1.22 |
| 20 | 4 | 306 | CLA | C1B-C2B | -3.42 | 1.35 | 1.43 |
| 20 | I | 102 | CLA | CHB-C1B | 3.42 | 1.47 | 1.39 |
| 20 | B | 810 | CLA | C1C-C2C | -3.42 | 1.38 | 1.44 |
| 20 | B | 839 | CLA | C4D-ND | -3.41 | 1.33 | 1.37 |
| 20 | A | 851 | CLA | C1B-NB | -3.41 | 1.33 | 1.37 |
| 20 | B | 824 | CLA | CHB-C1B | 3.41 | 1.47 | 1.39 |
| 20 | 4 | 310 | CLA | C1D-ND | -3.41 | 1.33 | 1.37 |
| 20 | 1 | 205 | CLA | C3A-C2A | -3.41 | 1.51 | 1.54 |
| 20 | 3 | 311 | CLA | C4C-C3C | -3.41 | 1.39 | 1.45 |
| 20 | L | 202 | CLA | C4C-C3C | -3.41 | 1.39 | 1.45 |
| 20 | B | 823 | CLA | CHB-C1B | 3.41 | 1.47 | 1.39 |
| 20 | A | 818 | CLA | C4B-NB | -3.40 | 1.33 | 1.37 |
| 20 | B | 833 | CLA | C1B-NB | -3.40 | 1.33 | 1.37 |
| 20 | A | 824 | CLA | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 20 | 4 | 304 | CLA | CHB-C1B | 3.40 | 1.47 | 1.39 |
| 20 | K | 101 | CLA | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 20 | B | 812 | CLA | C1C-C2C | -3.40 | 1.38 | 1.44 |
| 20 | A | 840 | CLA | CHB-C1B | 3.40 | 1.47 | 1.39 |
| 20 | B | 827 | CLA | CHB-C1B | 3.40 | 1.47 | 1.39 |
| 20 | B | 827 | CLA | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 20 | B | 803 | CLA | C1C-C2C | -3.40 | 1.38 | 1.44 |
| 20 | 4 | 301 | CLA | CHB-C1B | 3.40 | 1.47 | 1.39 |
| 20 | A | 849 | CLA | CHB-C1B | 3.39 | 1.47 | 1.39 |
| 20 | 2 | 315 | CLA | MG-NA | -3.39 | 1.98 | 2.06 |
| 20 | H | 110 | CLA | C4C-C3C | -3.39 | 1.39 | 1.45 |
| 20 | 4 | 302 | CLA | CHB-C1B | 3.39 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 307 | CLA | C1B-NB | -3.39 | 1.33 | 1.37 |
| 20 | F | 207 | CLA | CHB-C1B | 3.38 | 1.47 | 1.39 |
| 20 | B | 811 | CLA | CHD-C4C | 3.38 | 1.51 | 1.40 |
| 20 | 2 | 314 | CLA | MG-NA | -3.38 | 1.98 | 2.06 |
| 20 | B | 832 | CLA | C4C-C3C | -3.38 | 1.39 | 1.45 |
| 20 | 4 | 301 | CLA | C1B-NB | -3.38 | 1.33 | 1.37 |
| 20 | A | 832 | CLA | C1B-NB | -3.38 | 1.33 | 1.37 |
| 20 | 3 | 304 | CLA | CHC-C4B | 3.37 | 1.48 | 1.40 |
| 20 | 1 | 204 | CLA | C4B-NB | -3.37 | 1.33 | 1.37 |
| 20 | L | 208 | CLA | CHB-C1B | 3.37 | 1.47 | 1.39 |
| 20 | A | 849 | CLA | OBD-CAD | 3.37 | 1.28 | 1.22 |
| 20 | B | 835 | CLA | CHB-C1B | 3.37 | 1.47 | 1.39 |
| 20 | H | 101 | CLA | C1B-NB | -3.37 | 1.33 | 1.37 |
| 20 | A | 813 | CLA | C4C-C3C | -3.36 | 1.39 | 1.45 |
| 20 | A | 837 | CLA | C1C-C2C | -3.36 | 1.38 | 1.44 |
| 20 | A | 830 | CLA | C4C-C3C | -3.36 | 1.39 | 1.45 |
| 20 | K | 101 | CLA | C4C-C3C | -3.36 | 1.39 | 1.45 |
| 20 | A | 811 | CLA | C1C-C2C | -3.36 | 1.38 | 1.44 |
| 20 | 4 | 304 | CLA | C1C-C2C | -3.36 | 1.38 | 1.44 |
| 20 | 2 | 302 | CLA | C4B-NB | -3.35 | 1.33 | 1.37 |
| 20 | B | 820 | CLA | C4C-C3C | -3.35 | 1.39 | 1.45 |
| 20 | B | 818 | CLA | CHB-C1B | 3.35 | 1.46 | 1.39 |
| 20 | 1 | 203 | CLA | CHB-C1B | 3.35 | 1.46 | 1.39 |
| 20 | B | 828 | CLA | CHB-C1B | 3.34 | 1.46 | 1.39 |
| 20 | B | 838 | CLA | C4C-C3C | -3.34 | 1.39 | 1.45 |
| 20 | B | 839 | CLA | MG-NA | -3.34 | 1.98 | 2.06 |
| 20 | B | 833 | CLA | C4C-C3C | -3.34 | 1.39 | 1.45 |
| 20 | A | 851 | CLA | C4C-C3C | -3.34 | 1.39 | 1.45 |
| 20 | A | 827 | CLA | CHB-C1B | 3.34 | 1.46 | 1.39 |
| 20 | K | 102 | CLA | C1C-C2C | -3.34 | 1.38 | 1.44 |
| 20 | B | 835 | CLA | C4C-C3C | -3.34 | 1.39 | 1.45 |
| 20 | J | 101 | CLA | C1B-NB | -3.34 | 1.33 | 1.37 |
| 20 | L | 202 | CLA | CHB-C1B | 3.34 | 1.46 | 1.39 |
| 20 | 4 | 303 | CLA | C4D-ND | -3.34 | 1.33 | 1.37 |
| 20 | 1 | 201 | CLA | C4C-C3C | -3.34 | 1.39 | 1.45 |
| 20 | F | 206 | CLA | CHB-C1B | 3.34 | 1.46 | 1.39 |
| 20 | A | 836 | CLA | CHB-C1B | 3.33 | 1.46 | 1.39 |
| 22 | J | 102 | BCR | C20-C19 | -3.33 | 1.26 | 1.34 |
| 20 | B | 828 | CLA | OBD-CAD | 3.33 | 1.28 | 1.22 |
| 20 | L | 201 | CLA | CHB-C1B | 3.33 | 1.46 | 1.39 |
| 20 | H | 108 | CLA | OBD-CAD | 3.33 | 1.28 | 1.22 |
| 20 | B | 815 | CLA | CHB-C1B | 3.33 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | K | 104 | CLA | C4C-C3C | -3.32 | 1.39 | 1.45 |
| 20 | B | 836 | CLA | C1C-C2C | -3.32 | 1.38 | 1.44 |
| 20 | J | 101 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 20 | H | 109 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 20 | B | 826 | CLA | C4C-C3C | -3.32 | 1.39 | 1.45 |
| 20 | A | 812 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 20 | A | 824 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 20 | 4 | 309 | CLA | CHD-C4C | 3.32 | 1.51 | 1.40 |
| 20 | 4 | 311 | CLA | MG-NA | -3.32 | 1.98 | 2.06 |
| 20 | 1 | 211 | CLA | C1C-C2C | -3.32 | 1.38 | 1.44 |
| 20 | B | 808 | CLA | C1C-C2C | -3.32 | 1.38 | 1.44 |
| 20 | B | 850 | CLA | CHB-C1B | 3.32 | 1.46 | 1.39 |
| 20 | K | 104 | CLA | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 20 | B | 831 | CLA | C1B-NB | -3.31 | 1.33 | 1.37 |
| 20 | A | 850 | CLA | C4C-C3C | -3.31 | 1.39 | 1.45 |
| 20 | A | 823 | CLA | CHB-C1B | 3.31 | 1.46 | 1.39 |
| 20 | B | 807 | CLA | C1B-NB | -3.31 | 1.33 | 1.37 |
| 20 | A | 833 | CLA | C4C-C3C | -3.31 | 1.39 | 1.45 |
| 20 | F | 206 | CLA | C4C-C3C | -3.30 | 1.39 | 1.45 |
| 20 | B | 812 | CLA | C4B-NB | -3.30 | 1.33 | 1.37 |
| 20 | A | 833 | CLA | C1C-C2C | -3.30 | 1.38 | 1.44 |
| 20 | A | 803 | CLA | C4B-NB | -3.30 | 1.33 | 1.37 |
| 20 | B | 840 | CLA | CHB-C1B | 3.30 | 1.46 | 1.39 |
| 20 | 2 | 312 | CLA | C1B-NB | -3.30 | 1.33 | 1.37 |
| 20 | B | 802 | CLA | CHB-C1B | 3.30 | 1.46 | 1.39 |
| 20 | A | 806 | CLA | CHB-C1B | 3.30 | 1.46 | 1.39 |
| 20 | A | 824 | CLA | C1B-NB | -3.29 | 1.33 | 1.37 |
| 20 | L | 202 | CLA | C1B-NB | -3.29 | 1.33 | 1.37 |
| 20 | 3 | 312 | CLA | CHD-C4C | 3.29 | 1.51 | 1.40 |
| 20 | B | 850 | CLA | C4C-C3C | -3.28 | 1.39 | 1.45 |
| 20 | B | 810 | CLA | CHB-C1B | 3.28 | 1.46 | 1.39 |
| 20 | 3 | 315 | CLA | C3D-C4D | -3.28 | 1.37 | 1.44 |
| 20 | 1 | 207 | CLA | C2A-C1A | -3.28 | 1.44 | 1.52 |
| 20 | B | 808 | CLA | CHB-C1B | 3.28 | 1.46 | 1.39 |
| 20 | B | 834 | CLA | CHB-C1B | 3.28 | 1.46 | 1.39 |
| 20 | 1 | 214 | CLA | CHD-C4C | 3.27 | 1.51 | 1.40 |
| 20 | 2 | 316 | CLA | C1C-C2C | -3.27 | 1.38 | 1.44 |
| 20 | F | 207 | CLA | C4B-NB | -3.27 | 1.33 | 1.37 |
| 20 | B | 832 | CLA | CHB-C1B | 3.27 | 1.46 | 1.39 |
| 20 | R | 107 | CLA | C1B-NB | -3.27 | 1.33 | 1.37 |
| 20 | B | 803 | CLA | C4C-C3C | -3.27 | 1.39 | 1.45 |
| 20 | 4 | 312 | CLA | C3D-C4D | -3.27 | 1.37 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 828 | CLA | C4C-C3C | -3.26 | 1.39 | 1.45 |
| 20 | F | 201 | CLA | C1D-ND | -3.26 | 1.33 | 1.37 |
| 20 | B | 839 | CLA | C1D-ND | -3.26 | 1.33 | 1.37 |
| 22 | G | 104 | BCR | C20-C19 | -3.26 | 1.26 | 1.34 |
| 20 | A | 832 | CLA | CHB-C1B | 3.26 | 1.46 | 1.39 |
| 20 | 1 | 203 | CLA | MG-NA | -3.26 | 1.98 | 2.06 |
| 20 | 4 | 305 | CLA | C1C-C2C | -3.26 | 1.38 | 1.44 |
| 20 | I | 102 | CLA | C4C-C3C | -3.25 | 1.39 | 1.45 |
| 20 | 4 | 317 | CLA | CHB-C1B | 3.25 | 1.46 | 1.39 |
| 20 | K | 101 | CLA | C1B-NB | -3.25 | 1.33 | 1.37 |
| 20 | A | 825 | CLA | OBD-CAD | 3.25 | 1.28 | 1.22 |
| 20 | A | 816 | CLA | OBD-CAD | 3.25 | 1.28 | 1.22 |
| 20 | A | 830 | CLA | CHB-C1B | 3.25 | 1.46 | 1.39 |
| 20 | R | 108 | CLA | C1B-NB | -3.25 | 1.33 | 1.37 |
| 20 | 4 | 301 | CLA | C4C-C3C | -3.25 | 1.39 | 1.45 |
| 20 | A | 828 | CLA | C4C-C3C | -3.25 | 1.39 | 1.45 |
| 20 | B | 838 | CLA | C1B-NB | -3.25 | 1.33 | 1.37 |
| 20 | F | 206 | CLA | C1B-NB | -3.25 | 1.33 | 1.37 |
| 20 | 3 | 303 | CLA | C3A-C2A | -3.24 | 1.51 | 1.54 |
| 20 | A | 836 | CLA | C1B-NB | -3.24 | 1.33 | 1.37 |
| 20 | F | 207 | CLA | C1C-C2C | -3.24 | 1.38 | 1.44 |
| 20 | B | 819 | CLA | C1D-ND | -3.24 | 1.33 | 1.37 |
| 20 | 2 | 315 | CLA | C3D-C4D | -3.24 | 1.37 | 1.44 |
| 20 | A | 822 | CLA | C1B-NB | -3.23 | 1.33 | 1.37 |
| 20 | A | 813 | CLA | CHB-C1B | 3.23 | 1.46 | 1.39 |
| 20 | A | 805 | CLA | C1C-C2C | -3.23 | 1.38 | 1.44 |
| 20 | 3 | 302 | CLA | CHD-C4C | 3.23 | 1.51 | 1.40 |
| 20 | A | 828 | CLA | C1B-NB | -3.23 | 1.33 | 1.37 |
| 20 | A | 804 | CLA | CHB-C1B | 3.23 | 1.46 | 1.39 |
| 20 | B | 820 | CLA | OBD-CAD | 3.23 | 1.28 | 1.22 |
| 20 | 1 | 212 | CLA | CHD-C4C | 3.22 | 1.51 | 1.40 |
| 20 | A | 822 | CLA | CHB-C1B | 3.22 | 1.46 | 1.39 |
| 20 | B | 809 | CLA | OBD-CAD | 3.22 | 1.28 | 1.22 |
| 20 | H | 108 | CLA | CHB-C4A | -3.21 | 1.30 | 1.37 |
| 20 | B | 838 | CLA | OBD-CAD | 3.21 | 1.28 | 1.22 |
| 20 | A | 811 | CLA | CHB-C1B | 3.21 | 1.46 | 1.39 |
| 20 | 1 | 207 | CLA | C4C-C3C | -3.21 | 1.39 | 1.45 |
| 20 | 3 | 305 | CLA | CHD-C4C | 3.21 | 1.51 | 1.40 |
| 20 | 1 | 208 | CLA | CHD-C4C | 3.21 | 1.51 | 1.40 |
| 22 | I | 103 | BCR | C20-C19 | -3.21 | 1.26 | 1.34 |
| 20 | 4 | 312 | CLA | MG-NA | -3.21 | 1.98 | 2.06 |
| 20 | A | 825 | CLA | C1B-NB | -3.21 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 837 | CLA | C1B-NB | -3.21 | 1.33 | 1.37 |
| 20 | 3 | 304 | CLA | CHD-C4C | 3.20 | 1.51 | 1.40 |
| 20 | A | 851 | CLA | C1C-C2C | -3.20 | 1.38 | 1.44 |
| 20 | L | 201 | CLA | C1B-NB | -3.20 | 1.33 | 1.37 |
| 20 | A | 827 | CLA | C1B-NB | -3.20 | 1.33 | 1.37 |
| 20 | A | 813 | CLA | C1C-C2C | -3.20 | 1.38 | 1.44 |
| 20 | 4 | 317 | CLA | OBD-CAD | 3.19 | 1.28 | 1.22 |
| 20 | B | 807 | CLA | C4C-C3C | -3.19 | 1.39 | 1.45 |
| 20 | 2 | 311 | CLA | CHB-C1B | 3.19 | 1.46 | 1.39 |
| 20 | 2 | 310 | CLA | MG-NA | -3.19 | 1.98 | 2.06 |
| 20 | B | 814 | CLA | CHB-C1B | 3.19 | 1.46 | 1.39 |
| 20 | A | 835 | CLA | C4C-C3C | -3.19 | 1.39 | 1.45 |
| 20 | H | 108 | CLA | C4B-NB | -3.19 | 1.33 | 1.37 |
| 20 | F | 207 | CLA | C2A-C1A | -3.19 | 1.45 | 1.52 |
| 20 | 1 | 203 | CLA | O2A-CGA | 3.19 | 1.42 | 1.33 |
| 20 | L | 208 | CLA | C1B-NB | -3.18 | 1.33 | 1.37 |
| 20 | A | 839 | CLA | C3A-C2A | -3.18 | 1.45 | 1.54 |
| 20 | 3 | 311 | CLA | CHB-C1B | 3.18 | 1.46 | 1.39 |
| 20 | 4 | 313 | CLA | CHB-C1B | 3.18 | 1.46 | 1.39 |
| 20 | 2 | 301 | CLA | MG-NA | -3.18 | 1.98 | 2.06 |
| 20 | B | 826 | CLA | C1B-NB | -3.18 | 1.33 | 1.37 |
| 20 | A | 851 | CLA | CHB-C1B | 3.18 | 1.46 | 1.39 |
| 20 | A | 805 | CLA | OBD-CAD | 3.18 | 1.28 | 1.22 |
| 20 | B | 821 | CLA | C1B-NB | -3.18 | 1.33 | 1.37 |
| 20 | J | 101 | CLA | C4C-C3C | -3.17 | 1.39 | 1.45 |
| 20 | 4 | 306 | CLA | OBD-CAD | 3.17 | 1.27 | 1.22 |
| 20 | 1 | 202 | CLA | CHB-C1B | 3.17 | 1.46 | 1.39 |
| 20 | L | 208 | CLA | C4C-C3C | -3.17 | 1.39 | 1.45 |
| 22 | B | 844 | BCR | C20-C19 | -3.17 | 1.26 | 1.34 |
| 20 | 4 | 306 | CLA | CHB-C4A | -3.17 | 1.30 | 1.37 |
| 20 | B | 814 | CLA | OBD-CAD | 3.16 | 1.27 | 1.22 |
| 20 | B | 812 | CLA | MG-NA | -3.16 | 1.98 | 2.06 |
| 20 | 4 | 314 | CLA | CHD-C4C | 3.16 | 1.51 | 1.40 |
| 20 | 3 | 307 | CLA | MG-NA | -3.16 | 1.98 | 2.06 |
| 20 | 3 | 309 | CLA | CHD-C4C | 3.16 | 1.51 | 1.40 |
| 20 | A | 830 | CLA | C1C-C2C | -3.15 | 1.38 | 1.44 |
| 20 | 1 | 213 | CLA | C1B-C2B | -3.15 | 1.35 | 1.43 |
| 20 | B | 830 | CLA | C1C-C2C | -3.15 | 1.38 | 1.44 |
| 20 | A | 835 | CLA | C1B-NB | -3.15 | 1.33 | 1.37 |
| 20 | B | 809 | CLA | C4C-C3C | -3.15 | 1.39 | 1.45 |
| 20 | A | 837 | CLA | CHB-C1B | 3.15 | 1.46 | 1.39 |
| 20 | A | 824 | CLA | C4C-C3C | -3.15 | 1.39 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 312 | CLA | CHD-C4C | 3.15 | 1.51 | 1.40 |
| 20 | H | 101 | CLA | CHB-C1B | 3.15 | 1.46 | 1.39 |
| 20 | A | 812 | CLA | C4C-C3C | -3.14 | 1.39 | 1.45 |
| 20 | A | 826 | CLA | C4C-C3C | -3.14 | 1.39 | 1.45 |
| 20 | A | 820 | CLA | C1B-NB | -3.14 | 1.33 | 1.37 |
| 20 | 1 | 215 | CLA | C1D-C2D | -3.14 | 1.39 | 1.45 |
| 20 | B | 840 | CLA | C4C-C3C | -3.14 | 1.39 | 1.45 |
| 20 | 4 | 309 | CLA | MG-NA | -3.14 | 1.98 | 2.06 |
| 20 | B | 811 | CLA | MG-NA | -3.14 | 1.98 | 2.06 |
| 20 | A | 818 | CLA | C4D-ND | -3.13 | 1.33 | 1.37 |
| 20 | 3 | 308 | CLA | CHD-C4C | 3.13 | 1.51 | 1.40 |
| 20 | 2 | 314 | CLA | CHB-C1B | 3.13 | 1.46 | 1.39 |
| 20 | 4 | 311 | CLA | CHD-C4C | 3.13 | 1.51 | 1.40 |
| 20 | B | 836 | CLA | CHB-C1B | 3.13 | 1.46 | 1.39 |
| 20 | 4 | 314 | CLA | CHB-C1B | 3.13 | 1.47 | 1.40 |
| 20 | B | 803 | CLA | CHB-C1B | 3.13 | 1.46 | 1.39 |
| 20 | 4 | 302 | CLA | C1B-NB | -3.13 | 1.33 | 1.37 |
| 20 | 2 | 316 | CLA | C1C-NC | -3.12 | 1.33 | 1.37 |
| 20 | B | 822 | CLA | CHB-C1B | 3.12 | 1.46 | 1.39 |
| 20 | 2 | 306 | CLA | MG-NA | -3.12 | 1.98 | 2.06 |
| 20 | A | 801 | CLA | C1C-C2C | -3.12 | 1.38 | 1.44 |
| 20 | B | 821 | CLA | C4C-C3C | -3.12 | 1.39 | 1.45 |
| 20 | 4 | 307 | CLA | CHD-C4C | 3.11 | 1.50 | 1.40 |
| 20 | 3 | 312 | CLA | CHA-C1A | 3.11 | 1.49 | 1.40 |
| 20 | A | 819 | CLA | CHB-C1B | 3.11 | 1.46 | 1.39 |
| 20 | A | 811 | CLA | C4C-C3C | -3.11 | 1.39 | 1.45 |
| 20 | A | 823 | CLA | OBD-CAD | 3.11 | 1.27 | 1.22 |
| 20 | A | 840 | CLA | C1B-NB | -3.11 | 1.34 | 1.37 |
| 20 | K | 104 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 20 | 1 | 203 | CLA | C1C-C2C | -3.10 | 1.38 | 1.44 |
| 20 | B | 803 | CLA | C1B-NB | -3.10 | 1.34 | 1.37 |
| 20 | 2 | 306 | CLA | CHB-C1B | 3.10 | 1.47 | 1.40 |
| 20 | 4 | 307 | CLA | C3D-C4D | -3.10 | 1.37 | 1.44 |
| 20 | B | 839 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 20 | A | 826 | CLA | CHB-C1B | 3.10 | 1.46 | 1.39 |
| 20 | 4 | 318 | CLA | C1C-C2C | -3.09 | 1.38 | 1.44 |
| 20 | 2 | 312 | CLA | MG-NA | -3.09 | 1.98 | 2.06 |
| 20 | B | 834 | CLA | C1C-C2C | -3.09 | 1.38 | 1.44 |
| 20 | 4 | 318 | CLA | CHB-C1B | 3.08 | 1.46 | 1.39 |
| 20 | A | 806 | CLA | C4C-C3C | -3.08 | 1.39 | 1.45 |
| 20 | A | 831 | CLA | MG-ND | -3.08 | 1.99 | 2.05 |
| 20 | L | 207 | CLA | CHB-C1B | 3.08 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 825 | CLA | C4C-C3C | -3.07 | 1.39 | 1.45 |
| 20 | A | 839 | CLA | CHB-C1B | 3.07 | 1.46 | 1.39 |
| 20 | A | 814 | CLA | CHD-C4C | 3.07 | 1.50 | 1.40 |
| 20 | K | 103 | CLA | C1B-C2B | -3.07 | 1.36 | 1.43 |
| 20 | 3 | 315 | CLA | CHD-C4C | 3.07 | 1.50 | 1.40 |
| 20 | 1 | 210 | CLA | OBD-CAD | 3.07 | 1.27 | 1.22 |
| 20 | 4 | 308 | CLA | CHD-C4C | 3.07 | 1.50 | 1.40 |
| 20 | A | 836 | CLA | C4C-C3C | -3.06 | 1.39 | 1.45 |
| 20 | B | 810 | CLA | C4C-C3C | -3.06 | 1.39 | 1.45 |
| 20 | 2 | 309 | CLA | C3D-C4D | -3.06 | 1.37 | 1.44 |
| 20 | 3 | 316 | CLA | C3D-C4D | -3.06 | 1.37 | 1.44 |
| 20 | A | 807 | CLA | C4C-C3C | -3.06 | 1.39 | 1.45 |
| 20 | 4 | 317 | CLA | MG-NA | -3.06 | 1.99 | 2.06 |
| 20 | B | 802 | CLA | C4C-C3C | -3.06 | 1.39 | 1.45 |
| 20 | 1 | 209 | CLA | C3D-C4D | -3.06 | 1.37 | 1.44 |
| 20 | A | 808 | CLA | C4C-C3C | -3.05 | 1.39 | 1.45 |
| 20 | 2 | 310 | CLA | CHB-C1B | 3.05 | 1.46 | 1.39 |
| 20 | A | 816 | CLA | C1C-C2C | -3.05 | 1.38 | 1.44 |
| 20 | B | 830 | CLA | C1B-NB | -3.05 | 1.34 | 1.37 |
| 20 | L | 201 | CLA | C4C-C3C | -3.04 | 1.39 | 1.45 |
| 20 | 3 | 306 | CLA | CHD-C4C | 3.04 | 1.50 | 1.40 |
| 20 | 2 | 301 | CLA | C3D-C4D | -3.04 | 1.37 | 1.44 |
| 20 | 2 | 316 | CLA | OBD-CAD | 3.04 | 1.27 | 1.22 |
| 20 | B | 819 | CLA | C4B-NB | -3.04 | 1.34 | 1.37 |
| 20 | 2 | 306 | CLA | CHD-C4C | 3.03 | 1.50 | 1.40 |
| 20 | 1 | 206 | CLA | C1B-NB | -3.03 | 1.34 | 1.37 |
| 20 | 2 | 301 | CLA | CHD-C4C | 3.03 | 1.50 | 1.40 |
| 20 | F | 201 | CLA | C4B-NB | -3.03 | 1.34 | 1.37 |
| 20 | A | 817 | CLA | C4C-C3C | -3.02 | 1.39 | 1.45 |
| 20 | 1 | 201 | CLA | CHB-C1B | 3.02 | 1.46 | 1.39 |
| 20 | A | 817 | CLA | C1B-NB | -3.02 | 1.34 | 1.37 |
| 20 | B | 850 | CLA | C1D-ND | -3.02 | 1.34 | 1.37 |
| 20 | H | 110 | CLA | C1B-NB | -3.02 | 1.34 | 1.37 |
| 20 | K | 103 | CLA | MG-NA | -3.02 | 1.99 | 2.06 |
| 20 | 2 | 302 | CLA | C1B-C2B | -3.01 | 1.36 | 1.43 |
| 20 | A | 822 | CLA | C4C-C3C | -3.01 | 1.39 | 1.45 |
| 20 | 1 | 212 | CLA | MG-NA | -3.01 | 1.99 | 2.06 |
| 20 | 2 | 315 | CLA | CHB-C1B | 3.01 | 1.47 | 1.40 |
| 20 | J | 101 | CLA | C1C-C2C | -3.01 | 1.38 | 1.44 |
| 20 | 4 | 302 | CLA | C4C-C3C | -3.01 | 1.38 | 1.44 |
| 20 | A | 821 | CLA | C1C-C2C | -3.01 | 1.38 | 1.44 |
| 20 | B | 825 | CLA | CHB-C1B | 3.01 | 1.46 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 315 | CLA | C1C-C2C | -3.01 | 1.38 | 1.44 |
| 20 | 2 | 311 | CLA | C4C-C3C | -3.01 | 1.39 | 1.45 |
| 20 | B | 822 | CLA | C1B-NB | -3.01 | 1.34 | 1.37 |
| 20 | 3 | 306 | CLA | CHA-C1A | 3.00 | 1.49 | 1.40 |
| 20 | I | 102 | CLA | OBD-CAD | 3.00 | 1.27 | 1.22 |
| 20 | 1 | 208 | CLA | CHA-C1A | 3.00 | 1.49 | 1.40 |
| 20 | 1 | 203 | CLA | C1D-ND | -3.00 | 1.34 | 1.37 |
| 20 | 2 | 303 | CLA | CHB-C1B | 3.00 | 1.46 | 1.39 |
| 20 | B | 813 | CLA | C1C-C2C | -3.00 | 1.38 | 1.44 |
| 20 | B | 824 | CLA | MG-NA | -2.99 | 1.99 | 2.06 |
| 20 | A | 816 | CLA | C4B-NB | -2.99 | 1.34 | 1.37 |
| 20 | B | 809 | CLA | CHB-C1B | 2.99 | 1.46 | 1.39 |
| 20 | A | 807 | CLA | C1B-NB | -2.99 | 1.34 | 1.37 |
| 20 | B | 809 | CLA | C1B-NB | -2.99 | 1.34 | 1.37 |
| 20 | A | 841 | CLA | C3D-C4D | -2.99 | 1.37 | 1.44 |
| 20 | 3 | 302 | CLA | CHB-C1B | 2.99 | 1.47 | 1.40 |
| 20 | B | 828 | CLA | C1B-NB | -2.99 | 1.34 | 1.37 |
| 20 | B | 820 | CLA | C1B-NB | -2.99 | 1.34 | 1.37 |
| 20 | B | 809 | CLA | C4B-NB | -2.99 | 1.34 | 1.37 |
| 20 | B | 824 | CLA | C4D-ND | -2.98 | 1.33 | 1.37 |
| 20 | 3 | 302 | CLA | MG-NA | -2.98 | 1.99 | 2.06 |
| 20 | 3 | 314 | CLA | MG-NA | -2.98 | 1.99 | 2.06 |
| 20 | A | 839 | CLA | C1D-ND | -2.98 | 1.34 | 1.37 |
| 20 | A | 809 | CLA | C1B-NB | -2.98 | 1.34 | 1.37 |
| 20 | B | 806 | CLA | C4C-C3C | -2.97 | 1.39 | 1.45 |
| 20 | 3 | 301 | CLA | C3A-C2A | -2.97 | 1.51 | 1.54 |
| 20 | B | 840 | CLA | C1B-NB | -2.97 | 1.34 | 1.37 |
| 20 | 2 | 305 | CLA | C1B-NB | -2.97 | 1.34 | 1.37 |
| 20 | 2 | 302 | CLA | C4D-ND | -2.97 | 1.33 | 1.37 |
| 20 | B | 808 | CLA | MG-NA | -2.97 | 1.99 | 2.06 |
| 20 | 1 | 208 | CLA | CHB-C1B | 2.97 | 1.47 | 1.40 |
| 20 | J | 103 | CLA | MG-NA | -2.96 | 1.99 | 2.06 |
| 20 | B | 824 | CLA | C1C-C2C | -2.96 | 1.38 | 1.44 |
| 20 | 3 | 305 | CLA | CHB-C1B | 2.96 | 1.47 | 1.40 |
| 20 | 4 | 307 | CLA | CHB-C1B | 2.96 | 1.47 | 1.40 |
| 20 | 4 | 309 | CLA | CHB-C1B | 2.95 | 1.47 | 1.40 |
| 20 | 1 | 215 | CLA | CHB-C1B | 2.95 | 1.46 | 1.39 |
| 20 | 1 | 212 | CLA | CHA-C1A | 2.95 | 1.49 | 1.40 |
| 20 | 3 | 306 | CLA | CHB-C1B | 2.95 | 1.47 | 1.40 |
| 20 | B | 831 | CLA | CHB-C1B | 2.95 | 1.46 | 1.39 |
| 20 | 3 | 305 | CLA | MG-NA | -2.95 | 1.99 | 2.06 |
| 20 | B | 802 | CLA | C1B-NB | -2.94 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 310 | CLA | OBD-CAD | 2.94 | 1.27 | 1.22 |
| 21 | G | 101 | LMU | C4B-C3B | 2.94 | 1.59 | 1.52 |
| 20 | A | 833 | CLA | C1B-NB | -2.94 | 1.34 | 1.37 |
| 20 | B | 850 | CLA | C1B-NB | -2.94 | 1.34 | 1.37 |
| 20 | F | 205 | CLA | CHB-C1B | 2.94 | 1.46 | 1.39 |
| 20 | A | 831 | CLA | C4D-ND | -2.94 | 1.33 | 1.37 |
| 20 | 2 | 310 | CLA | OBD-CAD | 2.94 | 1.27 | 1.22 |
| 20 | A | 810 | CLA | C4C-C3C | -2.94 | 1.40 | 1.45 |
| 20 | B | 809 | CLA | MG-NA | -2.93 | 1.99 | 2.06 |
| 20 | 1 | 205 | CLA | C1B-NB | -2.93 | 1.34 | 1.37 |
| 20 | L | 203 | CLA | C4C-C3C | -2.93 | 1.40 | 1.45 |
| 20 | B | 817 | CLA | C4C-C3C | -2.93 | 1.40 | 1.45 |
| 20 | 1 | 210 | CLA | C1B-NB | -2.93 | 1.34 | 1.37 |
| 20 | B | 842 | CLA | C1B-NB | -2.93 | 1.34 | 1.37 |
| 20 | A | 818 | CLA | C1D-ND | -2.93 | 1.34 | 1.37 |
| 20 | 1 | 204 | CLA | C4D-ND | -2.93 | 1.33 | 1.37 |
| 20 | 1 | 209 | CLA | CHD-C4C | 2.93 | 1.50 | 1.40 |
| 20 | 4 | 314 | CLA | CHA-C1A | 2.93 | 1.48 | 1.40 |
| 20 | 2 | 312 | CLA | C1D-ND | -2.92 | 1.34 | 1.37 |
| 20 | A | 820 | CLA | C4C-C3C | -2.92 | 1.40 | 1.45 |
| 20 | A | 829 | CLA | C1B-NB | -2.92 | 1.34 | 1.37 |
| 20 | A | 850 | CLA | CHB-C1B | 2.92 | 1.46 | 1.39 |
| 20 | 4 | 305 | CLA | C1D-ND | -2.92 | 1.34 | 1.37 |
| 20 | A | 835 | CLA | CHB-C1B | 2.92 | 1.46 | 1.39 |
| 20 | 3 | 312 | CLA | CHB-C1B | 2.92 | 1.47 | 1.40 |
| 20 | B | 817 | CLA | C1C-C2C | -2.92 | 1.38 | 1.44 |
| 20 | A | 808 | CLA | CHB-C1B | 2.92 | 1.46 | 1.39 |
| 20 | 1 | 206 | CLA | C4C-C3C | -2.92 | 1.40 | 1.45 |
| 20 | B | 823 | CLA | C1C-C2C | -2.92 | 1.38 | 1.44 |
| 20 | H | 108 | CLA | C1B-C2B | -2.91 | 1.36 | 1.43 |
| 20 | 3 | 309 | CLA | CHA-C1A | 2.91 | 1.48 | 1.40 |
| 22 | F | 204 | BCR | C30-C25 | -2.91 | 1.49 | 1.53 |
| 20 | B | 807 | CLA | CHB-C1B | 2.91 | 1.45 | 1.39 |
| 20 | A | 819 | CLA | C1C-C2C | -2.91 | 1.38 | 1.44 |
| 20 | B | 838 | CLA | C1C-C2C | -2.91 | 1.38 | 1.44 |
| 20 | 2 | 304 | CLA | C3D-C4D | -2.91 | 1.38 | 1.44 |
| 20 | 3 | 305 | CLA | CHA-C1A | 2.90 | 1.48 | 1.40 |
| 20 | 4 | 311 | CLA | CHB-C1B | 2.90 | 1.47 | 1.40 |
| 21 | H | 105 | LMU | O1'-C1' | 2.90 | 1.45 | 1.40 |
| 20 | 3 | 317 | CLA | C1B-NB | -2.90 | 1.34 | 1.37 |
| 20 | 1 | 210 | CLA | C3A-C2A | -2.90 | 1.51 | 1.54 |
| 20 | 3 | 312 | CLA | MG-NA | -2.90 | 1.99 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | R | 107 | CLA | C4C-C3C | -2.90 | 1.40 | 1.45 |
| 21 | 2 | 321 | LMU | O1'-C1' | 2.90 | 1.45 | 1.40 |
| 20 | A | 835 | CLA | C1C-C2C | -2.90 | 1.39 | 1.44 |
| 20 | B | 824 | CLA | C4B-NB | -2.90 | 1.34 | 1.37 |
| 20 | 3 | 304 | CLA | C3D-C4D | -2.90 | 1.38 | 1.44 |
| 20 | F | 205 | CLA | C1C-C2C | -2.90 | 1.39 | 1.44 |
| 20 | A | 831 | CLA | CHB-C1B | 2.90 | 1.45 | 1.39 |
| 20 | B | 819 | CLA | MG-NA | -2.89 | 1.99 | 2.06 |
| 20 | 1 | 212 | CLA | CHB-C1B | 2.89 | 1.47 | 1.40 |
| 20 | A | 803 | CLA | OBD-CAD | 2.89 | 1.27 | 1.22 |
| 20 | H | 108 | CLA | MG-ND | -2.89 | 2.00 | 2.05 |
| 20 | A | 819 | CLA | C1B-NB | -2.89 | 1.34 | 1.37 |
| 20 | 3 | 307 | CLA | C4C-C3C | -2.89 | 1.40 | 1.45 |
| 20 | H | 101 | CLA | C4C-C3C | -2.89 | 1.40 | 1.45 |
| 20 | A | 818 | CLA | C1B-C2B | -2.89 | 1.36 | 1.43 |
| 20 | 4 | 308 | CLA | C3D-C4D | -2.88 | 1.38 | 1.44 |
| 20 | 2 | 316 | CLA | C1D-C2D | -2.88 | 1.39 | 1.45 |
| 20 | A | 831 | CLA | MG-NA | -2.88 | 1.99 | 2.06 |
| 20 | H | 109 | CLA | C1B-NB | -2.88 | 1.34 | 1.37 |
| 20 | 3 | 317 | CLA | C4C-C3C | -2.88 | 1.39 | 1.44 |
| 20 | A | 834 | CLA | C1C-C2C | -2.88 | 1.39 | 1.44 |
| 22 | B | 801 | BCR | C10-C9 | -2.88 | 1.32 | 1.35 |
| 20 | 2 | 309 | CLA | CHD-C4C | 2.88 | 1.50 | 1.40 |
| 20 | B | 819 | CLA | CHB-C1B | 2.88 | 1.45 | 1.39 |
| 20 | B | 812 | CLA | C1D-ND | -2.88 | 1.34 | 1.37 |
| 20 | A | 834 | CLA | C4C-C3C | -2.88 | 1.40 | 1.45 |
| 20 | B | 839 | CLA | OBD-CAD | 2.88 | 1.27 | 1.22 |
| 20 | 1 | 203 | CLA | C1B-NB | -2.87 | 1.34 | 1.37 |
| 20 | A | 839 | CLA | MG-NA | -2.87 | 1.99 | 2.06 |
| 20 | A | 826 | CLA | C1B-NB | -2.87 | 1.34 | 1.37 |
| 20 | L | 204 | CLA | C1B-NB | -2.87 | 1.34 | 1.37 |
| 20 | A | 804 | CLA | C4C-C3C | -2.87 | 1.40 | 1.45 |
| 20 | A | 819 | CLA | C4C-C3C | -2.87 | 1.40 | 1.45 |
| 20 | 3 | 306 | CLA | MG-NA | -2.87 | 1.99 | 2.06 |
| 20 | B | 824 | CLA | OBD-CAD | 2.87 | 1.27 | 1.22 |
| 20 | 3 | 316 | CLA | CHD-C4C | 2.86 | 1.50 | 1.40 |
| 20 | B | 832 | CLA | C1B-NB | -2.86 | 1.34 | 1.37 |
| 20 | A | 829 | CLA | C1C-C2C | -2.86 | 1.39 | 1.44 |
| 20 | A | 818 | CLA | CHB-C1B | 2.86 | 1.45 | 1.39 |
| 20 | B | 850 | CLA | C1C-C2C | -2.86 | 1.39 | 1.44 |
| 20 | B | 819 | CLA | C1C-NC | -2.86 | 1.33 | 1.37 |
| 20 | I | 102 | CLA | C1B-NB | -2.86 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 831 | CLA | C1D-C2D | -2.85 | 1.39 | 1.45 |
| 20 | A | 802 | CLA | C3D-C4D | -2.85 | 1.38 | 1.44 |
| 20 | 2 | 308 | CLA | C3D-C4D | -2.85 | 1.38 | 1.44 |
| 20 | 4 | 303 | CLA | MG-NA | -2.85 | 1.99 | 2.06 |
| 20 | 3 | 314 | CLA | CHB-C1B | 2.85 | 1.45 | 1.39 |
| 20 | J | 103 | CLA | CHB-C1B | 2.85 | 1.45 | 1.39 |
| 20 | 2 | 306 | CLA | CHA-C1A | 2.85 | 1.48 | 1.40 |
| 20 | 1 | 211 | CLA | C3D-CAD | -2.84 | 1.35 | 1.45 |
| 20 | A | 837 | CLA | MG-NA | -2.84 | 1.99 | 2.06 |
| 20 | A | 826 | CLA | C4B-NB | -2.84 | 1.34 | 1.37 |
| 20 | 3 | 311 | CLA | C1C-C2C | -2.84 | 1.39 | 1.44 |
| 20 | 3 | 302 | CLA | CHA-C1A | 2.84 | 1.48 | 1.40 |
| 20 | 4 | 311 | CLA | C3D-C4D | -2.84 | 1.38 | 1.44 |
| 20 | F | 201 | CLA | OBD-CAD | 2.84 | 1.27 | 1.22 |
| 20 | 1 | 205 | CLA | C1C-C2C | -2.84 | 1.39 | 1.44 |
| 20 | 2 | 312 | CLA | CHB-C1B | 2.83 | 1.45 | 1.39 |
| 20 | 3 | 317 | CLA | C1C-C2C | -2.83 | 1.39 | 1.44 |
| 20 | R | 108 | CLA | C4C-C3C | -2.83 | 1.40 | 1.45 |
| 20 | B | 836 | CLA | C1D-ND | -2.83 | 1.34 | 1.37 |
| 20 | J | 103 | CLA | C1D-ND | -2.83 | 1.34 | 1.37 |
| 20 | 4 | 312 | CLA | CHB-C1B | 2.83 | 1.47 | 1.40 |
| 20 | 2 | 315 | CLA | CHD-C4C | 2.82 | 1.49 | 1.40 |
| 20 | A | 839 | CLA | C4B-NB | -2.82 | 1.34 | 1.37 |
| 20 | A | 817 | CLA | C1C-C2C | -2.82 | 1.39 | 1.44 |
| 20 | B | 818 | CLA | C1C-C2C | -2.82 | 1.39 | 1.44 |
| 20 | 1 | 214 | CLA | C3D-C4D | -2.82 | 1.38 | 1.44 |
| 20 | 1 | 202 | CLA | C4C-C3C | -2.82 | 1.40 | 1.45 |
| 20 | A | 801 | CLA | C1B-NB | -2.82 | 1.34 | 1.37 |
| 20 | A | 806 | CLA | C1B-NB | -2.82 | 1.34 | 1.37 |
| 20 | 2 | 310 | CLA | C1B-C2B | -2.82 | 1.36 | 1.43 |
| 20 | A | 816 | CLA | C1B-C2B | -2.82 | 1.36 | 1.43 |
| 20 | A | 806 | CLA | C1C-C2C | -2.82 | 1.39 | 1.44 |
| 20 | 2 | 316 | CLA | CHB-C1B | 2.82 | 1.45 | 1.39 |
| 21 | 4 | 320 | LMU | O1'-C1' | 2.81 | 1.45 | 1.40 |
| 20 | A | 824 | CLA | C1C-C2C | -2.81 | 1.39 | 1.44 |
| 20 | 1 | 204 | CLA | C1D-ND | -2.81 | 1.34 | 1.37 |
| 20 | 3 | 314 | CLA | C1C-NC | -2.81 | 1.33 | 1.37 |
| 20 | A | 825 | CLA | C1C-C2C | -2.81 | 1.39 | 1.44 |
| 20 | B | 824 | CLA | C1B-C2B | -2.80 | 1.36 | 1.43 |
| 22 | B | 845 | BCR | C20-C19 | -2.80 | 1.27 | 1.34 |
| 20 | A | 832 | CLA | C1C-C2C | -2.80 | 1.39 | 1.44 |
| 20 | A | 808 | CLA | C1B-NB | -2.80 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | H | 102 | CLA | C4C-C3C | -2.80 | 1.40 | 1.45 |
| 20 | 2 | 305 | CLA | C4C-C3C | -2.80 | 1.40 | 1.45 |
| 20 | H | 108 | CLA | C1D-C2D | -2.80 | 1.39 | 1.45 |
| 20 | 4 | 302 | CLA | C4B-NB | -2.80 | 1.34 | 1.37 |
| 20 | 4 | 306 | CLA | C4B-NB | -2.80 | 1.34 | 1.37 |
| 20 | A | 815 | CLA | C1B-NB | -2.80 | 1.34 | 1.37 |
| 20 | H | 102 | CLA | C1B-NB | -2.80 | 1.34 | 1.37 |
| 20 | K | 103 | CLA | C1D-ND | -2.80 | 1.34 | 1.37 |
| 20 | A | 816 | CLA | MG-NA | -2.80 | 1.99 | 2.06 |
| 20 | A | 826 | CLA | C1C-C2C | -2.80 | 1.39 | 1.44 |
| 20 | 2 | 304 | CLA | CHD-C4C | 2.79 | 1.49 | 1.40 |
| 20 | 2 | 307 | CLA | C1D-ND | -2.79 | 1.34 | 1.37 |
| 20 | 4 | 301 | CLA | C1C-C2C | -2.79 | 1.39 | 1.44 |
| 20 | B | 835 | CLA | C1B-C2B | -2.79 | 1.36 | 1.43 |
| 20 | B | 818 | CLA | C4C-C3C | -2.79 | 1.40 | 1.45 |
| 20 | 2 | 302 | CLA | C1C-NC | -2.79 | 1.33 | 1.37 |
| 20 | 3 | 310 | CLA | MG-NA | -2.79 | 1.99 | 2.06 |
| 20 | A | 814 | CLA | CHB-C1B | 2.79 | 1.47 | 1.40 |
| 20 | 3 | 310 | CLA | C1D-ND | -2.79 | 1.34 | 1.37 |
| 20 | A | 841 | CLA | CHA-C1A | 2.79 | 1.48 | 1.40 |
| 20 | F | 207 | CLA | CMA-C3A | 2.79 | 1.59 | 1.53 |
| 20 | 1 | 201 | CLA | MG-NA | -2.79 | 1.99 | 2.06 |
| 20 | A | 814 | CLA | C3D-C4D | -2.78 | 1.38 | 1.44 |
| 20 | F | 206 | CLA | C1C-C2C | -2.78 | 1.39 | 1.44 |
| 20 | 3 | 308 | CLA | C3D-C4D | -2.78 | 1.38 | 1.44 |
| 20 | A | 822 | CLA | C1C-C2C | -2.78 | 1.39 | 1.44 |
| 20 | A | 815 | CLA | C4C-C3C | -2.78 | 1.40 | 1.45 |
| 20 | 2 | 316 | CLA | MG-NA | -2.78 | 1.99 | 2.06 |
| 20 | A | 812 | CLA | C1C-C2C | -2.78 | 1.39 | 1.44 |
| 20 | 3 | 314 | CLA | C3B-C4B | -2.78 | 1.36 | 1.42 |
| 20 | A | 835 | CLA | MG-NA | -2.77 | 1.99 | 2.06 |
| 20 | 2 | 310 | CLA | C1D-ND | -2.77 | 1.34 | 1.37 |
| 20 | 1 | 202 | CLA | C1C-C2C | -2.77 | 1.39 | 1.44 |
| 20 | 2 | 312 | CLA | C1C-C2C | -2.77 | 1.39 | 1.44 |
| 20 | A | 812 | CLA | C1B-NB | -2.77 | 1.34 | 1.37 |
| 20 | 2 | 306 | CLA | C3D-C4D | -2.77 | 1.38 | 1.44 |
| 20 | A | 836 | CLA | C1C-C2C | -2.77 | 1.39 | 1.44 |
| 20 | L | 207 | CLA | C1B-NB | -2.77 | 1.34 | 1.37 |
| 20 | B | 823 | CLA | C4C-C3C | -2.77 | 1.40 | 1.45 |
| 20 | 1 | 211 | CLA | CBD-CGD | -2.76 | 1.43 | 1.52 |
| 22 | I | 101 | BCR | C20-C19 | -2.76 | 1.27 | 1.34 |
| 20 | B | 830 | CLA | MG-NA | -2.76 | 1.99 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 211 | CLA | C4B-NB | -2.76 | 1.34 | 1.37 |
| 20 | B | 836 | CLA | MG-NA | -2.75 | 1.99 | 2.06 |
| 20 | H | 108 | CLA | C4D-ND | -2.75 | 1.33 | 1.37 |
| 20 | F | 201 | CLA | MG-NA | -2.75 | 1.99 | 2.06 |
| 20 | 2 | 316 | CLA | C1D-ND | -2.75 | 1.34 | 1.37 |
| 20 | 3 | 303 | CLA | C1B-NB | -2.75 | 1.34 | 1.37 |
| 20 | 4 | 305 | CLA | MG-NA | -2.75 | 1.99 | 2.06 |
| 20 | B | 825 | CLA | C1C-C2C | -2.75 | 1.39 | 1.44 |
| 20 | B | 813 | CLA | C4C-C3C | -2.75 | 1.40 | 1.45 |
| 20 | 1 | 213 | CLA | CAA-CBA | 2.74 | 1.61 | 1.52 |
| 20 | A | 849 | CLA | C1B-NB | -2.74 | 1.34 | 1.37 |
| 20 | 4 | 303 | CLA | C1B-C2B | -2.74 | 1.36 | 1.43 |
| 20 | 2 | 301 | CLA | CHA-C1A | 2.73 | 1.48 | 1.40 |
| 20 | 1 | 201 | CLA | C4B-NB | -2.73 | 1.34 | 1.37 |
| 20 | 3 | 310 | CLA | C1C-C2C | -2.73 | 1.39 | 1.44 |
| 21 | B | 849 | LMU | O1'-C1' | 2.73 | 1.44 | 1.40 |
| 20 | 2 | 308 | CLA | C3C-C4C | -2.72 | 1.36 | 1.43 |
| 20 | B | 812 | CLA | CHB-C1B | 2.72 | 1.45 | 1.39 |
| 20 | 4 | 313 | CLA | C1B-NB | -2.72 | 1.34 | 1.37 |
| 20 | G | 105 | CLA | CHB-C1B | 2.72 | 1.45 | 1.39 |
| 20 | 3 | 314 | CLA | C1B-C2B | -2.72 | 1.36 | 1.43 |
| 20 | A | 816 | CLA | CHB-C1B | 2.72 | 1.45 | 1.39 |
| 20 | 4 | 309 | CLA | CHA-C1A | 2.71 | 1.48 | 1.40 |
| 20 | 4 | 305 | CLA | C1D-C2D | -2.71 | 1.40 | 1.45 |
| 20 | 2 | 312 | CLA | C1D-C2D | -2.71 | 1.40 | 1.45 |
| 20 | B | 803 | CLA | MG-NA | -2.71 | 1.99 | 2.06 |
| 20 | A | 840 | CLA | C4C-C3C | -2.71 | 1.40 | 1.45 |
| 20 | B | 828 | CLA | C1C-C2C | -2.71 | 1.39 | 1.44 |
| 20 | B | 831 | CLA | C1C-C2C | -2.70 | 1.39 | 1.44 |
| 20 | 4 | 308 | CLA | CHA-C1A | 2.70 | 1.48 | 1.40 |
| 20 | 4 | 303 | CLA | CHB-C4A | -2.70 | 1.31 | 1.37 |
| 20 | A | 802 | CLA | CHA-C1A | 2.70 | 1.48 | 1.40 |
| 21 | B | 805 | LMU | O1'-C1' | 2.70 | 1.44 | 1.40 |
| 20 | B | 840 | CLA | C1C-C2C | -2.70 | 1.39 | 1.44 |
| 20 | A | 827 | CLA | C1C-C2C | -2.70 | 1.39 | 1.44 |
| 20 | B | 816 | CLA | C4C-C3C | -2.70 | 1.40 | 1.45 |
| 20 | 4 | 303 | CLA | C4B-NB | -2.70 | 1.34 | 1.37 |
| 20 | L | 207 | CLA | C1C-C2C | -2.70 | 1.39 | 1.44 |
| 20 | 4 | 311 | CLA | CHA-C1A | 2.70 | 1.48 | 1.40 |
| 20 | A | 821 | CLA | C4C-C3C | -2.70 | 1.40 | 1.45 |
| 20 | A | 810 | CLA | C1C-C2C | -2.70 | 1.39 | 1.44 |
| 20 | K | 101 | CLA | C1C-C2C | -2.70 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 823 | CLA | C1B-NB | -2.69 | 1.34 | 1.37 |
| 20 | B | 837 | CLA | C1B-NB | -2.69 | 1.34 | 1.37 |
| 20 | 3 | 303 | CLA | C4C-C3C | -2.69 | 1.39 | 1.44 |
| 20 | A | 834 | CLA | C1B-NB | -2.68 | 1.34 | 1.37 |
| 20 | A | 809 | CLA | C4B-NB | -2.68 | 1.34 | 1.37 |
| 20 | H | 101 | CLA | C1C-C2C | -2.68 | 1.39 | 1.44 |
| 20 | F | 207 | CLA | C1D-ND | -2.68 | 1.34 | 1.37 |
| 20 | B | 815 | CLA | C1C-C2C | -2.68 | 1.39 | 1.44 |
| 20 | B | 837 | CLA | C4C-C3C | -2.68 | 1.40 | 1.45 |
| 20 | B | 839 | CLA | C3D-CAD | -2.68 | 1.36 | 1.45 |
| 20 | B | 826 | CLA | C1C-C2C | -2.68 | 1.39 | 1.44 |
| 20 | A | 850 | CLA | C1C-C2C | -2.68 | 1.39 | 1.44 |
| 20 | 1 | 212 | CLA | C3D-C4D | -2.67 | 1.38 | 1.44 |
| 20 | B | 837 | CLA | C1C-C2C | -2.67 | 1.39 | 1.44 |
| 20 | 1 | 204 | CLA | CHB-C1B | 2.67 | 1.45 | 1.39 |
| 20 | 1 | 215 | CLA | MG-NA | -2.67 | 1.99 | 2.06 |
| 20 | 2 | 303 | CLA | C1C-NC | -2.67 | 1.33 | 1.37 |
| 20 | B | 819 | CLA | C1D-C2D | -2.66 | 1.40 | 1.45 |
| 20 | 3 | 313 | CLA | C4C-C3C | -2.66 | 1.40 | 1.45 |
| 20 | A | 813 | CLA | C1B-NB | -2.66 | 1.34 | 1.37 |
| 20 | B | 836 | CLA | C4D-ND | -2.66 | 1.34 | 1.37 |
| 20 | 3 | 309 | CLA | C3D-C4D | -2.66 | 1.38 | 1.44 |
| 20 | B | 812 | CLA | CHB-C4A | -2.66 | 1.31 | 1.37 |
| 20 | 2 | 316 | CLA | C1B-C2B | -2.66 | 1.37 | 1.43 |
| 20 | 2 | 304 | CLA | CHA-C1A | 2.66 | 1.48 | 1.40 |
| 20 | 1 | 215 | CLA | C1D-ND | -2.65 | 1.34 | 1.37 |
| 20 | 3 | 308 | CLA | CHA-C1A | 2.65 | 1.48 | 1.40 |
| 20 | 1 | 213 | CLA | CHB-C4A | -2.65 | 1.31 | 1.37 |
| 20 | 4 | 314 | CLA | C3D-C4D | -2.65 | 1.38 | 1.44 |
| 20 | 1 | 210 | CLA | C4C-C3C | -2.65 | 1.39 | 1.44 |
| 20 | F | 201 | CLA | C1D-C2D | -2.65 | 1.40 | 1.45 |
| 20 | 1 | 208 | CLA | MG-NA | -2.65 | 2.00 | 2.06 |
| 20 | G | 105 | CLA | C4B-NB | -2.65 | 1.34 | 1.37 |
| 20 | 4 | 315 | CLA | MG-NA | -2.65 | 2.00 | 2.06 |
| 20 | 4 | 315 | CLA | C4B-NB | -2.65 | 1.34 | 1.37 |
| 20 | 4 | 318 | CLA | C1D-ND | -2.65 | 1.34 | 1.37 |
| 21 | 2 | 319 | LMU | O1'-C1' | 2.65 | 1.44 | 1.40 |
| 20 | 2 | 302 | CLA | CHB-C4A | -2.64 | 1.31 | 1.37 |
| 21 | 4 | 316 | LMU | O1'-C1' | 2.64 | 1.44 | 1.40 |
| 20 | A | 818 | CLA | C1D-C2D | -2.64 | 1.40 | 1.45 |
| 20 | B | 819 | CLA | CHB-C4A | -2.64 | 1.31 | 1.37 |
| 20 | B | 811 | CLA | CHA-C1A | 2.64 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 828 | CLA | C1C-C2C | -2.64 | 1.39 | 1.44 |
| 20 | L | 202 | CLA | C1C-C2C | -2.63 | 1.39 | 1.44 |
| 20 | B | 819 | CLA | C1B-C2B | -2.63 | 1.37 | 1.43 |
| 20 | 3 | 316 | CLA | CHB-C1B | 2.63 | 1.46 | 1.40 |
| 20 | 3 | 314 | CLA | C1D-ND | -2.63 | 1.34 | 1.37 |
| 20 | A | 803 | CLA | MG-NA | -2.63 | 2.00 | 2.06 |
| 20 | H | 108 | CLA | C1C-NC | -2.63 | 1.33 | 1.37 |
| 20 | 3 | 304 | CLA | CHA-C1A | 2.63 | 1.48 | 1.40 |
| 20 | A | 815 | CLA | C1C-C2C | -2.63 | 1.39 | 1.44 |
| 20 | F | 205 | CLA | C4C-C3C | -2.63 | 1.39 | 1.44 |
| 20 | L | 207 | CLA | C4C-C3C | -2.62 | 1.40 | 1.45 |
| 20 | 2 | 308 | CLA | C1C-NC | -2.62 | 1.32 | 1.38 |
| 20 | 1 | 213 | CLA | C1C-NC | -2.62 | 1.33 | 1.37 |
| 21 | H | 103 | LMU | O1'-C1' | 2.62 | 1.44 | 1.40 |
| 20 | 2 | 304 | CLA | CHB-C1B | 2.62 | 1.46 | 1.40 |
| 20 | B | 812 | CLA | C1D-C2D | -2.61 | 1.40 | 1.45 |
| 20 | 3 | 312 | CLA | C3D-C4D | -2.61 | 1.38 | 1.44 |
| 20 | G | 105 | CLA | C1C-C2C | -2.61 | 1.39 | 1.44 |
| 20 | 4 | 309 | CLA | C3D-C4D | -2.61 | 1.38 | 1.44 |
| 20 | F | 206 | CLA | C4B-NB | -2.61 | 1.34 | 1.37 |
| 20 | K | 103 | CLA | CHB-C1B | 2.61 | 1.45 | 1.39 |
| 20 | B | 835 | CLA | C1C-C2C | -2.61 | 1.39 | 1.44 |
| 20 | 3 | 310 | CLA | C3B-C4B | -2.61 | 1.36 | 1.42 |
| 20 | A | 805 | CLA | C4C-C3C | -2.61 | 1.40 | 1.45 |
| 20 | B | 831 | CLA | C4C-C3C | -2.60 | 1.40 | 1.45 |
| 20 | A | 851 | CLA | MG-NA | -2.60 | 2.00 | 2.06 |
| 20 | B | 825 | CLA | C4B-NB | -2.60 | 1.34 | 1.37 |
| 20 | 1 | 205 | CLA | C4C-C3C | -2.60 | 1.39 | 1.44 |
| 20 | 4 | 310 | CLA | MG-NA | -2.60 | 2.00 | 2.06 |
| 20 | B | 815 | CLA | C4C-C3C | -2.60 | 1.40 | 1.45 |
| 20 | 3 | 313 | CLA | C1B-NB | -2.60 | 1.34 | 1.37 |
| 20 | A | 849 | CLA | C1D-ND | -2.60 | 1.34 | 1.37 |
| 20 | 3 | 307 | CLA | C1D-ND | -2.59 | 1.34 | 1.37 |
| 20 | A | 838 | CLA | C1D-ND | -2.59 | 1.34 | 1.37 |
| 20 | A | 818 | CLA | OBD-CAD | 2.59 | 1.26 | 1.22 |
| 20 | 3 | 304 | CLA | CHB-C1B | 2.59 | 1.46 | 1.40 |
| 20 | A | 832 | CLA | C4C-C3C | -2.59 | 1.40 | 1.45 |
| 20 | J | 103 | CLA | C1D-C2D | -2.58 | 1.40 | 1.45 |
| 20 | A | 823 | CLA | C1C-C2C | -2.58 | 1.39 | 1.44 |
| 20 | 2 | 301 | CLA | CHB-C1B | 2.58 | 1.46 | 1.40 |
| 20 | 3 | 301 | CLA | C1B-NB | -2.58 | 1.34 | 1.37 |
| 20 | K | 101 | CLA | MG-NA | -2.58 | 2.00 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 302 | CLA | C1C-C2C | -2.58 | 1.39 | 1.44 |
| 20 | 3 | 302 | CLA | C3D-C4D | -2.58 | 1.38 | 1.44 |
| 20 | A | 805 | CLA | C1B-NB | -2.57 | 1.34 | 1.37 |
| 20 | B | 822 | CLA | C1C-C2C | -2.57 | 1.39 | 1.44 |
| 20 | G | 105 | CLA | C1B-C2B | -2.57 | 1.37 | 1.43 |
| 20 | 1 | 203 | CLA | C2A-C1A | -2.56 | 1.46 | 1.52 |
| 20 | A | 850 | CLA | C1B-C2B | -2.56 | 1.37 | 1.43 |
| 20 | 2 | 308 | CLA | C2C-C1C | -2.56 | 1.37 | 1.43 |
| 20 | 2 | 309 | CLA | CHA-C1A | 2.56 | 1.47 | 1.40 |
| 20 | A | 838 | CLA | C1B-NB | -2.56 | 1.34 | 1.37 |
| 20 | 2 | 312 | CLA | C4B-NB | -2.55 | 1.34 | 1.37 |
| 20 | K | 104 | CLA | C1B-C2B | -2.55 | 1.37 | 1.43 |
| 20 | 4 | 305 | CLA | C4B-NB | -2.55 | 1.34 | 1.37 |
| 20 | B | 827 | CLA | C1C-C2C | -2.55 | 1.39 | 1.44 |
| 20 | 2 | 308 | CLA | CHA-C1A | 2.55 | 1.47 | 1.40 |
| 20 | 1 | 213 | CLA | MG-NA | -2.55 | 2.00 | 2.06 |
| 20 | G | 105 | CLA | CHB-C4A | -2.55 | 1.31 | 1.37 |
| 20 | B | 811 | CLA | CHB-C1B | 2.55 | 1.46 | 1.40 |
| 20 | 3 | 317 | CLA | C3A-C2A | -2.55 | 1.52 | 1.54 |
| 20 | B | 808 | CLA | C1D-ND | -2.55 | 1.34 | 1.37 |
| 20 | 1 | 213 | CLA | MG-ND | -2.55 | 2.00 | 2.05 |
| 20 | L | 208 | CLA | C4B-NB | -2.55 | 1.34 | 1.37 |
| 20 | A | 827 | CLA | C4C-C3C | -2.54 | 1.40 | 1.45 |
| 20 | 4 | 303 | CLA | CHB-C1B | 2.54 | 1.45 | 1.39 |
| 20 | R | 107 | CLA | C1C-C2C | -2.53 | 1.39 | 1.44 |
| 20 | A | 821 | CLA | C1B-NB | -2.53 | 1.34 | 1.37 |
| 20 | A | 850 | CLA | C4B-NB | -2.53 | 1.34 | 1.37 |
| 20 | A | 813 | CLA | MG-NA | -2.53 | 2.00 | 2.06 |
| 20 | A | 818 | CLA | C1C-NC | -2.53 | 1.34 | 1.37 |
| 20 | 4 | 315 | CLA | C1B-C2B | -2.52 | 1.37 | 1.43 |
| 20 | 1 | 214 | CLA | CHB-C1B | 2.52 | 1.46 | 1.40 |
| 20 | 4 | 313 | CLA | C1C-C2C | -2.52 | 1.39 | 1.44 |
| 20 | 2 | 308 | CLA | CHD-C4C | 2.52 | 1.48 | 1.40 |
| 20 | 1 | 206 | CLA | C1C-C2C | -2.51 | 1.39 | 1.44 |
| 20 | B | 841 | CLA | C1C-C2C | -2.51 | 1.39 | 1.44 |
| 20 | K | 104 | CLA | C4B-NB | -2.51 | 1.34 | 1.37 |
| 20 | 3 | 311 | CLA | MG-NA | -2.51 | 2.00 | 2.06 |
| 20 | 1 | 201 | CLA | C1D-C2D | -2.51 | 1.40 | 1.45 |
| 20 | 4 | 312 | CLA | CHA-C1A | 2.51 | 1.47 | 1.40 |
| 20 | 3 | 315 | CLA | CHB-C1B | 2.50 | 1.46 | 1.40 |
| 20 | B | 833 | CLA | C4B-NB | -2.50 | 1.34 | 1.37 |
| 20 | A | 802 | CLA | CHB-C1B | 2.50 | 1.46 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | A | 823 | CLA | C4C-C3C | -2.50 | 1.40 | 1.45 |
| 20 | 2 | 311 | CLA | C1C-C2C | -2.50 | 1.39 | 1.44 |
| 20 | 3 | 315 | CLA | CHA-C1A | 2.50 | 1.47 | 1.40 |
| 20 | A | 834 | CLA | C1D-ND | -2.50 | 1.34 | 1.37 |
| 20 | L | 201 | CLA | C1C-C2C | -2.49 | 1.39 | 1.44 |
| 20 | 1 | 215 | CLA | C1C-C2C | -2.49 | 1.39 | 1.44 |
| 20 | B | 832 | CLA | C1C-C2C | -2.49 | 1.39 | 1.44 |
| 20 | A | 849 | CLA | C1D-C2D | -2.49 | 1.40 | 1.45 |
| 20 | B | 839 | CLA | C1B-C2B | -2.49 | 1.37 | 1.43 |
| 20 | 2 | 307 | CLA | MG-NA | -2.49 | 2.00 | 2.06 |
| 20 | 2 | 312 | CLA | CHB-C4A | -2.49 | 1.31 | 1.37 |
| 21 | G | 101 | LMU | C6B-C5B | 2.48 | 1.60 | 1.51 |
| 20 | F | 207 | CLA | C1B-C2B | -2.48 | 1.37 | 1.43 |
| 20 | I | 102 | CLA | C1C-C2C | -2.48 | 1.39 | 1.44 |
| 20 | 2 | 309 | CLA | C2D-C1D | -2.48 | 1.38 | 1.44 |
| 20 | B | 802 | CLA | C1C-C2C | -2.48 | 1.39 | 1.44 |
| 20 | 1 | 204 | CLA | C1B-C2B | -2.48 | 1.37 | 1.43 |
| 20 | 1 | 207 | CLA | C3A-C2A | -2.48 | 1.47 | 1.54 |
| 20 | A | 809 | CLA | C4C-C3C | -2.48 | 1.40 | 1.45 |
| 20 | 1 | 207 | CLA | C1C-C2C | -2.47 | 1.39 | 1.44 |
| 20 | F | 205 | CLA | C1B-NB | -2.47 | 1.34 | 1.37 |
| 20 | 1 | 213 | CLA | CHB-C1B | 2.47 | 1.44 | 1.39 |
| 20 | L | 203 | CLA | C1B-NB | -2.46 | 1.34 | 1.37 |
| 20 | A | 820 | CLA | C1C-C2C | -2.46 | 1.39 | 1.44 |
| 20 | 4 | 318 | CLA | C4C-C3C | -2.46 | 1.40 | 1.45 |
| 20 | L | 203 | CLA | C1C-C2C | -2.46 | 1.39 | 1.44 |
| 20 | B | 839 | CLA | C1C-NC | -2.46 | 1.34 | 1.37 |
| 20 | B | 821 | CLA | C1C-C2C | -2.46 | 1.39 | 1.44 |
| 20 | 1 | 214 | CLA | CHA-C1A | 2.46 | 1.47 | 1.40 |
| 20 | 3 | 310 | CLA | C4D-ND | -2.45 | 1.34 | 1.37 |
| 20 | 3 | 305 | CLA | C3D-C4D | -2.45 | 1.39 | 1.44 |
| 20 | A | 804 | CLA | C1B-NB | -2.45 | 1.34 | 1.37 |
| 20 | A | 819 | CLA | C1B-C2B | -2.45 | 1.37 | 1.43 |
| 20 | 2 | 302 | CLA | C1D-ND | -2.45 | 1.34 | 1.37 |
| 20 | 1 | 202 | CLA | C1B-C2B | -2.45 | 1.37 | 1.43 |
| 20 | K | 103 | CLA | CHB-C4A | -2.45 | 1.31 | 1.37 |
| 20 | F | 201 | CLA | C1C-NC | -2.45 | 1.34 | 1.37 |
| 20 | 4 | 308 | CLA | CHB-C1B | 2.45 | 1.46 | 1.40 |
| 20 | F | 201 | CLA | C4D-ND | -2.45 | 1.34 | 1.37 |
| 20 | B | 814 | CLA | C1C-C2C | -2.44 | 1.39 | 1.44 |
| 20 | B | 836 | CLA | C1B-C2B | -2.44 | 1.37 | 1.43 |
| 20 | A | 839 | CLA | C1B-C2B | -2.44 | 1.37 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 812 | CLA | C1B-C2B | -2.44 | 1.37 | 1.43 |
| 20 | 1 | 208 | CLA | C3D-C4D | -2.44 | 1.39 | 1.44 |
| 20 | B | 836 | CLA | C4B-NB | -2.44 | 1.34 | 1.37 |
| 20 | A | 838 | CLA | C1C-C2C | -2.44 | 1.39 | 1.44 |
| 20 | 1 | 215 | CLA | C4D-ND | -2.44 | 1.34 | 1.37 |
| 20 | B | 834 | CLA | MG-NA | -2.44 | 2.00 | 2.06 |
| 20 | B | 812 | CLA | C3D-CAD | -2.43 | 1.36 | 1.45 |
| 20 | G | 105 | CLA | MG-NA | -2.43 | 2.00 | 2.06 |
| 20 | A | 803 | CLA | C1D-ND | -2.43 | 1.34 | 1.37 |
| 20 | 1 | 209 | CLA | CHA-C1A | 2.43 | 1.47 | 1.40 |
| 20 | A | 849 | CLA | C1C-C2C | -2.43 | 1.39 | 1.44 |
| 20 | B | 808 | CLA | OBD-CAD | 2.43 | 1.26 | 1.22 |
| 20 | B | 829 | CLA | C1C-C2C | -2.43 | 1.39 | 1.44 |
| 20 | 2 | 303 | CLA | C4D-ND | -2.43 | 1.34 | 1.37 |
| 20 | A | 831 | CLA | CHB-C4A | -2.43 | 1.31 | 1.37 |
| 20 | H | 102 | CLA | C1C-C2C | -2.43 | 1.39 | 1.44 |
| 20 | R | 108 | CLA | C1C-C2C | -2.43 | 1.39 | 1.44 |
| 20 | J | 103 | CLA | C4B-NB | -2.43 | 1.34 | 1.37 |
| 20 | K | 103 | CLA | C4B-NB | -2.42 | 1.34 | 1.37 |
| 20 | H | 109 | CLA | C1C-C2C | -2.42 | 1.39 | 1.44 |
| 20 | A | 831 | CLA | C1B-C2B | -2.42 | 1.37 | 1.43 |
| 20 | 1 | 210 | CLA | C1C-C2C | -2.42 | 1.39 | 1.44 |
| 20 | A | 814 | CLA | C2C-C1C | -2.42 | 1.37 | 1.43 |
| 20 | B | 832 | CLA | C1B-C2B | -2.42 | 1.37 | 1.43 |
| 20 | B | 826 | CLA | C4B-NB | -2.42 | 1.34 | 1.37 |
| 20 | A | 808 | CLA | MG-NA | -2.42 | 2.00 | 2.06 |
| 20 | B | 841 | CLA | C3B-C4B | -2.42 | 1.37 | 1.42 |
| 20 | A | 814 | CLA | CHA-C1A | 2.42 | 1.47 | 1.40 |
| 20 | 4 | 302 | CLA | C1B-C2B | -2.41 | 1.37 | 1.43 |
| 20 | B | 824 | CLA | C4D-CHA | -2.41 | 1.29 | 1.38 |
| 20 | A | 841 | CLA | CHB-C1B | 2.41 | 1.46 | 1.40 |
| 20 | A | 808 | CLA | C1C-C2C | -2.41 | 1.39 | 1.44 |
| 20 | 4 | 317 | CLA | C4B-NB | -2.41 | 1.34 | 1.37 |
| 20 | F | 207 | CLA | MG-NA | -2.41 | 2.00 | 2.06 |
| 20 | B | 827 | CLA | C1B-C2B | -2.41 | 1.37 | 1.43 |
| 20 | A | 804 | CLA | C1C-C2C | -2.41 | 1.39 | 1.44 |
| 20 | 1 | 213 | CLA | C1D-ND | -2.40 | 1.34 | 1.37 |
| 20 | L | 204 | CLA | C1C-C2C | -2.40 | 1.39 | 1.44 |
| 20 | A | 840 | CLA | C1C-C2C | -2.40 | 1.39 | 1.44 |
| 20 | B | 839 | CLA | C4D-CHA | -2.40 | 1.29 | 1.38 |
| 20 | 4 | 310 | CLA | C4B-NB | -2.40 | 1.34 | 1.37 |
| 20 | 1 | 215 | CLA | CHB-C4A | -2.40 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 841 | CLA | C4C-C3C | -2.40 | 1.40 | 1.45 |
| 20 | L | 202 | CLA | MG-NA | -2.40 | 2.00 | 2.06 |
| 20 | 4 | 305 | CLA | C4D-ND | -2.40 | 1.34 | 1.37 |
| 20 | A | 816 | CLA | C4D-ND | -2.40 | 1.34 | 1.37 |
| 20 | 2 | 309 | CLA | CHB-C1B | 2.39 | 1.46 | 1.40 |
| 20 | A | 808 | CLA | C1B-C2B | -2.39 | 1.37 | 1.43 |
| 20 | K | 104 | CLA | MG-NA | -2.39 | 2.00 | 2.06 |
| 20 | A | 835 | CLA | C1B-C2B | -2.39 | 1.37 | 1.43 |
| 20 | 1 | 213 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 20 | B | 850 | CLA | MG-NA | -2.39 | 2.00 | 2.06 |
| 20 | B | 807 | CLA | C1B-C2B | -2.39 | 1.37 | 1.43 |
| 20 | A | 832 | CLA | MG-NA | -2.39 | 2.00 | 2.06 |
| 20 | 3 | 301 | CLA | C1C-C2C | -2.38 | 1.40 | 1.44 |
| 20 | 1 | 215 | CLA | C4B-NB | -2.38 | 1.34 | 1.37 |
| 20 | B | 842 | CLA | C1C-C2C | -2.38 | 1.40 | 1.44 |
| 20 | B | 841 | CLA | C1B-NB | -2.38 | 1.34 | 1.37 |
| 20 | B | 807 | CLA | MG-NA | -2.38 | 2.00 | 2.06 |
| 20 | 3 | 310 | CLA | C1B-C2B | -2.38 | 1.37 | 1.43 |
| 20 | F | 205 | CLA | C1B-C2B | -2.38 | 1.37 | 1.43 |
| 20 | 2 | 316 | CLA | C4D-ND | -2.38 | 1.34 | 1.37 |
| 20 | 4 | 314 | CLA | MG-NA | -2.38 | 2.00 | 2.06 |
| 20 | 4 | 307 | CLA | CHA-C1A | 2.37 | 1.47 | 1.40 |
| 20 | A | 806 | CLA | MG-NA | -2.37 | 2.00 | 2.06 |
| 20 | A | 839 | CLA | C2A-C1A | -2.37 | 1.46 | 1.52 |
| 20 | 1 | 203 | CLA | C1B-C2B | -2.37 | 1.37 | 1.43 |
| 20 | B | 818 | CLA | C1B-C2B | -2.37 | 1.37 | 1.43 |
| 20 | 3 | 308 | CLA | CHB-C1B | 2.37 | 1.46 | 1.40 |
| 20 | 1 | 207 | CLA | C1B-NB | -2.36 | 1.34 | 1.37 |
| 20 | 2 | 315 | CLA | C2D-C1D | -2.36 | 1.39 | 1.44 |
| 20 | B | 808 | CLA | C4D-ND | -2.36 | 1.34 | 1.37 |
| 20 | B | 817 | CLA | C1B-NB | -2.36 | 1.34 | 1.37 |
| 20 | 1 | 211 | CLA | C4D-ND | -2.36 | 1.34 | 1.37 |
| 20 | A | 824 | CLA | MG-NA | -2.36 | 2.00 | 2.06 |
| 20 | B | 807 | CLA | C1C-C2C | -2.36 | 1.40 | 1.44 |
| 20 | B | 827 | CLA | MG-NA | -2.36 | 2.00 | 2.06 |
| 20 | 3 | 314 | CLA | CHB-C4A | -2.36 | 1.32 | 1.37 |
| 20 | 4 | 318 | CLA | C1B-C2B | -2.35 | 1.37 | 1.43 |
| 20 | A | 835 | CLA | CHB-C4A | -2.35 | 1.32 | 1.37 |
| 20 | A | 825 | CLA | MG-NA | -2.35 | 2.00 | 2.06 |
| 20 | A | 810 | CLA | C1B-NB | -2.35 | 1.34 | 1.37 |
| 20 | 3 | 301 | CLA | C4C-C3C | -2.35 | 1.40 | 1.44 |
| 20 | B | 828 | CLA | MG-NA | -2.35 | 2.00 | 2.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 819 | CLA | OBD-CAD | 2.35 | 1.26 | 1.22 |
| 20 | 2 | 316 | CLA | CHB-C4A | -2.35 | 1.32 | 1.37 |
| 20 | B | 808 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 20 | L | 201 | CLA | C1B-C2B | -2.34 | 1.37 | 1.43 |
| 20 | B | 819 | CLA | C4D-ND | -2.34 | 1.34 | 1.37 |
| 20 | 2 | 316 | CLA | C3D-CAD | -2.34 | 1.37 | 1.45 |
| 20 | B | 842 | CLA | C4C-C3C | -2.33 | 1.40 | 1.44 |
| 20 | 2 | 314 | CLA | C4B-NB | -2.33 | 1.34 | 1.37 |
| 20 | A | 816 | CLA | CHB-C4A | -2.33 | 1.32 | 1.37 |
| 20 | J | 101 | CLA | MG-NA | -2.33 | 2.00 | 2.06 |
| 20 | B | 831 | CLA | C1B-C2B | -2.33 | 1.37 | 1.43 |
| 20 | H | 101 | CLA | MG-NA | -2.33 | 2.00 | 2.06 |
| 20 | A | 833 | CLA | MG-NA | -2.33 | 2.00 | 2.06 |
| 20 | B | 823 | CLA | C4B-NB | -2.33 | 1.34 | 1.37 |
| 20 | A | 803 | CLA | C1B-C2B | -2.32 | 1.37 | 1.43 |
| 20 | B | 825 | CLA | C1B-C2B | -2.32 | 1.37 | 1.43 |
| 20 | 4 | 301 | CLA | MG-NA | -2.32 | 2.00 | 2.06 |
| 20 | B | 810 | CLA | C4B-NB | -2.32 | 1.34 | 1.37 |
| 20 | 1 | 204 | CLA | CHB-C4A | -2.32 | 1.32 | 1.37 |
| 20 | B | 806 | CLA | C1C-C2C | -2.32 | 1.40 | 1.44 |
| 20 | 2 | 304 | CLA | C3C-C4C | -2.32 | 1.37 | 1.43 |
| 20 | 4 | 318 | CLA | MG-NA | -2.32 | 2.00 | 2.06 |
| 20 | B | 806 | CLA | C1D-ND | -2.32 | 1.34 | 1.37 |
| 20 | B | 816 | CLA | C1C-C2C | -2.32 | 1.40 | 1.44 |
| 20 | A | 819 | CLA | C4B-NB | -2.31 | 1.34 | 1.37 |
| 20 | 2 | 305 | CLA | C1C-C2C | -2.31 | 1.40 | 1.44 |
| 20 | F | 201 | CLA | C3B-C4B | -2.31 | 1.37 | 1.42 |
| 20 | B | 808 | CLA | C4B-NB | -2.31 | 1.34 | 1.37 |
| 20 | B | 811 | CLA | C2C-C1C | -2.31 | 1.37 | 1.43 |
| 20 | K | 102 | CLA | MG-NA | -2.31 | 2.00 | 2.06 |
| 20 | 3 | 307 | CLA | C4B-NB | -2.31 | 1.34 | 1.37 |
| 20 | 1 | 215 | CLA | MG-ND | -2.31 | 2.01 | 2.05 |
| 20 | A | 808 | CLA | C1D-ND | -2.31 | 1.34 | 1.37 |
| 20 | 4 | 303 | CLA | CBD-CHA | -2.31 | 1.41 | 1.52 |
| 20 | A | 839 | CLA | C4D-ND | -2.30 | 1.34 | 1.37 |
| 20 | 2 | 302 | CLA | CHB-C1B | 2.30 | 1.44 | 1.39 |
| 20 | 3 | 314 | CLA | C3D-CAD | -2.30 | 1.37 | 1.45 |
| 20 | 3 | 315 | CLA | C2C-C1C | -2.30 | 1.37 | 1.43 |
| 20 | 1 | 204 | CLA | C3B-C4B | -2.30 | 1.37 | 1.42 |
| 20 | F | 206 | CLA | MG-NA | -2.29 | 2.00 | 2.06 |
| 22 | F | 204 | BCR | C1-C6 | -2.29 | 1.50 | 1.53 |
| 20 | B | 808 | CLA | C1B-C2B | -2.29 | 1.37 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 308 | CLA | C3C-C4C | -2.29 | 1.37 | 1.43 |
| 22 | A | 845 | BCR | C30-C25 | -2.28 | 1.50 | 1.53 |
| 20 | B | 814 | CLA | C1B-C2B | -2.28 | 1.37 | 1.43 |
| 20 | B | 811 | CLA | C2D-C1D | -2.28 | 1.39 | 1.44 |
| 20 | B | 819 | CLA | MG-ND | -2.28 | 2.01 | 2.05 |
| 20 | J | 103 | CLA | CHB-C4A | -2.28 | 1.32 | 1.37 |
| 20 | B | 833 | CLA | MG-NA | -2.28 | 2.00 | 2.06 |
| 20 | 4 | 315 | CLA | C1D-ND | -2.28 | 1.35 | 1.37 |
| 21 | R | 105 | LMU | O1'-C1' | 2.28 | 1.44 | 1.40 |
| 20 | B | 820 | CLA | C1C-C2C | -2.28 | 1.40 | 1.44 |
| 20 | B | 824 | CLA | C1C-NC | -2.28 | 1.34 | 1.37 |
| 20 | 4 | 306 | CLA | C4D-ND | -2.28 | 1.34 | 1.37 |
| 20 | A | 831 | CLA | C3B-C4B | -2.28 | 1.37 | 1.42 |
| 20 | 4 | 305 | CLA | C1C-NC | -2.28 | 1.34 | 1.37 |
| 20 | B | 807 | CLA | CHB-C4A | -2.28 | 1.32 | 1.37 |
| 20 | B | 832 | CLA | C4B-NB | -2.28 | 1.35 | 1.37 |
| 20 | 3 | 309 | CLA | CHB-C1B | 2.28 | 1.45 | 1.40 |
| 20 | L | 208 | CLA | C1B-C2B | -2.28 | 1.37 | 1.43 |
| 20 | 4 | 311 | CLA | C3C-C4C | -2.27 | 1.37 | 1.43 |
| 20 | 4 | 317 | CLA | C1B-C2B | -2.27 | 1.37 | 1.43 |
| 22 | I | 103 | BCR | C1-C6 | -2.27 | 1.50 | 1.53 |
| 20 | 3 | 304 | CLA | C2C-C1C | -2.27 | 1.37 | 1.43 |
| 20 | 1 | 207 | CLA | MG-NA | -2.27 | 2.00 | 2.06 |
| 20 | B | 812 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |
| 20 | 3 | 306 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 20 | F | 207 | CLA | CBD-CHA | -2.26 | 1.41 | 1.52 |
| 20 | 3 | 310 | CLA | C1C-NC | -2.26 | 1.34 | 1.37 |
| 20 | L | 208 | CLA | CBD-CGD | -2.26 | 1.45 | 1.52 |
| 20 | 4 | 313 | CLA | C4C-C3C | -2.26 | 1.40 | 1.44 |
| 20 | 4 | 318 | CLA | C4B-NB | -2.26 | 1.35 | 1.37 |
| 20 | L | 202 | CLA | C1B-C2B | -2.26 | 1.37 | 1.43 |
| 20 | 1 | 215 | CLA | C3D-CAD | -2.26 | 1.37 | 1.45 |
| 20 | A | 829 | CLA | C4C-C3C | -2.26 | 1.41 | 1.45 |
| 20 | B | 810 | CLA | MG-NA | -2.25 | 2.00 | 2.06 |
| 21 | 4 | 319 | LMU | O6B-C6B | 2.25 | 1.51 | 1.42 |
| 20 | 1 | 209 | CLA | CHB-C1B | 2.25 | 1.45 | 1.40 |
| 20 | B | 808 | CLA | MG-ND | -2.25 | 2.01 | 2.05 |
| 20 | 1 | 213 | CLA | C3A-C4A | -2.25 | 1.44 | 1.51 |
| 20 | 2 | 316 | CLA | CAA-C2A | -2.25 | 1.49 | 1.54 |
| 20 | H | 110 | CLA | C1C-C2C | -2.25 | 1.40 | 1.44 |
| 20 | A | 826 | CLA | C1B-C2B | -2.25 | 1.38 | 1.43 |
| 20 | 1 | 215 | CLA | C1B-C2B | -2.25 | 1.38 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 850 | CLA | C1D-C2D | -2.25 | 1.40 | 1.45 |
| 20 | B | 814 | CLA | MG-NA | -2.25 | 2.00 | 2.06 |
| 20 | L | 208 | CLA | C1C-C2C | -2.24 | 1.40 | 1.44 |
| 20 | F | 207 | CLA | CHB-C4A | -2.24 | 1.32 | 1.37 |
| 20 | J | 103 | CLA | C1B-C2B | -2.24 | 1.38 | 1.43 |
| 20 | A | 807 | CLA | C1C-C2C | -2.24 | 1.40 | 1.44 |
| 20 | H | 109 | CLA | C4C-C3C | -2.24 | 1.41 | 1.45 |
| 20 | 2 | 314 | CLA | C3D-CAD | -2.24 | 1.37 | 1.45 |
| 20 | A | 838 | CLA | MG-NA | -2.24 | 2.00 | 2.06 |
| 20 | A | 831 | CLA | C1C-NC | -2.24 | 1.34 | 1.37 |
| 20 | B | 823 | CLA | MG-NA | -2.24 | 2.00 | 2.06 |
| 20 | 1 | 201 | CLA | C1D-ND | -2.24 | 1.35 | 1.37 |
| 20 | F | 205 | CLA | CHB-C4A | -2.24 | 1.32 | 1.37 |
| 20 | B | 822 | CLA | C1B-C2B | -2.24 | 1.38 | 1.43 |
| 22 | B | 846 | BCR | C30-C25 | -2.23 | 1.50 | 1.53 |
| 20 | 3 | 309 | CLA | C2C-C1C | -2.23 | 1.38 | 1.43 |
| 20 | 4 | 306 | CLA | C1D-ND | -2.23 | 1.35 | 1.37 |
| 20 | B | 839 | CLA | C1D-C2D | -2.23 | 1.40 | 1.45 |
| 20 | A | 804 | CLA | C1B-C2B | -2.23 | 1.38 | 1.43 |
| 20 | A | 830 | CLA | MG-NA | -2.22 | 2.01 | 2.06 |
| 20 | B | 821 | CLA | MG-NA | -2.22 | 2.01 | 2.06 |
| 20 | 4 | 304 | CLA | MG-NA | -2.22 | 2.01 | 2.06 |
| 20 | A | 822 | CLA | C1B-C2B | -2.22 | 1.38 | 1.43 |
| 20 | A | 803 | CLA | C1C-NC | -2.22 | 1.34 | 1.37 |
| 20 | A | 827 | CLA | MG-NA | -2.22 | 2.01 | 2.06 |
| 20 | 4 | 301 | CLA | C4B-NB | -2.22 | 1.35 | 1.37 |
| 20 | 2 | 308 | CLA | C2D-C1D | -2.21 | 1.39 | 1.44 |
| 20 | 3 | 310 | CLA | C1D-C2D | -2.21 | 1.41 | 1.45 |
| 20 | K | 101 | CLA | C1B-C2B | -2.21 | 1.38 | 1.43 |
| 20 | A | 810 | CLA | MG-NA | -2.21 | 2.01 | 2.06 |
| 20 | B | 840 | CLA | MG-NA | -2.21 | 2.01 | 2.06 |
| 20 | A | 837 | CLA | C4B-NB | -2.21 | 1.35 | 1.37 |
| 20 | 1 | 213 | CLA | C4D-ND | -2.21 | 1.34 | 1.37 |
| 20 | B | 827 | CLA | C4B-NB | -2.21 | 1.35 | 1.37 |
| 20 | 2 | 312 | CLA | C1B-C2B | -2.20 | 1.38 | 1.43 |
| 20 | 4 | 313 | CLA | MG-NA | -2.20 | 2.01 | 2.06 |
| 20 | A | 830 | CLA | C1B-C2B | -2.20 | 1.38 | 1.43 |
| 20 | 3 | 311 | CLA | C1B-C2B | -2.20 | 1.38 | 1.43 |
| 20 | 4 | 310 | CLA | C1C-NC | -2.20 | 1.34 | 1.37 |
| 20 | 4 | 308 | CLA | C2C-C1C | -2.20 | 1.38 | 1.43 |
| 20 | B | 806 | CLA | C1B-NB | -2.20 | 1.35 | 1.37 |
| 20 | A | 850 | CLA | CHB-C4A | -2.20 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 820 | CLA | C1D-ND | -2.20 | 1.35 | 1.37 |
| 20 | 4 | 310 | CLA | C1B-C2B | -2.20 | 1.38 | 1.43 |
| 20 | 2 | 315 | CLA | CHA-C1A | 2.19 | 1.46 | 1.40 |
| 20 | 2 | 302 | CLA | MG-ND | -2.19 | 2.01 | 2.05 |
| 20 | B | 830 | CLA | C1D-ND | -2.19 | 1.35 | 1.37 |
| 20 | 2 | 312 | CLA | C4D-ND | -2.19 | 1.34 | 1.37 |
| 20 | K | 102 | CLA | C4B-NB | -2.19 | 1.35 | 1.37 |
| 20 | A | 849 | CLA | C1B-C2B | -2.19 | 1.38 | 1.43 |
| 20 | B | 830 | CLA | C3B-C4B | -2.18 | 1.37 | 1.42 |
| 20 | 4 | 306 | CLA | C3A-C2A | -2.18 | 1.48 | 1.54 |
| 20 | B | 826 | CLA | MG-NA | -2.18 | 2.01 | 2.06 |
| 20 | B | 831 | CLA | C1D-ND | -2.18 | 1.35 | 1.37 |
| 20 | A | 818 | CLA | CHB-C4A | -2.18 | 1.32 | 1.37 |
| 20 | B | 839 | CLA | CHB-C4A | -2.18 | 1.32 | 1.37 |
| 20 | A | 828 | CLA | C1B-C2B | -2.18 | 1.38 | 1.43 |
| 20 | 4 | 318 | CLA | CHB-C4A | -2.18 | 1.32 | 1.37 |
| 20 | K | 101 | CLA | C1D-ND | -2.18 | 1.35 | 1.37 |
| 20 | A | 823 | CLA | C1B-C2B | -2.18 | 1.38 | 1.43 |
| 20 | G | 105 | CLA | C4D-ND | -2.18 | 1.34 | 1.37 |
| 20 | A | 824 | CLA | C1B-C2B | -2.18 | 1.38 | 1.43 |
| 20 | 3 | 314 | CLA | MG-ND | -2.17 | 2.01 | 2.05 |
| 20 | 3 | 316 | CLA | C2D-C1D | -2.17 | 1.39 | 1.44 |
| 20 | A | 803 | CLA | C3D-CAD | -2.17 | 1.37 | 1.45 |
| 20 | A | 807 | CLA | C4B-NB | -2.17 | 1.35 | 1.37 |
| 21 | R | 101 | LMU | O2B-C2B | 2.17 | 1.48 | 1.43 |
| 20 | A | 819 | CLA | MG-NA | -2.17 | 2.01 | 2.06 |
| 21 | 4 | 319 | LMU | O1'-C1' | 2.17 | 1.43 | 1.40 |
| 20 | 4 | 304 | CLA | C4C-C3C | -2.17 | 1.41 | 1.45 |
| 20 | B | 828 | CLA | C1B-C2B | -2.17 | 1.38 | 1.43 |
| 20 | 2 | 307 | CLA | C4B-NB | -2.17 | 1.35 | 1.37 |
| 20 | B | 823 | CLA | C1D-ND | -2.17 | 1.35 | 1.37 |
| 21 | H | 106 | LMU | O1'-C1' | 2.17 | 1.43 | 1.40 |
| 20 | L | 208 | CLA | C4D-ND | -2.17 | 1.34 | 1.37 |
| 20 | A | 814 | CLA | C3C-C4C | -2.17 | 1.38 | 1.43 |
| 20 | B | 841 | CLA | C1D-ND | -2.17 | 1.35 | 1.37 |
| 20 | B | 829 | CLA | C1D-C2D | -2.17 | 1.41 | 1.45 |
| 20 | A | 820 | CLA | MG-NA | -2.16 | 2.01 | 2.06 |
| 20 | 3 | 306 | CLA | C3D-C2D | 2.16 | 1.40 | 1.35 |
| 20 | 3 | 317 | CLA | MG-NA | -2.16 | 2.01 | 2.06 |
| 20 | B | 813 | CLA | MG-NA | -2.16 | 2.01 | 2.06 |
| 21 | A | 847 | LMU | O1'-C1' | 2.16 | 1.43 | 1.40 |
| 22 | L | 209 | BCR | C17-C18 | -2.16 | 1.32 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | B | 801 | BCR | C14-C13 | -2.16 | 1.32 | 1.35 |
| 20 | A | 832 | CLA | C4B-NB | -2.15 | 1.35 | 1.37 |
| 20 | A | 822 | CLA | MG-NA | -2.15 | 2.01 | 2.06 |
| 20 | 2 | 303 | CLA | C1D-ND | -2.15 | 1.35 | 1.37 |
| 20 | A | 807 | CLA | MG-NA | -2.15 | 2.01 | 2.06 |
| 20 | 1 | 211 | CLA | C3B-C4B | -2.15 | 1.37 | 1.42 |
| 20 | 2 | 311 | CLA | C4B-NB | -2.15 | 1.35 | 1.37 |
| 20 | B | 839 | CLA | C4B-NB | -2.15 | 1.35 | 1.37 |
| 20 | 1 | 207 | CLA | CAA-C2A | -2.15 | 1.50 | 1.54 |
| 20 | 3 | 316 | CLA | C3C-C4C | -2.15 | 1.38 | 1.43 |
| 20 | 2 | 314 | CLA | C1D-ND | -2.15 | 1.35 | 1.37 |
| 20 | B | 833 | CLA | C1C-NC | -2.15 | 1.34 | 1.37 |
| 20 | B | 806 | CLA | MG-NA | -2.15 | 2.01 | 2.06 |
| 20 | L | 202 | CLA | C4B-NB | -2.14 | 1.35 | 1.37 |
| 20 | 2 | 306 | CLA | C2D-C1D | -2.14 | 1.39 | 1.44 |
| 20 | 2 | 314 | CLA | CHB-C4A | -2.14 | 1.32 | 1.37 |
| 20 | 4 | 315 | CLA | C1D-C2D | -2.14 | 1.41 | 1.45 |
| 20 | B | 824 | CLA | C1D-C2D | -2.14 | 1.41 | 1.45 |
| 20 | K | 104 | CLA | CHB-C4A | -2.14 | 1.32 | 1.37 |
| 20 | A | 834 | CLA | MG-NA | -2.14 | 2.01 | 2.06 |
| 20 | B | 813 | CLA | C1D-ND | -2.14 | 1.35 | 1.37 |
| 20 | A | 801 | CLA | C4C-C3C | -2.14 | 1.41 | 1.45 |
| 20 | 3 | 316 | CLA | CHA-C1A | 2.14 | 1.46 | 1.40 |
| 20 | B | 836 | CLA | CHB-C4A | -2.13 | 1.32 | 1.37 |
| 20 | 2 | 304 | CLA | C2D-C1D | -2.13 | 1.39 | 1.44 |
| 20 | 2 | 310 | CLA | C4B-NB | -2.13 | 1.35 | 1.37 |
| 20 | B | 835 | CLA | MG-NA | -2.13 | 2.01 | 2.06 |
| 20 | F | 201 | CLA | C1B-C2B | -2.13 | 1.38 | 1.43 |
| 20 | K | 102 | CLA | C1B-C2B | -2.13 | 1.38 | 1.43 |
| 20 | F | 205 | CLA | MG-NA | -2.13 | 2.01 | 2.06 |
| 20 | B | 819 | CLA | C3D-CAD | -2.13 | 1.37 | 1.45 |
| 20 | A | 825 | CLA | C1B-C2B | -2.13 | 1.38 | 1.43 |
| 20 | K | 103 | CLA | MG-ND | -2.12 | 2.01 | 2.05 |
| 20 | J | 101 | CLA | C1B-C2B | -2.12 | 1.38 | 1.43 |
| 20 | A | 816 | CLA | C3D-CAD | -2.12 | 1.38 | 1.45 |
| 20 | A | 822 | CLA | C4B-NB | -2.12 | 1.35 | 1.37 |
| 20 | 4 | 307 | CLA | C2C-C1C | -2.12 | 1.38 | 1.43 |
| 20 | A | 831 | CLA | C3D-CAD | -2.12 | 1.38 | 1.45 |
| 20 | A | 833 | CLA | C1B-C2B | -2.12 | 1.38 | 1.43 |
| 20 | 2 | 304 | CLA | C2C-C1C | -2.12 | 1.38 | 1.43 |
| 20 | A | 836 | CLA | C4B-NB | -2.11 | 1.35 | 1.37 |
| 20 | F | 201 | CLA | C2-C3 | 2.11 | 1.38 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 3 | 314 | CLA | MG-NB | -2.11 | 2.01 | 2.05 |
| 20 | A | 816 | CLA | C1C-NC | -2.11 | 1.34 | 1.37 |
| 20 | 4 | 311 | CLA | C2D-C1D | -2.11 | 1.39 | 1.44 |
| 20 | A | 801 | CLA | C2A-C1A | -2.11 | 1.47 | 1.52 |
| 20 | A | 824 | CLA | C4B-NB | -2.11 | 1.35 | 1.37 |
| 20 | A | 826 | CLA | MG-NA | -2.11 | 2.01 | 2.06 |
| 20 | B | 834 | CLA | C1B-C2B | -2.11 | 1.38 | 1.43 |
| 20 | B | 822 | CLA | MG-NA | -2.11 | 2.01 | 2.06 |
| 20 | B | 838 | CLA | C4B-NB | -2.11 | 1.35 | 1.37 |
| 20 | 4 | 310 | CLA | C1D-C2D | -2.11 | 1.41 | 1.45 |
| 20 | J | 101 | CLA | C4B-NB | -2.11 | 1.35 | 1.37 |
| 20 | 4 | 306 | CLA | CAA-C2A | -2.10 | 1.50 | 1.54 |
| 20 | 2 | 303 | CLA | CHB-C4A | -2.10 | 1.32 | 1.37 |
| 20 | B | 829 | CLA | MG-NA | -2.10 | 2.01 | 2.06 |
| 20 | 1 | 206 | CLA | MG-NA | -2.10 | 2.01 | 2.06 |
| 20 | 2 | 303 | CLA | C3D-CAD | -2.10 | 1.38 | 1.45 |
| 20 | 1 | 201 | CLA | C3B-C4B | -2.10 | 1.37 | 1.42 |
| 21 | L | 210 | LMU | O1'-C1' | 2.10 | 1.43 | 1.40 |
| 20 | B | 802 | CLA | MG-NA | -2.10 | 2.01 | 2.06 |
| 20 | A | 825 | CLA | C4B-NB | -2.10 | 1.35 | 1.37 |
| 20 | A | 807 | CLA | C1B-C2B | -2.09 | 1.38 | 1.43 |
| 20 | A | 817 | CLA | C4B-NB | -2.09 | 1.35 | 1.37 |
| 20 | A | 851 | CLA | C4B-NB | -2.09 | 1.35 | 1.37 |
| 20 | B | 832 | CLA | CHB-C4A | -2.09 | 1.32 | 1.37 |
| 20 | B | 815 | CLA | C1B-NB | -2.09 | 1.35 | 1.37 |
| 20 | 1 | 211 | CLA | C1D-C2D | -2.09 | 1.41 | 1.45 |
| 20 | A | 812 | CLA | MG-NA | -2.09 | 2.01 | 2.06 |
| 20 | K | 104 | CLA | C1D-ND | -2.09 | 1.35 | 1.37 |
| 21 | C | 101 | LMU | O1'-C1' | 2.09 | 1.43 | 1.40 |
| 20 | A | 804 | CLA | CHB-C4A | -2.08 | 1.32 | 1.37 |
| 20 | B | 826 | CLA | C1B-C2B | -2.08 | 1.38 | 1.43 |
| 20 | A | 827 | CLA | C1B-C2B | -2.08 | 1.38 | 1.43 |
| 20 | 4 | 302 | CLA | MG-NA | -2.08 | 2.01 | 2.06 |
| 20 | L | 201 | CLA | MG-NA | -2.08 | 2.01 | 2.06 |
| 20 | B | 836 | CLA | C1D-C2D | -2.08 | 1.41 | 1.45 |
| 20 | A | 803 | CLA | C4D-ND | -2.08 | 1.34 | 1.37 |
| 20 | 4 | 301 | CLA | C1B-C2B | -2.08 | 1.38 | 1.43 |
| 20 | K | 104 | CLA | C3D-CAD | -2.08 | 1.38 | 1.45 |
| 20 | A | 812 | CLA | C1B-C2B | -2.08 | 1.38 | 1.43 |
| 21 | R | 103 | LMU | O1'-C1' | 2.07 | 1.43 | 1.40 |
| 20 | B | 829 | CLA | C1D-ND | -2.07 | 1.35 | 1.37 |
| 20 | 1 | 211 | CLA | C1C-NC | -2.07 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 203 | CLA | C4D-CHA | -2.07 | 1.31 | 1.38 |
| 20 | B | 803 | CLA | C4B-NB | -2.07 | 1.35 | 1.37 |
| 20 | B | 842 | CLA | MG-NA | -2.07 | 2.01 | 2.06 |
| 20 | A | 819 | CLA | CHB-C4A | -2.07 | 1.32 | 1.37 |
| 20 | F | 201 | CLA | C3D-CAD | -2.07 | 1.38 | 1.45 |
| 20 | 2 | 315 | CLA | C3C-C4C | -2.07 | 1.38 | 1.43 |
| 20 | 4 | 302 | CLA | C1D-ND | -2.07 | 1.35 | 1.37 |
| 20 | F | 207 | CLA | C4D-ND | -2.07 | 1.34 | 1.37 |
| 21 | A | 852 | LMU | O1'-C1' | 2.07 | 1.43 | 1.40 |
| 20 | A | 817 | CLA | MG-NA | -2.06 | 2.01 | 2.06 |
| 20 | 4 | 306 | CLA | CHB-C1B | 2.06 | 1.44 | 1.39 |
| 20 | K | 101 | CLA | C4B-NB | -2.06 | 1.35 | 1.37 |
| 20 | B | 810 | CLA | C1B-C2B | -2.06 | 1.38 | 1.43 |
| 20 | H | 109 | CLA | C1B-C2B | -2.06 | 1.38 | 1.43 |
| 20 | 2 | 314 | CLA | C1D-C2D | -2.06 | 1.41 | 1.45 |
| 20 | 3 | 315 | CLA | C3C-C4C | -2.06 | 1.38 | 1.43 |
| 20 | 1 | 205 | CLA | C1B-C2B | -2.06 | 1.38 | 1.43 |
| 20 | 2 | 307 | CLA | C3B-C4B | -2.06 | 1.38 | 1.42 |
| 20 | I | 102 | CLA | C1B-C2B | -2.06 | 1.38 | 1.43 |
| 20 | A | 816 | CLA | C1D-ND | -2.06 | 1.35 | 1.37 |
| 20 | B | 825 | CLA | C1D-ND | -2.06 | 1.35 | 1.37 |
| 20 | 1 | 215 | CLA | C1C-NC | -2.06 | 1.34 | 1.37 |
| 20 | A | 841 | CLA | C2C-C1C | -2.06 | 1.38 | 1.43 |
| 20 | B | 837 | CLA | C4B-NB | -2.06 | 1.35 | 1.37 |
| 20 | B | 812 | CLA | C3A-C2A | -2.06 | 1.48 | 1.54 |
| 21 | K | 105 | LMU | O1'-C1' | 2.05 | 1.43 | 1.40 |
| 20 | A | 803 | CLA | C1D-C2D | -2.05 | 1.41 | 1.45 |
| 20 | A | 835 | CLA | C1D-ND | -2.05 | 1.35 | 1.37 |
| 20 | A | 813 | CLA | C1B-C2B | -2.05 | 1.38 | 1.43 |
| 20 | A | 818 | CLA | C3A-C2A | -2.05 | 1.48 | 1.54 |
| 21 | R | 101 | LMU | O1'-C1' | 2.05 | 1.43 | 1.40 |
| 20 | 3 | 311 | CLA | C4B-NB | -2.05 | 1.35 | 1.37 |
| 20 | A | 827 | CLA | C4B-NB | -2.05 | 1.35 | 1.37 |
| 20 | B | 836 | CLA | MG-ND | -2.05 | 2.01 | 2.05 |
| 21 | A | 855 | LMU | O1'-C1' | 2.05 | 1.43 | 1.40 |
| 20 | A | 808 | CLA | CHB-C4A | -2.05 | 1.32 | 1.37 |
| 21 | G | 101 | LMU | O4'-C4B | 2.04 | 1.47 | 1.43 |
| 20 | B | 806 | CLA | C1B-C2B | -2.04 | 1.38 | 1.43 |
| 20 | 3 | 304 | CLA | C3C-C4C | -2.04 | 1.38 | 1.43 |
| 20 | A | 839 | CLA | MG-ND | -2.04 | 2.01 | 2.05 |
| 20 | B | 811 | CLA | C3C-C4C | -2.04 | 1.38 | 1.43 |
| 20 | F | 207 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | F | 206 | CLA | C1B-C2B | -2.04 | 1.38 | 1.43 |
| 20 | 4 | 303 | CLA | C3A-C2A | -2.04 | 1.48 | 1.54 |
| 20 | 2 | 309 | CLA | C2C-C1C | -2.04 | 1.38 | 1.43 |
| 20 | A | 831 | CLA | C3A-C2A | -2.04 | 1.48 | 1.54 |
| 20 | A | 838 | CLA | C1B-C2B | -2.04 | 1.38 | 1.43 |
| 20 | B | 802 | CLA | C1B-C2B | -2.04 | 1.38 | 1.43 |
| 20 | B | 840 | CLA | C1B-C2B | -2.03 | 1.38 | 1.43 |
| 20 | A | 811 | CLA | C4B-NB | -2.03 | 1.35 | 1.37 |
| 20 | 2 | 303 | CLA | C1B-C2B | -2.03 | 1.38 | 1.43 |
| 20 | 1 | 213 | CLA | MG-NB | -2.03 | 2.01 | 2.05 |
| 20 | A | 826 | CLA | CHB-C4A | -2.03 | 1.32 | 1.37 |
| 20 | 1 | 204 | CLA | C2A-C1A | -2.03 | 1.47 | 1.52 |
| 20 | 1 | 201 | CLA | C3D-CAD | -2.03 | 1.38 | 1.45 |
| 20 | B | 825 | CLA | CHB-C4A | -2.03 | 1.32 | 1.37 |
| 20 | B | 831 | CLA | CHB-C4A | -2.03 | 1.32 | 1.37 |
| 20 | 2 | 311 | CLA | C1D-C2D | -2.03 | 1.41 | 1.45 |
| 20 | 4 | 311 | CLA | C2C-C1C | -2.03 | 1.38 | 1.43 |
| 20 | B | 825 | CLA | C1D-C2D | -2.03 | 1.41 | 1.45 |
| 20 | A | 840 | CLA | MG-NA | -2.03 | 2.01 | 2.06 |
| 20 | A | 812 | CLA | C4B-NB | -2.03 | 1.35 | 1.37 |
| 20 | A | 849 | CLA | MG-NA | -2.03 | 2.01 | 2.06 |
| 20 | 4 | 318 | CLA | C1D-C2D | -2.03 | 1.41 | 1.45 |
| 20 | H | 108 | CLA | C3D-CAD | -2.03 | 1.38 | 1.45 |
| 21 | G | 101 | LMU | C4B-C5B | 2.03 | 1.57 | 1.53 |
| 20 | B | 812 | CLA | C4D-CHA | -2.03 | 1.31 | 1.38 |
| 20 | 3 | 301 | CLA | MG-NA | -2.02 | 2.01 | 2.06 |
| 20 | 3 | 313 | CLA | C1C-C2C | -2.02 | 1.40 | 1.44 |
| 20 | B | 841 | CLA | MG-NA | -2.02 | 2.01 | 2.06 |
| 20 | 1 | 211 | CLA | MG-NA | -2.02 | 2.01 | 2.06 |
| 20 | 4 | 303 | CLA | C1D-ND | -2.02 | 1.35 | 1.37 |
| 20 | B | 833 | CLA | C1D-C2D | -2.02 | 1.41 | 1.45 |
| 20 | 4 | 313 | CLA | C4B-NB | -2.02 | 1.35 | 1.37 |
| 20 | B | 823 | CLA | C1B-C2B | -2.02 | 1.38 | 1.43 |
| 20 | H | 101 | CLA | C3A-C2A | -2.01 | 1.48 | 1.54 |
| 20 | 1 | 206 | CLA | C1D-ND | -2.01 | 1.35 | 1.37 |
| 20 | A | 837 | CLA | C1B-C2B | -2.01 | 1.38 | 1.43 |
| 20 | 3 | 316 | CLA | C2C-C1C | -2.01 | 1.38 | 1.43 |
| 20 | A | 817 | CLA | C1B-C2B | -2.01 | 1.38 | 1.43 |
| 20 | 3 | 312 | CLA | C3D-C2D | 2.01 | 1.39 | 1.35 |
| 20 | A | 801 | CLA | C3A-C2A | -2.01 | 1.48 | 1.54 |
| 20 | L | 204 | CLA | MG-NA | -2.01 | 2.01 | 2.06 |
| 20 | 1 | 211 | CLA | C1B-C2B | -2.00 | 1.38 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 824 | CLA | CHB-C4A | -2.00 | 1.32 | 1.37 |
| 20 | L | 208 | CLA | CHB-C4A | -2.00 | 1.32 | 1.37 |
| 20 | G | 105 | CLA | C3D-CAD | -2.00 | 1.38 | 1.45 |
| 20 | B | 835 | CLA | C1D-ND | -2.00 | 1.35 | 1.37 |
| 20 | J | 103 | CLA | MG-ND | -2.00 | 2.01 | 2.05 |
| 20 | 3 | 306 | CLA | C3C-C4C | -2.00 | 1.38 | 1.43 |
| 20 | 2 | 308 | CLA | CHB-C1B | 2.00 | 1.45 | 1.40 |
| 20 | B | 820 | CLA | C1D-C2D | -2.00 | 1.41 | 1.45 |
| 20 | 2 | 310 | CLA | CHB-C4A | -2.00 | 1.32 | 1.37 |
| 20 | 4 | 303 | CLA | C1C-NC | -2.00 | 1.34 | 1.37 |

All (5036) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | G | 104 | BCR | C20-C21-C22 | 36.27 | 179.07 | 127.31 |
| 22 | L | 209 | BCR | C20-C21-C22 | 35.78 | 178.38 | 127.31 |
| 22 | A | 845 | BCR | C20-C21-C22 | 35.54 | 178.03 | 127.31 |
| 22 | J | 102 | BCR | C20-C21-C22 | 35.47 | 177.93 | 127.31 |
| 22 | B | 846 | BCR | C20-C21-C22 | 35.39 | 177.82 | 127.31 |
| 22 | A | 844 | BCR | C20-C21-C22 | 35.34 | 177.74 | 127.31 |
| 22 | F | 204 | BCR | C20-C21-C22 | 35.23 | 177.59 | 127.31 |
| 22 | I | 103 | BCR | C20-C21-C22 | 35.19 | 177.54 | 127.31 |
| 22 | A | 843 | BCR | C20-C21-C22 | 34.78 | 176.95 | 127.31 |
| 22 | 2 | 317 | BCR | C20-C21-C22 | 34.60 | 176.70 | 127.31 |
| 22 | B | 801 | BCR | C20-C21-C22 | 34.47 | 176.50 | 127.31 |
| 22 | F | 203 | BCR | C20-C21-C22 | 34.38 | 176.38 | 127.31 |
| 22 | B | 847 | BCR | C20-C21-C22 | 34.25 | 176.20 | 127.31 |
| 22 | B | 844 | BCR | C20-C21-C22 | 31.07 | 171.65 | 127.31 |
| 22 | B | 845 | BCR | C20-C21-C22 | 29.37 | 169.23 | 127.31 |
| 22 | I | 101 | BCR | C20-C21-C22 | 20.43 | 156.47 | 127.31 |
| 22 | A | 845 | BCR | C21-C20-C19 | 17.67 | 178.37 | 123.22 |
| 22 | B | 847 | BCR | C21-C20-C19 | 17.62 | 178.22 | 123.22 |
| 22 | L | 209 | BCR | C21-C20-C19 | 17.52 | 177.89 | 123.22 |
| 22 | G | 104 | BCR | C21-C20-C19 | 17.50 | 177.84 | 123.22 |
| 22 | I | 103 | BCR | C21-C20-C19 | 17.48 | 177.76 | 123.22 |
| 22 | 2 | 317 | BCR | C21-C20-C19 | 17.36 | 177.39 | 123.22 |
| 22 | B | 801 | BCR | C21-C20-C19 | 17.21 | 176.93 | 123.22 |
| 22 | F | 203 | BCR | C21-C20-C19 | 17.11 | 176.60 | 123.22 |
| 22 | B | 846 | BCR | C21-C20-C19 | 16.91 | 175.98 | 123.22 |
| 22 | J | 102 | BCR | C21-C20-C19 | 16.88 | 175.90 | 123.22 |
| 22 | F | 204 | BCR | C21-C20-C19 | 16.85 | 175.80 | 123.22 |
| 22 | A | 843 | BCR | C21-C20-C19 | 16.45 | 174.54 | 123.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | A | 844 | BCR | C21-C20-C19 | 15.62 | 171.97 | 123.22 |
| 22 | B | 845 | BCR | C21-C20-C19 | 14.52 | 168.52 | 123.22 |
| 22 | B | 844 | BCR | C21-C20-C19 | 14.44 | 168.29 | 123.22 |
| 20 | A | 801 | CLA | CAB-C3B-C4B | -11.74 | 107.49 | 125.37 |
| 22 | I | 101 | BCR | C24-C23-C22 | -11.61 | 108.69 | 126.23 |
| 20 | 2 | 316 | CLA | OBD-CAD-C3D | -11.58 | 100.66 | 128.52 |
| 20 | A | 831 | CLA | OBD-CAD-C3D | -11.47 | 100.92 | 128.52 |
| 20 | 4 | 302 | CLA | CAB-C3B-C4B | -11.46 | 107.91 | 125.37 |
| 20 | B | 812 | CLA | CAB-C3B-C4B | -11.45 | 107.94 | 125.37 |
| 20 | 3 | 301 | CLA | CAB-C3B-C4B | -11.40 | 108.01 | 125.37 |
| 20 | 2 | 303 | CLA | OBD-CAD-C3D | -11.39 | 101.12 | 128.52 |
| 20 | B | 842 | CLA | CAB-C3B-C4B | -11.30 | 108.15 | 125.37 |
| 20 | 4 | 313 | CLA | CAB-C3B-C4B | -11.22 | 108.28 | 125.37 |
| 20 | B | 839 | CLA | OBD-CAD-C3D | -11.18 | 101.62 | 128.52 |
| 20 | 3 | 314 | CLA | OBD-CAD-C3D | -10.91 | 102.28 | 128.52 |
| 20 | 1 | 210 | CLA | CAB-C3B-C4B | -10.45 | 109.45 | 125.37 |
| 22 | B | 801 | BCR | C15-C16-C17 | -10.45 | 102.08 | 123.47 |
| 22 | B | 801 | BCR | C7-C8-C9 | -10.40 | 110.52 | 126.23 |
| 20 | A | 840 | CLA | CBB-CAB-C3B | 10.34 | 179.06 | 127.62 |
| 20 | 3 | 307 | CLA | CBB-CAB-C3B | 10.32 | 178.97 | 127.62 |
| 20 | 2 | 310 | CLA | OBD-CAD-C3D | -10.31 | 103.70 | 128.52 |
| 20 | B | 828 | CLA | OBD-CAD-C3D | -10.27 | 103.80 | 128.52 |
| 20 | A | 803 | CLA | OBD-CAD-C3D | -10.25 | 103.86 | 128.52 |
| 20 | B | 823 | CLA | CBB-CAB-C3B | 10.23 | 178.50 | 127.62 |
| 20 | 1 | 211 | CLA | OBD-CAD-C3D | -10.19 | 103.99 | 128.52 |
| 20 | I | 102 | CLA | CBB-CAB-C3B | 10.18 | 178.29 | 127.62 |
| 20 | 1 | 213 | CLA | OBD-CAD-C3D | -10.18 | 104.02 | 128.52 |
| 20 | L | 208 | CLA | CBB-CAB-C3B | 10.15 | 178.12 | 127.62 |
| 20 | J | 103 | CLA | CBB-CAB-C3B | 10.13 | 178.03 | 127.62 |
| 20 | A | 817 | CLA | CBB-CAB-C3B | 10.12 | 177.95 | 127.62 |
| 20 | A | 833 | CLA | OBD-CAD-C3D | -10.12 | 104.17 | 128.52 |
| 20 | K | 104 | CLA | OBD-CAD-C3D | -10.11 | 104.19 | 128.52 |
| 20 | A | 830 | CLA | CBB-CAB-C3B | 10.10 | 177.87 | 127.62 |
| 20 | H | 101 | CLA | CBB-CAB-C3B | 10.09 | 177.83 | 127.62 |
| 20 | 4 | 317 | CLA | CBB-CAB-C3B | 10.09 | 177.81 | 127.62 |
| 20 | 3 | 311 | CLA | CBB-CAB-C3B | 10.08 | 177.79 | 127.62 |
| 20 | 2 | 312 | CLA | CBB-CAB-C3B | 10.07 | 177.71 | 127.62 |
| 20 | 1 | 201 | CLA | CBB-CAB-C3B | 10.07 | 177.69 | 127.62 |
| 20 | K | 101 | CLA | CBB-CAB-C3B | 10.05 | 177.61 | 127.62 |
| 20 | H | 108 | CLA | C2B-C1B-NB | 10.04 | 116.96 | 110.23 |
| 20 | A | 849 | CLA | CBB-CAB-C3B | 10.01 | 177.40 | 127.62 |
| 20 | A | 815 | CLA | CBB-CAB-C3B | 10.00 | 177.36 | 127.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 301 | CLA | CBB-CAB-C3B | 9.98 | 177.26 | 127.62 |
| 20 | B | 822 | CLA | CBB-CAB-C3B | 9.97 | 177.24 | 127.62 |
| 20 | B | 824 | CLA | CBB-CAB-C3B | 9.96 | 177.18 | 127.62 |
| 20 | R | 108 | CLA | CBB-CAB-C3B | 9.96 | 177.18 | 127.62 |
| 20 | 3 | 313 | CLA | CBB-CAB-C3B | 9.95 | 177.12 | 127.62 |
| 20 | 3 | 317 | CLA | CAB-C3B-C4B | -9.94 | 110.23 | 125.37 |
| 20 | B | 820 | CLA | CBB-CAB-C3B | 9.93 | 177.03 | 127.62 |
| 20 | 4 | 305 | CLA | CBB-CAB-C3B | 9.92 | 176.95 | 127.62 |
| 20 | A | 851 | CLA | CBB-CAB-C3B | 9.91 | 176.94 | 127.62 |
| 20 | B | 803 | CLA | CBB-CAB-C3B | 9.90 | 176.88 | 127.62 |
| 20 | A | 829 | CLA | CBB-CAB-C3B | 9.90 | 176.86 | 127.62 |
| 20 | F | 201 | CLA | CBB-CAB-C3B | 9.89 | 176.80 | 127.62 |
| 20 | A | 850 | CLA | CBB-CAB-C3B | 9.87 | 176.71 | 127.62 |
| 20 | R | 107 | CLA | CBB-CAB-C3B | 9.83 | 176.54 | 127.62 |
| 20 | A | 832 | CLA | CBB-CAB-C3B | 9.83 | 176.52 | 127.62 |
| 20 | 3 | 310 | CLA | OBD-CAD-C3D | -9.83 | 104.87 | 128.52 |
| 20 | 2 | 314 | CLA | CBB-CAB-C3B | 9.82 | 176.46 | 127.62 |
| 20 | J | 101 | CLA | CBB-CAB-C3B | 9.81 | 176.45 | 127.62 |
| 20 | A | 801 | CLA | OBD-CAD-C3D | -9.79 | 104.95 | 128.52 |
| 20 | B | 812 | CLA | OBD-CAD-C3D | -9.79 | 104.97 | 128.52 |
| 20 | A | 826 | CLA | CBB-CAB-C3B | 9.78 | 176.29 | 127.62 |
| 20 | B | 834 | CLA | CBB-CAB-C3B | 9.77 | 176.24 | 127.62 |
| 20 | K | 102 | CLA | CBB-CAB-C3B | 9.77 | 176.21 | 127.62 |
| 20 | H | 110 | CLA | CBB-CAB-C3B | 9.75 | 176.13 | 127.62 |
| 20 | L | 202 | CLA | CBB-CAB-C3B | 9.75 | 176.10 | 127.62 |
| 20 | A | 836 | CLA | CBB-CAB-C3B | 9.73 | 176.01 | 127.62 |
| 20 | A | 833 | CLA | CBB-CAB-C3B | 9.72 | 176.00 | 127.62 |
| 20 | B | 825 | CLA | CBB-CAB-C3B | 9.72 | 175.99 | 127.62 |
| 20 | F | 206 | CLA | CBB-CAB-C3B | 9.71 | 175.94 | 127.62 |
| 20 | A | 816 | CLA | OBD-CAD-C3D | -9.71 | 105.15 | 128.52 |
| 20 | 4 | 301 | CLA | OBD-CAD-C3D | -9.70 | 105.17 | 128.52 |
| 20 | A | 820 | CLA | OBD-CAD-C3D | -9.69 | 105.20 | 128.52 |
| 20 | 1 | 203 | CLA | CBB-CAB-C3B | 9.69 | 175.82 | 127.62 |
| 20 | B | 826 | CLA | CBB-CAB-C3B | 9.68 | 175.80 | 127.62 |
| 22 | I | 101 | BCR | C21-C20-C19 | 9.68 | 153.42 | 123.22 |
| 20 | 1 | 204 | CLA | CBB-CAB-C3B | 9.68 | 175.75 | 127.62 |
| 20 | B | 821 | CLA | CBB-CAB-C3B | 9.66 | 175.70 | 127.62 |
| 20 | B | 819 | CLA | OBD-CAD-C3D | -9.62 | 105.37 | 128.52 |
| 20 | B | 822 | CLA | OBD-CAD-C3D | -9.60 | 105.41 | 128.52 |
| 20 | A | 806 | CLA | CBB-CAB-C3B | 9.60 | 175.37 | 127.62 |
| 20 | B | 818 | CLA | CBB-CAB-C3B | 9.59 | 175.35 | 127.62 |
| 20 | B | 809 | CLA | CBB-CAB-C3B | 9.59 | 175.31 | 127.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 837 | CLA | CBB-CAB-C3B | 9.57 | 175.25 | 127.62 |
| 20 | A | 829 | CLA | OBD-CAD-C3D | -9.56 | 105.50 | 128.52 |
| 20 | H | 102 | CLA | CBB-CAB-C3B | 9.55 | 175.14 | 127.62 |
| 20 | L | 201 | CLA | CBB-CAB-C3B | 9.53 | 175.05 | 127.62 |
| 20 | B | 810 | CLA | CBB-CAB-C3B | 9.51 | 174.94 | 127.62 |
| 20 | B | 833 | CLA | OBD-CAD-C3D | -9.50 | 105.65 | 128.52 |
| 20 | A | 810 | CLA | CBB-CAB-C3B | 9.50 | 174.86 | 127.62 |
| 20 | A | 834 | CLA | CBB-CAB-C3B | 9.49 | 174.83 | 127.62 |
| 20 | 1 | 211 | CLA | CBB-CAB-C3B | 9.49 | 174.82 | 127.62 |
| 20 | 2 | 316 | CLA | CBB-CAB-C3B | 9.49 | 174.82 | 127.62 |
| 20 | L | 207 | CLA | CBB-CAB-C3B | 9.48 | 174.78 | 127.62 |
| 20 | L | 204 | CLA | CBB-CAB-C3B | 9.47 | 174.76 | 127.62 |
| 20 | A | 824 | CLA | OBD-CAD-C3D | -9.47 | 105.74 | 128.52 |
| 20 | B | 839 | CLA | CBB-CAB-C3B | 9.44 | 174.60 | 127.62 |
| 20 | A | 837 | CLA | CBB-CAB-C3B | 9.43 | 174.52 | 127.62 |
| 20 | A | 810 | CLA | OBD-CAD-C3D | -9.43 | 105.83 | 128.52 |
| 20 | B | 815 | CLA | CBB-CAB-C3B | 9.42 | 174.47 | 127.62 |
| 20 | 2 | 311 | CLA | OBD-CAD-C3D | -9.39 | 105.93 | 128.52 |
| 20 | A | 808 | CLA | OBD-CAD-C3D | -9.39 | 105.93 | 128.52 |
| 20 | H | 109 | CLA | CBB-CAB-C3B | 9.37 | 174.25 | 127.62 |
| 20 | A | 805 | CLA | OBD-CAD-C3D | -9.37 | 105.98 | 128.52 |
| 20 | 4 | 303 | CLA | OBD-CAD-C3D | -9.36 | 106.00 | 128.52 |
| 20 | G | 105 | CLA | OBD-CAD-C3D | -9.36 | 106.01 | 128.52 |
| 20 | F | 207 | CLA | OBD-CAD-C3D | -9.35 | 106.03 | 128.52 |
| 20 | L | 203 | CLA | OBD-CAD-C3D | -9.35 | 106.03 | 128.52 |
| 20 | B | 802 | CLA | CBB-CAB-C3B | 9.33 | 174.04 | 127.62 |
| 20 | B | 806 | CLA | CBB-CAB-C3B | 9.33 | 174.04 | 127.62 |
| 20 | A | 835 | CLA | CBB-CAB-C3B | 9.33 | 174.03 | 127.62 |
| 20 | 4 | 315 | CLA | CBB-CAB-C3B | 9.32 | 173.97 | 127.62 |
| 20 | 1 | 203 | CLA | OBD-CAD-C3D | -9.31 | 106.11 | 128.52 |
| 20 | B | 836 | CLA | CBB-CAB-C3B | 9.31 | 173.95 | 127.62 |
| 20 | A | 819 | CLA | OBD-CAD-C3D | -9.29 | 106.16 | 128.52 |
| 20 | H | 101 | CLA | OBD-CAD-C3D | -9.29 | 106.17 | 128.52 |
| 20 | L | 202 | CLA | OBD-CAD-C3D | -9.28 | 106.19 | 128.52 |
| 20 | 3 | 307 | CLA | OBD-CAD-C3D | -9.27 | 106.21 | 128.52 |
| 20 | L | 203 | CLA | CBB-CAB-C3B | 9.27 | 173.72 | 127.62 |
| 20 | B | 827 | CLA | CBB-CAB-C3B | 9.25 | 173.66 | 127.62 |
| 20 | A | 807 | CLA | CBB-CAB-C3B | 9.25 | 173.66 | 127.62 |
| 20 | L | 208 | CLA | OBD-CAD-C3D | -9.25 | 106.26 | 128.52 |
| 20 | B | 850 | CLA | OBD-CAD-C3D | -9.24 | 106.28 | 128.52 |
| 20 | A | 826 | CLA | OBD-CAD-C3D | -9.24 | 106.28 | 128.52 |
| 20 | 2 | 302 | CLA | CBB-CAB-C3B | 9.21 | 173.43 | 127.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 306 | CLA | OBD-CAD-C3D | -9.20 | 106.39 | 128.52 |
| 20 | B | 826 | CLA | OBD-CAD-C3D | -9.18 | 106.42 | 128.52 |
| 20 | 1 | 207 | CLA | CBB-CAB-C3B | 9.18 | 173.27 | 127.62 |
| 20 | B | 813 | CLA | CBB-CAB-C3B | 9.17 | 173.26 | 127.62 |
| 20 | 2 | 307 | CLA | OBD-CAD-C3D | -9.17 | 106.45 | 128.52 |
| 20 | K | 103 | CLA | CBB-CAB-C3B | 9.17 | 173.23 | 127.62 |
| 20 | A | 813 | CLA | CBB-CAB-C3B | 9.16 | 173.20 | 127.62 |
| 20 | K | 102 | CLA | OBD-CAD-C3D | -9.13 | 106.54 | 128.52 |
| 20 | B | 831 | CLA | CBB-CAB-C3B | 9.12 | 172.97 | 127.62 |
| 20 | 1 | 202 | CLA | CBB-CAB-C3B | 9.11 | 172.95 | 127.62 |
| 20 | B | 807 | CLA | C2B-C1B-NB | 9.11 | 116.34 | 110.23 |
| 20 | 2 | 310 | CLA | CBB-CAB-C3B | 9.10 | 172.88 | 127.62 |
| 20 | B | 819 | CLA | CBB-CAB-C3B | 9.09 | 172.84 | 127.62 |
| 20 | 1 | 213 | CLA | CBB-CAB-C3B | 9.08 | 172.81 | 127.62 |
| 20 | A | 817 | CLA | OBD-CAD-C3D | -9.08 | 106.66 | 128.52 |
| 20 | B | 837 | CLA | OBD-CAD-C3D | -9.08 | 106.67 | 128.52 |
| 22 | I | 103 | BCR | C24-C23-C22 | -9.06 | 112.54 | 126.23 |
| 20 | 1 | 215 | CLA | OBD-CAD-C3D | -9.06 | 106.71 | 128.52 |
| 20 | A | 824 | CLA | CBB-CAB-C3B | 9.05 | 172.66 | 127.62 |
| 20 | A | 820 | CLA | CBB-CAB-C3B | 9.05 | 172.65 | 127.62 |
| 20 | F | 206 | CLA | OBD-CAD-C3D | -9.01 | 106.83 | 128.52 |
| 20 | 2 | 311 | CLA | CBB-CAB-C3B | 9.01 | 172.43 | 127.62 |
| 20 | 1 | 204 | CLA | OBD-CAD-C3D | -8.99 | 106.88 | 128.52 |
| 20 | 3 | 311 | CLA | OBD-CAD-C3D | -8.99 | 106.88 | 128.52 |
| 20 | B | 832 | CLA | CAA-C2A-C3A | -8.98 | 88.19 | 112.78 |
| 20 | 4 | 318 | CLA | CBB-CAB-C3B | 8.97 | 172.22 | 127.62 |
| 20 | I | 102 | CLA | OBD-CAD-C3D | -8.96 | 106.95 | 128.52 |
| 20 | B | 835 | CLA | CBB-CAB-C3B | 8.96 | 172.20 | 127.62 |
| 20 | 3 | 317 | CLA | OBD-CAD-C3D | -8.96 | 106.96 | 128.52 |
| 20 | 3 | 314 | CLA | CBB-CAB-C3B | 8.96 | 172.18 | 127.62 |
| 20 | A | 830 | CLA | OBD-CAD-C3D | -8.95 | 106.99 | 128.52 |
| 20 | A | 827 | CLA | CBB-CAB-C3B | 8.94 | 172.10 | 127.62 |
| 20 | R | 107 | CLA | OBD-CAD-C3D | -8.93 | 107.03 | 128.52 |
| 20 | H | 109 | CLA | OBD-CAD-C3D | -8.92 | 107.05 | 128.52 |
| 20 | B | 802 | CLA | OBD-CAD-C3D | -8.92 | 107.05 | 128.52 |
| 20 | B | 832 | CLA | CBB-CAB-C3B | 8.92 | 171.99 | 127.62 |
| 20 | A | 825 | CLA | OBD-CAD-C3D | -8.91 | 107.07 | 128.52 |
| 20 | 2 | 303 | CLA | CBB-CAB-C3B | 8.91 | 171.96 | 127.62 |
| 20 | B | 809 | CLA | OBD-CAD-C3D | -8.90 | 107.10 | 128.52 |
| 20 | A | 812 | CLA | CBB-CAB-C3B | 8.89 | 171.83 | 127.62 |
| 20 | A | 811 | CLA | CBB-CAB-C3B | 8.87 | 171.75 | 127.62 |
| 20 | B | 828 | CLA | CBB-CAB-C3B | 8.87 | 171.74 | 127.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | H | 108 | CLA | CBB-CAB-C3B | 8.85 | 171.65 | 127.62 |
| 20 | A | 850 | CLA | OBD-CAD-C3D | -8.85 | 107.23 | 128.52 |
| 20 | 4 | 302 | CLA | OBD-CAD-C3D | -8.84 | 107.24 | 128.52 |
| 22 | B | 801 | BCR | C15-C14-C13 | -8.84 | 114.69 | 127.31 |
| 20 | A | 822 | CLA | OBD-CAD-C3D | -8.84 | 107.25 | 128.52 |
| 20 | K | 101 | CLA | OBD-CAD-C3D | -8.81 | 107.32 | 128.52 |
| 20 | A | 828 | CLA | OBD-CAD-C3D | -8.81 | 107.33 | 128.52 |
| 20 | A | 837 | CLA | OBD-CAD-C3D | -8.79 | 107.37 | 128.52 |
| 20 | B | 813 | CLA | OBD-CAD-C3D | -8.79 | 107.37 | 128.52 |
| 20 | 2 | 305 | CLA | CBB-CAB-C3B | 8.79 | 171.34 | 127.62 |
| 20 | K | 103 | CLA | OBD-CAD-C3D | -8.78 | 107.38 | 128.52 |
| 20 | A | 819 | CLA | CBB-CAB-C3B | 8.78 | 171.32 | 127.62 |
| 20 | B | 816 | CLA | CBB-CAB-C3B | 8.78 | 171.31 | 127.62 |
| 20 | B | 814 | CLA | CBB-CAB-C3B | 8.78 | 171.30 | 127.62 |
| 20 | 3 | 303 | CLA | OBD-CAD-C3D | -8.77 | 107.41 | 128.52 |
| 20 | 2 | 312 | CLA | OBD-CAD-C3D | -8.76 | 107.44 | 128.52 |
| 20 | A | 803 | CLA | CBB-CAB-C3B | 8.74 | 171.08 | 127.62 |
| 20 | B | 830 | CLA | CBB-CAB-C3B | 8.72 | 171.01 | 127.62 |
| 20 | B | 829 | CLA | CBB-CAB-C3B | 8.72 | 171.00 | 127.62 |
| 20 | A | 806 | CLA | OBD-CAD-C3D | -8.72 | 107.54 | 128.52 |
| 20 | A | 821 | CLA | CBB-CAB-C3B | 8.72 | 170.99 | 127.62 |
| 20 | B | 807 | CLA | CBB-CAB-C3B | 8.71 | 170.97 | 127.62 |
| 20 | 4 | 305 | CLA | OBD-CAD-C3D | -8.71 | 107.55 | 128.52 |
| 20 | 1 | 206 | CLA | CBB-CAB-C3B | 8.71 | 170.96 | 127.62 |
| 20 | A | 838 | CLA | CBB-CAB-C3B | 8.69 | 170.87 | 127.62 |
| 20 | F | 201 | CLA | OBD-CAD-C3D | -8.67 | 107.64 | 128.52 |
| 20 | A | 851 | CLA | OBD-CAD-C3D | -8.67 | 107.66 | 128.52 |
| 20 | B | 834 | CLA | OBD-CAD-C3D | -8.67 | 107.66 | 128.52 |
| 20 | F | 205 | CLA | C2B-C1B-NB | 8.65 | 116.03 | 110.23 |
| 20 | B | 808 | CLA | CBB-CAB-C3B | 8.64 | 170.61 | 127.62 |
| 20 | L | 208 | CLA | O2D-CGD-CBD | 8.63 | 126.60 | 111.27 |
| 22 | 2 | 317 | BCR | C16-C17-C18 | -8.61 | 115.02 | 127.31 |
| 20 | J | 101 | CLA | OBD-CAD-C3D | -8.60 | 107.83 | 128.52 |
| 20 | A | 809 | CLA | CBB-CAB-C3B | 8.58 | 170.28 | 127.62 |
| 20 | 1 | 205 | CLA | OBD-CAD-C3D | -8.55 | 107.94 | 128.52 |
| 20 | B | 821 | CLA | OBD-CAD-C3D | -8.55 | 107.95 | 128.52 |
| 20 | L | 207 | CLA | OBD-CAD-C3D | -8.54 | 107.96 | 128.52 |
| 20 | B | 827 | CLA | OBD-CAD-C3D | -8.54 | 107.97 | 128.52 |
| 20 | A | 816 | CLA | CBB-CAB-C3B | 8.54 | 170.08 | 127.62 |
| 20 | 4 | 303 | CLA | CBB-CAB-C3B | 8.53 | 170.08 | 127.62 |
| 20 | A | 822 | CLA | CBB-CAB-C3B | 8.52 | 170.02 | 127.62 |
| 20 | K | 104 | CLA | CBB-CAB-C3B | 8.51 | 169.98 | 127.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 302 | CLA | OBD-CAD-C3D | -8.51 | 108.03 | 128.52 |
| 22 | I | 101 | BCR | C7-C8-C9 | -8.51 | 113.38 | 126.23 |
| 20 | 1 | 205 | CLA | CAB-C3B-C4B | -8.49 | 112.43 | 125.37 |
| 20 | A | 823 | CLA | CBB-CAB-C3B | 8.48 | 169.82 | 127.62 |
| 20 | B | 806 | CLA | C2B-C1B-NB | 8.48 | 115.91 | 110.23 |
| 20 | B | 841 | CLA | CBB-CAB-C3B | 8.47 | 169.78 | 127.62 |
| 20 | 1 | 201 | CLA | OBD-CAD-C3D | -8.43 | 108.22 | 128.52 |
| 20 | A | 804 | CLA | C2B-C1B-NB | 8.37 | 115.84 | 110.23 |
| 20 | 2 | 314 | CLA | OBD-CAD-C3D | -8.37 | 108.39 | 128.52 |
| 20 | B | 836 | CLA | OBD-CAD-C3D | -8.35 | 108.42 | 128.52 |
| 20 | B | 835 | CLA | OBD-CAD-C3D | -8.33 | 108.47 | 128.52 |
| 20 | H | 110 | CLA | OBD-CAD-C3D | -8.33 | 108.48 | 128.52 |
| 20 | 2 | 307 | CLA | CBB-CAB-C3B | 8.32 | 169.02 | 127.62 |
| 20 | B | 850 | CLA | CBB-CAB-C3B | 8.31 | 168.96 | 127.62 |
| 20 | A | 804 | CLA | CBB-CAB-C3B | 8.29 | 168.85 | 127.62 |
| 20 | 3 | 301 | CLA | OBD-CAD-C3D | -8.26 | 108.63 | 128.52 |
| 20 | A | 811 | CLA | C2B-C1B-NB | 8.26 | 115.77 | 110.23 |
| 20 | A | 839 | CLA | CBB-CAB-C3B | 8.25 | 168.65 | 127.62 |
| 20 | B | 833 | CLA | CBB-CAB-C3B | 8.23 | 168.59 | 127.62 |
| 20 | B | 824 | CLA | OBD-CAD-C3D | -8.23 | 108.72 | 128.52 |
| 22 | B | 844 | BCR | C24-C23-C22 | -8.21 | 113.82 | 126.23 |
| 20 | B | 816 | CLA | OBD-CAD-C3D | -8.16 | 108.89 | 128.52 |
| 20 | 4 | 304 | CLA | CBB-CAB-C3B | 8.15 | 168.16 | 127.62 |
| 20 | A | 831 | CLA | C2B-C1B-NB | 8.14 | 115.69 | 110.23 |
| 20 | B | 809 | CLA | C2B-C1B-NB | 8.13 | 115.68 | 110.23 |
| 20 | B | 819 | CLA | C2B-C1B-NB | 8.12 | 115.67 | 110.23 |
| 20 | 1 | 211 | CLA | CMD-C2D-C1D | 8.10 | 139.00 | 124.71 |
| 20 | A | 831 | CLA | CBB-CAB-C3B | 8.10 | 167.94 | 127.62 |
| 20 | A | 808 | CLA | CBB-CAB-C3B | 8.10 | 167.91 | 127.62 |
| 20 | B | 840 | CLA | CBB-CAB-C3B | 8.08 | 167.81 | 127.62 |
| 20 | A | 838 | CLA | OBD-CAD-C3D | -8.08 | 109.08 | 128.52 |
| 20 | H | 102 | CLA | OBD-CAD-C3D | -8.07 | 109.10 | 128.52 |
| 20 | B | 817 | CLA | CBB-CAB-C3B | 8.07 | 167.75 | 127.62 |
| 20 | 4 | 313 | CLA | OBD-CAD-C3D | -8.06 | 109.12 | 128.52 |
| 20 | B | 838 | CLA | CBB-CAB-C3B | 8.05 | 167.67 | 127.62 |
| 20 | A | 808 | CLA | C2B-C1B-NB | 8.04 | 115.62 | 110.23 |
| 20 | A | 835 | CLA | C2B-C1B-NB | 8.04 | 115.62 | 110.23 |
| 20 | A | 807 | CLA | OBD-CAD-C3D | -8.01 | 109.25 | 128.52 |
| 20 | 1 | 207 | CLA | OBD-CAD-C3D | -7.97 | 109.35 | 128.52 |
| 20 | 3 | 303 | CLA | CAB-C3B-C4B | -7.97 | 113.24 | 125.37 |
| 20 | G | 105 | CLA | C2B-C1B-NB | 7.96 | 115.57 | 110.23 |
| 20 | F | 207 | CLA | CBB-CAB-C3B | 7.96 | 167.22 | 127.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 803 | CLA | OBD-CAD-C3D | -7.95 | 109.39 | 128.52 |
| 20 | 1 | 207 | CLA | C3A-C2A-C1A | 7.94 | 113.24 | 101.34 |
| 20 | B | 839 | CLA | CMD-C2D-C1D | 7.93 | 138.69 | 124.71 |
| 20 | A | 827 | CLA | OBD-CAD-C3D | -7.92 | 109.45 | 128.52 |
| 20 | B | 820 | CLA | OBD-CAD-C3D | -7.92 | 109.47 | 128.52 |
| 20 | B | 840 | CLA | OBD-CAD-C3D | -7.91 | 109.48 | 128.52 |
| 20 | 2 | 302 | CLA | C2B-C1B-NB | 7.90 | 115.53 | 110.23 |
| 20 | A | 803 | CLA | O2D-CGD-CBD | 7.90 | 125.31 | 111.27 |
| 20 | A | 837 | CLA | C2B-C1B-NB | 7.90 | 115.53 | 110.23 |
| 20 | 1 | 201 | CLA | C4A-NA-C1A | 7.89 | 110.25 | 106.71 |
| 20 | A | 815 | CLA | OBD-CAD-C3D | -7.88 | 109.55 | 128.52 |
| 20 | 4 | 304 | CLA | OBD-CAD-C3D | -7.88 | 109.56 | 128.52 |
| 20 | A | 835 | CLA | OBD-CAD-C3D | -7.88 | 109.57 | 128.52 |
| 20 | B | 807 | CLA | OBD-CAD-C3D | -7.87 | 109.57 | 128.52 |
| 20 | B | 850 | CLA | C2B-C1B-NB | 7.87 | 115.51 | 110.23 |
| 22 | I | 103 | BCR | C30-C25-C26 | -7.84 | 111.57 | 122.61 |
| 20 | B | 823 | CLA | OBD-CAD-C3D | -7.83 | 109.67 | 128.52 |
| 20 | A | 819 | CLA | C2B-C1B-NB | 7.83 | 115.48 | 110.23 |
| 20 | A | 836 | CLA | C2B-C1B-NB | 7.83 | 115.48 | 110.23 |
| 20 | 4 | 306 | CLA | C2B-C1B-NB | 7.82 | 115.48 | 110.23 |
| 20 | A | 850 | CLA | C2B-C1B-NB | 7.80 | 115.46 | 110.23 |
| 20 | 1 | 204 | CLA | CMD-C2D-C1D | 7.78 | 138.43 | 124.71 |
| 20 | A | 840 | CLA | OBD-CAD-C3D | -7.77 | 109.82 | 128.52 |
| 20 | 1 | 210 | CLA | OBD-CAD-C3D | -7.75 | 109.87 | 128.52 |
| 20 | B | 831 | CLA | OBD-CAD-C3D | -7.74 | 109.89 | 128.52 |
| 20 | B | 828 | CLA | C2B-C1B-NB | 7.73 | 115.42 | 110.23 |
| 20 | A | 801 | CLA | C4D-C3D-CAD | 7.72 | 117.20 | 108.10 |
| 20 | L | 204 | CLA | OBD-CAD-C3D | -7.70 | 110.00 | 128.52 |
| 20 | A | 828 | CLA | CBB-CAB-C3B | 7.70 | 165.90 | 127.62 |
| 20 | A | 806 | CLA | C2B-C1B-NB | 7.69 | 115.39 | 110.23 |
| 20 | A | 818 | CLA | OBD-CAD-C3D | -7.69 | 110.02 | 128.52 |
| 20 | 1 | 206 | CLA | OBD-CAD-C3D | -7.68 | 110.05 | 128.52 |
| 20 | A | 849 | CLA | OBD-CAD-C3D | -7.67 | 110.06 | 128.52 |
| 20 | A | 826 | CLA | C2B-C1B-NB | 7.66 | 115.37 | 110.23 |
| 20 | B | 836 | CLA | C2B-C1B-NB | 7.66 | 115.36 | 110.23 |
| 20 | 4 | 318 | CLA | O2D-CGD-CBD | 7.65 | 124.87 | 111.27 |
| 20 | B | 810 | CLA | O2D-CGD-CBD | 7.65 | 124.86 | 111.27 |
| 20 | 3 | 303 | CLA | C2B-C1B-NB | 7.65 | 115.36 | 110.23 |
| 20 | A | 812 | CLA | OBD-CAD-C3D | -7.65 | 110.12 | 128.52 |
| 20 | B | 838 | CLA | OBD-CAD-C3D | -7.64 | 110.12 | 128.52 |
| 20 | B | 832 | CLA | OBD-CAD-C3D | -7.64 | 110.13 | 128.52 |
| 20 | 4 | 310 | CLA | OBD-CAD-C3D | -7.64 | 110.13 | 128.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 305 | CLA | C2B-C1B-NB | 7.63 | 115.35 | 110.23 |
| 20 | 4 | 317 | CLA | OBD-CAD-C3D | -7.62 | 110.17 | 128.52 |
| 20 | B | 842 | CLA | OBD-CAD-C3D | -7.61 | 110.20 | 128.52 |
| 20 | B | 841 | CLA | OBD-CAD-C3D | -7.60 | 110.24 | 128.52 |
| 20 | B | 840 | CLA | C2B-C1B-NB | 7.59 | 115.32 | 110.23 |
| 20 | 2 | 314 | CLA | C2B-C1B-NB | 7.58 | 115.31 | 110.23 |
| 20 | A | 813 | CLA | C2B-C1B-NB | 7.56 | 115.30 | 110.23 |
| 20 | A | 827 | CLA | O2D-CGD-CBD | 7.53 | 124.65 | 111.27 |
| 20 | 1 | 215 | CLA | C1D-CHD-C4C | -7.53 | 109.82 | 126.06 |
| 20 | A | 821 | CLA | O2D-CGD-CBD | 7.50 | 124.60 | 111.27 |
| 20 | A | 825 | CLA | CBB-CAB-C3B | 7.50 | 164.94 | 127.62 |
| 20 | A | 839 | CLA | OBD-CAD-C3D | -7.49 | 110.50 | 128.52 |
| 20 | L | 207 | CLA | C2B-C1B-NB | 7.44 | 115.22 | 110.23 |
| 20 | 1 | 202 | CLA | OBD-CAD-C3D | -7.43 | 110.63 | 128.52 |
| 20 | 1 | 215 | CLA | C4D-C3D-CAD | 7.43 | 116.86 | 108.10 |
| 20 | 1 | 213 | CLA | CAA-C2A-C1A | 7.43 | 136.32 | 111.97 |
| 20 | H | 101 | CLA | C2B-C1B-NB | 7.43 | 115.21 | 110.23 |
| 20 | B | 817 | CLA | OBD-CAD-C3D | -7.43 | 110.65 | 128.52 |
| 22 | I | 103 | BCR | C16-C15-C14 | -7.42 | 108.28 | 123.47 |
| 20 | 4 | 318 | CLA | OBD-CAD-C3D | -7.42 | 110.67 | 128.52 |
| 20 | A | 838 | CLA | C2B-C1B-NB | 7.41 | 115.20 | 110.23 |
| 20 | K | 103 | CLA | C2B-C1B-NB | 7.40 | 115.19 | 110.23 |
| 20 | A | 834 | CLA | OBD-CAD-C3D | -7.40 | 110.72 | 128.52 |
| 20 | 3 | 313 | CLA | C2B-C1B-NB | 7.40 | 115.19 | 110.23 |
| 20 | B | 803 | CLA | C2B-C1B-NB | 7.39 | 115.19 | 110.23 |
| 20 | A | 813 | CLA | OBD-CAD-C3D | -7.39 | 110.75 | 128.52 |
| 20 | B | 839 | CLA | O2D-CGD-CBD | 7.38 | 124.38 | 111.27 |
| 20 | B | 830 | CLA | OBD-CAD-C3D | -7.34 | 110.86 | 128.52 |
| 20 | 4 | 306 | CLA | CBB-CAB-C3B | 7.32 | 164.05 | 127.62 |
| 20 | B | 802 | CLA | C2B-C1B-NB | 7.32 | 115.14 | 110.23 |
| 20 | A | 839 | CLA | CMD-C2D-C1D | 7.31 | 137.59 | 124.71 |
| 20 | 4 | 317 | CLA | C4A-NA-C1A | 7.30 | 109.99 | 106.71 |
| 20 | A | 823 | CLA | OBD-CAD-C3D | -7.30 | 110.96 | 128.52 |
| 20 | A | 821 | CLA | OBD-CAD-C3D | -7.29 | 110.97 | 128.52 |
| 20 | A | 851 | CLA | C2B-C1B-NB | 7.28 | 115.11 | 110.23 |
| 20 | A | 809 | CLA | OBD-CAD-C3D | -7.26 | 111.05 | 128.52 |
| 20 | A | 832 | CLA | OBD-CAD-C3D | -7.25 | 111.08 | 128.52 |
| 20 | B | 814 | CLA | OBD-CAD-C3D | -7.25 | 111.08 | 128.52 |
| 20 | 2 | 312 | CLA | C2B-C1B-NB | 7.25 | 115.09 | 110.23 |
| 20 | 1 | 203 | CLA | CMD-C2D-C1D | 7.24 | 137.47 | 124.71 |
| 20 | B | 829 | CLA | OBD-CAD-C3D | -7.24 | 111.10 | 128.52 |
| 20 | A | 810 | CLA | C2B-C1B-NB | 7.23 | 115.08 | 110.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 303 | CLA | C2B-C1B-NB | 7.22 | 115.07 | 110.23 |
| 20 | A | 831 | CLA | C1D-CHD-C4C | -7.22 | 110.48 | 126.06 |
| 20 | A | 849 | CLA | C4D-C3D-CAD | 7.21 | 116.59 | 108.10 |
| 20 | K | 104 | CLA | CMD-C2D-C1D | 7.21 | 137.41 | 124.71 |
| 20 | A | 823 | CLA | C2B-C1B-NB | 7.21 | 115.06 | 110.23 |
| 20 | B | 841 | CLA | CHC-C4B-NB | 7.20 | 131.88 | 124.26 |
| 20 | L | 201 | CLA | C2B-C1B-NB | 7.19 | 115.05 | 110.23 |
| 20 | K | 104 | CLA | O2D-CGD-CBD | 7.18 | 124.03 | 111.27 |
| 20 | A | 840 | CLA | C2B-C1B-NB | 7.18 | 115.05 | 110.23 |
| 20 | A | 822 | CLA | C2B-C1B-NB | 7.17 | 115.04 | 110.23 |
| 20 | 4 | 318 | CLA | C4D-C3D-CAD | 7.17 | 116.54 | 108.10 |
| 22 | I | 103 | BCR | C16-C17-C18 | -7.16 | 117.08 | 127.31 |
| 20 | A | 815 | CLA | C2B-C1B-NB | 7.15 | 115.03 | 110.23 |
| 20 | B | 832 | CLA | C2B-C1B-NB | 7.13 | 115.02 | 110.23 |
| 20 | B | 818 | CLA | OBD-CAD-C3D | -7.13 | 111.37 | 128.52 |
| 20 | B | 825 | CLA | C2B-C1B-NB | 7.13 | 115.01 | 110.23 |
| 20 | A | 839 | CLA | C2B-C1B-NB | 7.12 | 115.00 | 110.23 |
| 20 | 1 | 207 | CLA | CMD-C2D-C1D | 7.11 | 137.25 | 124.71 |
| 21 | G | 101 | LMU | O1'-C1'-C2' | 7.11 | 119.41 | 108.30 |
| 20 | 2 | 302 | CLA | C1D-CHD-C4C | -7.11 | 110.72 | 126.06 |
| 20 | B | 831 | CLA | C2B-C1B-NB | 7.11 | 115.00 | 110.23 |
| 20 | B | 816 | CLA | C2B-C1B-NB | 7.08 | 114.98 | 110.23 |
| 20 | 3 | 314 | CLA | CMD-C2D-C1D | 7.07 | 137.18 | 124.71 |
| 20 | 2 | 314 | CLA | CMD-C2D-C1D | 7.06 | 137.15 | 124.71 |
| 20 | 3 | 310 | CLA | CHC-C4B-NB | 7.06 | 131.73 | 124.26 |
| 20 | 4 | 318 | CLA | C2B-C1B-NB | 7.06 | 114.96 | 110.23 |
| 21 | L | 205 | LMU | C1B-O1B-C4' | -7.05 | 100.53 | 117.96 |
| 20 | A | 818 | CLA | C2B-C1B-NB | 7.04 | 114.95 | 110.23 |
| 20 | F | 205 | CLA | OBD-CAD-C3D | -7.04 | 111.58 | 128.52 |
| 20 | A | 827 | CLA | C2B-C1B-NB | 7.03 | 114.95 | 110.23 |
| 20 | B | 836 | CLA | O2D-CGD-CBD | 7.01 | 123.72 | 111.27 |
| 20 | 3 | 311 | CLA | C2B-C1B-NB | 7.00 | 114.93 | 110.23 |
| 20 | 3 | 310 | CLA | O2D-CGD-CBD | 7.00 | 123.70 | 111.27 |
| 20 | F | 201 | CLA | O2D-CGD-CBD | 7.00 | 123.70 | 111.27 |
| 20 | 4 | 313 | CLA | C2B-C1B-NB | 6.99 | 114.92 | 110.23 |
| 20 | A | 805 | CLA | CBB-CAB-C3B | 6.99 | 162.39 | 127.62 |
| 20 | A | 849 | CLA | C2B-C1B-NB | 6.98 | 114.91 | 110.23 |
| 20 | 4 | 315 | CLA | C2B-C1B-NB | 6.98 | 114.91 | 110.23 |
| 20 | K | 104 | CLA | C2B-C1B-NB | 6.98 | 114.91 | 110.23 |
| 20 | H | 102 | CLA | CMD-C2D-C1D | 6.97 | 137.00 | 124.71 |
| 20 | 4 | 304 | CLA | C2B-C1B-NB | 6.97 | 114.91 | 110.23 |
| 20 | G | 105 | CLA | O2D-CGD-CBD | 6.95 | 123.62 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 822 | CLA | C2B-C1B-NB | 6.94 | 114.89 | 110.23 |
| 20 | B | 829 | CLA | O2D-CGD-CBD | 6.94 | 123.60 | 111.27 |
| 20 | A | 818 | CLA | C1D-CHD-C4C | -6.94 | 111.10 | 126.06 |
| 20 | B | 808 | CLA | OBD-CAD-C3D | -6.90 | 111.91 | 128.52 |
| 20 | 1 | 202 | CLA | C2B-C1B-NB | 6.89 | 114.85 | 110.23 |
| 20 | A | 820 | CLA | CMD-C2D-C1D | 6.88 | 136.83 | 124.71 |
| 20 | 1 | 204 | CLA | C2B-C1B-NB | 6.85 | 114.82 | 110.23 |
| 22 | F | 204 | BCR | C15-C14-C13 | -6.85 | 117.53 | 127.31 |
| 20 | 1 | 215 | CLA | CHD-C4C-C3C | -6.84 | 114.78 | 124.84 |
| 20 | 4 | 317 | CLA | C2B-C1B-NB | 6.84 | 114.82 | 110.23 |
| 20 | B | 839 | CLA | C4D-C3D-CAD | 6.84 | 116.15 | 108.10 |
| 20 | B | 837 | CLA | O2D-CGD-CBD | 6.82 | 123.39 | 111.27 |
| 20 | 1 | 215 | CLA | C2B-C1B-NB | 6.81 | 114.80 | 110.23 |
| 20 | B | 822 | CLA | CMD-C2D-C1D | 6.81 | 136.71 | 124.71 |
| 20 | A | 801 | CLA | CMD-C2D-C1D | 6.80 | 136.70 | 124.71 |
| 20 | G | 105 | CLA | CMD-C2D-C1D | 6.80 | 136.70 | 124.71 |
| 20 | G | 105 | CLA | CBB-CAB-C3B | 6.79 | 161.41 | 127.62 |
| 20 | B | 812 | CLA | CAB-C3B-C2B | -6.78 | 106.02 | 123.59 |
| 20 | 2 | 315 | CLA | CHA-C4D-ND | 6.77 | 131.06 | 124.52 |
| 20 | 3 | 314 | CLA | CHC-C4B-NB | 6.77 | 131.42 | 124.26 |
| 20 | H | 109 | CLA | C2B-C1B-NB | 6.76 | 114.77 | 110.23 |
| 20 | A | 816 | CLA | C2B-C1B-NB | 6.76 | 114.76 | 110.23 |
| 20 | A | 811 | CLA | CMD-C2D-C1D | 6.76 | 136.63 | 124.71 |
| 20 | B | 840 | CLA | CMD-C2D-C1D | 6.76 | 136.62 | 124.71 |
| 20 | B | 821 | CLA | CMD-C2D-C1D | 6.75 | 136.61 | 124.71 |
| 20 | A | 835 | CLA | O2D-CGD-CBD | 6.75 | 123.26 | 111.27 |
| 20 | H | 110 | CLA | C2B-C1B-NB | 6.75 | 114.76 | 110.23 |
| 20 | B | 814 | CLA | C2B-C1B-NB | 6.75 | 114.75 | 110.23 |
| 20 | 2 | 303 | CLA | O2D-CGD-CBD | 6.74 | 123.25 | 111.27 |
| 20 | B | 830 | CLA | O2D-CGD-CBD | 6.74 | 123.25 | 111.27 |
| 20 | 4 | 303 | CLA | CGD-CBD-CAD | 6.74 | 132.57 | 110.73 |
| 20 | 4 | 303 | CLA | C1D-CHD-C4C | -6.74 | 111.52 | 126.06 |
| 20 | B | 837 | CLA | CMD-C2D-C1D | 6.73 | 136.57 | 124.71 |
| 20 | 2 | 307 | CLA | O2D-CGD-CBD | 6.73 | 123.22 | 111.27 |
| 20 | B | 810 | CLA | C2B-C1B-NB | 6.73 | 114.74 | 110.23 |
| 20 | L | 201 | CLA | OBD-CAD-C3D | -6.71 | 112.38 | 128.52 |
| 20 | B | 812 | CLA | C1D-CHD-C4C | -6.70 | 111.60 | 126.06 |
| 20 | 4 | 315 | CLA | OBD-CAD-C3D | -6.70 | 112.40 | 128.52 |
| 20 | B | 833 | CLA | C2B-C1B-NB | 6.70 | 114.72 | 110.23 |
| 20 | B | 826 | CLA | CMD-C2D-C1D | 6.69 | 136.51 | 124.71 |
| 20 | 1 | 207 | CLA | C2B-C1B-NB | 6.69 | 114.72 | 110.23 |
| 20 | B | 807 | CLA | CMD-C2D-C1D | 6.69 | 136.51 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 812 | CLA | C2B-C1B-NB | 6.69 | 114.72 | 110.23 |
| 20 | A | 819 | CLA | CMD-C2D-C1D | 6.67 | 136.47 | 124.71 |
| 20 | B | 815 | CLA | CMD-C2D-C1D | 6.67 | 136.47 | 124.71 |
| 20 | K | 102 | CLA | CMD-C2D-C1D | 6.67 | 136.46 | 124.71 |
| 20 | 2 | 303 | CLA | CMD-C2D-C1D | 6.66 | 136.46 | 124.71 |
| 20 | 4 | 310 | CLA | C1D-CHD-C4C | -6.66 | 111.69 | 126.06 |
| 20 | B | 838 | CLA | O2D-CGD-CBD | 6.65 | 123.09 | 111.27 |
| 20 | F | 205 | CLA | CMD-C2D-C1D | 6.65 | 136.43 | 124.71 |
| 20 | 2 | 314 | CLA | C4D-C3D-CAD | 6.65 | 115.93 | 108.10 |
| 20 | A | 836 | CLA | O2D-CGD-CBD | 6.64 | 123.06 | 111.27 |
| 21 | H | 103 | LMU | C3'-C4'-C5' | -6.64 | 95.71 | 110.93 |
| 20 | A | 851 | CLA | CMD-C2D-C1D | 6.64 | 136.41 | 124.71 |
| 20 | L | 208 | CLA | C2B-C1B-NB | 6.63 | 114.68 | 110.23 |
| 20 | 2 | 314 | CLA | CHD-C4C-NC | 6.63 | 134.65 | 124.20 |
| 20 | 1 | 204 | CLA | C4D-C3D-CAD | 6.62 | 115.90 | 108.10 |
| 20 | B | 839 | CLA | CHD-C4C-NC | 6.62 | 134.64 | 124.20 |
| 20 | 2 | 303 | CLA | C2B-C1B-NB | 6.62 | 114.67 | 110.23 |
| 20 | B | 809 | CLA | O2D-CGD-CBD | 6.61 | 123.01 | 111.27 |
| 20 | A | 831 | CLA | C3B-C2B-C1B | -6.60 | 99.19 | 107.16 |
| 20 | 4 | 317 | CLA | C4D-C3D-CAD | 6.60 | 115.88 | 108.10 |
| 20 | A | 812 | CLA | C2B-C1B-NB | 6.59 | 114.65 | 110.23 |
| 20 | F | 206 | CLA | C2B-C1B-NB | 6.59 | 114.65 | 110.23 |
| 20 | 3 | 317 | CLA | CMD-C2D-C1D | 6.58 | 136.31 | 124.71 |
| 20 | 4 | 304 | CLA | O2D-CGD-CBD | 6.57 | 122.95 | 111.27 |
| 20 | R | 107 | CLA | CMD-C2D-C1D | 6.57 | 136.30 | 124.71 |
| 20 | B | 815 | CLA | OBD-CAD-C3D | -6.57 | 112.72 | 128.52 |
| 20 | A | 821 | CLA | C2B-C1B-NB | 6.56 | 114.63 | 110.23 |
| 20 | B | 818 | CLA | C2B-C1B-NB | 6.56 | 114.63 | 110.23 |
| 20 | I | 102 | CLA | C2B-C1B-NB | 6.56 | 114.63 | 110.23 |
| 20 | B | 839 | CLA | C2B-C1B-NB | 6.56 | 114.63 | 110.23 |
| 20 | 1 | 213 | CLA | C1D-CHD-C4C | -6.56 | 111.91 | 126.06 |
| 20 | B | 821 | CLA | C2B-C1B-NB | 6.56 | 114.63 | 110.23 |
| 20 | B | 825 | CLA | O2D-CGD-CBD | 6.55 | 122.92 | 111.27 |
| 20 | A | 817 | CLA | C2B-C1B-NB | 6.55 | 114.62 | 110.23 |
| 20 | A | 818 | CLA | CMD-C2D-C1D | 6.55 | 136.25 | 124.71 |
| 20 | 1 | 201 | CLA | CHC-C4B-NB | 6.55 | 131.19 | 124.26 |
| 20 | A | 818 | CLA | CHD-C4C-NC | 6.54 | 134.51 | 124.20 |
| 20 | A | 832 | CLA | C2B-C1B-NB | 6.54 | 114.61 | 110.23 |
| 20 | 1 | 210 | CLA | CAB-C3B-C2B | -6.53 | 106.66 | 123.59 |
| 20 | A | 811 | CLA | C3B-C2B-C1B | -6.53 | 99.28 | 107.16 |
| 22 | B | 801 | BCR | C3-C4-C5 | -6.52 | 102.43 | 114.08 |
| 20 | L | 202 | CLA | CMD-C2D-C1D | 6.52 | 136.20 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 310 | CLA | CMD-C2D-C1D | 6.52 | 136.20 | 124.71 |
| 20 | 4 | 301 | CLA | C2B-C1B-NB | 6.52 | 114.60 | 110.23 |
| 20 | A | 820 | CLA | C2B-C1B-NB | 6.51 | 114.60 | 110.23 |
| 20 | 3 | 310 | CLA | CHD-C4C-C3C | -6.50 | 115.29 | 124.84 |
| 20 | 1 | 201 | CLA | CMD-C2D-C1D | 6.49 | 136.16 | 124.71 |
| 20 | B | 839 | CLA | C1D-CHD-C4C | -6.49 | 112.05 | 126.06 |
| 20 | 4 | 312 | CLA | CHA-C4D-ND | 6.49 | 130.79 | 124.52 |
| 20 | A | 839 | CLA | O2D-CGD-CBD | 6.49 | 122.80 | 111.27 |
| 20 | 4 | 301 | CLA | CMD-C2D-C1D | 6.49 | 136.15 | 124.71 |
| 20 | 1 | 210 | CLA | CMD-C2D-C1D | 6.49 | 136.15 | 124.71 |
| 20 | 4 | 317 | CLA | CMD-C2D-C1D | 6.49 | 136.15 | 124.71 |
| 20 | A | 830 | CLA | C2B-C1B-NB | 6.48 | 114.58 | 110.23 |
| 20 | G | 105 | CLA | C1D-CHD-C4C | -6.48 | 112.08 | 126.06 |
| 20 | 4 | 303 | CLA | CMD-C2D-C1D | 6.47 | 136.12 | 124.71 |
| 20 | B | 812 | CLA | CMD-C2D-C1D | 6.47 | 136.12 | 124.71 |
| 20 | B | 830 | CLA | CMD-C2D-C1D | 6.47 | 136.12 | 124.71 |
| 20 | B | 828 | CLA | CMD-C2D-C1D | 6.47 | 136.12 | 124.71 |
| 20 | 4 | 310 | CLA | C4D-C3D-CAD | 6.47 | 115.72 | 108.10 |
| 20 | 1 | 213 | CLA | C2B-C1B-NB | 6.47 | 114.57 | 110.23 |
| 20 | A | 833 | CLA | C2B-C1B-NB | 6.46 | 114.56 | 110.23 |
| 20 | 4 | 310 | CLA | CHD-C4C-NC | 6.46 | 134.39 | 124.20 |
| 20 | 1 | 211 | CLA | C1D-CHD-C4C | -6.46 | 112.12 | 126.06 |
| 20 | A | 817 | CLA | CMD-C2D-C1D | 6.46 | 136.10 | 124.71 |
| 21 | R | 101 | LMU | C4B-C3B-C2B | -6.46 | 99.55 | 110.82 |
| 20 | B | 834 | CLA | CMD-C2D-C1D | 6.46 | 136.09 | 124.71 |
| 20 | B | 830 | CLA | CHC-C4B-NB | 6.45 | 131.09 | 124.26 |
| 20 | L | 202 | CLA | C2B-C1B-NB | 6.45 | 114.56 | 110.23 |
| 20 | B | 807 | CLA | O2D-CGD-CBD | 6.45 | 122.73 | 111.27 |
| 20 | 2 | 305 | CLA | OBD-CAD-C3D | -6.45 | 113.00 | 128.52 |
| 20 | 1 | 203 | CLA | C2B-C1B-NB | 6.44 | 114.55 | 110.23 |
| 20 | A | 834 | CLA | C2B-C1B-NB | 6.44 | 114.55 | 110.23 |
| 20 | 2 | 316 | CLA | C1D-CHD-C4C | -6.43 | 112.19 | 126.06 |
| 20 | A | 835 | CLA | CMD-C2D-C1D | 6.43 | 136.04 | 124.71 |
| 20 | A | 803 | CLA | CMD-C2D-C1D | 6.43 | 136.04 | 124.71 |
| 20 | 2 | 314 | CLA | C1D-CHD-C4C | -6.41 | 112.23 | 126.06 |
| 20 | F | 206 | CLA | CMD-C2D-C1D | 6.41 | 136.00 | 124.71 |
| 20 | 4 | 306 | CLA | C1D-CHD-C4C | -6.41 | 112.24 | 126.06 |
| 20 | K | 103 | CLA | CMD-C2D-C1D | 6.40 | 135.99 | 124.71 |
| 20 | F | 201 | CLA | CHC-C4B-NB | 6.39 | 131.02 | 124.26 |
| 20 | R | 108 | CLA | CMD-C2D-C1D | 6.38 | 135.96 | 124.71 |
| 20 | B | 817 | CLA | CMD-C2D-C1D | 6.38 | 135.95 | 124.71 |
| 20 | 2 | 305 | CLA | CMD-C2D-C1D | 6.38 | 135.95 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 810 | CLA | CMD-C2D-C1D | 6.38 | 135.95 | 124.71 |
| 20 | H | 108 | CLA | C1D-CHD-C4C | -6.37 | 112.31 | 126.06 |
| 20 | A | 832 | CLA | CMD-C2D-C1D | 6.37 | 135.94 | 124.71 |
| 20 | 1 | 201 | CLA | C2B-C1B-NB | 6.37 | 114.50 | 110.23 |
| 20 | F | 207 | CLA | CMA-C3A-C4A | 6.36 | 128.88 | 111.77 |
| 20 | A | 840 | CLA | O2D-CGD-CBD | 6.36 | 122.58 | 111.27 |
| 20 | 4 | 302 | CLA | C1D-CHD-C4C | -6.36 | 112.33 | 126.06 |
| 20 | 4 | 306 | CLA | CHD-C4C-NC | 6.36 | 134.22 | 124.20 |
| 20 | 3 | 314 | CLA | C1D-CHD-C4C | -6.36 | 112.34 | 126.06 |
| 20 | 4 | 305 | CLA | C1D-CHD-C4C | -6.36 | 112.35 | 126.06 |
| 20 | A | 804 | CLA | CMD-C2D-C1D | 6.35 | 135.91 | 124.71 |
| 20 | K | 102 | CLA | C2B-C1B-NB | 6.35 | 114.49 | 110.23 |
| 20 | B | 815 | CLA | C2B-C1B-NB | 6.35 | 114.49 | 110.23 |
| 20 | B | 806 | CLA | CMD-C2D-C1D | 6.35 | 135.90 | 124.71 |
| 20 | 1 | 202 | CLA | CMD-C2D-C1D | 6.35 | 135.90 | 124.71 |
| 20 | A | 801 | CLA | CAB-C3B-C2B | -6.35 | 107.14 | 123.59 |
| 20 | A | 824 | CLA | CMD-C2D-C1D | 6.34 | 135.89 | 124.71 |
| 20 | 1 | 215 | CLA | CBB-CAB-C3B | 6.34 | 159.18 | 127.62 |
| 20 | A | 804 | CLA | OBD-CAD-C3D | -6.34 | 113.26 | 128.52 |
| 20 | 3 | 313 | CLA | OBD-CAD-C3D | -6.34 | 113.26 | 128.52 |
| 20 | A | 829 | CLA | O2D-CGD-CBD | 6.34 | 122.53 | 111.27 |
| 20 | J | 103 | CLA | OBD-CAD-C3D | -6.33 | 113.28 | 128.52 |
| 20 | A | 816 | CLA | CMD-C2D-C1D | 6.33 | 135.87 | 124.71 |
| 20 | 2 | 310 | CLA | C2B-C1B-NB | 6.33 | 114.47 | 110.23 |
| 20 | B | 808 | CLA | C2B-C1B-NB | 6.33 | 114.47 | 110.23 |
| 20 | B | 819 | CLA | C1D-CHD-C4C | -6.33 | 112.41 | 126.06 |
| 20 | B | 813 | CLA | CMD-C2D-C1D | 6.32 | 135.86 | 124.71 |
| 20 | A | 811 | CLA | OBD-CAD-C3D | -6.32 | 113.31 | 128.52 |
| 20 | J | 103 | CLA | C2B-C1B-NB | 6.32 | 114.47 | 110.23 |
| 20 | 2 | 316 | CLA | CMD-C2D-C1D | 6.32 | 135.85 | 124.71 |
| 20 | B | 823 | CLA | C2B-C1B-NB | 6.31 | 114.46 | 110.23 |
| 20 | A | 805 | CLA | C2B-C1B-NB | 6.31 | 114.46 | 110.23 |
| 20 | 4 | 302 | CLA | C2B-C1B-NB | 6.31 | 114.46 | 110.23 |
| 20 | A | 824 | CLA | C2B-C1B-NB | 6.30 | 114.46 | 110.23 |
| 20 | B | 835 | CLA | CMD-C2D-C1D | 6.30 | 135.82 | 124.71 |
| 20 | A | 806 | CLA | CMD-C2D-C1D | 6.30 | 135.81 | 124.71 |
| 20 | B | 836 | CLA | CMD-C2D-C1D | 6.29 | 135.81 | 124.71 |
| 20 | A | 828 | CLA | O2D-CGD-CBD | 6.29 | 122.45 | 111.27 |
| 20 | 3 | 303 | CLA | CMD-C2D-C1D | 6.29 | 135.80 | 124.71 |
| 20 | A | 823 | CLA | CMD-C2D-C1D | 6.29 | 135.80 | 124.71 |
| 20 | B | 820 | CLA | O2D-CGD-CBD | 6.29 | 122.44 | 111.27 |
| 20 | 1 | 203 | CLA | C4D-C3D-CAD | 6.29 | 115.50 | 108.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | F | 205 | CLA | C1B-C2B-C3B | -6.28 | 101.06 | 107.03 |
| 20 | 3 | 310 | CLA | C1D-CHD-C4C | -6.28 | 112.51 | 126.06 |
| 20 | J | 101 | CLA | CMD-C2D-C1D | 6.28 | 135.78 | 124.71 |
| 20 | B | 834 | CLA | C2B-C1B-NB | 6.28 | 114.44 | 110.23 |
| 20 | 4 | 304 | CLA | CMD-C2D-C1D | 6.27 | 135.77 | 124.71 |
| 20 | A | 837 | CLA | CMD-C2D-C1D | 6.27 | 135.76 | 124.71 |
| 20 | L | 201 | CLA | CMD-C2D-C1D | 6.27 | 135.76 | 124.71 |
| 20 | K | 101 | CLA | C2B-C1B-NB | 6.27 | 114.43 | 110.23 |
| 20 | A | 834 | CLA | CMD-C2D-C1D | 6.26 | 135.74 | 124.71 |
| 20 | 1 | 207 | CLA | CBA-CAA-C2A | -6.26 | 95.40 | 113.86 |
| 20 | 3 | 307 | CLA | CHC-C1C-NC | 6.25 | 133.69 | 124.20 |
| 20 | 1 | 201 | CLA | C4D-C3D-CAD | 6.25 | 115.46 | 108.10 |
| 20 | A | 849 | CLA | CHC-C4B-NB | 6.25 | 130.87 | 124.26 |
| 20 | B | 833 | CLA | CMD-C2D-C1D | 6.25 | 135.72 | 124.71 |
| 20 | A | 833 | CLA | CMD-C2D-C1D | 6.25 | 135.72 | 124.71 |
| 22 | 2 | 317 | BCR | C11-C10-C9 | -6.25 | 118.40 | 127.31 |
| 20 | H | 110 | CLA | O2D-CGD-CBD | 6.24 | 122.36 | 111.27 |
| 22 | B | 801 | BCR | C10-C11-C12 | -6.23 | 103.78 | 123.22 |
| 20 | 2 | 302 | CLA | CMD-C2D-C1D | 6.23 | 135.69 | 124.71 |
| 20 | 4 | 306 | CLA | CMD-C2D-C1D | 6.22 | 135.68 | 124.71 |
| 20 | A | 822 | CLA | CMD-C2D-C1D | 6.22 | 135.68 | 124.71 |
| 20 | 3 | 310 | CLA | CHD-C4C-NC | 6.21 | 133.99 | 124.20 |
| 20 | A | 816 | CLA | C1D-CHD-C4C | -6.21 | 112.67 | 126.06 |
| 20 | A | 839 | CLA | C4D-C3D-CAD | 6.20 | 115.41 | 108.10 |
| 20 | 3 | 317 | CLA | C2B-C1B-NB | 6.20 | 114.39 | 110.23 |
| 20 | L | 203 | CLA | CMD-C2D-C1D | 6.20 | 135.63 | 124.71 |
| 20 | 1 | 205 | CLA | CMD-C2D-C1D | 6.19 | 135.62 | 124.71 |
| 20 | 2 | 312 | CLA | C1D-CHD-C4C | -6.18 | 112.72 | 126.06 |
| 20 | R | 107 | CLA | C2B-C1B-NB | 6.18 | 114.38 | 110.23 |
| 20 | B | 832 | CLA | CMD-C2D-C1D | 6.18 | 135.61 | 124.71 |
| 20 | B | 842 | CLA | CAB-C3B-C2B | -6.18 | 107.57 | 123.59 |
| 20 | 2 | 307 | CLA | CHC-C4B-NB | 6.18 | 130.79 | 124.26 |
| 20 | J | 101 | CLA | C2B-C1B-NB | 6.17 | 114.37 | 110.23 |
| 20 | 1 | 207 | CLA | C4D-C3D-CAD | 6.17 | 115.37 | 108.10 |
| 20 | A | 818 | CLA | O2D-CGD-CBD | 6.17 | 122.23 | 111.27 |
| 20 | L | 207 | CLA | CMD-C2D-C1D | 6.17 | 135.58 | 124.71 |
| 20 | 3 | 311 | CLA | CMD-C2D-C1D | 6.16 | 135.58 | 124.71 |
| 20 | 2 | 316 | CLA | C2B-C1B-NB | 6.16 | 114.36 | 110.23 |
| 20 | 1 | 204 | CLA | CHC-C4B-NB | 6.16 | 130.78 | 124.26 |
| 20 | 1 | 205 | CLA | C2B-C1B-NB | 6.15 | 114.36 | 110.23 |
| 20 | B | 836 | CLA | C1D-CHD-C4C | -6.15 | 112.78 | 126.06 |
| 20 | 1 | 215 | CLA | CHD-C4C-NC | 6.15 | 133.90 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 211 | CLA | C4D-C3D-CAD | 6.15 | 115.34 | 108.10 |
| 20 | B | 839 | CLA | CHD-C4C-C3C | -6.15 | 115.80 | 124.84 |
| 20 | B | 809 | CLA | CMD-C2D-C1D | 6.14 | 135.53 | 124.71 |
| 20 | 4 | 310 | CLA | O2D-CGD-CBD | 6.13 | 122.17 | 111.27 |
| 20 | H | 108 | CLA | O2D-CGD-CBD | 6.13 | 122.16 | 111.27 |
| 20 | 2 | 302 | CLA | CHD-C4C-NC | 6.13 | 133.86 | 124.20 |
| 20 | 1 | 211 | CLA | CHD-C4C-NC | 6.13 | 133.86 | 124.20 |
| 20 | F | 207 | CLA | C1D-CHD-C4C | -6.12 | 112.86 | 126.06 |
| 20 | 1 | 211 | CLA | CHD-C4C-C3C | -6.12 | 115.85 | 124.84 |
| 20 | R | 108 | CLA | OBD-CAD-C3D | -6.12 | 113.80 | 128.52 |
| 20 | 3 | 310 | CLA | CBB-CAB-C3B | 6.12 | 158.04 | 127.62 |
| 20 | A | 821 | CLA | CMD-C2D-C1D | 6.11 | 135.49 | 124.71 |
| 20 | A | 830 | CLA | CMD-C2D-C1D | 6.11 | 135.49 | 124.71 |
| 20 | A | 807 | CLA | C2B-C1B-NB | 6.11 | 114.33 | 110.23 |
| 20 | 4 | 309 | CLA | CHA-C4D-ND | 6.11 | 130.41 | 124.52 |
| 20 | B | 838 | CLA | C2B-C1B-NB | 6.11 | 114.33 | 110.23 |
| 20 | 2 | 309 | CLA | CHA-C4D-ND | 6.10 | 130.41 | 124.52 |
| 20 | A | 821 | CLA | C4D-C3D-CAD | 6.10 | 115.29 | 108.10 |
| 20 | 4 | 315 | CLA | C1D-CHD-C4C | -6.10 | 112.90 | 126.06 |
| 20 | B | 808 | CLA | C1D-CHD-C4C | -6.09 | 112.92 | 126.06 |
| 20 | 4 | 306 | CLA | CAA-C2A-C1A | 6.09 | 131.93 | 111.97 |
| 20 | B | 828 | CLA | O2D-CGD-CBD | 6.09 | 122.09 | 111.27 |
| 20 | A | 812 | CLA | CMD-C2D-C1D | 6.09 | 135.44 | 124.71 |
| 20 | B | 806 | CLA | C3B-C2B-C1B | -6.09 | 99.81 | 107.16 |
| 20 | A | 804 | CLA | C3B-C2B-C1B | -6.09 | 99.81 | 107.16 |
| 20 | B | 832 | CLA | O2D-CGD-CBD | 6.08 | 122.08 | 111.27 |
| 20 | B | 803 | CLA | CMD-C2D-C1D | 6.07 | 135.40 | 124.71 |
| 20 | H | 102 | CLA | C2B-C1B-NB | 6.06 | 114.30 | 110.23 |
| 20 | F | 205 | CLA | CAB-C3B-C4B | -6.06 | 116.14 | 125.37 |
| 20 | B | 838 | CLA | CMD-C2D-C1D | 6.06 | 135.39 | 124.71 |
| 20 | A | 801 | CLA | CAA-C2A-C3A | 6.06 | 129.36 | 112.78 |
| 20 | F | 201 | CLA | C1D-CHD-C4C | -6.05 | 113.00 | 126.06 |
| 20 | F | 207 | CLA | O2D-CGD-CBD | 6.05 | 122.02 | 111.27 |
| 20 | 2 | 312 | CLA | O2D-CGD-CBD | 6.05 | 122.02 | 111.27 |
| 20 | 2 | 306 | CLA | CHC-C4B-NB | 6.05 | 130.40 | 124.27 |
| 20 | A | 805 | CLA | CMD-C2D-C1D | 6.04 | 135.36 | 124.71 |
| 20 | A | 815 | CLA | CMD-C2D-C1D | 6.04 | 135.36 | 124.71 |
| 20 | L | 207 | CLA | O2D-CGD-CBD | 6.04 | 122.00 | 111.27 |
| 20 | 4 | 303 | CLA | CHD-C4C-NC | 6.04 | 133.71 | 124.20 |
| 20 | L | 208 | CLA | C1D-CHD-C4C | -6.03 | 113.04 | 126.06 |
| 20 | 1 | 210 | CLA | C2B-C1B-NB | 6.03 | 114.28 | 110.23 |
| 20 | H | 101 | CLA | CMD-C2D-C1D | 6.03 | 135.34 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 314 | CLA | CHA-C4D-ND | 6.03 | 130.34 | 124.52 |
| 20 | A | 851 | CLA | C4D-C3D-CAD | 6.03 | 115.20 | 108.10 |
| 20 | A | 807 | CLA | CMD-C2D-C1D | 6.03 | 135.34 | 124.71 |
| 20 | 1 | 209 | CLA | CHA-C4D-ND | 6.02 | 130.33 | 124.52 |
| 20 | I | 102 | CLA | CMD-C2D-C1D | 6.02 | 135.32 | 124.71 |
| 20 | A | 803 | CLA | C2B-C1B-NB | 6.01 | 114.26 | 110.23 |
| 20 | B | 820 | CLA | C2B-C1B-NB | 6.01 | 114.26 | 110.23 |
| 20 | B | 842 | CLA | CMD-C2D-C1D | 6.01 | 135.30 | 124.71 |
| 20 | A | 801 | CLA | O2D-CGD-CBD | 6.01 | 121.94 | 111.27 |
| 20 | A | 826 | CLA | CMD-C2D-C1D | 6.00 | 135.29 | 124.71 |
| 20 | F | 201 | CLA | CHD-C4C-C3C | -6.00 | 116.02 | 124.84 |
| 20 | A | 820 | CLA | O2D-CGD-CBD | 6.00 | 121.94 | 111.27 |
| 20 | B | 819 | CLA | CAA-C2A-C3A | -6.00 | 102.10 | 116.10 |
| 20 | A | 825 | CLA | C2B-C1B-NB | 6.00 | 114.25 | 110.23 |
| 20 | H | 101 | CLA | C4D-C3D-CAD | 5.99 | 115.16 | 108.10 |
| 20 | 3 | 301 | CLA | CMD-C2D-C1D | 5.99 | 135.26 | 124.71 |
| 20 | B | 823 | CLA | CMD-C2D-C1D | 5.98 | 135.26 | 124.71 |
| 20 | 1 | 201 | CLA | O2D-CGD-CBD | 5.98 | 121.89 | 111.27 |
| 20 | F | 201 | CLA | CHD-C4C-NC | 5.97 | 133.61 | 124.20 |
| 20 | 4 | 310 | CLA | CBB-CAB-C3B | 5.97 | 157.31 | 127.62 |
| 20 | B | 821 | CLA | C4D-C3D-CAD | 5.96 | 115.12 | 108.10 |
| 20 | 2 | 306 | CLA | CHA-C4D-ND | 5.96 | 130.27 | 124.52 |
| 20 | B | 830 | CLA | C4D-C3D-CAD | 5.95 | 115.11 | 108.10 |
| 20 | B | 827 | CLA | C2B-C1B-NB | 5.95 | 114.22 | 110.23 |
| 20 | J | 103 | CLA | C1D-CHD-C4C | -5.95 | 113.22 | 126.06 |
| 20 | B | 802 | CLA | CMD-C2D-C1D | 5.95 | 135.19 | 124.71 |
| 20 | H | 109 | CLA | O2D-CGD-CBD | 5.94 | 121.83 | 111.27 |
| 20 | A | 818 | CLA | CHD-C4C-C3C | -5.94 | 116.11 | 124.84 |
| 20 | B | 817 | CLA | C2B-C1B-NB | 5.94 | 114.21 | 110.23 |
| 20 | 4 | 302 | CLA | CMD-C2D-C1D | 5.94 | 135.18 | 124.71 |
| 20 | R | 107 | CLA | C4D-C3D-CAD | 5.93 | 115.09 | 108.10 |
| 21 | 1 | 218 | LMU | C1B-O1B-C4' | -5.93 | 103.29 | 117.96 |
| 20 | B | 818 | CLA | CMD-C2D-C1D | 5.92 | 135.16 | 124.71 |
| 20 | B | 822 | CLA | C1D-CHD-C4C | -5.92 | 113.30 | 126.06 |
| 20 | B | 810 | CLA | OBD-CAD-C3D | -5.92 | 114.28 | 128.52 |
| 20 | A | 809 | CLA | CHC-C4B-NB | 5.91 | 130.51 | 124.26 |
| 20 | 2 | 311 | CLA | C1D-CHD-C4C | -5.91 | 113.31 | 126.06 |
| 20 | 1 | 215 | CLA | CMD-C2D-C1D | 5.90 | 135.12 | 124.71 |
| 20 | K | 101 | CLA | C1D-CHD-C4C | -5.90 | 113.33 | 126.06 |
| 20 | 1 | 213 | CLA | O2D-CGD-CBD | 5.90 | 121.76 | 111.27 |
| 20 | B | 817 | CLA | O2D-CGD-CBD | 5.90 | 121.76 | 111.27 |
| 20 | 3 | 313 | CLA | CMD-C2D-C1D | 5.90 | 135.11 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | B | 844 | BCR | C1-C6-C5 | -5.90 | 114.30 | 122.61 |
| 20 | L | 208 | CLA | CMD-C2D-C1D | 5.90 | 135.10 | 124.71 |
| 20 | A | 808 | CLA | CMD-C2D-C1D | 5.89 | 135.09 | 124.71 |
| 20 | 4 | 318 | CLA | CMD-C2D-C1D | 5.88 | 135.08 | 124.71 |
| 20 | B | 827 | CLA | CMD-C2D-C1D | 5.88 | 135.08 | 124.71 |
| 20 | A | 809 | CLA | CMD-C2D-C1D | 5.88 | 135.08 | 124.71 |
| 20 | B | 833 | CLA | O2D-CGD-CBD | 5.88 | 121.72 | 111.27 |
| 20 | B | 806 | CLA | OBD-CAD-C3D | -5.88 | 114.37 | 128.52 |
| 20 | B | 814 | CLA | C1D-CHD-C4C | -5.88 | 113.38 | 126.06 |
| 20 | A | 829 | CLA | C2B-C1B-NB | 5.88 | 114.17 | 110.23 |
| 20 | B | 826 | CLA | C2B-C1B-NB | 5.88 | 114.17 | 110.23 |
| 20 | 2 | 301 | CLA | CHA-C4D-ND | 5.88 | 130.19 | 124.52 |
| 20 | B | 820 | CLA | CMD-C2D-C1D | 5.88 | 135.07 | 124.71 |
| 20 | B | 833 | CLA | C1D-CHD-C4C | -5.86 | 113.42 | 126.06 |
| 20 | L | 204 | CLA | CMD-C2D-C1D | 5.86 | 135.04 | 124.71 |
| 20 | A | 822 | CLA | C4D-C3D-CAD | 5.86 | 115.00 | 108.10 |
| 20 | B | 814 | CLA | CMD-C2D-C1D | 5.85 | 135.03 | 124.71 |
| 20 | B | 841 | CLA | C2B-C1B-NB | 5.85 | 114.15 | 110.23 |
| 20 | A | 810 | CLA | O2D-CGD-CBD | 5.84 | 121.65 | 111.27 |
| 20 | B | 833 | CLA | C4D-C3D-CAD | 5.84 | 114.98 | 108.10 |
| 20 | 4 | 307 | CLA | CHA-C4D-ND | 5.84 | 130.16 | 124.52 |
| 20 | 1 | 206 | CLA | CMD-C2D-C1D | 5.84 | 135.01 | 124.71 |
| 20 | B | 812 | CLA | C4D-C3D-CAD | 5.84 | 114.98 | 108.10 |
| 20 | A | 850 | CLA | C1D-CHD-C4C | -5.84 | 113.46 | 126.06 |
| 20 | B | 813 | CLA | C2B-C1B-NB | 5.83 | 114.14 | 110.23 |
| 20 | G | 105 | CLA | CHD-C4C-NC | 5.83 | 133.39 | 124.20 |
| 20 | A | 825 | CLA | C1D-CHD-C4C | -5.83 | 113.48 | 126.06 |
| 20 | B | 824 | CLA | CHD-C4C-C3C | -5.83 | 116.28 | 124.84 |
| 20 | A | 840 | CLA | CMD-C2D-C1D | 5.82 | 134.97 | 124.71 |
| 20 | 2 | 310 | CLA | CMD-C2D-C1D | 5.82 | 134.97 | 124.71 |
| 20 | B | 829 | CLA | C4A-NA-C1A | 5.81 | 109.32 | 106.71 |
| 20 | 3 | 316 | CLA | CHA-C4D-ND | 5.81 | 130.13 | 124.52 |
| 20 | A | 809 | CLA | C2B-C1B-NB | 5.81 | 114.13 | 110.23 |
| 20 | A | 813 | CLA | CMD-C2D-C1D | 5.81 | 134.95 | 124.71 |
| 20 | I | 102 | CLA | C1D-CHD-C4C | -5.81 | 113.53 | 126.06 |
| 20 | 2 | 308 | CLA | C4C-CHD-C1D | -5.80 | 111.76 | 126.11 |
| 20 | A | 809 | CLA | O2D-CGD-CBD | 5.80 | 121.58 | 111.27 |
| 20 | B | 830 | CLA | C1D-CHD-C4C | -5.80 | 113.55 | 126.06 |
| 20 | A | 828 | CLA | CMD-C2D-C1D | 5.80 | 134.93 | 124.71 |
| 20 | 1 | 201 | CLA | C1D-CHD-C4C | -5.79 | 113.56 | 126.06 |
| 20 | B | 825 | CLA | C1D-CHD-C4C | -5.79 | 113.57 | 126.06 |
| 20 | 1 | 206 | CLA | C4D-C3D-CAD | 5.79 | 114.92 | 108.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | G | 101 | LMU | C1'-O5'-C5' | -5.79 | 102.33 | 113.69 |
| 20 | A | 837 | CLA | C4D-C3D-CAD | 5.77 | 114.90 | 108.10 |
| 20 | B | 808 | CLA | CMD-C2D-C1D | 5.77 | 134.88 | 124.71 |
| 20 | A | 831 | CLA | O2D-CGD-CBD | 5.77 | 121.52 | 111.27 |
| 20 | 3 | 301 | CLA | CAB-C3B-C2B | -5.77 | 108.63 | 123.59 |
| 20 | 4 | 304 | CLA | C4D-C3D-CAD | 5.77 | 114.89 | 108.10 |
| 20 | B | 820 | CLA | C4D-C3D-CAD | 5.77 | 114.89 | 108.10 |
| 20 | B | 812 | CLA | O2D-CGD-CBD | 5.77 | 121.51 | 111.27 |
| 20 | 4 | 315 | CLA | O2D-CGD-CBD | 5.76 | 121.51 | 111.27 |
| 20 | 4 | 313 | CLA | CAB-C3B-C2B | -5.76 | 108.65 | 123.59 |
| 20 | B | 819 | CLA | CMD-C2D-C1D | 5.75 | 134.85 | 124.71 |
| 20 | B | 829 | CLA | C1D-CHD-C4C | -5.75 | 113.66 | 126.06 |
| 20 | A | 803 | CLA | C1D-CHD-C4C | -5.75 | 113.66 | 126.06 |
| 20 | 3 | 303 | CLA | C1D-CHD-C4C | -5.74 | 113.67 | 126.06 |
| 20 | B | 841 | CLA | C3B-C2B-C1B | -5.74 | 100.24 | 107.16 |
| 20 | 3 | 309 | CLA | C3A-C4A-CHB | -5.73 | 116.89 | 123.91 |
| 20 | 2 | 303 | CLA | C1D-CHD-C4C | -5.73 | 113.70 | 126.06 |
| 20 | B | 827 | CLA | C1D-CHD-C4C | -5.73 | 113.70 | 126.06 |
| 20 | 2 | 302 | CLA | O2D-CGD-CBD | 5.73 | 121.44 | 111.27 |
| 20 | B | 841 | CLA | CMD-C2D-C1D | 5.72 | 134.80 | 124.71 |
| 20 | A | 807 | CLA | O2D-CGD-CBD | 5.72 | 121.43 | 111.27 |
| 20 | 4 | 303 | CLA | C4D-CHA-C1A | 5.72 | 128.21 | 121.25 |
| 20 | 3 | 307 | CLA | C2B-C1B-NB | 5.71 | 114.06 | 110.23 |
| 20 | 3 | 311 | CLA | C1D-CHD-C4C | -5.71 | 113.75 | 126.06 |
| 20 | 3 | 314 | CLA | C2B-C1B-NB | 5.70 | 114.05 | 110.23 |
| 20 | A | 831 | CLA | CHD-C4C-NC | 5.70 | 133.18 | 124.20 |
| 20 | A | 813 | CLA | C1D-CHD-C4C | -5.69 | 113.78 | 126.06 |
| 20 | L | 204 | CLA | O2D-CGD-CBD | 5.69 | 121.38 | 111.27 |
| 20 | F | 206 | CLA | C1D-CHD-C4C | -5.68 | 113.80 | 126.06 |
| 20 | 3 | 310 | CLA | CMD-C2D-C1D | 5.68 | 134.73 | 124.71 |
| 20 | B | 842 | CLA | C2B-C1B-NB | 5.68 | 114.04 | 110.23 |
| 20 | A | 849 | CLA | CMD-C2D-C1D | 5.68 | 134.72 | 124.71 |
| 20 | 4 | 302 | CLA | C4D-C3D-CAD | 5.68 | 114.79 | 108.10 |
| 20 | A | 839 | CLA | C1D-CHD-C4C | -5.68 | 113.81 | 126.06 |
| 20 | 1 | 203 | CLA | CHD-C4C-NC | 5.67 | 133.14 | 124.20 |
| 20 | H | 108 | CLA | CMD-C2D-C1D | 5.67 | 134.71 | 124.71 |
| 20 | L | 207 | CLA | CAA-C2A-C3A | -5.67 | 97.25 | 112.78 |
| 20 | B | 813 | CLA | C4D-C3D-CAD | 5.67 | 114.78 | 108.10 |
| 20 | B | 807 | CLA | C4D-C3D-CAD | 5.67 | 114.78 | 108.10 |
| 20 | 3 | 301 | CLA | C4D-C3D-CAD | 5.67 | 114.78 | 108.10 |
| 20 | 1 | 205 | CLA | C1D-CHD-C4C | -5.66 | 113.84 | 126.06 |
| 20 | B | 840 | CLA | C4D-C3D-CAD | 5.66 | 114.77 | 108.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 303 | CLA | CHC-C1C-NC | 5.65 | 132.78 | 124.20 |
| 20 | J | 101 | CLA | C1D-CHD-C4C | -5.65 | 113.87 | 126.06 |
| 20 | B | 824 | CLA | CMD-C2D-C1D | 5.65 | 134.67 | 124.71 |
| 20 | B | 835 | CLA | C2B-C1B-NB | 5.65 | 114.02 | 110.23 |
| 20 | A | 829 | CLA | CMD-C2D-C1D | 5.65 | 134.67 | 124.71 |
| 20 | 3 | 315 | CLA | C3A-C4A-CHB | -5.65 | 117.00 | 123.91 |
| 20 | 2 | 308 | CLA | CHD-C4C-NC | 5.65 | 132.92 | 124.21 |
| 20 | 1 | 206 | CLA | C1D-CHD-C4C | -5.64 | 113.88 | 126.06 |
| 20 | B | 841 | CLA | C4D-C3D-CAD | 5.64 | 114.75 | 108.10 |
| 20 | 1 | 211 | CLA | CHC-C4B-NB | 5.64 | 130.23 | 124.26 |
| 20 | A | 833 | CLA | C1D-CHD-C4C | -5.64 | 113.89 | 126.06 |
| 20 | 2 | 307 | CLA | C1D-CHD-C4C | -5.64 | 113.90 | 126.06 |
| 20 | A | 805 | CLA | CHC-C4B-NB | 5.63 | 130.22 | 124.26 |
| 20 | 2 | 302 | CLA | CHD-C4C-C3C | -5.63 | 116.56 | 124.84 |
| 20 | 1 | 202 | CLA | C4D-C3D-CAD | 5.63 | 114.73 | 108.10 |
| 20 | 3 | 304 | CLA | C4A-NA-C1A | 5.63 | 109.24 | 106.71 |
| 20 | 1 | 205 | CLA | C4D-C3D-CAD | 5.63 | 114.73 | 108.10 |
| 20 | 3 | 317 | CLA | CAB-C3B-C2B | -5.63 | 108.99 | 123.59 |
| 20 | 1 | 206 | CLA | C2B-C1B-NB | 5.63 | 114.00 | 110.23 |
| 20 | 4 | 313 | CLA | C4D-C3D-CAD | 5.62 | 114.72 | 108.10 |
| 20 | F | 207 | CLA | CMD-C2D-C1D | 5.62 | 134.62 | 124.71 |
| 20 | A | 841 | CLA | CHC-C4B-NB | 5.62 | 129.97 | 124.27 |
| 20 | A | 849 | CLA | C3B-C2B-C1B | -5.61 | 100.38 | 107.16 |
| 20 | B | 803 | CLA | C4D-C3D-CAD | 5.61 | 114.71 | 108.10 |
| 20 | K | 104 | CLA | C4D-C3D-CAD | 5.61 | 114.71 | 108.10 |
| 20 | K | 102 | CLA | C1D-CHD-C4C | -5.61 | 113.96 | 126.06 |
| 20 | 2 | 308 | CLA | C3A-C4A-CHB | -5.61 | 117.04 | 123.91 |
| 20 | 3 | 308 | CLA | CHA-C4D-ND | 5.61 | 129.93 | 124.52 |
| 20 | J | 101 | CLA | C4D-C3D-CAD | 5.61 | 114.70 | 108.10 |
| 20 | F | 201 | CLA | C4A-NA-C1A | 5.60 | 109.22 | 106.71 |
| 20 | A | 817 | CLA | C4D-C3D-CAD | 5.60 | 114.69 | 108.10 |
| 20 | H | 108 | CLA | C3B-C2B-C1B | -5.60 | 100.41 | 107.16 |
| 20 | A | 820 | CLA | C4D-C3D-CAD | 5.59 | 114.69 | 108.10 |
| 20 | 3 | 311 | CLA | O2D-CGD-CBD | 5.59 | 121.21 | 111.27 |
| 20 | 4 | 310 | CLA | CHD-C4C-C3C | -5.59 | 116.62 | 124.84 |
| 20 | 3 | 302 | CLA | CHA-C4D-ND | 5.59 | 129.91 | 124.52 |
| 20 | H | 108 | CLA | OBD-CAD-C3D | -5.59 | 115.07 | 128.52 |
| 20 | 2 | 309 | CLA | CHC-C4B-NB | 5.59 | 129.93 | 124.27 |
| 20 | 4 | 313 | CLA | C1D-CHD-C4C | -5.59 | 114.00 | 126.06 |
| 20 | 4 | 310 | CLA | C2B-C1B-NB | 5.58 | 113.97 | 110.23 |
| 20 | B | 837 | CLA | C2B-C1B-NB | 5.58 | 113.97 | 110.23 |
| 20 | 2 | 302 | CLA | C4D-C3D-CAD | 5.58 | 114.67 | 108.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 824 | CLA | CHD-C4C-NC | 5.58 | 132.99 | 124.20 |
| 20 | K | 103 | CLA | C4D-C3D-CAD | 5.57 | 114.67 | 108.10 |
| 20 | B | 822 | CLA | C4D-C3D-CAD | 5.57 | 114.66 | 108.10 |
| 20 | 4 | 311 | CLA | CHA-C4D-ND | 5.57 | 129.90 | 124.52 |
| 20 | L | 204 | CLA | C1D-CHD-C4C | -5.57 | 114.05 | 126.06 |
| 20 | B | 829 | CLA | C4D-C3D-CAD | 5.57 | 114.66 | 108.10 |
| 20 | B | 832 | CLA | C1D-CHD-C4C | -5.57 | 114.05 | 126.06 |
| 20 | 4 | 313 | CLA | CMD-C2D-C1D | 5.57 | 134.52 | 124.71 |
| 20 | B | 811 | CLA | CHC-C4B-NB | 5.56 | 129.91 | 124.27 |
| 20 | A | 830 | CLA | C4D-C3D-CAD | 5.56 | 114.65 | 108.10 |
| 20 | A | 818 | CLA | C4D-C3D-CAD | 5.56 | 114.65 | 108.10 |
| 20 | B | 850 | CLA | C4D-C3D-CAD | 5.56 | 114.65 | 108.10 |
| 20 | A | 828 | CLA | C4D-C3D-CAD | 5.56 | 114.65 | 108.10 |
| 20 | 2 | 312 | CLA | C4D-C3D-CAD | 5.55 | 114.64 | 108.10 |
| 20 | 2 | 305 | CLA | C4D-C3D-CAD | 5.55 | 114.64 | 108.10 |
| 20 | 3 | 317 | CLA | C1D-CHD-C4C | -5.55 | 114.09 | 126.06 |
| 20 | B | 834 | CLA | C1D-CHD-C4C | -5.55 | 114.09 | 126.06 |
| 20 | A | 818 | CLA | CBB-CAB-C3B | 5.55 | 155.21 | 127.62 |
| 20 | B | 823 | CLA | C4D-C3D-CAD | 5.54 | 114.63 | 108.10 |
| 20 | 2 | 303 | CLA | C4D-C3D-CAD | 5.54 | 114.63 | 108.10 |
| 20 | 2 | 314 | CLA | CHD-C4C-C3C | -5.54 | 116.70 | 124.84 |
| 20 | B | 820 | CLA | C1D-CHD-C4C | -5.54 | 114.11 | 126.06 |
| 20 | A | 819 | CLA | C1D-CHD-C4C | -5.54 | 114.12 | 126.06 |
| 20 | L | 202 | CLA | C1D-CHD-C4C | -5.53 | 114.13 | 126.06 |
| 20 | 1 | 204 | CLA | C1D-CHD-C4C | -5.53 | 114.13 | 126.06 |
| 20 | A | 824 | CLA | O2D-CGD-CBD | 5.53 | 121.09 | 111.27 |
| 20 | B | 824 | CLA | C2B-C1B-NB | 5.53 | 113.94 | 110.23 |
| 20 | B | 809 | CLA | C1D-CHD-C4C | -5.53 | 114.13 | 126.06 |
| 20 | 4 | 310 | CLA | CHC-C1C-NC | 5.53 | 132.59 | 124.20 |
| 20 | F | 205 | CLA | C1D-CHD-C4C | -5.53 | 114.14 | 126.06 |
| 20 | 1 | 210 | CLA | C1D-CHD-C4C | -5.52 | 114.14 | 126.06 |
| 20 | A | 814 | CLA | CHB-C1B-NB | -5.52 | 118.68 | 124.27 |
| 20 | 4 | 301 | CLA | C1D-CHD-C4C | -5.52 | 114.14 | 126.06 |
| 20 | A | 817 | CLA | C1D-CHD-C4C | -5.52 | 114.14 | 126.06 |
| 20 | B | 826 | CLA | C4D-C3D-CAD | 5.52 | 114.61 | 108.10 |
| 20 | H | 102 | CLA | C4D-C3D-CAD | 5.52 | 114.61 | 108.10 |
| 20 | L | 202 | CLA | O2D-CGD-CBD | 5.52 | 121.08 | 111.27 |
| 20 | L | 203 | CLA | C4D-C3D-CAD | 5.52 | 114.60 | 108.10 |
| 20 | L | 208 | CLA | C4D-C3D-CAD | 5.51 | 114.59 | 108.10 |
| 20 | 1 | 209 | CLA | C3A-C4A-CHB | -5.51 | 117.16 | 123.91 |
| 20 | A | 831 | CLA | CMD-C2D-C1D | 5.51 | 134.42 | 124.71 |
| 20 | A | 837 | CLA | C1D-CHD-C4C | -5.51 | 114.17 | 126.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | I | 101 | BCR | C3-C4-C5 | -5.51 | 104.24 | 114.08 |
| 22 | I | 103 | BCR | C1-C6-C5 | -5.51 | 114.86 | 122.61 |
| 20 | 3 | 309 | CLA | C4A-NA-C1A | 5.51 | 109.18 | 106.71 |
| 20 | 3 | 301 | CLA | C2B-C1B-NB | 5.51 | 113.92 | 110.23 |
| 20 | A | 811 | CLA | CHC-C4B-NB | 5.51 | 130.09 | 124.26 |
| 20 | A | 835 | CLA | C4D-C3D-CAD | 5.50 | 114.58 | 108.10 |
| 20 | L | 203 | CLA | O2D-CGD-CBD | 5.50 | 121.05 | 111.27 |
| 20 | A | 802 | CLA | CHC-C4B-NB | 5.50 | 129.84 | 124.27 |
| 20 | A | 811 | CLA | C1D-CHD-C4C | -5.50 | 114.19 | 126.06 |
| 20 | B | 822 | CLA | CHD-C4C-NC | 5.50 | 132.87 | 124.20 |
| 20 | B | 816 | CLA | C1D-CHD-C4C | -5.50 | 114.20 | 126.06 |
| 20 | B | 819 | CLA | C4D-C3D-CAD | 5.50 | 114.58 | 108.10 |
| 20 | F | 206 | CLA | C4D-C3D-CAD | 5.50 | 114.58 | 108.10 |
| 20 | 4 | 306 | CLA | CHC-C1C-NC | 5.49 | 132.54 | 124.20 |
| 20 | A | 817 | CLA | O2D-CGD-CBD | 5.49 | 121.03 | 111.27 |
| 20 | 3 | 314 | CLA | CHC-C1C-NC | 5.49 | 132.53 | 124.20 |
| 20 | 2 | 311 | CLA | CHC-C4B-NB | 5.49 | 130.06 | 124.26 |
| 20 | A | 806 | CLA | C3B-C2B-C1B | -5.48 | 100.55 | 107.16 |
| 22 | B | 844 | BCR | C30-C25-C26 | -5.48 | 114.89 | 122.61 |
| 20 | B | 814 | CLA | CHD-C4C-NC | 5.48 | 132.84 | 124.20 |
| 20 | A | 812 | CLA | C1D-CHD-C4C | -5.48 | 114.24 | 126.06 |
| 20 | K | 101 | CLA | CMD-C2D-C1D | 5.47 | 134.36 | 124.71 |
| 20 | 4 | 301 | CLA | C4D-C3D-CAD | 5.47 | 114.55 | 108.10 |
| 20 | B | 836 | CLA | C4D-C3D-CAD | 5.47 | 114.54 | 108.10 |
| 20 | 1 | 213 | CLA | CMD-C2D-C1D | 5.47 | 134.35 | 124.71 |
| 20 | A | 805 | CLA | C1D-CHD-C4C | -5.47 | 114.27 | 126.06 |
| 20 | A | 826 | CLA | C1D-CHD-C4C | -5.46 | 114.27 | 126.06 |
| 21 | H | 104 | LMU | C1B-O5B-C5B | 5.46 | 124.41 | 113.69 |
| 20 | B | 811 | CLA | CHA-C4D-ND | 5.46 | 129.79 | 124.52 |
| 20 | H | 109 | CLA | CMD-C2D-C1D | 5.45 | 134.33 | 124.71 |
| 20 | B | 835 | CLA | O2D-CGD-CBD | 5.45 | 120.96 | 111.27 |
| 20 | A | 828 | CLA | C1D-CHD-C4C | -5.45 | 114.30 | 126.06 |
| 20 | B | 835 | CLA | C4D-C3D-CAD | 5.45 | 114.52 | 108.10 |
| 20 | H | 110 | CLA | C1D-CHD-C4C | -5.45 | 114.30 | 126.06 |
| 20 | B | 837 | CLA | C4D-C3D-CAD | 5.45 | 114.52 | 108.10 |
| 20 | B | 802 | CLA | O2D-CGD-CBD | 5.45 | 120.94 | 111.27 |
| 20 | L | 202 | CLA | C4D-C3D-CAD | 5.45 | 114.51 | 108.10 |
| 20 | A | 834 | CLA | C4D-C3D-CAD | 5.44 | 114.51 | 108.10 |
| 20 | B | 814 | CLA | CHD-C4C-C3C | -5.44 | 116.84 | 124.84 |
| 22 | I | 103 | BCR | C8-C9-C10 | 5.44 | 127.29 | 118.94 |
| 20 | L | 207 | CLA | C1D-CHD-C4C | -5.43 | 114.34 | 126.06 |
| 20 | B | 825 | CLA | CMD-C2D-C1D | 5.43 | 134.28 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 826 | CLA | C1D-CHD-C4C | -5.43 | 114.34 | 126.06 |
| 20 | 2 | 316 | CLA | C4D-C3D-CAD | 5.43 | 114.49 | 108.10 |
| 20 | B | 808 | CLA | C4D-C3D-CAD | 5.43 | 114.49 | 108.10 |
| 20 | L | 201 | CLA | O2D-CGD-CBD | 5.43 | 120.91 | 111.27 |
| 20 | 3 | 315 | CLA | CHC-C4B-NB | 5.42 | 129.77 | 124.27 |
| 20 | B | 803 | CLA | C1D-CHD-C4C | -5.42 | 114.36 | 126.06 |
| 20 | 2 | 311 | CLA | C2B-C1B-NB | 5.42 | 113.86 | 110.23 |
| 20 | A | 806 | CLA | C4D-C3D-CAD | 5.42 | 114.48 | 108.10 |
| 20 | K | 101 | CLA | C4D-C3D-CAD | 5.42 | 114.48 | 108.10 |
| 20 | A | 850 | CLA | CMD-C2D-C1D | 5.42 | 134.26 | 124.71 |
| 20 | R | 108 | CLA | C4D-C3D-CAD | 5.41 | 114.48 | 108.10 |
| 20 | B | 837 | CLA | C1D-CHD-C4C | -5.41 | 114.39 | 126.06 |
| 20 | B | 822 | CLA | CHD-C4C-C3C | -5.41 | 116.89 | 124.84 |
| 20 | B | 832 | CLA | C4D-C3D-CAD | 5.41 | 114.47 | 108.10 |
| 20 | B | 835 | CLA | C1D-CHD-C4C | -5.41 | 114.39 | 126.06 |
| 20 | 1 | 207 | CLA | CGD-CBD-CAD | -5.41 | 93.22 | 110.73 |
| 20 | A | 849 | CLA | CHD-C4C-C3C | -5.41 | 116.89 | 124.84 |
| 20 | B | 819 | CLA | O2D-CGD-CBD | 5.40 | 120.86 | 111.27 |
| 20 | 2 | 314 | CLA | CHC-C4B-NB | 5.40 | 129.97 | 124.26 |
| 20 | L | 203 | CLA | C2B-C1B-NB | 5.40 | 113.85 | 110.23 |
| 20 | 1 | 207 | CLA | C1D-CHD-C4C | -5.40 | 114.42 | 126.06 |
| 20 | 3 | 315 | CLA | CHA-C4D-ND | 5.39 | 129.73 | 124.52 |
| 20 | 3 | 303 | CLA | CAB-C3B-C2B | -5.39 | 109.60 | 123.59 |
| 21 | E | 101 | LMU | C1B-O5B-C5B | -5.39 | 103.10 | 113.69 |
| 20 | B | 807 | CLA | C1D-CHD-C4C | -5.39 | 114.42 | 126.06 |
| 20 | A | 833 | CLA | O2D-CGD-CBD | 5.39 | 120.85 | 111.27 |
| 20 | 2 | 310 | CLA | C4D-C3D-CAD | 5.39 | 114.45 | 108.10 |
| 20 | A | 831 | CLA | CHC-C4B-NB | 5.39 | 129.96 | 124.26 |
| 20 | H | 102 | CLA | C1D-CHD-C4C | -5.39 | 114.44 | 126.06 |
| 22 | I | 103 | BCR | C11-C10-C9 | -5.38 | 119.63 | 127.31 |
| 20 | A | 830 | CLA | C1D-CHD-C4C | -5.38 | 114.45 | 126.06 |
| 20 | 3 | 311 | CLA | C4D-C3D-CAD | 5.38 | 114.44 | 108.10 |
| 20 | 4 | 305 | CLA | CMD-C2D-C1D | 5.38 | 134.19 | 124.71 |
| 20 | A | 836 | CLA | C1D-CHD-C4C | -5.38 | 114.46 | 126.06 |
| 20 | 2 | 310 | CLA | C4B-CHC-C1C | -5.38 | 113.59 | 126.34 |
| 20 | 3 | 307 | CLA | CMD-C2D-C1D | 5.37 | 134.18 | 124.71 |
| 20 | B | 810 | CLA | C4D-C3D-CAD | 5.37 | 114.43 | 108.10 |
| 20 | B | 821 | CLA | C1D-CHD-C4C | -5.37 | 114.47 | 126.06 |
| 20 | 3 | 301 | CLA | C1D-CHD-C4C | -5.37 | 114.47 | 126.06 |
| 20 | A | 838 | CLA | C1D-CHD-C4C | -5.37 | 114.47 | 126.06 |
| 20 | G | 105 | CLA | CHD-C4C-C3C | -5.37 | 116.95 | 124.84 |
| 20 | B | 802 | CLA | C4-C3-C5 | 5.37 | 124.30 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 803 | CLA | C4A-NA-C1A | 5.36 | 109.12 | 106.71 |
| 20 | F | 205 | CLA | C4D-C3D-CAD | 5.36 | 114.42 | 108.10 |
| 20 | A | 823 | CLA | C1D-CHD-C4C | -5.36 | 114.50 | 126.06 |
| 20 | A | 840 | CLA | C1D-CHD-C4C | -5.36 | 114.50 | 126.06 |
| 20 | B | 815 | CLA | CHC-C4B-NB | 5.36 | 129.93 | 124.26 |
| 20 | B | 815 | CLA | C4D-C3D-CAD | 5.36 | 114.41 | 108.10 |
| 20 | A | 825 | CLA | O2D-CGD-CBD | 5.36 | 120.79 | 111.27 |
| 20 | 3 | 307 | CLA | C4B-CHC-C1C | -5.35 | 113.64 | 126.34 |
| 20 | A | 801 | CLA | C2B-C1B-NB | 5.35 | 113.82 | 110.23 |
| 20 | A | 827 | CLA | C1D-CHD-C4C | -5.35 | 114.52 | 126.06 |
| 20 | A | 806 | CLA | O2D-CGD-CBD | 5.35 | 120.77 | 111.27 |
| 20 | 2 | 301 | CLA | CHC-C4B-NB | 5.34 | 129.69 | 124.27 |
| 20 | A | 821 | CLA | CHC-C4B-NB | 5.34 | 129.91 | 124.26 |
| 20 | 4 | 315 | CLA | CHD-C4C-C3C | -5.34 | 116.99 | 124.84 |
| 20 | 3 | 313 | CLA | C1D-CHD-C4C | -5.34 | 114.53 | 126.06 |
| 20 | B | 825 | CLA | OBD-CAD-C3D | -5.34 | 115.66 | 128.52 |
| 20 | 3 | 317 | CLA | C4D-C3D-CAD | 5.34 | 114.39 | 108.10 |
| 20 | 3 | 308 | CLA | C4A-NA-C1A | 5.34 | 109.11 | 106.71 |
| 20 | 1 | 206 | CLA | O2D-CGD-CBD | 5.33 | 120.75 | 111.27 |
| 21 | R | 101 | LMU | O2B-C2B-C3B | 5.33 | 122.67 | 110.35 |
| 20 | B | 817 | CLA | C4D-C3D-CAD | 5.33 | 114.38 | 108.10 |
| 22 | B | 801 | BCR | C34-C9-C10 | -5.33 | 115.46 | 122.92 |
| 22 | F | 204 | BCR | C24-C23-C22 | -5.33 | 118.18 | 126.23 |
| 20 | B | 834 | CLA | C4D-C3D-CAD | 5.33 | 114.38 | 108.10 |
| 20 | B | 828 | CLA | C1D-CHD-C4C | -5.33 | 114.57 | 126.06 |
| 20 | A | 839 | CLA | CHC-C1C-NC | 5.33 | 132.28 | 124.20 |
| 20 | 2 | 314 | CLA | C4A-NA-C1A | 5.32 | 109.10 | 106.71 |
| 20 | H | 109 | CLA | C1D-CHD-C4C | -5.32 | 114.57 | 126.06 |
| 20 | A | 840 | CLA | C4D-C3D-CAD | 5.32 | 114.37 | 108.10 |
| 20 | 2 | 304 | CLA | CHD-C4C-NC | 5.32 | 132.42 | 124.21 |
| 20 | A | 824 | CLA | C1D-CHD-C4C | -5.32 | 114.58 | 126.06 |
| 20 | 2 | 307 | CLA | CHD-C4C-NC | 5.32 | 132.58 | 124.20 |
| 20 | H | 110 | CLA | C4D-C3D-CAD | 5.32 | 114.36 | 108.10 |
| 20 | A | 834 | CLA | O2D-CGD-CBD | 5.32 | 120.72 | 111.27 |
| 22 | A | 845 | BCR | C11-C10-C9 | -5.31 | 119.72 | 127.31 |
| 20 | 3 | 314 | CLA | CHD-C4C-NC | 5.31 | 132.57 | 124.20 |
| 20 | 4 | 317 | CLA | C1D-CHD-C4C | -5.30 | 114.61 | 126.06 |
| 20 | A | 836 | CLA | CMD-C2D-C1D | 5.30 | 134.06 | 124.71 |
| 22 | G | 104 | BCR | C11-C10-C9 | -5.30 | 119.74 | 127.31 |
| 20 | A | 831 | CLA | CHC-C1C-NC | 5.30 | 132.24 | 124.20 |
| 20 | 2 | 307 | CLA | C4B-CHC-C1C | -5.29 | 113.78 | 126.34 |
| 20 | 4 | 315 | CLA | CMD-C2D-C1D | 5.29 | 134.04 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 825 | CLA | CMD-C2D-C1D | 5.29 | 134.04 | 124.71 |
| 20 | L | 203 | CLA | C1D-CHD-C4C | -5.29 | 114.65 | 126.06 |
| 20 | A | 809 | CLA | C1D-CHD-C4C | -5.29 | 114.66 | 126.06 |
| 20 | B | 823 | CLA | C1D-CHD-C4C | -5.29 | 114.66 | 126.06 |
| 20 | 3 | 303 | CLA | CHD-C4C-C3C | -5.29 | 116.72 | 124.98 |
| 20 | B | 802 | CLA | C1D-CHD-C4C | -5.28 | 114.66 | 126.06 |
| 20 | H | 108 | CLA | CHD-C4C-NC | 5.28 | 132.53 | 124.20 |
| 20 | A | 815 | CLA | C4D-C3D-CAD | 5.28 | 114.32 | 108.10 |
| 20 | 2 | 303 | CLA | CHD-C4C-NC | 5.28 | 132.52 | 124.20 |
| 20 | A | 821 | CLA | C1D-CHD-C4C | -5.28 | 114.67 | 126.06 |
| 20 | A | 849 | CLA | C1D-CHD-C4C | -5.28 | 114.67 | 126.06 |
| 20 | 3 | 310 | CLA | C2B-C1B-NB | 5.28 | 113.77 | 110.23 |
| 20 | A | 838 | CLA | O2D-CGD-CBD | 5.28 | 120.65 | 111.27 |
| 20 | 3 | 301 | CLA | CHC-C4B-NB | 5.28 | 129.84 | 124.26 |
| 20 | 3 | 306 | CLA | CHA-C4D-ND | 5.28 | 129.61 | 124.52 |
| 20 | A | 820 | CLA | C1D-CHD-C4C | -5.28 | 114.68 | 126.06 |
| 20 | 3 | 314 | CLA | C4B-CHC-C1C | -5.27 | 113.83 | 126.34 |
| 20 | R | 107 | CLA | C1D-CHD-C4C | -5.27 | 114.68 | 126.06 |
| 20 | 3 | 306 | CLA | C4C-CHD-C1D | -5.27 | 113.07 | 126.11 |
| 20 | 3 | 313 | CLA | O2D-CGD-CBD | 5.27 | 120.63 | 111.27 |
| 20 | A | 826 | CLA | C4D-C3D-CAD | 5.27 | 114.31 | 108.10 |
| 20 | A | 819 | CLA | C4D-C3D-CAD | 5.27 | 114.30 | 108.10 |
| 20 | A | 811 | CLA | C4D-C3D-CAD | 5.27 | 114.30 | 108.10 |
| 20 | A | 837 | CLA | CHD-C4C-NC | 5.26 | 132.50 | 124.20 |
| 20 | A | 803 | CLA | CHD-C4C-NC | 5.26 | 132.50 | 124.20 |
| 20 | A | 835 | CLA | C1D-CHD-C4C | -5.26 | 114.71 | 126.06 |
| 20 | 4 | 305 | CLA | C4D-C3D-CAD | 5.26 | 114.30 | 108.10 |
| 20 | B | 842 | CLA | C4D-C3D-CAD | 5.26 | 114.30 | 108.10 |
| 20 | 3 | 303 | CLA | C4D-C3D-CAD | 5.26 | 114.29 | 108.10 |
| 20 | 4 | 311 | CLA | CHD-C4C-NC | 5.26 | 132.32 | 124.21 |
| 20 | A | 816 | CLA | O2D-CGD-CBD | 5.26 | 120.61 | 111.27 |
| 20 | 1 | 203 | CLA | C1D-CHD-C4C | -5.26 | 114.72 | 126.06 |
| 20 | B | 824 | CLA | C1D-CHD-C4C | -5.25 | 114.73 | 126.06 |
| 20 | B | 827 | CLA | O2D-CGD-CBD | 5.25 | 120.60 | 111.27 |
| 20 | B | 808 | CLA | CHC-C4B-NB | 5.25 | 129.81 | 124.26 |
| 20 | B | 850 | CLA | C3B-C2B-C1B | -5.24 | 100.83 | 107.16 |
| 20 | B | 829 | CLA | CHC-C4B-NB | 5.24 | 129.81 | 124.26 |
| 20 | A | 808 | CLA | C3B-C2B-C1B | -5.24 | 100.83 | 107.16 |
| 20 | J | 101 | CLA | O2D-CGD-CBD | 5.24 | 120.58 | 111.27 |
| 20 | 3 | 305 | CLA | CHA-C4D-ND | 5.24 | 129.58 | 124.52 |
| 20 | A | 810 | CLA | C3B-C2B-C1B | -5.24 | 100.84 | 107.16 |
| 20 | 4 | 303 | CLA | CAA-C2A-C3A | -5.24 | 98.44 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | A | 844 | BCR | C16-C17-C18 | -5.24 | 119.84 | 127.31 |
| 20 | 2 | 311 | CLA | O2D-CGD-CBD | 5.23 | 120.57 | 111.27 |
| 20 | 3 | 312 | CLA | CHA-C4D-ND | 5.23 | 129.57 | 124.52 |
| 20 | A | 814 | CLA | C4A-NA-C1A | 5.23 | 109.06 | 106.71 |
| 20 | B | 828 | CLA | C4D-C3D-CAD | 5.22 | 114.25 | 108.10 |
| 20 | 3 | 315 | CLA | C2A-C1A-CHA | -5.22 | 113.73 | 122.63 |
| 20 | A | 834 | CLA | CHC-C4B-NB | 5.22 | 129.78 | 124.26 |
| 20 | 1 | 212 | CLA | C3A-C4A-CHB | -5.22 | 117.52 | 123.91 |
| 20 | 3 | 303 | CLA | CHD-C4C-NC | 5.22 | 132.43 | 124.20 |
| 20 | B | 812 | CLA | CHD-C4C-NC | 5.22 | 132.43 | 124.20 |
| 20 | A | 838 | CLA | C4D-C3D-CAD | 5.22 | 114.25 | 108.10 |
| 20 | 2 | 304 | CLA | C4C-CHD-C1D | -5.22 | 113.21 | 126.11 |
| 20 | A | 832 | CLA | C1D-CHD-C4C | -5.21 | 114.81 | 126.06 |
| 20 | K | 102 | CLA | C4D-C3D-CAD | 5.21 | 114.24 | 108.10 |
| 20 | K | 104 | CLA | C1D-CHD-C4C | -5.21 | 114.81 | 126.06 |
| 20 | B | 817 | CLA | C1D-CHD-C4C | -5.21 | 114.81 | 126.06 |
| 20 | B | 819 | CLA | C3B-C2B-C1B | -5.21 | 100.87 | 107.16 |
| 20 | A | 841 | CLA | C3A-C4A-CHB | -5.21 | 117.53 | 123.91 |
| 20 | 4 | 303 | CLA | C4D-C3D-CAD | 5.21 | 114.24 | 108.10 |
| 20 | 1 | 207 | CLA | C4A-NA-C1A | 5.21 | 109.05 | 106.71 |
| 20 | H | 101 | CLA | C1D-CHD-C4C | -5.21 | 114.82 | 126.06 |
| 20 | R | 108 | CLA | C2B-C1B-NB | 5.21 | 113.72 | 110.23 |
| 21 | E | 101 | LMU | C4B-C3B-C2B | -5.20 | 101.74 | 110.82 |
| 20 | 3 | 304 | CLA | CHA-C4D-ND | 5.20 | 129.54 | 124.52 |
| 20 | 1 | 201 | CLA | C4B-CHC-C1C | -5.20 | 114.00 | 126.34 |
| 20 | B | 831 | CLA | O2D-CGD-CBD | 5.20 | 120.51 | 111.27 |
| 20 | B | 829 | CLA | CMD-C2D-C1D | 5.20 | 133.88 | 124.71 |
| 20 | B | 838 | CLA | C1D-CHD-C4C | -5.20 | 114.84 | 126.06 |
| 20 | 2 | 306 | CLA | C1C-CHC-C4B | -5.20 | 113.17 | 126.13 |
| 20 | K | 103 | CLA | O2D-CGD-CBD | 5.20 | 120.51 | 111.27 |
| 20 | A | 822 | CLA | C1D-CHD-C4C | -5.20 | 114.85 | 126.06 |
| 20 | 1 | 210 | CLA | C4D-C3D-CAD | 5.20 | 114.22 | 108.10 |
| 20 | 4 | 311 | CLA | C4C-CHD-C1D | -5.20 | 113.26 | 126.11 |
| 20 | A | 804 | CLA | C1D-CHD-C4C | -5.19 | 114.86 | 126.06 |
| 20 | 4 | 308 | CLA | C3A-C4A-CHB | -5.19 | 117.55 | 123.91 |
| 20 | 2 | 315 | CLA | C4C-CHD-C1D | -5.19 | 113.27 | 126.11 |
| 20 | 1 | 212 | CLA | CHA-C4D-ND | 5.19 | 129.53 | 124.52 |
| 21 | R | 101 | LMU | O1B-C1B-C2B | 5.19 | 121.55 | 108.10 |
| 20 | B | 822 | CLA | O2D-CGD-CBD | 5.19 | 120.49 | 111.27 |
| 20 | A | 816 | CLA | CHD-C4C-C3C | -5.19 | 117.22 | 124.84 |
| 22 | 2 | 317 | BCR | C38-C26-C25 | -5.19 | 118.70 | 124.53 |
| 20 | A | 802 | CLA | C2A-C1A-CHA | -5.19 | 113.79 | 122.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | I | 101 | BCR | C23-C22-C21 | 5.18 | 126.89 | 118.94 |
| 20 | 2 | 312 | CLA | CMD-C2D-C1D | 5.18 | 133.85 | 124.71 |
| 20 | B | 842 | CLA | C1D-CHD-C4C | -5.18 | 114.88 | 126.06 |
| 20 | B | 818 | CLA | O2D-CGD-CBD | 5.18 | 120.47 | 111.27 |
| 20 | B | 833 | CLA | CHC-C4B-NB | 5.18 | 129.74 | 124.26 |
| 20 | 1 | 202 | CLA | C1D-CHD-C4C | -5.18 | 114.89 | 126.06 |
| 20 | 4 | 315 | CLA | CHD-C4C-NC | 5.17 | 132.35 | 124.20 |
| 20 | B | 831 | CLA | CMD-C2D-C1D | 5.17 | 133.83 | 124.71 |
| 20 | B | 819 | CLA | CHD-C4C-NC | 5.17 | 132.35 | 124.20 |
| 20 | 2 | 308 | CLA | CHA-C4D-ND | 5.17 | 129.51 | 124.52 |
| 20 | B | 827 | CLA | C4D-C3D-CAD | 5.17 | 114.19 | 108.10 |
| 20 | I | 102 | CLA | O2D-CGD-CBD | 5.17 | 120.45 | 111.27 |
| 20 | A | 803 | CLA | C4D-C3D-CAD | 5.17 | 114.18 | 108.10 |
| 20 | B | 810 | CLA | C1D-CHD-C4C | -5.16 | 114.92 | 126.06 |
| 20 | 1 | 214 | CLA | CHA-C4D-ND | 5.16 | 129.50 | 124.52 |
| 20 | K | 103 | CLA | C1D-CHD-C4C | -5.16 | 114.92 | 126.06 |
| 20 | 1 | 211 | CLA | C4A-NA-C1A | 5.16 | 109.03 | 106.71 |
| 20 | B | 830 | CLA | C4A-NA-C1A | 5.16 | 109.03 | 106.71 |
| 20 | 3 | 314 | CLA | O2D-CGD-CBD | 5.16 | 120.43 | 111.27 |
| 20 | B | 827 | CLA | CHD-C4C-NC | 5.16 | 132.33 | 124.20 |
| 20 | A | 808 | CLA | O2D-CGD-CBD | 5.15 | 120.43 | 111.27 |
| 20 | L | 207 | CLA | C4D-C3D-CAD | 5.15 | 114.17 | 108.10 |
| 20 | A | 805 | CLA | C4D-C3D-CAD | 5.15 | 114.17 | 108.10 |
| 20 | 2 | 310 | CLA | CHC-C1C-NC | 5.15 | 132.02 | 124.20 |
| 20 | 1 | 208 | CLA | CHA-C4D-ND | 5.15 | 129.49 | 124.52 |
| 21 | B | 805 | LMU | C1B-O1B-C4' | -5.15 | 105.22 | 117.96 |
| 20 | B | 810 | CLA | CMD-C2D-C1D | 5.15 | 133.79 | 124.71 |
| 20 | A | 807 | CLA | C4D-C3D-CAD | 5.15 | 114.17 | 108.10 |
| 20 | F | 207 | CLA | CHD-C4C-NC | 5.15 | 132.31 | 124.20 |
| 21 | 2 | 320 | LMU | C4B-C3B-C2B | -5.14 | 101.84 | 110.82 |
| 21 | H | 103 | LMU | O5'-C5'-C6' | 5.14 | 119.22 | 106.44 |
| 20 | A | 825 | CLA | C4D-C3D-CAD | 5.14 | 114.15 | 108.10 |
| 20 | A | 816 | CLA | CHD-C4C-NC | 5.14 | 132.30 | 124.20 |
| 20 | 4 | 318 | CLA | CAA-C2A-C1A | 5.14 | 128.81 | 111.97 |
| 20 | 3 | 304 | CLA | CHC-C4B-NB | 5.14 | 129.47 | 124.27 |
| 20 | 2 | 309 | CLA | C3A-C4A-CHB | -5.14 | 117.62 | 123.91 |
| 20 | 2 | 311 | CLA | CMD-C2D-C1D | 5.13 | 133.76 | 124.71 |
| 20 | B | 806 | CLA | O2D-CGD-CBD | 5.13 | 120.39 | 111.27 |
| 20 | 2 | 311 | CLA | C4A-NA-C1A | 5.13 | 109.01 | 106.71 |
| 20 | 3 | 304 | CLA | CHC-C1C-NC | 5.13 | 131.81 | 124.23 |
| 20 | A | 837 | CLA | C3B-C2B-C1B | -5.13 | 100.97 | 107.16 |
| 20 | A | 831 | CLA | C4-C3-C5 | 5.13 | 123.90 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | K | 102 | CLA | CHD-C4C-NC | 5.13 | 132.28 | 124.20 |
| 20 | B | 816 | CLA | CMD-C2D-C1D | 5.13 | 133.75 | 124.71 |
| 23 | B | 843 | PQN | C11-C12-C13 | -5.13 | 118.26 | 126.79 |
| 20 | 1 | 204 | CLA | CHD-C4C-NC | 5.13 | 132.28 | 124.20 |
| 20 | A | 806 | CLA | C1D-CHD-C4C | -5.13 | 115.00 | 126.06 |
| 20 | K | 101 | CLA | O2D-CGD-CBD | 5.12 | 120.37 | 111.27 |
| 20 | A | 813 | CLA | C4D-C3D-CAD | 5.12 | 114.14 | 108.10 |
| 20 | B | 818 | CLA | C1D-CHD-C4C | -5.12 | 115.01 | 126.06 |
| 20 | H | 110 | CLA | CMD-C2D-C1D | 5.12 | 133.74 | 124.71 |
| 20 | 1 | 204 | CLA | C4B-CHC-C1C | -5.12 | 114.19 | 126.34 |
| 20 | 2 | 314 | CLA | C4B-CHC-C1C | -5.12 | 114.20 | 126.34 |
| 20 | L | 201 | CLA | C1D-CHD-C4C | -5.12 | 115.02 | 126.06 |
| 20 | 4 | 306 | CLA | C3A-C2A-C1A | 5.11 | 109.00 | 101.34 |
| 20 | 2 | 307 | CLA | CMD-C2D-C1D | 5.11 | 133.72 | 124.71 |
| 20 | A | 808 | CLA | C1D-CHD-C4C | -5.11 | 115.03 | 126.06 |
| 20 | A | 814 | CLA | C2A-C1A-CHA | -5.11 | 113.92 | 122.63 |
| 20 | 4 | 302 | CLA | CHD-C4C-NC | 5.11 | 132.25 | 124.20 |
| 20 | B | 837 | CLA | O2D-CGD-O1D | -5.11 | 113.85 | 123.84 |
| 20 | A | 808 | CLA | C4D-C3D-CAD | 5.11 | 114.11 | 108.10 |
| 20 | F | 201 | CLA | C4B-CHC-C1C | -5.11 | 114.23 | 126.34 |
| 20 | A | 851 | CLA | O2D-CGD-CBD | 5.10 | 120.34 | 111.27 |
| 20 | R | 108 | CLA | C1D-CHD-C4C | -5.10 | 115.05 | 126.06 |
| 20 | B | 841 | CLA | C1D-CHD-C4C | -5.10 | 115.05 | 126.06 |
| 20 | A | 838 | CLA | CMD-C2D-C1D | 5.10 | 133.70 | 124.71 |
| 20 | A | 831 | CLA | C4B-CHC-C1C | -5.10 | 114.25 | 126.34 |
| 20 | B | 808 | CLA | CHD-C4C-NC | 5.10 | 132.23 | 124.20 |
| 20 | A | 834 | CLA | C1D-CHD-C4C | -5.09 | 115.07 | 126.06 |
| 20 | 3 | 306 | CLA | C3A-C4A-CHB | -5.09 | 117.67 | 123.91 |
| 20 | 2 | 311 | CLA | C4D-C3D-CAD | 5.09 | 114.10 | 108.10 |
| 20 | A | 829 | CLA | C1D-CHD-C4C | -5.09 | 115.08 | 126.06 |
| 20 | 3 | 308 | CLA | C3A-C4A-CHB | -5.09 | 117.68 | 123.91 |
| 20 | A | 824 | CLA | C4D-C3D-CAD | 5.09 | 114.09 | 108.10 |
| 20 | A | 809 | CLA | CHC-C1C-NC | 5.09 | 131.92 | 124.20 |
| 22 | B | 845 | BCR | C24-C23-C22 | -5.09 | 118.55 | 126.23 |
| 20 | B | 813 | CLA | C1D-CHD-C4C | -5.09 | 115.09 | 126.06 |
| 20 | A | 849 | CLA | CHD-C4C-NC | 5.08 | 132.21 | 124.20 |
| 20 | F | 205 | CLA | CHD-C4C-NC | 5.08 | 132.21 | 124.20 |
| 20 | 3 | 305 | CLA | CHD-C4C-NC | 5.08 | 132.04 | 124.21 |
| 20 | A | 814 | CLA | CHA-C4D-ND | 5.07 | 129.42 | 124.52 |
| 20 | 2 | 316 | CLA | CHD-C4C-NC | 5.07 | 132.19 | 124.20 |
| 20 | 2 | 307 | CLA | CHC-C1C-NC | 5.06 | 131.88 | 124.20 |
| 20 | 3 | 305 | CLA | C4C-CHD-C1D | -5.06 | 113.60 | 126.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 204 | CLA | CMD-C2D-C3D | -5.06 | 115.98 | 127.61 |
| 20 | H | 108 | CLA | CHC-C1C-NC | 5.06 | 131.87 | 124.20 |
| 20 | 3 | 316 | CLA | C2A-C1A-CHA | -5.06 | 114.01 | 122.63 |
| 20 | A | 802 | CLA | C3A-C4A-CHB | -5.06 | 117.72 | 123.91 |
| 20 | B | 814 | CLA | C4D-C3D-CAD | 5.05 | 114.05 | 108.10 |
| 20 | A | 851 | CLA | C1D-CHD-C4C | -5.05 | 115.16 | 126.06 |
| 20 | A | 801 | CLA | C1D-CHD-C4C | -5.05 | 115.17 | 126.06 |
| 20 | L | 204 | CLA | CHD-C4C-NC | 5.04 | 132.15 | 124.20 |
| 20 | 4 | 302 | CLA | CAB-C3B-C2B | -5.04 | 110.52 | 123.59 |
| 21 | H | 105 | LMU | C1B-O5B-C5B | 5.04 | 123.58 | 113.69 |
| 20 | 2 | 309 | CLA | C4C-CHD-C1D | -5.04 | 113.65 | 126.11 |
| 20 | F | 207 | CLA | CHC-C4B-NB | 5.04 | 129.59 | 124.26 |
| 20 | A | 815 | CLA | C1D-CHD-C4C | -5.04 | 115.19 | 126.06 |
| 20 | A | 832 | CLA | C4D-C3D-CAD | 5.04 | 114.03 | 108.10 |
| 20 | A | 806 | CLA | CHC-C4B-NB | 5.03 | 129.59 | 124.26 |
| 20 | 3 | 316 | CLA | C3A-C4A-CHB | -5.03 | 117.75 | 123.91 |
| 20 | 2 | 301 | CLA | C3A-C4A-CHB | -5.02 | 117.76 | 123.91 |
| 20 | 4 | 317 | CLA | CHD-C4C-NC | 5.02 | 132.12 | 124.20 |
| 22 | G | 104 | BCR | C15-C14-C13 | -5.02 | 120.14 | 127.31 |
| 20 | 4 | 312 | CLA | CHC-C4B-NB | 5.02 | 129.36 | 124.27 |
| 20 | H | 102 | CLA | CHC-C4B-NB | 5.02 | 129.57 | 124.26 |
| 20 | B | 838 | CLA | C4D-C3D-CAD | 5.02 | 114.01 | 108.10 |
| 22 | F | 204 | BCR | C30-C25-C26 | -5.01 | 115.55 | 122.61 |
| 20 | A | 814 | CLA | C1B-NB-C4B | -5.01 | 102.77 | 106.33 |
| 20 | L | 208 | CLA | CHD-C4C-C3C | -5.01 | 117.47 | 124.84 |
| 20 | L | 208 | CLA | CHD-C4C-NC | 5.01 | 132.10 | 124.20 |
| 20 | K | 104 | CLA | C4-C3-C5 | 5.01 | 123.69 | 115.27 |
| 20 | A | 816 | CLA | C4D-C3D-CAD | 5.00 | 113.99 | 108.10 |
| 20 | 1 | 214 | CLA | C2A-C1A-CHA | -5.00 | 114.10 | 122.63 |
| 20 | 1 | 203 | CLA | C2A-C1A-CHA | -5.00 | 115.12 | 123.86 |
| 20 | A | 838 | CLA | CHD-C4C-NC | 5.00 | 132.07 | 124.20 |
| 20 | B | 839 | CLA | CMD-C2D-C3D | -4.99 | 116.12 | 127.61 |
| 20 | A | 823 | CLA | C4D-C3D-CAD | 4.99 | 113.98 | 108.10 |
| 20 | A | 813 | CLA | CHC-C1C-NC | 4.99 | 131.78 | 124.20 |
| 20 | B | 850 | CLA | CHC-C4B-NB | 4.99 | 129.54 | 124.26 |
| 20 | A | 833 | CLA | CHD-C4C-NC | 4.99 | 132.06 | 124.20 |
| 20 | A | 801 | CLA | C3A-C2A-C1A | 4.99 | 108.81 | 101.34 |
| 20 | B | 840 | CLA | O2D-CGD-CBD | 4.99 | 120.13 | 111.27 |
| 20 | A | 804 | CLA | CHC-C4B-NB | 4.99 | 129.54 | 124.26 |
| 20 | B | 836 | CLA | C4-C3-C5 | 4.99 | 121.68 | 115.98 |
| 20 | 4 | 308 | CLA | C4C-CHD-C1D | -4.98 | 113.78 | 126.11 |
| 20 | B | 824 | CLA | CHC-C4B-NB | 4.98 | 129.53 | 124.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 211 | CLA | O2A-CGA-CBA | 4.98 | 127.55 | 111.91 |
| 20 | 1 | 213 | CLA | CHD-C4C-NC | 4.98 | 132.05 | 124.20 |
| 20 | B | 810 | CLA | C4A-NA-C1A | 4.98 | 108.94 | 106.71 |
| 20 | B | 821 | CLA | CHD-C4C-NC | 4.97 | 132.04 | 124.20 |
| 20 | 3 | 304 | CLA | C1C-CHC-C4B | -4.97 | 113.73 | 126.13 |
| 20 | A | 809 | CLA | C4D-C3D-CAD | 4.97 | 113.95 | 108.10 |
| 20 | B | 809 | CLA | C3B-C2B-C1B | -4.97 | 101.16 | 107.16 |
| 20 | A | 810 | CLA | C1D-CHD-C4C | -4.97 | 115.34 | 126.06 |
| 20 | A | 837 | CLA | CHC-C4B-NB | 4.96 | 129.51 | 124.26 |
| 20 | L | 203 | CLA | CHC-C4B-NB | 4.96 | 129.51 | 124.26 |
| 20 | A | 818 | CLA | C3B-C2B-C1B | -4.96 | 101.17 | 107.16 |
| 21 | D | 201 | LMU | C1'-O5'-C5' | -4.96 | 103.96 | 113.69 |
| 20 | 4 | 307 | CLA | C2A-C1A-CHA | -4.96 | 114.18 | 122.63 |
| 20 | A | 839 | CLA | C4B-CHC-C1C | -4.95 | 114.59 | 126.34 |
| 20 | 3 | 304 | CLA | CHD-C4C-NC | 4.95 | 131.85 | 124.21 |
| 22 | A | 844 | BCR | C15-C14-C13 | -4.95 | 120.25 | 127.31 |
| 20 | A | 833 | CLA | C4D-C3D-CAD | 4.95 | 113.93 | 108.10 |
| 20 | 3 | 312 | CLA | C3A-C4A-CHB | -4.95 | 117.85 | 123.91 |
| 20 | 2 | 310 | CLA | O2D-CGD-CBD | 4.94 | 120.05 | 111.27 |
| 20 | A | 841 | CLA | C1C-CHC-C4B | -4.94 | 113.81 | 126.13 |
| 20 | A | 827 | CLA | C4D-C3D-CAD | 4.94 | 113.92 | 108.10 |
| 20 | 3 | 306 | CLA | CHD-C4C-NC | 4.94 | 131.83 | 124.21 |
| 21 | H | 105 | LMU | C1B-C2B-C3B | -4.94 | 99.71 | 110.00 |
| 20 | 2 | 312 | CLA | CHD-C4C-C3C | -4.94 | 117.58 | 124.84 |
| 20 | B | 820 | CLA | CHD-C4C-C3C | -4.94 | 117.58 | 124.84 |
| 20 | B | 829 | CLA | C2B-C1B-NB | 4.93 | 113.54 | 110.23 |
| 20 | B | 818 | CLA | C4D-C3D-CAD | 4.93 | 113.91 | 108.10 |
| 20 | A | 831 | CLA | C4D-C3D-CAD | 4.93 | 113.91 | 108.10 |
| 20 | 4 | 317 | CLA | CHC-C1C-NC | 4.93 | 131.68 | 124.20 |
| 20 | A | 813 | CLA | CHD-C4C-NC | 4.93 | 131.96 | 124.20 |
| 20 | 1 | 214 | CLA | C3A-C4A-CHB | -4.92 | 117.88 | 123.91 |
| 20 | 2 | 305 | CLA | C1D-CHD-C4C | -4.92 | 115.44 | 126.06 |
| 20 | A | 807 | CLA | C1D-CHD-C4C | -4.92 | 115.44 | 126.06 |
| 20 | H | 109 | CLA | C4D-C3D-CAD | 4.92 | 113.90 | 108.10 |
| 20 | 1 | 203 | CLA | CMD-C2D-C3D | -4.92 | 116.29 | 127.61 |
| 20 | B | 810 | CLA | CHC-C4B-NB | 4.91 | 129.46 | 124.26 |
| 20 | 3 | 310 | CLA | C4D-C3D-CAD | 4.91 | 113.89 | 108.10 |
| 20 | 4 | 305 | CLA | CHD-C4C-NC | 4.91 | 131.94 | 124.20 |
| 20 | B | 806 | CLA | CHD-C4C-NC | 4.91 | 131.94 | 124.20 |
| 20 | B | 816 | CLA | O2D-CGD-CBD | 4.91 | 119.99 | 111.27 |
| 20 | L | 204 | CLA | C4D-C3D-CAD | 4.91 | 113.88 | 108.10 |
| 20 | A | 804 | CLA | CHD-C4C-NC | 4.91 | 131.93 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 832 | CLA | O2D-CGD-CBD | 4.90 | 119.98 | 111.27 |
| 20 | 2 | 310 | CLA | CHD-C4C-NC | 4.90 | 131.93 | 124.20 |
| 20 | B | 809 | CLA | C4D-C3D-CAD | 4.90 | 113.87 | 108.10 |
| 20 | B | 850 | CLA | C1D-CHD-C4C | -4.90 | 115.49 | 126.06 |
| 20 | B | 808 | CLA | CHD-C4C-C3C | -4.90 | 117.64 | 124.84 |
| 20 | B | 806 | CLA | C1D-CHD-C4C | -4.90 | 115.49 | 126.06 |
| 20 | 2 | 312 | CLA | CHD-C4C-NC | 4.90 | 131.92 | 124.20 |
| 20 | B | 836 | CLA | CHD-C4C-NC | 4.90 | 131.92 | 124.20 |
| 22 | 2 | 317 | BCR | C16-C15-C14 | -4.89 | 113.45 | 123.47 |
| 20 | 4 | 308 | CLA | C3B-C2B-C1B | -4.89 | 101.45 | 106.75 |
| 22 | F | 203 | BCR | C11-C10-C9 | -4.89 | 120.33 | 127.31 |
| 20 | J | 103 | CLA | CMD-C2D-C1D | 4.89 | 133.34 | 124.71 |
| 22 | B | 847 | BCR | C15-C14-C13 | -4.89 | 120.33 | 127.31 |
| 20 | I | 102 | CLA | C4D-C3D-CAD | 4.89 | 113.86 | 108.10 |
| 20 | 3 | 315 | CLA | C1C-CHC-C4B | -4.89 | 113.94 | 126.13 |
| 20 | A | 802 | CLA | C2D-C3D-C4D | -4.89 | 101.86 | 107.28 |
| 20 | 2 | 316 | CLA | CHD-C4C-C3C | -4.89 | 117.65 | 124.84 |
| 20 | 3 | 317 | CLA | CHD-C4C-NC | 4.89 | 131.90 | 124.20 |
| 20 | 4 | 314 | CLA | CHC-C4B-NB | 4.89 | 129.22 | 124.27 |
| 20 | L | 204 | CLA | C2B-C1B-NB | 4.89 | 113.51 | 110.23 |
| 20 | 3 | 306 | CLA | CHC-C4B-NB | 4.88 | 129.22 | 124.27 |
| 20 | B | 831 | CLA | C4D-C3D-CAD | 4.88 | 113.85 | 108.10 |
| 20 | L | 204 | CLA | CHD-C4C-C3C | -4.88 | 117.67 | 124.84 |
| 20 | 4 | 306 | CLA | C4D-C3D-CAD | 4.88 | 113.85 | 108.10 |
| 20 | K | 103 | CLA | CHC-C1C-NC | 4.88 | 131.60 | 124.20 |
| 20 | 1 | 208 | CLA | C3A-C4A-CHB | -4.88 | 117.94 | 123.91 |
| 20 | 3 | 305 | CLA | CHC-C4B-NB | 4.88 | 129.21 | 124.27 |
| 20 | 1 | 207 | CLA | C2A-C3A-C4A | -4.88 | 93.99 | 101.87 |
| 20 | 1 | 204 | CLA | CHC-C1C-NC | 4.87 | 131.60 | 124.20 |
| 20 | B | 839 | CLA | CHC-C1C-NC | 4.87 | 131.59 | 124.20 |
| 20 | B | 806 | CLA | C4D-C3D-CAD | 4.87 | 113.84 | 108.10 |
| 20 | 3 | 311 | CLA | CHD-C4C-NC | 4.87 | 131.88 | 124.20 |
| 20 | 1 | 206 | CLA | CHD-C4C-C3C | -4.87 | 117.69 | 124.84 |
| 20 | B | 835 | CLA | CHD-C4C-NC | 4.87 | 131.87 | 124.20 |
| 20 | 4 | 308 | CLA | CHA-C4D-ND | 4.86 | 129.21 | 124.52 |
| 20 | 2 | 303 | CLA | C4A-NA-C1A | 4.86 | 108.89 | 106.71 |
| 21 | A | 855 | LMU | O1B-C4'-C3' | 4.86 | 120.22 | 107.28 |
| 20 | 3 | 316 | CLA | C4C-CHD-C1D | -4.86 | 114.09 | 126.11 |
| 20 | B | 829 | CLA | CHD-C4C-C3C | -4.86 | 117.69 | 124.84 |
| 20 | 4 | 304 | CLA | CHC-C4B-NB | 4.86 | 129.40 | 124.26 |
| 20 | 4 | 304 | CLA | CHC-C1C-NC | 4.86 | 131.57 | 124.20 |
| 20 | A | 835 | CLA | CHD-C4C-NC | 4.85 | 131.85 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | H | 108 | CLA | CHD-C4C-C3C | -4.85 | 117.72 | 124.84 |
| 20 | B | 824 | CLA | C4D-C3D-CAD | 4.85 | 113.81 | 108.10 |
| 20 | 2 | 314 | CLA | C1-C2-C3 | -4.85 | 118.91 | 126.75 |
| 20 | A | 802 | CLA | C1C-CHC-C4B | -4.84 | 114.06 | 126.13 |
| 20 | 3 | 305 | CLA | C3A-C4A-CHB | -4.84 | 117.98 | 123.91 |
| 20 | A | 831 | CLA | CHD-C4C-C3C | -4.84 | 117.72 | 124.84 |
| 20 | A | 812 | CLA | C4D-C3D-CAD | 4.84 | 113.80 | 108.10 |
| 20 | 1 | 213 | CLA | C4-C3-C5 | 4.84 | 121.51 | 115.98 |
| 20 | A | 839 | CLA | CHD-C4C-NC | 4.84 | 131.82 | 124.20 |
| 20 | 4 | 311 | CLA | CHC-C4B-NB | 4.84 | 129.17 | 124.27 |
| 20 | B | 816 | CLA | C3B-C2B-C1B | -4.83 | 101.33 | 107.16 |
| 20 | A | 805 | CLA | C4B-CHC-C1C | -4.83 | 114.88 | 126.34 |
| 20 | B | 821 | CLA | O2D-CGD-CBD | 4.83 | 119.85 | 111.27 |
| 20 | 3 | 307 | CLA | C1D-CHD-C4C | -4.83 | 115.64 | 126.06 |
| 20 | 1 | 201 | CLA | CHC-C1C-NC | 4.83 | 131.53 | 124.20 |
| 20 | A | 837 | CLA | CHC-C1C-NC | 4.83 | 131.52 | 124.20 |
| 20 | 4 | 304 | CLA | C4B-CHC-C1C | -4.83 | 114.89 | 126.34 |
| 20 | 4 | 305 | CLA | CHD-C4C-C3C | -4.82 | 117.75 | 124.84 |
| 20 | A | 803 | CLA | CHC-C1C-NC | 4.82 | 131.52 | 124.20 |
| 20 | A | 805 | CLA | CHC-C1C-NC | 4.82 | 131.52 | 124.20 |
| 20 | 4 | 312 | CLA | C2A-C1A-CHA | -4.82 | 114.41 | 122.63 |
| 20 | B | 802 | CLA | C4D-C3D-CAD | 4.82 | 113.78 | 108.10 |
| 20 | R | 107 | CLA | O2D-CGD-CBD | 4.82 | 119.84 | 111.27 |
| 20 | A | 841 | CLA | CHA-C4D-ND | 4.82 | 129.17 | 124.52 |
| 20 | A | 807 | CLA | CHC-C4B-NB | 4.82 | 129.36 | 124.26 |
| 20 | 1 | 213 | CLA | CHC-C1C-NC | 4.82 | 131.52 | 124.20 |
| 20 | 2 | 314 | CLA | CHC-C1C-NC | 4.82 | 131.52 | 124.20 |
| 20 | 3 | 309 | CLA | CHC-C4B-NB | 4.82 | 129.15 | 124.27 |
| 20 | B | 825 | CLA | C4D-C3D-CAD | 4.81 | 113.77 | 108.10 |
| 20 | A | 833 | CLA | CHC-C1C-NC | 4.81 | 131.50 | 124.20 |
| 20 | B | 820 | CLA | CHD-C4C-NC | 4.81 | 131.78 | 124.20 |
| 20 | 1 | 203 | CLA | O2D-CGD-CBD | 4.81 | 119.81 | 111.27 |
| 20 | A | 837 | CLA | C4B-CHC-C1C | -4.81 | 114.94 | 126.34 |
| 20 | 4 | 311 | CLA | C3A-C4A-CHB | -4.80 | 118.03 | 123.91 |
| 20 | 4 | 310 | CLA | C4B-CHC-C1C | -4.80 | 114.95 | 126.34 |
| 20 | A | 850 | CLA | C4D-C3D-CAD | 4.80 | 113.75 | 108.10 |
| 20 | 4 | 309 | CLA | C4C-CHD-C1D | -4.80 | 114.25 | 126.11 |
| 22 | A | 844 | BCR | C24-C23-C22 | -4.80 | 118.99 | 126.23 |
| 20 | A | 811 | CLA | CMB-C2B-C1B | 4.80 | 132.67 | 125.37 |
| 20 | B | 834 | CLA | CHD-C4C-NC | 4.80 | 131.76 | 124.20 |
| 20 | F | 201 | CLA | C2B-C1B-NB | 4.79 | 113.44 | 110.23 |
| 20 | B | 809 | CLA | CHC-C1C-NC | 4.79 | 131.47 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 839 | CLA | CHC-C4B-NB | 4.79 | 129.32 | 124.26 |
| 20 | H | 108 | CLA | C4B-CHC-C1C | -4.79 | 114.99 | 126.34 |
| 21 | G | 102 | LMU | C1B-O5B-C5B | -4.78 | 104.30 | 113.69 |
| 20 | A | 850 | CLA | CHD-C4C-NC | 4.78 | 131.74 | 124.20 |
| 20 | B | 838 | CLA | CHD-C4C-NC | 4.78 | 131.74 | 124.20 |
| 20 | B | 815 | CLA | C1D-CHD-C4C | -4.78 | 115.74 | 126.06 |
| 20 | 4 | 314 | CLA | C3A-C4A-CHB | -4.78 | 118.06 | 123.91 |
| 20 | B | 831 | CLA | C1D-CHD-C4C | -4.78 | 115.75 | 126.06 |
| 20 | A | 810 | CLA | C4D-C3D-CAD | 4.78 | 113.73 | 108.10 |
| 20 | L | 201 | CLA | CHD-C4C-NC | 4.78 | 131.73 | 124.20 |
| 20 | 1 | 205 | CLA | CAB-C3B-C2B | -4.78 | 111.20 | 123.59 |
| 20 | B | 850 | CLA | C4B-CHC-C1C | -4.78 | 115.01 | 126.34 |
| 20 | L | 202 | CLA | CHD-C4C-NC | 4.77 | 131.73 | 124.20 |
| 22 | B | 844 | BCR | C28-C27-C26 | -4.77 | 105.55 | 114.08 |
| 20 | B | 807 | CLA | CHD-C4C-NC | 4.77 | 131.72 | 124.20 |
| 20 | F | 207 | CLA | C2B-C1B-NB | 4.77 | 113.43 | 110.23 |
| 20 | A | 830 | CLA | CHC-C4B-NB | 4.77 | 129.30 | 124.26 |
| 20 | A | 850 | CLA | O2D-CGD-CBD | 4.77 | 119.74 | 111.27 |
| 21 | B | 804 | LMU | C3'-C4'-C5' | -4.77 | 100.00 | 110.93 |
| 20 | 2 | 304 | CLA | C3A-C4A-CHB | -4.76 | 118.08 | 123.91 |
| 20 | 4 | 301 | CLA | CHD-C4C-NC | 4.76 | 131.70 | 124.20 |
| 20 | 3 | 312 | CLA | C4C-CHD-C1D | -4.76 | 114.34 | 126.11 |
| 20 | 3 | 304 | CLA | C2A-C1A-CHA | -4.76 | 114.52 | 122.63 |
| 20 | 1 | 205 | CLA | CHD-C4C-NC | 4.75 | 131.69 | 124.20 |
| 20 | A | 825 | CLA | CHD-C4C-NC | 4.75 | 131.69 | 124.20 |
| 20 | B | 830 | CLA | CHD-C4C-NC | 4.75 | 131.69 | 124.20 |
| 20 | 2 | 315 | CLA | CHD-C4C-NC | 4.75 | 131.54 | 124.21 |
| 22 | B | 801 | BCR | C8-C9-C10 | 4.75 | 126.23 | 118.94 |
| 20 | 4 | 318 | CLA | C1D-CHD-C4C | -4.75 | 115.81 | 126.06 |
| 20 | 1 | 212 | CLA | C4C-CHD-C1D | -4.75 | 114.37 | 126.11 |
| 20 | A | 851 | CLA | CHD-C4C-NC | 4.75 | 131.68 | 124.20 |
| 22 | L | 209 | BCR | C7-C8-C9 | -4.75 | 119.06 | 126.23 |
| 20 | 4 | 315 | CLA | C4D-C3D-CAD | 4.74 | 113.69 | 108.10 |
| 20 | A | 826 | CLA | CHD-C4C-NC | 4.74 | 131.68 | 124.20 |
| 20 | 2 | 310 | CLA | C1D-CHD-C4C | -4.74 | 115.83 | 126.06 |
| 20 | 3 | 302 | CLA | C4C-CHD-C1D | -4.74 | 114.39 | 126.11 |
| 20 | A | 849 | CLA | C4B-CHC-C1C | -4.74 | 115.10 | 126.34 |
| 20 | 2 | 303 | CLA | CHD-C4C-C3C | -4.73 | 117.88 | 124.84 |
| 20 | A | 831 | CLA | CMB-C2B-C1B | 4.73 | 132.58 | 125.37 |
| 20 | 3 | 309 | CLA | C1B-NB-C4B | -4.73 | 102.97 | 106.33 |
| 20 | 1 | 207 | CLA | O2D-CGD-CBD | 4.73 | 119.67 | 111.27 |
| 20 | K | 101 | CLA | CHD-C4C-NC | 4.73 | 131.66 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 841 | CLA | C4B-CHC-C1C | -4.73 | 115.12 | 126.34 |
| 22 | A | 843 | BCR | C15-C14-C13 | -4.73 | 120.56 | 127.31 |
| 20 | J | 101 | CLA | CHD-C4C-NC | 4.73 | 131.65 | 124.20 |
| 20 | H | 110 | CLA | CHD-C4C-C3C | -4.72 | 117.89 | 124.84 |
| 20 | A | 838 | CLA | C3B-C2B-C1B | -4.72 | 101.46 | 107.16 |
| 20 | 3 | 308 | CLA | C2A-C1A-CHA | -4.72 | 114.58 | 122.63 |
| 20 | 1 | 209 | CLA | C4C-CHD-C1D | -4.72 | 114.44 | 126.11 |
| 20 | 2 | 314 | CLA | C3B-C2B-C1B | -4.72 | 101.46 | 107.16 |
| 20 | H | 110 | CLA | CHD-C4C-NC | 4.72 | 131.64 | 124.20 |
| 20 | 1 | 204 | CLA | CAA-C2A-C3A | -4.72 | 99.86 | 112.78 |
| 20 | A | 828 | CLA | CHD-C4C-NC | 4.71 | 131.63 | 124.20 |
| 20 | 4 | 313 | CLA | C1B-C2B-C3B | -4.71 | 102.56 | 107.03 |
| 20 | K | 103 | CLA | C4B-CHC-C1C | -4.71 | 115.16 | 126.34 |
| 20 | 4 | 317 | CLA | C4B-CHC-C1C | -4.71 | 115.17 | 126.34 |
| 20 | A | 839 | CLA | CMD-C2D-C3D | -4.71 | 116.79 | 127.61 |
| 20 | 2 | 316 | CLA | CHC-C4B-NB | 4.71 | 129.24 | 124.26 |
| 20 | 1 | 211 | CLA | O2D-CGD-CBD | 4.71 | 119.63 | 111.27 |
| 20 | B | 816 | CLA | C4D-C3D-CAD | 4.71 | 113.64 | 108.10 |
| 20 | A | 835 | CLA | CHC-C1C-NC | 4.70 | 131.34 | 124.20 |
| 22 | I | 103 | BCR | C38-C26-C27 | 4.70 | 122.64 | 113.62 |
| 20 | B | 840 | CLA | C1D-CHD-C4C | -4.70 | 115.92 | 126.06 |
| 20 | 4 | 309 | CLA | C2A-C1A-CHA | -4.69 | 114.63 | 122.63 |
| 20 | A | 804 | CLA | C1-O2A-CGA | 4.69 | 128.75 | 116.44 |
| 20 | B | 802 | CLA | CHD-C4C-NC | 4.69 | 131.59 | 124.20 |
| 20 | A | 804 | CLA | C4B-CHC-C1C | -4.69 | 115.22 | 126.34 |
| 21 | R | 103 | LMU | O1B-C4'-C3' | 4.69 | 119.75 | 107.28 |
| 20 | 1 | 207 | CLA | CAA-C2A-C3A | 4.69 | 125.61 | 112.78 |
| 20 | B | 803 | CLA | CHC-C1C-NC | 4.69 | 131.31 | 124.20 |
| 20 | B | 812 | CLA | CHD-C4C-C3C | -4.68 | 117.95 | 124.84 |
| 20 | 3 | 305 | CLA | CHC-C1C-NC | 4.68 | 131.14 | 124.23 |
| 20 | A | 804 | CLA | C3B-C4B-NB | -4.68 | 106.17 | 110.52 |
| 20 | A | 818 | CLA | CHC-C4B-NB | 4.68 | 129.21 | 124.26 |
| 20 | B | 824 | CLA | O2D-CGD-CBD | 4.68 | 119.58 | 111.27 |
| 20 | 4 | 314 | CLA | C4C-CHD-C1D | -4.68 | 114.55 | 126.11 |
| 20 | F | 201 | CLA | CMD-C2D-C1D | 4.67 | 132.95 | 124.71 |
| 20 | B | 819 | CLA | CHD-C4C-C3C | -4.67 | 117.97 | 124.84 |
| 20 | A | 809 | CLA | C4B-CHC-C1C | -4.67 | 115.26 | 126.34 |
| 20 | 2 | 312 | CLA | C1-C2-C3 | -4.67 | 117.97 | 126.04 |
| 20 | 1 | 202 | CLA | C4A-NA-C1A | 4.67 | 108.81 | 106.71 |
| 20 | A | 850 | CLA | CHD-C4C-C3C | -4.67 | 117.98 | 124.84 |
| 20 | A | 802 | CLA | CHA-C4D-ND | 4.67 | 129.02 | 124.52 |
| 20 | 4 | 307 | CLA | CHB-C1B-NB | -4.67 | 119.55 | 124.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | H | 103 | LMU | C1B-O1B-C4' | -4.67 | 106.42 | 117.96 |
| 20 | A | 801 | CLA | CMD-C2D-C3D | -4.66 | 116.88 | 127.61 |
| 20 | A | 818 | CLA | C1-C2-C3 | -4.66 | 117.98 | 126.04 |
| 22 | I | 103 | BCR | C7-C8-C9 | 4.66 | 133.28 | 126.23 |
| 20 | J | 103 | CLA | CHC-C1C-NC | 4.66 | 131.27 | 124.20 |
| 20 | 2 | 308 | CLA | CHC-C1C-NC | 4.66 | 131.11 | 124.23 |
| 20 | B | 820 | CLA | CHC-C4B-NB | 4.66 | 129.19 | 124.26 |
| 20 | B | 811 | CLA | C2A-C1A-CHA | -4.66 | 114.69 | 122.63 |
| 20 | A | 819 | CLA | O2D-CGD-CBD | 4.66 | 119.54 | 111.27 |
| 22 | B | 801 | BCR | C36-C18-C19 | 4.66 | 125.41 | 118.08 |
| 20 | R | 108 | CLA | CHC-C4B-NB | 4.65 | 129.18 | 124.26 |
| 20 | B | 828 | CLA | CHD-C4C-NC | 4.65 | 131.53 | 124.20 |
| 21 | D | 201 | LMU | O1'-C1'-C2' | 4.65 | 115.56 | 108.30 |
| 20 | 3 | 308 | CLA | CHC-C4B-NB | 4.65 | 128.98 | 124.27 |
| 20 | A | 803 | CLA | C4B-CHC-C1C | -4.65 | 115.32 | 126.34 |
| 20 | 1 | 214 | CLA | C4A-NA-C1A | 4.64 | 108.79 | 106.71 |
| 20 | F | 206 | CLA | CHD-C4C-NC | 4.64 | 131.52 | 124.20 |
| 20 | 1 | 208 | CLA | C4C-CHD-C1D | -4.64 | 114.63 | 126.11 |
| 20 | B | 827 | CLA | CHD-C4C-C3C | -4.64 | 118.02 | 124.84 |
| 20 | I | 102 | CLA | CHD-C4C-NC | 4.64 | 131.51 | 124.20 |
| 20 | 4 | 309 | CLA | CHC-C4B-NB | 4.64 | 128.97 | 124.27 |
| 20 | 2 | 308 | CLA | C4A-NA-C1A | 4.63 | 108.79 | 106.71 |
| 20 | B | 813 | CLA | O2D-CGD-CBD | 4.63 | 119.50 | 111.27 |
| 20 | 3 | 313 | CLA | C4D-C3D-CAD | 4.63 | 113.56 | 108.10 |
| 20 | 4 | 318 | CLA | C4B-CHC-C1C | -4.63 | 115.36 | 126.34 |
| 20 | 1 | 207 | CLA | CHD-C4C-NC | 4.63 | 131.50 | 124.20 |
| 20 | 4 | 305 | CLA | O2D-CGD-CBD | 4.63 | 119.50 | 111.27 |
| 20 | B | 838 | CLA | CHC-C4B-NB | 4.63 | 129.16 | 124.26 |
| 20 | A | 816 | CLA | CHC-C4B-NB | 4.63 | 129.16 | 124.26 |
| 20 | 4 | 302 | CLA | CHD-C4C-C3C | -4.63 | 117.75 | 124.98 |
| 20 | 4 | 308 | CLA | CHD-C4C-NC | 4.63 | 131.35 | 124.21 |
| 20 | 4 | 306 | CLA | C4B-CHC-C1C | -4.63 | 115.37 | 126.34 |
| 20 | L | 207 | CLA | CHD-C4C-NC | 4.63 | 131.49 | 124.20 |
| 20 | 3 | 314 | CLA | C4D-C3D-CAD | 4.62 | 113.55 | 108.10 |
| 20 | 1 | 213 | CLA | CHC-C4B-NB | 4.62 | 129.15 | 124.26 |
| 20 | 2 | 304 | CLA | CHC-C1C-NC | 4.62 | 131.06 | 124.23 |
| 20 | A | 811 | CLA | CHC-C1C-NC | 4.62 | 131.21 | 124.20 |
| 20 | B | 826 | CLA | CHD-C4C-NC | 4.62 | 131.48 | 124.20 |
| 20 | A | 829 | CLA | C4D-C3D-CAD | 4.62 | 113.54 | 108.10 |
| 20 | K | 102 | CLA | O2D-CGD-CBD | 4.62 | 119.47 | 111.27 |
| 20 | A | 801 | CLA | CHC-C1C-NC | 4.62 | 131.21 | 124.20 |
| 20 | B | 836 | CLA | CHC-C1C-NC | 4.62 | 131.21 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 814 | CLA | C2D-C3D-C4D | -4.62 | 102.17 | 107.28 |
| 20 | A | 812 | CLA | CHD-C4C-NC | 4.61 | 131.47 | 124.20 |
| 20 | B | 815 | CLA | C3B-C2B-C1B | -4.61 | 101.59 | 107.16 |
| 20 | K | 104 | CLA | CMD-C2D-C3D | -4.61 | 117.00 | 127.61 |
| 20 | B | 830 | CLA | C4B-CHC-C1C | -4.61 | 115.40 | 126.34 |
| 20 | 4 | 310 | CLA | C4A-NA-C1A | 4.61 | 108.78 | 106.71 |
| 20 | A | 823 | CLA | CHC-C4B-NB | 4.61 | 129.13 | 124.26 |
| 20 | 1 | 202 | CLA | C4B-CHC-C1C | -4.61 | 115.41 | 126.34 |
| 20 | 4 | 312 | CLA | C4C-CHD-C1D | -4.61 | 114.72 | 126.11 |
| 20 | B | 832 | CLA | CHD-C4C-NC | 4.61 | 131.46 | 124.20 |
| 20 | 1 | 206 | CLA | CHC-C4B-NB | 4.60 | 129.13 | 124.26 |
| 20 | A | 801 | CLA | O2D-CGD-O1D | -4.60 | 114.84 | 123.84 |
| 20 | A | 806 | CLA | CHD-C4C-NC | 4.60 | 131.46 | 124.20 |
| 20 | 2 | 307 | CLA | CHD-C4C-C3C | -4.60 | 118.07 | 124.84 |
| 20 | A | 827 | CLA | CMD-C2D-C1D | 4.60 | 132.82 | 124.71 |
| 20 | A | 805 | CLA | CHD-C4C-NC | 4.60 | 131.45 | 124.20 |
| 20 | A | 818 | CLA | CHC-C1C-NC | 4.60 | 131.18 | 124.20 |
| 20 | A | 813 | CLA | O2D-CGD-CBD | 4.60 | 119.44 | 111.27 |
| 20 | A | 821 | CLA | C4A-NA-C1A | 4.60 | 108.77 | 106.71 |
| 20 | B | 830 | CLA | C2B-C1B-NB | 4.60 | 113.31 | 110.23 |
| 20 | A | 838 | CLA | CHD-C4C-C3C | -4.60 | 118.08 | 124.84 |
| 20 | J | 103 | CLA | CHC-C4B-NB | 4.59 | 129.12 | 124.26 |
| 20 | A | 810 | CLA | CHD-C4C-NC | 4.59 | 131.44 | 124.20 |
| 22 | F | 204 | BCR | C10-C11-C12 | -4.59 | 108.89 | 123.22 |
| 20 | 3 | 309 | CLA | CHC-C1C-NC | 4.59 | 131.01 | 124.23 |
| 20 | A | 837 | CLA | O2D-CGD-CBD | 4.59 | 119.43 | 111.27 |
| 20 | 4 | 306 | CLA | CHD-C4C-C3C | -4.59 | 118.09 | 124.84 |
| 20 | 1 | 214 | CLA | C4C-CHD-C1D | -4.59 | 114.76 | 126.11 |
| 20 | A | 803 | CLA | O2D-CGD-O1D | -4.58 | 114.88 | 123.84 |
| 20 | B | 829 | CLA | CHD-C4C-NC | 4.58 | 131.43 | 124.20 |
| 20 | A | 804 | CLA | O2D-CGD-CBD | 4.58 | 119.41 | 111.27 |
| 20 | A | 841 | CLA | CHC-C1C-NC | 4.58 | 130.99 | 124.23 |
| 20 | 3 | 309 | CLA | CHD-C4C-NC | 4.58 | 131.27 | 124.21 |
| 20 | B | 829 | CLA | CHB-C1B-NB | -4.58 | 119.41 | 124.26 |
| 20 | A | 851 | CLA | CMD-C2D-C3D | -4.58 | 117.09 | 127.61 |
| 21 | 2 | 313 | LMU | O1'-C1'-C2' | 4.58 | 115.45 | 108.30 |
| 21 | H | 103 | LMU | O1B-C1B-C2B | 4.57 | 119.95 | 108.10 |
| 20 | A | 823 | CLA | O2D-CGD-CBD | 4.57 | 119.39 | 111.27 |
| 22 | F | 203 | BCR | C15-C14-C13 | -4.57 | 120.79 | 127.31 |
| 20 | 3 | 315 | CLA | CHC-C1C-NC | 4.57 | 130.98 | 124.23 |
| 21 | 2 | 313 | LMU | C1-O1'-C1' | -4.57 | 106.27 | 113.84 |
| 20 | 3 | 309 | CLA | C2D-C3D-C4D | -4.57 | 102.22 | 107.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 214 | CLA | CHD-C4C-NC | 4.57 | 131.25 | 124.21 |
| 20 | 3 | 316 | CLA | CHD-C4C-NC | 4.57 | 131.25 | 124.21 |
| 20 | K | 101 | CLA | CHC-C4B-NB | 4.56 | 129.09 | 124.26 |
| 20 | B | 808 | CLA | C4B-CHC-C1C | -4.56 | 115.52 | 126.34 |
| 20 | 1 | 203 | CLA | C4B-CHC-C1C | -4.56 | 115.52 | 126.34 |
| 20 | 4 | 303 | CLA | C4B-CHC-C1C | -4.56 | 115.52 | 126.34 |
| 20 | A | 828 | CLA | C2B-C1B-NB | 4.56 | 113.29 | 110.23 |
| 20 | 2 | 304 | CLA | C4A-NA-C1A | 4.56 | 108.76 | 106.71 |
| 20 | B | 825 | CLA | CHC-C4B-NB | 4.56 | 129.08 | 124.26 |
| 20 | 2 | 311 | CLA | CHD-C4C-C3C | -4.56 | 118.14 | 124.84 |
| 21 | 4 | 319 | LMU | C1B-O1B-C4' | -4.56 | 106.68 | 117.96 |
| 20 | B | 807 | CLA | CMD-C2D-C3D | -4.56 | 117.13 | 127.61 |
| 20 | 3 | 304 | CLA | C3A-C4A-CHB | -4.56 | 118.33 | 123.91 |
| 20 | B | 809 | CLA | C4A-NA-C1A | 4.56 | 108.75 | 106.71 |
| 20 | 1 | 209 | CLA | C2A-C1A-CHA | -4.56 | 114.86 | 122.63 |
| 20 | A | 830 | CLA | CHD-C4C-NC | 4.55 | 131.38 | 124.20 |
| 20 | 1 | 210 | CLA | CHD-C4C-NC | 4.55 | 131.38 | 124.20 |
| 20 | B | 840 | CLA | CHD-C4C-NC | 4.55 | 131.37 | 124.20 |
| 20 | 2 | 307 | CLA | C4D-C3D-CAD | 4.55 | 113.46 | 108.10 |
| 20 | B | 821 | CLA | CHC-C4B-NB | 4.55 | 129.07 | 124.26 |
| 20 | A | 805 | CLA | C4A-NA-C1A | 4.55 | 108.75 | 106.71 |
| 20 | A | 821 | CLA | C3B-C2B-C1B | -4.55 | 101.67 | 107.16 |
| 20 | A | 808 | CLA | CHC-C4B-NB | 4.55 | 129.07 | 124.26 |
| 20 | 2 | 314 | CLA | CMD-C2D-C3D | -4.55 | 117.16 | 127.61 |
| 20 | A | 822 | CLA | CHC-C4B-NB | 4.55 | 129.07 | 124.26 |
| 20 | B | 809 | CLA | CHD-C4C-NC | 4.54 | 131.36 | 124.20 |
| 20 | B | 834 | CLA | O2D-CGD-CBD | 4.54 | 119.34 | 111.27 |
| 20 | B | 833 | CLA | C3B-C2B-C1B | -4.54 | 101.68 | 107.16 |
| 20 | 3 | 315 | CLA | C2D-C3D-C4D | -4.54 | 102.25 | 107.28 |
| 20 | B | 833 | CLA | CHD-C4C-NC | 4.54 | 131.35 | 124.20 |
| 20 | A | 824 | CLA | CHD-C4C-NC | 4.54 | 131.35 | 124.20 |
| 20 | B | 803 | CLA | CHD-C4C-NC | 4.54 | 131.35 | 124.20 |
| 20 | 3 | 307 | CLA | CAC-C3C-C4C | 4.54 | 130.69 | 124.81 |
| 20 | A | 804 | CLA | O2A-CGA-CBA | 4.53 | 126.14 | 111.91 |
| 20 | 3 | 317 | CLA | CHC-C4B-NB | 4.53 | 129.06 | 124.26 |
| 20 | 1 | 207 | CLA | CHD-C4C-C3C | -4.53 | 118.18 | 124.84 |
| 20 | 4 | 318 | CLA | CHC-C1C-NC | 4.53 | 131.08 | 124.20 |
| 20 | 4 | 308 | CLA | C1B-NB-C4B | -4.53 | 103.12 | 106.33 |
| 20 | 1 | 214 | CLA | CHC-C1C-NC | 4.53 | 130.92 | 124.23 |
| 20 | 4 | 304 | CLA | C4A-NA-C1A | 4.53 | 108.74 | 106.71 |
| 22 | I | 103 | BCR | C34-C9-C10 | -4.53 | 116.58 | 122.92 |
| 20 | 3 | 308 | CLA | C4C-CHD-C1D | -4.52 | 114.92 | 126.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 840 | CLA | C4B-CHC-C1C | -4.52 | 115.61 | 126.34 |
| 20 | 4 | 306 | CLA | C4A-NA-C1A | 4.52 | 108.74 | 106.71 |
| 20 | 3 | 307 | CLA | CHC-C4B-NB | 4.52 | 129.04 | 124.26 |
| 20 | B | 813 | CLA | CHC-C4B-NB | 4.52 | 129.04 | 124.26 |
| 21 | B | 805 | LMU | O5B-C5B-C4B | -4.52 | 101.48 | 109.69 |
| 20 | A | 819 | CLA | CMD-C2D-C3D | -4.52 | 117.22 | 127.61 |
| 20 | B | 831 | CLA | CHC-C4B-NB | 4.52 | 129.04 | 124.26 |
| 20 | A | 812 | CLA | O2D-CGD-CBD | 4.52 | 119.30 | 111.27 |
| 20 | F | 201 | CLA | C4D-C3D-CAD | 4.52 | 113.42 | 108.10 |
| 20 | A | 825 | CLA | CHD-C4C-C3C | -4.52 | 118.20 | 124.84 |
| 20 | A | 810 | CLA | CHC-C4B-NB | 4.51 | 129.04 | 124.26 |
| 20 | 1 | 212 | CLA | CHC-C4B-NB | 4.51 | 128.84 | 124.27 |
| 20 | 1 | 204 | CLA | O2D-CGD-CBD | 4.51 | 119.28 | 111.27 |
| 20 | 2 | 316 | CLA | CAA-CBA-CGA | -4.51 | 100.07 | 113.25 |
| 20 | 3 | 302 | CLA | CHD-C4C-NC | 4.51 | 131.17 | 124.21 |
| 20 | B | 825 | CLA | CHD-C4C-NC | 4.51 | 131.31 | 124.20 |
| 20 | 4 | 309 | CLA | CHD-C4C-NC | 4.51 | 131.17 | 124.21 |
| 20 | B | 809 | CLA | CHB-C1B-NB | -4.51 | 119.48 | 124.26 |
| 20 | A | 841 | CLA | C2A-C1A-CHA | -4.51 | 114.94 | 122.63 |
| 20 | H | 102 | CLA | CHD-C4C-NC | 4.50 | 131.30 | 124.20 |
| 20 | 1 | 201 | CLA | CHD-C4C-NC | 4.50 | 131.30 | 124.20 |
| 20 | A | 811 | CLA | CHD-C4C-NC | 4.50 | 131.29 | 124.20 |
| 20 | A | 811 | CLA | CMD-C2D-C3D | -4.50 | 117.26 | 127.61 |
| 20 | L | 203 | CLA | CHD-C4C-C3C | -4.49 | 118.23 | 124.84 |
| 20 | B | 824 | CLA | C4B-CHC-C1C | -4.49 | 115.68 | 126.34 |
| 20 | 4 | 312 | CLA | C3A-C4A-CHB | -4.49 | 118.41 | 123.91 |
| 20 | A | 839 | CLA | CHD-C4C-C3C | -4.49 | 118.25 | 124.84 |
| 20 | 4 | 309 | CLA | CHC-C1C-NC | 4.48 | 130.85 | 124.23 |
| 20 | 3 | 310 | CLA | C4B-CHC-C1C | -4.48 | 115.70 | 126.34 |
| 20 | H | 102 | CLA | O2D-CGD-CBD | 4.48 | 119.23 | 111.27 |
| 20 | G | 105 | CLA | C4D-C3D-CAD | 4.48 | 113.38 | 108.10 |
| 20 | A | 803 | CLA | CHD-C4C-C3C | -4.48 | 118.25 | 124.84 |
| 20 | 2 | 315 | CLA | CHC-C4B-NB | 4.48 | 128.81 | 124.27 |
| 20 | B | 830 | CLA | CHD-C4C-C3C | -4.48 | 118.26 | 124.84 |
| 20 | 4 | 311 | CLA | CHC-C1C-NC | 4.48 | 130.84 | 124.23 |
| 20 | B | 837 | CLA | CHC-C4B-NB | 4.47 | 128.99 | 124.26 |
| 20 | A | 836 | CLA | CHD-C4C-NC | 4.47 | 131.25 | 124.20 |
| 20 | B | 815 | CLA | O2D-CGD-CBD | 4.47 | 119.22 | 111.27 |
| 20 | 3 | 312 | CLA | CHD-C4C-NC | 4.47 | 131.11 | 124.21 |
| 20 | F | 206 | CLA | O2D-CGD-CBD | 4.47 | 119.21 | 111.27 |
| 20 | 2 | 301 | CLA | C2A-C1A-CHA | -4.47 | 115.01 | 122.63 |
| 20 | 1 | 211 | CLA | C4B-CHC-C1C | -4.47 | 115.74 | 126.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | F | 201 | CLA | CHC-C1C-NC | 4.47 | 130.98 | 124.20 |
| 20 | A | 801 | CLA | C4A-NA-C1A | 4.47 | 108.71 | 106.71 |
| 20 | A | 834 | CLA | C4B-CHC-C1C | -4.46 | 115.75 | 126.34 |
| 22 | I | 101 | BCR | C4-C5-C6 | -4.46 | 116.25 | 122.73 |
| 20 | A | 821 | CLA | C4B-CHC-C1C | -4.46 | 115.75 | 126.34 |
| 20 | 2 | 315 | CLA | CHC-C1C-NC | 4.46 | 130.82 | 124.23 |
| 20 | 2 | 308 | CLA | CHC-C4B-NB | 4.46 | 128.79 | 124.27 |
| 20 | A | 849 | CLA | C3B-C4B-NB | -4.46 | 106.38 | 110.52 |
| 20 | 3 | 310 | CLA | C3B-C2B-C1B | -4.46 | 101.78 | 107.16 |
| 20 | A | 830 | CLA | O2D-CGD-CBD | 4.46 | 119.19 | 111.27 |
| 20 | 1 | 206 | CLA | CHD-C4C-NC | 4.46 | 131.23 | 124.20 |
| 20 | 3 | 307 | CLA | CHD-C4C-NC | 4.46 | 131.22 | 124.20 |
| 20 | A | 808 | CLA | CHD-C4C-NC | 4.46 | 131.22 | 124.20 |
| 20 | B | 826 | CLA | O2D-CGD-CBD | 4.46 | 119.19 | 111.27 |
| 20 | A | 804 | CLA | C4D-C3D-CAD | 4.45 | 113.35 | 108.10 |
| 20 | B | 816 | CLA | CHD-C4C-NC | 4.45 | 131.22 | 124.20 |
| 20 | A | 812 | CLA | CHC-C4B-NB | 4.45 | 128.97 | 124.26 |
| 20 | B | 835 | CLA | CHC-C4B-NB | 4.45 | 128.97 | 124.26 |
| 20 | B | 832 | CLA | CHD-C4C-C3C | -4.45 | 118.30 | 124.84 |
| 20 | B | 833 | CLA | CHD-C4C-C3C | -4.45 | 118.30 | 124.84 |
| 20 | 4 | 317 | CLA | CHC-C4B-NB | 4.45 | 128.97 | 124.26 |
| 20 | 2 | 310 | CLA | CHD-C4C-C3C | -4.45 | 118.30 | 124.84 |
| 20 | 1 | 209 | CLA | C3B-C2B-C1B | -4.45 | 101.93 | 106.75 |
| 20 | 1 | 203 | CLA | CHC-C1C-NC | 4.45 | 130.95 | 124.20 |
| 20 | 3 | 302 | CLA | C2A-C1A-CHA | -4.45 | 115.05 | 122.63 |
| 20 | H | 108 | CLA | C4D-C3D-CAD | 4.44 | 113.33 | 108.10 |
| 20 | 2 | 302 | CLA | CGD-CBD-CAD | 4.44 | 125.13 | 110.73 |
| 20 | A | 828 | CLA | C4A-NA-C1A | 4.44 | 108.70 | 106.71 |
| 22 | L | 209 | BCR | C11-C10-C9 | -4.44 | 120.97 | 127.31 |
| 20 | 1 | 213 | CLA | CMA-C3A-C4A | 4.44 | 123.71 | 111.77 |
| 21 | R | 101 | LMU | C1'-C2'-C3' | -4.44 | 100.75 | 110.00 |
| 20 | 3 | 316 | CLA | CHC-C1C-NC | 4.44 | 130.79 | 124.23 |
| 20 | A | 820 | CLA | CHD-C4C-NC | 4.44 | 131.20 | 124.20 |
| 20 | A | 802 | CLA | C4A-NA-C1A | 4.44 | 108.70 | 106.71 |
| 20 | B | 841 | CLA | CHB-C1B-NB | -4.43 | 119.56 | 124.26 |
| 20 | 1 | 202 | CLA | CHC-C1C-NC | 4.43 | 130.93 | 124.20 |
| 20 | A | 819 | CLA | CHD-C4C-NC | 4.43 | 131.19 | 124.20 |
| 20 | 1 | 202 | CLA | CHC-C4B-NB | 4.43 | 128.95 | 124.26 |
| 20 | 1 | 209 | CLA | CHC-C4B-NB | 4.43 | 128.76 | 124.27 |
| 20 | 4 | 315 | CLA | C4A-NA-C1A | 4.43 | 108.70 | 106.71 |
| 20 | 4 | 305 | CLA | C2B-C1B-NB | 4.43 | 113.20 | 110.23 |
| 20 | B | 842 | CLA | CHD-C4C-NC | 4.43 | 131.18 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | K | 102 | CLA | CHC-C1C-NC | 4.43 | 130.92 | 124.20 |
| 22 | A | 844 | BCR | C11-C10-C9 | -4.43 | 120.99 | 127.31 |
| 20 | 1 | 213 | CLA | C4B-CHC-C1C | -4.43 | 115.84 | 126.34 |
| 20 | B | 817 | CLA | CHD-C4C-NC | 4.43 | 131.18 | 124.20 |
| 20 | A | 834 | CLA | CMD-C2D-C3D | -4.43 | 117.43 | 127.61 |
| 20 | B | 838 | CLA | C4B-CHC-C1C | -4.43 | 115.84 | 126.34 |
| 22 | B | 847 | BCR | C16-C17-C18 | -4.43 | 120.99 | 127.31 |
| 20 | 4 | 313 | CLA | CHC-C4B-NB | 4.42 | 128.94 | 124.26 |
| 20 | 4 | 303 | CLA | CHD-C4C-C3C | -4.42 | 118.34 | 124.84 |
| 20 | B | 806 | CLA | CMD-C2D-C3D | -4.42 | 117.44 | 127.61 |
| 20 | A | 831 | CLA | C3B-C4B-NB | -4.42 | 106.42 | 110.52 |
| 20 | B | 829 | CLA | CMB-C2B-C1B | 4.42 | 132.10 | 125.37 |
| 20 | 4 | 310 | CLA | CMD-C2D-C3D | -4.42 | 117.46 | 127.61 |
| 20 | A | 815 | CLA | O2D-CGD-CBD | 4.41 | 119.11 | 111.27 |
| 20 | B | 836 | CLA | CHD-C4C-C3C | -4.41 | 118.36 | 124.84 |
| 20 | J | 103 | CLA | CHD-C4C-NC | 4.41 | 131.15 | 124.20 |
| 20 | 2 | 315 | CLA | C1C-CHC-C4B | -4.41 | 115.14 | 126.13 |
| 20 | B | 821 | CLA | CHD-C4C-C3C | -4.41 | 118.36 | 124.84 |
| 20 | 3 | 302 | CLA | CHC-C1C-NC | 4.41 | 130.74 | 124.23 |
| 20 | B | 840 | CLA | CHD-C4C-C3C | -4.41 | 118.36 | 124.84 |
| 20 | 1 | 205 | CLA | CHC-C4B-NB | 4.41 | 128.92 | 124.26 |
| 20 | 2 | 303 | CLA | CHC-C1C-NC | 4.41 | 130.89 | 124.20 |
| 20 | B | 812 | CLA | C1B-C2B-C3B | -4.41 | 102.84 | 107.03 |
| 20 | B | 835 | CLA | CHD-C4C-C3C | -4.41 | 118.36 | 124.84 |
| 20 | K | 102 | CLA | CHC-C4B-NB | 4.40 | 128.91 | 124.26 |
| 20 | A | 828 | CLA | CHD-C4C-C3C | -4.40 | 118.37 | 124.84 |
| 20 | B | 823 | CLA | CHC-C4B-NB | 4.40 | 128.91 | 124.26 |
| 20 | 3 | 302 | CLA | C3A-C4A-CHB | -4.40 | 118.52 | 123.91 |
| 20 | K | 104 | CLA | CHC-C1C-NC | 4.40 | 130.88 | 124.20 |
| 20 | K | 103 | CLA | CMD-C2D-C3D | -4.40 | 117.50 | 127.61 |
| 20 | K | 102 | CLA | C4B-CHC-C1C | -4.40 | 115.91 | 126.34 |
| 20 | 1 | 212 | CLA | CHD-C4C-NC | 4.40 | 130.99 | 124.21 |
| 20 | A | 827 | CLA | CHC-C4B-NB | 4.39 | 128.91 | 124.26 |
| 20 | R | 107 | CLA | CHD-C4C-NC | 4.39 | 131.12 | 124.20 |
| 20 | 3 | 306 | CLA | CHC-C1C-NC | 4.39 | 130.71 | 124.23 |
| 20 | B | 827 | CLA | CHC-C4B-NB | 4.39 | 128.90 | 124.26 |
| 20 | A | 818 | CLA | C4B-CHC-C1C | -4.39 | 115.93 | 126.34 |
| 22 | F | 204 | BCR | C8-C7-C6 | -4.39 | 114.88 | 127.20 |
| 20 | L | 202 | CLA | CHD-C4C-C3C | -4.39 | 118.39 | 124.84 |
| 20 | A | 841 | CLA | C2D-C3D-C4D | -4.39 | 102.42 | 107.28 |
| 20 | 1 | 212 | CLA | CHC-C1C-NC | 4.39 | 130.71 | 124.23 |
| 20 | A | 830 | CLA | C4B-CHC-C1C | -4.38 | 115.94 | 126.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 808 | CLA | C3B-C2B-C1B | -4.38 | 101.87 | 107.16 |
| 20 | 2 | 302 | CLA | CHC-C1C-NC | 4.38 | 130.85 | 124.20 |
| 20 | 4 | 309 | CLA | C3A-C4A-CHB | -4.38 | 118.55 | 123.91 |
| 20 | A | 851 | CLA | CHC-C4B-NB | 4.38 | 128.89 | 124.26 |
| 20 | A | 841 | CLA | C3B-C2B-C1B | -4.38 | 102.01 | 106.75 |
| 20 | 3 | 311 | CLA | CHD-C4C-C3C | -4.38 | 118.41 | 124.84 |
| 25 | B | 848 | LMG | O7-C10-C11 | 4.38 | 120.93 | 111.50 |
| 20 | 4 | 315 | CLA | CHC-C4B-NB | 4.38 | 128.89 | 124.26 |
| 20 | 1 | 207 | CLA | CHC-C4B-NB | 4.37 | 128.89 | 124.26 |
| 20 | 1 | 201 | CLA | CMD-C2D-C3D | -4.37 | 117.55 | 127.61 |
| 20 | 2 | 310 | CLA | CHC-C4B-NB | 4.37 | 128.89 | 124.26 |
| 20 | A | 829 | CLA | CHC-C4B-NB | 4.37 | 128.88 | 124.26 |
| 20 | 2 | 306 | CLA | CHC-C1C-NC | 4.37 | 130.68 | 124.23 |
| 20 | 2 | 308 | CLA | C2A-C1A-CHA | -4.37 | 115.18 | 122.63 |
| 20 | H | 102 | CLA | CMD-C2D-C3D | -4.37 | 117.57 | 127.61 |
| 20 | 3 | 304 | CLA | C4C-CHD-C1D | -4.37 | 115.31 | 126.11 |
| 20 | B | 810 | CLA | O1D-CGD-CBD | -4.37 | 115.55 | 124.48 |
| 20 | 1 | 203 | CLA | CHD-C4C-C3C | -4.37 | 118.42 | 124.84 |
| 20 | J | 103 | CLA | C4B-CHC-C1C | -4.36 | 115.99 | 126.34 |
| 20 | K | 104 | CLA | O2D-CGD-O1D | -4.36 | 115.31 | 123.84 |
| 20 | 3 | 308 | CLA | CHD-C4C-NC | 4.36 | 130.94 | 124.21 |
| 20 | A | 821 | CLA | CHC-C1C-NC | 4.36 | 130.82 | 124.20 |
| 20 | B | 819 | CLA | CHC-C1C-NC | 4.36 | 130.82 | 124.20 |
| 20 | 1 | 211 | CLA | CMD-C2D-C3D | -4.36 | 117.58 | 127.61 |
| 21 | G | 102 | LMU | C1B-C2B-C3B | -4.36 | 100.92 | 110.00 |
| 20 | B | 815 | CLA | C4B-CHC-C1C | -4.36 | 116.00 | 126.34 |
| 22 | J | 102 | BCR | C11-C10-C9 | -4.36 | 121.09 | 127.31 |
| 20 | A | 822 | CLA | CHD-C4C-NC | 4.36 | 131.07 | 124.20 |
| 20 | 3 | 309 | CLA | C1C-CHC-C4B | -4.36 | 115.27 | 126.13 |
| 20 | F | 206 | CLA | CHD-C4C-C3C | -4.36 | 118.44 | 124.84 |
| 20 | 3 | 309 | CLA | C2A-C1A-CHA | -4.36 | 115.20 | 122.63 |
| 20 | 1 | 208 | CLA | CHC-C4B-NB | 4.36 | 128.69 | 124.27 |
| 20 | R | 107 | CLA | CHC-C4B-NB | 4.36 | 128.87 | 124.26 |
| 20 | B | 817 | CLA | C4A-NA-C1A | 4.36 | 108.66 | 106.71 |
| 20 | 3 | 313 | CLA | CHD-C4C-NC | 4.35 | 131.06 | 124.20 |
| 20 | B | 815 | CLA | CMD-C2D-C3D | -4.35 | 117.60 | 127.61 |
| 20 | 3 | 305 | CLA | C4A-NA-C1A | 4.35 | 108.66 | 106.71 |
| 20 | 1 | 201 | CLA | CHB-C4A-NA | 4.35 | 130.53 | 124.51 |
| 20 | A | 819 | CLA | CHC-C1C-NC | 4.35 | 130.80 | 124.20 |
| 20 | A | 810 | CLA | C4B-CHC-C1C | -4.34 | 116.03 | 126.34 |
| 20 | A | 806 | CLA | C4B-CHC-C1C | -4.34 | 116.04 | 126.34 |
| 20 | 2 | 304 | CLA | C2A-C1A-CHA | -4.34 | 115.23 | 122.63 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 207 | CLA | CMD-C2D-C3D | -4.34 | 117.63 | 127.61 |
| 21 | K | 105 | LMU | O1'-C1'-C2' | 4.34 | 115.08 | 108.30 |
| 20 | 3 | 301 | CLA | CHD-C4C-NC | 4.34 | 131.03 | 124.20 |
| 20 | A | 840 | CLA | CHD-C4C-NC | 4.33 | 131.03 | 124.20 |
| 20 | B | 840 | CLA | CHC-C4B-NB | 4.33 | 128.84 | 124.26 |
| 20 | A | 836 | CLA | OBD-CAD-C3D | -4.33 | 118.10 | 128.52 |
| 20 | B | 808 | CLA | CAA-C2A-C3A | -4.33 | 100.93 | 112.78 |
| 20 | A | 817 | CLA | CHD-C4C-NC | 4.33 | 131.02 | 124.20 |
| 20 | 2 | 314 | CLA | CHB-C1B-NB | -4.33 | 119.68 | 124.26 |
| 20 | A | 820 | CLA | CMD-C2D-C3D | -4.32 | 117.67 | 127.61 |
| 20 | A | 835 | CLA | C3B-C2B-C1B | -4.32 | 101.94 | 107.16 |
| 20 | 3 | 316 | CLA | CHC-C4B-NB | 4.32 | 128.65 | 124.27 |
| 20 | 4 | 311 | CLA | C1C-CHC-C4B | -4.32 | 115.35 | 126.13 |
| 20 | B | 850 | CLA | CHC-C1C-NC | 4.32 | 130.76 | 124.20 |
| 20 | R | 108 | CLA | CHD-C4C-NC | 4.32 | 131.01 | 124.20 |
| 20 | B | 835 | CLA | C4B-CHC-C1C | -4.32 | 116.09 | 126.34 |
| 20 | 4 | 317 | CLA | CHD-C4C-C3C | -4.32 | 118.49 | 124.84 |
| 20 | B | 811 | CLA | C1C-CHC-C4B | -4.32 | 115.36 | 126.13 |
| 20 | 3 | 304 | CLA | C1B-NB-C4B | -4.32 | 103.27 | 106.33 |
| 20 | I | 102 | CLA | CHD-C4C-C3C | -4.32 | 118.49 | 124.84 |
| 21 | L | 210 | LMU | C3B-C4B-C5B | 4.32 | 117.94 | 110.24 |
| 20 | A | 821 | CLA | CHD-C4C-NC | 4.32 | 131.00 | 124.20 |
| 20 | A | 834 | CLA | CHD-C4C-NC | 4.32 | 131.00 | 124.20 |
| 20 | B | 839 | CLA | C4B-CHC-C1C | -4.31 | 116.11 | 126.34 |
| 20 | 3 | 302 | CLA | CHC-C4B-NB | 4.31 | 128.64 | 124.27 |
| 22 | B | 845 | BCR | C34-C9-C10 | -4.31 | 116.88 | 122.92 |
| 20 | A | 836 | CLA | CHC-C1C-NC | 4.31 | 130.74 | 124.20 |
| 20 | J | 103 | CLA | O2D-CGD-CBD | 4.31 | 118.92 | 111.27 |
| 20 | B | 842 | CLA | CHC-C4B-NB | 4.31 | 128.82 | 124.26 |
| 20 | 4 | 301 | CLA | CHD-C4C-C3C | -4.31 | 118.51 | 124.84 |
| 22 | J | 102 | BCR | C15-C14-C13 | -4.31 | 121.16 | 127.31 |
| 20 | 4 | 307 | CLA | C2D-C3D-C4D | -4.31 | 102.51 | 107.28 |
| 20 | L | 201 | CLA | C4D-C3D-CAD | 4.30 | 113.17 | 108.10 |
| 20 | 1 | 214 | CLA | CHC-C4B-NB | 4.30 | 128.63 | 124.27 |
| 20 | B | 818 | CLA | CHD-C4C-NC | 4.30 | 130.98 | 124.20 |
| 20 | A | 834 | CLA | C3B-C2B-C1B | -4.30 | 101.97 | 107.16 |
| 20 | B | 810 | CLA | CHC-C1C-NC | 4.30 | 130.73 | 124.20 |
| 22 | A | 845 | BCR | C15-C14-C13 | -4.30 | 121.17 | 127.31 |
| 20 | B | 836 | CLA | C4B-CHC-C1C | -4.30 | 116.14 | 126.34 |
| 20 | A | 835 | CLA | CMD-C2D-C3D | -4.30 | 117.73 | 127.61 |
| 20 | B | 826 | CLA | CHC-C4B-NB | 4.30 | 128.81 | 124.26 |
| 20 | A | 829 | CLA | CHC-C1C-NC | 4.30 | 130.72 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 810 | CLA | C4B-CHC-C1C | -4.30 | 116.15 | 126.34 |
| 20 | B | 837 | CLA | CHD-C4C-NC | 4.30 | 130.97 | 124.20 |
| 20 | 4 | 311 | CLA | C2A-C1A-CHA | -4.30 | 115.31 | 122.63 |
| 20 | 1 | 214 | CLA | C1B-NB-C4B | -4.29 | 103.28 | 106.33 |
| 20 | 4 | 307 | CLA | C3A-C4A-CHB | -4.29 | 118.65 | 123.91 |
| 20 | 4 | 317 | CLA | CHB-C1B-NB | -4.29 | 119.71 | 124.26 |
| 20 | A | 811 | CLA | C4B-CHC-C1C | -4.29 | 116.16 | 126.34 |
| 20 | A | 815 | CLA | CHD-C4C-NC | 4.29 | 130.96 | 124.20 |
| 20 | A | 822 | CLA | C4B-CHC-C1C | -4.29 | 116.16 | 126.34 |
| 20 | 4 | 313 | CLA | CHD-C4C-NC | 4.29 | 130.96 | 124.20 |
| 20 | 1 | 213 | CLA | CHD-C4C-C3C | -4.29 | 118.54 | 124.84 |
| 20 | A | 805 | CLA | C3B-C2B-C1B | -4.29 | 101.99 | 107.16 |
| 22 | B | 846 | BCR | C11-C10-C9 | -4.29 | 121.19 | 127.31 |
| 20 | B | 840 | CLA | C3B-C2B-C1B | -4.28 | 101.99 | 107.16 |
| 20 | A | 810 | CLA | CMD-C2D-C3D | -4.28 | 117.76 | 127.61 |
| 20 | 1 | 211 | CLA | O2A-CGA-O1A | -4.28 | 112.79 | 123.59 |
| 20 | A | 840 | CLA | C4A-NA-C1A | 4.28 | 108.63 | 106.71 |
| 20 | 4 | 306 | CLA | O2A-CGA-CBA | 4.28 | 125.34 | 111.91 |
| 20 | 3 | 308 | CLA | C3B-C2B-C1B | -4.28 | 102.11 | 106.75 |
| 20 | 3 | 312 | CLA | C2A-C1A-CHA | -4.28 | 115.34 | 122.63 |
| 20 | 4 | 309 | CLA | C1C-CHC-C4B | -4.28 | 115.47 | 126.13 |
| 20 | F | 205 | CLA | CMD-C2D-C3D | -4.28 | 117.77 | 127.61 |
| 20 | B | 807 | CLA | CHD-C4C-C3C | -4.28 | 118.55 | 124.84 |
| 20 | B | 850 | CLA | CHD-C4C-NC | 4.28 | 130.94 | 124.20 |
| 20 | 2 | 308 | CLA | C3B-C2B-C1B | -4.28 | 102.12 | 106.75 |
| 22 | F | 203 | BCR | C7-C8-C9 | -4.28 | 119.77 | 126.23 |
| 20 | A | 802 | CLA | CHC-C1C-NC | 4.27 | 130.54 | 124.23 |
| 20 | A | 807 | CLA | CHD-C4C-NC | 4.27 | 130.94 | 124.20 |
| 20 | 4 | 312 | CLA | C3D-C4D-CHA | -4.27 | 115.98 | 124.98 |
| 20 | R | 108 | CLA | C4B-CHC-C1C | -4.27 | 116.21 | 126.34 |
| 20 | A | 826 | CLA | O2D-CGD-CBD | 4.27 | 118.85 | 111.27 |
| 20 | 3 | 307 | CLA | C2A-C1A-CHA | -4.27 | 116.40 | 123.86 |
| 20 | A | 801 | CLA | CHC-C4B-NB | 4.27 | 128.77 | 124.26 |
| 20 | L | 203 | CLA | CHD-C4C-NC | 4.26 | 130.92 | 124.20 |
| 20 | A | 804 | CLA | CHC-C1C-NC | 4.26 | 130.67 | 124.20 |
| 20 | 3 | 312 | CLA | CHC-C4B-NB | 4.26 | 128.59 | 124.27 |
| 20 | 4 | 312 | CLA | C1C-CHC-C4B | -4.26 | 115.50 | 126.13 |
| 20 | B | 816 | CLA | CHD-C4C-C3C | -4.26 | 118.58 | 124.84 |
| 20 | B | 836 | CLA | O2D-CGD-O1D | -4.26 | 115.51 | 123.84 |
| 20 | 2 | 315 | CLA | C2A-C1A-CHA | -4.26 | 115.37 | 122.63 |
| 20 | B | 823 | CLA | CHD-C4C-NC | 4.26 | 130.91 | 124.20 |
| 20 | B | 814 | CLA | O2D-CGD-CBD | 4.26 | 118.83 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | F | 207 | CLA | C1-C2-C3 | -4.25 | 118.68 | 126.04 |
| 20 | L | 204 | CLA | CHC-C4B-NB | 4.25 | 128.76 | 124.26 |
| 20 | 4 | 312 | CLA | C2D-C3D-C4D | -4.25 | 102.57 | 107.28 |
| 20 | A | 833 | CLA | C4B-CHC-C1C | -4.25 | 116.25 | 126.34 |
| 20 | B | 809 | CLA | O2D-CGD-O1D | -4.25 | 115.52 | 123.84 |
| 20 | 3 | 317 | CLA | CHD-C4C-C3C | -4.25 | 118.34 | 124.98 |
| 20 | 1 | 214 | CLA | C1C-CHC-C4B | -4.25 | 115.54 | 126.13 |
| 20 | 3 | 314 | CLA | CHD-C4C-C3C | -4.25 | 118.59 | 124.84 |
| 20 | F | 205 | CLA | CHC-C1C-NC | 4.25 | 130.65 | 124.20 |
| 21 | 4 | 319 | LMU | C3B-C4B-C5B | 4.25 | 117.82 | 110.24 |
| 20 | 1 | 203 | CLA | CHC-C4B-NB | 4.25 | 128.75 | 124.26 |
| 20 | A | 827 | CLA | CHD-C4C-NC | 4.25 | 130.90 | 124.20 |
| 20 | B | 812 | CLA | CHC-C4B-NB | 4.25 | 128.75 | 124.26 |
| 20 | 3 | 305 | CLA | C1C-CHC-C4B | -4.25 | 115.55 | 126.13 |
| 22 | B | 844 | BCR | C38-C26-C27 | 4.25 | 121.77 | 113.62 |
| 20 | 3 | 303 | CLA | C1B-C2B-C3B | -4.24 | 103.00 | 107.03 |
| 20 | A | 827 | CLA | C4B-CHC-C1C | -4.24 | 116.28 | 126.34 |
| 20 | 1 | 210 | CLA | CMD-C2D-C3D | -4.24 | 117.86 | 127.61 |
| 20 | 4 | 301 | CLA | CED-O2D-CGD | 4.24 | 125.53 | 115.94 |
| 20 | 4 | 308 | CLA | C2A-C1A-CHA | -4.24 | 115.40 | 122.63 |
| 20 | K | 101 | CLA | CHD-C4C-C3C | -4.24 | 118.61 | 124.84 |
| 20 | 1 | 204 | CLA | C4A-NA-C1A | 4.24 | 108.61 | 106.71 |
| 20 | B | 834 | CLA | CMD-C2D-C3D | -4.24 | 117.86 | 127.61 |
| 20 | 4 | 314 | CLA | C2A-C1A-CHA | -4.24 | 115.41 | 122.63 |
| 20 | 2 | 305 | CLA | CMD-C2D-C3D | -4.24 | 117.87 | 127.61 |
| 20 | 3 | 307 | CLA | O2D-CGD-CBD | 4.24 | 118.80 | 111.27 |
| 20 | H | 101 | CLA | CHC-C1C-NC | 4.23 | 130.63 | 124.20 |
| 20 | 3 | 301 | CLA | C4B-CHC-C1C | -4.23 | 116.29 | 126.34 |
| 20 | 3 | 317 | CLA | CMD-C2D-C3D | -4.23 | 117.87 | 127.61 |
| 20 | R | 108 | CLA | O2D-CGD-CBD | 4.23 | 118.79 | 111.27 |
| 20 | 2 | 309 | CLA | CHD-C4C-NC | 4.23 | 130.74 | 124.21 |
| 20 | B | 840 | CLA | CMD-C2D-C3D | -4.23 | 117.88 | 127.61 |
| 20 | A | 835 | CLA | C4B-CHC-C1C | -4.23 | 116.30 | 126.34 |
| 20 | B | 834 | CLA | CHC-C4B-NB | 4.23 | 128.74 | 124.26 |
| 20 | R | 108 | CLA | O2A-CGA-CBA | 4.23 | 125.17 | 111.91 |
| 20 | 2 | 304 | CLA | C1B-NB-C4B | -4.23 | 103.33 | 106.33 |
| 20 | A | 803 | CLA | CHC-C4B-NB | 4.23 | 128.73 | 124.26 |
| 20 | H | 102 | CLA | CHD-C4C-C3C | -4.23 | 118.63 | 124.84 |
| 20 | B | 828 | CLA | CMD-C2D-C3D | -4.23 | 117.89 | 127.61 |
| 20 | 1 | 208 | CLA | CHD-C4C-NC | 4.23 | 130.73 | 124.21 |
| 21 | 2 | 319 | LMU | C1B-O1B-C4' | -4.22 | 107.51 | 117.96 |
| 20 | B | 841 | CLA | CHD-C4C-C3C | -4.22 | 118.63 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 311 | CLA | C4B-CHC-C1C | -4.22 | 116.32 | 126.34 |
| 20 | B | 838 | CLA | CHC-C1C-NC | 4.22 | 130.61 | 124.20 |
| 20 | A | 824 | CLA | CHC-C4B-NB | 4.22 | 128.73 | 124.26 |
| 20 | B | 813 | CLA | CHC-C1C-NC | 4.22 | 130.61 | 124.20 |
| 20 | A | 827 | CLA | CHC-C1C-NC | 4.22 | 130.61 | 124.20 |
| 20 | 4 | 314 | CLA | CHD-C4C-NC | 4.22 | 130.72 | 124.21 |
| 20 | A | 837 | CLA | CHD-C4C-C3C | -4.22 | 118.64 | 124.84 |
| 20 | B | 807 | CLA | C3B-C2B-C1B | -4.22 | 102.07 | 107.16 |
| 20 | 4 | 305 | CLA | O2A-CGA-CBA | 4.22 | 125.15 | 111.91 |
| 20 | A | 815 | CLA | CMD-C2D-C3D | -4.22 | 117.91 | 127.61 |
| 20 | H | 101 | CLA | CHD-C4C-NC | 4.22 | 130.85 | 124.20 |
| 20 | K | 102 | CLA | CMD-C2D-C3D | -4.22 | 117.92 | 127.61 |
| 20 | A | 801 | CLA | C4B-CHC-C1C | -4.22 | 116.34 | 126.34 |
| 20 | 2 | 309 | CLA | CHD-C1D-ND | 4.22 | 128.59 | 124.52 |
| 20 | 2 | 301 | CLA | C4C-CHD-C1D | -4.22 | 115.69 | 126.11 |
| 22 | 2 | 317 | BCR | C11-C12-C13 | -4.22 | 114.58 | 126.42 |
| 20 | 1 | 214 | CLA | C2D-C3D-C4D | -4.21 | 102.61 | 107.28 |
| 20 | A | 851 | CLA | C4B-CHC-C1C | -4.21 | 116.35 | 126.34 |
| 22 | 2 | 317 | BCR | C33-C5-C6 | -4.21 | 119.80 | 124.53 |
| 20 | A | 828 | CLA | CHC-C4B-NB | 4.21 | 128.71 | 124.26 |
| 20 | 4 | 307 | CLA | C1B-NB-C4B | -4.21 | 103.35 | 106.33 |
| 20 | R | 107 | CLA | C4B-CHC-C1C | -4.21 | 116.36 | 126.34 |
| 20 | A | 832 | CLA | CHC-C4B-NB | 4.21 | 128.71 | 124.26 |
| 20 | 1 | 203 | CLA | CGD-CBD-CAD | -4.20 | 97.12 | 110.73 |
| 20 | 3 | 316 | CLA | C4A-NA-C1A | 4.20 | 108.60 | 106.71 |
| 20 | 2 | 309 | CLA | C1C-CHC-C4B | -4.20 | 115.65 | 126.13 |
| 20 | B | 836 | CLA | C3B-C2B-C1B | -4.20 | 102.09 | 107.16 |
| 20 | B | 830 | CLA | CMD-C2D-C3D | -4.20 | 117.95 | 127.61 |
| 20 | A | 823 | CLA | C3B-C2B-C1B | -4.20 | 102.09 | 107.16 |
| 20 | A | 838 | CLA | CHC-C4B-NB | 4.20 | 128.70 | 124.26 |
| 20 | A | 830 | CLA | CHC-C1C-NC | 4.20 | 130.57 | 124.20 |
| 20 | A | 804 | CLA | CMD-C2D-C3D | -4.20 | 117.96 | 127.61 |
| 20 | 4 | 302 | CLA | C1B-C2B-C3B | -4.19 | 103.05 | 107.03 |
| 20 | B | 826 | CLA | CHD-C4C-C3C | -4.19 | 118.68 | 124.84 |
| 20 | B | 813 | CLA | C4B-CHC-C1C | -4.19 | 116.39 | 126.34 |
| 20 | B | 833 | CLA | C4B-CHC-C1C | -4.19 | 116.39 | 126.34 |
| 20 | B | 830 | CLA | CHC-C1C-NC | 4.19 | 130.56 | 124.20 |
| 20 | 2 | 304 | CLA | CHA-C4D-ND | 4.19 | 128.56 | 124.52 |
| 20 | B | 821 | CLA | C4B-CHC-C1C | -4.19 | 116.40 | 126.34 |
| 20 | 4 | 304 | CLA | CMD-C2D-C3D | -4.19 | 117.98 | 127.61 |
| 20 | 4 | 318 | CLA | CMD-C2D-C3D | -4.19 | 117.98 | 127.61 |
| 20 | 1 | 211 | CLA | CHC-C1C-NC | 4.19 | 130.56 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 832 | CLA | CHD-C4C-NC | 4.19 | 130.80 | 124.20 |
| 20 | 1 | 214 | CLA | C3B-C2B-C1B | -4.18 | 102.22 | 106.75 |
| 20 | B | 809 | CLA | CHC-C4B-NB | 4.18 | 128.69 | 124.26 |
| 21 | 3 | 319 | LMU | C1B-O1B-C4' | -4.18 | 107.61 | 117.96 |
| 20 | A | 814 | CLA | C1C-CHC-C4B | -4.18 | 115.71 | 126.13 |
| 20 | 4 | 317 | CLA | CAA-C2A-C3A | -4.18 | 101.33 | 112.78 |
| 20 | B | 811 | CLA | C2D-C3D-C4D | -4.18 | 102.65 | 107.28 |
| 20 | R | 107 | CLA | CHD-C4C-C3C | -4.18 | 118.70 | 124.84 |
| 20 | A | 802 | CLA | C3B-C2B-C1B | -4.18 | 102.22 | 106.75 |
| 20 | 4 | 309 | CLA | C4A-NA-C1A | 4.18 | 108.58 | 106.71 |
| 20 | A | 813 | CLA | CHD-C4C-C3C | -4.18 | 118.70 | 124.84 |
| 20 | B | 841 | CLA | CMB-C2B-C1B | 4.18 | 131.73 | 125.37 |
| 20 | 3 | 307 | CLA | CAC-C3C-C2C | -4.17 | 120.39 | 127.53 |
| 20 | B | 817 | CLA | CHC-C4B-NB | 4.17 | 128.67 | 124.26 |
| 20 | B | 802 | CLA | CHD-C4C-C3C | -4.17 | 118.71 | 124.84 |
| 22 | B | 847 | BCR | C11-C10-C9 | -4.17 | 121.36 | 127.31 |
| 20 | J | 101 | CLA | CHC-C4B-NB | 4.17 | 128.67 | 124.26 |
| 20 | B | 826 | CLA | CMD-C2D-C3D | -4.17 | 118.02 | 127.61 |
| 20 | 2 | 306 | CLA | CHD-C4C-NC | 4.17 | 130.64 | 124.21 |
| 20 | B | 819 | CLA | C4B-CHC-C1C | -4.17 | 116.45 | 126.34 |
| 20 | 2 | 307 | CLA | C2B-C1B-NB | 4.17 | 113.03 | 110.23 |
| 20 | L | 203 | CLA | C4B-CHC-C1C | -4.17 | 116.45 | 126.34 |
| 20 | B | 824 | CLA | C6-C5-C3 | -4.17 | 102.53 | 113.45 |
| 20 | A | 821 | CLA | CHB-C1B-NB | -4.16 | 119.85 | 124.26 |
| 21 | B | 804 | LMU | C1B-O5B-C5B | 4.16 | 121.86 | 113.69 |
| 20 | A | 833 | CLA | CHC-C4B-NB | 4.16 | 128.66 | 124.26 |
| 20 | 2 | 305 | CLA | CHD-C4C-NC | 4.16 | 130.76 | 124.20 |
| 20 | K | 101 | CLA | C4B-CHC-C1C | -4.16 | 116.47 | 126.34 |
| 20 | H | 102 | CLA | C4B-CHC-C1C | -4.16 | 116.48 | 126.34 |
| 22 | F | 204 | BCR | C8-C9-C10 | -4.16 | 112.56 | 118.94 |
| 20 | B | 806 | CLA | C4B-CHC-C1C | -4.15 | 116.49 | 126.34 |
| 20 | K | 103 | CLA | CHD-C4C-NC | 4.15 | 130.75 | 124.20 |
| 20 | 2 | 312 | CLA | CHC-C4B-NB | 4.15 | 128.65 | 124.26 |
| 20 | 3 | 309 | CLA | C4C-CHD-C1D | -4.15 | 115.84 | 126.11 |
| 20 | B | 821 | CLA | CMD-C2D-C3D | -4.15 | 118.07 | 127.61 |
| 20 | 1 | 210 | CLA | CHD-C4C-C3C | -4.15 | 118.50 | 124.98 |
| 20 | B | 807 | CLA | CHC-C1C-NC | 4.15 | 130.50 | 124.20 |
| 20 | R | 108 | CLA | CHD-C4C-C3C | -4.15 | 118.74 | 124.84 |
| 20 | F | 207 | CLA | CHD-C4C-C3C | -4.15 | 118.75 | 124.84 |
| 20 | A | 810 | CLA | CHC-C1C-NC | 4.15 | 130.49 | 124.20 |
| 20 | A | 804 | CLA | CHD-C4C-C3C | -4.15 | 118.75 | 124.84 |
| 20 | B | 840 | CLA | CHC-C1C-NC | 4.14 | 130.49 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 20 | A | 826 | CLA | C1-C2-C3 | -4.14 | 118.88 | 126.04 |
| 20 | A | 837 | CLA | CAA-CBA-CGA | -4.14 | 101.14 | 113.25 |
| 20 | A | 807 | CLA | C4B-CHC-C1C | -4.14 | 116.51 | 126.34 |
| 20 | A | 819 | CLA | CHD-C4C-C3C | -4.14 | 118.75 | 124.84 |
| 20 | 3 | 317 | CLA | C4B-CHC-C1C | -4.14 | 116.51 | 126.34 |
| 20 | 1 | 215 | CLA | C4A-NA-C1A | 4.14 | 108.57 | 106.71 |
| 20 | 3 | 302 | CLA | C1C-CHC-C4B | -4.14 | 115.81 | 126.13 |
| 20 | A | 829 | CLA | C4B-CHC-C1C | -4.14 | 116.52 | 126.34 |
| 20 | B | 837 | CLA | CMD-C2D-C3D | -4.14 | 118.09 | 127.61 |
| 20 | L | 207 | CLA | CHC-C4B-NB | 4.14 | 128.64 | 124.26 |
| 20 | B | 818 | CLA | CHC-C1C-NC | 4.14 | 130.48 | 124.20 |
| 20 | B | 818 | CLA | C4B-CHC-C1C | -4.14 | 116.52 | 126.34 |
| 22 | I | 103 | BCR | C15-C16-C17 | 4.14 | 131.95 | 123.47 |
| 20 | 3 | 315 | CLA | CHD-C4C-NC | 4.14 | 130.59 | 124.21 |
| 20 | A | 814 | CLA | CHC-C1C-NC | 4.14 | 130.34 | 124.23 |
| 20 | B | 803 | CLA | O2D-CGD-CBD | 4.14 | 118.62 | 111.27 |
| 22 | G | 104 | BCR | C7-C8-C9 | -4.13 | 119.99 | 126.23 |
| 20 | 3 | 316 | CLA | C1C-CHC-C4B | -4.13 | 115.83 | 126.13 |
| 20 | B | 816 | CLA | CHC-C4B-NB | 4.13 | 128.63 | 124.26 |
| 20 | B | 823 | CLA | C4B-CHC-C1C | -4.13 | 116.53 | 126.34 |
| 20 | 2 | 316 | CLA | CMD-C2D-C3D | -4.13 | 118.11 | 127.61 |
| 20 | J | 101 | CLA | CHD-C4C-C3C | -4.13 | 118.77 | 124.84 |
| 20 | 3 | 309 | CLA | C3B-C2B-C1B | -4.13 | 102.28 | 106.75 |
| 20 | B | 841 | CLA | O2A-CGA-CBA | 4.13 | 124.87 | 111.91 |
| 20 | A | 825 | CLA | CHC-C4B-NB | 4.13 | 128.63 | 124.26 |
| 20 | A | 817 | CLA | CHD-C4C-C3C | -4.13 | 118.77 | 124.84 |
| 20 | B | 850 | CLA | C4A-NA-C1A | 4.13 | 108.56 | 106.71 |
| 20 | 2 | 306 | CLA | C4C-CHD-C1D | -4.12 | 115.91 | 126.11 |
| 20 | A | 840 | CLA | CHD-C4C-C3C | -4.12 | 118.78 | 124.84 |
| 20 | 2 | 305 | CLA | O2D-CGD-CBD | 4.12 | 118.59 | 111.27 |
| 22 | F | 204 | BCR | C16-C17-C18 | -4.12 | 121.43 | 127.31 |
| 21 | 4 | 319 | LMU | O5B-C5B-C4B | 4.12 | 117.18 | 109.69 |
| 20 | B | 806 | CLA | C3B-C4B-NB | -4.12 | 106.69 | 110.52 |
| 20 | A | 811 | CLA | C4A-NA-C1A | 4.12 | 108.56 | 106.71 |
| 20 | 3 | 307 | CLA | CHC-C1C-C2C | -4.12 | 115.29 | 126.73 |
| 20 | K | 104 | CLA | CHD-C4C-NC | 4.12 | 130.69 | 124.20 |
| 20 | L | 201 | CLA | C4B-CHC-C1C | -4.12 | 116.57 | 126.34 |
| 20 | A | 806 | CLA | CHD-C4C-C3C | -4.12 | 118.79 | 124.84 |
| 20 | F | 207 | CLA | CBC-CAC-C3C | -4.12 | 101.08 | 112.43 |
| 20 | 3 | 308 | CLA | CHC-C1C-NC | 4.12 | 130.31 | 124.23 |
| 20 | A | 813 | CLA | C4A-NA-C1A | 4.11 | 108.56 | 106.71 |
| 20 | A | 808 | CLA | C4B-CHC-C1C | -4.11 | 116.58 | 126.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | H | 101 | CLA | C4B-CHC-C1C | -4.11 | 116.58 | 126.34 |
| 20 | 4 | 312 | CLA | CHC-C1C-NC | 4.11 | 130.30 | 124.23 |
| 20 | A | 825 | CLA | CHC-C1C-NC | 4.11 | 130.44 | 124.20 |
| 20 | 2 | 311 | CLA | CHD-C4C-NC | 4.11 | 130.68 | 124.20 |
| 22 | F | 204 | BCR | C34-C9-C8 | 4.11 | 124.55 | 118.08 |
| 20 | 1 | 212 | CLA | C4A-NA-C1A | 4.11 | 108.55 | 106.71 |
| 20 | A | 820 | CLA | CHD-C4C-C3C | -4.11 | 118.80 | 124.84 |
| 20 | L | 202 | CLA | CMD-C2D-C3D | -4.11 | 118.17 | 127.61 |
| 21 | 1 | 216 | LMU | C1'-O5'-C5' | -4.11 | 105.63 | 113.69 |
| 20 | F | 207 | CLA | C4D-C3D-CAD | 4.10 | 112.93 | 108.10 |
| 20 | 1 | 205 | CLA | C1B-C2B-C3B | -4.10 | 103.13 | 107.03 |
| 20 | B | 806 | CLA | CHD-C4C-C3C | -4.10 | 118.81 | 124.84 |
| 20 | A | 823 | CLA | C4B-CHC-C1C | -4.10 | 116.61 | 126.34 |
| 20 | A | 832 | CLA | CMD-C2D-C3D | -4.10 | 118.18 | 127.61 |
| 20 | 4 | 310 | CLA | CED-O2D-CGD | 4.10 | 125.21 | 115.94 |
| 20 | B | 831 | CLA | C4B-CHC-C1C | -4.10 | 116.62 | 126.34 |
| 20 | 1 | 203 | CLA | CAA-CBA-CGA | -4.10 | 101.28 | 113.25 |
| 20 | 2 | 301 | CLA | C3B-C2B-C1B | -4.10 | 102.31 | 106.75 |
| 20 | A | 802 | CLA | C1B-NB-C4B | -4.10 | 103.42 | 106.33 |
| 20 | B | 825 | CLA | O2D-CGD-O1D | -4.09 | 115.83 | 123.84 |
| 20 | 4 | 307 | CLA | C1C-CHC-C4B | -4.09 | 115.93 | 126.13 |
| 20 | 2 | 301 | CLA | C1C-CHC-C4B | -4.09 | 115.93 | 126.13 |
| 22 | A | 844 | BCR | C7-C8-C9 | -4.09 | 120.05 | 126.23 |
| 20 | J | 101 | CLA | CHC-C1C-NC | 4.09 | 130.41 | 124.20 |
| 20 | 3 | 307 | CLA | C4D-C3D-CAD | 4.09 | 112.92 | 108.10 |
| 20 | B | 815 | CLA | CHD-C4C-NC | 4.09 | 130.65 | 124.20 |
| 20 | B | 817 | CLA | CHC-C1C-NC | 4.09 | 130.41 | 124.20 |
| 20 | H | 102 | CLA | C4-C3-C5 | 4.09 | 122.15 | 115.27 |
| 20 | B | 836 | CLA | CHC-C4B-NB | 4.09 | 128.58 | 124.26 |
| 20 | B | 842 | CLA | C4A-NA-C1A | 4.08 | 108.54 | 106.71 |
| 20 | B | 823 | CLA | CHC-C1C-NC | 4.08 | 130.40 | 124.20 |
| 22 | I | 103 | BCR | C29-C30-C25 | -4.08 | 104.19 | 110.48 |
| 20 | B | 822 | CLA | C4B-CHC-C1C | -4.08 | 116.65 | 126.34 |
| 20 | L | 201 | CLA | CHC-C4B-NB | 4.08 | 128.58 | 124.26 |
| 20 | A | 832 | CLA | CHC-C1C-NC | 4.08 | 130.40 | 124.20 |
| 20 | 1 | 206 | CLA | CAC-C3C-C4C | 4.08 | 130.10 | 124.81 |
| 22 | I | 103 | BCR | C27-C26-C25 | -4.08 | 116.81 | 122.73 |
| 20 | A | 823 | CLA | CMD-C2D-C3D | -4.08 | 118.23 | 127.61 |
| 20 | 4 | 312 | CLA | CHD-C4C-NC | 4.08 | 130.50 | 124.21 |
| 20 | J | 103 | CLA | C4D-C3D-CAD | 4.08 | 112.90 | 108.10 |
| 20 | B | 834 | CLA | CHD-C4C-C3C | -4.08 | 118.85 | 124.84 |
| 20 | B | 836 | CLA | C1-C2-C3 | -4.08 | 118.99 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 806 | CLA | CMD-C2D-C3D | -4.08 | 118.24 | 127.61 |
| 20 | 3 | 311 | CLA | CHC-C1C-NC | 4.08 | 130.39 | 124.20 |
| 20 | 3 | 308 | CLA | C1C-CHC-C4B | -4.07 | 115.97 | 126.13 |
| 20 | 3 | 312 | CLA | C4A-NA-C1A | 4.07 | 108.54 | 106.71 |
| 20 | 4 | 318 | CLA | CHC-C4B-NB | 4.07 | 128.57 | 124.26 |
| 20 | K | 104 | CLA | C4B-CHC-C1C | -4.07 | 116.68 | 126.34 |
| 20 | B | 828 | CLA | CHD-C4C-C3C | -4.07 | 118.85 | 124.84 |
| 20 | L | 204 | CLA | C4A-NA-C1A | 4.07 | 108.54 | 106.71 |
| 20 | A | 823 | CLA | CHD-C4C-NC | 4.07 | 130.62 | 124.20 |
| 22 | B | 801 | BCR | C19-C18-C17 | -4.07 | 112.69 | 118.94 |
| 20 | 4 | 301 | CLA | CHC-C1C-NC | 4.07 | 130.38 | 124.20 |
| 20 | A | 814 | CLA | CHD-C4C-NC | 4.07 | 130.49 | 124.21 |
| 20 | B | 817 | CLA | CHD-C4C-C3C | -4.07 | 118.86 | 124.84 |
| 20 | B | 813 | CLA | CMD-C2D-C3D | -4.07 | 118.25 | 127.61 |
| 20 | B | 839 | CLA | C3B-C2B-C1B | -4.07 | 102.25 | 107.16 |
| 20 | A | 820 | CLA | CHC-C4B-NB | 4.07 | 128.56 | 124.26 |
| 20 | A | 821 | CLA | O1D-CGD-CBD | -4.07 | 116.16 | 124.48 |
| 20 | 4 | 308 | CLA | CHC-C1C-NC | 4.07 | 130.23 | 124.23 |
| 20 | G | 105 | CLA | O2D-CGD-O1D | -4.06 | 115.89 | 123.84 |
| 20 | B | 833 | CLA | CHC-C1C-NC | 4.06 | 130.37 | 124.20 |
| 20 | B | 827 | CLA | C4B-CHC-C1C | -4.06 | 116.70 | 126.34 |
| 20 | 1 | 212 | CLA | C1C-CHC-C4B | -4.06 | 116.01 | 126.13 |
| 20 | B | 817 | CLA | CAC-C3C-C4C | 4.06 | 130.08 | 124.81 |
| 20 | B | 842 | CLA | CHD-C4C-C3C | -4.06 | 118.64 | 124.98 |
| 20 | A | 813 | CLA | C4B-CHC-C1C | -4.06 | 116.71 | 126.34 |
| 21 | H | 106 | LMU | C1B-O5B-C5B | 4.06 | 121.65 | 113.69 |
| 20 | 4 | 307 | CLA | C3D-C4D-CHA | -4.06 | 116.44 | 124.98 |
| 20 | L | 207 | CLA | C4B-CHC-C1C | -4.06 | 116.72 | 126.34 |
| 20 | B | 841 | CLA | C4A-NA-C1A | 4.05 | 108.53 | 106.71 |
| 20 | A | 824 | CLA | C4B-CHC-C1C | -4.05 | 116.72 | 126.34 |
| 20 | A | 817 | CLA | CMD-C2D-C3D | -4.05 | 118.30 | 127.61 |
| 20 | A | 828 | CLA | C4B-CHC-C1C | -4.05 | 116.73 | 126.34 |
| 20 | A | 834 | CLA | CAA-C2A-C3A | -4.05 | 101.69 | 112.78 |
| 20 | 2 | 303 | CLA | CHC-C4B-NB | 4.05 | 128.54 | 124.26 |
| 20 | 1 | 206 | CLA | C4B-CHC-C1C | -4.05 | 116.74 | 126.34 |
| 20 | A | 836 | CLA | O2D-CGD-O1D | -4.05 | 115.93 | 123.84 |
| 20 | A | 812 | CLA | CHD-C4C-C3C | -4.05 | 118.89 | 124.84 |
| 20 | 3 | 301 | CLA | CHD-C4C-C3C | -4.04 | 118.66 | 124.98 |
| 20 | 1 | 202 | CLA | CHD-C4C-NC | 4.04 | 130.58 | 124.20 |
| 20 | 3 | 314 | CLA | CMD-C2D-C3D | -4.04 | 118.31 | 127.61 |
| 20 | A | 837 | CLA | CMD-C2D-C3D | -4.04 | 118.31 | 127.61 |
| 20 | R | 107 | CLA | CMD-C2D-C3D | -4.04 | 118.31 | 127.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | R | 103 | LMU | C1B-O5B-C5B | 4.04 | 121.62 | 113.69 |
| 20 | 4 | 317 | CLA | CMD-C2D-C3D | -4.04 | 118.32 | 127.61 |
| 20 | A | 814 | CLA | C3D-C4D-CHA | -4.04 | 116.48 | 124.98 |
| 20 | 2 | 301 | CLA | C2D-C3D-C4D | -4.04 | 102.81 | 107.28 |
| 20 | A | 825 | CLA | C4B-CHC-C1C | -4.04 | 116.76 | 126.34 |
| 20 | A | 850 | CLA | C4B-CHC-C1C | -4.04 | 116.76 | 126.34 |
| 20 | 2 | 316 | CLA | O2D-CGD-CBD | 4.04 | 118.44 | 111.27 |
| 20 | B | 850 | CLA | O2D-CGD-CBD | 4.03 | 118.44 | 111.27 |
| 22 | L | 209 | BCR | C15-C16-C17 | -4.03 | 115.21 | 123.47 |
| 20 | A | 836 | CLA | C4B-CHC-C1C | -4.03 | 116.77 | 126.34 |
| 20 | B | 820 | CLA | C4B-CHC-C1C | -4.03 | 116.77 | 126.34 |
| 20 | 4 | 305 | CLA | CHC-C1C-NC | 4.03 | 130.32 | 124.20 |
| 20 | 4 | 303 | CLA | CMD-C2D-C3D | -4.03 | 118.34 | 127.61 |
| 20 | 3 | 306 | CLA | C1C-CHC-C4B | -4.03 | 116.09 | 126.13 |
| 20 | 3 | 308 | CLA | C1B-NB-C4B | -4.03 | 103.47 | 106.33 |
| 20 | 4 | 308 | CLA | CHC-C4B-NB | 4.03 | 128.35 | 124.27 |
| 20 | A | 832 | CLA | C4B-CHC-C1C | -4.03 | 116.78 | 126.34 |
| 20 | 2 | 315 | CLA | C3D-C4D-CHA | -4.03 | 116.50 | 124.98 |
| 20 | A | 821 | CLA | CMD-C2D-C3D | -4.03 | 118.35 | 127.61 |
| 20 | B | 834 | CLA | C4B-CHC-C1C | -4.03 | 116.79 | 126.34 |
| 20 | 1 | 212 | CLA | C2A-C1A-CHA | -4.02 | 115.77 | 122.63 |
| 20 | A | 817 | CLA | CHC-C4B-NB | 4.02 | 128.52 | 124.26 |
| 20 | B | 807 | CLA | O2D-CGD-O1D | -4.02 | 115.97 | 123.84 |
| 20 | B | 811 | CLA | C3A-C4A-CHB | -4.02 | 118.98 | 123.91 |
| 20 | B | 822 | CLA | CMD-C2D-C3D | -4.02 | 118.36 | 127.61 |
| 20 | B | 813 | CLA | CHD-C4C-NC | 4.02 | 130.54 | 124.20 |
| 20 | A | 831 | CLA | C5-C3-C2 | -4.02 | 112.98 | 121.12 |
| 20 | 4 | 314 | CLA | C1C-CHC-C4B | -4.02 | 116.11 | 126.13 |
| 20 | 3 | 311 | CLA | C4B-CHC-C1C | -4.02 | 116.80 | 126.34 |
| 20 | A | 815 | CLA | CHC-C1C-NC | 4.02 | 130.30 | 124.20 |
| 20 | A | 810 | CLA | C3B-C4B-NB | -4.02 | 106.78 | 110.52 |
| 20 | H | 101 | CLA | CHB-C4A-NA | 4.02 | 130.07 | 124.51 |
| 20 | 4 | 305 | CLA | C4A-NA-C1A | 4.02 | 108.51 | 106.71 |
| 20 | A | 833 | CLA | CMD-C2D-C3D | -4.02 | 118.38 | 127.61 |
| 20 | B | 803 | CLA | CHD-C4C-C3C | -4.02 | 118.94 | 124.84 |
| 20 | B | 833 | CLA | CMD-C2D-C3D | -4.02 | 118.38 | 127.61 |
| 20 | B | 830 | CLA | CHB-C1B-NB | -4.02 | 120.01 | 124.26 |
| 20 | 1 | 215 | CLA | CHD-C1D-ND | 4.02 | 128.14 | 124.45 |
| 20 | B | 829 | CLA | C3B-C2B-C1B | -4.01 | 102.32 | 107.16 |
| 20 | 1 | 201 | CLA | CHB-C1B-NB | -4.01 | 120.01 | 124.26 |
| 20 | F | 201 | CLA | CHB-C1B-NB | -4.01 | 120.01 | 124.26 |
| 20 | 1 | 205 | CLA | CHD-C4C-C3C | -4.01 | 118.71 | 124.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 209 | CLA | C2D-C3D-C4D | -4.01 | 102.84 | 107.28 |
| 20 | L | 202 | CLA | CHC-C4B-NB | 4.01 | 128.50 | 124.26 |
| 20 | J | 101 | CLA | C4B-CHC-C1C | -4.01 | 116.83 | 126.34 |
| 20 | B | 802 | CLA | C4B-CHC-C1C | -4.01 | 116.83 | 126.34 |
| 20 | 2 | 303 | CLA | CMB-C2B-C1B | 4.01 | 131.47 | 125.37 |
| 20 | A | 841 | CLA | CHD-C4C-NC | 4.01 | 130.39 | 124.21 |
| 20 | 2 | 315 | CLA | CHD-C1D-ND | 4.00 | 128.38 | 124.52 |
| 20 | F | 206 | CLA | CHC-C4B-NB | 4.00 | 128.50 | 124.26 |
| 20 | A | 822 | CLA | CMD-C2D-C3D | -4.00 | 118.40 | 127.61 |
| 20 | R | 108 | CLA | CMD-C2D-C3D | -4.00 | 118.40 | 127.61 |
| 20 | A | 818 | CLA | CMD-C2D-C3D | -4.00 | 118.41 | 127.61 |
| 20 | 1 | 202 | CLA | CHD-C4C-C3C | -4.00 | 118.96 | 124.84 |
| 22 | I | 101 | BCR | C37-C22-C21 | -4.00 | 117.32 | 122.92 |
| 22 | B | 801 | BCR | C24-C23-C22 | -4.00 | 120.19 | 126.23 |
| 20 | B | 808 | CLA | CHC-C1C-NC | 4.00 | 130.27 | 124.20 |
| 20 | B | 802 | CLA | C4A-NA-C1A | 4.00 | 108.50 | 106.71 |
| 20 | 2 | 306 | CLA | C3A-C4A-CHB | -4.00 | 119.01 | 123.91 |
| 20 | 4 | 317 | CLA | CHB-C4A-NA | 4.00 | 130.04 | 124.51 |
| 20 | 1 | 209 | CLA | C3D-C4D-CHA | -4.00 | 116.56 | 124.98 |
| 20 | B | 822 | CLA | CHC-C4B-NB | 4.00 | 128.49 | 124.26 |
| 20 | 1 | 211 | CLA | CGD-CBD-CAD | -3.99 | 97.79 | 110.73 |
| 20 | B | 825 | CLA | C4B-CHC-C1C | -3.99 | 116.86 | 126.34 |
| 20 | B | 823 | CLA | CMD-C2D-C3D | -3.99 | 118.43 | 127.61 |
| 20 | A | 834 | CLA | CHC-C1C-NC | 3.99 | 130.26 | 124.20 |
| 20 | 1 | 205 | CLA | C4B-CHC-C1C | -3.99 | 116.87 | 126.34 |
| 20 | 3 | 312 | CLA | CHC-C1C-NC | 3.99 | 130.13 | 124.23 |
| 21 | 4 | 320 | LMU | C2'-C3'-C4' | 3.99 | 118.80 | 109.68 |
| 20 | B | 850 | CLA | CMD-C2D-C1D | 3.99 | 131.75 | 124.71 |
| 20 | 2 | 306 | CLA | C2A-C1A-CHA | -3.99 | 115.83 | 122.63 |
| 20 | 3 | 306 | CLA | C3B-C2B-C1B | -3.99 | 102.43 | 106.75 |
| 20 | A | 809 | CLA | CMD-C2D-C3D | -3.99 | 118.44 | 127.61 |
| 20 | 2 | 303 | CLA | C4B-CHC-C1C | -3.99 | 116.89 | 126.34 |
| 20 | A | 806 | CLA | CHC-C1C-NC | 3.98 | 130.25 | 124.20 |
| 20 | 1 | 207 | CLA | C3B-C2B-C1B | -3.98 | 102.35 | 107.16 |
| 20 | 3 | 306 | CLA | C2A-C1A-CHA | -3.98 | 115.84 | 122.63 |
| 20 | B | 829 | CLA | C4B-CHC-C1C | -3.98 | 116.89 | 126.34 |
| 20 | A | 824 | CLA | CHC-C1C-NC | 3.98 | 130.25 | 124.20 |
| 20 | L | 207 | CLA | CHC-C1C-NC | 3.98 | 130.25 | 124.20 |
| 20 | H | 102 | CLA | C4A-NA-C1A | 3.98 | 108.50 | 106.71 |
| 20 | 4 | 307 | CLA | CHC-C4B-NB | 3.98 | 128.31 | 124.27 |
| 20 | B | 832 | CLA | CHC-C4B-NB | 3.98 | 128.47 | 124.26 |
| 20 | L | 202 | CLA | C4B-CHC-C1C | -3.98 | 116.90 | 126.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 20 | B | 824 | CLA | C2A-C1A-CHA | -3.98 | 116.90 | 123.86 |
| 20 | B | 842 | CLA | CAA-C2A-C3A | -3.98 | 106.81 | 116.10 |
| 21 | H | 104 | LMU | C3'-C4'-C5' | -3.98 | 101.81 | 110.93 |
| 20 | 4 | 301 | CLA | C4B-CHC-C1C | -3.98 | 116.91 | 126.34 |
| 20 | A | 830 | CLA | CMD-C2D-C3D | -3.97 | 118.47 | 127.61 |
| 20 | H | 109 | CLA | C4B-CHC-C1C | -3.97 | 116.91 | 126.34 |
| 20 | 4 | 312 | CLA | CHD-C1D-ND | 3.97 | 128.35 | 124.52 |
| 20 | A | 833 | CLA | C4A-NA-C1A | 3.97 | 108.49 | 106.71 |
| 20 | K | 103 | CLA | CHC-C4B-NB | 3.97 | 128.46 | 124.26 |
| 20 | F | 205 | CLA | C4B-CHC-C1C | -3.97 | 116.92 | 126.34 |
| 20 | 1 | 207 | CLA | C4B-CHC-C1C | -3.97 | 116.92 | 126.34 |
| 20 | A | 841 | CLA | C1B-NB-C4B | -3.97 | 103.52 | 106.33 |
| 20 | J | 103 | CLA | C4A-NA-C1A | 3.97 | 108.49 | 106.71 |
| 20 | 4 | 315 | CLA | C4B-CHC-C1C | -3.97 | 116.93 | 126.34 |
| 20 | B | 828 | CLA | O2A-CGA-CBA | 3.97 | 124.36 | 111.91 |
| 20 | B | 809 | CLA | C4B-CHC-C1C | -3.97 | 116.93 | 126.34 |
| 20 | J | 101 | CLA | CMD-C2D-C3D | -3.97 | 118.49 | 127.61 |
| 20 | A | 838 | CLA | C4B-CHC-C1C | -3.96 | 116.93 | 126.34 |
| 20 | A | 807 | CLA | CMD-C2D-C3D | -3.96 | 118.49 | 127.61 |
| 20 | K | 101 | CLA | CMD-C2D-C3D | -3.96 | 118.50 | 127.61 |
| 20 | 1 | 205 | CLA | CMD-C2D-C3D | -3.96 | 118.50 | 127.61 |
| 21 | F | 202 | LMU | C2'-C3'-C4' | -3.96 | 100.64 | 109.68 |
| 20 | B | 819 | CLA | CMD-C2D-C3D | -3.96 | 118.50 | 127.61 |
| 20 | B | 810 | CLA | CHD-C4C-NC | 3.96 | 130.44 | 124.20 |
| 20 | B | 826 | CLA | C4B-CHC-C1C | -3.96 | 116.94 | 126.34 |
| 20 | L | 201 | CLA | CHD-C4C-C3C | -3.96 | 119.02 | 124.84 |
| 20 | 2 | 305 | CLA | C4B-CHC-C1C | -3.96 | 116.95 | 126.34 |
| 20 | 1 | 208 | CLA | C2A-C1A-CHA | -3.96 | 115.88 | 122.63 |
| 20 | A | 803 | CLA | CMA-C3A-C4A | -3.96 | 101.14 | 111.77 |
| 20 | 4 | 309 | CLA | C3D-C4D-CHA | -3.96 | 116.65 | 124.98 |
| 20 | 3 | 305 | CLA | C2A-C1A-CHA | -3.96 | 115.89 | 122.63 |
| 20 | A | 850 | CLA | CAA-C2A-C1A | 3.96 | 124.94 | 111.97 |
| 20 | 3 | 315 | CLA | C3D-C4D-CHA | -3.96 | 116.65 | 124.98 |
| 20 | B | 835 | CLA | CMD-C2D-C3D | -3.96 | 118.51 | 127.61 |
| 20 | B | 834 | CLA | CHC-C1C-NC | 3.95 | 130.20 | 124.20 |
| 20 | 1 | 208 | CLA | CHC-C1C-NC | 3.95 | 130.07 | 124.23 |
| 20 | B | 830 | CLA | C3B-C2B-C1B | -3.95 | 102.39 | 107.16 |
| 20 | 1 | 211 | CLA | CBA-CAA-C2A | 3.95 | 125.53 | 113.86 |
| 20 | 4 | 313 | CLA | CBD-CHA-C1A | 3.95 | 133.76 | 127.43 |
| 20 | 1 | 202 | CLA | CMD-C2D-C3D | -3.95 | 118.52 | 127.61 |
| 20 | B | 829 | CLA | O2D-CGD-O1D | -3.95 | 116.11 | 123.84 |
| 20 | B | 806 | CLA | CHC-C4B-NB | 3.95 | 128.44 | 124.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 835 | CLA | CHC-C1C-NC | 3.95 | 130.19 | 124.20 |
| 20 | A | 824 | CLA | CHD-C4C-C3C | -3.95 | 119.04 | 124.84 |
| 20 | B | 802 | CLA | CHC-C1C-NC | 3.95 | 130.19 | 124.20 |
| 22 | G | 104 | BCR | C16-C17-C18 | -3.95 | 121.68 | 127.31 |
| 20 | A | 826 | CLA | CHD-C4C-C3C | -3.95 | 119.04 | 124.84 |
| 20 | 3 | 312 | CLA | C3B-C2B-C1B | -3.94 | 102.48 | 106.75 |
| 20 | 3 | 301 | CLA | CMD-C2D-C3D | -3.94 | 118.54 | 127.61 |
| 20 | B | 836 | CLA | CMD-C2D-C3D | -3.94 | 118.54 | 127.61 |
| 20 | 4 | 307 | CLA | C4A-NA-C1A | 3.94 | 108.48 | 106.71 |
| 20 | B | 803 | CLA | CMD-C2D-C3D | -3.94 | 118.54 | 127.61 |
| 20 | 2 | 303 | CLA | CHB-C1B-NB | -3.94 | 120.08 | 124.26 |
| 20 | 4 | 306 | CLA | CMD-C2D-C3D | -3.94 | 118.55 | 127.61 |
| 20 | A | 820 | CLA | C4B-CHC-C1C | -3.94 | 116.99 | 126.34 |
| 20 | 1 | 206 | CLA | CHB-C1B-NB | -3.94 | 120.08 | 124.26 |
| 21 | F | 202 | LMU | C1B-O1B-C4' | -3.94 | 108.21 | 117.96 |
| 20 | 2 | 301 | CLA | C4A-NA-C1A | 3.94 | 108.48 | 106.71 |
| 20 | A | 839 | CLA | CHB-C1B-NB | -3.94 | 120.09 | 124.26 |
| 20 | 2 | 312 | CLA | C3B-C2B-C1B | -3.94 | 102.41 | 107.16 |
| 20 | A | 808 | CLA | CHD-C4C-C3C | -3.94 | 119.05 | 124.84 |
| 20 | 4 | 317 | CLA | C1-C2-C3 | -3.94 | 119.23 | 126.04 |
| 20 | 3 | 313 | CLA | CHD-C4C-C3C | -3.93 | 119.06 | 124.84 |
| 22 | J | 102 | BCR | C7-C8-C9 | -3.93 | 120.29 | 126.23 |
| 20 | 4 | 314 | CLA | CHC-C1C-NC | 3.93 | 130.04 | 124.23 |
| 20 | 3 | 315 | CLA | C4C-CHD-C1D | -3.93 | 116.39 | 126.11 |
| 21 | C | 101 | LMU | O1'-C1'-C2' | 3.93 | 114.44 | 108.30 |
| 20 | 3 | 316 | CLA | C3D-C4D-CHA | -3.93 | 116.70 | 124.98 |
| 20 | L | 203 | CLA | C4A-NA-C1A | 3.93 | 108.47 | 106.71 |
| 20 | B | 815 | CLA | CHC-C1C-NC | 3.93 | 130.16 | 124.20 |
| 20 | 3 | 307 | CLA | CHB-C1B-NB | -3.93 | 120.10 | 124.26 |
| 20 | R | 107 | CLA | CHC-C1C-NC | 3.93 | 130.16 | 124.20 |
| 20 | A | 814 | CLA | C3A-C4A-CHB | -3.93 | 119.10 | 123.91 |
| 20 | 3 | 301 | CLA | CBD-CHA-C1A | 3.93 | 133.72 | 127.43 |
| 21 | R | 102 | LMU | C3'-C4'-C5' | -3.93 | 101.93 | 110.93 |
| 20 | H | 108 | CLA | CHC-C4B-NB | 3.92 | 128.41 | 124.26 |
| 20 | G | 105 | CLA | CHC-C1C-NC | 3.92 | 130.16 | 124.20 |
| 20 | 3 | 306 | CLA | C4A-NA-C1A | 3.92 | 108.47 | 106.71 |
| 20 | B | 803 | CLA | CHB-C4A-NA | 3.92 | 129.94 | 124.51 |
| 20 | A | 807 | CLA | CHD-C4C-C3C | -3.92 | 119.08 | 124.84 |
| 20 | 4 | 302 | CLA | CMD-C2D-C3D | -3.92 | 118.59 | 127.61 |
| 20 | A | 851 | CLA | CHC-C1C-NC | 3.92 | 130.15 | 124.20 |
| 20 | 4 | 310 | CLA | O1D-CGD-CBD | -3.92 | 116.46 | 124.48 |
| 20 | 3 | 311 | CLA | CMD-C2D-C3D | -3.92 | 118.60 | 127.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 805 | CLA | CHB-C1B-NB | -3.92 | 120.11 | 124.26 |
| 20 | H | 108 | CLA | CHB-C4A-NA | 3.92 | 129.93 | 124.51 |
| 20 | 2 | 308 | CLA | C1C-CHC-C4B | -3.92 | 116.37 | 126.13 |
| 20 | B | 824 | CLA | CAA-C2A-C1A | -3.92 | 99.15 | 111.97 |
| 20 | 1 | 209 | CLA | CHD-C4C-NC | 3.91 | 130.25 | 124.21 |
| 20 | 1 | 208 | CLA | C3B-C2B-C1B | -3.91 | 102.51 | 106.75 |
| 20 | 2 | 312 | CLA | C4-C3-C5 | 3.91 | 121.85 | 115.27 |
| 20 | B | 838 | CLA | CMD-C2D-C3D | -3.91 | 118.61 | 127.61 |
| 20 | B | 809 | CLA | CMD-C2D-C3D | -3.91 | 118.62 | 127.61 |
| 22 | A | 845 | BCR | C33-C5-C6 | -3.91 | 120.14 | 124.53 |
| 20 | A | 817 | CLA | CHC-C1C-NC | 3.91 | 130.13 | 124.20 |
| 20 | 2 | 309 | CLA | C2A-C1A-CHA | -3.91 | 115.97 | 122.63 |
| 20 | 1 | 214 | CLA | C3D-C4D-CHA | -3.91 | 116.75 | 124.98 |
| 20 | B | 809 | CLA | CHB-C4A-NA | 3.91 | 129.91 | 124.51 |
| 20 | 3 | 315 | CLA | C4A-NA-C1A | 3.91 | 108.46 | 106.71 |
| 20 | A | 824 | CLA | CMD-C2D-C3D | -3.91 | 118.63 | 127.61 |
| 20 | L | 203 | CLA | C3B-C2B-C1B | -3.91 | 102.45 | 107.16 |
| 20 | B | 832 | CLA | C4B-CHC-C1C | -3.90 | 117.08 | 126.34 |
| 20 | 2 | 308 | CLA | C3C-C4C-CHD | -3.90 | 116.67 | 125.22 |
| 20 | H | 109 | CLA | CHC-C1C-NC | 3.90 | 130.13 | 124.20 |
| 20 | B | 803 | CLA | C4B-CHC-C1C | -3.90 | 117.08 | 126.34 |
| 20 | L | 208 | CLA | O2D-CGD-O1D | -3.90 | 116.20 | 123.84 |
| 20 | 2 | 310 | CLA | C4A-NA-C1A | 3.90 | 108.46 | 106.71 |
| 20 | 2 | 302 | CLA | CMD-C2D-C3D | -3.90 | 118.64 | 127.61 |
| 20 | B | 811 | CLA | C3D-C4D-CHA | -3.90 | 116.76 | 124.98 |
| 20 | 4 | 305 | CLA | CHC-C4B-NB | 3.90 | 128.39 | 124.26 |
| 20 | A | 802 | CLA | C3D-C4D-CHA | -3.90 | 116.77 | 124.98 |
| 20 | B | 819 | CLA | CGD-CBD-CAD | -3.90 | 98.10 | 110.73 |
| 20 | 3 | 315 | CLA | C3B-C2B-C1B | -3.90 | 102.53 | 106.75 |
| 21 | L | 205 | LMU | C4B-C3B-C2B | 3.90 | 117.63 | 110.82 |
| 21 | K | 105 | LMU | C3B-C4B-C5B | -3.90 | 103.28 | 110.24 |
| 20 | B | 817 | CLA | C4B-CHC-C1C | -3.90 | 117.09 | 126.34 |
| 20 | L | 201 | CLA | CHC-C1C-NC | 3.90 | 130.12 | 124.20 |
| 20 | B | 818 | CLA | CMD-C2D-C3D | -3.90 | 118.65 | 127.61 |
| 20 | 2 | 305 | CLA | CHC-C1C-NC | 3.90 | 130.11 | 124.20 |
| 20 | 4 | 307 | CLA | CHC-C1C-NC | 3.90 | 129.98 | 124.23 |
| 20 | 4 | 306 | CLA | C2A-C3A-C4A | -3.90 | 95.58 | 101.87 |
| 20 | A | 812 | CLA | CHC-C1C-NC | 3.90 | 130.11 | 124.20 |
| 20 | 4 | 304 | CLA | C1D-CHD-C4C | -3.89 | 117.66 | 126.06 |
| 20 | A | 812 | CLA | C4B-CHC-C1C | -3.89 | 117.10 | 126.34 |
| 20 | 2 | 307 | CLA | O2A-CGA-CBA | 3.89 | 124.13 | 111.91 |
| 20 | A | 811 | CLA | CAA-C2A-C3A | -3.89 | 102.12 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | F | 201 | CLA | O2D-CGD-O1D | -3.89 | 116.23 | 123.84 |
| 22 | A | 845 | BCR | C24-C23-C22 | -3.89 | 120.36 | 126.23 |
| 20 | 3 | 302 | CLA | C4A-NA-C1A | 3.89 | 108.45 | 106.71 |
| 20 | 4 | 305 | CLA | CHB-C1B-NB | -3.89 | 120.14 | 124.26 |
| 20 | K | 101 | CLA | CHC-C1C-NC | 3.89 | 130.10 | 124.20 |
| 22 | G | 104 | BCR | C33-C5-C6 | -3.89 | 120.16 | 124.53 |
| 20 | B | 850 | CLA | CHD-C4C-C3C | -3.89 | 119.13 | 124.84 |
| 20 | F | 206 | CLA | CMD-C2D-C3D | -3.89 | 118.67 | 127.61 |
| 20 | 4 | 303 | CLA | CHC-C4B-NB | 3.89 | 128.37 | 124.26 |
| 21 | 1 | 217 | LMU | O1B-C4'-C3' | 3.89 | 117.62 | 107.28 |
| 20 | H | 101 | CLA | CHD-C4C-C3C | -3.89 | 119.13 | 124.84 |
| 20 | B | 831 | CLA | C3B-C2B-C1B | -3.88 | 102.47 | 107.16 |
| 20 | A | 828 | CLA | CHC-C1C-NC | 3.88 | 130.09 | 124.20 |
| 20 | 4 | 301 | CLA | CMD-C2D-C3D | -3.88 | 118.69 | 127.61 |
| 20 | 4 | 302 | CLA | CHC-C4B-NB | 3.88 | 128.36 | 124.26 |
| 20 | 3 | 301 | CLA | C1B-C2B-C3B | -3.88 | 103.35 | 107.03 |
| 20 | H | 109 | CLA | CHD-C4C-NC | 3.88 | 130.31 | 124.20 |
| 20 | A | 840 | CLA | CHC-C1C-NC | 3.88 | 130.08 | 124.20 |
| 20 | A | 816 | CLA | C3B-C2B-C1B | -3.88 | 102.48 | 107.16 |
| 20 | 3 | 312 | CLA | C1B-NB-C4B | -3.87 | 103.58 | 106.33 |
| 20 | A | 827 | CLA | C3B-C2B-C1B | -3.87 | 102.49 | 107.16 |
| 20 | H | 108 | CLA | O2A-C1-C2 | 3.87 | 118.81 | 108.64 |
| 20 | B | 813 | CLA | C4A-NA-C1A | 3.87 | 108.45 | 106.71 |
| 20 | A | 822 | CLA | CHC-C1C-NC | 3.87 | 130.07 | 124.20 |
| 20 | F | 205 | CLA | CHC-C4B-NB | 3.87 | 128.35 | 124.26 |
| 20 | A | 830 | CLA | CHD-C4C-C3C | -3.87 | 119.16 | 124.84 |
| 20 | L | 203 | CLA | CMD-C2D-C3D | -3.87 | 118.72 | 127.61 |
| 20 | F | 205 | CLA | CHD-C4C-C3C | -3.86 | 118.94 | 124.98 |
| 20 | B | 838 | CLA | CHD-C4C-C3C | -3.86 | 119.16 | 124.84 |
| 20 | 3 | 302 | CLA | C1B-NB-C4B | -3.86 | 103.59 | 106.33 |
| 22 | B | 847 | BCR | C24-C23-C22 | -3.86 | 120.40 | 126.23 |
| 20 | 2 | 303 | CLA | CMD-C2D-C3D | -3.86 | 118.73 | 127.61 |
| 20 | B | 837 | CLA | CHD-C4C-C3C | -3.86 | 119.17 | 124.84 |
| 20 | 4 | 305 | CLA | C4B-CHC-C1C | -3.85 | 117.20 | 126.34 |
| 20 | B | 850 | CLA | CHB-C1B-NB | -3.85 | 120.18 | 124.26 |
| 20 | F | 207 | CLA | C4B-CHC-C1C | -3.85 | 117.20 | 126.34 |
| 20 | 4 | 310 | CLA | CBA-CAA-C2A | -3.85 | 102.50 | 113.86 |
| 22 | A | 844 | BCR | C33-C5-C6 | -3.85 | 120.20 | 124.53 |
| 20 | A | 840 | CLA | CHB-C1B-NB | -3.85 | 120.18 | 124.26 |
| 20 | B | 828 | CLA | C3B-C2B-C1B | -3.85 | 102.52 | 107.16 |
| 20 | B | 814 | CLA | C4B-CHC-C1C | -3.85 | 117.21 | 126.34 |
| 22 | A | 843 | BCR | C16-C17-C18 | -3.85 | 121.82 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 830 | CLA | CMB-C2B-C1B | 3.85 | 131.23 | 125.37 |
| 20 | B | 837 | CLA | C4B-CHC-C1C | -3.85 | 117.22 | 126.34 |
| 20 | F | 207 | CLA | CBA-CAA-C2A | -3.84 | 102.52 | 113.86 |
| 20 | 3 | 311 | CLA | CHC-C4B-NB | 3.84 | 128.32 | 124.26 |
| 20 | 4 | 315 | CLA | C3B-C2B-C1B | -3.84 | 102.53 | 107.16 |
| 21 | 4 | 321 | LMU | C4B-C3B-C2B | 3.84 | 117.53 | 110.82 |
| 20 | 1 | 208 | CLA | C1C-CHC-C4B | -3.84 | 116.56 | 126.13 |
| 20 | A | 826 | CLA | C3B-C2B-C1B | -3.84 | 102.53 | 107.16 |
| 20 | A | 829 | CLA | CHD-C4C-NC | 3.84 | 130.25 | 124.20 |
| 20 | B | 814 | CLA | CHC-C1C-NC | 3.84 | 130.03 | 124.20 |
| 20 | L | 202 | CLA | CHC-C1C-NC | 3.84 | 130.02 | 124.20 |
| 20 | 1 | 203 | CLA | C3B-C2B-C1B | -3.84 | 102.53 | 107.16 |
| 20 | 2 | 312 | CLA | C4B-CHC-C1C | -3.83 | 117.24 | 126.34 |
| 20 | B | 832 | CLA | CMD-C2D-C3D | -3.83 | 118.80 | 127.61 |
| 20 | A | 823 | CLA | CHD-C4C-C3C | -3.83 | 119.21 | 124.84 |
| 20 | L | 201 | CLA | C4-C3-C5 | 3.83 | 121.72 | 115.27 |
| 20 | 4 | 301 | CLA | CHC-C4B-NB | 3.83 | 128.31 | 124.26 |
| 22 | B | 845 | BCR | C30-C25-C26 | -3.83 | 117.22 | 122.61 |
| 20 | A | 850 | CLA | CHC-C4B-NB | 3.83 | 128.31 | 124.26 |
| 20 | A | 809 | CLA | CHC-C1C-C2C | -3.82 | 116.11 | 126.73 |
| 21 | 1 | 218 | LMU | C3B-C4B-C5B | 3.82 | 117.06 | 110.24 |
| 20 | 3 | 303 | CLA | CMD-C2D-C3D | -3.82 | 118.82 | 127.61 |
| 20 | B | 842 | CLA | C4B-CHC-C1C | -3.82 | 117.27 | 126.34 |
| 20 | 1 | 204 | CLA | CHD-C4C-C3C | -3.82 | 119.23 | 124.84 |
| 20 | B | 825 | CLA | CHD-C4C-C3C | -3.82 | 119.23 | 124.84 |
| 20 | 4 | 313 | CLA | CHB-C1B-NB | -3.82 | 120.22 | 124.26 |
| 20 | A | 805 | CLA | CMD-C2D-C3D | -3.82 | 118.83 | 127.61 |
| 20 | L | 207 | CLA | CMD-C2D-C3D | -3.82 | 118.83 | 127.61 |
| 20 | H | 109 | CLA | CHC-C4B-NB | 3.82 | 128.30 | 124.26 |
| 20 | 4 | 308 | CLA | C4A-NA-C1A | 3.82 | 108.42 | 106.71 |
| 20 | A | 817 | CLA | C4B-CHC-C1C | -3.82 | 117.29 | 126.34 |
| 20 | 1 | 204 | CLA | C3B-C2B-C1B | -3.82 | 102.56 | 107.16 |
| 20 | R | 108 | CLA | O2A-C1-C2 | 3.82 | 118.66 | 108.64 |
| 22 | B | 846 | BCR | C16-C17-C18 | -3.82 | 121.86 | 127.31 |
| 20 | 1 | 202 | CLA | O2D-CGD-CBD | 3.82 | 118.05 | 111.27 |
| 20 | B | 831 | CLA | CHC-C1C-NC | 3.81 | 129.99 | 124.20 |
| 20 | 2 | 304 | CLA | C1C-CHC-C4B | -3.81 | 116.63 | 126.13 |
| 20 | B | 822 | CLA | CHC-C1C-NC | 3.81 | 129.99 | 124.20 |
| 20 | A | 840 | CLA | C4B-CHC-C1C | -3.81 | 117.30 | 126.34 |
| 20 | B | 841 | CLA | CHD-C4C-NC | 3.81 | 130.21 | 124.20 |
| 20 | H | 102 | CLA | CHC-C1C-NC | 3.81 | 129.98 | 124.20 |
| 20 | B | 809 | CLA | CMB-C2B-C1B | 3.81 | 131.17 | 125.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | G | 102 | LMU | O1B-C1B-C2B | 3.81 | 117.97 | 108.10 |
| 20 | 3 | 317 | CLA | C1B-C2B-C3B | -3.81 | 103.41 | 107.03 |
| 20 | B | 821 | CLA | CHC-C1C-NC | 3.81 | 129.98 | 124.20 |
| 20 | H | 108 | CLA | CAA-C2A-C1A | 3.81 | 124.45 | 111.97 |
| 20 | 2 | 304 | CLA | CHB-C1B-NB | -3.81 | 120.42 | 124.27 |
| 20 | 1 | 207 | CLA | CHC-C1C-NC | 3.80 | 129.97 | 124.20 |
| 20 | L | 204 | CLA | CHB-C1B-NB | -3.80 | 120.23 | 124.26 |
| 20 | 3 | 317 | CLA | CHC-C1C-NC | 3.80 | 129.97 | 124.20 |
| 20 | B | 817 | CLA | CMD-C2D-C3D | -3.80 | 118.88 | 127.61 |
| 20 | K | 102 | CLA | CHD-C4C-C3C | -3.80 | 119.26 | 124.84 |
| 20 | 4 | 303 | CLA | CED-O2D-CGD | 3.80 | 124.53 | 115.94 |
| 20 | A | 850 | CLA | CHC-C1C-NC | 3.79 | 129.96 | 124.20 |
| 20 | I | 102 | CLA | CHC-C4B-NB | 3.79 | 128.27 | 124.26 |
| 20 | 1 | 211 | CLA | CHB-C1B-NB | -3.79 | 120.24 | 124.26 |
| 20 | B | 810 | CLA | C1-C2-C3 | -3.79 | 119.48 | 126.04 |
| 20 | B | 806 | CLA | CHC-C1C-NC | 3.79 | 129.95 | 124.20 |
| 20 | B | 812 | CLA | CHC-C1C-NC | 3.79 | 129.95 | 124.20 |
| 20 | 1 | 205 | CLA | CHC-C1C-NC | 3.79 | 129.95 | 124.20 |
| 20 | A | 841 | CLA | C4C-CHD-C1D | -3.79 | 116.75 | 126.11 |
| 20 | A | 823 | CLA | CHC-C1C-NC | 3.79 | 129.95 | 124.20 |
| 20 | 3 | 316 | CLA | C3B-C2B-C1B | -3.78 | 102.65 | 106.75 |
| 20 | 4 | 313 | CLA | CHD-C4C-C3C | -3.78 | 119.07 | 124.98 |
| 20 | 3 | 308 | CLA | C2D-C3D-C4D | -3.78 | 103.09 | 107.28 |
| 20 | A | 805 | CLA | CHD-C4C-C3C | -3.78 | 119.28 | 124.84 |
| 20 | A | 851 | CLA | CHD-C4C-C3C | -3.78 | 119.28 | 124.84 |
| 20 | 3 | 313 | CLA | CMD-C2D-C3D | -3.78 | 118.92 | 127.61 |
| 20 | A | 815 | CLA | C4B-CHC-C1C | -3.78 | 117.38 | 126.34 |
| 22 | B | 846 | BCR | C7-C8-C9 | -3.78 | 120.53 | 126.23 |
| 22 | A | 843 | BCR | C11-C10-C9 | -3.78 | 121.92 | 127.31 |
| 20 | 1 | 211 | CLA | C2B-C1B-NB | 3.78 | 112.76 | 110.23 |
| 20 | H | 101 | CLA | CMD-C2D-C3D | -3.78 | 118.93 | 127.61 |
| 22 | I | 101 | BCR | C38-C26-C27 | 3.77 | 120.87 | 113.62 |
| 20 | 2 | 305 | CLA | CHD-C4C-C3C | -3.77 | 119.29 | 124.84 |
| 20 | L | 204 | CLA | C4B-CHC-C1C | -3.77 | 117.39 | 126.34 |
| 20 | 1 | 208 | CLA | C2D-C3D-C4D | -3.77 | 103.10 | 107.28 |
| 20 | A | 836 | CLA | C3B-C2B-C1B | -3.77 | 102.61 | 107.16 |
| 20 | 1 | 212 | CLA | C2D-C3D-C4D | -3.77 | 103.10 | 107.28 |
| 20 | A | 841 | CLA | C3D-C4D-CHA | -3.77 | 117.04 | 124.98 |
| 20 | F | 201 | CLA | CGD-CBD-CAD | -3.77 | 98.52 | 110.73 |
| 20 | A | 840 | CLA | C4-C3-C5 | 3.77 | 121.61 | 115.27 |
| 22 | A | 843 | BCR | C7-C8-C9 | -3.77 | 120.54 | 126.23 |
| 20 | H | 108 | CLA | O2A-CGA-CBA | 3.77 | 123.74 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 311 | CLA | C3B-C2B-C1B | -3.77 | 102.67 | 106.75 |
| 20 | 4 | 311 | CLA | C4A-NA-C1A | 3.77 | 108.40 | 106.71 |
| 20 | 2 | 301 | CLA | C3D-C4D-CHA | -3.77 | 117.05 | 124.98 |
| 20 | B | 838 | CLA | C4-C3-C5 | 3.77 | 121.61 | 115.27 |
| 21 | B | 804 | LMU | C1'-O5'-C5' | 3.77 | 121.08 | 113.69 |
| 20 | B | 818 | CLA | CHD-C4C-C3C | -3.76 | 119.31 | 124.84 |
| 20 | A | 822 | CLA | O2D-CGD-CBD | 3.76 | 117.96 | 111.27 |
| 20 | B | 827 | CLA | C4-C3-C5 | 3.76 | 121.60 | 115.27 |
| 20 | 3 | 316 | CLA | C2D-C3D-C4D | -3.76 | 103.11 | 107.28 |
| 20 | A | 820 | CLA | CHC-C1C-NC | 3.76 | 129.91 | 124.20 |
| 20 | 2 | 303 | CLA | CAA-C2A-C3A | -3.76 | 102.48 | 112.78 |
| 20 | 3 | 301 | CLA | C4A-NA-C1A | 3.76 | 108.40 | 106.71 |
| 20 | J | 103 | CLA | CHB-C4A-NA | 3.76 | 129.71 | 124.51 |
| 20 | A | 805 | CLA | O2D-CGD-CBD | 3.76 | 117.95 | 111.27 |
| 20 | L | 201 | CLA | CMD-C2D-C3D | -3.76 | 118.97 | 127.61 |
| 20 | A | 803 | CLA | CHB-C1B-NB | -3.76 | 120.28 | 124.26 |
| 21 | 2 | 321 | LMU | O1B-C4'-C5' | 3.76 | 119.74 | 109.45 |
| 20 | 3 | 312 | CLA | C1C-CHC-C4B | -3.76 | 116.77 | 126.13 |
| 20 | A | 826 | CLA | CMD-C2D-C3D | -3.76 | 118.97 | 127.61 |
| 20 | 1 | 210 | CLA | CHC-C1C-NC | 3.76 | 129.90 | 124.20 |
| 20 | 1 | 210 | CLA | C4B-CHC-C1C | -3.75 | 117.44 | 126.34 |
| 21 | L | 205 | LMU | C1'-O5'-C5' | 3.75 | 121.05 | 113.69 |
| 20 | 4 | 302 | CLA | CHC-C1C-NC | 3.75 | 129.89 | 124.20 |
| 21 | A | 854 | LMU | C2'-C3'-C4' | 3.75 | 118.25 | 109.68 |
| 20 | 2 | 309 | CLA | CHC-C1C-NC | 3.75 | 129.76 | 124.23 |
| 20 | K | 103 | CLA | CHB-C4A-NA | 3.75 | 129.69 | 124.51 |
| 20 | 3 | 312 | CLA | C2D-C3D-C4D | -3.75 | 103.13 | 107.28 |
| 20 | A | 835 | CLA | CHD-C4C-C3C | -3.75 | 119.33 | 124.84 |
| 20 | B | 812 | CLA | CMD-C2D-C3D | -3.74 | 119.00 | 127.61 |
| 20 | A | 834 | CLA | CHD-C4C-C3C | -3.74 | 119.34 | 124.84 |
| 20 | L | 207 | CLA | CHD-C4C-C3C | -3.74 | 119.34 | 124.84 |
| 20 | K | 104 | CLA | CHC-C4B-NB | 3.74 | 128.22 | 124.26 |
| 20 | 1 | 212 | CLA | C1B-NB-C4B | -3.74 | 103.68 | 106.33 |
| 21 | 4 | 316 | LMU | C1B-O5B-C5B | 3.74 | 121.03 | 113.69 |
| 20 | 4 | 318 | CLA | O1D-CGD-CBD | -3.74 | 116.83 | 124.48 |
| 20 | 2 | 301 | CLA | CHD-C4C-NC | 3.74 | 129.98 | 124.21 |
| 20 | 1 | 206 | CLA | CHC-C1C-NC | 3.74 | 129.88 | 124.20 |
| 22 | B | 845 | BCR | C16-C17-C18 | -3.74 | 121.97 | 127.31 |
| 20 | B | 802 | CLA | CHC-C4B-NB | 3.74 | 128.21 | 124.26 |
| 20 | A | 839 | CLA | C3A-C2A-C1A | 3.74 | 106.94 | 101.34 |
| 20 | 2 | 304 | CLA | C2D-C3D-C4D | -3.74 | 103.14 | 107.28 |
| 21 | 2 | 313 | LMU | C1'-C2'-C3' | -3.73 | 102.22 | 110.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 3 | 306 | CLA | CHD-C1D-ND | 3.73 | 128.12 | 124.52 |
| 21 | R | 105 | LMU | O5B-C1B-C2B | 3.73 | 118.25 | 110.35 |
| 20 | H | 110 | CLA | C4B-CHC-C1C | -3.73 | 117.48 | 126.34 |
| 20 | A | 851 | CLA | C3B-C2B-C1B | -3.73 | 102.66 | 107.16 |
| 20 | L | 208 | CLA | O1D-CGD-CBD | -3.73 | 116.85 | 124.48 |
| 20 | 1 | 210 | CLA | CHC-C4B-NB | 3.73 | 128.21 | 124.26 |
| 20 | B | 827 | CLA | CMD-C2D-C3D | -3.73 | 119.04 | 127.61 |
| 20 | A | 803 | CLA | CHB-C4A-NA | 3.73 | 129.67 | 124.51 |
| 20 | 1 | 209 | CLA | CHD-C1D-ND | 3.73 | 128.12 | 124.52 |
| 21 | H | 103 | LMU | C2'-C3'-C4' | -3.73 | 101.17 | 109.68 |
| 20 | R | 108 | CLA | CHB-C1B-NB | -3.73 | 120.31 | 124.26 |
| 20 | B | 831 | CLA | CMD-C2D-C3D | -3.73 | 119.04 | 127.61 |
| 20 | A | 816 | CLA | C4B-CHC-C1C | -3.72 | 117.50 | 126.34 |
| 20 | B | 826 | CLA | CHC-C1C-NC | 3.72 | 129.85 | 124.20 |
| 21 | R | 102 | LMU | C1B-O5B-C5B | 3.72 | 121.00 | 113.69 |
| 20 | K | 104 | CLA | CAC-C3C-C4C | 3.72 | 129.64 | 124.81 |
| 20 | 4 | 313 | CLA | C4A-NA-C1A | 3.72 | 108.38 | 106.71 |
| 20 | A | 805 | CLA | CMB-C2B-C1B | 3.72 | 131.04 | 125.37 |
| 20 | 2 | 311 | CLA | CHC-C1C-NC | 3.72 | 129.85 | 124.20 |
| 20 | J | 103 | CLA | CHD-C4C-C3C | -3.72 | 119.37 | 124.84 |
| 20 | B | 832 | CLA | CHC-C1C-NC | 3.72 | 129.84 | 124.20 |
| 22 | G | 104 | BCR | C24-C23-C22 | -3.72 | 120.62 | 126.23 |
| 20 | A | 849 | CLA | CMD-C2D-C3D | -3.72 | 119.06 | 127.61 |
| 21 | 1 | 218 | LMU | O5'-C1'-C2' | 3.72 | 118.22 | 110.35 |
| 20 | 3 | 305 | CLA | C3B-C2B-C1B | -3.72 | 102.72 | 106.75 |
| 20 | A | 840 | CLA | CMD-C2D-C3D | -3.72 | 119.07 | 127.61 |
| 20 | L | 207 | CLA | C3B-C2B-C1B | -3.71 | 102.68 | 107.16 |
| 20 | 4 | 314 | CLA | C3D-C4D-CHA | -3.71 | 117.16 | 124.98 |
| 20 | B | 827 | CLA | CHC-C1C-NC | 3.71 | 129.84 | 124.20 |
| 20 | H | 101 | CLA | CHC-C4B-NB | 3.71 | 128.19 | 124.26 |
| 20 | B | 803 | CLA | C3B-C2B-C1B | -3.71 | 102.68 | 107.16 |
| 20 | L | 203 | CLA | C6-C5-C3 | -3.71 | 103.73 | 113.45 |
| 20 | H | 108 | CLA | O2D-CGD-O1D | -3.71 | 116.59 | 123.84 |
| 20 | B | 803 | CLA | CGD-CBD-CAD | 3.71 | 122.74 | 110.73 |
| 20 | 3 | 304 | CLA | C3B-C2B-C1B | -3.71 | 102.74 | 106.75 |
| 20 | B | 837 | CLA | CHC-C1C-NC | 3.70 | 129.82 | 124.20 |
| 20 | B | 811 | CLA | CHC-C1C-NC | 3.70 | 129.70 | 124.23 |
| 20 | A | 812 | CLA | CMD-C2D-C3D | -3.70 | 119.10 | 127.61 |
| 20 | A | 836 | CLA | CHD-C4C-C3C | -3.70 | 119.40 | 124.84 |
| 22 | I | 101 | BCR | C16-C15-C14 | -3.70 | 115.90 | 123.47 |
| 20 | B | 819 | CLA | CHC-C4B-NB | 3.70 | 128.17 | 124.26 |
| 20 | 4 | 312 | CLA | C3B-C2B-C1B | -3.70 | 102.75 | 106.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 310 | CLA | CMB-C2B-C1B | 3.70 | 131.00 | 125.37 |
| 20 | B | 808 | CLA | O2D-CGD-CBD | 3.70 | 117.83 | 111.27 |
| 23 | A | 842 | PQN | C14-C13-C15 | 3.69 | 121.49 | 115.27 |
| 20 | 4 | 315 | CLA | CHC-C1C-NC | 3.69 | 129.81 | 124.20 |
| 21 | E | 101 | LMU | C1B-O1B-C4' | -3.69 | 108.82 | 117.96 |
| 20 | B | 807 | CLA | C4B-CHC-C1C | -3.69 | 117.58 | 126.34 |
| 20 | R | 108 | CLA | CHC-C1C-NC | 3.69 | 129.80 | 124.20 |
| 20 | 4 | 309 | CLA | C1B-NB-C4B | -3.69 | 103.71 | 106.33 |
| 20 | 2 | 307 | CLA | O2D-CGD-O1D | -3.69 | 116.62 | 123.84 |
| 20 | 4 | 309 | CLA | C3B-C2B-C1B | -3.69 | 102.75 | 106.75 |
| 20 | 2 | 316 | CLA | C3B-C2B-C1B | -3.69 | 102.71 | 107.16 |
| 20 | B | 838 | CLA | O2D-CGD-O1D | -3.69 | 116.63 | 123.84 |
| 20 | B | 841 | CLA | CHC-C1C-NC | 3.69 | 129.80 | 124.20 |
| 20 | 3 | 314 | CLA | CHC-C1C-C2C | -3.69 | 116.49 | 126.73 |
| 20 | 4 | 302 | CLA | CAA-C2A-C3A | -3.69 | 107.50 | 116.10 |
| 20 | 4 | 314 | CLA | CHD-C1D-ND | 3.69 | 128.07 | 124.52 |
| 20 | 4 | 309 | CLA | C2D-C3D-C4D | -3.69 | 103.20 | 107.28 |
| 20 | 1 | 208 | CLA | C1B-NB-C4B | -3.69 | 103.72 | 106.33 |
| 20 | B | 811 | CLA | C4C-CHD-C1D | -3.69 | 117.00 | 126.11 |
| 20 | 2 | 315 | CLA | C3A-C4A-CHB | -3.68 | 119.40 | 123.91 |
| 22 | 2 | 317 | BCR | C7-C8-C9 | -3.68 | 120.67 | 126.23 |
| 20 | 1 | 215 | CLA | CMA-C3A-C4A | -3.68 | 101.89 | 111.77 |
| 20 | 3 | 301 | CLA | CHC-C1C-NC | 3.68 | 129.78 | 124.20 |
| 20 | B | 828 | CLA | C4B-CHC-C1C | -3.68 | 117.62 | 126.34 |
| 20 | 4 | 304 | CLA | CHB-C1B-NB | -3.68 | 120.37 | 124.26 |
| 20 | B | 816 | CLA | C4B-CHC-C1C | -3.67 | 117.62 | 126.34 |
| 22 | B | 845 | BCR | C8-C9-C10 | 3.67 | 124.58 | 118.94 |
| 21 | H | 103 | LMU | O1B-C4'-C3' | 3.67 | 117.05 | 107.28 |
| 20 | A | 811 | CLA | O2D-CGD-CBD | 3.67 | 117.79 | 111.27 |
| 20 | 1 | 201 | CLA | C3B-C2B-C1B | -3.67 | 102.73 | 107.16 |
| 20 | L | 203 | CLA | CHB-C1B-NB | -3.67 | 120.37 | 124.26 |
| 20 | A | 819 | CLA | C4B-CHC-C1C | -3.67 | 117.63 | 126.34 |
| 20 | A | 801 | CLA | O2A-CGA-CBA | 3.67 | 123.42 | 111.91 |
| 20 | 1 | 201 | CLA | CHD-C4C-C3C | -3.67 | 119.45 | 124.84 |
| 21 | G | 101 | LMU | C1-O1'-C1' | -3.67 | 107.76 | 113.84 |
| 20 | 2 | 310 | CLA | CMD-C2D-C3D | -3.67 | 119.18 | 127.61 |
| 20 | B | 828 | CLA | CHC-C1C-NC | 3.67 | 129.76 | 124.20 |
| 20 | 1 | 211 | CLA | CMB-C2B-C1B | 3.66 | 130.95 | 125.37 |
| 20 | A | 840 | CLA | O2D-CGD-O1D | -3.66 | 116.68 | 123.84 |
| 20 | 3 | 302 | CLA | C3D-C4D-CHA | -3.66 | 117.27 | 124.98 |
| 20 | 3 | 308 | CLA | C3D-C4D-CHA | -3.66 | 117.28 | 124.98 |
| 20 | A | 803 | CLA | CMD-C2D-C3D | -3.66 | 119.20 | 127.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | F | 207 | CLA | O2D-CGD-O1D | -3.65 | 116.70 | 123.84 |
| 20 | B | 803 | CLA | CHB-C1B-NB | -3.65 | 120.39 | 124.26 |
| 20 | A | 831 | CLA | CBC-CAC-C3C | -3.65 | 102.36 | 112.43 |
| 20 | 2 | 301 | CLA | CHC-C1C-NC | 3.65 | 129.62 | 124.23 |
| 20 | 1 | 205 | CLA | CBD-CHA-C1A | 3.65 | 133.28 | 127.43 |
| 20 | F | 207 | CLA | CED-O2D-CGD | 3.65 | 124.19 | 115.94 |
| 20 | 4 | 307 | CLA | C4C-CHD-C1D | -3.65 | 117.08 | 126.11 |
| 20 | A | 829 | CLA | CMD-C2D-C3D | -3.65 | 119.22 | 127.61 |
| 20 | A | 849 | CLA | CED-O2D-CGD | 3.65 | 124.19 | 115.94 |
| 22 | A | 845 | BCR | C30-C25-C26 | -3.65 | 117.47 | 122.61 |
| 20 | H | 101 | CLA | O2D-CGD-CBD | 3.65 | 117.75 | 111.27 |
| 20 | 1 | 201 | CLA | CAC-C3C-C4C | 3.65 | 129.54 | 124.81 |
| 20 | B | 839 | CLA | O2D-CGD-O1D | -3.65 | 116.71 | 123.84 |
| 20 | 4 | 313 | CLA | C4B-CHC-C1C | -3.64 | 117.69 | 126.34 |
| 20 | A | 818 | CLA | C6-C5-C3 | -3.64 | 103.90 | 113.45 |
| 20 | 4 | 311 | CLA | C3D-C4D-CHA | -3.64 | 117.31 | 124.98 |
| 20 | 3 | 305 | CLA | C1B-NB-C4B | -3.64 | 103.75 | 106.33 |
| 20 | A | 813 | CLA | CMD-C2D-C3D | -3.64 | 119.24 | 127.61 |
| 20 | A | 828 | CLA | CMD-C2D-C3D | -3.64 | 119.24 | 127.61 |
| 20 | B | 817 | CLA | CHB-C1B-NB | -3.64 | 120.40 | 124.26 |
| 20 | R | 108 | CLA | C1-C2-C3 | 3.64 | 132.34 | 126.04 |
| 20 | B | 832 | CLA | C3B-C2B-C1B | -3.64 | 102.77 | 107.16 |
| 22 | I | 103 | BCR | C8-C7-C6 | -3.64 | 116.99 | 127.20 |
| 20 | 2 | 305 | CLA | C3B-C2B-C1B | -3.64 | 102.77 | 107.16 |
| 20 | A | 816 | CLA | CMD-C2D-C3D | -3.63 | 119.25 | 127.61 |
| 20 | B | 810 | CLA | C3B-C2B-C1B | -3.63 | 102.78 | 107.16 |
| 20 | A | 832 | CLA | CHB-C1B-NB | -3.63 | 120.41 | 124.26 |
| 20 | B | 825 | CLA | C4A-NA-C1A | 3.63 | 108.34 | 106.71 |
| 20 | 1 | 201 | CLA | CHC-C1C-C2C | -3.63 | 116.65 | 126.73 |
| 20 | B | 842 | CLA | CBD-CHA-C1A | 3.63 | 133.24 | 127.43 |
| 21 | G | 101 | LMU | C1B-C2B-C3B | -3.63 | 102.44 | 110.00 |
| 20 | 1 | 207 | CLA | CAA-CBA-CGA | 3.63 | 123.85 | 113.25 |
| 20 | 4 | 307 | CLA | C3B-C2B-C1B | -3.63 | 102.82 | 106.75 |
| 20 | A | 801 | CLA | CBA-CAA-C2A | 3.63 | 124.57 | 113.86 |
| 20 | A | 850 | CLA | C3B-C2B-C1B | -3.63 | 102.78 | 107.16 |
| 20 | 1 | 212 | CLA | C3B-C2B-C1B | -3.63 | 102.82 | 106.75 |
| 21 | H | 105 | LMU | C2'-C3'-C4' | 3.62 | 117.96 | 109.68 |
| 20 | B | 814 | CLA | CMD-C2D-C3D | -3.62 | 119.28 | 127.61 |
| 20 | 3 | 313 | CLA | C4B-CHC-C1C | -3.62 | 117.75 | 126.34 |
| 20 | A | 822 | CLA | CHD-C4C-C3C | -3.62 | 119.52 | 124.84 |
| 20 | 4 | 302 | CLA | C4B-CHC-C1C | -3.62 | 117.75 | 126.34 |
| 20 | B | 812 | CLA | C4B-CHC-C1C | -3.62 | 117.75 | 126.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 312 | CLA | CHC-C1C-NC | 3.62 | 129.69 | 124.20 |
| 20 | B | 808 | CLA | CMD-C2D-C3D | -3.61 | 119.30 | 127.61 |
| 20 | L | 207 | CLA | O2D-CGD-O1D | -3.61 | 116.77 | 123.84 |
| 20 | A | 850 | CLA | O2A-CGA-CBA | 3.61 | 123.25 | 111.91 |
| 20 | A | 841 | CLA | C4A-NA-C1A | 3.61 | 108.33 | 106.71 |
| 21 | C | 101 | LMU | C1B-C2B-C3B | 3.61 | 117.52 | 110.00 |
| 20 | 1 | 202 | CLA | CED-O2D-CGD | 3.61 | 124.10 | 115.94 |
| 21 | H | 106 | LMU | O5B-C5B-C4B | 3.61 | 116.25 | 109.69 |
| 20 | 3 | 304 | CLA | C2D-C3D-C4D | -3.61 | 103.28 | 107.28 |
| 20 | A | 810 | CLA | CHD-C4C-C3C | -3.61 | 119.54 | 124.84 |
| 22 | I | 103 | BCR | C38-C26-C25 | -3.61 | 120.48 | 124.53 |
| 20 | B | 810 | CLA | CHB-C1B-NB | -3.61 | 120.44 | 124.26 |
| 20 | 1 | 214 | CLA | CHB-C1B-NB | -3.60 | 120.62 | 124.27 |
| 20 | I | 102 | CLA | CHC-C1C-NC | 3.60 | 129.67 | 124.20 |
| 22 | B | 844 | BCR | C38-C26-C25 | -3.60 | 120.48 | 124.53 |
| 20 | A | 802 | CLA | CHD-C4C-NC | 3.60 | 129.77 | 124.21 |
| 20 | 4 | 308 | CLA | C1C-CHC-C4B | -3.60 | 117.15 | 126.13 |
| 22 | A | 843 | BCR | C33-C5-C6 | -3.60 | 120.48 | 124.53 |
| 20 | A | 835 | CLA | O2D-CGD-O1D | -3.60 | 116.80 | 123.84 |
| 21 | R | 101 | LMU | C1B-O1B-C4' | -3.60 | 109.06 | 117.96 |
| 20 | L | 201 | CLA | C3B-C2B-C1B | -3.60 | 102.82 | 107.16 |
| 20 | A | 816 | CLA | C4-C3-C5 | 3.60 | 121.32 | 115.27 |
| 20 | B | 838 | CLA | C3B-C2B-C1B | -3.60 | 102.82 | 107.16 |
| 20 | 2 | 309 | CLA | C3D-C4D-CHA | -3.60 | 117.40 | 124.98 |
| 22 | L | 209 | BCR | C36-C18-C19 | 3.60 | 123.75 | 118.08 |
| 20 | A | 837 | CLA | C4A-NA-C1A | 3.60 | 108.32 | 106.71 |
| 20 | J | 103 | CLA | O2A-CGA-CBA | 3.60 | 123.19 | 111.91 |
| 20 | L | 203 | CLA | CHC-C1C-NC | 3.60 | 129.66 | 124.20 |
| 20 | A | 809 | CLA | O2A-C1-C2 | 3.59 | 118.07 | 108.64 |
| 20 | 4 | 307 | CLA | CHD-C4C-NC | 3.59 | 129.75 | 124.21 |
| 20 | L | 207 | CLA | CHB-C4A-NA | 3.59 | 129.47 | 124.51 |
| 20 | 3 | 307 | CLA | CMD-C2D-C3D | -3.59 | 119.36 | 127.61 |
| 20 | G | 105 | CLA | CMD-C2D-C3D | -3.58 | 119.37 | 127.61 |
| 20 | A | 823 | CLA | C4-C3-C5 | 3.58 | 121.30 | 115.27 |
| 20 | A | 817 | CLA | O2A-CGA-CBA | 3.58 | 123.15 | 111.91 |
| 20 | 3 | 314 | CLA | C3B-C2B-C1B | -3.58 | 102.84 | 107.16 |
| 20 | B | 820 | CLA | CMD-C2D-C3D | -3.58 | 119.38 | 127.61 |
| 20 | B | 811 | CLA | CHD-C4C-NC | 3.58 | 129.73 | 124.21 |
| 20 | I | 102 | CLA | C4B-CHC-C1C | -3.58 | 117.86 | 126.34 |
| 20 | A | 808 | CLA | CMD-C2D-C3D | -3.58 | 119.39 | 127.61 |
| 20 | 4 | 304 | CLA | CHC-C1C-C2C | -3.57 | 116.80 | 126.73 |
| 20 | B | 842 | CLA | CHB-C1B-NB | -3.57 | 120.47 | 124.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 818 | CLA | CHC-C4B-NB | 3.57 | 128.04 | 124.26 |
| 20 | B | 802 | CLA | CMD-C2D-C3D | -3.57 | 119.40 | 127.61 |
| 20 | B | 823 | CLA | O2D-CGD-CBD | 3.57 | 117.61 | 111.27 |
| 20 | 4 | 308 | CLA | C2D-C3D-C4D | -3.57 | 103.33 | 107.28 |
| 20 | A | 840 | CLA | CHC-C4B-NB | 3.57 | 128.03 | 124.26 |
| 20 | 3 | 313 | CLA | CHC-C1C-NC | 3.57 | 129.61 | 124.20 |
| 20 | B | 825 | CLA | CHC-C1C-NC | 3.57 | 129.61 | 124.20 |
| 20 | B | 832 | CLA | C4-C3-C5 | 3.56 | 121.27 | 115.27 |
| 22 | L | 209 | BCR | C24-C23-C22 | -3.56 | 120.85 | 126.23 |
| 20 | 1 | 215 | CLA | C4B-CHC-C1C | -3.56 | 117.89 | 126.34 |
| 20 | 2 | 308 | CLA | CHD-C1D-ND | 3.56 | 127.95 | 124.52 |
| 20 | A | 811 | CLA | CHB-C1B-NB | -3.56 | 120.49 | 124.26 |
| 20 | A | 827 | CLA | CHD-C4C-C3C | -3.56 | 119.61 | 124.84 |
| 20 | A | 813 | CLA | C3B-C2B-C1B | -3.56 | 102.86 | 107.16 |
| 20 | B | 819 | CLA | C3B-C4B-NB | -3.56 | 107.21 | 110.52 |
| 20 | B | 810 | CLA | CMD-C2D-C3D | -3.56 | 119.43 | 127.61 |
| 20 | 2 | 308 | CLA | C1B-NB-C4B | -3.56 | 103.81 | 106.33 |
| 20 | A | 808 | CLA | CHC-C1C-NC | 3.56 | 129.60 | 124.20 |
| 21 | A | 847 | LMU | C3B-C4B-C5B | -3.56 | 103.89 | 110.24 |
| 20 | 2 | 307 | CLA | CHC-C1C-C2C | -3.56 | 116.85 | 126.73 |
| 20 | 1 | 212 | CLA | C3D-C4D-CHA | -3.56 | 117.49 | 124.98 |
| 20 | I | 102 | CLA | CMD-C2D-C3D | -3.55 | 119.44 | 127.61 |
| 20 | 2 | 307 | CLA | C4A-NA-C1A | 3.55 | 108.30 | 106.71 |
| 20 | B | 809 | CLA | C6-C5-C3 | -3.55 | 104.15 | 113.45 |
| 22 | L | 209 | BCR | C30-C25-C26 | -3.55 | 117.61 | 122.61 |
| 20 | B | 838 | CLA | CHB-C1B-NB | -3.55 | 120.50 | 124.26 |
| 20 | 2 | 302 | CLA | C4B-CHC-C1C | -3.55 | 117.92 | 126.34 |
| 20 | 1 | 215 | CLA | C1-C2-C3 | -3.55 | 119.91 | 126.04 |
| 20 | B | 841 | CLA | CMD-C2D-C3D | -3.55 | 119.45 | 127.61 |
| 20 | 2 | 309 | CLA | C2D-C3D-C4D | -3.55 | 103.35 | 107.28 |
| 22 | B | 844 | BCR | C3-C4-C5 | -3.54 | 107.75 | 114.08 |
| 20 | L | 208 | CLA | CHC-C4B-NB | 3.54 | 128.00 | 124.26 |
| 20 | A | 815 | CLA | CHD-C4C-C3C | -3.53 | 119.65 | 124.84 |
| 20 | 4 | 318 | CLA | C4A-NA-C1A | 3.53 | 108.29 | 106.71 |
| 20 | 4 | 306 | CLA | C6-C5-C3 | -3.53 | 108.84 | 114.62 |
| 20 | 3 | 304 | CLA | C3D-C4D-CHA | -3.53 | 117.55 | 124.98 |
| 21 | L | 205 | LMU | O5B-C5B-C4B | -3.53 | 103.28 | 109.69 |
| 22 | B | 845 | BCR | C37-C22-C21 | -3.53 | 117.98 | 122.92 |
| 20 | 4 | 309 | CLA | CHD-C1D-ND | 3.53 | 127.92 | 124.52 |
| 20 | L | 203 | CLA | CMB-C2B-C1B | 3.53 | 130.74 | 125.37 |
| 20 | A | 814 | CLA | C4C-CHD-C1D | -3.53 | 117.39 | 126.11 |
| 20 | 4 | 313 | CLA | CMD-C2D-C3D | -3.53 | 119.50 | 127.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 824 | CLA | O2D-CGD-O1D | -3.53 | 116.94 | 123.84 |
| 20 | B | 829 | CLA | CHC-C1C-NC | 3.52 | 129.55 | 124.20 |
| 20 | 3 | 314 | CLA | C4A-NA-C1A | 3.52 | 108.29 | 106.71 |
| 20 | 1 | 215 | CLA | CHB-C4A-NA | 3.52 | 129.38 | 124.51 |
| 20 | H | 110 | CLA | CHC-C1C-NC | 3.52 | 129.55 | 124.20 |
| 20 | 4 | 311 | CLA | C1B-NB-C4B | -3.52 | 103.83 | 106.33 |
| 22 | B | 844 | BCR | C27-C26-C25 | -3.52 | 117.62 | 122.73 |
| 20 | 4 | 310 | CLA | CHC-C4B-NB | 3.52 | 127.98 | 124.26 |
| 20 | 4 | 306 | CLA | O2D-CGD-CBD | 3.52 | 117.52 | 111.27 |
| 20 | A | 821 | CLA | CMB-C2B-C1B | 3.52 | 130.72 | 125.37 |
| 20 | 1 | 208 | CLA | C3D-C4D-CHA | -3.52 | 117.58 | 124.98 |
| 20 | L | 204 | CLA | CMD-C2D-C3D | -3.51 | 119.53 | 127.61 |
| 20 | 2 | 304 | CLA | C3C-C4C-CHD | -3.51 | 117.53 | 125.22 |
| 20 | B | 831 | CLA | CHD-C4C-NC | 3.51 | 129.74 | 124.20 |
| 20 | A | 807 | CLA | C3B-C2B-C1B | -3.51 | 102.92 | 107.16 |
| 20 | H | 109 | CLA | CMD-C2D-C3D | -3.51 | 119.54 | 127.61 |
| 20 | A | 809 | CLA | CHB-C1B-NB | -3.51 | 120.54 | 124.26 |
| 20 | 4 | 314 | CLA | C4A-NA-C1A | 3.51 | 108.28 | 106.71 |
| 20 | 1 | 215 | CLA | CED-O2D-CGD | 3.51 | 123.88 | 115.94 |
| 20 | A | 818 | CLA | O2D-CGD-O1D | -3.51 | 116.98 | 123.84 |
| 20 | 1 | 213 | CLA | CBA-CAA-C2A | -3.50 | 103.52 | 113.86 |
| 22 | A | 845 | BCR | C16-C17-C18 | -3.50 | 122.31 | 127.31 |
| 20 | A | 851 | CLA | CHB-C1B-NB | -3.50 | 120.55 | 124.26 |
| 20 | A | 801 | CLA | CHD-C4C-NC | 3.50 | 129.72 | 124.20 |
| 20 | A | 839 | CLA | C3B-C2B-C1B | -3.50 | 102.94 | 107.16 |
| 20 | A | 816 | CLA | C1-C2-C3 | -3.50 | 119.99 | 126.04 |
| 20 | 3 | 312 | CLA | C3D-C4D-CHA | -3.50 | 117.61 | 124.98 |
| 20 | A | 838 | CLA | O2D-CGD-O1D | -3.50 | 117.00 | 123.84 |
| 22 | B | 845 | BCR | C27-C26-C25 | -3.49 | 117.66 | 122.73 |
| 20 | 2 | 306 | CLA | C3D-C4D-CHA | -3.49 | 117.62 | 124.98 |
| 22 | J | 102 | BCR | C24-C23-C22 | -3.49 | 120.96 | 126.23 |
| 20 | 1 | 208 | CLA | C4A-NA-C1A | 3.49 | 108.28 | 106.71 |
| 20 | B | 833 | CLA | C4A-NA-C1A | 3.49 | 108.28 | 106.71 |
| 20 | A | 822 | CLA | C3B-C2B-C1B | -3.49 | 102.95 | 107.16 |
| 20 | A | 816 | CLA | CHC-C1C-NC | 3.49 | 129.50 | 124.20 |
| 20 | A | 832 | CLA | CHD-C4C-C3C | -3.49 | 119.71 | 124.84 |
| 20 | B | 842 | CLA | CMD-C2D-C3D | -3.49 | 119.58 | 127.61 |
| 20 | 3 | 303 | CLA | C4B-CHC-C1C | -3.49 | 118.07 | 126.34 |
| 20 | B | 842 | CLA | CHC-C1C-NC | 3.49 | 129.49 | 124.20 |
| 20 | 4 | 308 | CLA | CHB-C1B-NB | -3.49 | 120.75 | 124.27 |
| 20 | B | 816 | CLA | CHC-C1C-NC | 3.48 | 129.49 | 124.20 |
| 21 | 2 | 313 | LMU | O5'-C5'-C4' | -3.48 | 102.41 | 109.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 20 | B | 842 | CLA | C1B-C2B-C3B | -3.48 | 103.72 | 107.03 |
| 22 | I | 101 | BCR | C38-C26-C25 | -3.48 | 120.62 | 124.50 |
| 20 | A | 821 | CLA | CHD-C4C-C3C | -3.48 | 119.72 | 124.84 |
| 20 | A | 811 | CLA | C3B-C4B-NB | -3.48 | 107.28 | 110.52 |
| 20 | 3 | 316 | CLA | C1B-NB-C4B | -3.48 | 103.86 | 106.33 |
| 20 | F | 207 | CLA | CMD-C2D-C3D | -3.48 | 119.61 | 127.61 |
| 20 | B | 821 | CLA | C4A-NA-C1A | 3.48 | 108.27 | 106.71 |
| 20 | 4 | 313 | CLA | CHC-C1C-NC | 3.48 | 129.48 | 124.20 |
| 20 | 4 | 318 | CLA | CHB-C4A-NA | 3.48 | 129.32 | 124.51 |
| 21 | A | 847 | LMU | O5B-C1B-C2B | 3.48 | 117.71 | 110.35 |
| 20 | A | 821 | CLA | CAA-C2A-C1A | 3.47 | 119.83 | 112.14 |
| 20 | A | 814 | CLA | CHC-C4B-NB | 3.47 | 127.79 | 124.27 |
| 21 | R | 106 | LMU | C1B-O5B-C5B | 3.47 | 120.50 | 113.69 |
| 20 | 2 | 304 | CLA | CHC-C4B-NB | 3.47 | 127.79 | 124.27 |
| 20 | 4 | 304 | CLA | CAC-C3C-C4C | 3.47 | 129.31 | 124.81 |
| 20 | A | 826 | CLA | CHC-C1C-NC | 3.47 | 129.47 | 124.20 |
| 20 | F | 206 | CLA | C4B-CHC-C1C | -3.47 | 118.11 | 126.34 |
| 20 | A | 835 | CLA | CHC-C4B-NB | 3.47 | 127.93 | 124.26 |
| 20 | 1 | 204 | CLA | CED-O2D-CGD | 3.47 | 123.78 | 115.94 |
| 20 | H | 110 | CLA | CED-O2D-CGD | 3.47 | 123.78 | 115.94 |
| 20 | 2 | 302 | CLA | C3B-C2B-C1B | -3.47 | 102.98 | 107.16 |
| 20 | A | 816 | CLA | C4A-NA-C1A | 3.47 | 108.26 | 106.71 |
| 20 | B | 802 | CLA | CHB-C4A-NA | 3.47 | 129.30 | 124.51 |
| 20 | H | 101 | CLA | CHB-C1B-NB | -3.46 | 120.59 | 124.26 |
| 20 | 1 | 215 | CLA | CHC-C1C-NC | 3.46 | 129.46 | 124.20 |
| 21 | L | 206 | LMU | C1B-O1B-C4' | -3.46 | 109.40 | 117.96 |
| 20 | B | 802 | CLA | C5-C3-C2 | -3.46 | 114.12 | 121.12 |
| 20 | 3 | 310 | CLA | C4A-NA-C1A | 3.46 | 108.26 | 106.71 |
| 20 | 1 | 209 | CLA | C1C-CHC-C4B | -3.46 | 117.52 | 126.13 |
| 20 | B | 825 | CLA | O2A-CGA-CBA | 3.46 | 122.75 | 111.91 |
| 20 | B | 830 | CLA | O2D-CGD-O1D | -3.46 | 117.08 | 123.84 |
| 20 | 1 | 206 | CLA | CMD-C2D-C3D | -3.46 | 119.67 | 127.61 |
| 22 | F | 203 | BCR | C33-C5-C6 | -3.45 | 120.65 | 124.53 |
| 22 | A | 843 | BCR | C33-C5-C4 | 3.45 | 120.25 | 113.62 |
| 20 | 3 | 301 | CLA | CHB-C1B-NB | -3.45 | 120.60 | 124.26 |
| 20 | A | 831 | CLA | CAC-C3C-C4C | 3.45 | 129.29 | 124.81 |
| 20 | B | 839 | CLA | C1D-ND-C4D | -3.45 | 103.89 | 106.33 |
| 20 | 2 | 307 | CLA | CHB-C1B-NB | -3.44 | 120.61 | 124.26 |
| 20 | 1 | 209 | CLA | C1B-NB-C4B | -3.44 | 103.89 | 106.33 |
| 20 | B | 813 | CLA | CHD-C4C-C3C | -3.44 | 119.78 | 124.84 |
| 20 | G | 105 | CLA | C4B-CHC-C1C | -3.44 | 118.17 | 126.34 |
| 20 | 2 | 306 | CLA | C1B-NB-C4B | -3.44 | 103.89 | 106.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 819 | CLA | C3B-C2B-C1B | -3.44 | 103.01 | 107.16 |
| 20 | 3 | 302 | CLA | C3B-C2B-C1B | -3.44 | 103.02 | 106.75 |
| 20 | B | 811 | CLA | C4A-NA-C1A | 3.44 | 108.25 | 106.71 |
| 20 | A | 808 | CLA | CAA-C2A-C1A | -3.44 | 100.70 | 111.97 |
| 20 | B | 825 | CLA | CMD-C2D-C3D | -3.44 | 119.70 | 127.61 |
| 20 | A | 807 | CLA | CHC-C1C-NC | 3.44 | 129.42 | 124.20 |
| 20 | 4 | 305 | CLA | CAC-C3C-C4C | 3.44 | 129.27 | 124.81 |
| 20 | A | 809 | CLA | CHD-C4C-NC | 3.44 | 129.62 | 124.20 |
| 20 | K | 103 | CLA | O2A-CGA-CBA | 3.44 | 122.69 | 111.91 |
| 20 | 4 | 311 | CLA | C2D-C3D-C4D | -3.43 | 103.47 | 107.28 |
| 22 | I | 103 | BCR | C15-C14-C13 | 3.43 | 132.21 | 127.31 |
| 20 | 2 | 312 | CLA | CAA-C2A-C3A | -3.43 | 103.38 | 112.78 |
| 20 | 4 | 317 | CLA | CAA-CBA-CGA | -3.43 | 103.23 | 113.25 |
| 20 | R | 107 | CLA | CED-O2D-CGD | 3.43 | 123.69 | 115.94 |
| 22 | B | 801 | BCR | C33-C5-C4 | 3.43 | 120.20 | 113.62 |
| 20 | 3 | 314 | CLA | C4-C3-C5 | 3.43 | 121.04 | 115.27 |
| 21 | K | 105 | LMU | C1B-C2B-C3B | 3.43 | 117.14 | 110.00 |
| 21 | B | 805 | LMU | C3B-C4B-C5B | -3.42 | 104.13 | 110.24 |
| 20 | 1 | 210 | CLA | C1B-C2B-C3B | -3.42 | 103.78 | 107.03 |
| 20 | B | 802 | CLA | C3B-C2B-C1B | -3.42 | 103.03 | 107.16 |
| 20 | B | 825 | CLA | C3B-C2B-C1B | -3.42 | 103.03 | 107.16 |
| 21 | A | 853 | LMU | C2'-C3'-C4' | 3.42 | 117.49 | 109.68 |
| 21 | G | 101 | LMU | C1'-C2'-C3' | -3.42 | 102.87 | 110.00 |
| 22 | A | 844 | BCR | C33-C5-C4 | 3.42 | 120.18 | 113.62 |
| 20 | F | 207 | CLA | CHC-C1C-NC | 3.42 | 129.39 | 124.20 |
| 20 | A | 839 | CLA | O2A-CGA-CBA | 3.42 | 122.63 | 111.91 |
| 20 | A | 839 | CLA | CHC-C1C-C2C | -3.42 | 117.24 | 126.73 |
| 20 | 1 | 215 | CLA | CMD-C2D-C3D | -3.42 | 119.76 | 127.61 |
| 20 | 3 | 304 | CLA | CHB-C1B-NB | -3.41 | 120.82 | 124.27 |
| 20 | B | 810 | CLA | O2A-CGA-CBA | 3.41 | 122.61 | 111.91 |
| 20 | B | 824 | CLA | CMD-C2D-C3D | -3.41 | 119.77 | 127.61 |
| 20 | A | 809 | CLA | C4A-NA-C1A | 3.41 | 108.24 | 106.71 |
| 20 | B | 820 | CLA | C4A-NA-C1A | 3.41 | 108.24 | 106.71 |
| 20 | B | 850 | CLA | CHB-C4A-NA | 3.41 | 129.22 | 124.51 |
| 20 | 4 | 312 | CLA | C4A-NA-C1A | 3.41 | 108.24 | 106.71 |
| 20 | B | 802 | CLA | CHB-C1B-NB | -3.40 | 120.66 | 124.26 |
| 20 | 3 | 307 | CLA | C3C-C4C-NC | -3.40 | 106.76 | 110.57 |
| 20 | B | 811 | CLA | C3B-C2B-C1B | -3.40 | 103.07 | 106.75 |
| 20 | B | 813 | CLA | CHB-C1B-NB | -3.40 | 120.66 | 124.26 |
| 20 | 2 | 316 | CLA | C4B-CHC-C1C | -3.40 | 118.27 | 126.34 |
| 20 | 4 | 308 | CLA | C3D-C4D-CHA | -3.40 | 117.82 | 124.98 |
| 20 | A | 826 | CLA | O2A-CGA-CBA | 3.40 | 122.57 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | F | 202 | LMU | C1B-O5B-C5B | 3.40 | 120.36 | 113.69 |
| 20 | 1 | 211 | CLA | C1-C2-C3 | -3.40 | 120.17 | 126.04 |
| 21 | A | 853 | LMU | O1'-C1'-C2' | 3.40 | 113.61 | 108.30 |
| 21 | A | 853 | LMU | C1B-C2B-C3B | 3.40 | 117.07 | 110.00 |
| 20 | 3 | 317 | CLA | CHB-C1B-NB | -3.39 | 120.67 | 124.26 |
| 20 | 1 | 203 | CLA | O2D-CGD-O1D | -3.39 | 117.21 | 123.84 |
| 20 | 1 | 210 | CLA | CHB-C1B-NB | -3.39 | 120.67 | 124.26 |
| 20 | 2 | 312 | CLA | CAA-C2A-C1A | -3.39 | 100.86 | 111.97 |
| 20 | B | 822 | CLA | CHB-C4A-NA | 3.39 | 129.20 | 124.51 |
| 20 | A | 839 | CLA | O2D-CGD-O1D | -3.39 | 117.21 | 123.84 |
| 20 | B | 829 | CLA | O2A-CGA-CBA | 3.39 | 122.54 | 111.91 |
| 21 | R | 102 | LMU | C1B-C2B-C3B | 3.39 | 117.05 | 110.00 |
| 20 | 2 | 301 | CLA | C1B-NB-C4B | -3.39 | 103.93 | 106.33 |
| 20 | B | 815 | CLA | CMB-C2B-C1B | 3.39 | 130.53 | 125.37 |
| 20 | A | 814 | CLA | C3B-C2B-C1B | -3.38 | 103.09 | 106.75 |
| 21 | 4 | 319 | LMU | C1'-C2'-C3' | 3.38 | 117.04 | 110.00 |
| 20 | L | 208 | CLA | C4B-CHC-C1C | -3.38 | 118.32 | 126.34 |
| 20 | 1 | 206 | CLA | C4A-NA-C1A | 3.38 | 108.22 | 106.71 |
| 20 | B | 823 | CLA | CHD-C4C-C3C | -3.38 | 119.88 | 124.84 |
| 21 | H | 106 | LMU | C1B-C2B-C3B | 3.37 | 117.02 | 110.00 |
| 20 | A | 809 | CLA | O2A-CGA-CBA | 3.37 | 122.49 | 111.91 |
| 22 | F | 203 | BCR | C16-C17-C18 | -3.37 | 122.50 | 127.31 |
| 20 | A | 809 | CLA | C3B-C2B-C1B | -3.37 | 103.09 | 107.16 |
| 20 | L | 204 | CLA | CHC-C1C-NC | 3.37 | 129.32 | 124.20 |
| 20 | B | 829 | CLA | CHB-C4A-NA | 3.37 | 129.17 | 124.51 |
| 20 | A | 833 | CLA | CHD-C4C-C3C | -3.37 | 119.89 | 124.84 |
| 20 | 2 | 308 | CLA | C3D-C4D-CHA | -3.37 | 117.88 | 124.98 |
| 21 | R | 105 | LMU | C2'-C3'-C4' | 3.37 | 117.37 | 109.68 |
| 20 | B | 810 | CLA | CHB-C4A-NA | 3.37 | 129.17 | 124.51 |
| 20 | A | 851 | CLA | O2D-CGD-O1D | -3.36 | 117.26 | 123.84 |
| 20 | A | 818 | CLA | C4A-NA-C1A | 3.36 | 108.22 | 106.71 |
| 20 | 2 | 309 | CLA | C3B-C2B-C1B | -3.36 | 103.11 | 106.75 |
| 20 | H | 102 | CLA | CHB-C1B-NB | -3.36 | 120.70 | 124.26 |
| 20 | H | 108 | CLA | CAA-C2A-C3A | -3.36 | 103.58 | 112.78 |
| 20 | A | 836 | CLA | CHC-C4B-NB | 3.36 | 127.81 | 124.26 |
| 20 | A | 827 | CLA | C1-O2A-CGA | 3.36 | 125.25 | 116.44 |
| 20 | 3 | 309 | CLA | C3D-C4D-CHA | -3.35 | 117.92 | 124.98 |
| 20 | 4 | 314 | CLA | C2D-C3D-C4D | -3.35 | 103.56 | 107.28 |
| 20 | H | 108 | CLA | CMD-C2D-C3D | -3.35 | 119.90 | 127.61 |
| 20 | F | 206 | CLA | C3B-C2B-C1B | -3.35 | 103.12 | 107.16 |
| 20 | 4 | 313 | CLA | CMB-C2B-C1B | 3.35 | 130.47 | 125.37 |
| 21 | A | 846 | LMU | C1B-O5B-C5B | 3.35 | 120.26 | 113.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 850 | CLA | O2A-CGA-CBA | 3.35 | 122.41 | 111.91 |
| 20 | B | 832 | CLA | O2D-CGD-O1D | -3.35 | 117.29 | 123.84 |
| 20 | B | 820 | CLA | C3B-C2B-C1B | -3.35 | 103.12 | 107.16 |
| 20 | 2 | 307 | CLA | CMD-C2D-C3D | -3.35 | 119.92 | 127.61 |
| 22 | 2 | 317 | BCR | C15-C14-C13 | -3.35 | 122.53 | 127.31 |
| 20 | B | 821 | CLA | C3B-C2B-C1B | -3.35 | 103.12 | 107.16 |
| 20 | B | 808 | CLA | O2A-CGA-CBA | 3.35 | 122.41 | 111.91 |
| 22 | B | 844 | BCR | C16-C17-C18 | -3.34 | 122.54 | 127.31 |
| 20 | K | 103 | CLA | CMA-C3A-C4A | -3.34 | 102.79 | 111.77 |
| 20 | I | 102 | CLA | O2A-CGA-CBA | 3.34 | 122.39 | 111.91 |
| 20 | A | 815 | CLA | O2A-CGA-CBA | 3.34 | 122.39 | 111.91 |
| 22 | B | 846 | BCR | C28-C27-C26 | -3.34 | 108.11 | 114.08 |
| 20 | 2 | 315 | CLA | C1B-NB-C4B | -3.34 | 103.97 | 106.33 |
| 20 | H | 108 | CLA | C1-C2-C3 | 3.34 | 131.81 | 126.04 |
| 20 | 4 | 318 | CLA | CHD-C4C-NC | 3.34 | 129.46 | 124.20 |
| 20 | B | 820 | CLA | C1-C2-C3 | -3.33 | 120.28 | 126.04 |
| 20 | B | 803 | CLA | CHC-C4B-NB | 3.33 | 127.79 | 124.26 |
| 20 | A | 824 | CLA | CAC-C3C-C4C | 3.33 | 129.13 | 124.81 |
| 20 | 4 | 311 | CLA | CHD-C1D-ND | 3.33 | 127.73 | 124.52 |
| 20 | B | 818 | CLA | O2D-CGD-O1D | -3.33 | 117.33 | 123.84 |
| 20 | A | 832 | CLA | CHB-C4A-NA | 3.33 | 129.12 | 124.51 |
| 20 | 4 | 305 | CLA | O2D-CGD-O1D | -3.33 | 117.33 | 123.84 |
| 22 | B | 846 | BCR | C24-C23-C22 | -3.33 | 121.20 | 126.23 |
| 20 | A | 801 | CLA | CHC-C1C-C2C | -3.33 | 117.48 | 126.73 |
| 20 | A | 818 | CLA | CMB-C2B-C1B | 3.33 | 130.44 | 125.37 |
| 20 | F | 201 | CLA | C1-O2A-CGA | 3.33 | 125.17 | 116.44 |
| 20 | H | 102 | CLA | C3B-C2B-C1B | -3.33 | 103.15 | 107.16 |
| 21 | K | 105 | LMU | O5B-C5B-C6B | 3.33 | 114.70 | 106.44 |
| 20 | 3 | 302 | CLA | C2D-C3D-C4D | -3.33 | 103.60 | 107.28 |
| 20 | A | 806 | CLA | CHB-C1B-NB | -3.32 | 120.74 | 124.26 |
| 20 | 2 | 306 | CLA | C2C-C1C-CHC | -3.32 | 117.71 | 125.67 |
| 20 | 3 | 301 | CLA | CMB-C2B-C1B | 3.32 | 130.43 | 125.37 |
| 20 | A | 811 | CLA | CHD-C4C-C3C | -3.32 | 119.95 | 124.84 |
| 20 | 3 | 306 | CLA | C3D-C4D-CHA | -3.32 | 117.98 | 124.98 |
| 20 | A | 849 | CLA | CHB-C1B-NB | -3.32 | 120.74 | 124.26 |
| 20 | R | 108 | CLA | C4A-NA-C1A | 3.32 | 108.20 | 106.71 |
| 20 | 2 | 303 | CLA | C3B-C2B-C1B | -3.32 | 103.15 | 107.16 |
| 20 | A | 813 | CLA | CHB-C1B-NB | -3.32 | 120.74 | 124.26 |
| 20 | A | 838 | CLA | O2A-CGA-CBA | 3.32 | 122.32 | 111.91 |
| 20 | B | 831 | CLA | O2D-CGD-O1D | -3.31 | 117.36 | 123.84 |
| 21 | 2 | 320 | LMU | C3B-C4B-C5B | -3.31 | 104.33 | 110.24 |
| 22 | B | 847 | BCR | C7-C8-C9 | -3.31 | 121.23 | 126.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | F | 206 | CLA | CMA-C3A-C2A | -3.31 | 108.37 | 116.10 |
| 20 | L | 208 | CLA | CMD-C2D-C3D | -3.31 | 120.00 | 127.61 |
| 20 | 1 | 206 | CLA | C3B-C2B-C1B | -3.31 | 103.17 | 107.16 |
| 20 | 1 | 212 | CLA | CHD-C1D-ND | 3.31 | 127.71 | 124.52 |
| 20 | 2 | 304 | CLA | C3D-C4D-CHA | -3.31 | 118.02 | 124.98 |
| 20 | 3 | 306 | CLA | C2D-C3D-C4D | -3.31 | 103.62 | 107.28 |
| 20 | B | 806 | CLA | O2D-CGD-O1D | -3.31 | 117.38 | 123.84 |
| 20 | A | 827 | CLA | O2D-CGD-O1D | -3.30 | 117.38 | 123.84 |
| 20 | 2 | 315 | CLA | C3C-C4C-CHD | -3.30 | 117.98 | 125.22 |
| 20 | A | 838 | CLA | CMD-C2D-C3D | -3.30 | 120.01 | 127.61 |
| 20 | L | 203 | CLA | C1-C2-C3 | -3.30 | 120.33 | 126.04 |
| 20 | A | 826 | CLA | C4B-CHC-C1C | -3.30 | 118.50 | 126.34 |
| 20 | R | 107 | CLA | C4-C3-C5 | 3.30 | 120.83 | 115.27 |
| 20 | A | 838 | CLA | C4A-NA-C1A | 3.30 | 108.19 | 106.71 |
| 20 | A | 836 | CLA | CHB-C1B-NB | -3.30 | 120.76 | 124.26 |
| 20 | 2 | 310 | CLA | CHC-C1C-C2C | -3.30 | 117.57 | 126.73 |
| 20 | B | 806 | CLA | C4-C3-C5 | 3.30 | 120.82 | 115.27 |
| 20 | 3 | 302 | CLA | CHB-C1B-NB | -3.29 | 120.94 | 124.27 |
| 21 | H | 103 | LMU | O1B-C4'-C5' | 3.29 | 118.47 | 109.45 |
| 20 | A | 801 | CLA | CHB-C1B-NB | -3.29 | 120.77 | 124.26 |
| 20 | 3 | 303 | CLA | CHC-C1C-NC | 3.29 | 129.20 | 124.20 |
| 21 | B | 804 | LMU | O1B-C4'-C3' | 3.29 | 116.03 | 107.28 |
| 20 | 3 | 316 | CLA | C3C-C4C-CHD | -3.29 | 118.02 | 125.22 |
| 20 | 3 | 303 | CLA | CBD-CHA-C1A | 3.29 | 132.69 | 127.43 |
| 20 | H | 101 | CLA | CMA-C3A-C2A | -3.29 | 100.57 | 113.83 |
| 22 | B | 844 | BCR | C34-C9-C10 | -3.29 | 118.32 | 122.92 |
| 20 | A | 840 | CLA | C1-C2-C3 | -3.29 | 120.36 | 126.04 |
| 20 | A | 802 | CLA | C4C-CHD-C1D | -3.28 | 117.99 | 126.11 |
| 20 | 1 | 203 | CLA | CAA-C2A-C1A | -3.28 | 101.22 | 111.97 |
| 20 | A | 815 | CLA | C3B-C2B-C1B | -3.28 | 103.20 | 107.16 |
| 20 | K | 103 | CLA | CHD-C4C-C3C | -3.28 | 120.02 | 124.84 |
| 20 | A | 838 | CLA | CHC-C1C-NC | 3.28 | 129.18 | 124.20 |
| 20 | 2 | 311 | CLA | CAA-C2A-C1A | 3.28 | 122.73 | 111.97 |
| 22 | F | 204 | BCR | C3-C4-C5 | -3.28 | 108.22 | 114.08 |
| 20 | R | 107 | CLA | O2A-CGA-CBA | 3.28 | 122.20 | 111.91 |
| 20 | B | 815 | CLA | CHD-C4C-C3C | -3.28 | 120.02 | 124.84 |
| 20 | A | 818 | CLA | C3B-C4B-NB | -3.28 | 107.47 | 110.52 |
| 20 | 2 | 305 | CLA | CHC-C4B-NB | 3.28 | 127.73 | 124.26 |
| 20 | 1 | 203 | CLA | C4A-NA-C1A | 3.28 | 108.18 | 106.71 |
| 20 | 3 | 309 | CLA | C3D-C4D-ND | 3.28 | 114.41 | 109.46 |
| 22 | L | 209 | BCR | C27-C26-C25 | -3.28 | 117.97 | 122.73 |
| 20 | 4 | 315 | CLA | CHB-C1B-NB | -3.28 | 120.79 | 124.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 315 | CLA | CHB-C1B-NB | -3.28 | 120.95 | 124.27 |
| 20 | A | 831 | CLA | CMD-C2D-C3D | -3.28 | 120.08 | 127.61 |
| 21 | K | 105 | LMU | O5B-C5B-C4B | -3.28 | 103.75 | 109.69 |
| 22 | B | 801 | BCR | C33-C5-C6 | -3.28 | 120.85 | 124.53 |
| 21 | B | 805 | LMU | O1B-C1B-C2B | 3.27 | 116.58 | 108.10 |
| 20 | A | 813 | CLA | C1-C2-C3 | -3.27 | 121.46 | 126.75 |
| 20 | B | 814 | CLA | CHC-C4B-NB | 3.27 | 127.72 | 124.26 |
| 20 | 3 | 306 | CLA | C3C-C4C-CHD | -3.27 | 118.06 | 125.22 |
| 20 | 3 | 309 | CLA | CHA-C4D-ND | 3.27 | 127.67 | 124.52 |
| 21 | H | 104 | LMU | O1B-C1B-C2B | 3.27 | 116.57 | 108.10 |
| 20 | B | 836 | CLA | CAA-CBA-CGA | -3.27 | 103.71 | 113.25 |
| 20 | 2 | 304 | CLA | C3B-C2B-C1B | -3.26 | 103.21 | 106.75 |
| 20 | 2 | 316 | CLA | CHC-C1C-NC | 3.26 | 129.16 | 124.20 |
| 20 | A | 805 | CLA | CHC-C1C-C2C | -3.26 | 117.67 | 126.73 |
| 20 | B | 841 | CLA | O2D-CGD-CBD | 3.26 | 117.07 | 111.27 |
| 20 | A | 808 | CLA | C3B-C4B-NB | -3.26 | 107.49 | 110.52 |
| 20 | B | 806 | CLA | CED-O2D-CGD | 3.26 | 123.31 | 115.94 |
| 20 | F | 201 | CLA | CMB-C2B-C1B | 3.26 | 130.34 | 125.37 |
| 20 | A | 818 | CLA | O2A-CGA-CBA | 3.26 | 122.14 | 111.91 |
| 20 | A | 803 | CLA | CHC-C1C-C2C | -3.26 | 117.68 | 126.73 |
| 20 | 2 | 306 | CLA | C1C-NC-C4C | -3.26 | 105.24 | 106.71 |
| 20 | A | 832 | CLA | C4A-NA-C1A | 3.26 | 108.17 | 106.71 |
| 20 | A | 813 | CLA | CHB-C4A-NA | 3.26 | 129.02 | 124.51 |
| 20 | B | 817 | CLA | C3B-C2B-C1B | -3.26 | 103.23 | 107.16 |
| 20 | 3 | 316 | CLA | CHD-C1D-ND | 3.26 | 127.66 | 124.52 |
| 20 | F | 205 | CLA | CAB-C3B-C2B | -3.26 | 115.15 | 123.59 |
| 20 | A | 812 | CLA | C3B-C2B-C1B | -3.26 | 103.23 | 107.16 |
| 20 | B | 824 | CLA | C3B-C2B-C1B | -3.26 | 103.23 | 107.16 |
| 20 | A | 810 | CLA | C2A-C1A-CHA | -3.26 | 118.17 | 123.86 |
| 20 | 3 | 304 | CLA | C2C-C1C-CHC | -3.26 | 117.88 | 125.67 |
| 21 | 4 | 319 | LMU | O2'-C2'-C3' | -3.25 | 102.83 | 110.35 |
| 20 | F | 201 | CLA | C3B-C2B-C1B | -3.25 | 103.23 | 107.16 |
| 20 | 2 | 303 | CLA | CHB-C4A-NA | 3.25 | 129.01 | 124.51 |
| 22 | F | 203 | BCR | C38-C26-C25 | -3.25 | 120.88 | 124.53 |
| 20 | 3 | 313 | CLA | C3B-C2B-C1B | -3.25 | 103.24 | 107.16 |
| 20 | 3 | 312 | CLA | CHD-C1D-ND | 3.25 | 127.66 | 124.52 |
| 20 | B | 839 | CLA | C4A-NA-C1A | 3.25 | 108.17 | 106.71 |
| 20 | G | 105 | CLA | C3B-C2B-C1B | -3.25 | 103.24 | 107.16 |
| 20 | 3 | 313 | CLA | CHC-C4B-NB | 3.24 | 127.69 | 124.26 |
| 20 | B | 812 | CLA | CMB-C2B-C1B | 3.24 | 130.31 | 125.37 |
| 20 | 4 | 310 | CLA | O2A-CGA-CBA | 3.24 | 122.08 | 111.91 |
| 20 | B | 840 | CLA | O2A-CGA-CBA | 3.24 | 122.07 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 20 | 3 | 312 | CLA | CHB-C1B-NB | -3.24 | 120.99 | 124.27 |
| 20 | 4 | 303 | CLA | O2A-CGA-CBA | 3.24 | 122.07 | 111.91 |
| 20 | A | 850 | CLA | CHB-C4A-NA | 3.24 | 128.99 | 124.51 |
| 21 | R | 105 | LMU | C1B-O5B-C5B | 3.24 | 120.04 | 113.69 |
| 21 | C | 101 | LMU | C4B-C3B-C2B | 3.24 | 116.47 | 110.82 |
| 20 | A | 839 | CLA | CGD-CBD-CAD | -3.24 | 100.25 | 110.73 |
| 20 | B | 839 | CLA | CHC-C4B-NB | 3.23 | 127.68 | 124.26 |
| 20 | A | 836 | CLA | CMD-C2D-C3D | -3.23 | 120.18 | 127.61 |
| 20 | K | 104 | CLA | CHD-C4C-C3C | -3.23 | 120.09 | 124.84 |
| 20 | 1 | 203 | CLA | C1D-ND-C4D | -3.23 | 104.04 | 106.33 |
| 20 | 3 | 309 | CLA | CHB-C4A-NA | 3.23 | 129.29 | 124.34 |
| 20 | B | 822 | CLA | C3B-C2B-C1B | -3.23 | 103.26 | 107.16 |
| 20 | A | 839 | CLA | C1-O2A-CGA | 3.23 | 124.92 | 116.44 |
| 20 | 1 | 213 | CLA | CMD-C2D-C3D | -3.23 | 120.18 | 127.61 |
| 20 | 4 | 318 | CLA | CBA-CAA-C2A | -3.23 | 104.33 | 113.86 |
| 20 | 3 | 308 | CLA | CHB-C1B-NB | -3.23 | 121.00 | 124.27 |
| 20 | B | 825 | CLA | CHB-C4A-NA | 3.23 | 128.98 | 124.51 |
| 20 | 3 | 311 | CLA | O2A-CGA-CBA | 3.23 | 122.04 | 111.91 |
| 23 | B | 843 | PQN | C2M-C2-C3 | -3.23 | 119.14 | 124.40 |
| 20 | A | 840 | CLA | C3B-C2B-C1B | -3.23 | 103.27 | 107.16 |
| 20 | B | 819 | CLA | O2D-CGD-O1D | -3.23 | 117.53 | 123.84 |
| 20 | A | 827 | CLA | CMD-C2D-C3D | -3.23 | 120.19 | 127.61 |
| 20 | B | 812 | CLA | C4A-NA-C1A | 3.23 | 108.16 | 106.71 |
| 20 | A | 825 | CLA | CMD-C2D-C3D | -3.22 | 120.20 | 127.61 |
| 21 | K | 107 | LMU | C1B-O1B-C4' | -3.22 | 109.98 | 117.96 |
| 20 | 2 | 301 | CLA | CHD-C1D-ND | 3.22 | 127.63 | 124.52 |
| 20 | A | 850 | CLA | CMD-C2D-C3D | -3.22 | 120.20 | 127.61 |
| 20 | 4 | 313 | CLA | CAA-C2A-C3A | -3.22 | 108.58 | 116.10 |
| 20 | B | 831 | CLA | C1-O2A-CGA | 3.22 | 124.89 | 116.44 |
| 20 | J | 101 | CLA | C4A-NA-C1A | 3.22 | 108.15 | 106.71 |
| 21 | R | 104 | LMU | O1B-C4'-C3' | 3.22 | 115.84 | 107.28 |
| 20 | 2 | 311 | CLA | CHB-C4A-NA | 3.22 | 128.96 | 124.51 |
| 20 | B | 814 | CLA | C4A-NA-C1A | 3.22 | 108.15 | 106.71 |
| 20 | B | 850 | CLA | CAA-C2A-C3A | -3.22 | 103.97 | 112.78 |
| 20 | 3 | 309 | CLA | C4D-ND-C1D | -3.22 | 104.05 | 106.33 |
| 21 | H | 106 | LMU | O5B-C1B-C2B | 3.21 | 117.15 | 110.35 |
| 21 | H | 106 | LMU | C1'-C2'-C3' | 3.21 | 116.69 | 110.00 |
| 20 | B | 802 | CLA | O2D-CGD-O1D | -3.21 | 117.55 | 123.84 |
| 20 | 1 | 209 | CLA | CHB-C1B-NB | -3.21 | 121.02 | 124.27 |
| 20 | 4 | 304 | CLA | CHB-C4A-NA | 3.21 | 128.95 | 124.51 |
| 21 | B | 804 | LMU | C2'-C3'-C4' | -3.21 | 102.35 | 109.68 |
| 22 | A | 845 | BCR | C33-C5-C4 | 3.21 | 119.78 | 113.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 824 | CLA | O2D-CGD-O1D | -3.21 | 117.56 | 123.84 |
| 20 | K | 101 | CLA | O2D-CGD-O1D | -3.21 | 117.57 | 123.84 |
| 20 | 1 | 206 | CLA | C4-C3-C5 | 3.21 | 120.67 | 115.27 |
| 20 | 4 | 318 | CLA | C3B-C2B-C1B | -3.21 | 103.29 | 107.16 |
| 20 | 1 | 213 | CLA | CHC-C1C-C2C | -3.20 | 117.83 | 126.73 |
| 20 | B | 808 | CLA | C4A-NA-C1A | 3.20 | 108.15 | 106.71 |
| 20 | J | 103 | CLA | CHC-C1C-C2C | -3.20 | 117.84 | 126.73 |
| 22 | A | 843 | BCR | C24-C23-C22 | -3.20 | 121.40 | 126.23 |
| 20 | A | 829 | CLA | O2A-CGA-CBA | 3.20 | 121.95 | 111.91 |
| 20 | 2 | 306 | CLA | C4A-NA-C1A | 3.20 | 108.14 | 106.71 |
| 20 | A | 828 | CLA | O2D-CGD-O1D | -3.20 | 117.59 | 123.84 |
| 20 | I | 102 | CLA | C3B-C2B-C1B | -3.20 | 103.30 | 107.16 |
| 20 | A | 830 | CLA | C3B-C2B-C1B | -3.19 | 103.31 | 107.16 |
| 22 | I | 103 | BCR | C2-C1-C6 | -3.19 | 105.56 | 110.48 |
| 22 | A | 844 | BCR | C30-C25-C26 | -3.19 | 118.11 | 122.61 |
| 20 | B | 809 | CLA | CHD-C4C-C3C | -3.19 | 120.15 | 124.84 |
| 20 | 2 | 310 | CLA | C1-C2-C3 | -3.19 | 121.58 | 126.75 |
| 20 | A | 817 | CLA | CHB-C1B-NB | -3.19 | 120.88 | 124.26 |
| 20 | 4 | 308 | CLA | CHD-C1D-ND | 3.19 | 127.60 | 124.52 |
| 22 | F | 204 | BCR | C37-C22-C21 | -3.19 | 118.45 | 122.92 |
| 20 | A | 809 | CLA | CAC-C3C-C4C | 3.19 | 128.95 | 124.81 |
| 21 | B | 805 | LMU | O3'-C3'-C2' | -3.19 | 102.97 | 110.35 |
| 20 | A | 838 | CLA | CHB-C1B-NB | -3.19 | 120.88 | 124.26 |
| 20 | A | 827 | CLA | O1D-CGD-CBD | -3.19 | 117.96 | 124.48 |
| 20 | A | 817 | CLA | C3B-C2B-C1B | -3.19 | 103.32 | 107.16 |
| 21 | 4 | 319 | LMU | C2'-C3'-C4' | 3.19 | 116.95 | 109.68 |
| 20 | B | 826 | CLA | C3B-C2B-C1B | -3.18 | 103.32 | 107.16 |
| 21 | A | 847 | LMU | C1B-O5B-C5B | 3.18 | 119.93 | 113.69 |
| 20 | A | 838 | CLA | CAA-C2A-C3A | -3.18 | 104.07 | 112.78 |
| 20 | 2 | 311 | CLA | CHB-C1B-NB | -3.18 | 120.89 | 124.26 |
| 21 | H | 105 | LMU | C3B-C4B-C5B | -3.18 | 104.57 | 110.24 |
| 21 | A | 855 | LMU | C3'-C4'-C5' | -3.18 | 103.64 | 110.93 |
| 20 | 4 | 303 | CLA | CHC-C1C-C2C | -3.18 | 117.90 | 126.73 |
| 20 | A | 801 | CLA | CED-O2D-CGD | 3.18 | 123.12 | 115.94 |
| 20 | 4 | 318 | CLA | CHC-C1C-C2C | -3.17 | 117.91 | 126.73 |
| 20 | 2 | 307 | CLA | C4-C3-C5 | 3.17 | 120.61 | 115.27 |
| 20 | 4 | 304 | CLA | C4-C3-C5 | 3.17 | 120.61 | 115.27 |
| 20 | F | 206 | CLA | CHC-C1C-NC | 3.17 | 129.02 | 124.20 |
| 21 | R | 104 | LMU | O1B-C1B-C2B | 3.17 | 116.32 | 108.10 |
| 20 | A | 806 | CLA | O2D-CGD-O1D | -3.17 | 117.64 | 123.84 |
| 20 | 4 | 305 | CLA | CMD-C2D-C3D | -3.17 | 120.32 | 127.61 |
| 20 | B | 820 | CLA | CHB-C1B-NB | -3.17 | 120.90 | 124.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 833 | CLA | CHB-C1B-NB | -3.17 | 120.90 | 124.26 |
| 20 | L | 207 | CLA | C4A-NA-C1A | 3.17 | 108.13 | 106.71 |
| 20 | B | 820 | CLA | CHC-C1C-NC | 3.17 | 129.01 | 124.20 |
| 22 | B | 846 | BCR | C15-C14-C13 | -3.17 | 122.78 | 127.31 |
| 20 | K | 103 | CLA | C2D-C1D-ND | -3.17 | 107.77 | 110.10 |
| 20 | A | 827 | CLA | CMB-C2B-C1B | 3.17 | 130.19 | 125.37 |
| 20 | 1 | 209 | CLA | CHC-C1C-NC | 3.17 | 128.91 | 124.23 |
| 20 | A | 804 | CLA | CMB-C2B-C1B | 3.17 | 130.19 | 125.37 |
| 21 | H | 104 | LMU | O2B-C2B-C1B | 3.17 | 117.74 | 110.05 |
| 20 | 1 | 203 | CLA | C3D-C4D-ND | 3.17 | 115.36 | 110.24 |
| 20 | 4 | 301 | CLA | C4A-NA-C1A | 3.16 | 108.13 | 106.71 |
| 21 | A | 847 | LMU | O1'-C1'-C2' | 3.16 | 113.24 | 108.30 |
| 20 | B | 842 | CLA | CMA-C3A-C2A | -3.16 | 108.72 | 116.10 |
| 20 | 3 | 311 | CLA | O2D-CGD-O1D | -3.16 | 117.66 | 123.84 |
| 20 | A | 821 | CLA | CHC-C1C-C2C | -3.16 | 117.95 | 126.73 |
| 20 | A | 820 | CLA | O2D-CGD-O1D | -3.16 | 117.66 | 123.84 |
| 20 | B | 831 | CLA | CED-O2D-CGD | 3.16 | 123.08 | 115.94 |
| 22 | G | 104 | BCR | C33-C5-C4 | 3.16 | 119.68 | 113.62 |
| 20 | G | 105 | CLA | CHB-C4A-NA | 3.16 | 128.88 | 124.51 |
| 20 | A | 829 | CLA | O2D-CGD-O1D | -3.16 | 117.67 | 123.84 |
| 20 | L | 208 | CLA | C3B-C2B-C1B | -3.16 | 103.35 | 107.16 |
| 20 | B | 821 | CLA | CHB-C1B-NB | -3.15 | 120.92 | 124.26 |
| 20 | A | 837 | CLA | CAA-C2A-C1A | -3.15 | 101.64 | 111.97 |
| 20 | A | 815 | CLA | CHB-C1B-NB | -3.15 | 120.92 | 124.26 |
| 20 | A | 826 | CLA | CHC-C4B-NB | 3.15 | 127.59 | 124.26 |
| 21 | A | 853 | LMU | C1'-O5'-C5' | -3.15 | 107.50 | 113.69 |
| 20 | 3 | 308 | CLA | CHD-C1D-ND | 3.15 | 127.56 | 124.52 |
| 20 | 1 | 210 | CLA | CBD-CHA-C1A | 3.15 | 132.47 | 127.43 |
| 20 | F | 205 | CLA | CMB-C2B-C3B | 3.15 | 131.75 | 123.59 |
| 20 | 4 | 304 | CLA | C3B-C2B-C1B | -3.15 | 103.36 | 107.16 |
| 20 | H | 110 | CLA | CMD-C2D-C3D | -3.15 | 120.37 | 127.61 |
| 20 | 3 | 311 | CLA | C3B-C2B-C1B | -3.15 | 103.36 | 107.16 |
| 20 | 3 | 306 | CLA | C1B-NB-C4B | -3.15 | 104.10 | 106.33 |
| 22 | L | 209 | BCR | C37-C22-C21 | -3.15 | 118.51 | 122.92 |
| 20 | A | 802 | CLA | C3D-C4D-ND | 3.15 | 114.21 | 109.46 |
| 21 | 2 | 319 | LMU | O1'-C1'-C2' | 3.14 | 113.21 | 108.30 |
| 20 | A | 832 | CLA | C1-C2-C3 | -3.14 | 121.67 | 126.75 |
| 20 | B | 818 | CLA | C4A-NA-C1A | 3.14 | 108.12 | 106.71 |
| 21 | 4 | 321 | LMU | O2B-C2B-C3B | -3.14 | 103.08 | 110.35 |
| 20 | H | 110 | CLA | CHB-C1B-NB | -3.14 | 120.93 | 124.26 |
| 20 | H | 109 | CLA | CHD-C4C-C3C | -3.14 | 120.22 | 124.84 |
| 20 | L | 208 | CLA | CHC-C1C-NC | 3.14 | 128.97 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 311 | CLA | O2A-CGA-CBA | 3.14 | 121.76 | 111.91 |
| 21 | R | 102 | LMU | C1-O1'-C1' | -3.14 | 108.64 | 113.84 |
| 20 | A | 815 | CLA | O2D-CGD-O1D | -3.14 | 117.70 | 123.84 |
| 20 | A | 805 | CLA | C4-C3-C5 | 3.14 | 120.55 | 115.27 |
| 20 | 3 | 310 | CLA | C4-C3-C5 | 3.14 | 120.55 | 115.27 |
| 20 | 1 | 208 | CLA | CHD-C1D-ND | 3.14 | 127.54 | 124.52 |
| 20 | 3 | 316 | CLA | CHB-C1B-NB | -3.14 | 121.10 | 124.27 |
| 21 | G | 101 | LMU | O5B-C5B-C4B | -3.13 | 104.00 | 109.69 |
| 20 | B | 828 | CLA | CHC-C4B-NB | 3.13 | 127.57 | 124.26 |
| 20 | 2 | 314 | CLA | CMB-C2B-C1B | 3.13 | 130.14 | 125.37 |
| 20 | 3 | 317 | CLA | CBD-CHA-C1A | 3.13 | 132.44 | 127.43 |
| 20 | B | 809 | CLA | CHC-C1C-C2C | -3.13 | 118.03 | 126.73 |
| 20 | A | 832 | CLA | CMB-C2B-C1B | 3.13 | 130.13 | 125.37 |
| 20 | 3 | 314 | CLA | C1-C2-C3 | -3.13 | 120.64 | 126.04 |
| 20 | B | 809 | CLA | C1-C2-C3 | -3.13 | 120.64 | 126.04 |
| 21 | 4 | 321 | LMU | C1B-O5B-C5B | -3.13 | 107.55 | 113.69 |
| 20 | A | 830 | CLA | O2A-CGA-CBA | 3.12 | 121.71 | 111.91 |
| 21 | E | 101 | LMU | O5B-C5B-C6B | 3.12 | 114.20 | 106.44 |
| 20 | B | 810 | CLA | CHD-C4C-C3C | -3.12 | 120.25 | 124.84 |
| 20 | A | 849 | CLA | CHC-C1C-NC | 3.12 | 128.94 | 124.20 |
| 20 | F | 205 | CLA | CHB-C4A-NA | 3.12 | 128.83 | 124.51 |
| 20 | 4 | 317 | CLA | CHC-C1C-C2C | -3.12 | 118.06 | 126.73 |
| 20 | B | 809 | CLA | O2A-CGA-CBA | 3.12 | 121.70 | 111.91 |
| 20 | B | 824 | CLA | CBA-CAA-C2A | 3.12 | 123.07 | 113.86 |
| 20 | 1 | 206 | CLA | O2A-CGA-CBA | 3.12 | 121.69 | 111.91 |
| 20 | 3 | 305 | CLA | C2C-C1C-CHC | -3.12 | 118.20 | 125.67 |
| 20 | 2 | 308 | CLA | C2D-C3D-C4D | -3.12 | 103.83 | 107.28 |
| 21 | A | 846 | LMU | C2'-C3'-C4' | 3.12 | 116.80 | 109.68 |
| 20 | 3 | 305 | CLA | C3C-C4C-CHD | -3.12 | 118.40 | 125.22 |
| 20 | A | 815 | CLA | CHC-C4B-NB | 3.12 | 127.56 | 124.26 |
| 20 | B | 819 | CLA | CMB-C2B-C1B | 3.11 | 130.11 | 125.37 |
| 20 | A | 812 | CLA | C4A-NA-C1A | 3.11 | 108.11 | 106.71 |
| 20 | 2 | 302 | CLA | O2A-CGA-CBA | 3.11 | 121.68 | 111.91 |
| 20 | 4 | 309 | CLA | CHB-C1B-NB | -3.11 | 121.12 | 124.27 |
| 20 | L | 202 | CLA | C1-C2-C3 | -3.11 | 120.66 | 126.04 |
| 20 | 1 | 202 | CLA | CHC-C1C-C2C | -3.11 | 118.09 | 126.73 |
| 20 | H | 102 | CLA | CMB-C2B-C1B | 3.11 | 130.10 | 125.37 |
| 20 | 1 | 201 | CLA | O2D-CGD-O1D | -3.11 | 117.76 | 123.84 |
| 20 | L | 204 | CLA | O2D-CGD-O1D | -3.11 | 117.76 | 123.84 |
| 20 | B | 829 | CLA | CMD-C2D-C3D | -3.11 | 120.47 | 127.61 |
| 20 | 2 | 311 | CLA | CMD-C2D-C3D | -3.11 | 120.47 | 127.61 |
| 20 | F | 205 | CLA | C4B-C3B-C2B | 3.10 | 109.97 | 107.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 833 | CLA | CHC-C1C-C2C | -3.10 | 118.11 | 126.73 |
| 20 | 3 | 310 | CLA | CMD-C2D-C3D | -3.10 | 120.47 | 127.61 |
| 20 | H | 102 | CLA | O2A-CGA-CBA | 3.10 | 121.65 | 111.91 |
| 21 | 1 | 216 | LMU | O1'-C1'-C2' | 3.10 | 113.15 | 108.30 |
| 20 | 2 | 306 | CLA | C2D-C3D-C4D | -3.10 | 103.84 | 107.28 |
| 20 | B | 808 | CLA | CGD-CBD-CAD | -3.10 | 100.69 | 110.73 |
| 22 | I | 101 | BCR | C33-C5-C4 | 3.10 | 119.57 | 113.62 |
| 20 | A | 832 | CLA | C3B-C2B-C1B | -3.10 | 103.42 | 107.16 |
| 20 | B | 829 | CLA | C1-C2-C3 | -3.10 | 120.68 | 126.04 |
| 20 | A | 825 | CLA | C3B-C2B-C1B | -3.10 | 103.42 | 107.16 |
| 20 | K | 101 | CLA | C3B-C2B-C1B | -3.10 | 103.42 | 107.16 |
| 20 | B | 828 | CLA | O1D-CGD-CBD | -3.10 | 118.15 | 124.48 |
| 20 | A | 850 | CLA | O2A-C1-C2 | 3.10 | 116.77 | 108.64 |
| 20 | 3 | 307 | CLA | O2D-CGD-O1D | -3.09 | 117.79 | 123.84 |
| 20 | 3 | 310 | CLA | O2D-CGD-O1D | -3.09 | 117.79 | 123.84 |
| 20 | 3 | 315 | CLA | C1B-NB-C4B | -3.09 | 104.14 | 106.33 |
| 20 | B | 803 | CLA | C1-O2A-CGA | 3.09 | 124.56 | 116.44 |
| 20 | 4 | 305 | CLA | CMB-C2B-C1B | 3.09 | 130.08 | 125.37 |
| 20 | J | 103 | CLA | CMD-C2D-C3D | -3.09 | 120.50 | 127.61 |
| 20 | 1 | 215 | CLA | C3B-C2B-C1B | -3.09 | 103.43 | 107.16 |
| 20 | H | 101 | CLA | O2A-CGA-CBA | 3.09 | 121.61 | 111.91 |
| 20 | B | 812 | CLA | CBA-CAA-C2A | -3.09 | 104.74 | 113.86 |
| 20 | 2 | 302 | CLA | CHB-C4A-NA | 3.09 | 128.78 | 124.51 |
| 20 | B | 819 | CLA | C2D-C1D-ND | -3.09 | 107.83 | 110.10 |
| 20 | B | 830 | CLA | C2A-C1A-CHA | -3.09 | 118.46 | 123.86 |
| 20 | A | 831 | CLA | O2A-CGA-CBA | 3.09 | 121.59 | 111.91 |
| 20 | B | 841 | CLA | C3B-C4B-NB | -3.09 | 107.65 | 110.52 |
| 20 | K | 104 | CLA | C3B-C2B-C1B | -3.08 | 103.44 | 107.16 |
| 20 | A | 833 | CLA | CHB-C1B-NB | -3.08 | 120.99 | 124.26 |
| 20 | A | 824 | CLA | C3B-C2B-C1B | -3.08 | 103.44 | 107.16 |
| 22 | 2 | 317 | BCR | C23-C24-C25 | -3.08 | 118.55 | 127.20 |
| 20 | 4 | 304 | CLA | O2D-CGD-O1D | -3.08 | 117.82 | 123.84 |
| 20 | H | 108 | CLA | CHC-C1C-C2C | -3.08 | 118.18 | 126.73 |
| 20 | A | 814 | CLA | C3D-C4D-ND | 3.08 | 114.11 | 109.46 |
| 20 | 1 | 201 | CLA | CBA-CAA-C2A | -3.08 | 104.78 | 113.86 |
| 20 | A | 812 | CLA | CHB-C1B-NB | -3.08 | 121.00 | 124.26 |
| 20 | 3 | 311 | CLA | C4-C3-C5 | 3.07 | 120.44 | 115.27 |
| 20 | A | 813 | CLA | CHC-C4B-NB | 3.07 | 127.51 | 124.26 |
| 20 | A | 816 | CLA | O2A-CGA-CBA | 3.07 | 121.55 | 111.91 |
| 20 | A | 831 | CLA | CHC-C1C-C2C | -3.07 | 118.20 | 126.73 |
| 20 | 4 | 301 | CLA | C4-C3-C5 | 3.07 | 120.43 | 115.27 |
| 20 | L | 207 | CLA | CHB-C1B-NB | -3.07 | 121.01 | 124.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 312 | CLA | CHB-C4A-NA | 3.07 | 128.75 | 124.51 |
| 20 | 3 | 315 | CLA | CHB-C1B-NB | -3.06 | 121.17 | 124.27 |
| 20 | B | 813 | CLA | CHC-C1C-C2C | -3.06 | 118.22 | 126.73 |
| 20 | A | 808 | CLA | O2D-CGD-O1D | -3.06 | 117.85 | 123.84 |
| 20 | A | 831 | CLA | CHD-C1D-ND | 3.06 | 127.27 | 124.45 |
| 20 | B | 837 | CLA | C3B-C2B-C1B | -3.06 | 103.47 | 107.16 |
| 22 | A | 845 | BCR | C7-C8-C9 | -3.06 | 121.61 | 126.23 |
| 21 | E | 101 | LMU | O4'-C4B-C5B | 3.06 | 116.90 | 109.30 |
| 20 | L | 201 | CLA | O2A-CGA-CBA | 3.06 | 121.51 | 111.91 |
| 21 | 2 | 319 | LMU | C6B-C5B-C4B | 3.06 | 120.17 | 113.00 |
| 20 | H | 109 | CLA | O2D-CGD-O1D | -3.06 | 117.86 | 123.84 |
| 22 | B | 801 | BCR | C1-C6-C7 | 3.06 | 124.43 | 115.78 |
| 20 | B | 813 | CLA | C4-C3-C2 | -3.06 | 115.84 | 123.68 |
| 20 | A | 828 | CLA | C4-C3-C5 | 3.06 | 120.41 | 115.27 |
| 20 | K | 103 | CLA | O2D-CGD-O1D | -3.06 | 117.86 | 123.84 |
| 20 | A | 801 | CLA | C1B-C2B-C3B | -3.05 | 104.13 | 107.03 |
| 20 | A | 840 | CLA | CED-O2D-CGD | 3.05 | 122.84 | 115.94 |
| 20 | 4 | 306 | CLA | CHB-C4A-NA | 3.05 | 128.73 | 124.51 |
| 20 | B | 818 | CLA | O2A-CGA-CBA | 3.05 | 121.48 | 111.91 |
| 20 | A | 851 | CLA | CHB-C4A-NA | 3.05 | 128.73 | 124.51 |
| 20 | A | 811 | CLA | C11-C12-C13 | -3.05 | 106.06 | 115.92 |
| 22 | B | 844 | BCR | C11-C10-C9 | -3.05 | 122.96 | 127.31 |
| 20 | 4 | 312 | CLA | CHB-C1B-NB | -3.05 | 121.19 | 124.27 |
| 20 | 2 | 307 | CLA | C1-O2A-CGA | 3.05 | 124.43 | 116.44 |
| 20 | 2 | 311 | CLA | CGD-CBD-CAD | -3.04 | 100.87 | 110.73 |
| 20 | A | 803 | CLA | C3B-C2B-C1B | -3.04 | 103.49 | 107.16 |
| 20 | 2 | 305 | CLA | CHB-C1B-NB | -3.04 | 121.04 | 124.26 |
| 20 | A | 802 | CLA | CHB-C1B-NB | -3.04 | 121.19 | 124.27 |
| 20 | 4 | 311 | CLA | C2C-C1C-CHC | -3.04 | 118.39 | 125.67 |
| 20 | A | 818 | CLA | C6-C7-C8 | -3.04 | 106.09 | 115.92 |
| 20 | A | 808 | CLA | CHB-C4A-NA | 3.04 | 128.71 | 124.51 |
| 20 | 3 | 302 | CLA | CHD-C1D-ND | 3.04 | 127.45 | 124.52 |
| 20 | B | 837 | CLA | CHB-C1B-NB | -3.04 | 121.04 | 124.26 |
| 20 | B | 823 | CLA | C3B-C2B-C1B | -3.04 | 103.50 | 107.16 |
| 20 | 3 | 317 | CLA | C4A-NA-C1A | 3.04 | 108.07 | 106.71 |
| 20 | A | 824 | CLA | C4A-NA-C1A | 3.04 | 108.07 | 106.71 |
| 20 | A | 805 | CLA | CED-O2D-CGD | 3.04 | 122.80 | 115.94 |
| 22 | B | 801 | BCR | C37-C22-C23 | 3.03 | 122.86 | 118.08 |
| 20 | 1 | 215 | CLA | CMB-C2B-C1B | 3.03 | 129.99 | 125.37 |
| 20 | B | 834 | CLA | C3B-C2B-C1B | -3.03 | 103.50 | 107.16 |
| 20 | L | 207 | CLA | CGD-CBD-CAD | -3.03 | 100.91 | 110.73 |
| 20 | 2 | 316 | CLA | CHB-C4A-NA | 3.03 | 128.71 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 312 | CLA | CBA-CAA-C2A | -3.03 | 104.91 | 113.86 |
| 20 | A | 829 | CLA | C3B-C2B-C1B | -3.03 | 103.50 | 107.16 |
| 20 | L | 202 | CLA | O2D-CGD-O1D | -3.03 | 117.92 | 123.84 |
| 20 | A | 811 | CLA | CHB-C4A-NA | 3.03 | 128.70 | 124.51 |
| 20 | B | 820 | CLA | O1D-CGD-CBD | -3.03 | 118.29 | 124.48 |
| 20 | A | 833 | CLA | CHB-C4A-NA | 3.02 | 128.69 | 124.51 |
| 20 | 2 | 312 | CLA | C4A-NA-C1A | 3.02 | 108.06 | 106.71 |
| 20 | B | 824 | CLA | CHC-C1C-NC | 3.02 | 128.79 | 124.20 |
| 20 | 2 | 312 | CLA | O2D-CGD-O1D | -3.02 | 117.93 | 123.84 |
| 22 | J | 102 | BCR | C16-C17-C18 | -3.02 | 123.00 | 127.31 |
| 20 | B | 823 | CLA | C4-C3-C5 | 3.02 | 120.35 | 115.27 |
| 20 | 4 | 314 | CLA | C3B-C2B-C1B | -3.02 | 103.48 | 106.75 |
| 20 | B | 830 | CLA | CHC-C1C-C2C | -3.02 | 118.35 | 126.73 |
| 22 | J | 102 | BCR | C38-C26-C25 | -3.02 | 121.14 | 124.53 |
| 20 | F | 205 | CLA | C4A-NA-C1A | 3.02 | 108.06 | 106.71 |
| 20 | 4 | 310 | CLA | CHC-C1C-C2C | -3.02 | 118.36 | 126.73 |
| 20 | 3 | 302 | CLA | C3C-C4C-CHD | -3.01 | 118.62 | 125.22 |
| 20 | 3 | 305 | CLA | CHD-C1D-ND | 3.01 | 127.43 | 124.52 |
| 20 | 4 | 306 | CLA | O2A-CGA-O1A | -3.01 | 115.98 | 123.59 |
| 20 | K | 103 | CLA | CHC-C1C-C2C | -3.01 | 118.36 | 126.73 |
| 20 | 3 | 308 | CLA | CHB-C4A-NA | 3.01 | 128.95 | 124.34 |
| 20 | B | 837 | CLA | C1-O2A-CGA | 3.01 | 124.34 | 116.44 |
| 21 | K | 107 | LMU | C4B-C3B-C2B | -3.01 | 105.57 | 110.82 |
| 22 | B | 847 | BCR | C11-C12-C13 | -3.01 | 117.97 | 126.42 |
| 20 | A | 840 | CLA | CHB-C4A-NA | 3.01 | 128.67 | 124.51 |
| 20 | 4 | 310 | CLA | C1D-ND-C4D | -3.01 | 104.20 | 106.33 |
| 20 | A | 811 | CLA | CHC-C1C-C2C | -3.01 | 118.38 | 126.73 |
| 20 | A | 837 | CLA | CHC-C1C-C2C | -3.01 | 118.38 | 126.73 |
| 20 | B | 850 | CLA | CBA-CAA-C2A | -3.01 | 104.99 | 113.86 |
| 21 | R | 101 | LMU | O1'-C1'-C2' | 3.01 | 113.00 | 108.30 |
| 20 | B | 803 | CLA | C4A-NA-C1A | 3.01 | 108.06 | 106.71 |
| 20 | A | 816 | CLA | CHB-C4A-NA | 3.00 | 128.67 | 124.51 |
| 22 | F | 204 | BCR | C33-C5-C6 | -3.00 | 121.15 | 124.53 |
| 20 | 3 | 309 | CLA | C2C-C1C-CHC | -3.00 | 118.48 | 125.67 |
| 20 | A | 849 | CLA | CHB-C4A-NA | 3.00 | 128.67 | 124.51 |
| 20 | A | 825 | CLA | O2D-CGD-O1D | -3.00 | 117.97 | 123.84 |
| 20 | 4 | 301 | CLA | C3B-C2B-C1B | -3.00 | 103.54 | 107.16 |
| 20 | B | 816 | CLA | CMD-C2D-C3D | -3.00 | 120.71 | 127.61 |
| 20 | 4 | 303 | CLA | C3B-C2B-C1B | -3.00 | 103.54 | 107.16 |
| 20 | A | 819 | CLA | CHC-C4B-NB | 3.00 | 127.43 | 124.26 |
| 20 | 4 | 315 | CLA | O1D-CGD-CBD | -3.00 | 118.35 | 124.48 |
| 21 | 2 | 319 | LMU | C1'-C2'-C3' | 3.00 | 116.24 | 110.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | E | 101 | LMU | C3B-C4B-C5B | -3.00 | 104.89 | 110.24 |
| 20 | 2 | 309 | CLA | C1C-NC-C4C | -3.00 | 105.36 | 106.71 |
| 20 | A | 838 | CLA | CHB-C4A-NA | 3.00 | 128.66 | 124.51 |
| 20 | 4 | 311 | CLA | CHB-C1B-NB | -3.00 | 121.24 | 124.27 |
| 22 | L | 209 | BCR | C38-C26-C27 | 2.99 | 119.37 | 113.62 |
| 20 | K | 103 | CLA | O2A-CGA-O1A | -2.99 | 116.04 | 123.59 |
| 20 | 2 | 303 | CLA | O2D-CGD-O1D | -2.99 | 117.99 | 123.84 |
| 20 | J | 103 | CLA | CHB-C1B-NB | -2.99 | 121.09 | 124.26 |
| 20 | 3 | 307 | CLA | C4A-NA-C1A | 2.99 | 108.05 | 106.71 |
| 22 | B | 846 | BCR | C38-C26-C25 | -2.99 | 121.17 | 124.53 |
| 21 | A | 847 | LMU | C2'-C3'-C4' | 2.99 | 116.51 | 109.68 |
| 20 | F | 207 | CLA | CHB-C4A-NA | 2.99 | 128.65 | 124.51 |
| 21 | B | 804 | LMU | O5B-C5B-C4B | 2.99 | 115.12 | 109.69 |
| 20 | H | 108 | CLA | C6-C5-C3 | -2.99 | 105.61 | 113.45 |
| 20 | A | 827 | CLA | CHB-C1B-NB | -2.99 | 121.09 | 124.26 |
| 20 | B | 813 | CLA | CAC-C3C-C4C | 2.99 | 128.69 | 124.81 |
| 20 | A | 811 | CLA | C1-C2-C3 | -2.99 | 120.88 | 126.04 |
| 20 | 4 | 318 | CLA | CHB-C1B-NB | -2.98 | 121.10 | 124.26 |
| 20 | R | 107 | CLA | CHB-C1B-NB | -2.98 | 121.10 | 124.26 |
| 20 | A | 804 | CLA | O2D-CGD-O1D | -2.98 | 118.00 | 123.84 |
| 21 | L | 205 | LMU | C1B-O5B-C5B | -2.98 | 107.83 | 113.69 |
| 20 | A | 829 | CLA | CHC-C1C-C2C | -2.98 | 118.45 | 126.73 |
| 20 | A | 831 | CLA | CAA-C2A-C3A | -2.98 | 104.61 | 112.78 |
| 20 | A | 835 | CLA | C1-C2-C3 | -2.98 | 120.89 | 126.04 |
| 22 | F | 204 | BCR | C15-C16-C17 | -2.98 | 117.37 | 123.47 |
| 20 | A | 831 | CLA | CHB-C1B-NB | -2.98 | 121.11 | 124.26 |
| 20 | 1 | 204 | CLA | CHC-C1C-C2C | -2.98 | 118.46 | 126.73 |
| 20 | 3 | 315 | CLA | C2C-C1C-CHC | -2.98 | 118.54 | 125.67 |
| 20 | B | 807 | CLA | CHB-C4A-NA | 2.98 | 128.63 | 124.51 |
| 21 | 2 | 319 | LMU | C2'-C3'-C4' | 2.98 | 116.48 | 109.68 |
| 21 | R | 105 | LMU | C1'-C2'-C3' | 2.97 | 116.19 | 110.00 |
| 20 | 3 | 307 | CLA | C3D-C4D-ND | 2.97 | 115.05 | 110.24 |
| 20 | 2 | 312 | CLA | CMD-C2D-C3D | -2.97 | 120.77 | 127.61 |
| 20 | B | 831 | CLA | CHD-C4C-C3C | -2.97 | 120.47 | 124.84 |
| 20 | 1 | 212 | CLA | CHB-C1B-NB | -2.97 | 121.27 | 124.27 |
| 20 | B | 822 | CLA | C4A-NA-C1A | 2.97 | 108.04 | 106.71 |
| 20 | 1 | 213 | CLA | O2D-CGD-O1D | -2.97 | 118.03 | 123.84 |
| 20 | A | 841 | CLA | CHB-C1B-NB | -2.97 | 121.27 | 124.27 |
| 20 | A | 851 | CLA | CMB-C2B-C1B | 2.97 | 129.89 | 125.37 |
| 20 | A | 837 | CLA | CHB-C1B-NB | -2.97 | 121.12 | 124.26 |
| 20 | A | 824 | CLA | O2A-CGA-CBA | 2.97 | 121.22 | 111.91 |
| 20 | 1 | 201 | CLA | CAA-C2A-C3A | -2.97 | 104.66 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 3 | 311 | CLA | O2A-CGA-O1A | -2.97 | 116.11 | 123.59 |
| 20 | A | 815 | CLA | CAA-C2A-C3A | -2.97 | 104.66 | 112.78 |
| 20 | 4 | 314 | CLA | C3C-C4C-CHD | -2.96 | 118.73 | 125.22 |
| 20 | A | 829 | CLA | CHD-C4C-C3C | -2.96 | 120.48 | 124.84 |
| 20 | B | 810 | CLA | CHC-C1C-C2C | -2.96 | 118.50 | 126.73 |
| 20 | B | 808 | CLA | CHB-C1B-NB | -2.96 | 121.12 | 124.26 |
| 20 | A | 822 | CLA | C1-C2-C3 | -2.96 | 121.96 | 126.75 |
| 20 | 3 | 310 | CLA | CHC-C1C-NC | 2.96 | 128.69 | 124.20 |
| 20 | F | 201 | CLA | CHC-C1C-C2C | -2.96 | 118.52 | 126.73 |
| 22 | A | 845 | BCR | C40-C30-C25 | -2.96 | 105.50 | 110.30 |
| 20 | K | 102 | CLA | CHC-C1C-C2C | -2.96 | 118.52 | 126.73 |
| 20 | H | 101 | CLA | CAA-C2A-C3A | -2.96 | 104.68 | 112.78 |
| 20 | B | 850 | CLA | CMD-C2D-C3D | -2.96 | 120.81 | 127.61 |
| 21 | B | 804 | LMU | O5'-C1'-C2' | 2.95 | 116.60 | 110.35 |
| 20 | 2 | 309 | CLA | C2A-C3A-C4A | -2.95 | 99.55 | 104.18 |
| 21 | 2 | 320 | LMU | O1B-C1B-C2B | 2.95 | 115.75 | 108.10 |
| 20 | H | 110 | CLA | O2D-CGD-O1D | -2.95 | 118.07 | 123.84 |
| 20 | R | 107 | CLA | C4A-NA-C1A | 2.95 | 108.03 | 106.71 |
| 21 | B | 849 | LMU | O1'-C1'-C2' | 2.95 | 112.91 | 108.30 |
| 20 | 4 | 313 | CLA | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 21 | 2 | 313 | LMU | O1B-C4'-C5' | 2.95 | 117.53 | 109.45 |
| 20 | 2 | 308 | CLA | C2C-C1C-CHC | -2.95 | 118.61 | 125.67 |
| 22 | A | 843 | BCR | C23-C24-C25 | -2.95 | 118.92 | 127.20 |
| 20 | I | 102 | CLA | C4A-NA-C1A | 2.95 | 108.03 | 106.71 |
| 20 | 3 | 314 | CLA | CHB-C4A-NA | 2.95 | 128.59 | 124.51 |
| 20 | 2 | 304 | CLA | C2C-C1C-CHC | -2.95 | 118.61 | 125.67 |
| 20 | 1 | 211 | CLA | CAA-C2A-C1A | -2.95 | 102.32 | 111.97 |
| 20 | A | 801 | CLA | CAC-C3C-C4C | 2.94 | 128.63 | 124.81 |
| 20 | 2 | 314 | CLA | CHB-C4A-NA | 2.94 | 128.58 | 124.51 |
| 20 | A | 822 | CLA | CHB-C4A-NA | 2.94 | 128.58 | 124.51 |
| 20 | 1 | 215 | CLA | CHB-C1B-NB | -2.94 | 121.14 | 124.26 |
| 20 | L | 201 | CLA | O2D-CGD-O1D | -2.94 | 118.09 | 123.84 |
| 20 | K | 102 | CLA | C4A-NA-C1A | 2.94 | 108.03 | 106.71 |
| 20 | A | 828 | CLA | CMB-C2B-C1B | 2.94 | 129.84 | 125.37 |
| 20 | 4 | 315 | CLA | CMD-C2D-C3D | -2.94 | 120.86 | 127.61 |
| 20 | F | 207 | CLA | C4A-NA-C1A | 2.94 | 108.03 | 106.71 |
| 20 | 4 | 315 | CLA | CGD-CBD-CAD | -2.94 | 101.23 | 110.73 |
| 20 | 2 | 309 | CLA | C1B-NB-C4B | -2.94 | 104.25 | 106.33 |
| 20 | A | 830 | CLA | CHC-C1C-C2C | -2.93 | 118.58 | 126.73 |
| 20 | 2 | 307 | CLA | C2A-C1A-CHA | -2.93 | 118.73 | 123.86 |
| 20 | 2 | 303 | CLA | O2A-CGA-CBA | 2.93 | 121.11 | 111.91 |
| 20 | 2 | 302 | CLA | CHC-C4B-NB | 2.93 | 127.36 | 124.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | B | 845 | BCR | C38-C26-C27 | 2.93 | 119.25 | 113.62 |
| 20 | A | 831 | CLA | O2D-CGD-O1D | -2.93 | 118.11 | 123.84 |
| 20 | L | 204 | CLA | O2A-CGA-CBA | 2.93 | 121.11 | 111.91 |
| 20 | B | 822 | CLA | O1D-CGD-CBD | -2.93 | 118.49 | 124.48 |
| 20 | A | 826 | CLA | CHB-C4A-NA | 2.93 | 128.56 | 124.51 |
| 20 | H | 110 | CLA | CHC-C4B-NB | 2.93 | 127.36 | 124.26 |
| 21 | H | 103 | LMU | O5'-C1'-C2' | 2.93 | 116.55 | 110.35 |
| 20 | B | 807 | CLA | C4A-NA-C1A | 2.93 | 108.02 | 106.71 |
| 20 | B | 838 | CLA | CMB-C2B-C1B | 2.93 | 129.83 | 125.37 |
| 21 | R | 103 | LMU | O1'-C1'-C2' | 2.93 | 112.87 | 108.30 |
| 20 | H | 101 | CLA | C3B-C2B-C1B | -2.93 | 103.63 | 107.16 |
| 20 | 3 | 303 | CLA | CHC-C4B-NB | 2.92 | 127.35 | 124.26 |
| 20 | J | 103 | CLA | C4-C3-C5 | 2.92 | 120.19 | 115.27 |
| 20 | A | 840 | CLA | CMB-C2B-C1B | 2.92 | 129.82 | 125.37 |
| 20 | K | 102 | CLA | C3B-C2B-C1B | -2.92 | 103.63 | 107.16 |
| 20 | 3 | 310 | CLA | O1D-CGD-CBD | -2.92 | 118.50 | 124.48 |
| 20 | 1 | 208 | CLA | C3C-C4C-CHD | -2.92 | 118.82 | 125.22 |
| 22 | 2 | 317 | BCR | C38-C26-C27 | 2.92 | 119.23 | 113.62 |
| 20 | L | 202 | CLA | C3B-C2B-C1B | -2.92 | 103.64 | 107.16 |
| 22 | B | 801 | BCR | C37-C22-C21 | -2.92 | 118.83 | 122.92 |
| 20 | H | 101 | CLA | C1-O2A-CGA | 2.92 | 124.11 | 116.44 |
| 20 | 3 | 313 | CLA | O2A-CGA-CBA | 2.92 | 121.07 | 111.91 |
| 20 | 3 | 310 | CLA | CHB-C1B-NB | -2.92 | 121.17 | 124.26 |
| 21 | R | 105 | LMU | O5'-C5'-C6' | 2.92 | 113.69 | 106.44 |
| 20 | A | 809 | CLA | O2D-CGD-O1D | -2.92 | 118.13 | 123.84 |
| 20 | 3 | 311 | CLA | C4A-NA-C1A | 2.92 | 108.02 | 106.71 |
| 20 | A | 801 | CLA | C2A-C3A-C4A | -2.92 | 97.16 | 101.87 |
| 20 | A | 804 | CLA | O2A-CGA-O1A | -2.92 | 116.23 | 123.59 |
| 22 | I | 101 | BCR | C27-C26-C25 | -2.92 | 118.51 | 122.70 |
| 20 | B | 808 | CLA | C6-C5-C3 | -2.91 | 105.81 | 113.45 |
| 20 | A | 814 | CLA | C4D-ND-C1D | -2.91 | 104.27 | 106.33 |
| 20 | B | 803 | CLA | CHC-C1C-C2C | -2.91 | 118.64 | 126.73 |
| 20 | B | 841 | CLA | CHC-C1C-C2C | -2.91 | 118.64 | 126.73 |
| 20 | R | 107 | CLA | O2A-CGA-O1A | -2.91 | 116.25 | 123.59 |
| 20 | H | 101 | CLA | CHC-C1C-C2C | -2.91 | 118.65 | 126.73 |
| 20 | B | 839 | CLA | C3B-C4B-NB | -2.91 | 107.82 | 110.52 |
| 20 | 2 | 311 | CLA | CHC-C1C-C2C | -2.91 | 118.66 | 126.73 |
| 20 | L | 208 | CLA | C4D-CHA-C1A | 2.91 | 124.78 | 121.25 |
| 20 | A | 816 | CLA | O2A-CGA-O1A | -2.90 | 116.26 | 123.59 |
| 20 | K | 104 | CLA | C4-C3-C2 | -2.90 | 116.23 | 123.68 |
| 20 | K | 102 | CLA | O2A-CGA-CBA | 2.90 | 121.02 | 111.91 |
| 21 | R | 101 | LMU | O5'-C1'-O1' | 2.90 | 116.85 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 816 | CLA | C4-C3-C5 | 2.90 | 120.16 | 115.27 |
| 20 | B | 818 | CLA | C1-C2-C3 | -2.90 | 121.02 | 126.04 |
| 22 | I | 101 | BCR | C28-C27-C26 | -2.90 | 108.89 | 114.08 |
| 20 | 2 | 309 | CLA | C3C-C4C-CHD | -2.90 | 118.86 | 125.22 |
| 20 | 1 | 201 | CLA | CAC-C3C-C2C | -2.90 | 122.57 | 127.53 |
| 20 | 3 | 313 | CLA | CED-O2D-CGD | 2.90 | 122.50 | 115.94 |
| 20 | B | 812 | CLA | CHB-C1B-NB | -2.90 | 121.19 | 124.26 |
| 20 | B | 833 | CLA | CHC-C1C-C2C | -2.90 | 118.67 | 126.73 |
| 20 | 3 | 309 | CLA | CHB-C1B-NB | -2.90 | 121.34 | 124.27 |
| 21 | 4 | 319 | LMU | O1B-C4'-C5' | -2.90 | 101.50 | 109.45 |
| 21 | K | 106 | LMU | C4B-C3B-C2B | -2.90 | 105.76 | 110.82 |
| 20 | 2 | 316 | CLA | C4A-NA-C1A | 2.90 | 108.01 | 106.71 |
| 20 | 4 | 304 | CLA | O2A-CGA-CBA | 2.90 | 121.00 | 111.91 |
| 20 | A | 835 | CLA | O2A-CGA-CBA | 2.90 | 121.00 | 111.91 |
| 20 | A | 820 | CLA | C3B-C2B-C1B | -2.90 | 103.66 | 107.16 |
| 20 | B | 827 | CLA | C1-C2-C3 | -2.90 | 121.03 | 126.04 |
| 25 | B | 848 | LMG | O8-C28-C29 | 2.90 | 121.00 | 111.91 |
| 21 | L | 205 | LMU | O5B-C5B-C6B | 2.90 | 113.64 | 106.44 |
| 20 | L | 204 | CLA | C1D-ND-C4D | -2.90 | 104.28 | 106.33 |
| 20 | 4 | 318 | CLA | O2D-CGD-O1D | -2.89 | 118.18 | 123.84 |
| 20 | 2 | 308 | CLA | CHB-C4A-NA | 2.89 | 128.77 | 124.34 |
| 20 | 2 | 310 | CLA | O2A-CGA-CBA | 2.89 | 120.99 | 111.91 |
| 20 | B | 827 | CLA | C3B-C2B-C1B | -2.89 | 103.67 | 107.16 |
| 20 | H | 109 | CLA | C3B-C2B-C1B | -2.89 | 103.67 | 107.16 |
| 20 | 1 | 209 | CLA | C3C-C4C-CHD | -2.89 | 118.89 | 125.22 |
| 20 | J | 103 | CLA | C3B-C2B-C1B | -2.89 | 103.68 | 107.16 |
| 20 | B | 838 | CLA | C4A-NA-C1A | 2.89 | 108.00 | 106.71 |
| 20 | 2 | 314 | CLA | CBC-CAC-C3C | -2.89 | 104.47 | 112.43 |
| 20 | B | 832 | CLA | CHB-C4A-NA | 2.89 | 128.50 | 124.51 |
| 20 | B | 821 | CLA | O2A-CGA-CBA | 2.89 | 120.97 | 111.91 |
| 20 | A | 818 | CLA | O2A-CGA-O1A | -2.89 | 116.31 | 123.59 |
| 20 | 1 | 213 | CLA | CGD-CBD-CAD | -2.88 | 101.39 | 110.73 |
| 20 | 1 | 210 | CLA | CMB-C2B-C1B | 2.88 | 129.76 | 125.37 |
| 20 | 4 | 308 | CLA | C3C-C4C-CHD | -2.88 | 118.90 | 125.22 |
| 20 | 4 | 312 | CLA | C1B-NB-C4B | -2.88 | 104.29 | 106.33 |
| 20 | A | 813 | CLA | CHC-C1C-C2C | -2.88 | 118.72 | 126.73 |
| 20 | B | 823 | CLA | CHB-C1B-NB | -2.88 | 121.21 | 124.26 |
| 20 | A | 832 | CLA | CHC-C1C-C2C | -2.88 | 118.73 | 126.73 |
| 20 | 1 | 214 | CLA | C3C-C4C-CHD | -2.88 | 118.91 | 125.22 |
| 20 | 4 | 311 | CLA | C3C-C4C-CHD | -2.88 | 118.92 | 125.22 |
| 20 | 4 | 309 | CLA | C3C-C4C-CHD | -2.88 | 118.92 | 125.22 |
| 23 | A | 842 | PQN | C21-C20-C18 | -2.88 | 106.61 | 115.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 306 | CLA | CHC-C1C-C2C | -2.88 | 118.73 | 126.73 |
| 20 | A | 830 | CLA | C4A-NA-C1A | 2.88 | 108.00 | 106.71 |
| 20 | A | 834 | CLA | O2D-CGD-O1D | -2.88 | 118.22 | 123.84 |
| 20 | A | 836 | CLA | C4D-C3D-CAD | 2.87 | 111.48 | 108.10 |
| 20 | 3 | 316 | CLA | CHB-C4A-NA | 2.87 | 128.74 | 124.34 |
| 20 | K | 103 | CLA | C1-C2-C3 | -2.87 | 122.10 | 126.75 |
| 20 | B | 823 | CLA | CED-O2D-CGD | 2.87 | 122.44 | 115.94 |
| 21 | A | 853 | LMU | C4B-C3B-C2B | 2.87 | 115.84 | 110.82 |
| 20 | 3 | 310 | CLA | CMC-C2C-C1C | 2.87 | 129.41 | 125.04 |
| 20 | B | 836 | CLA | CAC-C3C-C4C | 2.87 | 128.53 | 124.81 |
| 22 | B | 844 | BCR | C37-C22-C21 | -2.87 | 118.90 | 122.92 |
| 20 | J | 101 | CLA | C3B-C2B-C1B | -2.87 | 103.70 | 107.16 |
| 20 | 4 | 318 | CLA | C2D-C1D-ND | -2.87 | 107.99 | 110.10 |
| 20 | L | 207 | CLA | CHC-C1C-C2C | -2.87 | 118.76 | 126.73 |
| 20 | H | 108 | CLA | CMA-C3A-C4A | -2.87 | 104.07 | 111.77 |
| 20 | B | 838 | CLA | CHC-C1C-C2C | -2.86 | 118.77 | 126.73 |
| 20 | A | 841 | CLA | C3D-C4D-ND | 2.86 | 113.78 | 109.46 |
| 20 | 2 | 315 | CLA | C2C-C1C-CHC | -2.86 | 118.81 | 125.67 |
| 20 | 1 | 210 | CLA | C4A-NA-C1A | 2.86 | 107.99 | 106.71 |
| 20 | A | 802 | CLA | CHB-C4A-NA | 2.86 | 128.72 | 124.34 |
| 20 | 3 | 304 | CLA | C3C-C4C-CHD | -2.86 | 118.95 | 125.22 |
| 20 | 4 | 317 | CLA | C3B-C2B-C1B | -2.86 | 103.71 | 107.16 |
| 20 | 2 | 311 | CLA | C3B-C2B-C1B | -2.86 | 103.71 | 107.16 |
| 20 | 1 | 203 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 20 | H | 109 | CLA | CHB-C4A-NA | 2.86 | 128.47 | 124.51 |
| 20 | A | 817 | CLA | C1-O2A-CGA | 2.86 | 123.95 | 116.44 |
| 20 | B | 808 | CLA | C11-C10-C8 | -2.86 | 106.68 | 115.92 |
| 20 | H | 101 | CLA | C4A-NA-C1A | 2.86 | 107.99 | 106.71 |
| 20 | 3 | 314 | CLA | C4D-CHA-C1A | 2.86 | 124.73 | 121.25 |
| 20 | B | 826 | CLA | CAC-C3C-C4C | 2.86 | 128.52 | 124.81 |
| 20 | K | 103 | CLA | C3B-C2B-C1B | -2.86 | 103.71 | 107.16 |
| 21 | R | 106 | LMU | C1'-C2'-C3' | 2.85 | 115.94 | 110.00 |
| 20 | B | 831 | CLA | C2D-C1D-ND | -2.85 | 108.00 | 110.10 |
| 20 | 4 | 301 | CLA | C1-C2-C3 | -2.85 | 121.11 | 126.04 |
| 20 | B | 813 | CLA | C5-C3-C2 | 2.85 | 126.89 | 121.12 |
| 20 | 1 | 207 | CLA | C1D-ND-C4D | -2.85 | 104.31 | 106.33 |
| 20 | B | 823 | CLA | CHC-C1C-C2C | -2.85 | 118.81 | 126.73 |
| 20 | A | 809 | CLA | C4-C3-C5 | 2.85 | 120.06 | 115.27 |
| 20 | L | 201 | CLA | C1-O2A-CGA | 2.85 | 123.92 | 116.44 |
| 20 | F | 205 | CLA | CBD-CHA-C1A | 2.85 | 131.99 | 127.43 |
| 20 | A | 849 | CLA | C4A-NA-C1A | 2.85 | 107.99 | 106.71 |
| 20 | A | 814 | CLA | C2C-C1C-CHC | -2.85 | 118.85 | 125.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 824 | CLA | C3D-C4D-ND | 2.85 | 114.84 | 110.24 |
| 22 | B | 846 | BCR | C38-C26-C27 | 2.85 | 119.08 | 113.62 |
| 20 | A | 805 | CLA | C1-O2A-CGA | 2.84 | 123.90 | 116.44 |
| 20 | A | 832 | CLA | CMA-C3A-C4A | -2.84 | 104.13 | 111.77 |
| 21 | A | 854 | LMU | O1'-C1'-C2' | 2.84 | 112.74 | 108.30 |
| 22 | 2 | 317 | BCR | C35-C13-C12 | 2.84 | 122.56 | 118.08 |
| 20 | 4 | 315 | CLA | CHB-C4A-NA | 2.84 | 128.44 | 124.51 |
| 20 | B | 817 | CLA | C1D-ND-C4D | -2.84 | 104.32 | 106.33 |
| 20 | B | 815 | CLA | CHC-C1C-C2C | -2.84 | 118.84 | 126.73 |
| 21 | 1 | 218 | LMU | C4B-C3B-C2B | 2.84 | 115.78 | 110.82 |
| 21 | 4 | 319 | LMU | C1B-C2B-C3B | -2.84 | 104.08 | 110.00 |
| 20 | 1 | 204 | CLA | CHB-C1B-NB | -2.84 | 121.25 | 124.26 |
| 20 | 1 | 215 | CLA | CAA-C2A-C1A | 2.84 | 121.28 | 111.97 |
| 20 | H | 110 | CLA | C3B-C2B-C1B | -2.84 | 103.73 | 107.16 |
| 20 | B | 834 | CLA | C4A-NA-C1A | 2.84 | 107.98 | 106.71 |
| 20 | 1 | 214 | CLA | C3D-C4D-ND | 2.84 | 113.74 | 109.46 |
| 20 | 1 | 207 | CLA | O2A-CGA-CBA | 2.84 | 120.81 | 111.91 |
| 20 | A | 833 | CLA | C3B-C2B-C1B | -2.84 | 103.74 | 107.16 |
| 22 | F | 204 | BCR | C33-C5-C4 | 2.84 | 119.06 | 113.62 |
| 21 | G | 101 | LMU | O5B-C5B-C6B | 2.84 | 113.49 | 106.44 |
| 20 | B | 816 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 20 | 4 | 305 | CLA | O2A-CGA-O1A | -2.84 | 116.44 | 123.59 |
| 20 | A | 835 | CLA | CHC-C1C-C2C | -2.83 | 118.86 | 126.73 |
| 20 | B | 833 | CLA | O1D-CGD-CBD | -2.83 | 118.69 | 124.48 |
| 20 | A | 825 | CLA | C4A-NA-C1A | 2.83 | 107.98 | 106.71 |
| 20 | A | 827 | CLA | C4A-NA-C1A | 2.83 | 107.98 | 106.71 |
| 20 | A | 827 | CLA | CHC-C1C-C2C | -2.83 | 118.86 | 126.73 |
| 20 | 2 | 314 | CLA | CHC-C1C-C2C | -2.83 | 118.86 | 126.73 |
| 20 | 4 | 312 | CLA | C3C-C4C-CHD | -2.83 | 119.02 | 125.22 |
| 22 | G | 104 | BCR | C38-C26-C25 | -2.83 | 121.35 | 124.53 |
| 20 | 1 | 213 | CLA | C3B-C2B-C1B | -2.83 | 103.75 | 107.16 |
| 20 | A | 806 | CLA | C4A-NA-C1A | 2.83 | 107.98 | 106.71 |
| 20 | B | 836 | CLA | CHC-C1C-C2C | -2.83 | 118.88 | 126.73 |
| 20 | 1 | 204 | CLA | CHB-C4A-NA | 2.83 | 128.42 | 124.51 |
| 22 | F | 203 | BCR | C23-C24-C25 | -2.82 | 119.27 | 127.20 |
| 20 | A | 836 | CLA | O2A-CGA-CBA | 2.82 | 120.76 | 111.91 |
| 20 | A | 836 | CLA | CHC-C1C-C2C | -2.82 | 118.89 | 126.73 |
| 21 | L | 210 | LMU | O5B-C5B-C4B | 2.82 | 114.82 | 109.69 |
| 20 | B | 850 | CLA | CHC-C1C-C2C | -2.82 | 118.90 | 126.73 |
| 20 | 1 | 212 | CLA | C2C-C1C-CHC | -2.82 | 118.92 | 125.67 |
| 20 | F | 206 | CLA | CHB-C1B-NB | -2.82 | 121.27 | 124.26 |
| 20 | A | 851 | CLA | C1-C2-C3 | 2.82 | 130.92 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 3 | 311 | CLA | CHB-C4A-NA | 2.82 | 128.41 | 124.51 |
| 20 | B | 828 | CLA | CHB-C4A-NA | 2.82 | 128.41 | 124.51 |
| 20 | 4 | 304 | CLA | CHD-C4C-NC | 2.82 | 128.64 | 124.20 |
| 20 | B | 814 | CLA | CBA-CAA-C2A | -2.82 | 105.55 | 113.86 |
| 21 | E | 101 | LMU | O5'-C5'-C6' | 2.82 | 113.44 | 106.44 |
| 20 | J | 101 | CLA | O2A-CGA-CBA | 2.81 | 120.74 | 111.91 |
| 20 | 4 | 301 | CLA | CHB-C1B-NB | -2.81 | 121.28 | 124.26 |
| 21 | 4 | 319 | LMU | O1B-C4'-C3' | -2.81 | 99.80 | 107.28 |
| 20 | G | 105 | CLA | C4A-NA-C1A | 2.81 | 107.97 | 106.71 |
| 20 | 4 | 317 | CLA | O2D-CGD-CBD | 2.81 | 116.27 | 111.27 |
| 21 | D | 201 | LMU | C1'-C2'-C3' | -2.81 | 104.14 | 110.00 |
| 20 | A | 807 | CLA | C2A-C1A-CHA | -2.81 | 118.94 | 123.86 |
| 20 | 1 | 204 | CLA | CAA-C2A-C1A | -2.81 | 102.76 | 111.97 |
| 20 | B | 816 | CLA | CMB-C2B-C1B | 2.81 | 129.65 | 125.37 |
| 20 | A | 808 | CLA | C6-C5-C3 | -2.81 | 106.09 | 113.45 |
| 21 | H | 105 | LMU | C3'-C4'-C5' | 2.81 | 117.37 | 110.93 |
| 20 | 1 | 205 | CLA | C4A-NA-C1A | 2.81 | 107.97 | 106.71 |
| 20 | 1 | 205 | CLA | CHB-C1B-NB | -2.81 | 121.28 | 124.26 |
| 20 | 1 | 215 | CLA | CHC-C4B-NB | 2.81 | 127.23 | 124.26 |
| 21 | R | 101 | LMU | O5B-C5B-C6B | 2.81 | 113.42 | 106.44 |
| 22 | F | 203 | BCR | C1-C6-C5 | -2.81 | 118.66 | 122.61 |
| 20 | R | 107 | CLA | C3B-C2B-C1B | -2.81 | 103.77 | 107.16 |
| 21 | D | 201 | LMU | O5B-C5B-C6B | 2.81 | 113.42 | 106.44 |
| 20 | B | 840 | CLA | C4A-NA-C1A | 2.81 | 107.97 | 106.71 |
| 21 | 4 | 319 | LMU | C3'-C4'-C5' | 2.80 | 117.36 | 110.93 |
| 20 | 3 | 312 | CLA | C3C-C4C-CHD | -2.80 | 119.08 | 125.22 |
| 20 | F | 207 | CLA | CHC-C1C-C2C | -2.80 | 118.94 | 126.73 |
| 20 | 1 | 211 | CLA | CHC-C1C-C2C | -2.80 | 118.94 | 126.73 |
| 20 | 1 | 201 | CLA | CMB-C2B-C1B | 2.80 | 129.64 | 125.37 |
| 20 | A | 827 | CLA | CHB-C4A-NA | 2.80 | 128.39 | 124.51 |
| 20 | 2 | 312 | CLA | C11-C10-C8 | -2.80 | 106.86 | 115.92 |
| 20 | A | 837 | CLA | O2D-CGD-O1D | -2.80 | 118.36 | 123.84 |
| 20 | 4 | 303 | CLA | CBC-CAC-C3C | -2.80 | 104.70 | 112.43 |
| 20 | B | 810 | CLA | CAA-C2A-C3A | -2.80 | 105.10 | 112.78 |
| 20 | L | 208 | CLA | CAA-C2A-C1A | 2.80 | 121.16 | 111.97 |
| 20 | 1 | 213 | CLA | C4D-C3D-CAD | 2.80 | 111.40 | 108.10 |
| 21 | R | 103 | LMU | C1B-O1B-C4' | 2.80 | 124.90 | 117.96 |
| 20 | 2 | 306 | CLA | C3C-C4C-CHD | -2.80 | 119.09 | 125.22 |
| 22 | I | 103 | BCR | C30-C25-C24 | 2.80 | 123.69 | 115.78 |
| 20 | B | 820 | CLA | O2A-CGA-CBA | 2.80 | 120.69 | 111.91 |
| 20 | 1 | 211 | CLA | O2A-C1-C2 | 2.80 | 115.99 | 108.64 |
| 20 | B | 837 | CLA | CMB-C2B-C1B | 2.80 | 129.63 | 125.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 306 | CLA | CHC-C4B-NB | 2.80 | 127.22 | 124.26 |
| 20 | F | 205 | CLA | C3B-C4B-NB | -2.80 | 108.36 | 110.23 |
| 20 | 2 | 308 | CLA | CHB-C1B-NB | -2.80 | 121.44 | 124.27 |
| 20 | 1 | 215 | CLA | C4-C3-C5 | 2.80 | 119.18 | 115.98 |
| 20 | 2 | 303 | CLA | O1D-CGD-CBD | -2.80 | 118.77 | 124.48 |
| 21 | R | 102 | LMU | O5B-C1B-C2B | 2.79 | 116.27 | 110.35 |
| 22 | A | 845 | BCR | C38-C26-C27 | 2.79 | 118.98 | 113.62 |
| 20 | A | 851 | CLA | O2A-CGA-CBA | 2.79 | 120.67 | 111.91 |
| 20 | A | 812 | CLA | O2A-CGA-CBA | 2.79 | 120.67 | 111.91 |
| 20 | F | 207 | CLA | CMA-C3A-C2A | 2.79 | 125.10 | 113.83 |
| 20 | 2 | 309 | CLA | C2C-C1C-CHC | -2.79 | 118.98 | 125.67 |
| 20 | L | 207 | CLA | O2A-CGA-CBA | 2.79 | 120.67 | 111.91 |
| 20 | H | 109 | CLA | C4-C3-C5 | 2.79 | 119.97 | 115.27 |
| 20 | B | 830 | CLA | CMA-C3A-C2A | -2.79 | 102.56 | 113.83 |
| 21 | A | 846 | LMU | C3B-C4B-C5B | 2.79 | 115.22 | 110.24 |
| 20 | A | 841 | CLA | C2C-C1C-CHC | -2.79 | 118.98 | 125.67 |
| 20 | B | 825 | CLA | CHC-C1C-C2C | -2.79 | 118.98 | 126.73 |
| 20 | 1 | 202 | CLA | CAA-C2A-C1A | 2.79 | 118.70 | 111.81 |
| 21 | A | 846 | LMU | O5'-C5'-C4' | 2.79 | 115.63 | 109.75 |
| 20 | B | 816 | CLA | O2A-CGA-CBA | 2.79 | 120.66 | 111.91 |
| 22 | L | 209 | BCR | C33-C5-C6 | -2.79 | 121.40 | 124.53 |
| 20 | 4 | 303 | CLA | C1-C2-C3 | -2.79 | 121.22 | 126.04 |
| 20 | B | 838 | CLA | CBC-CAC-C3C | -2.78 | 104.75 | 112.43 |
| 20 | 3 | 308 | CLA | C3C-C4C-CHD | -2.78 | 119.12 | 125.22 |
| 20 | A | 801 | CLA | CHD-C4C-C3C | -2.78 | 120.75 | 124.84 |
| 21 | K | 106 | LMU | O1B-C1B-C2B | 2.78 | 115.31 | 108.10 |
| 21 | 1 | 216 | LMU | C1B-O5B-C5B | -2.78 | 108.23 | 113.69 |
| 20 | F | 206 | CLA | CAA-C2A-C3A | -2.78 | 109.61 | 116.10 |
| 20 | 3 | 303 | CLA | CHB-C1B-NB | -2.78 | 121.31 | 124.26 |
| 20 | A | 833 | CLA | CAC-C3C-C4C | 2.78 | 128.42 | 124.81 |
| 20 | 2 | 305 | CLA | CHB-C4A-NA | 2.78 | 128.36 | 124.51 |
| 20 | 4 | 313 | CLA | CMA-C3A-C2A | -2.78 | 109.61 | 116.10 |
| 20 | F | 206 | CLA | O2D-CGD-O1D | -2.78 | 118.41 | 123.84 |
| 20 | B | 834 | CLA | CHB-C4A-NA | 2.78 | 128.35 | 124.51 |
| 20 | A | 806 | CLA | C2A-C1A-CHA | -2.78 | 119.00 | 123.86 |
| 20 | A | 810 | CLA | CMA-C3A-C2A | -2.77 | 102.64 | 113.83 |
| 20 | A | 830 | CLA | O2D-CGD-O1D | -2.77 | 118.42 | 123.84 |
| 20 | 2 | 301 | CLA | C1C-NC-C4C | -2.77 | 105.46 | 106.71 |
| 20 | A | 823 | CLA | O2A-CGA-CBA | 2.77 | 120.61 | 111.91 |
| 20 | B | 826 | CLA | CHB-C1B-NB | -2.77 | 121.32 | 124.26 |
| 21 | L | 205 | LMU | C3B-C4B-C5B | 2.77 | 115.19 | 110.24 |
| 20 | B | 850 | CLA | C3B-C4B-NB | -2.77 | 107.94 | 110.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 815 | CLA | C4A-NA-C1A | 2.77 | 107.95 | 106.71 |
| 20 | H | 102 | CLA | C1-O2A-CGA | 2.77 | 123.71 | 116.44 |
| 20 | A | 812 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 20 | 3 | 313 | CLA | CHB-C1B-NB | -2.77 | 121.33 | 124.26 |
| 20 | B | 816 | CLA | CHB-C1B-NB | -2.77 | 121.33 | 124.26 |
| 20 | A | 801 | CLA | CAA-C2A-C1A | 2.77 | 121.04 | 111.97 |
| 20 | H | 109 | CLA | O2A-CGA-CBA | 2.77 | 120.59 | 111.91 |
| 22 | F | 203 | BCR | C33-C5-C4 | 2.77 | 118.93 | 113.62 |
| 20 | 4 | 307 | CLA | CHD-C1D-ND | 2.77 | 127.19 | 124.52 |
| 20 | A | 823 | CLA | CHB-C4A-NA | 2.77 | 128.34 | 124.51 |
| 20 | A | 820 | CLA | CHB-C1B-NB | -2.77 | 121.33 | 124.26 |
| 20 | 2 | 301 | CLA | C2C-C1C-CHC | -2.77 | 119.05 | 125.67 |
| 20 | B | 802 | CLA | CAA-C2A-C1A | 2.77 | 121.04 | 111.97 |
| 21 | H | 105 | LMU | C4B-C3B-C2B | -2.77 | 106.00 | 110.82 |
| 20 | 1 | 206 | CLA | C1-O2A-CGA | 2.76 | 123.69 | 116.44 |
| 20 | J | 101 | CLA | O2D-CGD-O1D | -2.76 | 118.44 | 123.84 |
| 20 | K | 102 | CLA | CBC-CAC-C3C | -2.76 | 104.81 | 112.43 |
| 22 | F | 204 | BCR | C2-C1-C6 | 2.76 | 114.73 | 110.48 |
| 20 | K | 104 | CLA | CHC-C1C-C2C | -2.76 | 119.06 | 126.73 |
| 20 | J | 101 | CLA | CHC-C1C-C2C | -2.76 | 119.06 | 126.73 |
| 20 | 3 | 315 | CLA | C3D-C4D-ND | 2.76 | 113.62 | 109.46 |
| 20 | 1 | 203 | CLA | CHB-C1B-NB | -2.76 | 121.34 | 124.26 |
| 20 | 2 | 302 | CLA | O2D-CGD-O1D | -2.76 | 118.45 | 123.84 |
| 20 | 4 | 318 | CLA | O2A-CGA-CBA | 2.76 | 120.56 | 111.91 |
| 20 | 2 | 303 | CLA | CHC-C1C-C2C | -2.76 | 119.07 | 126.73 |
| 20 | B | 802 | CLA | C1-O2A-CGA | 2.76 | 123.67 | 116.44 |
| 20 | B | 812 | CLA | CHB-C4A-NA | 2.76 | 128.32 | 124.51 |
| 21 | L | 206 | LMU | O1'-C1'-C2' | 2.76 | 112.61 | 108.30 |
| 20 | R | 108 | CLA | C4-C3-C2 | -2.75 | 116.61 | 123.68 |
| 20 | 4 | 301 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |
| 20 | 2 | 312 | CLA | CAA-CBA-CGA | -2.75 | 105.20 | 113.25 |
| 20 | 3 | 314 | CLA | O2D-CGD-O1D | -2.75 | 118.45 | 123.84 |
| 20 | A | 850 | CLA | O2A-CGA-O1A | -2.75 | 116.64 | 123.59 |
| 20 | 4 | 301 | CLA | O2A-CGA-CBA | 2.75 | 120.55 | 111.91 |
| 20 | L | 204 | CLA | CMB-C2B-C1B | 2.75 | 129.56 | 125.37 |
| 20 | B | 825 | CLA | CGD-CBD-CAD | -2.75 | 101.82 | 110.73 |
| 20 | 4 | 307 | CLA | C2C-C1C-CHC | -2.75 | 119.08 | 125.67 |
| 20 | 3 | 305 | CLA | C3D-C4D-CHA | -2.75 | 119.19 | 124.98 |
| 20 | B | 808 | CLA | CMB-C2B-C1B | 2.75 | 129.56 | 125.37 |
| 22 | A | 844 | BCR | C11-C12-C13 | -2.75 | 118.69 | 126.42 |
| 21 | E | 101 | LMU | O1B-C1B-O5B | 2.75 | 118.36 | 110.67 |
| 20 | B | 831 | CLA | C1-C2-C3 | -2.75 | 122.30 | 126.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 303 | CLA | C1D-ND-C4D | -2.75 | 104.38 | 106.33 |
| 22 | J | 102 | BCR | C38-C26-C27 | 2.75 | 118.90 | 113.62 |
| 22 | F | 203 | BCR | C37-C22-C21 | -2.75 | 119.07 | 122.92 |
| 20 | A | 835 | CLA | CAA-C2A-C1A | -2.75 | 102.97 | 111.97 |
| 20 | B | 803 | CLA | O2A-CGA-CBA | 2.75 | 120.53 | 111.91 |
| 20 | B | 811 | CLA | C1B-NB-C4B | -2.74 | 104.39 | 106.33 |
| 20 | A | 806 | CLA | C1-C2-C3 | -2.74 | 121.30 | 126.04 |
| 20 | B | 839 | CLA | CMB-C2B-C1B | 2.74 | 129.54 | 125.37 |
| 23 | A | 842 | PQN | C2M-C2-C3 | -2.74 | 119.93 | 124.40 |
| 20 | 3 | 306 | CLA | C2C-C1C-CHC | -2.74 | 119.11 | 125.67 |
| 20 | 4 | 309 | CLA | C2C-C1C-CHC | -2.74 | 119.11 | 125.67 |
| 20 | A | 819 | CLA | C4-C3-C5 | 2.74 | 119.88 | 115.27 |
| 20 | A | 820 | CLA | O2A-CGA-CBA | 2.74 | 120.50 | 111.91 |
| 20 | 2 | 310 | CLA | C1D-ND-C4D | -2.74 | 104.39 | 106.33 |
| 20 | 3 | 315 | CLA | CHB-C4A-NA | 2.74 | 128.53 | 124.34 |
| 20 | A | 829 | CLA | CHB-C1B-NB | -2.74 | 121.36 | 124.26 |
| 20 | B | 834 | CLA | CHB-C1B-NB | -2.74 | 121.36 | 124.26 |
| 20 | 1 | 206 | CLA | C1D-ND-C4D | -2.74 | 104.39 | 106.33 |
| 20 | A | 828 | CLA | C1-C2-C3 | -2.73 | 121.31 | 126.04 |
| 20 | A | 849 | CLA | CAA-C2A-C3A | -2.73 | 105.29 | 112.78 |
| 20 | 1 | 214 | CLA | CHB-C4A-NA | 2.73 | 128.52 | 124.34 |
| 20 | R | 108 | CLA | CHC-C1C-C2C | -2.73 | 119.14 | 126.73 |
| 20 | B | 815 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 20 | 3 | 311 | CLA | CHB-C1B-NB | -2.73 | 121.36 | 124.26 |
| 20 | B | 815 | CLA | C3B-C4B-NB | -2.73 | 107.98 | 110.52 |
| 20 | 2 | 306 | CLA | CHD-C1D-ND | 2.73 | 127.15 | 124.52 |
| 20 | 1 | 204 | CLA | C1D-ND-C4D | -2.73 | 104.39 | 106.33 |
| 20 | 2 | 305 | CLA | C4A-NA-C1A | 2.73 | 107.93 | 106.71 |
| 20 | K | 104 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 20 | A | 817 | CLA | CHC-C1C-C2C | -2.73 | 119.15 | 126.73 |
| 20 | A | 819 | CLA | CED-O2D-CGD | 2.73 | 122.11 | 115.94 |
| 22 | I | 101 | BCR | C10-C11-C12 | -2.73 | 114.70 | 123.22 |
| 20 | B | 824 | CLA | C1D-ND-C4D | -2.73 | 104.40 | 106.33 |
| 20 | H | 109 | CLA | CHC-C1C-C2C | -2.73 | 119.16 | 126.73 |
| 20 | A | 811 | CLA | CAA-C2A-C1A | -2.73 | 103.05 | 111.97 |
| 20 | B | 839 | CLA | O1D-CGD-CBD | -2.72 | 118.91 | 124.48 |
| 20 | 4 | 301 | CLA | CAC-C3C-C4C | 2.72 | 128.34 | 124.81 |
| 20 | 4 | 310 | CLA | CHB-C1B-NB | -2.72 | 121.38 | 124.26 |
| 20 | B | 833 | CLA | O2A-CGA-CBA | 2.72 | 120.45 | 111.91 |
| 20 | 2 | 306 | CLA | C3B-C4B-CHC | -2.72 | 118.33 | 126.24 |
| 20 | R | 108 | CLA | CMB-C2B-C1B | 2.72 | 129.51 | 125.37 |
| 20 | 2 | 312 | CLA | O2A-C1-C2 | -2.72 | 101.49 | 108.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 810 | CLA | O2A-C1-C2 | 2.72 | 115.78 | 108.64 |
| 20 | A | 837 | CLA | C4-C3-C5 | 2.72 | 119.09 | 115.98 |
| 20 | K | 101 | CLA | C2D-C1D-ND | -2.72 | 108.10 | 110.10 |
| 20 | A | 839 | CLA | CAA-C2A-C3A | 2.72 | 120.22 | 112.78 |
| 20 | 4 | 306 | CLA | CBA-CAA-C2A | -2.72 | 105.85 | 113.86 |
| 20 | B | 808 | CLA | CHB-C4A-NA | 2.72 | 128.27 | 124.51 |
| 21 | H | 106 | LMU | C1'-O5'-C5' | 2.72 | 119.02 | 113.69 |
| 20 | B | 817 | CLA | CHB-C4A-NA | 2.71 | 128.26 | 124.51 |
| 20 | 3 | 302 | CLA | C2C-C1C-CHC | -2.71 | 119.17 | 125.67 |
| 20 | A | 840 | CLA | CHC-C1C-C2C | -2.71 | 119.20 | 126.73 |
| 20 | B | 818 | CLA | CHC-C1C-C2C | -2.71 | 119.20 | 126.73 |
| 20 | 3 | 317 | CLA | CMB-C2B-C1B | 2.71 | 129.50 | 125.37 |
| 20 | B | 814 | CLA | C3B-C2B-C1B | -2.71 | 103.89 | 107.16 |
| 20 | J | 101 | CLA | CHB-C1B-NB | -2.71 | 121.39 | 124.26 |
| 20 | 3 | 310 | CLA | O2A-CGA-CBA | 2.71 | 120.41 | 111.91 |
| 21 | E | 101 | LMU | O2'-C2'-C1' | -2.71 | 103.47 | 110.05 |
| 20 | 3 | 315 | CLA | CHD-C1D-ND | 2.71 | 127.13 | 124.52 |
| 20 | B | 816 | CLA | CED-O2D-CGD | 2.70 | 122.06 | 115.94 |
| 20 | B | 817 | CLA | O1D-CGD-CBD | -2.70 | 118.95 | 124.48 |
| 20 | A | 836 | CLA | CHB-C4A-NA | 2.70 | 128.25 | 124.51 |
| 20 | A | 820 | CLA | CED-O2D-CGD | 2.70 | 122.05 | 115.94 |
| 20 | A | 815 | CLA | CHC-C1C-C2C | -2.70 | 119.22 | 126.73 |
| 20 | K | 101 | CLA | CHB-C1B-NB | -2.70 | 121.39 | 124.26 |
| 22 | G | 104 | BCR | C38-C26-C27 | 2.70 | 118.81 | 113.62 |
| 20 | 4 | 303 | CLA | C11-C10-C8 | -2.70 | 107.18 | 115.92 |
| 20 | H | 101 | CLA | CED-O2D-CGD | 2.70 | 122.05 | 115.94 |
| 20 | A | 809 | CLA | C2D-C1D-ND | -2.70 | 108.11 | 110.10 |
| 20 | B | 837 | CLA | CHC-C1C-C2C | -2.70 | 119.23 | 126.73 |
| 21 | F | 202 | LMU | O5B-C5B-C6B | 2.70 | 113.15 | 106.44 |
| 22 | J | 102 | BCR | C30-C25-C26 | -2.70 | 118.81 | 122.61 |
| 20 | A | 805 | CLA | CAC-C3C-C4C | 2.70 | 128.31 | 124.81 |
| 20 | 3 | 301 | CLA | CAA-C2A-C3A | -2.70 | 109.80 | 116.10 |
| 20 | 1 | 214 | CLA | C2C-C1C-CHC | -2.70 | 119.21 | 125.67 |
| 20 | R | 107 | CLA | CHC-C1C-C2C | -2.70 | 119.23 | 126.73 |
| 22 | L | 209 | BCR | C3-C4-C5 | -2.70 | 109.26 | 114.08 |
| 20 | B | 841 | CLA | O2A-CGA-O1A | -2.70 | 116.78 | 123.59 |
| 20 | 3 | 316 | CLA | C2C-C1C-CHC | -2.70 | 119.21 | 125.67 |
| 20 | I | 102 | CLA | CHB-C1B-NB | -2.69 | 121.40 | 124.26 |
| 22 | A | 845 | BCR | C1-C6-C5 | -2.69 | 118.82 | 122.61 |
| 20 | B | 812 | CLA | O2D-CGD-O1D | -2.69 | 118.57 | 123.84 |
| 22 | B | 846 | BCR | C33-C5-C6 | -2.69 | 121.50 | 124.53 |
| 21 | 4 | 320 | LMU | C1'-C2'-C3' | 2.69 | 115.61 | 110.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 806 | CLA | CHB-C4A-NA | 2.69 | 128.24 | 124.51 |
| 20 | 3 | 310 | CLA | C1-O2A-CGA | 2.69 | 123.51 | 116.44 |
| 20 | H | 101 | CLA | CMA-C3A-C4A | -2.69 | 104.54 | 111.77 |
| 20 | F | 206 | CLA | CMB-C2B-C1B | 2.69 | 129.47 | 125.37 |
| 20 | A | 806 | CLA | CHC-C1C-C2C | -2.69 | 119.26 | 126.73 |
| 20 | A | 834 | CLA | CHC-C1C-C2C | -2.69 | 119.26 | 126.73 |
| 22 | A | 845 | BCR | C3-C4-C5 | -2.69 | 109.28 | 114.08 |
| 20 | B | 831 | CLA | CHC-C1C-C2C | -2.69 | 119.26 | 126.73 |
| 20 | B | 821 | CLA | C1D-ND-C4D | -2.69 | 104.43 | 106.33 |
| 20 | 1 | 204 | CLA | C2A-C1A-CHA | -2.69 | 119.16 | 123.86 |
| 20 | 4 | 318 | CLA | CHD-C4C-C3C | -2.69 | 120.89 | 124.84 |
| 20 | 1 | 202 | CLA | C3B-C2B-C1B | -2.68 | 103.92 | 107.16 |
| 20 | A | 830 | CLA | CHB-C1B-NB | -2.68 | 121.42 | 124.26 |
| 20 | B | 825 | CLA | CHB-C1B-NB | -2.68 | 121.42 | 124.26 |
| 20 | B | 828 | CLA | C4-C3-C5 | 2.68 | 119.78 | 115.27 |
| 20 | 2 | 315 | CLA | C2D-C3D-C4D | -2.68 | 104.31 | 107.28 |
| 20 | A | 817 | CLA | O2A-C1-C2 | 2.68 | 115.69 | 108.64 |
| 20 | A | 820 | CLA | C4-C3-C5 | 2.68 | 119.05 | 115.98 |
| 20 | A | 818 | CLA | CAA-C2A-C3A | -2.68 | 105.44 | 112.78 |
| 20 | A | 825 | CLA | CHB-C1B-NB | -2.68 | 121.42 | 124.26 |
| 20 | A | 805 | CLA | O2A-CGA-CBA | 2.68 | 120.31 | 111.91 |
| 20 | 1 | 212 | CLA | C2A-C3A-C4A | -2.68 | 99.98 | 104.18 |
| 20 | 2 | 308 | CLA | C2A-C3A-C4A | -2.68 | 99.98 | 104.18 |
| 20 | B | 802 | CLA | CMB-C2B-C1B | 2.68 | 129.45 | 125.37 |
| 20 | B | 810 | CLA | CMB-C2B-C1B | 2.68 | 129.45 | 125.37 |
| 20 | A | 826 | CLA | O2D-CGD-O1D | -2.68 | 118.60 | 123.84 |
| 20 | 1 | 213 | CLA | O2A-CGA-CBA | 2.68 | 120.31 | 111.91 |
| 20 | A | 802 | CLA | C2C-C1C-CHC | -2.68 | 119.26 | 125.67 |
| 20 | B | 802 | CLA | CAC-C3C-C4C | 2.68 | 128.28 | 124.81 |
| 21 | 4 | 316 | LMU | O1'-C1'-C2' | 2.67 | 112.48 | 108.30 |
| 20 | 4 | 315 | CLA | C1D-ND-C4D | -2.67 | 104.44 | 106.33 |
| 20 | 3 | 307 | CLA | CHB-C4A-NA | 2.67 | 128.21 | 124.51 |
| 20 | L | 204 | CLA | C4-C3-C5 | 2.67 | 119.77 | 115.27 |
| 22 | B | 844 | BCR | C33-C5-C4 | 2.67 | 118.75 | 113.62 |
| 21 | 2 | 319 | LMU | C1'-O5'-C5' | 2.67 | 118.93 | 113.69 |
| 21 | R | 103 | LMU | C6B-C5B-C4B | -2.67 | 106.75 | 113.00 |
| 20 | A | 804 | CLA | C4-C3-C5 | 2.67 | 119.76 | 115.27 |
| 20 | A | 801 | CLA | CHC-C4B-C3B | -2.67 | 119.70 | 127.24 |
| 20 | F | 207 | CLA | C3B-C2B-C1B | -2.67 | 103.94 | 107.16 |
| 20 | A | 823 | CLA | CHC-C1C-C2C | -2.67 | 119.32 | 126.73 |
| 20 | B | 831 | CLA | CGD-CBD-CAD | 2.67 | 119.37 | 110.73 |
| 20 | 1 | 208 | CLA | CHB-C1B-NB | -2.67 | 121.57 | 124.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 835 | CLA | C2A-C1A-CHA | -2.67 | 119.19 | 123.86 |
| 20 | A | 831 | CLA | C11-C10-C8 | -2.67 | 107.30 | 115.92 |
| 20 | 3 | 309 | CLA | C3C-C4C-CHD | -2.67 | 119.38 | 125.22 |
| 20 | 4 | 317 | CLA | CAA-C2A-C1A | -2.67 | 103.24 | 111.97 |
| 22 | B | 845 | BCR | C15-C14-C13 | -2.67 | 123.51 | 127.31 |
| 20 | 3 | 304 | CLA | CHB-C4A-NA | 2.67 | 128.42 | 124.34 |
| 22 | B | 845 | BCR | C23-C22-C21 | 2.66 | 123.03 | 118.94 |
| 20 | A | 851 | CLA | O2A-C1-C2 | 2.66 | 115.64 | 108.64 |
| 21 | 1 | 216 | LMU | O5'-C1'-C2' | -2.66 | 104.71 | 110.35 |
| 20 | B | 840 | CLA | CAA-C2A-C3A | -2.66 | 105.48 | 112.78 |
| 20 | A | 806 | CLA | CED-O2D-CGD | 2.66 | 121.96 | 115.94 |
| 21 | D | 201 | LMU | C4B-C3B-C2B | -2.66 | 106.17 | 110.82 |
| 20 | 3 | 308 | CLA | C2C-C1C-CHC | -2.66 | 119.29 | 125.67 |
| 20 | B | 840 | CLA | C4-C3-C5 | 2.66 | 119.75 | 115.27 |
| 20 | H | 108 | CLA | CHB-C1B-NB | -2.66 | 121.44 | 124.26 |
| 21 | B | 849 | LMU | C2'-C3'-C4' | 2.66 | 115.75 | 109.68 |
| 20 | A | 801 | CLA | CGD-CBD-CAD | 2.66 | 119.35 | 110.73 |
| 20 | 2 | 304 | CLA | C4D-ND-C1D | -2.66 | 104.45 | 106.33 |
| 20 | 3 | 301 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 20 | B | 841 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 22 | A | 843 | BCR | C8-C7-C6 | -2.66 | 119.74 | 127.20 |
| 20 | 1 | 209 | CLA | C2A-C3A-C4A | -2.66 | 100.01 | 104.18 |
| 20 | B | 832 | CLA | CAA-CBA-CGA | -2.66 | 105.49 | 113.25 |
| 20 | 1 | 212 | CLA | C3C-C4C-CHD | -2.66 | 119.40 | 125.22 |
| 20 | B | 811 | CLA | C2C-C1C-CHC | -2.66 | 119.31 | 125.67 |
| 20 | A | 812 | CLA | CHC-C1C-C2C | -2.66 | 119.35 | 126.73 |
| 20 | 2 | 306 | CLA | C3B-C2B-C1B | -2.66 | 103.87 | 106.75 |
| 20 | 4 | 303 | CLA | O2D-CGD-CBD | 2.66 | 115.99 | 111.27 |
| 20 | B | 813 | CLA | O2D-CGD-O1D | -2.65 | 118.65 | 123.84 |
| 20 | A | 826 | CLA | CHB-C1B-NB | -2.65 | 121.45 | 124.26 |
| 20 | A | 826 | CLA | C4A-NA-C1A | 2.65 | 107.90 | 106.71 |
| 20 | A | 815 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 20 | A | 851 | CLA | CHC-C1C-C2C | -2.65 | 119.36 | 126.73 |
| 22 | A | 845 | BCR | C35-C13-C14 | -2.65 | 119.21 | 122.92 |
| 20 | B | 820 | CLA | C4-C3-C5 | 2.65 | 119.73 | 115.27 |
| 20 | B | 817 | CLA | CHC-C1C-C2C | -2.65 | 119.36 | 126.73 |
| 21 | 4 | 320 | LMU | C3'-C4'-C5' | 2.65 | 117.00 | 110.93 |
| 20 | A | 819 | CLA | CHC-C1C-C2C | -2.65 | 119.37 | 126.73 |
| 20 | 2 | 302 | CLA | C1-C2-C3 | -2.65 | 121.46 | 126.04 |
| 20 | 3 | 312 | CLA | CHB-C4A-NA | 2.65 | 128.40 | 124.34 |
| 20 | B | 813 | CLA | C3B-C2B-C1B | -2.65 | 103.96 | 107.16 |
| 20 | 1 | 203 | CLA | CMB-C2B-C1B | 2.65 | 129.40 | 125.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 3 | 311 | CLA | CHC-C1C-C2C | -2.65 | 119.37 | 126.73 |
| 21 | A | 846 | LMU | C3'-C4'-C5' | 2.65 | 117.00 | 110.93 |
| 20 | B | 824 | CLA | O2A-CGA-CBA | 2.65 | 120.22 | 111.91 |
| 20 | 1 | 202 | CLA | CHB-C4A-NA | 2.65 | 128.17 | 124.51 |
| 21 | B | 849 | LMU | O5B-C5B-C4B | 2.65 | 114.50 | 109.69 |
| 20 | A | 818 | CLA | C1D-ND-C4D | -2.65 | 104.45 | 106.33 |
| 22 | 2 | 317 | BCR | C36-C18-C17 | -2.65 | 119.22 | 122.92 |
| 20 | A | 825 | CLA | CHC-C1C-C2C | -2.64 | 119.38 | 126.73 |
| 20 | 3 | 310 | CLA | C6-C5-C3 | -2.64 | 106.52 | 113.45 |
| 20 | A | 806 | CLA | C3B-C4B-NB | -2.64 | 108.06 | 110.52 |
| 20 | B | 811 | CLA | C3D-C4D-ND | 2.64 | 113.45 | 109.46 |
| 20 | A | 841 | CLA | C2A-C3A-C4A | -2.64 | 100.03 | 104.18 |
| 20 | B | 808 | CLA | CHC-C1C-C2C | -2.64 | 119.40 | 126.73 |
| 22 | B | 801 | BCR | C7-C6-C5 | -2.64 | 115.07 | 121.46 |
| 22 | G | 104 | BCR | C23-C24-C25 | -2.64 | 119.79 | 127.20 |
| 21 | R | 106 | LMU | C2'-C3'-C4' | 2.64 | 115.70 | 109.68 |
| 20 | 1 | 204 | CLA | C3D-C4D-ND | 2.64 | 114.50 | 110.24 |
| 20 | A | 826 | CLA | CMA-C3A-C4A | -2.64 | 104.69 | 111.77 |
| 20 | L | 208 | CLA | O2A-CGA-CBA | 2.64 | 120.18 | 111.91 |
| 20 | B | 812 | CLA | CAA-C2A-C3A | -2.63 | 105.56 | 112.78 |
| 20 | A | 817 | CLA | CHB-C4A-NA | 2.63 | 128.15 | 124.51 |
| 21 | K | 107 | LMU | C1'-C2'-C3' | -2.63 | 104.52 | 110.00 |
| 20 | 2 | 314 | CLA | O2D-CGD-CBD | 2.63 | 115.94 | 111.27 |
| 20 | A | 806 | CLA | O2A-CGA-CBA | 2.63 | 120.16 | 111.91 |
| 20 | H | 102 | CLA | CED-O2D-CGD | 2.63 | 121.88 | 115.94 |
| 20 | B | 842 | CLA | CMB-C2B-C1B | 2.63 | 129.37 | 125.37 |
| 22 | A | 844 | BCR | C38-C26-C27 | 2.63 | 118.66 | 113.62 |
| 20 | 1 | 213 | CLA | C2D-C1D-ND | -2.63 | 108.17 | 110.10 |
| 20 | A | 802 | CLA | C4D-ND-C1D | -2.62 | 104.47 | 106.33 |
| 20 | 3 | 317 | CLA | CHC-C1C-C2C | -2.62 | 119.44 | 126.73 |
| 20 | F | 205 | CLA | CAA-C2A-C3A | -2.62 | 109.98 | 116.10 |
| 20 | 2 | 304 | CLA | C3D-C4D-ND | 2.62 | 113.42 | 109.46 |
| 20 | H | 102 | CLA | CHC-C1C-C2C | -2.62 | 119.44 | 126.73 |
| 20 | B | 842 | CLA | CHB-C4A-NA | 2.62 | 128.14 | 124.51 |
| 20 | A | 851 | CLA | C2A-C1A-CHA | -2.62 | 119.28 | 123.86 |
| 20 | A | 836 | CLA | CMB-C2B-C1B | 2.62 | 129.36 | 125.37 |
| 20 | B | 803 | CLA | CMB-C2B-C1B | 2.62 | 129.36 | 125.37 |
| 22 | B | 844 | BCR | C33-C5-C6 | -2.62 | 121.59 | 124.53 |
| 20 | 3 | 312 | CLA | C2C-C1C-CHC | -2.62 | 119.40 | 125.67 |
| 21 | H | 103 | LMU | O3'-C3'-C2' | 2.62 | 116.40 | 110.35 |
| 20 | 1 | 214 | CLA | C4D-ND-C1D | -2.62 | 104.48 | 106.33 |
| 20 | 1 | 211 | CLA | O2D-CGD-O1D | -2.62 | 118.72 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 20 | B | 809 | CLA | CAA-C2A-C3A | -2.61 | 105.62 | 112.78 |
| 20 | A | 830 | CLA | CHB-C4A-NA | 2.61 | 128.13 | 124.51 |
| 22 | F | 204 | BCR | C1-C6-C5 | -2.61 | 118.93 | 122.61 |
| 20 | 4 | 307 | CLA | C3D-C4D-ND | 2.61 | 113.41 | 109.46 |
| 20 | 1 | 213 | CLA | CHB-C4A-NA | 2.61 | 128.12 | 124.51 |
| 20 | F | 207 | CLA | CMB-C2B-C1B | 2.61 | 129.35 | 125.37 |
| 22 | A | 845 | BCR | C27-C26-C25 | -2.61 | 118.94 | 122.73 |
| 20 | 3 | 301 | CLA | CHC-C4B-C3B | -2.61 | 119.86 | 127.24 |
| 20 | A | 801 | CLA | CMB-C2B-C1B | 2.61 | 129.34 | 125.37 |
| 20 | A | 837 | CLA | CHB-C4A-NA | 2.61 | 128.12 | 124.51 |
| 20 | 2 | 301 | CLA | CHB-C4A-NA | 2.61 | 128.33 | 124.34 |
| 20 | A | 828 | CLA | CHB-C1B-NB | -2.61 | 121.50 | 124.26 |
| 20 | B | 836 | CLA | CHB-C1B-NB | -2.61 | 121.50 | 124.26 |
| 20 | 1 | 214 | CLA | CHD-C1D-ND | 2.61 | 127.03 | 124.52 |
| 20 | 2 | 307 | CLA | C3B-C2B-C1B | -2.61 | 104.02 | 107.16 |
| 22 | B | 801 | BCR | C4-C5-C6 | -2.61 | 118.95 | 122.73 |
| 20 | B | 814 | CLA | C4-C3-C5 | 2.61 | 119.65 | 115.27 |
| 20 | 2 | 301 | CLA | C3C-C4C-CHD | -2.60 | 119.52 | 125.22 |
| 20 | 4 | 313 | CLA | CHC-C1C-C2C | -2.60 | 119.50 | 126.73 |
| 21 | 4 | 321 | LMU | O1'-C1'-C2' | 2.60 | 112.37 | 108.30 |
| 20 | K | 102 | CLA | O2A-CGA-O1A | -2.60 | 117.03 | 123.59 |
| 21 | G | 101 | LMU | O4'-C4B-C5B | 2.60 | 115.76 | 109.30 |
| 20 | 2 | 316 | CLA | C4-C3-C5 | 2.60 | 119.65 | 115.27 |
| 21 | G | 101 | LMU | O1B-C1B-C2B | 2.60 | 114.83 | 108.10 |
| 21 | H | 104 | LMU | O1B-C4'-C5' | 2.60 | 116.57 | 109.45 |
| 20 | B | 806 | CLA | CHB-C1B-NB | -2.60 | 121.51 | 124.26 |
| 20 | A | 851 | CLA | C4A-NA-C1A | 2.60 | 107.87 | 106.71 |
| 20 | B | 815 | CLA | CHB-C1B-NB | -2.60 | 121.51 | 124.26 |
| 20 | A | 822 | CLA | CHC-C1C-C2C | -2.60 | 119.52 | 126.73 |
| 20 | 4 | 310 | CLA | C3B-C2B-C1B | -2.60 | 104.03 | 107.16 |
| 21 | 2 | 319 | LMU | O1B-C1B-C2B | 2.59 | 114.82 | 108.10 |
| 20 | 2 | 315 | CLA | C3B-C2B-C1B | -2.59 | 103.94 | 106.75 |
| 20 | 4 | 304 | CLA | C1-O2A-CGA | 2.59 | 123.25 | 116.44 |
| 20 | B | 809 | CLA | C16-C15-C13 | -2.59 | 107.54 | 115.92 |
| 21 | L | 205 | LMU | O5'-C5'-C6' | 2.59 | 112.88 | 106.44 |
| 20 | 2 | 306 | CLA | CHB-C1B-NB | -2.59 | 121.65 | 124.27 |
| 20 | B | 806 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |
| 20 | 2 | 307 | CLA | C3D-C4D-ND | 2.59 | 114.42 | 110.24 |
| 20 | A | 827 | CLA | O2A-CGA-CBA | 2.59 | 120.03 | 111.91 |
| 20 | 2 | 309 | CLA | C4A-NA-C1A | 2.59 | 107.87 | 106.71 |
| 20 | A | 822 | CLA | C4A-NA-C1A | 2.59 | 107.87 | 106.71 |
| 21 | B | 804 | LMU | O5'-C5'-C6' | 2.59 | 112.87 | 106.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 312 | CLA | C3D-C2D-C1D | 2.59 | 110.14 | 107.28 |
| 20 | A | 819 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |
| 20 | A | 832 | CLA | O2D-CGD-O1D | -2.58 | 118.79 | 123.84 |
| 20 | 3 | 310 | CLA | C6-C7-C8 | -2.58 | 107.57 | 115.92 |
| 20 | 1 | 208 | CLA | C2C-C1C-CHC | -2.58 | 119.48 | 125.67 |
| 20 | H | 110 | CLA | C4A-NA-C1A | 2.58 | 107.87 | 106.71 |
| 20 | A | 812 | CLA | O2D-CGD-O1D | -2.58 | 118.79 | 123.84 |
| 22 | B | 844 | BCR | C1-C6-C7 | 2.58 | 123.08 | 115.78 |
| 20 | A | 849 | CLA | CMB-C2B-C1B | 2.58 | 129.30 | 125.37 |
| 20 | A | 835 | CLA | C4A-NA-C1A | 2.58 | 107.87 | 106.71 |
| 20 | 3 | 305 | CLA | CHB-C1B-NB | -2.58 | 121.66 | 124.27 |
| 20 | A | 814 | CLA | CHB-C4A-NA | 2.58 | 128.29 | 124.34 |
| 20 | A | 827 | CLA | C4-C3-C5 | 2.58 | 119.61 | 115.27 |
| 20 | A | 839 | CLA | C4A-NA-C1A | 2.58 | 107.86 | 106.71 |
| 20 | 4 | 306 | CLA | C3C-C4C-NC | -2.58 | 107.68 | 110.57 |
| 20 | B | 839 | CLA | CHB-C1B-NB | -2.58 | 121.53 | 124.26 |
| 20 | A | 850 | CLA | CED-O2D-CGD | 2.58 | 121.77 | 115.94 |
| 20 | A | 839 | CLA | CHB-C4A-NA | 2.58 | 128.07 | 124.51 |
| 20 | 3 | 313 | CLA | O2A-CGA-O1A | -2.58 | 117.09 | 123.59 |
| 20 | A | 829 | CLA | CMB-C2B-C1B | 2.58 | 129.29 | 125.37 |
| 20 | 3 | 305 | CLA | CHB-C4A-NA | 2.57 | 128.28 | 124.34 |
| 22 | F | 203 | BCR | C20-C19-C18 | -2.57 | 119.19 | 126.42 |
| 20 | A | 824 | CLA | CHB-C1B-NB | -2.57 | 121.53 | 124.26 |
| 20 | 4 | 314 | CLA | C2C-C1C-CHC | -2.57 | 119.51 | 125.67 |
| 20 | B | 813 | CLA | CHB-C4A-NA | 2.57 | 128.07 | 124.51 |
| 20 | B | 831 | CLA | CMB-C2B-C1B | 2.57 | 129.29 | 125.37 |
| 20 | J | 101 | CLA | CHB-C4A-NA | 2.57 | 128.07 | 124.51 |
| 20 | B | 832 | CLA | C4A-NA-C1A | 2.57 | 107.86 | 106.71 |
| 20 | I | 102 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 22 | I | 103 | BCR | C35-C13-C12 | 2.57 | 122.12 | 118.08 |
| 20 | 3 | 303 | CLA | C1D-ND-C4D | -2.57 | 104.51 | 106.33 |
| 20 | 4 | 304 | CLA | O1D-CGD-CBD | -2.57 | 119.23 | 124.48 |
| 20 | A | 810 | CLA | CED-O2D-CGD | 2.57 | 121.74 | 115.94 |
| 20 | B | 829 | CLA | CHC-C1C-C2C | -2.57 | 119.60 | 126.73 |
| 20 | B | 823 | CLA | CHB-C4A-NA | 2.56 | 128.06 | 124.51 |
| 20 | 2 | 305 | CLA | CHC-C1C-C2C | -2.56 | 119.61 | 126.73 |
| 20 | A | 808 | CLA | CAA-C2A-C3A | -2.56 | 105.76 | 112.78 |
| 20 | A | 831 | CLA | CAC-C3C-C2C | -2.56 | 123.14 | 127.53 |
| 20 | L | 202 | CLA | C4A-NA-C1A | 2.56 | 107.86 | 106.71 |
| 20 | A | 805 | CLA | CHB-C4A-NA | 2.56 | 128.06 | 124.51 |
| 20 | 2 | 304 | CLA | CHB-C4A-NA | 2.56 | 128.26 | 124.34 |
| 22 | F | 204 | BCR | C35-C13-C14 | -2.56 | 119.34 | 122.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | A | 844 | BCR | C8-C7-C6 | -2.56 | 120.01 | 127.20 |
| 20 | 1 | 205 | CLA | CHC-C1C-C2C | -2.56 | 119.62 | 126.73 |
| 20 | 1 | 211 | CLA | CED-O2D-CGD | 2.56 | 121.73 | 115.94 |
| 20 | 2 | 310 | CLA | CHB-C4A-NA | 2.56 | 128.05 | 124.51 |
| 20 | A | 833 | CLA | CAC-C3C-C2C | -2.56 | 123.15 | 127.53 |
| 20 | B | 828 | CLA | CHB-C1B-NB | -2.56 | 121.55 | 124.26 |
| 20 | 2 | 307 | CLA | CGD-CBD-CAD | 2.56 | 119.02 | 110.73 |
| 20 | 4 | 318 | CLA | O2A-CGA-O1A | -2.56 | 117.14 | 123.59 |
| 22 | F | 204 | BCR | C27-C26-C25 | -2.56 | 119.02 | 122.73 |
| 20 | 2 | 315 | CLA | C4A-NA-C1A | 2.56 | 107.86 | 106.71 |
| 20 | B | 807 | CLA | CHB-C1B-NB | -2.55 | 121.55 | 124.26 |
| 22 | I | 103 | BCR | C33-C5-C6 | -2.55 | 121.66 | 124.53 |
| 20 | A | 835 | CLA | CHB-C4A-NA | 2.55 | 128.04 | 124.51 |
| 22 | B | 846 | BCR | C33-C5-C4 | 2.55 | 118.52 | 113.62 |
| 21 | 1 | 218 | LMU | C3'-C4'-C5' | -2.55 | 105.08 | 110.93 |
| 20 | B | 833 | CLA | CAA-CBA-CGA | -2.55 | 105.80 | 113.25 |
| 20 | 4 | 308 | CLA | C2C-C1C-CHC | -2.55 | 119.56 | 125.67 |
| 20 | 3 | 303 | CLA | C4A-NA-C1A | 2.55 | 107.85 | 106.71 |
| 23 | B | 843 | PQN | C2M-C2-C1 | 2.55 | 120.50 | 116.27 |
| 21 | 2 | 313 | LMU | O1B-C1B-C2B | 2.55 | 114.71 | 108.10 |
| 20 | A | 808 | CLA | C1-O2A-CGA | 2.55 | 123.13 | 116.44 |
| 20 | A | 808 | CLA | C4A-NA-C1A | 2.55 | 107.85 | 106.71 |
| 20 | A | 807 | CLA | CAA-C2A-C1A | -2.55 | 103.62 | 111.97 |
| 20 | 4 | 306 | CLA | CMA-C3A-C4A | -2.55 | 104.93 | 111.77 |
| 20 | B | 839 | CLA | CAA-CBA-CGA | -2.55 | 105.81 | 113.25 |
| 20 | A | 824 | CLA | CHC-C1C-C2C | -2.55 | 119.66 | 126.73 |
| 20 | B | 834 | CLA | CHC-C1C-C2C | -2.55 | 119.66 | 126.73 |
| 21 | A | 854 | LMU | C1'-O5'-C5' | -2.54 | 108.69 | 113.69 |
| 20 | 2 | 304 | CLA | CHD-C1D-ND | 2.54 | 126.97 | 124.52 |
| 20 | A | 810 | CLA | O2D-CGD-O1D | -2.54 | 118.86 | 123.84 |
| 20 | A | 828 | CLA | CHC-C1C-C2C | -2.54 | 119.67 | 126.73 |
| 20 | 2 | 310 | CLA | C3D-C4D-ND | 2.54 | 114.35 | 110.24 |
| 20 | A | 811 | CLA | CAA-CBA-CGA | 2.54 | 120.68 | 113.25 |
| 20 | 4 | 301 | CLA | CHC-C1C-C2C | -2.54 | 119.67 | 126.73 |
| 20 | A | 838 | CLA | C3B-C4B-NB | -2.54 | 108.16 | 110.52 |
| 20 | A | 824 | CLA | CHB-C4A-NA | 2.54 | 128.02 | 124.51 |
| 20 | 2 | 307 | CLA | C1D-ND-C4D | -2.54 | 104.53 | 106.33 |
| 20 | B | 815 | CLA | CAC-C3C-C4C | 2.54 | 128.10 | 124.81 |
| 20 | A | 827 | CLA | CGD-CBD-CAD | 2.54 | 118.95 | 110.73 |
| 20 | L | 204 | CLA | C3B-C2B-C1B | -2.54 | 104.10 | 107.16 |
| 20 | B | 839 | CLA | CED-O2D-CGD | 2.54 | 121.67 | 115.94 |
| 20 | A | 804 | CLA | CHC-C1C-C2C | -2.53 | 119.69 | 126.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | F | 205 | CLA | CHC-C1C-C2C | -2.53 | 119.69 | 126.73 |
| 20 | R | 107 | CLA | O2D-CGD-O1D | -2.53 | 118.88 | 123.84 |
| 20 | B | 831 | CLA | CAC-C3C-C4C | 2.53 | 128.10 | 124.81 |
| 21 | B | 805 | LMU | O1'-C1'-C2' | 2.53 | 112.26 | 108.30 |
| 20 | 3 | 303 | CLA | CAA-C2A-C3A | -2.53 | 110.19 | 116.10 |
| 20 | B | 833 | CLA | CED-O2D-CGD | 2.53 | 121.66 | 115.94 |
| 20 | H | 102 | CLA | CGD-CBD-CAD | -2.53 | 102.53 | 110.73 |
| 20 | A | 817 | CLA | C4A-NA-C1A | 2.53 | 107.84 | 106.71 |
| 20 | A | 820 | CLA | C4A-NA-C1A | 2.53 | 107.84 | 106.71 |
| 20 | 3 | 317 | CLA | CHB-C4A-NA | 2.53 | 128.01 | 124.51 |
| 20 | B | 829 | CLA | C11-C12-C13 | -2.53 | 107.74 | 115.92 |
| 20 | 3 | 301 | CLA | CHC-C1C-C2C | -2.53 | 119.70 | 126.73 |
| 20 | A | 850 | CLA | CHC-C1C-C2C | -2.53 | 119.70 | 126.73 |
| 20 | 2 | 307 | CLA | CMB-C2B-C1B | 2.53 | 129.22 | 125.37 |
| 20 | A | 829 | CLA | CAC-C3C-C4C | 2.53 | 128.09 | 124.81 |
| 20 | 1 | 215 | CLA | O2D-CGD-CBD | 2.53 | 115.76 | 111.27 |
| 20 | B | 823 | CLA | C4A-NA-C1A | 2.53 | 107.84 | 106.71 |
| 20 | A | 823 | CLA | O2A-CGA-O1A | -2.53 | 117.22 | 123.59 |
| 20 | L | 203 | CLA | CAC-C3C-C4C | 2.53 | 128.09 | 124.81 |
| 20 | 4 | 306 | CLA | CED-O2D-CGD | 2.52 | 121.65 | 115.94 |
| 21 | G | 103 | LMU | C1B-O1B-C4' | -2.52 | 111.72 | 117.96 |
| 20 | H | 108 | CLA | C3B-C4B-NB | -2.52 | 108.17 | 110.52 |
| 20 | B | 818 | CLA | CHB-C4A-NA | 2.52 | 128.00 | 124.51 |
| 20 | R | 108 | CLA | CAA-CBA-CGA | 2.52 | 120.63 | 113.25 |
| 20 | B | 839 | CLA | C2A-C1A-CHA | -2.52 | 119.45 | 123.86 |
| 20 | H | 108 | CLA | C4A-NA-C1A | 2.52 | 107.84 | 106.71 |
| 20 | K | 101 | CLA | CHC-C1C-C2C | -2.52 | 119.72 | 126.73 |
| 22 | B | 845 | BCR | C35-C13-C14 | -2.52 | 119.39 | 122.92 |
| 20 | A | 850 | CLA | CHB-C1B-NB | -2.52 | 121.59 | 124.26 |
| 20 | 3 | 306 | CLA | C2A-C3A-C4A | -2.52 | 100.22 | 104.18 |
| 20 | A | 835 | CLA | CAA-C2A-C3A | -2.52 | 105.88 | 112.78 |
| 20 | 3 | 309 | CLA | C2A-C3A-C4A | -2.52 | 100.22 | 104.18 |
| 20 | 2 | 310 | CLA | C2A-C1A-CHA | -2.52 | 119.45 | 123.86 |
| 20 | 3 | 315 | CLA | C2A-C3A-C4A | -2.52 | 100.23 | 104.18 |
| 20 | 4 | 308 | CLA | C2A-C3A-C4A | -2.52 | 100.23 | 104.18 |
| 21 | H | 104 | LMU | O5B-C5B-C6B | 2.52 | 112.70 | 106.44 |
| 20 | A | 809 | CLA | CMB-C2B-C1B | 2.52 | 129.21 | 125.37 |
| 20 | 2 | 311 | CLA | C1-O2A-CGA | 2.52 | 123.05 | 116.44 |
| 20 | A | 810 | CLA | CHC-C1C-C2C | -2.52 | 119.74 | 126.73 |
| 20 | 2 | 311 | CLA | CHD-C1D-ND | 2.52 | 126.77 | 124.45 |
| 21 | K | 107 | LMU | C1'-O5'-C5' | -2.52 | 108.75 | 113.69 |
| 20 | A | 839 | CLA | CMB-C2B-C1B | 2.52 | 129.20 | 125.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 838 | CLA | O2A-CGA-O1A | -2.51 | 117.25 | 123.59 |
| 21 | B | 804 | LMU | O1B-C1B-C2B | 2.51 | 114.61 | 108.10 |
| 20 | 4 | 310 | CLA | C3D-C4D-ND | 2.51 | 114.30 | 110.24 |
| 20 | A | 831 | CLA | O2A-CGA-O1A | -2.51 | 117.25 | 123.59 |
| 20 | 1 | 203 | CLA | C4D-CHA-C1A | -2.51 | 118.19 | 121.25 |
| 20 | 1 | 203 | CLA | CHC-C1C-C2C | -2.51 | 119.75 | 126.73 |
| 20 | 2 | 305 | CLA | CED-O2D-CGD | 2.51 | 121.62 | 115.94 |
| 20 | A | 808 | CLA | CHB-C1B-NB | -2.51 | 121.60 | 124.26 |
| 20 | 3 | 306 | CLA | CHB-C4A-NA | 2.51 | 128.18 | 124.34 |
| 20 | A | 806 | CLA | CAA-C2A-C1A | -2.51 | 103.75 | 111.97 |
| 22 | B | 847 | BCR | C30-C25-C26 | -2.51 | 119.08 | 122.61 |
| 20 | L | 202 | CLA | CHB-C1B-NB | -2.51 | 121.60 | 124.26 |
| 20 | 3 | 307 | CLA | CED-O2D-CGD | 2.51 | 121.61 | 115.94 |
| 21 | F | 202 | LMU | C4B-C3B-C2B | -2.51 | 106.44 | 110.82 |
| 20 | B | 821 | CLA | CHC-C1C-C2C | -2.51 | 119.76 | 126.73 |
| 20 | B | 850 | CLA | CMB-C2B-C1B | 2.51 | 129.19 | 125.37 |
| 20 | H | 110 | CLA | C1D-ND-C4D | -2.51 | 104.55 | 106.33 |
| 20 | B | 826 | CLA | O2D-CGD-O1D | -2.51 | 118.94 | 123.84 |
| 20 | 2 | 302 | CLA | C3D-C4D-ND | 2.51 | 114.29 | 110.24 |
| 22 | I | 101 | BCR | C35-C13-C12 | 2.51 | 122.02 | 118.08 |
| 20 | G | 105 | CLA | O2A-CGA-CBA | 2.51 | 119.77 | 111.91 |
| 20 | 1 | 208 | CLA | C2A-C3A-C4A | -2.51 | 100.25 | 104.18 |
| 20 | 4 | 309 | CLA | CHB-C4A-NA | 2.50 | 128.17 | 124.34 |
| 20 | 3 | 315 | CLA | C3C-C4C-CHD | -2.50 | 119.74 | 125.22 |
| 20 | B | 850 | CLA | O2D-CGD-O1D | -2.50 | 118.94 | 123.84 |
| 20 | A | 811 | CLA | O2A-CGA-CBA | 2.50 | 119.76 | 111.91 |
| 20 | 1 | 209 | CLA | C4A-NA-C1A | 2.50 | 107.83 | 106.71 |
| 20 | B | 819 | CLA | CHC-C1C-C2C | -2.50 | 119.78 | 126.73 |
| 20 | B | 820 | CLA | CAA-C2A-C1A | 2.50 | 120.17 | 111.97 |
| 21 | L | 205 | LMU | O5'-C1'-C2' | 2.50 | 115.64 | 110.35 |
| 20 | F | 207 | CLA | C4-C3-C5 | 2.50 | 119.48 | 115.27 |
| 20 | H | 101 | CLA | CGD-CBD-CAD | 2.50 | 118.83 | 110.73 |
| 20 | 4 | 305 | CLA | CHC-C1C-C2C | -2.50 | 119.79 | 126.73 |
| 20 | L | 203 | CLA | CHC-C1C-C2C | -2.50 | 119.79 | 126.73 |
| 20 | A | 818 | CLA | CGD-CBD-CAD | 2.50 | 118.83 | 110.73 |
| 20 | A | 839 | CLA | O2A-CGA-O1A | -2.50 | 117.29 | 123.59 |
| 20 | B | 829 | CLA | O2A-CGA-O1A | -2.50 | 117.29 | 123.59 |
| 22 | J | 102 | BCR | C8-C7-C6 | -2.50 | 120.19 | 127.20 |
| 20 | 4 | 312 | CLA | C3D-C4D-ND | 2.50 | 113.23 | 109.46 |
| 22 | A | 845 | BCR | C37-C22-C21 | -2.50 | 119.43 | 122.92 |
| 20 | 1 | 207 | CLA | CHC-C1C-C2C | -2.50 | 119.80 | 126.73 |
| 22 | A | 843 | BCR | C38-C26-C25 | -2.50 | 121.73 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 3 | 310 | CLA | C2A-C1A-CHA | -2.50 | 119.50 | 123.86 |
| 22 | I | 101 | BCR | C16-C17-C18 | -2.50 | 123.75 | 127.31 |
| 20 | G | 105 | CLA | C1-C2-C3 | -2.49 | 121.73 | 126.04 |
| 20 | 4 | 312 | CLA | C2C-C1C-CHC | -2.49 | 119.70 | 125.67 |
| 20 | B | 815 | CLA | CED-O2D-CGD | 2.49 | 121.58 | 115.94 |
| 20 | B | 842 | CLA | CHC-C1C-C2C | -2.49 | 119.80 | 126.73 |
| 20 | H | 108 | CLA | O2A-CGA-O1A | -2.49 | 117.30 | 123.59 |
| 20 | B | 825 | CLA | CMB-C2B-C1B | 2.49 | 129.16 | 125.37 |
| 20 | 3 | 313 | CLA | CHB-C4A-NA | 2.49 | 127.96 | 124.51 |
| 20 | B | 835 | CLA | CHC-C1C-C2C | -2.49 | 119.81 | 126.73 |
| 21 | R | 105 | LMU | C3B-C4B-C5B | -2.49 | 105.79 | 110.24 |
| 20 | 2 | 303 | CLA | CAA-C2A-C1A | -2.49 | 103.81 | 111.97 |
| 22 | A | 843 | BCR | C38-C26-C27 | 2.49 | 118.40 | 113.62 |
| 20 | A | 809 | CLA | CHD-C4C-C3C | -2.49 | 121.18 | 124.84 |
| 20 | F | 206 | CLA | CHC-C1C-C2C | -2.49 | 119.81 | 126.73 |
| 20 | 4 | 302 | CLA | CMA-C3A-C2A | -2.49 | 110.29 | 116.10 |
| 21 | K | 105 | LMU | O1B-C4'-C5' | 2.49 | 116.27 | 109.45 |
| 20 | 2 | 312 | CLA | CHB-C1B-NB | -2.49 | 121.62 | 124.26 |
| 20 | B | 808 | CLA | C3B-C4B-NB | -2.49 | 108.21 | 110.52 |
| 22 | I | 101 | BCR | C24-C25-C26 | -2.49 | 115.43 | 121.46 |
| 20 | B | 840 | CLA | O1D-CGD-CBD | -2.49 | 119.39 | 124.48 |
| 20 | 4 | 308 | CLA | CHB-C4A-NA | 2.49 | 128.15 | 124.34 |
| 20 | R | 107 | CLA | C1D-ND-C4D | -2.49 | 104.57 | 106.33 |
| 20 | B | 824 | CLA | C9-C8-C10 | 2.49 | 120.30 | 111.29 |
| 20 | B | 828 | CLA | O2A-CGA-O1A | -2.49 | 117.32 | 123.59 |
| 20 | A | 820 | CLA | CHB-C4A-NA | 2.48 | 127.95 | 124.51 |
| 20 | 2 | 305 | CLA | O2A-CGA-CBA | 2.48 | 119.70 | 111.91 |
| 21 | A | 855 | LMU | O5'-C1'-C2' | 2.48 | 115.61 | 110.35 |
| 20 | 1 | 206 | CLA | CHC-C1C-C2C | -2.48 | 119.83 | 126.73 |
| 20 | A | 821 | CLA | CHB-C4A-NA | 2.48 | 127.95 | 124.51 |
| 20 | L | 202 | CLA | C1-O2A-CGA | 2.48 | 122.96 | 116.44 |
| 20 | A | 807 | CLA | O2D-CGD-O1D | -2.48 | 118.98 | 123.84 |
| 21 | R | 101 | LMU | O2B-C2B-C1B | 2.48 | 116.07 | 110.05 |
| 20 | A | 804 | CLA | CBA-CAA-C2A | 2.48 | 121.19 | 113.86 |
| 20 | 1 | 212 | CLA | CHB-C4A-NA | 2.48 | 128.14 | 124.34 |
| 20 | B | 840 | CLA | CHB-C4A-NA | 2.48 | 127.94 | 124.51 |
| 20 | A | 850 | CLA | C4-C3-C5 | 2.48 | 119.44 | 115.27 |
| 20 | G | 105 | CLA | C4-C3-C5 | 2.48 | 118.82 | 115.98 |
| 20 | B | 822 | CLA | CHC-C1C-C2C | -2.48 | 119.84 | 126.73 |
| 20 | B | 816 | CLA | CHB-C4A-NA | 2.48 | 127.94 | 124.51 |
| 21 | L | 205 | LMU | O4'-C4B-C5B | -2.48 | 103.14 | 109.30 |
| 20 | I | 102 | CLA | CHC-C1C-C2C | -2.48 | 119.85 | 126.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 209 | CLA | CHB-C4A-NA | 2.48 | 128.13 | 124.34 |
| 20 | B | 819 | CLA | CMA-C3A-C2A | -2.48 | 110.32 | 116.10 |
| 20 | A | 815 | CLA | C1-O2A-CGA | 2.48 | 122.94 | 116.44 |
| 20 | 1 | 204 | CLA | CAC-C3C-C4C | 2.47 | 128.02 | 124.81 |
| 20 | 4 | 317 | CLA | C4D-CHA-C1A | -2.47 | 118.24 | 121.25 |
| 20 | B | 803 | CLA | CAA-C2A-C3A | -2.47 | 106.00 | 112.78 |
| 20 | L | 203 | CLA | O1D-CGD-CBD | -2.47 | 119.42 | 124.48 |
| 20 | 1 | 205 | CLA | CHB-C4A-NA | 2.47 | 127.93 | 124.51 |
| 20 | 3 | 303 | CLA | CMC-C2C-C1C | 2.47 | 128.80 | 125.04 |
| 22 | A | 844 | BCR | C23-C24-C25 | -2.47 | 120.26 | 127.20 |
| 20 | 4 | 303 | CLA | C3D-C4D-ND | 2.47 | 114.23 | 110.24 |
| 20 | 4 | 314 | CLA | CHB-C4A-NA | 2.47 | 128.12 | 124.34 |
| 20 | L | 201 | CLA | CHC-C1C-C2C | -2.47 | 119.87 | 126.73 |
| 20 | A | 823 | CLA | C4A-NA-C1A | 2.47 | 107.82 | 106.71 |
| 20 | 2 | 309 | CLA | C3A-C4A-NA | 2.47 | 115.10 | 109.92 |
| 20 | B | 830 | CLA | CHB-C4A-NA | 2.47 | 127.93 | 124.51 |
| 20 | A | 810 | CLA | C3D-C4D-ND | 2.47 | 114.23 | 110.24 |
| 20 | B | 806 | CLA | C3D-C4D-ND | 2.47 | 114.23 | 110.24 |
| 21 | 4 | 320 | LMU | O5'-C5'-C4' | 2.47 | 114.95 | 109.75 |
| 20 | 3 | 307 | CLA | C3B-C2B-C1B | -2.47 | 104.19 | 107.16 |
| 20 | B | 827 | CLA | O2A-CGA-CBA | 2.47 | 119.65 | 111.91 |
| 20 | A | 828 | CLA | CAA-C2A-C1A | -2.47 | 103.89 | 111.97 |
| 21 | 4 | 321 | LMU | C1B-C2B-C3B | 2.47 | 115.13 | 110.00 |
| 20 | A | 825 | CLA | CHB-C4A-NA | 2.47 | 127.92 | 124.51 |
| 20 | 1 | 211 | CLA | C1D-ND-C4D | -2.46 | 104.58 | 106.33 |
| 22 | B | 844 | BCR | C23-C22-C21 | 2.46 | 122.72 | 118.94 |
| 20 | L | 202 | CLA | CHC-C1C-C2C | -2.46 | 119.89 | 126.73 |
| 20 | B | 809 | CLA | CAC-C3C-C4C | 2.46 | 128.00 | 124.81 |
| 20 | B | 816 | CLA | C3B-C4B-NB | -2.46 | 108.23 | 110.52 |
| 21 | 4 | 319 | LMU | O5'-C5'-C6' | 2.46 | 112.56 | 106.44 |
| 20 | F | 206 | CLA | CHB-C4A-NA | 2.46 | 127.92 | 124.51 |
| 20 | 4 | 317 | CLA | C1D-ND-C4D | -2.46 | 104.59 | 106.33 |
| 20 | B | 814 | CLA | O2A-CGA-CBA | 2.46 | 119.62 | 111.91 |
| 20 | A | 832 | CLA | O2A-CGA-CBA | 2.46 | 119.62 | 111.91 |
| 20 | 3 | 316 | CLA | C3D-C4D-ND | 2.46 | 113.17 | 109.46 |
| 20 | A | 840 | CLA | C1-O2A-CGA | 2.46 | 122.89 | 116.44 |
| 20 | A | 817 | CLA | O2D-CGD-O1D | -2.46 | 119.03 | 123.84 |
| 21 | G | 101 | LMU | O5'-C1'-C2' | -2.46 | 105.15 | 110.35 |
| 21 | H | 106 | LMU | C6'-C5'-C4' | -2.46 | 106.18 | 113.33 |
| 20 | 1 | 206 | CLA | C1-C2-C3 | -2.46 | 121.80 | 126.04 |
| 20 | A | 815 | CLA | C1-C2-C3 | -2.45 | 122.78 | 126.75 |
| 20 | B | 840 | CLA | CHC-C1C-C2C | -2.45 | 119.92 | 126.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | A | 845 | BCR | C28-C27-C26 | -2.45 | 109.70 | 114.08 |
| 20 | B | 825 | CLA | CBC-CAC-C3C | -2.45 | 105.68 | 112.43 |
| 20 | A | 803 | CLA | CMB-C2B-C1B | 2.45 | 129.10 | 125.37 |
| 20 | B | 814 | CLA | CHB-C1B-NB | -2.45 | 121.66 | 124.26 |
| 20 | I | 102 | CLA | O1D-CGD-CBD | -2.45 | 119.47 | 124.48 |
| 20 | 2 | 314 | CLA | CED-O2D-CGD | 2.45 | 121.48 | 115.94 |
| 20 | 2 | 312 | CLA | C4-C3-C2 | -2.45 | 117.40 | 123.68 |
| 21 | R | 105 | LMU | O5B-C5B-C6B | 2.45 | 112.52 | 106.44 |
| 21 | R | 105 | LMU | O1'-C1'-C2' | 2.45 | 112.12 | 108.30 |
| 20 | G | 105 | CLA | CHB-C1B-NB | -2.45 | 121.67 | 124.26 |
| 20 | I | 102 | CLA | C1-O2A-CGA | 2.45 | 122.86 | 116.44 |
| 22 | G | 104 | BCR | C8-C7-C6 | -2.45 | 120.33 | 127.20 |
| 20 | 3 | 303 | CLA | CHB-C4A-NA | 2.45 | 127.89 | 124.51 |
| 20 | K | 102 | CLA | CHB-C1B-NB | -2.45 | 121.67 | 124.26 |
| 21 | B | 804 | LMU | C6B-C5B-C4B | -2.45 | 107.28 | 113.00 |
| 20 | B | 839 | CLA | C3D-C4D-ND | 2.45 | 114.19 | 110.24 |
| 20 | A | 810 | CLA | O1D-CGD-CBD | -2.45 | 119.48 | 124.48 |
| 20 | A | 835 | CLA | C3D-C4D-ND | 2.44 | 114.19 | 110.24 |
| 21 | R | 102 | LMU | C1'-O5'-C5' | -2.44 | 108.89 | 113.69 |
| 20 | B | 814 | CLA | C1D-ND-C4D | -2.44 | 104.60 | 106.33 |
| 20 | B | 836 | CLA | O2A-CGA-CBA | 2.44 | 119.58 | 111.91 |
| 20 | 4 | 306 | CLA | C3B-C2B-C1B | -2.44 | 104.21 | 107.16 |
| 21 | 4 | 321 | LMU | C1B-O1B-C4' | -2.44 | 111.92 | 117.96 |
| 20 | K | 102 | CLA | CHB-C4A-NA | 2.44 | 127.89 | 124.51 |
| 22 | A | 843 | BCR | C28-C27-C26 | -2.44 | 109.72 | 114.08 |
| 20 | A | 819 | CLA | O2D-CGD-O1D | -2.44 | 119.07 | 123.84 |
| 20 | A | 802 | CLA | C3D-C2D-C1D | 2.44 | 109.98 | 107.28 |
| 20 | B | 827 | CLA | C2A-C1A-CHA | -2.44 | 119.60 | 123.86 |
| 20 | 2 | 316 | CLA | C4-C3-C2 | -2.44 | 117.43 | 123.68 |
| 20 | 1 | 206 | CLA | O2D-CGD-O1D | -2.43 | 119.08 | 123.84 |
| 20 | A | 808 | CLA | CHC-C1C-C2C | -2.43 | 119.97 | 126.73 |
| 20 | B | 819 | CLA | CHB-C4A-NA | 2.43 | 127.88 | 124.51 |
| 20 | K | 101 | CLA | C4A-NA-C1A | 2.43 | 107.80 | 106.71 |
| 20 | A | 850 | CLA | O1D-CGD-CBD | -2.43 | 119.51 | 124.48 |
| 20 | A | 813 | CLA | C1D-ND-C4D | -2.43 | 104.61 | 106.33 |
| 20 | K | 103 | CLA | C4A-NA-C1A | 2.43 | 107.80 | 106.71 |
| 20 | L | 203 | CLA | C6-C7-C8 | -2.43 | 108.06 | 115.92 |
| 20 | A | 826 | CLA | C1-O2A-CGA | 2.43 | 122.82 | 116.44 |
| 22 | F | 203 | BCR | C30-C25-C26 | -2.43 | 119.19 | 122.61 |
| 20 | A | 807 | CLA | CMC-C2C-C1C | 2.43 | 128.74 | 125.04 |
| 20 | L | 201 | CLA | C4A-NA-C1A | 2.43 | 107.80 | 106.71 |
| 20 | A | 822 | CLA | CHB-C1B-NB | -2.43 | 121.69 | 124.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 22 | F | 203 | BCR | C38-C26-C27 | 2.43 | 118.28 | 113.62 |
| 20 | K | 101 | CLA | CHB-C4A-NA | 2.43 | 127.87 | 124.51 |
| 20 | B | 816 | CLA | C4-C3-C2 | -2.43 | 117.45 | 123.68 |
| 21 | A | 854 | LMU | C1-O1'-C1' | -2.43 | 109.82 | 113.84 |
| 20 | A | 826 | CLA | O2A-CGA-O1A | -2.43 | 117.47 | 123.59 |
| 20 | B | 839 | CLA | CHC-C1C-C2C | -2.42 | 119.99 | 126.73 |
| 20 | B | 806 | CLA | C2A-C1A-CHA | -2.42 | 119.62 | 123.86 |
| 20 | A | 807 | CLA | C3D-C4D-ND | 2.42 | 114.16 | 110.24 |
| 21 | A | 855 | LMU | O5'-C5'-C4' | -2.42 | 104.65 | 109.75 |
| 22 | I | 103 | BCR | C29-C28-C27 | 2.42 | 116.79 | 111.38 |
| 21 | H | 104 | LMU | C3B-C4B-C5B | -2.42 | 105.92 | 110.24 |
| 20 | A | 823 | CLA | CHB-C1B-NB | -2.42 | 121.69 | 124.26 |
| 21 | E | 101 | LMU | O1B-C1B-C2B | 2.42 | 114.37 | 108.10 |
| 20 | K | 101 | CLA | C2A-C1A-CHA | -2.42 | 119.63 | 123.86 |
| 20 | 4 | 311 | CLA | C2A-C3A-C4A | -2.42 | 100.38 | 104.18 |
| 20 | 2 | 302 | CLA | CHC-C1C-C2C | -2.42 | 120.02 | 126.73 |
| 20 | L | 202 | CLA | CHB-C4A-NA | 2.42 | 127.85 | 124.51 |
| 21 | A | 847 | LMU | C1'-C2'-C3' | 2.42 | 115.03 | 110.00 |
| 20 | A | 823 | CLA | CMB-C2B-C1B | 2.42 | 129.05 | 125.37 |
| 20 | 2 | 316 | CLA | CHB-C1B-NB | -2.42 | 121.70 | 124.26 |
| 22 | B | 846 | BCR | C11-C12-C13 | -2.41 | 119.63 | 126.42 |
| 21 | 2 | 319 | LMU | O5'-C5'-C6' | 2.41 | 112.44 | 106.44 |
| 20 | 2 | 306 | CLA | C2A-C3A-C4A | -2.41 | 100.39 | 104.18 |
| 20 | 1 | 209 | CLA | C3D-C4D-ND | 2.41 | 113.10 | 109.46 |
| 20 | L | 202 | CLA | O2A-CGA-CBA | 2.41 | 119.48 | 111.91 |
| 20 | A | 804 | CLA | CHB-C4A-NA | 2.41 | 127.85 | 124.51 |
| 20 | B | 803 | CLA | CMA-C3A-C4A | -2.41 | 105.29 | 111.77 |
| 21 | L | 206 | LMU | O5B-C5B-C6B | 2.41 | 112.43 | 106.44 |
| 20 | 4 | 317 | CLA | C4-C3-C5 | 2.41 | 119.33 | 115.27 |
| 20 | H | 110 | CLA | O1D-CGD-CBD | -2.41 | 119.55 | 124.48 |
| 20 | B | 808 | CLA | O2D-CGD-O1D | -2.41 | 119.13 | 123.84 |
| 20 | B | 815 | CLA | O2A-CGA-CBA | 2.41 | 119.46 | 111.91 |
| 20 | B | 807 | CLA | C1D-ND-C4D | -2.41 | 104.62 | 106.33 |
| 21 | 1 | 218 | LMU | O5'-C5'-C6' | 2.41 | 112.42 | 106.44 |
| 20 | 2 | 301 | CLA | CHB-C1B-NB | -2.41 | 121.84 | 124.27 |
| 20 | J | 103 | CLA | O2D-CGD-O1D | -2.41 | 119.14 | 123.84 |
| 20 | L | 201 | CLA | CHB-C4A-NA | 2.41 | 127.84 | 124.51 |
| 20 | 1 | 210 | CLA | CHC-C1C-C2C | -2.40 | 120.05 | 126.73 |
| 22 | A | 844 | BCR | C27-C26-C25 | -2.40 | 119.24 | 122.73 |
| 20 | A | 835 | CLA | CMB-C2B-C1B | 2.40 | 129.03 | 125.37 |
| 20 | 1 | 204 | CLA | O2A-CGA-O1A | -2.40 | 115.61 | 123.14 |
| 20 | B | 826 | CLA | CHC-C1C-C2C | -2.40 | 120.06 | 126.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | B | 801 | BCR | C23-C24-C25 | -2.40 | 120.46 | 127.20 |
| 20 | B | 835 | CLA | O2D-CGD-O1D | -2.40 | 119.15 | 123.84 |
| 20 | B | 838 | CLA | O2A-CGA-CBA | 2.40 | 119.44 | 111.91 |
| 20 | B | 807 | CLA | CMB-C2B-C1B | 2.40 | 129.02 | 125.37 |
| 20 | A | 807 | CLA | O1D-CGD-CBD | -2.40 | 119.58 | 124.48 |
| 20 | 3 | 308 | CLA | C2A-C3A-C4A | -2.40 | 100.42 | 104.18 |
| 20 | 2 | 302 | CLA | O2A-CGA-O1A | -2.40 | 117.54 | 123.59 |
| 20 | B | 835 | CLA | C3B-C2B-C1B | -2.40 | 104.27 | 107.16 |
| 20 | R | 108 | CLA | O2A-CGA-O1A | -2.40 | 117.55 | 123.59 |
| 20 | 3 | 304 | CLA | C3B-C4B-CHC | -2.40 | 119.28 | 126.24 |
| 20 | B | 827 | CLA | O2D-CGD-O1D | -2.40 | 119.15 | 123.84 |
| 23 | B | 843 | PQN | C14-C13-C15 | 2.40 | 119.30 | 115.27 |
| 22 | A | 844 | BCR | C28-C27-C26 | -2.40 | 109.80 | 114.08 |
| 22 | F | 204 | BCR | C36-C18-C17 | -2.40 | 119.57 | 122.92 |
| 20 | 3 | 317 | CLA | CHC-C4B-C3B | -2.39 | 120.47 | 127.24 |
| 20 | B | 842 | CLA | CHC-C4B-C3B | -2.39 | 120.48 | 127.24 |
| 20 | 1 | 207 | CLA | CHB-C1B-NB | -2.39 | 121.72 | 124.26 |
| 20 | B | 818 | CLA | C3B-C2B-C1B | -2.39 | 104.27 | 107.16 |
| 20 | L | 204 | CLA | C4-C3-C2 | -2.39 | 117.54 | 123.68 |
| 20 | B | 832 | CLA | CHC-C1C-C2C | -2.39 | 120.09 | 126.73 |
| 20 | A | 818 | CLA | CHC-C1C-C2C | -2.39 | 120.09 | 126.73 |
| 20 | 3 | 302 | CLA | CHB-C4A-NA | 2.39 | 128.00 | 124.34 |
| 20 | A | 814 | CLA | C3C-C4C-CHD | -2.39 | 119.99 | 125.22 |
| 20 | B | 828 | CLA | CAA-C2A-C1A | -2.39 | 104.15 | 111.97 |
| 20 | 4 | 315 | CLA | CBA-CAA-C2A | -2.39 | 106.81 | 113.86 |
| 20 | A | 833 | CLA | O2D-CGD-O1D | -2.39 | 119.17 | 123.84 |
| 20 | A | 813 | CLA | CAA-C2A-C1A | -2.39 | 104.15 | 111.97 |
| 20 | 2 | 311 | CLA | O1D-CGD-CBD | -2.39 | 119.60 | 124.48 |
| 20 | A | 823 | CLA | O2D-CGD-O1D | -2.39 | 119.17 | 123.84 |
| 20 | B | 817 | CLA | CMB-C2B-C1B | 2.39 | 129.01 | 125.37 |
| 22 | A | 843 | BCR | C4-C5-C6 | -2.39 | 119.26 | 122.73 |
| 20 | B | 806 | CLA | C1D-ND-C4D | -2.39 | 104.64 | 106.33 |
| 21 | 2 | 321 | LMU | C1'-O5'-C5' | 2.39 | 118.37 | 113.69 |
| 20 | A | 820 | CLA | CHC-C1C-C2C | -2.39 | 120.10 | 126.73 |
| 20 | 1 | 211 | CLA | CHB-C4A-NA | 2.39 | 127.81 | 124.51 |
| 20 | A | 849 | CLA | O2A-CGA-CBA | 2.39 | 119.39 | 111.91 |
| 20 | A | 811 | CLA | C2D-C1D-ND | -2.39 | 108.35 | 110.10 |
| 20 | 3 | 315 | CLA | C3D-C2D-C1D | 2.39 | 109.92 | 107.28 |
| 20 | B | 820 | CLA | CHC-C1C-C2C | -2.39 | 120.10 | 126.73 |
| 20 | 3 | 304 | CLA | CHD-C1D-ND | 2.39 | 126.82 | 124.52 |
| 20 | L | 208 | CLA | C1-C2-C3 | -2.38 | 122.90 | 126.75 |
| 21 | G | 102 | LMU | O5B-C5B-C6B | -2.38 | 100.51 | 106.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 20 | 4 | 304 | CLA | CAC-C3C-C2C | -2.38 | 123.45 | 127.53 |
| 20 | 3 | 313 | CLA | CHC-C1C-C2C | -2.38 | 120.11 | 126.73 |
| 20 | 3 | 313 | CLA | O2D-CGD-O1D | -2.38 | 119.18 | 123.84 |
| 20 | B | 831 | CLA | CHB-C4A-NA | 2.38 | 127.80 | 124.51 |
| 20 | A | 838 | CLA | C1D-ND-C4D | -2.38 | 104.64 | 106.33 |
| 20 | 4 | 318 | CLA | CAA-C2A-C3A | 2.38 | 119.29 | 112.78 |
| 20 | A | 836 | CLA | C4A-NA-C1A | 2.38 | 107.78 | 106.71 |
| 20 | A | 807 | CLA | CAC-C3C-C4C | 2.38 | 127.90 | 124.81 |
| 22 | A | 843 | BCR | C1-C6-C5 | -2.38 | 119.27 | 122.61 |
| 21 | 1 | 216 | LMU | C1B-C2B-C3B | -2.38 | 105.05 | 110.00 |
| 22 | B | 846 | BCR | C23-C24-C25 | -2.38 | 120.53 | 127.20 |
| 21 | 3 | 319 | LMU | O1'-C1'-C2' | 2.38 | 112.01 | 108.30 |
| 20 | 3 | 314 | CLA | C11-C10-C8 | -2.38 | 108.24 | 115.92 |
| 20 | 4 | 301 | CLA | C1D-ND-C4D | -2.37 | 104.65 | 106.33 |
| 21 | A | 855 | LMU | O5'-C5'-C6' | 2.37 | 112.34 | 106.44 |
| 20 | 1 | 209 | CLA | C1C-NC-C4C | -2.37 | 105.64 | 106.71 |
| 20 | B | 806 | CLA | O2A-CGA-CBA | 2.37 | 119.35 | 111.91 |
| 20 | 4 | 315 | CLA | CHC-C1C-C2C | -2.37 | 120.14 | 126.73 |
| 20 | A | 834 | CLA | C3D-C4D-ND | 2.37 | 114.07 | 110.24 |
| 20 | 2 | 303 | CLA | O2A-CGA-O1A | -2.37 | 117.61 | 123.59 |
| 20 | 4 | 311 | CLA | CHB-C4A-NA | 2.37 | 127.97 | 124.34 |
| 20 | B | 802 | CLA | O2A-CGA-CBA | 2.37 | 119.34 | 111.91 |
| 21 | A | 848 | LMU | C1-O1'-C1' | -2.37 | 109.91 | 113.84 |
| 21 | H | 106 | LMU | O5'-C5'-C6' | 2.37 | 112.32 | 106.44 |
| 20 | A | 834 | CLA | CHB-C1B-NB | -2.36 | 121.75 | 124.26 |
| 20 | 4 | 306 | CLA | CGD-CBD-CAD | 2.36 | 118.39 | 110.73 |
| 20 | 1 | 207 | CLA | O2D-CGD-O1D | -2.36 | 119.22 | 123.84 |
| 20 | R | 108 | CLA | C3B-C2B-C1B | -2.36 | 104.31 | 107.16 |
| 20 | A | 808 | CLA | CMB-C2B-C1B | 2.36 | 128.97 | 125.37 |
| 20 | B | 802 | CLA | CHC-C1C-C2C | -2.36 | 120.17 | 126.73 |
| 20 | A | 827 | CLA | CAC-C3C-C4C | 2.36 | 127.88 | 124.81 |
| 20 | 4 | 317 | CLA | O2D-CGD-O1D | -2.36 | 119.22 | 123.84 |
| 20 | 4 | 306 | CLA | CHB-C1B-C2B | -2.36 | 120.57 | 127.24 |
| 20 | 2 | 303 | CLA | CED-O2D-CGD | 2.36 | 121.28 | 115.94 |
| 20 | A | 811 | CLA | O2D-CGD-O1D | -2.36 | 119.22 | 123.84 |
| 22 | A | 843 | BCR | C15-C16-C17 | -2.36 | 118.64 | 123.47 |
| 21 | L | 210 | LMU | O5'-C5'-C6' | 2.36 | 112.30 | 106.44 |
| 20 | A | 821 | CLA | O2D-CGD-O1D | -2.36 | 119.23 | 123.84 |
| 20 | J | 103 | CLA | C1-C2-C3 | -2.36 | 121.97 | 126.04 |
| 20 | B | 840 | CLA | CHB-C1B-NB | -2.36 | 121.76 | 124.26 |
| 20 | A | 829 | CLA | C2D-C1D-ND | -2.36 | 108.37 | 110.10 |
| 21 | K | 105 | LMU | O3B-C3B-C4B | -2.36 | 104.90 | 110.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 806 | CLA | CHC-C1C-C2C | -2.36 | 120.19 | 126.73 |
| 20 | A | 810 | CLA | CMB-C2B-C1B | 2.36 | 128.96 | 125.37 |
| 20 | K | 104 | CLA | C1-C2-C3 | -2.35 | 121.97 | 126.04 |
| 20 | B | 830 | CLA | O1D-CGD-CBD | -2.35 | 119.67 | 124.48 |
| 20 | 4 | 302 | CLA | CMB-C2B-C3B | 2.35 | 129.69 | 123.59 |
| 22 | I | 103 | BCR | C19-C18-C17 | 2.35 | 122.55 | 118.94 |
| 21 | K | 106 | LMU | C1B-O5B-C5B | -2.35 | 109.07 | 113.69 |
| 20 | 1 | 210 | CLA | CHB-C4A-NA | 2.35 | 127.77 | 124.51 |
| 20 | 3 | 306 | CLA | CHB-C1B-NB | -2.35 | 121.89 | 124.27 |
| 20 | K | 103 | CLA | C5-C3-C4 | 2.35 | 119.80 | 114.60 |
| 20 | A | 828 | CLA | CHB-C4A-NA | 2.35 | 127.76 | 124.51 |
| 20 | B | 827 | CLA | CHB-C4A-NA | 2.35 | 127.76 | 124.51 |
| 20 | B | 832 | CLA | O2A-CGA-CBA | 2.35 | 119.28 | 111.91 |
| 20 | B | 806 | CLA | CMB-C2B-C1B | 2.35 | 128.95 | 125.37 |
| 20 | H | 102 | CLA | CHB-C4A-NA | 2.35 | 127.76 | 124.51 |
| 20 | 3 | 307 | CLA | CMB-C2B-C1B | 2.35 | 128.95 | 125.37 |
| 20 | B | 826 | CLA | C4A-NA-C1A | 2.35 | 107.76 | 106.71 |
| 20 | J | 101 | CLA | CED-O2D-CGD | 2.35 | 121.25 | 115.94 |
| 20 | A | 815 | CLA | CGD-CBD-CAD | 2.35 | 118.34 | 110.73 |
| 21 | G | 101 | LMU | O1B-C1B-O5B | 2.35 | 117.23 | 110.67 |
| 20 | F | 201 | CLA | O2A-CGA-CBA | 2.35 | 119.27 | 111.91 |
| 20 | J | 103 | CLA | C1-O2A-CGA | 2.35 | 122.60 | 116.44 |
| 20 | 1 | 208 | CLA | CHB-C4A-NA | 2.35 | 127.93 | 124.34 |
| 20 | B | 841 | CLA | O2D-CGD-O1D | -2.35 | 119.25 | 123.84 |
| 20 | B | 827 | CLA | CHB-C1B-NB | -2.35 | 121.77 | 124.26 |
| 20 | 2 | 309 | CLA | C3B-C4B-CHC | -2.35 | 119.43 | 126.24 |
| 21 | A | 848 | LMU | C1B-O1B-C4' | -2.34 | 112.16 | 117.96 |
| 23 | B | 843 | PQN | C16-C15-C13 | -2.34 | 107.31 | 113.45 |
| 20 | A | 849 | CLA | CMC-C2C-C1C | 2.34 | 128.60 | 125.04 |
| 20 | A | 828 | CLA | O2A-CGA-CBA | 2.34 | 119.25 | 111.91 |
| 20 | B | 820 | CLA | O2D-CGD-O1D | -2.34 | 119.26 | 123.84 |
| 20 | B | 820 | CLA | CMC-C2C-C1C | 2.34 | 128.60 | 125.04 |
| 22 | B | 846 | BCR | C37-C22-C21 | -2.34 | 119.65 | 122.92 |
| 20 | 4 | 303 | CLA | C3C-C4C-NC | -2.34 | 107.95 | 110.57 |
| 22 | 2 | 317 | BCR | C8-C7-C6 | -2.34 | 120.63 | 127.20 |
| 20 | A | 838 | CLA | C2A-C1A-CHA | -2.34 | 119.77 | 123.86 |
| 20 | B | 827 | CLA | C4A-NA-C1A | 2.34 | 107.76 | 106.71 |
| 21 | A | 848 | LMU | O5'-C5'-C6' | 2.34 | 112.25 | 106.44 |
| 20 | B | 816 | CLA | CHC-C1C-C2C | -2.34 | 120.24 | 126.73 |
| 20 | 4 | 303 | CLA | C1D-ND-C4D | -2.34 | 104.67 | 106.33 |
| 20 | A | 807 | CLA | CHB-C1B-NB | -2.34 | 121.78 | 124.26 |
| 20 | 4 | 306 | CLA | C3D-C4D-ND | 2.34 | 114.02 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | K | 102 | CLA | CED-O2D-CGD | 2.34 | 121.22 | 115.94 |
| 20 | 2 | 305 | CLA | CAA-C2A-C3A | -2.34 | 106.38 | 112.78 |
| 20 | A | 833 | CLA | CED-O2D-CGD | 2.33 | 121.22 | 115.94 |
| 20 | B | 827 | CLA | CHC-C1C-C2C | -2.33 | 120.25 | 126.73 |
| 20 | A | 808 | CLA | C1-C2-C3 | -2.33 | 122.01 | 126.04 |
| 22 | A | 845 | BCR | C8-C7-C6 | -2.33 | 120.65 | 127.20 |
| 21 | 1 | 216 | LMU | C1B-O1B-C4' | -2.33 | 112.19 | 117.96 |
| 20 | B | 828 | CLA | CHC-C1C-C2C | -2.33 | 120.25 | 126.73 |
| 20 | A | 809 | CLA | O2A-CGA-O1A | -2.33 | 117.71 | 123.59 |
| 20 | A | 834 | CLA | C2A-C1A-CHA | -2.33 | 119.78 | 123.86 |
| 20 | B | 807 | CLA | CHC-C1C-C2C | -2.33 | 120.26 | 126.73 |
| 20 | 4 | 307 | CLA | C3C-C4C-CHD | -2.33 | 120.12 | 125.22 |
| 20 | 1 | 212 | CLA | C3D-C4D-ND | 2.33 | 112.97 | 109.46 |
| 20 | H | 108 | CLA | CMB-C2B-C3B | 2.33 | 132.22 | 126.59 |
| 20 | H | 109 | CLA | CED-O2D-CGD | 2.33 | 121.20 | 115.94 |
| 21 | A | 853 | LMU | C1-O1'-C1' | -2.33 | 109.98 | 113.84 |
| 20 | 4 | 306 | CLA | CBC-CAC-C3C | -2.33 | 106.02 | 112.43 |
| 20 | B | 817 | CLA | O2D-CGD-O1D | -2.33 | 119.29 | 123.84 |
| 20 | F | 201 | CLA | C1D-ND-C4D | -2.33 | 104.68 | 106.33 |
| 20 | G | 105 | CLA | CMB-C2B-C1B | 2.33 | 128.91 | 125.37 |
| 20 | B | 841 | CLA | C4-C3-C5 | 2.32 | 119.18 | 115.27 |
| 20 | 2 | 310 | CLA | O1D-CGD-CBD | -2.32 | 119.73 | 124.48 |
| 22 | L | 209 | BCR | C8-C7-C6 | -2.32 | 120.68 | 127.20 |
| 21 | H | 106 | LMU | O5'-C1'-C2' | 2.32 | 115.26 | 110.35 |
| 20 | 4 | 305 | CLA | C1-C2-C3 | -2.32 | 123.00 | 126.75 |
| 20 | 1 | 201 | CLA | C4D-CHA-C1A | -2.32 | 118.42 | 121.25 |
| 20 | 4 | 308 | CLA | C3D-C4D-ND | 2.32 | 112.96 | 109.46 |
| 20 | B | 818 | CLA | CED-O2D-CGD | 2.32 | 121.18 | 115.94 |
| 21 | H | 106 | LMU | O1B-C4'-C3' | 2.32 | 113.45 | 107.28 |
| 20 | A | 841 | CLA | C3C-C4C-CHD | -2.32 | 120.14 | 125.22 |
| 20 | H | 110 | CLA | C1-O2A-CGA | 2.32 | 122.53 | 116.44 |
| 20 | 4 | 303 | CLA | O2A-CGA-O1A | -2.32 | 117.74 | 123.59 |
| 20 | A | 816 | CLA | CHC-C1C-C2C | -2.32 | 120.29 | 126.73 |
| 20 | A | 818 | CLA | CHB-C1B-NB | -2.32 | 121.80 | 124.26 |
| 22 | B | 844 | BCR | C29-C30-C25 | -2.32 | 106.91 | 110.48 |
| 22 | A | 844 | BCR | C3-C4-C5 | -2.32 | 109.94 | 114.08 |
| 22 | B | 847 | BCR | C20-C19-C18 | -2.32 | 119.91 | 126.42 |
| 20 | 4 | 313 | CLA | CAC-C3C-C4C | 2.32 | 128.57 | 125.04 |
| 20 | B | 828 | CLA | CAA-C2A-C3A | -2.32 | 106.44 | 112.78 |
| 20 | 3 | 305 | CLA | C2A-C3A-C4A | -2.32 | 100.55 | 104.18 |
| 20 | B | 829 | CLA | CMA-C3A-C2A | -2.32 | 104.49 | 113.83 |
| 20 | 2 | 316 | CLA | CED-O2D-CGD | 2.32 | 121.17 | 115.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | I | 101 | BCR | C12-C13-C14 | -2.31 | 115.39 | 118.94 |
| 20 | A | 818 | CLA | CAA-C2A-C1A | -2.31 | 104.39 | 111.97 |
| 20 | B | 803 | CLA | CED-O2D-CGD | 2.31 | 121.17 | 115.94 |
| 20 | A | 813 | CLA | C3D-C4D-ND | 2.31 | 113.98 | 110.24 |
| 20 | B | 813 | CLA | O2A-CGA-CBA | 2.31 | 119.16 | 111.91 |
| 20 | 2 | 316 | CLA | CHC-C1C-C2C | -2.31 | 120.31 | 126.73 |
| 23 | A | 842 | PQN | C2M-C2-C1 | 2.31 | 120.10 | 116.27 |
| 20 | A | 819 | CLA | CGD-CBD-CAD | 2.31 | 118.22 | 110.73 |
| 20 | F | 206 | CLA | C4A-NA-C1A | 2.31 | 107.75 | 106.71 |
| 20 | 4 | 310 | CLA | CBC-CAC-C3C | -2.31 | 106.06 | 112.43 |
| 20 | A | 804 | CLA | C1D-ND-C4D | -2.31 | 104.69 | 106.33 |
| 20 | B | 807 | CLA | C3D-C4D-ND | 2.31 | 113.97 | 110.24 |
| 20 | L | 202 | CLA | C4-C3-C5 | 2.31 | 119.16 | 115.27 |
| 21 | H | 103 | LMU | O5'-C5'-C4' | -2.31 | 104.89 | 109.75 |
| 20 | 1 | 201 | CLA | CHD-C1D-ND | 2.31 | 126.58 | 124.45 |
| 21 | B | 805 | LMU | O5B-C1B-C2B | 2.31 | 115.23 | 110.35 |
| 20 | 4 | 302 | CLA | CHB-C4A-NA | 2.31 | 127.70 | 124.51 |
| 20 | G | 105 | CLA | CHC-C1C-C2C | -2.31 | 120.32 | 126.73 |
| 20 | 4 | 318 | CLA | CMB-C2B-C1B | 2.31 | 128.88 | 125.37 |
| 20 | L | 201 | CLA | C1D-ND-C4D | -2.31 | 104.70 | 106.33 |
| 20 | 1 | 201 | CLA | C2D-C1D-ND | -2.31 | 108.40 | 110.10 |
| 20 | F | 205 | CLA | C3D-C4D-ND | 2.31 | 113.97 | 110.24 |
| 20 | B | 803 | CLA | C3D-C4D-ND | 2.31 | 113.97 | 110.24 |
| 21 | H | 105 | LMU | O5'-C1'-C2' | -2.31 | 105.47 | 110.35 |
| 20 | 2 | 312 | CLA | CHC-C1C-C2C | -2.30 | 120.33 | 126.73 |
| 20 | B | 828 | CLA | O2A-C1-C2 | 2.30 | 114.69 | 108.64 |
| 20 | 2 | 310 | CLA | CAA-C2A-C3A | -2.30 | 106.47 | 112.78 |
| 20 | A | 831 | CLA | C11-C12-C13 | -2.30 | 108.47 | 115.92 |
| 20 | 4 | 309 | CLA | C3D-C4D-ND | 2.30 | 112.94 | 109.46 |
| 20 | 2 | 310 | CLA | CAA-C2A-C1A | -2.30 | 104.43 | 111.97 |
| 20 | B | 810 | CLA | O2A-CGA-O1A | -2.30 | 117.78 | 123.59 |
| 22 | 2 | 317 | BCR | C37-C22-C21 | -2.30 | 119.70 | 122.92 |
| 21 | 4 | 320 | LMU | O5B-C5B-C6B | 2.30 | 112.16 | 106.44 |
| 20 | B | 824 | CLA | O2A-CGA-O1A | -2.30 | 117.79 | 123.59 |
| 20 | B | 832 | CLA | CMB-C2B-C1B | 2.30 | 128.87 | 125.37 |
| 20 | B | 811 | CLA | C3C-C4C-CHD | -2.30 | 120.18 | 125.22 |
| 20 | 2 | 316 | CLA | O2A-CGA-CBA | 2.30 | 119.12 | 111.91 |
| 20 | L | 204 | CLA | CHC-C1C-C2C | -2.30 | 120.34 | 126.73 |
| 20 | 1 | 208 | CLA | C3D-C4D-ND | 2.30 | 112.93 | 109.46 |
| 20 | 2 | 303 | CLA | C3D-C4D-ND | 2.30 | 113.96 | 110.24 |
| 20 | A | 822 | CLA | CAC-C3C-C4C | 2.30 | 127.79 | 124.81 |
| 20 | B | 812 | CLA | CHC-C1C-C2C | -2.30 | 120.35 | 126.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | A | 845 | BCR | C23-C24-C25 | -2.30 | 120.75 | 127.20 |
| 20 | A | 826 | CLA | C11-C10-C8 | -2.29 | 108.51 | 115.92 |
| 20 | B | 821 | CLA | CHB-C4A-NA | 2.29 | 127.68 | 124.51 |
| 20 | A | 829 | CLA | O1D-CGD-CBD | -2.29 | 119.79 | 124.48 |
| 20 | B | 836 | CLA | CHB-C4A-NA | 2.29 | 127.68 | 124.51 |
| 21 | B | 804 | LMU | O3'-C3'-C2' | 2.29 | 115.64 | 110.35 |
| 20 | L | 204 | CLA | C1-O2A-CGA | 2.29 | 122.45 | 116.44 |
| 20 | B | 821 | CLA | C3D-C4D-ND | 2.29 | 113.94 | 110.24 |
| 20 | A | 807 | CLA | CHC-C1C-C2C | -2.29 | 120.38 | 126.73 |
| 20 | G | 105 | CLA | CHC-C4B-NB | 2.29 | 126.68 | 124.26 |
| 20 | 2 | 316 | CLA | C2D-C1D-ND | -2.29 | 108.42 | 110.10 |
| 20 | 2 | 301 | CLA | C3D-C2D-C1D | 2.29 | 109.81 | 107.28 |
| 20 | 4 | 302 | CLA | CHC-C1C-C2C | -2.29 | 120.38 | 126.73 |
| 20 | H | 110 | CLA | CHC-C1C-C2C | -2.29 | 120.38 | 126.73 |
| 20 | A | 812 | CLA | CED-O2D-CGD | 2.29 | 121.11 | 115.94 |
| 20 | 3 | 304 | CLA | C3D-C4D-ND | 2.29 | 112.91 | 109.46 |
| 20 | A | 818 | CLA | CHB-C4A-NA | 2.29 | 127.67 | 124.51 |
| 22 | A | 845 | BCR | C34-C9-C10 | -2.28 | 119.72 | 122.92 |
| 20 | F | 201 | CLA | CHB-C4A-NA | 2.28 | 127.67 | 124.51 |
| 20 | A | 803 | CLA | O1D-CGD-CBD | -2.28 | 119.81 | 124.48 |
| 20 | 4 | 306 | CLA | C4-C3-C2 | -2.28 | 117.82 | 123.68 |
| 20 | B | 840 | CLA | C1D-ND-C4D | -2.28 | 104.71 | 106.33 |
| 22 | B | 844 | BCR | C30-C25-C24 | 2.28 | 122.23 | 115.78 |
| 22 | J | 102 | BCR | C23-C24-C25 | -2.28 | 120.79 | 127.20 |
| 20 | 1 | 209 | CLA | C3A-C4A-NA | 2.28 | 114.71 | 109.92 |
| 20 | A | 835 | CLA | C1D-ND-C4D | -2.28 | 104.72 | 106.33 |
| 20 | 1 | 201 | CLA | CGD-CBD-CAD | -2.28 | 103.35 | 110.73 |
| 20 | A | 828 | CLA | C2A-C1A-CHA | -2.28 | 119.87 | 123.86 |
| 21 | A | 852 | LMU | O5'-C5'-C6' | 2.28 | 112.10 | 106.44 |
| 20 | A | 841 | CLA | CHB-C4A-NA | 2.28 | 127.83 | 124.34 |
| 20 | A | 834 | CLA | CHB-C4A-NA | 2.28 | 127.66 | 124.51 |
| 20 | H | 109 | CLA | CHB-C1B-NB | -2.28 | 121.84 | 124.26 |
| 22 | F | 203 | BCR | C11-C12-C13 | -2.28 | 120.02 | 126.42 |
| 20 | A | 838 | CLA | C6-C7-C8 | -2.28 | 108.56 | 115.92 |
| 20 | 4 | 317 | CLA | CMB-C2B-C1B | 2.28 | 128.84 | 125.37 |
| 20 | A | 806 | CLA | CMB-C2B-C1B | 2.28 | 128.84 | 125.37 |
| 20 | B | 830 | CLA | C1D-ND-C4D | -2.28 | 104.72 | 106.33 |
| 21 | R | 102 | LMU | C3B-C4B-C5B | -2.28 | 106.18 | 110.24 |
| 20 | B | 828 | CLA | C2A-C1A-CHA | -2.28 | 119.88 | 123.86 |
| 20 | F | 201 | CLA | CMD-C2D-C3D | -2.28 | 122.38 | 127.61 |
| 20 | B | 842 | CLA | CGD-CBD-CAD | -2.27 | 104.97 | 114.30 |
| 20 | 1 | 204 | CLA | O1D-CGD-CBD | -2.27 | 119.83 | 124.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 815 | CLA | O2A-CGA-O1A | -2.27 | 117.85 | 123.59 |
| 20 | 3 | 314 | CLA | CHC-C4B-C3B | -2.27 | 117.60 | 127.71 |
| 21 | R | 101 | LMU | C1-O1'-C1' | -2.27 | 110.07 | 113.84 |
| 21 | A | 855 | LMU | O1B-C4'-C5' | 2.27 | 115.67 | 109.45 |
| 20 | 2 | 310 | CLA | CHB-C1B-NB | -2.27 | 121.85 | 124.26 |
| 20 | A | 816 | CLA | CED-O2D-CGD | 2.27 | 121.08 | 115.94 |
| 20 | L | 204 | CLA | C2A-C1A-CHA | -2.27 | 119.89 | 123.86 |
| 22 | B | 846 | BCR | C29-C30-C25 | -2.27 | 106.98 | 110.48 |
| 20 | B | 832 | CLA | C1-O2A-CGA | 2.27 | 122.40 | 116.44 |
| 20 | B | 819 | CLA | CHB-C1B-NB | -2.27 | 121.85 | 124.26 |
| 22 | B | 847 | BCR | C38-C26-C27 | 2.27 | 117.98 | 113.62 |
| 20 | 2 | 309 | CLA | CHB-C1B-NB | -2.27 | 121.98 | 124.27 |
| 20 | A | 838 | CLA | O2A-C1-C2 | 2.27 | 114.60 | 108.64 |
| 20 | A | 813 | CLA | C5-C3-C4 | 2.27 | 119.61 | 114.60 |
| 20 | A | 819 | CLA | CAA-C2A-C3A | -2.27 | 106.57 | 112.78 |
| 20 | B | 826 | CLA | CHB-C4A-NA | 2.27 | 127.65 | 124.51 |
| 22 | F | 203 | BCR | C24-C23-C22 | -2.27 | 122.81 | 126.23 |
| 20 | F | 206 | CLA | C2A-C1A-CHA | -2.26 | 119.90 | 123.85 |
| 20 | K | 104 | CLA | C1-O2A-CGA | 2.26 | 122.39 | 116.44 |
| 20 | 4 | 317 | CLA | C3A-C2A-C1A | 2.26 | 104.73 | 101.34 |
| 21 | R | 103 | LMU | O5B-C5B-C4B | 2.26 | 113.81 | 109.69 |
| 20 | 4 | 312 | CLA | CHB-C4A-NA | 2.26 | 127.81 | 124.34 |
| 20 | R | 107 | CLA | C1-O2A-CGA | 2.26 | 122.38 | 116.44 |
| 21 | 2 | 319 | LMU | C3'-C4'-C5' | 2.26 | 116.11 | 110.93 |
| 20 | A | 826 | CLA | CHC-C1C-C2C | -2.26 | 120.45 | 126.73 |
| 21 | A | 846 | LMU | O5B-C5B-C4B | 2.26 | 113.80 | 109.69 |
| 20 | L | 208 | CLA | CAC-C3C-C4C | 2.26 | 127.74 | 124.81 |
| 20 | A | 822 | CLA | CAA-C2A-C3A | -2.26 | 106.59 | 112.78 |
| 20 | B | 811 | CLA | CHD-C1D-ND | 2.26 | 126.70 | 124.52 |
| 20 | A | 810 | CLA | C2D-C1D-ND | -2.26 | 108.44 | 110.10 |
| 20 | B | 807 | CLA | CHC-C4B-NB | 2.26 | 126.65 | 124.26 |
| 20 | A | 826 | CLA | C7-C6-C5 | -2.26 | 107.23 | 113.36 |
| 20 | A | 829 | CLA | CHB-C4A-NA | 2.26 | 127.63 | 124.51 |
| 20 | L | 201 | CLA | C3D-C4D-ND | 2.26 | 113.89 | 110.24 |
| 20 | 1 | 211 | CLA | C3B-C2B-C1B | -2.25 | 104.44 | 107.16 |
| 21 | 1 | 218 | LMU | O5B-C5B-C6B | 2.25 | 112.04 | 106.44 |
| 20 | 1 | 203 | CLA | CBC-CAC-C3C | -2.25 | 106.22 | 112.43 |
| 22 | L | 209 | BCR | C28-C27-C26 | -2.25 | 110.05 | 114.08 |
| 20 | B | 840 | CLA | C3B-C4B-NB | -2.25 | 108.42 | 110.52 |
| 20 | A | 815 | CLA | C2D-C1D-ND | -2.25 | 108.44 | 110.10 |
| 20 | A | 816 | CLA | C1-O2A-CGA | 2.25 | 122.35 | 116.44 |
| 20 | A | 851 | CLA | CGD-CBD-CAD | 2.25 | 118.03 | 110.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 841 | CLA | C3A-C4A-NA | 2.25 | 114.64 | 109.92 |
| 22 | A | 844 | BCR | C15-C16-C17 | -2.25 | 118.86 | 123.47 |
| 20 | K | 104 | CLA | C2D-C1D-ND | -2.25 | 108.45 | 110.10 |
| 22 | B | 844 | BCR | C15-C14-C13 | -2.25 | 124.10 | 127.31 |
| 20 | B | 826 | CLA | O2A-CGA-CBA | 2.25 | 118.96 | 111.91 |
| 20 | A | 833 | CLA | C3C-C4C-NC | -2.25 | 108.05 | 110.57 |
| 20 | 4 | 301 | CLA | CMB-C2B-C1B | 2.25 | 128.79 | 125.37 |
| 20 | A | 834 | CLA | CMB-C2B-C1B | 2.25 | 128.79 | 125.37 |
| 20 | 3 | 312 | CLA | C2A-C3A-C4A | -2.25 | 100.66 | 104.18 |
| 21 | E | 101 | LMU | C1'-C2'-C3' | 2.25 | 114.67 | 110.00 |
| 20 | A | 835 | CLA | O1D-CGD-CBD | -2.24 | 119.89 | 124.48 |
| 20 | A | 819 | CLA | O2A-CGA-CBA | 2.24 | 118.95 | 111.91 |
| 20 | A | 809 | CLA | CHC-C4B-C3B | -2.24 | 117.74 | 127.71 |
| 20 | B | 835 | CLA | O1D-CGD-CBD | -2.24 | 119.90 | 124.48 |
| 20 | 3 | 314 | CLA | CMB-C2B-C1B | 2.24 | 128.78 | 125.37 |
| 22 | A | 845 | BCR | C11-C12-C13 | -2.24 | 120.12 | 126.42 |
| 20 | A | 837 | CLA | CBC-CAC-C3C | -2.24 | 106.25 | 112.43 |
| 20 | A | 816 | CLA | O2D-CGD-O1D | -2.24 | 119.46 | 123.84 |
| 20 | 1 | 202 | CLA | CHB-C1B-NB | -2.24 | 121.89 | 124.26 |
| 21 | B | 805 | LMU | O3B-C3B-C2B | -2.24 | 105.17 | 110.35 |
| 20 | 4 | 306 | CLA | C4-C3-C5 | 2.24 | 119.04 | 115.27 |
| 20 | B | 824 | CLA | C10-C8-C7 | 2.24 | 123.89 | 112.13 |
| 20 | 1 | 213 | CLA | CMA-C3A-C2A | 2.24 | 122.85 | 113.83 |
| 20 | 2 | 312 | CLA | O1D-CGD-CBD | -2.24 | 119.91 | 124.48 |
| 20 | B | 823 | CLA | CAC-C3C-C4C | 2.24 | 127.71 | 124.81 |
| 20 | L | 201 | CLA | CED-O2D-CGD | 2.24 | 120.99 | 115.94 |
| 20 | 2 | 301 | CLA | C2A-C3A-C4A | -2.23 | 100.67 | 104.18 |
| 20 | B | 812 | CLA | O1D-CGD-CBD | -2.23 | 119.91 | 124.48 |
| 22 | B | 846 | BCR | C37-C22-C23 | 2.23 | 121.60 | 118.08 |
| 20 | A | 832 | CLA | CED-O2D-CGD | 2.23 | 120.99 | 115.94 |
| 25 | B | 848 | LMG | O7-C10-O9 | -2.23 | 118.30 | 123.70 |
| 20 | B | 837 | CLA | O2A-CGA-CBA | 2.23 | 118.92 | 111.91 |
| 20 | 4 | 318 | CLA | CMA-C3A-C4A | -2.23 | 105.77 | 111.77 |
| 21 | E | 101 | LMU | O3B-C3B-C2B | 2.23 | 115.51 | 110.35 |
| 20 | A | 824 | CLA | C1-C2-C3 | -2.23 | 122.19 | 126.04 |
| 20 | 2 | 305 | CLA | C1-O2A-CGA | 2.23 | 122.30 | 116.44 |
| 20 | 2 | 304 | CLA | C2A-C3A-C4A | -2.23 | 100.68 | 104.18 |
| 20 | A | 816 | CLA | O1D-CGD-CBD | -2.23 | 119.92 | 124.48 |
| 20 | A | 839 | CLA | O1D-CGD-CBD | -2.23 | 119.92 | 124.48 |
| 20 | 4 | 317 | CLA | C4-C3-C2 | -2.23 | 117.96 | 123.68 |
| 20 | A | 817 | CLA | O1D-CGD-CBD | -2.23 | 119.92 | 124.48 |
| 20 | L | 208 | CLA | CHB-C1B-NB | -2.23 | 121.90 | 124.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 20 | B | 833 | CLA | CMB-C2B-C1B | 2.23 | 128.76 | 125.37 |
| 20 | L | 208 | CLA | CHB-C4A-NA | 2.23 | 127.59 | 124.51 |
| 21 | 1 | 218 | LMU | C1'-C2'-C3' | 2.23 | 114.63 | 110.00 |
| 20 | A | 825 | CLA | O2A-CGA-CBA | 2.23 | 118.89 | 111.91 |
| 22 | B | 845 | BCR | C16-C15-C14 | -2.23 | 118.92 | 123.47 |
| 20 | 4 | 305 | CLA | C1D-ND-C4D | -2.23 | 104.75 | 106.33 |
| 20 | 3 | 312 | CLA | C3D-C4D-ND | 2.22 | 112.82 | 109.46 |
| 20 | 2 | 310 | CLA | C5-C3-C4 | 2.22 | 119.52 | 114.60 |
| 20 | K | 104 | CLA | CMB-C2B-C1B | 2.22 | 128.76 | 125.37 |
| 21 | K | 107 | LMU | O5B-C5B-C6B | 2.22 | 111.96 | 106.44 |
| 22 | 2 | 317 | BCR | C20-C19-C18 | -2.22 | 120.17 | 126.42 |
| 20 | 3 | 302 | CLA | C3D-C4D-ND | 2.22 | 112.81 | 109.46 |
| 20 | 2 | 314 | CLA | C1D-ND-C4D | -2.22 | 104.76 | 106.33 |
| 20 | 4 | 314 | CLA | CHB-C1B-NB | -2.22 | 122.03 | 124.27 |
| 20 | 1 | 215 | CLA | C1-O2A-CGA | 2.22 | 122.27 | 116.44 |
| 20 | B | 821 | CLA | CMA-C3A-C2A | -2.22 | 104.88 | 113.83 |
| 20 | B | 830 | CLA | O2A-CGA-CBA | 2.22 | 118.87 | 111.91 |
| 20 | L | 203 | CLA | O2D-CGD-O1D | -2.22 | 119.50 | 123.84 |
| 20 | A | 805 | CLA | O1D-CGD-CBD | -2.22 | 119.95 | 124.48 |
| 20 | A | 813 | CLA | CMB-C2B-C1B | 2.22 | 128.75 | 125.37 |
| 20 | A | 813 | CLA | O2D-CGD-O1D | -2.22 | 119.50 | 123.84 |
| 22 | B | 844 | BCR | C36-C18-C19 | 2.22 | 121.57 | 118.08 |
| 20 | L | 201 | CLA | O2A-CGA-O1A | -2.22 | 118.00 | 123.59 |
| 20 | 2 | 302 | CLA | O1D-CGD-CBD | -2.22 | 119.95 | 124.48 |
| 20 | 1 | 206 | CLA | CED-O2D-CGD | 2.22 | 120.95 | 115.94 |
| 21 | 2 | 321 | LMU | O1'-C1'-C2' | 2.22 | 111.76 | 108.30 |
| 22 | J | 102 | BCR | C30-C25-C24 | 2.22 | 122.05 | 115.78 |
| 20 | A | 828 | CLA | O2A-CGA-O1A | -2.21 | 118.00 | 123.59 |
| 20 | 4 | 303 | CLA | C7-C6-C5 | -2.21 | 107.35 | 113.36 |
| 20 | A | 815 | CLA | CED-O2D-CGD | 2.21 | 120.94 | 115.94 |
| 21 | A | 846 | LMU | O1'-C1'-C2' | 2.21 | 111.75 | 108.30 |
| 20 | A | 834 | CLA | C2D-C1D-ND | -2.21 | 108.47 | 110.10 |
| 20 | B | 824 | CLA | CHB-C1B-NB | -2.21 | 121.92 | 124.26 |
| 20 | A | 801 | CLA | O2A-CGA-O1A | -2.21 | 118.01 | 123.59 |
| 20 | A | 828 | CLA | O1D-CGD-CBD | -2.21 | 119.96 | 124.48 |
| 20 | 3 | 308 | CLA | C3D-C4D-ND | 2.21 | 112.80 | 109.46 |
| 20 | A | 850 | CLA | C1-C2-C3 | -2.21 | 122.22 | 126.04 |
| 20 | 4 | 311 | CLA | C3D-C4D-ND | 2.21 | 112.79 | 109.46 |
| 20 | 4 | 302 | CLA | C2D-C1D-ND | -2.21 | 108.48 | 110.10 |
| 20 | A | 838 | CLA | CHC-C1C-C2C | -2.21 | 120.60 | 126.73 |
| 20 | R | 108 | CLA | CGD-CBD-CAD | -2.21 | 103.59 | 110.73 |
| 20 | B | 840 | CLA | O2A-CGA-O1A | -2.21 | 118.02 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | F | 205 | CLA | C1D-ND-C4D | -2.21 | 104.77 | 106.33 |
| 22 | A | 845 | BCR | C38-C26-C25 | -2.21 | 122.05 | 124.53 |
| 20 | R | 108 | CLA | CAA-C2A-C1A | 2.21 | 119.20 | 111.97 |
| 20 | A | 833 | CLA | O1D-CGD-CBD | -2.21 | 119.97 | 124.48 |
| 20 | 2 | 311 | CLA | O2A-CGA-O1A | -2.20 | 118.03 | 123.59 |
| 20 | H | 102 | CLA | O2A-CGA-O1A | -2.20 | 118.03 | 123.59 |
| 20 | 2 | 312 | CLA | C11-C12-C13 | -2.20 | 108.80 | 115.92 |
| 20 | B | 812 | CLA | CAC-C3C-C4C | 2.20 | 127.67 | 124.81 |
| 20 | B | 826 | CLA | CMB-C2B-C1B | 2.20 | 128.72 | 125.37 |
| 20 | A | 832 | CLA | O2A-CGA-O1A | -2.20 | 118.03 | 123.59 |
| 20 | 3 | 316 | CLA | C2A-C3A-C4A | -2.20 | 100.72 | 104.18 |
| 20 | 3 | 317 | CLA | CAA-C2A-C3A | -2.20 | 110.96 | 116.10 |
| 20 | 4 | 313 | CLA | CHC-C4B-C3B | -2.20 | 121.02 | 127.24 |
| 20 | 4 | 314 | CLA | C1C-NC-C4C | -2.20 | 105.72 | 106.71 |
| 20 | 4 | 302 | CLA | CBD-CHA-C1A | 2.20 | 130.95 | 127.43 |
| 21 | 3 | 319 | LMU | C1'-O5'-C5' | 2.20 | 118.00 | 113.69 |
| 21 | 4 | 321 | LMU | C3B-C4B-C5B | 2.20 | 114.16 | 110.24 |
| 20 | L | 203 | CLA | O2A-CGA-CBA | 2.20 | 118.81 | 111.91 |
| 20 | 1 | 201 | CLA | CHC-C4B-C3B | -2.20 | 117.93 | 127.71 |
| 20 | A | 849 | CLA | C6-C7-C8 | -2.20 | 108.82 | 115.92 |
| 20 | B | 811 | CLA | C3B-C4B-CHC | -2.20 | 119.86 | 126.24 |
| 20 | B | 813 | CLA | C2A-C1A-CHA | -2.20 | 120.02 | 123.86 |
| 20 | K | 103 | CLA | CED-O2D-CGD | 2.20 | 120.90 | 115.94 |
| 20 | 4 | 314 | CLA | C2A-C3A-C4A | -2.20 | 100.73 | 104.18 |
| 20 | B | 809 | CLA | O2A-CGA-O1A | -2.20 | 118.05 | 123.59 |
| 20 | B | 850 | CLA | CAC-C3C-C4C | 2.20 | 127.66 | 124.81 |
| 20 | F | 201 | CLA | O1D-CGD-CBD | -2.19 | 119.99 | 124.48 |
| 20 | 2 | 312 | CLA | CMB-C2B-C1B | 2.19 | 128.71 | 125.37 |
| 20 | A | 829 | CLA | C1-O2A-CGA | 2.19 | 122.20 | 116.44 |
| 20 | B | 825 | CLA | C1-O2A-CGA | 2.19 | 122.20 | 116.44 |
| 21 | R | 102 | LMU | O1'-C1'-C2' | 2.19 | 111.73 | 108.30 |
| 20 | B | 840 | CLA | C1-C2-C3 | -2.19 | 122.25 | 126.04 |
| 21 | G | 102 | LMU | O5B-C1B-C2B | -2.19 | 105.71 | 110.35 |
| 20 | 2 | 307 | CLA | CED-O2D-CGD | 2.19 | 120.90 | 115.94 |
| 20 | A | 839 | CLA | CED-O2D-CGD | 2.19 | 120.90 | 115.94 |
| 22 | B | 801 | BCR | C20-C19-C18 | -2.19 | 120.26 | 126.42 |
| 22 | B | 844 | BCR | C36-C18-C17 | -2.19 | 119.85 | 122.92 |
| 20 | A | 841 | CLA | C3D-C2D-C1D | 2.19 | 109.70 | 107.28 |
| 20 | A | 833 | CLA | C3D-C4D-ND | 2.19 | 113.78 | 110.24 |
| 21 | 3 | 318 | LMU | C1B-O1B-C4' | -2.19 | 112.55 | 117.96 |
| 20 | 1 | 213 | CLA | O2A-CGA-O1A | -2.19 | 118.07 | 123.59 |
| 20 | 4 | 317 | CLA | O2A-CGA-CBA | 2.19 | 118.77 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 20 | 1 | 214 | CLA | C2A-C3A-C4A | -2.19 | 100.75 | 104.18 |
| 20 | 2 | 301 | CLA | C3B-C4B-CHC | -2.19 | 119.89 | 126.24 |
| 20 | B | 817 | CLA | CAC-C3C-C2C | -2.19 | 123.79 | 127.53 |
| 20 | 2 | 301 | CLA | C3D-C4D-ND | 2.19 | 112.76 | 109.46 |
| 20 | B | 808 | CLA | C4-C3-C5 | 2.18 | 118.95 | 115.27 |
| 20 | B | 835 | CLA | O2A-CGA-O1A | -2.18 | 117.85 | 123.30 |
| 20 | B | 814 | CLA | CHC-C1C-C2C | -2.18 | 120.67 | 126.73 |
| 20 | B | 833 | CLA | O2A-CGA-O1A | -2.18 | 118.08 | 123.59 |
| 20 | A | 838 | CLA | C3D-C4D-ND | 2.18 | 113.77 | 110.24 |
| 21 | G | 102 | LMU | O4'-C4B-C3B | 2.18 | 115.39 | 110.35 |
| 21 | 3 | 319 | LMU | C1'-C2'-C3' | -2.18 | 105.45 | 110.00 |
| 22 | G | 104 | BCR | C28-C27-C26 | -2.18 | 110.18 | 114.08 |
| 20 | A | 802 | CLA | C3B-C4B-CHC | -2.18 | 119.91 | 126.24 |
| 20 | A | 849 | CLA | CHC-C1C-C2C | -2.18 | 120.67 | 126.73 |
| 20 | B | 825 | CLA | CAA-CBA-CGA | -2.18 | 106.88 | 113.25 |
| 20 | B | 810 | CLA | CAC-C3C-C4C | 2.18 | 127.64 | 124.81 |
| 20 | K | 104 | CLA | C4A-NA-C1A | 2.18 | 107.69 | 106.71 |
| 20 | A | 825 | CLA | C2A-C1A-CHA | -2.18 | 120.05 | 123.86 |
| 20 | K | 104 | CLA | CAC-C3C-C2C | -2.18 | 123.80 | 127.53 |
| 20 | 3 | 309 | CLA | C3B-C4B-CHC | -2.18 | 119.91 | 126.24 |
| 22 | A | 844 | BCR | C38-C26-C25 | -2.18 | 122.08 | 124.53 |
| 20 | 3 | 310 | CLA | CBC-CAC-C3C | -2.18 | 106.43 | 112.43 |
| 20 | B | 834 | CLA | O1D-CGD-CBD | -2.18 | 120.03 | 124.48 |
| 20 | 4 | 307 | CLA | C3D-C2D-C1D | 2.18 | 109.69 | 107.28 |
| 21 | B | 849 | LMU | O1B-C4'-C3' | 2.18 | 113.07 | 107.28 |
| 20 | A | 802 | CLA | C3C-C4C-CHD | -2.18 | 120.45 | 125.22 |
| 20 | I | 102 | CLA | CMB-C2B-C1B | 2.18 | 128.68 | 125.37 |
| 20 | 1 | 209 | CLA | C2C-C1C-CHC | -2.18 | 120.46 | 125.67 |
| 20 | 4 | 303 | CLA | CAC-C3C-C4C | 2.17 | 127.63 | 124.81 |
| 20 | B | 850 | CLA | C7-C6-C5 | -2.17 | 107.45 | 113.36 |
| 20 | B | 810 | CLA | O2D-CGD-O1D | -2.17 | 119.59 | 123.84 |
| 20 | B | 833 | CLA | O2D-CGD-O1D | -2.17 | 119.59 | 123.84 |
| 22 | J | 102 | BCR | C33-C5-C6 | -2.17 | 122.09 | 124.53 |
| 20 | 2 | 315 | CLA | C2A-C3A-C4A | -2.17 | 100.77 | 104.18 |
| 20 | B | 829 | CLA | C16-C15-C13 | -2.17 | 108.90 | 115.92 |
| 20 | B | 838 | CLA | C3D-C4D-ND | 2.17 | 113.75 | 110.24 |
| 22 | 2 | 317 | BCR | C37-C22-C23 | 2.17 | 121.50 | 118.08 |
| 21 | L | 205 | LMU | O1B-C1B-C2B | 2.17 | 113.73 | 108.10 |
| 20 | H | 108 | CLA | CHD-C1D-ND | 2.17 | 126.45 | 124.45 |
| 20 | L | 204 | CLA | CMC-C2C-C1C | 2.17 | 128.34 | 125.04 |
| 20 | A | 825 | CLA | CMB-C2B-C1B | 2.17 | 128.68 | 125.37 |
| 20 | A | 841 | CLA | C3B-C4B-CHC | -2.17 | 119.94 | 126.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 3 | 315 | CLA | C3A-C4A-NA | 2.17 | 114.47 | 109.92 |
| 20 | A | 804 | CLA | C3D-C4D-ND | 2.17 | 113.75 | 110.24 |
| 22 | B | 846 | BCR | C30-C25-C26 | -2.17 | 119.56 | 122.61 |
| 20 | 2 | 311 | CLA | C5-C3-C4 | 2.17 | 119.39 | 114.60 |
| 20 | 2 | 307 | CLA | CHC-C4B-C3B | -2.17 | 118.07 | 127.71 |
| 20 | L | 204 | CLA | C3D-C4D-ND | 2.17 | 113.74 | 110.24 |
| 20 | F | 207 | CLA | O2A-CGA-CBA | 2.17 | 118.70 | 111.91 |
| 20 | A | 819 | CLA | C1-O2A-CGA | 2.17 | 122.12 | 116.44 |
| 20 | B | 823 | CLA | O2A-CGA-CBA | 2.17 | 118.70 | 111.91 |
| 20 | 3 | 314 | CLA | CHB-C1B-NB | -2.17 | 121.97 | 124.26 |
| 20 | B | 822 | CLA | CHB-C1B-NB | -2.17 | 121.97 | 124.26 |
| 20 | A | 811 | CLA | C3A-C2A-C1A | 2.16 | 104.58 | 101.34 |
| 20 | K | 101 | CLA | CMB-C2B-C1B | 2.16 | 128.66 | 125.37 |
| 20 | 1 | 203 | CLA | C3B-C4B-NB | -2.16 | 108.51 | 110.52 |
| 20 | B | 817 | CLA | C3D-C4D-ND | 2.16 | 113.74 | 110.24 |
| 20 | 1 | 205 | CLA | CMB-C2B-C1B | 2.16 | 128.66 | 125.37 |
| 20 | A | 833 | CLA | C2A-C1A-CHA | -2.16 | 120.08 | 123.86 |
| 20 | 1 | 210 | CLA | CHC-C4B-C3B | -2.16 | 121.14 | 127.24 |
| 21 | L | 205 | LMU | O5B-C1B-C2B | 2.16 | 114.92 | 110.35 |
| 20 | 2 | 303 | CLA | C6-C7-C8 | -2.16 | 108.94 | 115.92 |
| 20 | K | 102 | CLA | C2A-C1A-CHA | -2.16 | 120.08 | 123.86 |
| 22 | A | 843 | BCR | C30-C25-C26 | -2.16 | 119.57 | 122.61 |
| 20 | B | 842 | CLA | C1D-ND-C4D | -2.16 | 104.80 | 106.33 |
| 20 | A | 824 | CLA | C4-C3-C5 | 2.16 | 118.90 | 115.27 |
| 20 | A | 851 | CLA | O2A-CGA-O1A | -2.16 | 118.14 | 123.59 |
| 21 | B | 805 | LMU | C1'-C2'-C3' | 2.16 | 114.49 | 110.00 |
| 21 | B | 849 | LMU | C3B-C4B-C5B | 2.16 | 114.09 | 110.24 |
| 20 | 1 | 215 | CLA | O2A-CGA-CBA | 2.16 | 118.68 | 111.91 |
| 20 | A | 818 | CLA | C2A-C1A-CHA | -2.15 | 120.09 | 123.86 |
| 20 | A | 819 | CLA | C2D-C1D-ND | -2.15 | 108.52 | 110.10 |
| 21 | G | 102 | LMU | O5B-C5B-C4B | -2.15 | 105.78 | 109.69 |
| 20 | 2 | 302 | CLA | C2A-C1A-CHA | -2.15 | 120.09 | 123.86 |
| 20 | A | 851 | CLA | C3D-C4D-ND | 2.15 | 113.72 | 110.24 |
| 20 | 3 | 314 | CLA | CED-O2D-CGD | 2.15 | 120.81 | 115.94 |
| 20 | 3 | 307 | CLA | C2D-C1D-ND | -2.15 | 108.52 | 110.10 |
| 20 | 2 | 314 | CLA | CAC-C3C-C4C | -2.15 | 122.02 | 124.81 |
| 20 | F | 207 | CLA | C2A-C3A-C4A | 2.15 | 105.34 | 101.87 |
| 20 | 2 | 302 | CLA | C4D-CHA-C1A | 2.15 | 123.87 | 121.25 |
| 20 | B | 802 | CLA | CMC-C2C-C1C | 2.15 | 128.31 | 125.04 |
| 20 | H | 101 | CLA | CAA-C2A-C1A | 2.15 | 119.02 | 111.97 |
| 20 | F | 207 | CLA | C3D-C4D-ND | 2.15 | 113.72 | 110.24 |
| 20 | 4 | 302 | CLA | CHB-C1B-NB | -2.15 | 121.98 | 124.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | H | 103 | LMU | O6'-C6'-C5' | -2.15 | 103.92 | 111.29 |
| 22 | A | 844 | BCR | C4-C5-C6 | -2.15 | 119.61 | 122.73 |
| 22 | I | 103 | BCR | C23-C22-C21 | 2.15 | 122.24 | 118.94 |
| 20 | A | 804 | CLA | CHB-C1B-NB | -2.15 | 121.98 | 124.26 |
| 20 | A | 803 | CLA | CBC-CAC-C3C | -2.15 | 106.51 | 112.43 |
| 20 | L | 204 | CLA | CED-O2D-CGD | 2.15 | 120.79 | 115.94 |
| 22 | A | 845 | BCR | C1-C6-C7 | 2.15 | 121.85 | 115.78 |
| 20 | A | 835 | CLA | O2A-C1-C2 | 2.14 | 114.27 | 108.64 |
| 20 | 3 | 310 | CLA | CHB-C4A-NA | 2.14 | 127.48 | 124.51 |
| 20 | B | 814 | CLA | C3A-C2A-C1A | 2.14 | 104.55 | 101.34 |
| 21 | B | 805 | LMU | C1B-C2B-C3B | 2.14 | 114.46 | 110.00 |
| 22 | A | 843 | BCR | C1-C6-C7 | 2.14 | 121.84 | 115.78 |
| 20 | B | 833 | CLA | CAC-C3C-C4C | 2.14 | 127.59 | 124.81 |
| 22 | A | 845 | BCR | C20-C19-C18 | -2.14 | 120.40 | 126.42 |
| 20 | B | 829 | CLA | CHD-C1D-ND | 2.14 | 126.42 | 124.45 |
| 20 | I | 102 | CLA | O2A-CGA-O1A | -2.14 | 118.19 | 123.59 |
| 20 | A | 851 | CLA | C16-C15-C13 | -2.14 | 109.00 | 115.92 |
| 20 | B | 835 | CLA | CHB-C4A-NA | 2.14 | 127.47 | 124.51 |
| 22 | J | 102 | BCR | C28-C27-C26 | -2.14 | 110.25 | 114.08 |
| 20 | A | 806 | CLA | C3D-C4D-ND | 2.14 | 113.70 | 110.24 |
| 22 | J | 102 | BCR | C15-C16-C17 | -2.14 | 119.09 | 123.47 |
| 20 | 1 | 205 | CLA | CAA-C2A-C3A | -2.14 | 111.11 | 116.10 |
| 20 | 2 | 315 | CLA | C3B-C4B-CHC | -2.14 | 120.03 | 126.24 |
| 20 | B | 841 | CLA | CAA-CBA-CGA | 2.14 | 119.49 | 113.25 |
| 20 | B | 830 | CLA | C3D-C4D-ND | 2.14 | 113.69 | 110.24 |
| 20 | A | 822 | CLA | O2D-CGD-O1D | -2.13 | 119.66 | 123.84 |
| 20 | A | 808 | CLA | O2A-CGA-CBA | 2.13 | 118.61 | 111.91 |
| 20 | A | 809 | CLA | C2C-C1C-NC | 2.13 | 111.97 | 109.97 |
| 20 | H | 110 | CLA | O2A-CGA-CBA | 2.13 | 118.60 | 111.91 |
| 20 | A | 824 | CLA | C2A-C1A-CHA | -2.13 | 120.13 | 123.86 |
| 22 | J | 102 | BCR | C11-C12-C13 | -2.13 | 120.43 | 126.42 |
| 20 | 3 | 310 | CLA | C11-C10-C8 | -2.13 | 109.03 | 115.92 |
| 20 | B | 850 | CLA | C1D-ND-C4D | -2.13 | 104.82 | 106.33 |
| 20 | 1 | 204 | CLA | CHC-C4B-C3B | -2.13 | 118.24 | 127.71 |
| 20 | R | 107 | CLA | CAA-CBA-CGA | 2.13 | 119.47 | 113.25 |
| 20 | L | 208 | CLA | CHC-C1C-C2C | -2.13 | 120.82 | 126.73 |
| 20 | A | 838 | CLA | CMB-C2B-C1B | 2.13 | 128.61 | 125.37 |
| 21 | K | 107 | LMU | O5'-C5'-C6' | 2.13 | 111.72 | 106.44 |
| 20 | B | 817 | CLA | O2A-CGA-CBA | 2.13 | 120.63 | 112.23 |
| 20 | 2 | 307 | CLA | O1D-CGD-CBD | -2.12 | 120.14 | 124.48 |
| 20 | 3 | 314 | CLA | O2A-CGA-CBA | 2.12 | 118.57 | 111.91 |
| 21 | R | 109 | LMU | O1'-C1'-C2' | 2.12 | 111.62 | 108.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | 2 | 306 | CLA | C3A-C4A-NA | 2.12 | 114.38 | 109.92 |
| 21 | 2 | 319 | LMU | C3B-C4B-C5B | 2.12 | 114.03 | 110.24 |
| 20 | A | 835 | CLA | CHB-C1B-NB | -2.12 | 122.01 | 124.26 |
| 21 | K | 105 | LMU | C4B-C3B-C2B | 2.12 | 114.53 | 110.82 |
| 20 | B | 814 | CLA | CHB-C4A-NA | 2.12 | 127.45 | 124.51 |
| 20 | L | 203 | CLA | CHB-C4A-NA | 2.12 | 127.45 | 124.51 |
| 20 | 4 | 301 | CLA | O2A-CGA-O1A | -2.12 | 118.23 | 123.59 |
| 20 | A | 823 | CLA | C1-C2-C3 | -2.12 | 122.37 | 126.04 |
| 20 | B | 839 | CLA | CHB-C4A-NA | 2.12 | 127.45 | 124.51 |
| 22 | I | 103 | BCR | C7-C6-C5 | 2.12 | 126.60 | 121.46 |
| 20 | 2 | 311 | CLA | CED-O2D-CGD | 2.12 | 120.74 | 115.94 |
| 22 | B | 844 | BCR | C4-C5-C6 | -2.12 | 119.65 | 122.73 |
| 22 | A | 844 | BCR | C1-C6-C7 | 2.12 | 121.78 | 115.78 |
| 20 | L | 204 | CLA | CHB-C4A-NA | 2.12 | 127.44 | 124.51 |
| 20 | A | 839 | CLA | C3D-C4D-ND | 2.12 | 113.67 | 110.24 |
| 20 | A | 819 | CLA | C3A-C2A-C1A | 2.12 | 104.52 | 101.34 |
| 20 | 3 | 303 | CLA | CMB-C2B-C3B | 2.12 | 129.08 | 123.59 |
| 20 | B | 832 | CLA | C1-C2-C3 | -2.12 | 122.38 | 126.04 |
| 21 | C | 101 | LMU | O5B-C5B-C4B | -2.12 | 105.84 | 109.69 |
| 20 | L | 202 | CLA | C2A-C1A-CHA | -2.12 | 120.15 | 123.86 |
| 20 | 1 | 206 | CLA | CMB-C2B-C1B | 2.12 | 128.60 | 125.37 |
| 20 | B | 850 | CLA | C3D-C4D-ND | 2.12 | 113.67 | 110.24 |
| 20 | B | 831 | CLA | CHB-C1B-NB | -2.12 | 122.01 | 124.26 |
| 20 | A | 851 | CLA | C2D-C1D-ND | -2.12 | 108.54 | 110.10 |
| 20 | L | 207 | CLA | CMB-C2B-C1B | 2.12 | 128.59 | 125.37 |
| 20 | 3 | 307 | CLA | CMA-C3A-C4A | -2.12 | 106.08 | 111.77 |
| 20 | 3 | 310 | CLA | C1D-ND-C4D | -2.12 | 104.83 | 106.33 |
| 20 | B | 814 | CLA | C3D-C4D-ND | 2.12 | 113.66 | 110.24 |
| 20 | B | 809 | CLA | CMA-C3A-C2A | -2.12 | 105.29 | 113.83 |
| 20 | B | 809 | CLA | C4-C3-C5 | 2.12 | 118.83 | 115.27 |
| 22 | B | 845 | BCR | C33-C5-C6 | -2.11 | 122.15 | 124.53 |
| 20 | B | 818 | CLA | CHB-C1B-NB | -2.11 | 122.02 | 124.26 |
| 20 | F | 207 | CLA | C1C-C2C-C3C | -2.11 | 104.73 | 106.96 |
| 21 | A | 854 | LMU | C1B-C2B-C3B | 2.11 | 114.40 | 110.00 |
| 21 | R | 101 | LMU | O5B-C1B-C2B | -2.11 | 105.87 | 110.35 |
| 20 | K | 101 | CLA | C3D-C4D-ND | 2.11 | 113.66 | 110.24 |
| 21 | D | 201 | LMU | O5'-C1'-C2' | -2.11 | 105.88 | 110.35 |
| 20 | A | 849 | CLA | CGD-CBD-CAD | 2.11 | 117.57 | 110.73 |
| 20 | A | 837 | CLA | CMB-C2B-C1B | 2.11 | 128.59 | 125.37 |
| 20 | 4 | 315 | CLA | CMB-C2B-C1B | 2.11 | 128.58 | 125.37 |
| 20 | 4 | 305 | CLA | CHB-C4A-NA | 2.11 | 127.43 | 124.51 |
| 21 | A | 854 | LMU | O5B-C5B-C6B | 2.11 | 111.68 | 106.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 808 | CLA | CBC-CAC-C3C | -2.11 | 106.61 | 112.43 |
| 20 | B | 826 | CLA | C2A-C1A-CHA | -2.11 | 120.17 | 123.86 |
| 20 | 1 | 206 | CLA | O1D-CGD-CBD | -2.11 | 120.17 | 124.48 |
| 20 | A | 850 | CLA | CMB-C2B-C1B | 2.11 | 128.58 | 125.37 |
| 20 | G | 105 | CLA | CBA-CAA-C2A | -2.11 | 107.64 | 113.86 |
| 20 | H | 110 | CLA | CHB-C4A-NA | 2.11 | 127.43 | 124.51 |
| 20 | H | 102 | CLA | O2D-CGD-O1D | -2.11 | 119.71 | 123.84 |
| 22 | J | 102 | BCR | C20-C19-C18 | -2.11 | 120.49 | 126.42 |
| 20 | 1 | 212 | CLA | C3A-C4A-NA | 2.11 | 114.34 | 109.92 |
| 20 | 2 | 307 | CLA | O2A-CGA-O1A | -2.11 | 118.28 | 123.59 |
| 20 | A | 809 | CLA | C1-C2-C3 | 2.11 | 129.69 | 126.04 |
| 22 | B | 846 | BCR | C16-C15-C14 | -2.10 | 119.16 | 123.47 |
| 22 | 2 | 317 | BCR | C24-C23-C22 | -2.10 | 123.06 | 126.23 |
| 20 | B | 815 | CLA | O1D-CGD-CBD | -2.10 | 120.18 | 124.48 |
| 20 | 3 | 313 | CLA | O1D-CGD-CBD | -2.10 | 120.18 | 124.48 |
| 21 | A | 847 | LMU | C1B-C2B-C3B | 2.10 | 114.38 | 110.00 |
| 20 | A | 835 | CLA | O2A-CGA-O1A | -2.10 | 118.28 | 123.59 |
| 20 | 3 | 314 | CLA | CAC-C3C-C4C | 2.10 | 127.54 | 124.81 |
| 20 | 3 | 312 | CLA | C3D-C2D-C1D | 2.10 | 109.61 | 107.28 |
| 20 | A | 815 | CLA | C3D-C4D-ND | 2.10 | 113.64 | 110.24 |
| 20 | A | 813 | CLA | CAC-C3C-C4C | 2.10 | 127.54 | 124.81 |
| 21 | 2 | 321 | LMU | C1B-C2B-C3B | 2.10 | 114.37 | 110.00 |
| 20 | B | 809 | CLA | C3D-C4D-ND | 2.10 | 113.63 | 110.24 |
| 20 | B | 823 | CLA | C2A-C1A-CHA | -2.10 | 120.19 | 123.86 |
| 20 | A | 829 | CLA | O2A-CGA-O1A | -2.10 | 118.30 | 123.59 |
| 21 | B | 805 | LMU | O2'-C2'-C3' | -2.10 | 105.50 | 110.35 |
| 20 | 4 | 307 | CLA | C2A-C3A-C4A | -2.10 | 100.89 | 104.18 |
| 20 | A | 839 | CLA | C1D-ND-C4D | -2.10 | 104.85 | 106.33 |
| 20 | 4 | 307 | CLA | CHB-C4A-NA | 2.10 | 127.55 | 124.34 |
| 20 | A | 834 | CLA | C3B-C4B-NB | -2.10 | 108.57 | 110.52 |
| 20 | 3 | 317 | CLA | C2A-C1A-CHA | -2.10 | 120.19 | 123.85 |
| 20 | B | 850 | CLA | CGD-CBD-CAD | 2.09 | 117.52 | 110.73 |
| 22 | B | 847 | BCR | C28-C27-C26 | -2.09 | 110.34 | 114.08 |
| 20 | 4 | 312 | CLA | C2A-C3A-C4A | -2.09 | 100.89 | 104.18 |
| 20 | A | 817 | CLA | CMB-C2B-C1B | 2.09 | 128.56 | 125.37 |
| 20 | 3 | 311 | CLA | C1-C2-C3 | -2.09 | 122.42 | 126.04 |
| 21 | B | 804 | LMU | C4B-C3B-C2B | -2.09 | 107.17 | 110.82 |
| 20 | 2 | 312 | CLA | C2A-C1A-CHA | -2.09 | 120.20 | 123.86 |
| 22 | G | 104 | BCR | C11-C12-C13 | -2.09 | 120.54 | 126.42 |
| 20 | A | 808 | CLA | C2A-C1A-CHA | -2.09 | 120.20 | 123.86 |
| 20 | A | 837 | CLA | C1-O2A-CGA | 2.09 | 121.93 | 116.44 |
| 20 | B | 803 | CLA | O2D-CGD-O1D | -2.09 | 119.75 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | B | 814 | CLA | C16-C15-C13 | -2.09 | 109.17 | 115.92 |
| 20 | 1 | 213 | CLA | O1D-CGD-CBD | -2.09 | 120.21 | 124.48 |
| 20 | A | 838 | CLA | CMC-C2C-C1C | 2.09 | 128.22 | 125.04 |
| 20 | B | 842 | CLA | CMC-C2C-C1C | 2.09 | 128.22 | 125.04 |
| 20 | 4 | 308 | CLA | C3A-C4A-NA | 2.09 | 114.30 | 109.92 |
| 21 | 2 | 319 | LMU | O5'-C1'-C2' | 2.09 | 114.77 | 110.35 |
| 20 | B | 812 | CLA | CAA-CBA-CGA | -2.09 | 107.15 | 113.25 |
| 20 | B | 823 | CLA | C2D-C1D-ND | -2.09 | 108.57 | 110.10 |
| 20 | R | 107 | CLA | CHB-C4A-NA | 2.09 | 127.40 | 124.51 |
| 20 | B | 825 | CLA | CMC-C2C-C1C | 2.09 | 128.22 | 125.04 |
| 21 | H | 103 | LMU | O1'-C1'-C2' | 2.09 | 111.56 | 108.30 |
| 20 | B | 828 | CLA | O2D-CGD-O1D | -2.08 | 119.76 | 123.84 |
| 20 | 1 | 202 | CLA | O2D-CGD-O1D | -2.08 | 119.76 | 123.84 |
| 20 | B | 816 | CLA | C4A-NA-C1A | 2.08 | 107.64 | 106.71 |
| 20 | B | 837 | CLA | CHB-C4A-NA | 2.08 | 127.39 | 124.51 |
| 20 | 2 | 308 | CLA | C3D-C4D-ND | 2.08 | 112.61 | 109.46 |
| 20 | B | 850 | CLA | O2A-CGA-O1A | -2.08 | 118.33 | 123.59 |
| 21 | E | 101 | LMU | O1'-C1'-C2' | -2.08 | 105.05 | 108.30 |
| 20 | 3 | 313 | CLA | CAA-C2A-C1A | 2.08 | 118.80 | 111.97 |
| 20 | B | 827 | CLA | O1D-CGD-CBD | -2.08 | 120.22 | 124.48 |
| 20 | B | 806 | CLA | C4A-NA-C1A | 2.08 | 107.64 | 106.71 |
| 20 | B | 837 | CLA | C4A-NA-C1A | 2.08 | 107.64 | 106.71 |
| 20 | A | 836 | CLA | CAA-CBA-CGA | -2.08 | 107.18 | 113.25 |
| 20 | 1 | 206 | CLA | CBC-CAC-C3C | 2.08 | 118.16 | 112.43 |
| 22 | F | 203 | BCR | C8-C7-C6 | -2.08 | 121.37 | 127.20 |
| 20 | 2 | 305 | CLA | C1D-ND-C4D | -2.08 | 104.86 | 106.33 |
| 20 | 4 | 306 | CLA | CAA-C2A-C3A | 2.08 | 118.46 | 112.78 |
| 20 | J | 103 | CLA | CHD-C1D-ND | 2.08 | 126.36 | 124.45 |
| 20 | A | 828 | CLA | C3B-C2B-C1B | -2.08 | 104.66 | 107.16 |
| 20 | 1 | 201 | CLA | O1D-CGD-CBD | -2.08 | 120.24 | 124.48 |
| 20 | 4 | 303 | CLA | C6-C5-C3 | -2.08 | 108.01 | 113.45 |
| 20 | B | 827 | CLA | C3D-C4D-ND | 2.07 | 113.59 | 110.24 |
| 20 | B | 821 | CLA | O1D-CGD-CBD | -2.07 | 120.24 | 124.48 |
| 20 | 3 | 313 | CLA | C3D-C4D-ND | 2.07 | 113.59 | 110.24 |
| 22 | I | 103 | BCR | C12-C13-C14 | -2.07 | 115.76 | 118.94 |
| 20 | 3 | 315 | CLA | C3B-C4B-CHC | -2.07 | 120.22 | 126.24 |
| 22 | F | 204 | BCR | C28-C27-C26 | -2.07 | 110.38 | 114.08 |
| 20 | A | 827 | CLA | C2D-C1D-ND | -2.07 | 108.58 | 110.10 |
| 20 | R | 108 | CLA | O2D-CGD-O1D | -2.07 | 119.79 | 123.84 |
| 20 | B | 823 | CLA | CMB-C2B-C1B | 2.07 | 128.52 | 125.37 |
| 20 | A | 834 | CLA | CED-O2D-CGD | 2.07 | 120.62 | 115.94 |
| 21 | A | 854 | LMU | C3'-C4'-C5' | 2.07 | 115.67 | 110.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | R | 107 | CLA | C4-C3-C2 | -2.07 | 118.37 | 123.68 |
| 20 | A | 830 | CLA | C3D-C4D-ND | 2.07 | 113.58 | 110.24 |
| 20 | 4 | 305 | CLA | CAC-C3C-C2C | -2.07 | 123.99 | 127.53 |
| 21 | R | 104 | LMU | C1B-O1B-C4' | 2.07 | 123.08 | 117.96 |
| 21 | 4 | 320 | LMU | O2'-C2'-C3' | -2.07 | 105.57 | 110.35 |
| 20 | L | 202 | CLA | C1D-ND-C4D | -2.07 | 104.87 | 106.33 |
| 22 | A | 843 | BCR | C11-C12-C13 | -2.07 | 120.61 | 126.42 |
| 20 | B | 812 | CLA | CHC-C4B-C3B | -2.07 | 121.40 | 127.24 |
| 22 | A | 843 | BCR | C36-C18-C17 | -2.07 | 120.03 | 122.92 |
| 20 | 3 | 317 | CLA | C1D-ND-C4D | -2.07 | 104.87 | 106.33 |
| 20 | A | 815 | CLA | C4A-NA-C1A | 2.06 | 107.63 | 106.71 |
| 20 | A | 809 | CLA | O1D-CGD-CBD | -2.06 | 120.26 | 124.48 |
| 20 | A | 833 | CLA | C1D-ND-C4D | -2.06 | 104.87 | 106.33 |
| 20 | 3 | 310 | CLA | C4-C3-C2 | -2.06 | 118.39 | 123.68 |
| 20 | B | 831 | CLA | C3D-C4D-ND | 2.06 | 113.57 | 110.24 |
| 20 | B | 850 | CLA | C11-C10-C8 | -2.06 | 109.26 | 115.92 |
| 20 | B | 822 | CLA | O2A-CGA-CBA | 2.06 | 120.37 | 112.23 |
| 20 | B | 829 | CLA | O1D-CGD-CBD | -2.06 | 120.27 | 124.48 |
| 22 | F | 204 | BCR | C38-C26-C27 | 2.06 | 117.57 | 113.62 |
| 20 | A | 824 | CLA | C1D-ND-C4D | -2.06 | 104.87 | 106.33 |
| 22 | F | 203 | BCR | C3-C4-C5 | -2.06 | 110.40 | 114.08 |
| 20 | B | 814 | CLA | O1D-CGD-CBD | -2.06 | 120.27 | 124.48 |
| 21 | H | 105 | LMU | O5B-C5B-C6B | 2.06 | 111.55 | 106.44 |
| 21 | B | 805 | LMU | C2'-C3'-C4' | 2.06 | 114.38 | 109.68 |
| 22 | B | 847 | BCR | C33-C5-C6 | -2.06 | 122.22 | 124.53 |
| 20 | B | 838 | CLA | O1D-CGD-CBD | -2.06 | 120.28 | 124.48 |
| 20 | A | 841 | CLA | CHD-C1D-ND | 2.06 | 126.50 | 124.52 |
| 20 | A | 838 | CLA | C4D-CHA-C1A | -2.06 | 118.75 | 121.25 |
| 22 | B | 847 | BCR | C27-C26-C25 | -2.06 | 119.75 | 122.73 |
| 21 | L | 210 | LMU | O1B-C4'-C3' | 2.06 | 112.75 | 107.28 |
| 20 | 2 | 302 | CLA | C1D-ND-C4D | -2.06 | 104.87 | 106.33 |
| 20 | B | 814 | CLA | C11-C10-C8 | -2.06 | 109.27 | 115.92 |
| 20 | 2 | 316 | CLA | CMA-C3A-C4A | -2.06 | 106.25 | 111.77 |
| 20 | 4 | 305 | CLA | C2A-C1A-CHA | -2.06 | 120.26 | 123.86 |
| 22 | B | 847 | BCR | C1-C6-C5 | -2.06 | 119.72 | 122.61 |
| 20 | A | 809 | CLA | C3D-C4D-ND | 2.06 | 113.56 | 110.24 |
| 22 | B | 845 | BCR | C1-C6-C7 | 2.06 | 121.59 | 115.78 |
| 22 | B | 846 | BCR | C27-C26-C25 | -2.06 | 119.75 | 122.73 |
| 20 | 1 | 213 | CLA | CHA-C4D-ND | 2.06 | 136.80 | 132.50 |
| 21 | A | 855 | LMU | C1'-C2'-C3' | 2.06 | 114.28 | 110.00 |
| 20 | 2 | 305 | CLA | CMB-C2B-C1B | 2.05 | 128.50 | 125.37 |
| 20 | B | 819 | CLA | CHD-C1D-ND | 2.05 | 126.34 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A | 817 | CLA | C3D-C4D-ND | 2.05 | 113.56 | 110.24 |
| 20 | B | 840 | CLA | C3D-C4D-ND | 2.05 | 113.56 | 110.24 |
| 22 | L | 209 | BCR | C33-C5-C4 | 2.05 | 117.56 | 113.62 |
| 20 | 3 | 313 | CLA | C4A-NA-C1A | 2.05 | 107.63 | 106.71 |
| 20 | B | 828 | CLA | CMB-C2B-C1B | 2.05 | 128.49 | 125.37 |
| 20 | F | 201 | CLA | CAA-C2A-C3A | -2.05 | 107.17 | 112.78 |
| 20 | 2 | 311 | CLA | O2D-CGD-O1D | -2.05 | 119.83 | 123.84 |
| 20 | 4 | 313 | CLA | CMC-C2C-C1C | 2.05 | 128.16 | 125.04 |
| 20 | A | 809 | CLA | CMA-C3A-C4A | 2.05 | 117.28 | 111.77 |
| 20 | A | 828 | CLA | CED-O2D-CGD | 2.05 | 120.57 | 115.94 |
| 20 | A | 826 | CLA | CMB-C2B-C1B | 2.05 | 128.49 | 125.37 |
| 20 | A | 849 | CLA | O2A-C1-C2 | 2.05 | 114.02 | 108.64 |
| 20 | A | 810 | CLA | CHB-C1B-NB | -2.05 | 122.09 | 124.26 |
| 21 | B | 849 | LMU | O5'-C5'-C4' | 2.05 | 114.07 | 109.75 |
| 20 | 1 | 205 | CLA | CHC-C4B-C3B | -2.05 | 121.46 | 127.24 |
| 20 | A | 808 | CLA | O2A-C1-C2 | 2.05 | 114.01 | 108.64 |
| 20 | A | 803 | CLA | O2A-CGA-CBA | 2.05 | 120.32 | 112.23 |
| 22 | B | 846 | BCR | C20-C19-C18 | -2.05 | 120.67 | 126.42 |
| 21 | L | 205 | LMU | O3'-C3'-C2' | -2.05 | 105.62 | 110.35 |
| 20 | 3 | 310 | CLA | CHC-C4B-C3B | -2.05 | 118.61 | 127.71 |
| 20 | 3 | 310 | CLA | CHC-C1C-C2C | -2.05 | 121.05 | 126.73 |
| 21 | G | 102 | LMU | C4B-C3B-C2B | -2.04 | 107.25 | 110.82 |
| 21 | R | 104 | LMU | O1B-C1B-O5B | -2.04 | 104.96 | 110.67 |
| 20 | A | 809 | CLA | C5-C3-C2 | -2.04 | 116.98 | 121.12 |
| 22 | F | 204 | BCR | C20-C19-C18 | -2.04 | 120.67 | 126.42 |
| 22 | B | 845 | BCR | C3-C4-C5 | -2.04 | 110.43 | 114.08 |
| 20 | H | 109 | CLA | O1D-CGD-CBD | -2.04 | 120.30 | 124.48 |
| 20 | A | 807 | CLA | O2A-CGA-CBA | 2.04 | 120.30 | 112.23 |
| 20 | R | 107 | CLA | C3D-C4D-ND | 2.04 | 113.54 | 110.24 |
| 20 | 4 | 318 | CLA | CAC-C3C-C4C | 2.04 | 127.46 | 124.81 |
| 20 | A | 839 | CLA | CAC-C3C-C4C | 2.04 | 127.46 | 124.81 |
| 20 | B | 834 | CLA | CED-O2D-CGD | 2.04 | 120.55 | 115.94 |
| 21 | K | 106 | LMU | C6B-C5B-C4B | -2.04 | 108.22 | 113.00 |
| 21 | R | 102 | LMU | C6'-C5'-C4' | 2.04 | 119.26 | 113.33 |
| 20 | K | 102 | CLA | C3D-C4D-ND | 2.04 | 113.54 | 110.24 |
| 20 | 4 | 304 | CLA | C4D-CHA-C1A | -2.04 | 118.77 | 121.25 |
| 20 | H | 109 | CLA | C4-C3-C2 | -2.04 | 118.45 | 123.68 |
| 20 | R | 108 | CLA | CHB-C4A-NA | 2.04 | 127.33 | 124.51 |
| 22 | B | 847 | BCR | C8-C7-C6 | -2.04 | 121.48 | 127.20 |
| 21 | R | 104 | LMU | O5'-C5'-C4' | 2.04 | 114.05 | 109.75 |
| 20 | H | 110 | CLA | C2A-C1A-CHA | -2.04 | 120.30 | 123.86 |
| 20 | B | 808 | CLA | C6-C7-C8 | -2.04 | 109.33 | 115.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 20 | B | 832 | CLA | C3A-C2A-C1A | 2.04 | 104.39 | 101.34 |
| 22 | B | 845 | BCR | C8-C7-C6 | -2.04 | 121.48 | 127.20 |
| 20 | 1 | 209 | CLA | C3D-C2D-C1D | 2.04 | 109.53 | 107.28 |
| 20 | 1 | 210 | CLA | C1D-ND-C4D | -2.04 | 104.89 | 106.33 |
| 20 | A | 818 | CLA | C3D-C4D-ND | 2.04 | 113.53 | 110.24 |
| 20 | 1 | 213 | CLA | CED-O2D-CGD | 2.04 | 120.54 | 115.94 |
| 22 | G | 104 | BCR | C20-C19-C18 | -2.04 | 120.70 | 126.42 |
| 20 | B | 821 | CLA | C1-C2-C3 | -2.03 | 123.46 | 126.75 |
| 20 | B | 815 | CLA | C3D-C4D-ND | 2.03 | 113.53 | 110.24 |
| 20 | 2 | 311 | CLA | CMB-C2B-C1B | 2.03 | 128.47 | 125.37 |
| 21 | H | 105 | LMU | O1'-C1-C2 | 2.03 | 116.69 | 109.56 |
| 22 | F | 204 | BCR | C4-C5-C6 | -2.03 | 119.78 | 122.73 |
| 20 | 2 | 308 | CLA | C3A-C4A-NA | 2.03 | 114.19 | 109.92 |
| 22 | A | 845 | BCR | C15-C16-C17 | -2.03 | 119.31 | 123.47 |
| 20 | H | 109 | CLA | O2A-CGA-O1A | -2.03 | 118.46 | 123.59 |
| 20 | 1 | 203 | CLA | O2A-CGA-CBA | 2.03 | 118.29 | 111.91 |
| 20 | L | 203 | CLA | C4-C3-C5 | 2.03 | 118.69 | 115.27 |
| 20 | A | 802 | CLA | C2A-C3A-C4A | -2.03 | 100.99 | 104.18 |
| 20 | 4 | 303 | CLA | CMB-C2B-C1B | 2.03 | 128.46 | 125.37 |
| 20 | B | 838 | CLA | C1D-ND-C4D | -2.03 | 104.89 | 106.33 |
| 20 | 3 | 305 | CLA | C3B-C4B-CHC | -2.03 | 120.34 | 126.24 |
| 20 | J | 101 | CLA | CMB-C2B-C1B | 2.03 | 128.46 | 125.37 |
| 20 | B | 826 | CLA | C4-C3-C5 | 2.03 | 118.69 | 115.27 |
| 20 | A | 813 | CLA | O2A-CGA-CBA | 2.03 | 118.27 | 111.91 |
| 20 | K | 104 | CLA | CHB-C1B-NB | -2.03 | 122.11 | 124.26 |
| 20 | B | 836 | CLA | C4-C3-C2 | -2.03 | 118.48 | 123.68 |
| 21 | R | 106 | LMU | O2'-C2'-C3' | -2.03 | 105.66 | 110.35 |
| 20 | 4 | 302 | CLA | C2A-C1A-CHA | -2.03 | 120.32 | 123.85 |
| 21 | 4 | 316 | LMU | O5'-C5'-C6' | 2.03 | 111.47 | 106.44 |
| 23 | A | 842 | PQN | C12-C11-C3 | -2.03 | 106.58 | 112.05 |
| 21 | 4 | 320 | LMU | C1B-C2B-C3B | 2.02 | 114.21 | 110.00 |
| 20 | 2 | 311 | CLA | CHC-C4B-C3B | -2.02 | 118.71 | 127.71 |
| 20 | B | 811 | CLA | CHB-C4A-NA | 2.02 | 127.44 | 124.34 |
| 20 | B | 823 | CLA | C5-C3-C2 | -2.02 | 117.02 | 121.12 |
| 20 | H | 108 | CLA | CBA-CAA-C2A | -2.02 | 107.89 | 113.86 |
| 20 | 4 | 311 | CLA | C3B-C4B-CHC | -2.02 | 120.37 | 126.24 |
| 20 | 3 | 304 | CLA | C2A-C3A-C4A | -2.02 | 101.01 | 104.18 |
| 20 | 2 | 305 | CLA | O2D-CGD-O1D | -2.02 | 119.89 | 123.84 |
| 20 | B | 816 | CLA | CAC-C3C-C4C | 2.02 | 127.43 | 124.81 |
| 20 | K | 103 | CLA | C4D-CHA-C1A | -2.02 | 118.79 | 121.25 |
| 20 | A | 835 | CLA | C3A-C2A-C1A | 2.02 | 104.36 | 101.34 |
| 20 | 1 | 206 | CLA | O2A-CGA-O1A | -2.02 | 118.50 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | H | 109 | CLA | C2D-C1D-ND | -2.02 | 108.62 | 110.10 |
| 20 | 4 | 303 | CLA | CHA-C1A-NA | -2.02 | 121.77 | 126.40 |
| 20 | 1 | 206 | CLA | C3D-C4D-ND | 2.02 | 113.50 | 110.24 |
| 20 | L | 202 | CLA | C3D-C4D-ND | 2.02 | 113.50 | 110.24 |
| 22 | L | 209 | BCR | C19-C18-C17 | -2.02 | 115.84 | 118.94 |
| 20 | 3 | 303 | CLA | C3D-C4D-ND | 2.02 | 113.50 | 110.24 |
| 20 | A | 849 | CLA | CMA-C3A-C2A | -2.02 | 105.69 | 113.83 |
| 20 | 4 | 302 | CLA | CHC-C4B-C3B | -2.02 | 121.54 | 127.24 |
| 20 | B | 821 | CLA | O2A-CGA-O1A | -2.02 | 118.51 | 123.59 |
| 21 | H | 106 | LMU | C4B-C3B-C2B | -2.02 | 107.31 | 110.82 |
| 20 | 2 | 316 | CLA | CAC-C3C-C4C | 2.01 | 127.42 | 124.81 |
| 20 | A | 824 | CLA | C3D-C4D-ND | 2.01 | 113.50 | 110.24 |
| 20 | B | 823 | CLA | C3D-C4D-ND | 2.01 | 113.50 | 110.24 |
| 20 | A | 807 | CLA | CHB-C4A-NA | 2.01 | 127.30 | 124.51 |
| 20 | B | 850 | CLA | C16-C17-C18 | -2.01 | 106.49 | 115.98 |
| 20 | B | 830 | CLA | C7-C6-C5 | -2.01 | 107.89 | 113.36 |
| 22 | G | 104 | BCR | C3-C4-C5 | -2.01 | 110.48 | 114.08 |
| 22 | I | 103 | BCR | C37-C22-C21 | -2.01 | 120.10 | 122.92 |
| 20 | 3 | 306 | CLA | C3A-C4A-NA | 2.01 | 114.14 | 109.92 |
| 20 | 4 | 314 | CLA | C3D-C4D-ND | 2.01 | 112.50 | 109.46 |
| 20 | B | 811 | CLA | C3D-C2D-C1D | 2.01 | 109.51 | 107.28 |
| 20 | A | 822 | CLA | O2A-CGA-CBA | 2.01 | 118.22 | 111.91 |
| 20 | A | 831 | CLA | O1D-CGD-CBD | -2.01 | 120.37 | 124.48 |
| 20 | A | 810 | CLA | CHB-C4A-NA | 2.01 | 127.29 | 124.51 |
| 20 | B | 821 | CLA | O2D-CGD-O1D | -2.01 | 119.91 | 123.84 |
| 20 | L | 207 | CLA | CAC-C3C-C4C | 2.01 | 127.42 | 124.81 |
| 20 | B | 820 | CLA | CHB-C4A-NA | 2.01 | 127.29 | 124.51 |
| 20 | 4 | 306 | CLA | C1D-ND-C4D | -2.01 | 104.91 | 106.33 |
| 20 | B | 838 | CLA | C2A-C1A-CHA | -2.01 | 120.35 | 123.86 |
| 20 | 3 | 317 | CLA | C3D-C4D-ND | 2.01 | 113.49 | 110.24 |
| 20 | 4 | 305 | CLA | CBC-CAC-C3C | -2.01 | 106.90 | 112.43 |
| 20 | B | 830 | CLA | C1-O2A-CGA | 2.01 | 121.71 | 116.44 |
| 20 | 1 | 208 | CLA | C3A-C4A-NA | 2.01 | 114.13 | 109.92 |
| 23 | B | 843 | PQN | C14-C13-C12 | -2.01 | 118.53 | 123.68 |
| 22 | B | 847 | BCR | C38-C26-C25 | -2.01 | 122.28 | 124.53 |
| 20 | A | 823 | CLA | CAC-C3C-C4C | 2.01 | 127.41 | 124.81 |
| 20 | H | 101 | CLA | O2D-CGD-O1D | -2.00 | 119.92 | 123.84 |
| 20 | A | 822 | CLA | C5-C3-C4 | 2.00 | 119.03 | 114.60 |
| 20 | A | 816 | CLA | C1D-ND-C4D | -2.00 | 104.91 | 106.33 |
| 20 | B | 812 | CLA | CGD-CBD-CAD | -2.00 | 104.24 | 110.73 |
| 20 | 3 | 311 | CLA | CED-O2D-CGD | 2.00 | 120.47 | 115.94 |
| 20 | L | 203 | CLA | CED-O2D-CGD | 2.00 | 120.47 | 115.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | L | 207 | CLA | CED-O2D-CGD | 2.00 | 120.47 | 115.94 |
| 20 | L | 207 | CLA | O2A-CGA-O1A | -2.00 | 118.54 | 123.59 |
| 20 | L | 203 | CLA | C2A-C1A-CHA | -2.00 | 120.36 | 123.86 |
| 20 | A | 824 | CLA | O2A-CGA-O1A | -2.00 | 118.54 | 123.59 |
| 20 | 1 | 201 | CLA | CBC-CAC-C3C | -2.00 | 106.91 | 112.43 |
| 20 | F | 205 | CLA | CHB-C1B-C2B | -2.00 | 121.59 | 127.24 |
| 22 | B | 845 | BCR | C2-C1-C6 | 2.00 | 113.56 | 110.48 |
| 20 | B | 817 | CLA | CAA-C2A-C1A | 2.00 | 118.53 | 111.97 |
| 20 | H | 110 | CLA | C3D-C4D-ND | 2.00 | 113.47 | 110.24 |
| 20 | A | 824 | CLA | CAC-C3C-C2C | -2.00 | 124.11 | 127.53 |

All (85) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 20 | 1 | 206 | CLA | C8 |
| 20 | 1 | 207 | CLA | C2A |
| 20 | 1 | 211 | CLA | CBD |
| 20 | 1 | 213 | CLA | C2A |
| 20 | 1 | 213 | CLA | C3A |
| 20 | 1 | 215 | CLA | CBD |
| 20 | 2 | 303 | CLA | C8 |
| 20 | 2 | 307 | CLA | C8 |
| 20 | 2 | 312 | CLA | C8 |
| 20 | 2 | 316 | CLA | C8 |
| 20 | 3 | 310 | CLA | C8 |
| 20 | 3 | 311 | CLA | C8 |
| 20 | 3 | 314 | CLA | C8 |
| 20 | 4 | 301 | CLA | C8 |
| 20 | 4 | 303 | CLA | CBD |
| 20 | 4 | 303 | CLA | C8 |
| 20 | 4 | 304 | CLA | C8 |
| 20 | 4 | 306 | CLA | C2A |
| 20 | A | 801 | CLA | C2A |
| 20 | A | 801 | CLA | CBD |
| 20 | A | 804 | CLA | C8 |
| 20 | A | 806 | CLA | C8 |
| 20 | A | 808 | CLA | C8 |
| 20 | A | 811 | CLA | C8 |
| 20 | A | 818 | CLA | C8 |
| 20 | A | 819 | CLA | C8 |
| 20 | A | 823 | CLA | C8 |
| 20 | A | 824 | CLA | C8 |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 20 | A | 825 | CLA | C8 |
| 20 | A | 826 | CLA | C8 |
| 20 | A | 827 | CLA | C8 |
| 20 | A | 828 | CLA | C8 |
| 20 | A | 830 | CLA | C8 |
| 20 | A | 831 | CLA | C8 |
| 20 | A | 835 | CLA | C8 |
| 20 | A | 838 | CLA | C8 |
| 20 | A | 839 | CLA | C2A |
| 20 | A | 840 | CLA | C8 |
| 20 | A | 849 | CLA | C8 |
| 20 | A | 850 | CLA | C8 |
| 20 | A | 851 | CLA | C8 |
| 20 | B | 803 | CLA | C8 |
| 20 | B | 806 | CLA | C8 |
| 20 | B | 808 | CLA | C8 |
| 20 | B | 809 | CLA | C8 |
| 20 | B | 810 | CLA | C8 |
| 20 | B | 812 | CLA | C8 |
| 20 | B | 813 | CLA | C8 |
| 20 | B | 814 | CLA | C8 |
| 20 | B | 815 | CLA | C8 |
| 20 | B | 816 | CLA | C8 |
| 20 | B | 820 | CLA | C8 |
| 20 | B | 823 | CLA | C8 |
| 20 | B | 824 | CLA | C8 |
| 20 | B | 826 | CLA | C8 |
| 20 | B | 827 | CLA | C8 |
| 20 | B | 828 | CLA | C8 |
| 20 | B | 829 | CLA | C8 |
| 20 | B | 830 | CLA | C8 |
| 20 | B | 832 | CLA | C8 |
| 20 | B | 837 | CLA | C8 |
| 20 | B | 838 | CLA | C8 |
| 20 | B | 840 | CLA | C8 |
| 20 | B | 841 | CLA | C8 |
| 20 | B | 850 | CLA | C8 |
| 20 | F | 207 | CLA | C2A |
| 20 | F | 207 | CLA | C3A |
| 20 | F | 207 | CLA | CBD |
| 20 | H | 101 | CLA | CBD |
| 20 | H | 101 | CLA | C8 |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 20 | H | 102 | CLA | C8 |
| 20 | H | 108 | CLA | C8 |
| 20 | H | 109 | CLA | C8 |
| 20 | I | 102 | CLA | C8 |
| 20 | J | 103 | CLA | C8 |
| 20 | K | 104 | CLA | C8 |
| 20 | L | 201 | CLA | C8 |
| 20 | L | 202 | CLA | C8 |
| 20 | L | 203 | CLA | C8 |
| 20 | L | 204 | CLA | C8 |
| 20 | L | 208 | CLA | CBD |
| 20 | R | 107 | CLA | C8 |
| 20 | R | 108 | CLA | C8 |
| 23 | A | 842 | PQN | C23 |
| 23 | B | 843 | PQN | C23 |

All (2678) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 1 | 201 | CLA | C1A-C2A-CAA-CBA |
| 20 | 1 | 201 | CLA | C3A-C2A-CAA-CBA |
| 20 | 1 | 201 | CLA | CBA-CGA-O2A-C1 |
| 20 | 1 | 201 | CLA | CHA-CBD-CGD-O1D |
| 20 | 1 | 201 | CLA | CHA-CBD-CGD-O2D |
| 20 | 1 | 202 | CLA | C4B-C3B-CAB-CBB |
| 20 | 1 | 202 | CLA | CBD-CGD-O2D-CED |
| 20 | 1 | 203 | CLA | C2B-C3B-CAB-CBB |
| 20 | 1 | 203 | CLA | CBD-CGD-O2D-CED |
| 20 | 1 | 204 | CLA | C1A-C2A-CAA-CBA |
| 20 | 1 | 204 | CLA | CBA-CGA-O2A-C1 |
| 20 | 1 | 204 | CLA | O1A-CGA-O2A-C1 |
| 20 | 1 | 204 | CLA | CHA-CBD-CGD-O1D |
| 20 | 1 | 204 | CLA | CBD-CGD-O2D-CED |
| 20 | 1 | 206 | CLA | C4B-C3B-CAB-CBB |
| 20 | 1 | 206 | CLA | C2C-C3C-CAC-CBC |
| 20 | 1 | 206 | CLA | C4C-C3C-CAC-CBC |
| 20 | 1 | 206 | CLA | CHA-CBD-CGD-O1D |
| 20 | 1 | 206 | CLA | CHA-CBD-CGD-O2D |
| 20 | 1 | 207 | CLA | C2B-C3B-CAB-CBB |
| 20 | 1 | 207 | CLA | CBD-CGD-O2D-CED |
| 20 | 1 | 207 | CLA | C2-C3-C5-C6 |
| 20 | 1 | 207 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 1 | 211 | CLA | C2B-C3B-CAB-CBB |
| 20 | 1 | 211 | CLA | CBD-CGD-O2D-CED |
| 20 | 1 | 213 | CLA | C3A-C2A-CAA-CBA |
| 20 | 1 | 213 | CLA | C4B-C3B-CAB-CBB |
| 20 | 1 | 213 | CLA | C2-C3-C5-C6 |
| 20 | 1 | 213 | CLA | C4-C3-C5-C6 |
| 20 | 1 | 215 | CLA | C2B-C3B-CAB-CBB |
| 20 | 1 | 215 | CLA | CAD-CBD-CGD-O1D |
| 20 | 1 | 215 | CLA | CAD-CBD-CGD-O2D |
| 20 | 1 | 215 | CLA | C2-C3-C5-C6 |
| 20 | 1 | 215 | CLA | C4-C3-C5-C6 |
| 20 | 2 | 302 | CLA | C1A-C2A-CAA-CBA |
| 20 | 2 | 302 | CLA | C3A-C2A-CAA-CBA |
| 20 | 2 | 302 | CLA | C4B-C3B-CAB-CBB |
| 20 | 2 | 302 | CLA | O2A-C1-C2-C3 |
| 20 | 2 | 302 | CLA | C2-C3-C5-C6 |
| 20 | 2 | 302 | CLA | C4-C3-C5-C6 |
| 20 | 2 | 303 | CLA | C1A-C2A-CAA-CBA |
| 20 | 2 | 303 | CLA | C3A-C2A-CAA-CBA |
| 20 | 2 | 303 | CLA | C2-C1-O2A-CGA |
| 20 | 2 | 303 | CLA | C4B-C3B-CAB-CBB |
| 20 | 2 | 303 | CLA | CAD-CBD-CGD-O1D |
| 20 | 2 | 303 | CLA | CAD-CBD-CGD-O2D |
| 20 | 2 | 305 | CLA | C2-C1-O2A-CGA |
| 20 | 2 | 307 | CLA | CBA-CGA-O2A-C1 |
| 20 | 2 | 307 | CLA | O1A-CGA-O2A-C1 |
| 20 | 2 | 307 | CLA | C6-C7-C8-C9 |
| 20 | 2 | 310 | CLA | C4B-C3B-CAB-CBB |
| 20 | 2 | 311 | CLA | CBA-CGA-O2A-C1 |
| 20 | 2 | 311 | CLA | O1A-CGA-O2A-C1 |
| 20 | 2 | 312 | CLA | C4B-C3B-CAB-CBB |
| 20 | 2 | 312 | CLA | CAD-CBD-CGD-O1D |
| 20 | 2 | 312 | CLA | CBD-CGD-O2D-CED |
| 20 | 2 | 314 | CLA | C2B-C3B-CAB-CBB |
| 20 | 2 | 314 | CLA | CBD-CGD-O2D-CED |
| 20 | 2 | 314 | CLA | O1D-CGD-O2D-CED |
| 20 | 2 | 316 | CLA | C4B-C3B-CAB-CBB |
| 20 | 3 | 307 | CLA | C1A-C2A-CAA-CBA |
| 20 | 3 | 307 | CLA | C3A-C2A-CAA-CBA |
| 20 | 3 | 307 | CLA | CBD-CGD-O2D-CED |
| 20 | 3 | 310 | CLA | C1A-C2A-CAA-CBA |
| 20 | 3 | 310 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 3 | 310 | CLA | CAD-CBD-CGD-O1D |
| 20 | 3 | 314 | CLA | CBA-CGA-O2A-C1 |
| 20 | 3 | 314 | CLA | O1A-CGA-O2A-C1 |
| 20 | 3 | 314 | CLA | C2B-C3B-CAB-CBB |
| 20 | 4 | 303 | CLA | C3A-C2A-CAA-CBA |
| 20 | 4 | 303 | CLA | CHA-CBD-CGD-O1D |
| 20 | 4 | 303 | CLA | CHA-CBD-CGD-O2D |
| 20 | 4 | 303 | CLA | C6-C7-C8-C9 |
| 20 | 4 | 304 | CLA | C4B-C3B-CAB-CBB |
| 20 | 4 | 306 | CLA | C2-C1-O2A-CGA |
| 20 | 4 | 306 | CLA | C2B-C3B-CAB-CBB |
| 20 | 4 | 310 | CLA | C1A-C2A-CAA-CBA |
| 20 | 4 | 310 | CLA | C2B-C3B-CAB-CBB |
| 20 | 4 | 310 | CLA | CBD-CGD-O2D-CED |
| 20 | 4 | 315 | CLA | C1A-C2A-CAA-CBA |
| 20 | 4 | 315 | CLA | C4B-C3B-CAB-CBB |
| 20 | 4 | 317 | CLA | C4B-C3B-CAB-CBB |
| 20 | 4 | 318 | CLA | C2B-C3B-CAB-CBB |
| 20 | 4 | 318 | CLA | CHA-CBD-CGD-O2D |
| 20 | 4 | 318 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 801 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 801 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 801 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 801 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 804 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 804 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 804 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 804 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 805 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 805 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 805 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 805 | CLA | C2-C3-C5-C6 |
| 20 | A | 805 | CLA | C4-C3-C5-C6 |
| 20 | A | 806 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 806 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 806 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 807 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 807 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 807 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 808 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 808 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 809 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | A | 809 | CLA | O2A-C1-C2-C3 |
| 20 | A | 811 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 812 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 813 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 813 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 813 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 813 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 815 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 815 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 815 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 815 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 815 | CLA | CHA-CBD-CGD-O2D |
| 20 | A | 815 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 816 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 816 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 816 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 816 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 817 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 817 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 817 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 817 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 817 | CLA | CHA-CBD-CGD-O2D |
| 20 | A | 818 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 818 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 818 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 818 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 818 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 818 | CLA | O2A-C1-C2-C3 |
| 20 | A | 820 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 820 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 820 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 821 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 821 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 821 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 822 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 822 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 823 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 824 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 824 | CLA | C4C-C3C-CAC-CBC |
| 20 | A | 824 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 824 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 825 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | A | 825 | CLA | O2A-C1-C2-C3 |
| 20 | A | 828 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 828 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 828 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 828 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 828 | CLA | CHA-CBD-CGD-O2D |
| 20 | A | 829 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 830 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 830 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 831 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 831 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 832 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 832 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 832 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 833 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 833 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 833 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 833 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 834 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 834 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 834 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 835 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 835 | CLA | CHA-CBD-CGD-O2D |
| 20 | A | 835 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 836 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 837 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 837 | CLA | O2A-C1-C2-C3 |
| 20 | A | 837 | CLA | C2-C3-C5-C6 |
| 20 | A | 837 | CLA | C4-C3-C5-C6 |
| 20 | A | 838 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 838 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 838 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 839 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 839 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 839 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 839 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 839 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 839 | CLA | C4C-C3C-CAC-CBC |
| 20 | A | 839 | CLA | C2-C3-C5-C6 |
| 20 | A | 839 | CLA | C4-C3-C5-C6 |
| 20 | A | 840 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 840 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | A | 849 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 849 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 850 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 850 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 850 | CLA | C6-C7-C8-C9 |
| 20 | A | 851 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 851 | CLA | CHA-CBD-CGD-O2D |
| 20 | A | 851 | CLA | O2A-C1-C2-C3 |
| 20 | B | 802 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 802 | CLA | C2-C3-C5-C6 |
| 20 | B | 802 | CLA | C4-C3-C5-C6 |
| 20 | B | 803 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 806 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 807 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 807 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 808 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 808 | CLA | C2-C1-O2A-CGA |
| 20 | B | 808 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 808 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 809 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 809 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 810 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 810 | CLA | C11-C10-C8-C9 |
| 20 | B | 812 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 812 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 812 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 814 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 814 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 814 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 814 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 814 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 815 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 815 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 815 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 816 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 816 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 816 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 816 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 816 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 817 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 817 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 817 | CLA | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 817 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 817 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 818 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 818 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 818 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 820 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 820 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 820 | CLA | C2-C3-C5-C6 |
| 20 | B | 820 | CLA | C4-C3-C5-C6 |
| 20 | B | 821 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 821 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 822 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 822 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 823 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 823 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 823 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 824 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 824 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 824 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 824 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 824 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 826 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 826 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 826 | CLA | C4C-C3C-CAC-CBC |
| 20 | B | 826 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 826 | CLA | C2-C3-C5-C6 |
| 20 | B | 826 | CLA | C4-C3-C5-C6 |
| 20 | B | 826 | CLA | C11-C10-C8-C9 |
| 20 | B | 827 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 827 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 827 | CLA | C11-C12-C13-C14 |
| 20 | B | 828 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 828 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 829 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 829 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 829 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 830 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 830 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 830 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 830 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 831 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 831 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 831 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 831 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 831 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 832 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 833 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 833 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 834 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 834 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 834 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 834 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 834 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 835 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 835 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 836 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 836 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 836 | CLA | C4C-C3C-CAC-CBC |
| 20 | B | 836 | CLA | C2-C3-C5-C6 |
| 20 | B | 836 | CLA | C4-C3-C5-C6 |
| 20 | B | 837 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 839 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 839 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 839 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 840 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 840 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 841 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 850 | CLA | C4B-C3B-CAB-CBB |
| 20 | F | 201 | CLA | C2C-C3C-CAC-CBC |
| 20 | F | 201 | CLA | C4C-C3C-CAC-CBC |
| 20 | F | 201 | CLA | O2A-C1-C2-C3 |
| 20 | F | 206 | CLA | CBD-CGD-O2D-CED |
| 20 | F | 207 | CLA | C1A-C2A-CAA-CBA |
| 20 | F | 207 | CLA | C4B-C3B-CAB-CBB |
| 20 | F | 207 | CLA | CBD-CGD-O2D-CED |
| 20 | F | 207 | CLA | O1D-CGD-O2D-CED |
| 20 | G | 105 | CLA | C2B-C3B-CAB-CBB |
| 20 | G | 105 | CLA | CAD-CBD-CGD-O1D |
| 20 | G | 105 | CLA | CAD-CBD-CGD-O2D |
| 20 | G | 105 | CLA | CBD-CGD-O2D-CED |
| 20 | H | 101 | CLA | C1A-C2A-CAA-CBA |
| 20 | H | 101 | CLA | C3A-C2A-CAA-CBA |
| 20 | H | 101 | CLA | CBD-CGD-O2D-CED |
| 20 | H | 102 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | H | 102 | CLA | C2B-C3B-CAB-CBB |
| 20 | H | 102 | CLA | C2-C3-C5-C6 |
| 20 | H | 102 | CLA | C4-C3-C5-C6 |
| 20 | H | 108 | CLA | C2B-C3B-CAB-CBB |
| 20 | H | 108 | CLA | CHA-CBD-CGD-O1D |
| 20 | H | 108 | CLA | CHA-CBD-CGD-O2D |
| 20 | H | 109 | CLA | CAD-CBD-CGD-O1D |
| 20 | H | 109 | CLA | CAD-CBD-CGD-O2D |
| 20 | H | 109 | CLA | CBD-CGD-O2D-CED |
| 20 | H | 110 | CLA | C1A-C2A-CAA-CBA |
| 20 | H | 110 | CLA | C3A-C2A-CAA-CBA |
| 20 | H | 110 | CLA | C2B-C3B-CAB-CBB |
| 20 | H | 110 | CLA | CBD-CGD-O2D-CED |
| 20 | I | 102 | CLA | C4B-C3B-CAB-CBB |
| 20 | I | 102 | CLA | CHA-CBD-CGD-O1D |
| 20 | I | 102 | CLA | CHA-CBD-CGD-O2D |
| 20 | J | 101 | CLA | C1A-C2A-CAA-CBA |
| 20 | J | 101 | CLA | CBD-CGD-O2D-CED |
| 20 | J | 103 | CLA | C3A-C2A-CAA-CBA |
| 20 | J | 103 | CLA | C4B-C3B-CAB-CBB |
| 20 | J | 103 | CLA | CBD-CGD-O2D-CED |
| 20 | J | 103 | CLA | O1D-CGD-O2D-CED |
| 20 | K | 101 | CLA | C2B-C3B-CAB-CBB |
| 20 | K | 102 | CLA | C2B-C3B-CAB-CBB |
| 20 | K | 102 | CLA | O2A-C1-C2-C3 |
| 20 | K | 104 | CLA | C1A-C2A-CAA-CBA |
| 20 | L | 201 | CLA | C1A-C2A-CAA-CBA |
| 20 | L | 201 | CLA | C2A-CAA-CBA-CGA |
| 20 | L | 201 | CLA | CHA-CBD-CGD-O1D |
| 20 | L | 201 | CLA | CHA-CBD-CGD-O2D |
| 20 | L | 201 | CLA | CBD-CGD-O2D-CED |
| 20 | L | 201 | CLA | O1D-CGD-O2D-CED |
| 20 | L | 201 | CLA | C2-C3-C5-C6 |
| 20 | L | 201 | CLA | C4-C3-C5-C6 |
| 20 | L | 202 | CLA | C2-C1-O2A-CGA |
| 20 | L | 202 | CLA | CBD-CGD-O2D-CED |
| 20 | L | 203 | CLA | C2B-C3B-CAB-CBB |
| 20 | L | 204 | CLA | C2B-C3B-CAB-CBB |
| 20 | L | 204 | CLA | CBD-CGD-O2D-CED |
| 20 | L | 204 | CLA | C2-C3-C5-C6 |
| 20 | L | 204 | CLA | C4-C3-C5-C6 |
| 20 | L | 207 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | L | 207 | CLA | CBD-CGD-O2D-CED |
| 20 | L | 208 | CLA | C1A-C2A-CAA-CBA |
| 20 | L | 208 | CLA | C2B-C3B-CAB-CBB |
| 20 | L | 208 | CLA | C4C-C3C-CAC-CBC |
| 20 | R | 107 | CLA | C1A-C2A-CAA-CBA |
| 20 | R | 107 | CLA | CHA-CBD-CGD-O1D |
| 20 | R | 107 | CLA | CHA-CBD-CGD-O2D |
| 20 | R | 107 | CLA | CBD-CGD-O2D-CED |
| 20 | R | 107 | CLA | C2-C3-C5-C6 |
| 20 | R | 107 | CLA | C4-C3-C5-C6 |
| 20 | R | 108 | CLA | C1A-C2A-CAA-CBA |
| 20 | R | 108 | CLA | O1A-CGA-O2A-C1 |
| 20 | R | 108 | CLA | O2A-C1-C2-C3 |
| 21 | 1 | 216 | LMU | O5B-C1B-O1B-C4' |
| 21 | 1 | 217 | LMU | C2-C1-O1'-C1' |
| 21 | 2 | 318 | LMU | C2'-C1'-O1'-C1 |
| 21 | 2 | 318 | LMU | O5'-C1'-O1'-C1 |
| 21 | 2 | 319 | LMU | O5'-C1'-O1'-C1 |
| 21 | 2 | 320 | LMU | C2B-C1B-O1B-C4' |
| 21 | 2 | 320 | LMU | C2'-C1'-O1'-C1 |
| 21 | 2 | 320 | LMU | O5'-C1'-O1'-C1 |
| 21 | 2 | 321 | LMU | C2-C1-O1'-C1' |
| 21 | 3 | 318 | LMU | C2'-C1'-O1'-C1 |
| 21 | 3 | 318 | LMU | O5'-C1'-O1'-C1 |
| 21 | 4 | 316 | LMU | C2'-C1'-O1'-C1 |
| 21 | 4 | 316 | LMU | O5'-C1'-O1'-C1 |
| 21 | 4 | 319 | LMU | C2'-C1'-O1'-C1 |
| 21 | 4 | 319 | LMU | O5'-C1'-O1'-C1 |
| 21 | 4 | 319 | LMU | C2-C1-O1'-C1' |
| 21 | 4 | 320 | LMU | C2'-C1'-O1'-C1 |
| 21 | 4 | 320 | LMU | O5'-C1'-O1'-C1 |
| 21 | 4 | 321 | LMU | C2-C1-O1'-C1' |
| 21 | A | 846 | LMU | C2-C1-O1'-C1' |
| 21 | A | 847 | LMU | C2-C1-O1'-C1' |
| 21 | A | 848 | LMU | C2'-C1'-O1'-C1 |
| 21 | A | 848 | LMU | O5'-C1'-O1'-C1 |
| 21 | A | 848 | LMU | C2-C1-O1'-C1' |
| 21 | A | 852 | LMU | C2'-C1'-O1'-C1 |
| 21 | A | 852 | LMU | O5'-C1'-O1'-C1 |
| 21 | A | 852 | LMU | C2-C1-O1'-C1' |
| 21 | A | 854 | LMU | C2'-C1'-O1'-C1 |
| 21 | A | 854 | LMU | O5'-C1'-O1'-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 805 | LMU | C2'-C1'-O1'-C1 |
| 21 | B | 805 | LMU | O5'-C1'-O1'-C1 |
| 21 | C | 101 | LMU | C2'-C1'-O1'-C1 |
| 21 | C | 101 | LMU | O5'-C1'-O1'-C1 |
| 21 | D | 201 | LMU | C2-C1-O1'-C1' |
| 21 | E | 101 | LMU | C2'-C1'-O1'-C1 |
| 21 | E | 101 | LMU | O5'-C1'-O1'-C1 |
| 21 | E | 101 | LMU | C2-C1-O1'-C1' |
| 21 | F | 202 | LMU | C2'-C1'-O1'-C1 |
| 21 | F | 202 | LMU | O5'-C1'-O1'-C1 |
| 21 | H | 103 | LMU | C2'-C1'-O1'-C1 |
| 21 | H | 103 | LMU | O5'-C1'-O1'-C1 |
| 21 | H | 104 | LMU | C2B-C1B-O1B-C4' |
| 21 | H | 104 | LMU | C2-C1-O1'-C1' |
| 21 | H | 105 | LMU | O5'-C1'-O1'-C1 |
| 21 | H | 106 | LMU | O5'-C1'-O1'-C1 |
| 21 | K | 106 | LMU | C2B-C1B-O1B-C4' |
| 21 | K | 106 | LMU | C2'-C1'-O1'-C1 |
| 21 | K | 106 | LMU | O5'-C1'-O1'-C1 |
| 21 | K | 107 | LMU | C3'-C4'-O1B-C1B |
| 21 | K | 107 | LMU | O5'-C1'-O1'-C1 |
| 21 | L | 205 | LMU | C2-C1-O1'-C1' |
| 21 | L | 206 | LMU | C2-C1-O1'-C1' |
| 21 | L | 210 | LMU | C2'-C1'-O1'-C1 |
| 21 | L | 210 | LMU | O5'-C1'-O1'-C1 |
| 21 | L | 210 | LMU | C2-C1-O1'-C1' |
| 21 | R | 101 | LMU | C2'-C1'-O1'-C1 |
| 21 | R | 101 | LMU | O5'-C1'-O1'-C1 |
| 21 | R | 102 | LMU | C2-C1-O1'-C1' |
| 21 | R | 104 | LMU | O5'-C1'-O1'-C1 |
| 21 | R | 104 | LMU | C2-C1-O1'-C1' |
| 21 | R | 105 | LMU | C2'-C1'-O1'-C1 |
| 21 | R | 106 | LMU | C2'-C1'-O1'-C1 |
| 21 | R | 106 | LMU | O5'-C1'-O1'-C1 |
| 21 | R | 106 | LMU | C2-C1-O1'-C1' |
| 21 | R | 109 | LMU | O5B-C1B-O1B-C4' |
| 21 | R | 109 | LMU | C2'-C1'-O1'-C1 |
| 21 | R | 109 | LMU | O5'-C1'-O1'-C1 |
| 21 | R | 109 | LMU | C2-C1-O1'-C1' |
| 22 | 2 | 317 | BCR | C36-C18-C19-C20 |
| 22 | 2 | 317 | BCR | C18-C19-C20-C21 |
| 22 | 2 | 317 | BCR | C20-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | 2 | 317 | BCR | C20-C21-C22-C37 |
| 22 | A | 843 | BCR | C7-C8-C9-C10 |
| 22 | A | 843 | BCR | C7-C8-C9-C34 |
| 22 | A | 843 | BCR | C18-C19-C20-C21 |
| 22 | A | 843 | BCR | C20-C21-C22-C23 |
| 22 | A | 843 | BCR | C20-C21-C22-C37 |
| 22 | A | 843 | BCR | C21-C22-C23-C24 |
| 22 | A | 843 | BCR | C37-C22-C23-C24 |
| 22 | A | 844 | BCR | C11-C12-C13-C14 |
| 22 | A | 844 | BCR | C11-C12-C13-C35 |
| 22 | A | 844 | BCR | C17-C18-C19-C20 |
| 22 | A | 844 | BCR | C36-C18-C19-C20 |
| 22 | A | 844 | BCR | C21-C22-C23-C24 |
| 22 | A | 844 | BCR | C37-C22-C23-C24 |
| 22 | A | 845 | BCR | C7-C8-C9-C34 |
| 22 | A | 845 | BCR | C18-C19-C20-C21 |
| 22 | A | 845 | BCR | C23-C24-C25-C26 |
| 22 | B | 801 | BCR | C11-C12-C13-C14 |
| 22 | B | 801 | BCR | C11-C12-C13-C35 |
| 22 | B | 801 | BCR | C13-C14-C15-C16 |
| 22 | B | 801 | BCR | C15-C16-C17-C18 |
| 22 | B | 801 | BCR | C18-C19-C20-C21 |
| 22 | B | 801 | BCR | C20-C21-C22-C23 |
| 22 | B | 801 | BCR | C20-C21-C22-C37 |
| 22 | B | 801 | BCR | C21-C22-C23-C24 |
| 22 | B | 801 | BCR | C37-C22-C23-C24 |
| 22 | B | 845 | BCR | C19-C20-C21-C22 |
| 22 | B | 845 | BCR | C20-C21-C22-C23 |
| 22 | B | 845 | BCR | C20-C21-C22-C37 |
| 22 | B | 845 | BCR | C21-C22-C23-C24 |
| 22 | B | 845 | BCR | C37-C22-C23-C24 |
| 22 | B | 845 | BCR | C23-C24-C25-C26 |
| 22 | B | 845 | BCR | C23-C24-C25-C30 |
| 22 | B | 846 | BCR | C11-C12-C13-C14 |
| 22 | B | 846 | BCR | C11-C12-C13-C35 |
| 22 | B | 846 | BCR | C17-C18-C19-C20 |
| 22 | B | 846 | BCR | C36-C18-C19-C20 |
| 22 | B | 846 | BCR | C18-C19-C20-C21 |
| 22 | B | 846 | BCR | C20-C21-C22-C23 |
| 22 | B | 846 | BCR | C20-C21-C22-C37 |
| 22 | B | 846 | BCR | C37-C22-C23-C24 |
| 22 | B | 847 | BCR | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | B | 847 | BCR | C7-C8-C9-C34 |
| 22 | B | 847 | BCR | C18-C19-C20-C21 |
| 22 | B | 847 | BCR | C20-C21-C22-C23 |
| 22 | B | 847 | BCR | C20-C21-C22-C37 |
| 22 | B | 847 | BCR | C21-C22-C23-C24 |
| 22 | B | 847 | BCR | C37-C22-C23-C24 |
| 22 | F | 204 | BCR | C7-C8-C9-C10 |
| 22 | F | 204 | BCR | C7-C8-C9-C34 |
| 22 | F | 204 | BCR | C9-C10-C11-C12 |
| 22 | F | 204 | BCR | C18-C19-C20-C21 |
| 22 | G | 104 | BCR | C7-C8-C9-C10 |
| 22 | G | 104 | BCR | C7-C8-C9-C34 |
| 22 | G | 104 | BCR | C17-C18-C19-C20 |
| 22 | G | 104 | BCR | C36-C18-C19-C20 |
| 22 | G | 104 | BCR | C18-C19-C20-C21 |
| 22 | G | 104 | BCR | C20-C21-C22-C23 |
| 22 | G | 104 | BCR | C20-C21-C22-C37 |
| 22 | I | 101 | BCR | C5-C6-C7-C8 |
| 22 | I | 101 | BCR | C9-C10-C11-C12 |
| 22 | I | 101 | BCR | C21-C22-C23-C24 |
| 22 | I | 101 | BCR | C37-C22-C23-C24 |
| 22 | I | 103 | BCR | C9-C10-C11-C12 |
| 22 | I | 103 | BCR | C11-C12-C13-C14 |
| 22 | I | 103 | BCR | C11-C12-C13-C35 |
| 22 | I | 103 | BCR | C17-C18-C19-C20 |
| 22 | I | 103 | BCR | C36-C18-C19-C20 |
| 22 | I | 103 | BCR | C18-C19-C20-C21 |
| 22 | I | 103 | BCR | C20-C21-C22-C23 |
| 22 | I | 103 | BCR | C20-C21-C22-C37 |
| 22 | J | 102 | BCR | C7-C8-C9-C10 |
| 22 | J | 102 | BCR | C7-C8-C9-C34 |
| 22 | J | 102 | BCR | C17-C18-C19-C20 |
| 22 | J | 102 | BCR | C36-C18-C19-C20 |
| 22 | J | 102 | BCR | C18-C19-C20-C21 |
| 22 | L | 209 | BCR | C1-C6-C7-C8 |
| 22 | L | 209 | BCR | C7-C8-C9-C10 |
| 22 | L | 209 | BCR | C7-C8-C9-C34 |
| 22 | L | 209 | BCR | C20-C21-C22-C23 |
| 22 | L | 209 | BCR | C20-C21-C22-C37 |
| 22 | L | 209 | BCR | C21-C22-C23-C24 |
| 22 | L | 209 | BCR | C37-C22-C23-C24 |
| 23 | A | 842 | PQN | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | B | 843 | PQN | C14-C13-C15-C16 |
| 25 | B | 848 | LMG | O6-C1-O1-C7 |
| 25 | B | 848 | LMG | C11-C10-O7-C8 |
| 20 | 2 | 311 | CLA | C4C-C3C-CAC-CBC |
| 20 | 3 | 311 | CLA | C4C-C3C-CAC-CBC |
| 20 | 4 | 301 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 824 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 826 | CLA | C2C-C3C-CAC-CBC |
| 20 | L | 208 | CLA | C2C-C3C-CAC-CBC |
| 21 | 2 | 313 | LMU | C5'-C4'-O1B-C1B |
| 21 | H | 106 | LMU | C3'-C4'-O1B-C1B |
| 20 | 1 | 204 | CLA | O1D-CGD-O2D-CED |
| 20 | 1 | 206 | CLA | O1D-CGD-O2D-CED |
| 20 | 1 | 207 | CLA | O1D-CGD-O2D-CED |
| 20 | 1 | 213 | CLA | O1D-CGD-O2D-CED |
| 20 | 4 | 315 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 806 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 815 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 816 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 817 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 823 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 837 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 812 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 816 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 818 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 821 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 822 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 833 | CLA | O1D-CGD-O2D-CED |
| 20 | H | 102 | CLA | O1D-CGD-O2D-CED |
| 20 | L | 202 | CLA | O1D-CGD-O2D-CED |
| 20 | L | 204 | CLA | O1D-CGD-O2D-CED |
| 20 | R | 107 | CLA | O1D-CGD-O2D-CED |
| 21 | K | 107 | LMU | O5B-C1B-O1B-C4' |
| 20 | 2 | 311 | CLA | C2C-C3C-CAC-CBC |
| 20 | 3 | 311 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 801 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 801 | CLA | C4C-C3C-CAC-CBC |
| 20 | A | 825 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 825 | CLA | C4C-C3C-CAC-CBC |
| 20 | H | 101 | CLA | C2C-C3C-CAC-CBC |
| 20 | K | 104 | CLA | C2C-C3C-CAC-CBC |
| 21 | 2 | 318 | LMU | C5'-C4'-O1B-C1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 4 | 321 | LMU | C5'-C4'-O1B-C1B |
| 20 | 1 | 202 | CLA | O1D-CGD-O2D-CED |
| 20 | 1 | 203 | CLA | O1D-CGD-O2D-CED |
| 20 | 2 | 312 | CLA | O1D-CGD-O2D-CED |
| 20 | 3 | 307 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 801 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 811 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 826 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 819 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 828 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 839 | CLA | O1D-CGD-O2D-CED |
| 20 | F | 206 | CLA | O1D-CGD-O2D-CED |
| 20 | G | 105 | CLA | O1D-CGD-O2D-CED |
| 20 | H | 101 | CLA | O1D-CGD-O2D-CED |
| 20 | H | 110 | CLA | O1D-CGD-O2D-CED |
| 20 | 1 | 206 | CLA | CBD-CGD-O2D-CED |
| 20 | 1 | 213 | CLA | CBD-CGD-O2D-CED |
| 20 | 2 | 311 | CLA | CBD-CGD-O2D-CED |
| 20 | 3 | 313 | CLA | CBD-CGD-O2D-CED |
| 20 | 4 | 305 | CLA | CBD-CGD-O2D-CED |
| 20 | 4 | 315 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 807 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 809 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 810 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 817 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 823 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 825 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 826 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 828 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 832 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 837 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 839 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 806 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 816 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 819 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 820 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 830 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 833 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 834 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 837 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 850 | CLA | CBD-CGD-O2D-CED |
| 20 | H | 102 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | L | 208 | CLA | CBD-CGD-O2D-CED |
| 20 | 2 | 316 | CLA | O1A-CGA-O2A-C1 |
| 20 | 3 | 311 | CLA | O1A-CGA-O2A-C1 |
| 20 | 4 | 317 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 849 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 825 | CLA | O1A-CGA-O2A-C1 |
| 20 | H | 102 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 807 | CLA | O1A-CGA-O2A-C1 |
| 21 | D | 201 | LMU | O5B-C1B-O1B-C4' |
| 21 | G | 102 | LMU | O5B-C1B-O1B-C4' |
| 21 | H | 103 | LMU | O5B-C1B-O1B-C4' |
| 21 | E | 101 | LMU | C2B-C1B-O1B-C4' |
| 20 | 2 | 303 | CLA | C2C-C3C-CAC-CBC |
| 20 | 4 | 301 | CLA | C4C-C3C-CAC-CBC |
| 20 | 4 | 304 | CLA | C2C-C3C-CAC-CBC |
| 20 | 4 | 304 | CLA | C4C-C3C-CAC-CBC |
| 20 | H | 101 | CLA | C4C-C3C-CAC-CBC |
| 21 | 1 | 217 | LMU | C3'-C4'-O1B-C1B |
| 21 | B | 849 | LMU | C3'-C4'-O1B-C1B |
| 21 | R | 101 | LMU | C3'-C4'-O1B-C1B |
| 21 | R | 103 | LMU | C3'-C4'-O1B-C1B |
| 20 | 4 | 305 | CLA | O1D-CGD-O2D-CED |
| 20 | 4 | 318 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 810 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 830 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 840 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 809 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 834 | CLA | O1D-CGD-O2D-CED |
| 20 | L | 207 | CLA | O1D-CGD-O2D-CED |
| 20 | 2 | 312 | CLA | C5-C6-C7-C8 |
| 20 | 4 | 315 | CLA | CBA-CGA-O2A-C1 |
| 20 | K | 101 | CLA | CBA-CGA-O2A-C1 |
| 20 | 1 | 203 | CLA | C2-C1-O2A-CGA |
| 20 | 1 | 204 | CLA | C2C-C3C-CAC-CBC |
| 20 | 1 | 204 | CLA | C4C-C3C-CAC-CBC |
| 20 | 1 | 213 | CLA | C4C-C3C-CAC-CBC |
| 20 | B | 828 | CLA | C4C-C3C-CAC-CBC |
| 20 | B | 841 | CLA | C4C-C3C-CAC-CBC |
| 20 | K | 104 | CLA | C4C-C3C-CAC-CBC |
| 21 | K | 105 | LMU | C5'-C4'-O1B-C1B |
| 25 | B | 848 | LMG | C8-C9-O8-C28 |
| 21 | A | 847 | LMU | O5B-C1B-O1B-C4' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 804 | LMU | O5B-C1B-O1B-C4' |
| 21 | E | 101 | LMU | O5B-C1B-O1B-C4' |
| 21 | L | 210 | LMU | O5B-C1B-O1B-C4' |
| 21 | R | 102 | LMU | O5B-C1B-O1B-C4' |
| 21 | R | 105 | LMU | O5B-C1B-O1B-C4' |
| 21 | B | 804 | LMU | C2B-C1B-O1B-C4' |
| 21 | K | 107 | LMU | C2B-C1B-O1B-C4' |
| 20 | 1 | 211 | CLA | O1D-CGD-O2D-CED |
| 20 | 4 | 310 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 807 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 809 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 813 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 833 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 834 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 806 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 824 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 826 | CLA | O1D-CGD-O2D-CED |
| 20 | 2 | 316 | CLA | CBA-CGA-O2A-C1 |
| 20 | 3 | 311 | CLA | CBA-CGA-O2A-C1 |
| 20 | 4 | 317 | CLA | CBA-CGA-O2A-C1 |
| 20 | H | 102 | CLA | CBA-CGA-O2A-C1 |
| 20 | R | 108 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 846 | LMU | C4B-C5B-C6B-O6B |
| 20 | 4 | 304 | CLA | CBD-CGD-O2D-CED |
| 20 | 4 | 317 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 835 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 803 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 808 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 815 | CLA | CBD-CGD-O2D-CED |
| 20 | H | 108 | CLA | CBD-CGD-O2D-CED |
| 20 | I | 102 | CLA | CBD-CGD-O2D-CED |
| 20 | R | 108 | CLA | CBD-CGD-O2D-CED |
| 20 | 1 | 202 | CLA | C4C-C3C-CAC-CBC |
| 20 | 1 | 213 | CLA | C2C-C3C-CAC-CBC |
| 20 | 4 | 318 | CLA | C2C-C3C-CAC-CBC |
| 20 | 4 | 318 | CLA | C4C-C3C-CAC-CBC |
| 20 | A | 819 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 819 | CLA | C4C-C3C-CAC-CBC |
| 20 | B | 803 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 803 | CLA | C4C-C3C-CAC-CBC |
| 20 | B | 828 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 839 | CLA | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 839 | CLA | C4C-C3C-CAC-CBC |
| 21 | 2 | 321 | LMU | C5'-C4'-O1B-C1B |
| 21 | A | 847 | LMU | C5'-C4'-O1B-C1B |
| 20 | 1 | 206 | CLA | O1A-CGA-O2A-C1 |
| 20 | 1 | 207 | CLA | O1A-CGA-O2A-C1 |
| 20 | 2 | 314 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 809 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 817 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 826 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 832 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 851 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 818 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 821 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 850 | CLA | O1A-CGA-O2A-C1 |
| 20 | J | 103 | CLA | O1A-CGA-O2A-C1 |
| 20 | K | 102 | CLA | O1A-CGA-O2A-C1 |
| 20 | L | 203 | CLA | O1A-CGA-O2A-C1 |
| 20 | R | 107 | CLA | O1A-CGA-O2A-C1 |
| 20 | 1 | 201 | CLA | O1A-CGA-O2A-C1 |
| 20 | 4 | 315 | CLA | O1A-CGA-O2A-C1 |
| 20 | K | 101 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 835 | CLA | O1D-CGD-O2D-CED |
| 20 | J | 101 | CLA | O1D-CGD-O2D-CED |
| 21 | 4 | 321 | LMU | O5B-C1B-O1B-C4' |
| 21 | G | 103 | LMU | O5B-C1B-O1B-C4' |
| 20 | 3 | 314 | CLA | C15-C16-C17-C18 |
| 20 | A | 832 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 824 | CLA | C4C-C3C-CAC-CBC |
| 20 | B | 837 | CLA | C4C-C3C-CAC-CBC |
| 20 | K | 103 | CLA | C4C-C3C-CAC-CBC |
| 21 | 4 | 316 | LMU | O5'-C5'-C6'-O6' |
| 20 | A | 822 | CLA | O1D-CGD-O2D-CED |
| 20 | H | 109 | CLA | O1D-CGD-O2D-CED |
| 20 | 1 | 202 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 832 | CLA | C4C-C3C-CAC-CBC |
| 20 | B | 822 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 830 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 830 | CLA | C4C-C3C-CAC-CBC |
| 20 | B | 841 | CLA | C2C-C3C-CAC-CBC |
| 20 | K | 103 | CLA | C2C-C3C-CAC-CBC |
| 21 | R | 104 | LMU | C3'-C4'-O1B-C1B |
| 20 | 1 | 201 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 3 | 311 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 820 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 836 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 804 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 839 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 832 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 848 | LMG | O9-C10-O7-C8 |
| 20 | B | 817 | CLA | CBA-CGA-O2A-C1 |
| 20 | 2 | 303 | CLA | C4C-C3C-CAC-CBC |
| 20 | 4 | 318 | CLA | C2-C1-O2A-CGA |
| 20 | B | 824 | CLA | C2C-C3C-CAC-CBC |
| 21 | A | 855 | LMU | C3'-C4'-O1B-C1B |
| 20 | B | 817 | CLA | O1A-CGA-O2A-C1 |
| 20 | 2 | 307 | CLA | C3-C5-C6-C7 |
| 20 | 2 | 316 | CLA | C3-C5-C6-C7 |
| 20 | 3 | 314 | CLA | C3-C5-C6-C7 |
| 20 | 4 | 301 | CLA | C3-C5-C6-C7 |
| 20 | 4 | 304 | CLA | C3-C5-C6-C7 |
| 20 | A | 805 | CLA | C3-C5-C6-C7 |
| 20 | A | 818 | CLA | C3-C5-C6-C7 |
| 20 | A | 819 | CLA | C3-C5-C6-C7 |
| 20 | A | 828 | CLA | C3-C5-C6-C7 |
| 20 | A | 838 | CLA | C3-C5-C6-C7 |
| 20 | B | 823 | CLA | C3-C5-C6-C7 |
| 20 | B | 840 | CLA | C3-C5-C6-C7 |
| 20 | H | 102 | CLA | C3-C5-C6-C7 |
| 20 | 1 | 206 | CLA | CBA-CGA-O2A-C1 |
| 20 | 1 | 207 | CLA | CBA-CGA-O2A-C1 |
| 20 | 2 | 314 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 828 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 836 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 851 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 806 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 813 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 818 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 825 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 850 | CLA | CBA-CGA-O2A-C1 |
| 20 | J | 103 | CLA | CBA-CGA-O2A-C1 |
| 20 | K | 102 | CLA | CBA-CGA-O2A-C1 |
| 20 | L | 203 | CLA | CBA-CGA-O2A-C1 |
| 20 | R | 107 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 837 | CLA | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 1 | 218 | LMU | O5'-C5'-C6'-O6' |
| 21 | 2 | 320 | LMU | O5B-C1B-O1B-C4' |
| 20 | A | 805 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 802 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 825 | CLA | CBD-CGD-O2D-CED |
| 20 | 3 | 307 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 816 | CLA | C2C-C3C-CAC-CBC |
| 21 | 2 | 313 | LMU | O5'-C5'-C6'-O6' |
| 21 | R | 104 | LMU | O5B-C5B-C6B-O6B |
| 21 | K | 106 | LMU | O5B-C1B-O1B-C4' |
| 21 | B | 805 | LMU | C3'-C4'-O1B-C1B |
| 20 | A | 834 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 817 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 831 | CLA | C4-C3-C5-C6 |
| 23 | A | 842 | PQN | C12-C13-C15-C16 |
| 20 | B | 841 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 805 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 817 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 830 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 832 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 849 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 806 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 814 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 815 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 818 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 822 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 823 | CLA | C2A-CAA-CBA-CGA |
| 20 | K | 103 | CLA | C2A-CAA-CBA-CGA |
| 20 | 3 | 313 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 825 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 828 | CLA | O1D-CGD-O2D-CED |
| 21 | 1 | 218 | LMU | C3'-C4'-O1B-C1B |
| 21 | A | 852 | LMU | C3'-C4'-O1B-C1B |
| 20 | B | 822 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 826 | CLA | C3-C5-C6-C7 |
| 20 | A | 827 | CLA | C3-C5-C6-C7 |
| 20 | A | 830 | CLA | C3-C5-C6-C7 |
| 20 | B | 802 | CLA | C3-C5-C6-C7 |
| 20 | B | 837 | CLA | C3-C5-C6-C7 |
| 20 | B | 841 | CLA | C3-C5-C6-C7 |
| 20 | A | 801 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 809 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | A | 817 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 826 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 832 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 821 | CLA | CBA-CGA-O2A-C1 |
| 20 | G | 105 | CLA | CBA-CGA-O2A-C1 |
| 20 | H | 109 | CLA | CBA-CGA-O2A-C1 |
| 20 | L | 208 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 854 | LMU | O5B-C5B-C6B-O6B |
| 21 | K | 106 | LMU | C4'-C5'-C6'-O6' |
| 21 | R | 103 | LMU | C4B-C5B-C6B-O6B |
| 21 | 4 | 320 | LMU | O5B-C1B-O1B-C4' |
| 21 | 4 | 320 | LMU | C2B-C1B-O1B-C4' |
| 21 | 4 | 321 | LMU | C2B-C1B-O1B-C4' |
| 20 | B | 822 | CLA | C4C-C3C-CAC-CBC |
| 21 | 3 | 319 | LMU | C3'-C4'-O1B-C1B |
| 21 | G | 102 | LMU | C11-C10-C9-C8 |
| 20 | B | 850 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 836 | CLA | CBD-CGD-O2D-CED |
| 20 | 2 | 311 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 830 | CLA | O1D-CGD-O2D-CED |
| 21 | G | 102 | LMU | O5'-C5'-C6'-O6' |
| 21 | 2 | 319 | LMU | C4B-C5B-C6B-O6B |
| 21 | K | 107 | LMU | C4B-C5B-C6B-O6B |
| 21 | R | 101 | LMU | C4'-C5'-C6'-O6' |
| 20 | A | 828 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 836 | CLA | O1A-CGA-O2A-C1 |
| 20 | F | 207 | CLA | O1A-CGA-O2A-C1 |
| 20 | 4 | 305 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 816 | CLA | C4C-C3C-CAC-CBC |
| 20 | J | 101 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 834 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 843 | BCR | C9-C10-C11-C12 |
| 22 | B | 846 | BCR | C9-C10-C11-C12 |
| 22 | F | 203 | BCR | C19-C20-C21-C22 |
| 22 | I | 101 | BCR | C19-C20-C21-C22 |
| 22 | J | 102 | BCR | C19-C20-C21-C22 |
| 22 | L | 209 | BCR | C19-C20-C21-C22 |
| 21 | 1 | 216 | LMU | O5'-C5'-C6'-O6' |
| 21 | B | 804 | LMU | O5B-C5B-C6B-O6B |
| 21 | R | 106 | LMU | O5B-C5B-C6B-O6B |
| 21 | 4 | 319 | LMU | C5'-C4'-O1B-C1B |
| 21 | K | 105 | LMU | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | A | 812 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 813 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 832 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 820 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 812 | CLA | C3-C5-C6-C7 |
| 20 | H | 108 | CLA | C3-C5-C6-C7 |
| 23 | A | 842 | PQN | C13-C15-C16-C17 |
| 20 | 2 | 305 | CLA | CBA-CGA-O2A-C1 |
| 20 | 4 | 310 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 808 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 820 | CLA | CBA-CGA-O2A-C1 |
| 25 | B | 848 | LMG | C29-C28-O8-C9 |
| 21 | R | 104 | LMU | C11-C10-C9-C8 |
| 20 | A | 801 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 806 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 813 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 820 | CLA | O1A-CGA-O2A-C1 |
| 20 | L | 208 | CLA | O1A-CGA-O2A-C1 |
| 21 | 4 | 320 | LMU | O5B-C5B-C6B-O6B |
| 21 | F | 202 | LMU | O5'-C5'-C6'-O6' |
| 21 | R | 105 | LMU | O5B-C5B-C6B-O6B |
| 21 | R | 105 | LMU | O5'-C5'-C6'-O6' |
| 21 | 4 | 316 | LMU | C4'-C5'-C6'-O6' |
| 21 | B | 804 | LMU | C4B-C5B-C6B-O6B |
| 21 | B | 849 | LMU | C4'-C5'-C6'-O6' |
| 20 | A | 811 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 836 | CLA | C2C-C3C-CAC-CBC |
| 21 | 2 | 318 | LMU | O5B-C1B-O1B-C4' |
| 21 | G | 101 | LMU | C2B-C1B-O1B-C4' |
| 21 | 4 | 320 | LMU | O5'-C5'-C6'-O6' |
| 21 | A | 855 | LMU | O5'-C5'-C6'-O6' |
| 21 | F | 202 | LMU | O5B-C5B-C6B-O6B |
| 21 | 2 | 313 | LMU | C4'-C5'-C6'-O6' |
| 21 | 2 | 313 | LMU | C4-C5-C6-C7 |
| 21 | R | 109 | LMU | C7-C8-C9-C10 |
| 21 | 1 | 217 | LMU | C1-C2-C3-C4 |
| 20 | H | 109 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 840 | CLA | C2C-C3C-CAC-CBC |
| 21 | 2 | 313 | LMU | C2-C3-C4-C5 |
| 21 | 3 | 319 | LMU | C4-C5-C6-C7 |
| 21 | 4 | 319 | LMU | C5-C6-C7-C8 |
| 21 | 4 | 320 | LMU | C7-C8-C9-C10 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 846 | LMU | C2-C3-C4-C5 |
| 21 | A | 853 | LMU | C2-C3-C4-C5 |
| 21 | A | 853 | LMU | C11-C10-C9-C8 |
| 21 | H | 106 | LMU | C7-C8-C9-C10 |
| 21 | R | 102 | LMU | C6-C7-C8-C9 |
| 21 | R | 106 | LMU | C6-C7-C8-C9 |
| 21 | A | 846 | LMU | O5'-C5'-C6'-O6' |
| 21 | A | 846 | LMU | C4'-C5'-C6'-O6' |
| 21 | A | 854 | LMU | C4B-C5B-C6B-O6B |
| 21 | F | 202 | LMU | C4'-C5'-C6'-O6' |
| 21 | G | 102 | LMU | C4'-C5'-C6'-O6' |
| 20 | B | 837 | CLA | O1D-CGD-O2D-CED |
| 21 | H | 105 | LMU | C5-C6-C7-C8 |
| 20 | A | 816 | CLA | C3-C5-C6-C7 |
| 20 | A | 849 | CLA | C3-C5-C6-C7 |
| 20 | B | 830 | CLA | C3-C5-C6-C7 |
| 20 | L | 204 | CLA | C3-C5-C6-C7 |
| 20 | 3 | 313 | CLA | CBA-CGA-O2A-C1 |
| 20 | F | 207 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 846 | LMU | O5B-C5B-C6B-O6B |
| 21 | A | 852 | LMU | O5'-C5'-C6'-O6' |
| 21 | H | 103 | LMU | O5B-C5B-C6B-O6B |
| 21 | K | 105 | LMU | O5'-C5'-C6'-O6' |
| 21 | L | 205 | LMU | O5'-C5'-C6'-O6' |
| 21 | R | 101 | LMU | O5'-C5'-C6'-O6' |
| 21 | R | 104 | LMU | C4B-C5B-C6B-O6B |
| 21 | R | 106 | LMU | C4B-C5B-C6B-O6B |
| 20 | 2 | 305 | CLA | O1A-CGA-O2A-C1 |
| 20 | 4 | 317 | CLA | C3-C5-C6-C7 |
| 21 | 4 | 319 | LMU | C7-C8-C9-C10 |
| 21 | A | 846 | LMU | C3'-C4'-O1B-C1B |
| 21 | H | 105 | LMU | O1'-C1-C2-C3 |
| 21 | 2 | 319 | LMU | O5B-C5B-C6B-O6B |
| 21 | 3 | 318 | LMU | O5'-C5'-C6'-O6' |
| 21 | K | 107 | LMU | O5B-C5B-C6B-O6B |
| 21 | L | 205 | LMU | O5B-C5B-C6B-O6B |
| 21 | L | 206 | LMU | O5B-C5B-C6B-O6B |
| 20 | 2 | 307 | CLA | C4-C3-C5-C6 |
| 20 | 3 | 311 | CLA | C4-C3-C5-C6 |
| 20 | A | 850 | CLA | C4-C3-C5-C6 |
| 20 | B | 827 | CLA | C4-C3-C5-C6 |
| 21 | 1 | 218 | LMU | C4'-C5'-C6'-O6' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 2 | 307 | CLA | C2-C3-C5-C6 |
| 20 | 3 | 311 | CLA | C2-C3-C5-C6 |
| 20 | A | 831 | CLA | C2-C3-C5-C6 |
| 20 | A | 850 | CLA | C2-C3-C5-C6 |
| 20 | B | 827 | CLA | C2-C3-C5-C6 |
| 23 | B | 843 | PQN | C12-C13-C15-C16 |
| 20 | A | 807 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 837 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 838 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 831 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 835 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 804 | LMU | C6-C7-C8-C9 |
| 21 | E | 101 | LMU | C1-C2-C3-C4 |
| 21 | B | 849 | LMU | O5'-C5'-C6'-O6' |
| 21 | K | 106 | LMU | O5'-C5'-C6'-O6' |
| 21 | R | 103 | LMU | O5B-C5B-C6B-O6B |
| 20 | 4 | 310 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 837 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 808 | CLA | O1A-CGA-O2A-C1 |
| 20 | G | 105 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 848 | LMG | O10-C28-O8-C9 |
| 21 | H | 106 | LMU | C4B-C5B-C6B-O6B |
| 21 | 4 | 321 | LMU | O5'-C1'-O1'-C1 |
| 21 | A | 853 | LMU | O5'-C1'-O1'-C1 |
| 21 | R | 105 | LMU | O5'-C1'-O1'-C1 |
| 21 | D | 201 | LMU | O1'-C1-C2-C3 |
| 20 | A | 837 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 839 | CLA | CBA-CGA-O2A-C1 |
| 20 | K | 104 | CLA | CBA-CGA-O2A-C1 |
| 20 | 1 | 201 | CLA | C2C-C3C-CAC-CBC |
| 20 | 1 | 207 | CLA | C2C-C3C-CAC-CBC |
| 21 | L | 210 | LMU | O5B-C5B-C6B-O6B |
| 21 | 2 | 313 | LMU | C2B-C1B-O1B-C4' |
| 20 | 3 | 307 | CLA | C4C-C3C-CAC-CBC |
| 20 | A | 817 | CLA | C4C-C3C-CAC-CBC |
| 21 | L | 210 | LMU | C5-C6-C7-C8 |
| 20 | I | 102 | CLA | O1D-CGD-O2D-CED |
| 21 | 3 | 318 | LMU | C4'-C5'-C6'-O6' |
| 21 | A | 855 | LMU | C4'-C5'-C6'-O6' |
| 21 | E | 101 | LMU | C3-C4-C5-C6 |
| 20 | 4 | 304 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 815 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | L | 208 | CLA | O1D-CGD-O2D-CED |
| 20 | R | 108 | CLA | O1D-CGD-O2D-CED |
| 20 | K | 103 | CLA | CBD-CGD-O2D-CED |
| 21 | 4 | 316 | LMU | O5B-C5B-C6B-O6B |
| 21 | R | 104 | LMU | O5'-C5'-C6'-O6' |
| 21 | K | 105 | LMU | C4'-C5'-C6'-O6' |
| 21 | 2 | 319 | LMU | C3-C4-C5-C6 |
| 20 | 1 | 211 | CLA | CBA-CGA-O2A-C1 |
| 20 | 2 | 310 | CLA | CBA-CGA-O2A-C1 |
| 20 | 3 | 310 | CLA | CBA-CGA-O2A-C1 |
| 20 | 4 | 304 | CLA | CBA-CGA-O2A-C1 |
| 20 | 4 | 318 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 812 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 838 | CLA | CBA-CGA-O2A-C1 |
| 20 | H | 108 | CLA | CBA-CGA-O2A-C1 |
| 20 | H | 110 | CLA | CBA-CGA-O2A-C1 |
| 21 | F | 202 | LMU | C4B-C5B-C6B-O6B |
| 21 | L | 205 | LMU | C4B-C5B-C6B-O6B |
| 21 | L | 210 | LMU | C4'-C5'-C6'-O6' |
| 21 | R | 105 | LMU | C4'-C5'-C6'-O6' |
| 21 | A | 852 | LMU | C2-C3-C4-C5 |
| 21 | K | 107 | LMU | C3-C4-C5-C6 |
| 22 | F | 204 | BCR | C13-C14-C15-C16 |
| 22 | F | 204 | BCR | C15-C16-C17-C18 |
| 20 | A | 811 | CLA | C5-C6-C7-C8 |
| 21 | 1 | 216 | LMU | C4'-C5'-C6'-O6' |
| 21 | R | 104 | LMU | C4'-C5'-C6'-O6' |
| 21 | 2 | 313 | LMU | O5B-C1B-O1B-C4' |
| 20 | J | 101 | CLA | C4C-C3C-CAC-CBC |
| 21 | R | 105 | LMU | C4B-C5B-C6B-O6B |
| 20 | B | 838 | CLA | C13-C15-C16-C17 |
| 20 | A | 817 | CLA | C3-C5-C6-C7 |
| 21 | 4 | 321 | LMU | C2'-C1'-O1'-C1 |
| 21 | G | 101 | LMU | C2'-C1'-O1'-C1 |
| 21 | H | 105 | LMU | C2'-C1'-O1'-C1 |
| 21 | H | 106 | LMU | C2'-C1'-O1'-C1 |
| 21 | L | 206 | LMU | C2'-C1'-O1'-C1 |
| 21 | 1 | 216 | LMU | C7-C8-C9-C10 |
| 21 | A | 846 | LMU | C5'-C4'-O1B-C1B |
| 20 | 3 | 313 | CLA | O1A-CGA-O2A-C1 |
| 20 | 4 | 304 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 838 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 1 | 206 | CLA | C4-C3-C5-C6 |
| 21 | L | 206 | LMU | C4B-C5B-C6B-O6B |
| 21 | L | 210 | LMU | C4B-C5B-C6B-O6B |
| 20 | 2 | 303 | CLA | C11-C10-C8-C9 |
| 20 | A | 811 | CLA | C14-C13-C15-C16 |
| 20 | A | 825 | CLA | C11-C10-C8-C9 |
| 20 | A | 825 | CLA | C14-C13-C15-C16 |
| 20 | A | 828 | CLA | C11-C10-C8-C9 |
| 20 | A | 831 | CLA | C6-C7-C8-C9 |
| 20 | A | 831 | CLA | C11-C12-C13-C14 |
| 20 | A | 851 | CLA | C6-C7-C8-C9 |
| 20 | A | 851 | CLA | C11-C10-C8-C9 |
| 20 | B | 803 | CLA | C14-C13-C15-C16 |
| 20 | B | 806 | CLA | C11-C10-C8-C9 |
| 20 | B | 806 | CLA | C14-C13-C15-C16 |
| 20 | B | 808 | CLA | C11-C10-C8-C9 |
| 20 | B | 808 | CLA | C11-C12-C13-C14 |
| 20 | B | 824 | CLA | C11-C10-C8-C9 |
| 20 | B | 824 | CLA | C14-C13-C15-C16 |
| 20 | B | 828 | CLA | C6-C7-C8-C9 |
| 20 | B | 830 | CLA | C11-C10-C8-C9 |
| 20 | B | 832 | CLA | C11-C10-C8-C9 |
| 20 | B | 838 | CLA | C11-C12-C13-C14 |
| 20 | B | 850 | CLA | C11-C12-C13-C14 |
| 20 | H | 108 | CLA | C6-C7-C8-C9 |
| 20 | R | 108 | CLA | C11-C10-C8-C9 |
| 20 | R | 108 | CLA | C11-C12-C13-C14 |
| 23 | A | 842 | PQN | C21-C22-C23-C24 |
| 20 | B | 803 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 819 | CLA | CBD-CGD-O2D-CED |
| 20 | B | 827 | CLA | CBD-CGD-O2D-CED |
| 21 | K | 107 | LMU | C5-C6-C7-C8 |
| 20 | 3 | 311 | CLA | C13-C15-C16-C17 |
| 20 | 4 | 305 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 830 | CLA | C2A-CAA-CBA-CGA |
| 20 | J | 103 | CLA | C2A-CAA-CBA-CGA |
| 20 | K | 101 | CLA | C2A-CAA-CBA-CGA |
| 22 | 2 | 317 | BCR | C37-C22-C23-C24 |
| 22 | A | 844 | BCR | C7-C8-C9-C34 |
| 22 | I | 101 | BCR | C36-C18-C19-C20 |
| 22 | 2 | 317 | BCR | C17-C18-C19-C20 |
| 22 | 2 | 317 | BCR | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | A | 844 | BCR | C7-C8-C9-C10 |
| 22 | B | 847 | BCR | C7-C8-C9-C10 |
| 22 | F | 203 | BCR | C21-C22-C23-C24 |
| 20 | B | 808 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 854 | LMU | O5'-C5'-C6'-O6' |
| 21 | R | 103 | LMU | O5'-C5'-C6'-O6' |
| 21 | A | 853 | LMU | C4-C5-C6-C7 |
| 21 | D | 201 | LMU | C2-C3-C4-C5 |
| 21 | B | 849 | LMU | C4B-C5B-C6B-O6B |
| 21 | H | 103 | LMU | C4B-C5B-C6B-O6B |
| 21 | K | 107 | LMU | C4'-C5'-C6'-O6' |
| 20 | A | 851 | CLA | C8-C10-C11-C12 |
| 20 | B | 806 | CLA | C15-C16-C17-C18 |
| 20 | B | 815 | CLA | C10-C11-C12-C13 |
| 20 | R | 108 | CLA | C8-C10-C11-C12 |
| 21 | H | 104 | LMU | C3-C4-C5-C6 |
| 21 | L | 206 | LMU | O5'-C5'-C6'-O6' |
| 21 | A | 852 | LMU | C4'-C5'-C6'-O6' |
| 20 | A | 851 | CLA | C2C-C3C-CAC-CBC |
| 20 | 4 | 317 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 824 | CLA | C3-C5-C6-C7 |
| 20 | F | 201 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 808 | CLA | C5-C6-C7-C8 |
| 20 | A | 819 | CLA | C5-C6-C7-C8 |
| 20 | A | 849 | CLA | C10-C11-C12-C13 |
| 20 | B | 815 | CLA | C5-C6-C7-C8 |
| 20 | B | 824 | CLA | C13-C15-C16-C17 |
| 20 | B | 828 | CLA | C8-C10-C11-C12 |
| 20 | B | 837 | CLA | C5-C6-C7-C8 |
| 20 | B | 841 | CLA | C15-C16-C17-C18 |
| 20 | L | 201 | CLA | C5-C6-C7-C8 |
| 21 | E | 101 | LMU | O5'-C5'-C6'-O6' |
| 20 | A | 835 | CLA | O1D-CGD-O2D-CED |
| 21 | R | 101 | LMU | C4B-C5B-C6B-O6B |
| 20 | 2 | 302 | CLA | CBD-CGD-O2D-CED |
| 20 | 2 | 305 | CLA | C2C-C3C-CAC-CBC |
| 21 | R | 109 | LMU | C3'-C4'-O1B-C1B |
| 20 | 1 | 206 | CLA | C8-C10-C11-C12 |
| 20 | 3 | 314 | CLA | C10-C11-C12-C13 |
| 20 | A | 818 | CLA | C5-C6-C7-C8 |
| 20 | A | 827 | CLA | C5-C6-C7-C8 |
| 20 | A | 831 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | A | 849 | CLA | C5-C6-C7-C8 |
| 20 | B | 803 | CLA | C13-C15-C16-C17 |
| 20 | B | 820 | CLA | C10-C11-C12-C13 |
| 20 | L | 203 | CLA | C8-C10-C11-C12 |
| 20 | 2 | 310 | CLA | O1A-CGA-O2A-C1 |
| 20 | H | 110 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 840 | CLA | C4C-C3C-CAC-CBC |
| 21 | F | 202 | LMU | O1'-C1-C2-C3 |
| 20 | 2 | 307 | CLA | C5-C6-C7-C8 |
| 20 | 3 | 314 | CLA | C13-C15-C16-C17 |
| 20 | B | 823 | CLA | C5-C6-C7-C8 |
| 20 | L | 202 | CLA | C5-C6-C7-C8 |
| 23 | B | 843 | PQN | C18-C20-C21-C22 |
| 20 | 4 | 305 | CLA | C4C-C3C-CAC-CBC |
| 21 | L | 206 | LMU | O1'-C1-C2-C3 |
| 21 | 1 | 216 | LMU | O5B-C5B-C6B-O6B |
| 21 | B | 805 | LMU | O5'-C5'-C6'-O6' |
| 20 | 1 | 206 | CLA | C2-C1-O2A-CGA |
| 20 | A | 805 | CLA | C2-C1-O2A-CGA |
| 20 | A | 823 | CLA | C2-C1-O2A-CGA |
| 20 | A | 824 | CLA | C2-C1-O2A-CGA |
| 20 | A | 837 | CLA | C2-C1-O2A-CGA |
| 21 | 1 | 217 | LMU | O1'-C1-C2-C3 |
| 21 | R | 103 | LMU | C7-C8-C9-C10 |
| 20 | A | 851 | CLA | C15-C16-C17-C18 |
| 20 | B | 840 | CLA | C10-C11-C12-C13 |
| 20 | I | 102 | CLA | C5-C6-C7-C8 |
| 23 | A | 842 | PQN | C25-C26-C27-C28 |
| 20 | K | 104 | CLA | O1A-CGA-O2A-C1 |
| 20 | R | 107 | CLA | C8-C10-C11-C12 |
| 20 | A | 831 | CLA | C15-C16-C17-C18 |
| 20 | A | 838 | CLA | C13-C15-C16-C17 |
| 20 | B | 827 | CLA | C15-C16-C17-C18 |
| 23 | B | 843 | PQN | C20-C21-C22-C23 |
| 20 | 3 | 311 | CLA | O1D-CGD-O2D-CED |
| 21 | 4 | 319 | LMU | C4'-C5'-C6'-O6' |
| 20 | 2 | 312 | CLA | C11-C12-C13-C15 |
| 20 | 2 | 316 | CLA | C12-C13-C15-C16 |
| 20 | 3 | 314 | CLA | C11-C10-C8-C7 |
| 20 | 4 | 303 | CLA | C12-C13-C15-C16 |
| 20 | A | 811 | CLA | C12-C13-C15-C16 |
| 20 | A | 849 | CLA | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 815 | CLA | C11-C10-C8-C7 |
| 20 | B | 824 | CLA | C11-C12-C13-C15 |
| 20 | B | 850 | CLA | C6-C7-C8-C10 |
| 20 | L | 203 | CLA | C11-C10-C8-C7 |
| 20 | L | 203 | CLA | C11-C12-C13-C15 |
| 20 | A | 812 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 839 | CLA | O1A-CGA-O2A-C1 |
| 20 | H | 108 | CLA | O1A-CGA-O2A-C1 |
| 20 | 2 | 302 | CLA | C2C-C3C-CAC-CBC |
| 22 | A | 845 | BCR | C19-C20-C21-C22 |
| 22 | G | 104 | BCR | C19-C20-C21-C22 |
| 22 | I | 103 | BCR | C19-C20-C21-C22 |
| 20 | A | 822 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 824 | CLA | C2A-CAA-CBA-CGA |
| 20 | R | 107 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 836 | CLA | O1D-CGD-O2D-CED |
| 20 | H | 108 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 811 | CLA | C10-C11-C12-C13 |
| 20 | B | 803 | CLA | C10-C11-C12-C13 |
| 20 | B | 810 | CLA | C8-C10-C11-C12 |
| 20 | B | 813 | CLA | C5-C6-C7-C8 |
| 23 | B | 843 | PQN | C15-C16-C17-C18 |
| 21 | 1 | 218 | LMU | O1'-C1-C2-C3 |
| 21 | A | 854 | LMU | O1'-C1-C2-C3 |
| 20 | 4 | 318 | CLA | O1A-CGA-O2A-C1 |
| 20 | F | 201 | CLA | O1A-CGA-O2A-C1 |
| 21 | G | 101 | LMU | O5'-C1'-O1'-C1 |
| 21 | L | 206 | LMU | O5'-C1'-O1'-C1 |
| 20 | B | 830 | CLA | C15-C16-C17-C18 |
| 20 | 2 | 312 | CLA | C2C-C3C-CAC-CBC |
| 21 | G | 101 | LMU | O5B-C1B-O1B-C4' |
| 22 | B | 844 | BCR | C18-C19-C20-C21 |
| 21 | 1 | 218 | LMU | C3-C4-C5-C6 |
| 21 | A | 852 | LMU | O1'-C1-C2-C3 |
| 21 | R | 102 | LMU | C11-C10-C9-C8 |
| 21 | R | 105 | LMU | O1'-C1-C2-C3 |
| 21 | 2 | 313 | LMU | O5B-C5B-C6B-O6B |
| 20 | A | 826 | CLA | C15-C16-C17-C18 |
| 20 | A | 850 | CLA | C13-C15-C16-C17 |
| 20 | B | 806 | CLA | C13-C15-C16-C17 |
| 20 | B | 838 | CLA | C8-C10-C11-C12 |
| 20 | R | 108 | CLA | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 804 | LMU | O1'-C1-C2-C3 |
| 20 | 1 | 211 | CLA | O1A-CGA-O2A-C1 |
| 20 | 3 | 310 | CLA | O1A-CGA-O2A-C1 |
| 21 | 2 | 318 | LMU | O1'-C1-C2-C3 |
| 21 | H | 104 | LMU | O1'-C1-C2-C3 |
| 21 | K | 107 | LMU | O1'-C1-C2-C3 |
| 20 | A | 830 | CLA | C13-C15-C16-C17 |
| 20 | A | 851 | CLA | C10-C11-C12-C13 |
| 20 | B | 814 | CLA | C5-C6-C7-C8 |
| 21 | H | 106 | LMU | O5B-C5B-C6B-O6B |
| 21 | L | 210 | LMU | O5'-C5'-C6'-O6' |
| 20 | A | 820 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 841 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 805 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 806 | CLA | C5-C6-C7-C8 |
| 20 | B | 814 | CLA | C10-C11-C12-C13 |
| 20 | B | 830 | CLA | C5-C6-C7-C8 |
| 20 | H | 102 | CLA | C5-C6-C7-C8 |
| 20 | L | 203 | CLA | C15-C16-C17-C18 |
| 20 | 3 | 311 | CLA | C3-C5-C6-C7 |
| 20 | A | 811 | CLA | C3-C5-C6-C7 |
| 20 | B | 830 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 802 | CLA | O1D-CGD-O2D-CED |
| 20 | 3 | 311 | CLA | C5-C6-C7-C8 |
| 20 | A | 828 | CLA | C13-C15-C16-C17 |
| 20 | A | 849 | CLA | C8-C10-C11-C12 |
| 21 | 4 | 320 | LMU | C4B-C5B-C6B-O6B |
| 20 | F | 207 | CLA | C4-C3-C5-C6 |
| 21 | L | 205 | LMU | C4'-C5'-C6'-O6' |
| 20 | A | 836 | CLA | C4C-C3C-CAC-CBC |
| 20 | L | 201 | CLA | C10-C11-C12-C13 |
| 23 | A | 842 | PQN | C20-C21-C22-C23 |
| 21 | 1 | 218 | LMU | C7-C8-C9-C10 |
| 20 | 1 | 215 | CLA | C2A-CAA-CBA-CGA |
| 20 | 2 | 312 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 812 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 827 | CLA | C2A-CAA-CBA-CGA |
| 20 | 3 | 311 | CLA | C16-C17-C18-C20 |
| 20 | L | 202 | CLA | C6-C7-C8-C10 |
| 20 | A | 825 | CLA | CBA-CGA-O2A-C1 |
| 21 | H | 105 | LMU | O5'-C5'-C6'-O6' |
| 21 | 4 | 321 | LMU | C4'-C5'-C6'-O6' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | A | 811 | CLA | C4C-C3C-CAC-CBC |
| 21 | A | 855 | LMU | C6-C7-C8-C9 |
| 21 | H | 105 | LMU | C3'-C4'-O1B-C1B |
| 22 | F | 203 | BCR | C20-C21-C22-C37 |
| 20 | J | 103 | CLA | C3-C5-C6-C7 |
| 21 | 4 | 320 | LMU | C6-C7-C8-C9 |
| 21 | 4 | 321 | LMU | C3-C4-C5-C6 |
| 21 | A | 848 | LMU | C7-C8-C9-C10 |
| 21 | B | 805 | LMU | C4-C5-C6-C7 |
| 21 | D | 201 | LMU | C11-C10-C9-C8 |
| 21 | E | 101 | LMU | C11-C10-C9-C8 |
| 21 | K | 107 | LMU | C4-C5-C6-C7 |
| 21 | L | 205 | LMU | C6-C7-C8-C9 |
| 20 | A | 811 | CLA | C16-C17-C18-C19 |
| 20 | A | 818 | CLA | C11-C12-C13-C15 |
| 20 | A | 827 | CLA | C6-C7-C8-C9 |
| 20 | A | 835 | CLA | C16-C17-C18-C19 |
| 21 | 1 | 217 | LMU | C3-C4-C5-C6 |
| 21 | 2 | 313 | LMU | C9-C10-C11-C12 |
| 21 | 4 | 316 | LMU | C2-C3-C4-C5 |
| 21 | 4 | 321 | LMU | C5-C6-C7-C8 |
| 21 | A | 848 | LMU | C5-C6-C7-C8 |
| 21 | H | 103 | LMU | C4-C5-C6-C7 |
| 21 | K | 107 | LMU | C6-C7-C8-C9 |
| 21 | L | 206 | LMU | C6-C7-C8-C9 |
| 21 | L | 210 | LMU | C11-C10-C9-C8 |
| 21 | R | 101 | LMU | C2-C3-C4-C5 |
| 21 | R | 106 | LMU | O1'-C1-C2-C3 |
| 21 | R | 106 | LMU | C2-C3-C4-C5 |
| 25 | B | 848 | LMG | C32-C33-C34-C35 |
| 21 | H | 104 | LMU | C4B-C5B-C6B-O6B |
| 21 | 2 | 320 | LMU | C4-C5-C6-C7 |
| 21 | C | 101 | LMU | C7-C8-C9-C10 |
| 21 | H | 106 | LMU | C6-C7-C8-C9 |
| 21 | K | 106 | LMU | C4-C5-C6-C7 |
| 21 | R | 104 | LMU | C5-C6-C7-C8 |
| 21 | R | 109 | LMU | C5'-C4'-O1B-C1B |
| 25 | B | 848 | LMG | C17-C18-C19-C20 |
| 25 | B | 848 | LMG | C33-C34-C35-C36 |
| 20 | B | 825 | CLA | O1D-CGD-O2D-CED |
| 21 | D | 201 | LMU | O5B-C5B-C6B-O6B |
| 21 | R | 101 | LMU | O5B-C5B-C6B-O6B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 2 | 318 | LMU | C7-C8-C9-C10 |
| 21 | 3 | 318 | LMU | C2-C3-C4-C5 |
| 21 | 3 | 318 | LMU | C4-C5-C6-C7 |
| 21 | C | 101 | LMU | C11-C10-C9-C8 |
| 21 | G | 101 | LMU | C7-C8-C9-C10 |
| 21 | G | 103 | LMU | C2-C3-C4-C5 |
| 21 | H | 103 | LMU | C6-C7-C8-C9 |
| 21 | L | 205 | LMU | C7-C8-C9-C10 |
| 20 | A | 831 | CLA | C2C-C3C-CAC-CBC |
| 21 | 2 | 320 | LMU | C5-C6-C7-C8 |
| 21 | G | 101 | LMU | C2-C3-C4-C5 |
| 20 | A | 824 | CLA | C3-C5-C6-C7 |
| 20 | 4 | 306 | CLA | CBD-CGD-O2D-CED |
| 25 | B | 848 | LMG | C10-C11-C12-C13 |
| 20 | 1 | 201 | CLA | O1D-CGD-O2D-CED |
| 21 | 3 | 319 | LMU | C2'-C1'-O1'-C1 |
| 22 | F | 203 | BCR | C20-C21-C22-C23 |
| 25 | B | 848 | LMG | C2-C1-O1-C7 |
| 21 | 4 | 321 | LMU | C6-C7-C8-C9 |
| 21 | A | 852 | LMU | C7-C8-C9-C10 |
| 21 | H | 105 | LMU | C4-C5-C6-C7 |
| 20 | 3 | 310 | CLA | C13-C15-C16-C17 |
| 20 | A | 838 | CLA | C10-C11-C12-C13 |
| 20 | B | 809 | CLA | C10-C11-C12-C13 |
| 20 | 3 | 314 | CLA | C16-C17-C18-C20 |
| 20 | B | 837 | CLA | C11-C12-C13-C14 |
| 20 | B | 840 | CLA | C16-C17-C18-C19 |
| 20 | I | 102 | CLA | C11-C12-C13-C14 |
| 20 | L | 203 | CLA | C16-C17-C18-C20 |
| 20 | A | 812 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 836 | CLA | O1D-CGD-O2D-CED |
| 21 | A | 852 | LMU | O5B-C1B-O1B-C4' |
| 20 | B | 825 | CLA | C5-C6-C7-C8 |
| 21 | 2 | 313 | LMU | C11-C10-C9-C8 |
| 21 | 2 | 321 | LMU | C7-C8-C9-C10 |
| 21 | 4 | 316 | LMU | C7-C8-C9-C10 |
| 21 | 4 | 320 | LMU | C3-C4-C5-C6 |
| 21 | A | 848 | LMU | C11-C10-C9-C8 |
| 21 | A | 854 | LMU | C3-C4-C5-C6 |
| 21 | A | 855 | LMU | C7-C8-C9-C10 |
| 21 | G | 103 | LMU | C5-C6-C7-C8 |
| 20 | F | 207 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 2 | 312 | CLA | C11-C12-C13-C14 |
| 20 | 3 | 310 | CLA | C11-C12-C13-C14 |
| 20 | A | 850 | CLA | C11-C12-C13-C14 |
| 20 | B | 840 | CLA | C14-C13-C15-C16 |
| 20 | B | 850 | CLA | C11-C10-C8-C9 |
| 20 | B | 850 | CLA | C14-C13-C15-C16 |
| 21 | A | 846 | LMU | C5-C6-C7-C8 |
| 21 | B | 805 | LMU | C5-C6-C7-C8 |
| 21 | C | 101 | LMU | C6-C7-C8-C9 |
| 21 | G | 103 | LMU | C7-C8-C9-C10 |
| 21 | 3 | 319 | LMU | O5'-C5'-C6'-O6' |
| 21 | K | 107 | LMU | O5'-C5'-C6'-O6' |
| 20 | 1 | 211 | CLA | C2A-CAA-CBA-CGA |
| 20 | 3 | 313 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 823 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 829 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 836 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 840 | CLA | C2A-CAA-CBA-CGA |
| 20 | H | 108 | CLA | C2A-CAA-CBA-CGA |
| 22 | 2 | 317 | BCR | C11-C12-C13-C35 |
| 22 | B | 844 | BCR | C7-C8-C9-C34 |
| 22 | F | 203 | BCR | C37-C22-C23-C24 |
| 22 | G | 104 | BCR | C37-C22-C23-C24 |
| 22 | I | 103 | BCR | C37-C22-C23-C24 |
| 22 | J | 102 | BCR | C37-C22-C23-C24 |
| 20 | 1 | 207 | CLA | C4C-C3C-CAC-CBC |
| 21 | 3 | 319 | LMU | C7-C8-C9-C10 |
| 21 | 4 | 319 | LMU | C6-C7-C8-C9 |
| 21 | A | 846 | LMU | C11-C10-C9-C8 |
| 21 | A | 848 | LMU | C6-C7-C8-C9 |
| 21 | A | 852 | LMU | C5-C6-C7-C8 |
| 21 | H | 104 | LMU | C5'-C4'-O1B-C1B |
| 21 | K | 106 | LMU | C3-C4-C5-C6 |
| 21 | L | 206 | LMU | C2-C3-C4-C5 |
| 22 | A | 845 | BCR | C7-C8-C9-C10 |
| 22 | B | 844 | BCR | C7-C8-C9-C10 |
| 22 | G | 104 | BCR | C21-C22-C23-C24 |
| 22 | I | 101 | BCR | C17-C18-C19-C20 |
| 22 | I | 103 | BCR | C21-C22-C23-C24 |
| 22 | J | 102 | BCR | C21-C22-C23-C24 |
| 20 | K | 104 | CLA | C3-C5-C6-C7 |
| 20 | A | 831 | CLA | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 4 | 316 | LMU | C11-C10-C9-C8 |
| 21 | A | 846 | LMU | C3-C4-C5-C6 |
| 21 | H | 105 | LMU | C7-C8-C9-C10 |
| 21 | A | 852 | LMU | C2B-C1B-O1B-C4' |
| 21 | 3 | 318 | LMU | C11-C10-C9-C8 |
| 21 | A | 847 | LMU | C5-C6-C7-C8 |
| 21 | A | 847 | LMU | C6-C7-C8-C9 |
| 21 | A | 855 | LMU | C4-C5-C6-C7 |
| 21 | G | 103 | LMU | C3-C4-C5-C6 |
| 21 | H | 104 | LMU | C2-C3-C4-C5 |
| 21 | K | 105 | LMU | C7-C8-C9-C10 |
| 21 | R | 105 | LMU | C2-C3-C4-C5 |
| 21 | R | 105 | LMU | C7-C8-C9-C10 |
| 21 | R | 109 | LMU | C5-C6-C7-C8 |
| 21 | R | 109 | LMU | C11-C10-C9-C8 |
| 21 | 2 | 319 | LMU | C1-C2-C3-C4 |
| 20 | 1 | 201 | CLA | C4B-C3B-CAB-CBB |
| 20 | 2 | 307 | CLA | C4B-C3B-CAB-CBB |
| 20 | 3 | 313 | CLA | C4B-C3B-CAB-CBB |
| 20 | 4 | 301 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 803 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 807 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 811 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 834 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 809 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 815 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 817 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 818 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 822 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 825 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 829 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 830 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 833 | CLA | C4B-C3B-CAB-CBB |
| 20 | F | 201 | CLA | C4B-C3B-CAB-CBB |
| 20 | H | 108 | CLA | C4B-C3B-CAB-CBB |
| 20 | R | 107 | CLA | C4B-C3B-CAB-CBB |
| 20 | 3 | 311 | CLA | C16-C17-C18-C19 |
| 20 | 3 | 314 | CLA | C16-C17-C18-C19 |
| 20 | A | 828 | CLA | C16-C17-C18-C19 |
| 20 | A | 828 | CLA | C16-C17-C18-C20 |
| 20 | A | 850 | CLA | C16-C17-C18-C19 |
| 20 | L | 203 | CLA | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | A | 842 | PQN | C26-C27-C28-C30 |
| 20 | A | 828 | CLA | C8-C10-C11-C12 |
| 20 | A | 815 | CLA | C2C-C3C-CAC-CBC |
| 21 | 1 | 218 | LMU | C6-C7-C8-C9 |
| 21 | 2 | 320 | LMU | C6-C7-C8-C9 |
| 21 | L | 210 | LMU | C6-C7-C8-C9 |
| 21 | R | 103 | LMU | O1'-C1-C2-C3 |
| 25 | B | 848 | LMG | C11-C12-C13-C14 |
| 25 | B | 848 | LMG | C37-C38-C39-C40 |
| 20 | 2 | 310 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 807 | CLA | C2C-C3C-CAC-CBC |
| 21 | B | 804 | LMU | C5-C6-C7-C8 |
| 21 | B | 804 | LMU | C11-C10-C9-C8 |
| 20 | 3 | 310 | CLA | C10-C11-C12-C13 |
| 20 | A | 825 | CLA | C8-C10-C11-C12 |
| 20 | B | 830 | CLA | O1A-CGA-O2A-C1 |
| 21 | 2 | 320 | LMU | C3-C4-C5-C6 |
| 21 | L | 205 | LMU | C4-C5-C6-C7 |
| 21 | L | 206 | LMU | C5-C6-C7-C8 |
| 21 | R | 109 | LMU | C2-C3-C4-C5 |
| 20 | B | 814 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 840 | CLA | CBA-CGA-O2A-C1 |
| 20 | K | 103 | CLA | CBA-CGA-O2A-C1 |
| 21 | 4 | 316 | LMU | C4-C5-C6-C7 |
| 21 | G | 102 | LMU | C2-C3-C4-C5 |
| 21 | G | 102 | LMU | C4-C5-C6-C7 |
| 21 | K | 106 | LMU | O1'-C1-C2-C3 |
| 21 | L | 210 | LMU | C3-C4-C5-C6 |
| 25 | B | 848 | LMG | C40-C41-C42-C43 |
| 20 | B | 813 | CLA | O1D-CGD-O2D-CED |
| 20 | 1 | 203 | CLA | C3A-C2A-CAA-CBA |
| 20 | 3 | 311 | CLA | C3A-C2A-CAA-CBA |
| 20 | 4 | 310 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 806 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 809 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 815 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 825 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 814 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 816 | CLA | C3A-C2A-CAA-CBA |
| 20 | F | 201 | CLA | C3A-C2A-CAA-CBA |
| 20 | K | 104 | CLA | C3A-C2A-CAA-CBA |
| 20 | L | 201 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | L | 207 | CLA | C3A-C2A-CAA-CBA |
| 20 | L | 208 | CLA | C3A-C2A-CAA-CBA |
| 20 | R | 107 | CLA | C3A-C2A-CAA-CBA |
| 20 | 2 | 303 | CLA | C5-C6-C7-C8 |
| 20 | A | 830 | CLA | C15-C16-C17-C18 |
| 20 | A | 838 | CLA | C5-C6-C7-C8 |
| 20 | B | 850 | CLA | C10-C11-C12-C13 |
| 21 | G | 102 | LMU | C2-C1-O1'-C1' |
| 21 | G | 103 | LMU | C2-C1-O1'-C1' |
| 21 | 2 | 318 | LMU | C5-C6-C7-C8 |
| 21 | 3 | 318 | LMU | O1'-C1-C2-C3 |
| 21 | F | 202 | LMU | C5-C6-C7-C8 |
| 21 | K | 107 | LMU | C11-C10-C9-C8 |
| 20 | A | 825 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 850 | CLA | C16-C17-C18-C20 |
| 20 | A | 839 | CLA | C8-C10-C11-C12 |
| 21 | G | 101 | LMU | C3-C4-C5-C6 |
| 21 | 2 | 313 | LMU | C1-C2-C3-C4 |
| 21 | R | 102 | LMU | C1-C2-C3-C4 |
| 20 | B | 833 | CLA | O2A-C1-C2-C3 |
| 20 | 2 | 303 | CLA | C3-C5-C6-C7 |
| 20 | B | 825 | CLA | C3-C5-C6-C7 |
| 21 | R | 105 | LMU | C5-C6-C7-C8 |
| 20 | 3 | 314 | CLA | C8-C10-C11-C12 |
| 20 | A | 825 | CLA | C4-C3-C5-C6 |
| 20 | A | 823 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 835 | CLA | C2-C3-C5-C6 |
| 21 | R | 103 | LMU | C1-C2-C3-C4 |
| 21 | 1 | 216 | LMU | C4B-C5B-C6B-O6B |
| 21 | 2 | 319 | LMU | C2-C3-C4-C5 |
| 21 | 4 | 321 | LMU | C2-C3-C4-C5 |
| 21 | A | 847 | LMU | C11-C10-C9-C8 |
| 21 | A | 853 | LMU | O1'-C1-C2-C3 |
| 21 | A | 854 | LMU | C7-C8-C9-C10 |
| 21 | G | 101 | LMU | C11-C10-C9-C8 |
| 20 | B | 837 | CLA | C11-C12-C13-C15 |
| 21 | B | 805 | LMU | C11-C10-C9-C8 |
| 21 | L | 210 | LMU | C1-C2-C3-C4 |
| 20 | 2 | 311 | CLA | C2B-C3B-CAB-CBB |
| 20 | 3 | 307 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 811 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 807 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 816 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 833 | CLA | C2B-C3B-CAB-CBB |
| 20 | L | 207 | CLA | C2B-C3B-CAB-CBB |
| 21 | 2 | 320 | LMU | O5'-C5'-C6'-O6' |
| 21 | A | 852 | LMU | C1-C2-C3-C4 |
| 20 | A | 851 | CLA | C4C-C3C-CAC-CBC |
| 25 | B | 848 | LMG | C15-C16-C17-C18 |
| 20 | B | 838 | CLA | C15-C16-C17-C18 |
| 20 | 1 | 201 | CLA | C4C-C3C-CAC-CBC |
| 21 | 3 | 319 | LMU | C5'-C4'-O1B-C1B |
| 21 | R | 109 | LMU | C1-C2-C3-C4 |
| 20 | 2 | 302 | CLA | C2-C1-O2A-CGA |
| 20 | 2 | 316 | CLA | C2-C1-O2A-CGA |
| 20 | B | 832 | CLA | C2-C1-O2A-CGA |
| 21 | 1 | 217 | LMU | C5-C6-C7-C8 |
| 21 | 3 | 319 | LMU | C3-C4-C5-C6 |
| 25 | B | 848 | LMG | C35-C36-C37-C38 |
| 20 | B | 820 | CLA | C8-C10-C11-C12 |
| 20 | H | 101 | CLA | C5-C6-C7-C8 |
| 21 | L | 206 | LMU | C4'-C5'-C6'-O6' |
| 21 | H | 105 | LMU | C5'-C4'-O1B-C1B |
| 20 | L | 202 | CLA | C6-C7-C8-C9 |
| 22 | 2 | 317 | BCR | C23-C24-C25-C26 |
| 22 | 2 | 317 | BCR | C23-C24-C25-C30 |
| 22 | A | 843 | BCR | C23-C24-C25-C26 |
| 22 | A | 843 | BCR | C23-C24-C25-C30 |
| 22 | A | 844 | BCR | C1-C6-C7-C8 |
| 22 | A | 844 | BCR | C5-C6-C7-C8 |
| 22 | A | 844 | BCR | C23-C24-C25-C26 |
| 22 | A | 845 | BCR | C23-C24-C25-C30 |
| 22 | B | 847 | BCR | C1-C6-C7-C8 |
| 22 | B | 847 | BCR | C23-C24-C25-C26 |
| 22 | B | 847 | BCR | C23-C24-C25-C30 |
| 22 | F | 203 | BCR | C1-C6-C7-C8 |
| 22 | F | 203 | BCR | C5-C6-C7-C8 |
| 22 | F | 203 | BCR | C23-C24-C25-C26 |
| 22 | F | 203 | BCR | C23-C24-C25-C30 |
| 22 | G | 104 | BCR | C23-C24-C25-C26 |
| 22 | G | 104 | BCR | C23-C24-C25-C30 |
| 22 | I | 101 | BCR | C1-C6-C7-C8 |
| 22 | J | 102 | BCR | C1-C6-C7-C8 |
| 22 | J | 102 | BCR | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | L | 209 | BCR | C5-C6-C7-C8 |
| 21 | H | 103 | LMU | C2-C3-C4-C5 |
| 20 | 1 | 215 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 803 | CLA | C15-C16-C17-C18 |
| 20 | B | 814 | CLA | C15-C16-C17-C18 |
| 20 | B | 829 | CLA | C10-C11-C12-C13 |
| 20 | I | 102 | CLA | C8-C10-C11-C12 |
| 20 | R | 108 | CLA | C10-C11-C12-C13 |
| 21 | R | 103 | LMU | C4'-C5'-C6'-O6' |
| 21 | 1 | 217 | LMU | C6-C7-C8-C9 |
| 21 | 3 | 319 | LMU | C9-C10-C11-C12 |
| 21 | A | 852 | LMU | C4-C5-C6-C7 |
| 21 | G | 102 | LMU | C5-C6-C7-C8 |
| 21 | R | 109 | LMU | C9-C10-C11-C12 |
| 20 | B | 814 | CLA | O1A-CGA-O2A-C1 |
| 21 | 4 | 319 | LMU | C4-C5-C6-C7 |
| 21 | A | 853 | LMU | C5-C6-C7-C8 |
| 21 | A | 853 | LMU | C6-C7-C8-C9 |
| 21 | F | 202 | LMU | C7-C8-C9-C10 |
| 20 | A | 831 | CLA | C10-C11-C12-C13 |
| 20 | A | 812 | CLA | C5-C6-C7-C8 |
| 21 | 1 | 218 | LMU | C11-C10-C9-C8 |
| 21 | L | 205 | LMU | C11-C10-C9-C8 |
| 21 | R | 101 | LMU | C11-C10-C9-C8 |
| 20 | A | 835 | CLA | C4-C3-C5-C6 |
| 20 | B | 808 | CLA | C4-C3-C5-C6 |
| 20 | B | 815 | CLA | C4-C3-C5-C6 |
| 20 | 2 | 316 | CLA | C11-C12-C13-C15 |
| 20 | A | 808 | CLA | C6-C7-C8-C10 |
| 20 | A | 823 | CLA | C11-C10-C8-C7 |
| 20 | A | 825 | CLA | C2-C3-C5-C6 |
| 20 | A | 828 | CLA | C11-C10-C8-C7 |
| 20 | A | 838 | CLA | C6-C7-C8-C10 |
| 20 | A | 850 | CLA | C11-C12-C13-C15 |
| 20 | A | 851 | CLA | C6-C7-C8-C10 |
| 20 | B | 808 | CLA | C2-C3-C5-C6 |
| 20 | B | 809 | CLA | C11-C10-C8-C7 |
| 20 | B | 809 | CLA | C11-C12-C13-C15 |
| 20 | B | 814 | CLA | C12-C13-C15-C16 |
| 20 | B | 815 | CLA | C2-C3-C5-C6 |
| 20 | B | 828 | CLA | C6-C7-C8-C10 |
| 20 | B | 828 | CLA | C11-C10-C8-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 850 | CLA | C11-C10-C8-C7 |
| 20 | B | 850 | CLA | C12-C13-C15-C16 |
| 20 | H | 108 | CLA | C11-C10-C8-C7 |
| 23 | B | 843 | PQN | C21-C22-C23-C25 |
| 20 | A | 823 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 840 | CLA | O1A-CGA-O2A-C1 |
| 21 | 1 | 218 | LMU | C5'-C4'-O1B-C1B |
| 20 | B | 841 | CLA | C10-C11-C12-C13 |
| 20 | A | 835 | CLA | C16-C17-C18-C20 |
| 20 | B | 840 | CLA | C16-C17-C18-C20 |
| 20 | I | 102 | CLA | C11-C12-C13-C15 |
| 20 | A | 813 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 823 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 827 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 847 | LMU | C3-C4-C5-C6 |
| 20 | A | 808 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 808 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 834 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 836 | CLA | C2A-CAA-CBA-CGA |
| 20 | F | 201 | CLA | C2A-CAA-CBA-CGA |
| 20 | 4 | 304 | CLA | C5-C6-C7-C8 |
| 20 | B | 840 | CLA | C8-C10-C11-C12 |
| 21 | 2 | 319 | LMU | C4-C5-C6-C7 |
| 21 | A | 847 | LMU | C2-C3-C4-C5 |
| 21 | R | 104 | LMU | O1'-C1-C2-C3 |
| 21 | C | 101 | LMU | O5'-C5'-C6'-O6' |
| 20 | 4 | 306 | CLA | O1D-CGD-O2D-CED |
| 20 | A | 850 | CLA | C15-C16-C17-C18 |
| 21 | R | 105 | LMU | C1-C2-C3-C4 |
| 21 | R | 106 | LMU | C1-C2-C3-C4 |
| 20 | B | 815 | CLA | C3-C5-C6-C7 |
| 20 | 2 | 305 | CLA | C4C-C3C-CAC-CBC |
| 20 | 3 | 310 | CLA | C2C-C3C-CAC-CBC |
| 20 | 3 | 314 | CLA | C2C-C3C-CAC-CBC |
| 21 | A | 855 | LMU | C11-C10-C9-C8 |
| 20 | B | 838 | CLA | C16-C17-C18-C19 |
| 21 | A | 854 | LMU | C4'-C5'-C6'-O6' |
| 20 | 4 | 303 | CLA | C8-C10-C11-C12 |
| 20 | B | 850 | CLA | C8-C10-C11-C12 |
| 21 | L | 205 | LMU | C1-C2-C3-C4 |
| 21 | B | 804 | LMU | C3-C4-C5-C6 |
| 21 | K | 105 | LMU | C11-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | K | 106 | LMU | C11-C10-C9-C8 |
| 21 | L | 210 | LMU | C7-C8-C9-C10 |
| 25 | B | 848 | LMG | C39-C40-C41-C42 |
| 21 | G | 101 | LMU | C6-C7-C8-C9 |
| 21 | L | 210 | LMU | C2-C3-C4-C5 |
| 21 | 4 | 321 | LMU | C1-C2-C3-C4 |
| 20 | 2 | 307 | CLA | C10-C11-C12-C13 |
| 20 | B | 809 | CLA | C8-C10-C11-C12 |
| 20 | B | 850 | CLA | C5-C6-C7-C8 |
| 21 | 2 | 321 | LMU | C2-C3-C4-C5 |
| 21 | 4 | 321 | LMU | C11-C10-C9-C8 |
| 21 | H | 103 | LMU | C7-C8-C9-C10 |
| 20 | A | 808 | CLA | C3-C5-C6-C7 |
| 21 | A | 855 | LMU | C2'-C1'-O1'-C1 |
| 21 | K | 107 | LMU | C2'-C1'-O1'-C1 |
| 21 | R | 104 | LMU | C2'-C1'-O1'-C1 |
| 21 | B | 804 | LMU | O5'-C5'-C6'-O6' |
| 21 | 2 | 313 | LMU | O1'-C1-C2-C3 |
| 21 | A | 852 | LMU | C11-C10-C9-C8 |
| 20 | A | 827 | CLA | CBD-CGD-O2D-CED |
| 20 | 1 | 215 | CLA | O1A-CGA-O2A-C1 |
| 21 | 3 | 318 | LMU | C5-C6-C7-C8 |
| 21 | A | 848 | LMU | C3-C4-C5-C6 |
| 21 | B | 804 | LMU | C7-C8-C9-C10 |
| 21 | 2 | 321 | LMU | O5B-C5B-C6B-O6B |
| 21 | R | 102 | LMU | O5'-C5'-C6'-O6' |
| 20 | A | 849 | CLA | C13-C15-C16-C17 |
| 20 | A | 851 | CLA | C13-C15-C16-C17 |
| 20 | B | 829 | CLA | C5-C6-C7-C8 |
| 20 | 4 | 301 | CLA | C4-C3-C5-C6 |
| 20 | 1 | 206 | CLA | C2-C3-C5-C6 |
| 20 | A | 830 | CLA | C2-C3-C5-C6 |
| 20 | B | 810 | CLA | C2-C3-C5-C6 |
| 20 | 4 | 303 | CLA | C14-C13-C15-C16 |
| 20 | A | 811 | CLA | C11-C12-C13-C14 |
| 20 | A | 818 | CLA | C6-C7-C8-C9 |
| 20 | A | 823 | CLA | C11-C10-C8-C9 |
| 20 | A | 825 | CLA | C6-C7-C8-C9 |
| 20 | A | 838 | CLA | C6-C7-C8-C9 |
| 20 | B | 803 | CLA | C6-C7-C8-C9 |
| 20 | B | 809 | CLA | C11-C10-C8-C9 |
| 20 | B | 809 | CLA | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 814 | CLA | C14-C13-C15-C16 |
| 20 | B | 824 | CLA | C11-C12-C13-C14 |
| 20 | B | 828 | CLA | C11-C10-C8-C9 |
| 20 | H | 108 | CLA | C11-C10-C8-C9 |
| 20 | L | 203 | CLA | C11-C10-C8-C9 |
| 20 | L | 203 | CLA | C11-C12-C13-C14 |
| 23 | B | 843 | PQN | C21-C22-C23-C24 |
| 21 | G | 103 | LMU | O5'-C5'-C6'-O6' |
| 20 | K | 103 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 831 | CLA | C3-C5-C6-C7 |
| 20 | 2 | 314 | CLA | C2A-CAA-CBA-CGA |
| 20 | 4 | 301 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 827 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 829 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 853 | LMU | C1-C2-C3-C4 |
| 20 | B | 827 | CLA | C8-C10-C11-C12 |
| 20 | L | 207 | CLA | C2C-C3C-CAC-CBC |
| 21 | L | 205 | LMU | C5-C6-C7-C8 |
| 22 | 2 | 317 | BCR | C11-C12-C13-C14 |
| 22 | B | 846 | BCR | C21-C22-C23-C24 |
| 20 | B | 827 | CLA | O1A-CGA-O2A-C1 |
| 20 | 1 | 203 | CLA | C1A-C2A-CAA-CBA |
| 20 | 1 | 206 | CLA | C1A-C2A-CAA-CBA |
| 20 | 1 | 213 | CLA | C1A-C2A-CAA-CBA |
| 20 | 3 | 313 | CLA | C1A-C2A-CAA-CBA |
| 20 | 4 | 303 | CLA | C1A-C2A-CAA-CBA |
| 20 | 4 | 318 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 804 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 820 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 825 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 837 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 840 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 849 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 802 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 816 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 817 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 828 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 839 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 841 | CLA | C1A-C2A-CAA-CBA |
| 20 | F | 201 | CLA | C1A-C2A-CAA-CBA |
| 20 | J | 103 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 811 | CLA | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | A | 818 | CLA | C11-C12-C13-C14 |
| 20 | B | 813 | CLA | C6-C7-C8-C9 |
| 20 | B | 813 | CLA | C6-C7-C8-C10 |
| 21 | 2 | 319 | LMU | C5-C6-C7-C8 |
| 21 | 2 | 319 | LMU | C7-C8-C9-C10 |
| 22 | F | 203 | BCR | C13-C14-C15-C16 |
| 20 | 4 | 303 | CLA | C5-C6-C7-C8 |
| 20 | B | 809 | CLA | C13-C15-C16-C17 |
| 20 | B | 820 | CLA | C5-C6-C7-C8 |
| 21 | 4 | 316 | LMU | C1-C2-C3-C4 |
| 21 | A | 852 | LMU | C5'-C4'-O1B-C1B |
| 21 | A | 852 | LMU | C4B-C5B-C6B-O6B |
| 21 | H | 104 | LMU | C6-C7-C8-C9 |
| 21 | H | 104 | LMU | C11-C10-C9-C8 |
| 21 | G | 101 | LMU | C1-C2-C3-C4 |
| 20 | 2 | 312 | CLA | C8-C10-C11-C12 |
| 20 | B | 803 | CLA | CBA-CGA-O2A-C1 |
| 20 | K | 103 | CLA | O1D-CGD-O2D-CED |
| 21 | K | 105 | LMU | C1-C2-C3-C4 |
| 20 | 4 | 304 | CLA | C6-C7-C8-C10 |
| 21 | A | 848 | LMU | O5B-C5B-C6B-O6B |
| 21 | L | 206 | LMU | C11-C10-C9-C8 |
| 20 | 1 | 206 | CLA | C3-C5-C6-C7 |
| 21 | 2 | 318 | LMU | C4'-C5'-C6'-O6' |
| 20 | 2 | 302 | CLA | C4C-C3C-CAC-CBC |
| 21 | 2 | 320 | LMU | O1'-C1-C2-C3 |
| 20 | A | 830 | CLA | C4-C3-C5-C6 |
| 20 | B | 810 | CLA | C4-C3-C5-C6 |
| 21 | 2 | 318 | LMU | C2-C3-C4-C5 |
| 21 | 2 | 321 | LMU | C6-C7-C8-C9 |
| 21 | H | 103 | LMU | C3-C4-C5-C6 |
| 21 | K | 106 | LMU | C6-C7-C8-C9 |
| 21 | R | 103 | LMU | C4-C5-C6-C7 |
| 20 | A | 813 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 823 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 855 | LMU | C5-C6-C7-C8 |
| 20 | B | 815 | CLA | C11-C12-C13-C15 |
| 20 | B | 829 | CLA | C16-C17-C18-C20 |
| 21 | H | 103 | LMU | O5'-C5'-C6'-O6' |
| 20 | R | 108 | CLA | C3-C5-C6-C7 |
| 20 | B | 832 | CLA | C10-C11-C12-C13 |
| 21 | 4 | 319 | LMU | C11-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 846 | LMU | C9-C10-C11-C12 |
| 25 | B | 848 | LMG | O1-C7-C8-C9 |
| 20 | B | 825 | CLA | C6-C7-C8-C9 |
| 21 | H | 105 | LMU | C9-C10-C11-C12 |
| 21 | C | 101 | LMU | C5-C6-C7-C8 |
| 21 | H | 104 | LMU | C9-C10-C11-C12 |
| 21 | R | 101 | LMU | C9-C10-C11-C12 |
| 21 | B | 804 | LMU | C4-C5-C6-C7 |
| 21 | G | 101 | LMU | C4-C5-C6-C7 |
| 21 | 2 | 321 | LMU | O5'-C1'-O1'-C1 |
| 21 | 2 | 318 | LMU | C9-C10-C11-C12 |
| 21 | F | 202 | LMU | C11-C10-C9-C8 |
| 21 | H | 106 | LMU | C9-C10-C11-C12 |
| 20 | A | 809 | CLA | C2C-C3C-CAC-CBC |
| 21 | 1 | 217 | LMU | O5'-C5'-C6'-O6' |
| 21 | 4 | 319 | LMU | O1'-C1-C2-C3 |
| 21 | E | 101 | LMU | C9-C10-C11-C12 |
| 21 | A | 854 | LMU | C1-C2-C3-C4 |
| 20 | 2 | 303 | CLA | C10-C11-C12-C13 |
| 20 | A | 819 | CLA | C10-C11-C12-C13 |
| 21 | H | 106 | LMU | C11-C10-C9-C8 |
| 20 | B | 828 | CLA | C10-C11-C12-C13 |
| 21 | E | 101 | LMU | O5B-C5B-C6B-O6B |
| 21 | K | 105 | LMU | O5B-C5B-C6B-O6B |
| 20 | A | 812 | CLA | C4-C3-C5-C6 |
| 20 | B | 850 | CLA | C4-C3-C5-C6 |
| 21 | R | 105 | LMU | C5'-C4'-O1B-C1B |
| 20 | 2 | 307 | CLA | C16-C17-C18-C20 |
| 20 | A | 827 | CLA | C6-C7-C8-C10 |
| 20 | A | 830 | CLA | C16-C17-C18-C19 |
| 23 | B | 843 | PQN | C26-C27-C28-C30 |
| 20 | 4 | 305 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 811 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 829 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 847 | LMU | C9-C10-C11-C12 |
| 20 | A | 816 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 826 | CLA | C2A-CAA-CBA-CGA |
| 20 | 1 | 215 | CLA | C2-C1-O2A-CGA |
| 20 | 3 | 310 | CLA | C2-C1-O2A-CGA |
| 20 | A | 804 | CLA | C2-C1-O2A-CGA |
| 20 | B | 838 | CLA | C2-C1-O2A-CGA |
| 21 | B | 805 | LMU | C5'-C4'-O1B-C1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | R | 104 | LMU | C9-C10-C11-C12 |
| 21 | 3 | 319 | LMU | O5B-C5B-C6B-O6B |
| 21 | B | 805 | LMU | O5B-C5B-C6B-O6B |
| 20 | A | 816 | CLA | C6-C7-C8-C9 |
| 21 | H | 104 | LMU | C3'-C4'-O1B-C1B |
| 21 | 4 | 316 | LMU | C4B-C5B-C6B-O6B |
| 20 | 2 | 316 | CLA | C8-C10-C11-C12 |
| 20 | 2 | 312 | CLA | C4C-C3C-CAC-CBC |
| 20 | L | 204 | CLA | CBA-CGA-O2A-C1 |
| 21 | 4 | 321 | LMU | O5'-C5'-C6'-O6' |
| 21 | 1 | 216 | LMU | C5-C6-C7-C8 |
| 21 | D | 201 | LMU | C3-C4-C5-C6 |
| 21 | E | 101 | LMU | C4-C5-C6-C7 |
| 21 | A | 847 | LMU | O1'-C1-C2-C3 |
| 21 | K | 105 | LMU | C9-C10-C11-C12 |
| 20 | B | 803 | CLA | O1A-CGA-O2A-C1 |
| 21 | A | 854 | LMU | C4-C5-C6-C7 |
| 21 | 2 | 319 | LMU | C2'-C1'-O1'-C1 |
| 20 | B | 828 | CLA | C5-C6-C7-C8 |
| 20 | B | 840 | CLA | C5-C6-C7-C8 |
| 20 | 4 | 305 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 848 | LMG | O6-C5-C6-O5 |
| 20 | B | 813 | CLA | C4-C3-C5-C6 |
| 20 | J | 103 | CLA | C4-C3-C5-C6 |
| 20 | 2 | 310 | CLA | C4C-C3C-CAC-CBC |
| 20 | B | 807 | CLA | C4C-C3C-CAC-CBC |
| 21 | 4 | 319 | LMU | C3'-C4'-O1B-C1B |
| 20 | 2 | 303 | CLA | C11-C10-C8-C7 |
| 20 | 3 | 310 | CLA | C11-C12-C13-C15 |
| 20 | 3 | 311 | CLA | C11-C10-C8-C7 |
| 20 | A | 812 | CLA | C2-C3-C5-C6 |
| 20 | A | 825 | CLA | C6-C7-C8-C10 |
| 20 | A | 851 | CLA | C11-C10-C8-C7 |
| 20 | A | 851 | CLA | C11-C12-C13-C15 |
| 20 | B | 806 | CLA | C12-C13-C15-C16 |
| 20 | B | 808 | CLA | C6-C7-C8-C10 |
| 20 | B | 808 | CLA | C11-C12-C13-C15 |
| 20 | B | 809 | CLA | C12-C13-C15-C16 |
| 20 | B | 813 | CLA | C2-C3-C5-C6 |
| 20 | B | 815 | CLA | C6-C7-C8-C10 |
| 20 | B | 820 | CLA | C11-C12-C13-C15 |
| 20 | B | 826 | CLA | C11-C10-C8-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 830 | CLA | C6-C7-C8-C10 |
| 20 | B | 830 | CLA | C11-C10-C8-C7 |
| 20 | B | 830 | CLA | C12-C13-C15-C16 |
| 20 | B | 837 | CLA | C6-C7-C8-C10 |
| 20 | B | 840 | CLA | C11-C10-C8-C7 |
| 20 | R | 108 | CLA | C6-C7-C8-C10 |
| 20 | R | 108 | CLA | C11-C10-C8-C7 |
| 20 | R | 108 | CLA | C11-C12-C13-C15 |
| 21 | B | 849 | LMU | O5B-C5B-C6B-O6B |
| 21 | 1 | 217 | LMU | C7-C8-C9-C10 |
| 20 | 2 | 312 | CLA | C6-C7-C8-C9 |
| 20 | 2 | 312 | CLA | C11-C10-C8-C9 |
| 20 | 2 | 316 | CLA | C11-C12-C13-C14 |
| 20 | 3 | 311 | CLA | C11-C10-C8-C9 |
| 20 | 4 | 303 | CLA | C11-C12-C13-C14 |
| 20 | A | 851 | CLA | C14-C13-C15-C16 |
| 20 | B | 809 | CLA | C6-C7-C8-C9 |
| 20 | B | 809 | CLA | C14-C13-C15-C16 |
| 20 | B | 815 | CLA | C6-C7-C8-C9 |
| 20 | B | 816 | CLA | C6-C7-C8-C9 |
| 20 | B | 820 | CLA | C11-C10-C8-C9 |
| 20 | B | 829 | CLA | C11-C12-C13-C14 |
| 20 | B | 830 | CLA | C6-C7-C8-C9 |
| 20 | B | 837 | CLA | C6-C7-C8-C9 |
| 20 | J | 103 | CLA | C6-C7-C8-C9 |
| 20 | J | 103 | CLA | C11-C10-C8-C9 |
| 22 | B | 801 | BCR | C19-C20-C21-C22 |
| 20 | 2 | 302 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 822 | CLA | CBA-CGA-O2A-C1 |
| 20 | J | 101 | CLA | CBA-CGA-O2A-C1 |
| 20 | L | 208 | CLA | C2A-CAA-CBA-CGA |
| 22 | I | 103 | BCR | C7-C8-C9-C34 |
| 20 | B | 830 | CLA | C13-C15-C16-C17 |
| 20 | H | 102 | CLA | C6-C7-C8-C9 |
| 20 | H | 101 | CLA | C3-C5-C6-C7 |
| 21 | 1 | 216 | LMU | C4-C5-C6-C7 |
| 21 | 2 | 318 | LMU | C3-C4-C5-C6 |
| 20 | 4 | 306 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 841 | CLA | CBA-CGA-O2A-C1 |
| 21 | 1 | 218 | LMU | C1-C2-C3-C4 |
| 20 | B | 814 | CLA | C13-C15-C16-C17 |
| 20 | R | 108 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 846 | LMU | C6-C7-C8-C9 |
| 21 | G | 101 | LMU | C9-C10-C11-C12 |
| 20 | 3 | 311 | CLA | C4B-C3B-CAB-CBB |
| 20 | 4 | 305 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 815 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 832 | CLA | C4B-C3B-CAB-CBB |
| 20 | F | 206 | CLA | C4B-C3B-CAB-CBB |
| 20 | H | 108 | CLA | C8-C10-C11-C12 |
| 20 | B | 810 | CLA | C3-C5-C6-C7 |
| 21 | B | 805 | LMU | C1-C2-C3-C4 |
| 21 | 3 | 318 | LMU | C7-C8-C9-C10 |
| 20 | A | 811 | CLA | C8-C10-C11-C12 |
| 20 | A | 819 | CLA | O1D-CGD-O2D-CED |
| 20 | B | 830 | CLA | C4-C3-C5-C6 |
| 20 | B | 850 | CLA | C2-C3-C5-C6 |
| 20 | J | 103 | CLA | C2-C3-C5-C6 |
| 20 | B | 815 | CLA | C8-C10-C11-C12 |
| 20 | B | 827 | CLA | C13-C15-C16-C17 |
| 20 | 1 | 206 | CLA | C14-C13-C15-C16 |
| 20 | J | 103 | CLA | C14-C13-C15-C16 |
| 20 | A | 805 | CLA | C5-C6-C7-C8 |
| 21 | A | 855 | LMU | C1-C2-C3-C4 |
| 21 | G | 103 | LMU | C1-C2-C3-C4 |
| 20 | A | 815 | CLA | C4C-C3C-CAC-CBC |
| 21 | D | 201 | LMU | C6-C7-C8-C9 |
| 21 | G | 102 | LMU | C5'-C4'-O1B-C1B |
| 25 | B | 848 | LMG | C13-C14-C15-C16 |
| 20 | 1 | 203 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 830 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 855 | LMU | C2-C3-C4-C5 |
| 21 | F | 202 | LMU | C2-C3-C4-C5 |
| 20 | 2 | 307 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 820 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 837 | CLA | C3A-C2A-CAA-CBA |
| 20 | F | 207 | CLA | C3A-C2A-CAA-CBA |
| 20 | H | 108 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 819 | CLA | C8-C10-C11-C12 |
| 21 | L | 205 | LMU | C2-C3-C4-C5 |
| 21 | R | 102 | LMU | C9-C10-C11-C12 |
| 21 | R | 105 | LMU | C3'-C4'-O1B-C1B |
| 21 | H | 105 | LMU | C4B-C5B-C6B-O6B |
| 22 | A | 844 | BCR | C19-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 2 | 313 | LMU | C2-C1-O1'-C1' |
| 21 | 2 | 318 | LMU | C2-C1-O1'-C1' |
| 21 | 2 | 320 | LMU | C2-C1-O1'-C1' |
| 21 | 3 | 318 | LMU | C2-C1-O1'-C1' |
| 21 | 4 | 320 | LMU | C2-C1-O1'-C1' |
| 21 | A | 853 | LMU | C2-C1-O1'-C1' |
| 21 | C | 101 | LMU | C2-C1-O1'-C1' |
| 21 | F | 202 | LMU | C2-C1-O1'-C1' |
| 21 | H | 103 | LMU | C2-C1-O1'-C1' |
| 21 | K | 107 | LMU | C2-C1-O1'-C1' |
| 21 | R | 103 | LMU | C2-C1-O1'-C1' |
| 20 | B | 812 | CLA | C5-C6-C7-C8 |
| 20 | B | 830 | CLA | C8-C10-C11-C12 |
| 21 | A | 854 | LMU | C2-C3-C4-C5 |
| 21 | L | 206 | LMU | C7-C8-C9-C10 |
| 20 | 2 | 307 | CLA | C16-C17-C18-C19 |
| 21 | C | 101 | LMU | C9-C10-C11-C12 |
| 21 | A | 846 | LMU | O1'-C1-C2-C3 |
| 21 | G | 103 | LMU | C3'-C4'-O1B-C1B |
| 21 | 2 | 321 | LMU | C9-C10-C11-C12 |
| 20 | B | 815 | CLA | C11-C12-C13-C14 |
| 20 | B | 830 | CLA | C2-C3-C5-C6 |
| 20 | A | 824 | CLA | C10-C11-C12-C13 |
| 21 | G | 103 | LMU | C6-C7-C8-C9 |
| 21 | G | 102 | LMU | C9-C10-C11-C12 |
| 20 | F | 207 | CLA | C5-C6-C7-C8 |
| 21 | 2 | 320 | LMU | C1-C2-C3-C4 |
| 20 | B | 827 | CLA | O1D-CGD-O2D-CED |
| 20 | L | 204 | CLA | O1A-CGA-O2A-C1 |
| 20 | 4 | 304 | CLA | C6-C7-C8-C9 |
| 20 | A | 830 | CLA | C16-C17-C18-C20 |
| 20 | 4 | 310 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 806 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 817 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 828 | CLA | C2B-C3B-CAB-CBB |
| 20 | H | 109 | CLA | C2B-C3B-CAB-CBB |
| 20 | K | 103 | CLA | C2B-C3B-CAB-CBB |
| 20 | 2 | 302 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 822 | CLA | O1A-CGA-O2A-C1 |
| 20 | J | 101 | CLA | O1A-CGA-O2A-C1 |
| 21 | K | 105 | LMU | C6-C7-C8-C9 |
| 21 | 2 | 318 | LMU | O5B-C5B-C6B-O6B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 4 | 315 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 820 | CLA | CBA-CGA-O2A-C1 |
| 20 | 3 | 311 | CLA | C10-C11-C12-C13 |
| 22 | 2 | 317 | BCR | C19-C20-C21-C22 |
| 22 | F | 204 | BCR | C19-C20-C21-C22 |
| 20 | A | 804 | CLA | C6-C7-C8-C10 |
| 21 | 1 | 216 | LMU | O5'-C1'-O1'-C1 |
| 20 | B | 809 | CLA | C5-C6-C7-C8 |
| 20 | B | 832 | CLA | C11-C12-C13-C14 |
| 21 | E | 101 | LMU | O1'-C1-C2-C3 |
| 20 | L | 202 | CLA | C3-C5-C6-C7 |
| 20 | A | 838 | CLA | C2-C1-O2A-CGA |
| 20 | B | 827 | CLA | C2-C1-O2A-CGA |
| 20 | F | 207 | CLA | C2-C1-O2A-CGA |
| 20 | L | 203 | CLA | C2-C1-O2A-CGA |
| 20 | B | 826 | CLA | C5-C6-C7-C8 |
| 20 | 3 | 314 | CLA | C11-C10-C8-C9 |
| 20 | 3 | 314 | CLA | C14-C13-C15-C16 |
| 20 | A | 808 | CLA | C6-C7-C8-C9 |
| 20 | A | 826 | CLA | C6-C7-C8-C9 |
| 20 | B | 814 | CLA | C6-C7-C8-C9 |
| 20 | B | 820 | CLA | C11-C12-C13-C14 |
| 20 | B | 827 | CLA | C6-C7-C8-C9 |
| 20 | B | 829 | CLA | C6-C7-C8-C9 |
| 20 | B | 840 | CLA | C11-C10-C8-C9 |
| 20 | B | 850 | CLA | C6-C7-C8-C9 |
| 21 | G | 102 | LMU | C3'-C4'-O1B-C1B |
| 21 | 1 | 218 | LMU | C9-C10-C11-C12 |
| 20 | B | 835 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 807 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 838 | CLA | C16-C17-C18-C20 |
| 20 | B | 829 | CLA | C16-C17-C18-C19 |
| 23 | A | 842 | PQN | C26-C27-C28-C29 |
| 22 | 2 | 317 | BCR | C5-C6-C7-C8 |
| 22 | A | 844 | BCR | C23-C24-C25-C30 |
| 20 | B | 832 | CLA | C8-C10-C11-C12 |
| 21 | L | 206 | LMU | C1-C2-C3-C4 |
| 20 | A | 850 | CLA | C5-C6-C7-C8 |
| 20 | 4 | 303 | CLA | C16-C17-C18-C20 |
| 20 | B | 838 | CLA | C16-C17-C18-C20 |
| 20 | 3 | 314 | CLA | CBD-CGD-O2D-CED |
| 21 | 3 | 319 | LMU | C2-C3-C4-C5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 852 | LMU | C6-C7-C8-C9 |
| 21 | G | 103 | LMU | C5'-C4'-O1B-C1B |
| 20 | H | 108 | CLA | C2C-C3C-CAC-CBC |
| 23 | B | 843 | PQN | C23-C25-C26-C27 |
| 20 | 2 | 307 | CLA | C6-C7-C8-C10 |
| 20 | 2 | 312 | CLA | C6-C7-C8-C10 |
| 20 | 2 | 312 | CLA | C11-C10-C8-C7 |
| 20 | 3 | 310 | CLA | C6-C7-C8-C10 |
| 20 | 3 | 310 | CLA | C11-C10-C8-C7 |
| 20 | 4 | 303 | CLA | C11-C12-C13-C15 |
| 20 | A | 826 | CLA | C6-C7-C8-C10 |
| 20 | A | 831 | CLA | C6-C7-C8-C10 |
| 20 | A | 835 | CLA | C12-C13-C15-C16 |
| 20 | A | 851 | CLA | C12-C13-C15-C16 |
| 20 | B | 803 | CLA | C6-C7-C8-C10 |
| 20 | B | 809 | CLA | C6-C7-C8-C10 |
| 20 | B | 810 | CLA | C11-C10-C8-C7 |
| 20 | B | 816 | CLA | C6-C7-C8-C10 |
| 20 | B | 820 | CLA | C11-C10-C8-C7 |
| 20 | B | 824 | CLA | C6-C7-C8-C10 |
| 20 | B | 827 | CLA | C11-C12-C13-C15 |
| 20 | B | 829 | CLA | C6-C7-C8-C10 |
| 20 | B | 829 | CLA | C11-C12-C13-C15 |
| 20 | B | 841 | CLA | C11-C12-C13-C15 |
| 20 | B | 841 | CLA | C12-C13-C15-C16 |
| 20 | H | 108 | CLA | C6-C7-C8-C10 |
| 20 | I | 102 | CLA | C11-C10-C8-C7 |
| 20 | J | 103 | CLA | C6-C7-C8-C10 |
| 20 | J | 103 | CLA | C11-C10-C8-C7 |
| 20 | J | 103 | CLA | C11-C12-C13-C15 |
| 23 | A | 842 | PQN | C22-C23-C25-C26 |
| 21 | A | 854 | LMU | C5-C6-C7-C8 |
| 20 | A | 811 | CLA | C13-C15-C16-C17 |
| 20 | A | 838 | CLA | C15-C16-C17-C18 |
| 20 | B | 808 | CLA | C8-C10-C11-C12 |
| 22 | A | 843 | BCR | C19-C20-C21-C22 |
| 22 | B | 844 | BCR | C19-C20-C21-C22 |
| 22 | G | 104 | BCR | C15-C16-C17-C18 |
| 22 | I | 101 | BCR | C15-C16-C17-C18 |
| 20 | 4 | 301 | CLA | C6-C7-C8-C10 |
| 20 | B | 810 | CLA | C11-C12-C13-C15 |
| 23 | B | 843 | PQN | C26-C27-C28-C29 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 854 | LMU | O5B-C1B-O1B-C4' |
| 21 | K | 105 | LMU | C2-C3-C4-C5 |
| 20 | B | 802 | CLA | C5-C6-C7-C8 |
| 20 | A | 823 | CLA | C8-C10-C11-C12 |
| 20 | 2 | 307 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 831 | CLA | C4C-C3C-CAC-CBC |
| 21 | G | 103 | LMU | C4-C5-C6-C7 |
| 21 | 2 | 313 | LMU | C4B-C5B-C6B-O6B |
| 20 | A | 831 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 832 | CLA | CBA-CGA-O2A-C1 |
| 20 | 1 | 206 | CLA | C12-C13-C15-C16 |
| 20 | 2 | 312 | CLA | C12-C13-C15-C16 |
| 20 | J | 103 | CLA | C12-C13-C15-C16 |
| 21 | 2 | 313 | LMU | C5-C6-C7-C8 |
| 20 | 2 | 307 | CLA | CAD-CBD-CGD-O2D |
| 20 | 2 | 312 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 804 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 812 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 819 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 834 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 813 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 814 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 817 | CLA | CAD-CBD-CGD-O2D |
| 20 | K | 103 | CLA | CAD-CBD-CGD-O2D |
| 20 | L | 208 | CLA | CAD-CBD-CGD-O2D |
| 25 | B | 848 | LMG | C9-C8-O7-C10 |
| 21 | G | 102 | LMU | C1-C2-C3-C4 |
| 20 | H | 108 | CLA | C10-C11-C12-C13 |
| 20 | A | 823 | CLA | C5-C6-C7-C8 |
| 20 | H | 102 | CLA | C6-C7-C8-C10 |
| 21 | C | 101 | LMU | C3'-C4'-O1B-C1B |
| 21 | H | 103 | LMU | C5-C6-C7-C8 |
| 20 | A | 811 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 830 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 823 | CLA | C3-C5-C6-C7 |
| 20 | B | 850 | CLA | C3-C5-C6-C7 |
| 21 | C | 101 | LMU | C5'-C4'-O1B-C1B |
| 20 | A | 851 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 808 | CLA | C11-C12-C13-C15 |
| 21 | E | 101 | LMU | C7-C8-C9-C10 |
| 21 | R | 101 | LMU | O1'-C1-C2-C3 |
| 20 | 1 | 204 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 2 | 311 | CLA | CHA-CBD-CGD-O1D |
| 20 | 2 | 311 | CLA | CHA-CBD-CGD-O2D |
| 20 | 2 | 312 | CLA | CHA-CBD-CGD-O1D |
| 20 | 2 | 316 | CLA | CHA-CBD-CGD-O1D |
| 20 | 2 | 316 | CLA | CHA-CBD-CGD-O2D |
| 20 | 3 | 311 | CLA | CHA-CBD-CGD-O1D |
| 20 | 3 | 311 | CLA | CHA-CBD-CGD-O2D |
| 20 | 4 | 318 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 808 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 808 | CLA | CHA-CBD-CGD-O2D |
| 20 | A | 849 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 849 | CLA | CHA-CBD-CGD-O2D |
| 20 | A | 850 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 850 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 822 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 822 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 824 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 829 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 829 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 850 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 850 | CLA | CHA-CBD-CGD-O2D |
| 20 | J | 103 | CLA | CHA-CBD-CGD-O1D |
| 20 | J | 103 | CLA | CHA-CBD-CGD-O2D |
| 20 | L | 203 | CLA | CHA-CBD-CGD-O1D |
| 20 | L | 203 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 828 | CLA | C3-C5-C6-C7 |
| 20 | 1 | 203 | CLA | O1A-CGA-O2A-C1 |
| 20 | 4 | 306 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 820 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 841 | CLA | O1A-CGA-O2A-C1 |
| 21 | 2 | 320 | LMU | C9-C10-C11-C12 |
| 20 | B | 832 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 823 | CLA | C10-C11-C12-C13 |
| 20 | 4 | 317 | CLA | C4-C3-C5-C6 |
| 20 | 4 | 301 | CLA | C2-C3-C5-C6 |
| 20 | B | 841 | CLA | C11-C12-C13-C14 |
| 20 | J | 103 | CLA | C11-C12-C13-C14 |
| 20 | R | 108 | CLA | C14-C13-C15-C16 |
| 21 | A | 854 | LMU | C2B-C1B-O1B-C4' |
| 21 | G | 102 | LMU | O1'-C1-C2-C3 |
| 20 | A | 831 | CLA | O1A-CGA-O2A-C1 |
| 20 | B | 816 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 802 | CLA | C2A-CAA-CBA-CGA |
| 20 | J | 101 | CLA | CAA-CBA-CGA-O2A |
| 21 | 2 | 320 | LMU | C7-C8-C9-C10 |
| 21 | 4 | 316 | LMU | C3-C4-C5-C6 |
| 22 | I | 103 | BCR | C7-C8-C9-C10 |
| 20 | 3 | 311 | CLA | C1A-C2A-CAA-CBA |
| 20 | 4 | 306 | CLA | C1A-C2A-CAA-CBA |
| 20 | 2 | 316 | CLA | C16-C17-C18-C19 |
| 20 | 4 | 303 | CLA | C2-C1-O2A-CGA |
| 20 | A | 816 | CLA | C2-C1-O2A-CGA |
| 22 | A | 843 | BCR | C13-C14-C15-C16 |
| 22 | F | 203 | BCR | C15-C16-C17-C18 |
| 21 | K | 106 | LMU | C1-C2-C3-C4 |
| 20 | 3 | 310 | CLA | C4C-C3C-CAC-CBC |
| 21 | H | 105 | LMU | O5B-C5B-C6B-O6B |
| 20 | 1 | 204 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 827 | CLA | C4B-C3B-CAB-CBB |
| 22 | I | 101 | BCR | C23-C24-C25-C30 |
| 20 | A | 849 | CLA | C16-C17-C18-C19 |
| 21 | G | 103 | LMU | C11-C10-C9-C8 |
| 21 | K | 106 | LMU | C9-C10-C11-C12 |
| 20 | F | 207 | CLA | C3-C5-C6-C7 |
| 21 | H | 103 | LMU | C11-C10-C9-C8 |
| 21 | R | 102 | LMU | C4-C5-C6-C7 |
| 20 | A | 808 | CLA | C11-C12-C13-C14 |
| 20 | B | 806 | CLA | C16-C17-C18-C19 |
| 20 | B | 816 | CLA | C11-C12-C13-C14 |
| 21 | C | 101 | LMU | O1'-C1-C2-C3 |
| 20 | 1 | 211 | CLA | C2-C3-C5-C6 |
| 20 | 3 | 307 | CLA | CAD-CBD-CGD-O1D |
| 20 | 3 | 314 | CLA | CAD-CBD-CGD-O1D |
| 20 | 4 | 301 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 826 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 832 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 850 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 802 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 834 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 836 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 837 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 839 | CLA | CAD-CBD-CGD-O1D |
| 20 | F | 206 | CLA | CAD-CBD-CGD-O1D |
| 20 | H | 101 | CLA | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | R | 108 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 804 | CLA | C2C-C3C-CAC-CBC |
| 21 | R | 109 | LMU | O1'-C1-C2-C3 |
| 21 | 2 | 320 | LMU | C11-C10-C9-C8 |
| 21 | H | 105 | LMU | C2-C3-C4-C5 |
| 21 | R | 106 | LMU | C3'-C4'-O1B-C1B |
| 20 | 2 | 307 | CLA | C11-C10-C8-C7 |
| 20 | 4 | 315 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 808 | CLA | C11-C10-C8-C7 |
| 20 | A | 824 | CLA | C11-C10-C8-C7 |
| 20 | A | 828 | CLA | C6-C7-C8-C10 |
| 20 | A | 830 | CLA | C11-C10-C8-C7 |
| 20 | A | 850 | CLA | C6-C7-C8-C10 |
| 20 | B | 803 | CLA | C12-C13-C15-C16 |
| 20 | B | 806 | CLA | C11-C10-C8-C7 |
| 20 | B | 808 | CLA | C11-C10-C8-C7 |
| 20 | B | 814 | CLA | C11-C10-C8-C7 |
| 20 | B | 816 | CLA | C11-C10-C8-C7 |
| 20 | B | 824 | CLA | C12-C13-C15-C16 |
| 20 | B | 826 | CLA | C6-C7-C8-C10 |
| 20 | B | 830 | CLA | C11-C12-C13-C15 |
| 20 | K | 104 | CLA | C6-C7-C8-C10 |
| 23 | A | 842 | PQN | C21-C22-C23-C25 |
| 21 | G | 101 | LMU | C2-C1-O1'-C1' |
| 21 | R | 102 | LMU | C7-C8-C9-C10 |
| 20 | A | 835 | CLA | C8-C10-C11-C12 |
| 20 | 2 | 316 | CLA | C16-C17-C18-C20 |
| 20 | B | 803 | CLA | C16-C17-C18-C20 |
| 20 | B | 829 | CLA | C3-C5-C6-C7 |
| 21 | 4 | 319 | LMU | O5'-C5'-C6'-O6' |
| 20 | A | 801 | CLA | CAA-CBA-CGA-O2A |
| 20 | A | 824 | CLA | C8-C10-C11-C12 |
| 20 | B | 824 | CLA | C5-C6-C7-C8 |
| 20 | A | 849 | CLA | C4-C3-C5-C6 |
| 21 | K | 105 | LMU | C3'-C4'-O1B-C1B |
| 20 | 3 | 310 | CLA | C11-C10-C8-C9 |
| 20 | A | 826 | CLA | C11-C12-C13-C14 |
| 20 | A | 831 | CLA | C11-C10-C8-C9 |
| 20 | A | 835 | CLA | C14-C13-C15-C16 |
| 20 | A | 849 | CLA | C14-C13-C15-C16 |
| 20 | B | 815 | CLA | C11-C10-C8-C9 |
| 21 | 2 | 320 | LMU | C5'-C4'-O1B-C1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | A | 838 | CLA | C16-C17-C18-C19 |
| 20 | B | 806 | CLA | C16-C17-C18-C20 |
| 20 | B | 810 | CLA | C11-C12-C13-C14 |
| 20 | B | 809 | CLA | C15-C16-C17-C18 |
| 20 | B | 817 | CLA | CAA-CBA-CGA-O2A |
| 20 | L | 207 | CLA | C4C-C3C-CAC-CBC |
| 21 | 2 | 319 | LMU | O5B-C1B-O1B-C4' |
| 20 | A | 826 | CLA | C13-C15-C16-C17 |
| 20 | 1 | 201 | CLA | C2B-C3B-CAB-CBB |
| 20 | 4 | 303 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 803 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 807 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 808 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 810 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 831 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 835 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 808 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 809 | CLA | C2B-C3B-CAB-CBB |
| 20 | F | 206 | CLA | C2B-C3B-CAB-CBB |
| 20 | R | 108 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 850 | CLA | C8-C10-C11-C12 |
| 21 | 4 | 320 | LMU | C4-C5-C6-C7 |
| 25 | B | 848 | LMG | C38-C39-C40-C41 |
| 20 | A | 840 | CLA | C2C-C3C-CAC-CBC |
| 20 | B | 838 | CLA | C3-C5-C6-C7 |
| 20 | 4 | 305 | CLA | CAA-CBA-CGA-O2A |
| 20 | 1 | 204 | CLA | C2A-CAA-CBA-CGA |
| 20 | A | 818 | CLA | C2A-CAA-CBA-CGA |
| 20 | H | 101 | CLA | C2A-CAA-CBA-CGA |
| 20 | H | 110 | CLA | C2A-CAA-CBA-CGA |
| 20 | L | 202 | CLA | C2A-CAA-CBA-CGA |
| 20 | L | 207 | CLA | C2A-CAA-CBA-CGA |
| 20 | 2 | 307 | CLA | C2-C1-O2A-CGA |
| 20 | 2 | 310 | CLA | C2-C1-O2A-CGA |
| 20 | H | 101 | CLA | C2-C1-O2A-CGA |
| 20 | R | 107 | CLA | C2-C1-O2A-CGA |
| 20 | A | 804 | CLA | C3-C5-C6-C7 |
| 20 | A | 840 | CLA | C3-C5-C6-C7 |
| 21 | 4 | 320 | LMU | C9-C10-C11-C12 |
| 20 | A | 819 | CLA | CBA-CGA-O2A-C1 |
| 20 | 3 | 310 | CLA | C8-C10-C11-C12 |
| 20 | 4 | 317 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | A | 809 | CLA | C4C-C3C-CAC-CBC |
| 20 | L | 202 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 827 | CLA | O1D-CGD-O2D-CED |
| 20 | 1 | 213 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 819 | CLA | O1A-CGA-O2A-C1 |
| 20 | 2 | 312 | CLA | C14-C13-C15-C16 |
| 20 | B | 806 | CLA | C5-C6-C7-C8 |
| 21 | A | 847 | LMU | C7-C8-C9-C10 |
| 20 | A | 811 | CLA | C4-C3-C5-C6 |
| 20 | 3 | 314 | CLA | C12-C13-C15-C16 |
| 20 | A | 811 | CLA | C6-C7-C8-C10 |
| 20 | A | 811 | CLA | C11-C12-C13-C15 |
| 20 | B | 814 | CLA | C6-C7-C8-C10 |
| 20 | B | 837 | CLA | C11-C10-C8-C7 |
| 20 | B | 840 | CLA | C12-C13-C15-C16 |
| 20 | 2 | 316 | CLA | C14-C13-C15-C16 |
| 20 | 3 | 310 | CLA | C6-C7-C8-C9 |
| 20 | A | 808 | CLA | C11-C10-C8-C9 |
| 20 | A | 824 | CLA | C11-C10-C8-C9 |
| 20 | A | 830 | CLA | C11-C10-C8-C9 |
| 20 | A | 851 | CLA | C11-C12-C13-C14 |
| 20 | B | 814 | CLA | C11-C10-C8-C9 |
| 20 | B | 830 | CLA | C14-C13-C15-C16 |
| 20 | B | 841 | CLA | C14-C13-C15-C16 |
| 23 | A | 842 | PQN | C24-C23-C25-C26 |
| 20 | A | 849 | CLA | C16-C17-C18-C20 |
| 20 | 4 | 317 | CLA | C2C-C3C-CAC-CBC |
| 21 | C | 101 | LMU | C4B-C5B-C6B-O6B |
| 20 | B | 829 | CLA | CBD-CGD-O2D-CED |
| 20 | A | 824 | CLA | C11-C12-C13-C14 |
| 20 | B | 813 | CLA | C3-C5-C6-C7 |
| 20 | B | 832 | CLA | C3-C5-C6-C7 |
| 21 | B | 805 | LMU | C4'-C5'-C6'-O6' |
| 21 | 1 | 218 | LMU | C2-C3-C4-C5 |
| 20 | A | 812 | CLA | C6-C7-C8-C9 |
| 20 | A | 829 | CLA | O1D-CGD-O2D-CED |
| 21 | R | 106 | LMU | C5'-C4'-O1B-C1B |
| 20 | 3 | 311 | CLA | C8-C10-C11-C12 |
| 20 | B | 850 | CLA | CAA-CBA-CGA-O2A |
| 21 | L | 205 | LMU | C3'-C4'-O1B-C1B |
| 20 | 3 | 307 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 824 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 855 | LMU | O5'-C1'-O1'-C1 |
| 22 | 2 | 317 | BCR | C15-C16-C17-C18 |
| 22 | A | 844 | BCR | C13-C14-C15-C16 |
| 22 | B | 844 | BCR | C15-C16-C17-C18 |
| 21 | B | 804 | LMU | C2-C3-C4-C5 |
| 21 | R | 102 | LMU | C3'-C4'-O1B-C1B |
| 22 | F | 203 | BCR | C18-C19-C20-C21 |
| 20 | 2 | 316 | CLA | C4-C3-C5-C6 |
| 20 | L | 203 | CLA | C4-C3-C5-C6 |
| 20 | B | 835 | CLA | CAA-CBA-CGA-O1A |
| 20 | 1 | 213 | CLA | O1A-CGA-O2A-C1 |
| 20 | 2 | 307 | CLA | C15-C16-C17-C18 |
| 20 | A | 833 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 828 | CLA | CAA-CBA-CGA-O2A |
| 20 | 4 | 310 | CLA | C2-C1-O2A-CGA |
| 20 | B | 802 | CLA | C2-C1-O2A-CGA |
| 20 | B | 806 | CLA | C2-C1-O2A-CGA |
| 20 | A | 825 | CLA | C10-C11-C12-C13 |
| 20 | B | 824 | CLA | C16-C17-C18-C20 |
| 20 | A | 850 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 828 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 812 | CLA | C2C-C3C-CAC-CBC |
| 21 | B | 804 | LMU | C9-C10-C11-C12 |
| 20 | 4 | 306 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 812 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 834 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 806 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 808 | CLA | C3A-C2A-CAA-CBA |
| 20 | K | 103 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 840 | CLA | C4C-C3C-CAC-CBC |
| 22 | G | 104 | BCR | C13-C14-C15-C16 |
| 20 | A | 824 | CLA | CBA-CGA-O2A-C1 |
| 20 | B | 835 | CLA | CAA-CBA-CGA-O2A |
| 20 | 2 | 307 | CLA | C13-C15-C16-C17 |
| 20 | A | 811 | CLA | C6-C7-C8-C9 |
| 20 | A | 849 | CLA | C11-C12-C13-C14 |
| 20 | B | 830 | CLA | C11-C12-C13-C14 |
| 20 | K | 104 | CLA | C6-C7-C8-C9 |
| 20 | L | 201 | CLA | C11-C10-C8-C9 |
| 21 | 4 | 320 | LMU | C2-C3-C4-C5 |
| 21 | K | 107 | LMU | C9-C10-C11-C12 |
| 22 | A | 845 | BCR | C35-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | B | 801 | BCR | C11-C10-C9-C34 |
| 22 | B | 845 | BCR | C11-C10-C9-C34 |
| 22 | F | 204 | BCR | C16-C17-C18-C36 |
| 21 | H | 105 | LMU | C4'-C5'-C6'-O6' |
| 20 | A | 851 | CLA | C16-C17-C18-C20 |
| 20 | B | 826 | CLA | O2A-C1-C2-C3 |
| 20 | L | 203 | CLA | O2A-C1-C2-C3 |
| 21 | F | 202 | LMU | C3'-C4'-O1B-C1B |
| 20 | A | 810 | CLA | CAA-CBA-CGA-O2A |
| 22 | A | 843 | BCR | C36-C18-C19-C20 |
| 20 | A | 810 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 814 | CLA | C4-C3-C5-C6 |
| 20 | 2 | 307 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 806 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 832 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 837 | CLA | C1A-C2A-CAA-CBA |
| 20 | H | 108 | CLA | C1A-C2A-CAA-CBA |
| 20 | K | 103 | CLA | C1A-C2A-CAA-CBA |
| 20 | 4 | 303 | CLA | C6-C7-C8-C10 |
| 20 | 4 | 303 | CLA | C11-C10-C8-C7 |
| 20 | A | 825 | CLA | C11-C10-C8-C7 |
| 20 | A | 825 | CLA | C11-C12-C13-C15 |
| 20 | A | 825 | CLA | C12-C13-C15-C16 |
| 20 | A | 835 | CLA | C11-C10-C8-C7 |
| 20 | A | 849 | CLA | C6-C7-C8-C10 |
| 20 | A | 849 | CLA | C11-C10-C8-C7 |
| 20 | B | 832 | CLA | C11-C10-C8-C7 |
| 20 | B | 838 | CLA | C11-C10-C8-C7 |
| 20 | B | 840 | CLA | C6-C7-C8-C10 |
| 20 | A | 824 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 801 | BCR | C9-C10-C11-C12 |
| 20 | 4 | 310 | CLA | C2A-CAA-CBA-CGA |
| 20 | I | 102 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 847 | LMU | C1-C2-C3-C4 |
| 20 | 2 | 312 | CLA | C10-C11-C12-C13 |
| 20 | A | 830 | CLA | C8-C10-C11-C12 |
| 20 | B | 814 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 831 | CLA | CAA-CBA-CGA-O2A |
| 20 | A | 826 | CLA | C10-C11-C12-C13 |
| 25 | B | 848 | LMG | C31-C32-C33-C34 |
| 20 | 3 | 314 | CLA | C4C-C3C-CAC-CBC |
| 20 | 2 | 307 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 852 | LMU | O5B-C5B-C6B-O6B |
| 21 | H | 104 | LMU | O5B-C5B-C6B-O6B |
| 20 | 4 | 303 | CLA | C16-C17-C18-C19 |
| 20 | A | 804 | CLA | C6-C7-C8-C9 |
| 20 | A | 851 | CLA | C16-C17-C18-C19 |
| 21 | R | 101 | LMU | C4-C5-C6-C7 |
| 20 | A | 835 | CLA | C13-C15-C16-C17 |
| 20 | 4 | 305 | CLA | C2B-C3B-CAB-CBB |
| 20 | A | 809 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 850 | CLA | C2B-C3B-CAB-CBB |
| 20 | F | 201 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 852 | LMU | C9-C10-C11-C12 |
| 22 | A | 845 | BCR | C12-C13-C14-C15 |
| 22 | B | 801 | BCR | C11-C10-C9-C8 |
| 22 | B | 845 | BCR | C11-C10-C9-C8 |
| 22 | F | 204 | BCR | C16-C17-C18-C19 |
| 21 | R | 104 | LMU | O5B-C1B-O1B-C4' |
| 21 | B | 804 | LMU | C1-C2-C3-C4 |
| 21 | 2 | 320 | LMU | C3'-C4'-O1B-C1B |
| 20 | A | 825 | CLA | C5-C6-C7-C8 |
| 20 | A | 851 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 846 | BCR | C19-C20-C21-C22 |
| 22 | J | 102 | BCR | C15-C16-C17-C18 |
| 22 | L | 209 | BCR | C15-C16-C17-C18 |
| 21 | R | 104 | LMU | C2-C3-C4-C5 |
| 20 | B | 827 | CLA | C5-C6-C7-C8 |
| 20 | A | 833 | CLA | CAA-CBA-CGA-O1A |
| 20 | 4 | 301 | CLA | C2-C1-O2A-CGA |
| 20 | A | 808 | CLA | C2-C1-O2A-CGA |
| 20 | A | 809 | CLA | C2-C1-O2A-CGA |
| 20 | A | 832 | CLA | C2-C1-O2A-CGA |
| 20 | B | 831 | CLA | C2-C1-O2A-CGA |
| 20 | A | 811 | CLA | C2-C3-C5-C6 |
| 20 | L | 203 | CLA | C2-C3-C5-C6 |
| 21 | B | 805 | LMU | C9-C10-C11-C12 |
| 21 | A | 848 | LMU | C2-C3-C4-C5 |
| 21 | B | 805 | LMU | C3-C4-C5-C6 |
| 20 | A | 829 | CLA | O1A-CGA-O2A-C1 |
| 20 | 1 | 211 | CLA | C4-C3-C5-C6 |
| 20 | B | 826 | CLA | C10-C11-C12-C13 |
| 20 | 2 | 302 | CLA | O1D-CGD-O2D-CED |
| 20 | R | 107 | CLA | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | H | 105 | LMU | O5B-C1B-O1B-C4' |
| 22 | 2 | 317 | BCR | C1-C6-C7-C8 |
| 22 | B | 844 | BCR | C23-C24-C25-C30 |
| 22 | B | 846 | BCR | C23-C24-C25-C30 |
| 20 | A | 830 | CLA | C10-C11-C12-C13 |
| 20 | R | 108 | CLA | CAA-CBA-CGA-O2A |
| 21 | R | 101 | LMU | C6-C7-C8-C9 |
| 20 | B | 803 | CLA | C4-C3-C5-C6 |
| 20 | B | 825 | CLA | C4-C3-C5-C6 |
| 20 | B | 829 | CLA | C4-C3-C5-C6 |
| 20 | B | 832 | CLA | C4-C3-C5-C6 |
| 21 | R | 103 | LMU | C6-C7-C8-C9 |
| 20 | A | 849 | CLA | C2-C3-C5-C6 |
| 21 | 1 | 218 | LMU | C5-C6-C7-C8 |
| 20 | 4 | 303 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 827 | CLA | O1A-CGA-O2A-C1 |
| 21 | C | 101 | LMU | C1-C2-C3-C4 |
| 20 | 1 | 206 | CLA | C2A-CAA-CBA-CGA |
| 21 | 4 | 320 | LMU | C4'-C5'-C6'-O6' |
| 21 | B | 804 | LMU | C3'-C4'-O1B-C1B |
| 25 | B | 848 | LMG | C12-C13-C14-C15 |
| 20 | A | 830 | CLA | C4B-C3B-CAB-CBB |
| 20 | K | 103 | CLA | C4B-C3B-CAB-CBB |
| 20 | L | 207 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 853 | LMU | O5'-C5'-C6'-O6' |
| 21 | A | 853 | LMU | C7-C8-C9-C10 |
| 20 | A | 826 | CLA | C4-C3-C5-C6 |
| 20 | A | 849 | CLA | C11-C12-C13-C15 |
| 20 | B | 814 | CLA | C2-C3-C5-C6 |
| 20 | B | 832 | CLA | C2-C3-C5-C6 |
| 22 | F | 203 | BCR | C9-C10-C11-C12 |
| 20 | 2 | 314 | CLA | CAA-CBA-CGA-O2A |
| 21 | 1 | 216 | LMU | C2'-C1'-O1'-C1 |
| 20 | L | 201 | CLA | C11-C12-C13-C15 |
| 20 | 4 | 303 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 829 | CLA | CBA-CGA-O2A-C1 |
| 20 | A | 805 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 839 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 846 | LMU | C4-C5-C6-C7 |
| 21 | 4 | 320 | LMU | C1-C2-C3-C4 |
| 20 | 2 | 316 | CLA | C2-C3-C5-C6 |
| 21 | A | 846 | LMU | C1-C2-C3-C4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 4 | 301 | CLA | C6-C7-C8-C9 |
| 20 | F | 201 | CLA | O1D-CGD-O2D-CED |
| 20 | 4 | 303 | CLA | CAA-CBA-CGA-O2A |
| 20 | A | 849 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 821 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 822 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 836 | CLA | CAA-CBA-CGA-O2A |
| 20 | H | 102 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 847 | LMU | C4-C5-C6-C7 |
| 21 | A | 854 | LMU | C9-C10-C11-C12 |
| 20 | 2 | 307 | CLA | C11-C10-C8-C9 |
| 20 | A | 828 | CLA | C6-C7-C8-C9 |
| 20 | B | 816 | CLA | C11-C10-C8-C9 |
| 20 | B | 826 | CLA | C6-C7-C8-C9 |
| 20 | B | 838 | CLA | C11-C10-C8-C9 |
| 20 | I | 102 | CLA | C11-C10-C8-C9 |
| 20 | B | 834 | CLA | CAA-CBA-CGA-O1A |
| 20 | 1 | 206 | CLA | C3A-C2A-CAA-CBA |
| 20 | 2 | 305 | CLA | C3A-C2A-CAA-CBA |
| 20 | 4 | 301 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 837 | CLA | C3A-C2A-CAA-CBA |
| 20 | 2 | 303 | CLA | CAA-CBA-CGA-O2A |
| 20 | 1 | 203 | CLA | CAD-CBD-CGD-O2D |
| 20 | 2 | 311 | CLA | CAD-CBD-CGD-O2D |
| 20 | 3 | 310 | CLA | CAD-CBD-CGD-O2D |
| 20 | 3 | 313 | CLA | CAD-CBD-CGD-O2D |
| 20 | 4 | 317 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 803 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 805 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 813 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 818 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 835 | CLA | CAD-CBD-CGD-O2D |
| 20 | A | 837 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 825 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 826 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 827 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 833 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 838 | CLA | CAD-CBD-CGD-O2D |
| 20 | K | 101 | CLA | CAD-CBD-CGD-O2D |
| 20 | B | 827 | CLA | C10-C11-C12-C13 |
| 25 | B | 848 | LMG | C28-C29-C30-C31 |
| 20 | 2 | 311 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 806 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 827 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 826 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 846 | LMU | O5'-C1'-O1'-C1 |
| 20 | 1 | 206 | CLA | CAA-CBA-CGA-O2A |
| 20 | I | 102 | CLA | CAA-CBA-CGA-O2A |
| 20 | L | 202 | CLA | CAA-CBA-CGA-O2A |
| 22 | A | 843 | BCR | C17-C18-C19-C20 |
| 21 | A | 855 | LMU | C5'-C4'-O1B-C1B |
| 20 | A | 827 | CLA | CBA-CGA-O2A-C1 |
| 21 | 2 | 313 | LMU | C3-C4-C5-C6 |
| 20 | A | 837 | CLA | CAA-CBA-CGA-O2A |
| 20 | K | 102 | CLA | C2C-C3C-CAC-CBC |
| 20 | A | 817 | CLA | O2A-C1-C2-C3 |
| 20 | A | 838 | CLA | O2A-C1-C2-C3 |
| 20 | B | 803 | CLA | O2A-C1-C2-C3 |
| 20 | H | 108 | CLA | O2A-C1-C2-C3 |
| 20 | B | 812 | CLA | C4C-C3C-CAC-CBC |
| 20 | A | 851 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 839 | CLA | C2A-CAA-CBA-CGA |
| 20 | 4 | 318 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 823 | CLA | C6-C7-C8-C9 |
| 21 | 4 | 321 | LMU | C7-C8-C9-C10 |
| 20 | 2 | 303 | CLA | CHA-CBD-CGD-O2D |
| 20 | 2 | 312 | CLA | CHA-CBD-CGD-O2D |
| 20 | 4 | 304 | CLA | CHA-CBD-CGD-O1D |
| 20 | 4 | 304 | CLA | CHA-CBD-CGD-O2D |
| 20 | A | 827 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 831 | CLA | CHA-CBD-CGD-O1D |
| 20 | A | 831 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 806 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 810 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 810 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 831 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 831 | CLA | CHA-CBD-CGD-O2D |
| 20 | B | 841 | CLA | CHA-CBD-CGD-O1D |
| 20 | B | 841 | CLA | CHA-CBD-CGD-O2D |
| 20 | G | 105 | CLA | CHA-CBD-CGD-O1D |
| 20 | G | 105 | CLA | CHA-CBD-CGD-O2D |
| 20 | L | 202 | CLA | CHA-CBD-CGD-O1D |
| 20 | L | 202 | CLA | CHA-CBD-CGD-O2D |
| 20 | L | 207 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | L | 207 | CLA | CHA-CBD-CGD-O2D |
| 20 | A | 803 | CLA | CAA-CBA-CGA-O2A |
| 20 | A | 838 | CLA | CAA-CBA-CGA-O2A |
| 21 | H | 105 | LMU | C2B-C1B-O1B-C4' |
| 21 | 3 | 319 | LMU | C11-C10-C9-C8 |
| 20 | 3 | 313 | CLA | CAA-CBA-CGA-O2A |
| 20 | 4 | 315 | CLA | CAA-CBA-CGA-O2A |
| 20 | 4 | 317 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 848 | LMU | C2B-C1B-O1B-C4' |
| 21 | H | 105 | LMU | C11-C10-C9-C8 |
| 25 | B | 848 | LMG | C41-C42-C43-C44 |
| 21 | D | 201 | LMU | C4B-C5B-C6B-O6B |
| 20 | B | 834 | CLA | CAA-CBA-CGA-O2A |
| 20 | B | 823 | CLA | CAA-CBA-CGA-O2A |
| 21 | R | 102 | LMU | C2-C3-C4-C5 |
| 20 | B | 826 | CLA | O1A-CGA-O2A-C1 |
| 20 | A | 818 | CLA | C11-C10-C8-C7 |
| 20 | L | 201 | CLA | C11-C12-C13-C14 |
| 20 | A | 813 | CLA | CAA-CBA-CGA-O2A |
| 20 | A | 839 | CLA | C6-C7-C8-C10 |
| 20 | A | 818 | CLA | C11-C10-C8-C9 |
| 20 | A | 849 | CLA | C6-C7-C8-C9 |
| 20 | B | 803 | CLA | C11-C10-C8-C9 |
| 20 | 3 | 313 | CLA | C2B-C3B-CAB-CBB |
| 20 | B | 803 | CLA | CAA-CBA-CGA-O2A |
| 20 | 4 | 310 | CLA | CAA-CBA-CGA-O1A |
| 21 | L | 210 | LMU | C9-C10-C11-C12 |
| 20 | 2 | 303 | CLA | CAA-CBA-CGA-O1A |
| 20 | I | 102 | CLA | CAA-CBA-CGA-O1A |
| 21 | G | 103 | LMU | O1'-C1-C2-C3 |
| 21 | R | 106 | LMU | C3-C4-C5-C6 |
| 20 | B | 818 | CLA | CAA-CBA-CGA-O2A |
| 20 | 1 | 206 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 821 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 836 | CLA | CAA-CBA-CGA-O1A |
| 20 | L | 202 | CLA | CAA-CBA-CGA-O1A |
| 20 | A | 817 | CLA | C4-C3-C5-C6 |
| 20 | 4 | 303 | CLA | CAA-CBA-CGA-O1A |
| 20 | A | 803 | CLA | CAA-CBA-CGA-O1A |
| 20 | A | 849 | CLA | CAA-CBA-CGA-O1A |
| 22 | A | 845 | BCR | C17-C18-C19-C20 |
| 20 | 4 | 301 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 1 | 207 | CLA | C1A-C2A-CAA-CBA |
| 20 | 2 | 305 | CLA | C1A-C2A-CAA-CBA |
| 20 | 2 | 314 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 812 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 812 | CLA | C1A-C2A-CAA-CBA |
| 20 | B | 822 | CLA | C1A-C2A-CAA-CBA |
| 20 | K | 101 | CLA | C1A-C2A-CAA-CBA |
| 20 | L | 202 | CLA | C1A-C2A-CAA-CBA |
| 20 | A | 805 | CLA | CAA-CBA-CGA-O1A |
| 21 | 3 | 318 | LMU | C9-C10-C11-C12 |
| 20 | B | 839 | CLA | CAA-CBA-CGA-O1A |
| 20 | H | 102 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 813 | CLA | C2A-CAA-CBA-CGA |
| 20 | B | 817 | CLA | C2A-CAA-CBA-CGA |
| 20 | 4 | 318 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 822 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 838 | CLA | CAA-CBA-CGA-O2A |
| 20 | A | 826 | CLA | C2-C3-C5-C6 |
| 21 | R | 109 | LMU | C3-C4-C5-C6 |
| 21 | G | 102 | LMU | C2'-C1'-O1'-C1 |
| 20 | 1 | 203 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 813 | CLA | C4B-C3B-CAB-CBB |
| 20 | B | 841 | CLA | C4B-C3B-CAB-CBB |
| 20 | A | 813 | CLA | CAA-CBA-CGA-O1A |
| 20 | A | 837 | CLA | CAA-CBA-CGA-O1A |
| 20 | A | 838 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 827 | CLA | CAA-CBA-CGA-O1A |
| 20 | 4 | 301 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 845 | BCR | C5-C6-C7-C8 |
| 22 | B | 844 | BCR | C23-C24-C25-C26 |
| 22 | B | 846 | BCR | C1-C6-C7-C8 |
| 22 | B | 846 | BCR | C5-C6-C7-C8 |
| 22 | I | 103 | BCR | C1-C6-C7-C8 |
| 22 | I | 103 | BCR | C5-C6-C7-C8 |
| 21 | A | 848 | LMU | O5B-C1B-O1B-C4' |
| 20 | B | 806 | CLA | CAA-CBA-CGA-O1A |
| 25 | B | 848 | LMG | C42-C43-C44-C45 |
| 20 | 2 | 311 | CLA | CAA-CBA-CGA-O1A |
| 20 | 4 | 315 | CLA | CAA-CBA-CGA-O1A |
| 20 | 4 | 317 | CLA | CAA-CBA-CGA-O1A |
| 20 | 2 | 312 | CLA | C4-C3-C5-C6 |
| 20 | B | 829 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | 1 | 211 | CLA | CAD-CBD-CGD-O1D |
| 20 | 4 | 305 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 808 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 825 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 828 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 839 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 849 | CLA | CAD-CBD-CGD-O1D |
| 20 | A | 851 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 831 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 835 | CLA | CAD-CBD-CGD-O1D |
| 20 | H | 102 | CLA | CAD-CBD-CGD-O1D |
| 20 | J | 101 | CLA | CAD-CBD-CGD-O1D |
| 20 | B | 829 | CLA | C13-C15-C16-C17 |
| 20 | 4 | 303 | CLA | C11-C10-C8-C9 |
| 20 | A | 828 | CLA | C11-C12-C13-C14 |
| 20 | B | 808 | CLA | C6-C7-C8-C9 |
| 20 | B | 840 | CLA | C6-C7-C8-C9 |
| 20 | K | 104 | CLA | C11-C10-C8-C9 |
| 20 | B | 823 | CLA | CAA-CBA-CGA-O1A |
| 21 | 4 | 316 | LMU | C6-C7-C8-C9 |
| 20 | A | 811 | CLA | CAA-CBA-CGA-O2A |
| 20 | A | 825 | CLA | CAA-CBA-CGA-O2A |
| 20 | A | 830 | CLA | CAA-CBA-CGA-O2A |
| 20 | A | 801 | CLA | C2-C1-O2A-CGA |
| 21 | 2 | 320 | LMU | C2-C3-C4-C5 |
| 20 | A | 828 | CLA | C10-C11-C12-C13 |
| 20 | 2 | 314 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 826 | CLA | C11-C12-C13-C15 |
| 20 | B | 824 | CLA | C11-C10-C8-C7 |
| 20 | B | 832 | CLA | C3A-C2A-CAA-CBA |
| 20 | B | 850 | CLA | C11-C12-C13-C15 |
| 20 | J | 101 | CLA | C3A-C2A-CAA-CBA |
| 20 | K | 101 | CLA | C3A-C2A-CAA-CBA |
| 20 | R | 108 | CLA | C3A-C2A-CAA-CBA |
| 20 | A | 825 | CLA | CAA-CBA-CGA-O1A |
| 20 | H | 109 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 841 | CLA | CAA-CBA-CGA-O2A |
| 20 | G | 105 | CLA | CAA-CBA-CGA-O2A |
| 20 | H | 109 | CLA | CAA-CBA-CGA-O2A |
| 20 | H | 110 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 847 | BCR | C17-C18-C19-C20 |
| 20 | A | 830 | CLA | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | B | 803 | CLA | CAA-CBA-CGA-O1A |
| 20 | G | 105 | CLA | CAA-CBA-CGA-O1A |
| 20 | 2 | 312 | CLA | CAA-CBA-CGA-O2A |
| 20 | K | 104 | CLA | CAA-CBA-CGA-O2A |
| 20 | A | 811 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 838 | CLA | CAA-CBA-CGA-O1A |
| 20 | B | 832 | CLA | C2A-CAA-CBA-CGA |
| 20 | 4 | 303 | CLA | C15-C16-C17-C18 |
| 21 | 1 | 216 | LMU | C11-C10-C9-C8 |

There are no ring outliers.

222 monomers are involved in 2653 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 20 | A | 822 | CLA | 19 | 0 |
| 20 | A | 851 | CLA | 26 | 0 |
| 20 | A | 808 | CLA | 19 | 0 |
| 21 | D | 201 | LMU | 3 | 0 |
| 21 | 4 | 321 | LMU | 13 | 0 |
| 21 | L | 210 | LMU | 1 | 0 |
| 21 | R | 106 | LMU | 9 | 0 |
| 21 | R | 101 | LMU | 3 | 0 |
| 21 | B | 849 | LMU | 1 | 0 |
| 20 | K | 103 | CLA | 8 | 0 |
| 20 | A | 821 | CLA | 8 | 0 |
| 20 | B | 831 | CLA | 8 | 0 |
| 20 | 1 | 206 | CLA | 10 | 0 |
| 20 | B | 802 | CLA | 16 | 0 |
| 20 | J | 101 | CLA | 12 | 0 |
| 20 | B | 818 | CLA | 15 | 0 |
| 20 | L | 204 | CLA | 14 | 0 |
| 20 | B | 842 | CLA | 2 | 0 |
| 20 | 3 | 307 | CLA | 14 | 0 |
| 20 | 2 | 314 | CLA | 17 | 0 |
| 20 | A | 817 | CLA | 6 | 0 |
| 20 | 4 | 301 | CLA | 36 | 0 |
| 20 | B | 806 | CLA | 24 | 0 |
| 20 | K | 104 | CLA | 17 | 0 |
| 20 | B | 810 | CLA | 18 | 0 |
| 21 | 2 | 313 | LMU | 29 | 0 |
| 21 | 4 | 319 | LMU | 8 | 3 |
| 20 | A | 801 | CLA | 9 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 24 | C | 103 | SF4 | 1 | 0 |
| 21 | A | 847 | LMU | 4 | 0 |
| 20 | 2 | 304 | CLA | 2 | 0 |
| 21 | B | 805 | LMU | 3 | 0 |
| 20 | L | 202 | CLA | 10 | 0 |
| 20 | A | 841 | CLA | 1 | 0 |
| 20 | B | 809 | CLA | 21 | 0 |
| 20 | A | 816 | CLA | 20 | 0 |
| 21 | H | 104 | LMU | 9 | 0 |
| 20 | B | 832 | CLA | 22 | 0 |
| 21 | 4 | 320 | LMU | 2 | 0 |
| 21 | R | 103 | LMU | 9 | 0 |
| 20 | B | 836 | CLA | 9 | 0 |
| 20 | 4 | 314 | CLA | 10 | 0 |
| 20 | B | 825 | CLA | 24 | 0 |
| 22 | B | 845 | BCR | 16 | 0 |
| 21 | A | 852 | LMU | 4 | 0 |
| 21 | K | 105 | LMU | 12 | 0 |
| 21 | E | 101 | LMU | 11 | 0 |
| 20 | B | 835 | CLA | 34 | 0 |
| 20 | H | 109 | CLA | 13 | 0 |
| 20 | A | 807 | CLA | 33 | 0 |
| 21 | K | 106 | LMU | 8 | 0 |
| 21 | R | 104 | LMU | 5 | 0 |
| 20 | B | 814 | CLA | 28 | 0 |
| 20 | B | 807 | CLA | 8 | 0 |
| 20 | A | 805 | CLA | 13 | 0 |
| 20 | 4 | 304 | CLA | 21 | 0 |
| 21 | 3 | 318 | LMU | 2 | 0 |
| 20 | A | 830 | CLA | 30 | 0 |
| 21 | H | 103 | LMU | 6 | 0 |
| 21 | G | 102 | LMU | 7 | 0 |
| 21 | R | 109 | LMU | 9 | 3 |
| 20 | L | 208 | CLA | 8 | 0 |
| 22 | B | 801 | BCR | 24 | 0 |
| 22 | B | 847 | BCR | 34 | 0 |
| 20 | A | 836 | CLA | 4 | 0 |
| 21 | F | 202 | LMU | 8 | 0 |
| 20 | 4 | 311 | CLA | 3 | 0 |
| 20 | A | 828 | CLA | 14 | 0 |
| 20 | 3 | 305 | CLA | 3 | 0 |
| 20 | A | 835 | CLA | 15 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 20 | 1 | 215 | CLA | 1 | 0 |
| 20 | 2 | 316 | CLA | 11 | 0 |
| 20 | A | 806 | CLA | 12 | 0 |
| 20 | K | 101 | CLA | 15 | 1 |
| 20 | B | 824 | CLA | 32 | 0 |
| 20 | A | 814 | CLA | 14 | 0 |
| 20 | H | 102 | CLA | 2 | 0 |
| 20 | B | 833 | CLA | 15 | 0 |
| 20 | 1 | 204 | CLA | 14 | 0 |
| 21 | A | 846 | LMU | 5 | 0 |
| 22 | I | 101 | BCR | 7 | 0 |
| 20 | G | 105 | CLA | 4 | 0 |
| 20 | 3 | 304 | CLA | 2 | 0 |
| 21 | 1 | 216 | LMU | 3 | 0 |
| 20 | H | 101 | CLA | 14 | 0 |
| 20 | 4 | 318 | CLA | 13 | 0 |
| 20 | B | 829 | CLA | 26 | 0 |
| 20 | A | 834 | CLA | 7 | 0 |
| 22 | B | 844 | BCR | 7 | 0 |
| 20 | 4 | 305 | CLA | 5 | 0 |
| 20 | 4 | 312 | CLA | 4 | 0 |
| 20 | 3 | 314 | CLA | 11 | 0 |
| 20 | B | 823 | CLA | 15 | 0 |
| 20 | H | 110 | CLA | 3 | 0 |
| 20 | A | 824 | CLA | 46 | 0 |
| 20 | A | 826 | CLA | 47 | 0 |
| 22 | G | 104 | BCR | 4 | 0 |
| 20 | 2 | 303 | CLA | 23 | 0 |
| 20 | 3 | 311 | CLA | 10 | 0 |
| 20 | K | 102 | CLA | 25 | 0 |
| 20 | B | 811 | CLA | 4 | 0 |
| 25 | B | 848 | LMG | 16 | 0 |
| 20 | I | 102 | CLA | 11 | 0 |
| 20 | 2 | 312 | CLA | 19 | 0 |
| 20 | B | 821 | CLA | 8 | 0 |
| 22 | F | 203 | BCR | 27 | 0 |
| 20 | A | 804 | CLA | 36 | 0 |
| 20 | 1 | 211 | CLA | 7 | 0 |
| 20 | B | 819 | CLA | 9 | 0 |
| 21 | H | 105 | LMU | 18 | 0 |
| 20 | B | 834 | CLA | 23 | 0 |
| 20 | B | 822 | CLA | 15 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 24 | A | 856 | SF4 | 18 | 0 |
| 20 | B | 850 | CLA | 18 | 0 |
| 20 | R | 107 | CLA | 10 | 0 |
| 20 | R | 108 | CLA | 4 | 0 |
| 21 | R | 102 | LMU | 8 | 0 |
| 24 | C | 102 | SF4 | 4 | 0 |
| 20 | B | 841 | CLA | 17 | 0 |
| 20 | 1 | 209 | CLA | 1 | 0 |
| 20 | F | 201 | CLA | 30 | 0 |
| 20 | F | 205 | CLA | 1 | 0 |
| 20 | 3 | 310 | CLA | 16 | 0 |
| 20 | L | 201 | CLA | 21 | 0 |
| 20 | 4 | 315 | CLA | 5 | 0 |
| 20 | A | 818 | CLA | 44 | 0 |
| 22 | A | 845 | BCR | 48 | 0 |
| 23 | A | 842 | PQN | 7 | 0 |
| 20 | F | 206 | CLA | 6 | 0 |
| 20 | B | 827 | CLA | 33 | 0 |
| 20 | A | 837 | CLA | 16 | 0 |
| 20 | L | 203 | CLA | 27 | 0 |
| 20 | A | 819 | CLA | 34 | 0 |
| 20 | 2 | 310 | CLA | 20 | 0 |
| 20 | 3 | 313 | CLA | 1 | 0 |
| 20 | A | 850 | CLA | 28 | 0 |
| 21 | 4 | 316 | LMU | 1 | 0 |
| 20 | 1 | 212 | CLA | 2 | 0 |
| 22 | A | 844 | BCR | 23 | 0 |
| 20 | B | 840 | CLA | 13 | 0 |
| 20 | F | 207 | CLA | 12 | 0 |
| 20 | A | 838 | CLA | 31 | 0 |
| 20 | A | 823 | CLA | 11 | 0 |
| 20 | A | 815 | CLA | 3 | 0 |
| 20 | L | 207 | CLA | 24 | 0 |
| 21 | B | 804 | LMU | 7 | 0 |
| 21 | 2 | 320 | LMU | 5 | 0 |
| 20 | B | 826 | CLA | 40 | 0 |
| 20 | A | 827 | CLA | 20 | 0 |
| 20 | 3 | 303 | CLA | 3 | 0 |
| 20 | 3 | 308 | CLA | 2 | 0 |
| 21 | 1 | 217 | LMU | 20 | 0 |
| 20 | A | 810 | CLA | 5 | 0 |
| 21 | 2 | 318 | LMU | 6 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | G | 101 | LMU | 4 | 28 |
| 22 | A | 843 | BCR | 32 | 0 |
| 20 | 2 | 305 | CLA | 15 | 0 |
| 20 | 4 | 317 | CLA | 3 | 0 |
| 20 | J | 103 | CLA | 14 | 0 |
| 20 | 4 | 310 | CLA | 26 | 0 |
| 21 | 3 | 319 | LMU | 14 | 0 |
| 22 | J | 102 | BCR | 34 | 0 |
| 20 | 2 | 311 | CLA | 5 | 0 |
| 20 | B | 838 | CLA | 42 | 0 |
| 20 | A | 849 | CLA | 17 | 0 |
| 20 | A | 812 | CLA | 2 | 0 |
| 20 | 2 | 308 | CLA | 1 | 0 |
| 20 | A | 832 | CLA | 20 | 0 |
| 20 | A | 840 | CLA | 8 | 0 |
| 23 | B | 843 | PQN | 27 | 0 |
| 20 | 4 | 303 | CLA | 19 | 0 |
| 22 | L | 209 | BCR | 36 | 0 |
| 21 | 2 | 319 | LMU | 5 | 0 |
| 20 | A | 825 | CLA | 51 | 0 |
| 20 | 4 | 306 | CLA | 17 | 0 |
| 20 | B | 813 | CLA | 7 | 0 |
| 20 | B | 828 | CLA | 15 | 0 |
| 20 | 1 | 201 | CLA | 12 | 0 |
| 20 | 1 | 205 | CLA | 7 | 0 |
| 20 | A | 839 | CLA | 28 | 0 |
| 20 | 4 | 302 | CLA | 3 | 0 |
| 21 | K | 107 | LMU | 21 | 0 |
| 21 | H | 106 | LMU | 9 | 0 |
| 20 | A | 829 | CLA | 5 | 0 |
| 20 | 2 | 302 | CLA | 13 | 0 |
| 20 | B | 803 | CLA | 41 | 0 |
| 20 | 1 | 203 | CLA | 8 | 0 |
| 20 | B | 812 | CLA | 7 | 0 |
| 21 | L | 205 | LMU | 1 | 0 |
| 20 | 1 | 210 | CLA | 8 | 0 |
| 20 | 2 | 307 | CLA | 21 | 0 |
| 20 | A | 820 | CLA | 6 | 0 |
| 20 | B | 808 | CLA | 31 | 0 |
| 22 | B | 846 | BCR | 36 | 0 |
| 20 | 4 | 313 | CLA | 4 | 0 |
| 20 | A | 813 | CLA | 16 | 0 |

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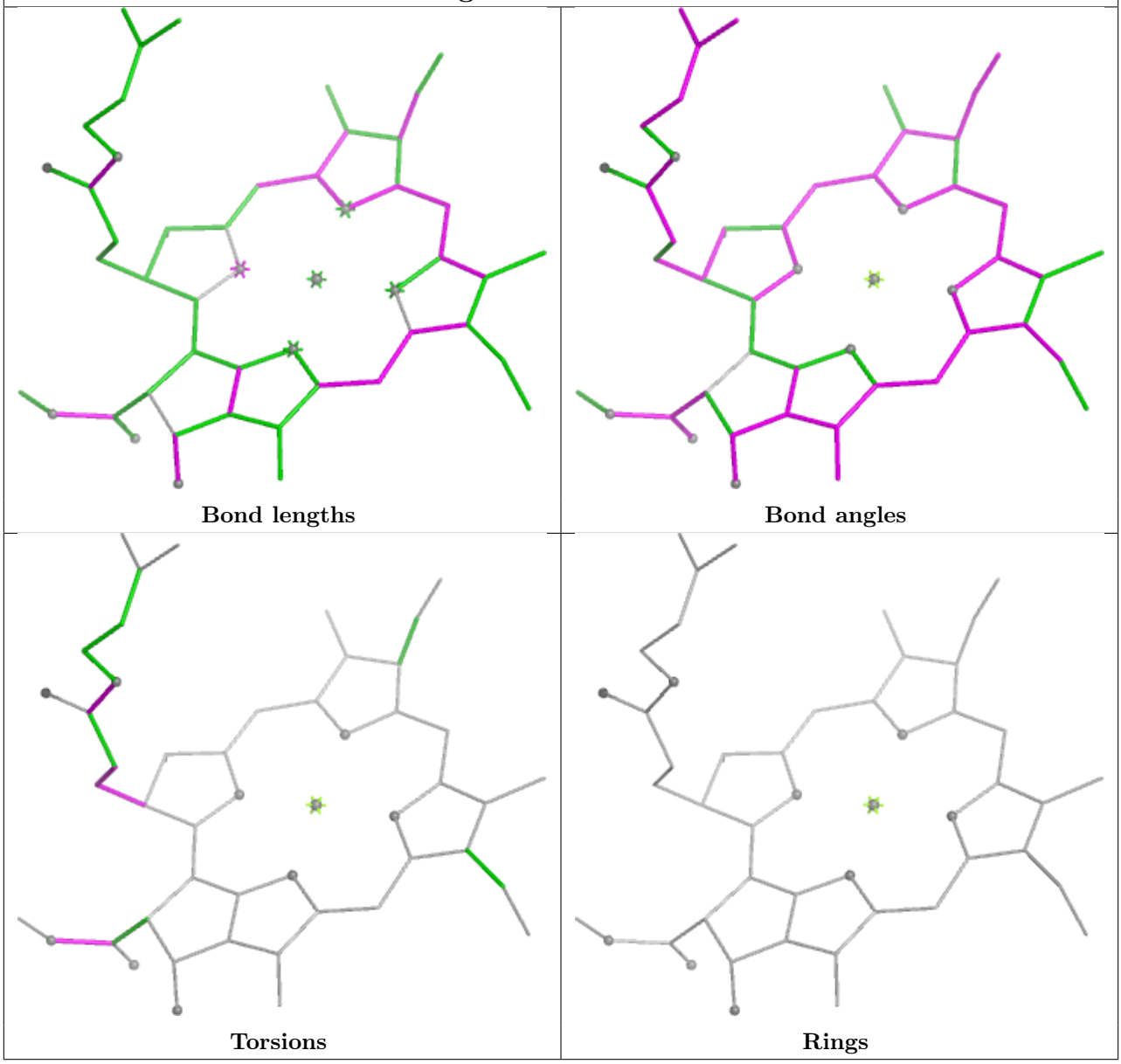
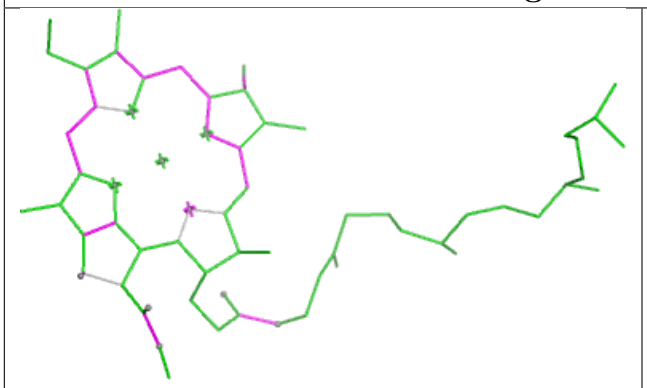
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | 1 | 218 | LMU | 9 | 0 |
| 22 | I | 103 | BCR | 38 | 0 |
| 20 | 1 | 207 | CLA | 5 | 1 |
| 20 | 3 | 306 | CLA | 7 | 0 |
| 20 | B | 816 | CLA | 7 | 0 |
| 21 | A | 854 | LMU | 16 | 0 |
| 20 | 3 | 309 | CLA | 1 | 0 |
| 20 | A | 833 | CLA | 13 | 0 |
| 22 | F | 204 | BCR | 34 | 0 |
| 20 | A | 811 | CLA | 19 | 0 |
| 20 | B | 815 | CLA | 17 | 0 |
| 20 | A | 831 | CLA | 36 | 0 |
| 20 | B | 820 | CLA | 18 | 0 |
| 20 | B | 839 | CLA | 49 | 0 |
| 21 | G | 103 | LMU | 16 | 0 |
| 20 | B | 837 | CLA | 10 | 0 |
| 20 | A | 809 | CLA | 30 | 0 |
| 20 | 1 | 208 | CLA | 4 | 0 |
| 20 | B | 830 | CLA | 25 | 0 |
| 20 | H | 108 | CLA | 26 | 0 |
| 20 | A | 803 | CLA | 19 | 0 |
| 21 | A | 848 | LMU | 4 | 0 |
| 21 | A | 853 | LMU | 21 | 0 |
| 20 | B | 817 | CLA | 19 | 0 |
| 22 | 2 | 317 | BCR | 9 | 0 |
| 20 | 1 | 213 | CLA | 18 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

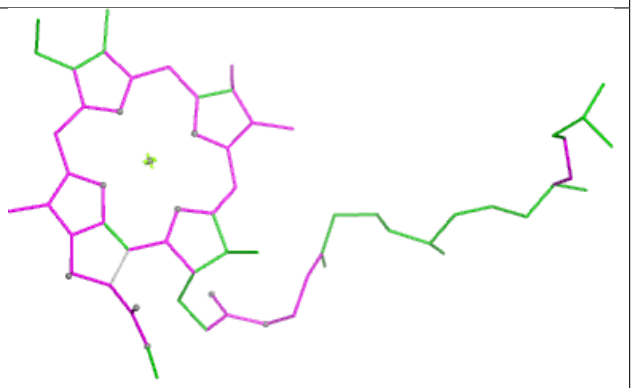
**Ligand CLA A 822**



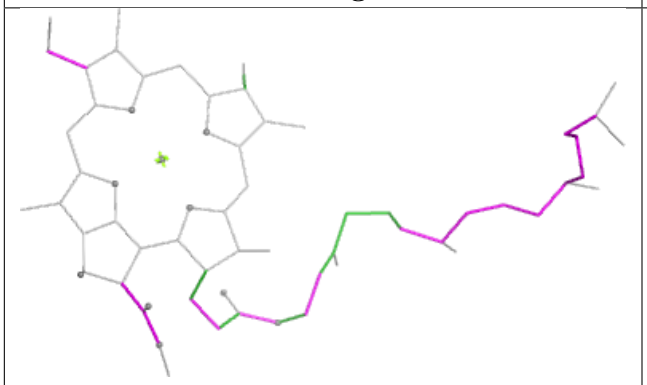
## Ligand CLA A 851



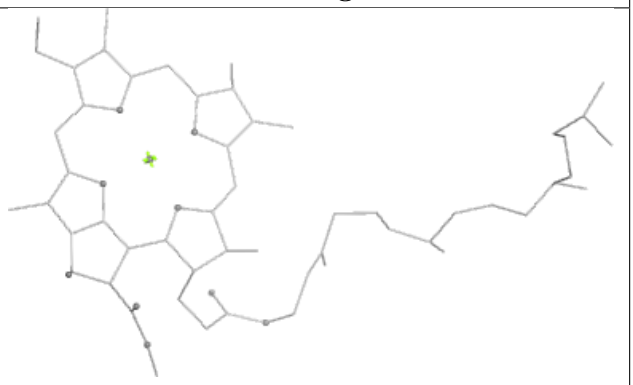
Bond lengths



Bond angles

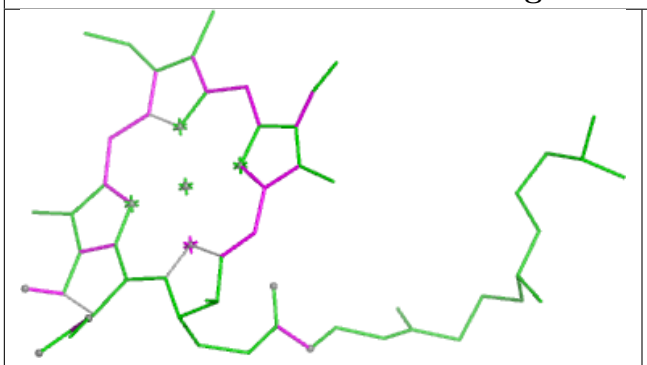


Torsions

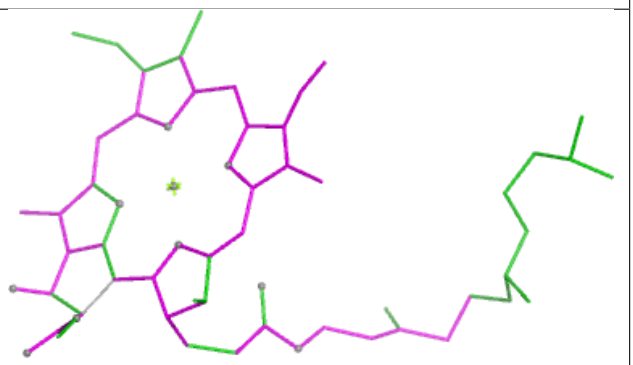


Rings

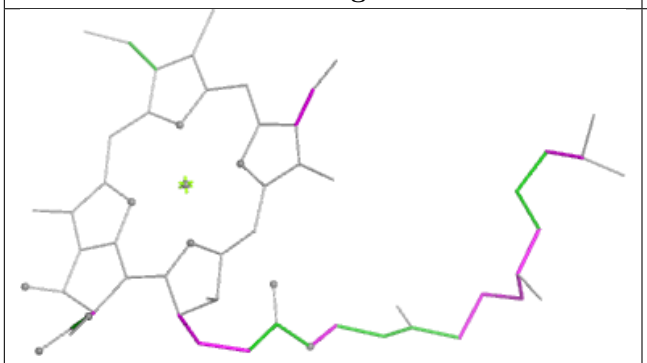
## Ligand CLA A 808



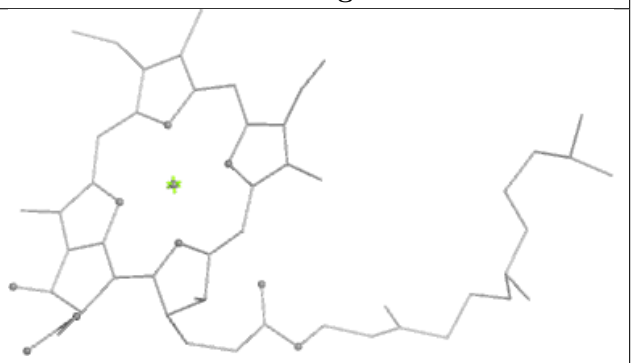
Bond lengths



Bond angles

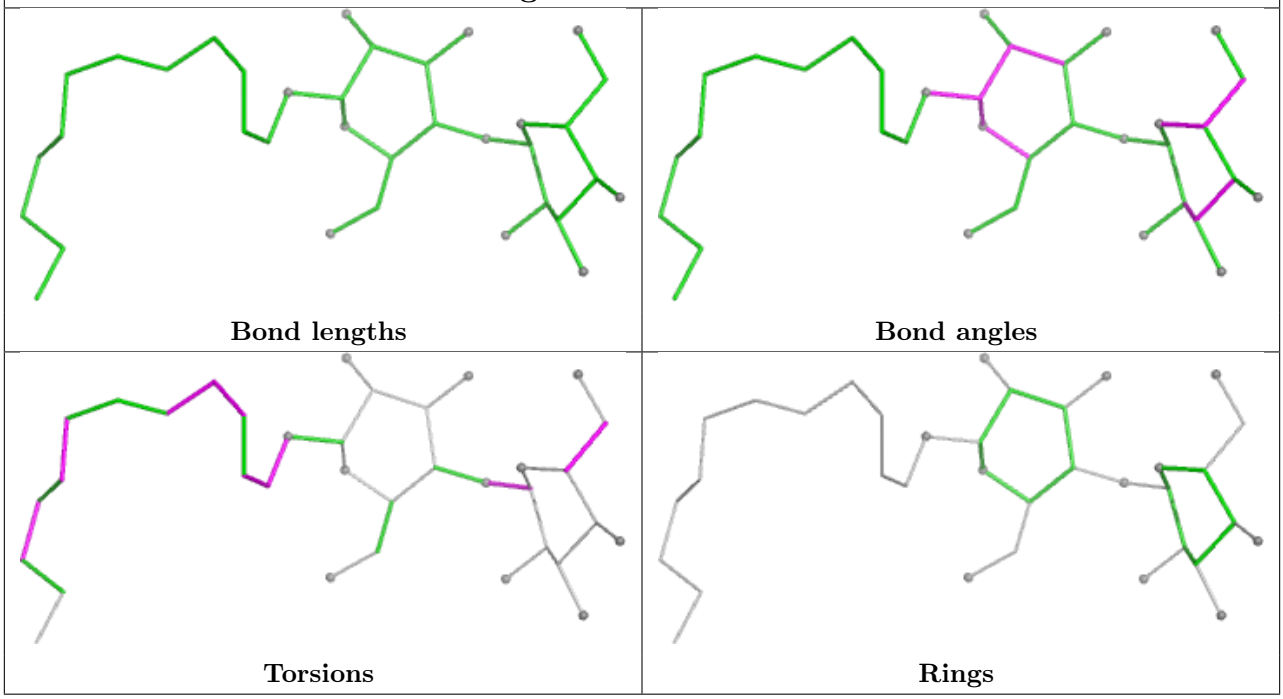


Torsions

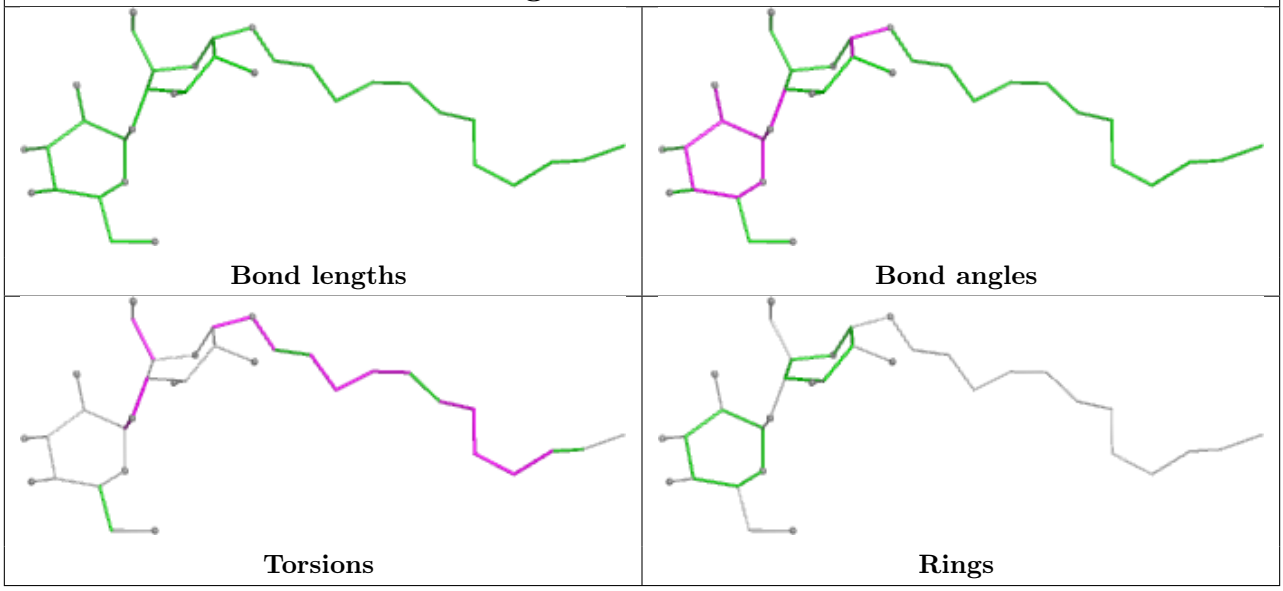


Rings

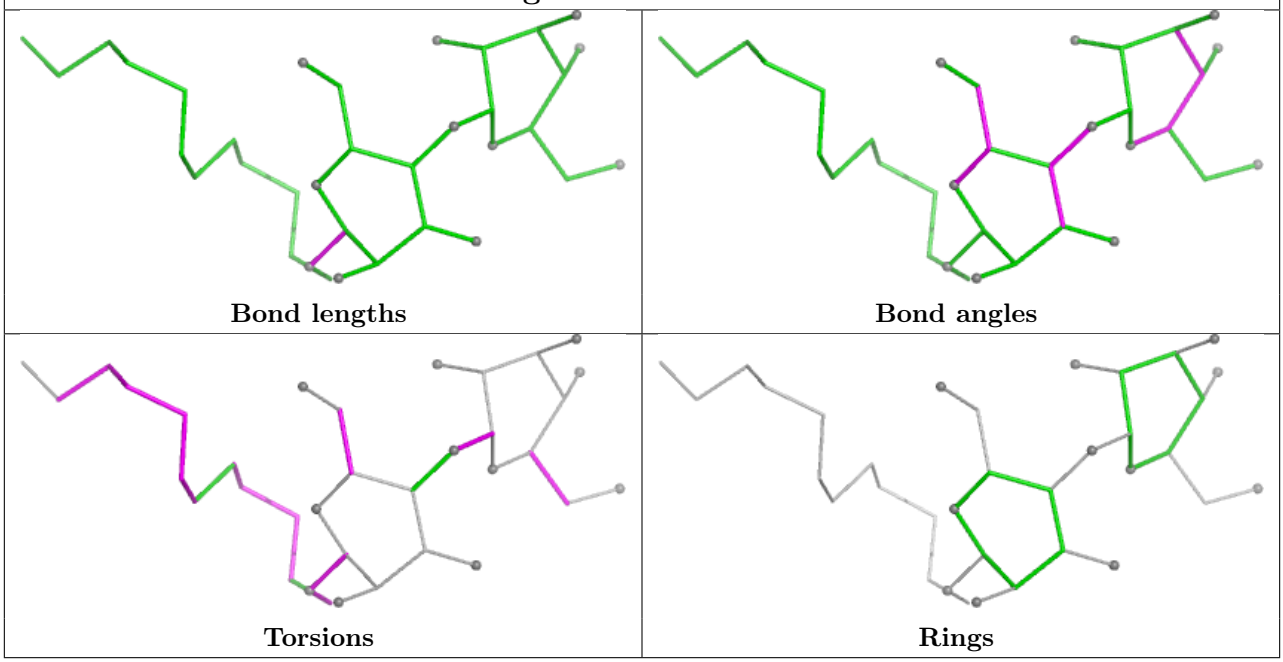
## Ligand LMU D 201



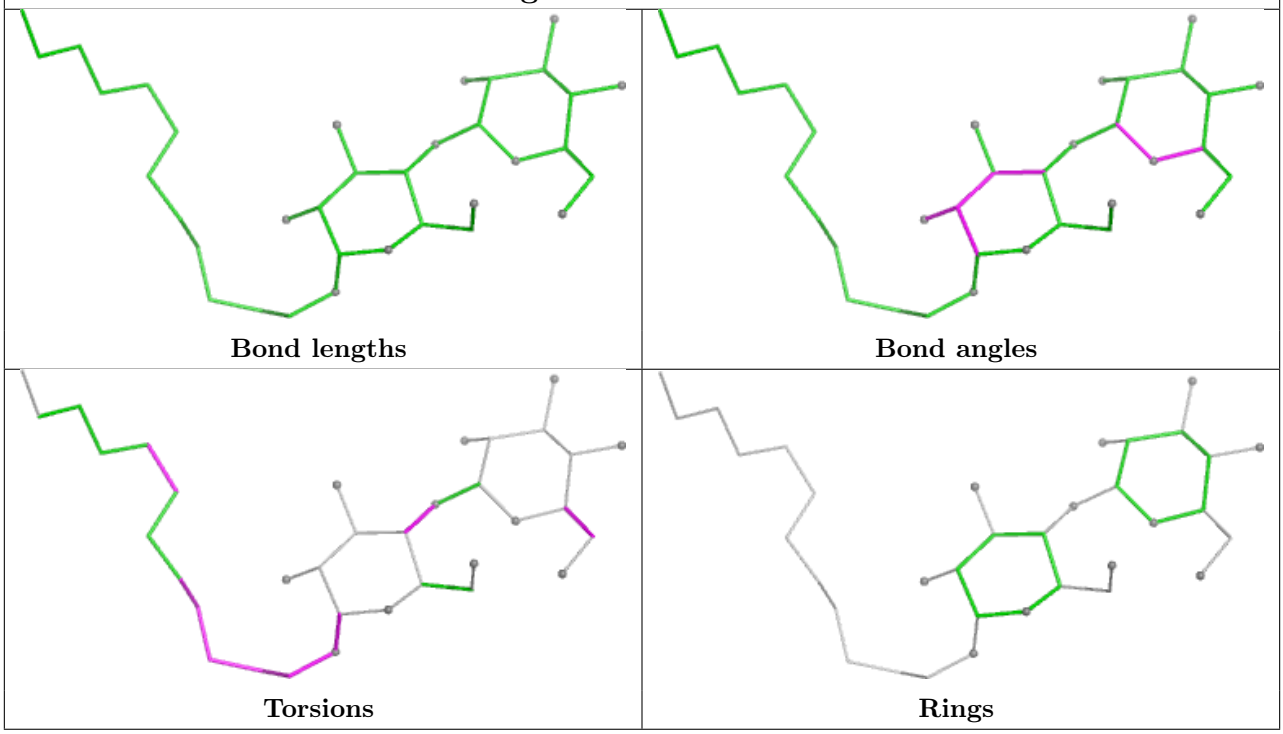

## Ligand LMU 4 321



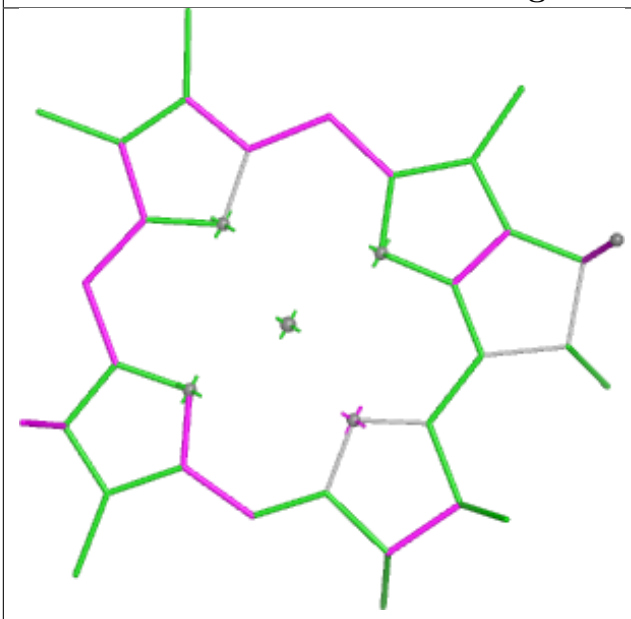
## Ligand LMU L 210



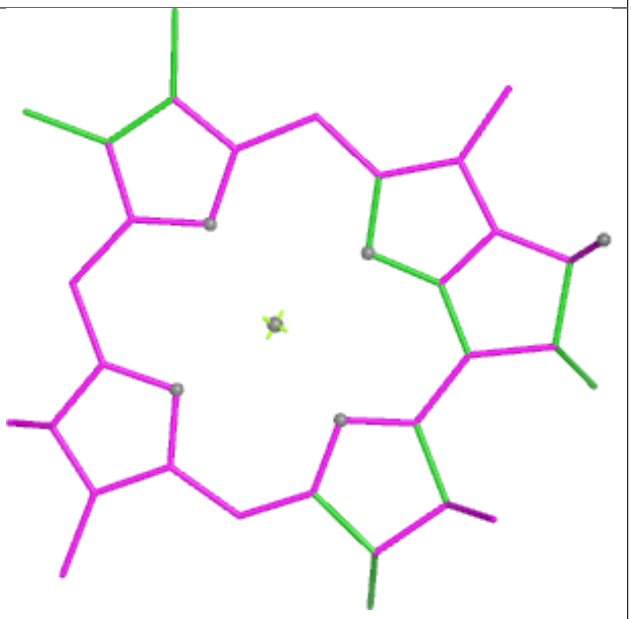

## Ligand LMU R 106



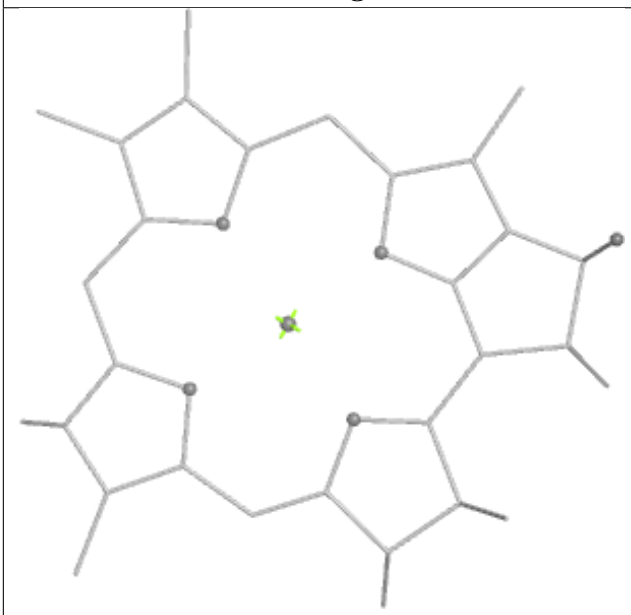
**Ligand CLA 3 301**



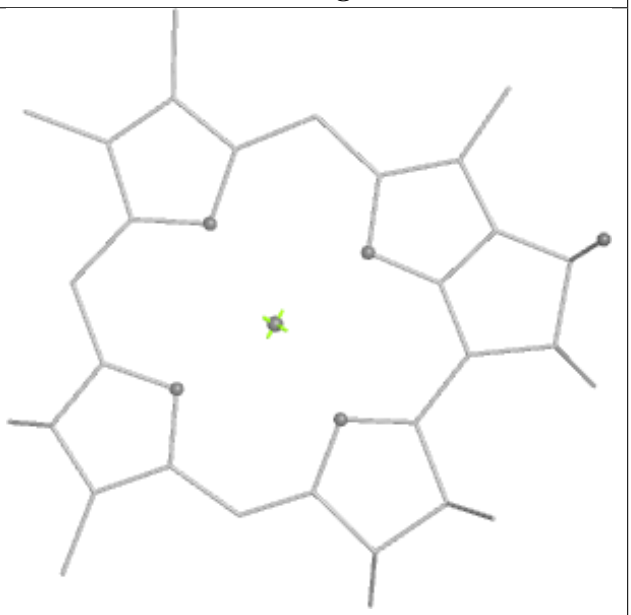
**Bond lengths**



**Bond angles**

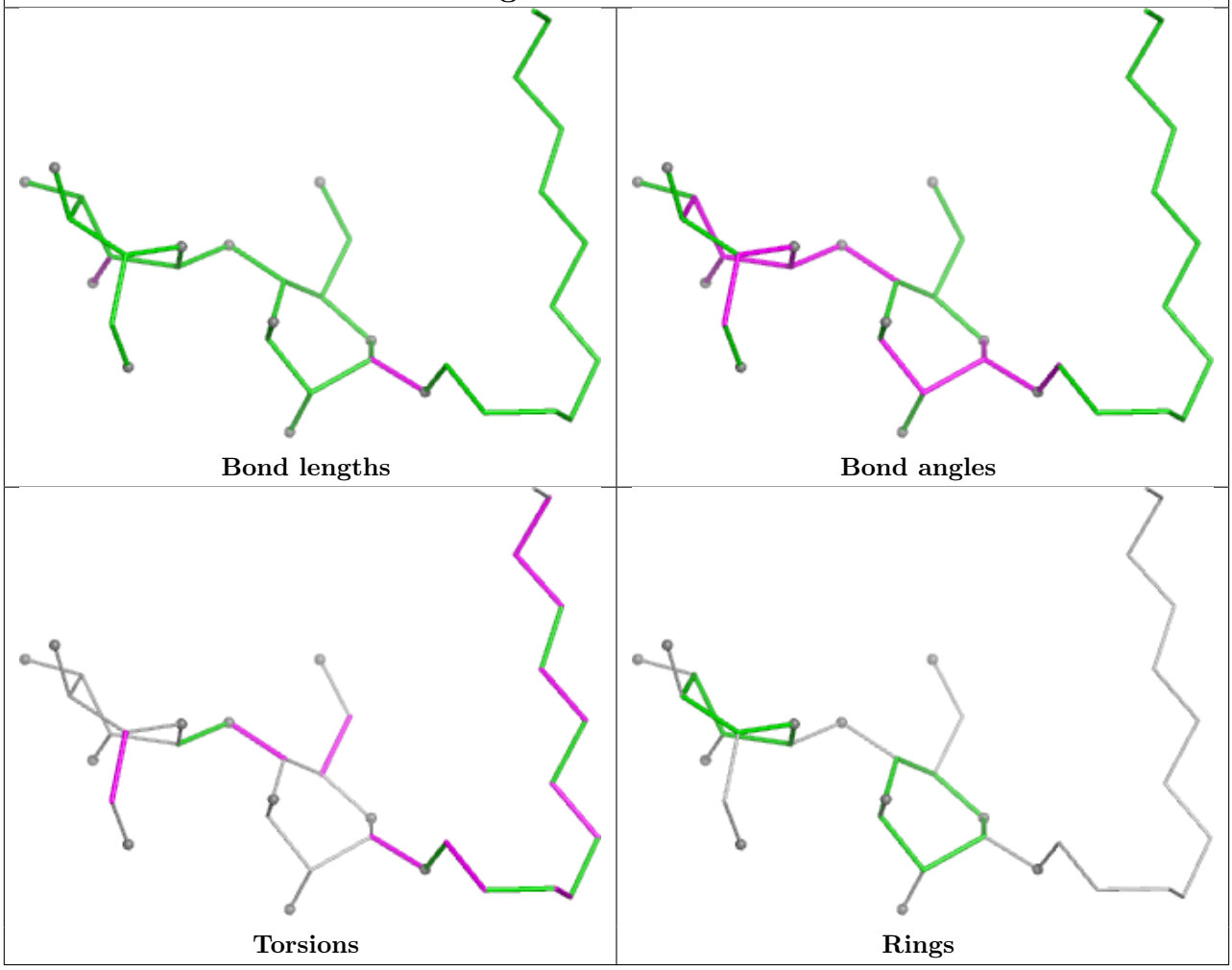


**Torsions**

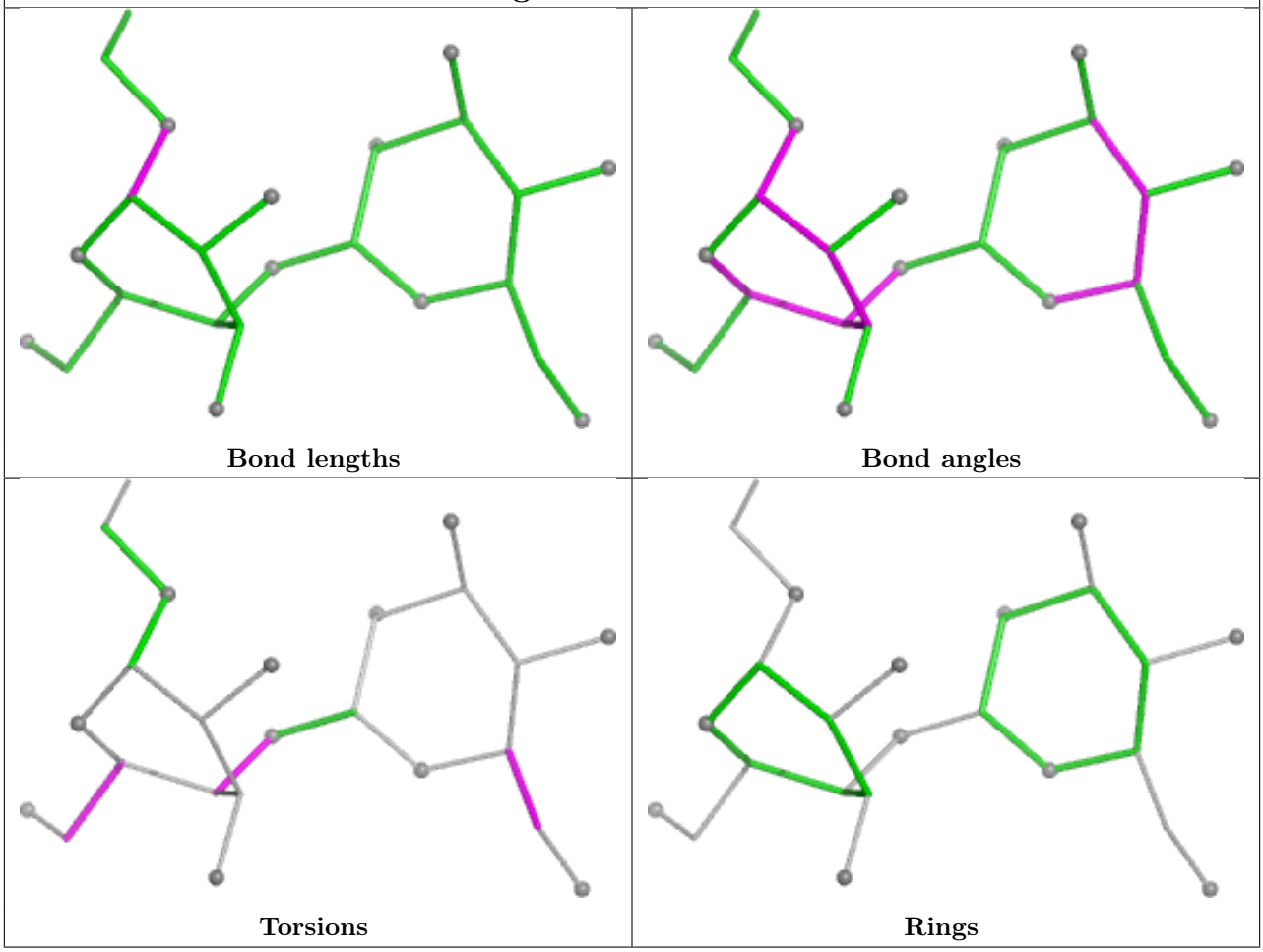


**Rings**

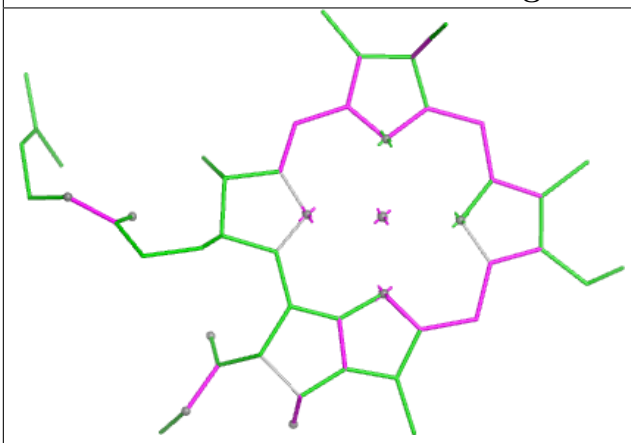
**Ligand LMU R 101**



**Ligand LMU B 849**



**Ligand CLA K 103**



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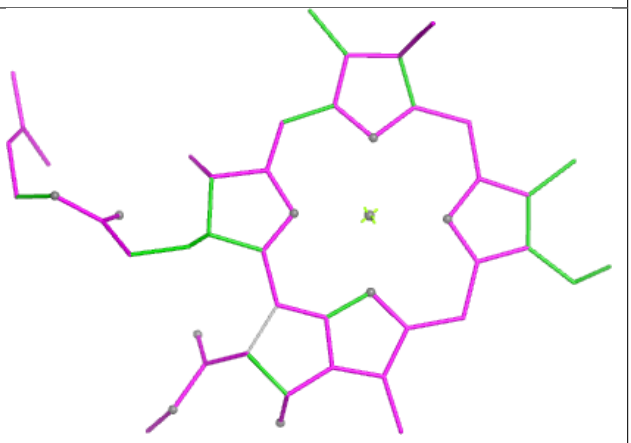
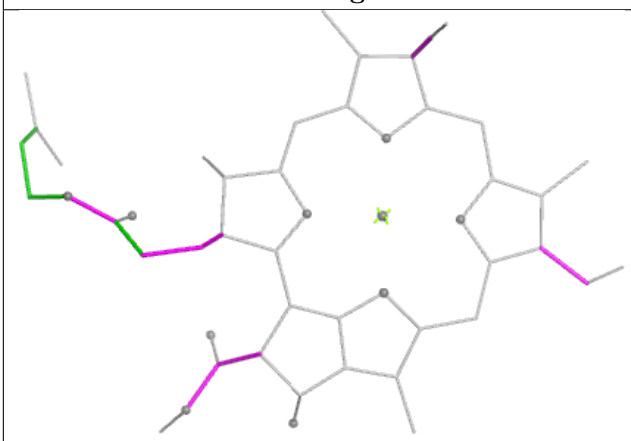
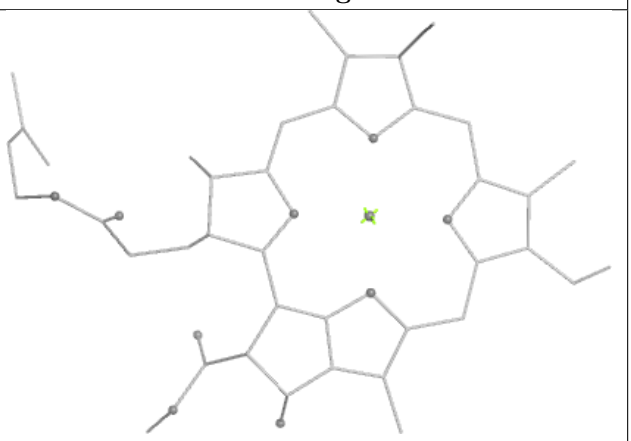


**Bond angles**

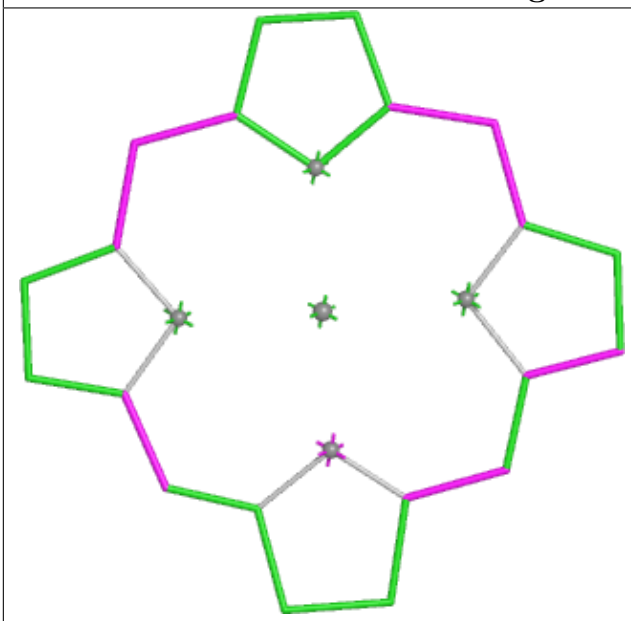


**Torsions**



**Rings**

**Ligand CLA 1 214**



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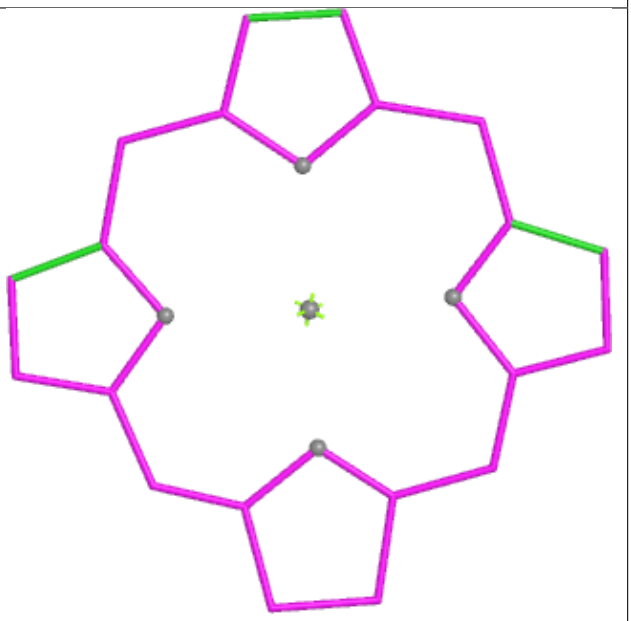
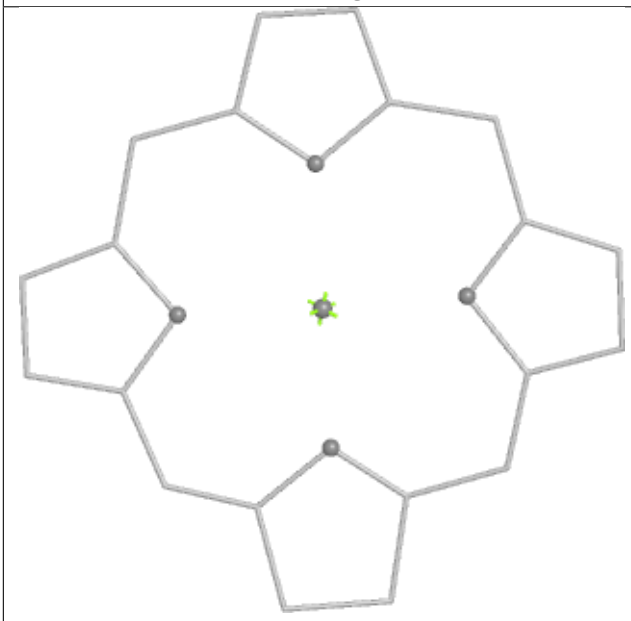
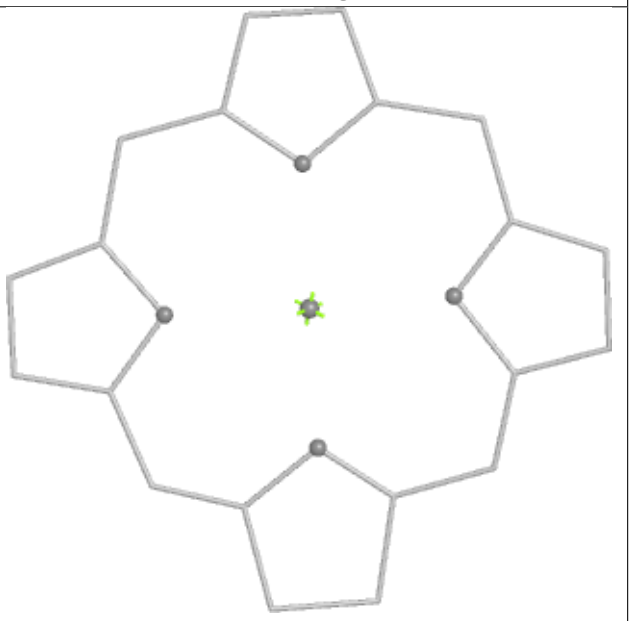


**Bond angles**

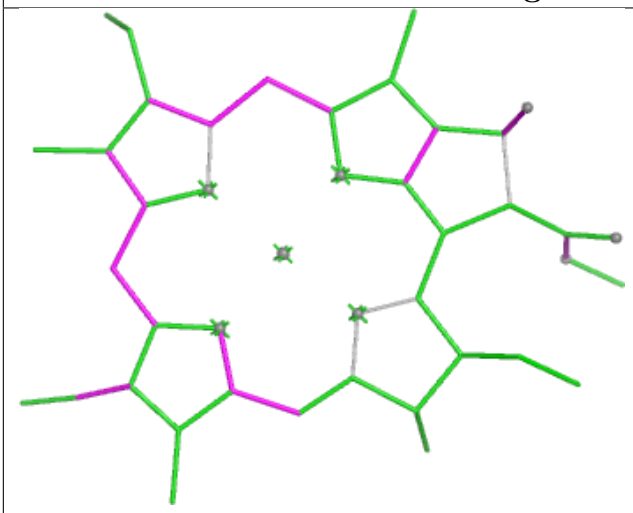


**Torsions**



**Rings**

**Ligand CLA A 821**



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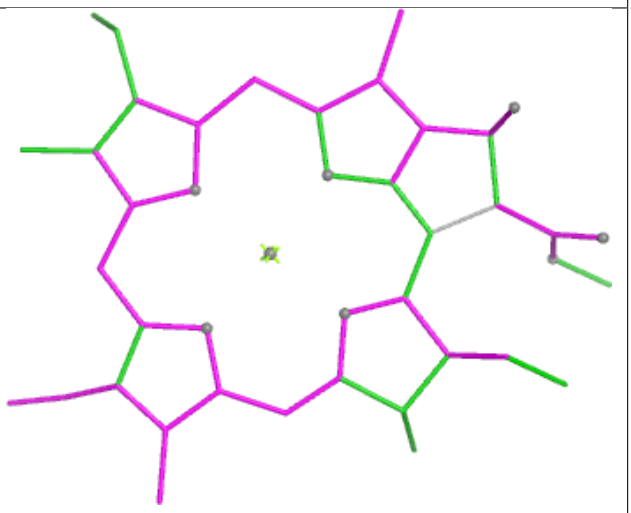
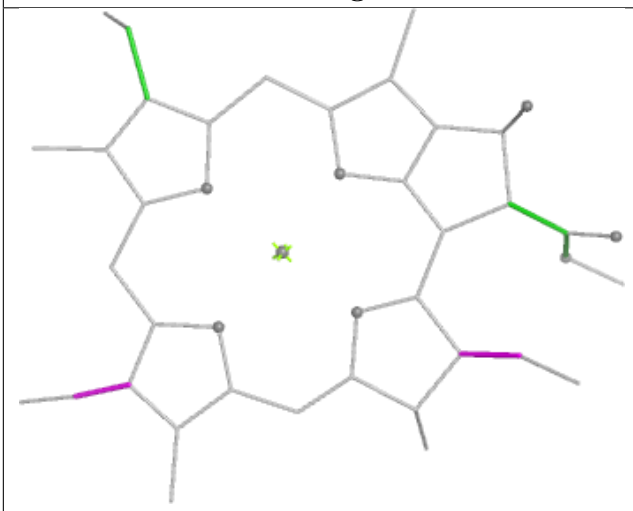
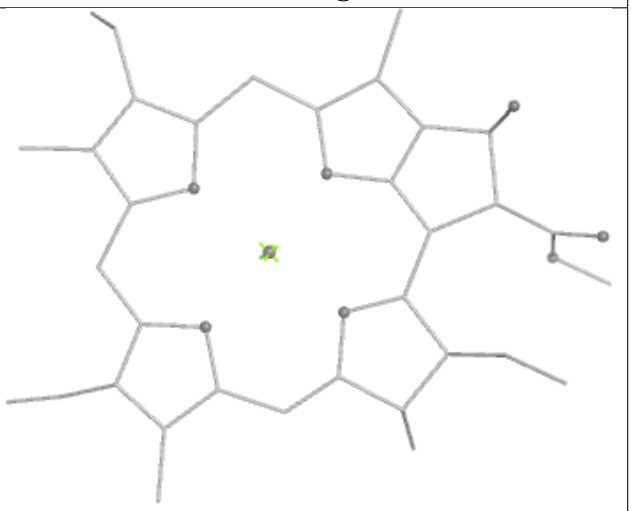


**Bond angles**

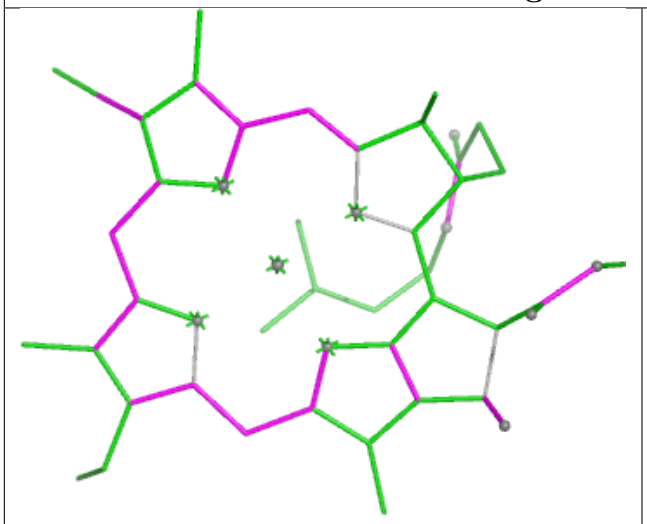


**Torsions**



**Rings**

**Ligand CLA B 831**



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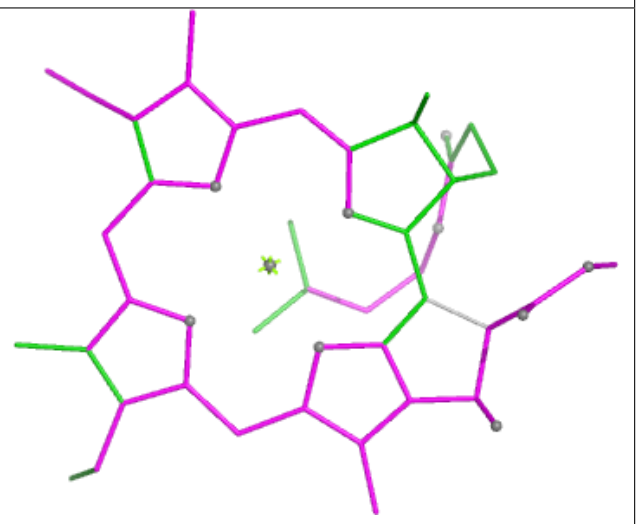

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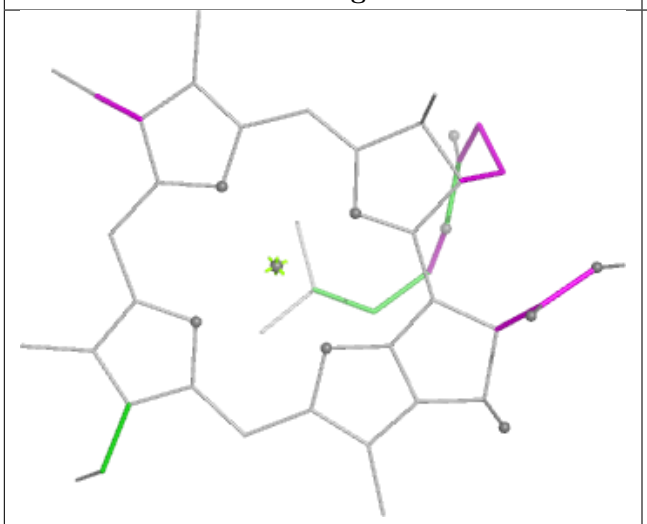
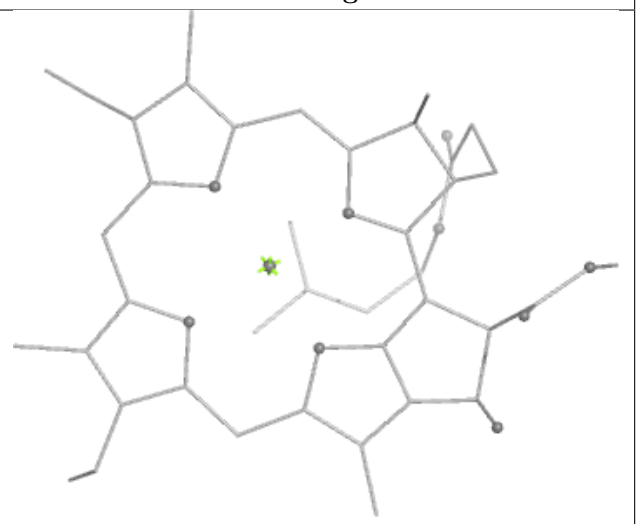
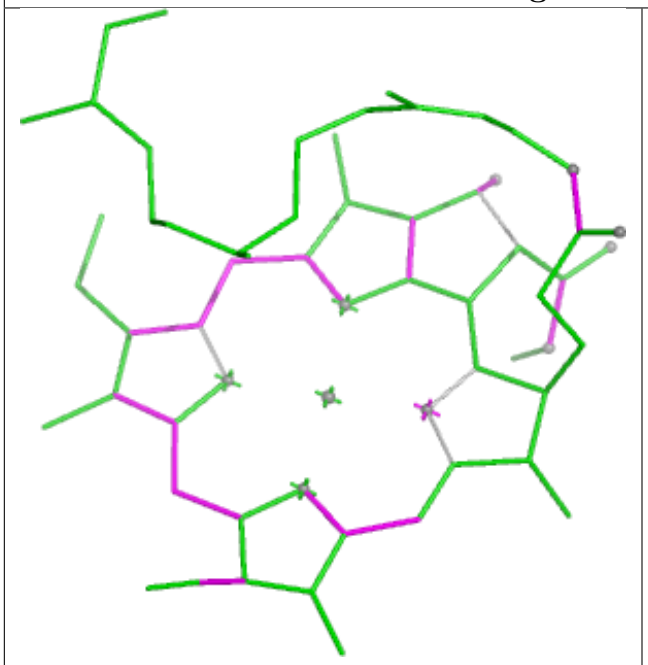


**Torsions**



**Rings**

**Ligand CLA 1 206**



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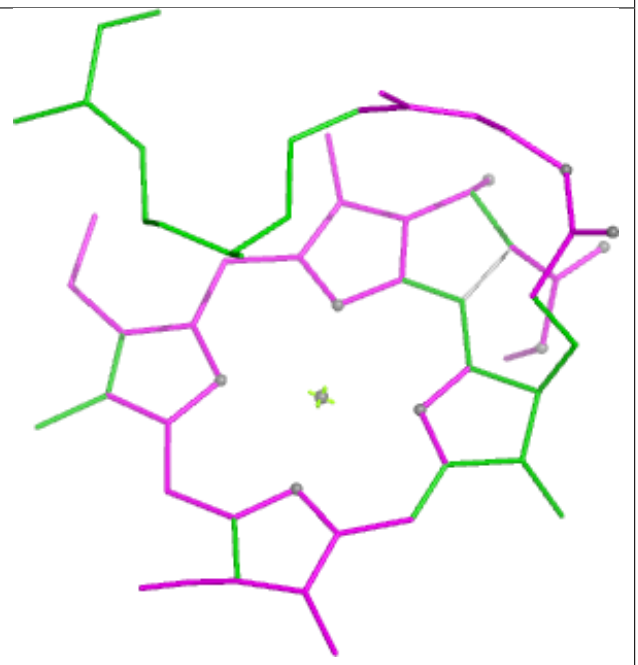

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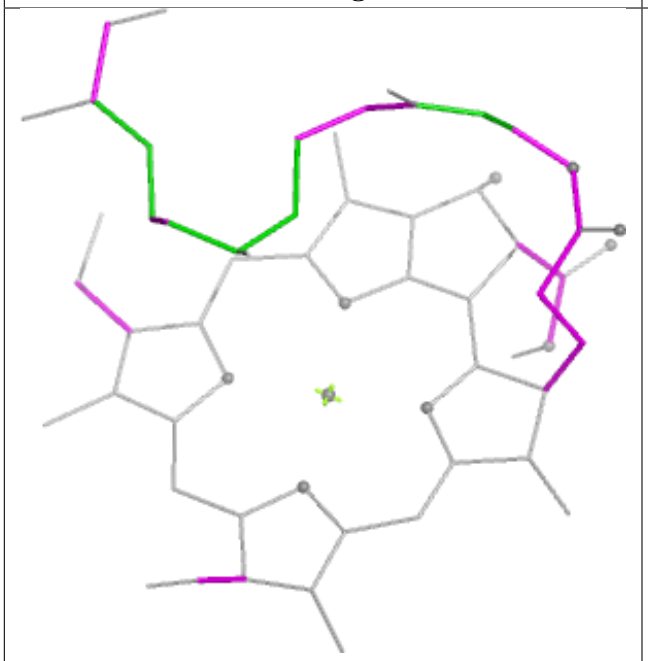
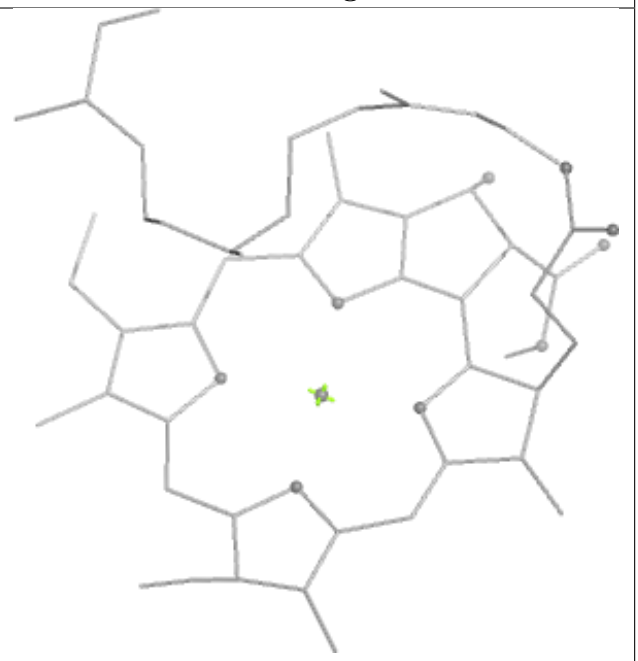
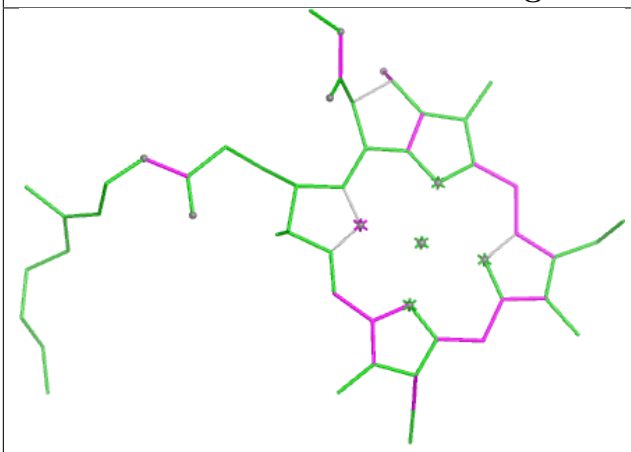


**Torsions**



**Rings**

**Ligand CLA B 802**



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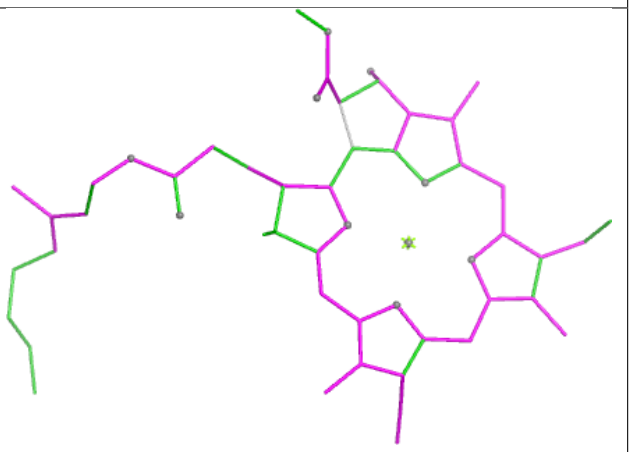

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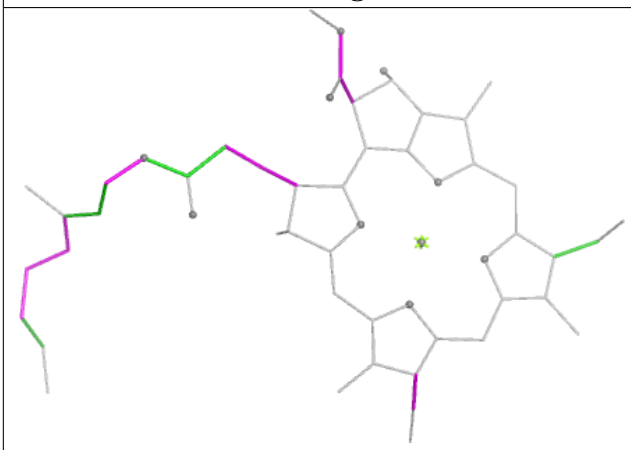
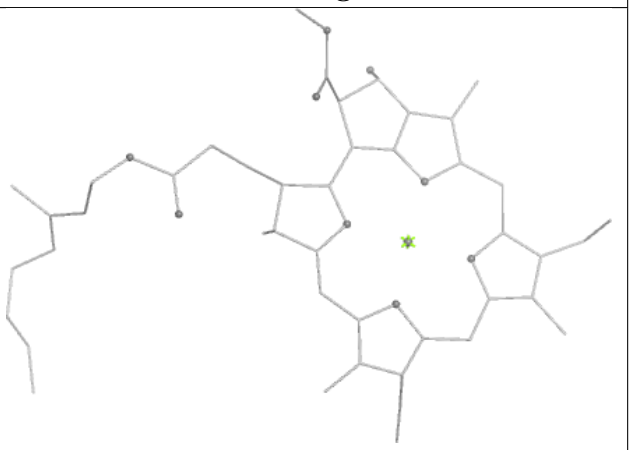
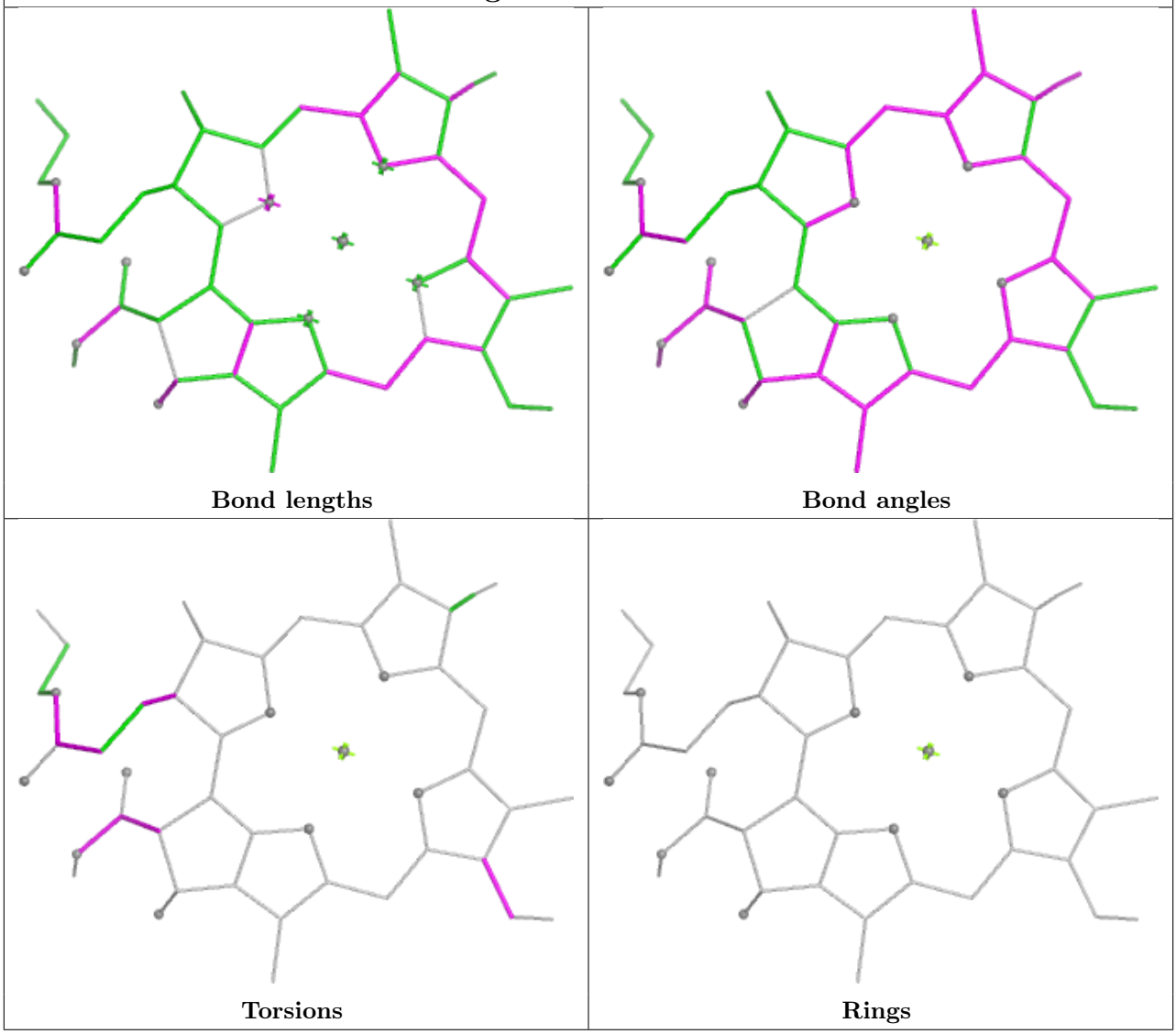


**Torsions**

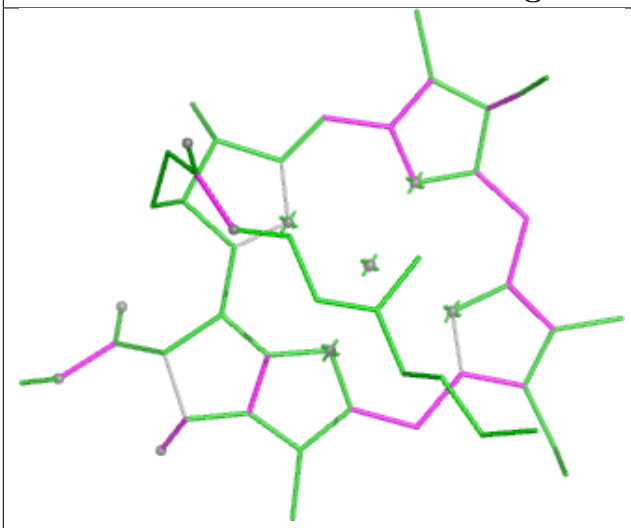


**Rings**

**Ligand CLA J 101**



**Ligand CLA B 818**



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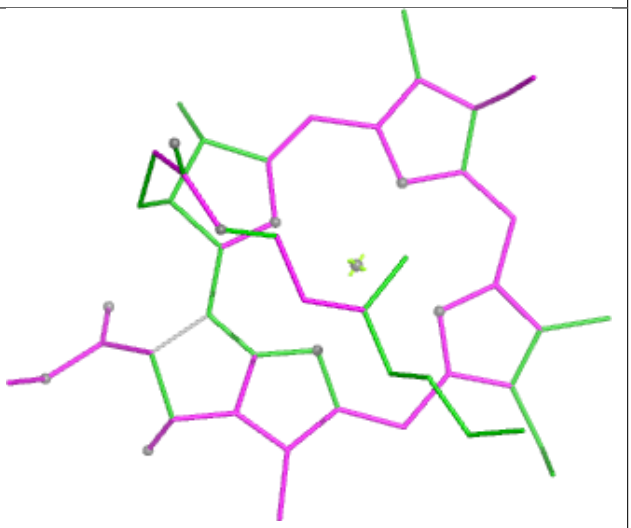
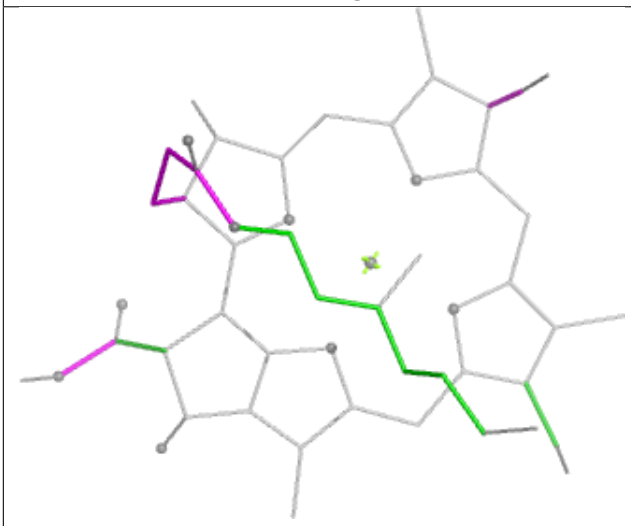


**Bond angles**



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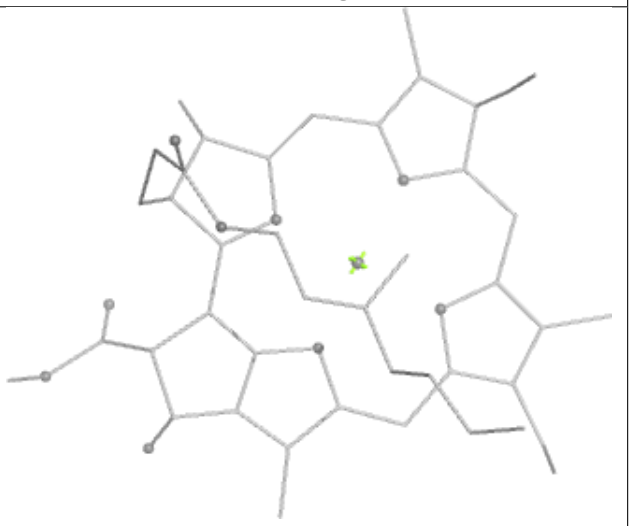
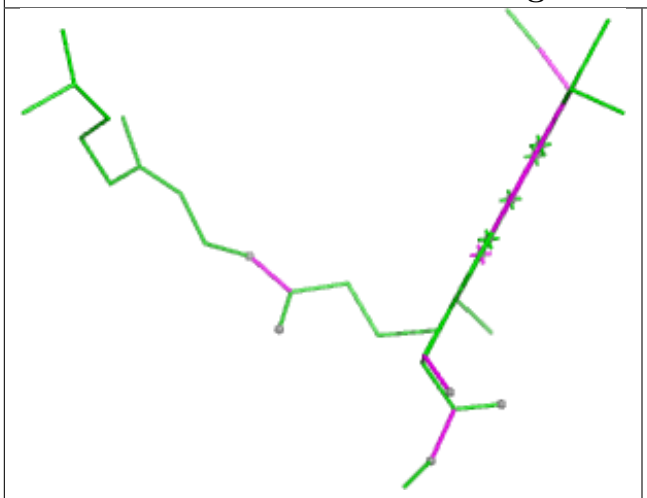


**Rings**

**Ligand CLA L 204**



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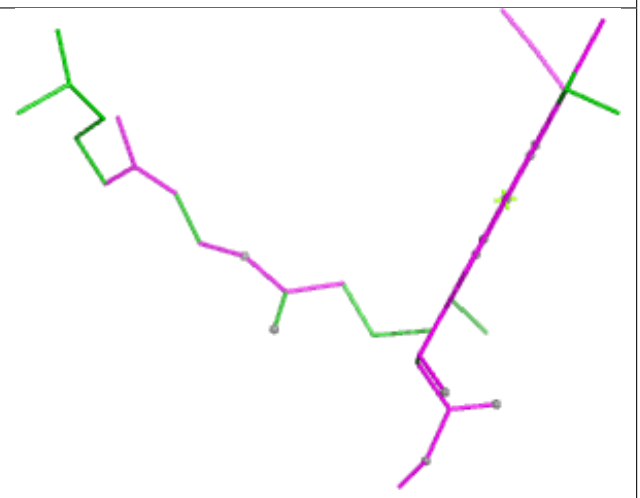
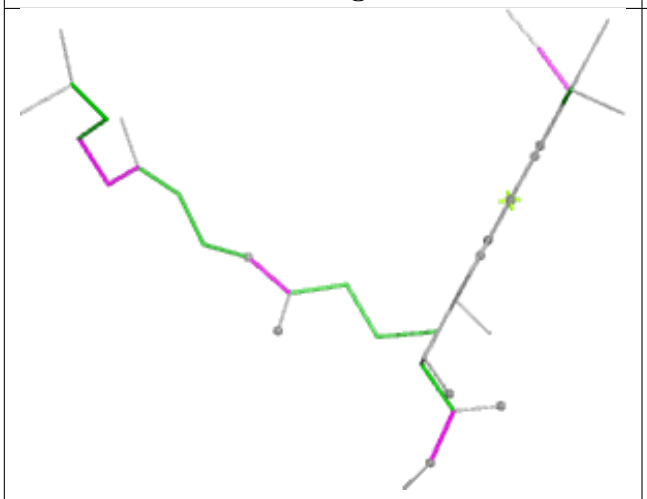


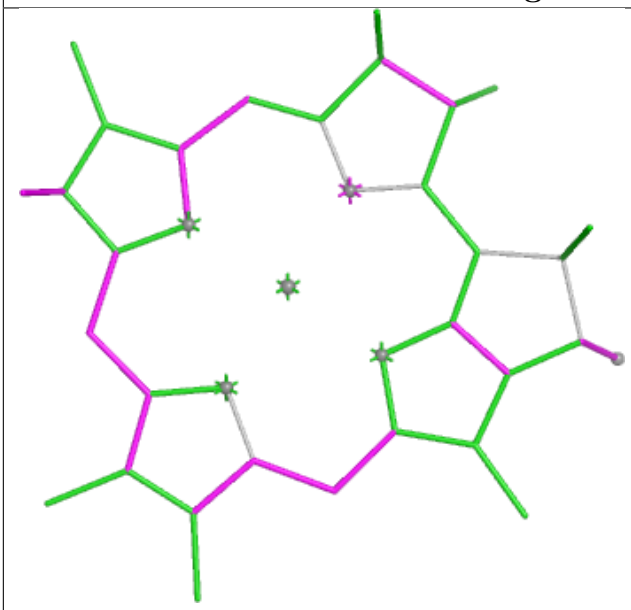
**Bond angles**



**Torsions**

**Rings**

**Ligand CLA B 842**



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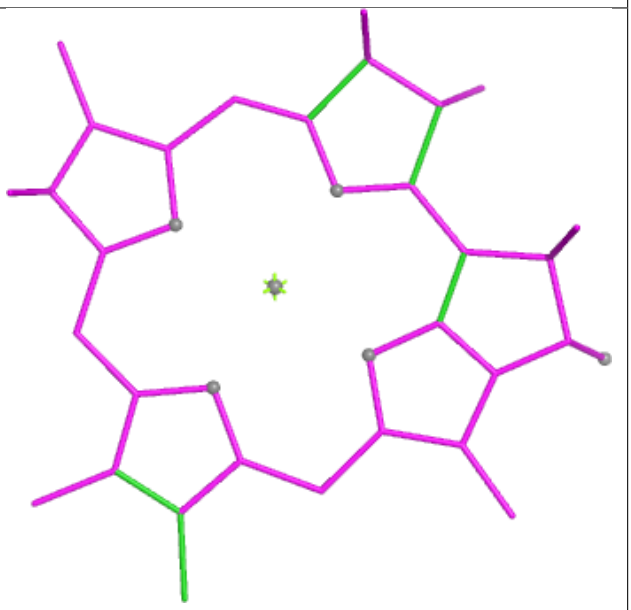
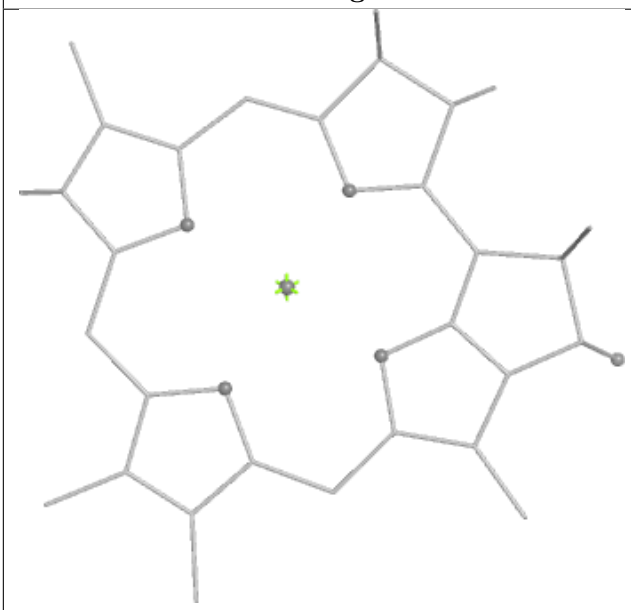
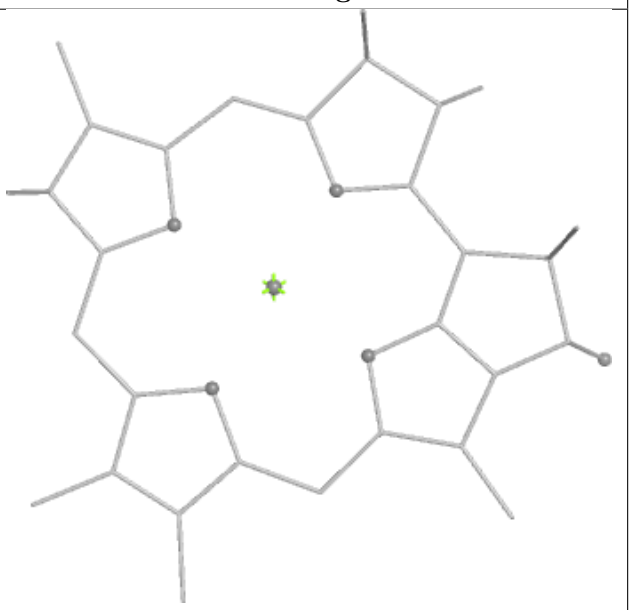


**Bond angles**

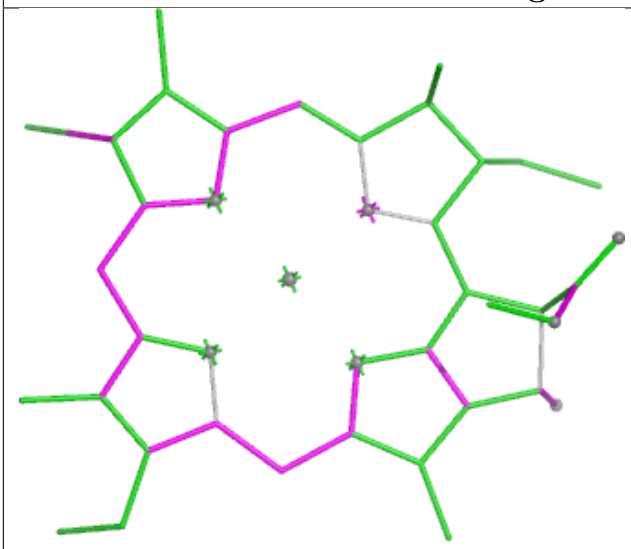


**Torsions**



**Rings**

**Ligand CLA 3 307**



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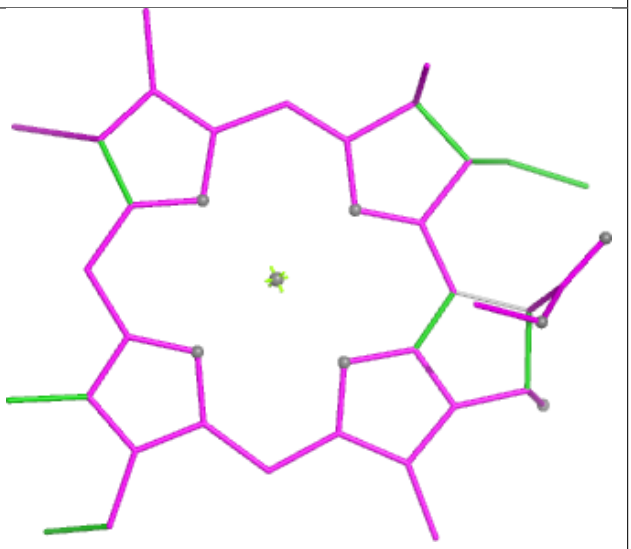
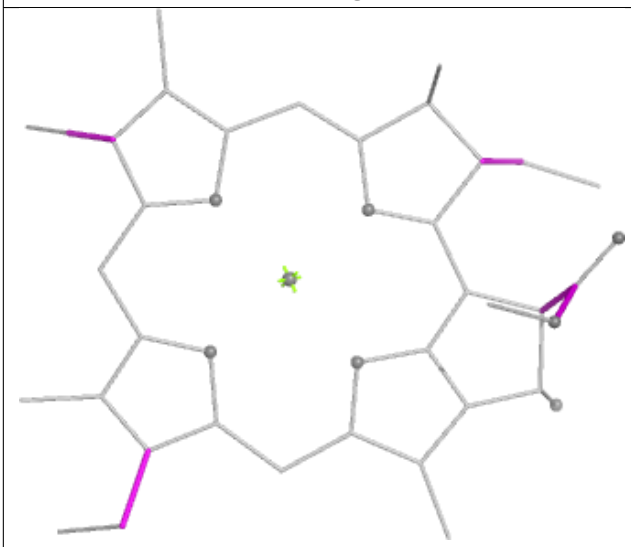
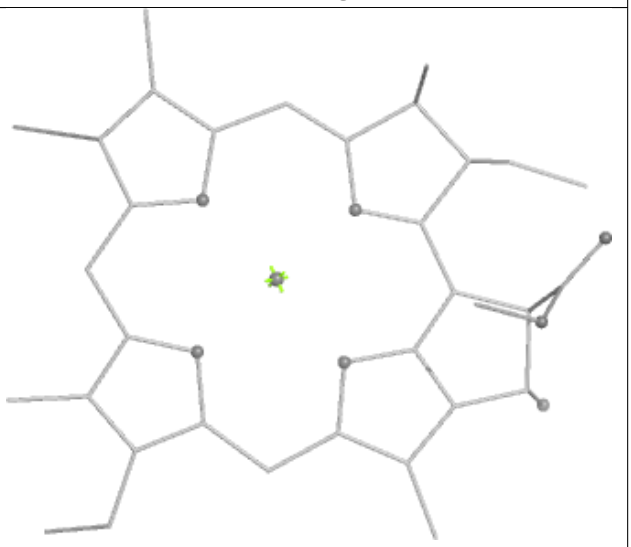


**Bond angles**

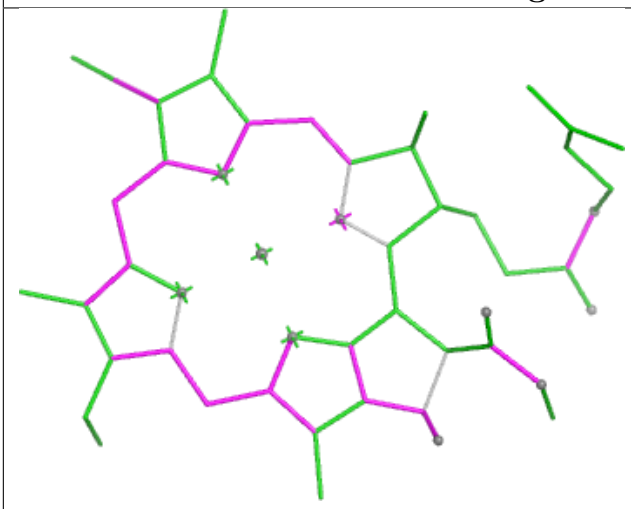


**Torsions**



**Rings**

**Ligand CLA 2 314**



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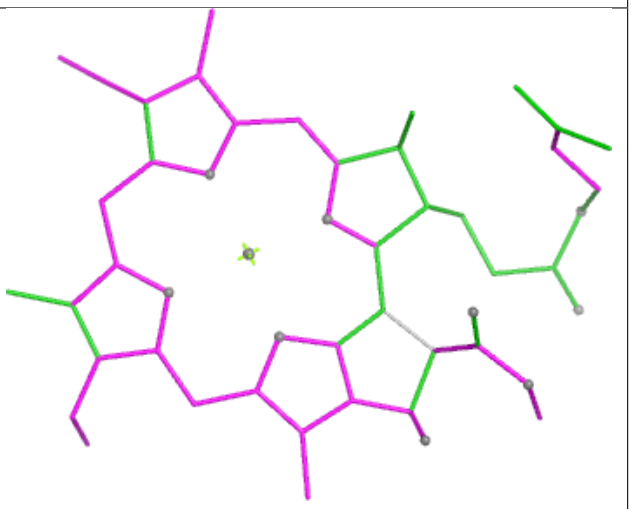
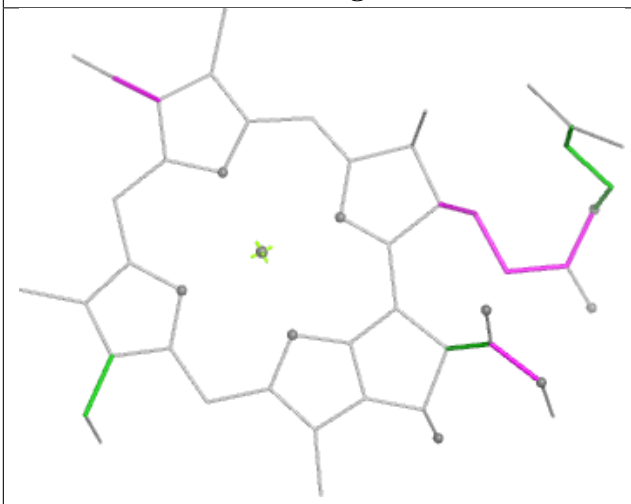
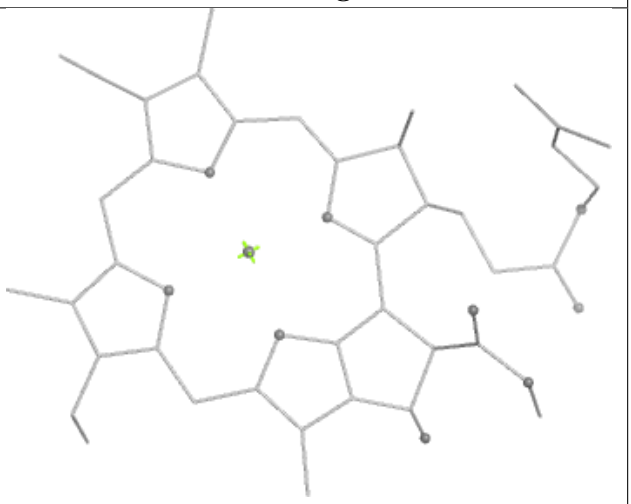


**Bond angles**

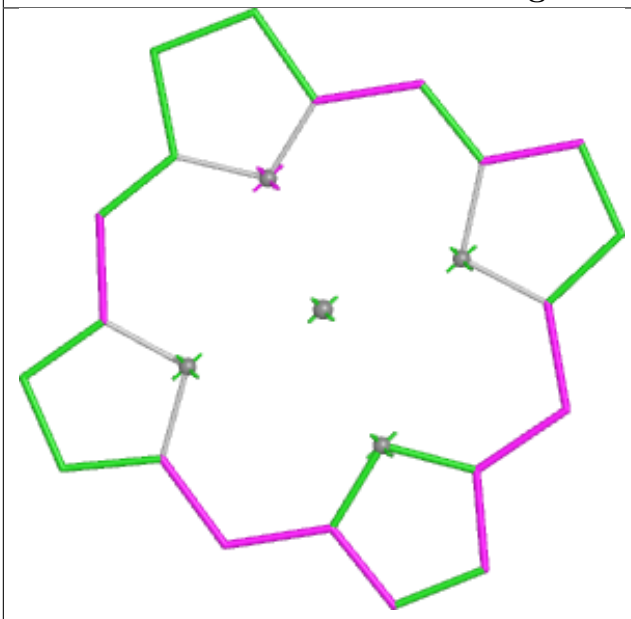


**Torsions**



**Rings**

**Ligand CLA 4 308**



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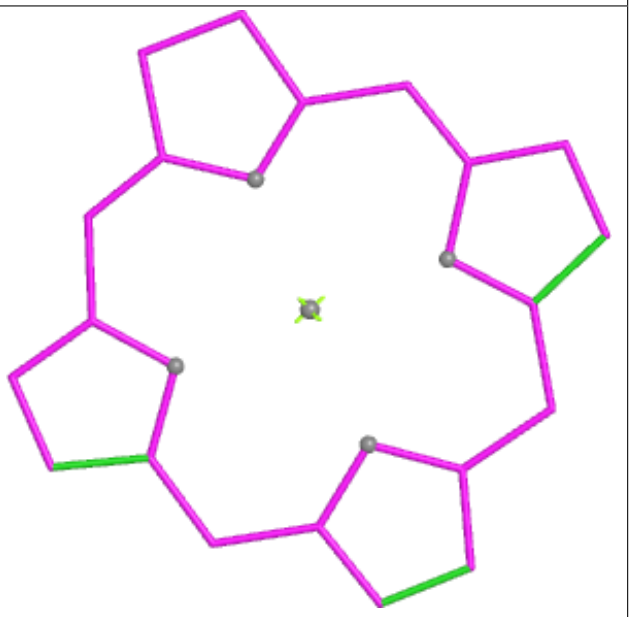
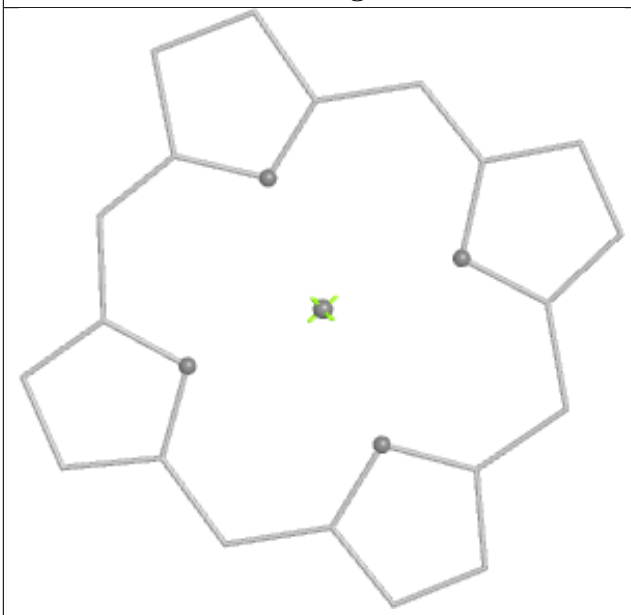
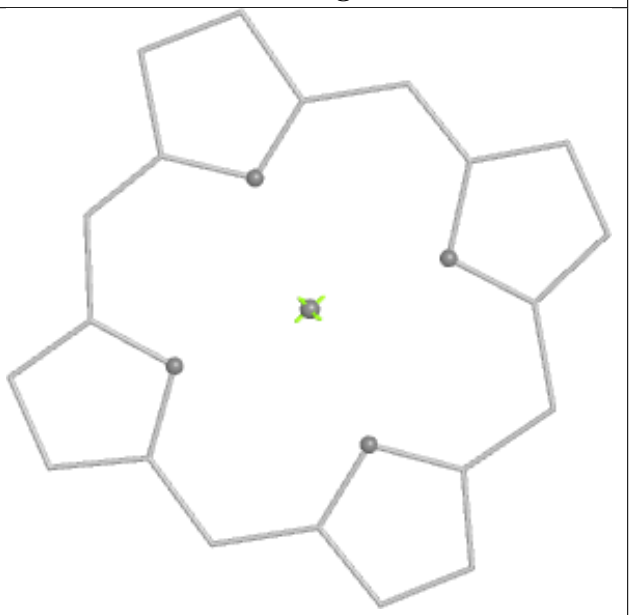


**Bond angles**

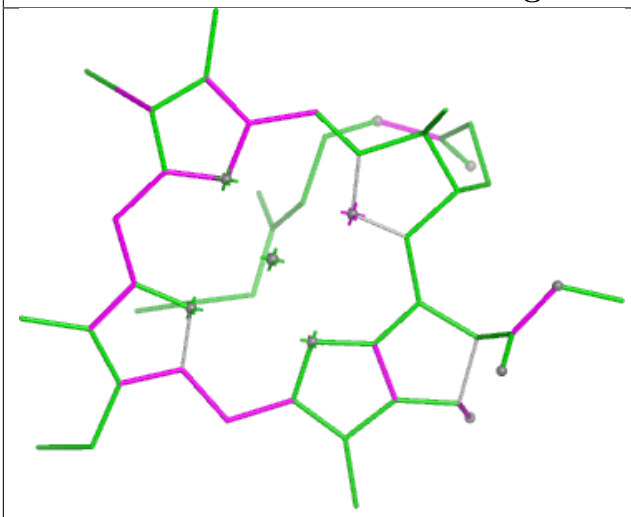


**Torsions**

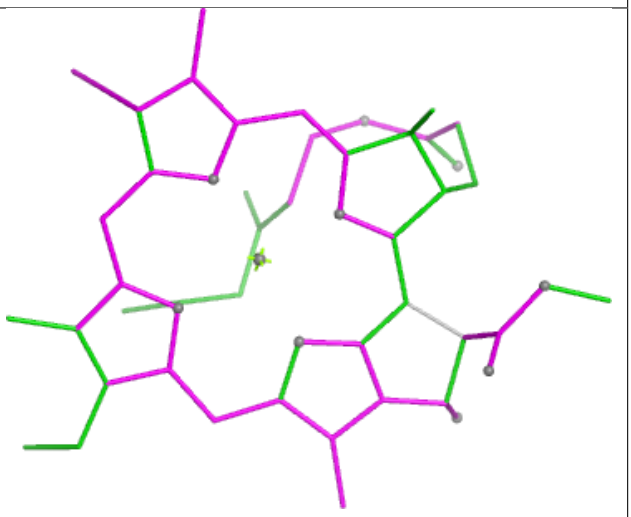


**Rings**

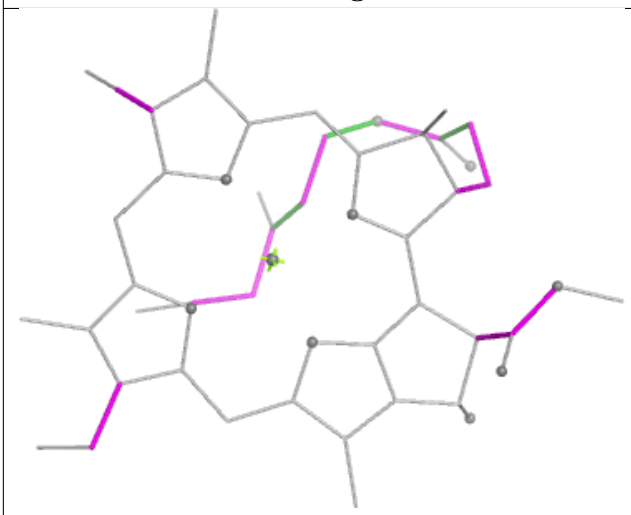
**Ligand CLA A 817**



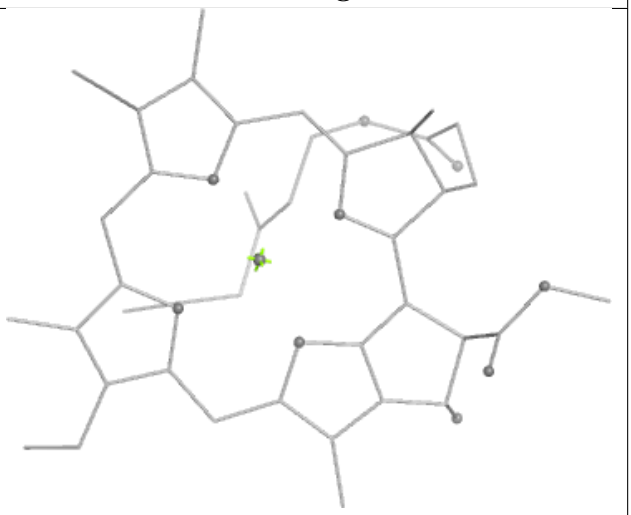
**Bond lengths**



**Bond angles**

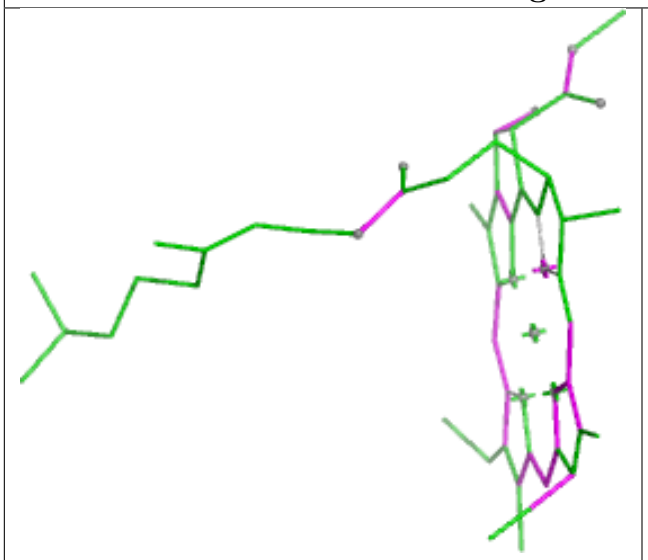


**Torsions**

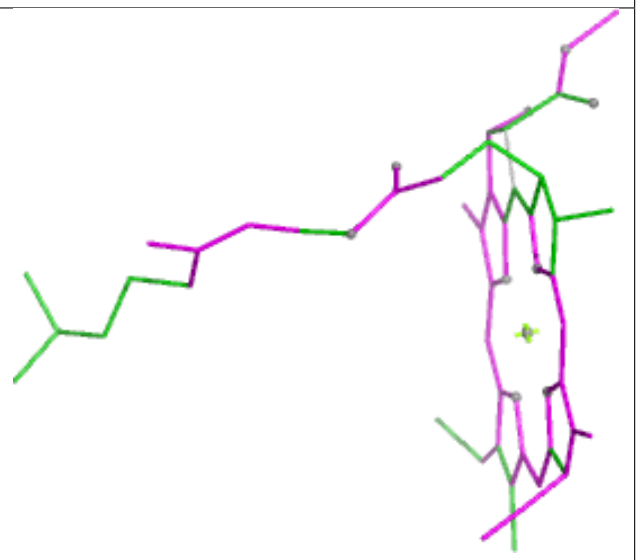


**Rings**

**Ligand CLA 4 301**

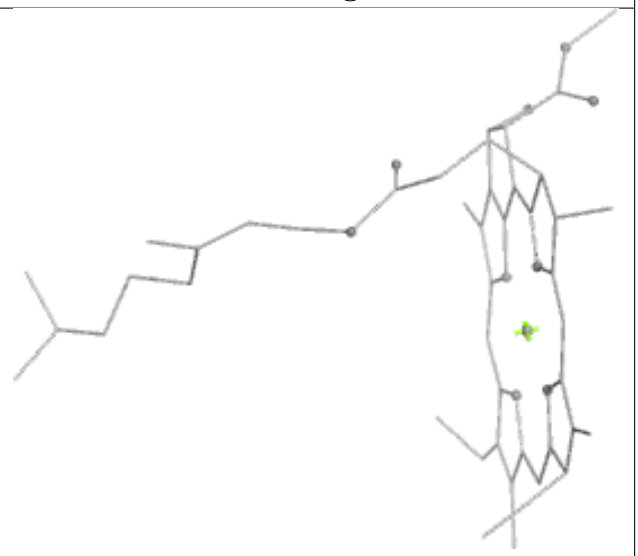


**Bond lengths**



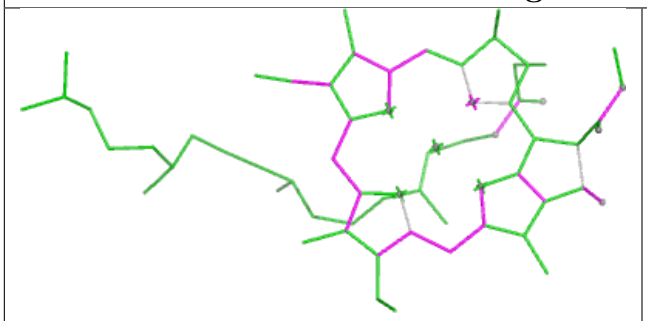
**Bond angles**

**Torsions**

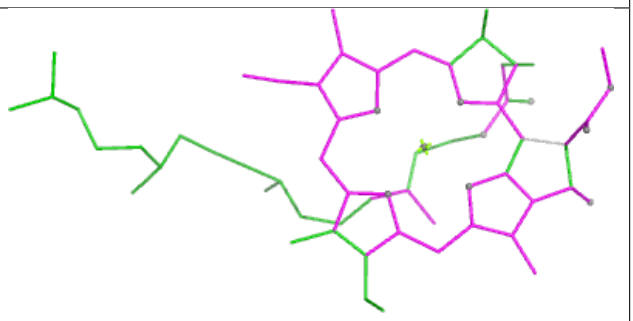


**Rings**

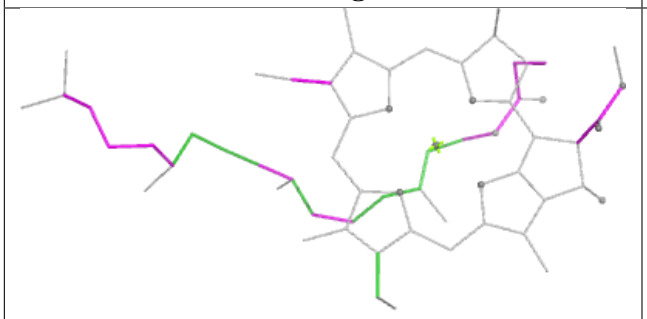
## Ligand CLA B 806



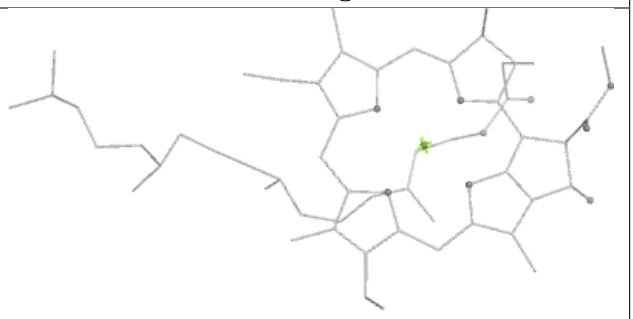
Bond lengths



Bond angles

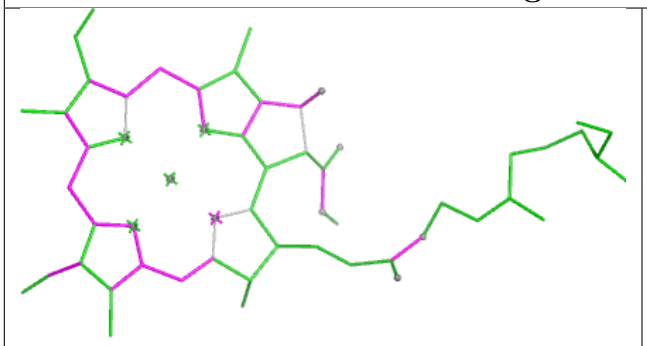


Torsions

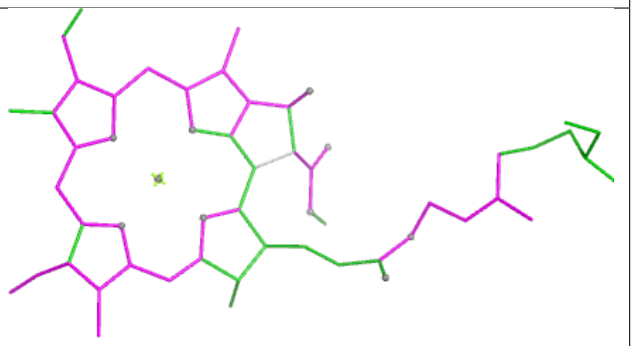


Rings

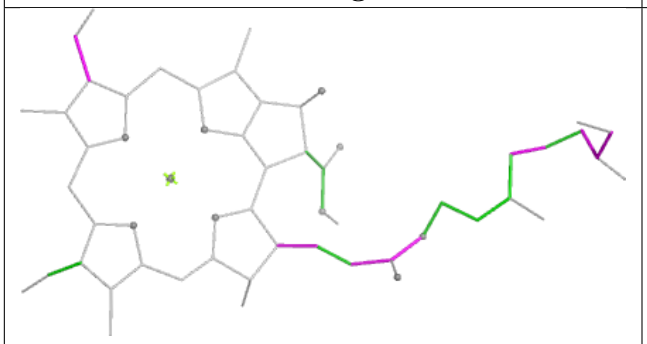
## Ligand CLA K 104



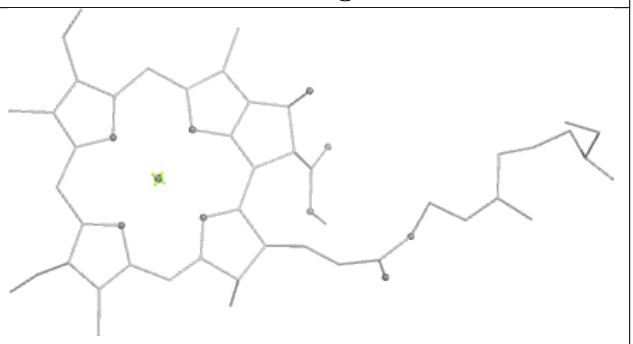
Bond lengths



Bond angles

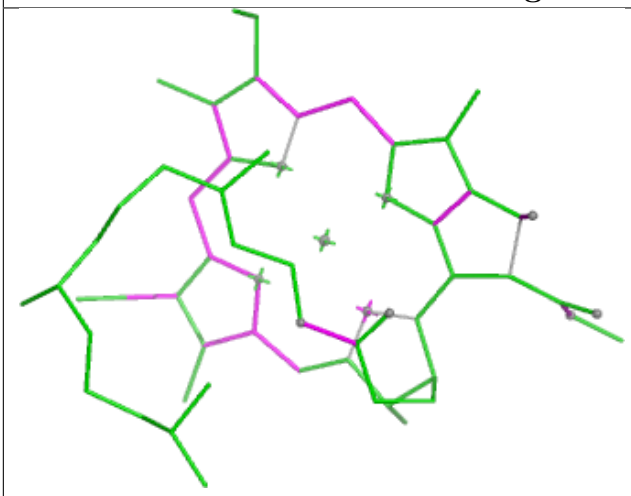


Torsions

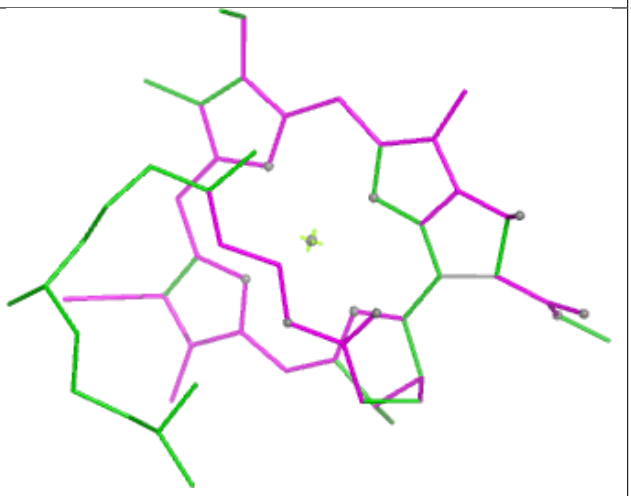


Rings

## Ligand CLA B 810

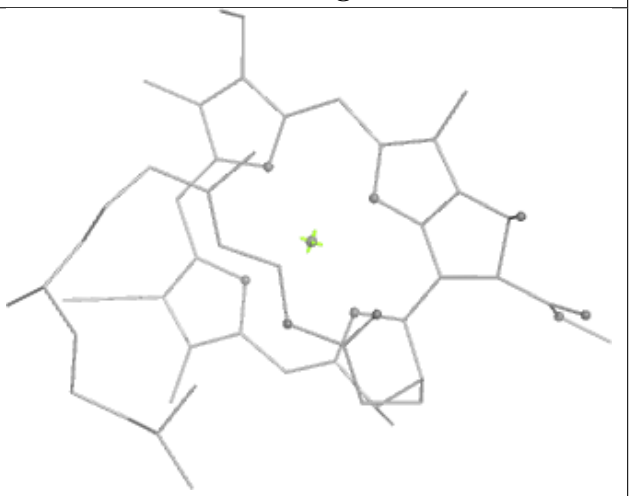


Bond lengths



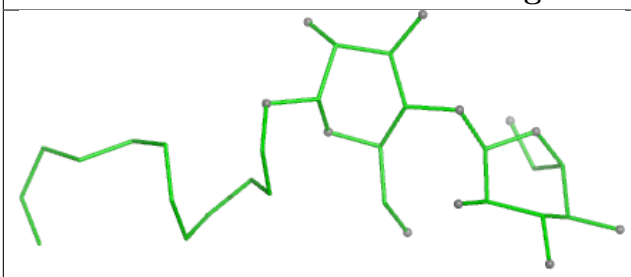
Bond angles

Torsions

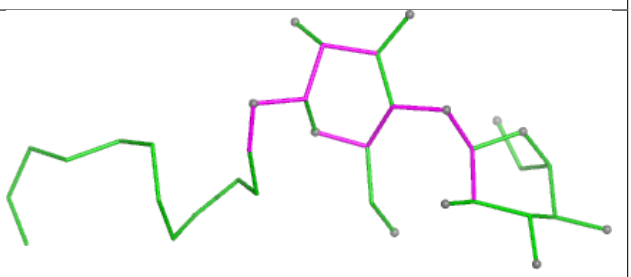


Rings

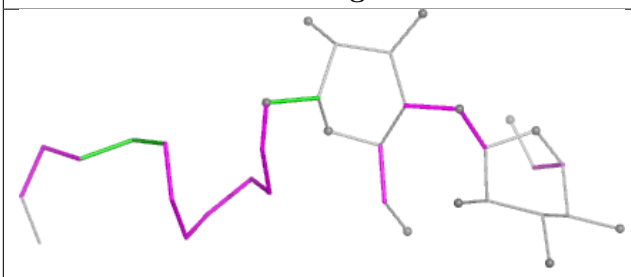
## Ligand LMU 2 313



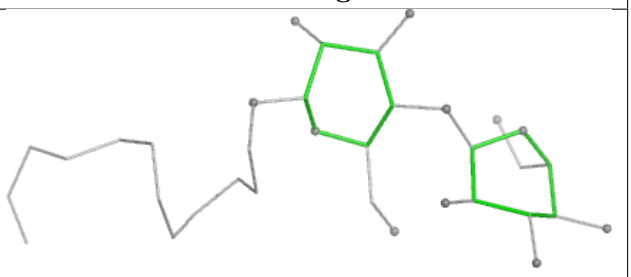
Bond lengths



Bond angles

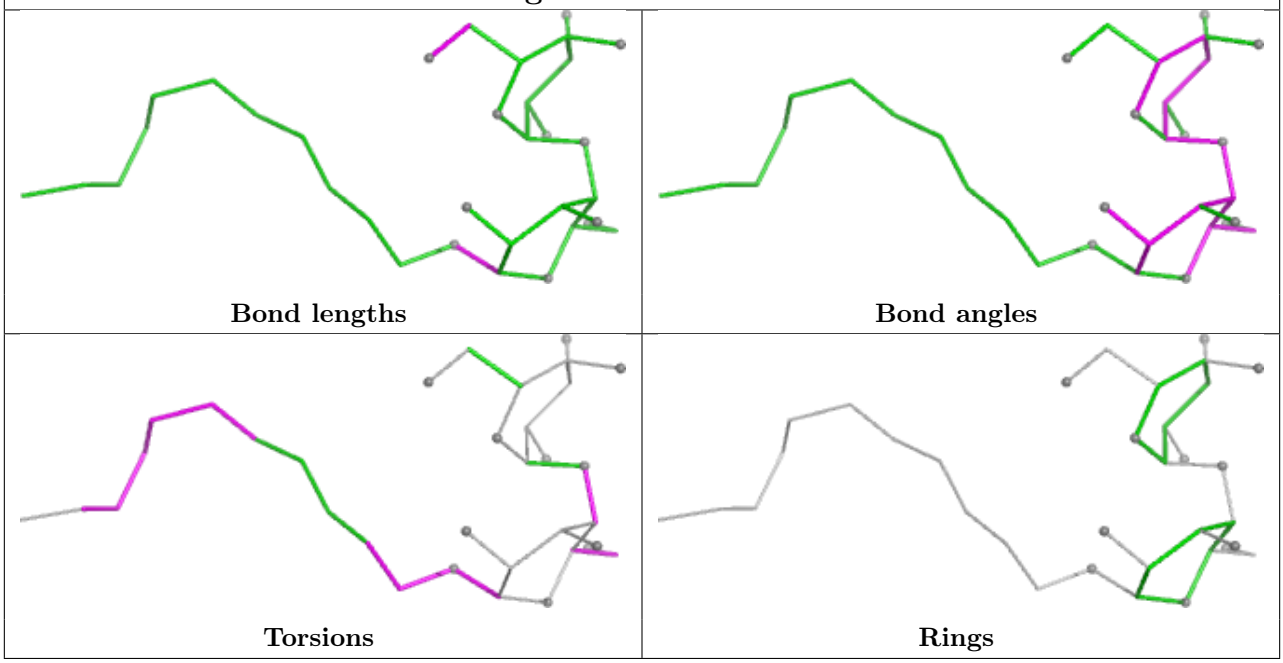


Torsions

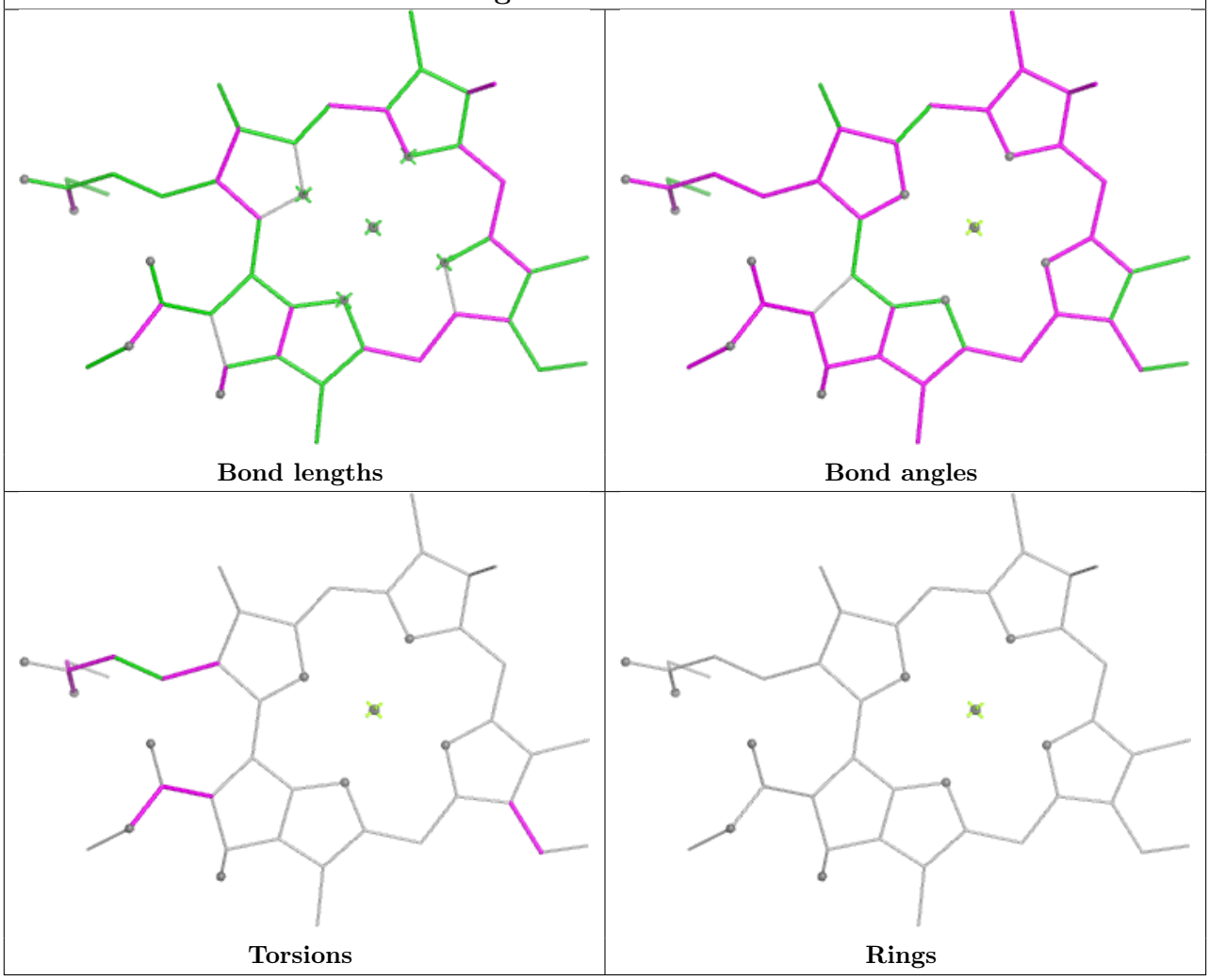


Rings

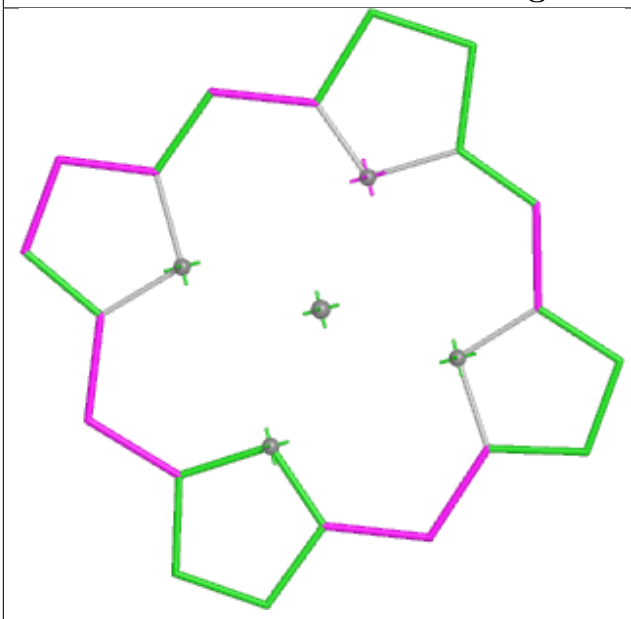
## Ligand LMU 4 319



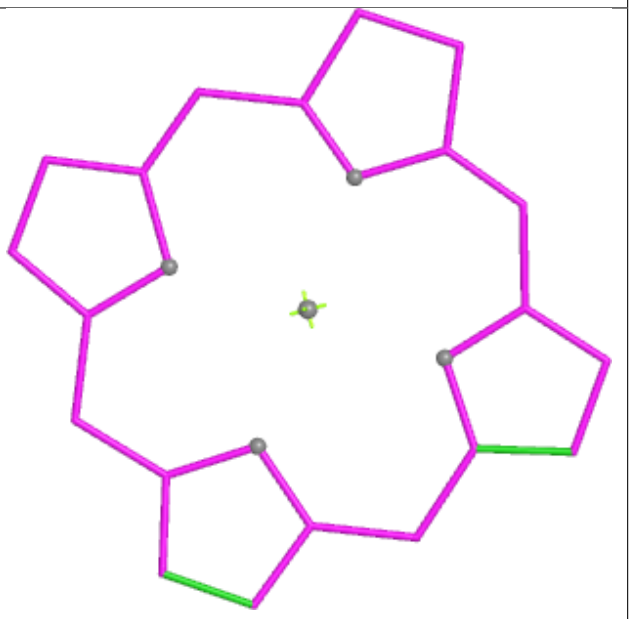

## Ligand CLA A 801



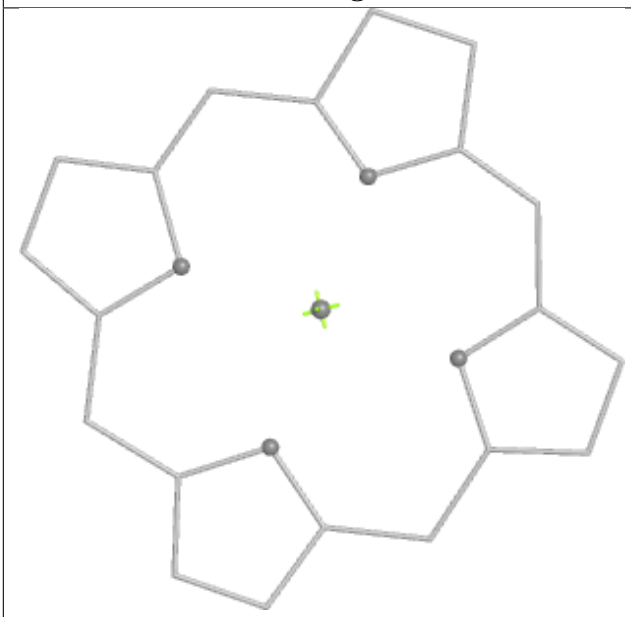
**Ligand CLA 3 312**



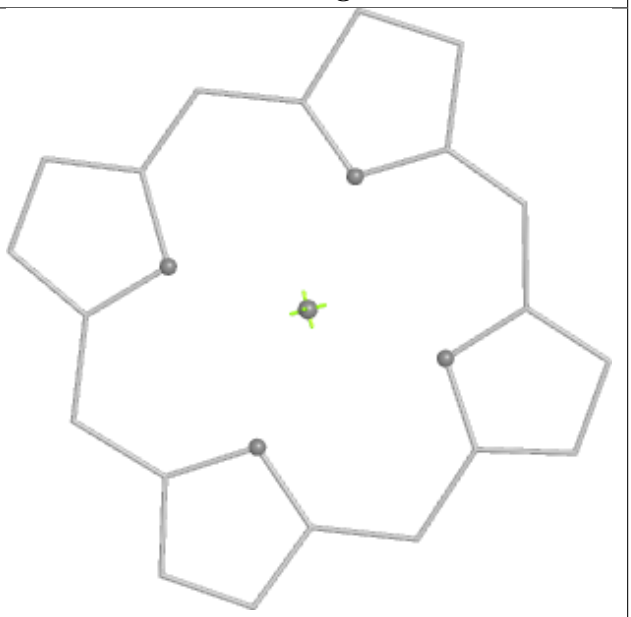
**Bond lengths**



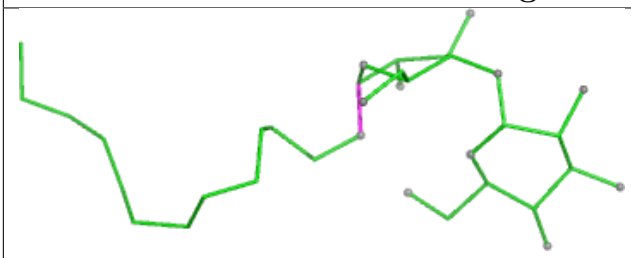
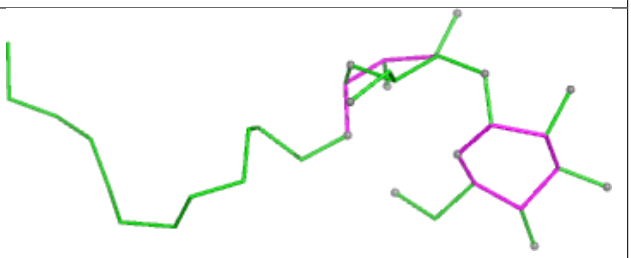
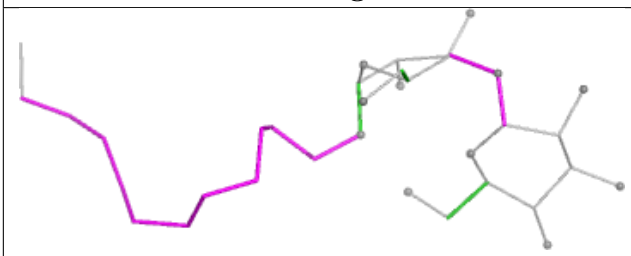
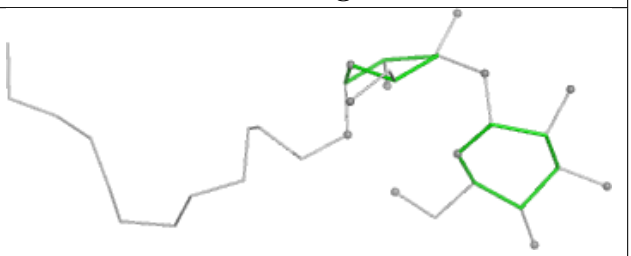
**Bond angles**



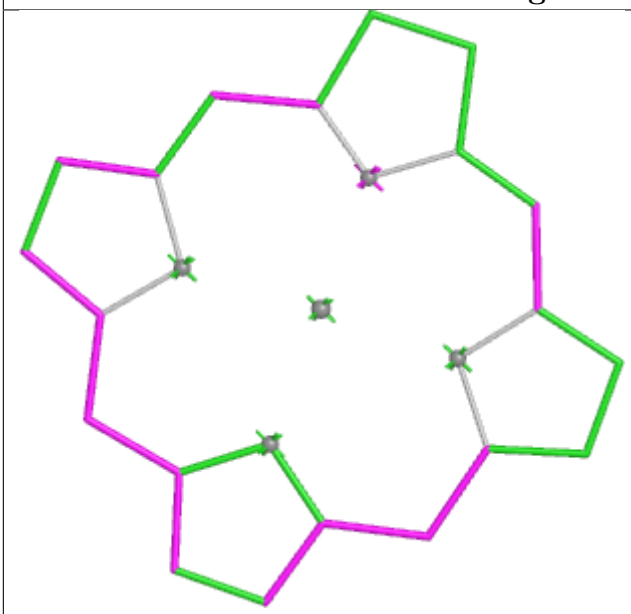
**Torsions**



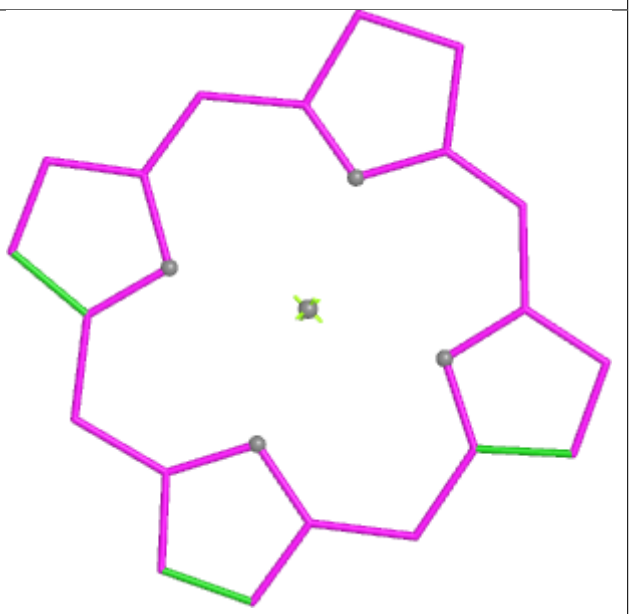
**Rings**

| Ligand LMU A 847 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

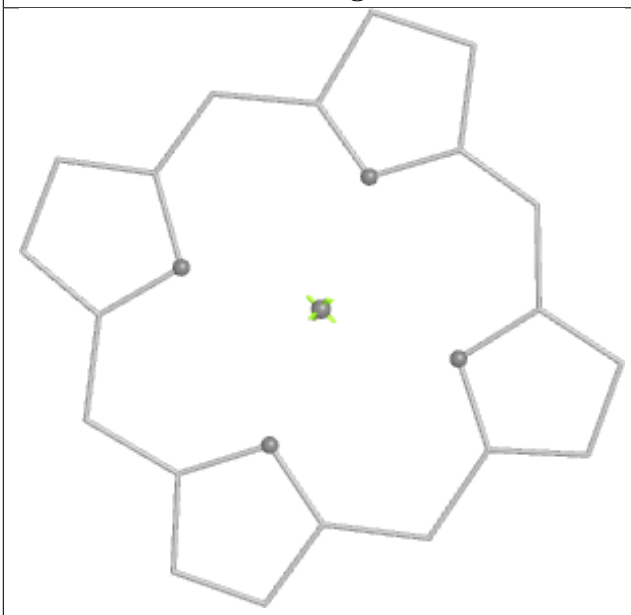
## Ligand CLA 2 304



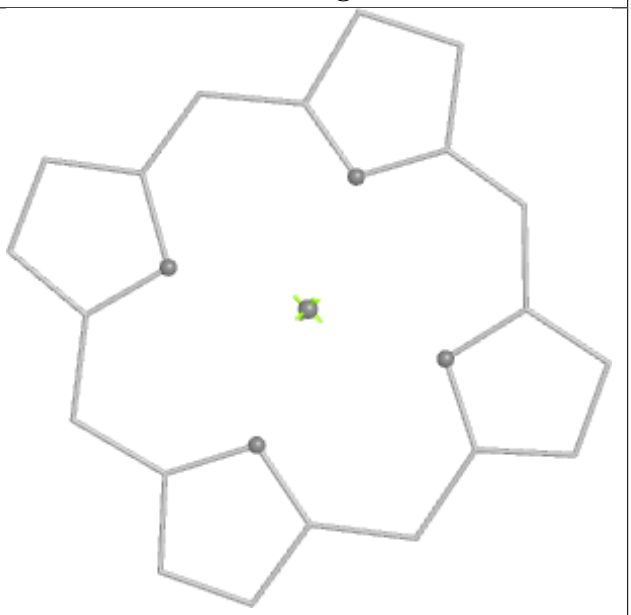
Bond lengths



Bond angles

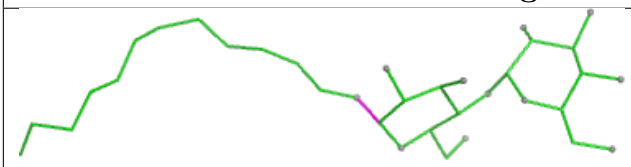


Torsions

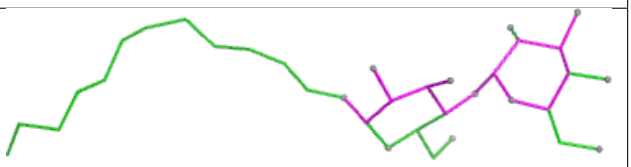


Rings

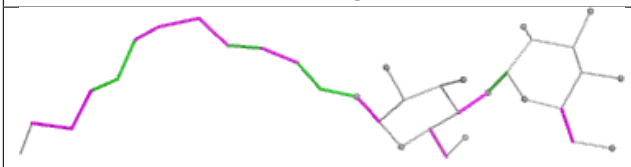
## Ligand LMU B 805



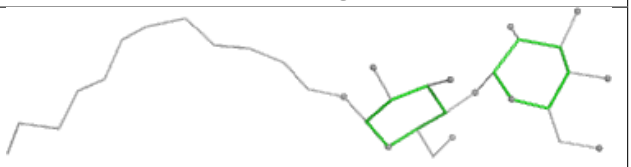
Bond lengths



Bond angles

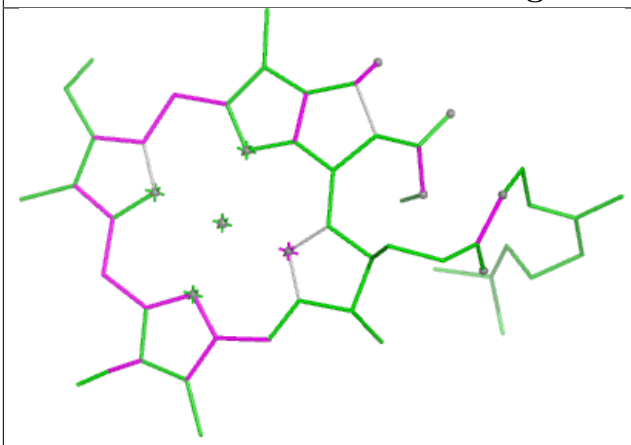


Torsions

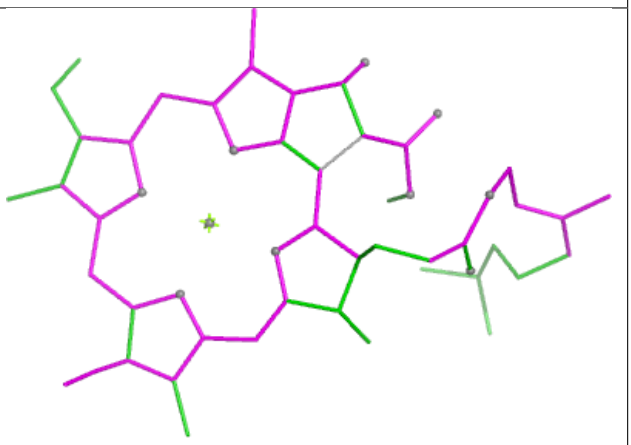


Rings

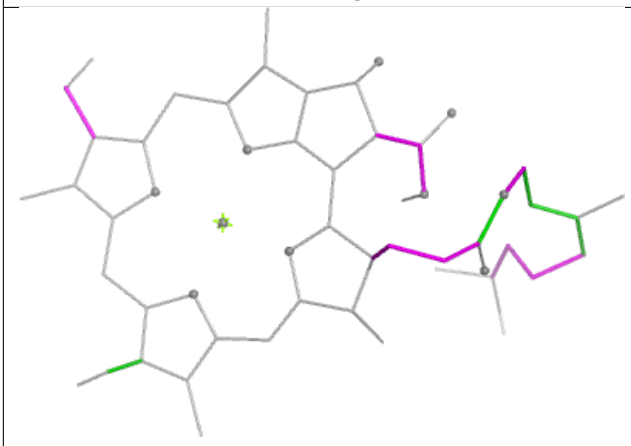
**Ligand CLA L 202**



**Bond lengths**



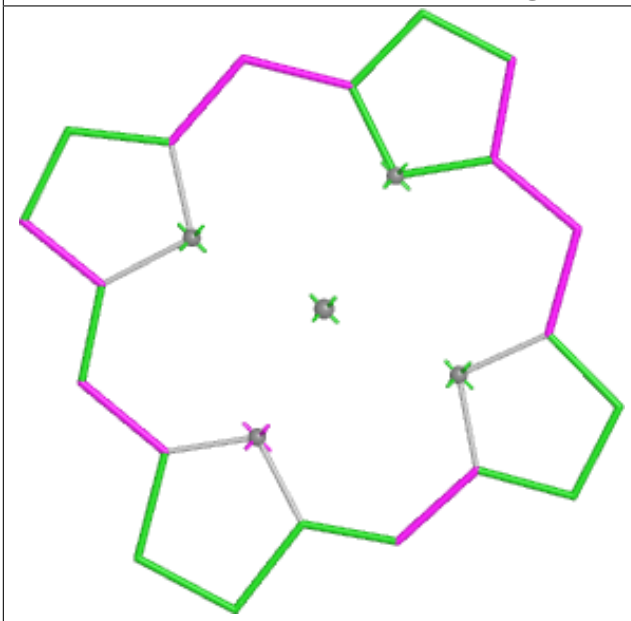
**Bond angles**



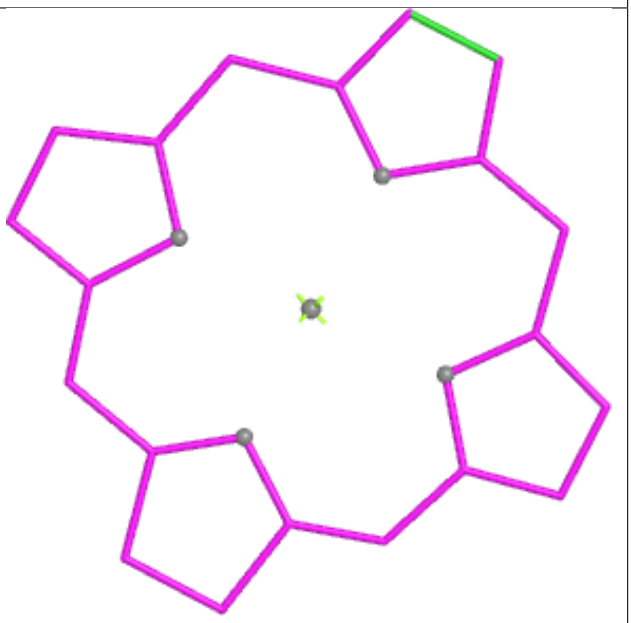
**Torsions**

**Rings**

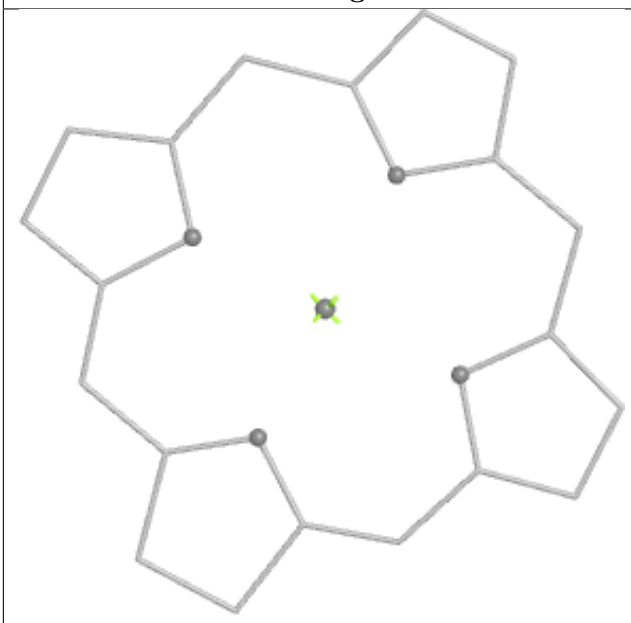
**Ligand CLA A 841**



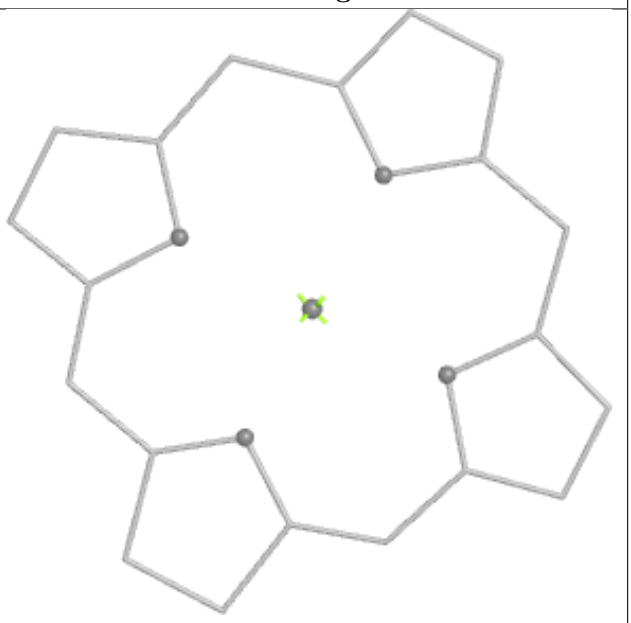
**Bond lengths**



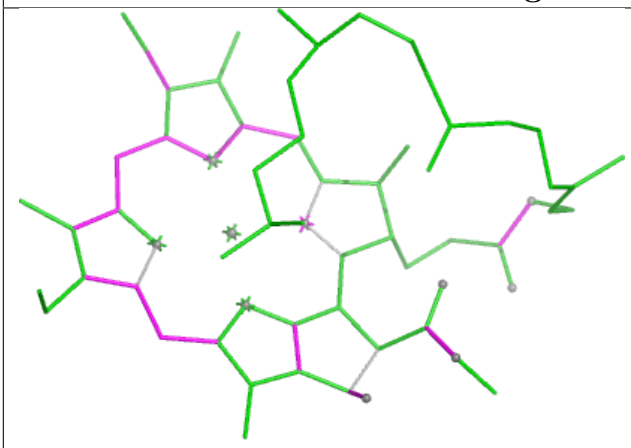
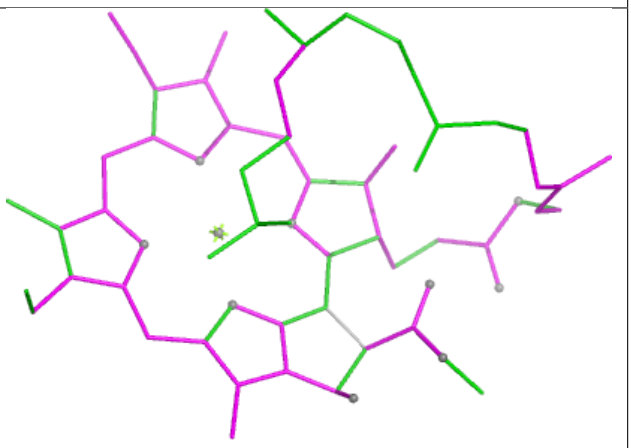
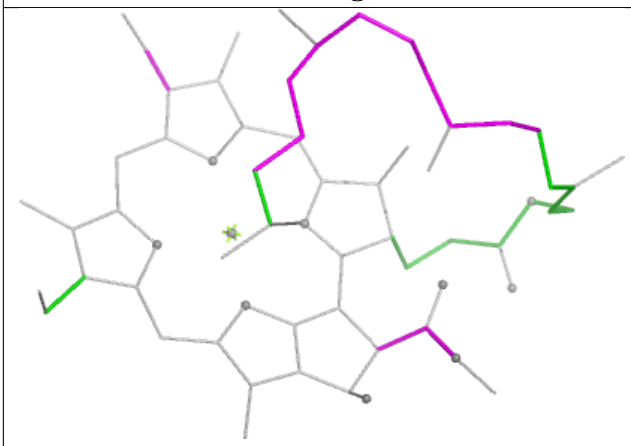
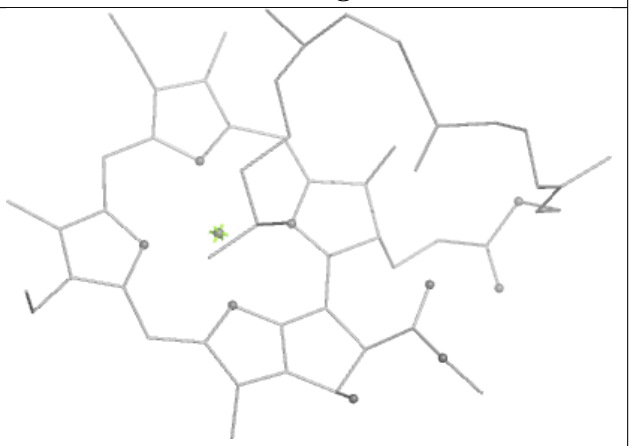
**Bond angles**



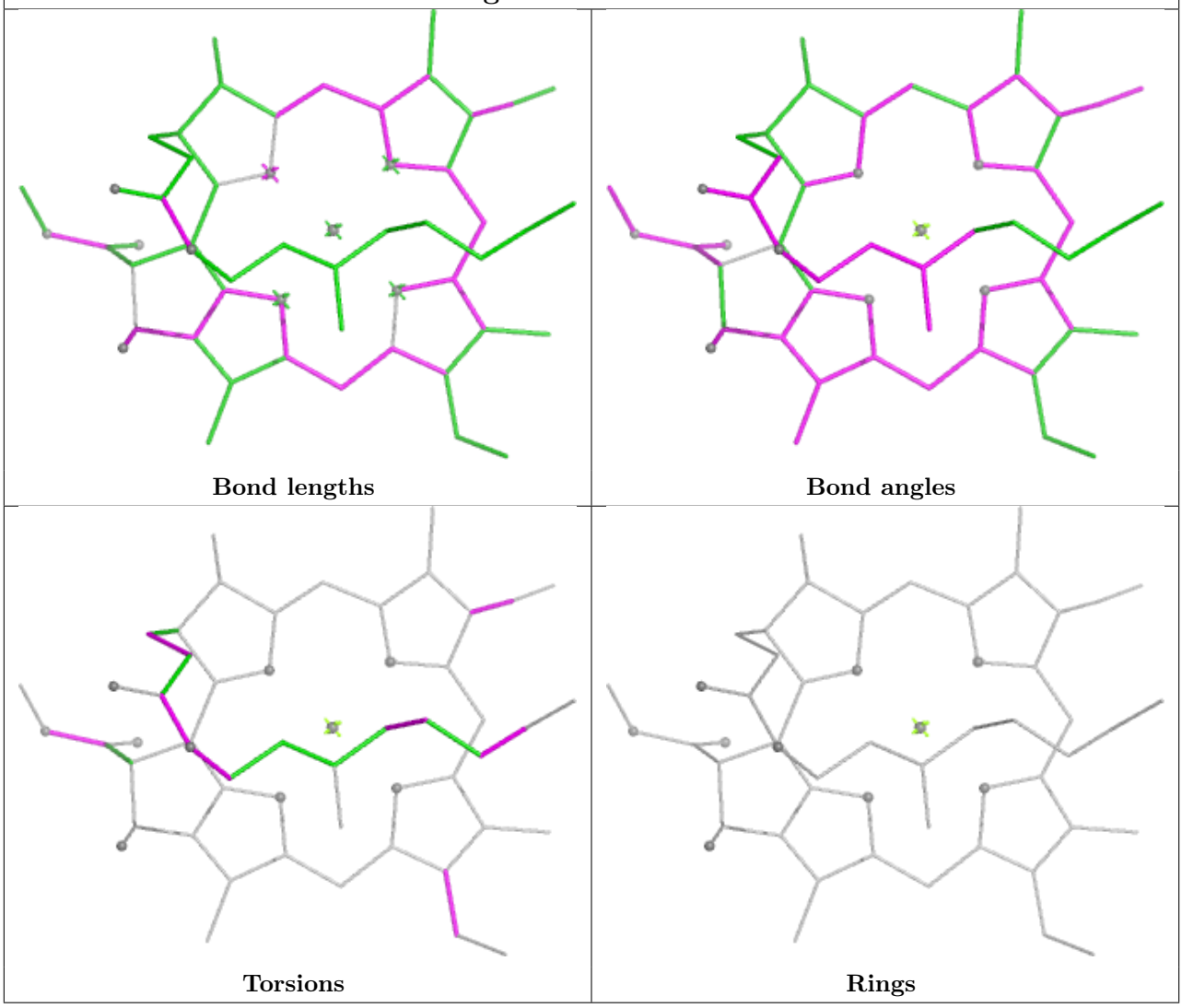
**Torsions**



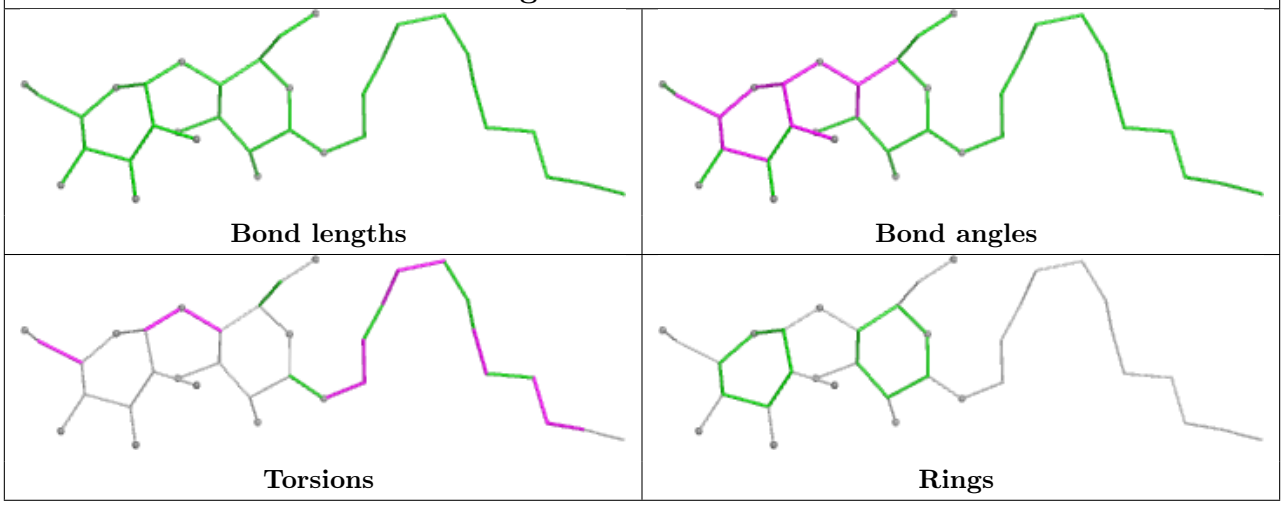
**Rings**

| Ligand CLA B 809 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

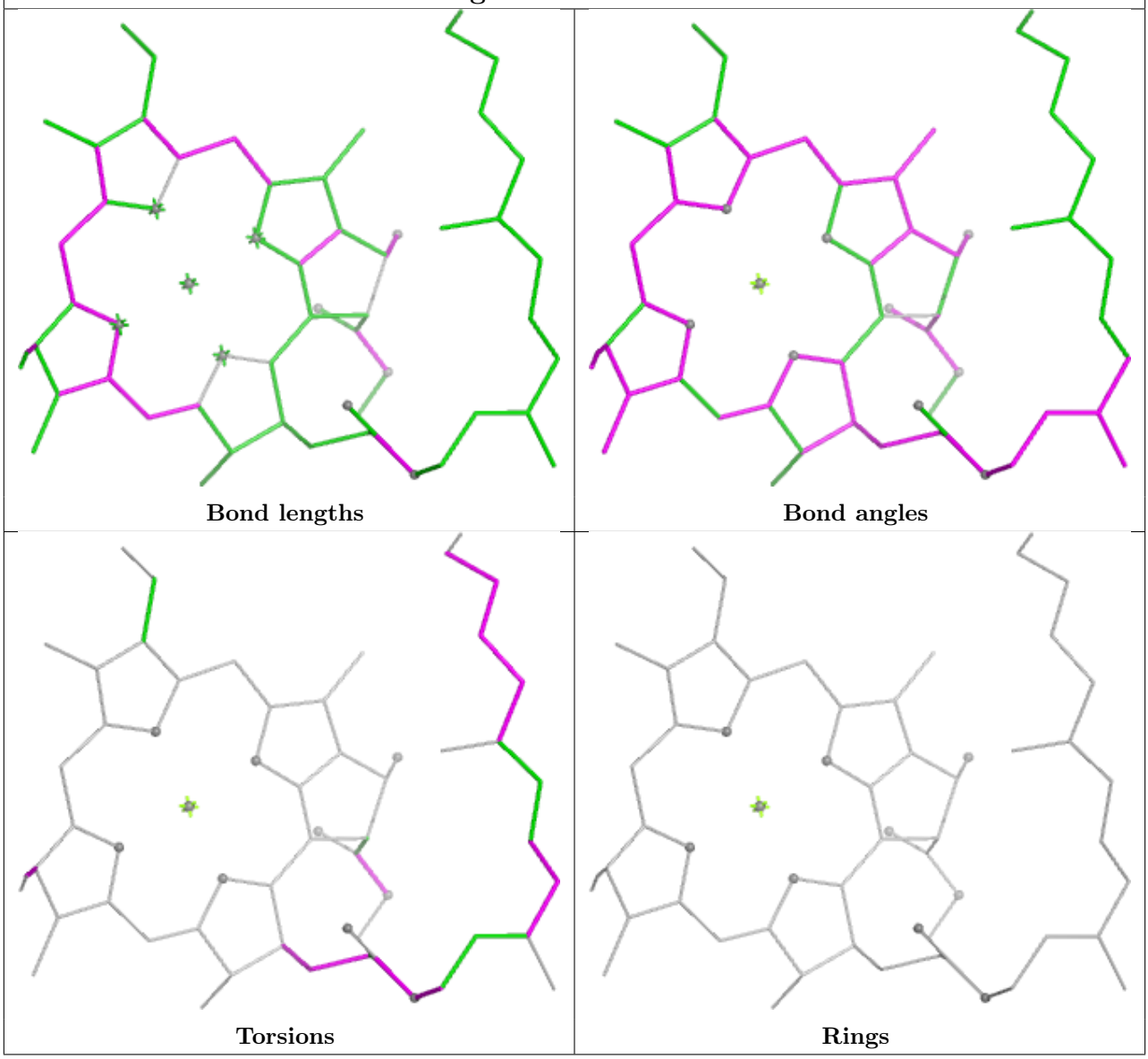
## Ligand CLA A 816



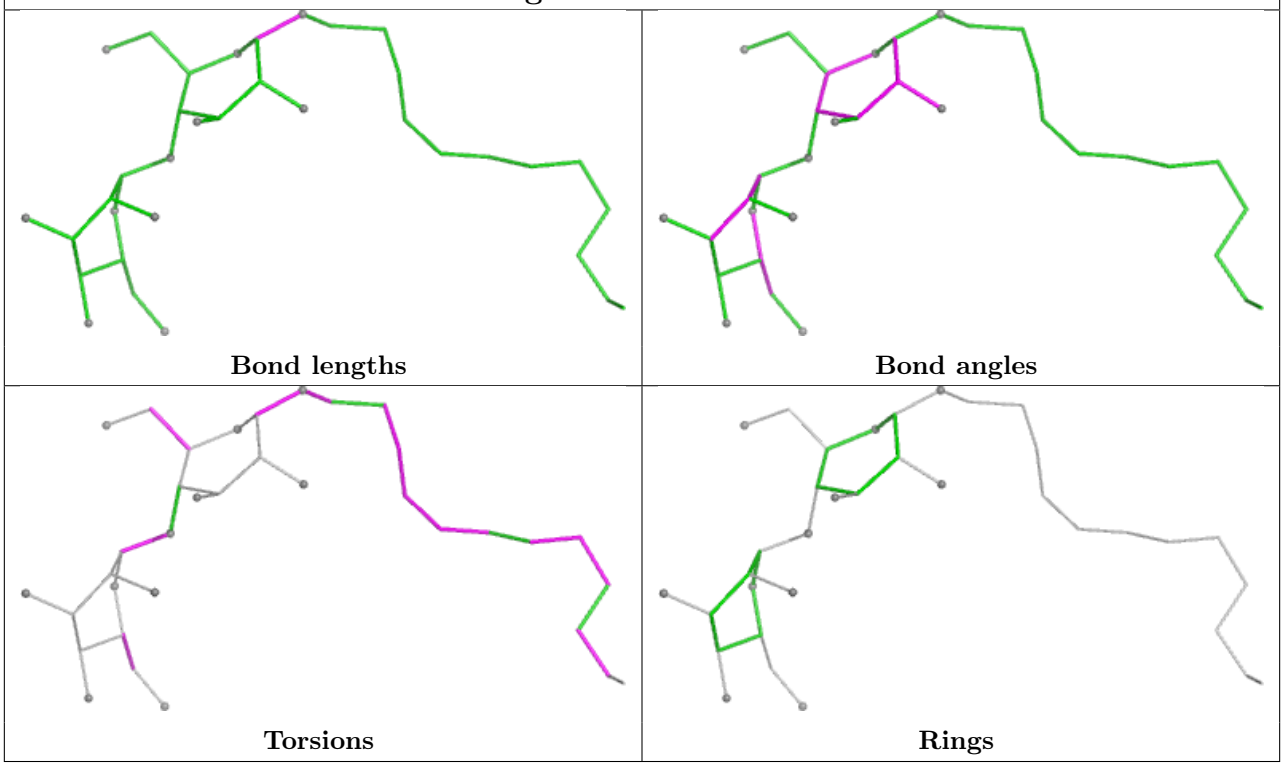

## Ligand LMU H 104



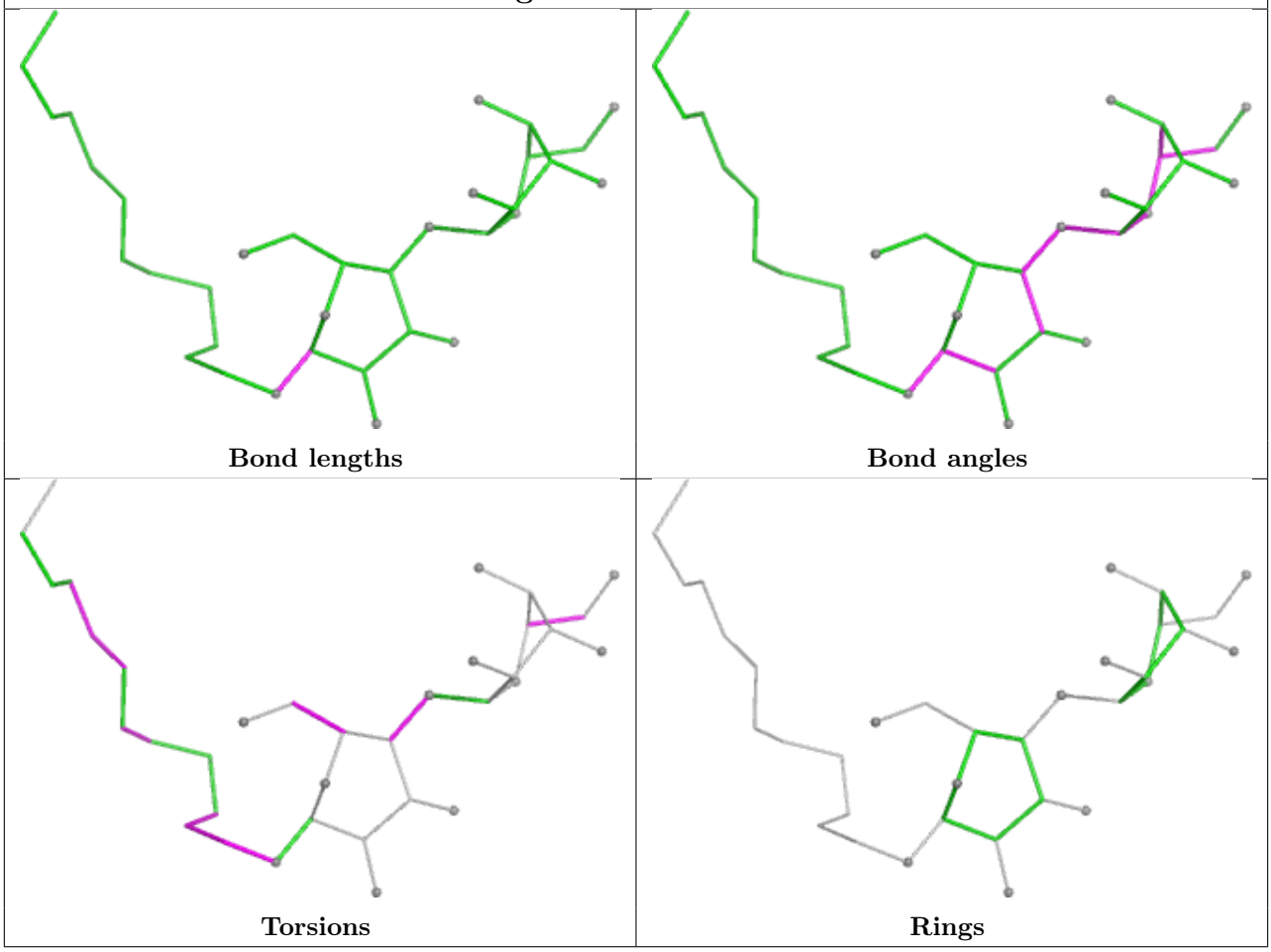
**Ligand CLA B 832**



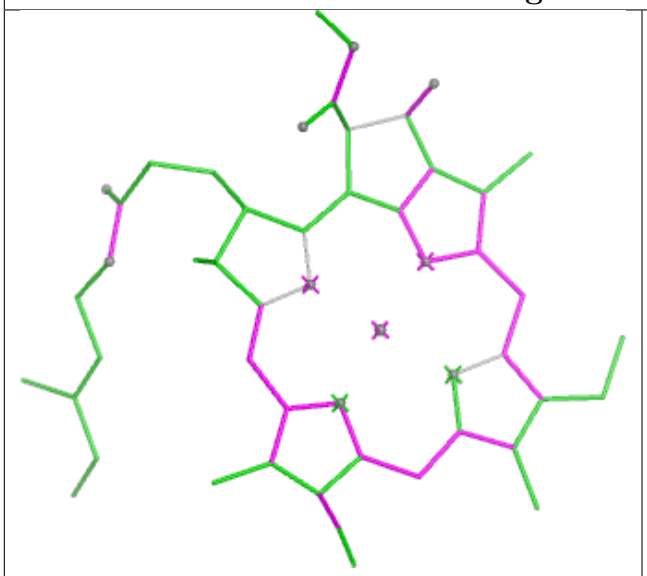
## Ligand LMU 4 320



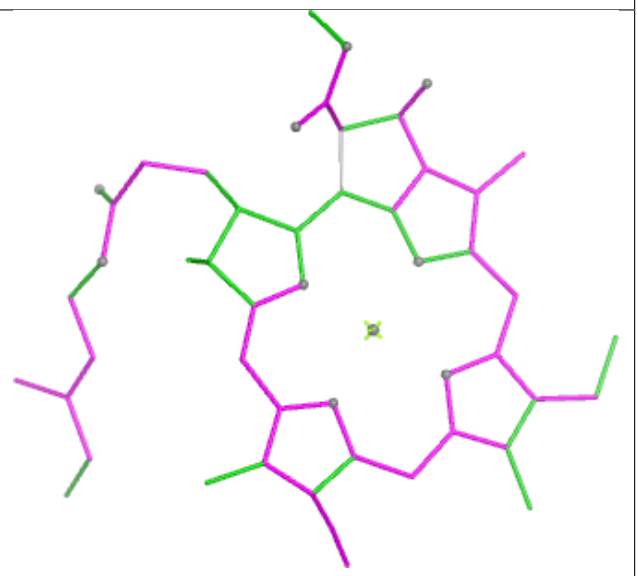

## Ligand LMU R 103



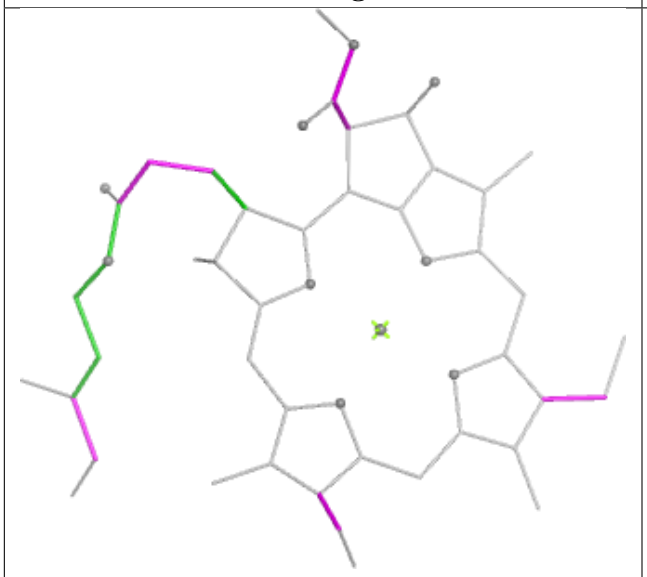
**Ligand CLA B 836**



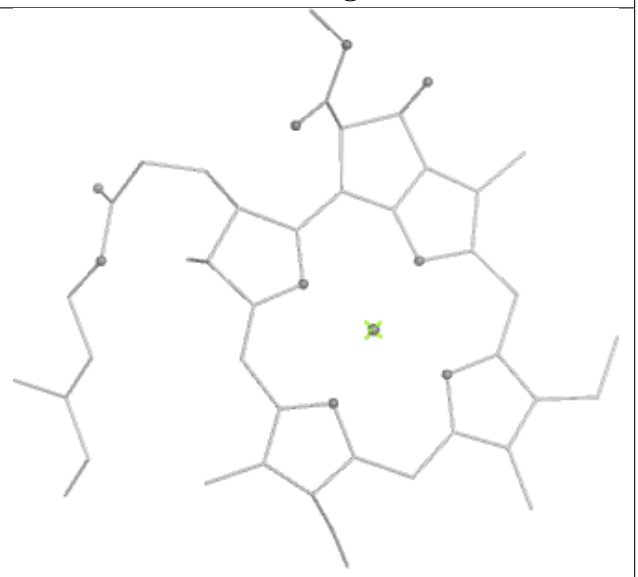
**Bond lengths**



**Bond angles**

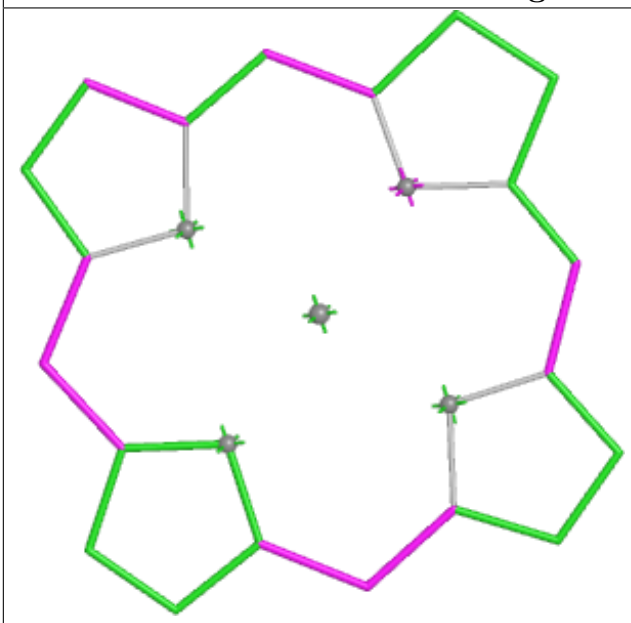


**Torsions**

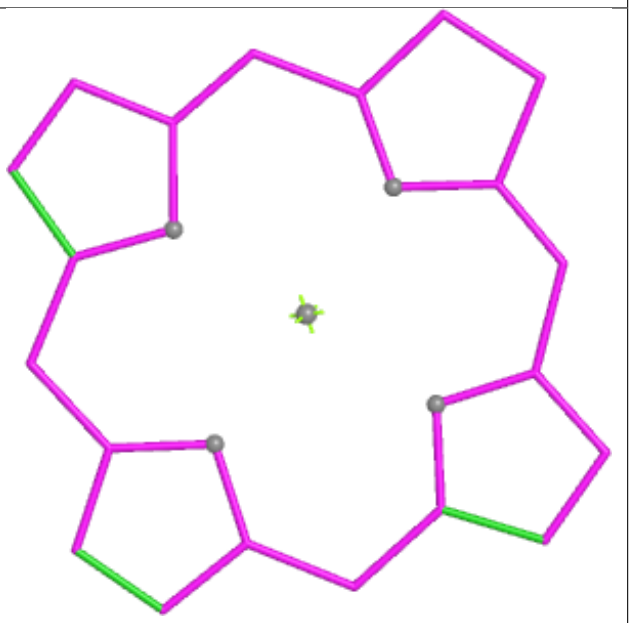


**Rings**

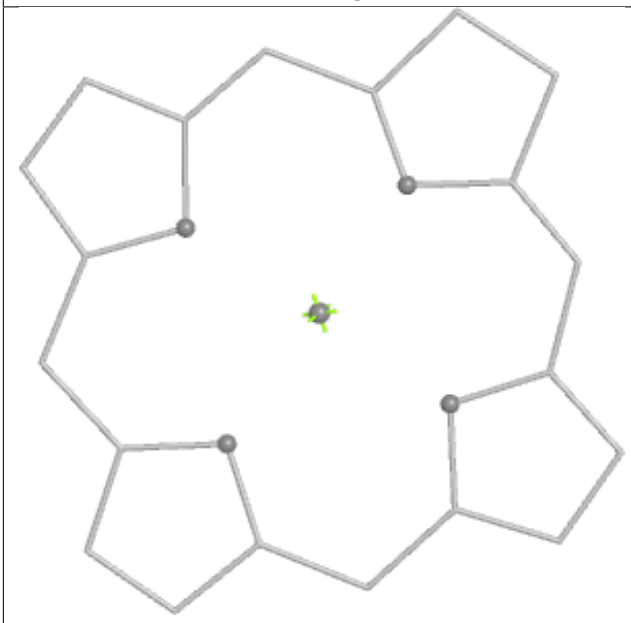
**Ligand CLA 4 314**



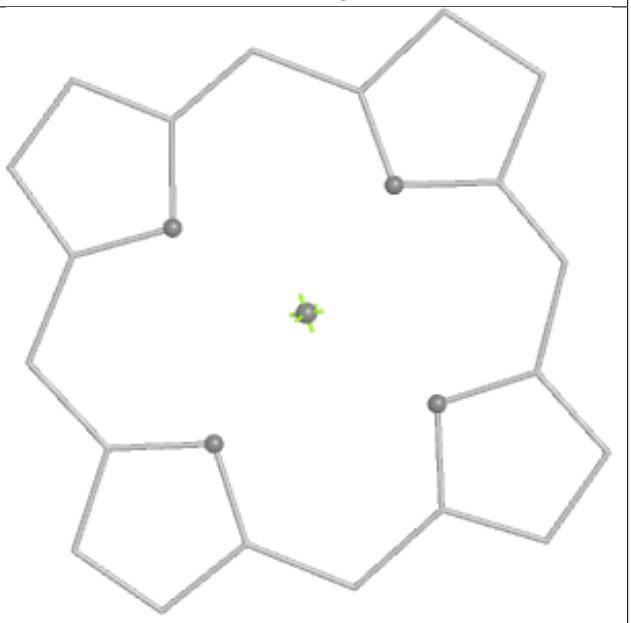
**Bond lengths**



**Bond angles**

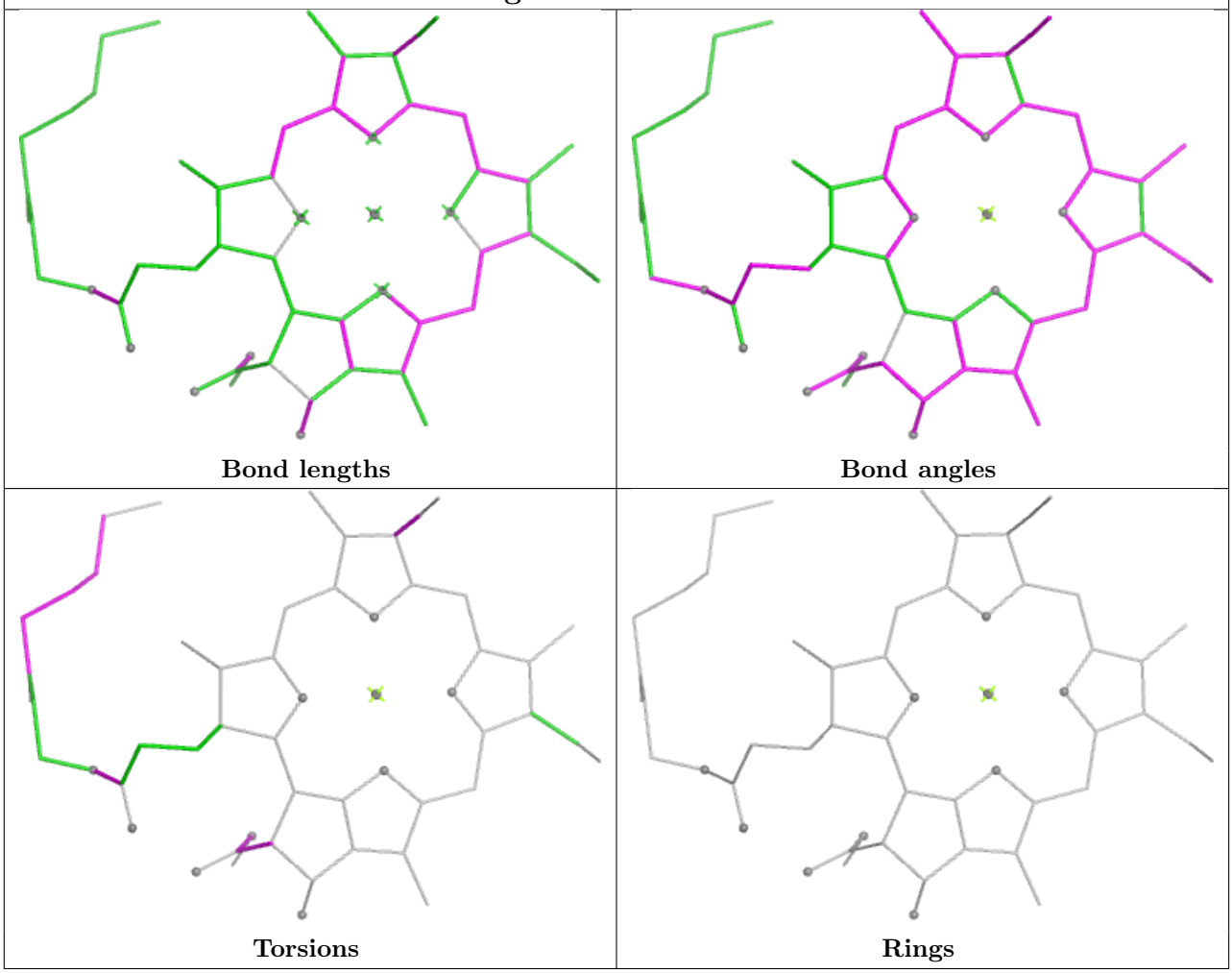


**Torsions**

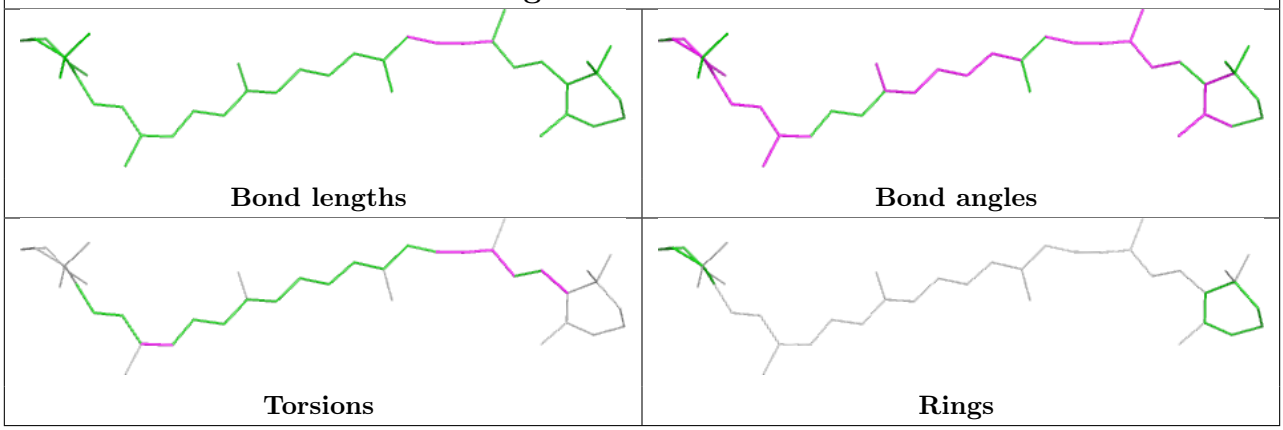


**Rings**

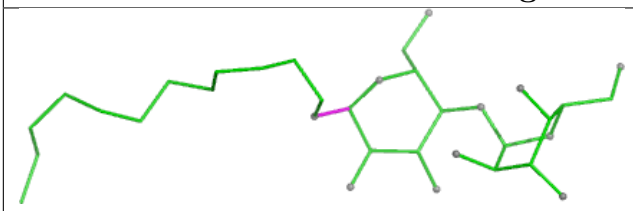
## Ligand CLA B 825



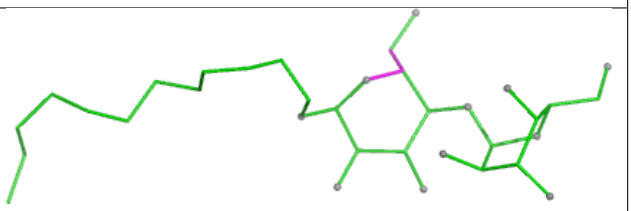

## Ligand BCR B 845



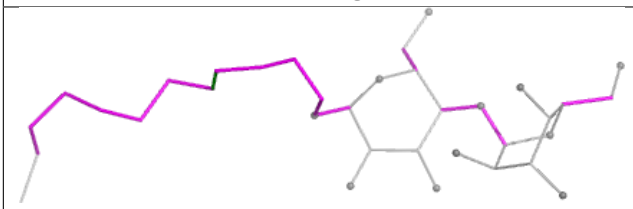
## Ligand LMU A 852



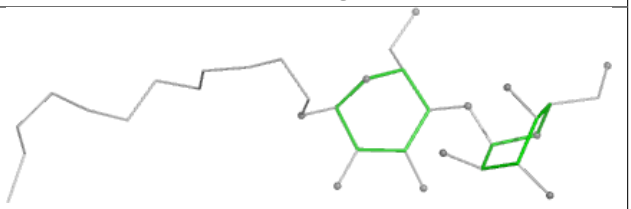
Bond lengths



Bond angles



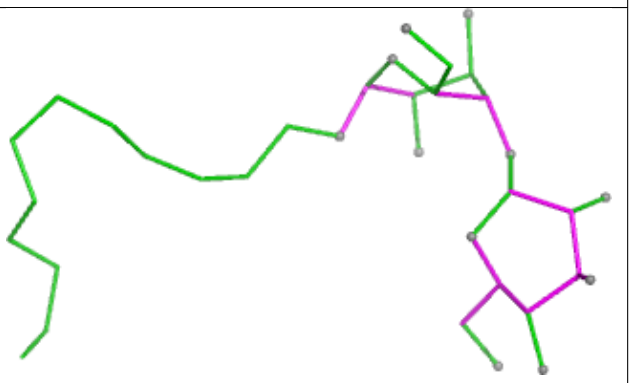
Torsions



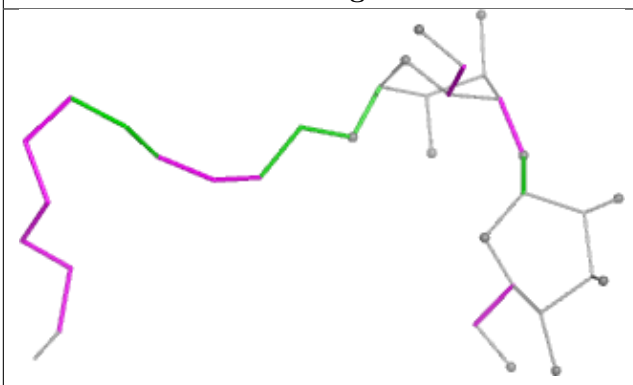
Rings

## Ligand LMU K 105

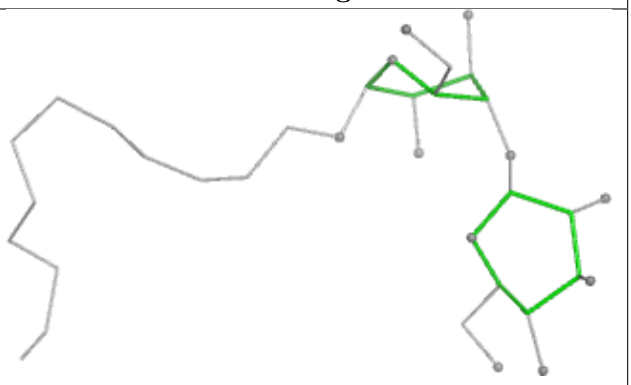
Bond lengths



Bond angles

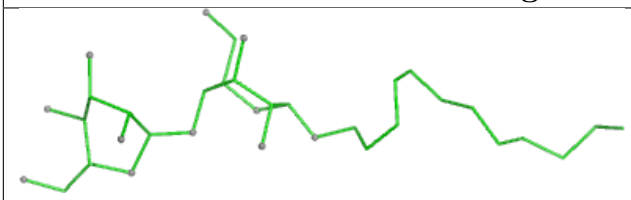


Torsions

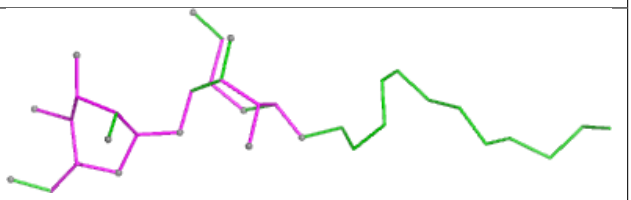


Rings

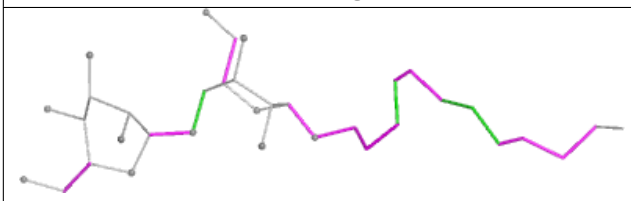
## Ligand LMU E 101



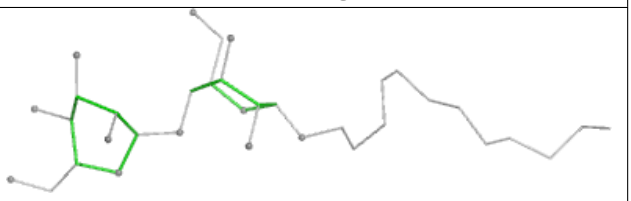
Bond lengths



Bond angles

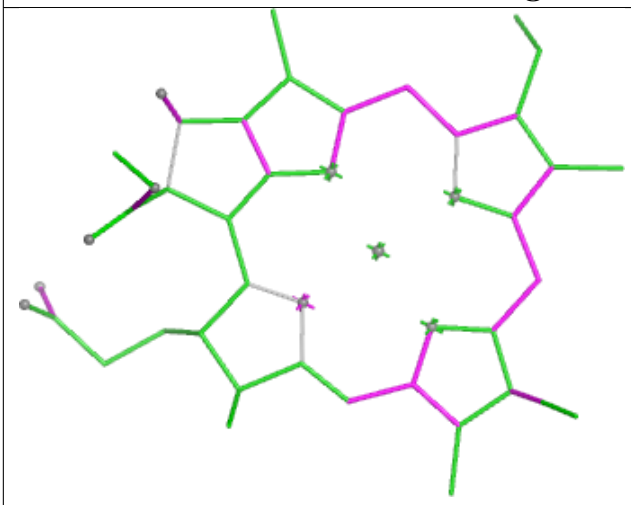


Torsions

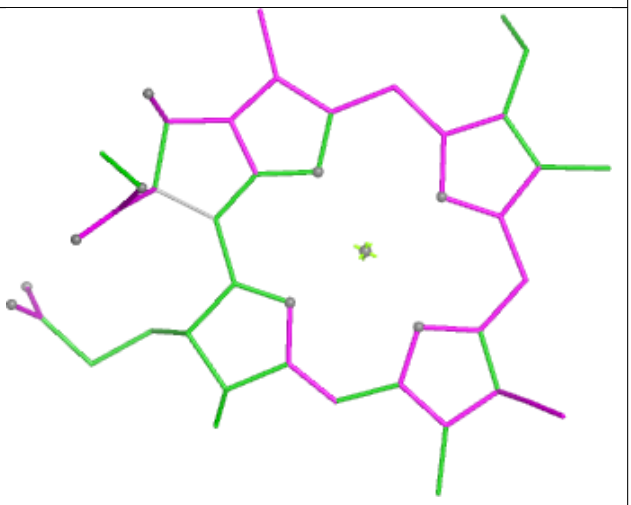


Rings

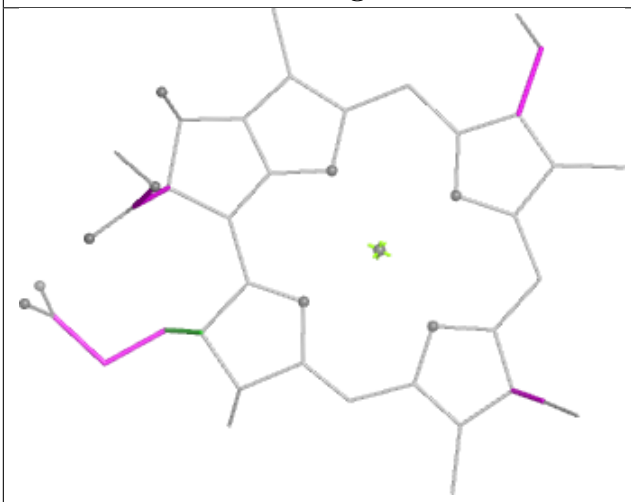
## Ligand CLA B 835



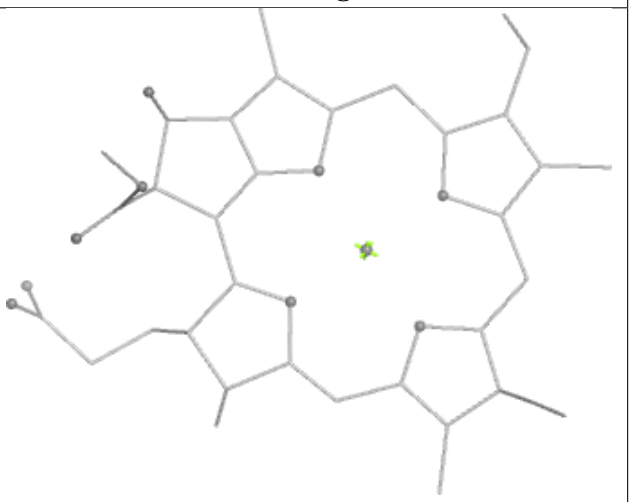
Bond lengths



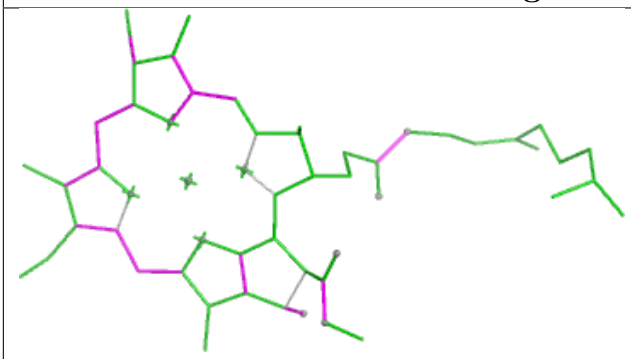
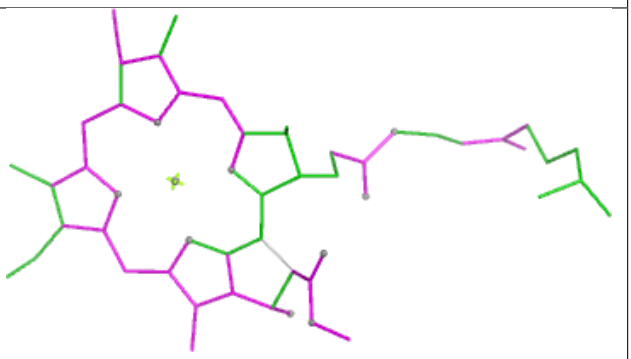
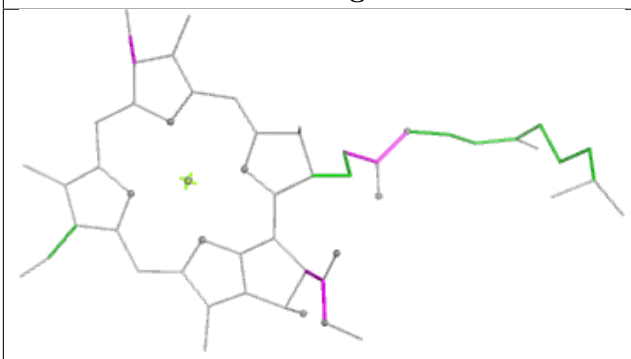
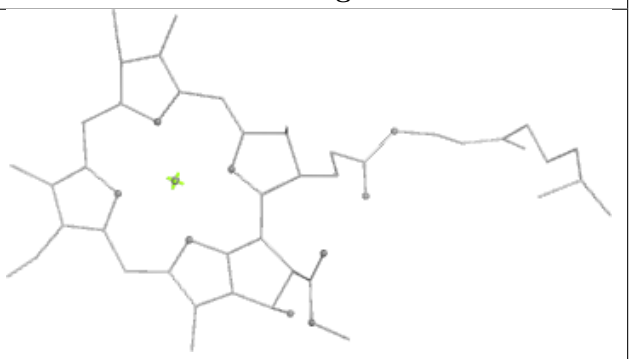
Bond angles



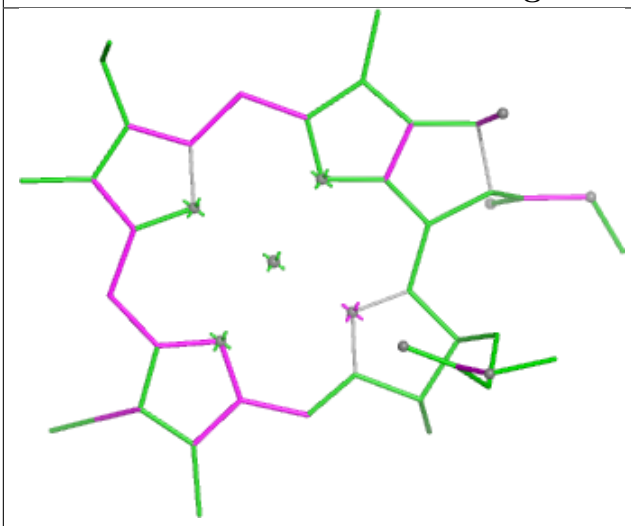
Torsions



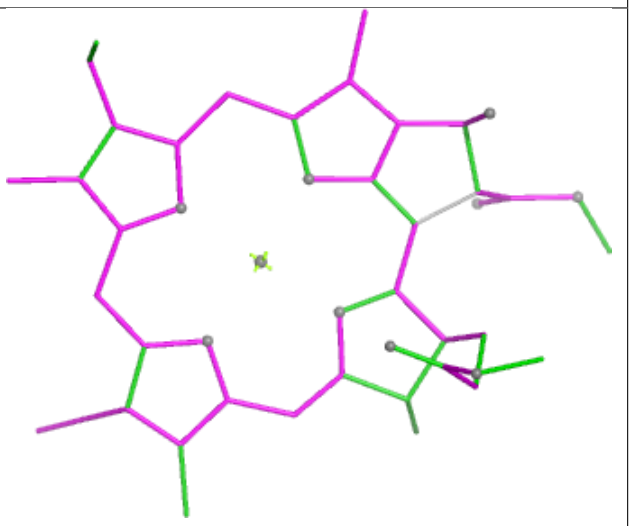
Rings

| Ligand CLA H 109 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

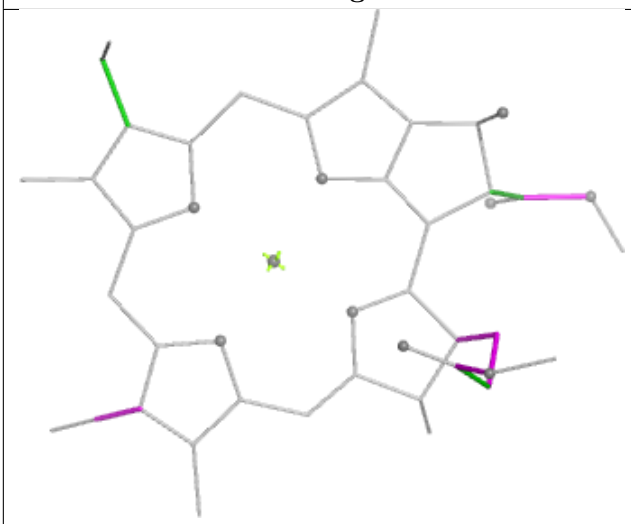
## Ligand CLA A 807



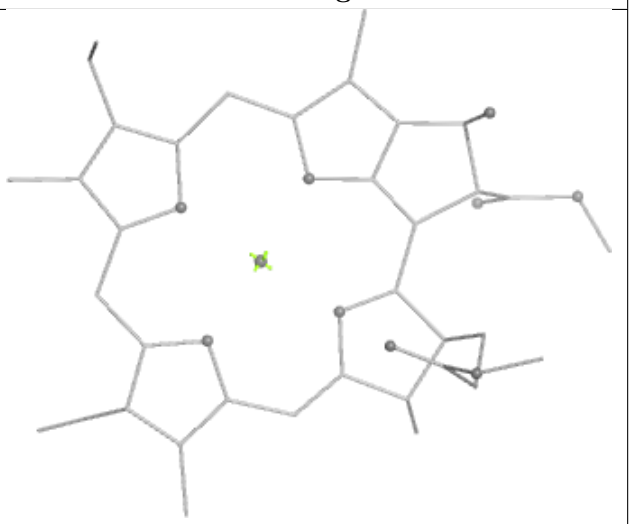
Bond lengths



Bond angles

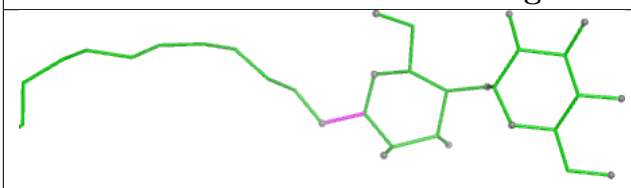


Torsions



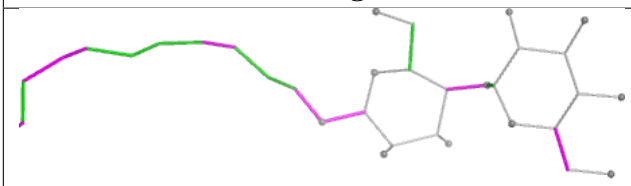
Rings

## Ligand LMU 2 321

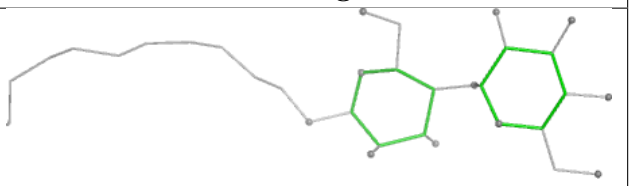


Bond lengths

Bond angles

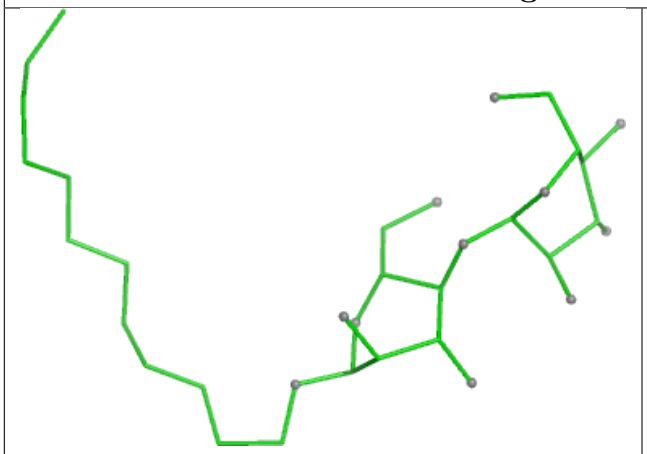


Torsions

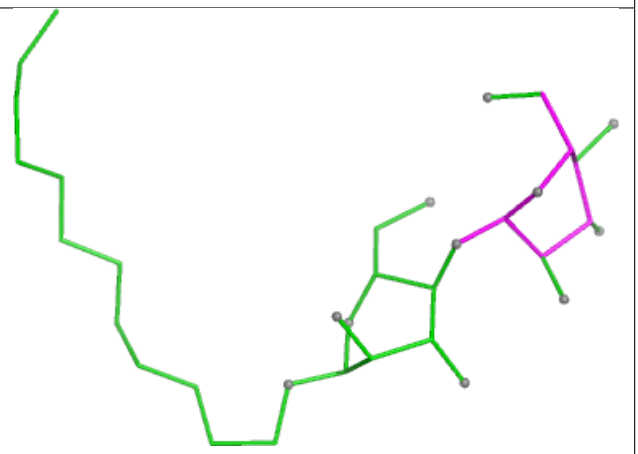


Rings

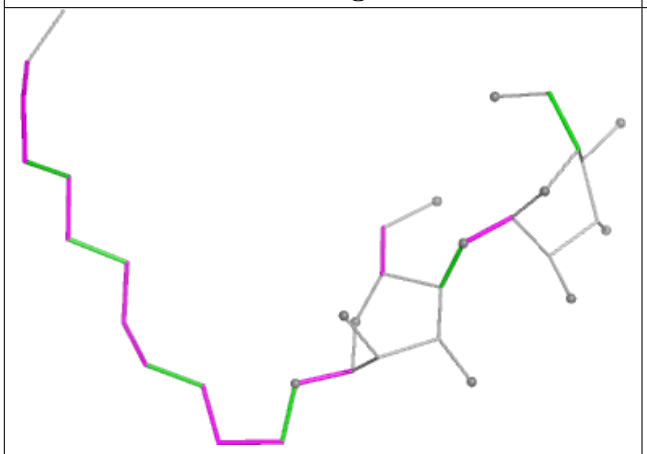
## Ligand LMU K 106



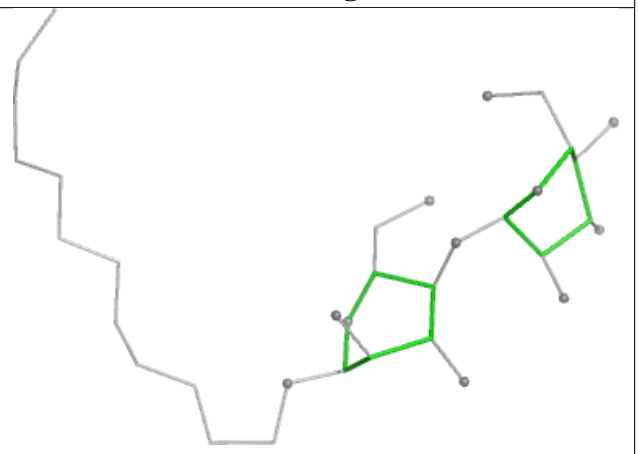
Bond lengths



Bond angles

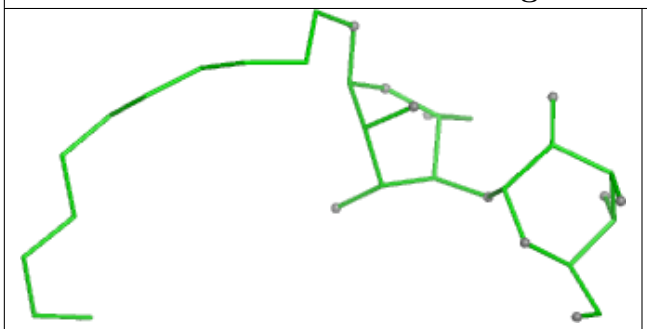


Torsions



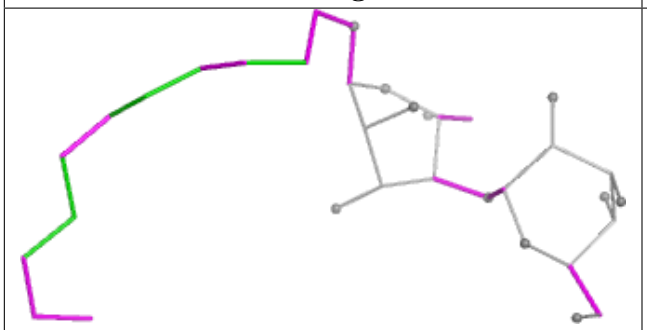
Rings

## Ligand LMU R 104



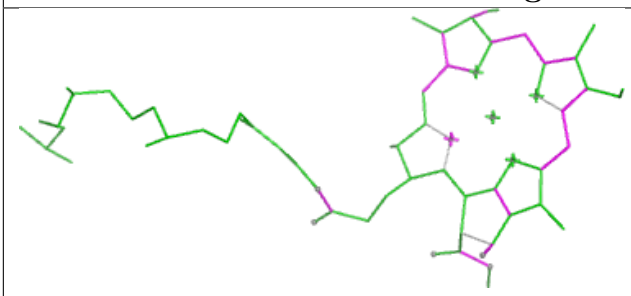
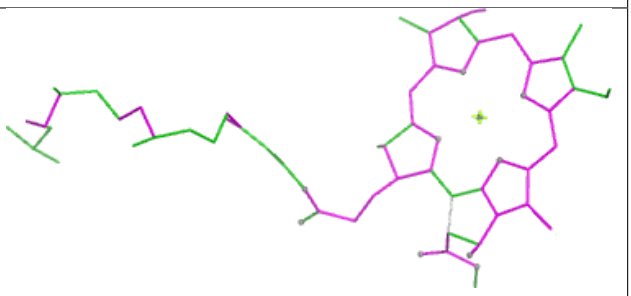
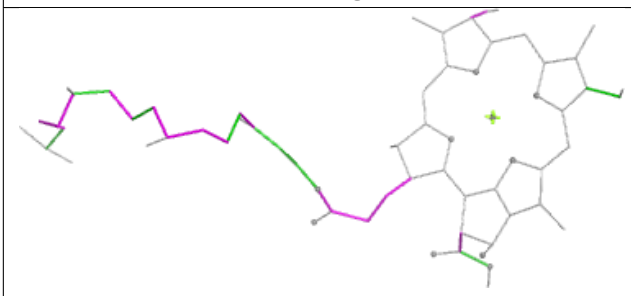
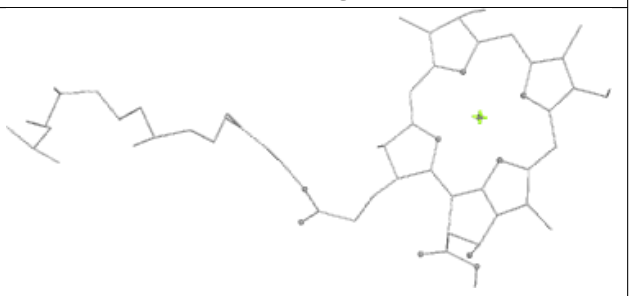
Bond lengths

Bond angles

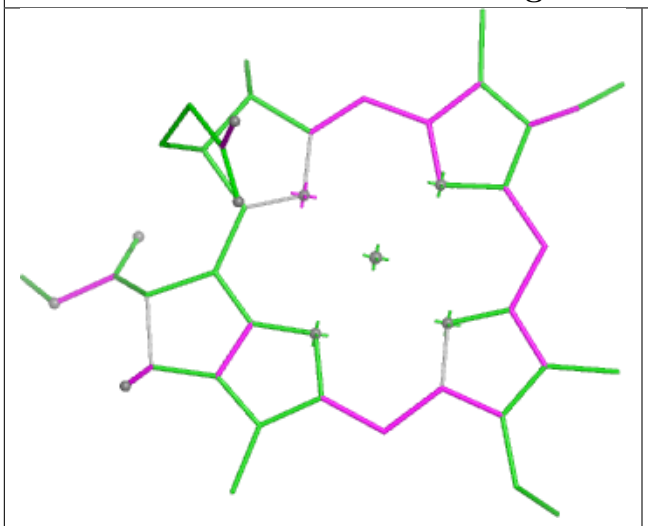


Torsions

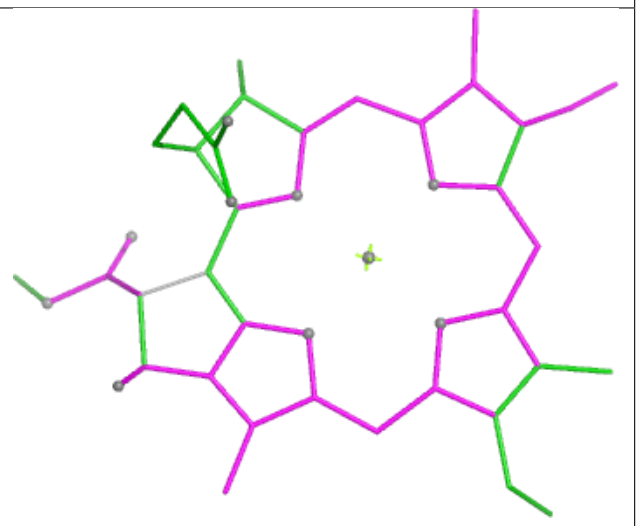
Rings

| Ligand CLA B 814 | |
|---|---|
|  **Bond lengths** |  **Bond angles** |
|  **Torsions** |  **Rings** |

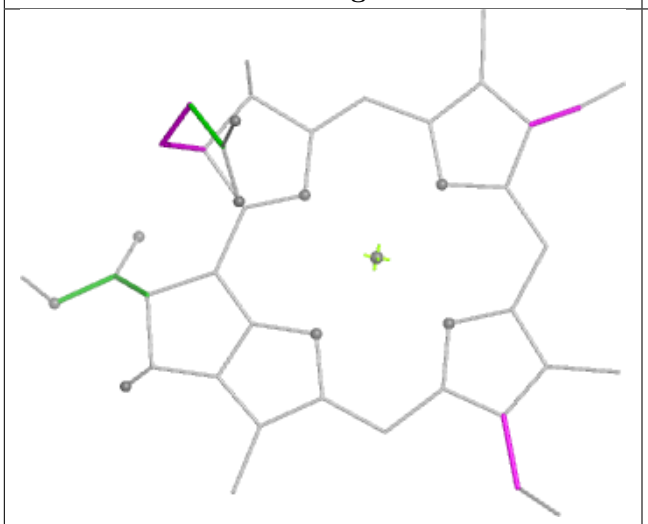
**Ligand CLA B 807**



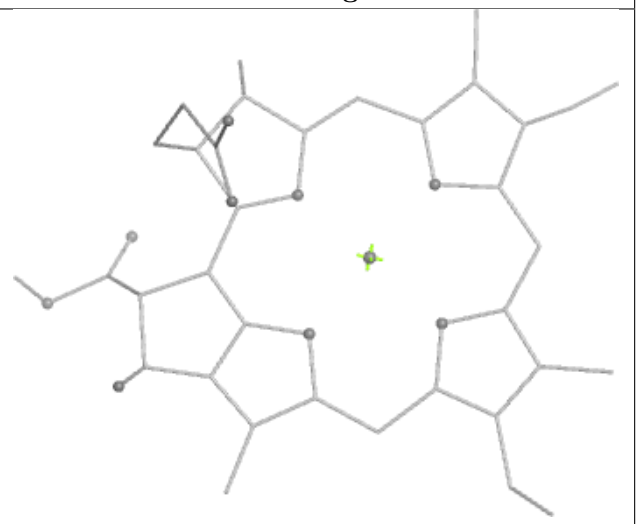
**Bond lengths**



**Bond angles**

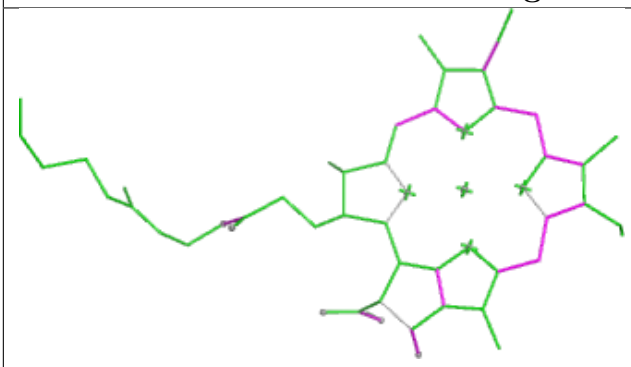


**Torsions**

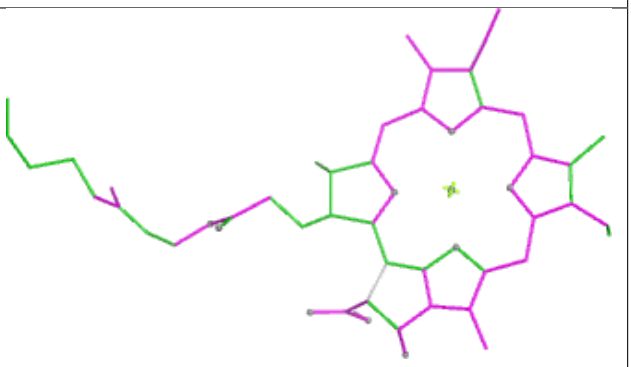


**Rings**

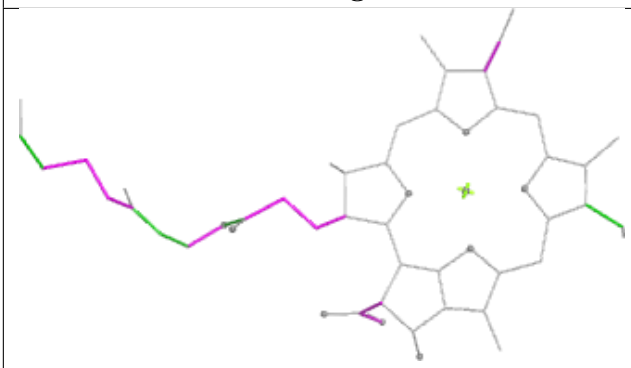
**Ligand CLA A 805**



**Bond lengths**



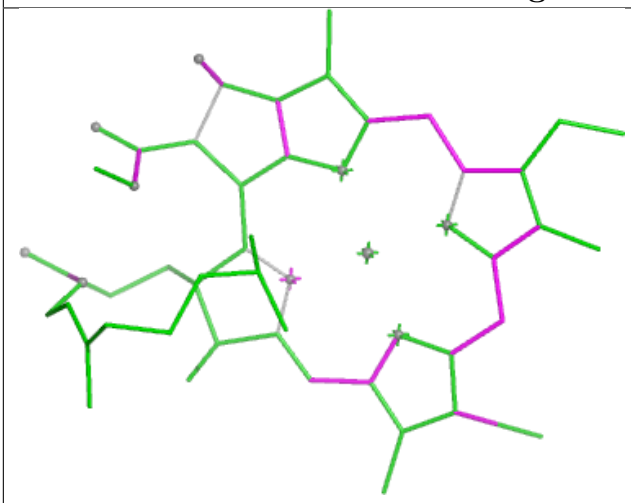
**Bond angles**



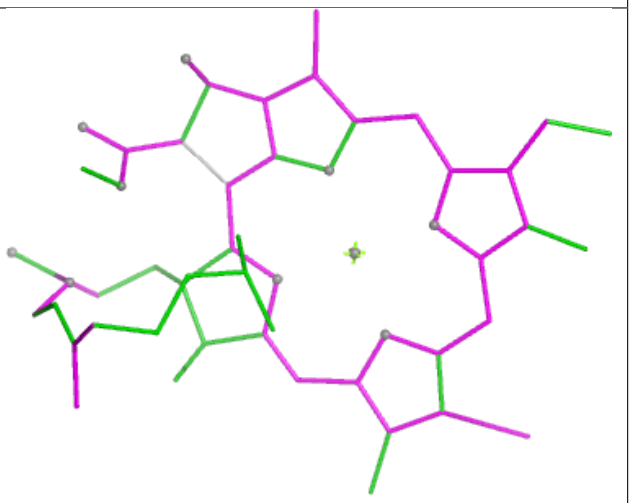
**Torsions**

**Rings**

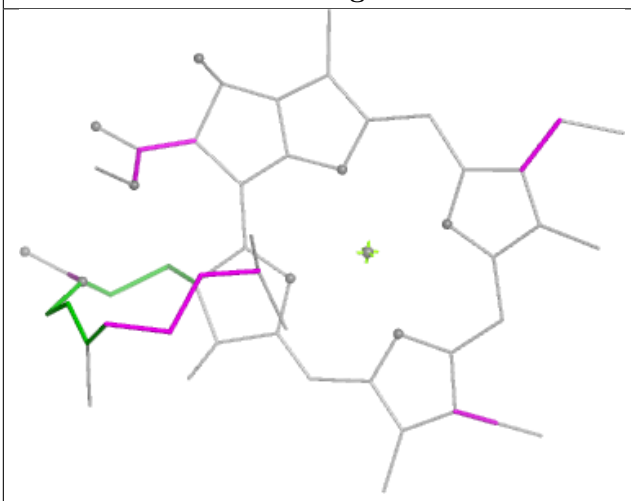
**Ligand CLA 4 304**



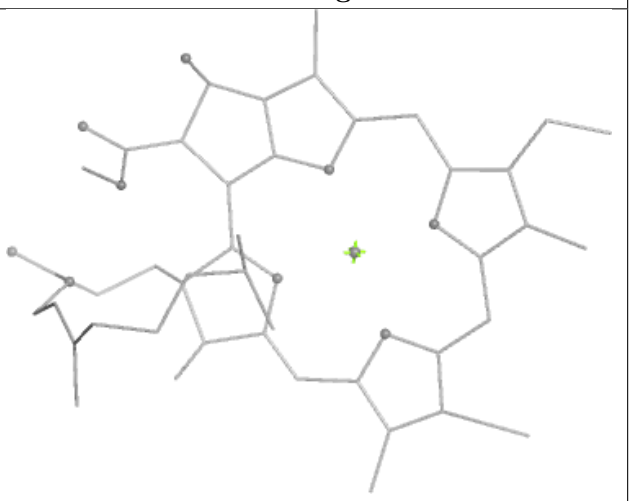
**Bond lengths**



**Bond angles**

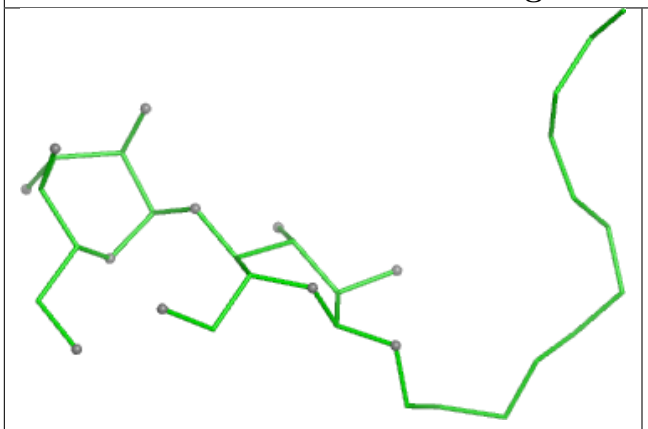


**Torsions**

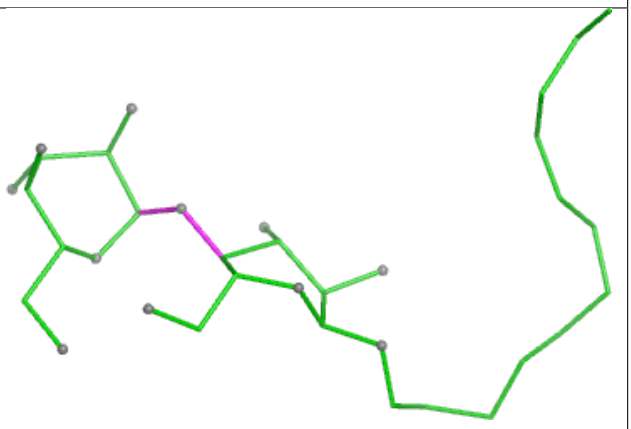


**Rings**

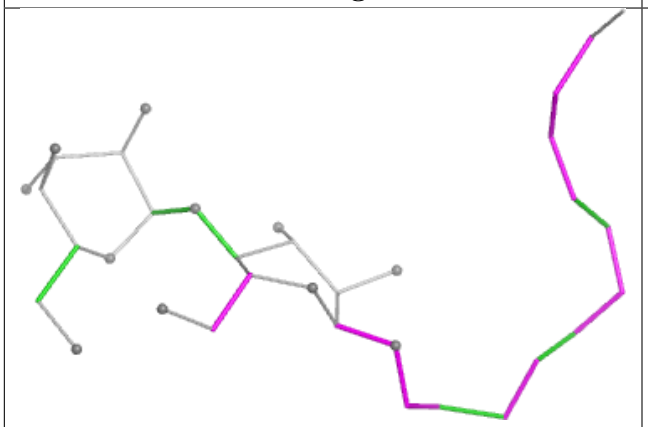
## Ligand LMU 3 318



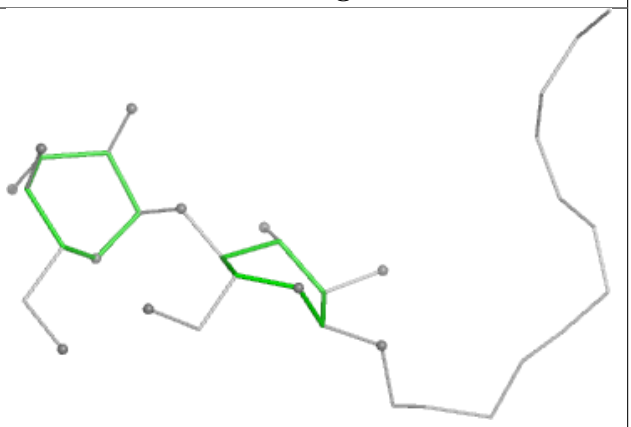
Bond lengths



Bond angles

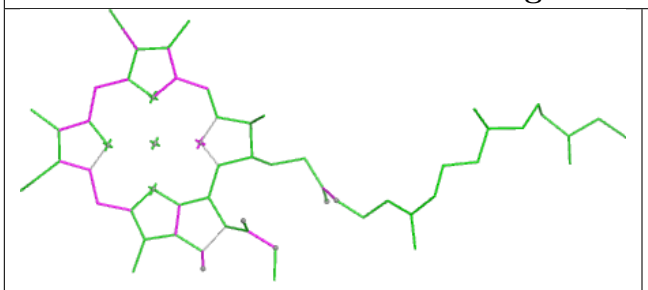


Torsions

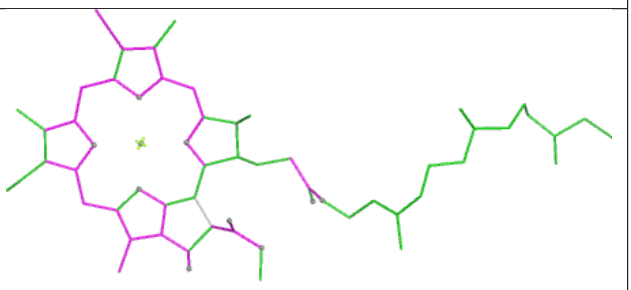


Rings

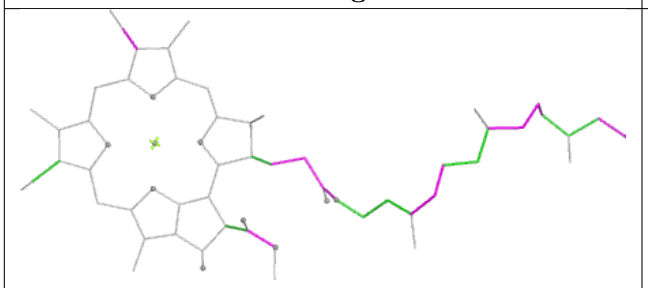
## Ligand CLA A 830



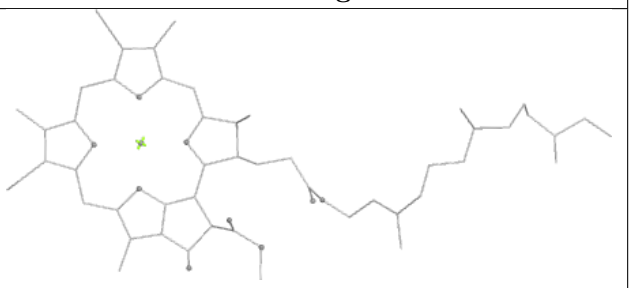
Bond lengths



Bond angles

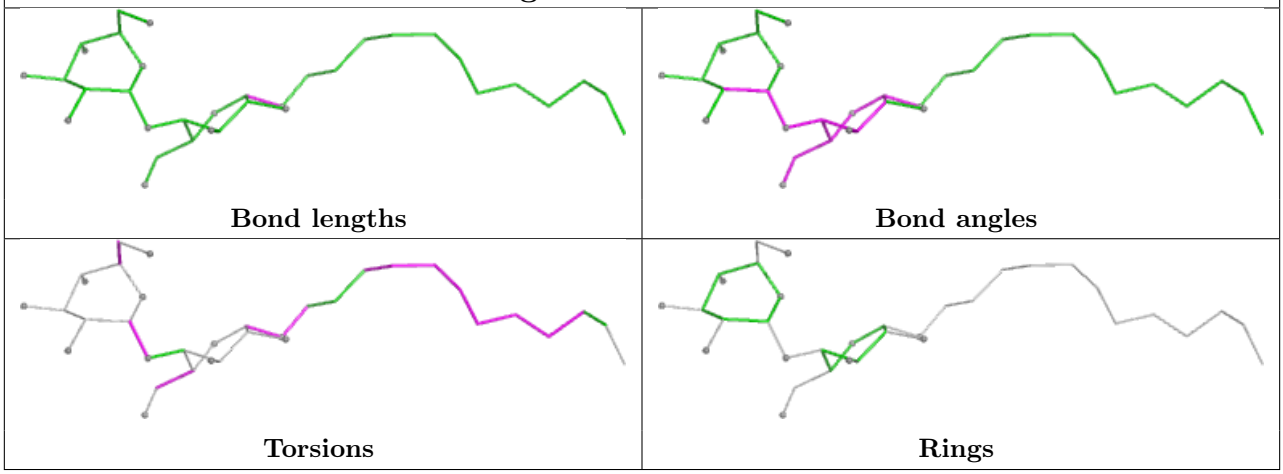


Torsions

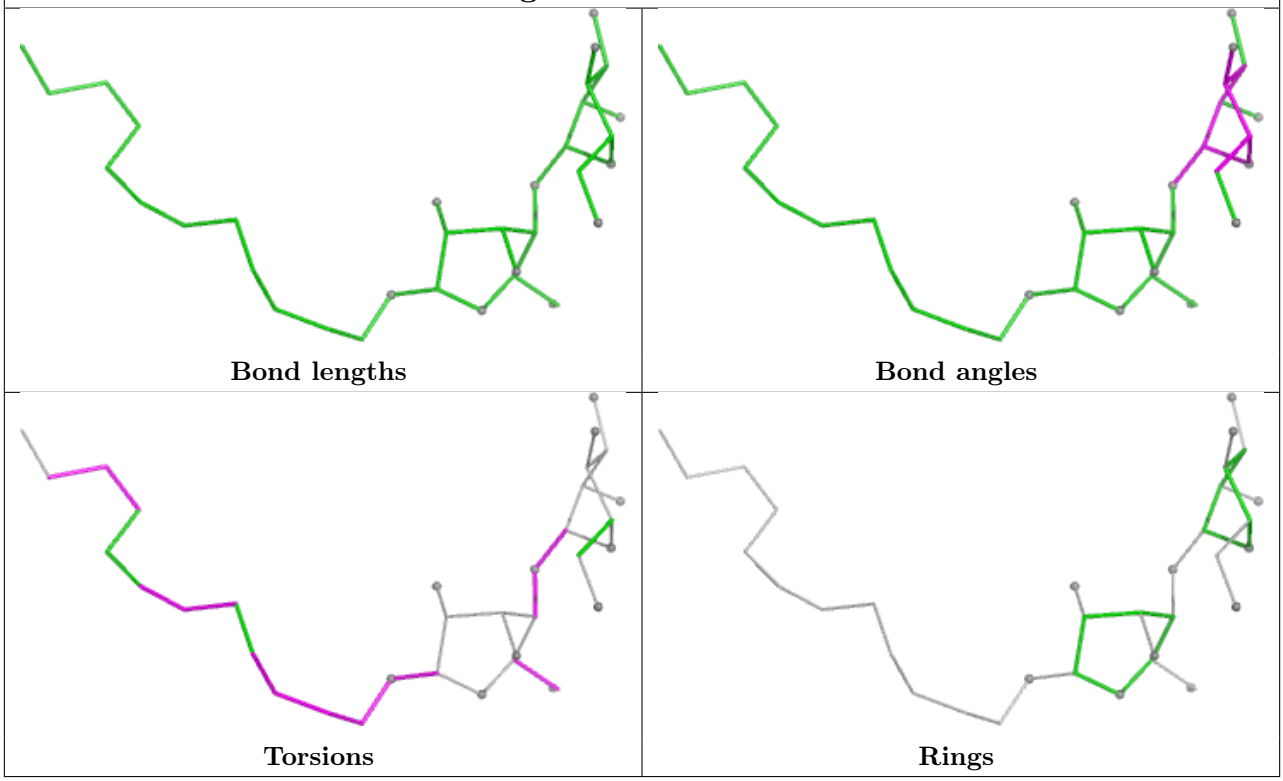


Rings

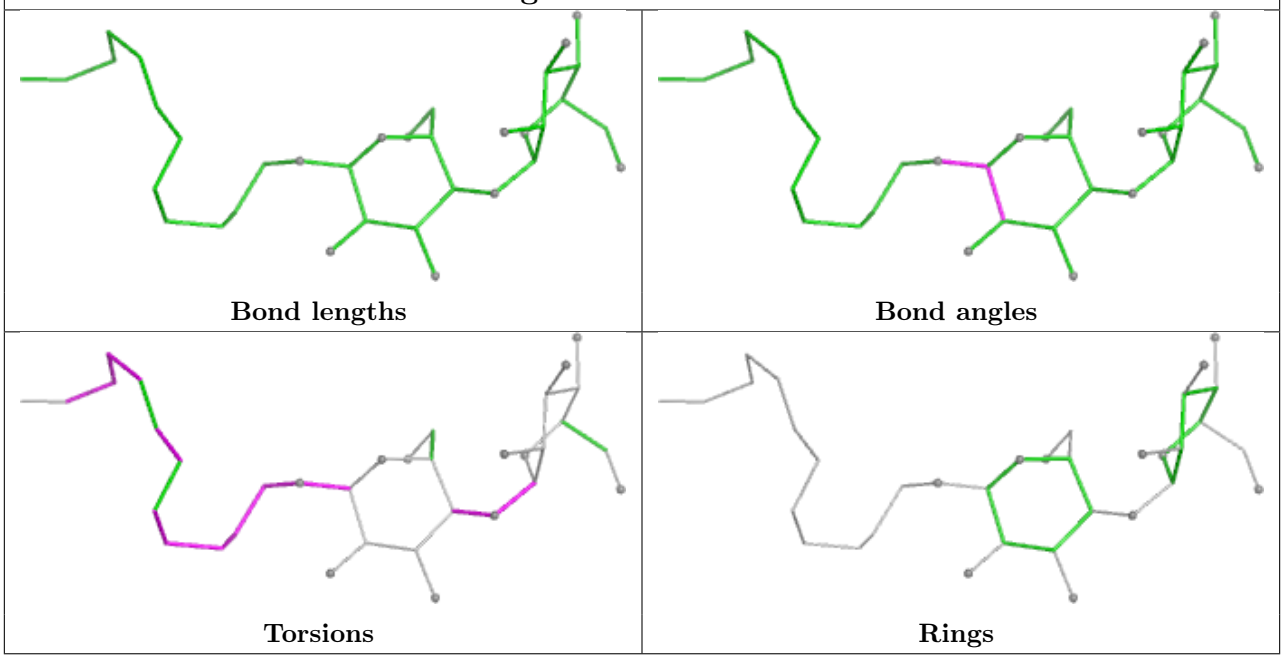
## Ligand LMU H 103



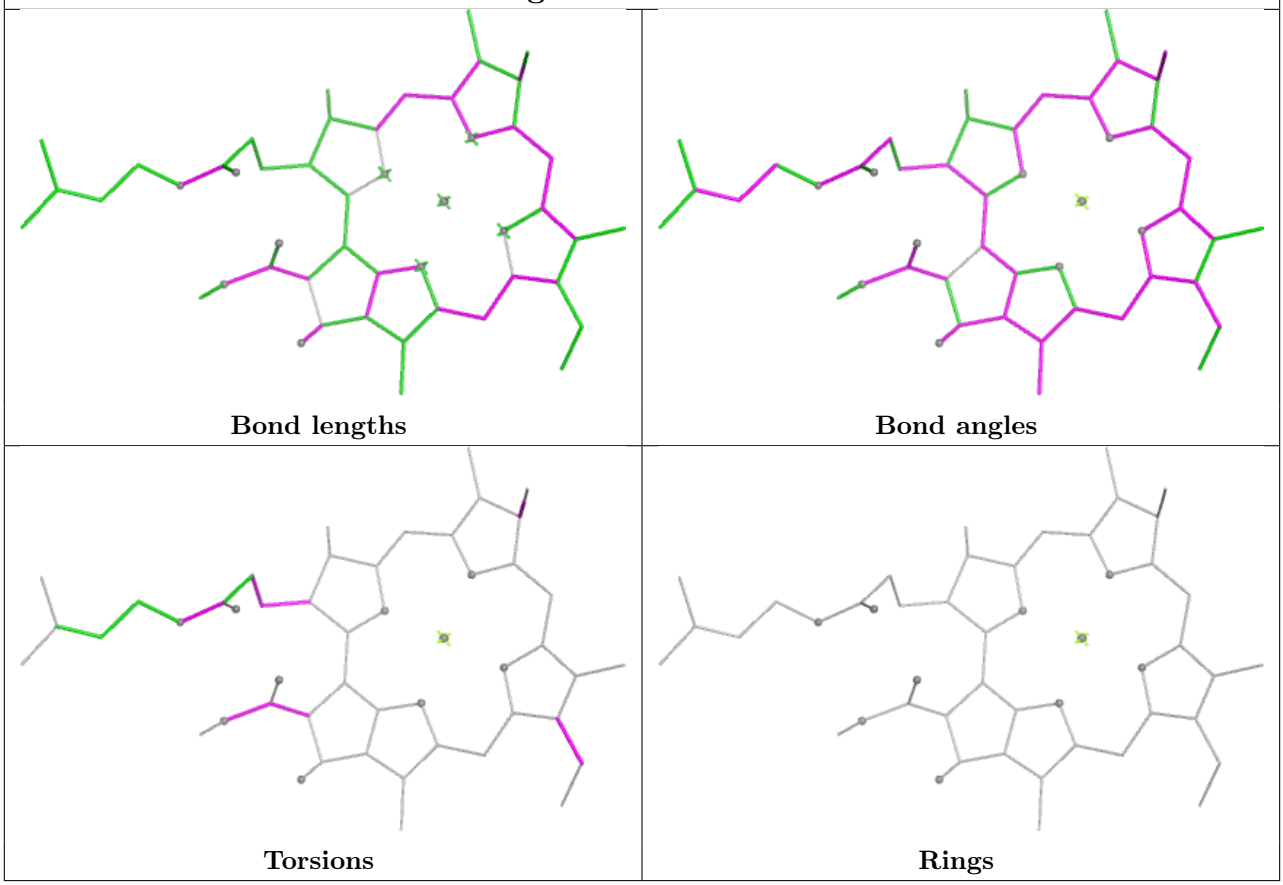

## Ligand LMU G 102



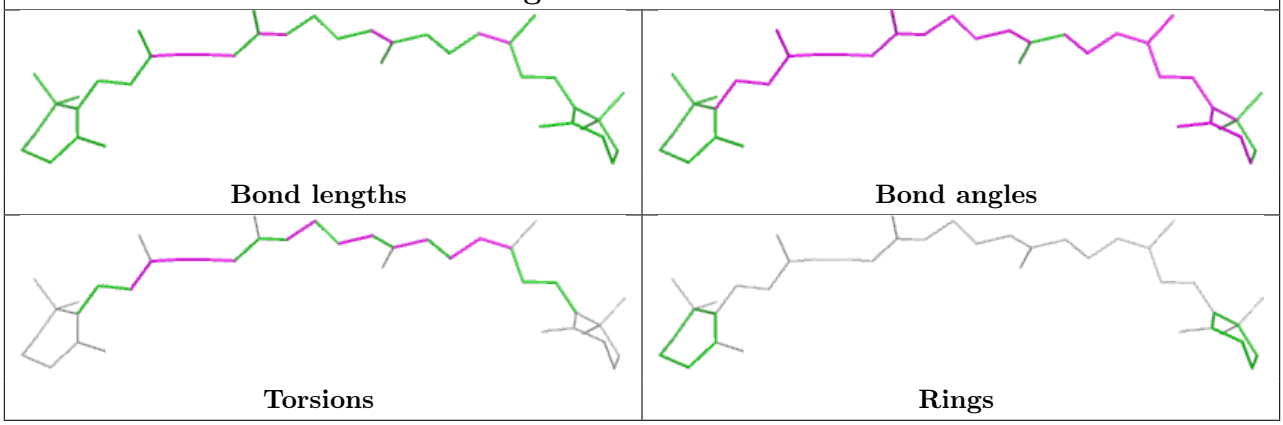
## Ligand LMU R 109



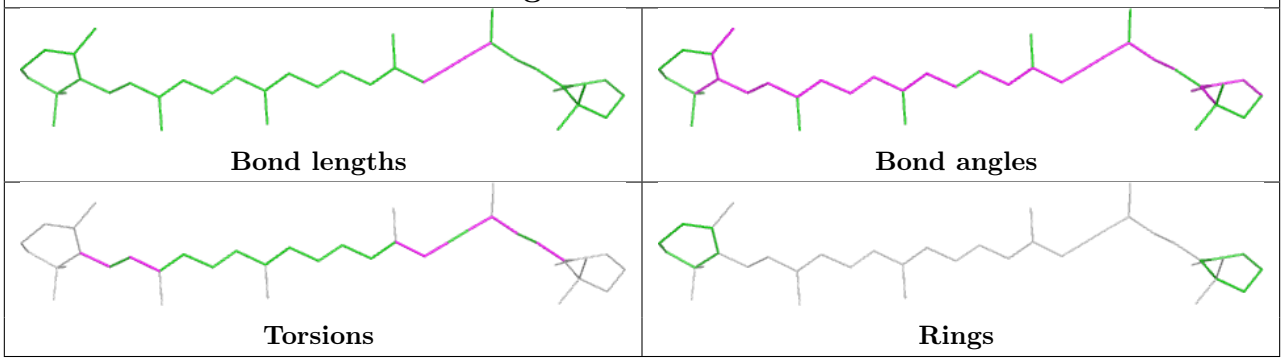

## Ligand CLA L 208



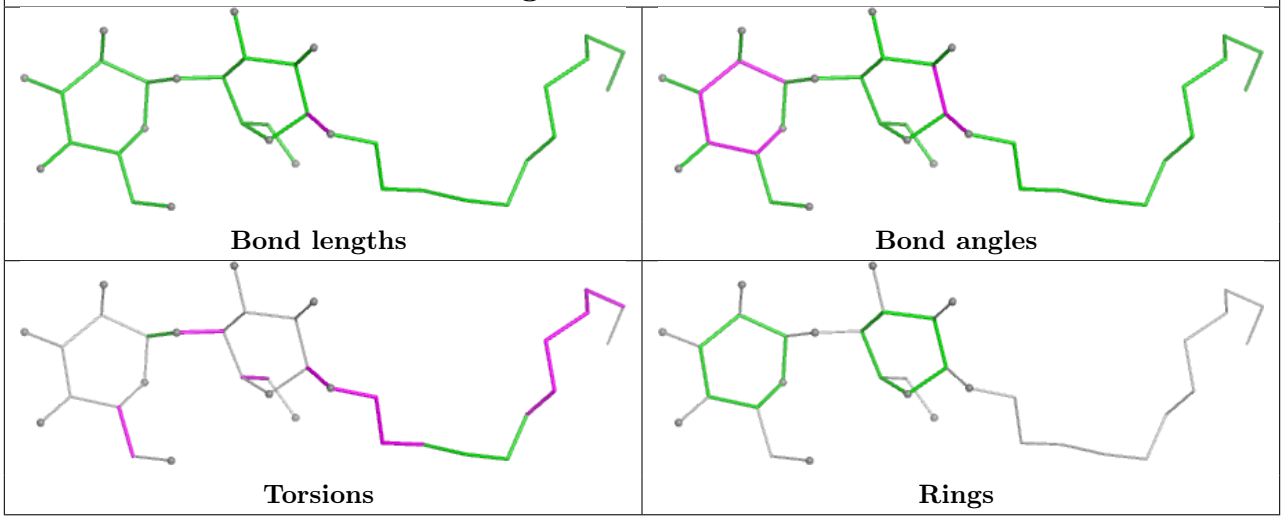
## Ligand BCR B 801



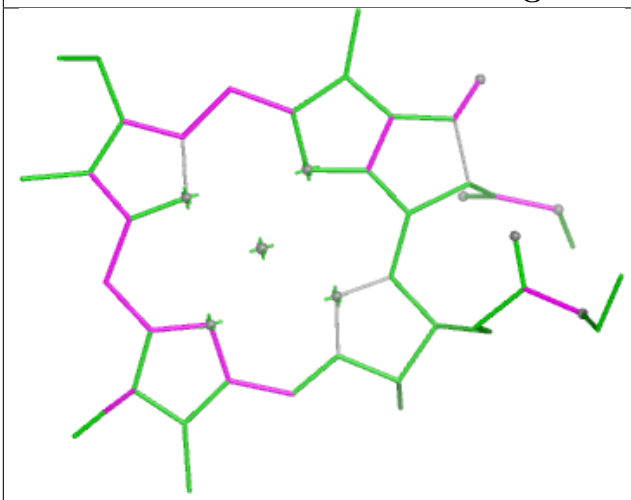

## Ligand BCR B 847



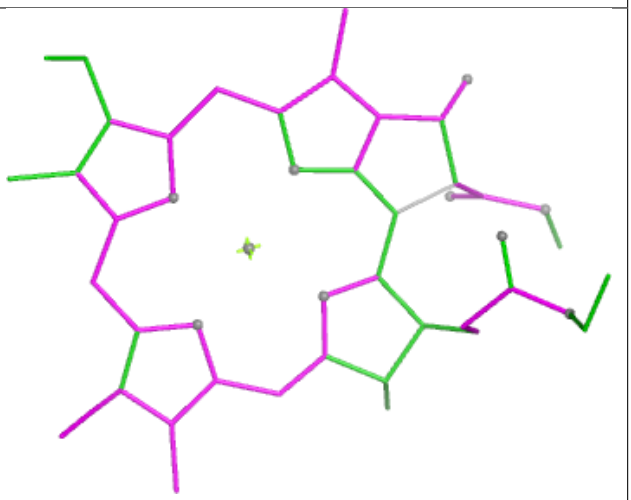

## Ligand LMU C 101



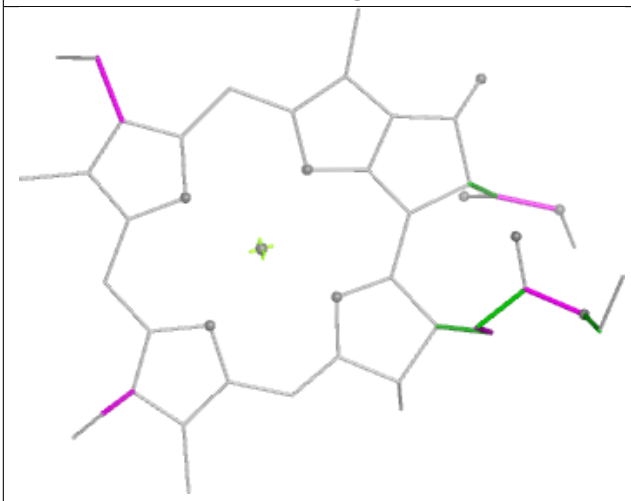
**Ligand CLA A 836**



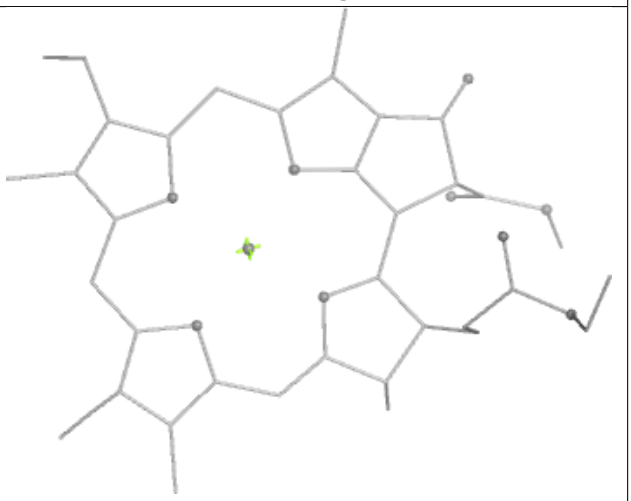
**Bond lengths**



**Bond angles**

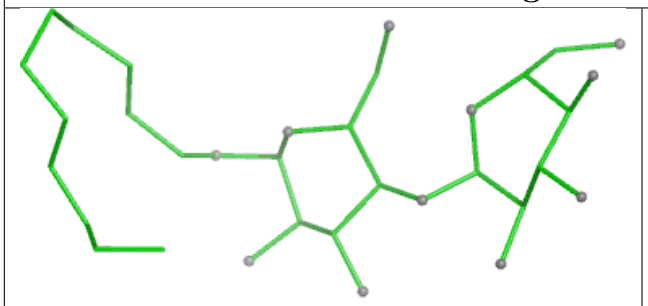


**Torsions**

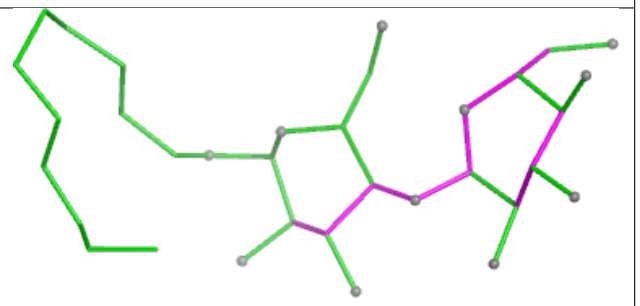


**Rings**

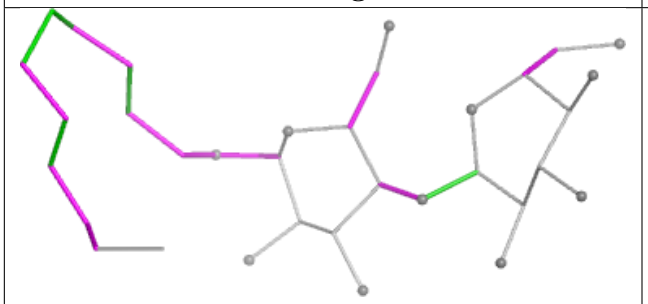
**Ligand LMU F 202**



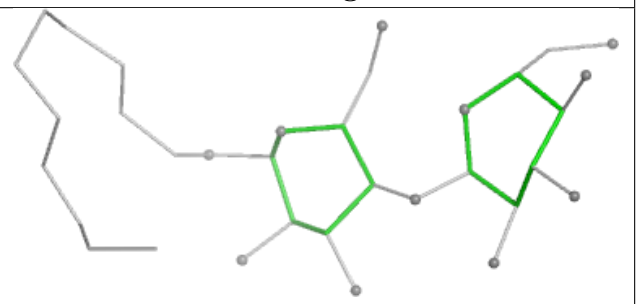
**Bond lengths**



**Bond angles**

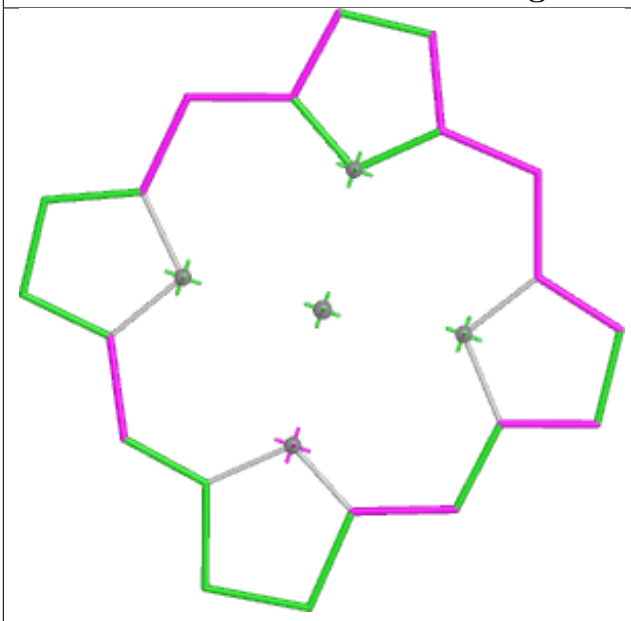


**Torsions**

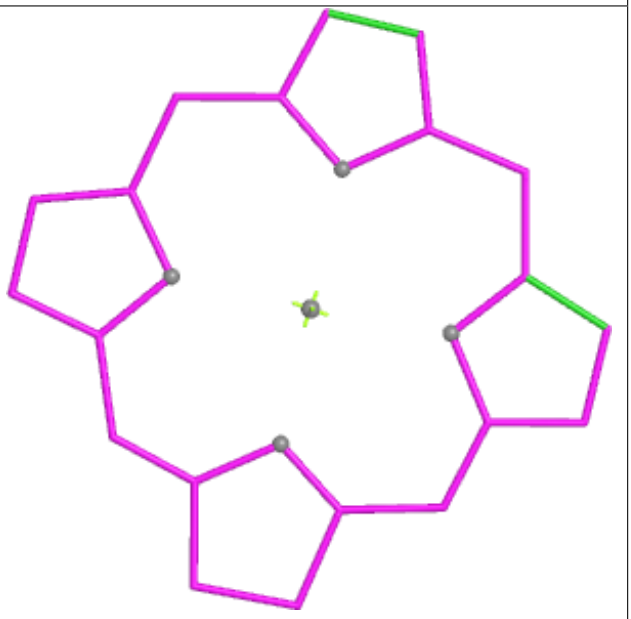


**Rings**

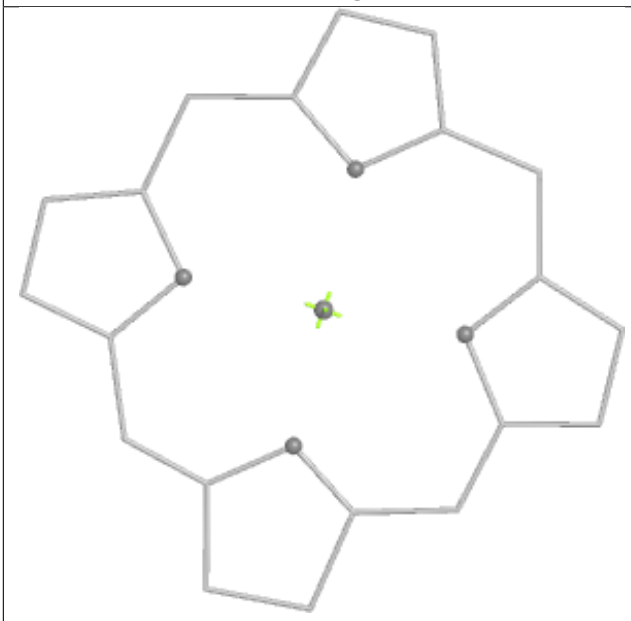
**Ligand CLA 4 311**



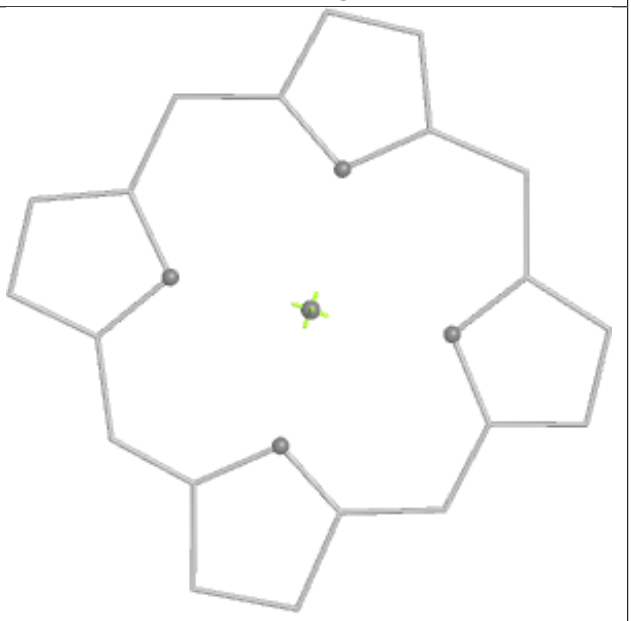
**Bond lengths**



**Bond angles**

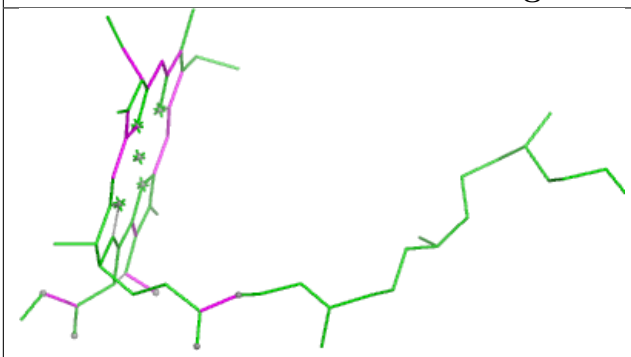


**Torsions**

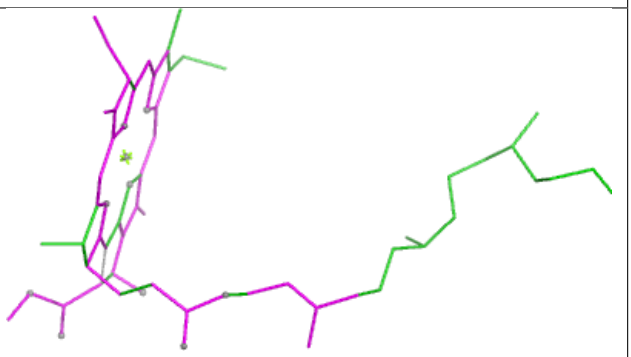


**Rings**

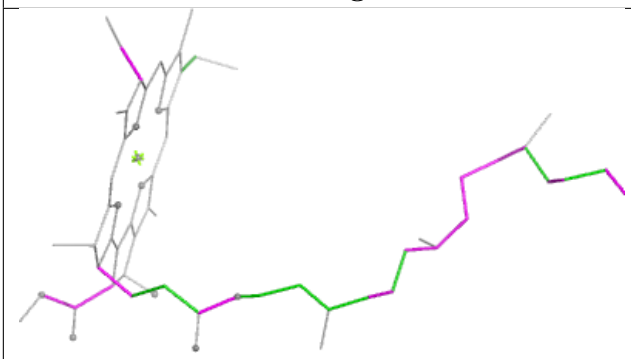
**Ligand CLA A 828**



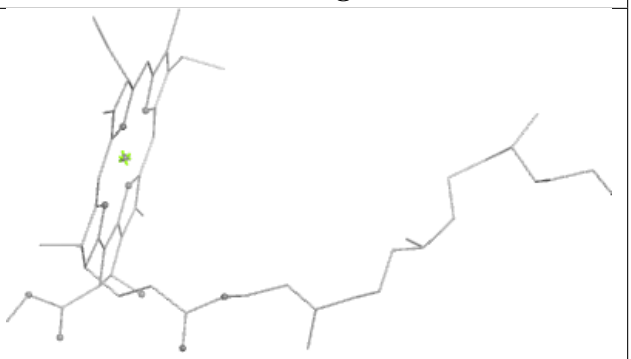
**Bond lengths**



**Bond angles**

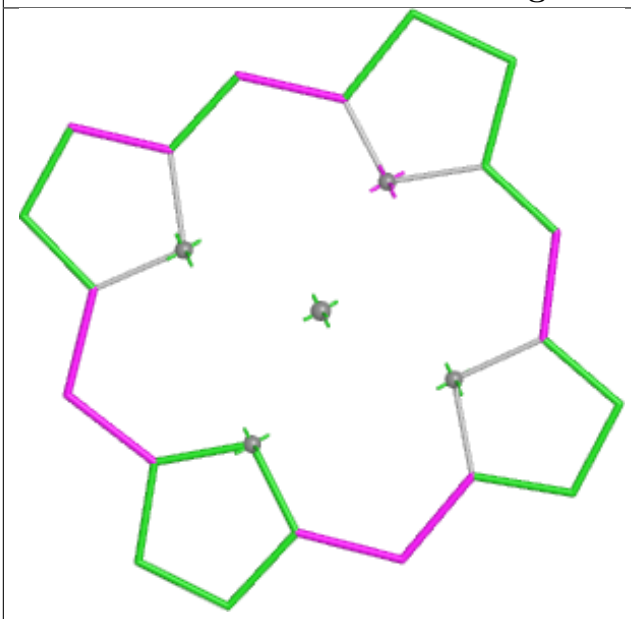


**Torsions**

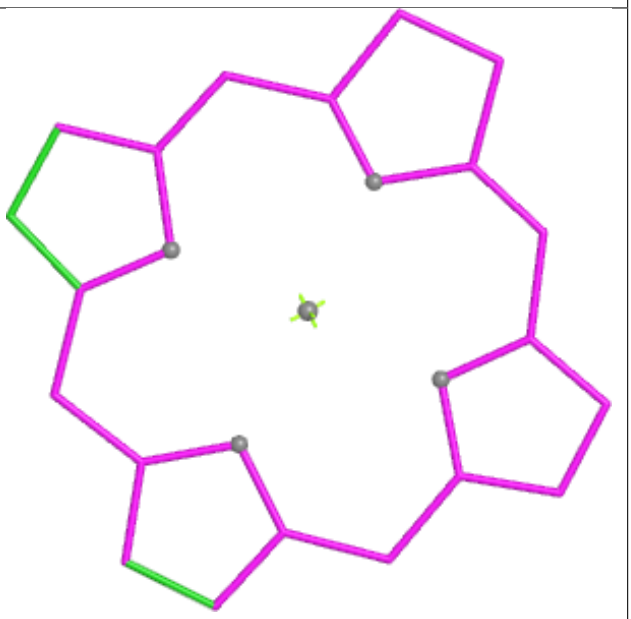


**Rings**

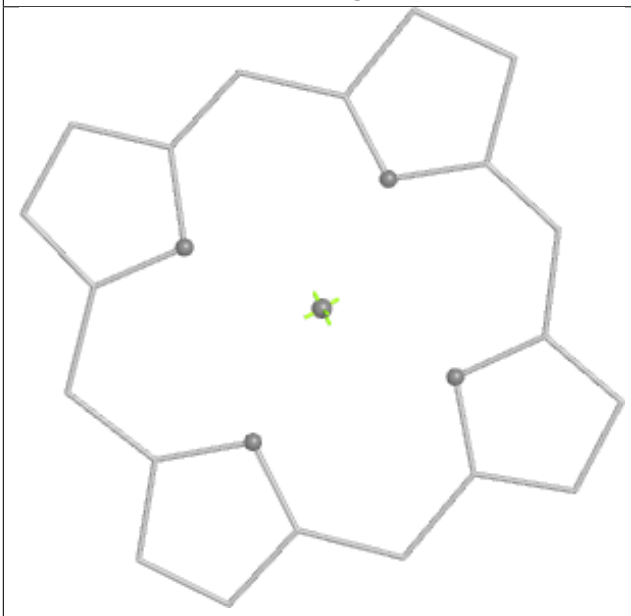
**Ligand CLA 3 305**



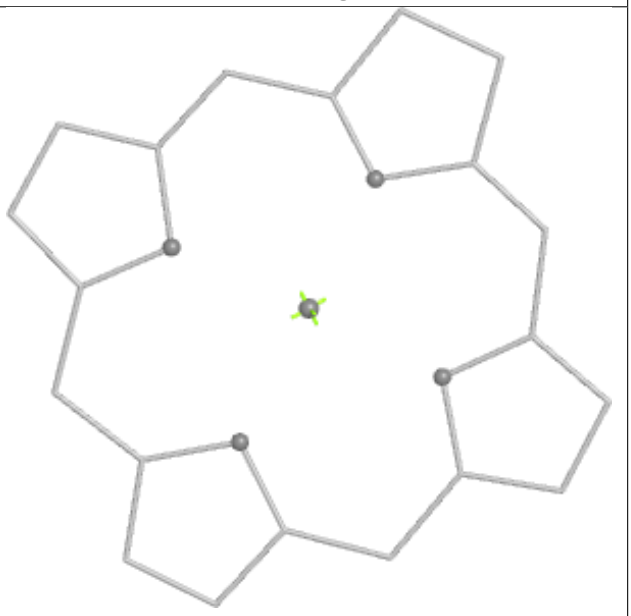
**Bond lengths**



**Bond angles**

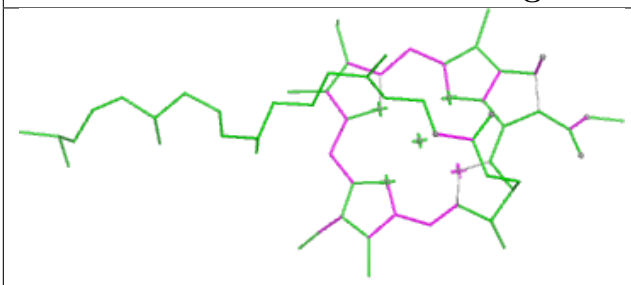


**Torsions**

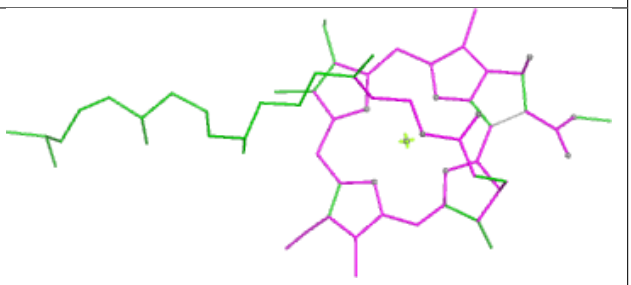


**Rings**

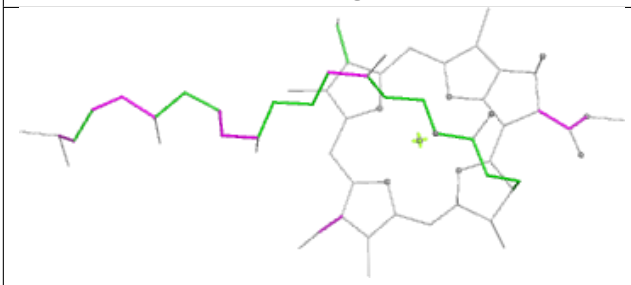
## Ligand CLA A 835



Bond lengths



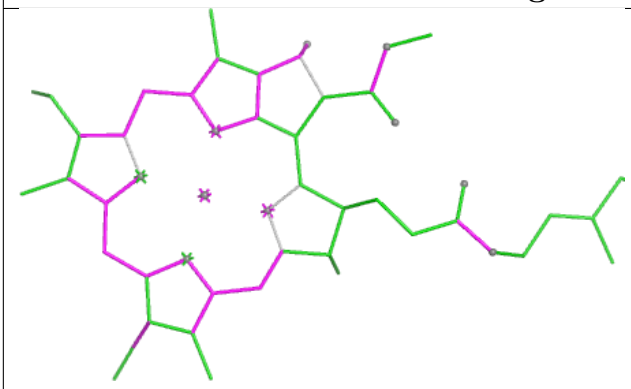
Bond angles



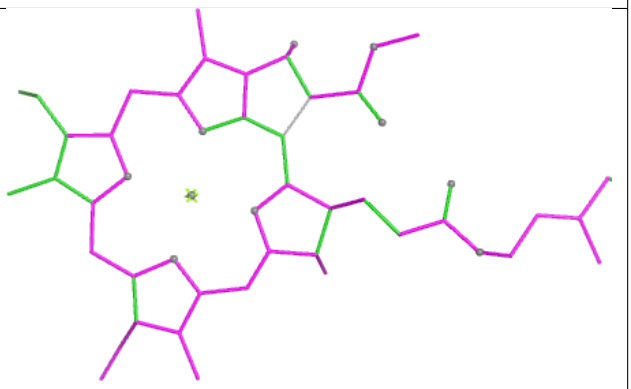
Torsions

Rings

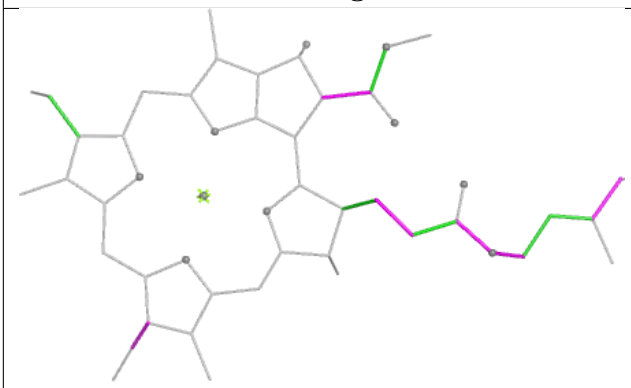
## Ligand CLA 1 215



Bond lengths



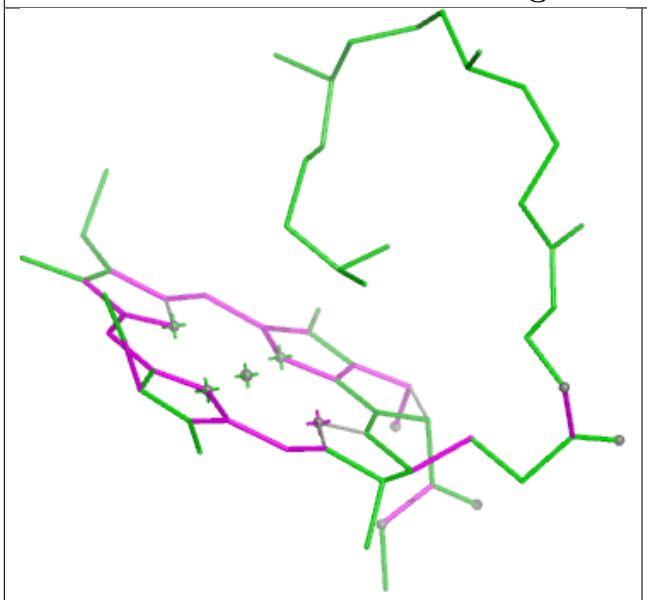
Bond angles



Torsions

Rings

**Ligand CLA 2 316**



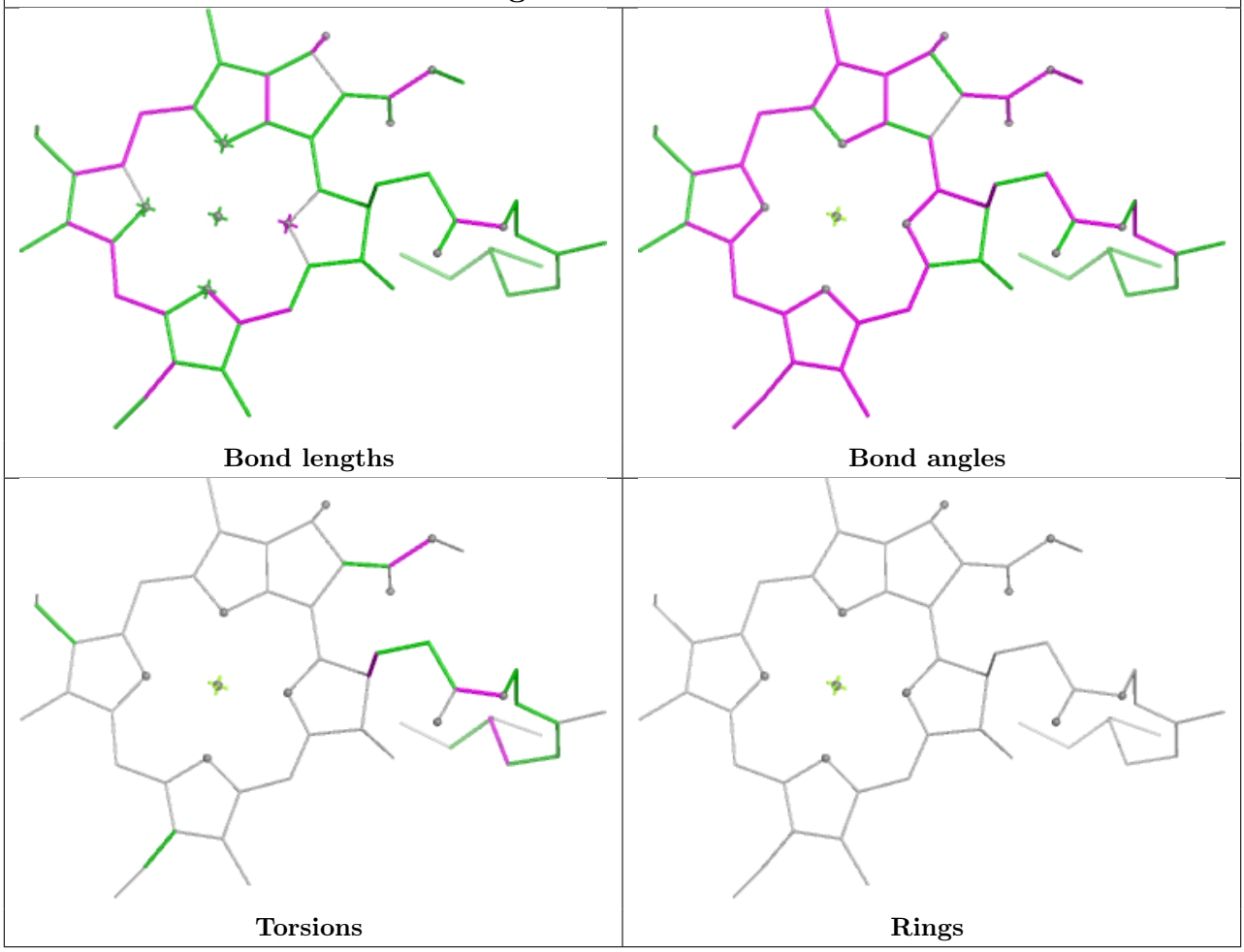
**Bond lengths**

**Bond angles**

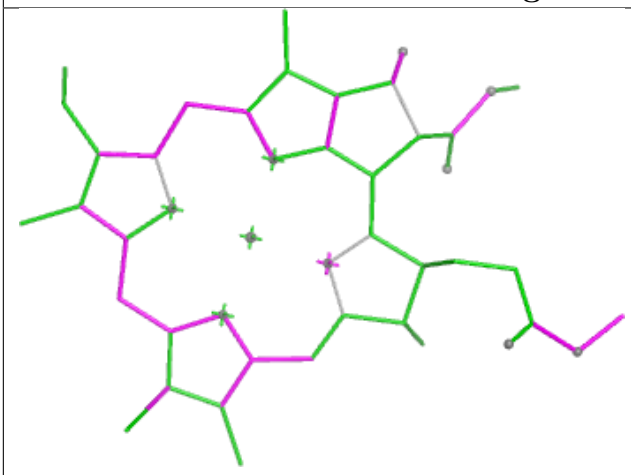
**Torsions**

**Rings**

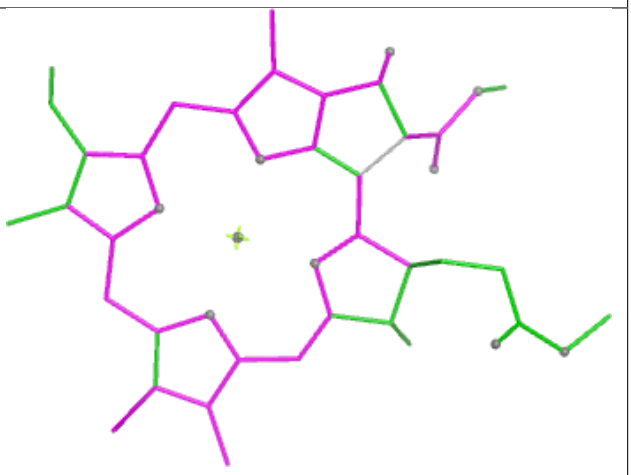
**Ligand CLA A 806**



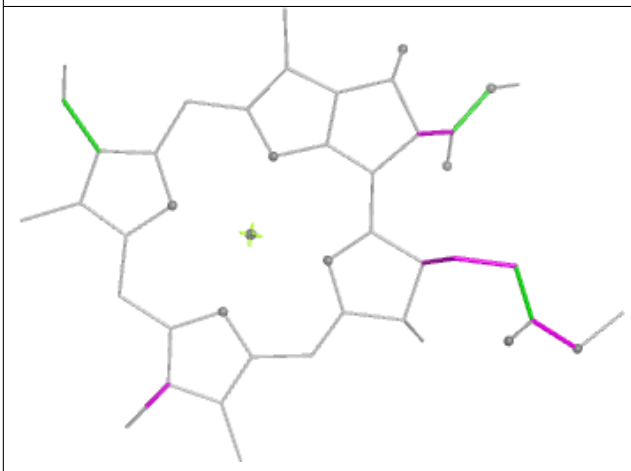
**Ligand CLA K 101**



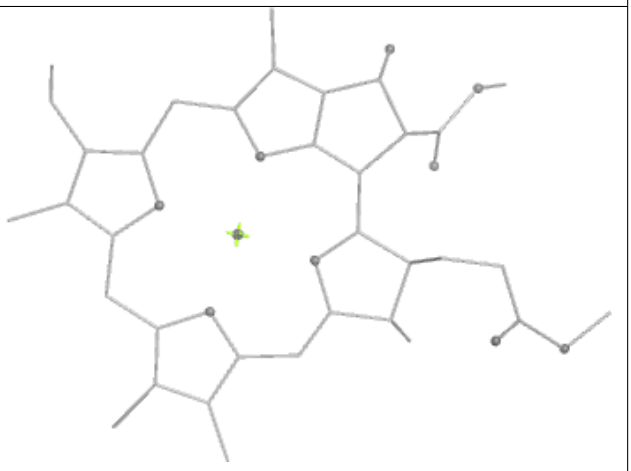
**Bond lengths**



**Bond angles**

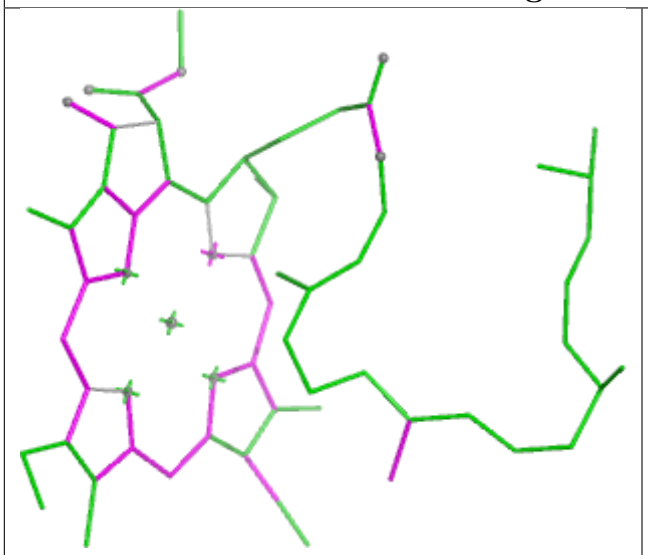


**Torsions**

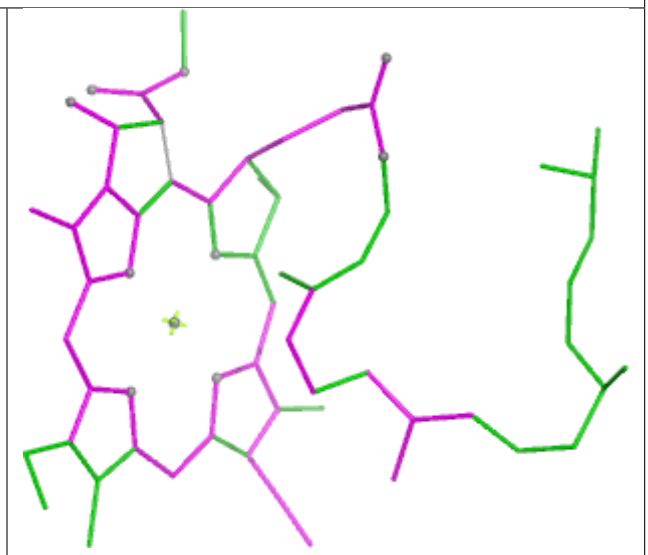


**Rings**

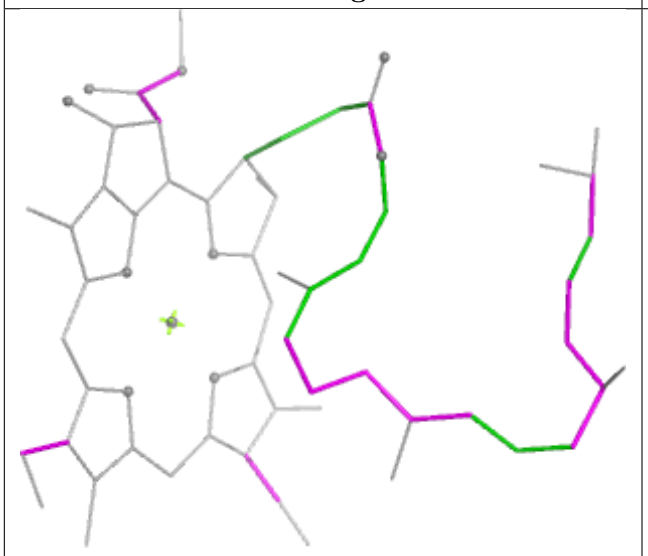
**Ligand CLA B 824**



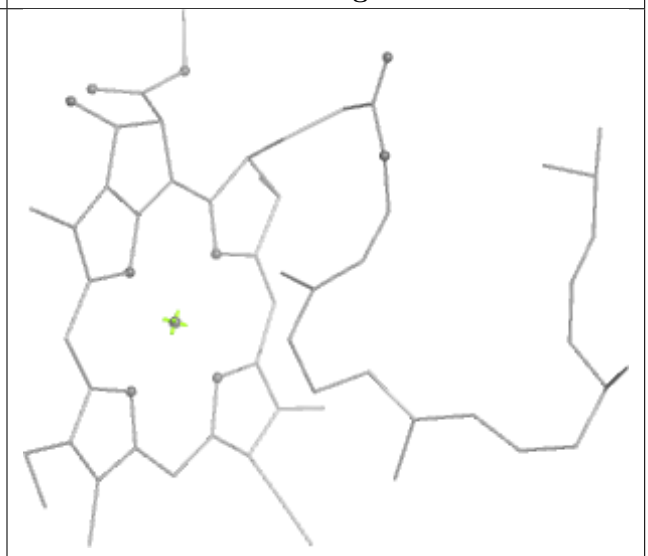
**Bond lengths**



**Bond angles**

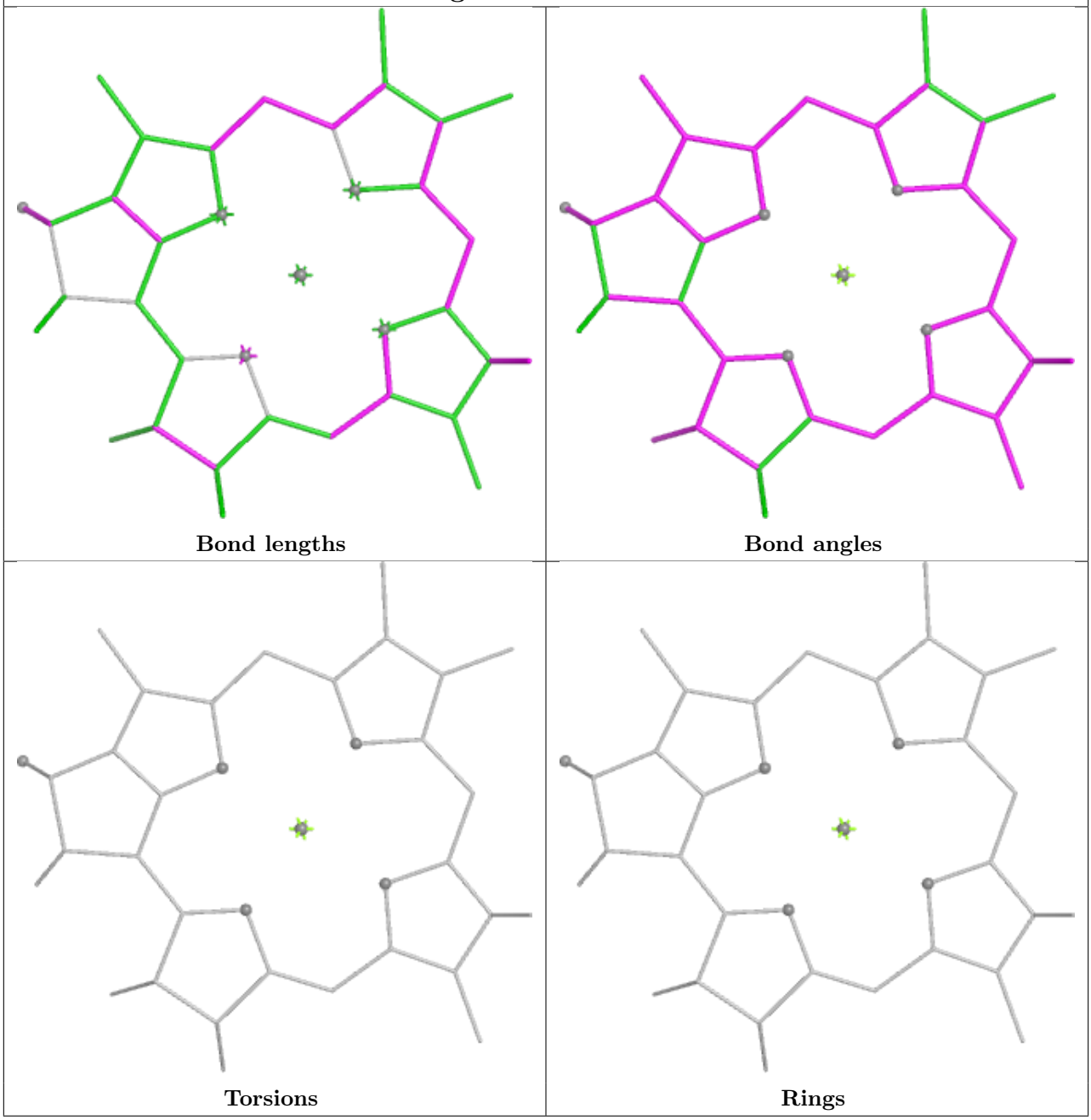


**Torsions**

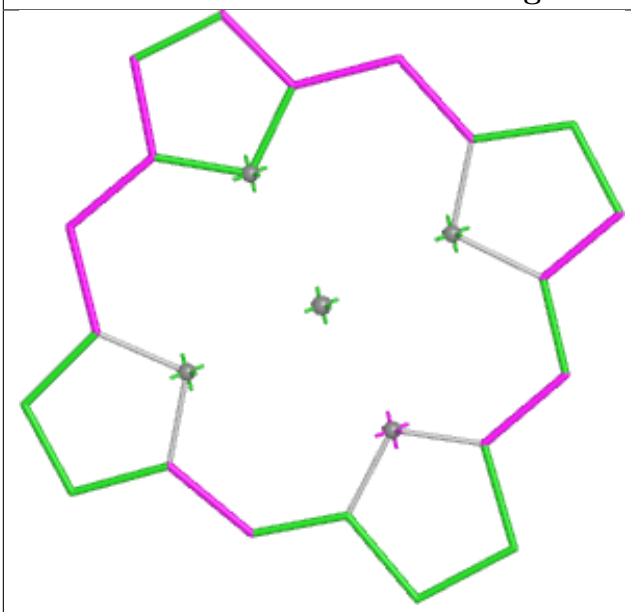


**Rings**

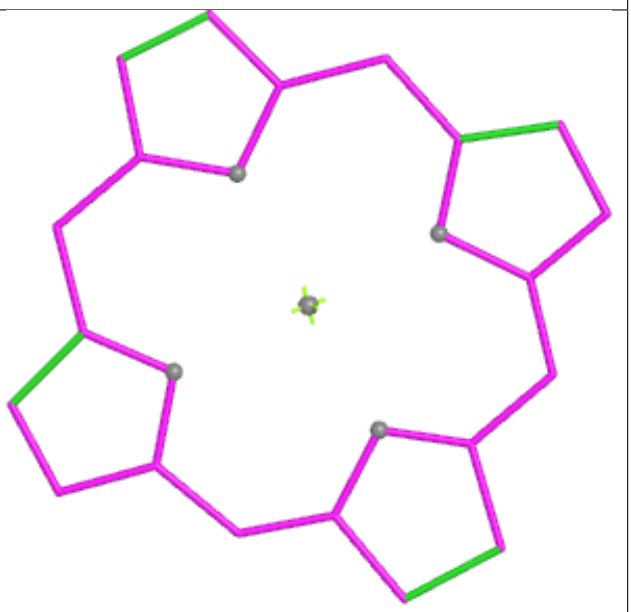
**Ligand CLA 3 317**



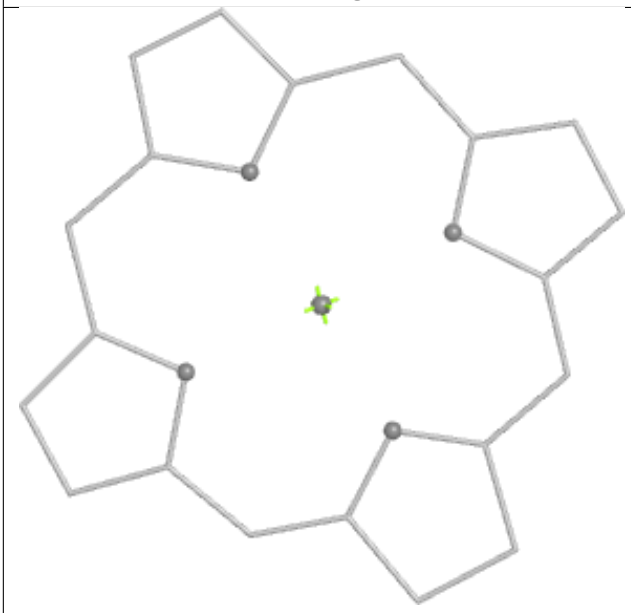
**Ligand CLA A 814**



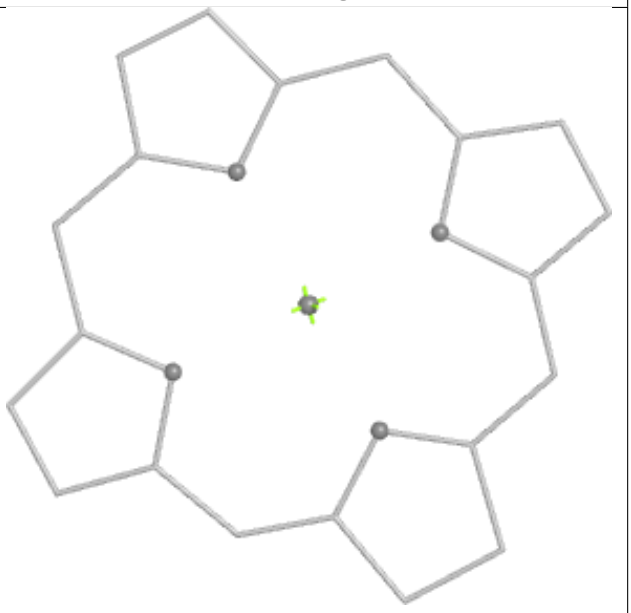
**Bond lengths**



**Bond angles**

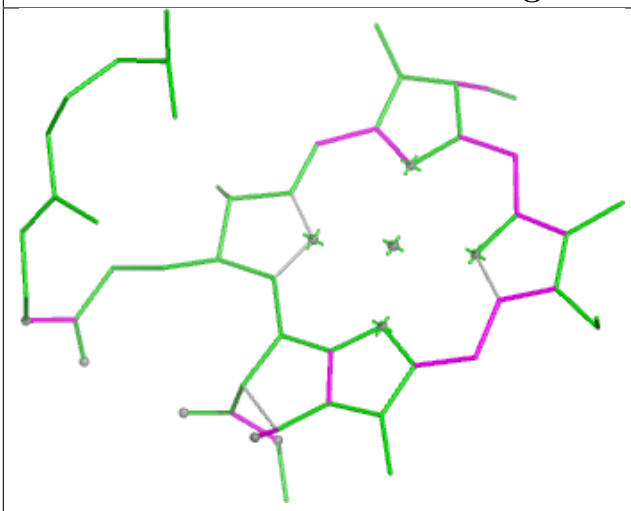


**Torsions**

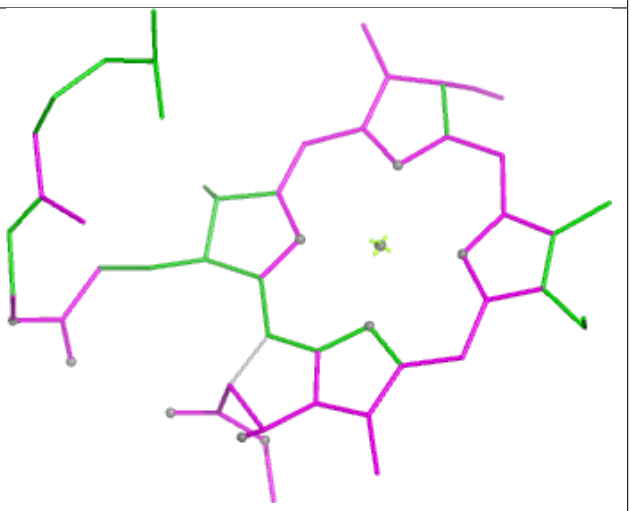


**Rings**

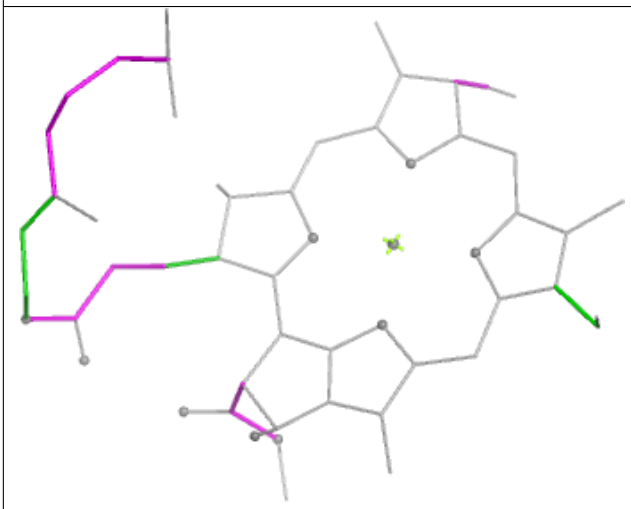
**Ligand CLA H 102**



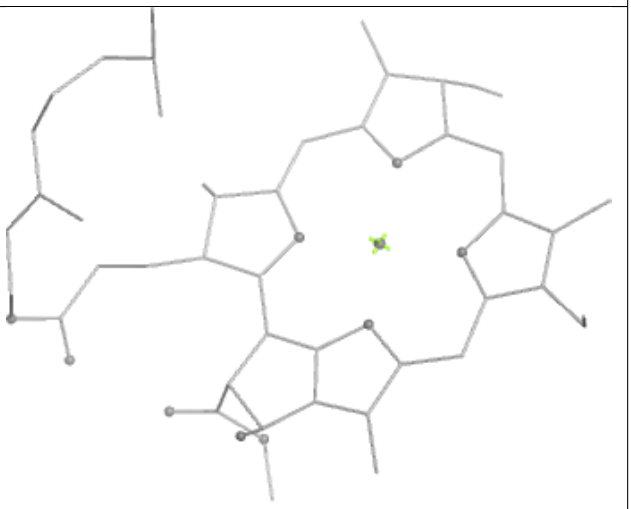
**Bond lengths**



**Bond angles**

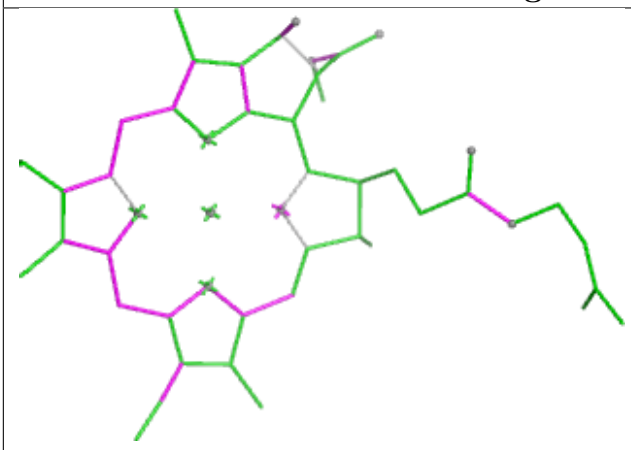


**Torsions**



**Rings**

**Ligand CLA B 833**



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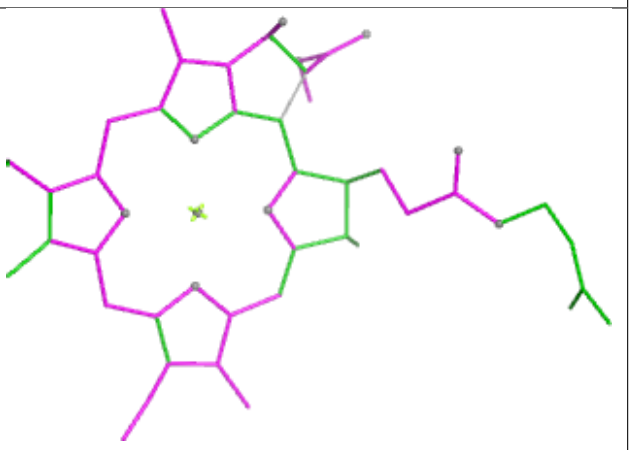
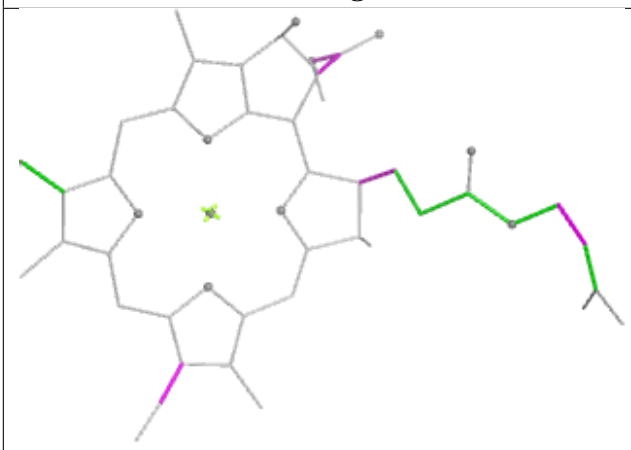


**Bond angles**



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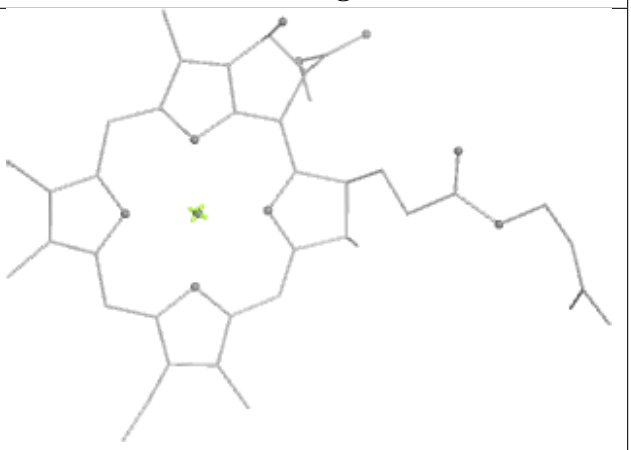
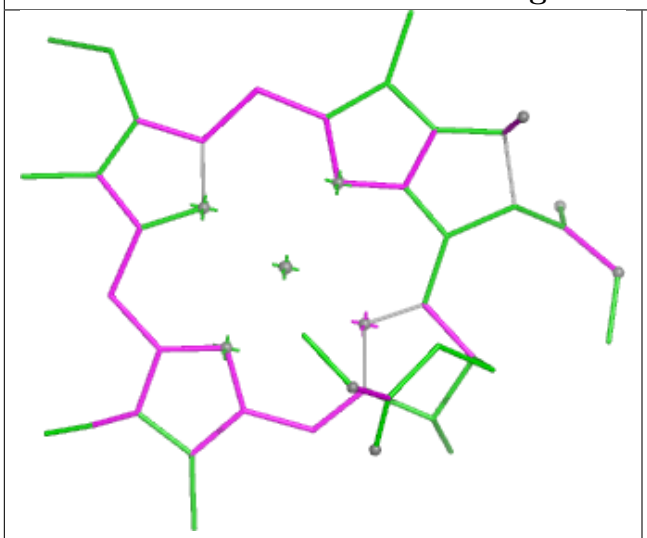


**Rings**

## Ligand CLA 1 204



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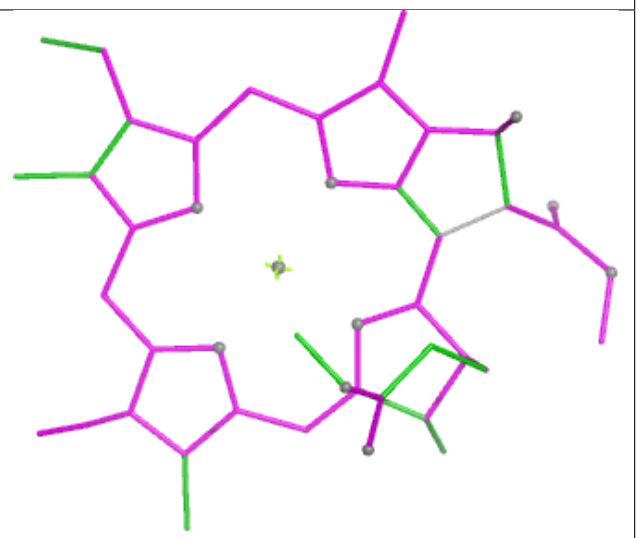
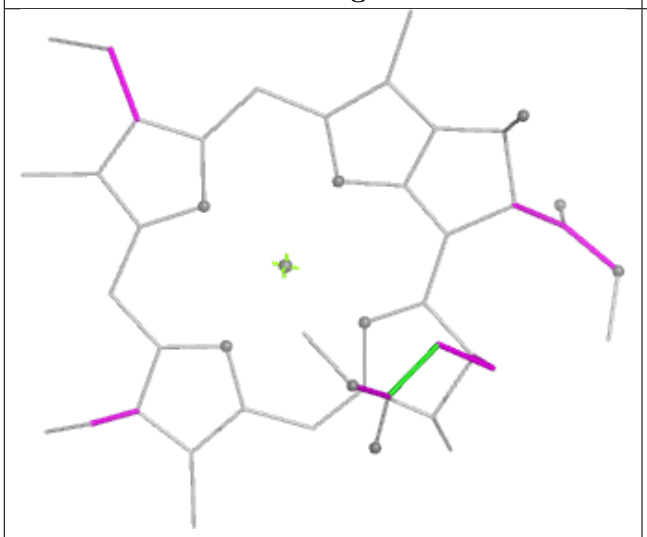


Bond angles



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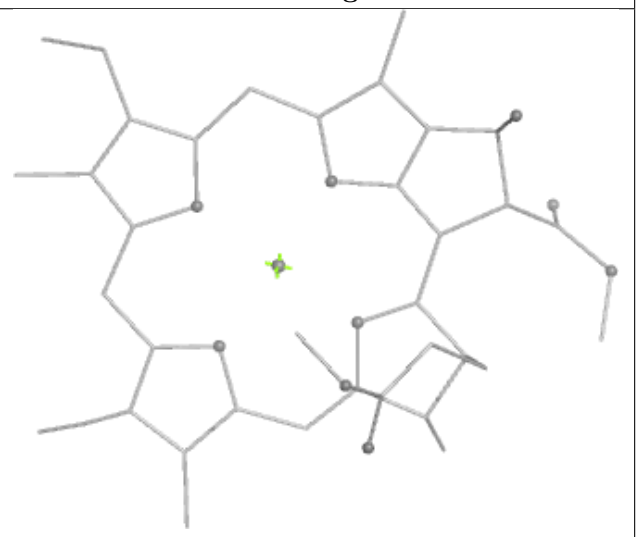
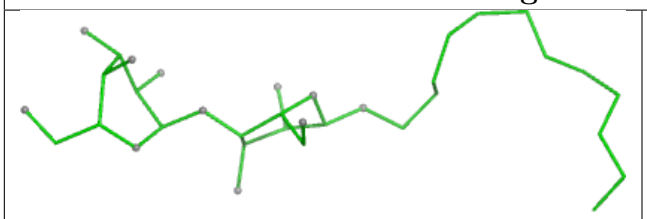


Rings

## Ligand LMU A 846



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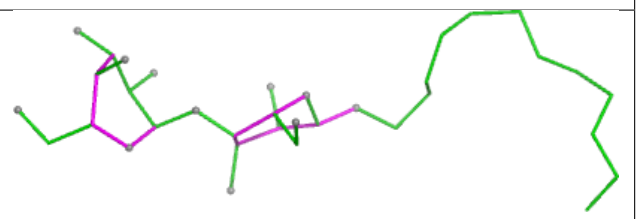
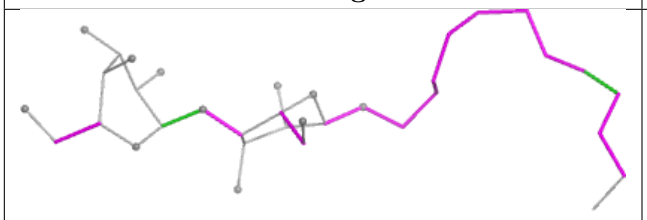


Bond angles



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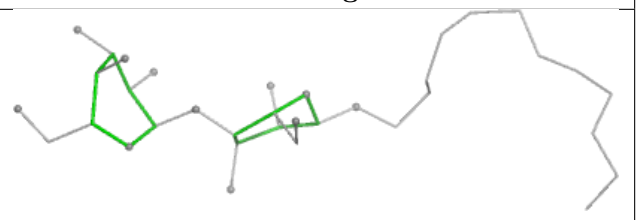
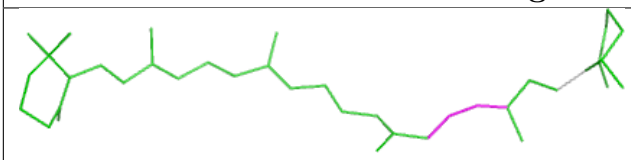
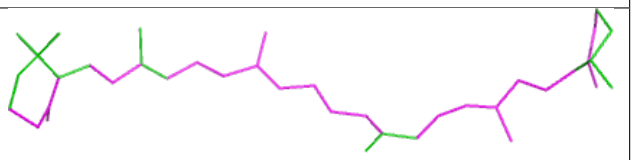


Rings

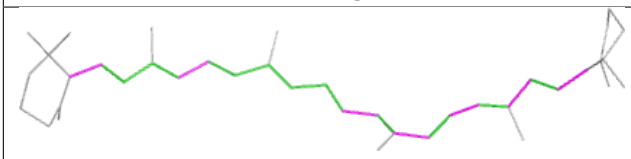
## Ligand BCR I 101



Bond lengths



Bond angles



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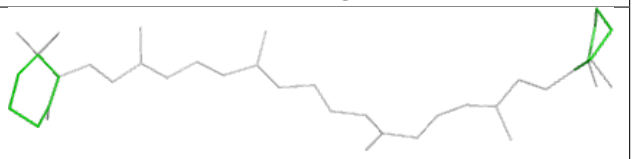
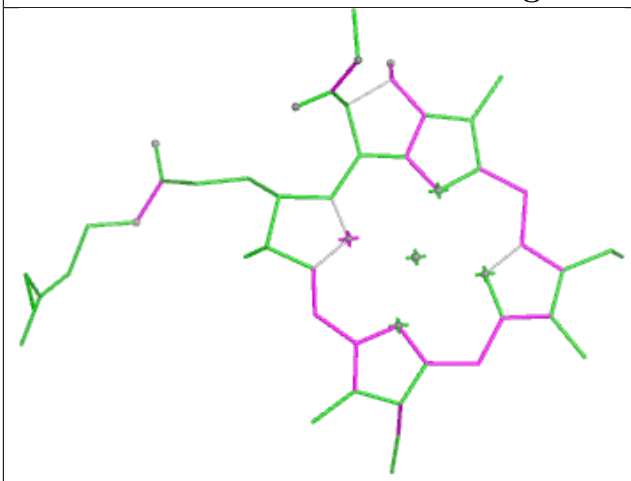


Rings

## Ligand CLA G 105



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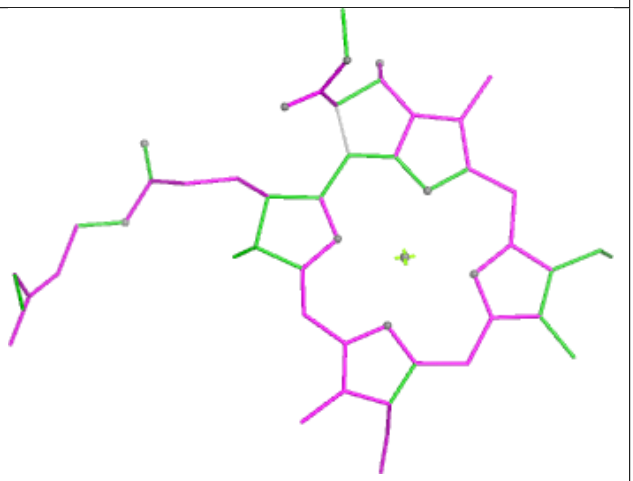
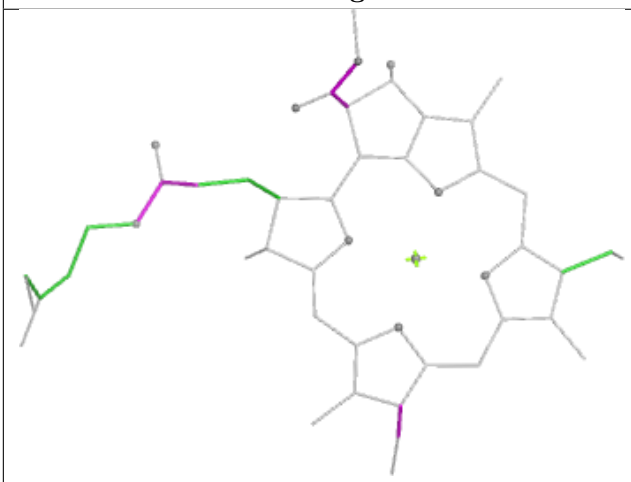


Bond angles



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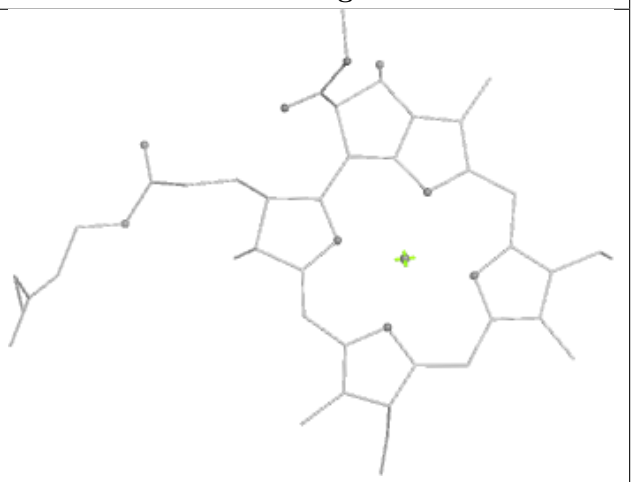
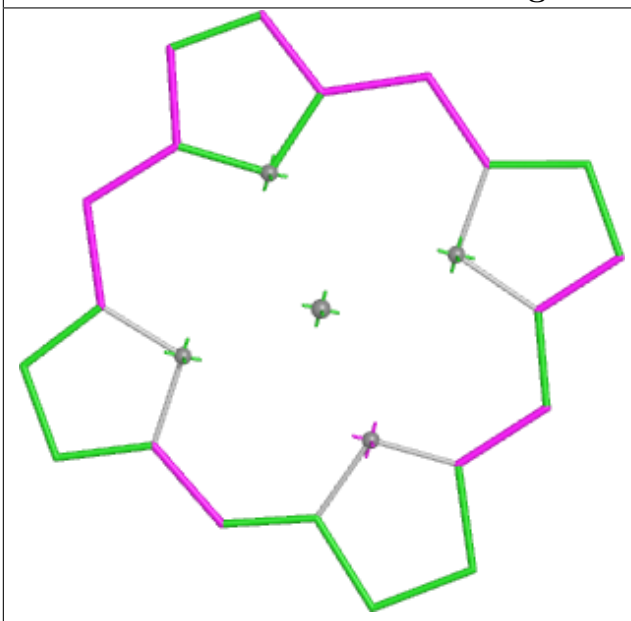
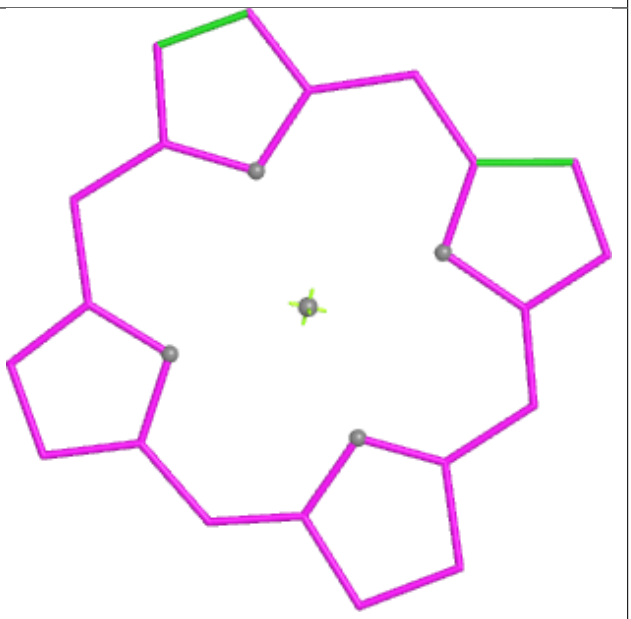


Rings

**Ligand CLA 3 304**



**Bond lengths**



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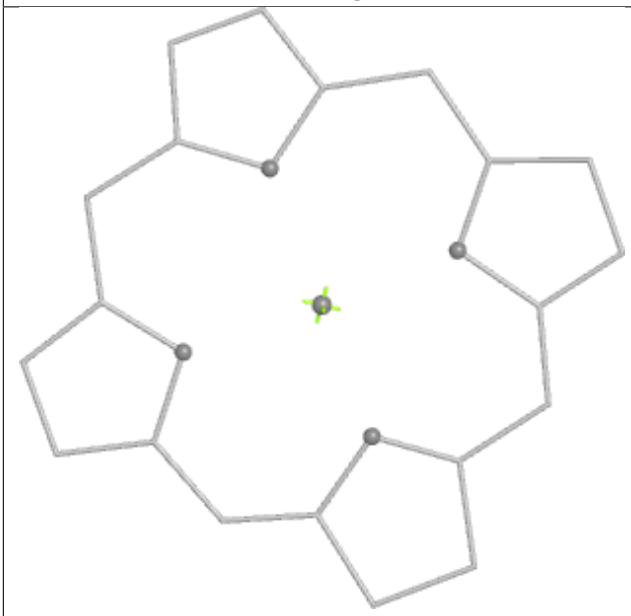

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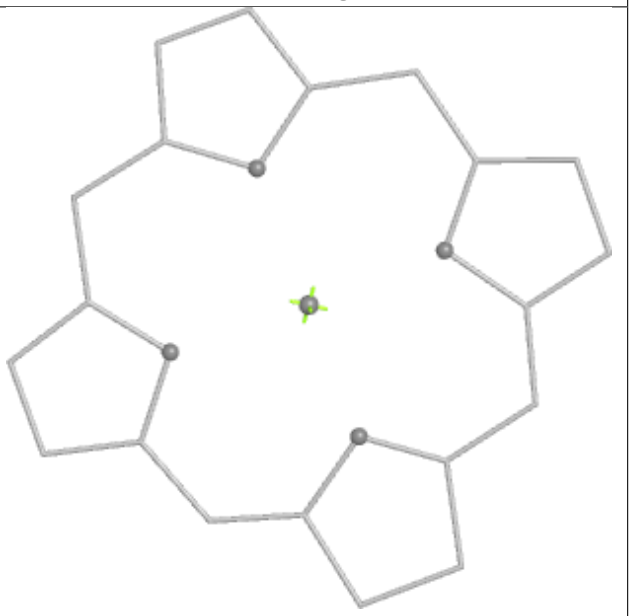
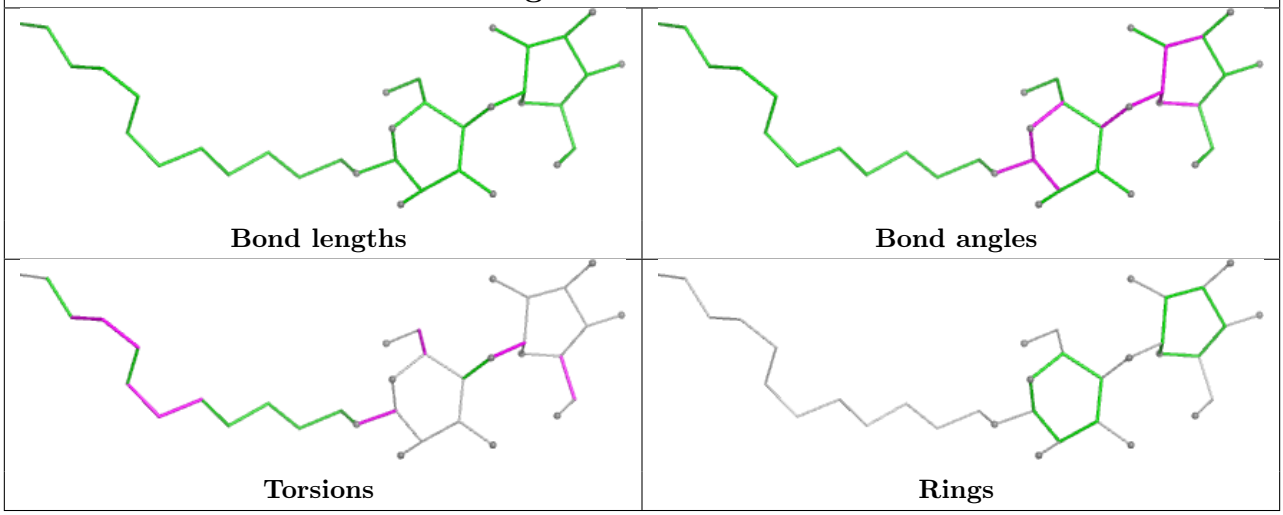
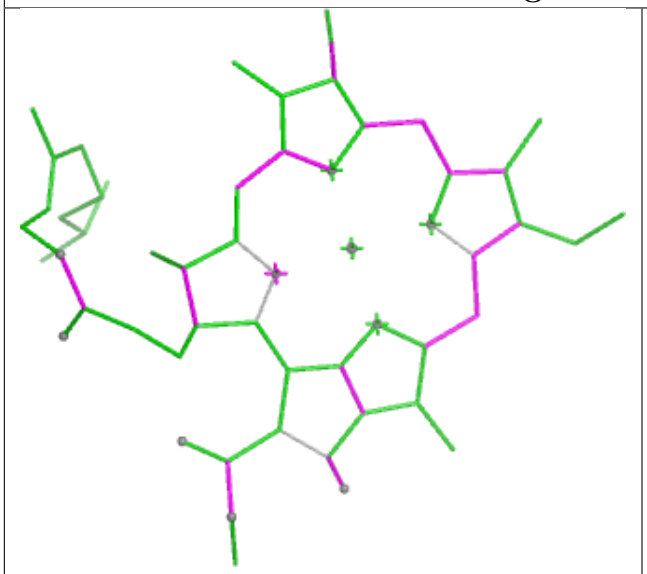


**Rings**

**Ligand LMU 1 216**



**Ligand CLA H 101**



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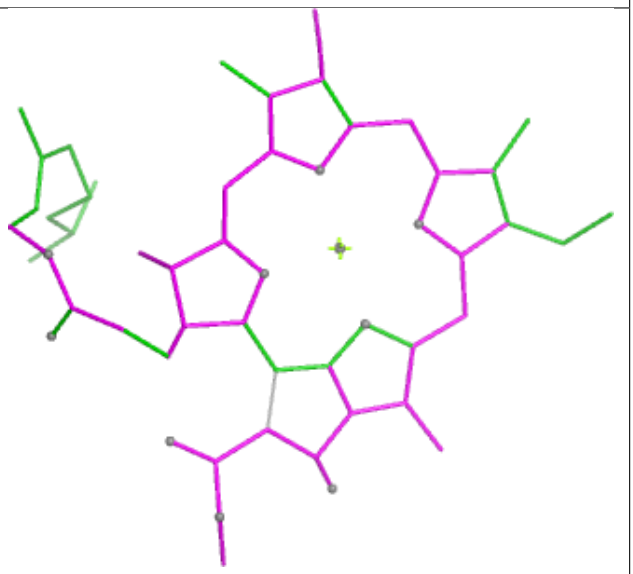
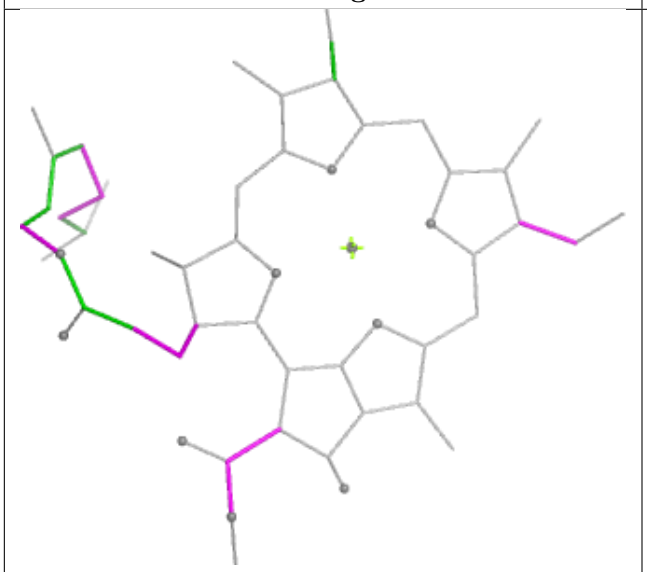


**Bond angles**



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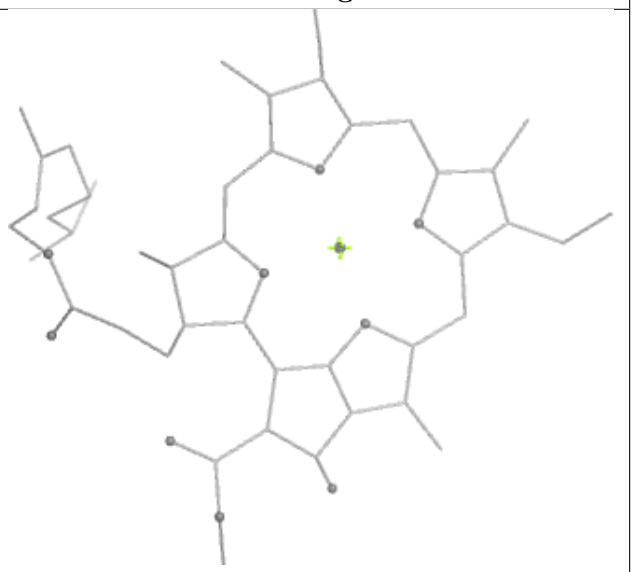
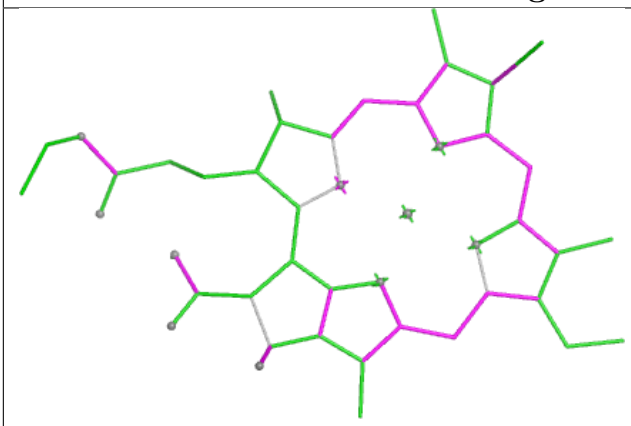
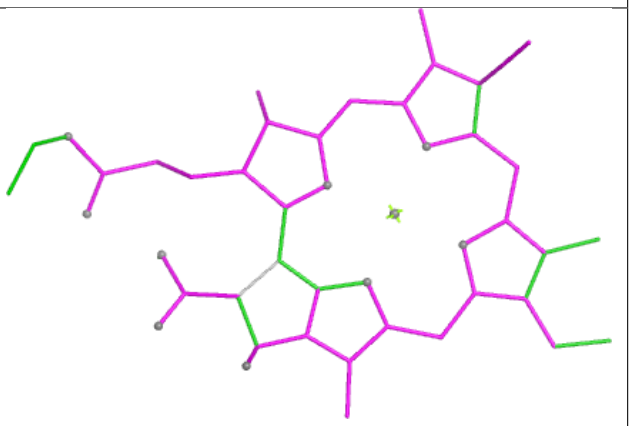


**Rings**

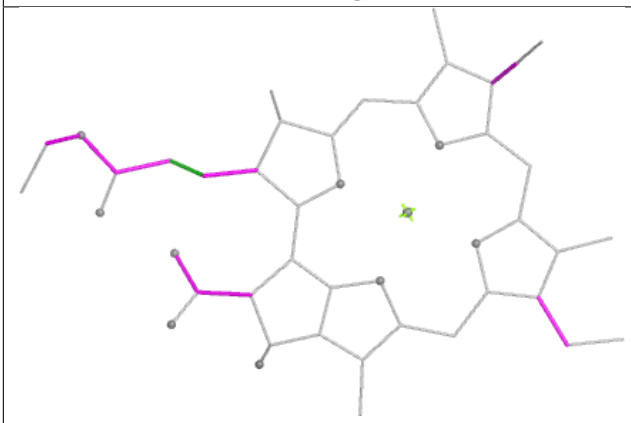
## Ligand CLA 4 318



Bond lengths



Bond angles



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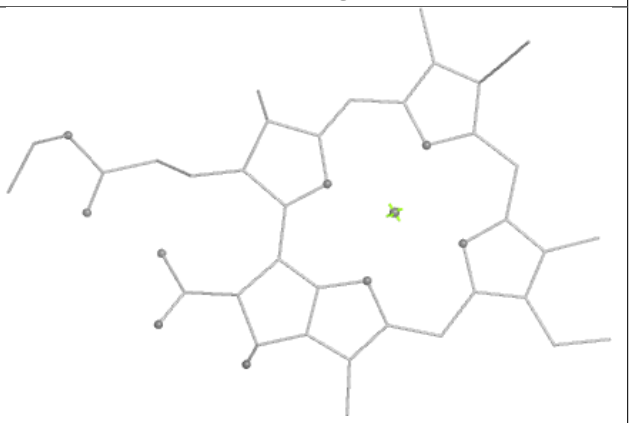
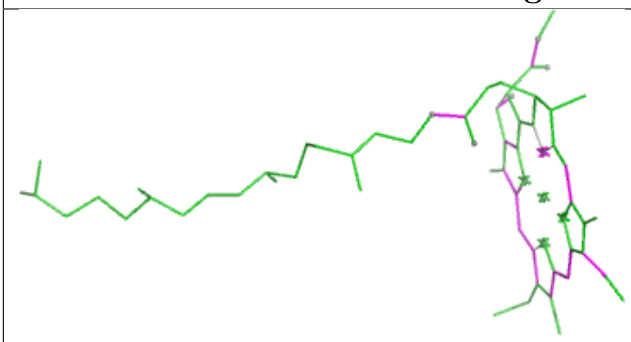
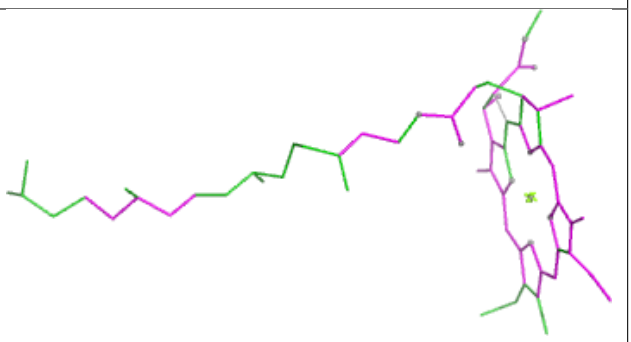


Rings

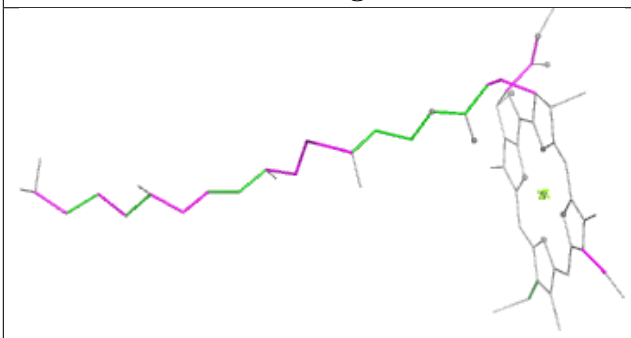
## Ligand CLA B 829



Bond lengths



Bond angles



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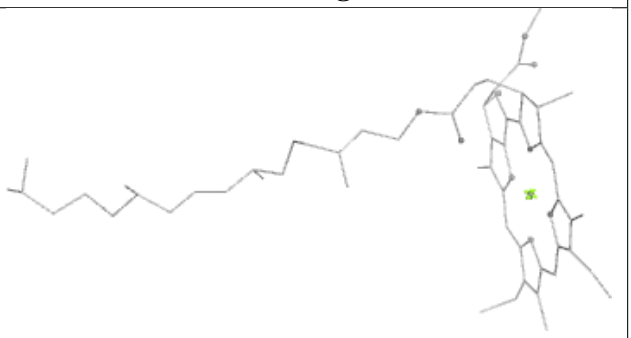
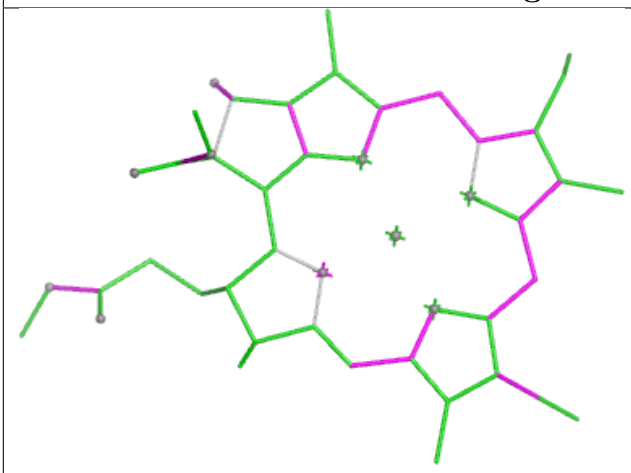


Rings

## Ligand CLA A 834



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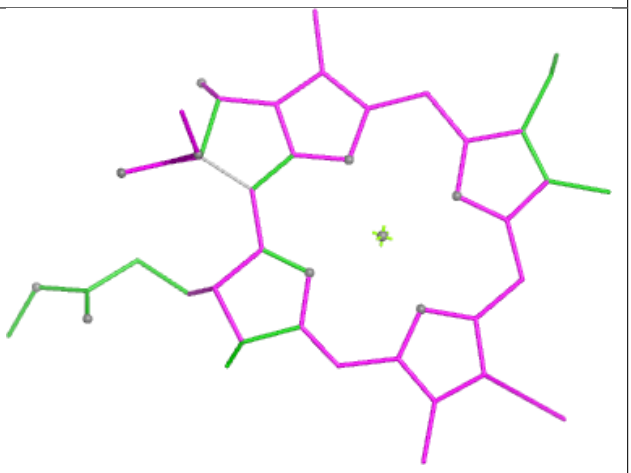
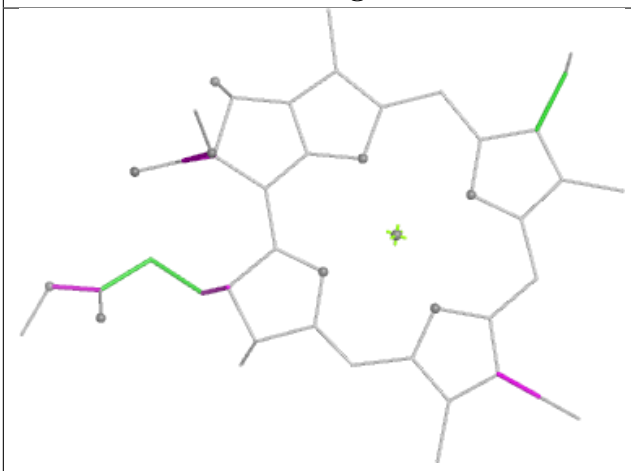


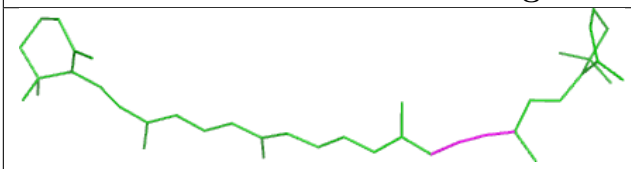
Bond angles



Torsions

Rings

## Ligand BCR B 844



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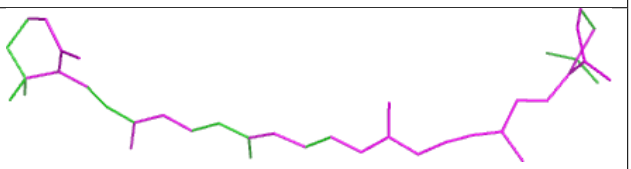
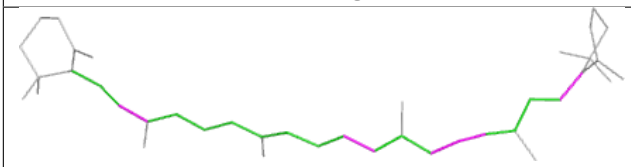
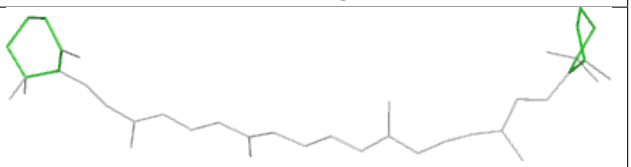


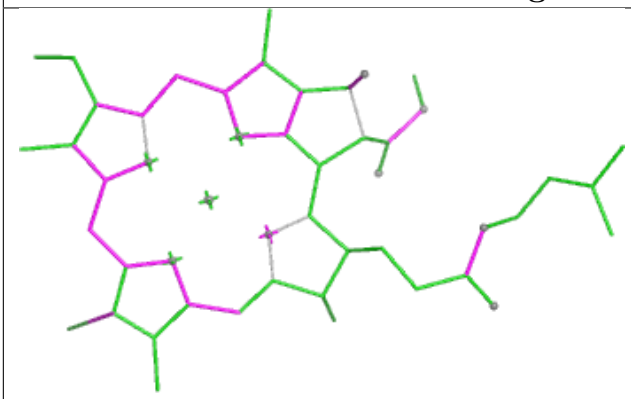
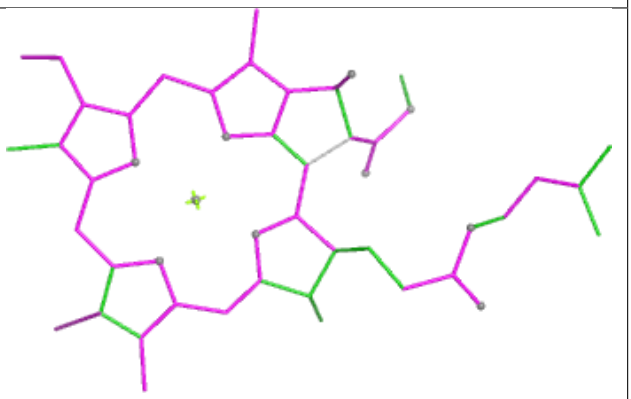
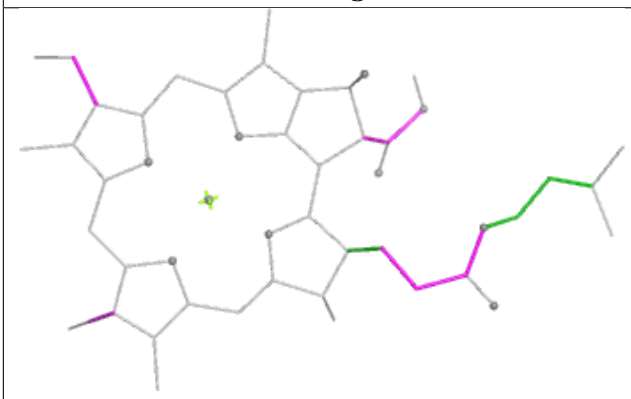
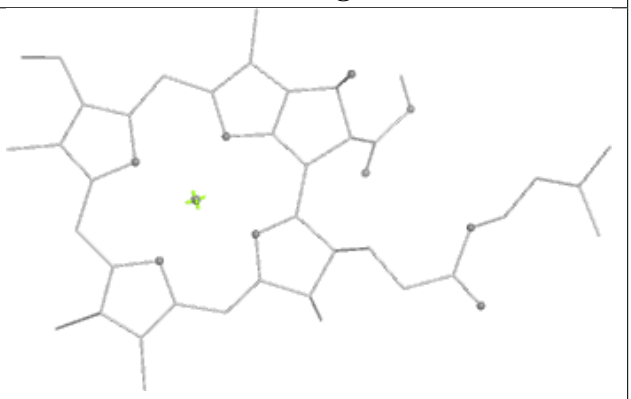
Bond angles



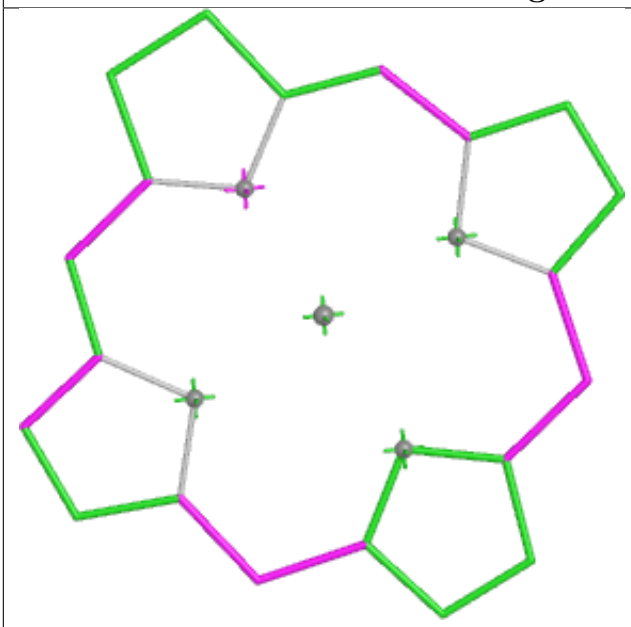
Torsions



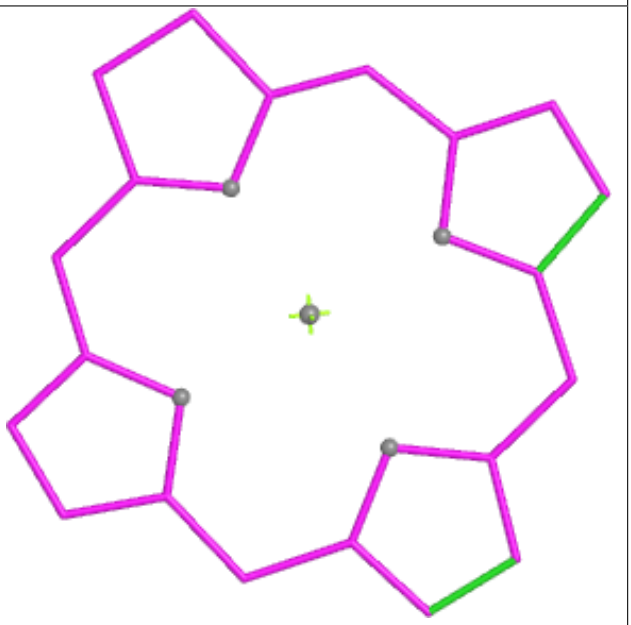
Rings

| Ligand CLA 4 305 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

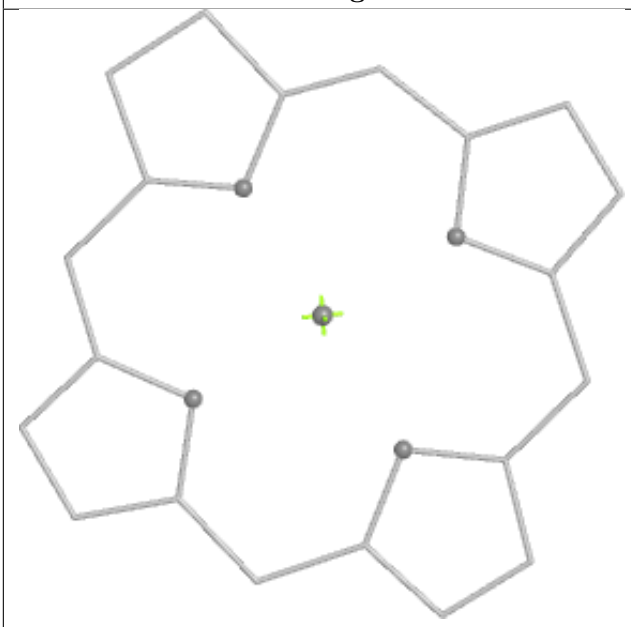
**Ligand CLA 4 312**



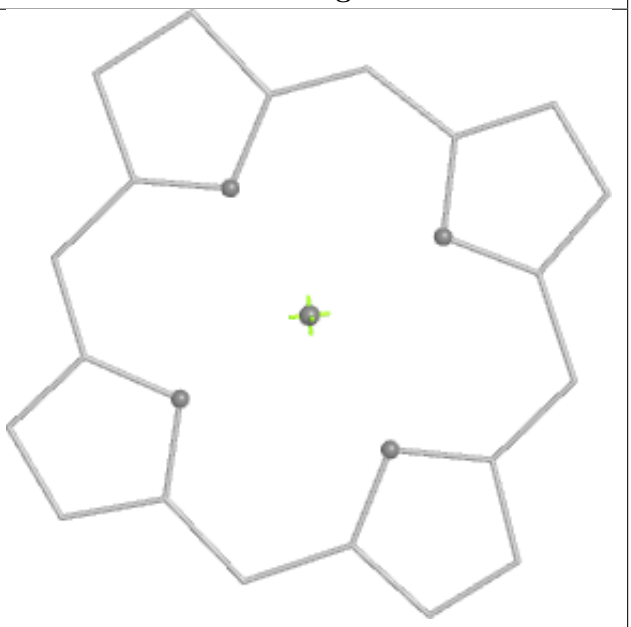
**Bond lengths**



**Bond angles**

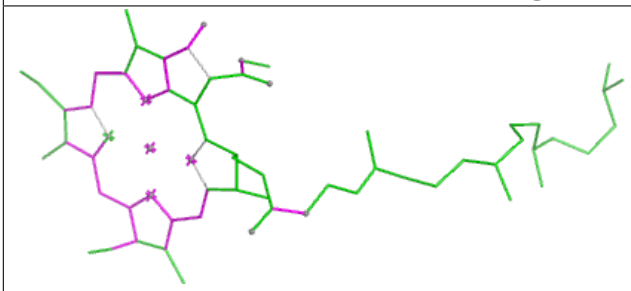


**Torsions**

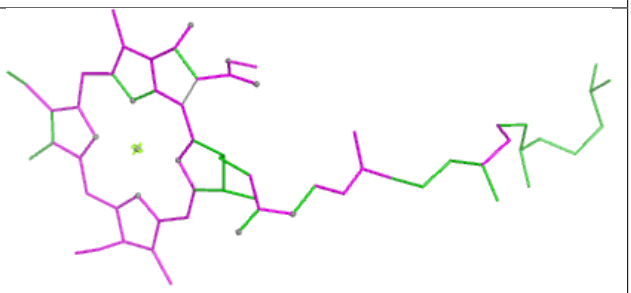


**Rings**

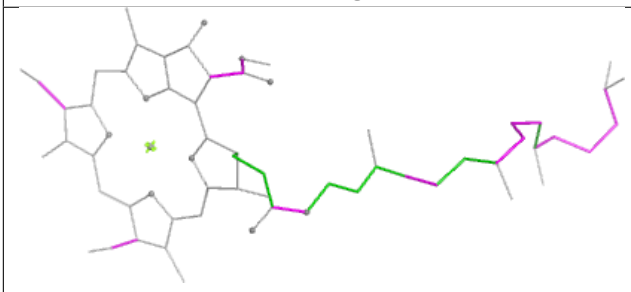
## Ligand CLA 3 314



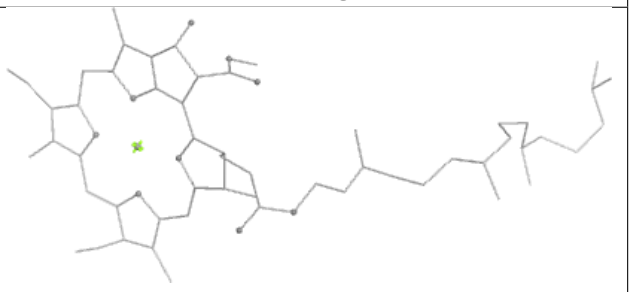
Bond lengths



Bond angles

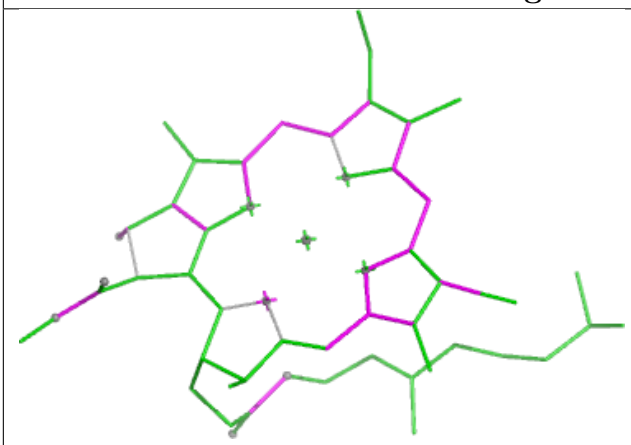


Torsions

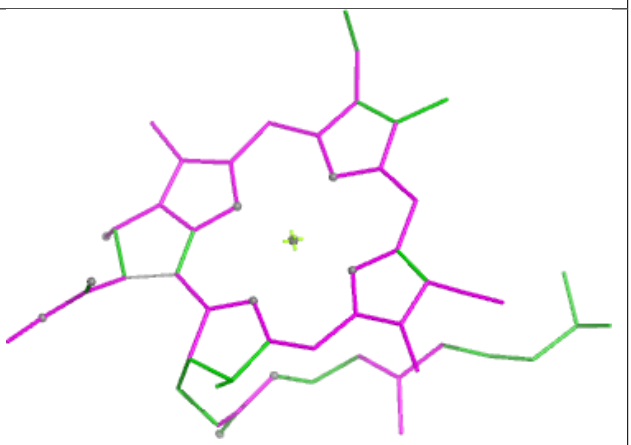


Rings

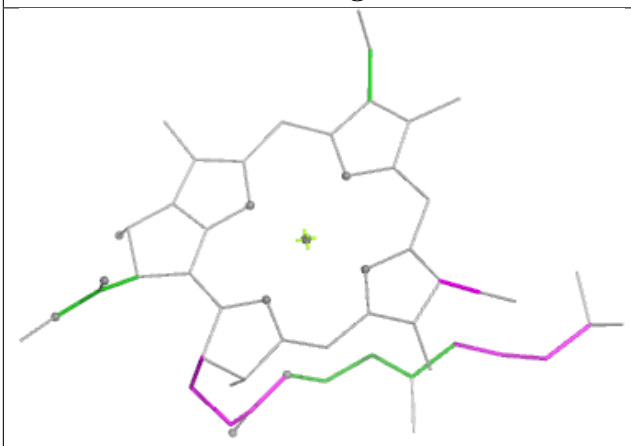
## Ligand CLA B 823



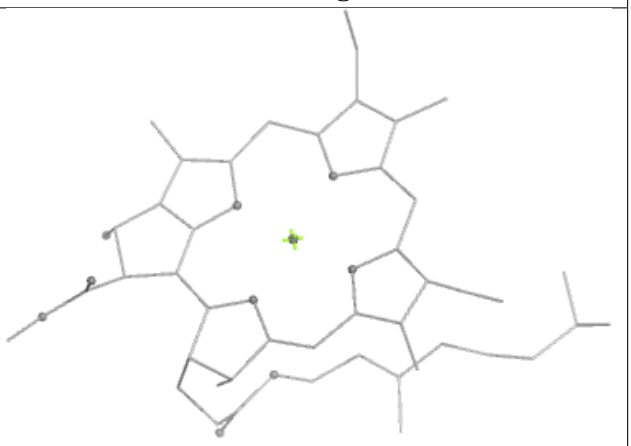
Bond lengths



Bond angles

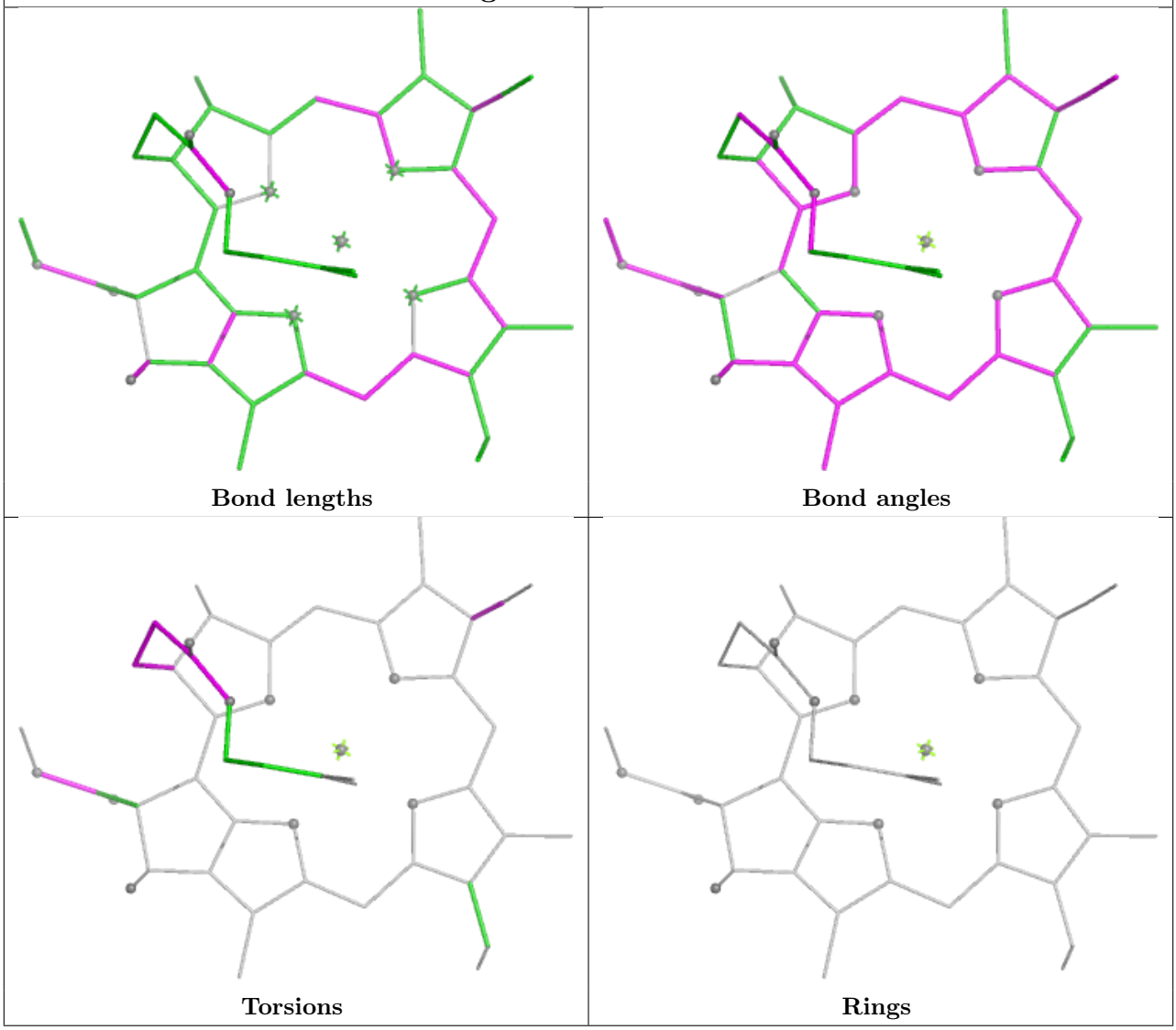


Torsions

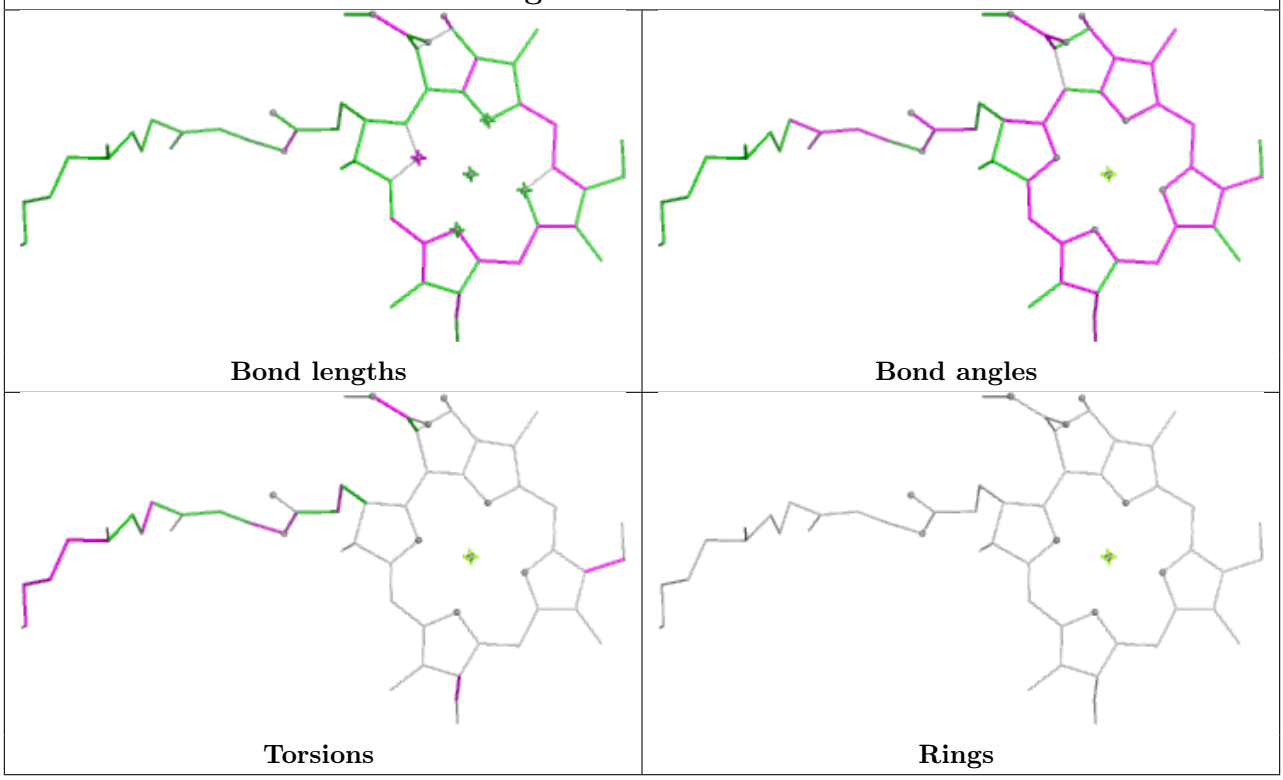


Rings

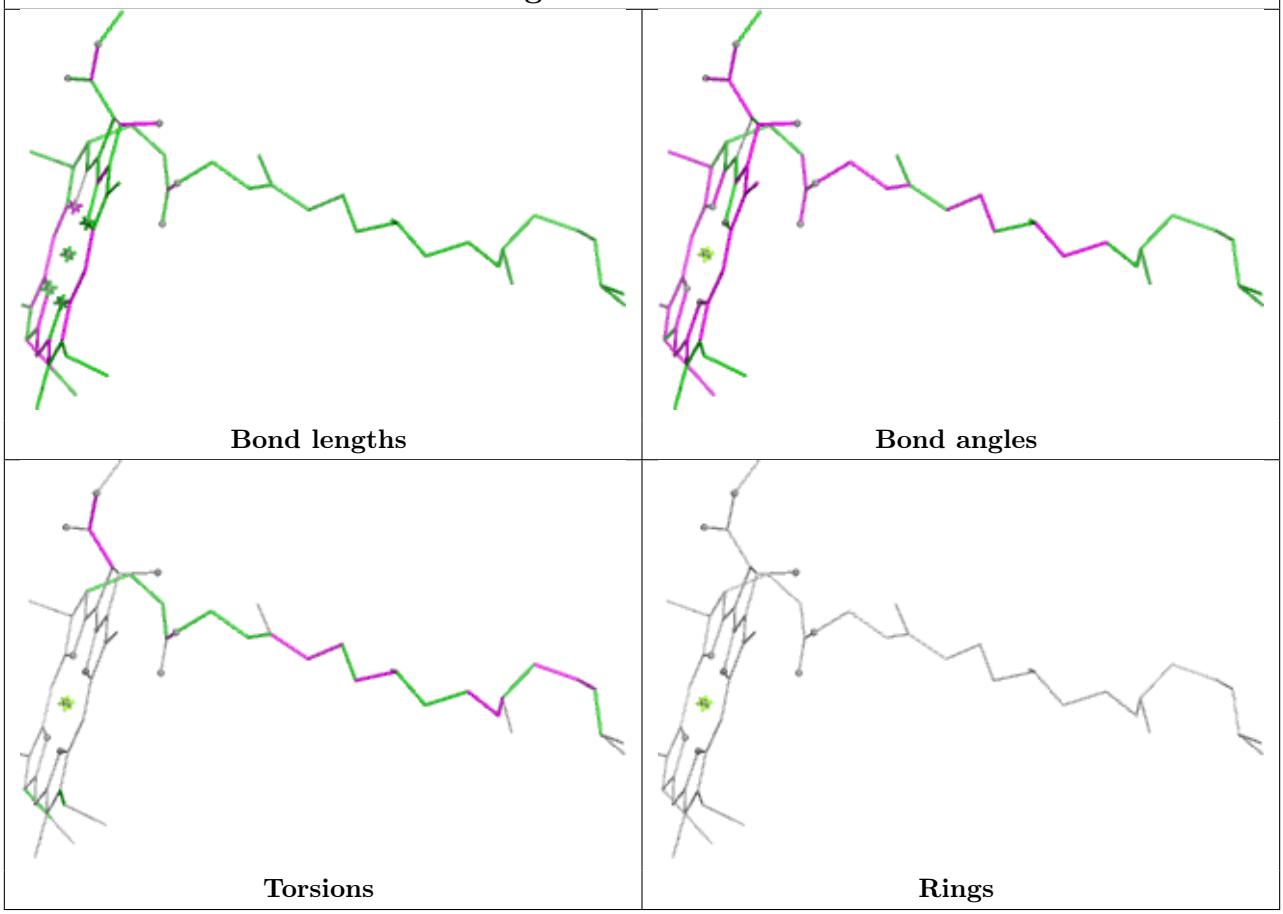
**Ligand CLA H 110**



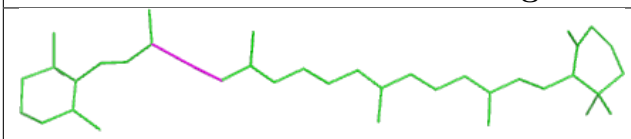
## Ligand CLA A 824



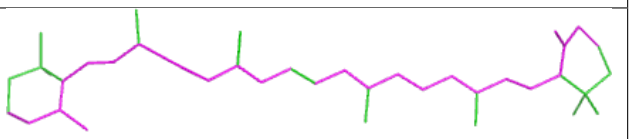

## Ligand CLA A 826



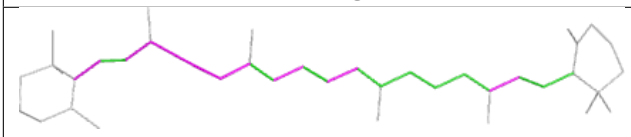
## Ligand BCR G 104



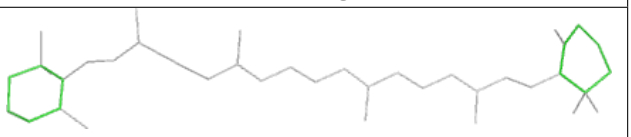
Bond lengths



Bond angles

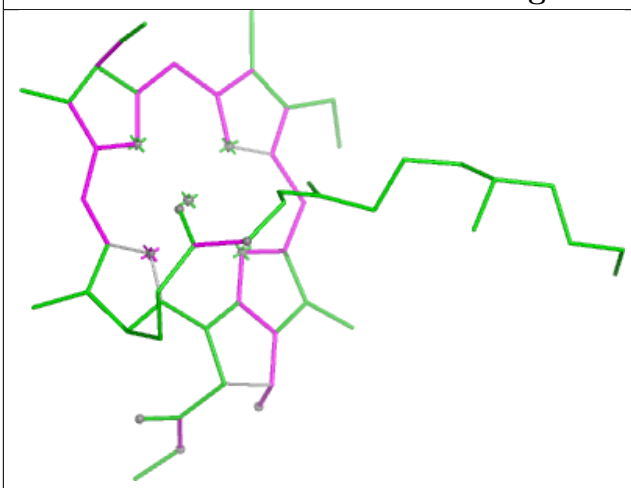


Torsions

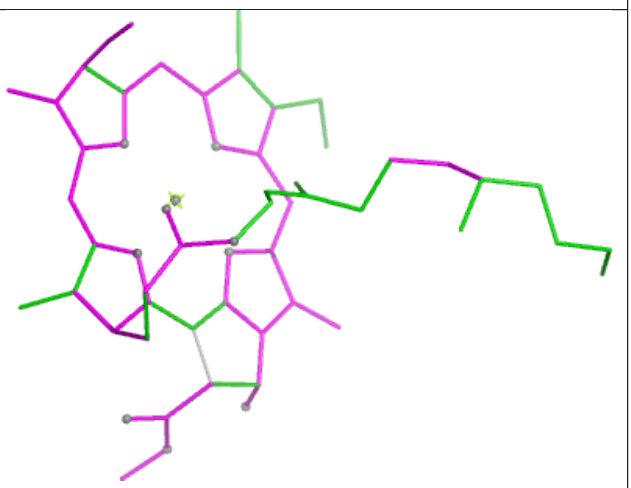


Rings

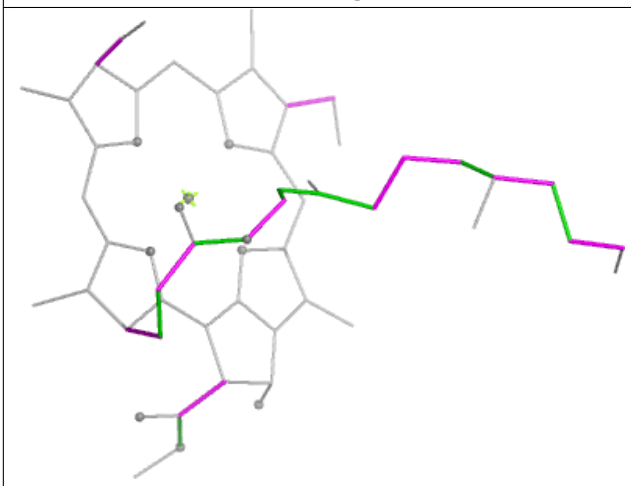
## Ligand CLA 2 303



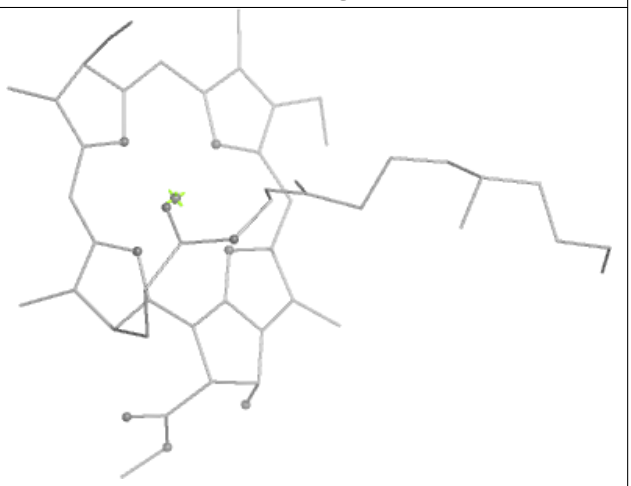
Bond lengths



Bond angles

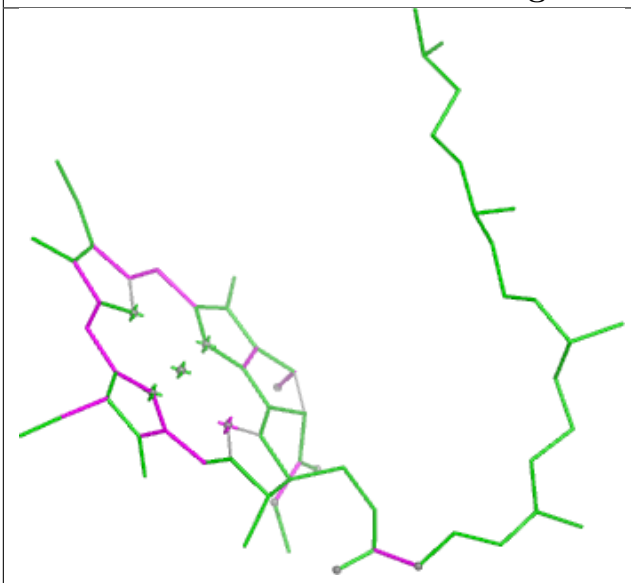


Torsions

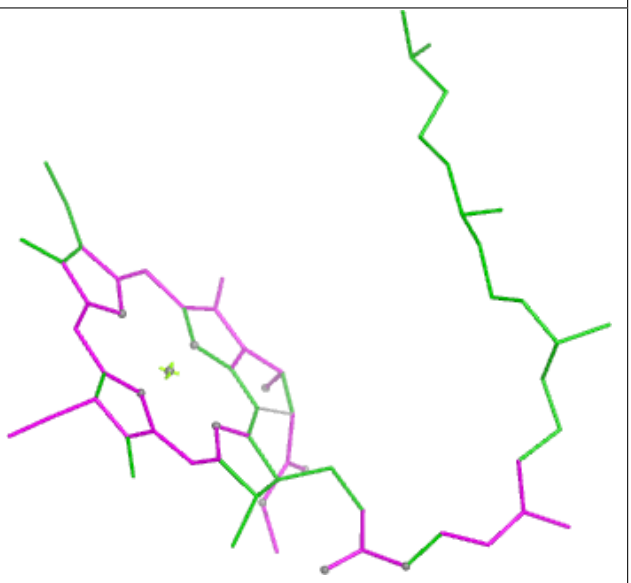


Rings

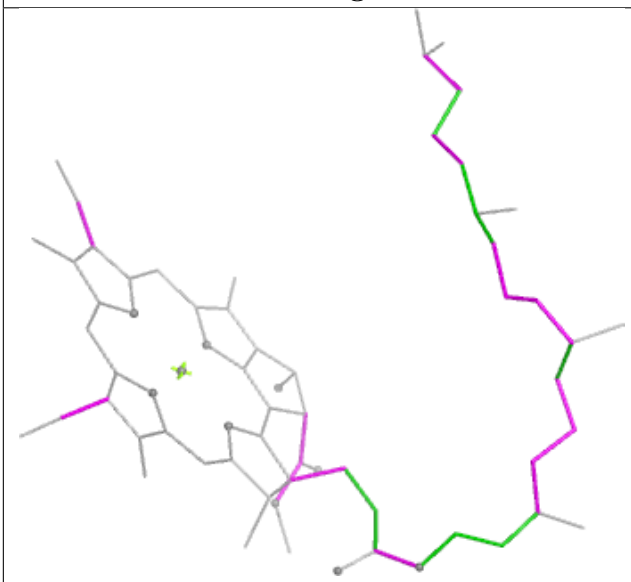
**Ligand CLA 3 311**



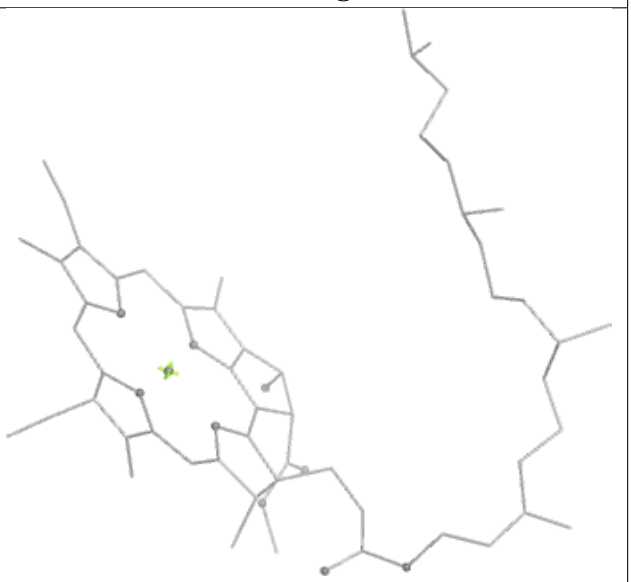
**Bond lengths**



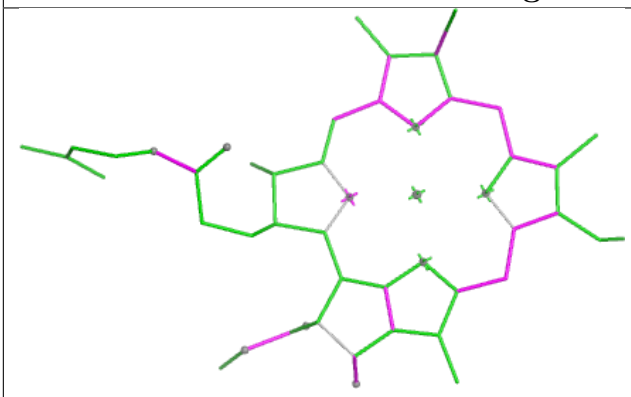
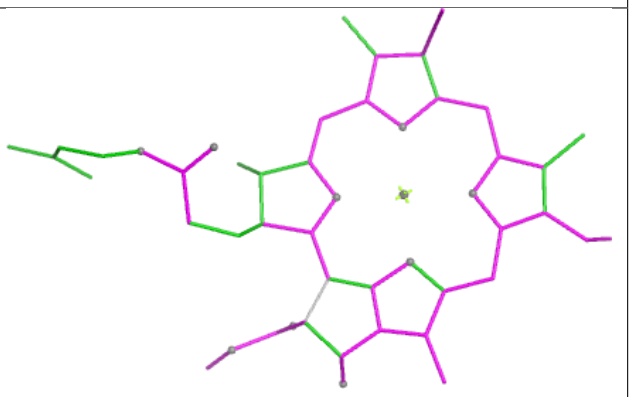
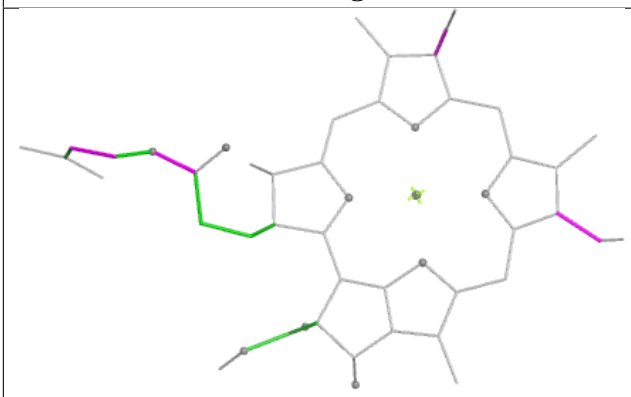
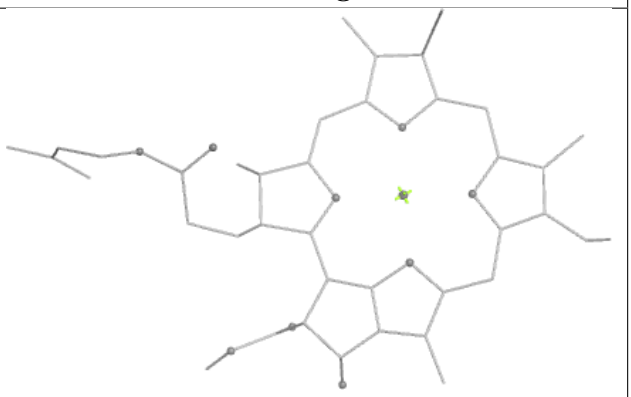
**Bond angles**



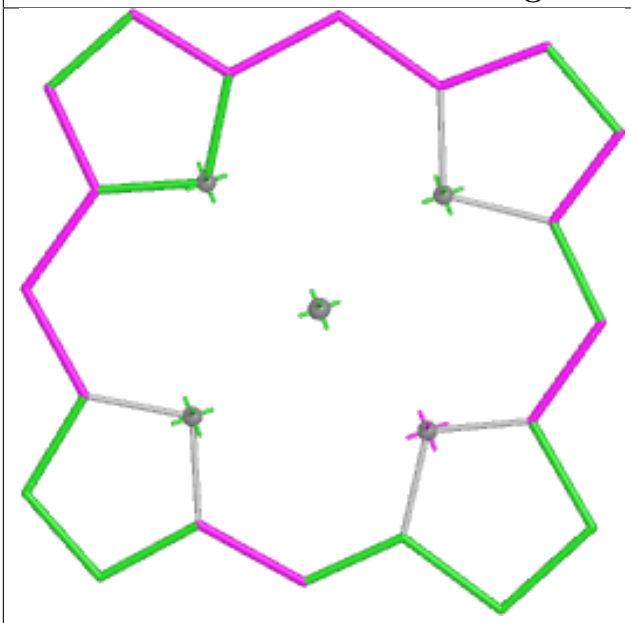
**Torsions**



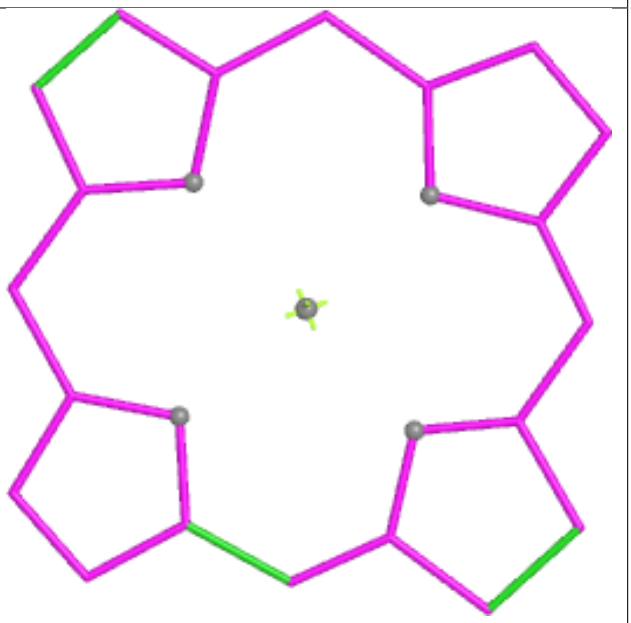
**Rings**

| Ligand CLA K 102 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

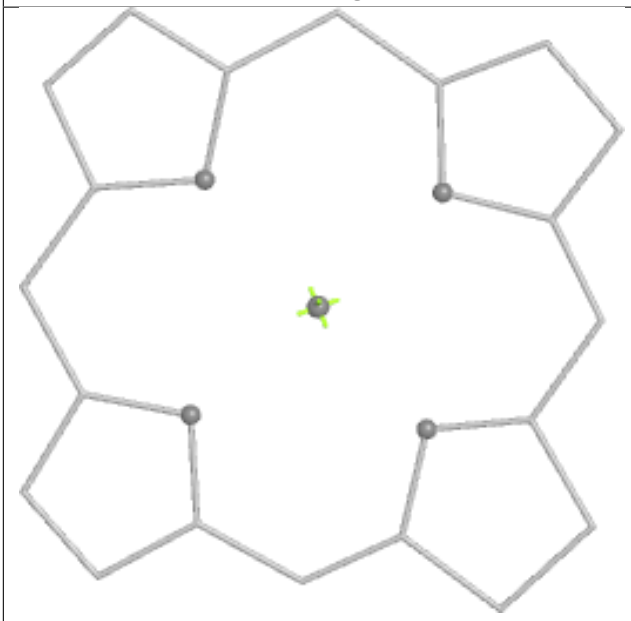
**Ligand CLA B 811**



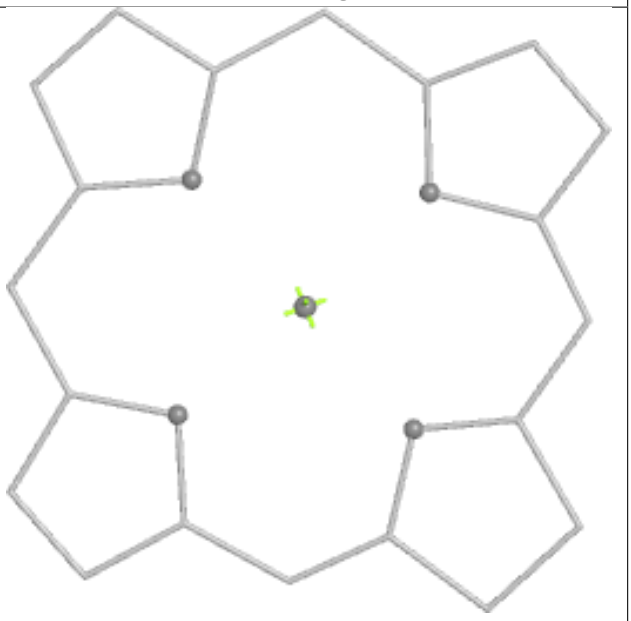
**Bond lengths**



**Bond angles**

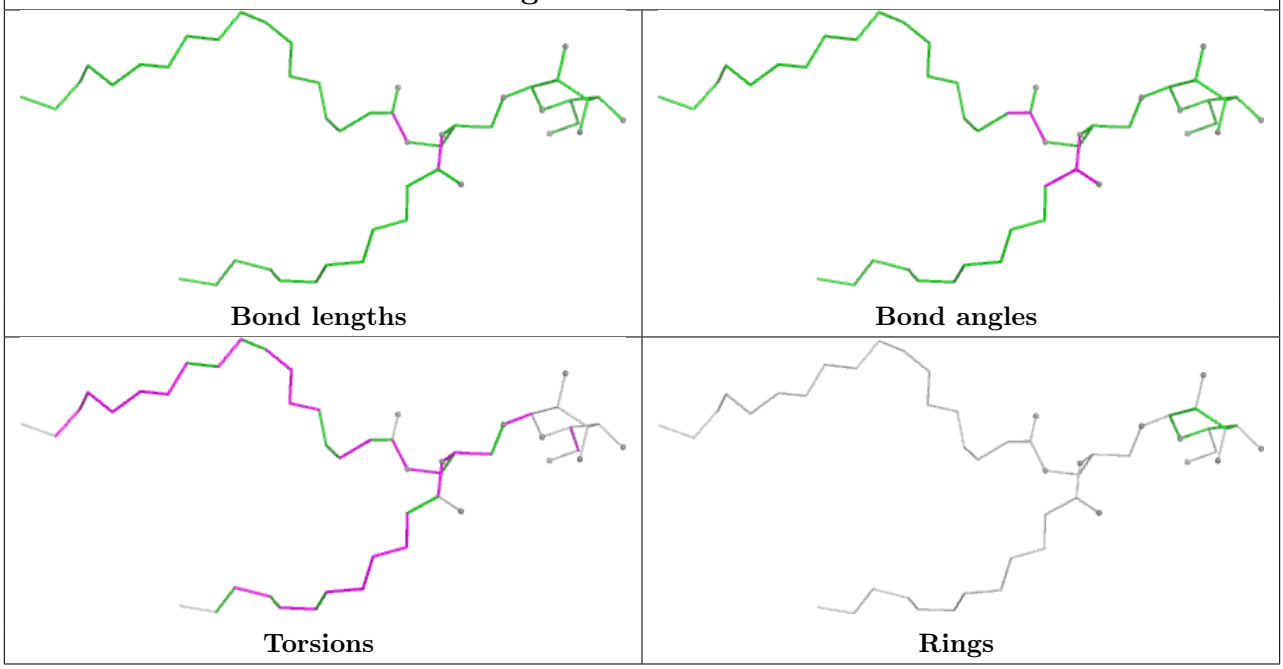


**Torsions**

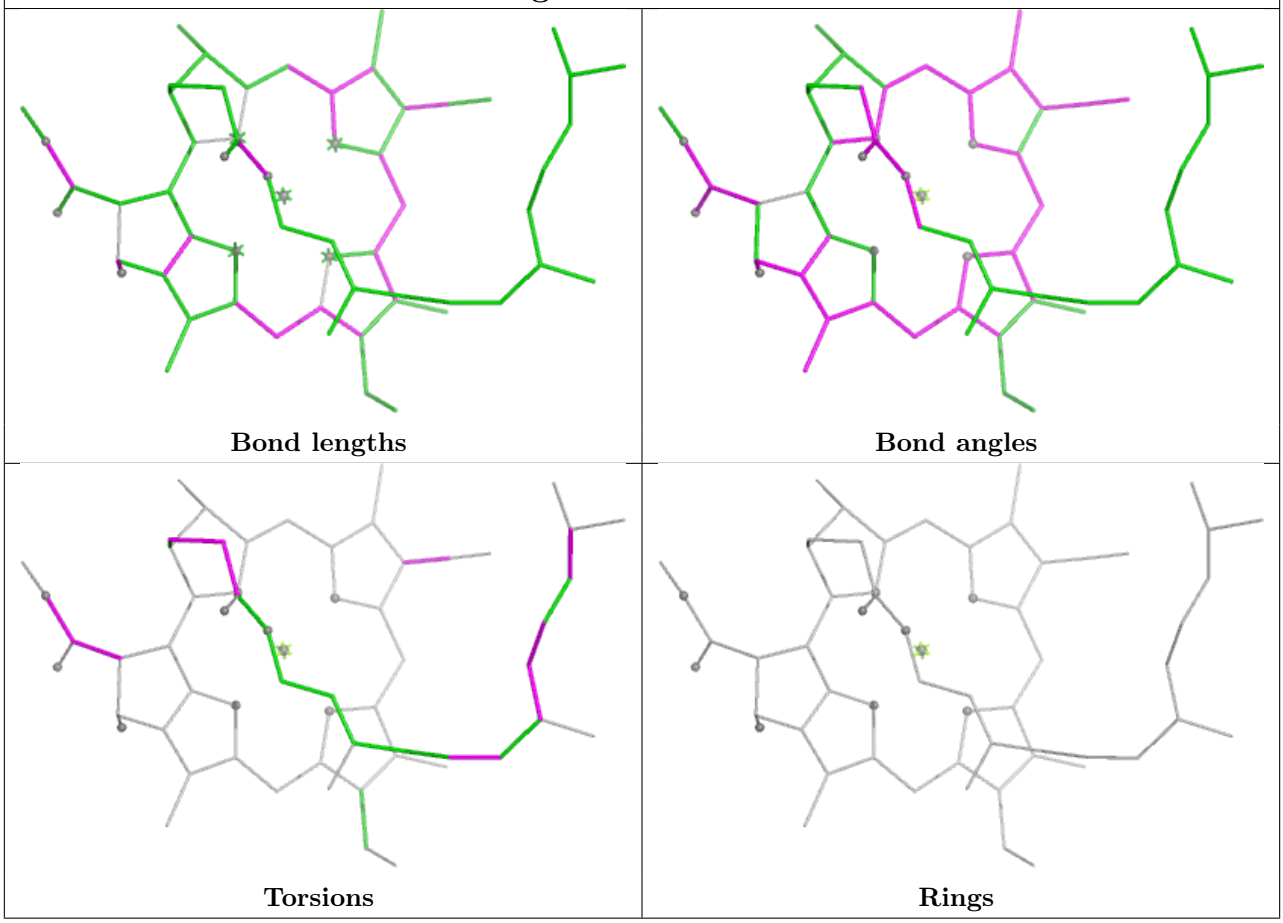


**Rings**

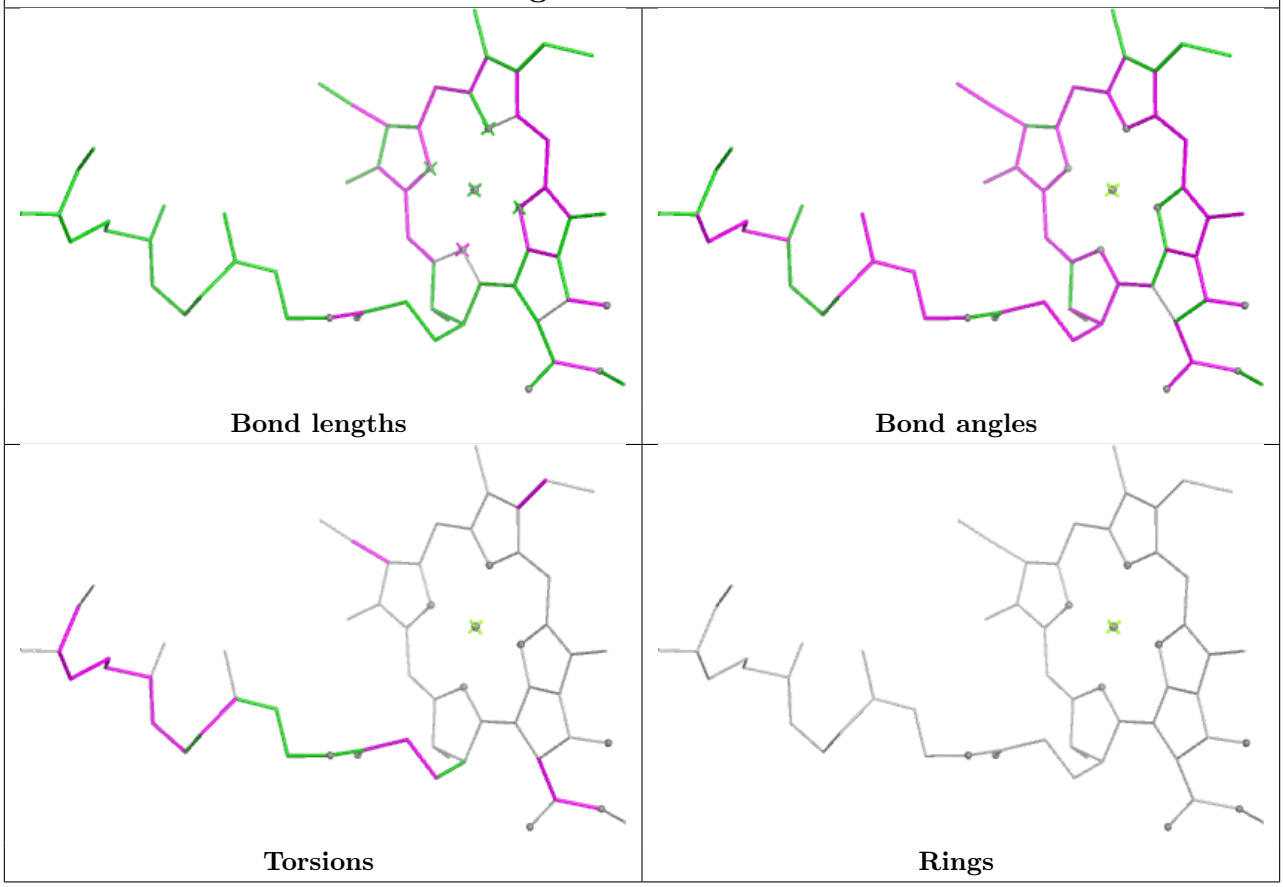
## Ligand LMG B 848



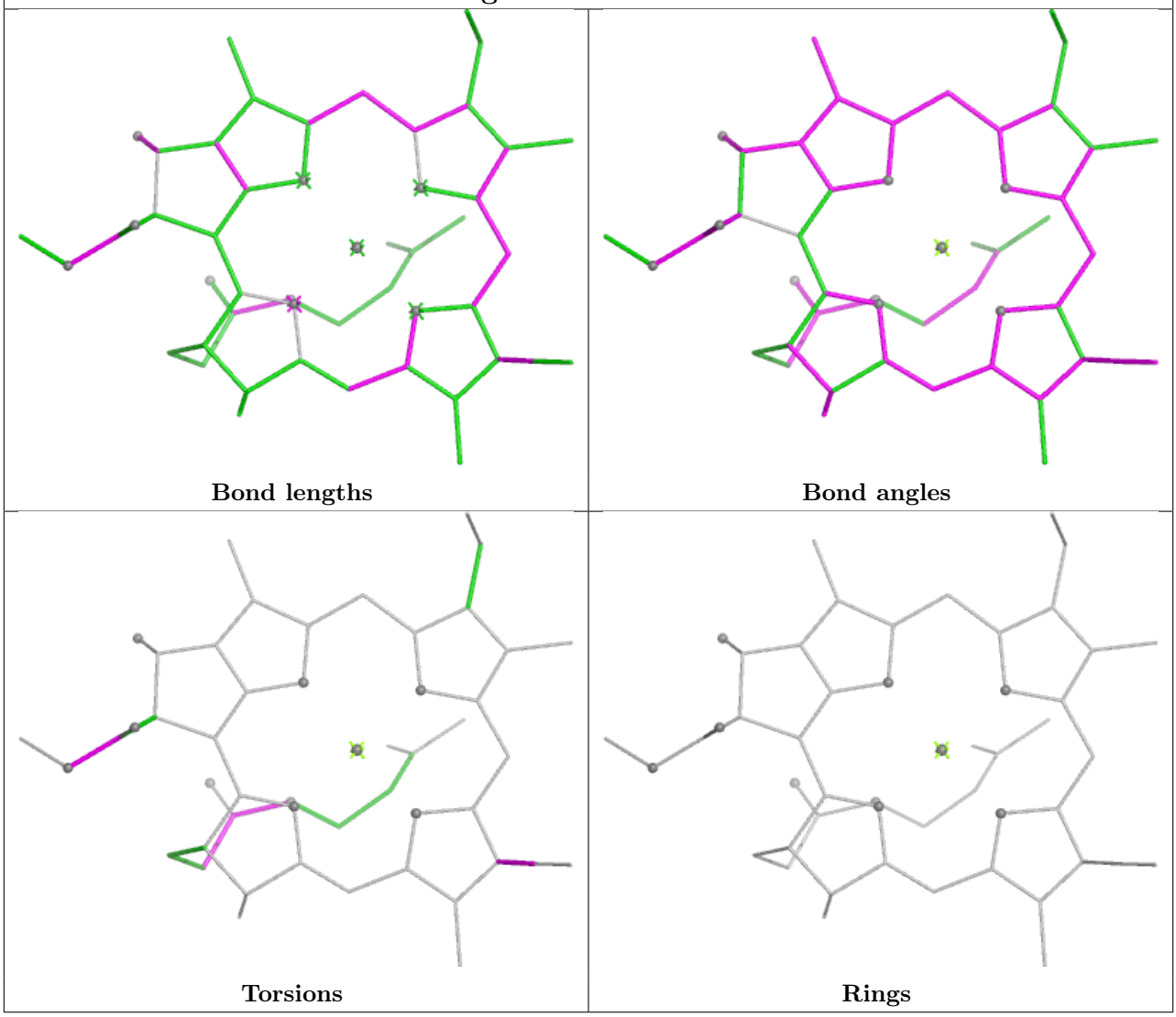

## Ligand CLA I 102



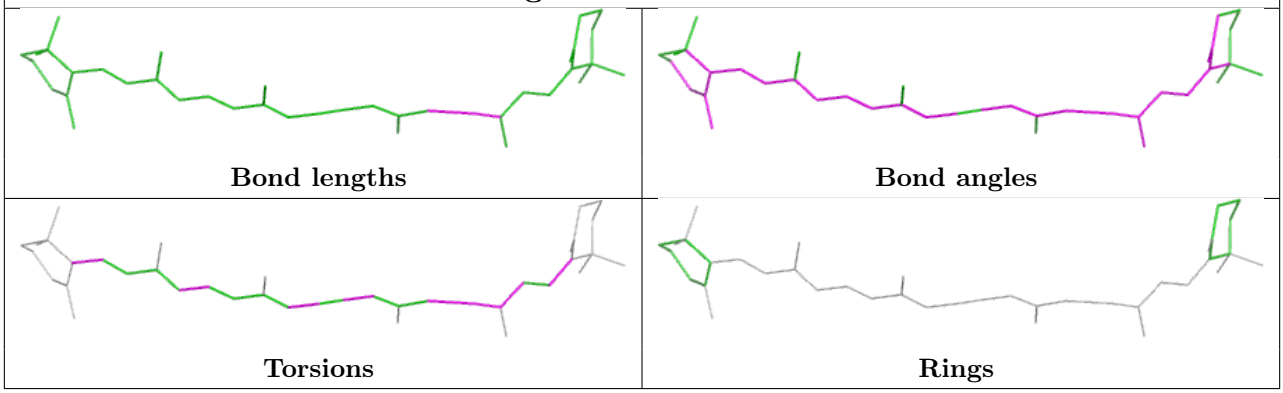
**Ligand CLA 2 312**



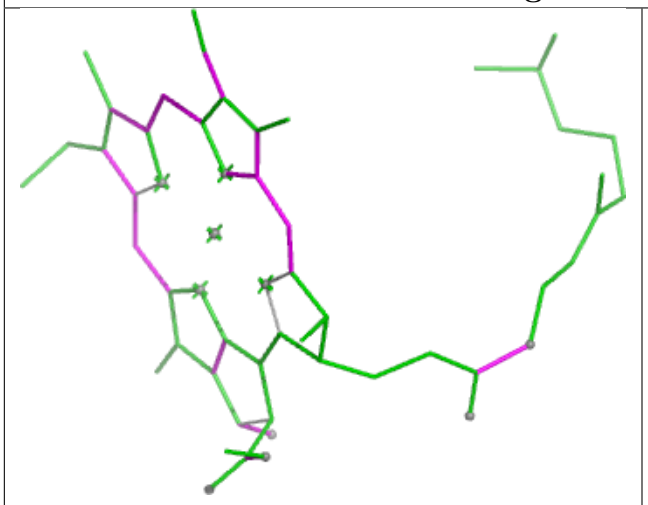
## Ligand CLA B 821



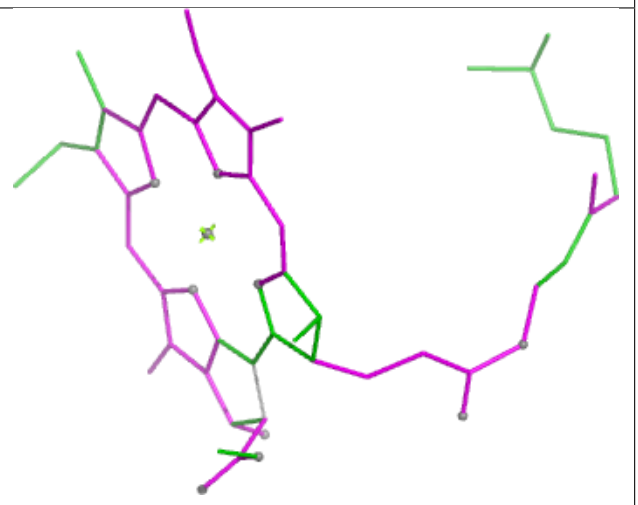

## Ligand BCR F 203



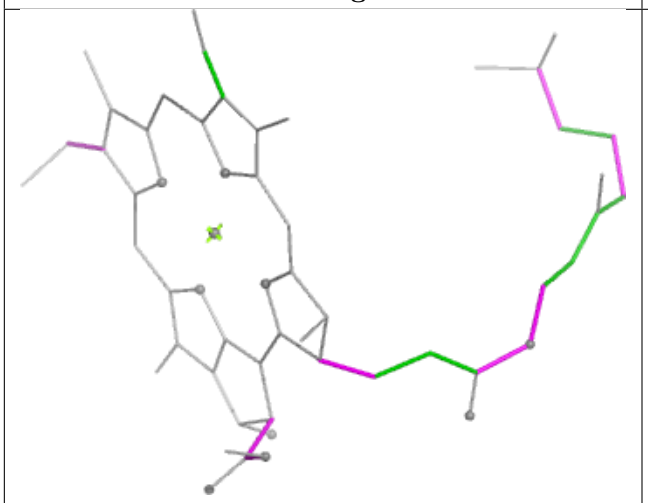
**Ligand CLA A 804**



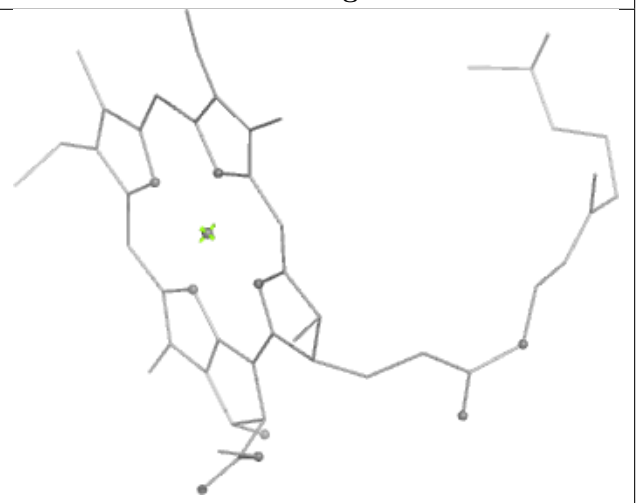
**Bond lengths**



**Bond angles**

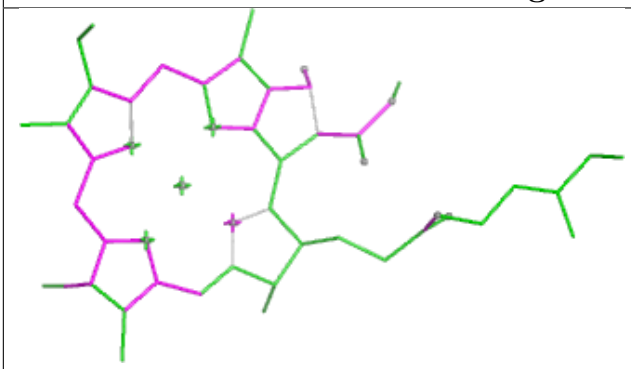


**Torsions**

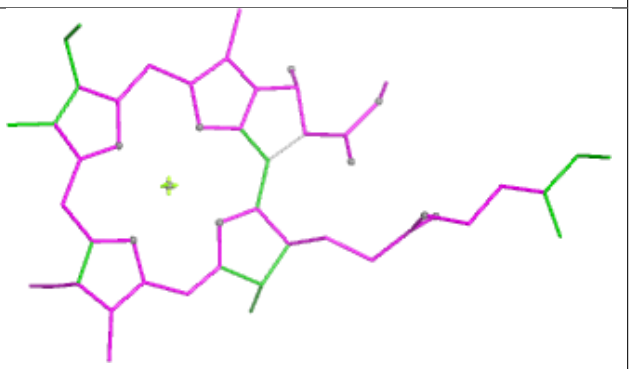


**Rings**

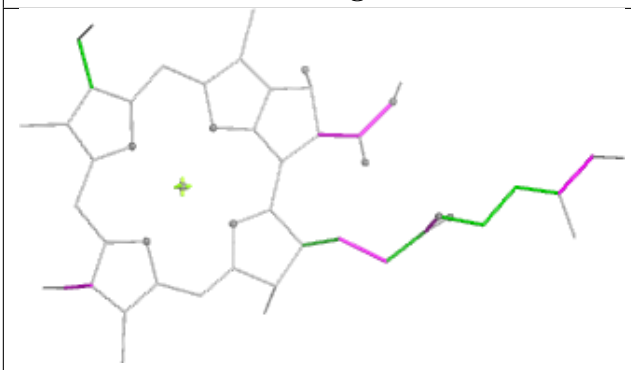
**Ligand CLA 1 211**



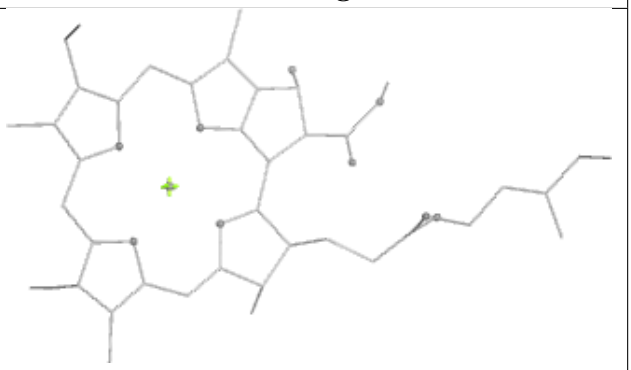
**Bond lengths**



**Bond angles**

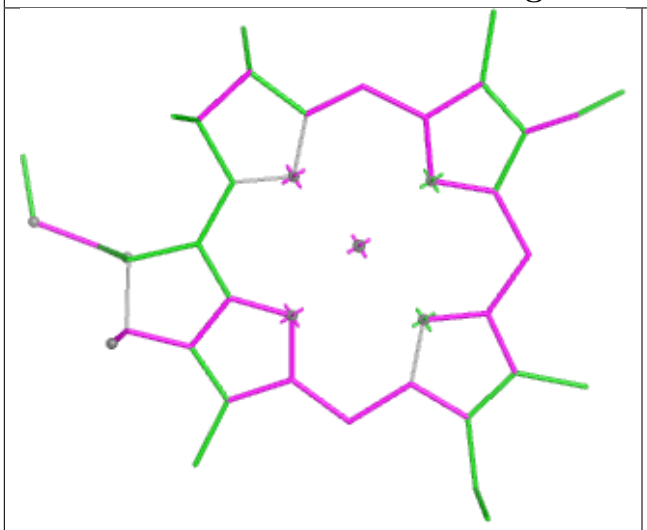


**Torsions**

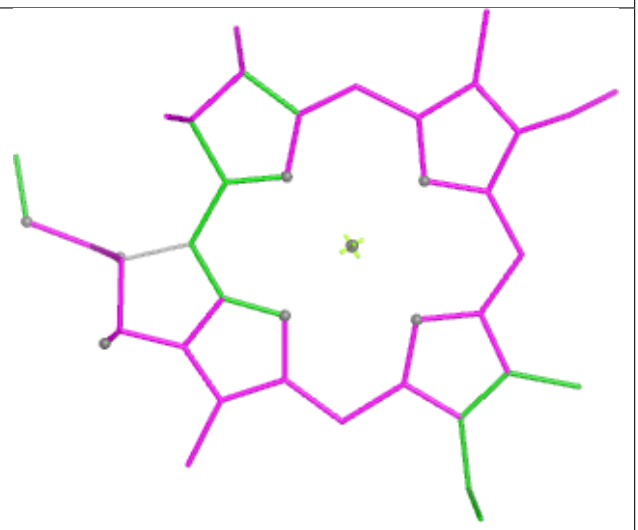


**Rings**

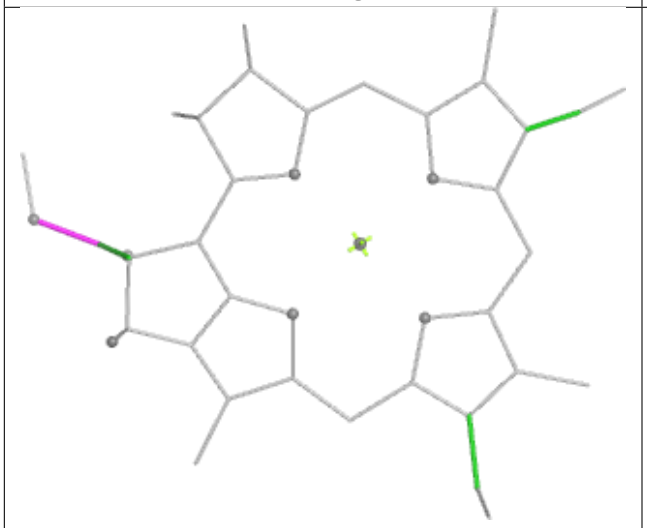
**Ligand CLA B 819**



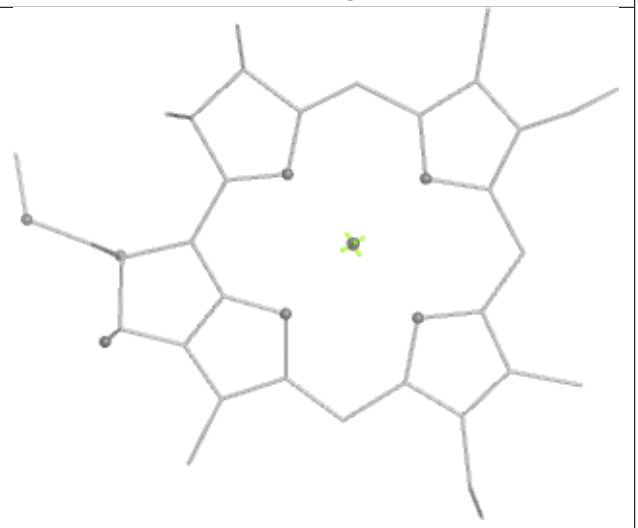
**Bond lengths**



**Bond angles**

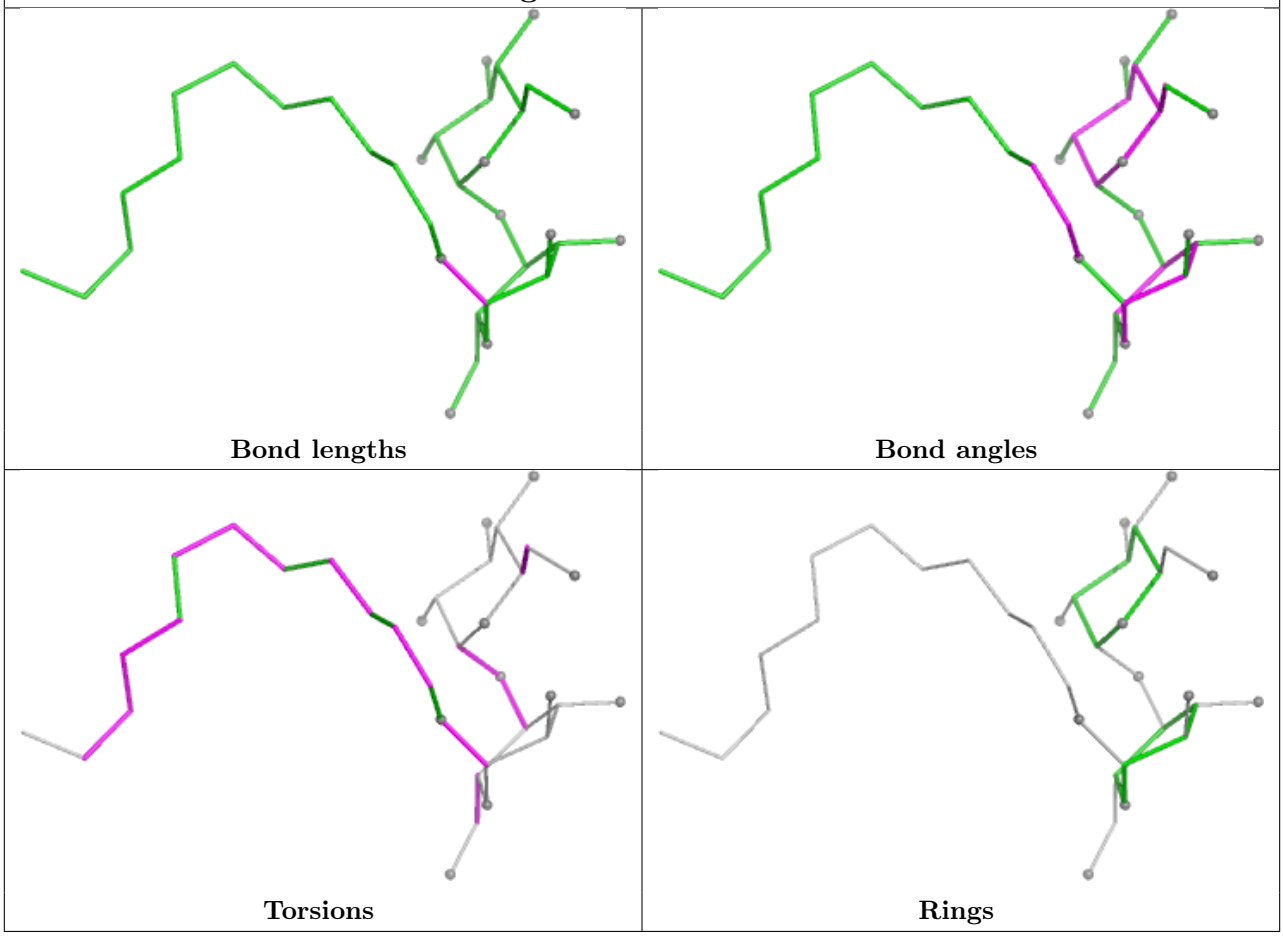


**Torsions**

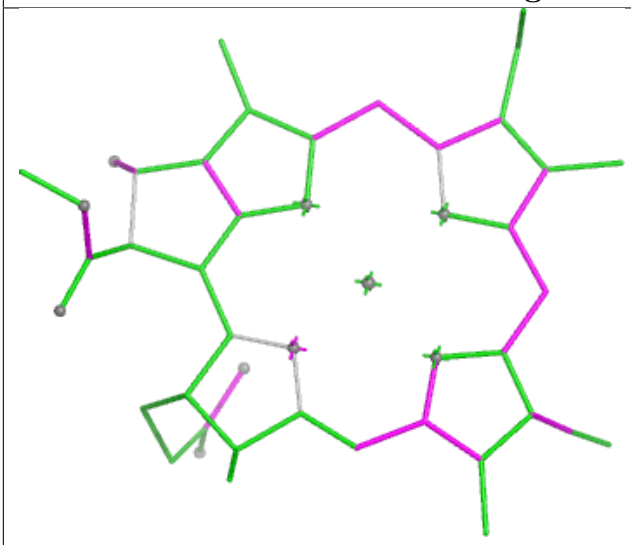


**Rings**

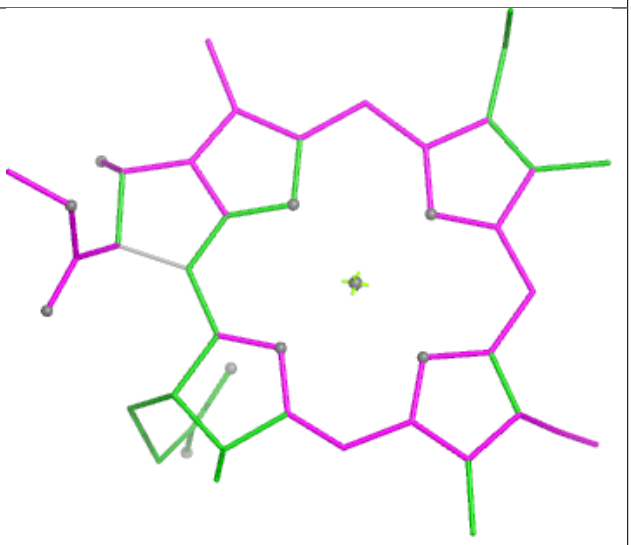
**Ligand LMU H 105**



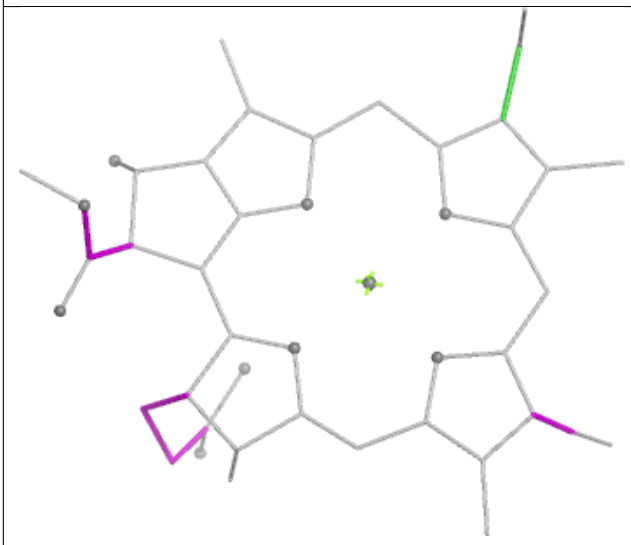
**Ligand CLA B 834**



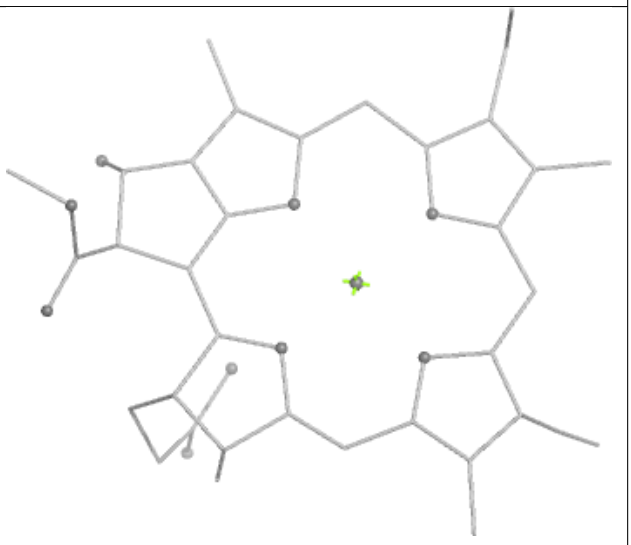
**Bond lengths**



**Bond angles**

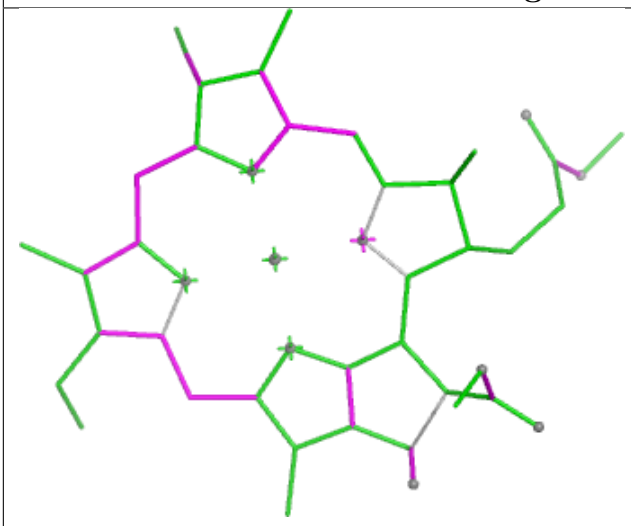


**Torsions**

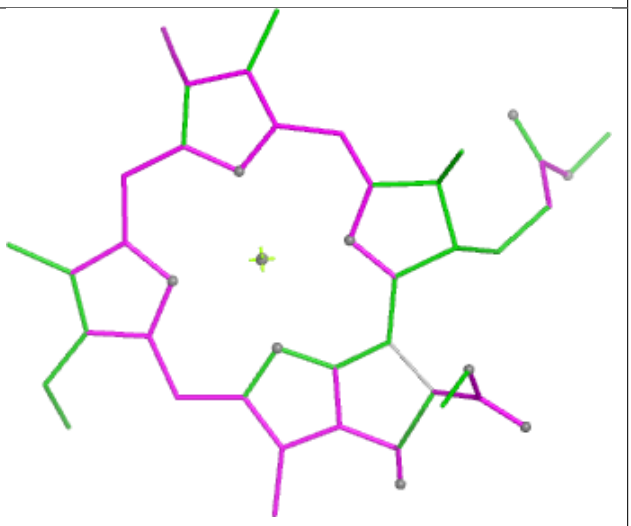


**Rings**

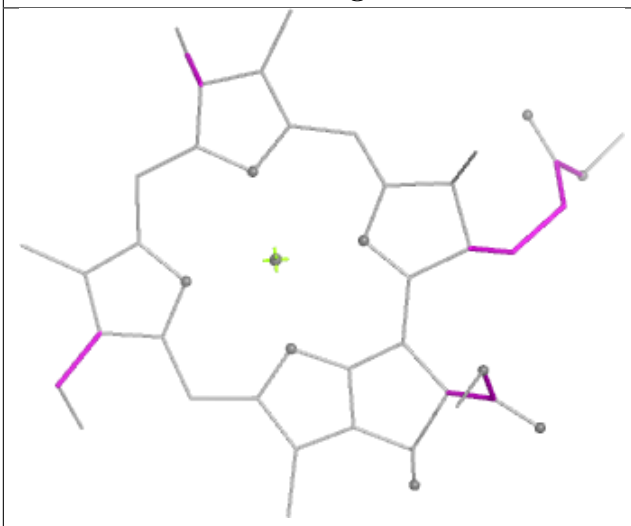
**Ligand CLA B 822**



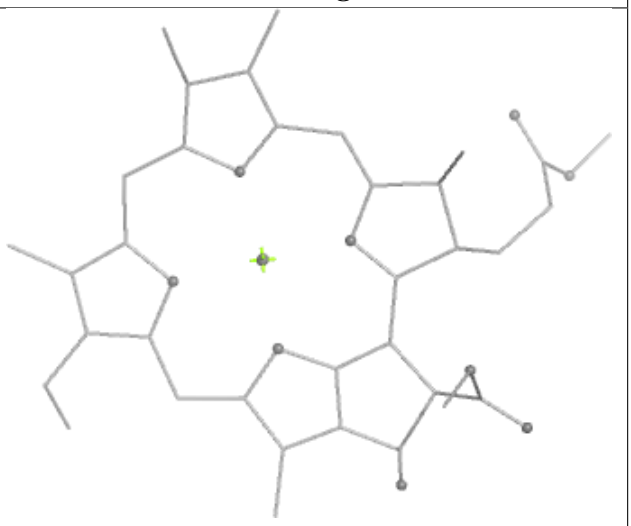
**Bond lengths**



**Bond angles**

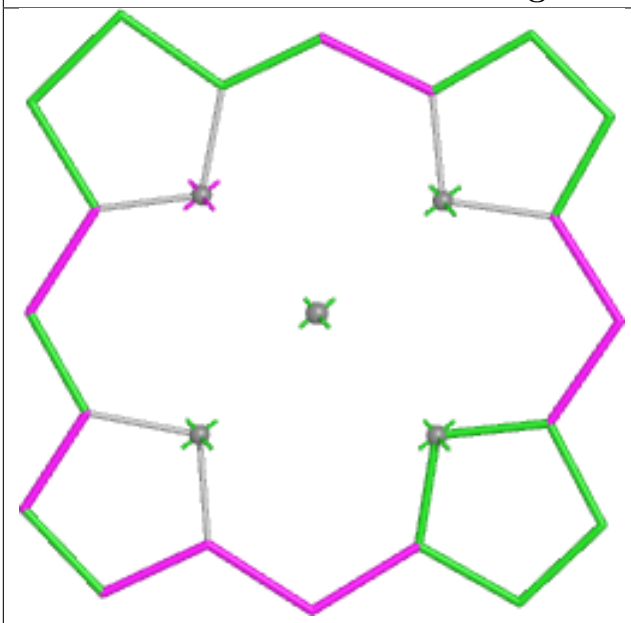


**Torsions**

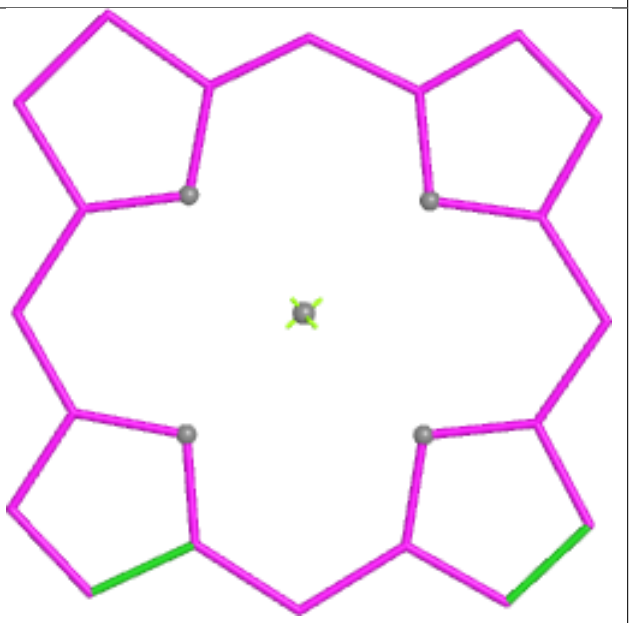


**Rings**

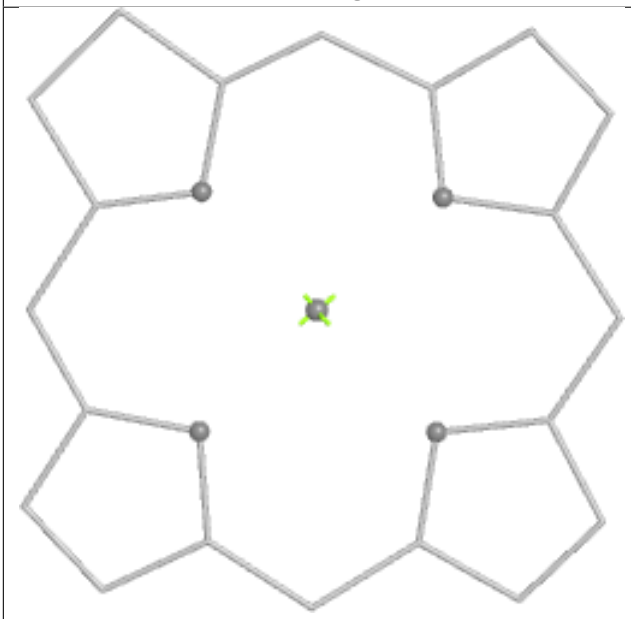
**Ligand CLA 2 306**



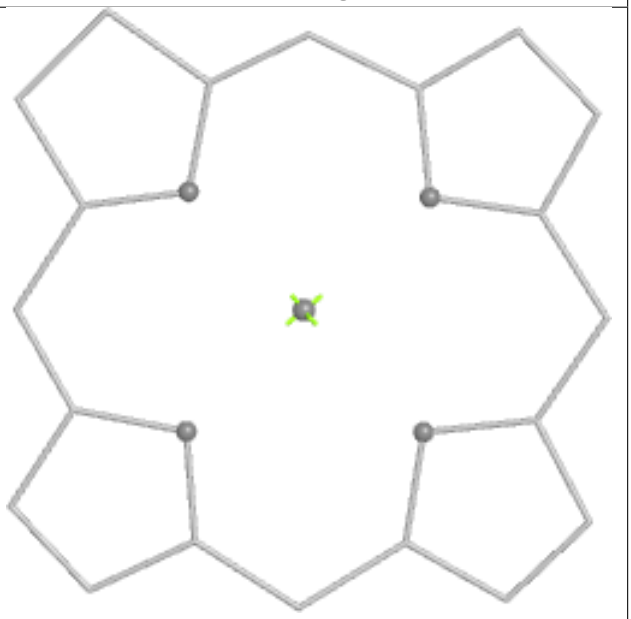
**Bond lengths**



**Bond angles**

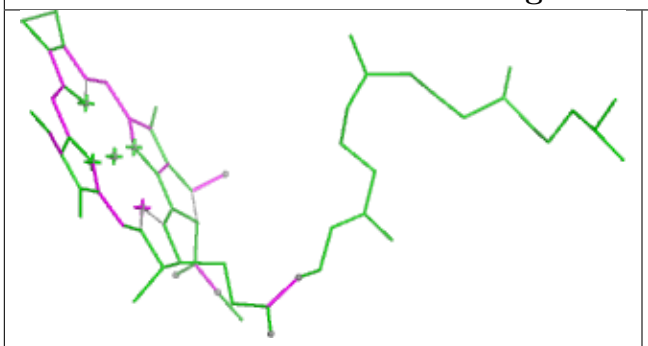


**Torsions**

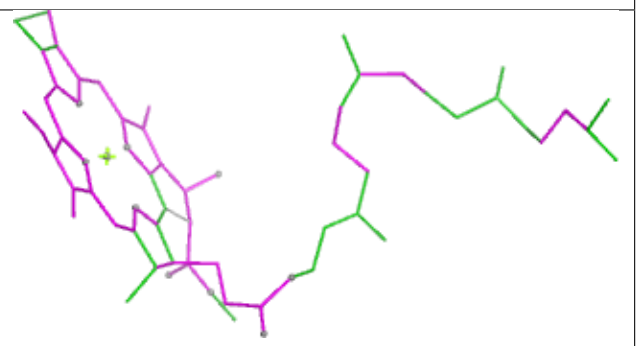


**Rings**

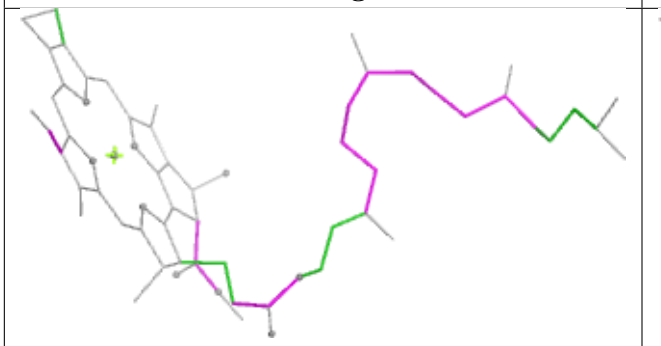
## Ligand CLA B 850



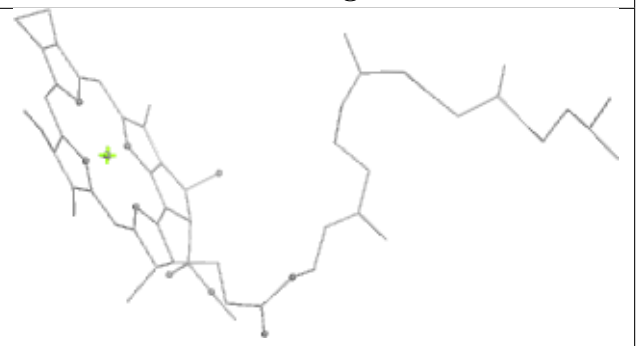
Bond lengths



Bond angles

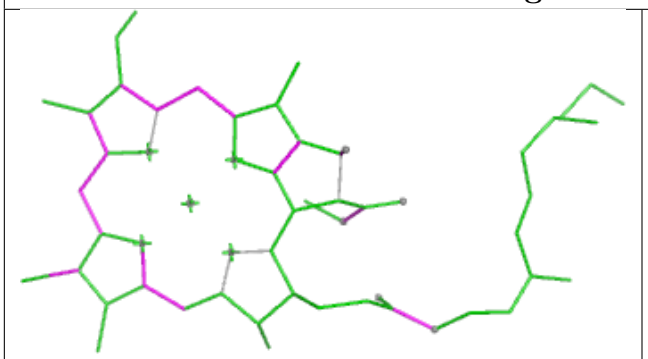


Torsions



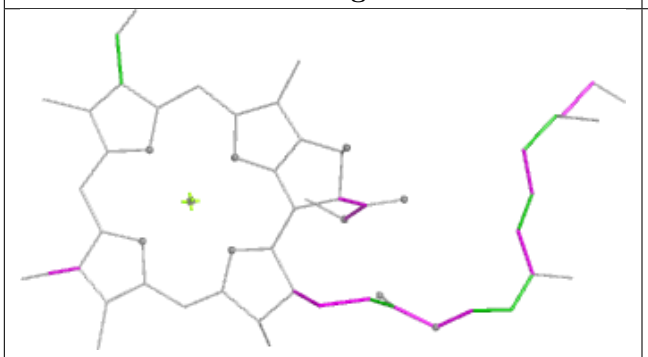
Rings

## Ligand CLA R 107

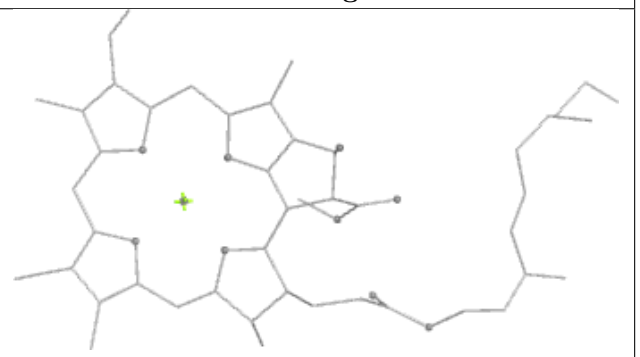


Bond lengths

Bond angles

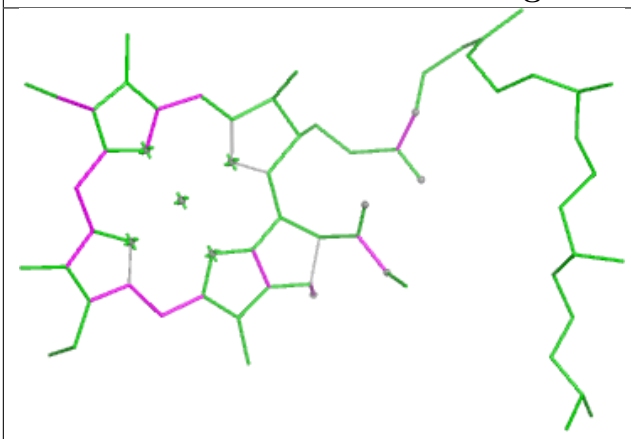


Torsions

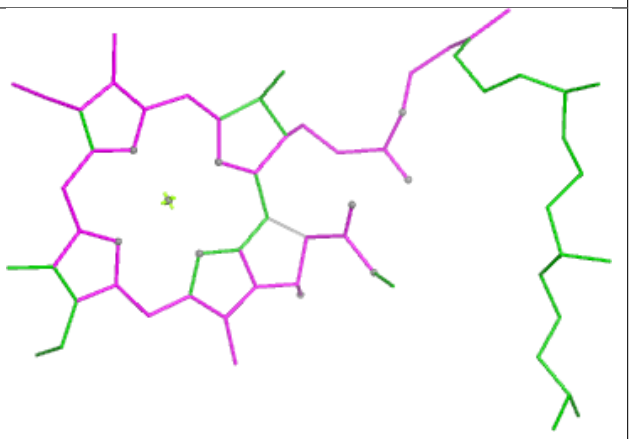


Rings

## Ligand CLA R 108



Bond lengths

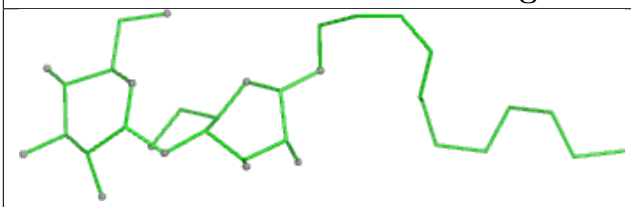


Bond angles

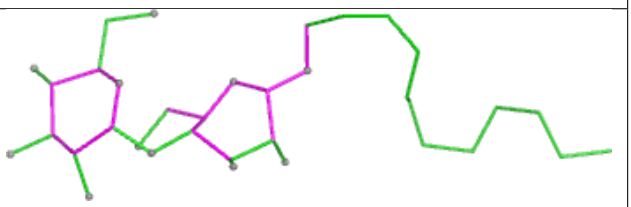
Torsions

Rings

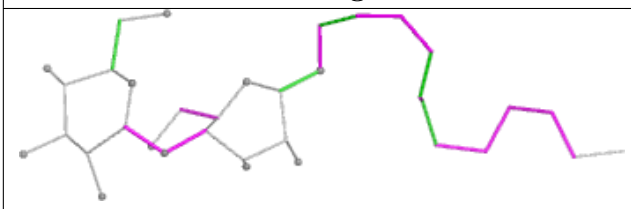
## Ligand LMU R 102



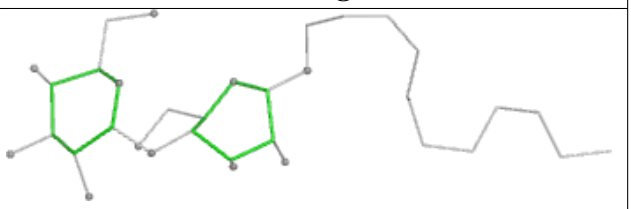
Bond lengths



Bond angles

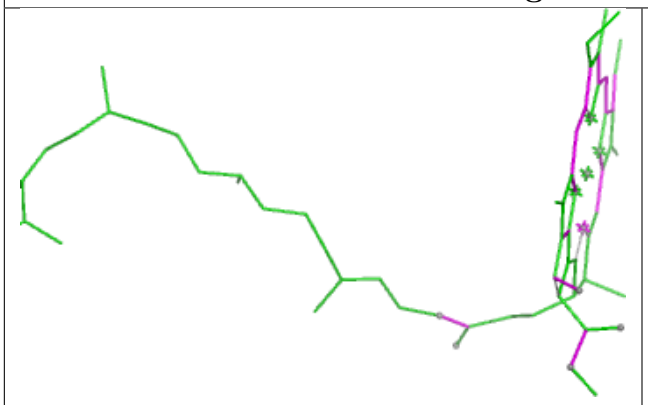


Torsions

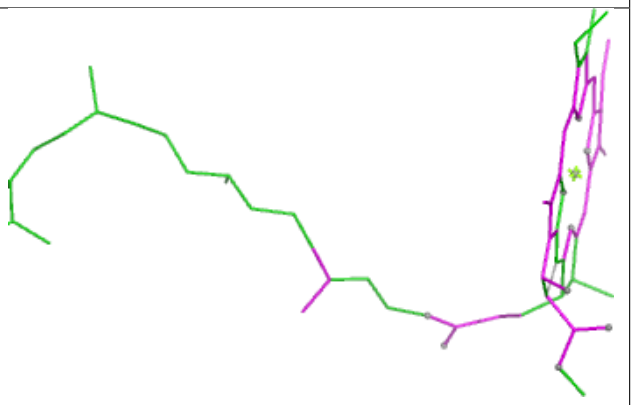


Rings

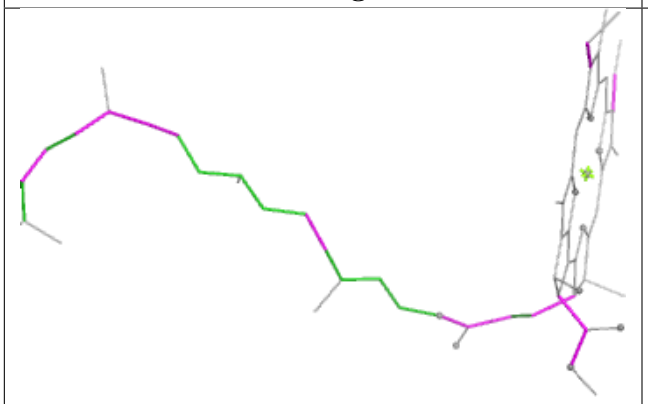
**Ligand CLA B 841**



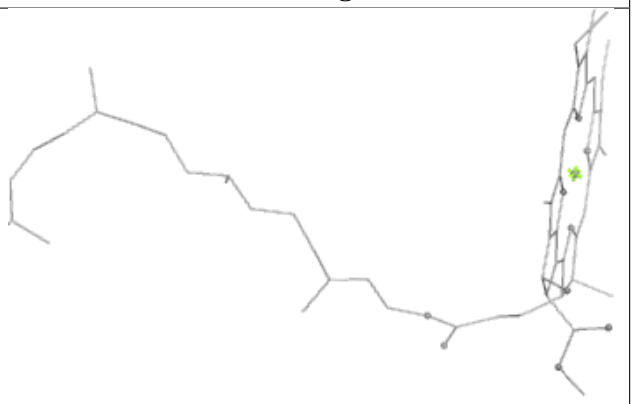
**Bond lengths**



**Bond angles**

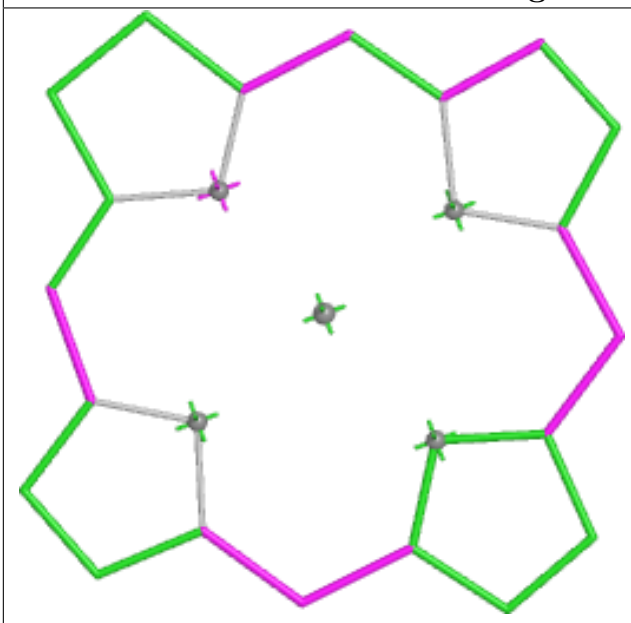


**Torsions**



**Rings**

**Ligand CLA 1 209**



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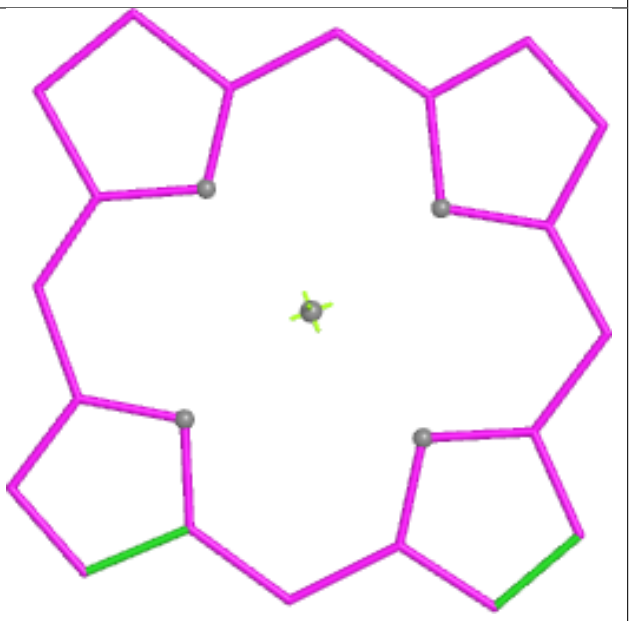
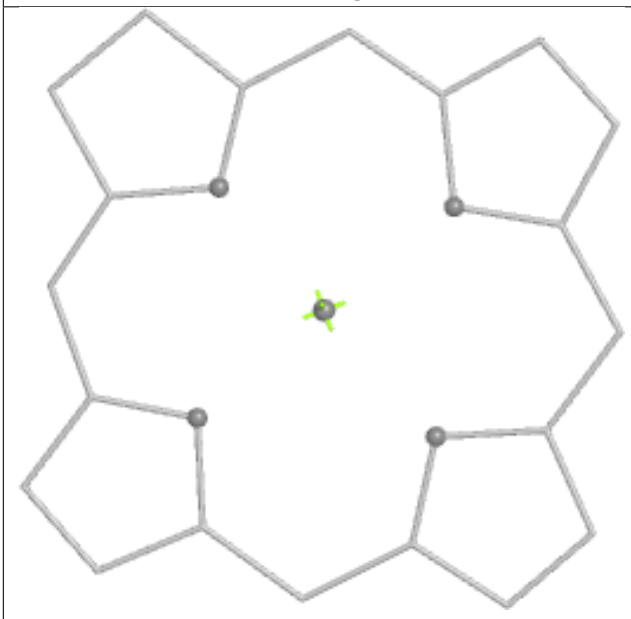
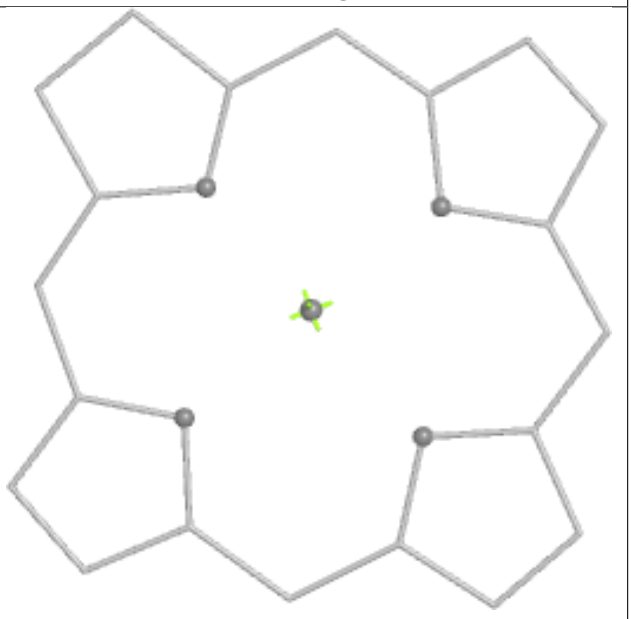


**Bond angles**

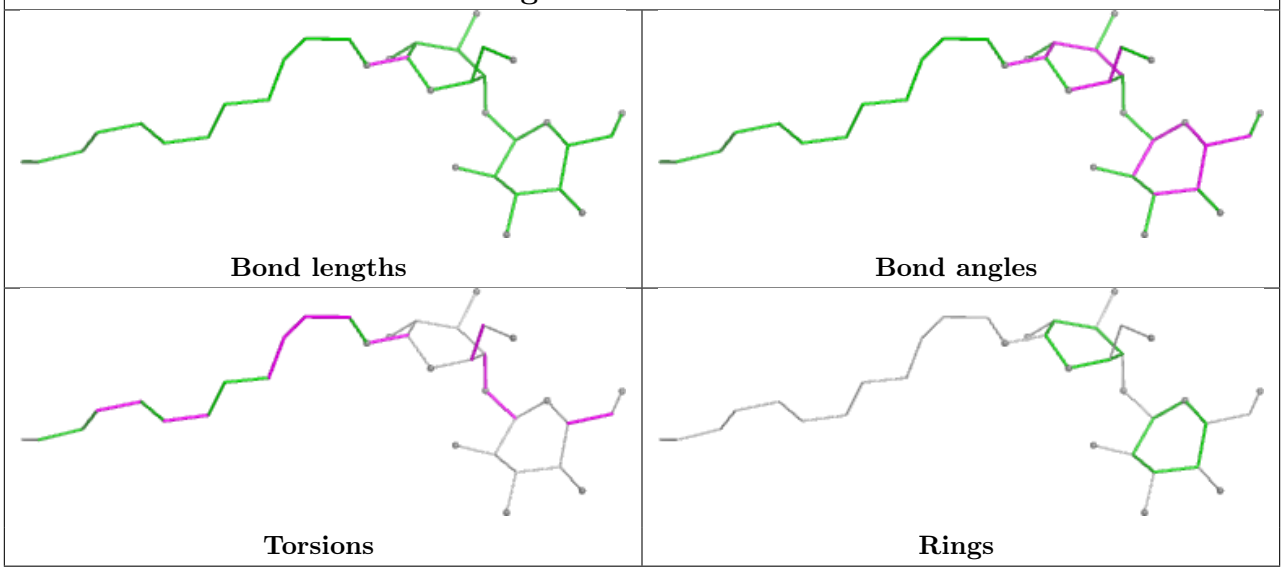


**Torsions**

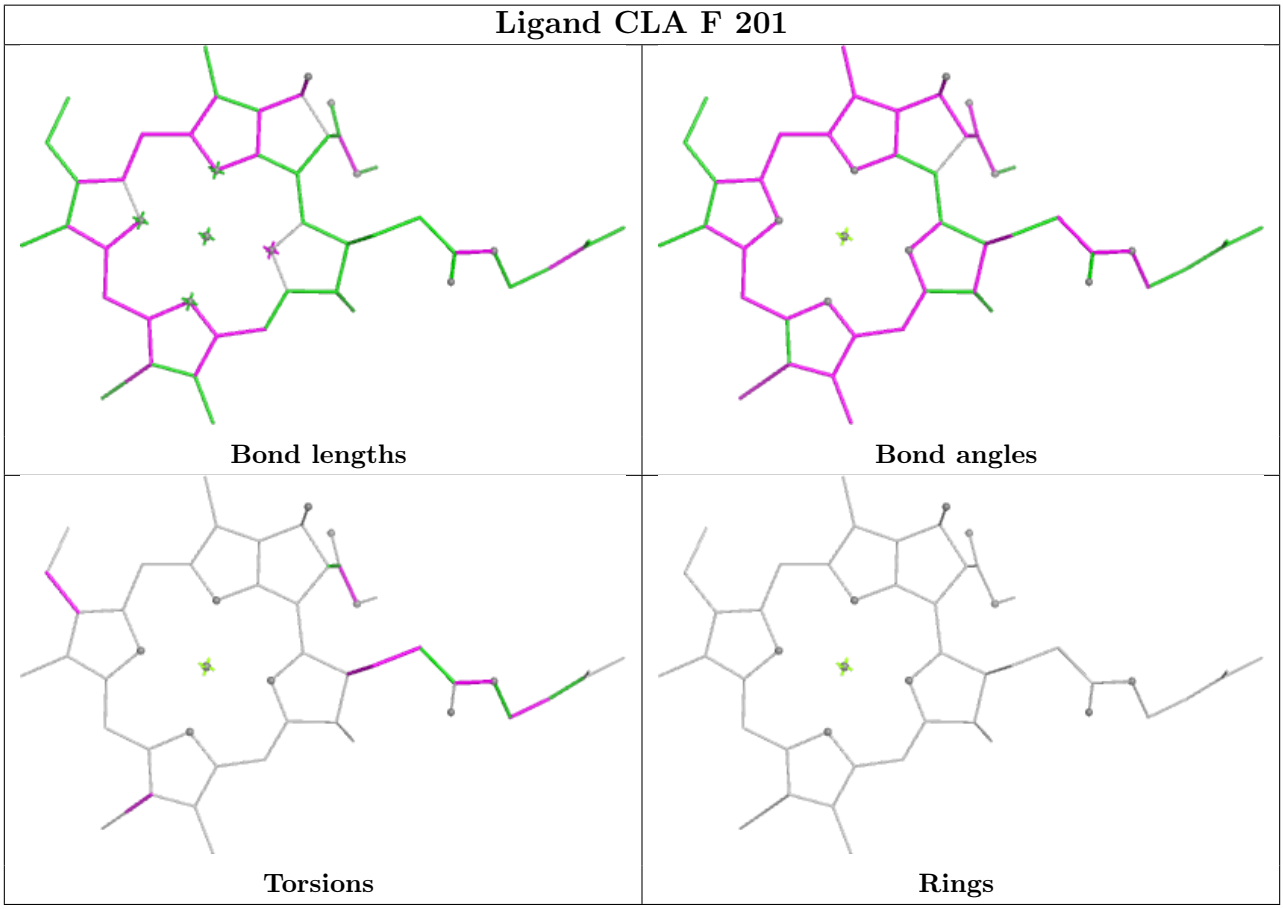


**Rings**

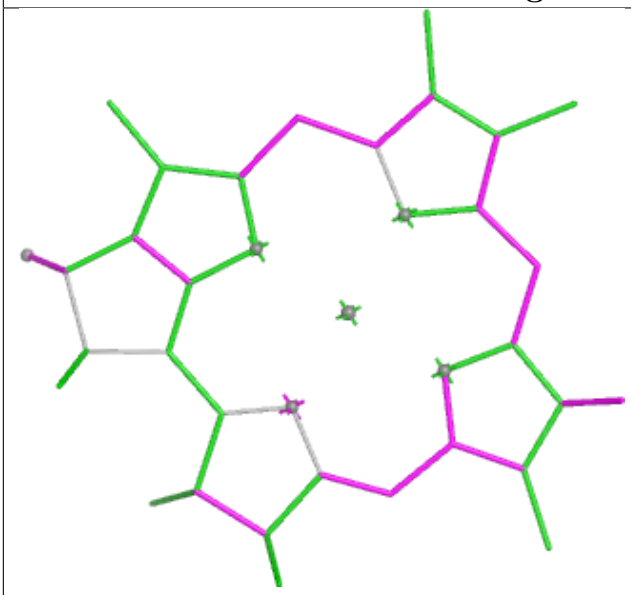
## Ligand LMU R 105



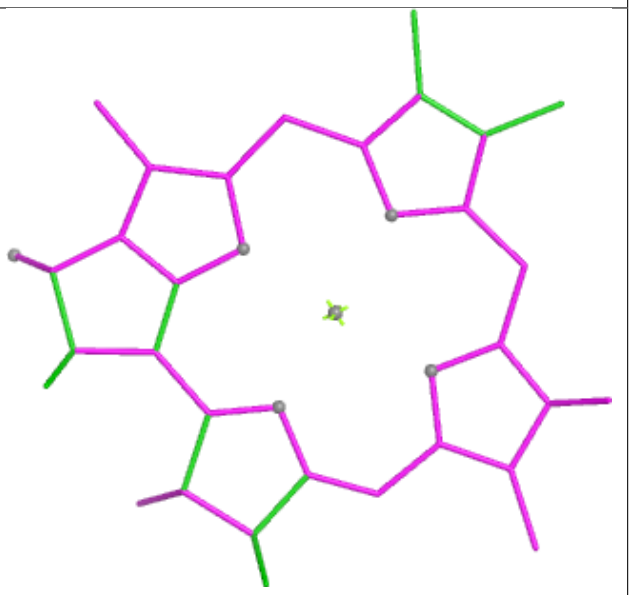

## Ligand CLA F 201



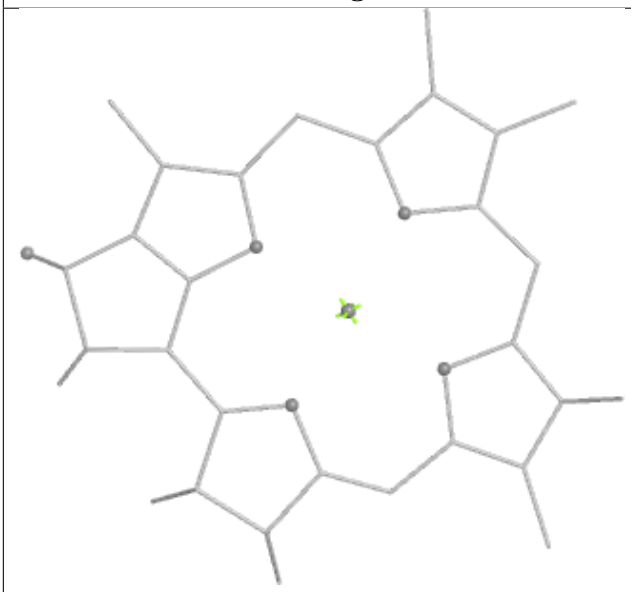
**Ligand CLA F 205**



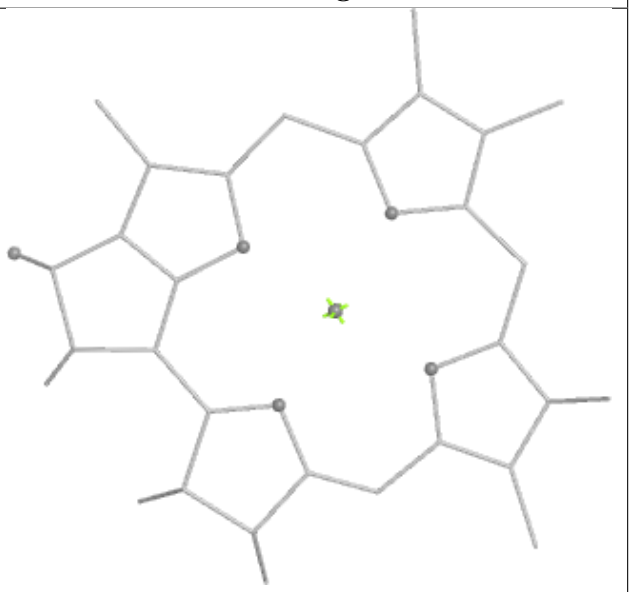
**Bond lengths**



**Bond angles**

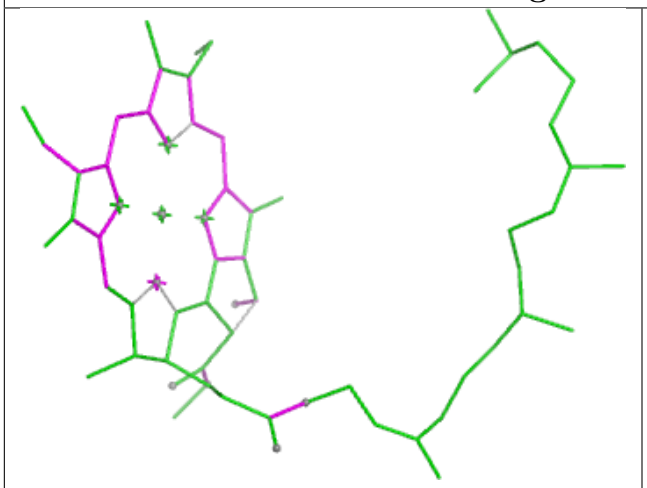


**Torsions**

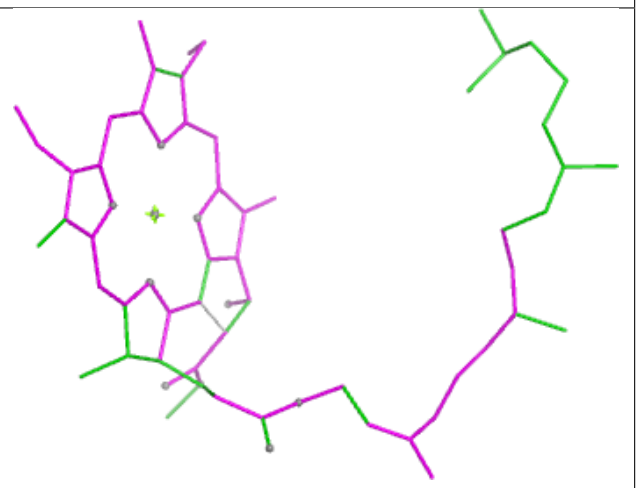


**Rings**

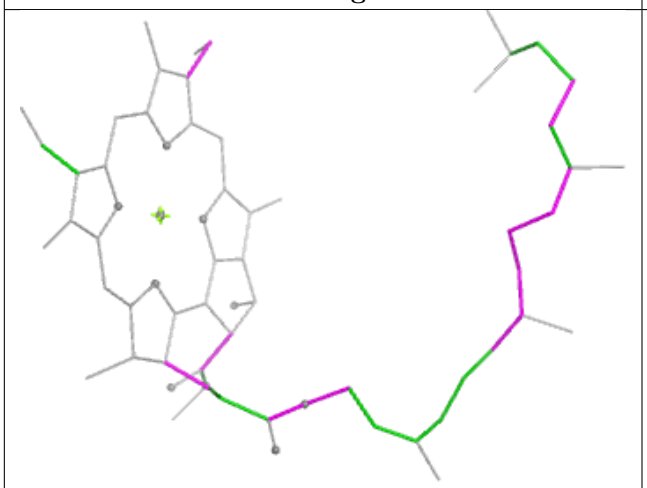
**Ligand CLA 3 310**



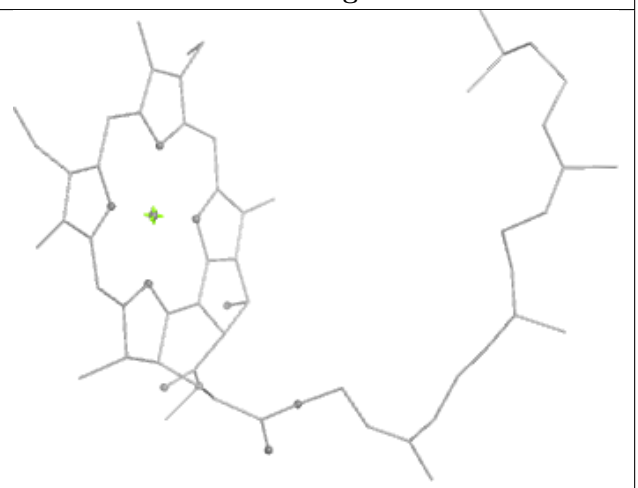
**Bond lengths**



**Bond angles**

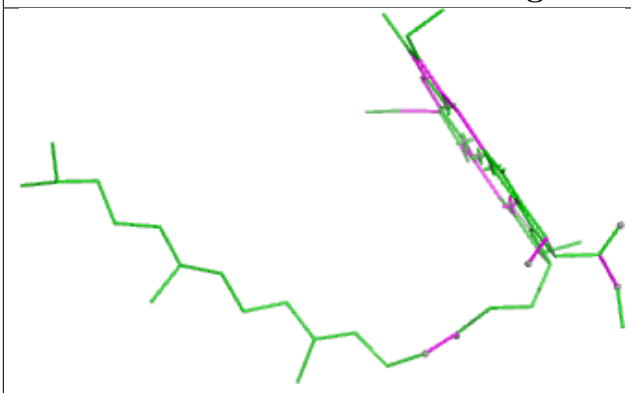


**Torsions**



**Rings**

**Ligand CLA L 201**



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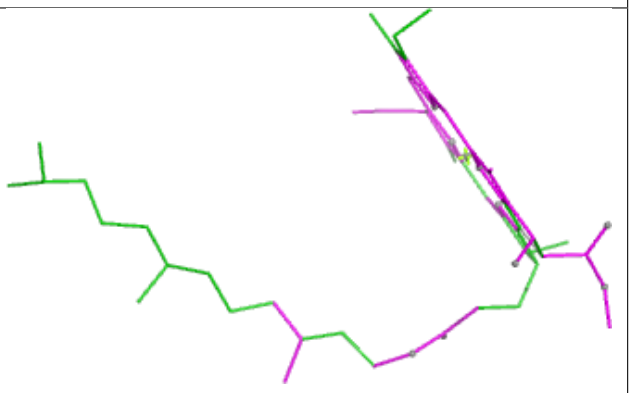
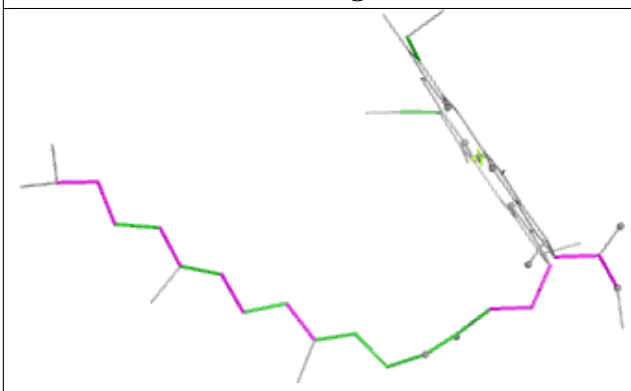


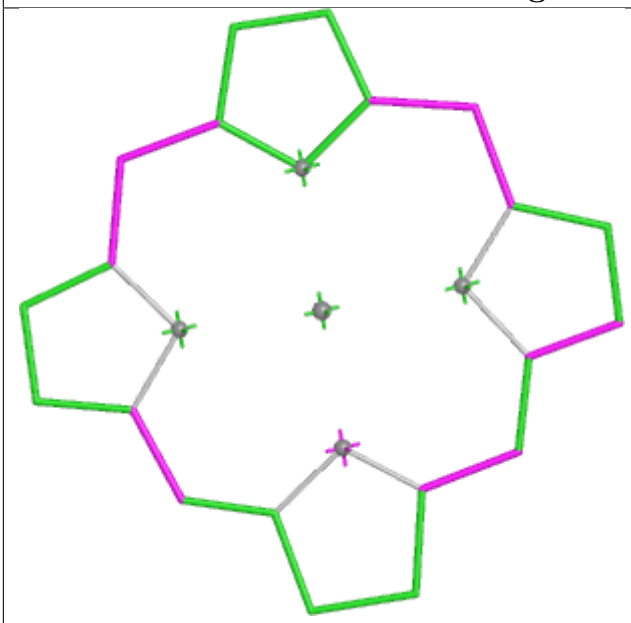
**Bond angles**



**Torsions**

**Rings**

**Ligand CLA 4 309**



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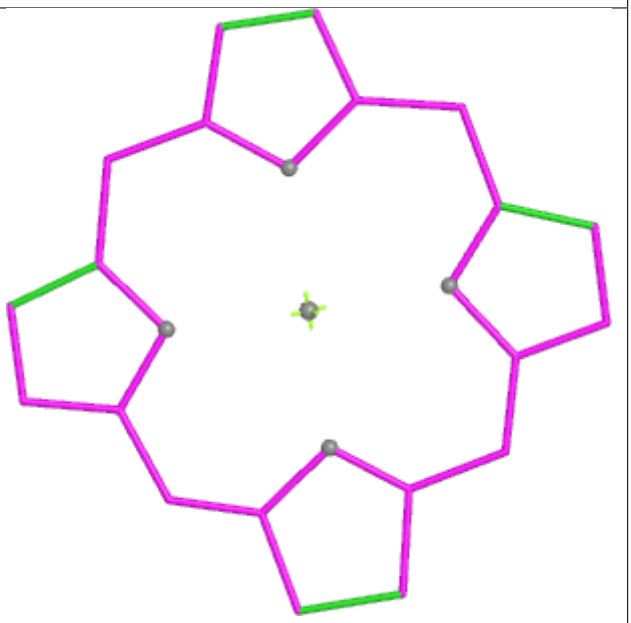
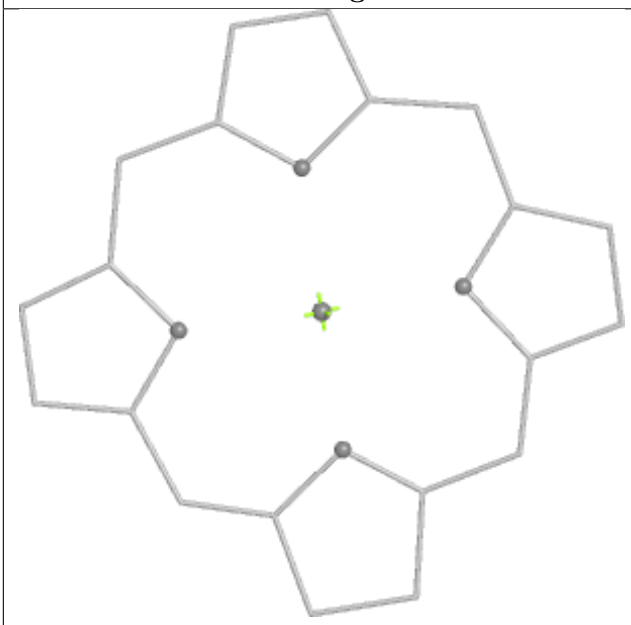
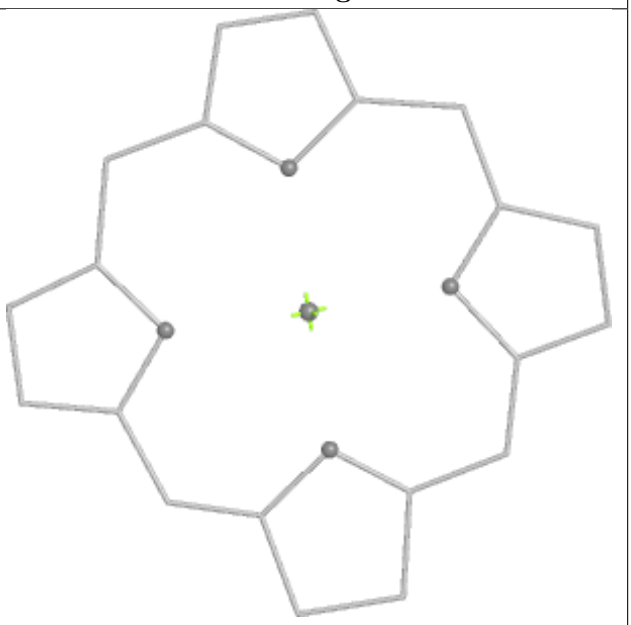


**Bond angles**

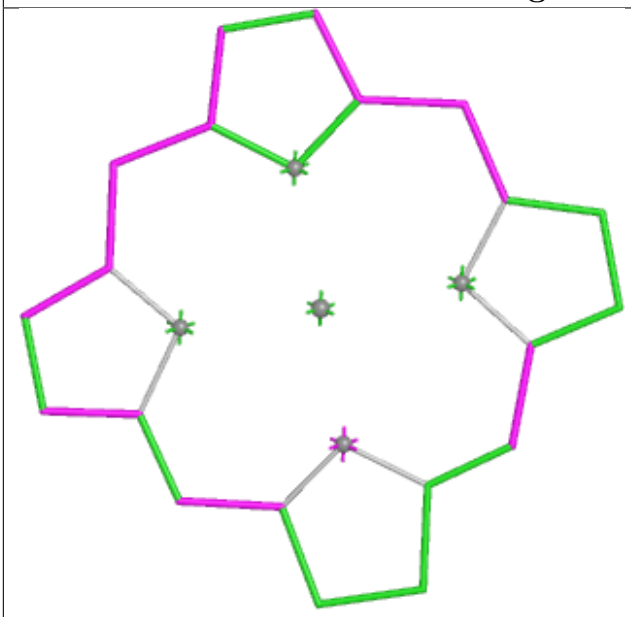


**Torsions**

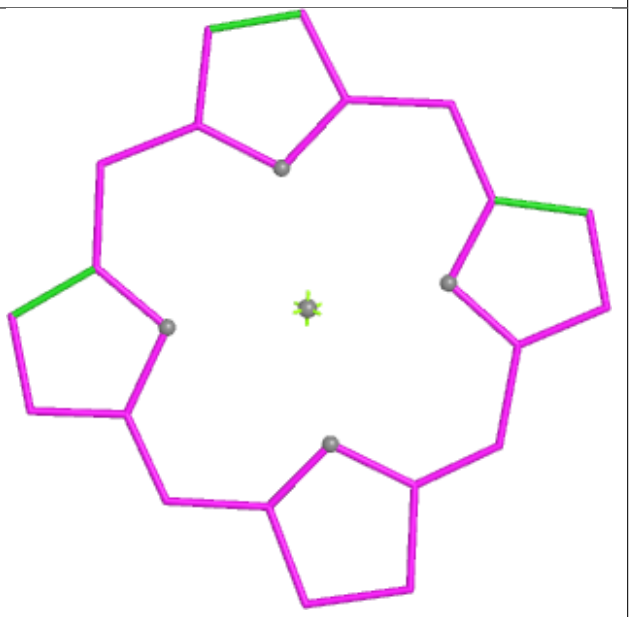


**Rings**

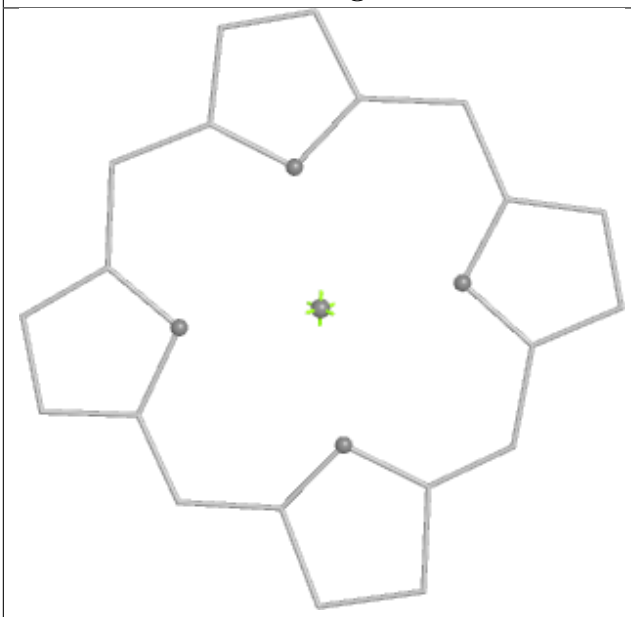
**Ligand CLA 3 316**



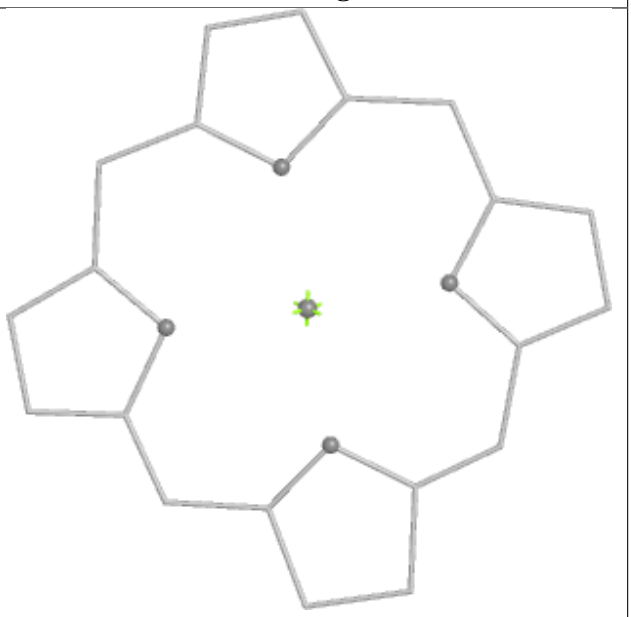
**Bond lengths**



**Bond angles**

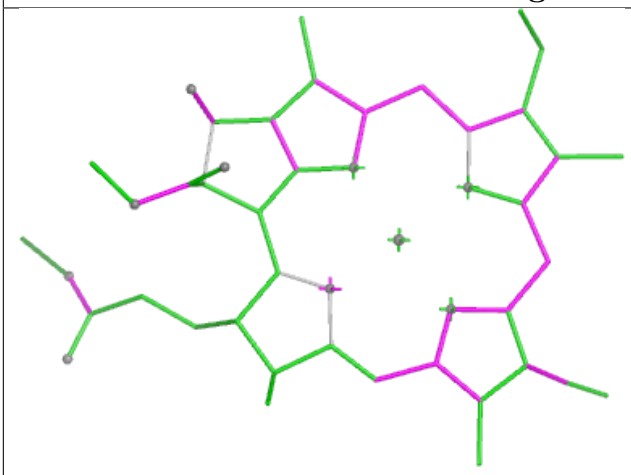


**Torsions**

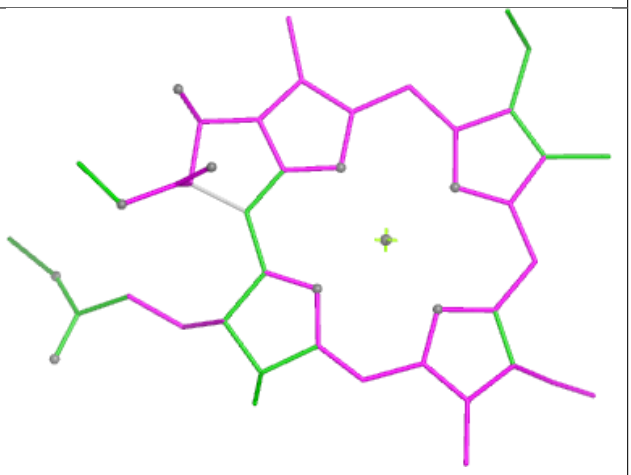


**Rings**

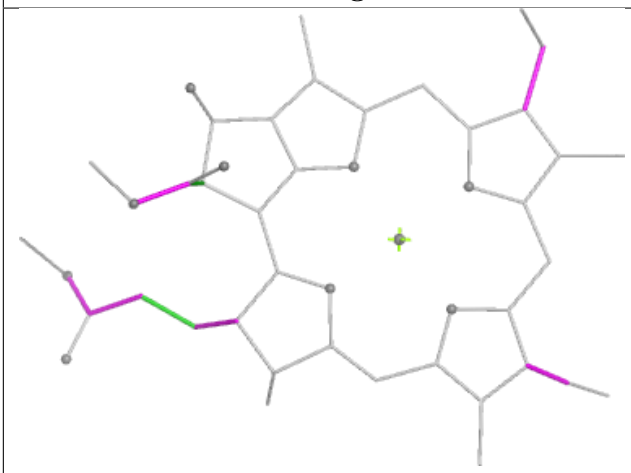
**Ligand CLA 4 315**



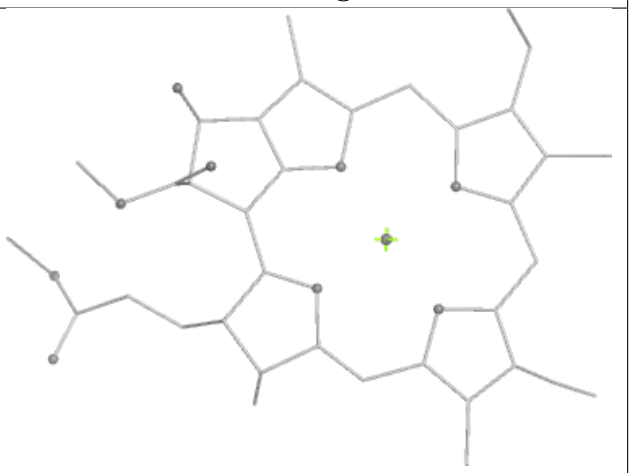
**Bond lengths**



**Bond angles**

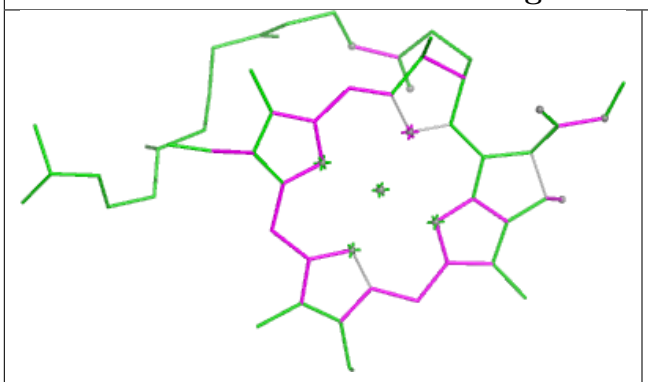


**Torsions**

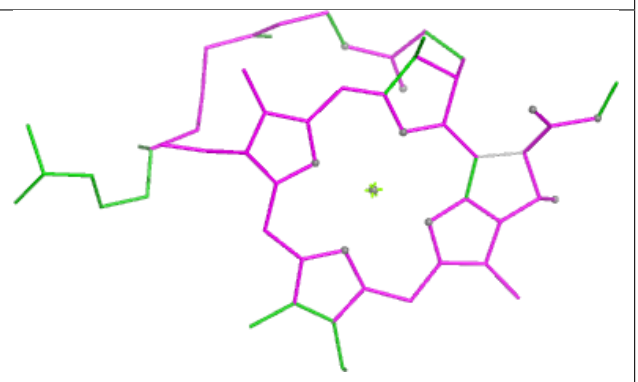


**Rings**

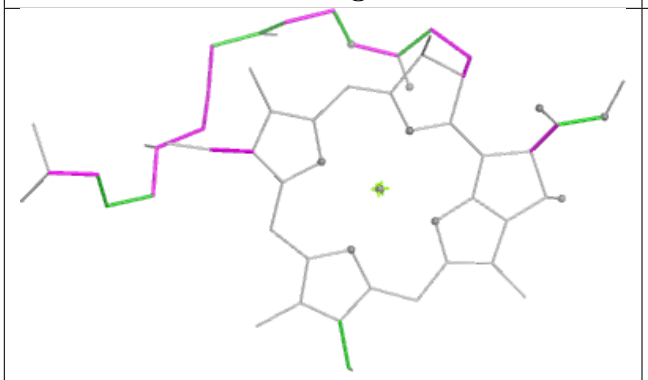
## Ligand CLA A 818



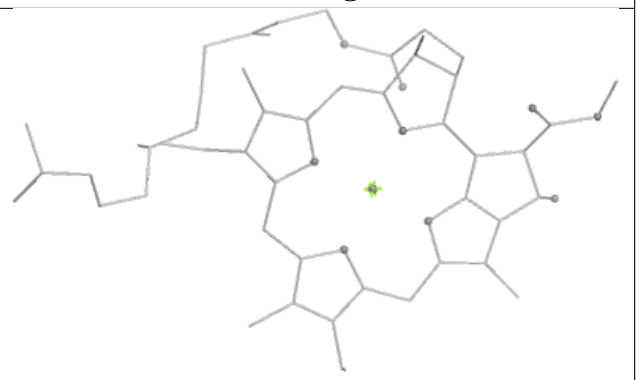
Bond lengths



Bond angles

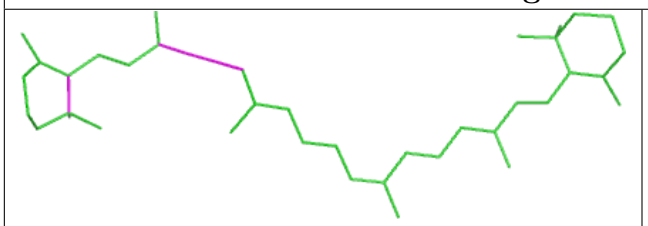


Torsions

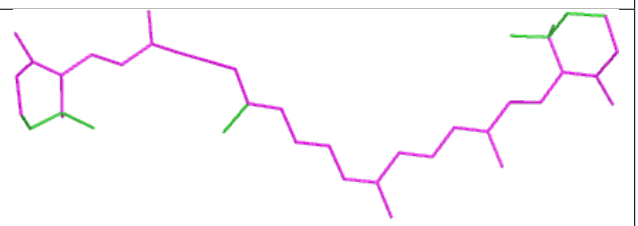


Rings

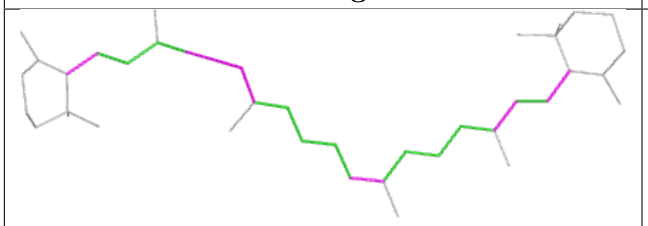
## Ligand BCR A 845



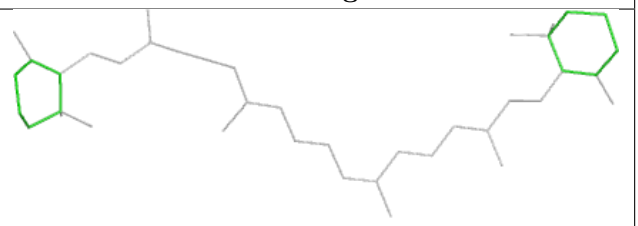
Bond lengths



Bond angles

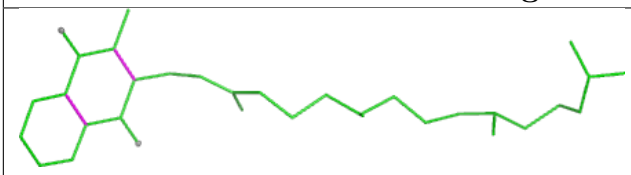


Torsions

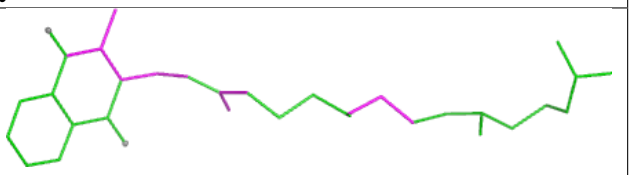


Rings

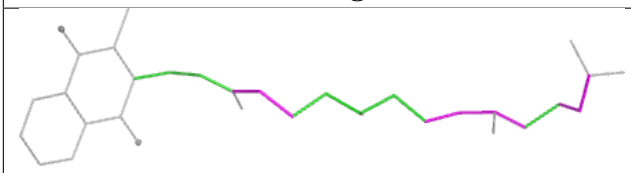
## Ligand PQN A 842



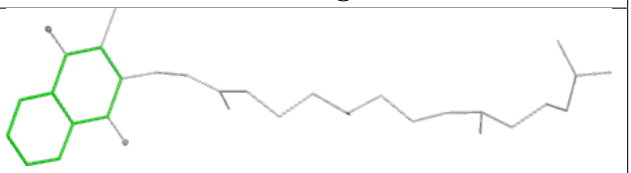
Bond lengths



Bond angles

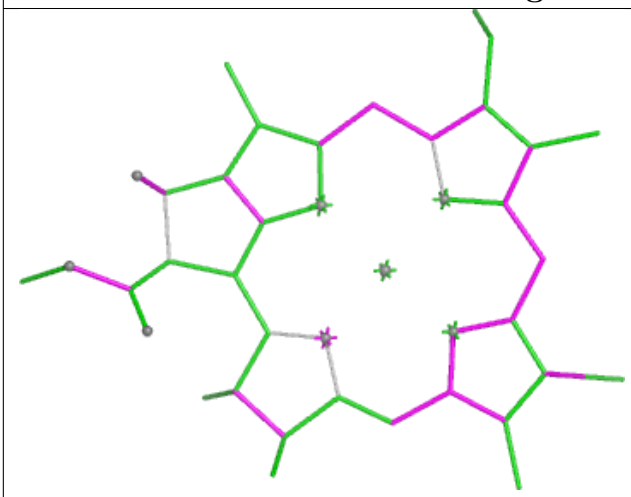


Torsions

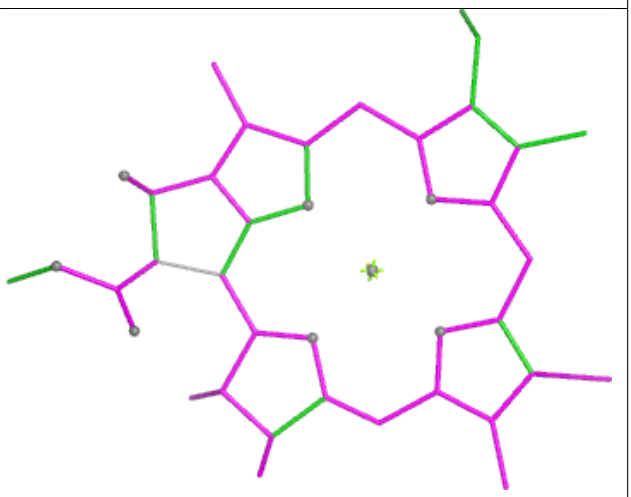


Rings

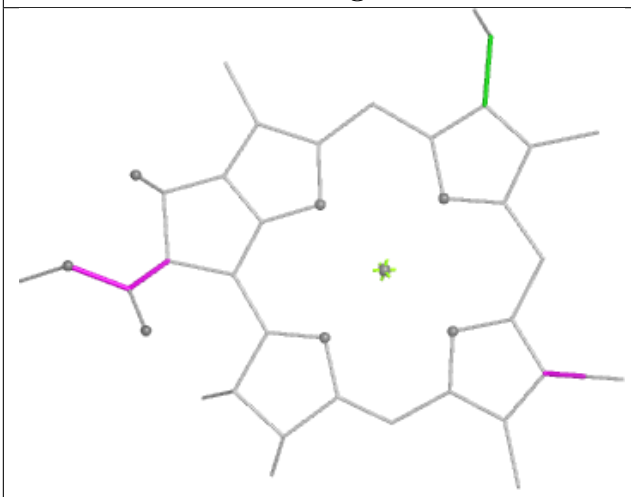
## Ligand CLA F 206



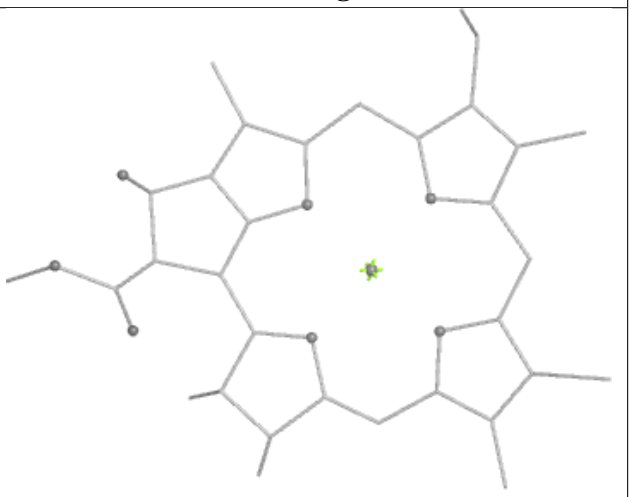
Bond lengths



Bond angles

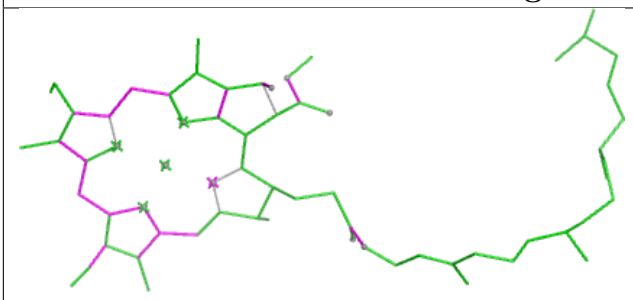


Torsions

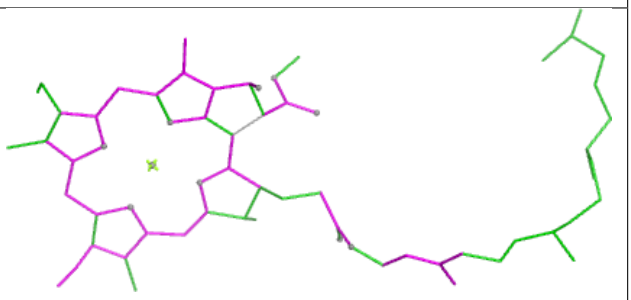


Rings

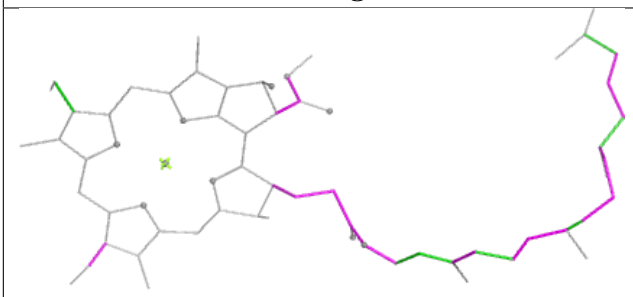
## Ligand CLA B 827



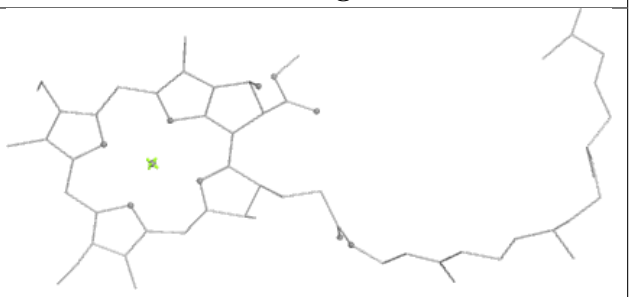
Bond lengths



Bond angles

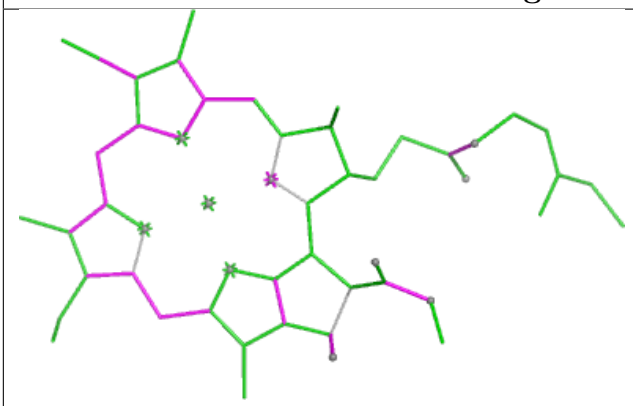


Torsions

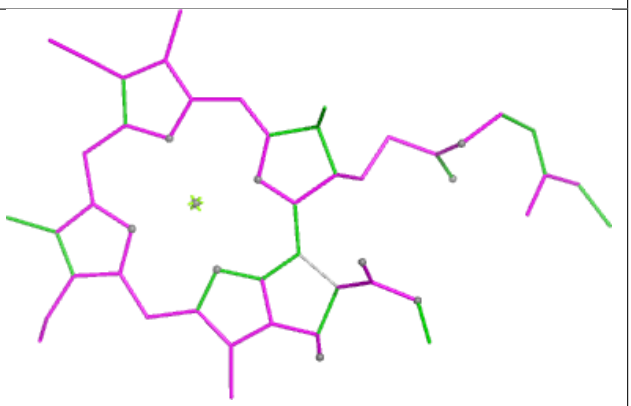


Rings

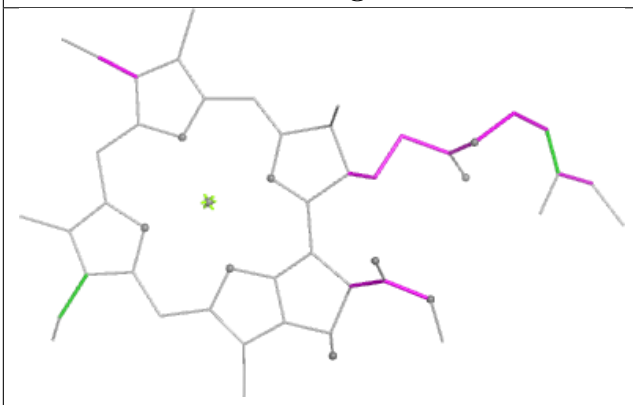
## Ligand CLA A 837



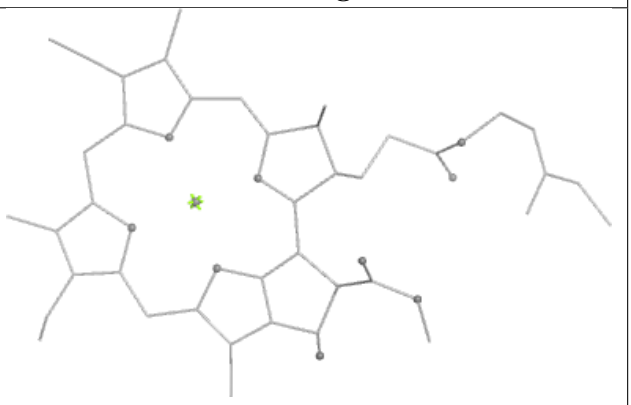
Bond lengths



Bond angles

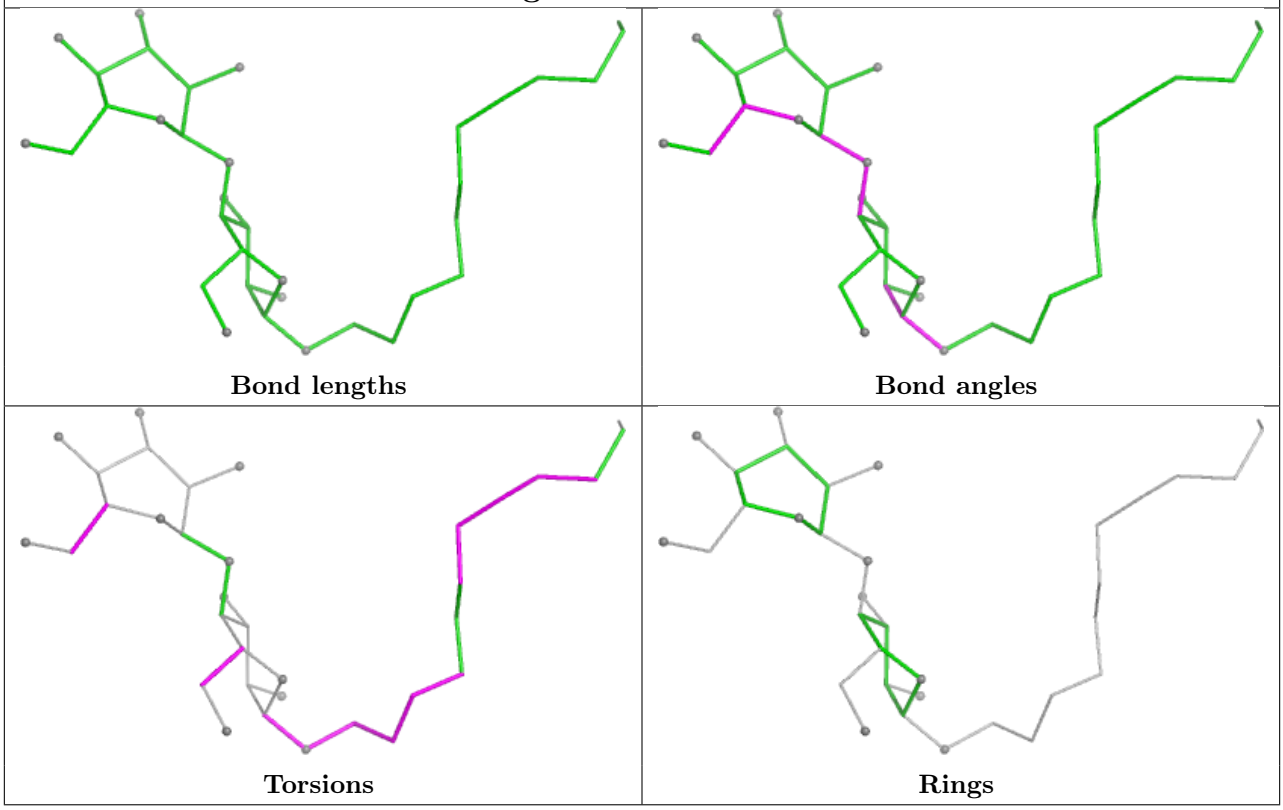


Torsions

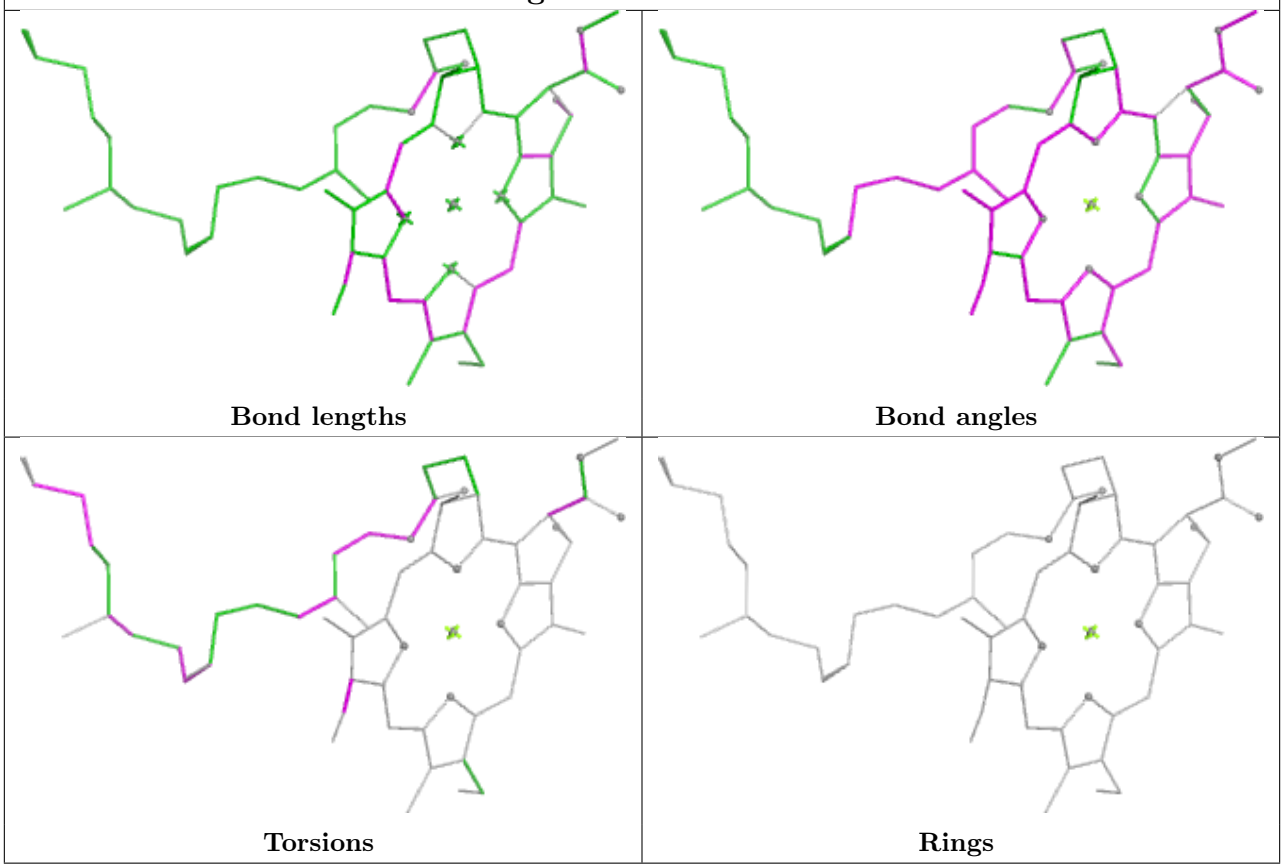


Rings

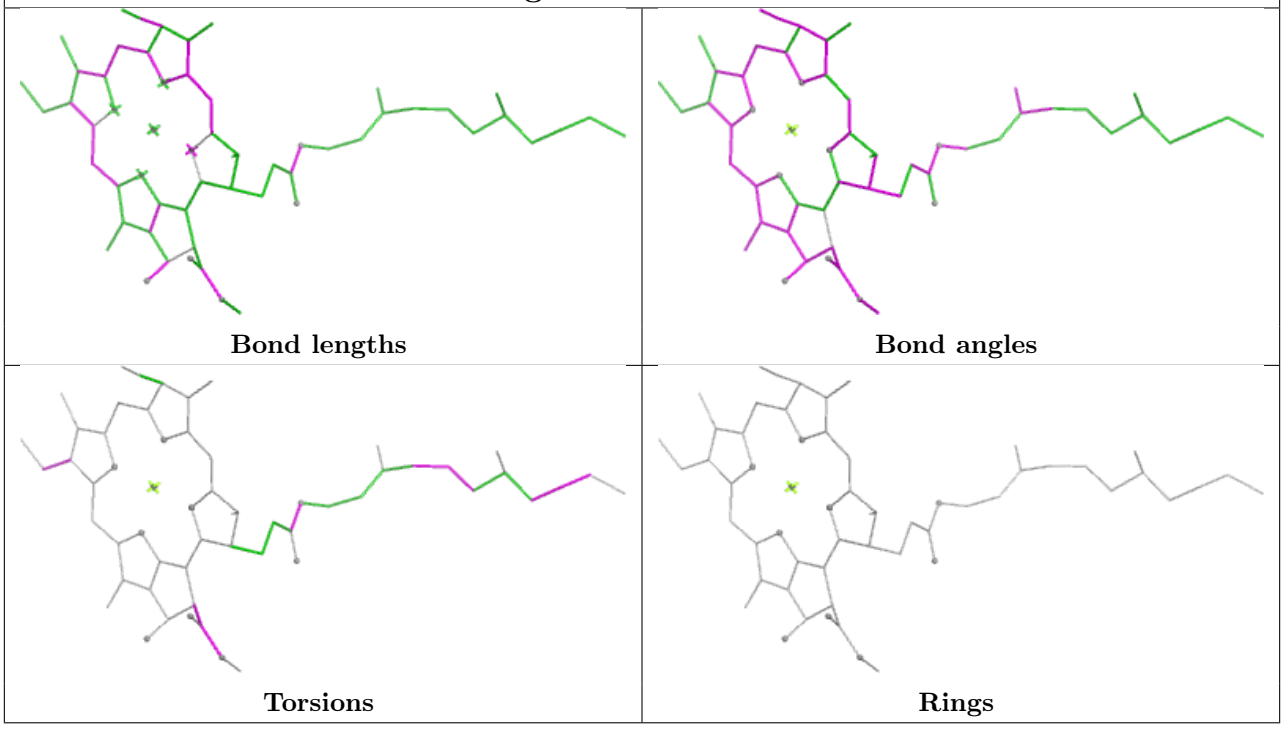
## Ligand LMU L 206



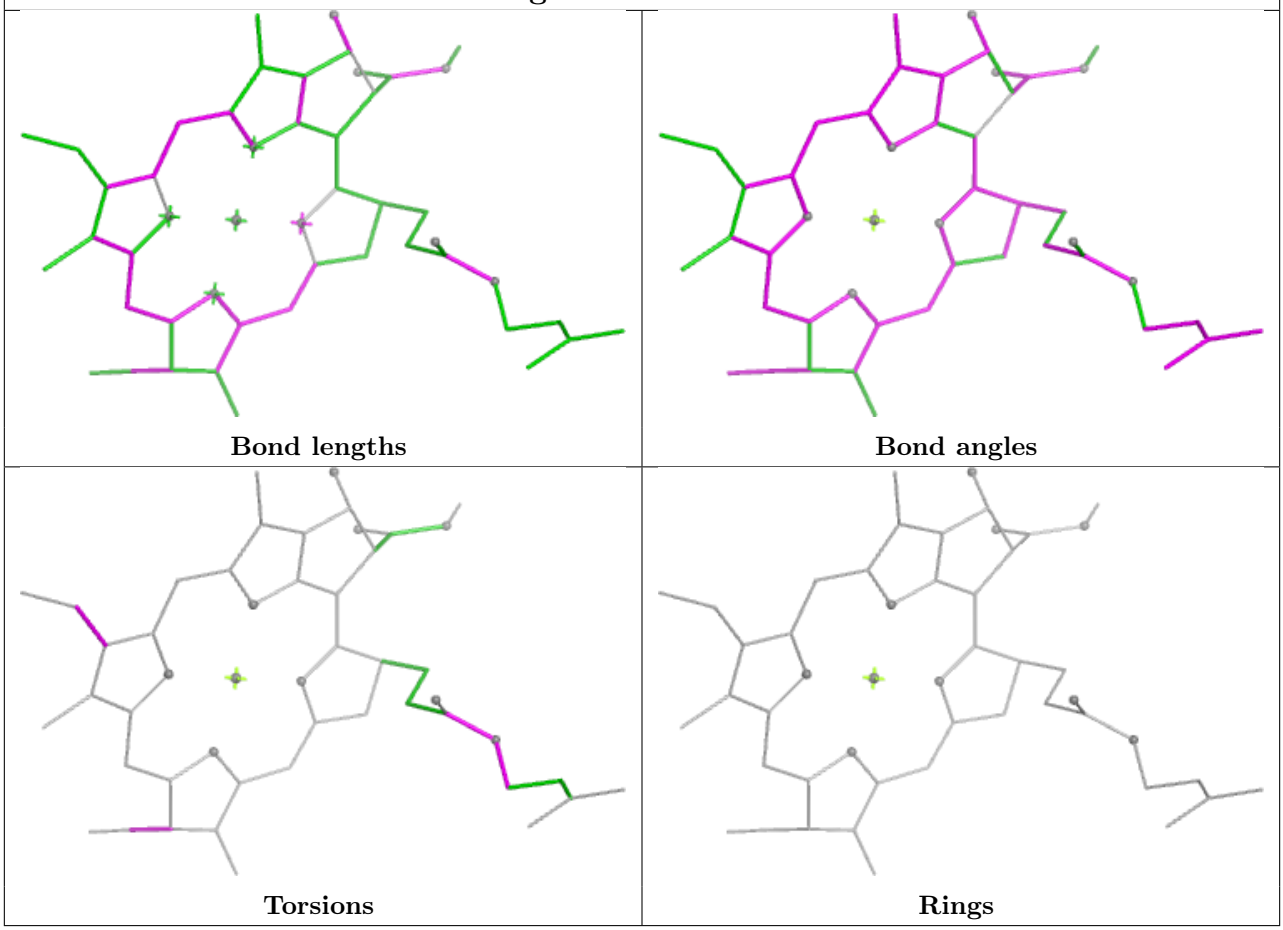

## Ligand CLA L 203



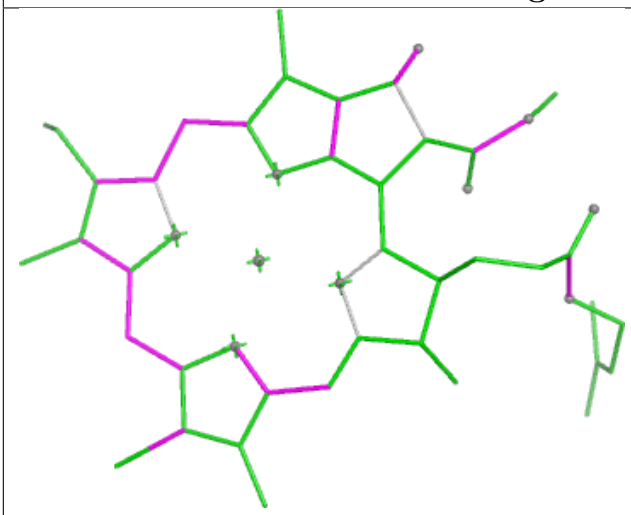
## Ligand CLA A 819



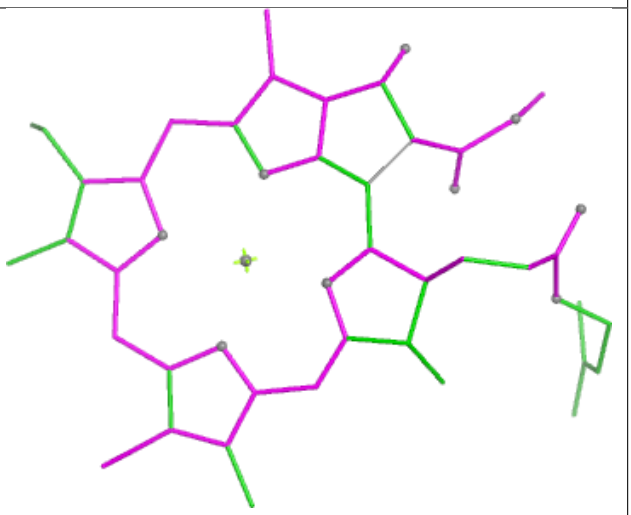

## Ligand CLA 2 310



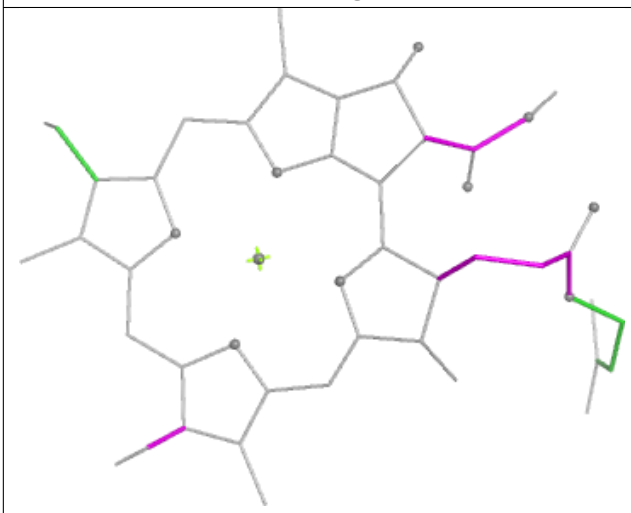
**Ligand CLA 3 313**



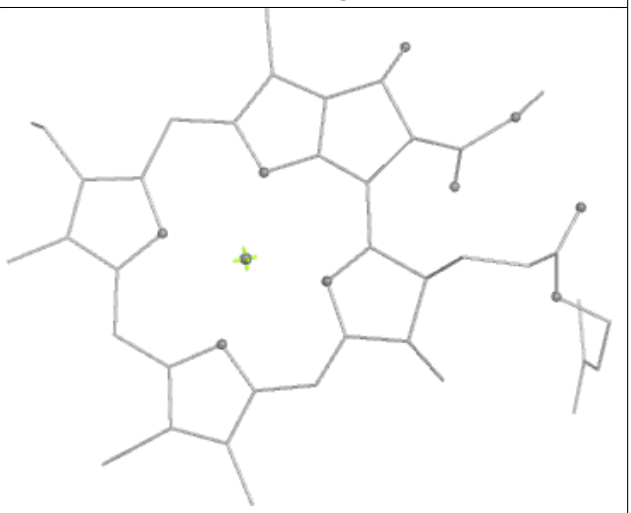
**Bond lengths**



**Bond angles**

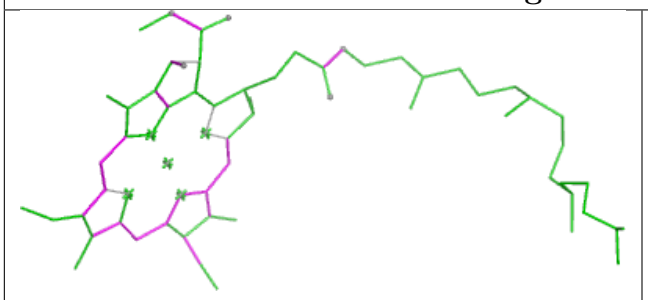


**Torsions**

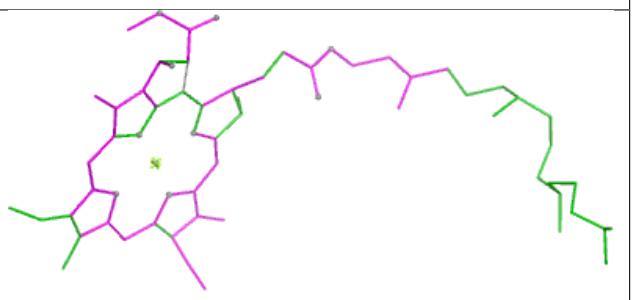


**Rings**

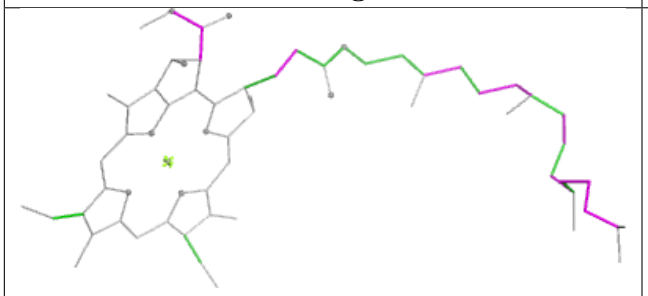
## Ligand CLA A 850



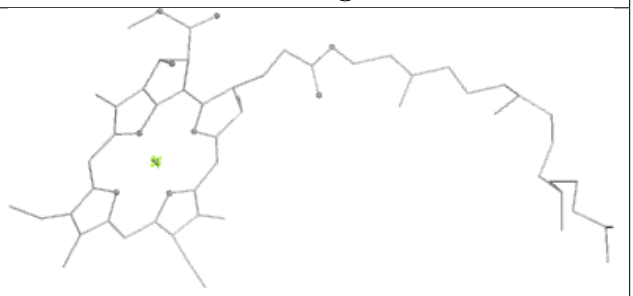
Bond lengths



Bond angles

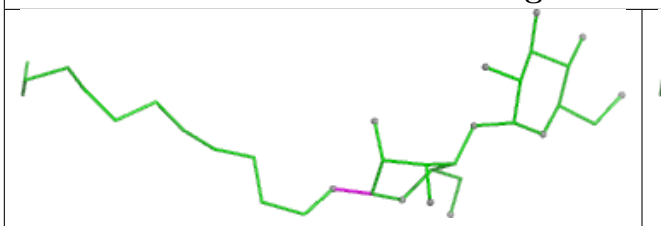


Torsions

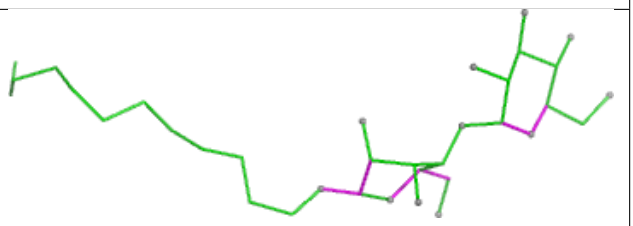


Rings

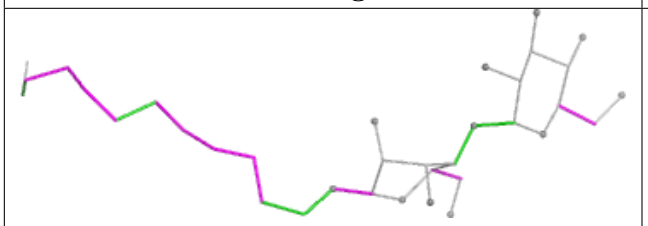
## Ligand LMU 4 316



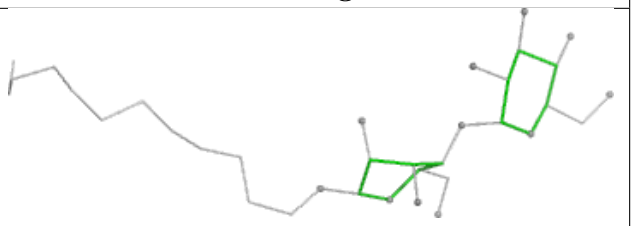
Bond lengths



Bond angles

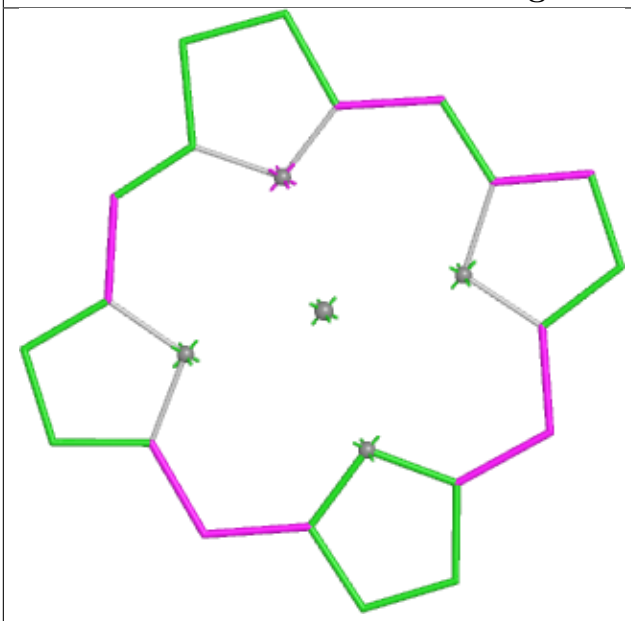


Torsions

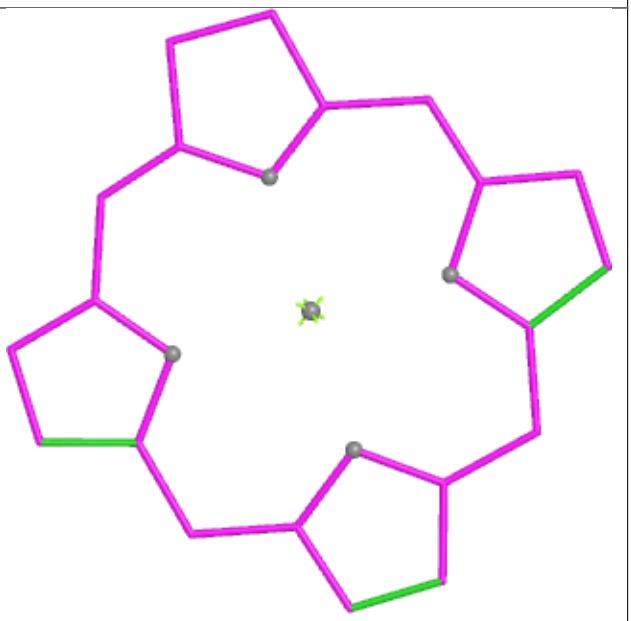


Rings

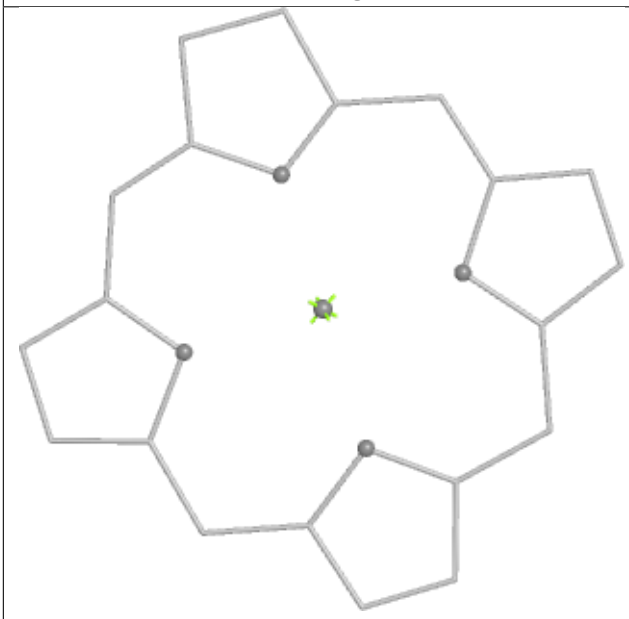
**Ligand CLA 1 212**



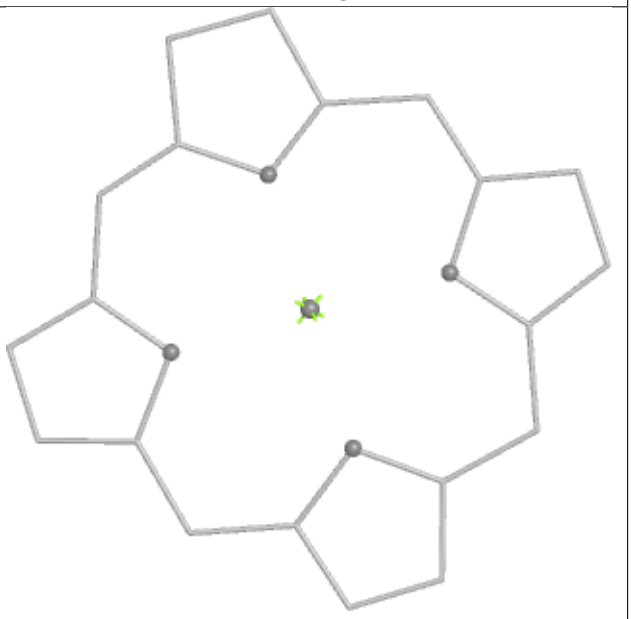
**Bond lengths**



**Bond angles**

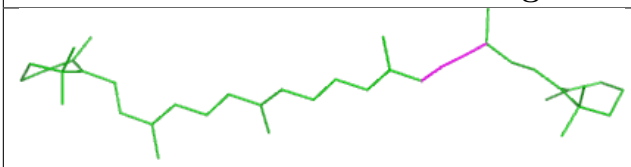


**Torsions**

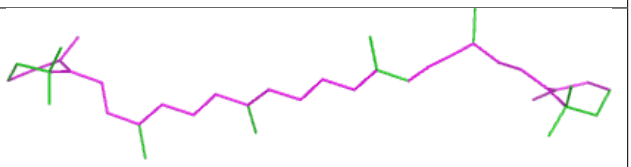


**Rings**

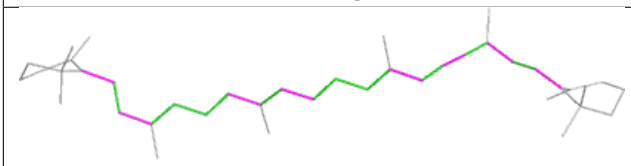
## Ligand BCR A 844



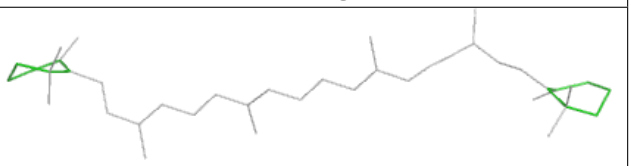
Bond lengths



Bond angles

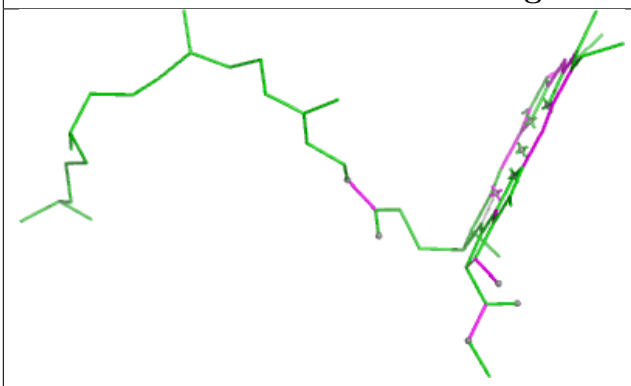


Torsions

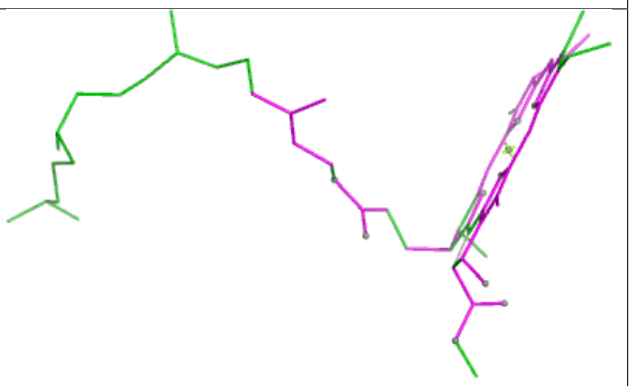


Rings

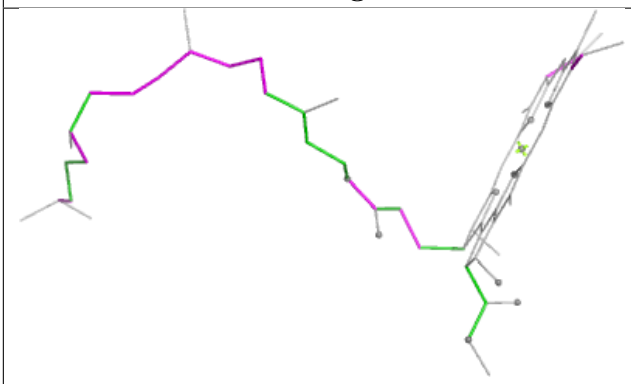
## Ligand CLA B 840



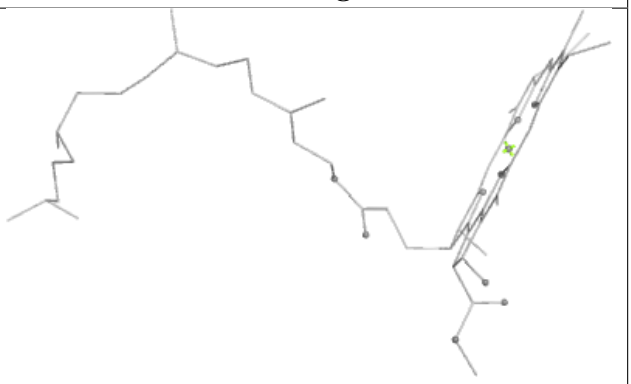
Bond lengths



Bond angles

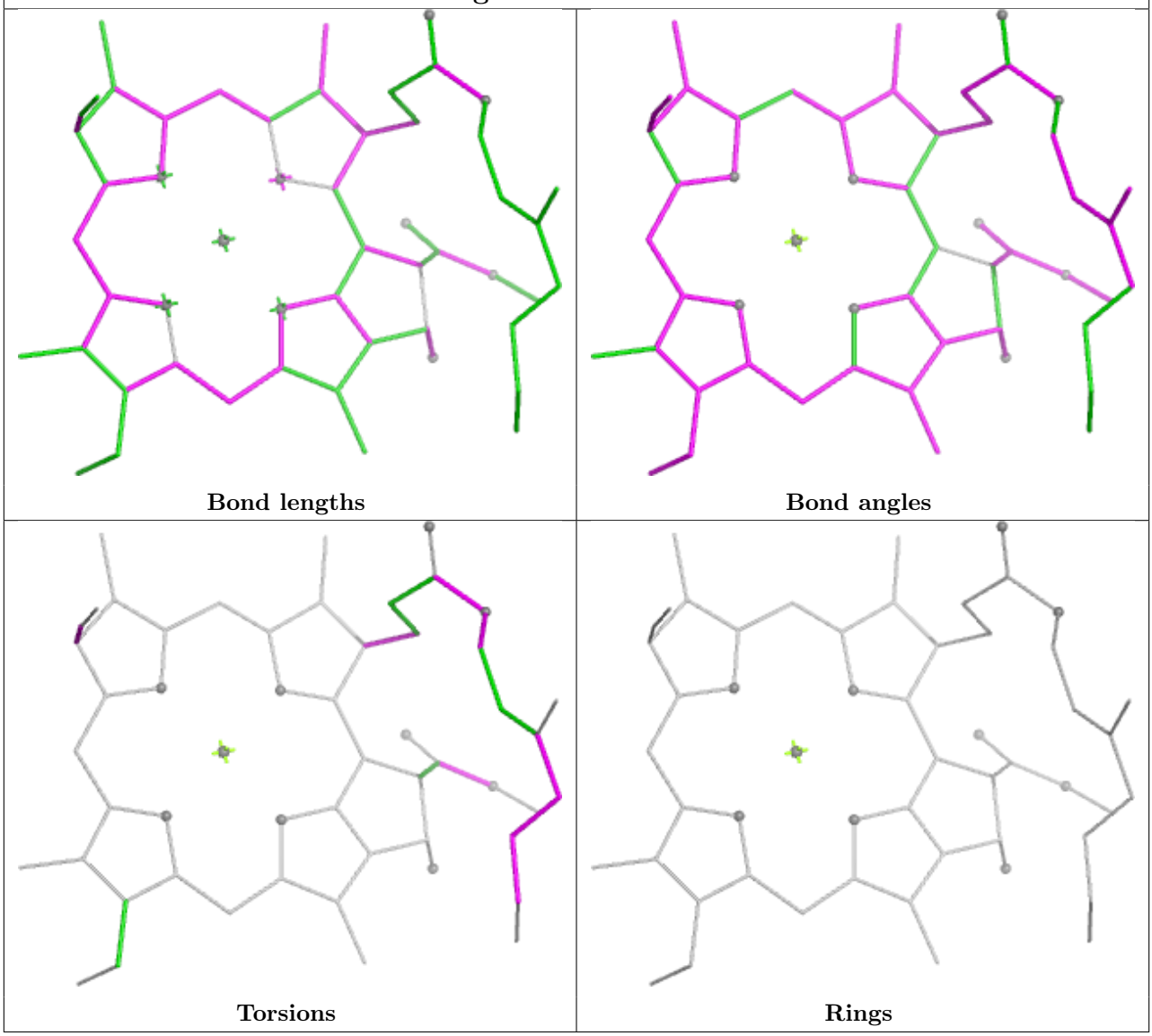


Torsions

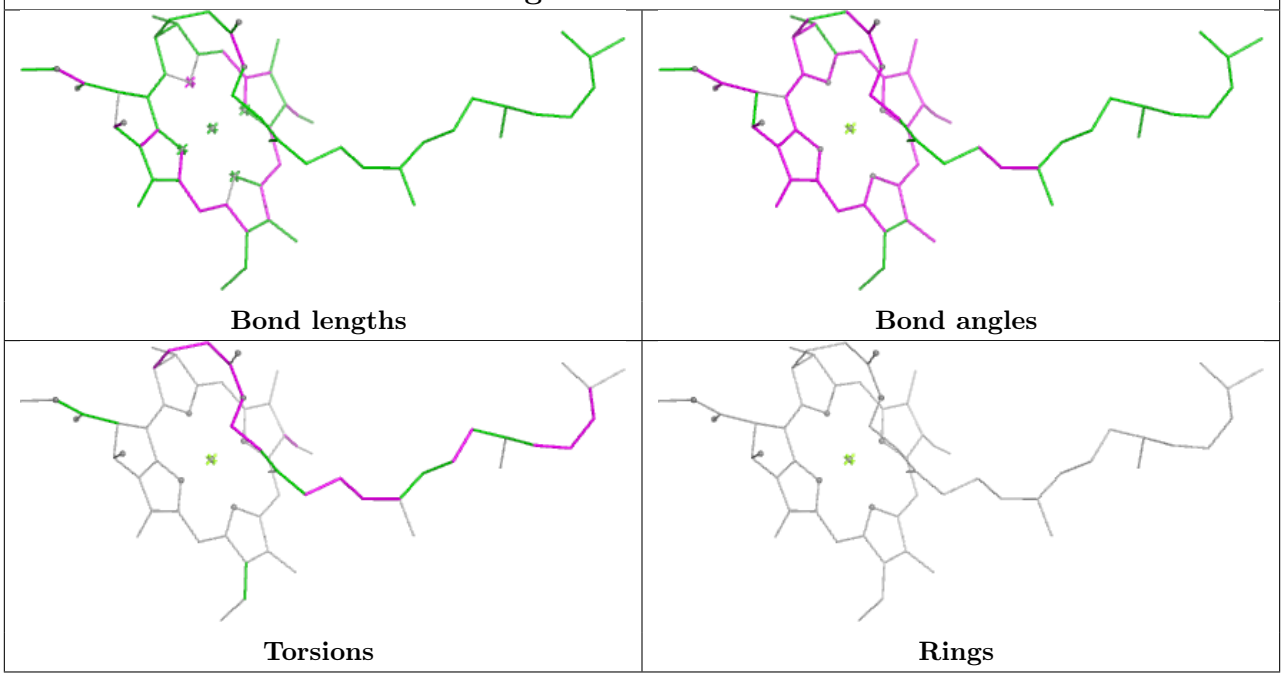


Rings

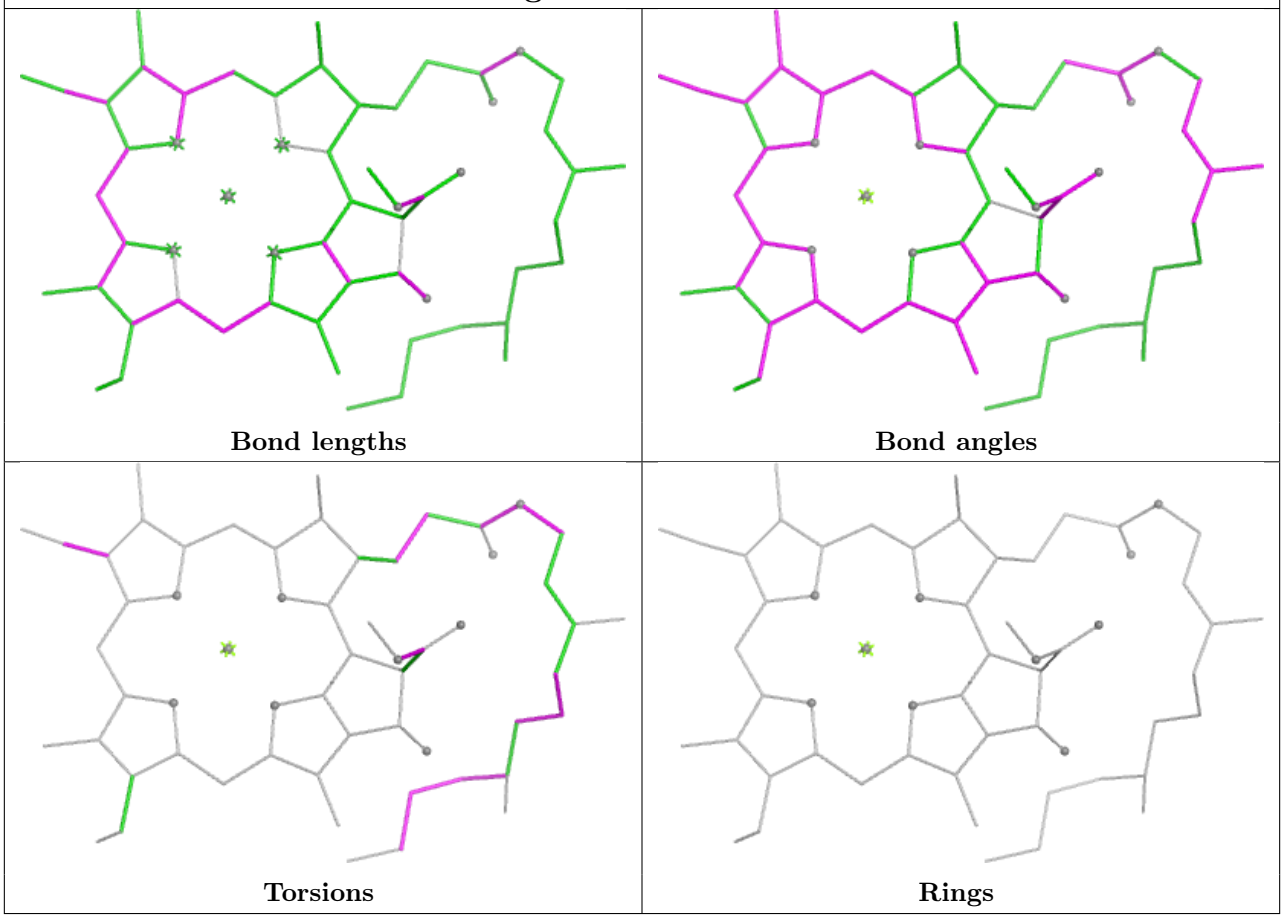
**Ligand CLA F 207**



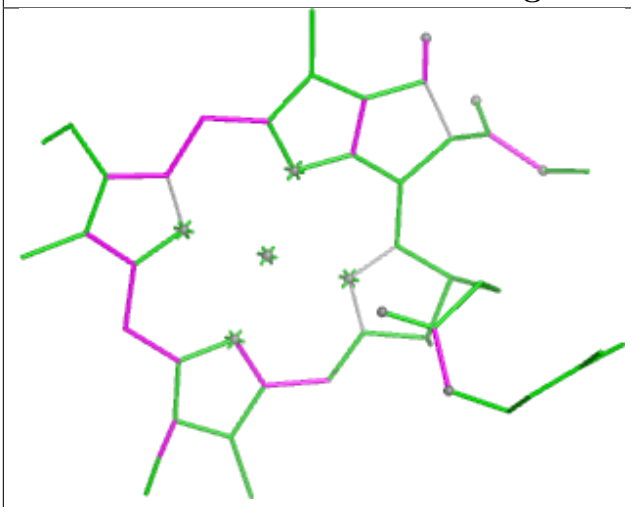
## Ligand CLA A 838



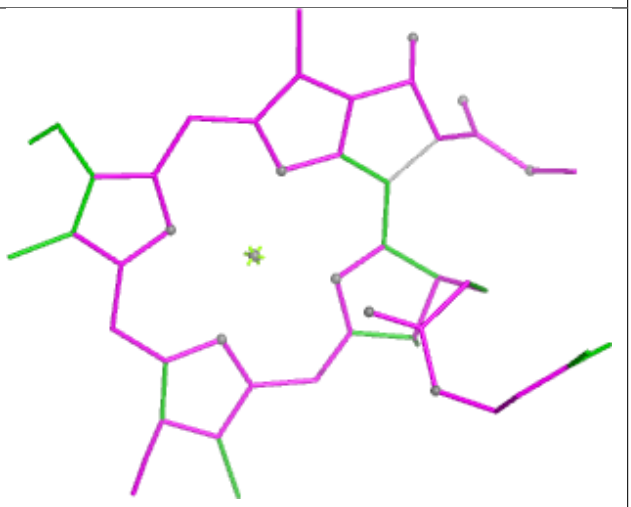

## Ligand CLA A 823



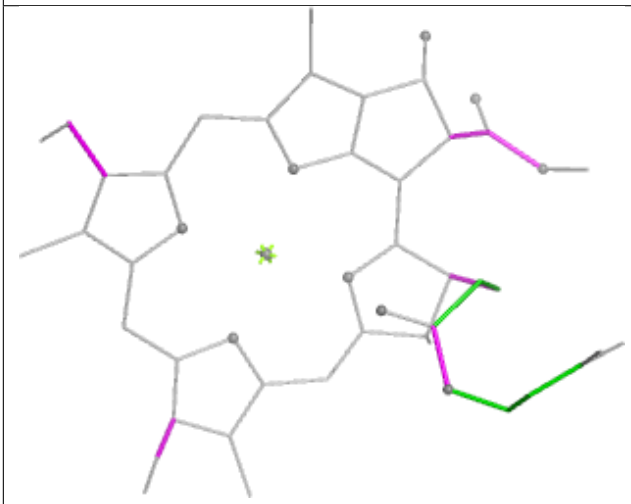
**Ligand CLA A 815**



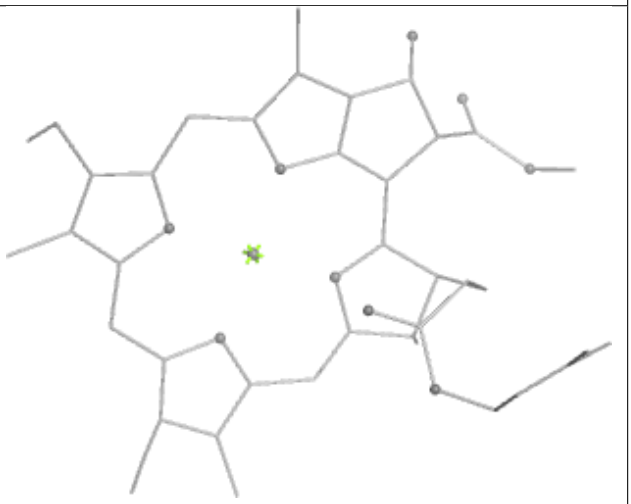
**Bond lengths**



**Bond angles**

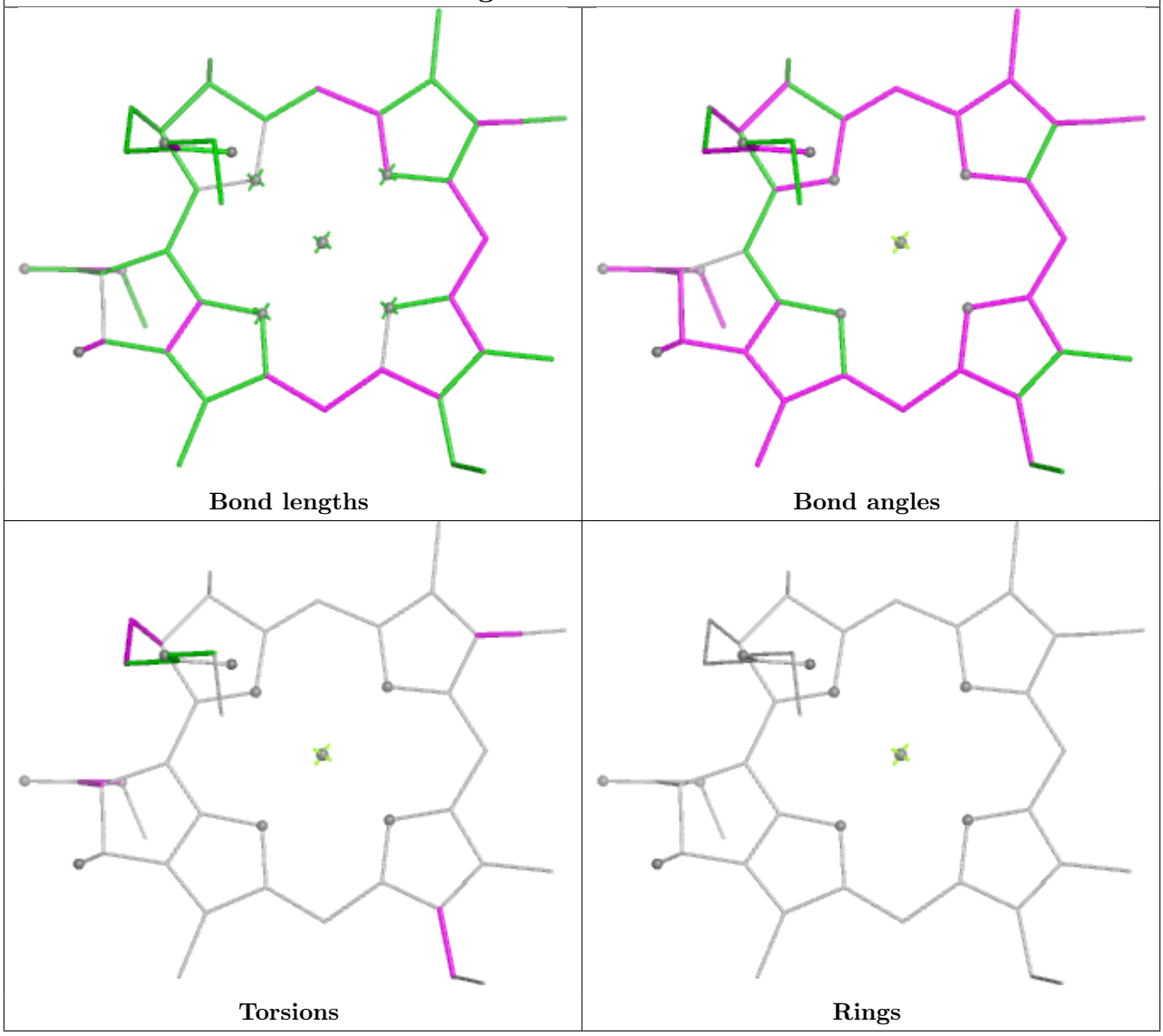


**Torsions**

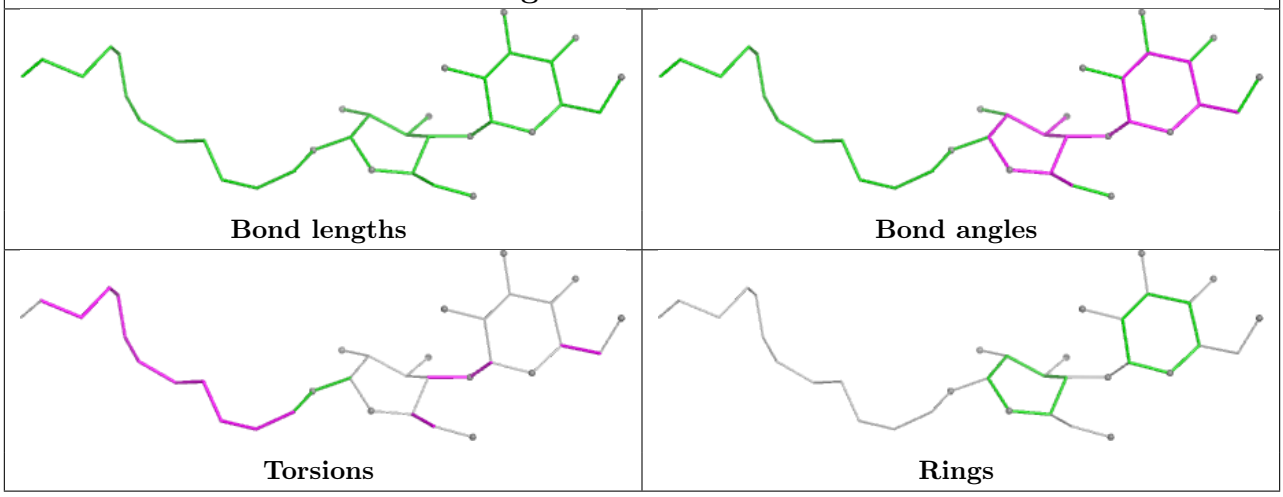


**Rings**

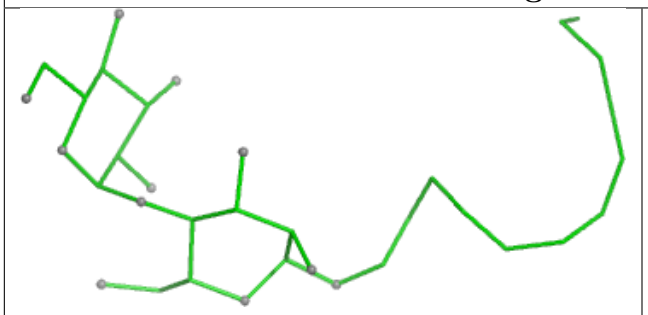
## Ligand CLA L 207



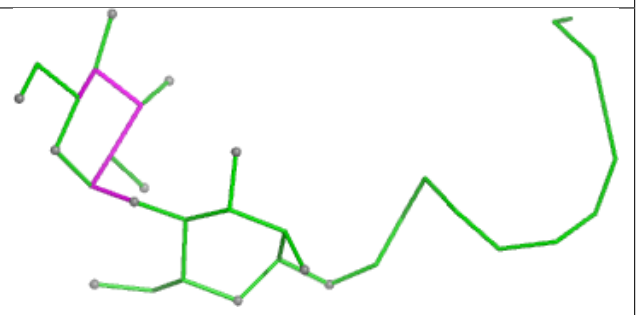

## Ligand LMU B 804



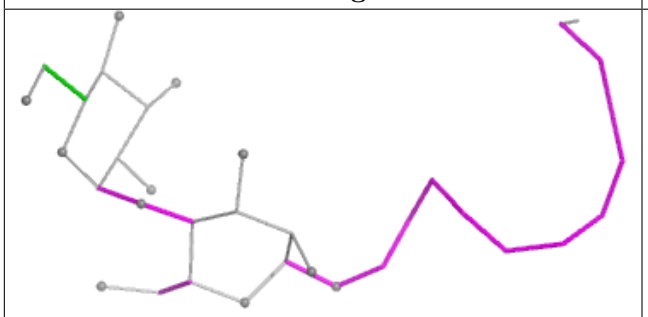
## Ligand LMU 2 320



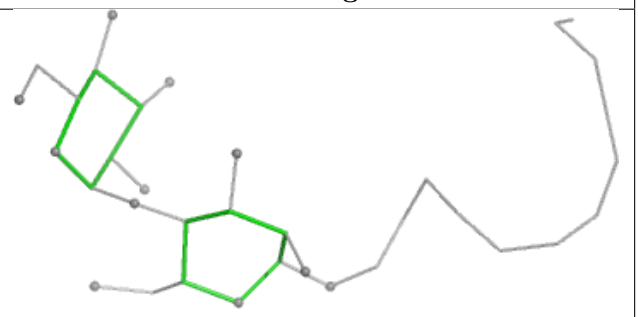
Bond lengths



Bond angles

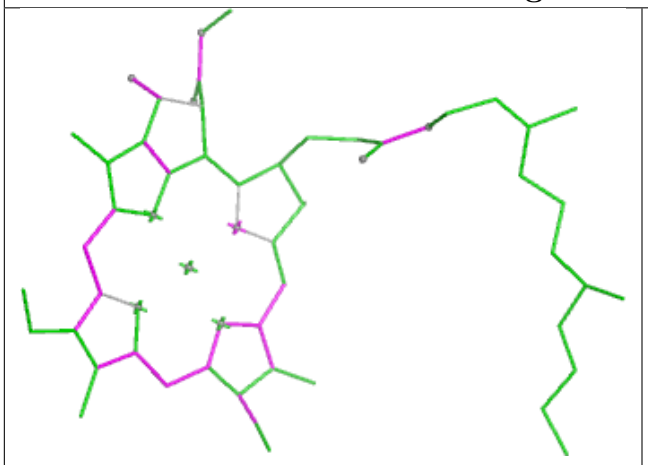


Torsions

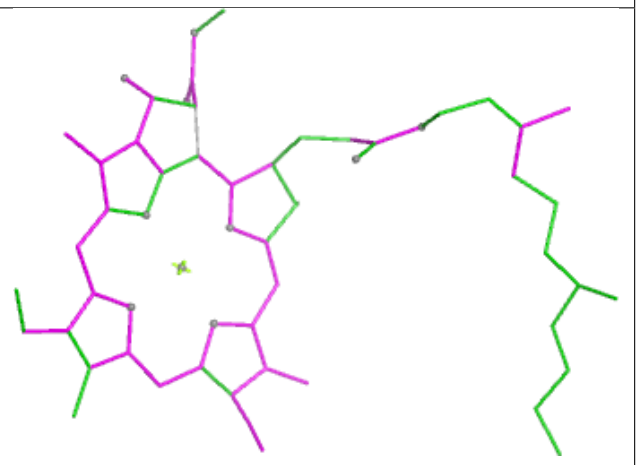


Rings

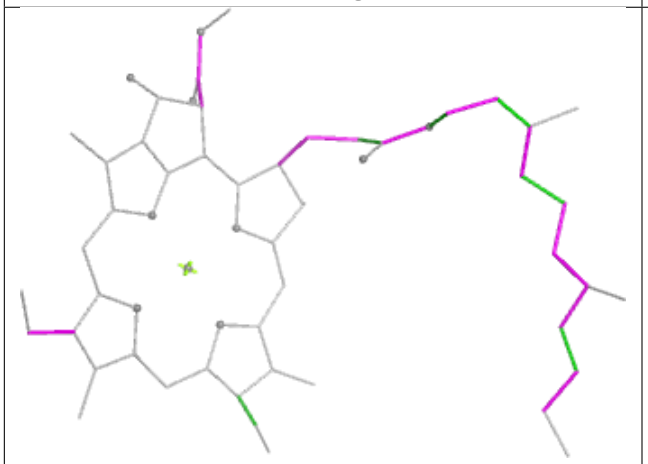
## Ligand CLA B 826



Bond lengths



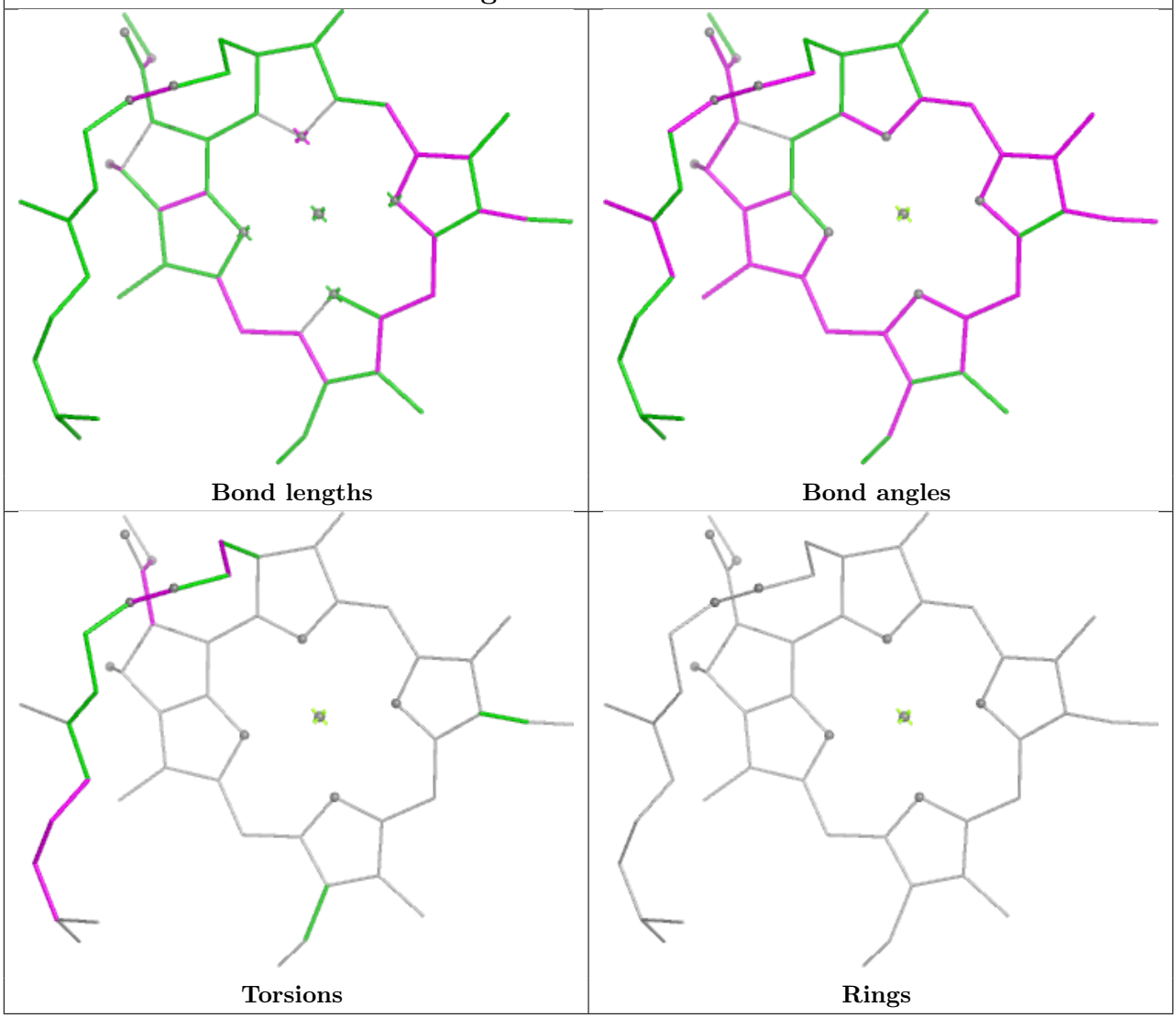
Bond angles



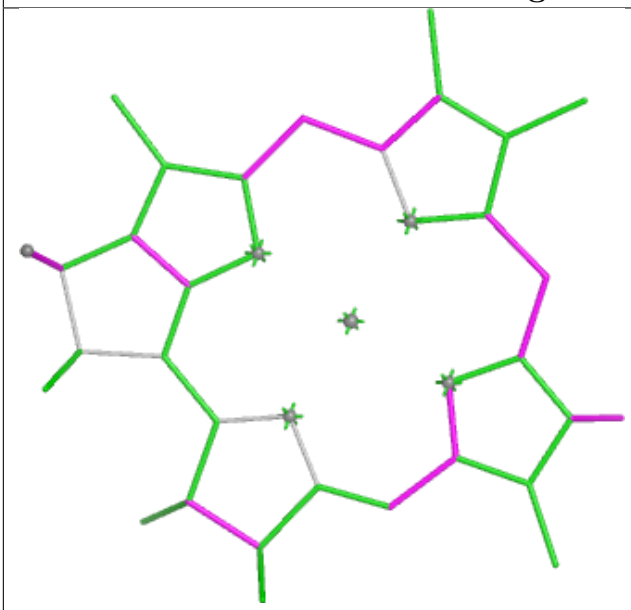
Torsions

Rings

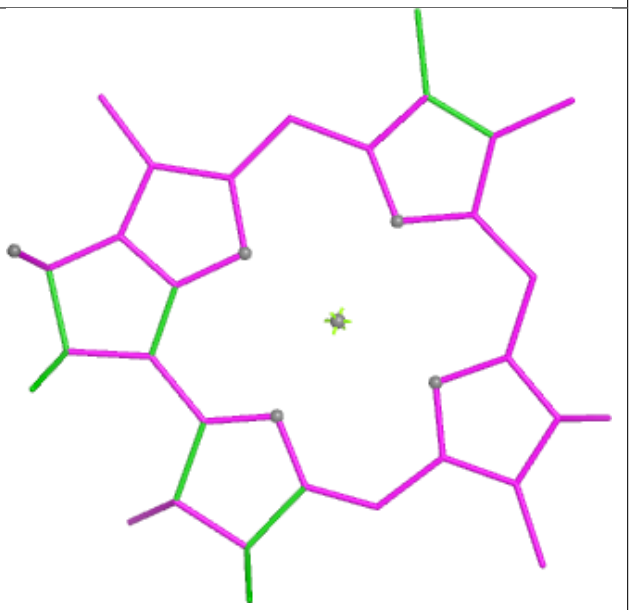
**Ligand CLA A 827**



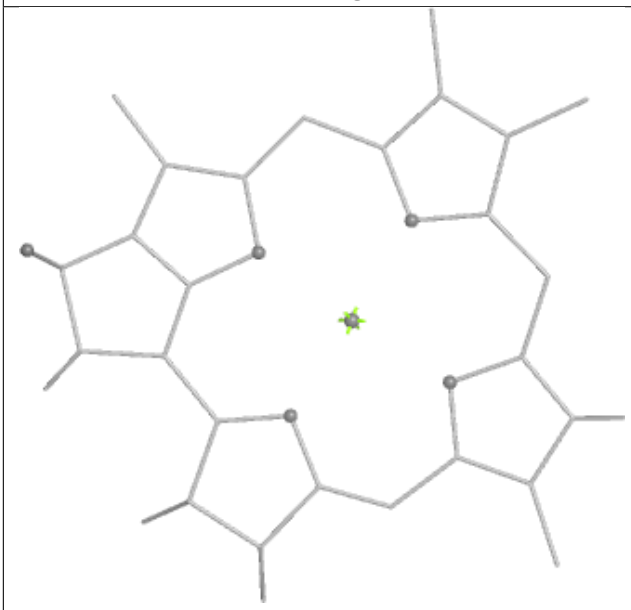
**Ligand CLA 3 303**



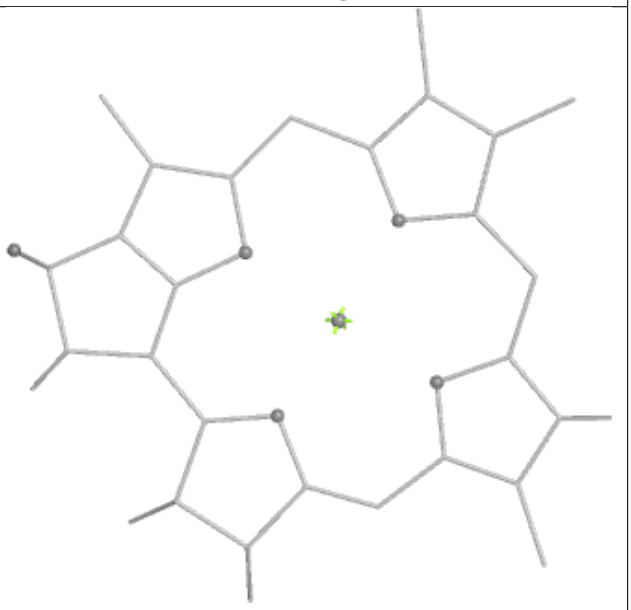
**Bond lengths**



**Bond angles**

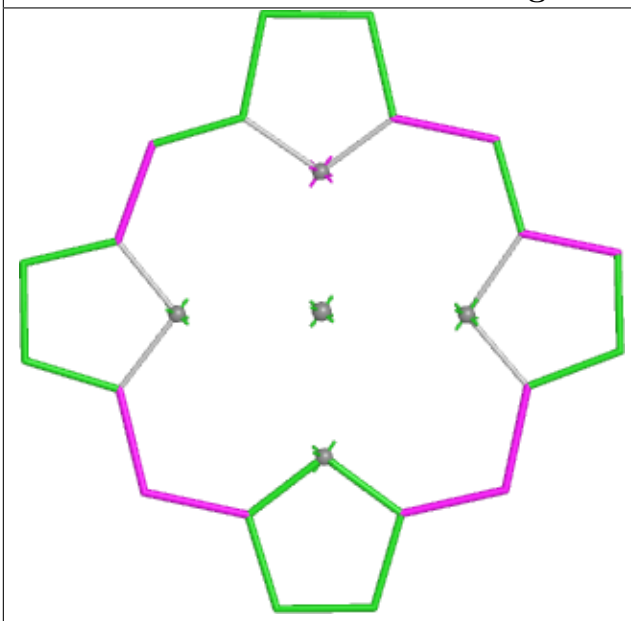


**Torsions**

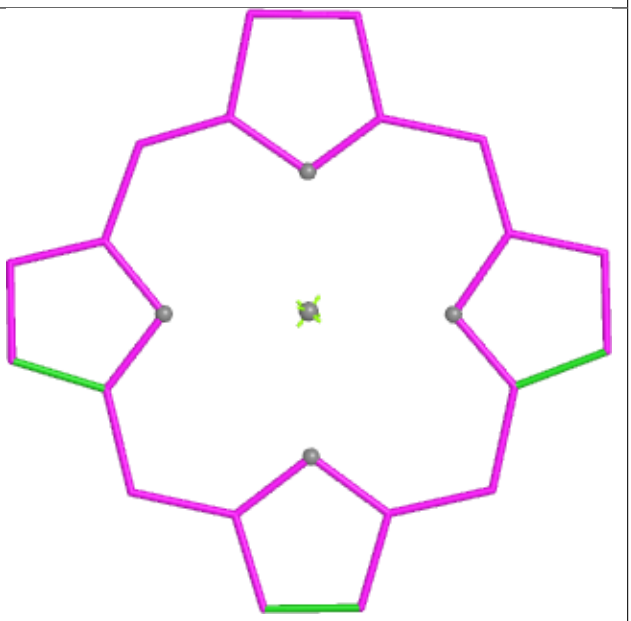


**Rings**

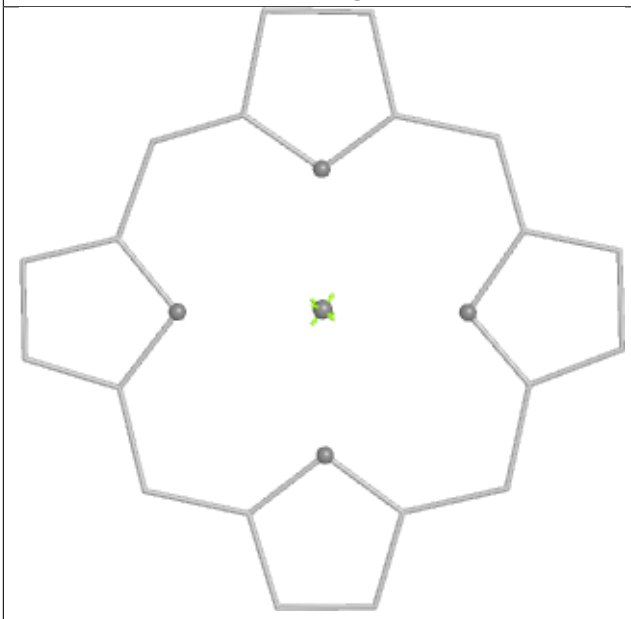
**Ligand CLA 3 308**



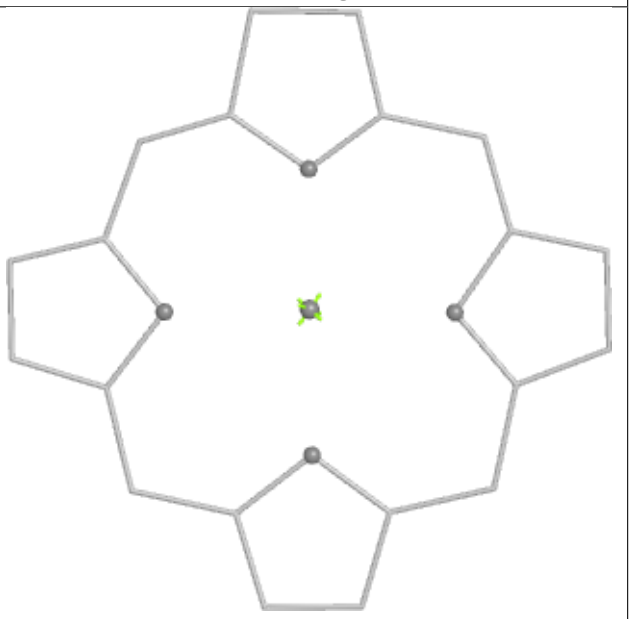
**Bond lengths**



**Bond angles**

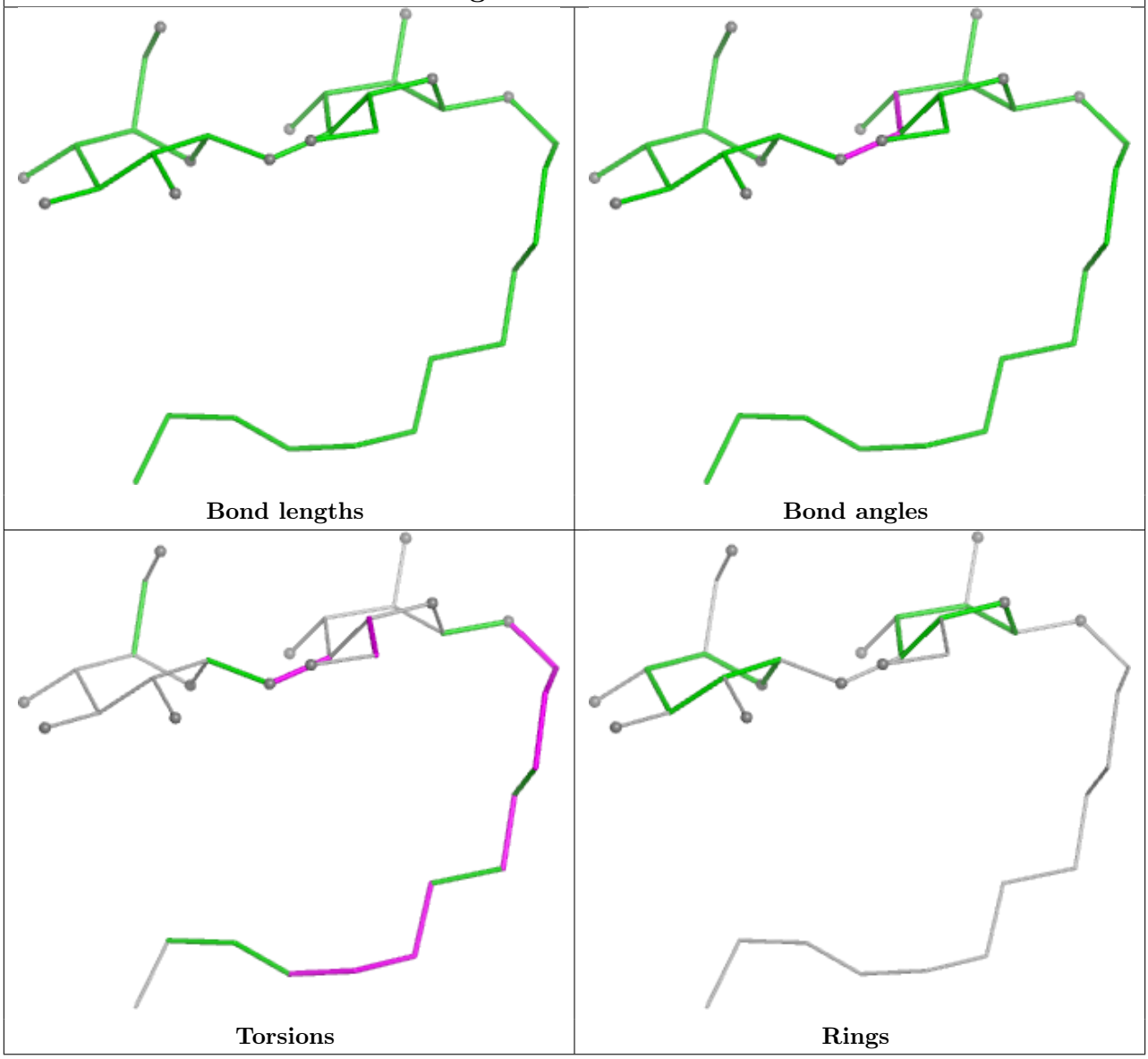


**Torsions**

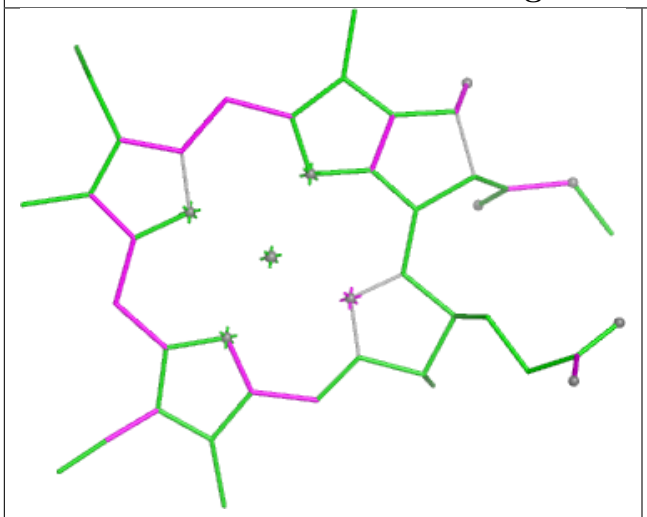


**Rings**

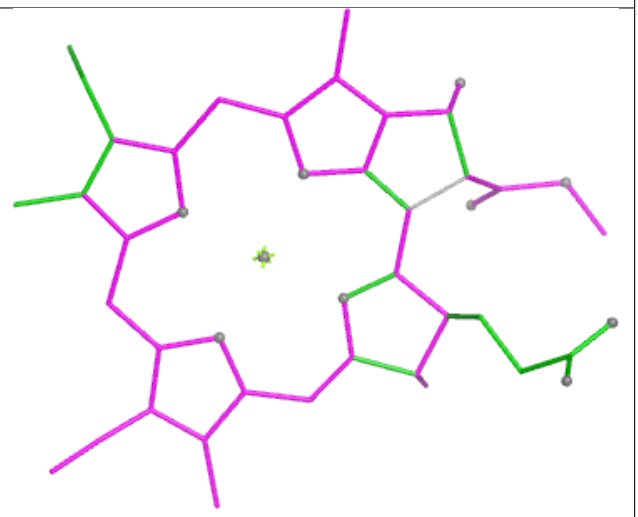
**Ligand LMU 1 217**



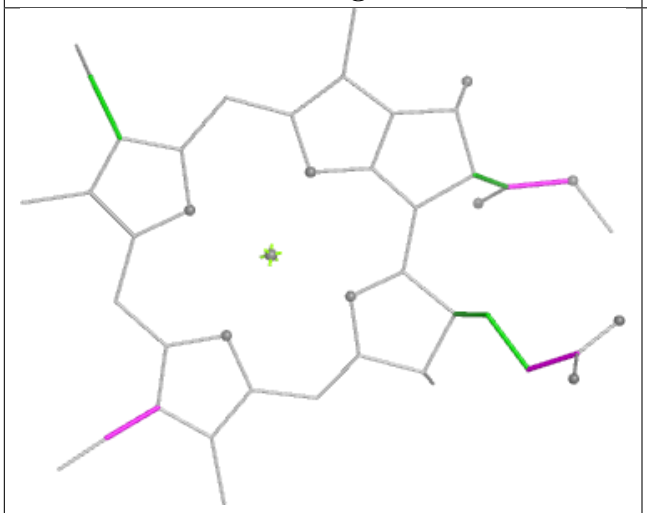
**Ligand CLA A 810**



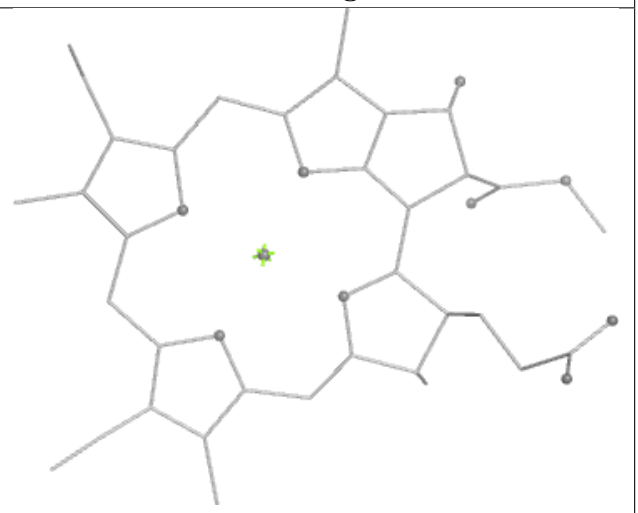
**Bond lengths**



**Bond angles**

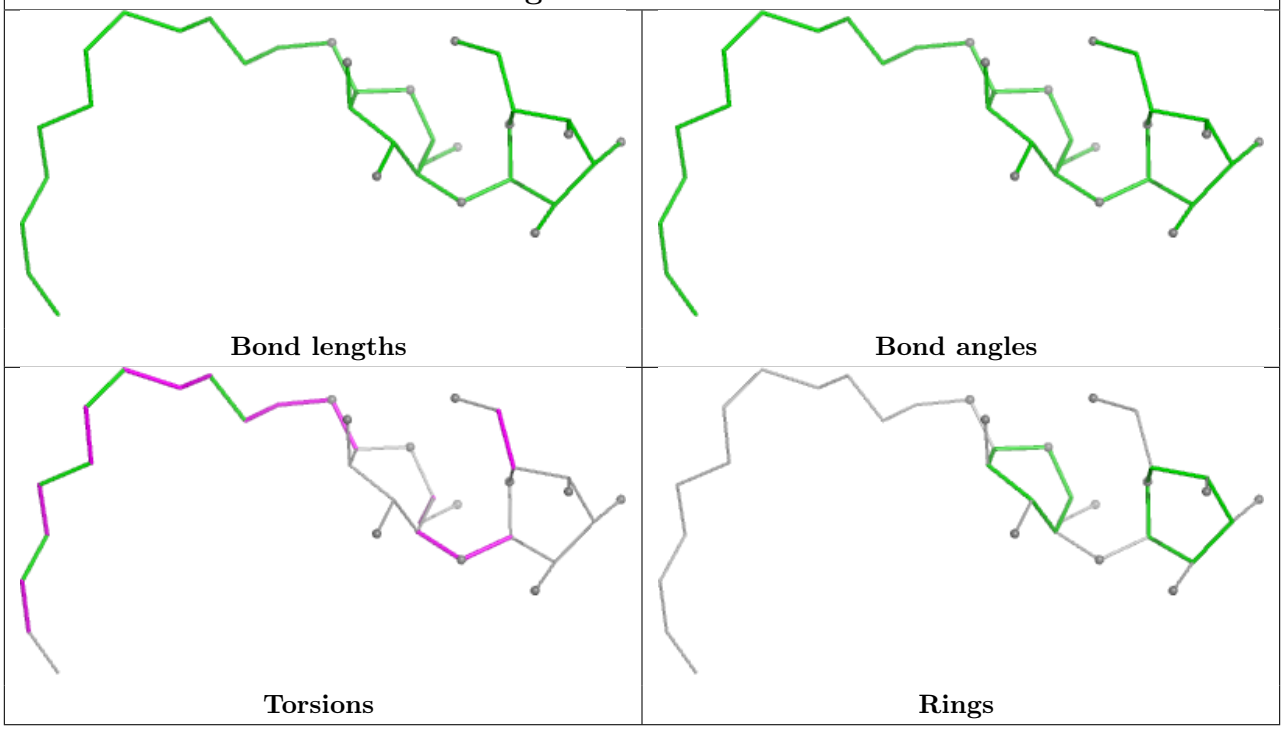


**Torsions**

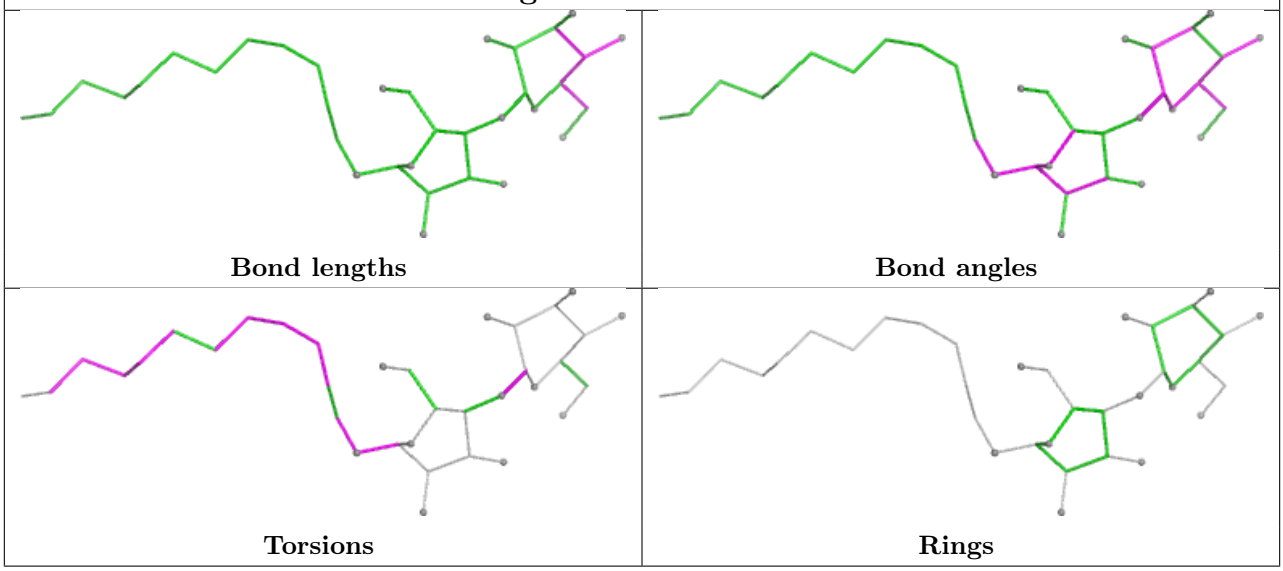


**Rings**

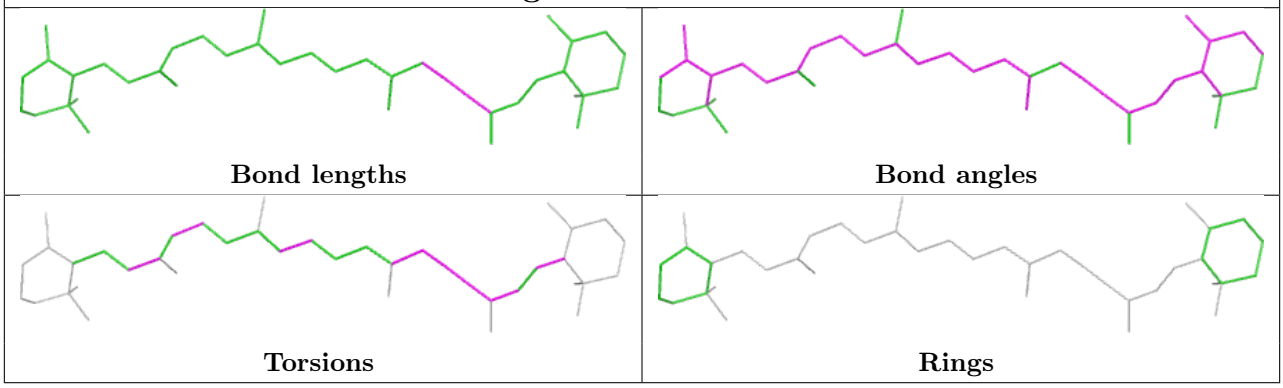
## Ligand LMU 2 318



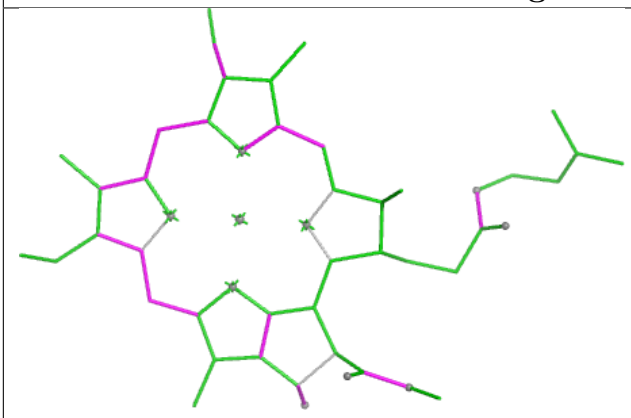

## Ligand LMU G 101



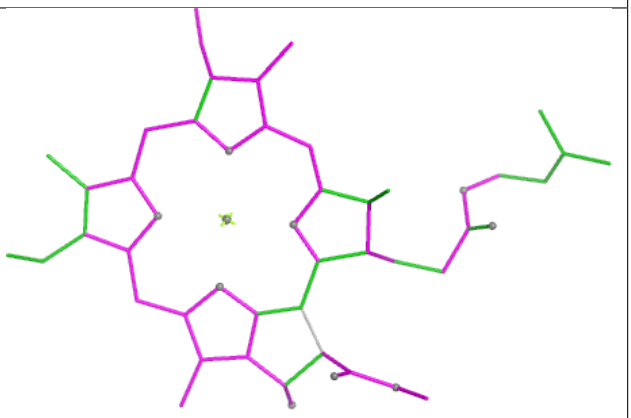

## Ligand BCR A 843



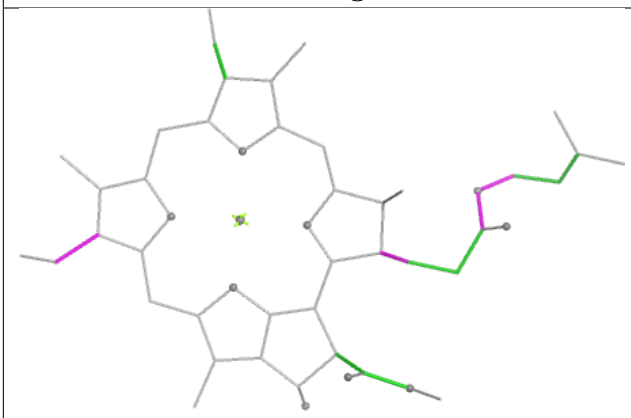
**Ligand CLA 2 305**



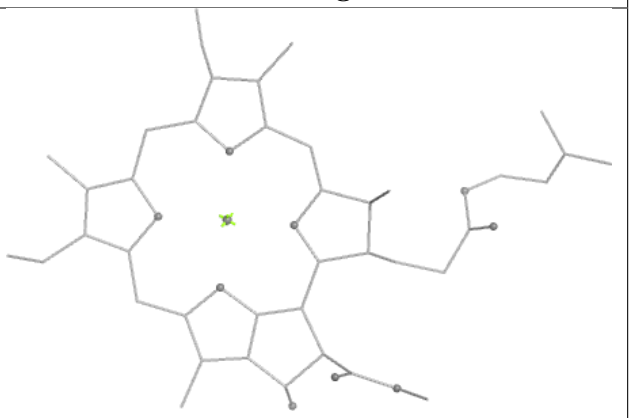
**Bond lengths**



**Bond angles**

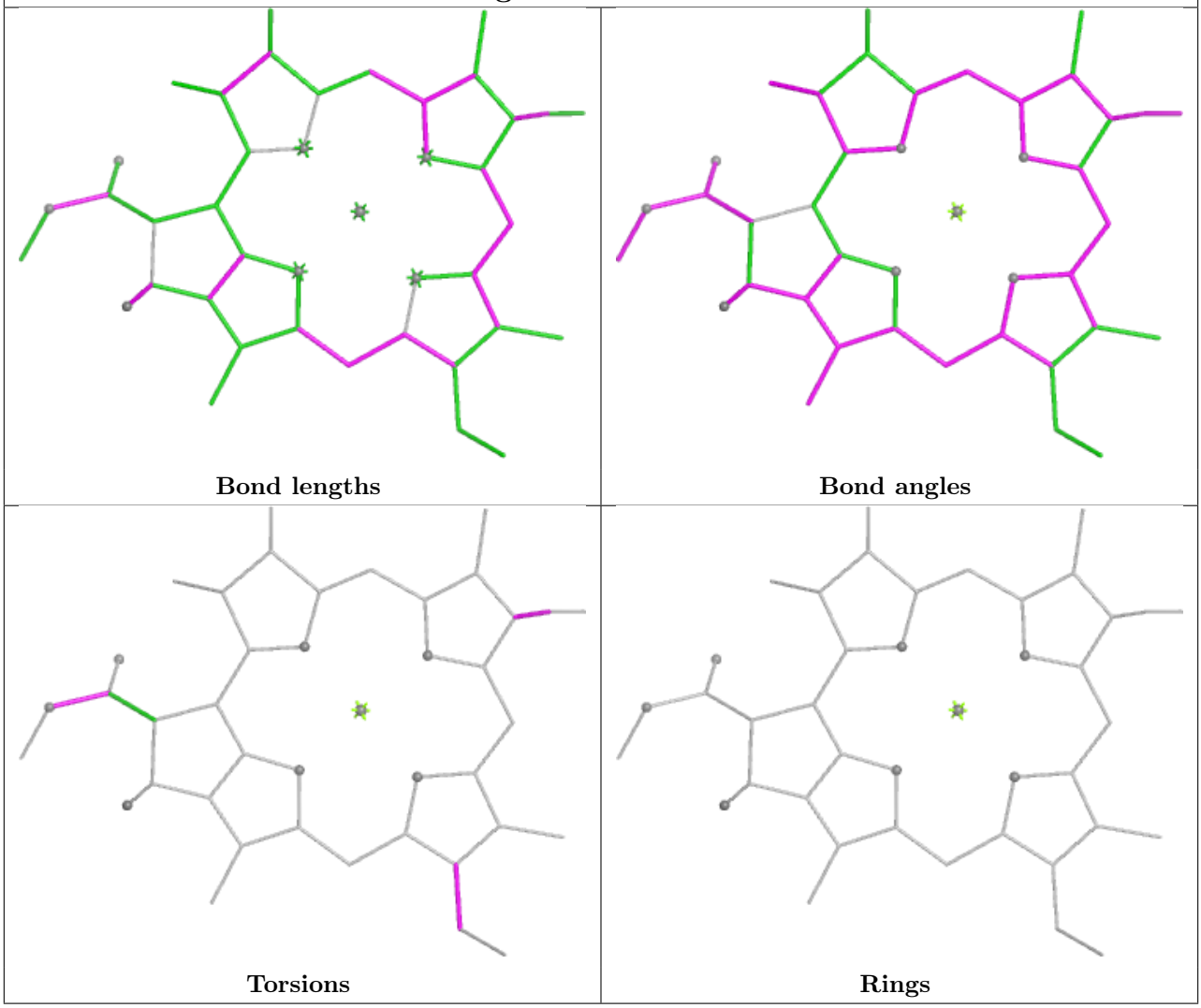


**Torsions**

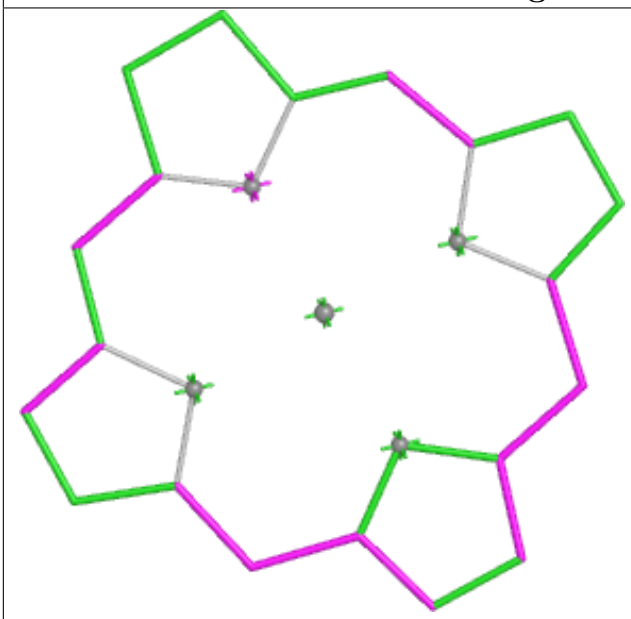


**Rings**

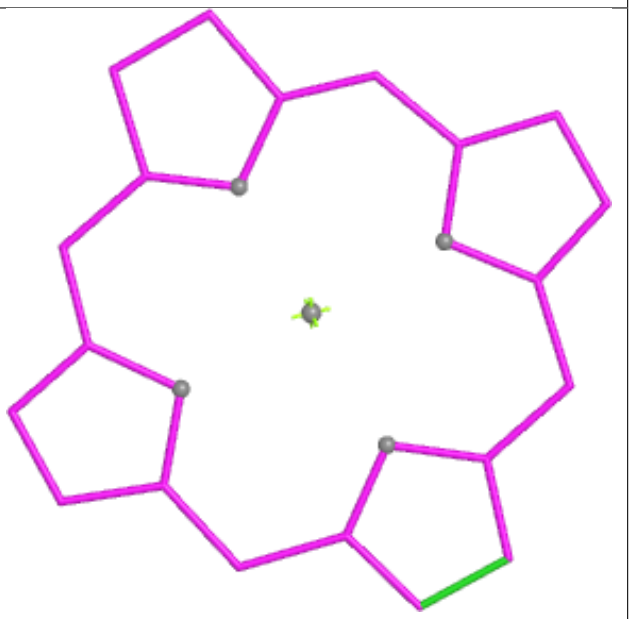
**Ligand CLA 1 202**



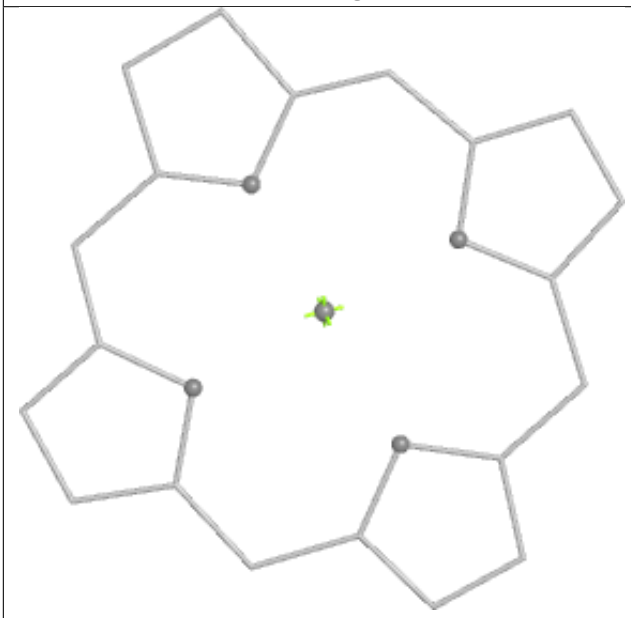
**Ligand CLA 3 315**



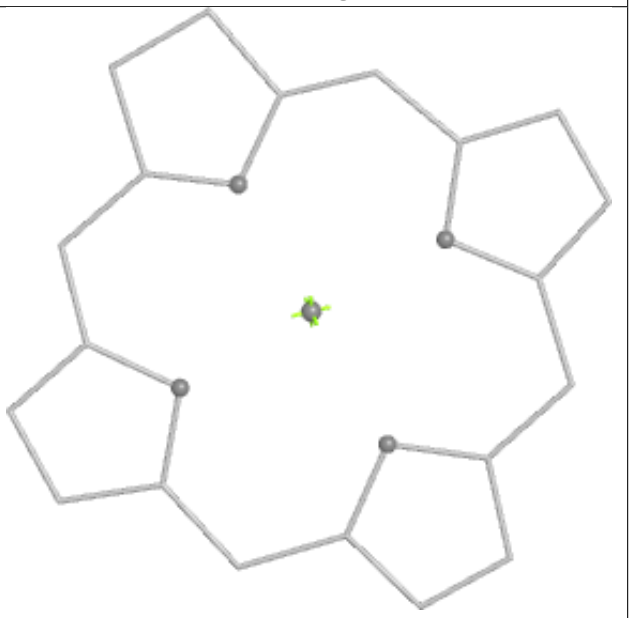
**Bond lengths**



**Bond angles**

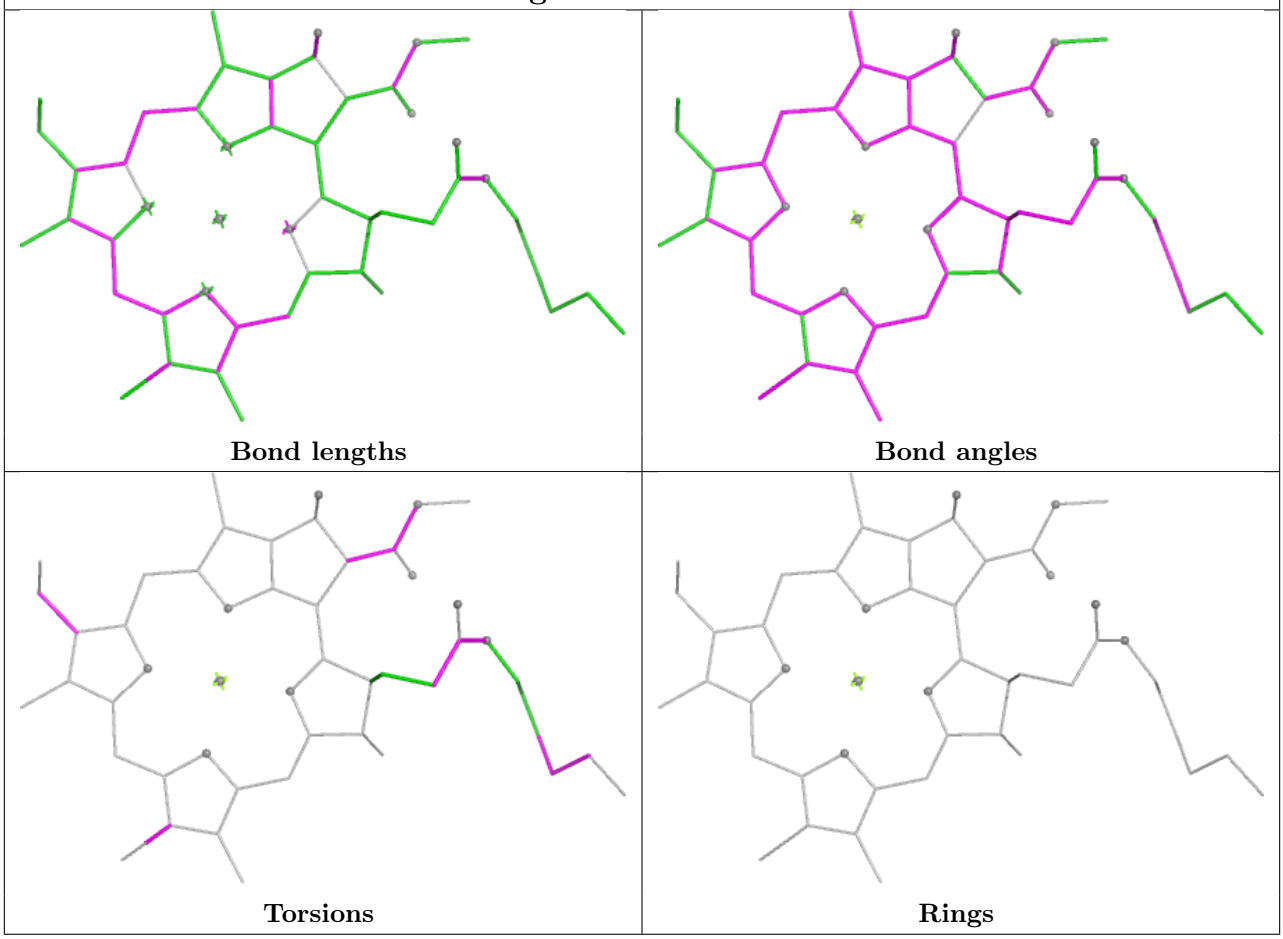


**Torsions**

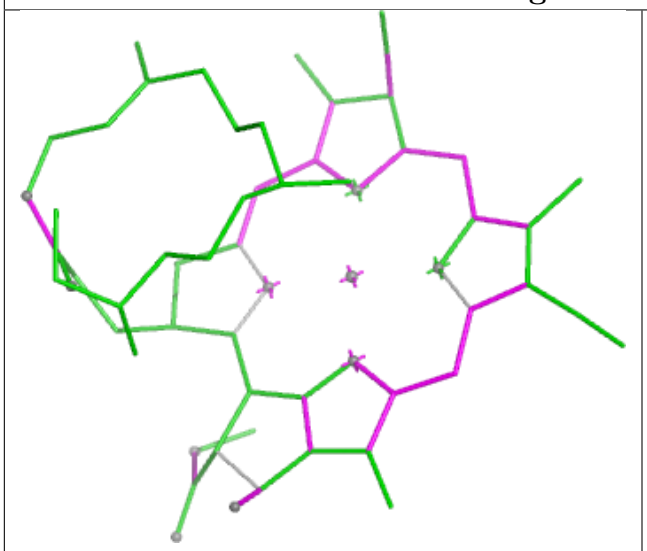


**Rings**

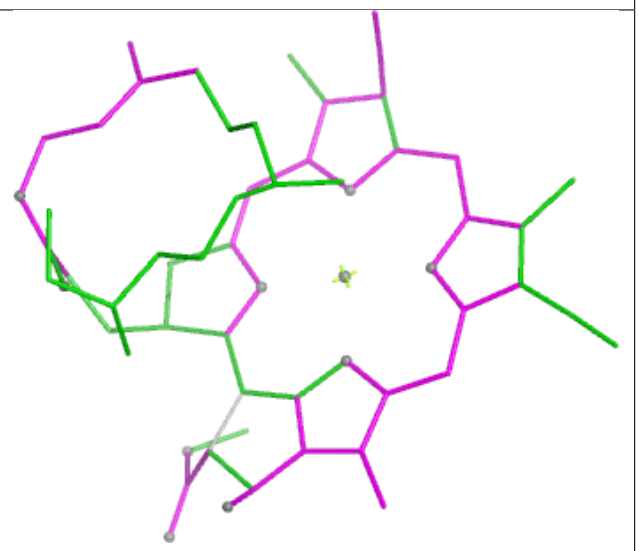
**Ligand CLA 4 317**



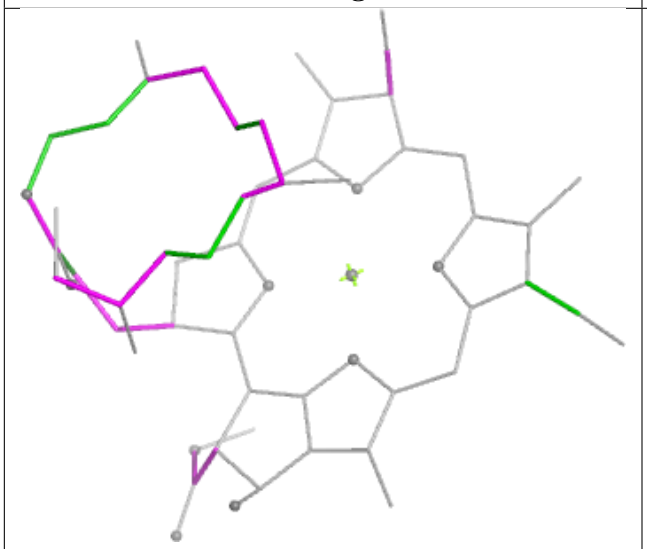
**Ligand CLA J 103**



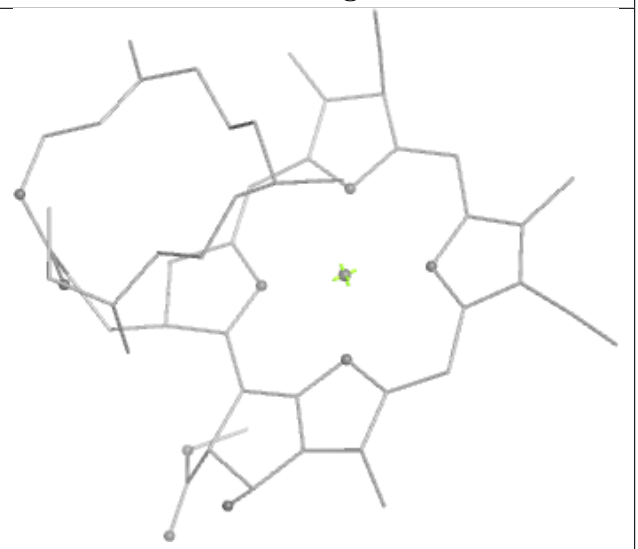
**Bond lengths**



**Bond angles**

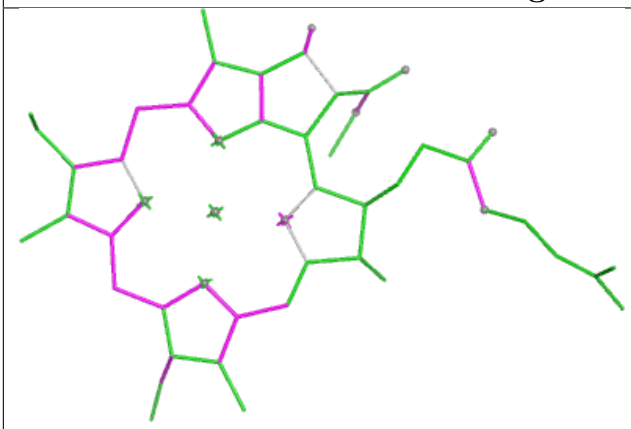


**Torsions**

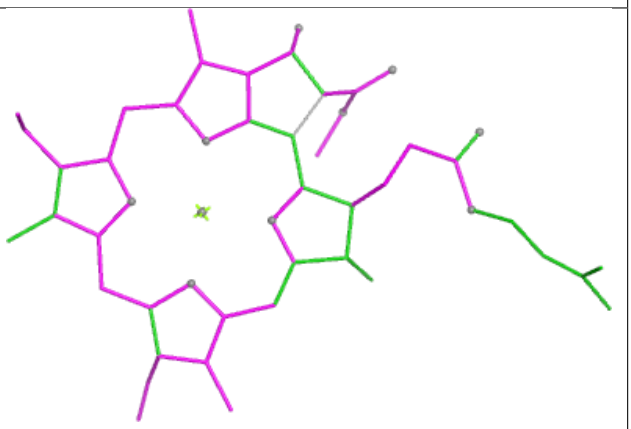


**Rings**

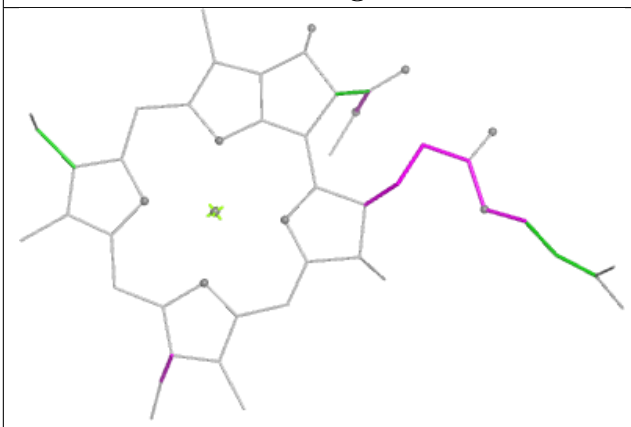
## Ligand CLA 4 310



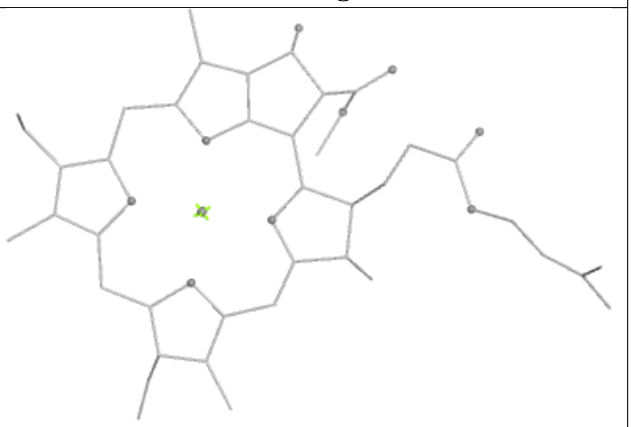
Bond lengths



Bond angles

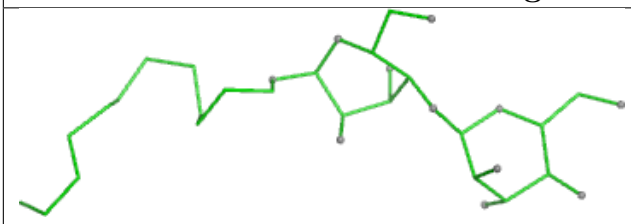


Torsions

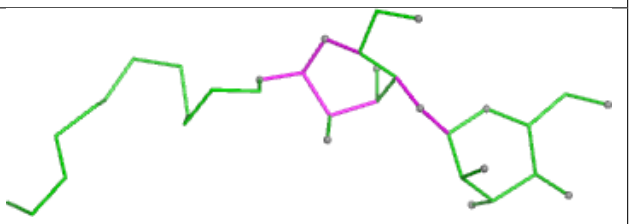


Rings

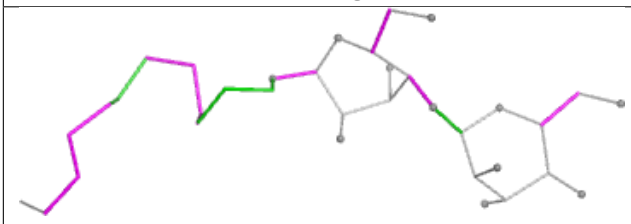
## Ligand LMU 3 319



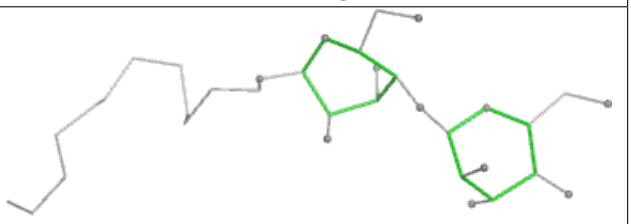
Bond lengths



Bond angles

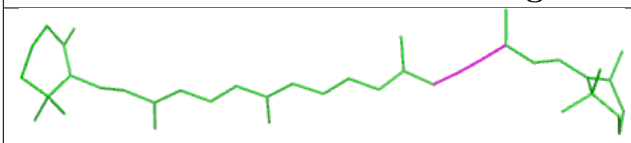


Torsions

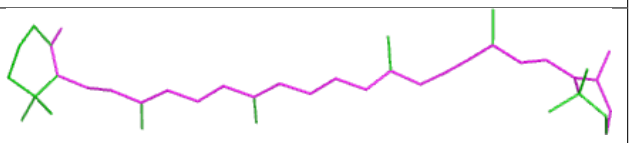


Rings

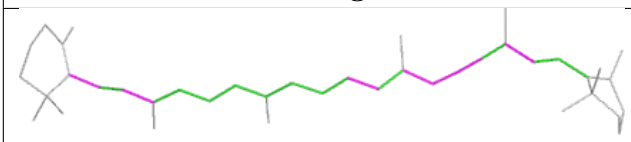
## Ligand BCR J 102



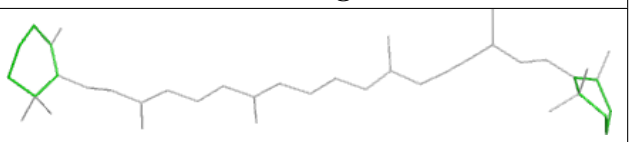
Bond lengths



Bond angles

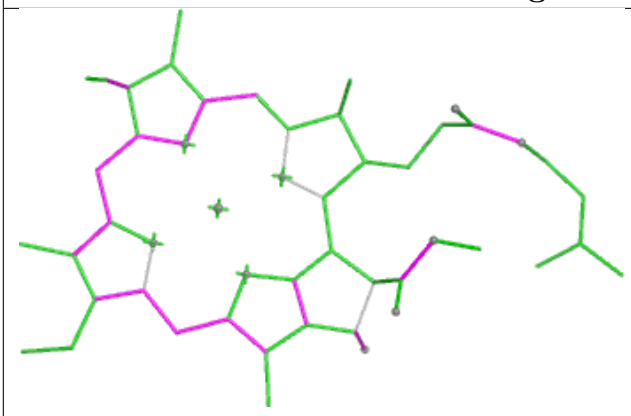


Torsions

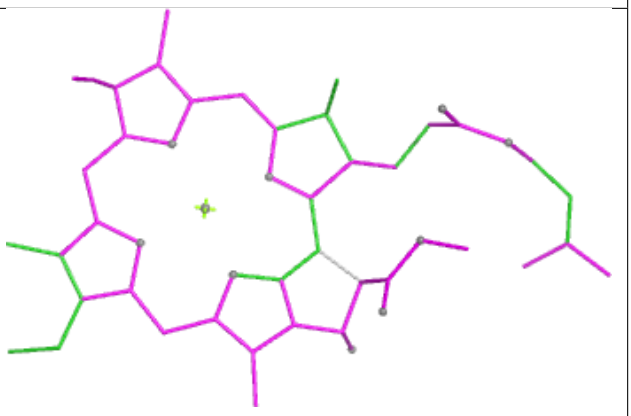


Rings

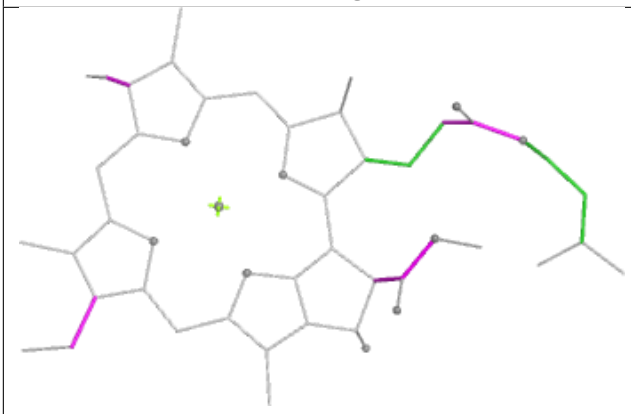
## Ligand CLA 2 311



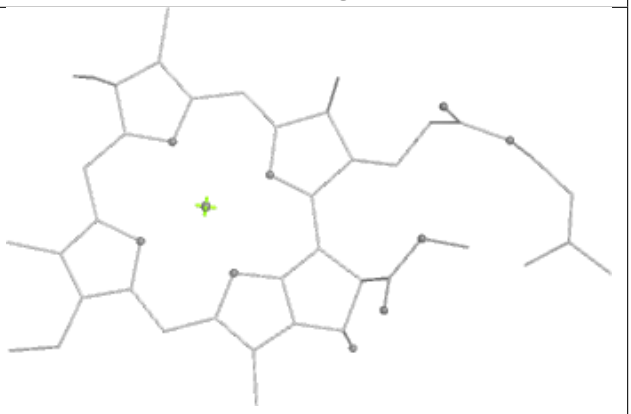
Bond lengths



Bond angles

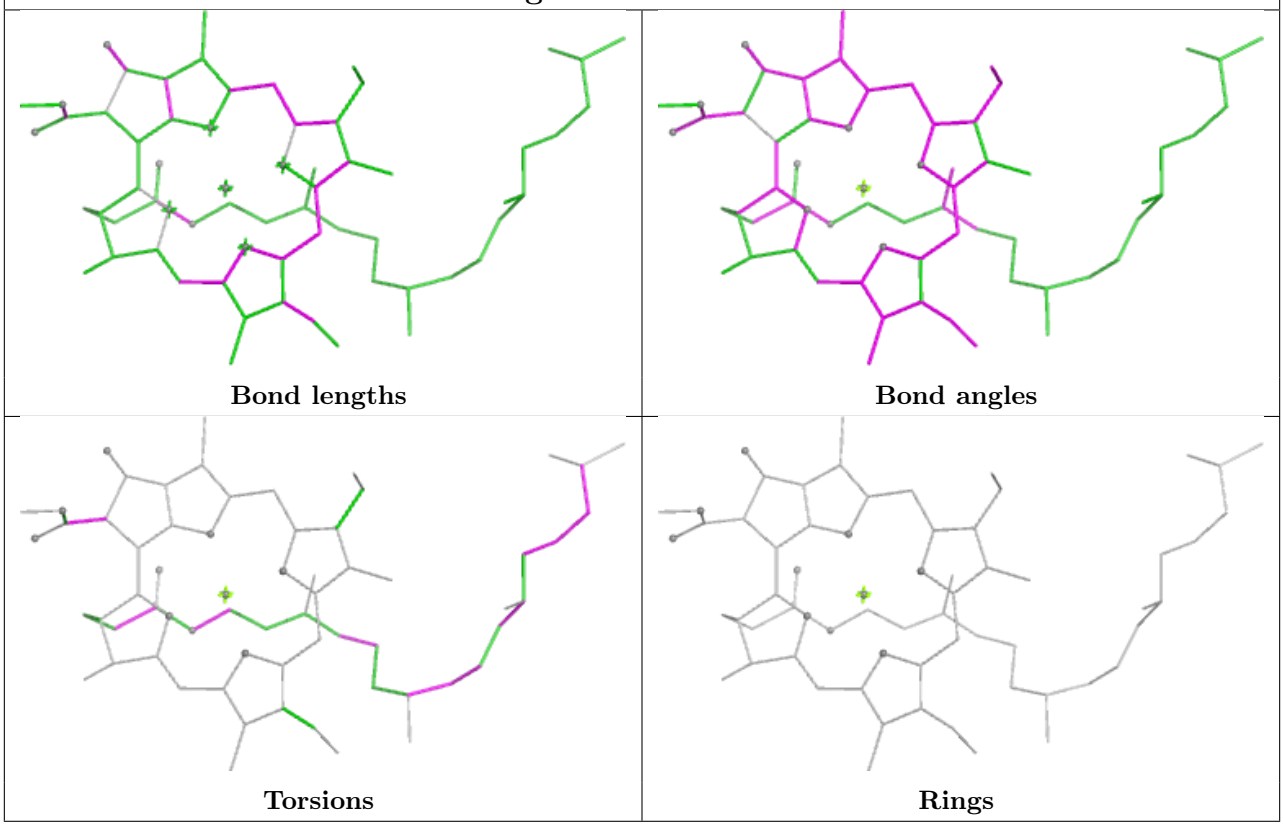


Torsions

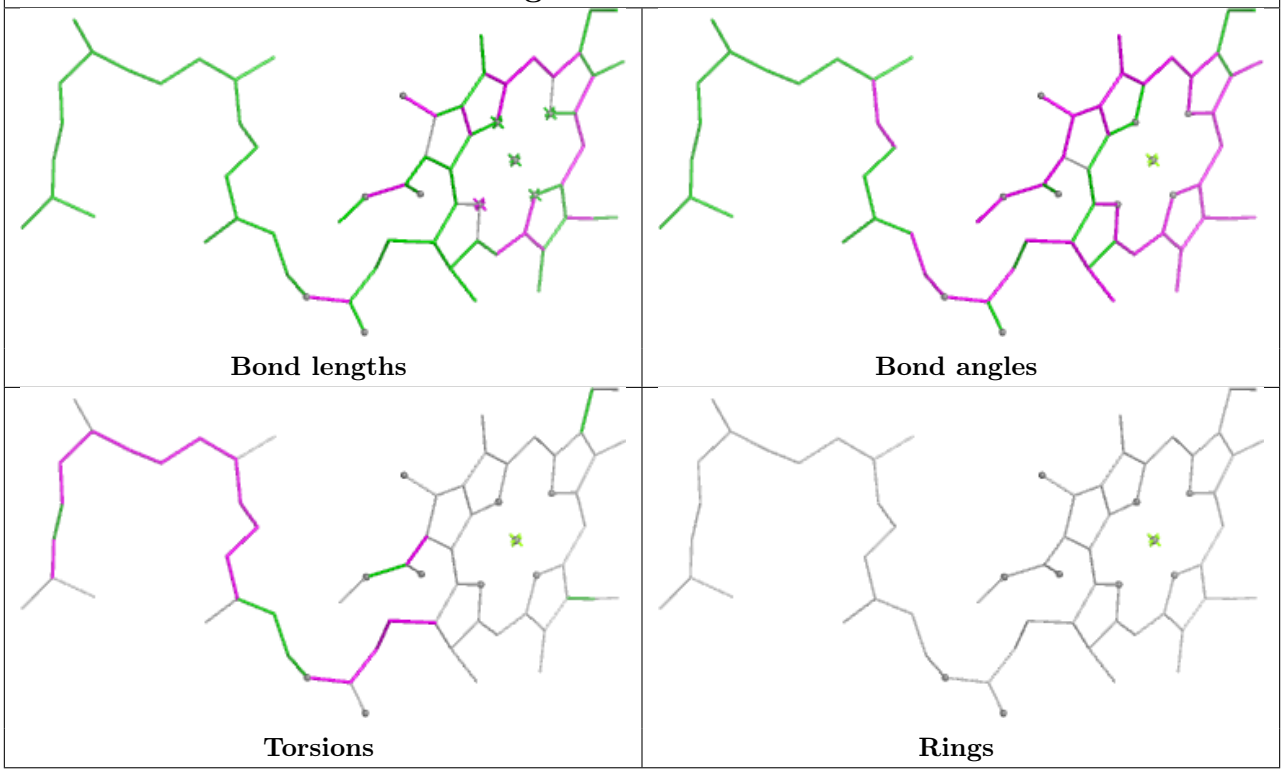


Rings

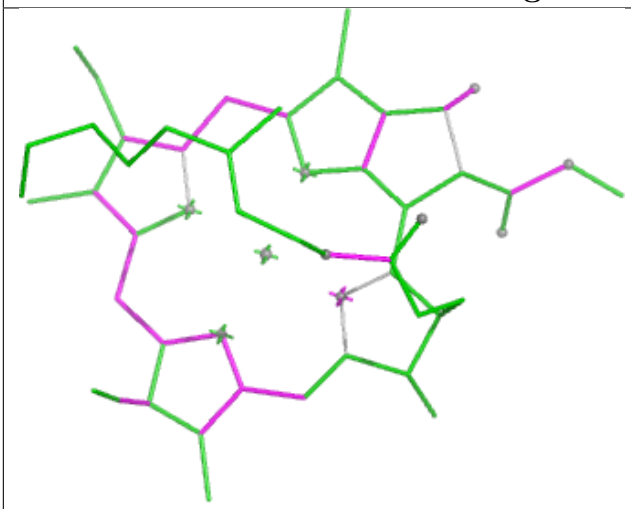
## Ligand CLA B 838



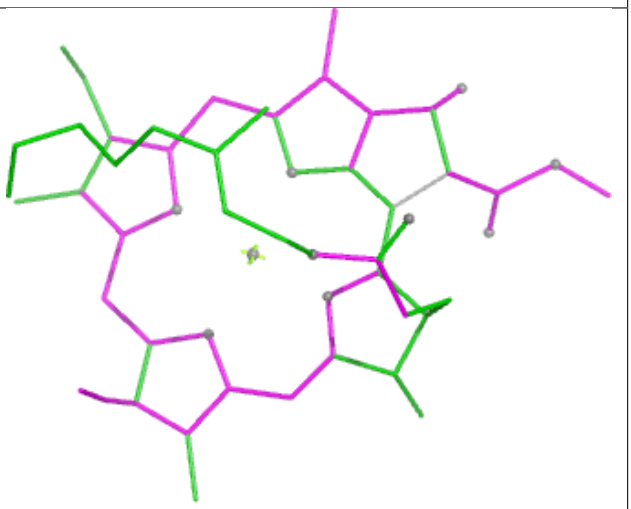

## Ligand CLA A 849



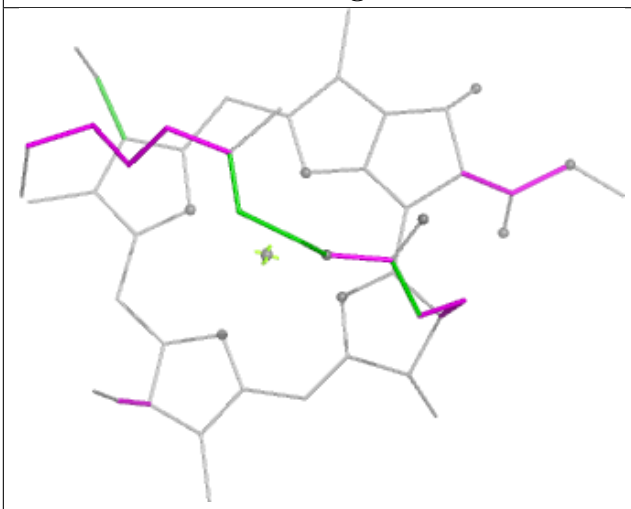
**Ligand CLA A 812**



**Bond lengths**



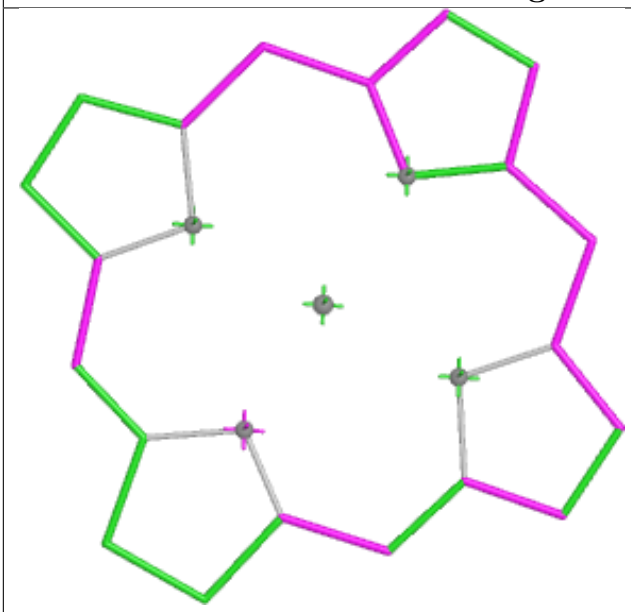
**Bond angles**



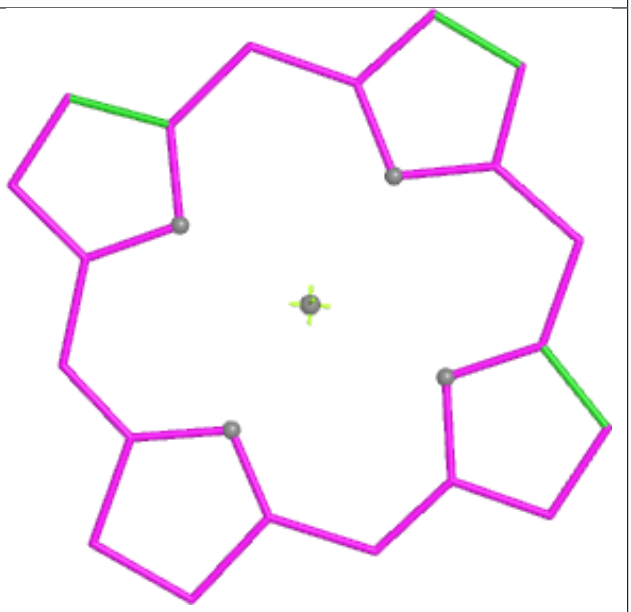
**Torsions**

**Rings**

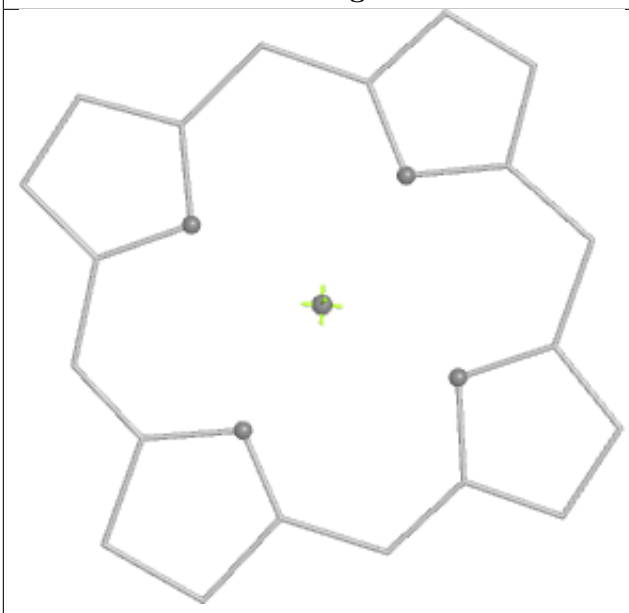
**Ligand CLA 2 308**



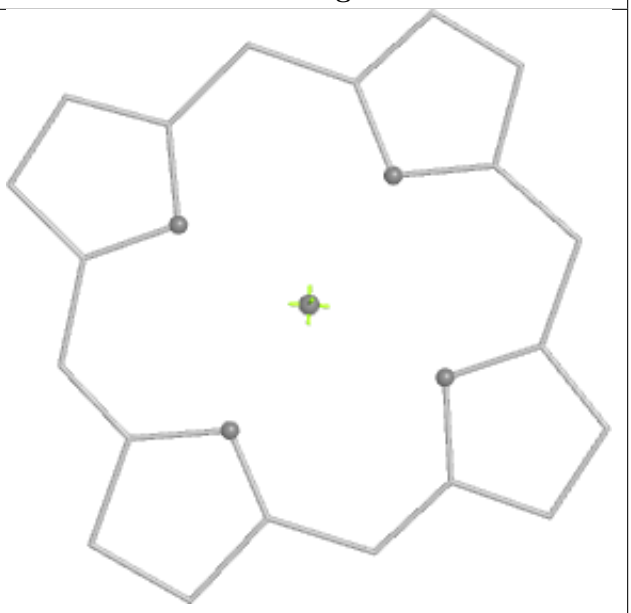
**Bond lengths**



**Bond angles**

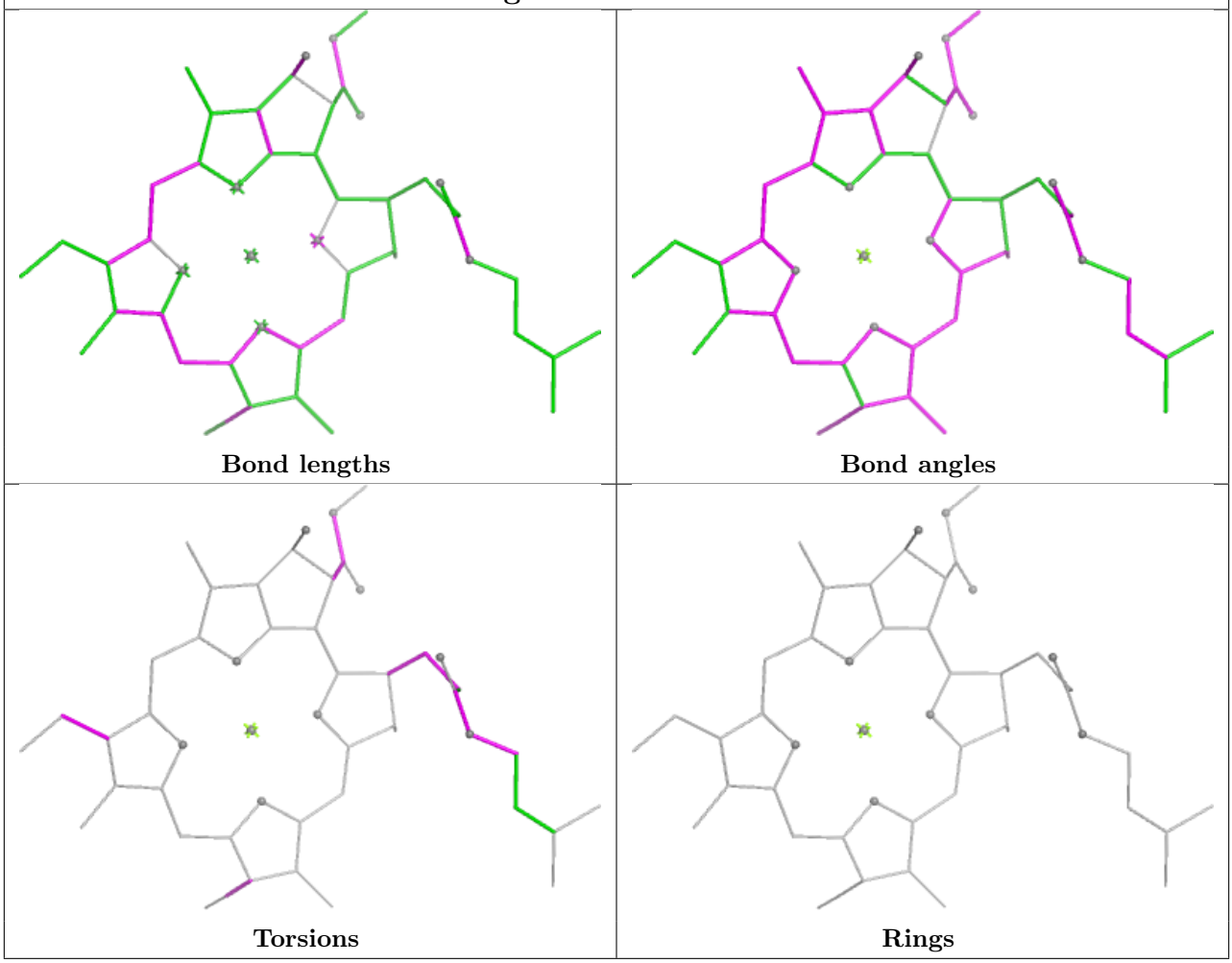


**Torsions**

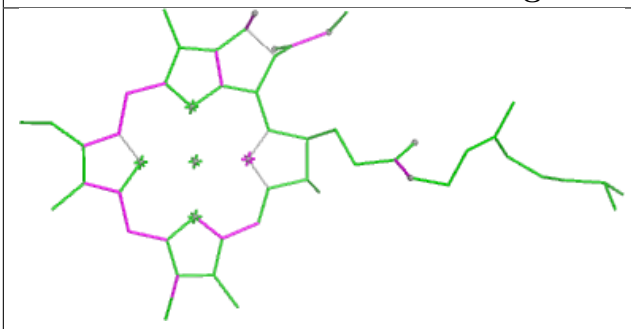


**Rings**

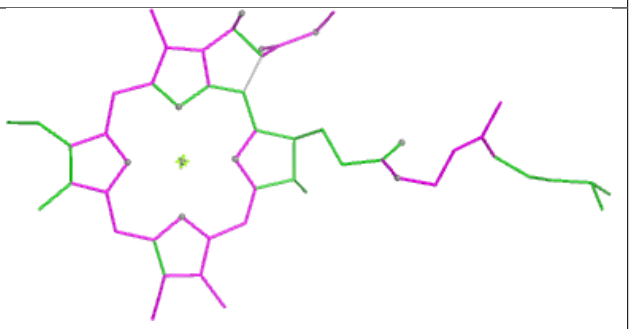
**Ligand CLA A 832**



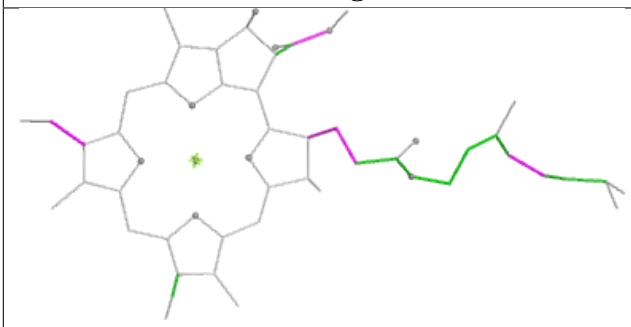
## Ligand CLA A 840



Bond lengths



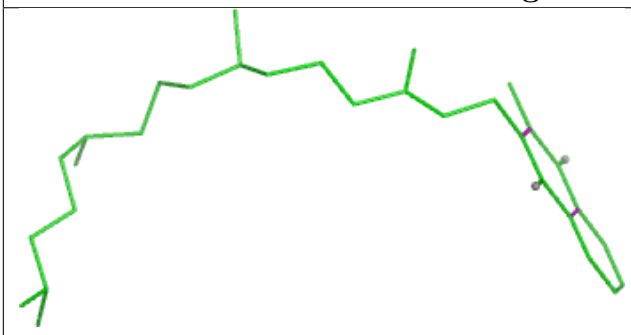
Bond angles



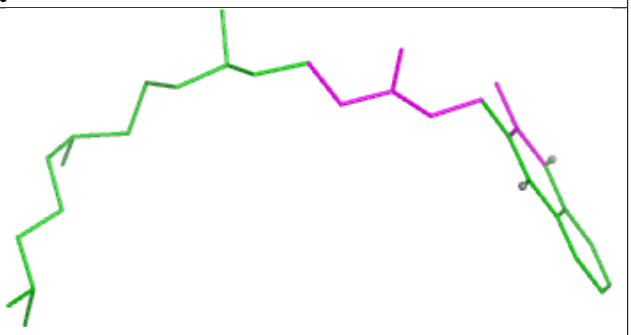
Torsions

Rings

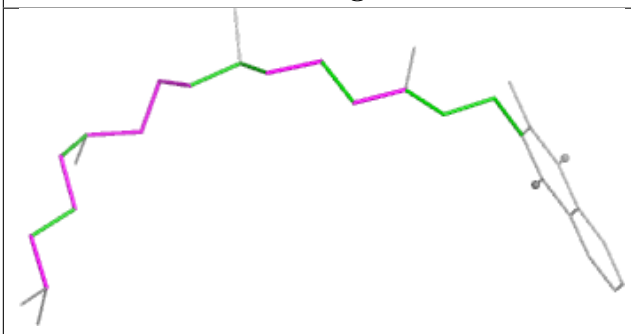
## Ligand PQN B 843



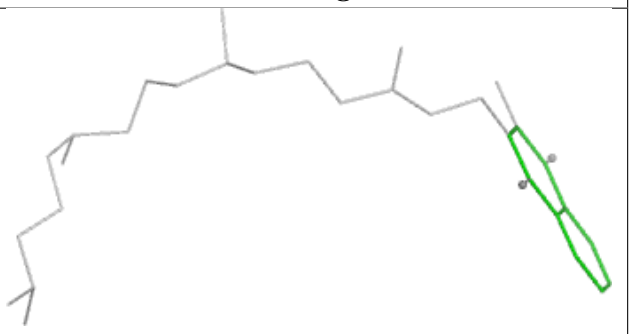
Bond lengths



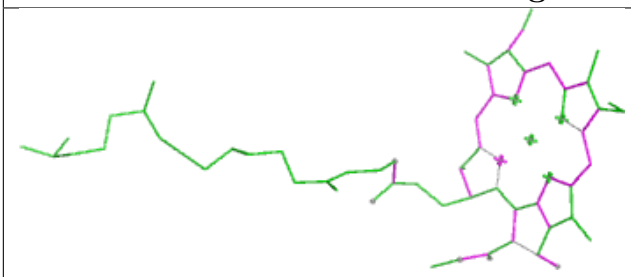
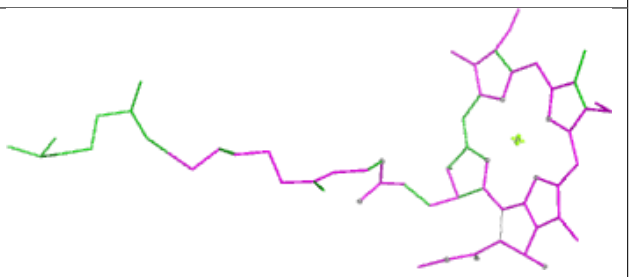
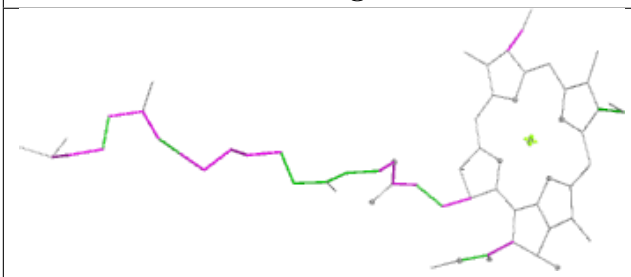
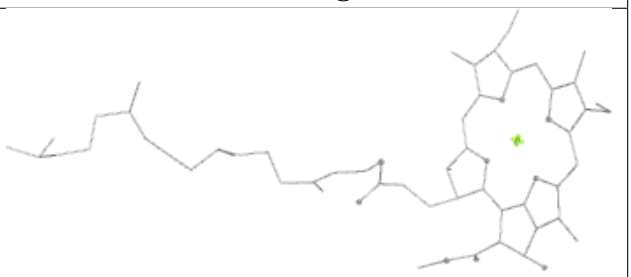
Bond angles



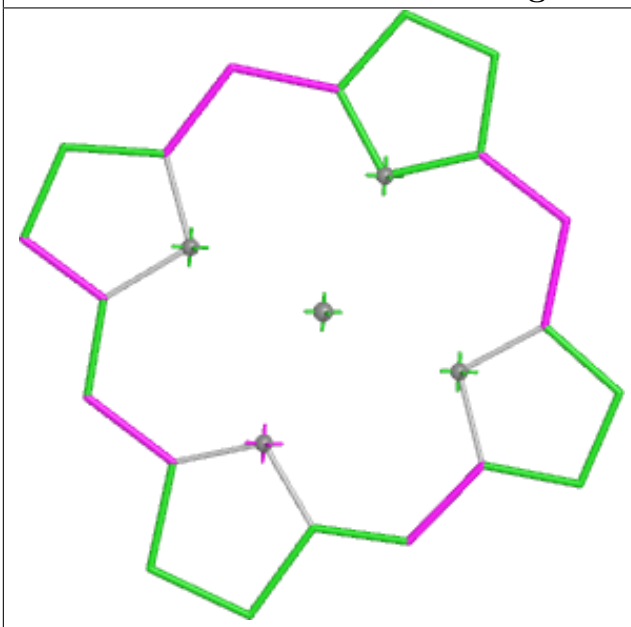
Torsions



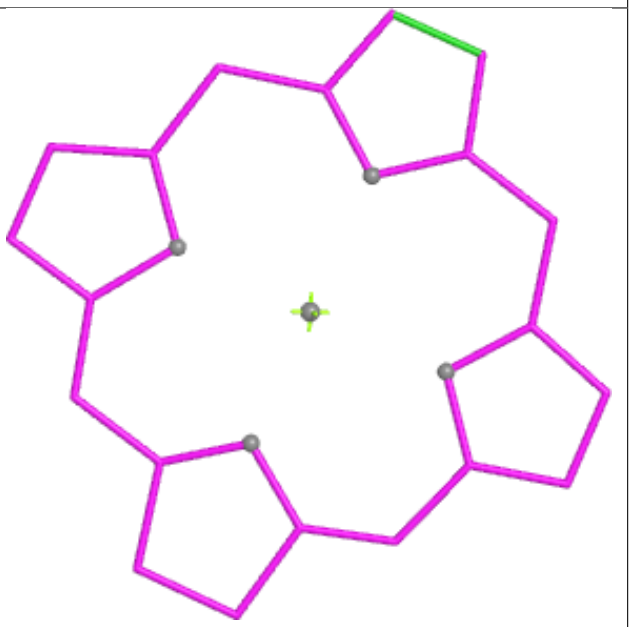
Rings

| Ligand CLA 4 303 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

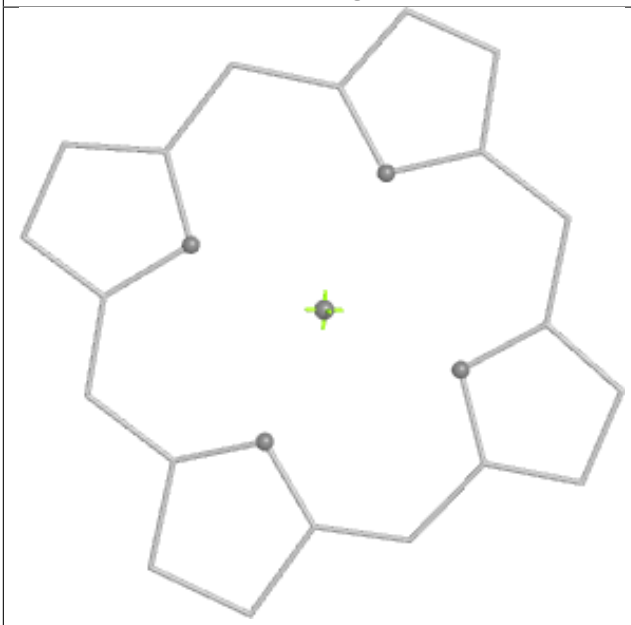
## Ligand CLA 2 301



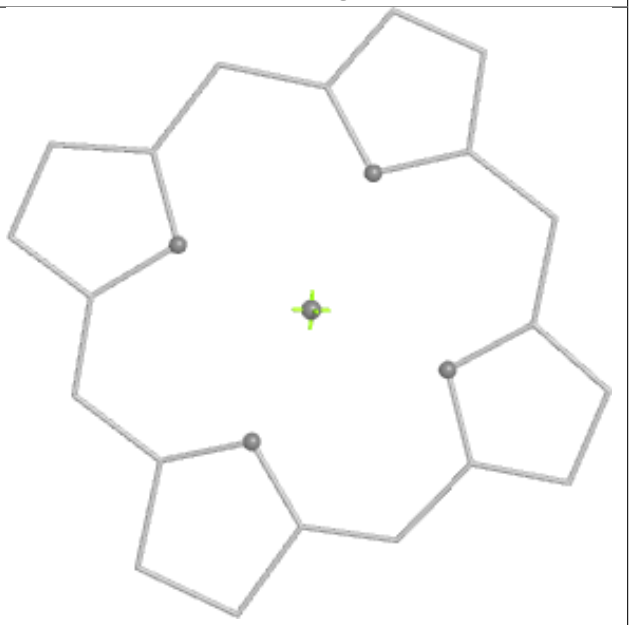
Bond lengths



Bond angles

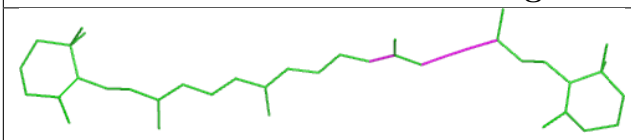


Torsions

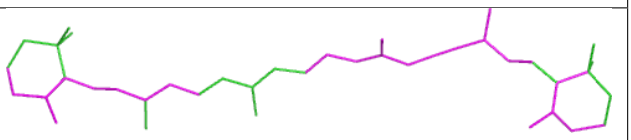


Rings

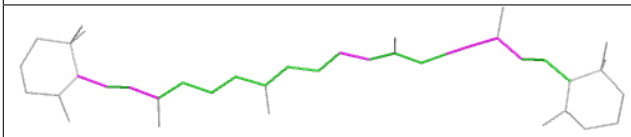
## Ligand BCR L 209



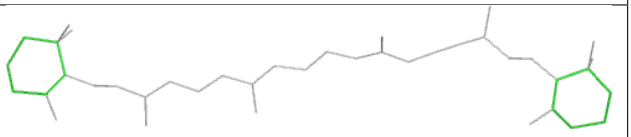
Bond lengths



Bond angles

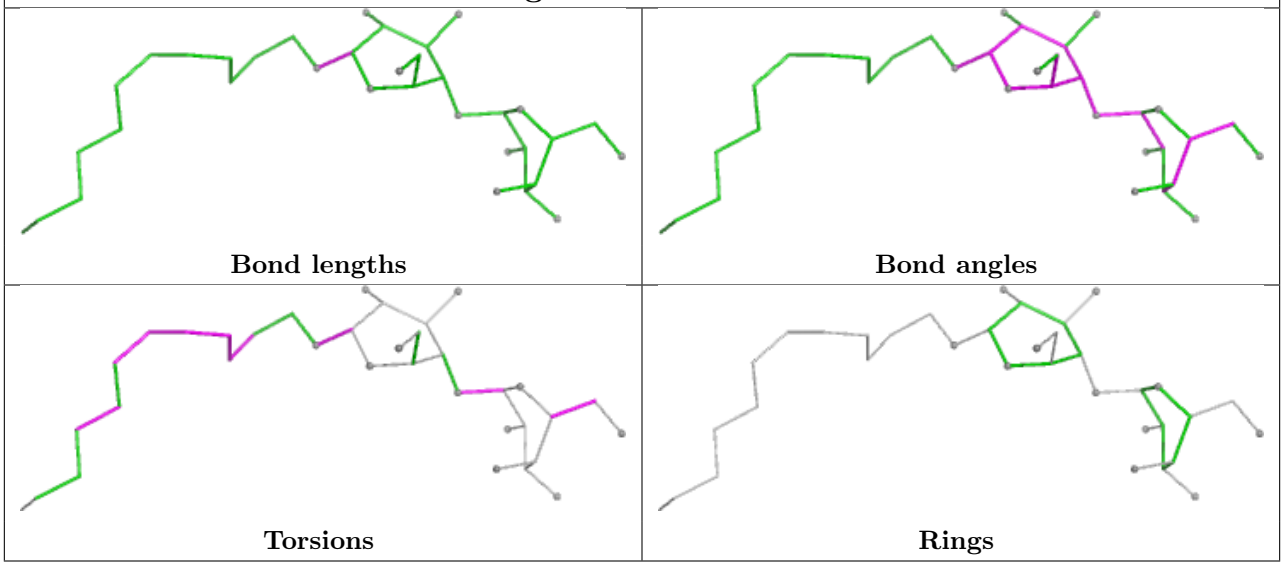


Torsions

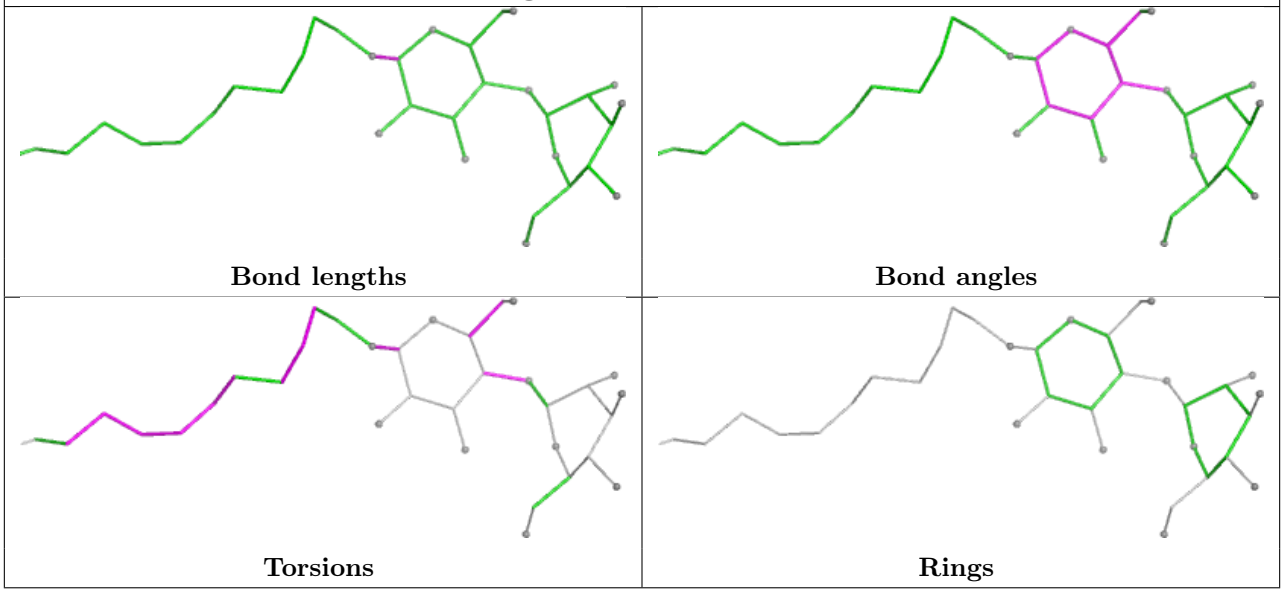


Rings

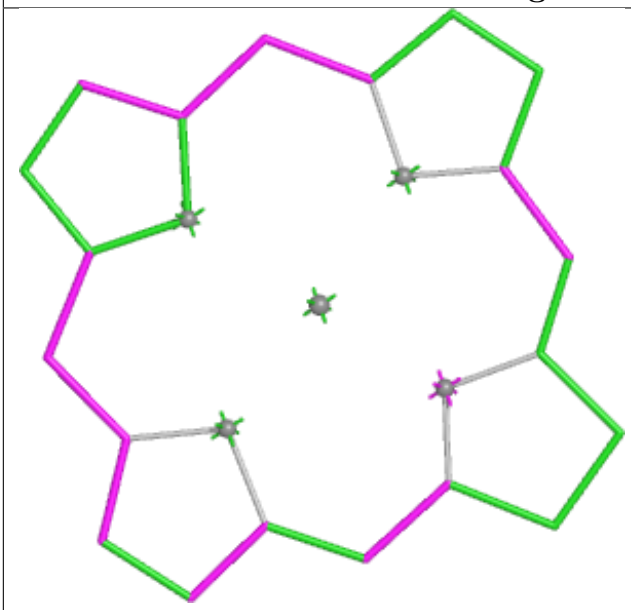
**Ligand LMU 2 319**



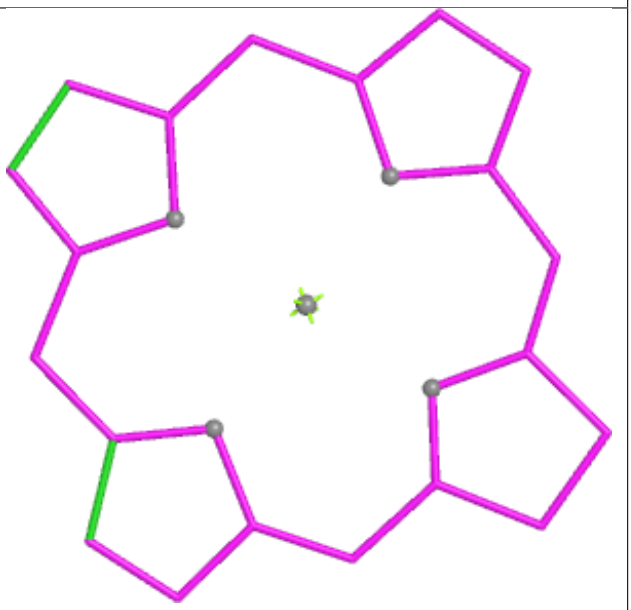

**Ligand LMU A 855**



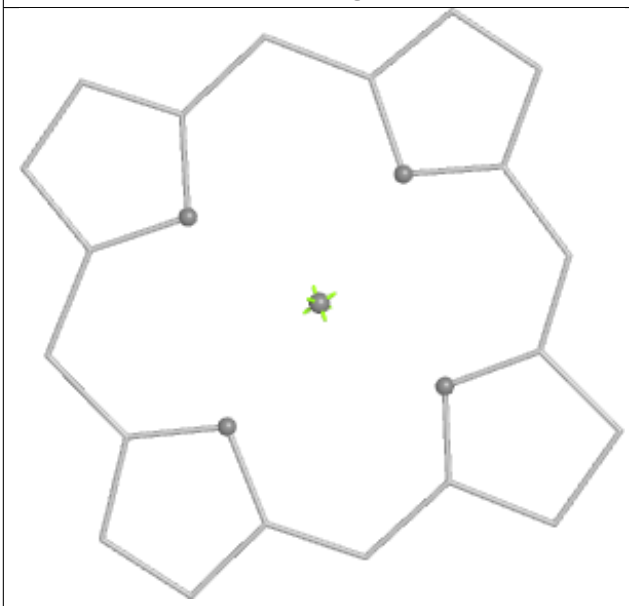
**Ligand CLA 2 309**



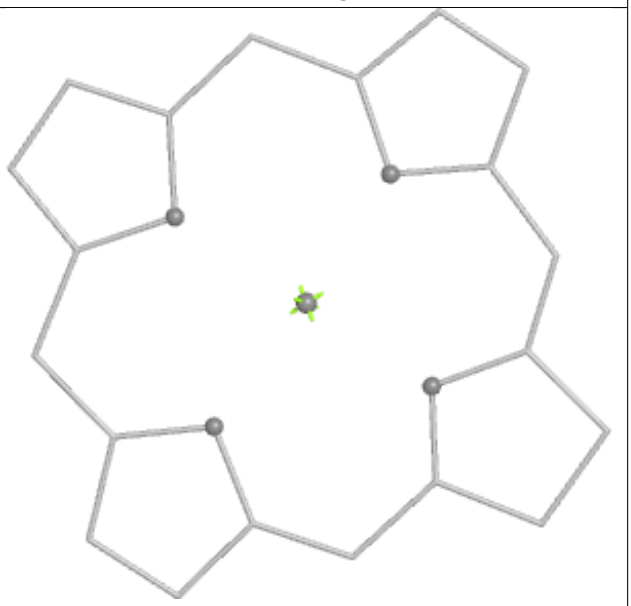
**Bond lengths**



**Bond angles**

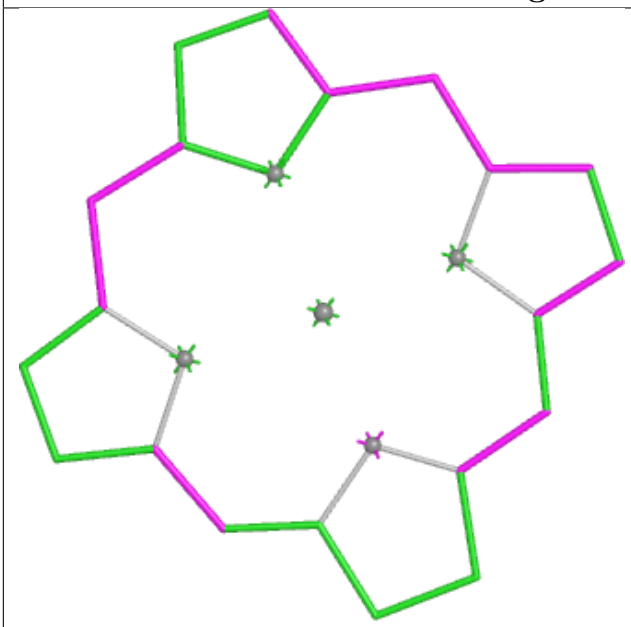


**Torsions**

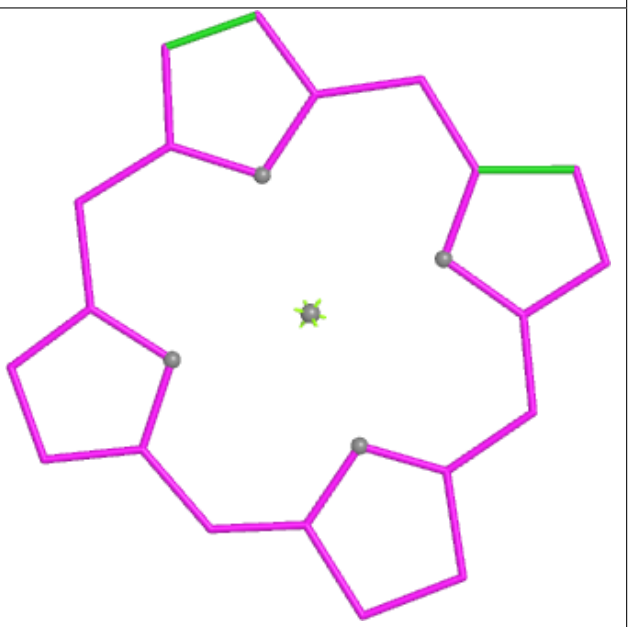


**Rings**

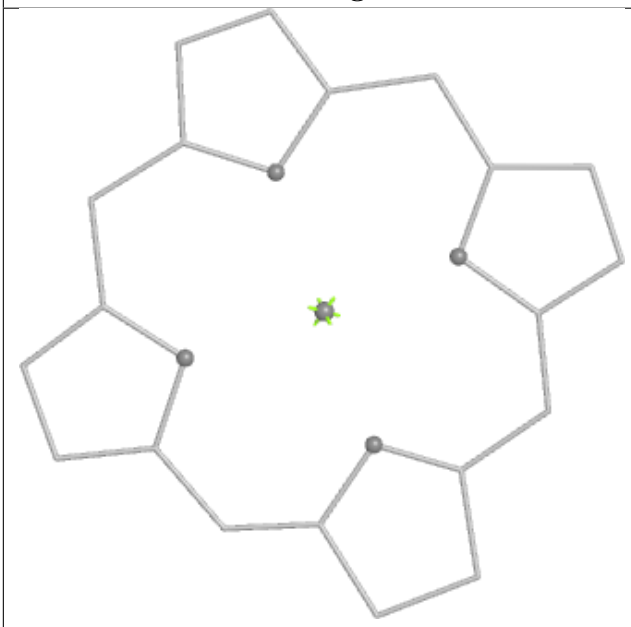
**Ligand CLA 2 315**



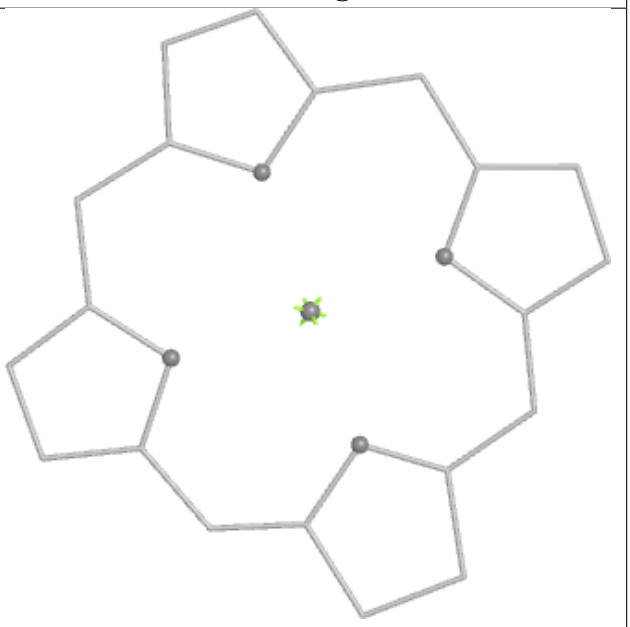
**Bond lengths**



**Bond angles**

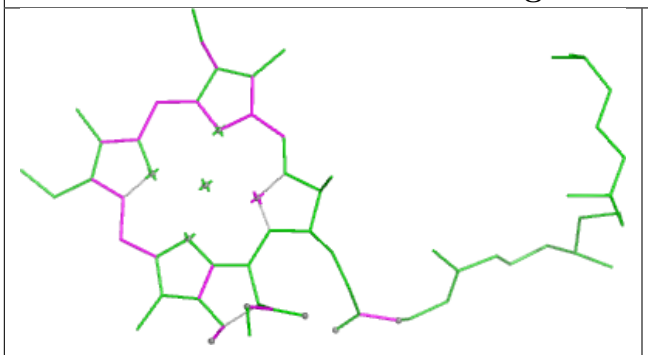


**Torsions**



**Rings**

**Ligand CLA A 825**



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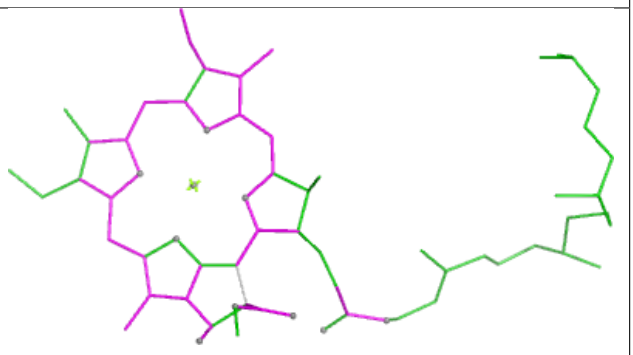
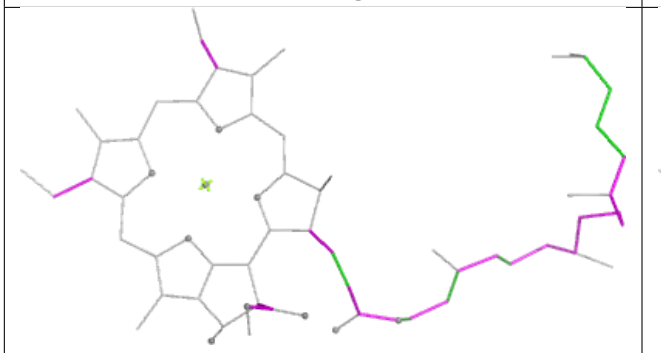


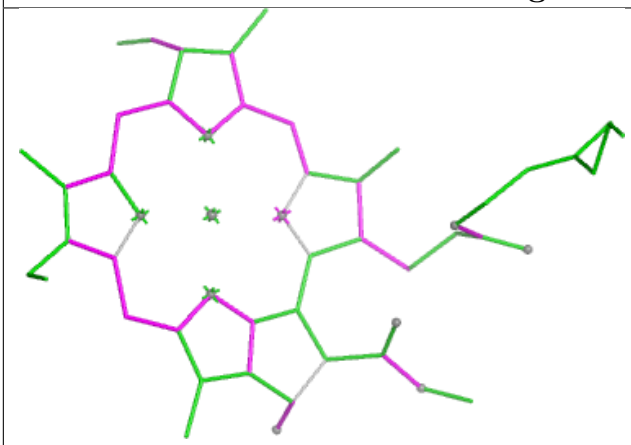
**Bond angles**



**Torsions**

**Rings**

**Ligand CLA 4 306**



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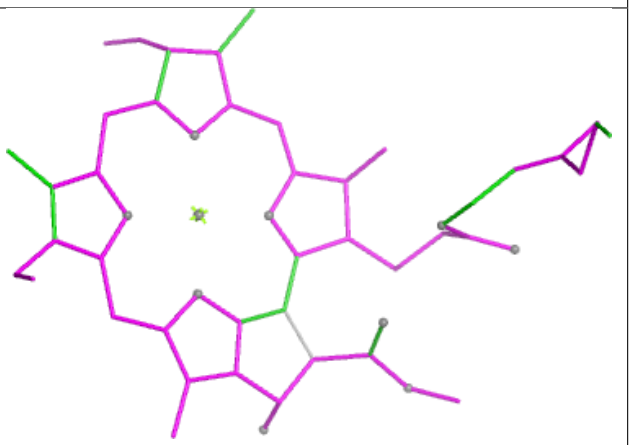
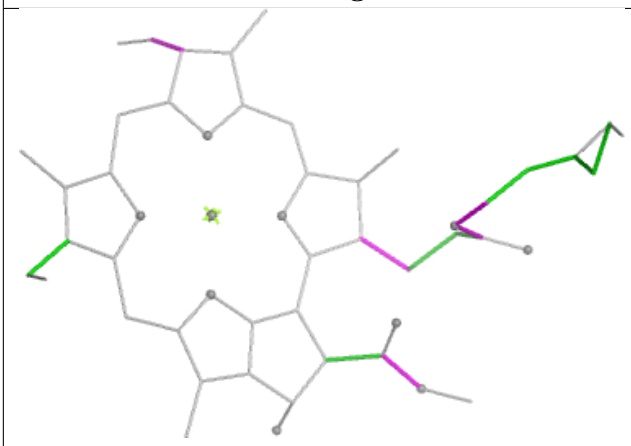
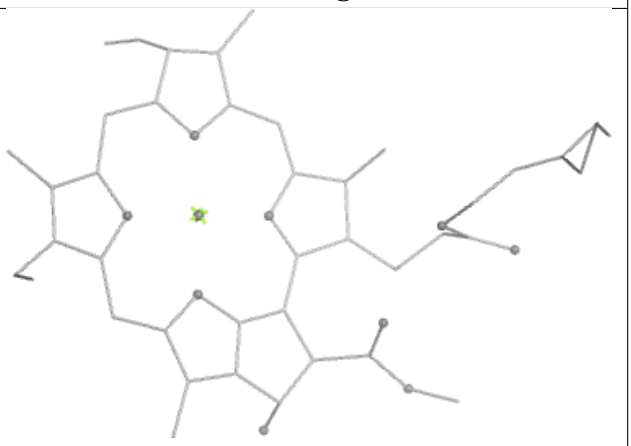


**Bond angles**

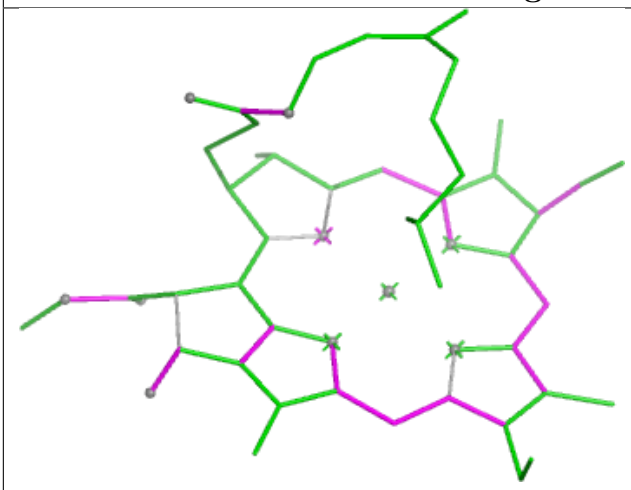


**Torsions**

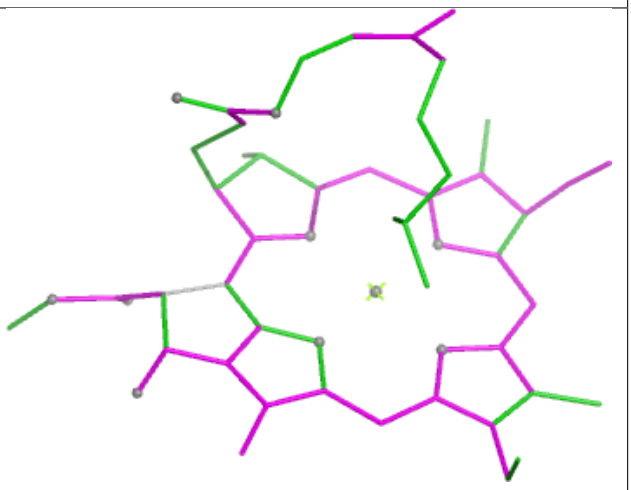


**Rings**

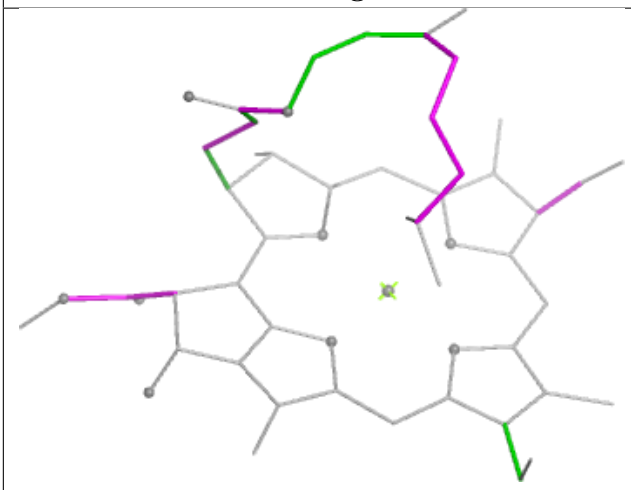
**Ligand CLA B 813**



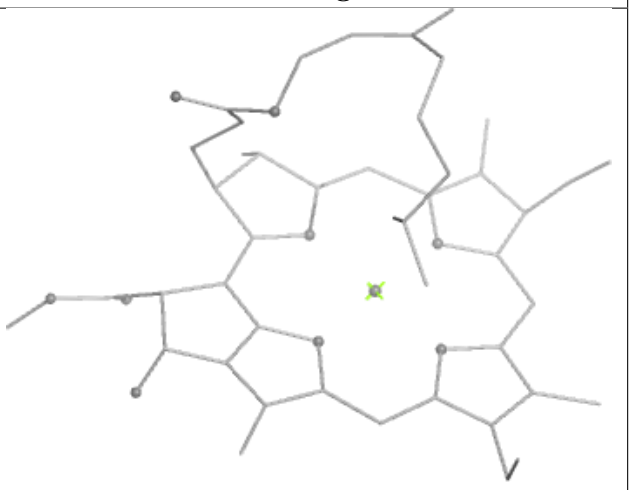
**Bond lengths**



**Bond angles**

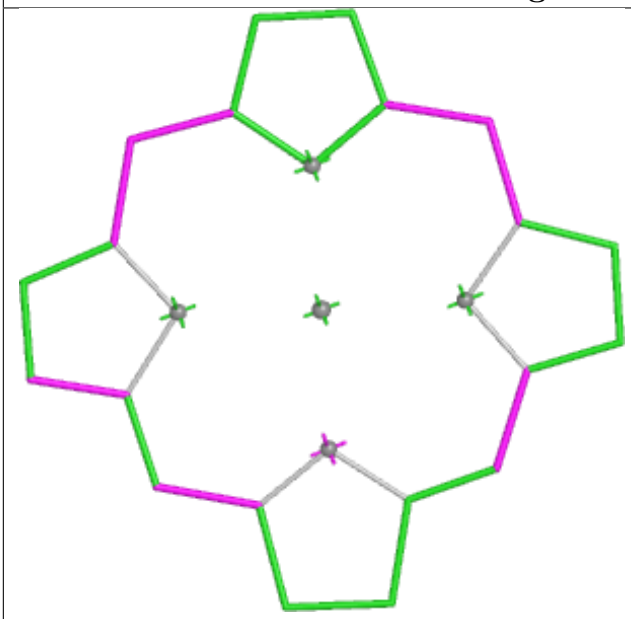


**Torsions**

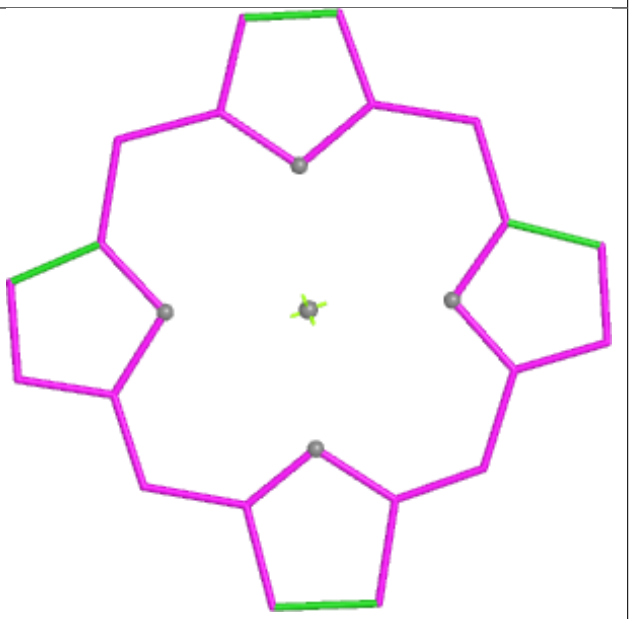


**Rings**

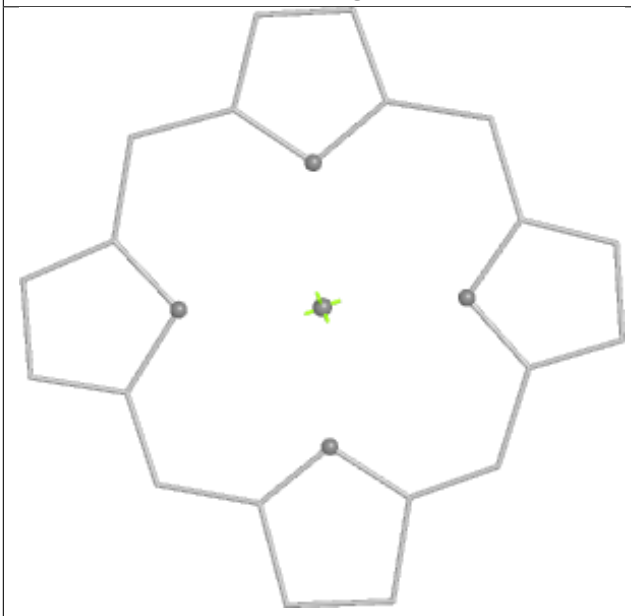
**Ligand CLA 3 302**



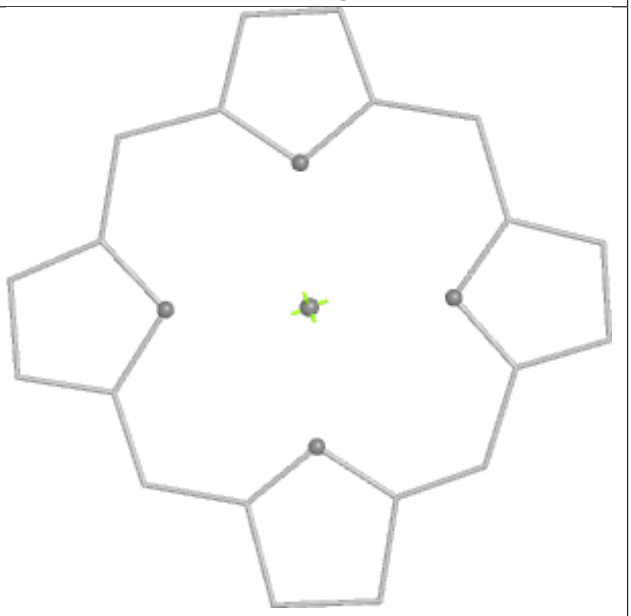
**Bond lengths**



**Bond angles**

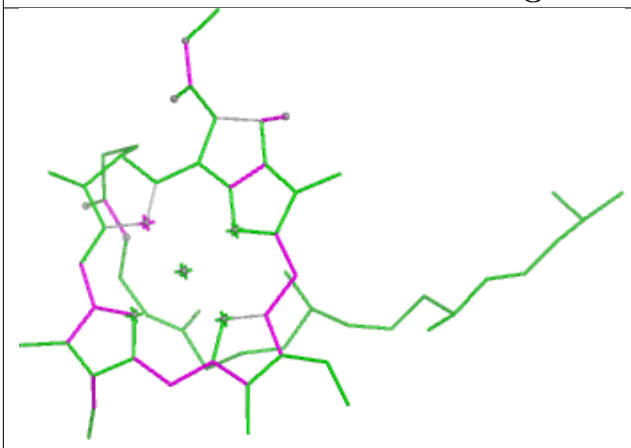


**Torsions**

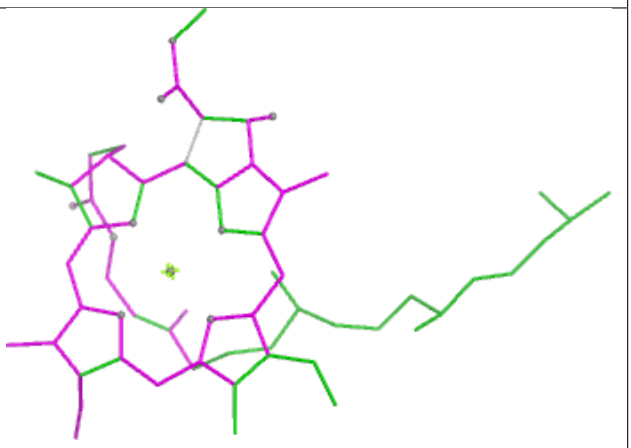


**Rings**

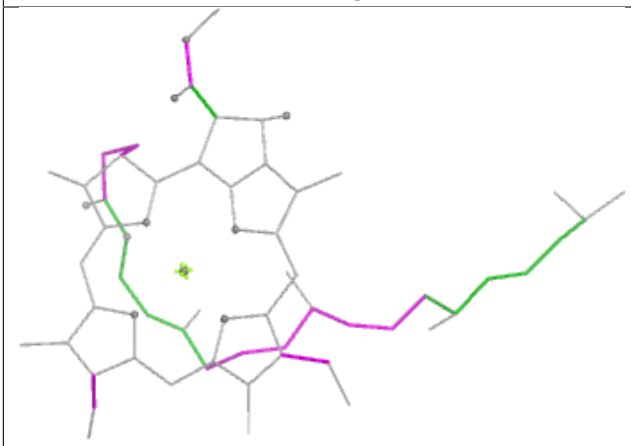
**Ligand CLA B 828**



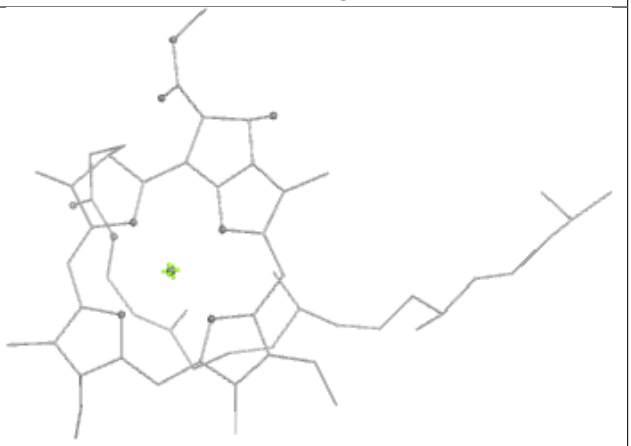
**Bond lengths**



**Bond angles**

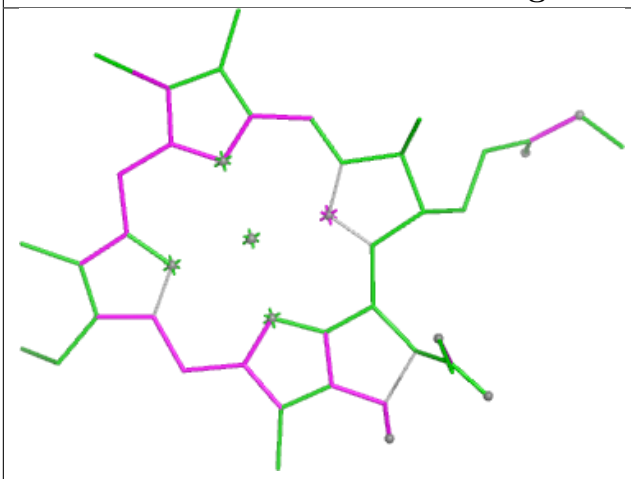


**Torsions**

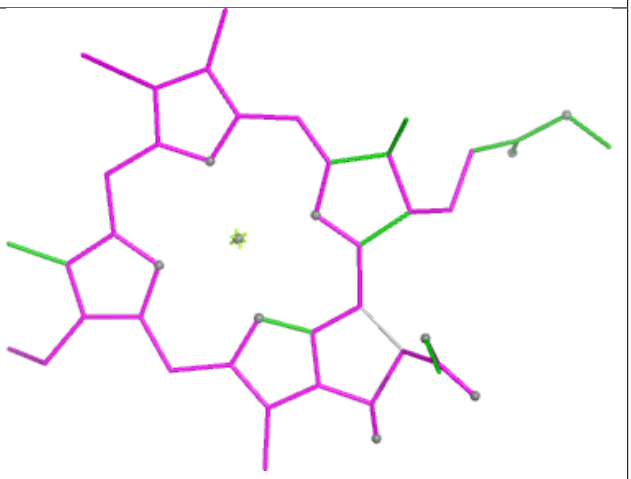


**Rings**

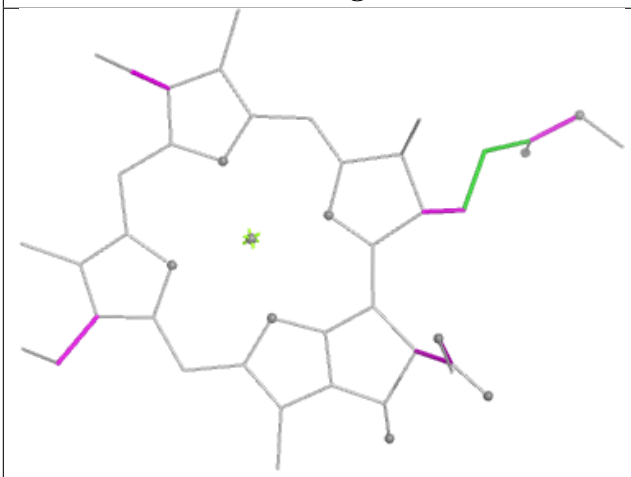
**Ligand CLA 1 201**



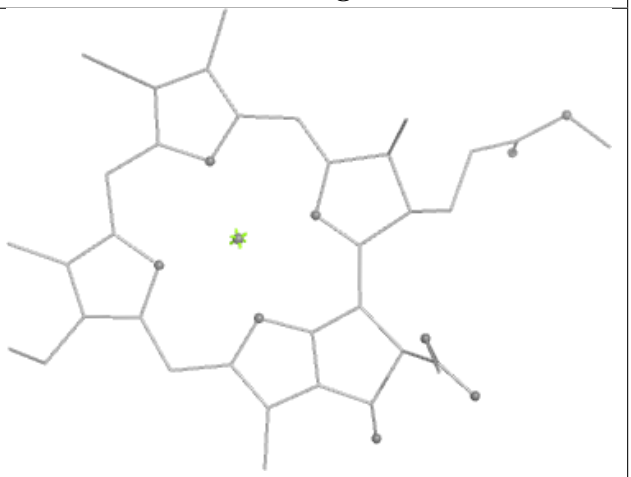
**Bond lengths**



**Bond angles**

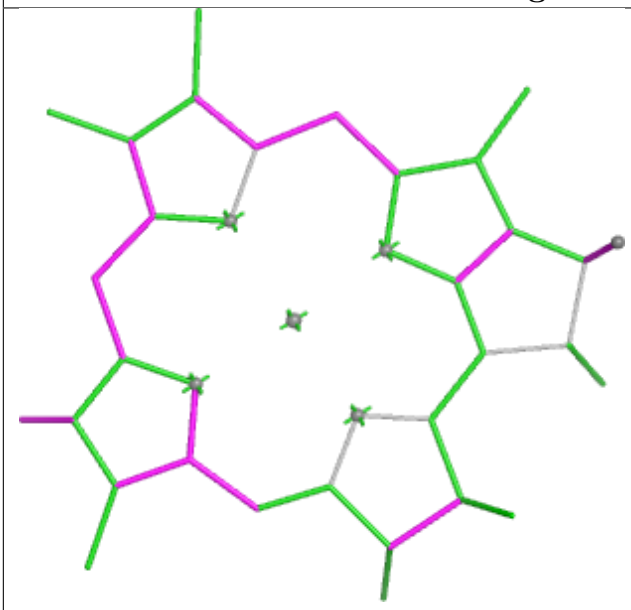


**Torsions**

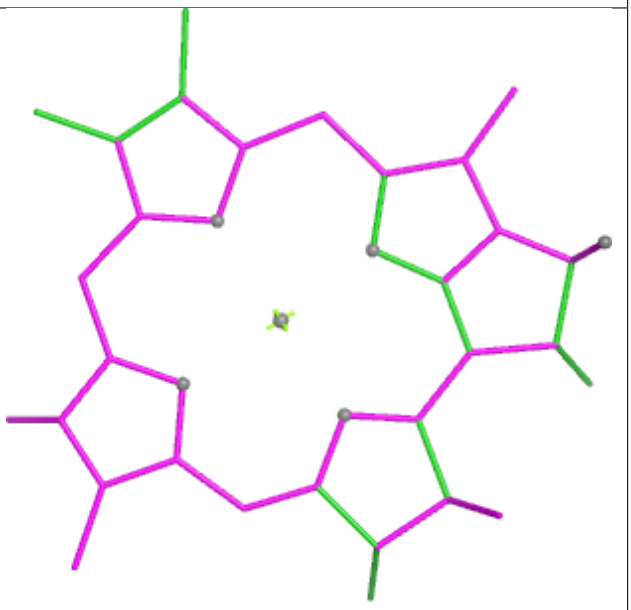


**Rings**

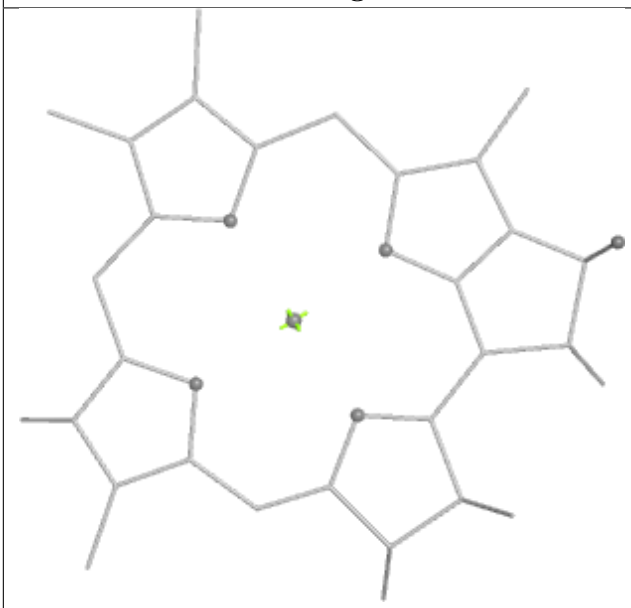
**Ligand CLA 1 205**



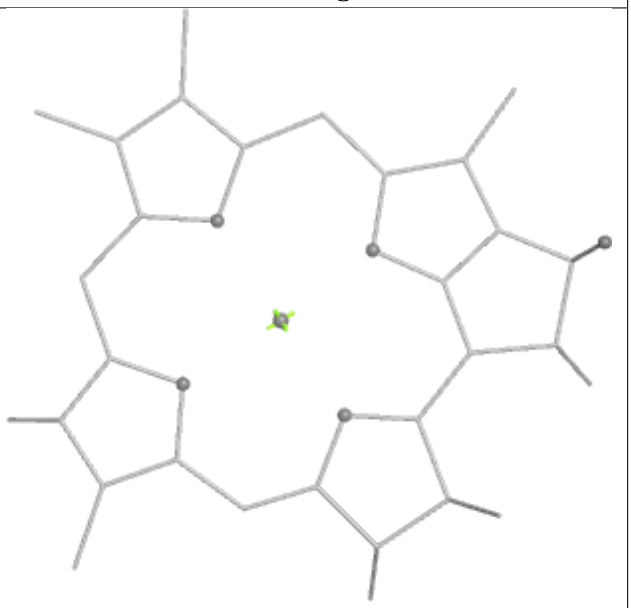
**Bond lengths**



**Bond angles**

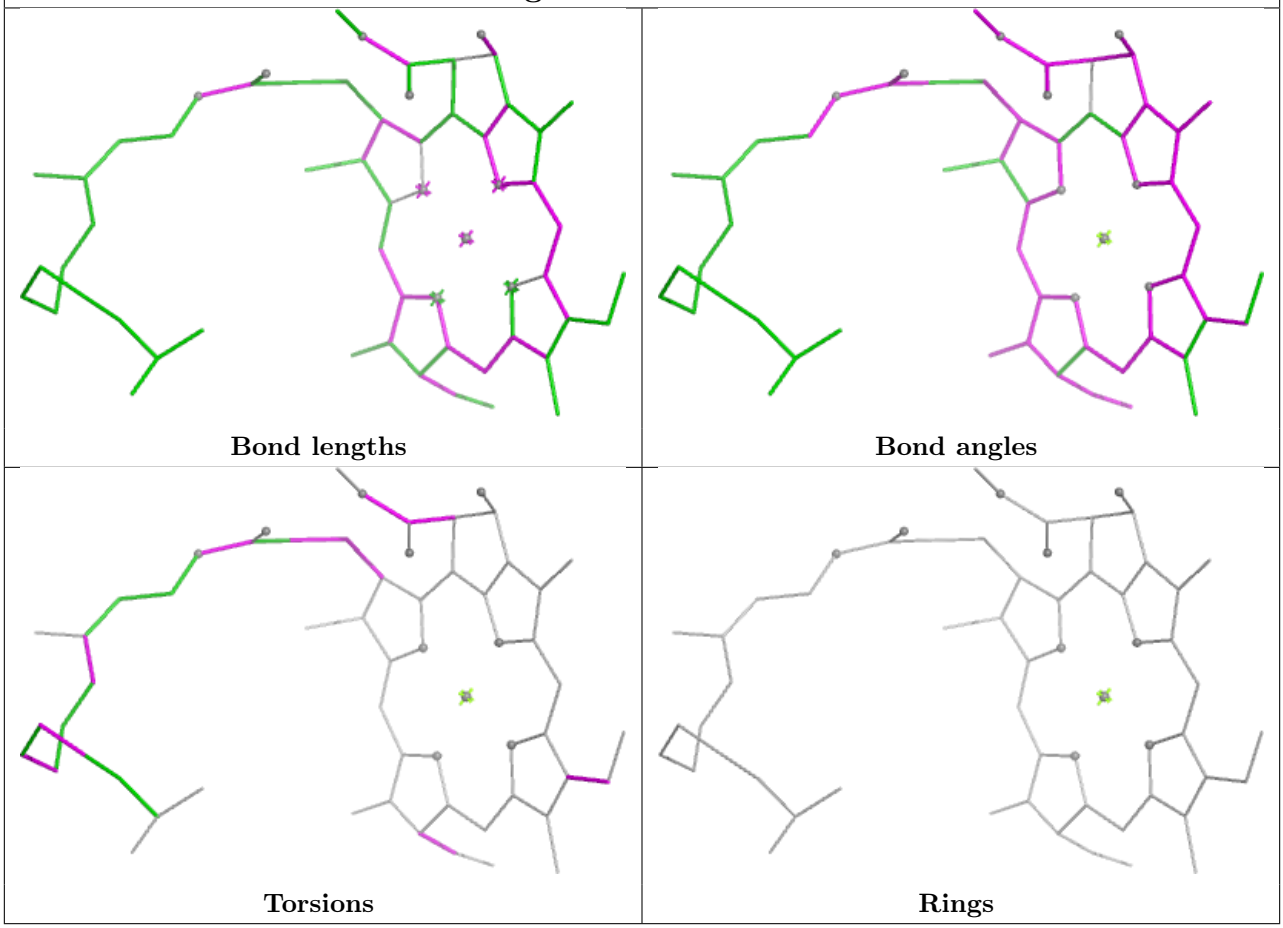


**Torsions**

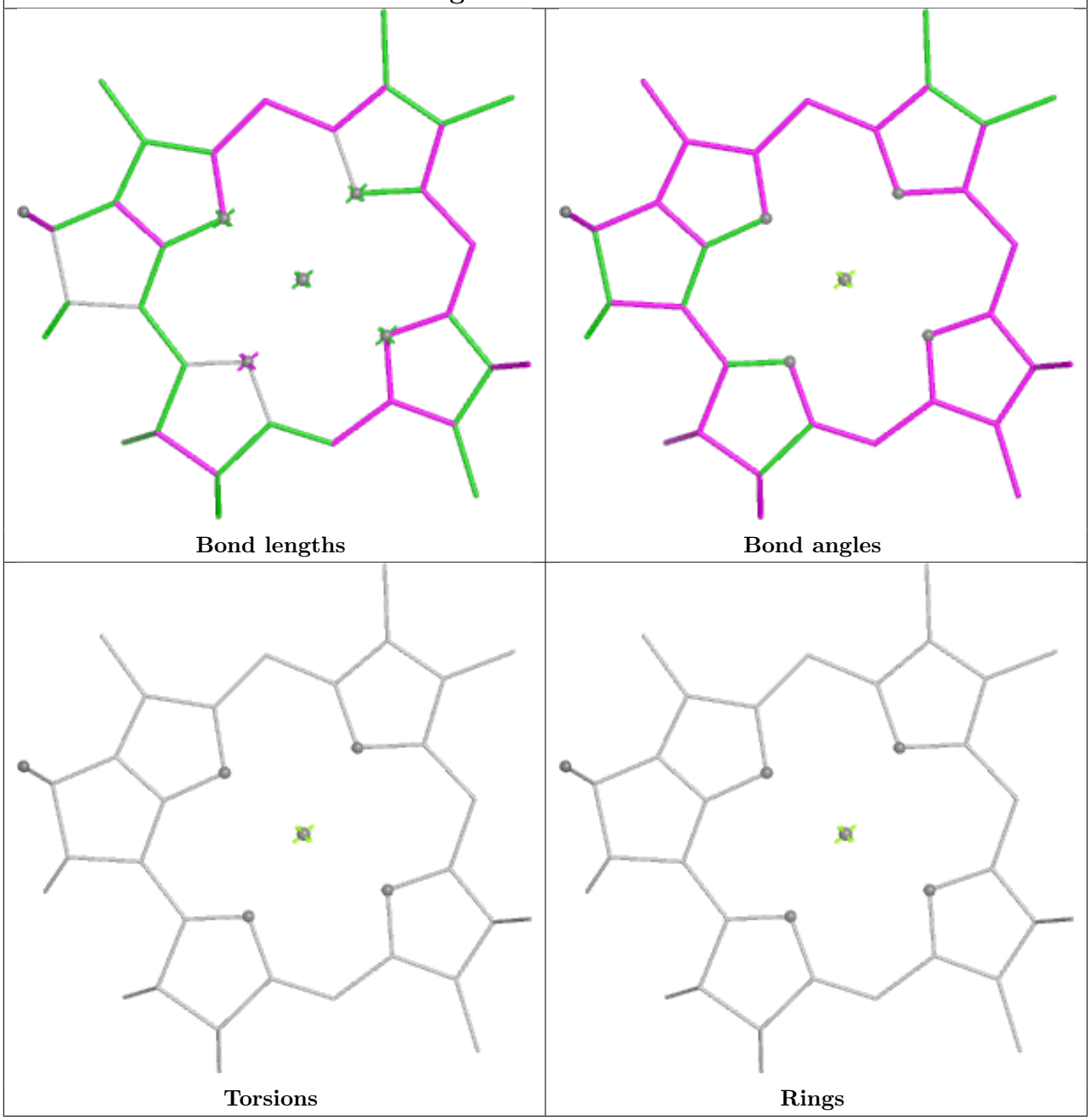


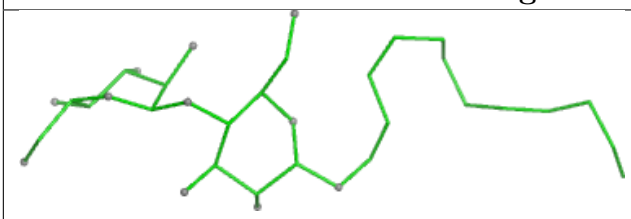
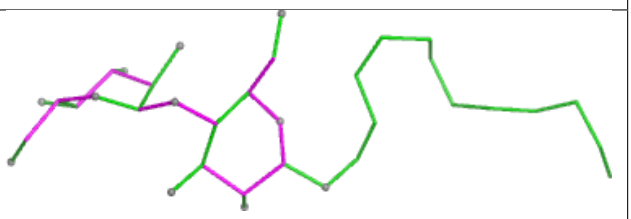
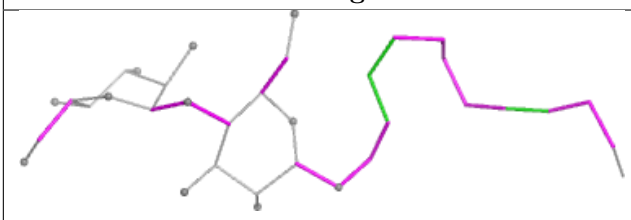
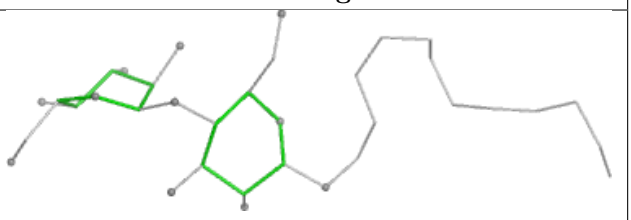
**Rings**

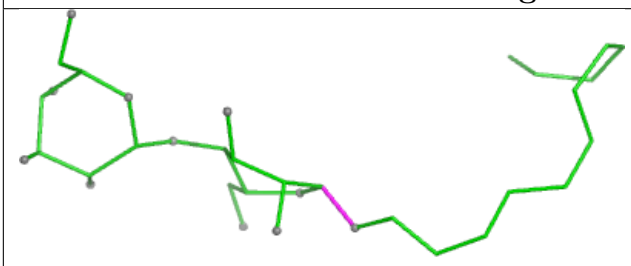
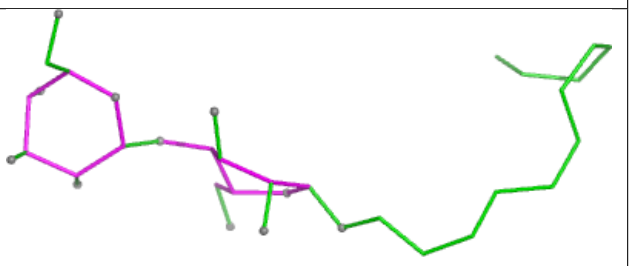
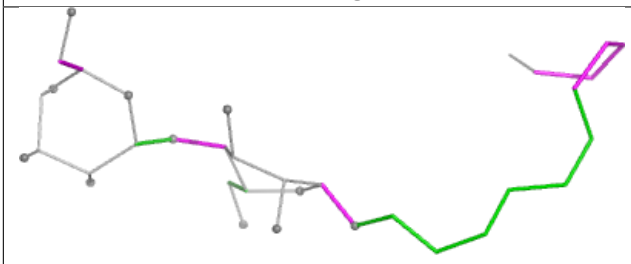
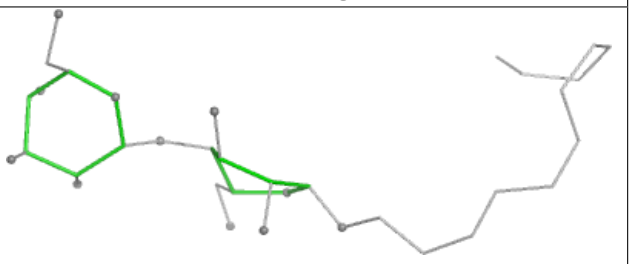
**Ligand CLA A 839**



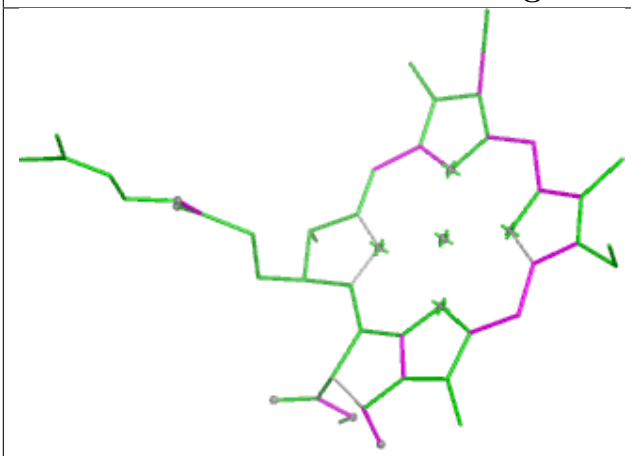
**Ligand CLA 4 302**



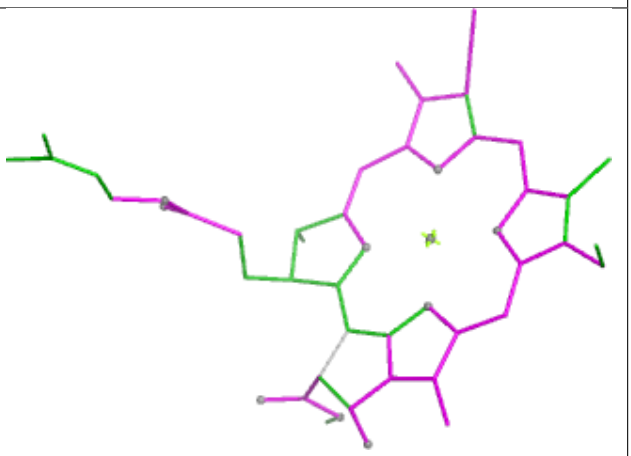
| Ligand LMU K 107 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand LMU H 106 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

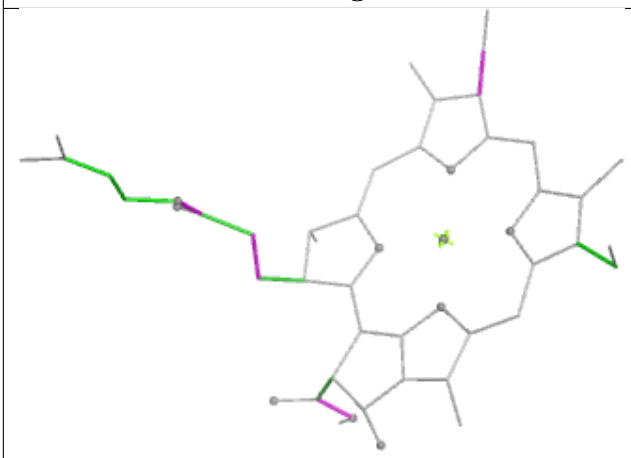
**Ligand CLA A 829**



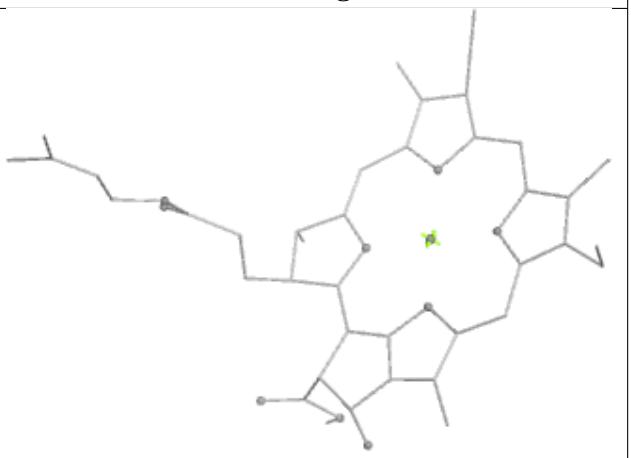
**Bond lengths**



**Bond angles**



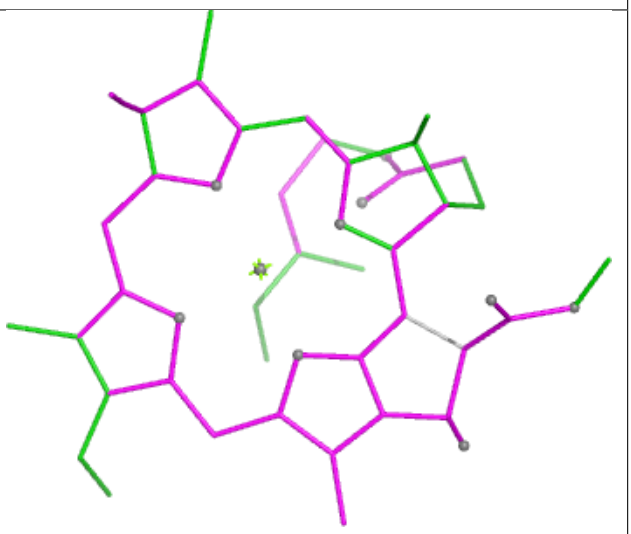
**Torsions**



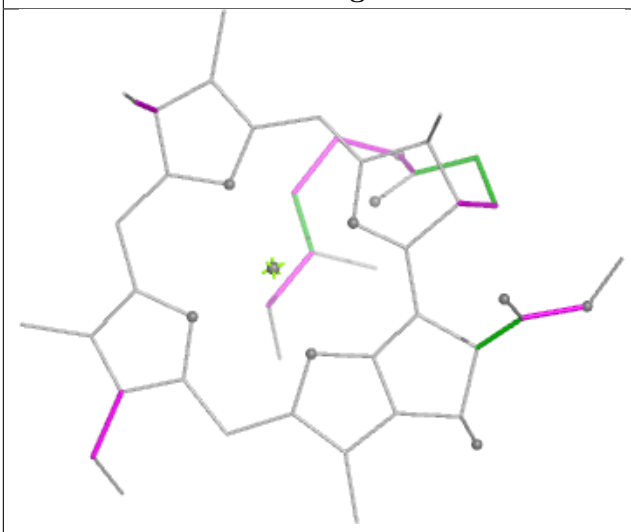
**Rings**

**Ligand CLA 2 302**

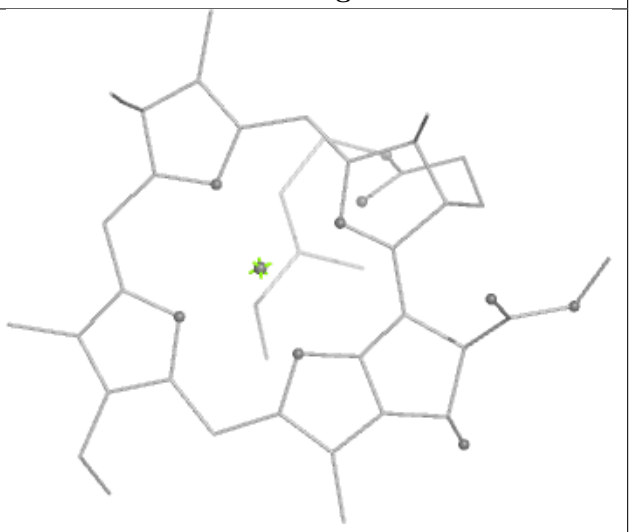
**Bond lengths**



**Bond angles**

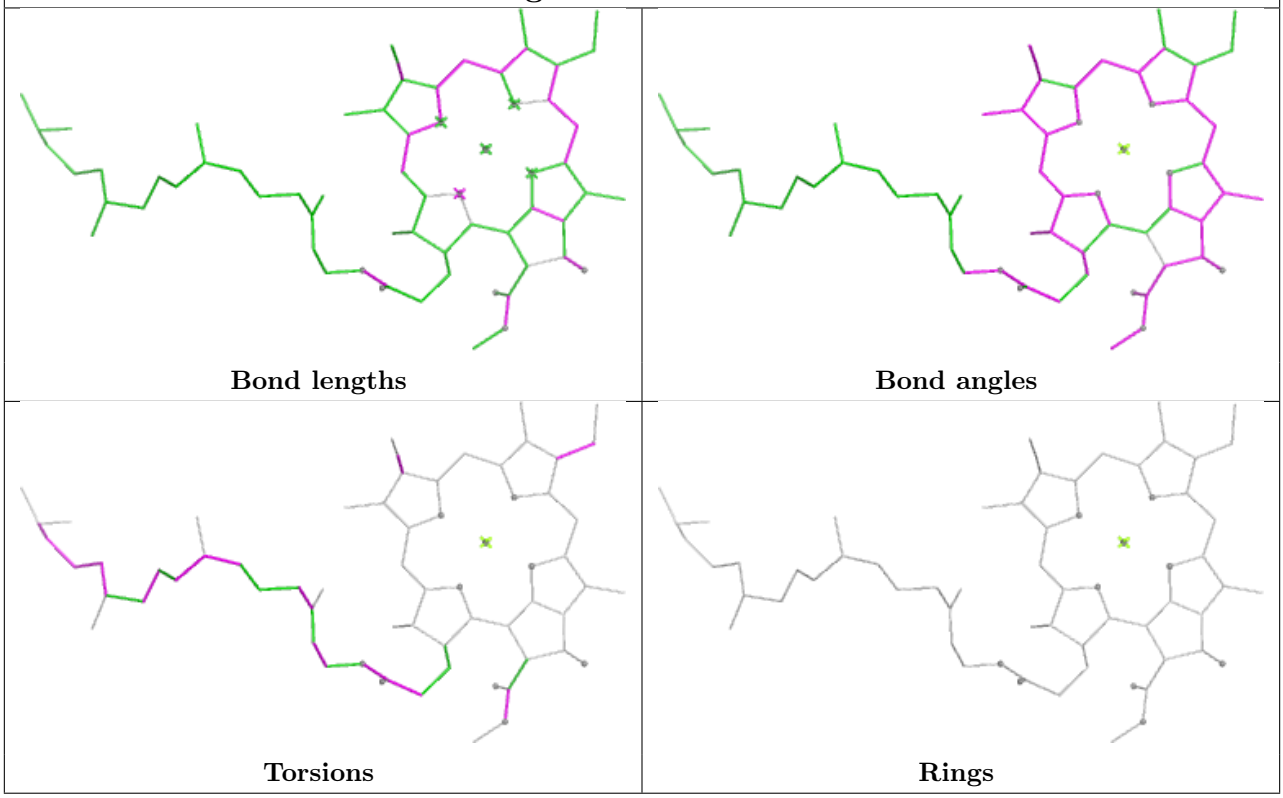


**Torsions**

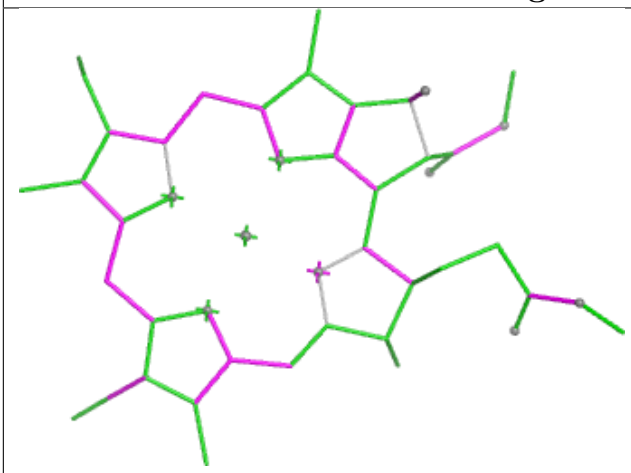


**Rings**

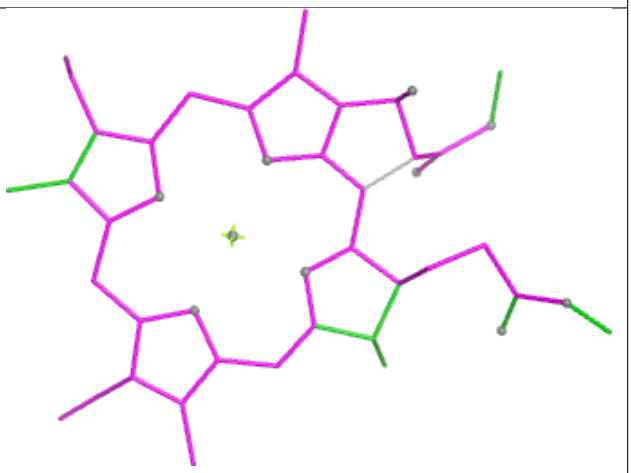
**Ligand CLA B 803**



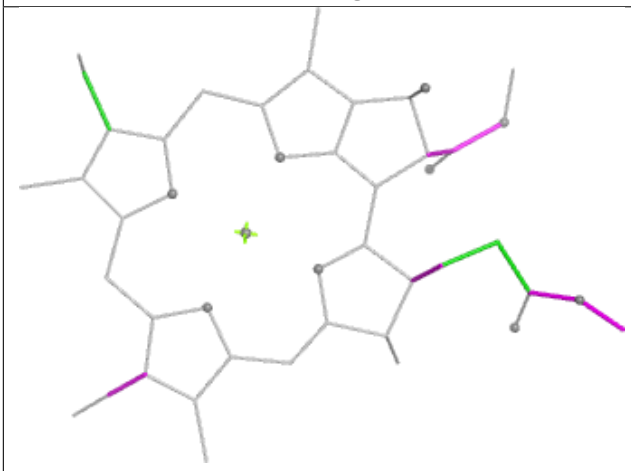
**Ligand CLA 1 203**



**Bond lengths**



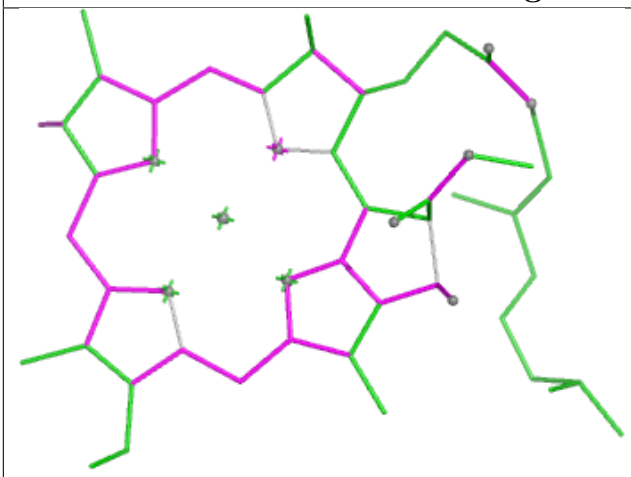
**Bond angles**



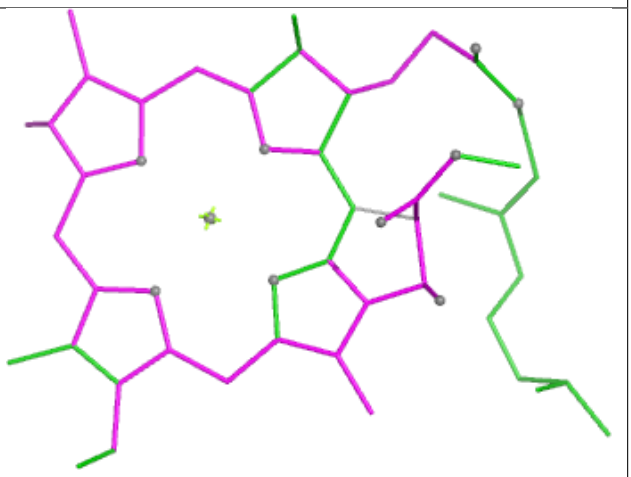
**Torsions**

**Rings**

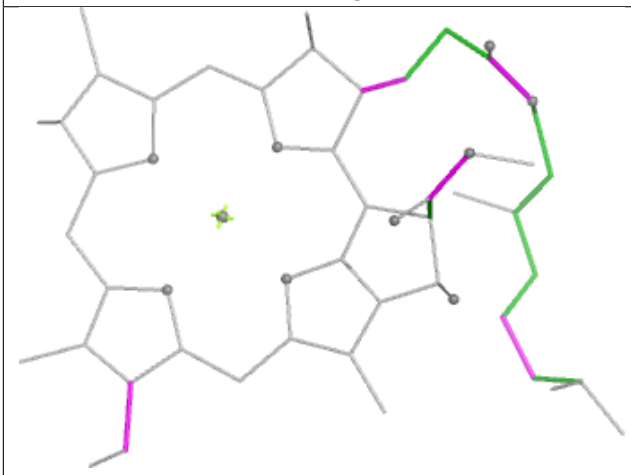
## Ligand CLA B 812



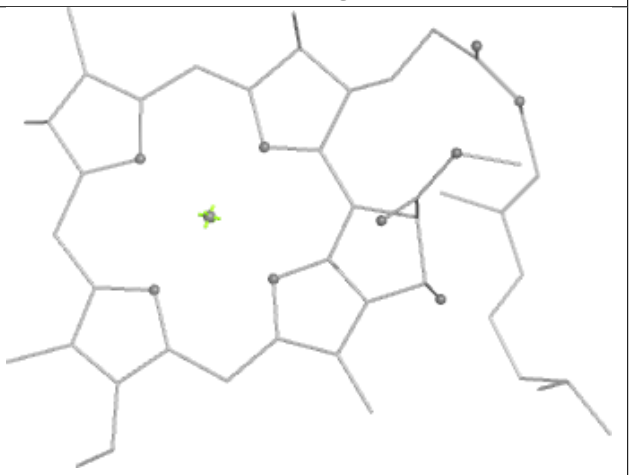
Bond lengths



Bond angles

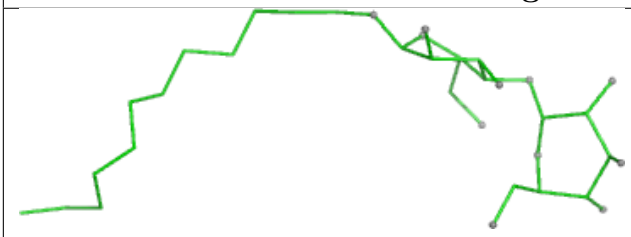


Torsions

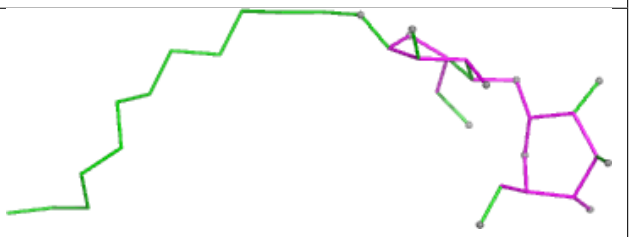


Rings

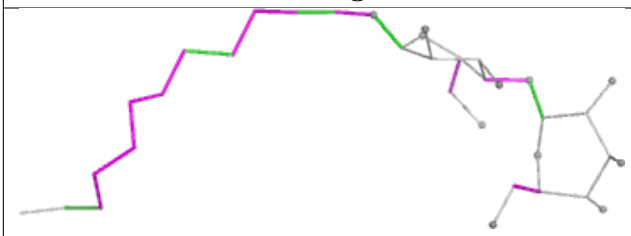
## Ligand LMU L 205



Bond lengths



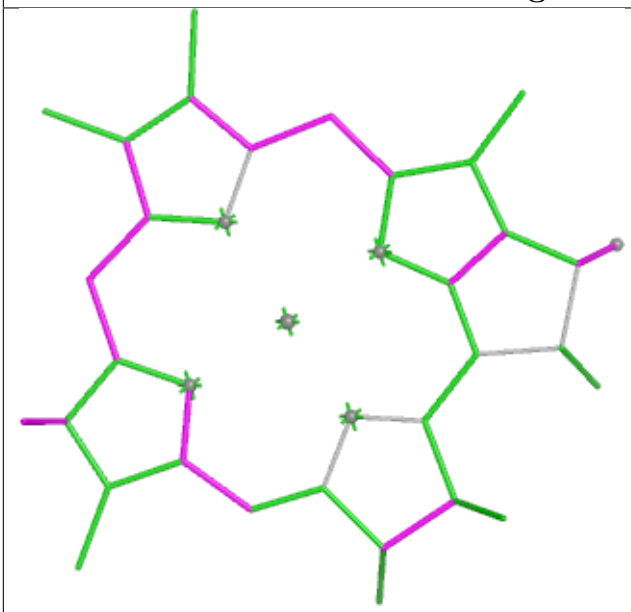
Bond angles



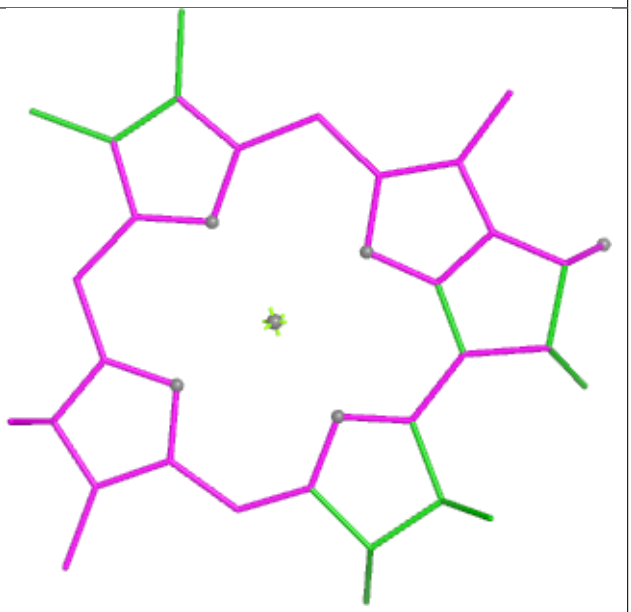
Torsions

Rings

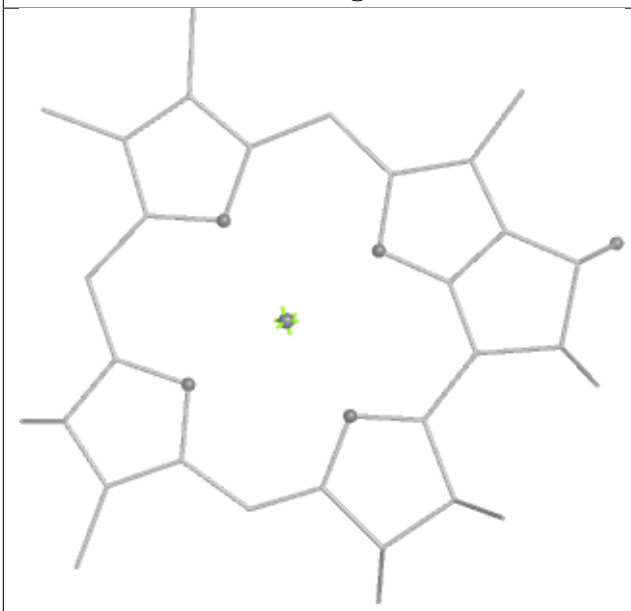
**Ligand CLA 1 210**



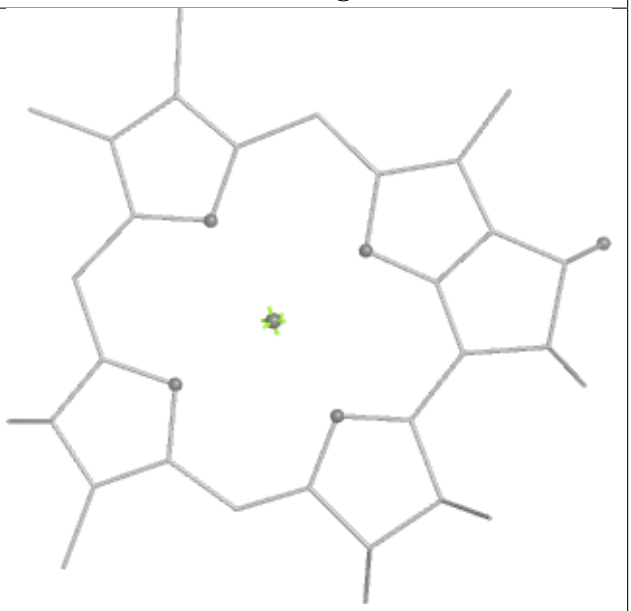
**Bond lengths**



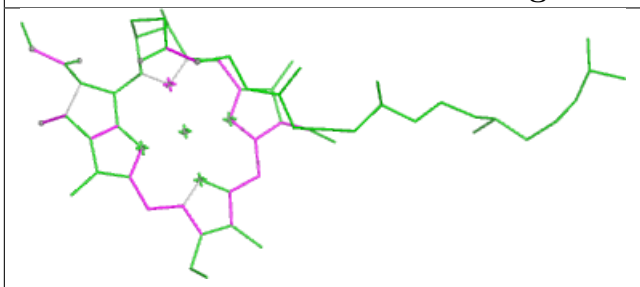
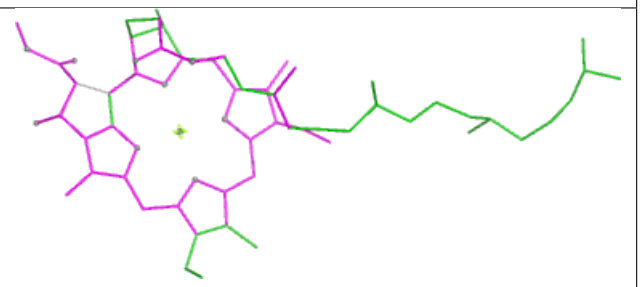
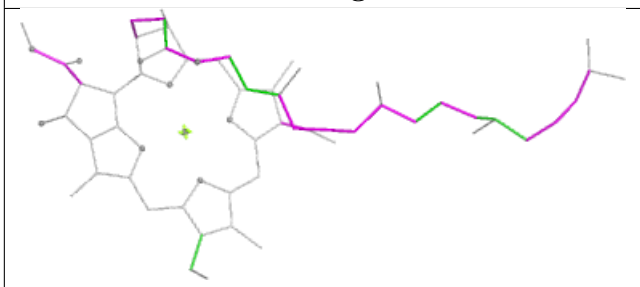
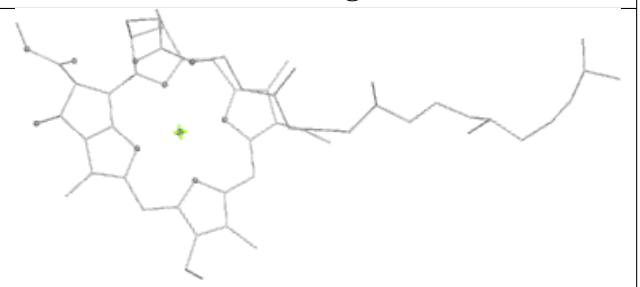
**Bond angles**



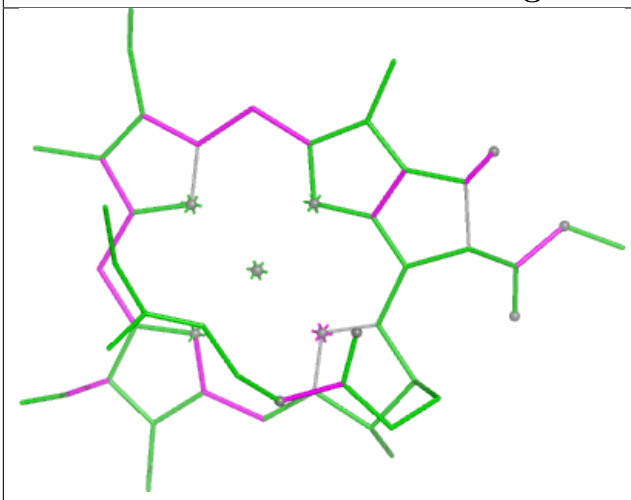
**Torsions**



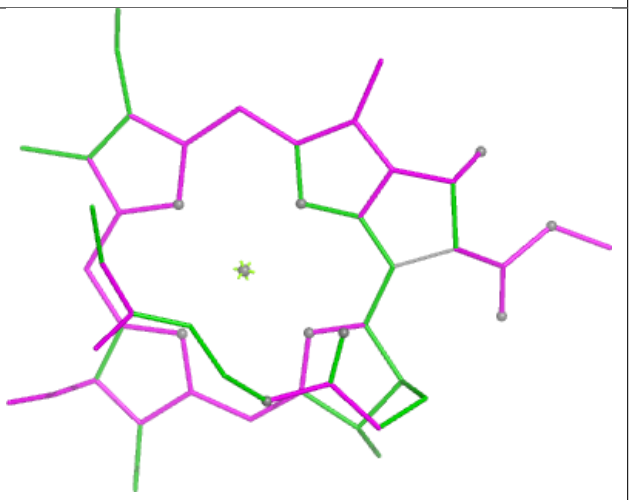
**Rings**

| Ligand CLA 2 307 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

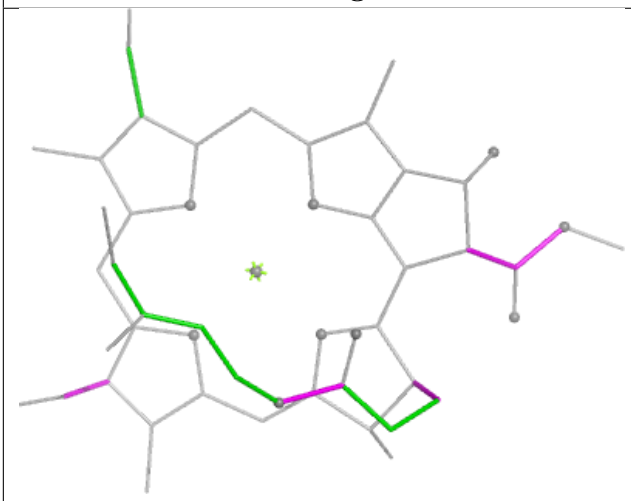
**Ligand CLA A 820**



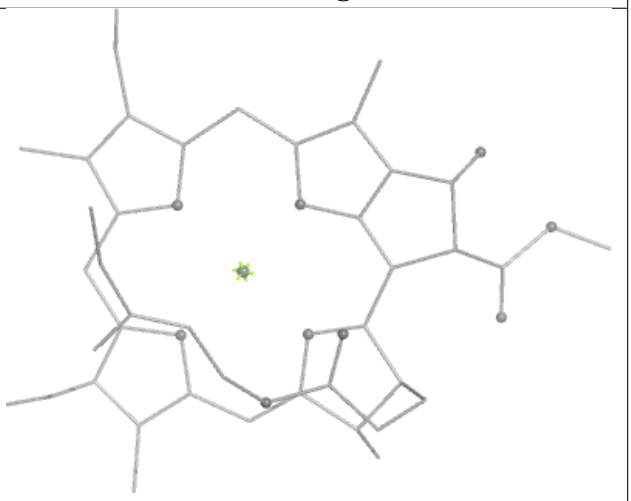
**Bond lengths**



**Bond angles**

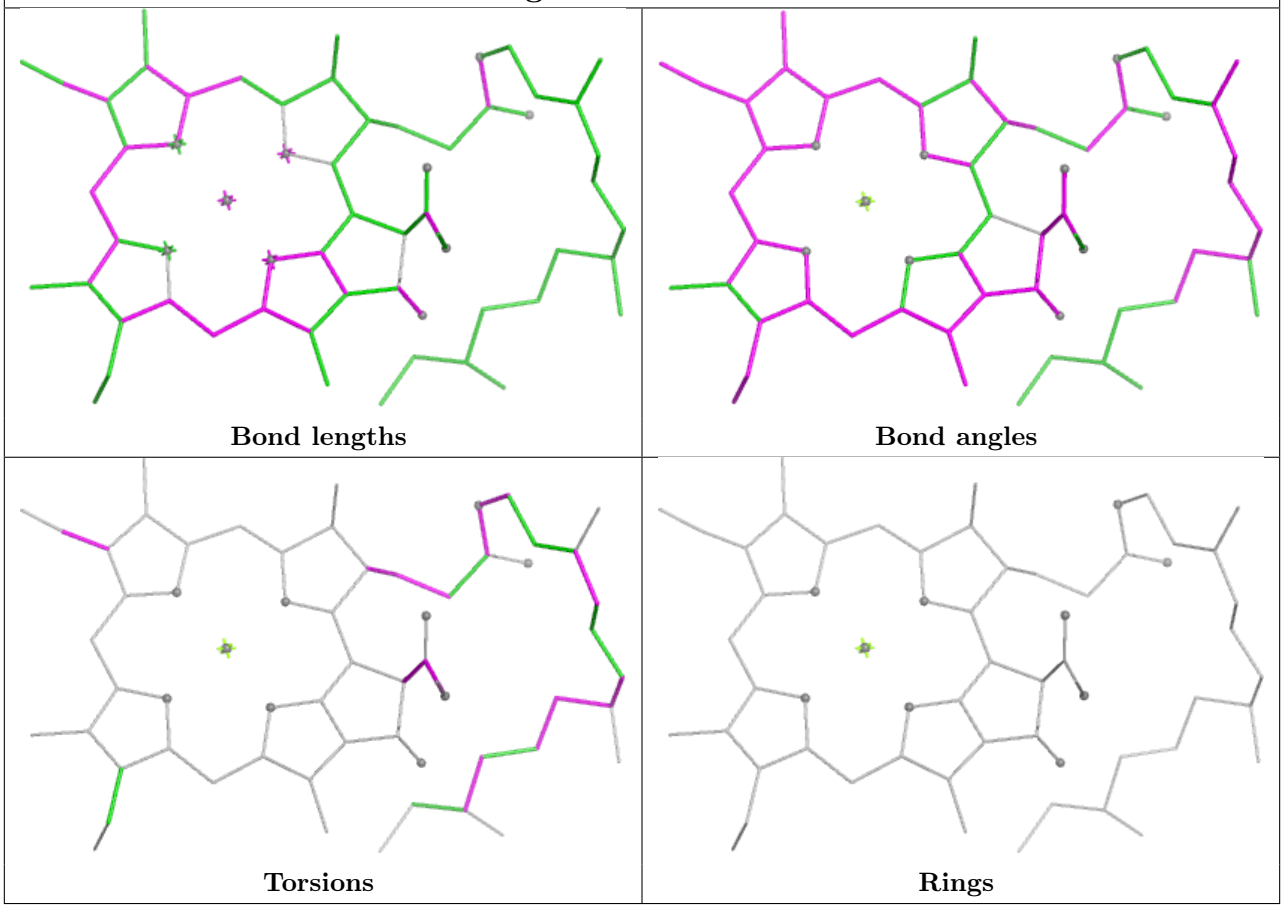


**Torsions**

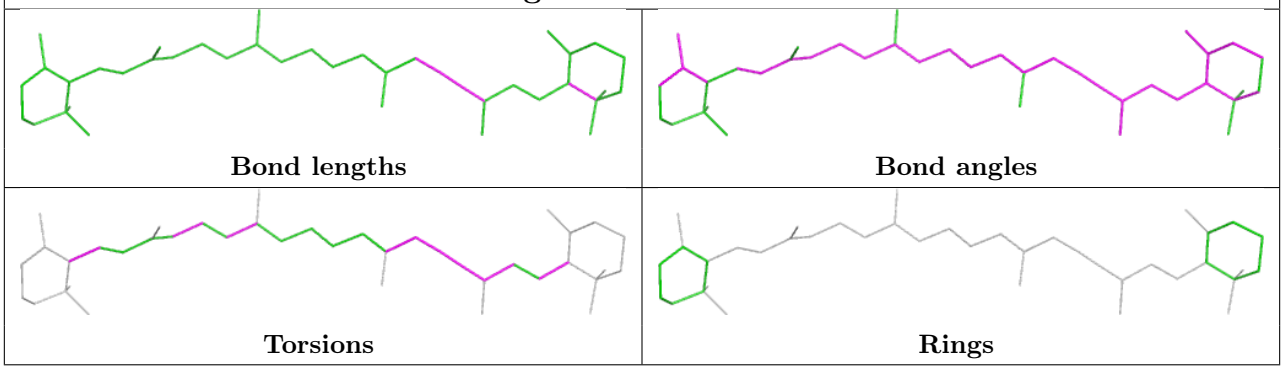


**Rings**

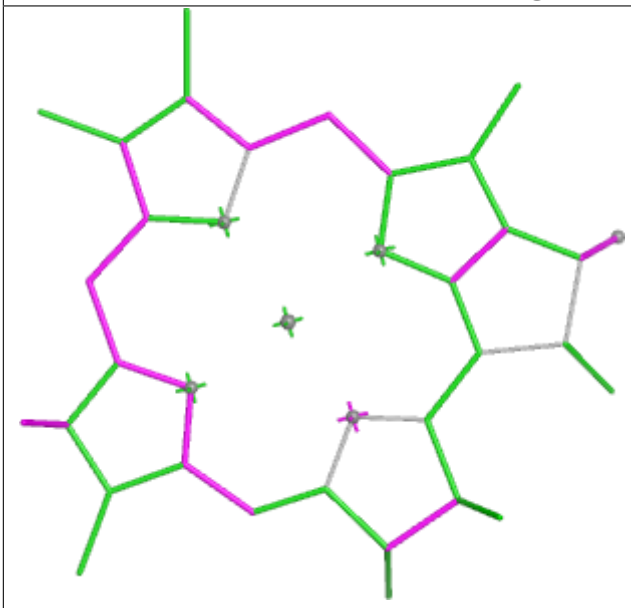
## Ligand CLA B 808



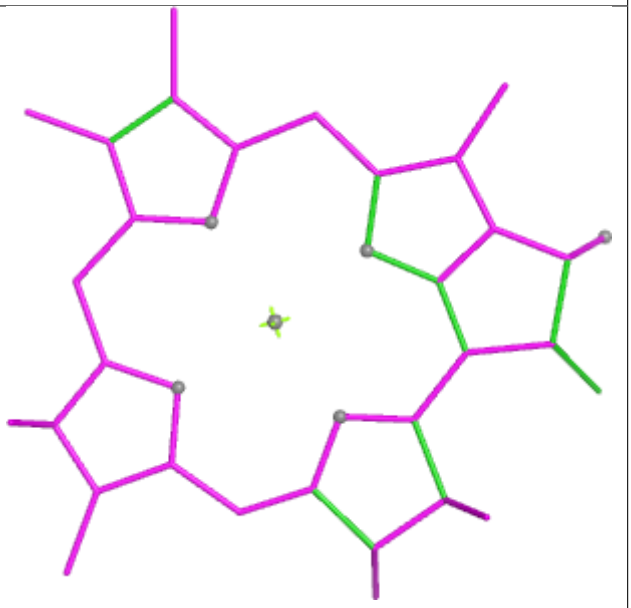

## Ligand BCR B 846



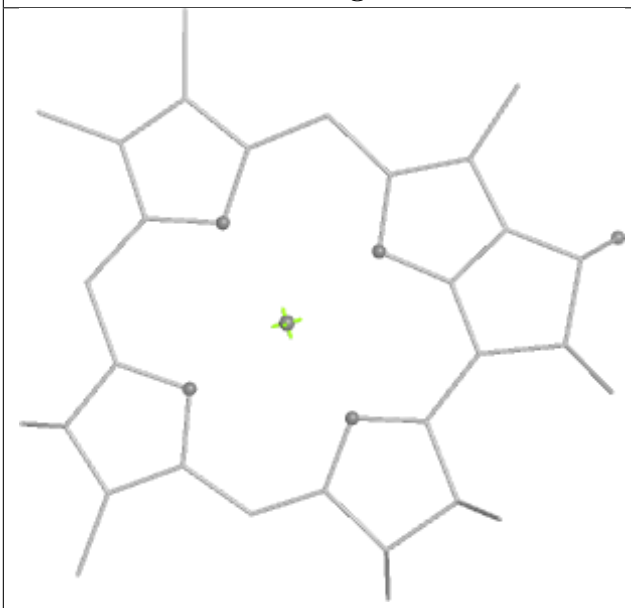
**Ligand CLA 4 313**



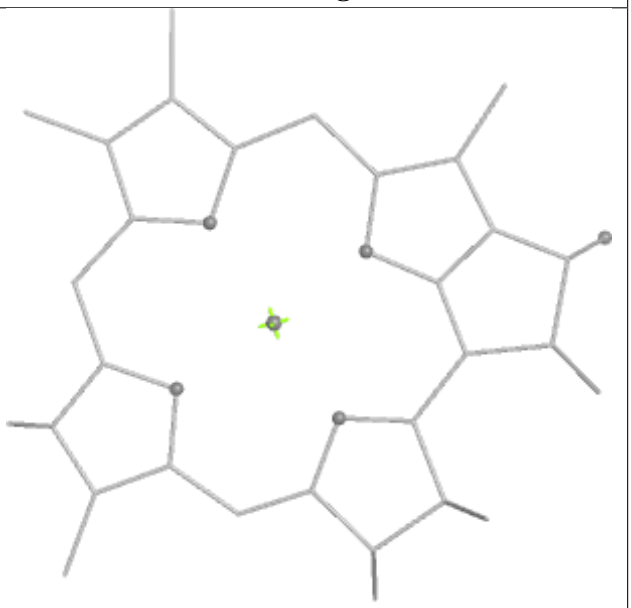
**Bond lengths**



**Bond angles**

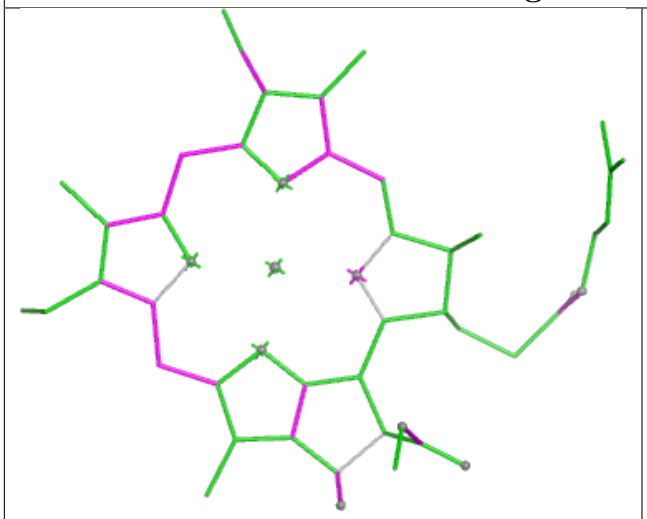


**Torsions**

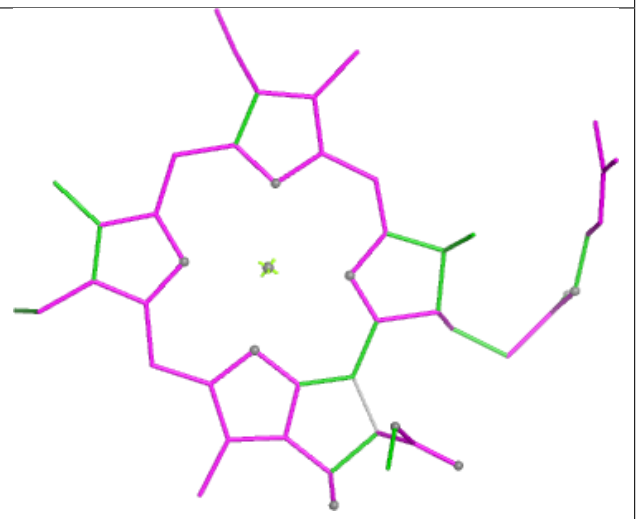


**Rings**

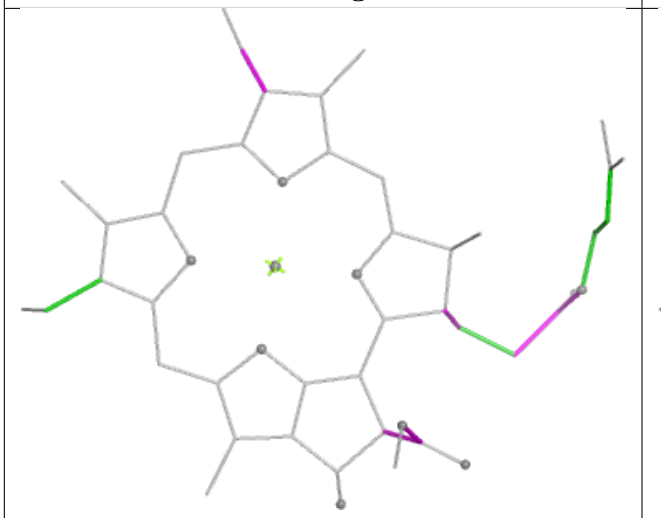
## Ligand CLA A 813



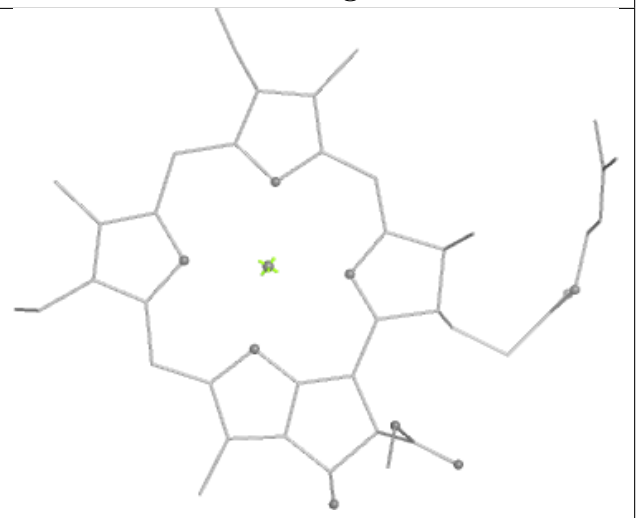
Bond lengths



Bond angles

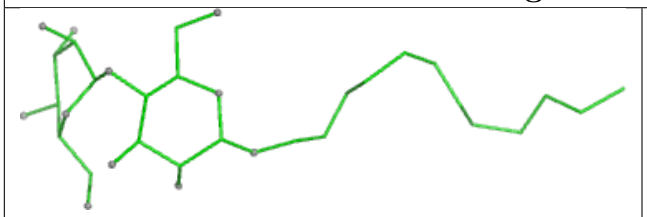


Torsions

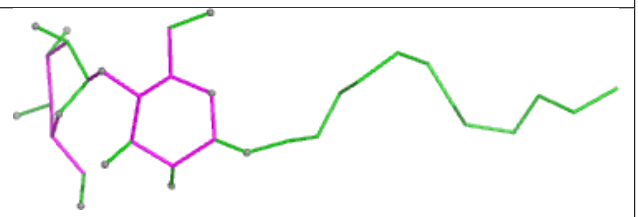


Rings

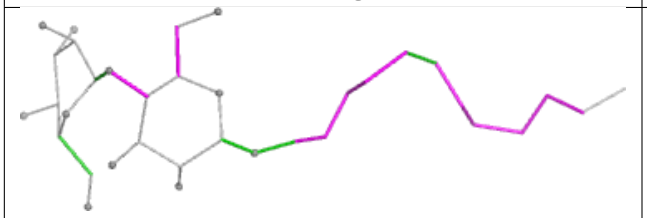
## Ligand LMU 1 218



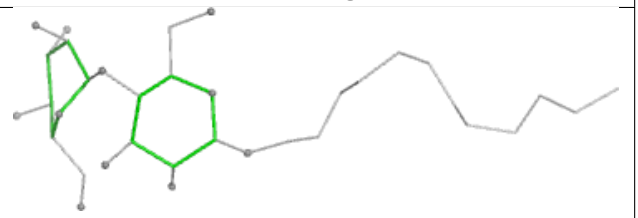
Bond lengths



Bond angles

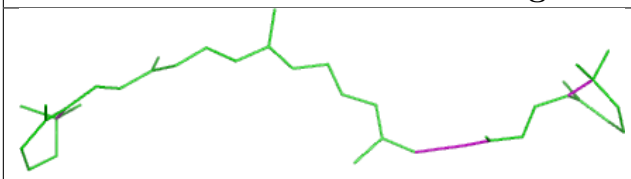


Torsions

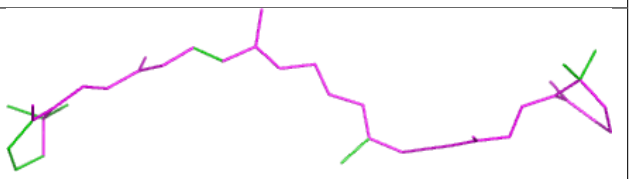


Rings

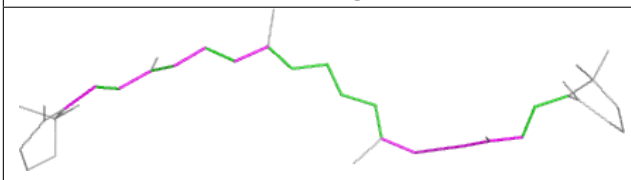
## Ligand BCR I 103



Bond lengths



Bond angles



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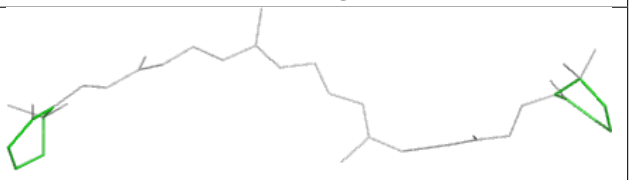
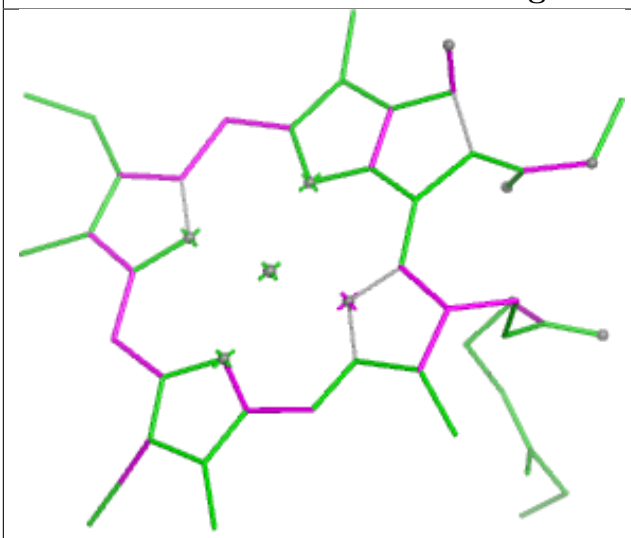
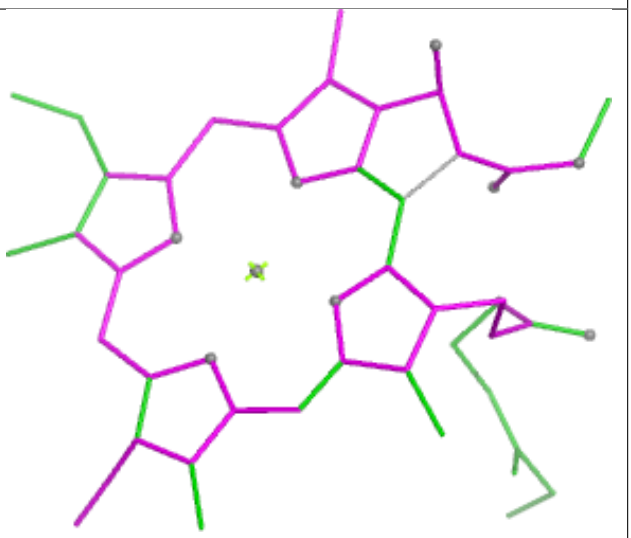


Rings

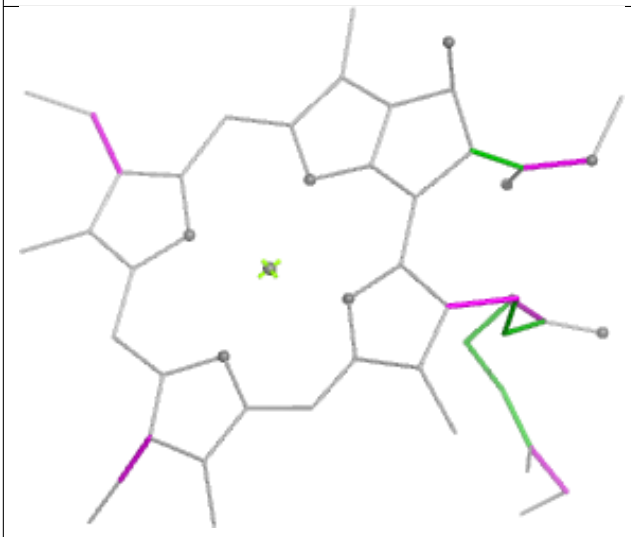
## Ligand CLA 1 207



Bond lengths



Bond angles



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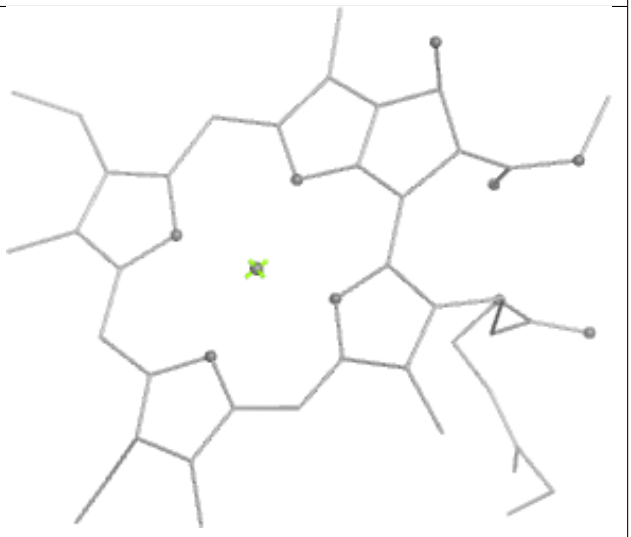
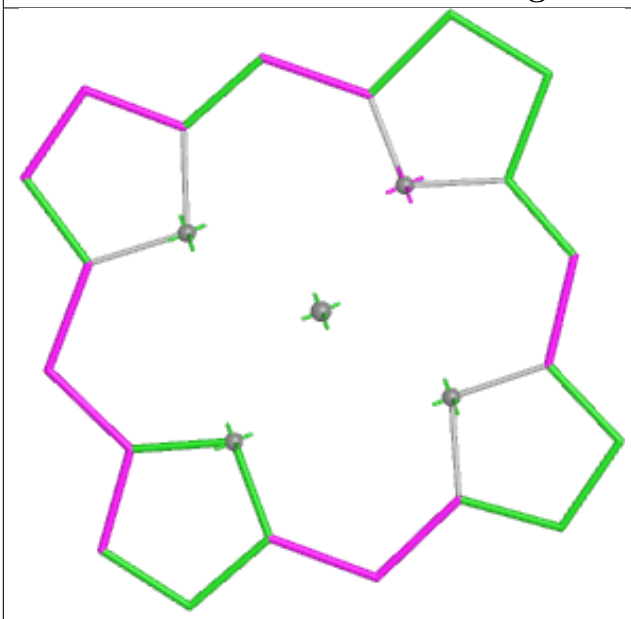
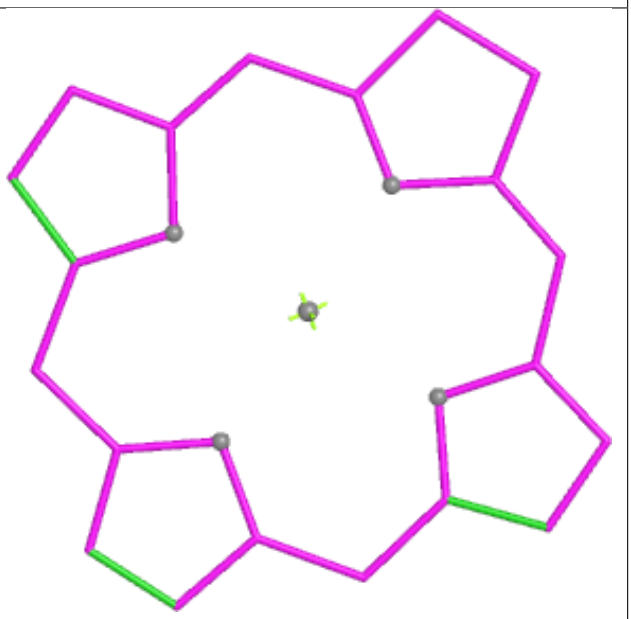


Rings

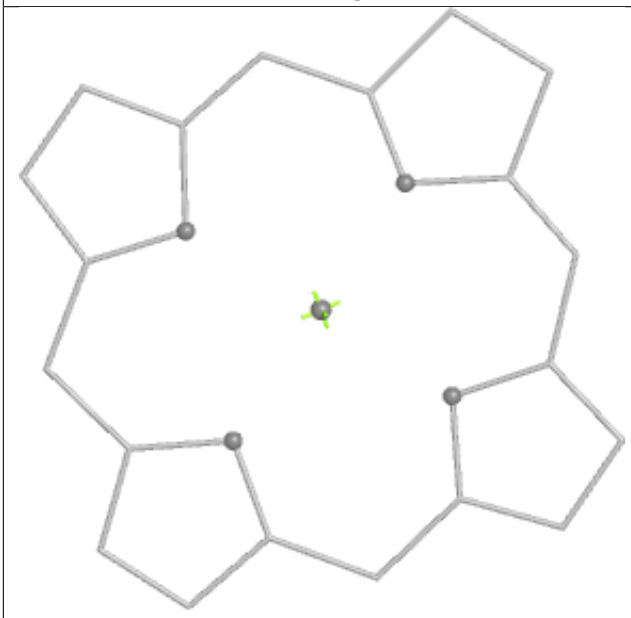
**Ligand CLA 3 306**



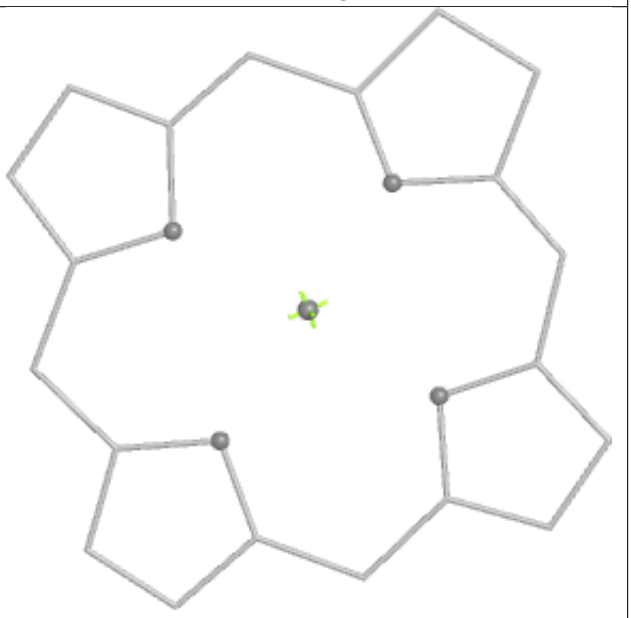
**Bond lengths**



**Bond angles**

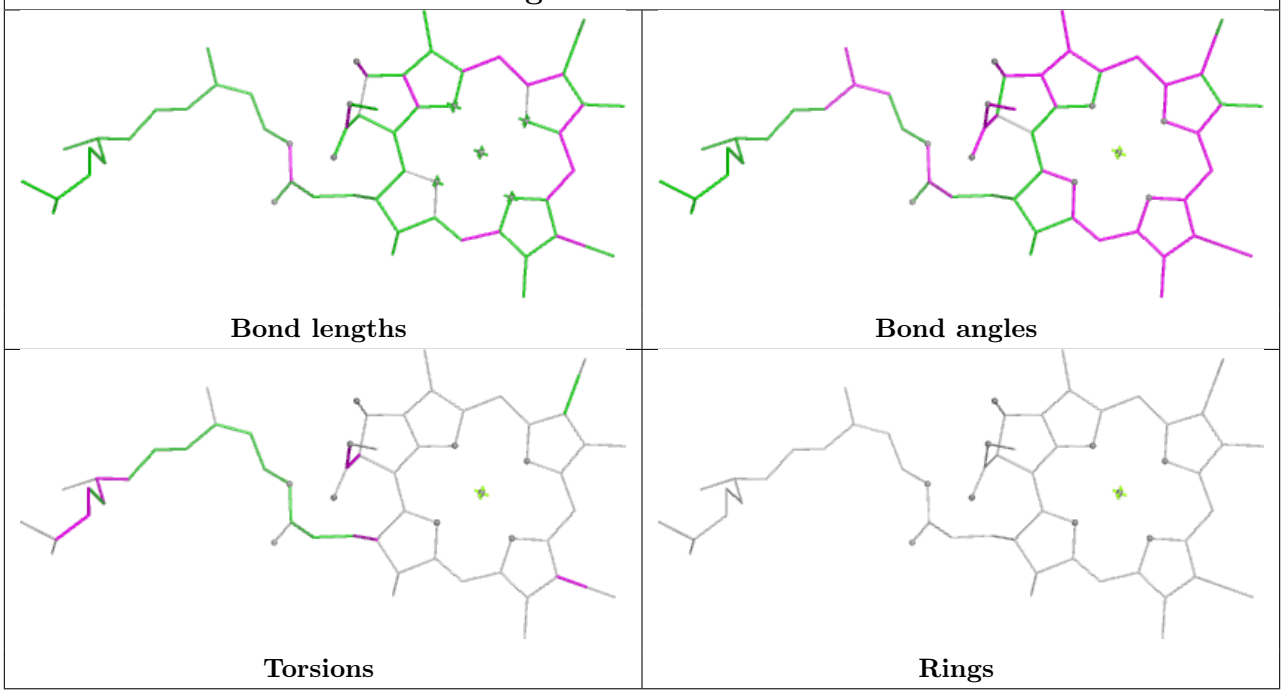


**Torsions**

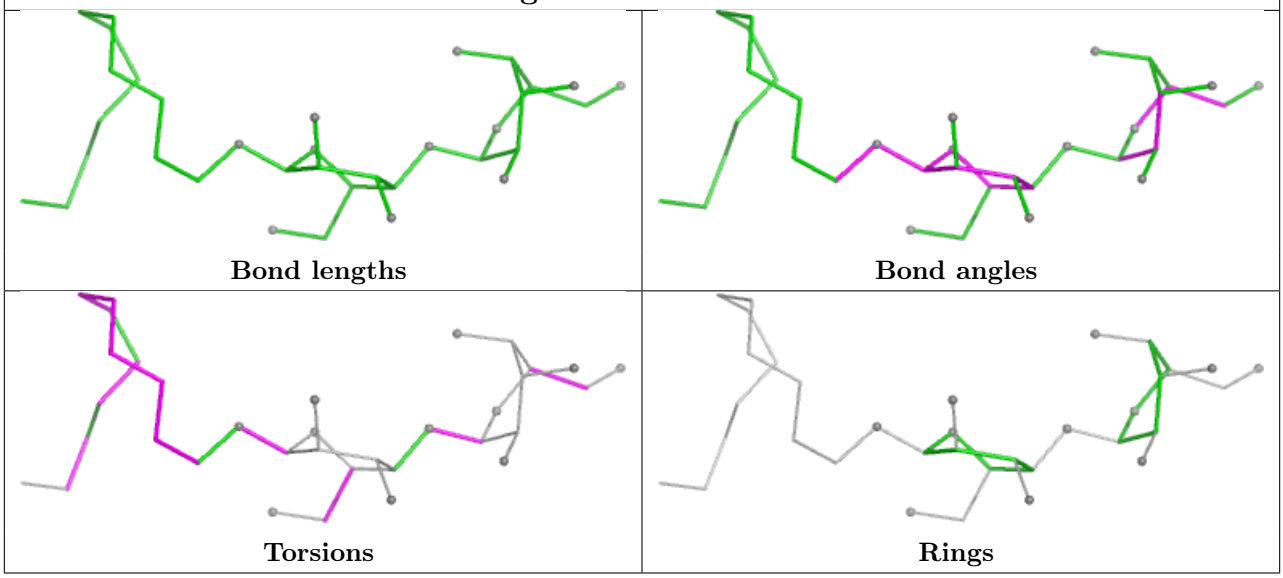


**Rings**

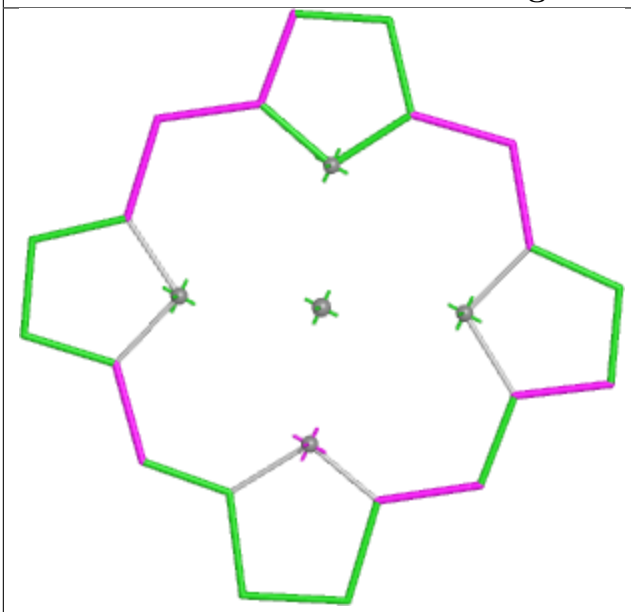
## Ligand CLA B 816



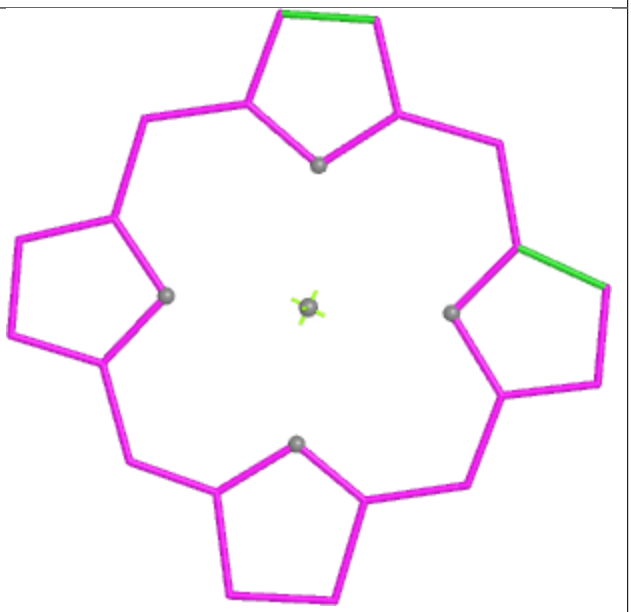

## Ligand LMU A 854



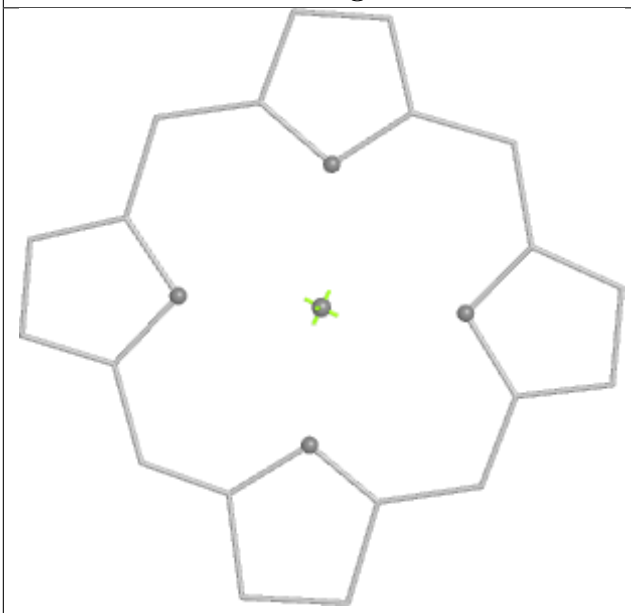
**Ligand CLA 3 309**



**Bond lengths**



**Bond angles**



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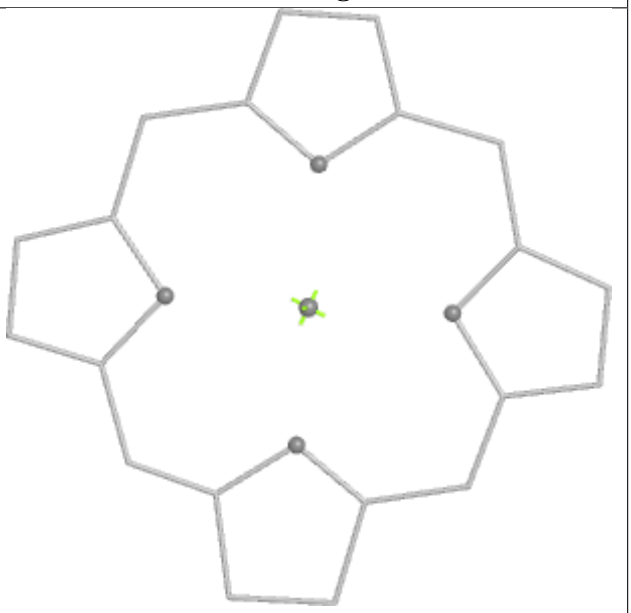
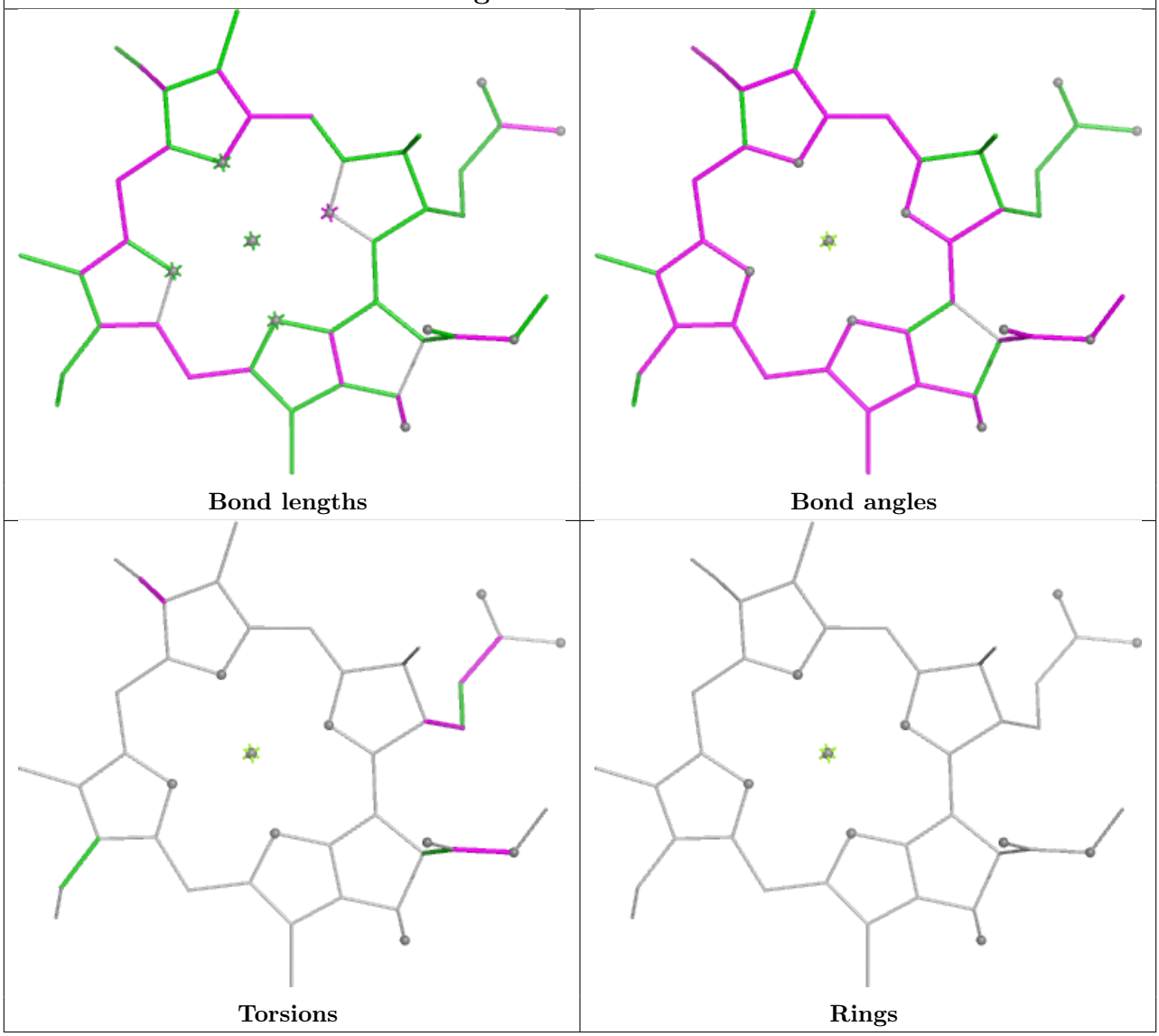
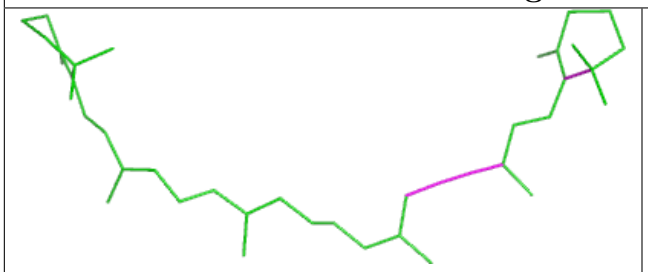


**Rings**

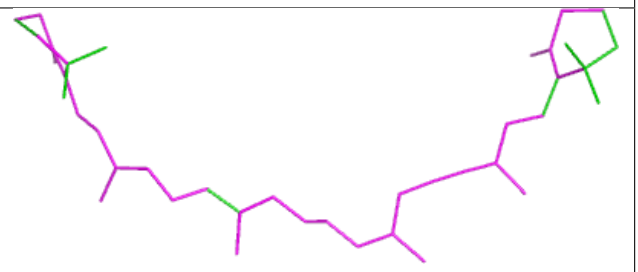
**Ligand CLA A 833**



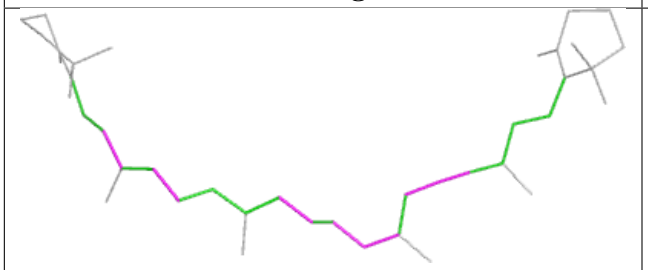
## Ligand BCR F 204



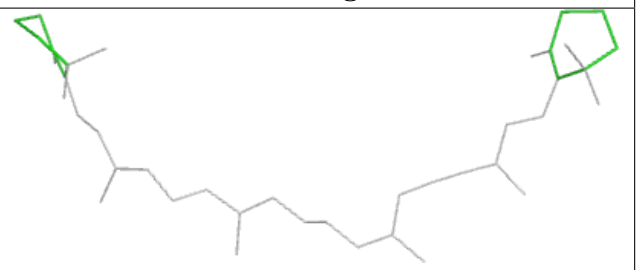
Bond lengths



Bond angles

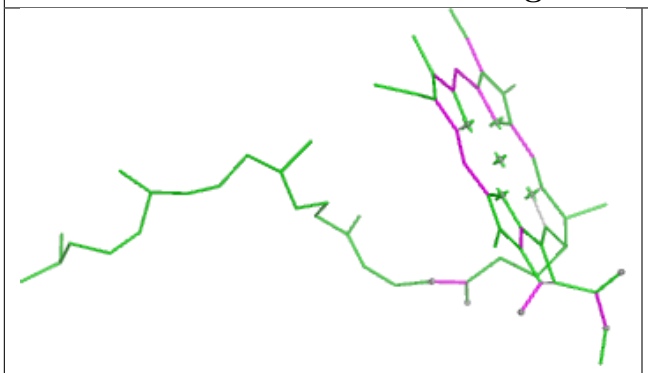


Torsions

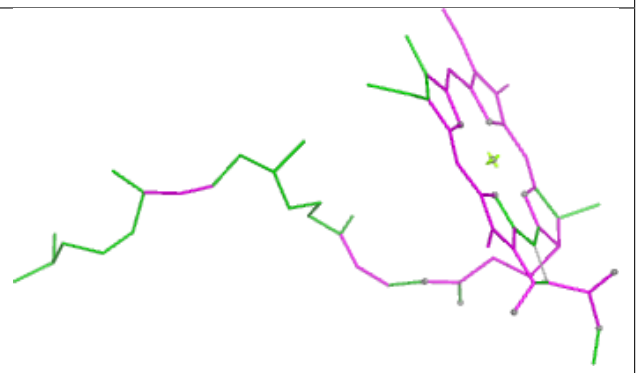


Rings

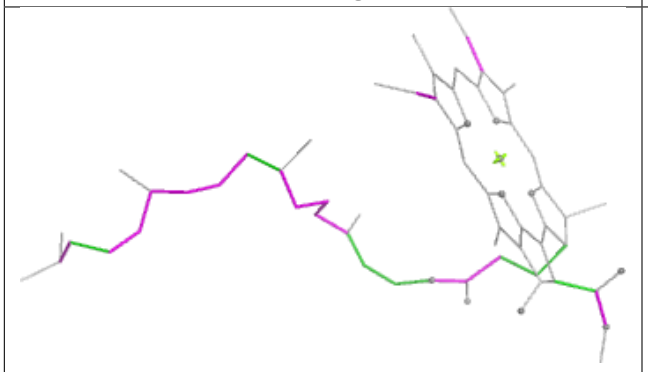
## Ligand CLA A 811



Bond lengths



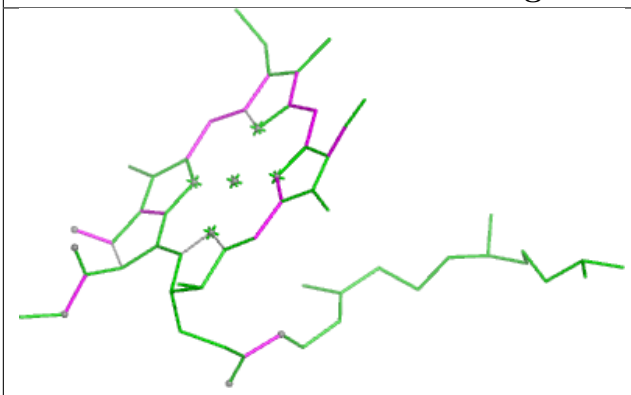
Bond angles



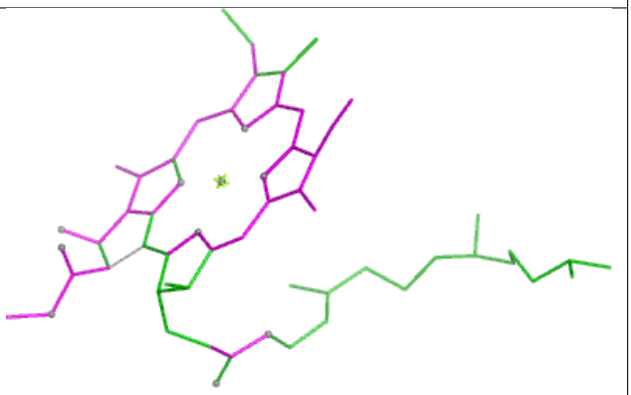
Torsions

Rings

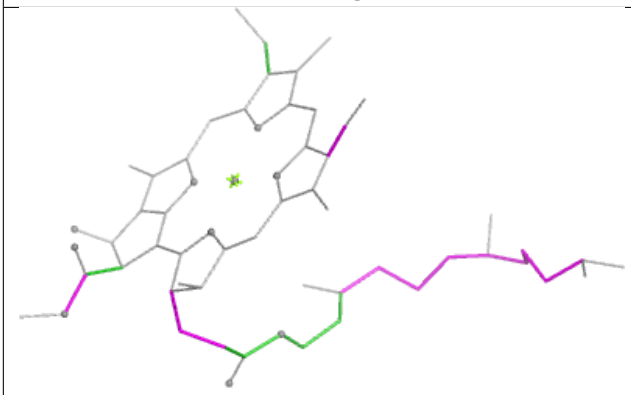
## Ligand CLA B 815



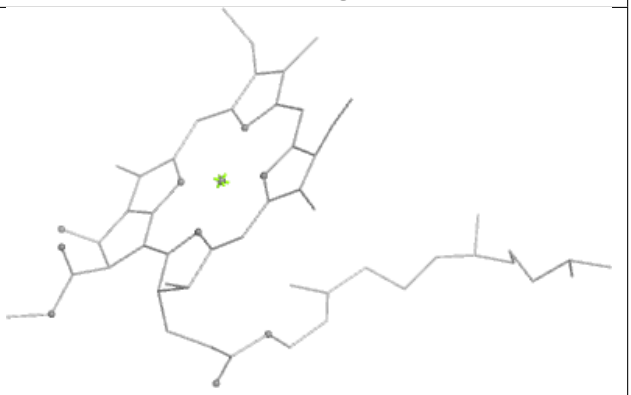
Bond lengths



Bond angles

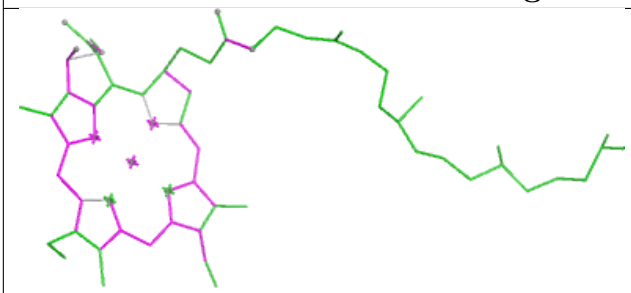


Torsions

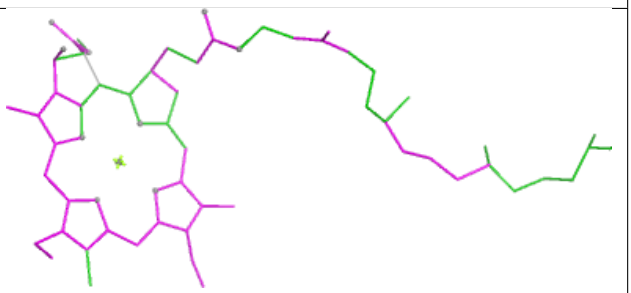


Rings

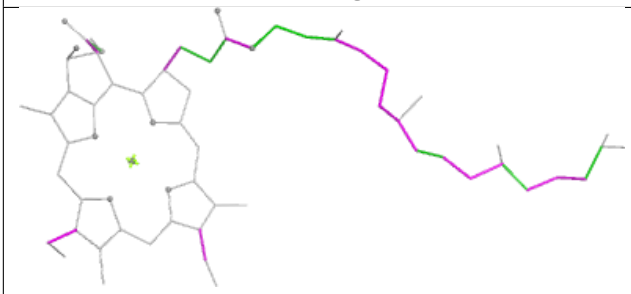
## Ligand CLA A 831



Bond lengths



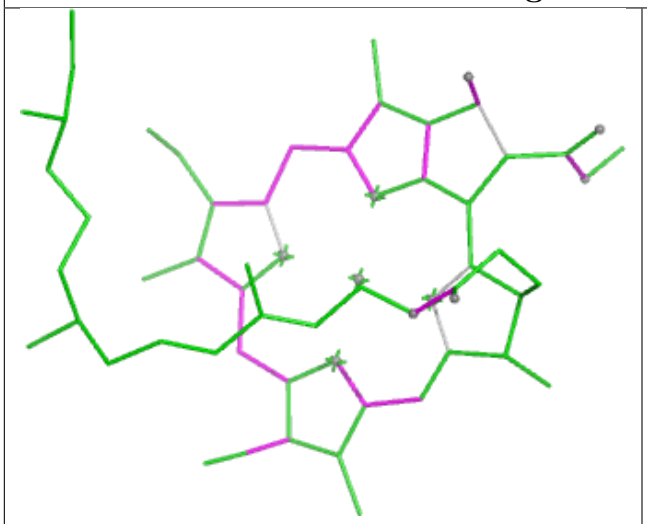
Bond angles



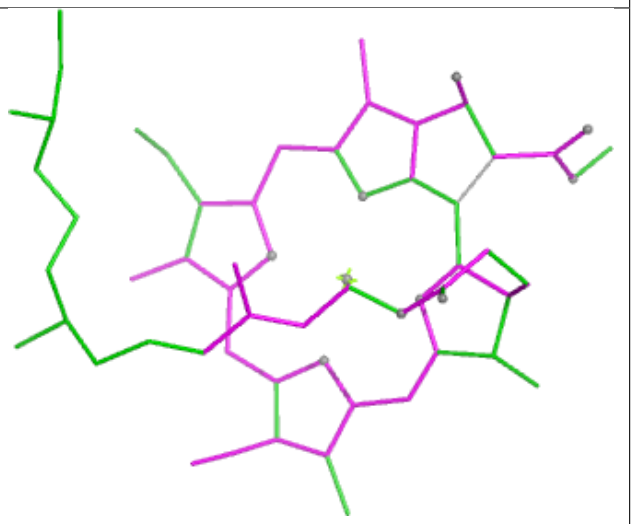
Torsions

Rings

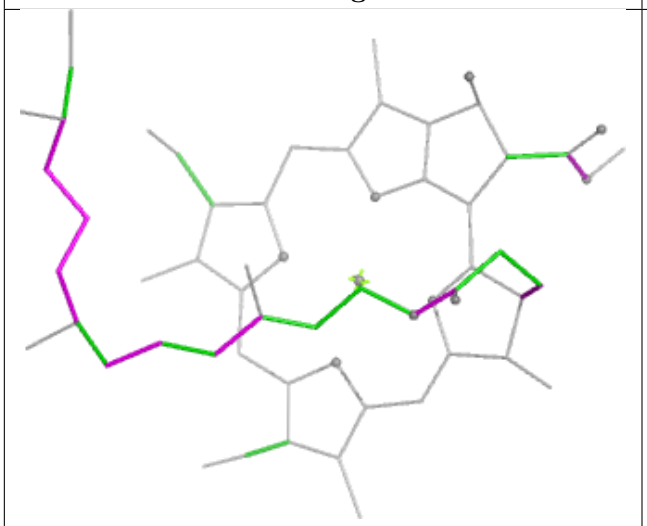
**Ligand CLA B 820**



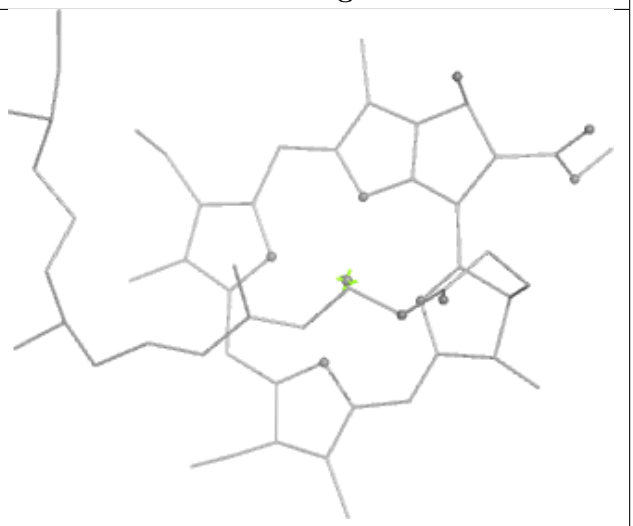
**Bond lengths**



**Bond angles**

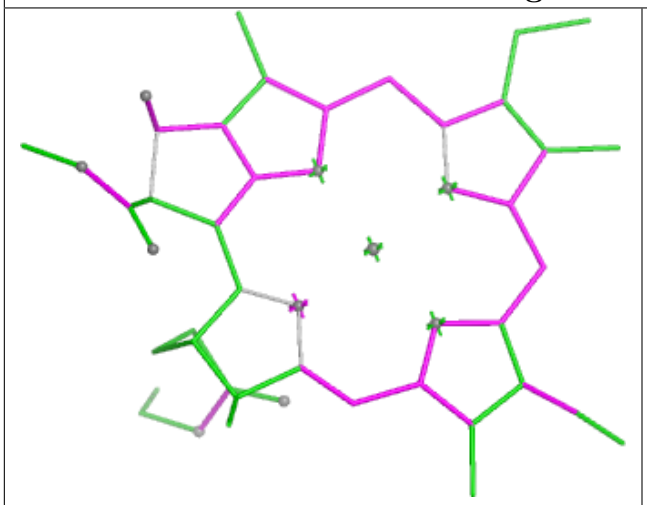


**Torsions**



**Rings**

## Ligand CLA B 839



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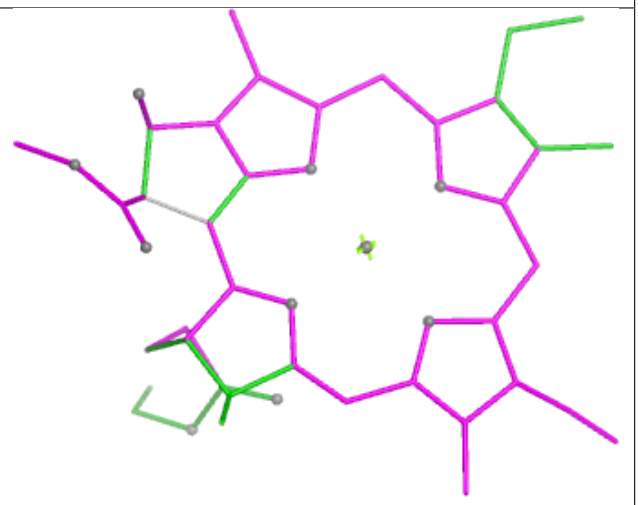
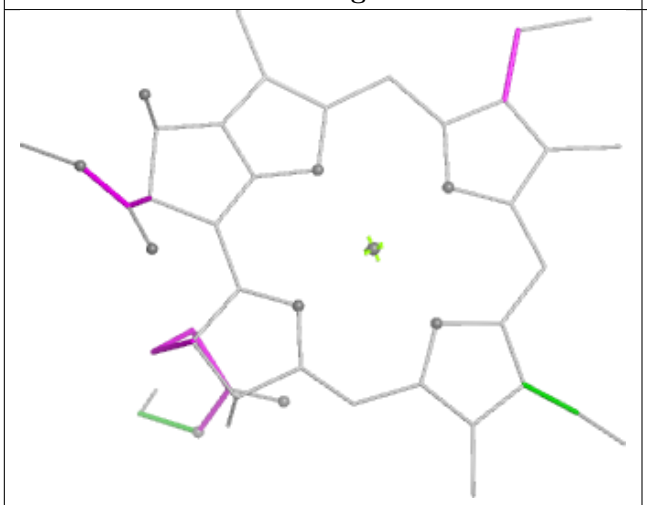
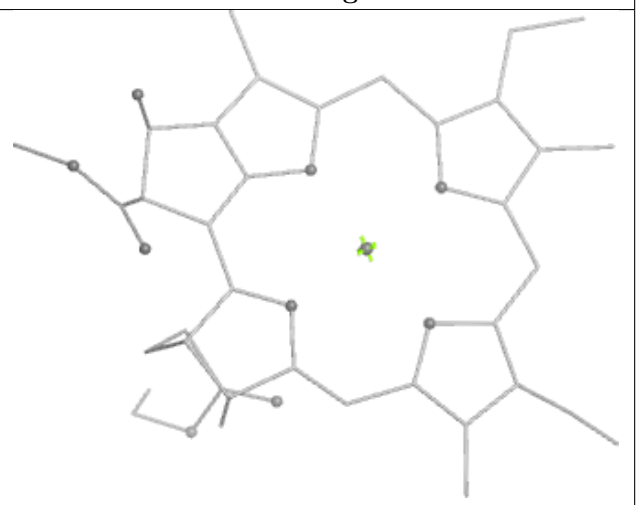


Bond angles

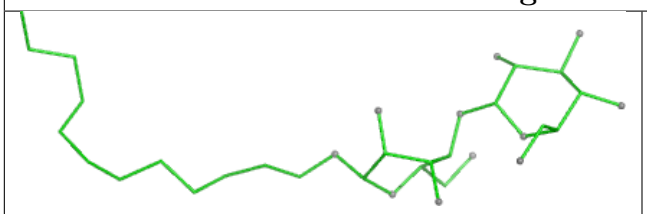


Torsions

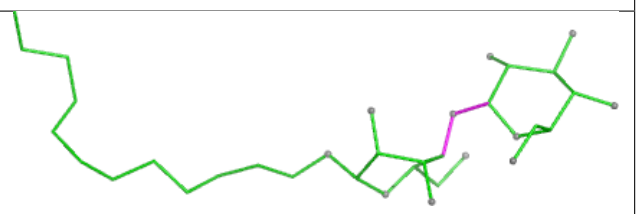


Rings

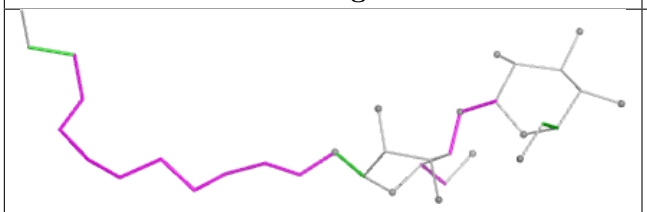
## Ligand LMU G 103



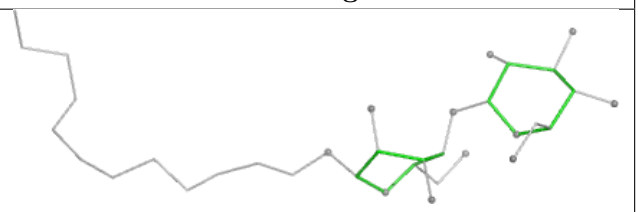
Bond lengths



Bond angles

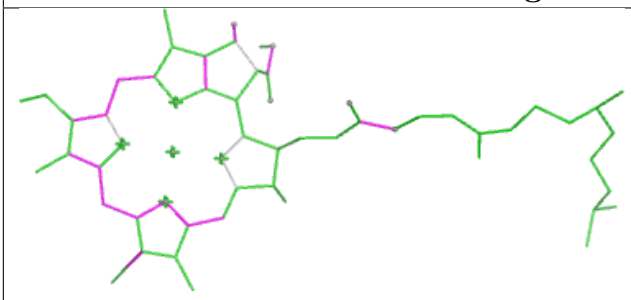


Torsions

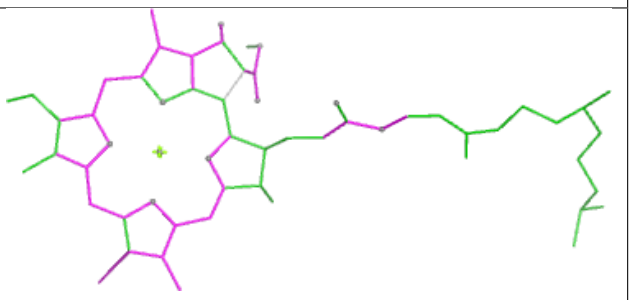


Rings

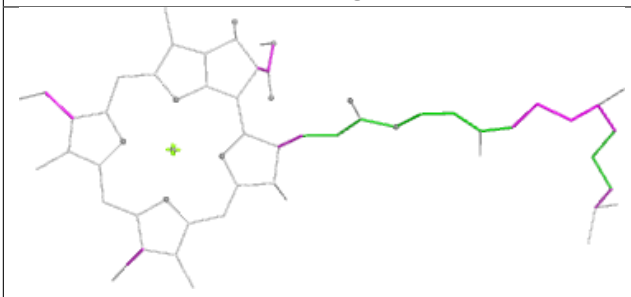
## Ligand CLA B 837



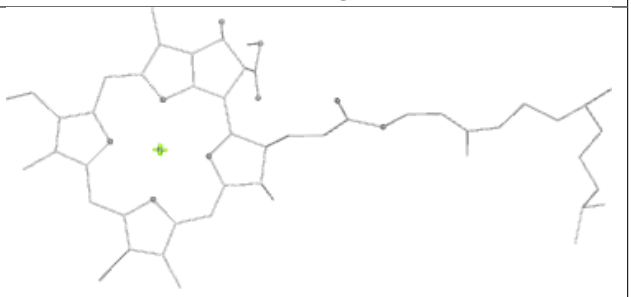
Bond lengths



Bond angles

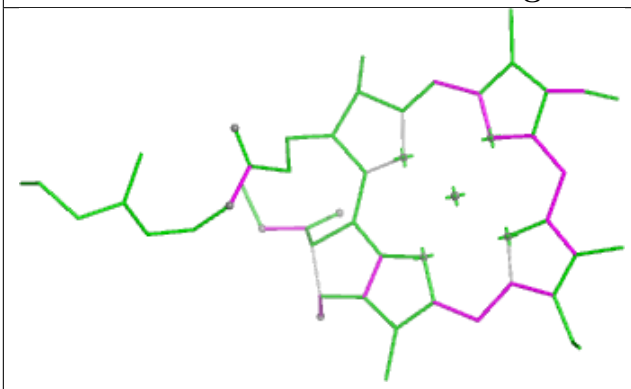


Torsions

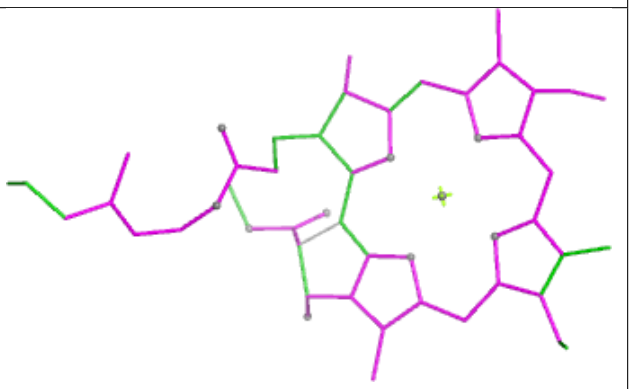


Rings

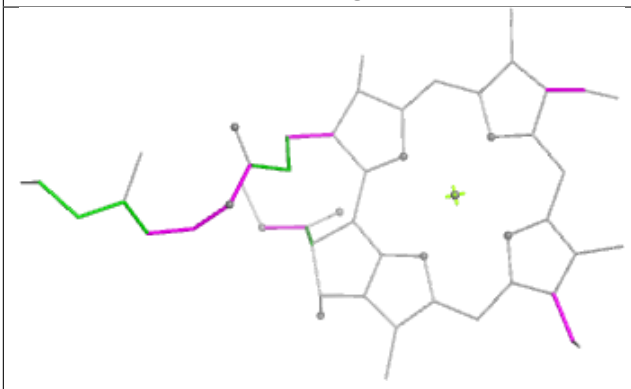
## Ligand CLA A 809



Bond lengths



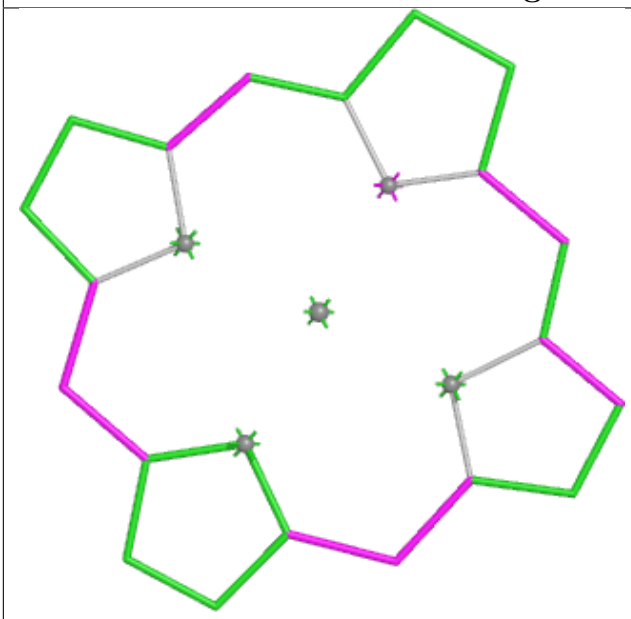
Bond angles



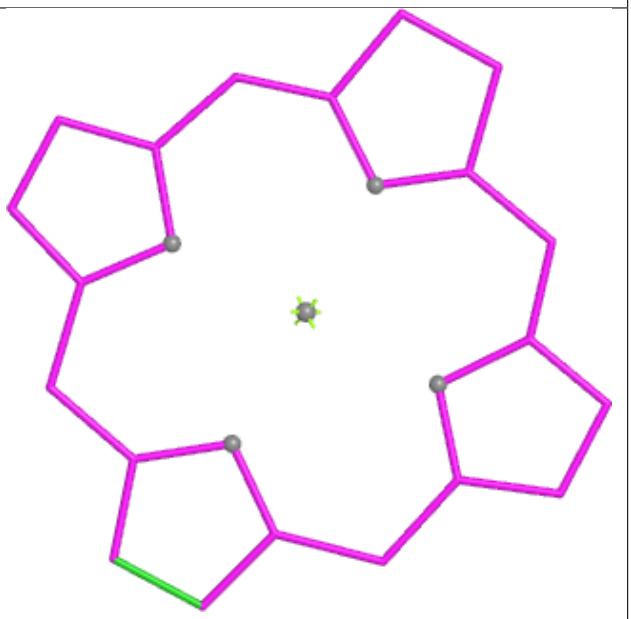
Torsions

Rings

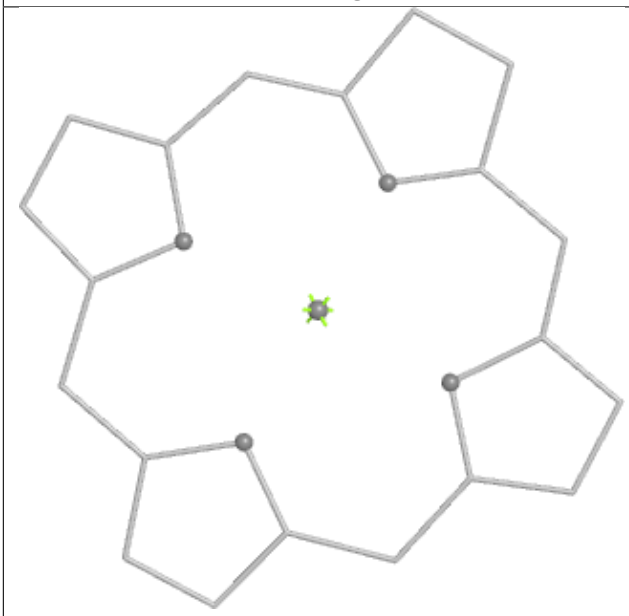
**Ligand CLA A 802**



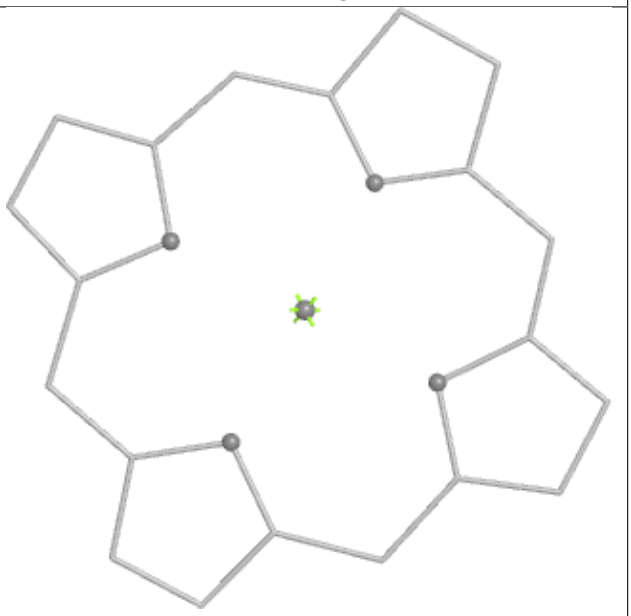
**Bond lengths**



**Bond angles**

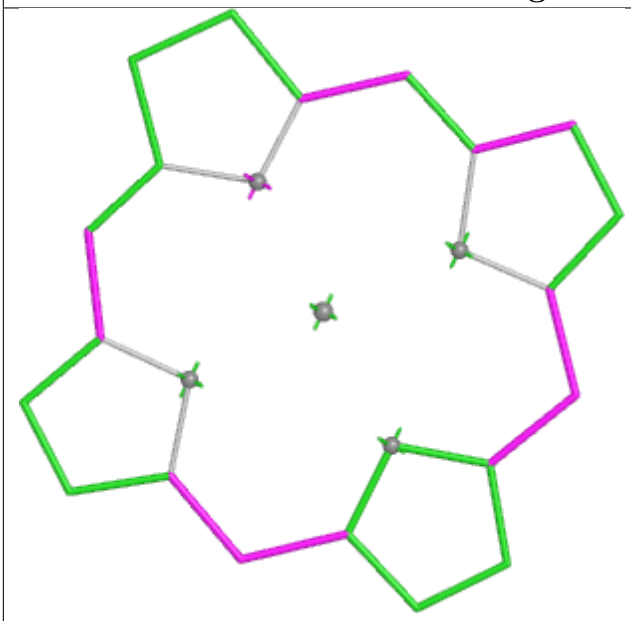


**Torsions**

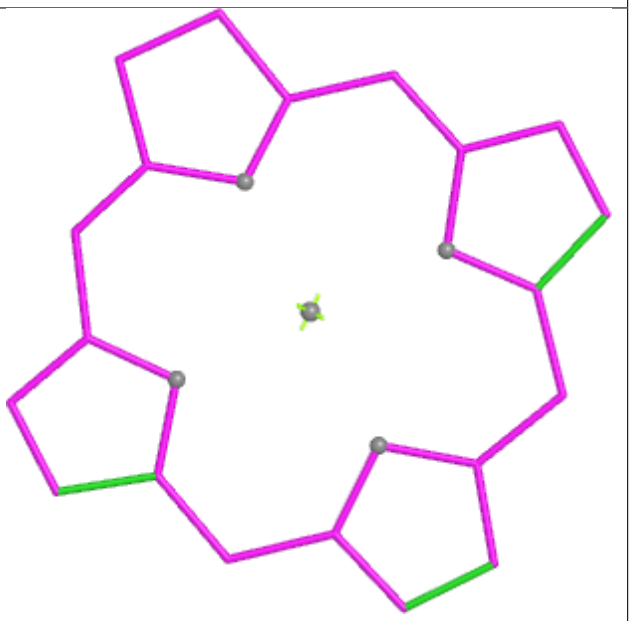


**Rings**

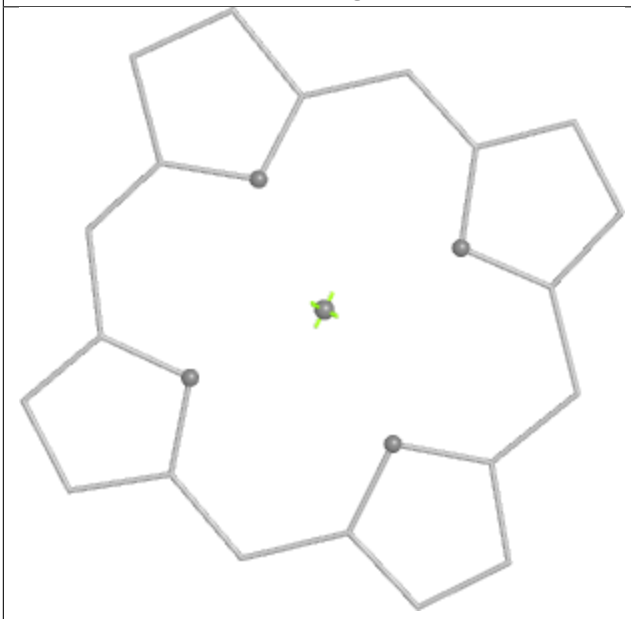
**Ligand CLA 1 208**



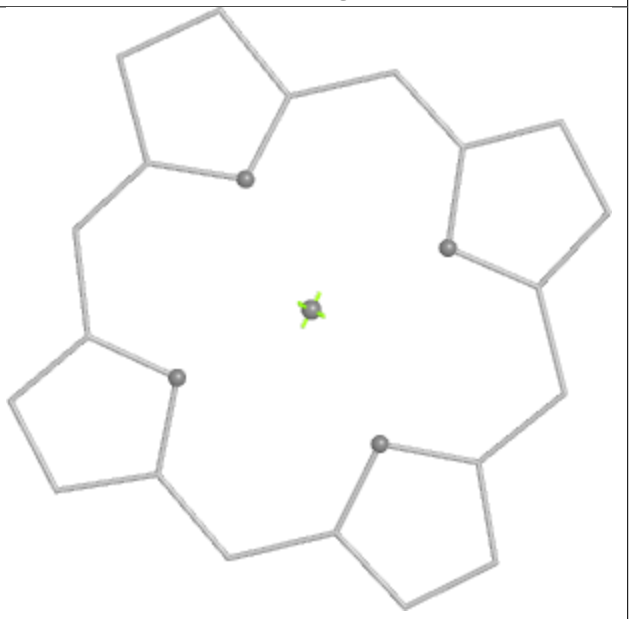
**Bond lengths**



**Bond angles**

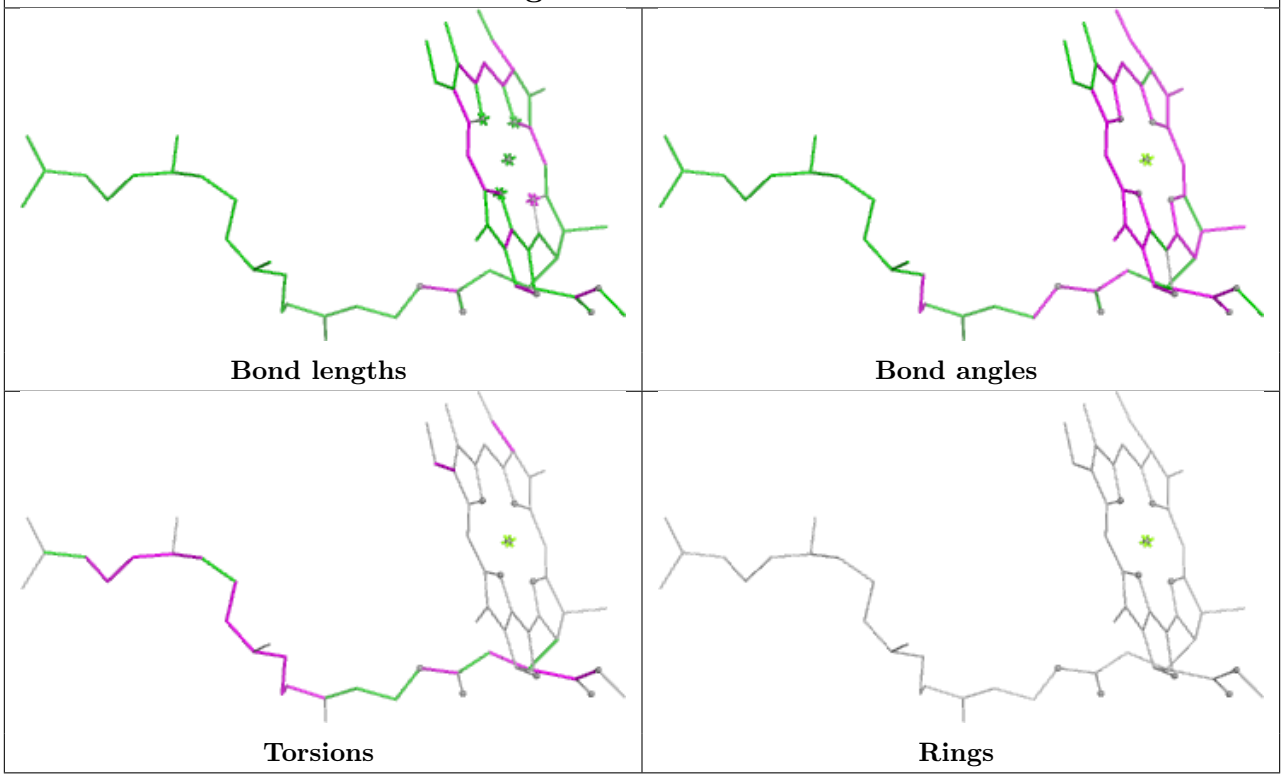


**Torsions**

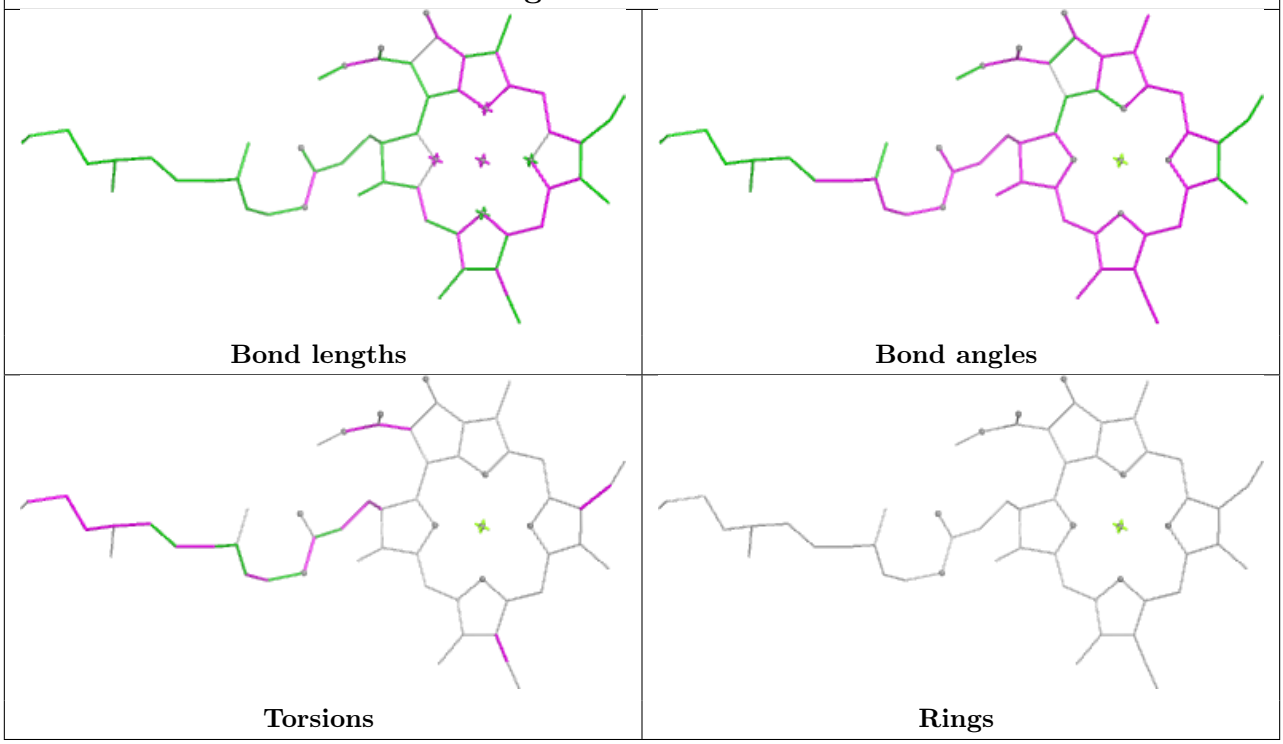


**Rings**

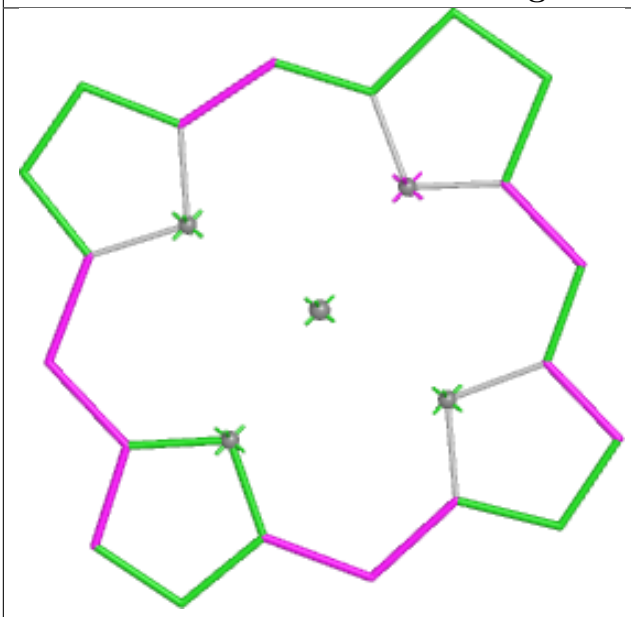
## Ligand CLA B 830



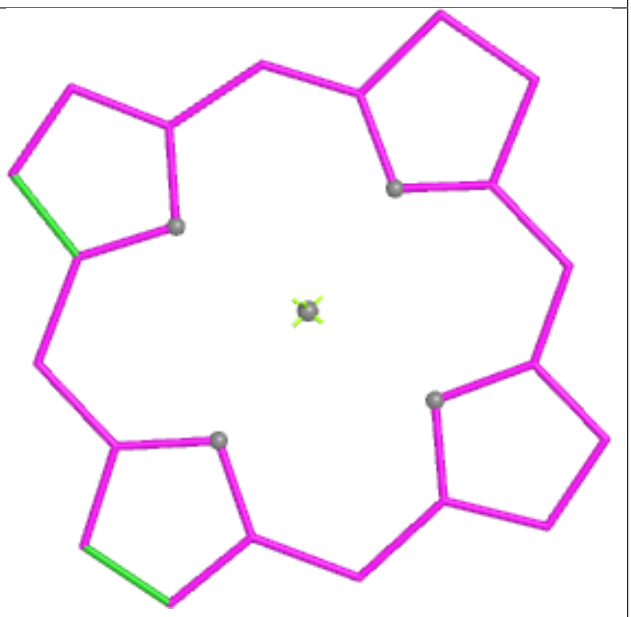

## Ligand CLA H 108



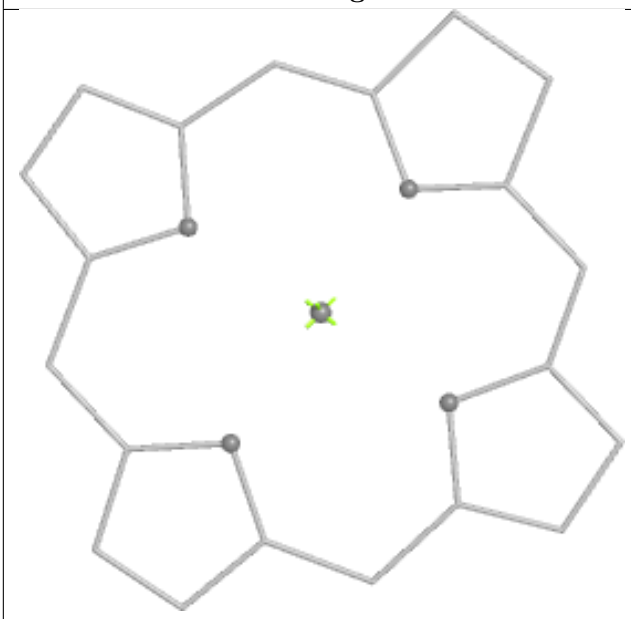
**Ligand CLA 4 307**



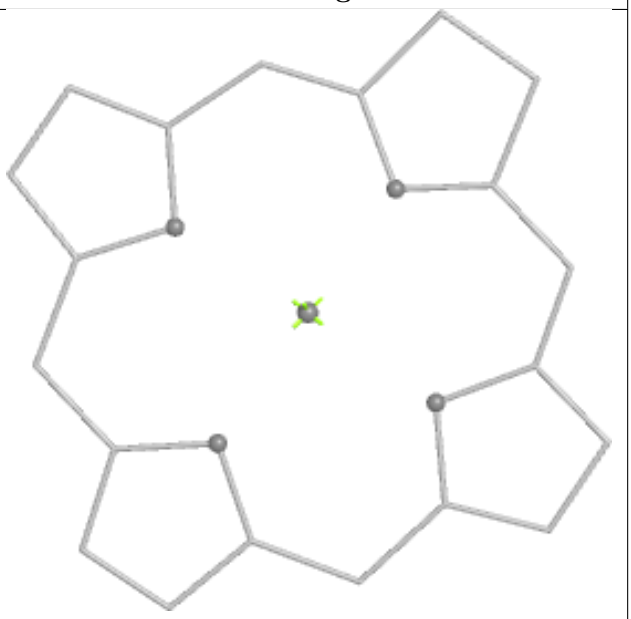
**Bond lengths**



**Bond angles**

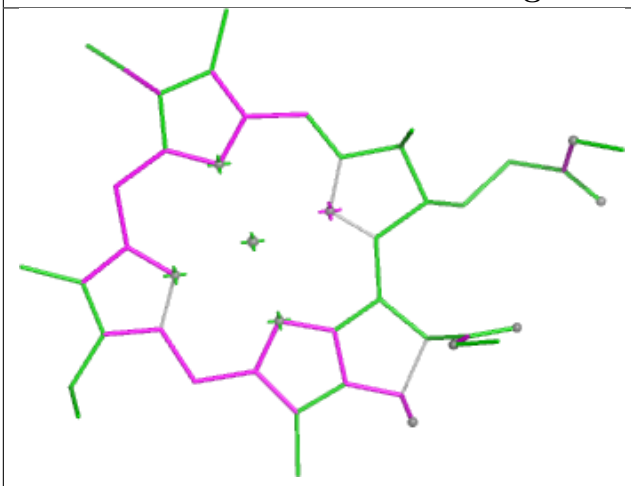


**Torsions**

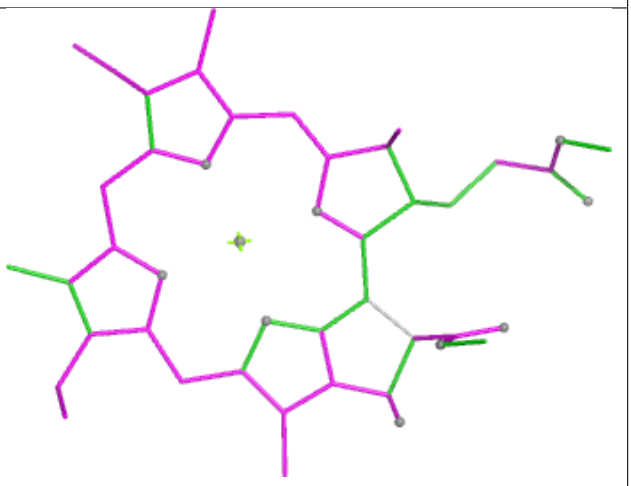


**Rings**

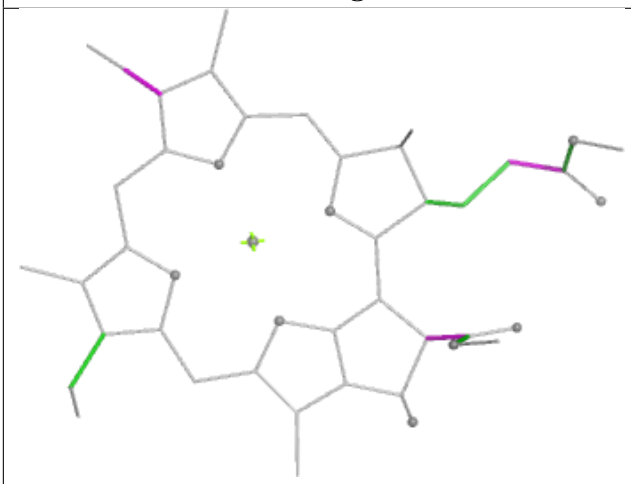
**Ligand CLA A 803**



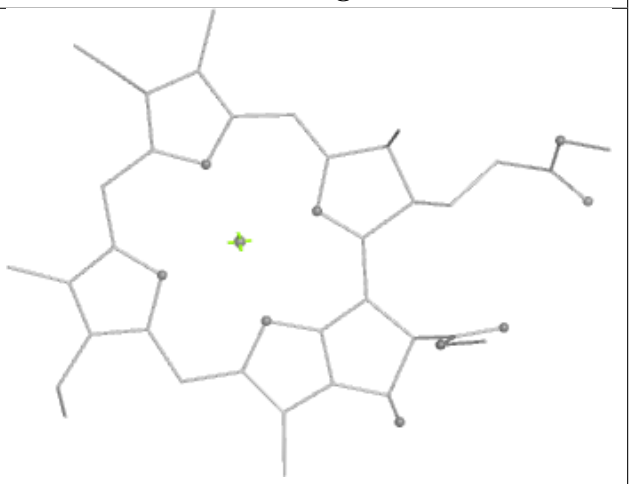
**Bond lengths**



**Bond angles**

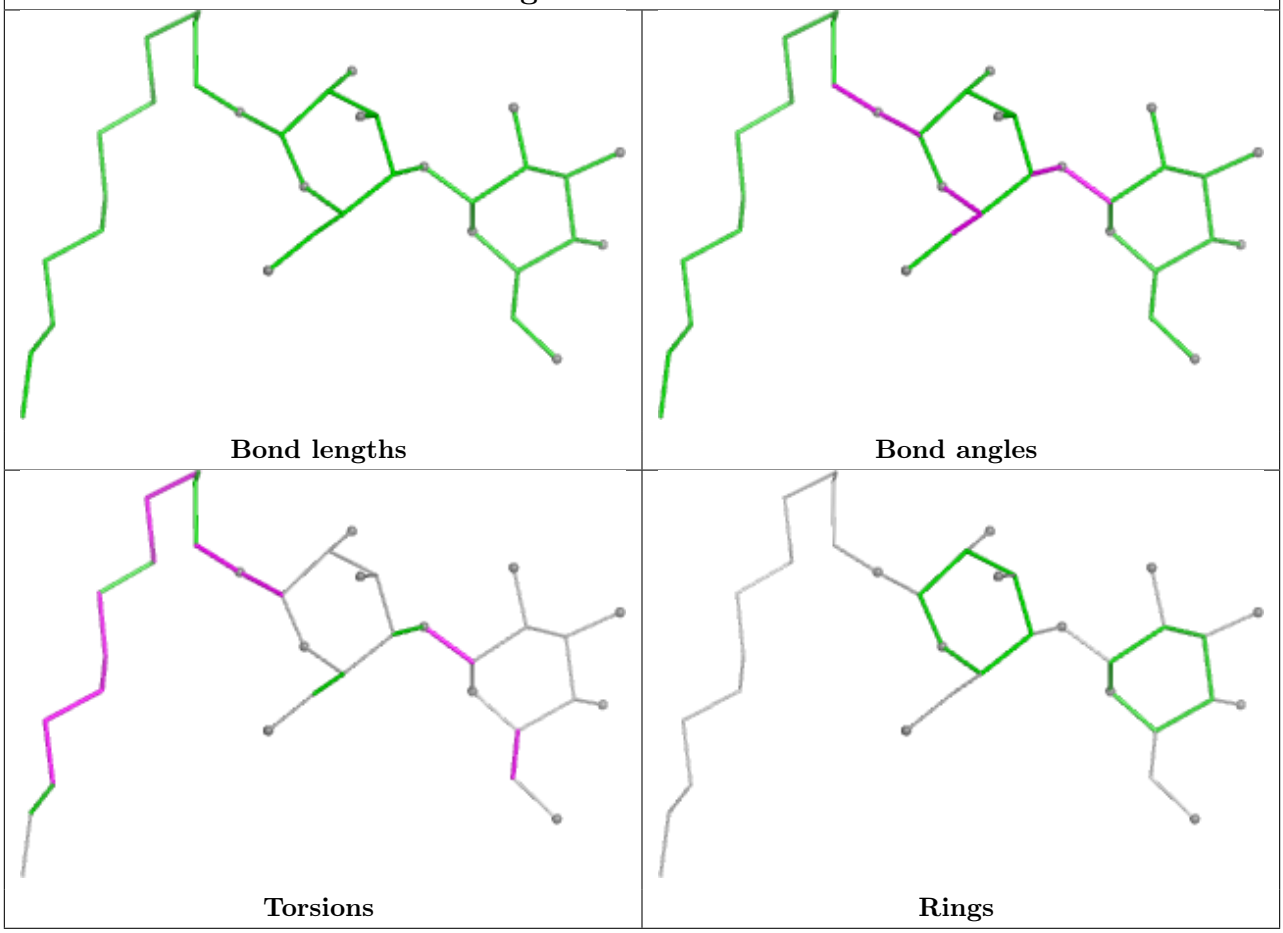


**Torsions**

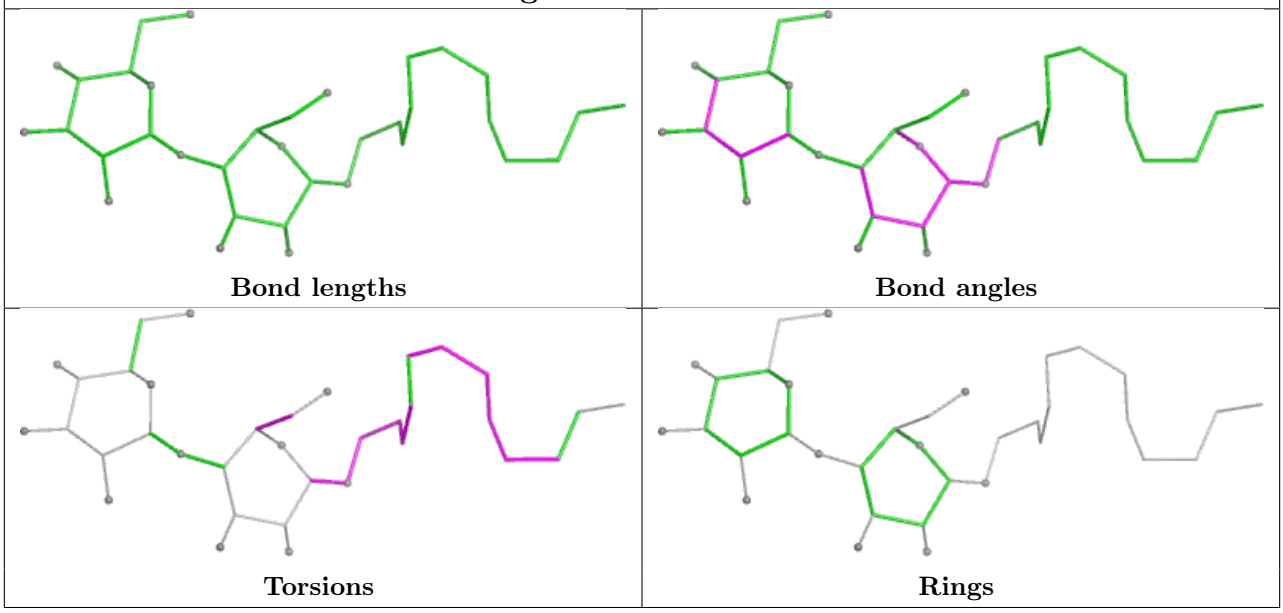


**Rings**

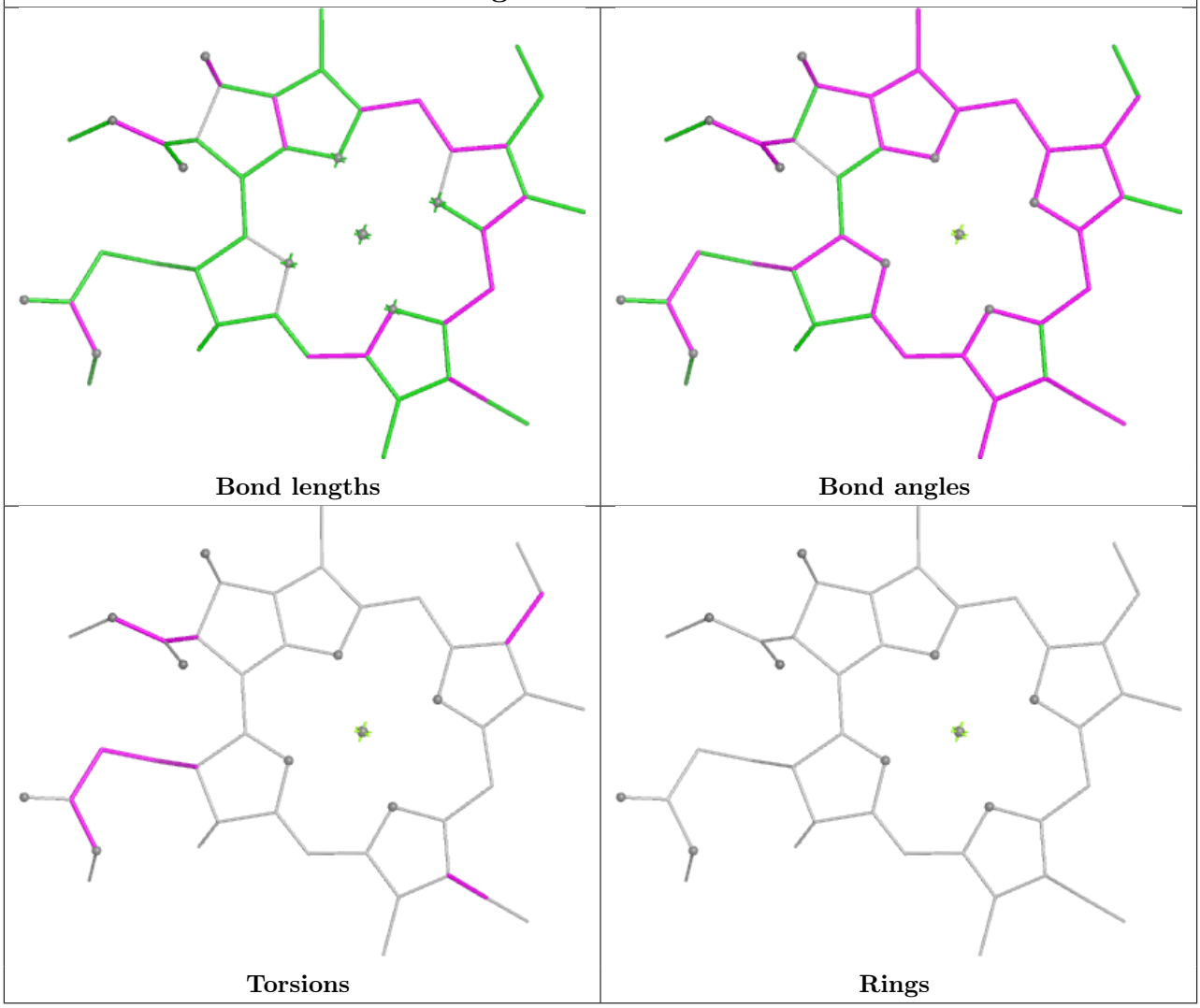
**Ligand LMU A 848**



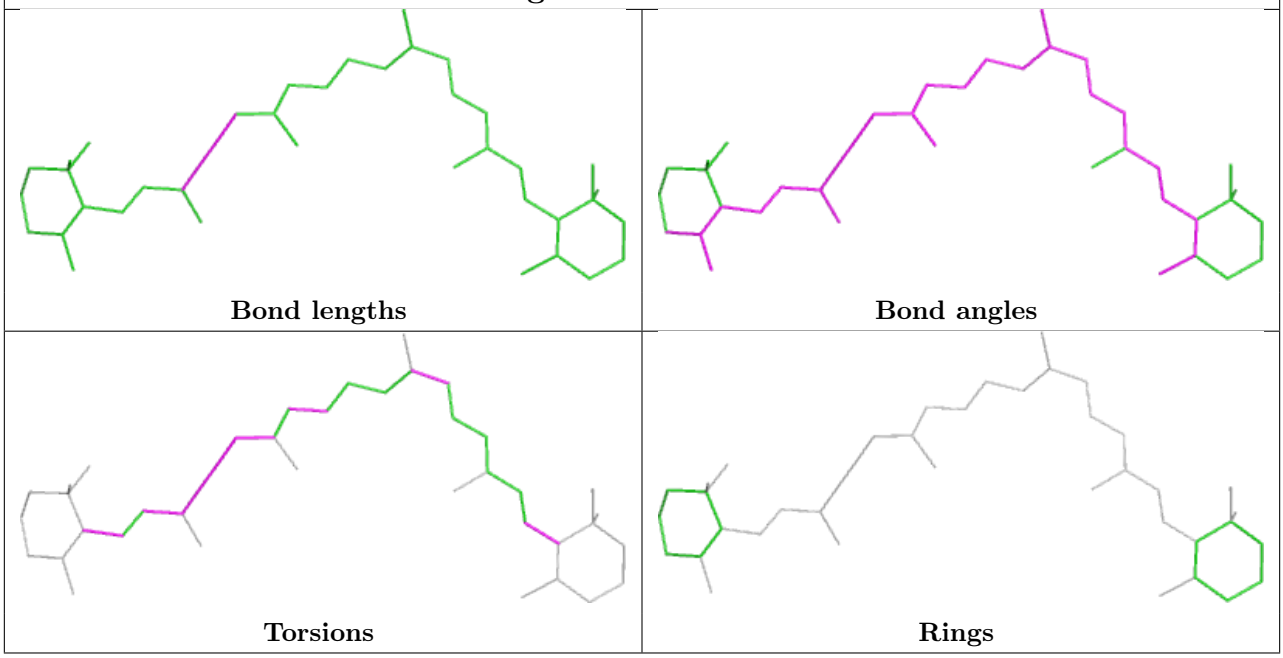

**Ligand LMU A 853**



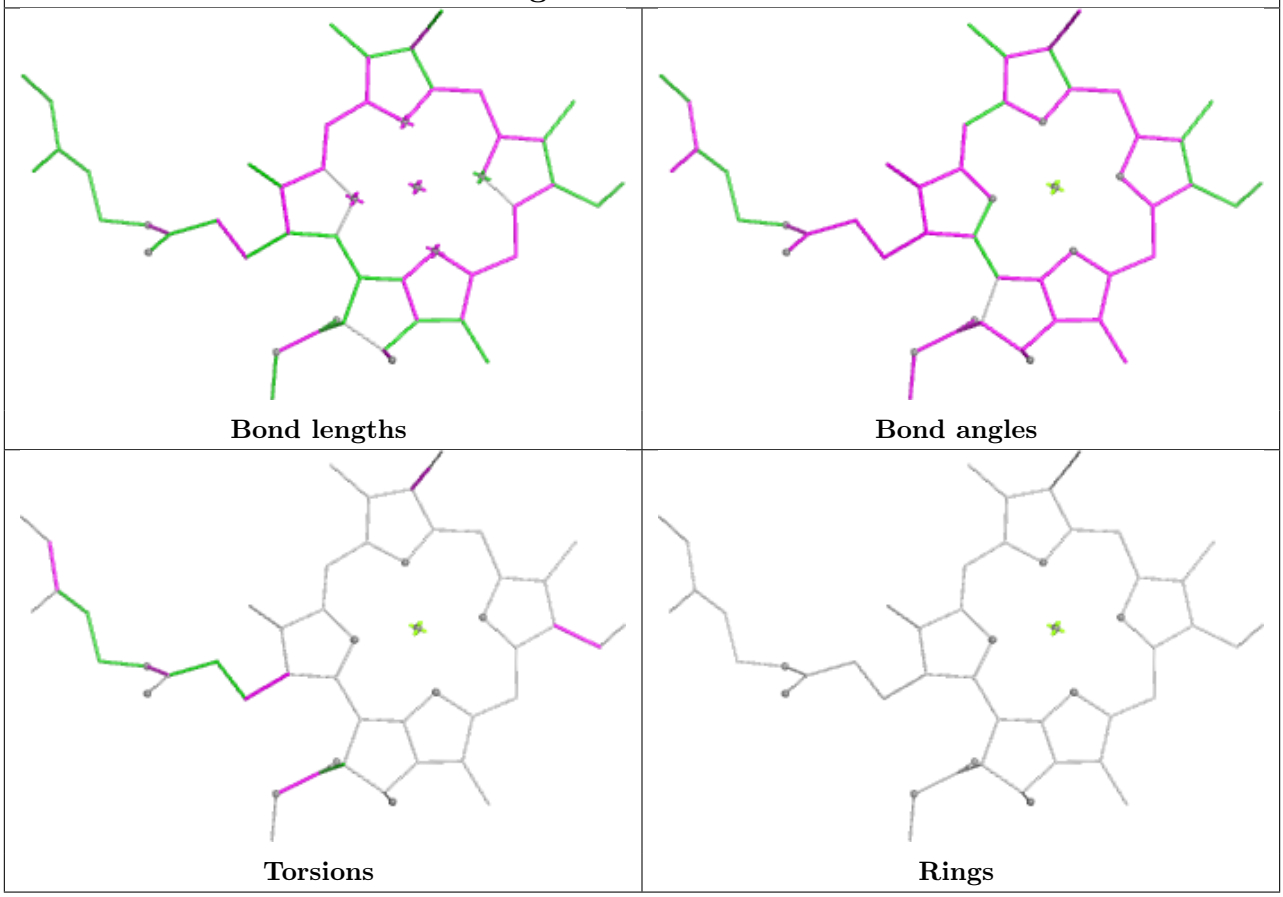
## Ligand CLA B 817




## Ligand BCR 2 317



**Ligand CLA 1 213**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 165/241 (68%) | 2.01 | 62 (37%) | 1 | 1 | 21, 24, 25, 25 | 0 |
| 2 | 2 | 176/269 (65%) | 1.61 | 50 (28%) | 1 | 2 | 21, 23, 24, 25 | 0 |
| 3 | 3 | 153/276 (55%) | 2.87 | 99 (64%) | 0 | 0 | 49, 78, 110, 112 | 0 |
| 4 | 4 | 166/251 (66%) | 1.67 | 51 (30%) | 1 | 2 | 21, 23, 24, 25 | 0 |
| 5 | A | 730/758 (96%) | 2.29 | 356 (48%) | 0 | 1 | 20, 22, 23, 25 | 0 |
| 6 | B | 733/734 (99%) | 2.38 | 403 (54%) | 0 | 0 | 20, 22, 24, 25 | 0 |
| 7 | C | 81/81 (100%) | 2.19 | 42 (51%) | 0 | 1 | 21, 22, 23, 23 | 0 |
| 8 | D | 138/212 (65%) | 1.93 | 54 (39%) | 1 | 1 | 21, 23, 24, 25 | 0 |
| 9 | E | 65/143 (45%) | 1.78 | 22 (33%) | 1 | 1 | 21, 22, 24, 24 | 0 |
| 10 | F | 154/231 (66%) | 1.73 | 50 (32%) | 1 | 1 | 21, 22, 23, 24 | 0 |
| 11 | G | 95/167 (56%) | 1.87 | 34 (35%) | 1 | 1 | 21, 23, 24, 25 | 0 |
| 12 | H | 69/144 (47%) | 1.54 | 21 (30%) | 1 | 2 | 21, 23, 24, 25 | 0 |
| 13 | I | 30/40 (75%) | 1.40 | 7 (23%) | 2 | 2 | 21, 22, 23, 23 | 0 |
| 14 | J | 42/44 (95%) | 1.85 | 16 (38%) | 1 | 1 | 21, 23, 23, 24 | 0 |
| 15 | K | 84/131 (64%) | 1.47 | 18 (21%) | 2 | 3 | 21, 24, 24, 26 | 0 |
| 16 | L | 162/216 (75%) | 1.94 | 55 (33%) | 1 | 1 | 20, 23, 24, 25 | 0 |
| 17 | N | 85/170 (50%) | 1.24 | 16 (18%) | 3 | 3 | 22, 23, 24, 25 | 0 |
| 18 | R | 0/53 | - | - | | | - | - |
| All | All | 3128/4161 (75%) | 2.08 | 1356 (43%) | 0 | 1 | 20, 23, 25, 112 | 0 |

All (1356) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | B | 204 | GLY | 10.5 |
| 16 | L | 141 | GLY | 10.3 |
| 6 | B | 197 | VAL | 10.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 130 | GLU | 10.0 |
| 6 | B | 566 | GLY | 9.4 |
| 16 | L | 142 | GLY | 9.3 |
| 5 | A | 752 | ALA | 9.1 |
| 6 | B | 517 | PHE | 9.0 |
| 16 | L | 140 | THR | 8.9 |
| 3 | 3 | 40 | SER | 8.8 |
| 5 | A | 344 | LYS | 8.7 |
| 1 | 1 | 88 | PRO | 8.7 |
| 1 | 1 | 92 | GLY | 8.6 |
| 3 | 3 | 58 | GLU | 8.5 |
| 5 | A | 582 | ASP | 8.5 |
| 5 | A | 126 | ILE | 8.5 |
| 3 | 3 | 123 | PHE | 8.4 |
| 16 | L | 96 | SER | 8.4 |
| 15 | K | 16 | THR | 8.4 |
| 2 | 2 | 123 | PRO | 8.2 |
| 5 | A | 746 | THR | 8.1 |
| 6 | B | 40 | GLY | 8.0 |
| 5 | A | 124 | TRP | 7.8 |
| 6 | B | 258 | LEU | 7.8 |
| 5 | A | 236 | GLY | 7.8 |
| 5 | A | 433 | ASP | 7.8 |
| 6 | B | 321 | GLY | 7.7 |
| 3 | 3 | 116 | PHE | 7.6 |
| 12 | H | 47 | PHE | 7.6 |
| 5 | A | 391 | THR | 7.5 |
| 6 | B | 252 | THR | 7.5 |
| 11 | G | 74 | TRP | 7.3 |
| 5 | A | 460 | LEU | 7.3 |
| 5 | A | 589 | THR | 7.3 |
| 6 | B | 562 | PRO | 7.3 |
| 10 | F | 124 | PRO | 7.2 |
| 5 | A | 505 | PRO | 7.2 |
| 6 | B | 487 | ASN | 7.2 |
| 6 | B | 354 | SER | 7.2 |
| 6 | B | 170 | ASN | 7.1 |
| 5 | A | 232 | PHE | 7.1 |
| 6 | B | 94 | PRO | 6.9 |
| 3 | 3 | 55 | ALA | 6.9 |
| 1 | 1 | 87 | ASN | 6.9 |
| 4 | 4 | 114 | SER | 6.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | B | 334 | LEU | 6.8 |
| 5 | A | 751 | LEU | 6.8 |
| 3 | 3 | 113 | LEU | 6.8 |
| 8 | D | 141 | VAL | 6.7 |
| 5 | A | 33 | GLN | 6.7 |
| 6 | B | 200 | PRO | 6.7 |
| 6 | B | 147 | PHE | 6.6 |
| 5 | A | 575 | LEU | 6.5 |
| 5 | A | 217 | SER | 6.4 |
| 3 | 3 | 126 | HIS | 6.4 |
| 10 | F | 38 | PRO | 6.4 |
| 10 | F | 152 | ASN | 6.4 |
| 5 | A | 647 | ILE | 6.3 |
| 5 | A | 586 | ARG | 6.2 |
| 11 | G | 59 | LYS | 6.2 |
| 6 | B | 486 | LEU | 6.1 |
| 5 | A | 617 | SER | 6.1 |
| 5 | A | 34 | TRP | 6.1 |
| 5 | A | 388 | ASP | 6.1 |
| 5 | A | 134 | GLY | 6.0 |
| 6 | B | 457 | PRO | 6.0 |
| 6 | B | 210 | ASN | 6.0 |
| 6 | B | 413 | GLU | 6.0 |
| 1 | 1 | 113 | SER | 6.0 |
| 5 | A | 659 | ALA | 5.9 |
| 6 | B | 263 | PRO | 5.9 |
| 5 | A | 506 | GLY | 5.9 |
| 6 | B | 558 | PRO | 5.8 |
| 6 | B | 251 | GLY | 5.8 |
| 16 | L | 98 | CYS | 5.8 |
| 6 | B | 271 | THR | 5.8 |
| 2 | 2 | 61 | GLY | 5.7 |
| 5 | A | 371 | VAL | 5.7 |
| 1 | 1 | 39 | TYR | 5.7 |
| 5 | A | 53 | TRP | 5.7 |
| 8 | D | 61 | PRO | 5.7 |
| 6 | B | 511 | THR | 5.7 |
| 2 | 2 | 110 | TRP | 5.7 |
| 6 | B | 93 | ASP | 5.7 |
| 5 | A | 61 | ALA | 5.6 |
| 6 | B | 358 | TYR | 5.6 |
| 2 | 2 | 43 | TRP | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 538 | ASP | 5.6 |
| 6 | B | 527 | LEU | 5.5 |
| 3 | 3 | 193 | ALA | 5.5 |
| 5 | A | 461 | TYR | 5.5 |
| 6 | B | 534 | LEU | 5.4 |
| 6 | B | 700 | LEU | 5.4 |
| 6 | B | 234 | ALA | 5.4 |
| 11 | G | 75 | GLY | 5.4 |
| 5 | A | 191 | PRO | 5.4 |
| 5 | A | 32 | GLU | 5.3 |
| 5 | A | 470 | LEU | 5.3 |
| 6 | B | 96 | PHE | 5.3 |
| 5 | A | 724 | ALA | 5.3 |
| 6 | B | 387 | PHE | 5.3 |
| 6 | B | 491 | ASN | 5.3 |
| 5 | A | 122 | VAL | 5.3 |
| 10 | F | 121 | ILE | 5.3 |
| 6 | B | 300 | SER | 5.2 |
| 3 | 3 | 80 | LYS | 5.2 |
| 5 | A | 220 | ARG | 5.2 |
| 5 | A | 283 | PHE | 5.2 |
| 15 | K | 64 | GLY | 5.2 |
| 6 | B | 217 | PRO | 5.2 |
| 6 | B | 183 | PHE | 5.1 |
| 6 | B | 682 | HIS | 5.1 |
| 5 | A | 464 | ASN | 5.1 |
| 16 | L | 95 | LEU | 5.1 |
| 5 | A | 195 | TRP | 5.1 |
| 6 | B | 364 | ASP | 5.1 |
| 5 | A | 718 | PRO | 5.1 |
| 3 | 3 | 124 | ALA | 5.1 |
| 7 | C | 4 | SER | 5.1 |
| 8 | D | 86 | LEU | 5.1 |
| 3 | 3 | 108 | ALA | 5.0 |
| 6 | B | 372 | TYR | 5.0 |
| 5 | A | 719 | ALA | 5.0 |
| 16 | L | 145 | PHE | 5.0 |
| 6 | B | 430 | GLY | 5.0 |
| 6 | B | 214 | ASP | 5.0 |
| 6 | B | 724 | PHE | 5.0 |
| 5 | A | 286 | GLY | 5.0 |
| 6 | B | 148 | ILE | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | B | 212 | PHE | 5.0 |
| 6 | B | 702 | ILE | 4.9 |
| 1 | 1 | 111 | GLN | 4.9 |
| 5 | A | 247 | GLU | 4.9 |
| 7 | C | 1 | MET | 4.9 |
| 3 | 3 | 117 | GLU | 4.9 |
| 7 | C | 57 | ALA | 4.9 |
| 6 | B | 645 | VAL | 4.9 |
| 8 | D | 63 | GLY | 4.9 |
| 6 | B | 514 | PRO | 4.9 |
| 5 | A | 750 | PHE | 4.9 |
| 6 | B | 264 | GLN | 4.8 |
| 7 | C | 60 | THR | 4.8 |
| 6 | B | 368 | GLN | 4.8 |
| 5 | A | 159 | THR | 4.8 |
| 6 | B | 520 | HIS | 4.8 |
| 3 | 3 | 79 | GLY | 4.8 |
| 5 | A | 685 | VAL | 4.8 |
| 6 | B | 590 | VAL | 4.8 |
| 3 | 3 | 53 | TRP | 4.8 |
| 6 | B | 493 | TRP | 4.8 |
| 3 | 3 | 112 | THR | 4.8 |
| 7 | C | 78 | GLY | 4.8 |
| 10 | F | 37 | ALA | 4.8 |
| 3 | 3 | 111 | TYR | 4.7 |
| 1 | 1 | 115 | GLU | 4.7 |
| 8 | D | 108 | GLU | 4.7 |
| 5 | A | 574 | ASN | 4.7 |
| 6 | B | 541 | ALA | 4.7 |
| 5 | A | 576 | GLY | 4.7 |
| 6 | B | 455 | ILE | 4.7 |
| 16 | L | 20 | ILE | 4.7 |
| 3 | 3 | 120 | LEU | 4.7 |
| 5 | A | 304 | LEU | 4.7 |
| 8 | D | 136 | SER | 4.7 |
| 14 | J | 36 | ALA | 4.7 |
| 1 | 1 | 163 | VAL | 4.7 |
| 6 | B | 92 | TRP | 4.6 |
| 5 | A | 76 | ARG | 4.6 |
| 6 | B | 194 | LEU | 4.6 |
| 1 | 1 | 42 | SER | 4.6 |
| 5 | A | 281 | LEU | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | 3 | 196 | GLY | 4.6 |
| 5 | A | 542 | HIS | 4.6 |
| 5 | A | 329 | ASP | 4.6 |
| 5 | A | 266 | ALA | 4.6 |
| 5 | A | 186 | TYR | 4.6 |
| 7 | C | 68 | TYR | 4.6 |
| 6 | B | 118 | SER | 4.6 |
| 6 | B | 249 | GLY | 4.6 |
| 5 | A | 101 | ALA | 4.6 |
| 6 | B | 353 | TYR | 4.5 |
| 6 | B | 670 | TYR | 4.5 |
| 5 | A | 485 | GLN | 4.5 |
| 6 | B | 366 | THR | 4.5 |
| 6 | B | 337 | ALA | 4.5 |
| 7 | C | 20 | ALA | 4.5 |
| 3 | 3 | 122 | GLY | 4.5 |
| 3 | 3 | 42 | PRO | 4.5 |
| 1 | 1 | 28 | GLY | 4.5 |
| 3 | 3 | 114 | PHE | 4.5 |
| 9 | E | 64 | PRO | 4.5 |
| 3 | 3 | 104 | TYR | 4.4 |
| 10 | F | 73 | VAL | 4.4 |
| 7 | C | 56 | SER | 4.4 |
| 5 | A | 345 | GLY | 4.4 |
| 6 | B | 16 | PRO | 4.4 |
| 16 | L | 73 | PRO | 4.4 |
| 1 | 1 | 17 | SER | 4.4 |
| 3 | 3 | 95 | THR | 4.4 |
| 6 | B | 561 | GLY | 4.4 |
| 7 | C | 9 | ASP | 4.4 |
| 15 | K | 63 | CYS | 4.4 |
| 5 | A | 385 | LEU | 4.3 |
| 6 | B | 209 | TRP | 4.3 |
| 4 | 4 | 134 | PRO | 4.3 |
| 11 | G | 4 | PRO | 4.3 |
| 6 | B | 576 | PHE | 4.3 |
| 5 | A | 484 | LEU | 4.3 |
| 5 | A | 686 | TRP | 4.3 |
| 6 | B | 67 | HIS | 4.3 |
| 7 | C | 55 | GLU | 4.3 |
| 3 | 3 | 61 | ASN | 4.3 |
| 7 | C | 50 | GLY | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | B | 205 | GLU | 4.3 |
| 9 | E | 79 | THR | 4.3 |
| 6 | B | 272 | ASP | 4.3 |
| 5 | A | 341 | GLN | 4.3 |
| 5 | A | 209 | GLY | 4.2 |
| 6 | B | 346 | SER | 4.2 |
| 2 | 2 | 139 | GLY | 4.2 |
| 5 | A | 161 | GLU | 4.2 |
| 16 | L | 134 | ASP | 4.2 |
| 5 | A | 376 | MET | 4.2 |
| 16 | L | 144 | PHE | 4.2 |
| 6 | B | 679 | ALA | 4.2 |
| 4 | 4 | 89 | THR | 4.2 |
| 3 | 3 | 64 | TYR | 4.2 |
| 5 | A | 123 | VAL | 4.2 |
| 5 | A | 287 | LEU | 4.2 |
| 5 | A | 80 | SER | 4.2 |
| 10 | F | 76 | ASP | 4.2 |
| 6 | B | 199 | ILE | 4.2 |
| 6 | B | 331 | HIS | 4.2 |
| 5 | A | 699 | TYR | 4.2 |
| 8 | D | 135 | ARG | 4.2 |
| 5 | A | 393 | LEU | 4.1 |
| 6 | B | 261 | PHE | 4.1 |
| 4 | 4 | 157 | GLY | 4.1 |
| 14 | J | 6 | THR | 4.1 |
| 6 | B | 341 | LEU | 4.1 |
| 5 | A | 249 | ILE | 4.1 |
| 16 | L | 116 | PRO | 4.1 |
| 4 | 4 | 174 | GLY | 4.1 |
| 5 | A | 731 | ARG | 4.1 |
| 3 | 3 | 54 | LEU | 4.1 |
| 2 | 2 | 104 | TRP | 4.1 |
| 5 | A | 500 | PRO | 4.1 |
| 5 | A | 541 | VAL | 4.1 |
| 6 | B | 127 | ILE | 4.1 |
| 5 | A | 697 | ARG | 4.1 |
| 4 | 4 | 125 | SER | 4.1 |
| 6 | B | 690 | LEU | 4.1 |
| 5 | A | 278 | ALA | 4.1 |
| 6 | B | 250 | ALA | 4.1 |
| 6 | B | 621 | ARG | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 9 | E | 30 | PRO | 4.1 |
| 1 | 1 | 80 | GLY | 4.1 |
| 6 | B | 220 | GLN | 4.0 |
| 5 | A | 742 | GLY | 4.0 |
| 15 | K | 5 | SER | 4.0 |
| 8 | D | 25 | PRO | 4.0 |
| 16 | L | 101 | MET | 4.0 |
| 5 | A | 160 | SER | 4.0 |
| 5 | A | 440 | ASP | 4.0 |
| 5 | A | 706 | SER | 4.0 |
| 3 | 3 | 44 | GLY | 4.0 |
| 5 | A | 185 | HIS | 4.0 |
| 3 | 3 | 49 | ILE | 4.0 |
| 9 | E | 73 | ASN | 4.0 |
| 6 | B | 196 | HIS | 4.0 |
| 6 | B | 332 | PHE | 4.0 |
| 6 | B | 533 | ILE | 4.0 |
| 3 | 3 | 81 | ALA | 4.0 |
| 16 | L | 42 | ALA | 4.0 |
| 11 | G | 5 | SER | 4.0 |
| 6 | B | 213 | LEU | 4.0 |
| 10 | F | 62 | LEU | 4.0 |
| 12 | H | 76 | VAL | 3.9 |
| 5 | A | 368 | LEU | 3.9 |
| 6 | B | 195 | VAL | 3.9 |
| 7 | C | 66 | ARG | 3.9 |
| 6 | B | 484 | PRO | 3.9 |
| 5 | A | 493 | GLN | 3.9 |
| 8 | D | 151 | LYS | 3.9 |
| 5 | A | 168 | ALA | 3.9 |
| 5 | A | 640 | GLY | 3.9 |
| 16 | L | 99 | LEU | 3.9 |
| 3 | 3 | 142 | TYR | 3.9 |
| 4 | 4 | 36 | ASN | 3.9 |
| 6 | B | 627 | ASN | 3.9 |
| 5 | A | 257 | GLN | 3.9 |
| 5 | A | 62 | HIS | 3.9 |
| 6 | B | 242 | HIS | 3.9 |
| 5 | A | 223 | VAL | 3.8 |
| 1 | 1 | 169 | PRO | 3.8 |
| 8 | D | 34 | GLY | 3.8 |
| 16 | L | 81 | GLY | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 744 | ALA | 3.8 |
| 7 | C | 65 | VAL | 3.8 |
| 13 | I | 9 | VAL | 3.8 |
| 16 | L | 69 | VAL | 3.8 |
| 5 | A | 335 | LYS | 3.8 |
| 14 | J | 38 | THR | 3.8 |
| 14 | J | 4 | PHE | 3.8 |
| 6 | B | 270 | LEU | 3.8 |
| 6 | B | 292 | ARG | 3.8 |
| 16 | L | 106 | SER | 3.8 |
| 9 | E | 87 | VAL | 3.8 |
| 3 | 3 | 76 | GLU | 3.8 |
| 3 | 3 | 173 | GLU | 3.8 |
| 6 | B | 456 | GLU | 3.8 |
| 7 | C | 17 | CYS | 3.8 |
| 6 | B | 203 | ARG | 3.8 |
| 6 | B | 674 | LEU | 3.8 |
| 16 | L | 23 | LEU | 3.8 |
| 3 | 3 | 43 | GLU | 3.8 |
| 5 | A | 486 | PRO | 3.8 |
| 6 | B | 565 | GLY | 3.8 |
| 5 | A | 294 | LEU | 3.8 |
| 6 | B | 579 | ALA | 3.8 |
| 6 | B | 319 | HIS | 3.8 |
| 6 | B | 574 | ASP | 3.8 |
| 1 | 1 | 64 | GLY | 3.8 |
| 3 | 3 | 57 | GLY | 3.8 |
| 6 | B | 676 | GLU | 3.8 |
| 5 | A | 536 | THR | 3.8 |
| 6 | B | 559 | CYS | 3.8 |
| 12 | H | 44 | ALA | 3.7 |
| 5 | A | 527 | VAL | 3.7 |
| 5 | A | 272 | LEU | 3.7 |
| 6 | B | 530 | THR | 3.7 |
| 4 | 4 | 86 | SER | 3.7 |
| 5 | A | 610 | SER | 3.7 |
| 6 | B | 512 | ILE | 3.7 |
| 3 | 3 | 181 | LEU | 3.7 |
| 5 | A | 106 | TYR | 3.7 |
| 1 | 1 | 18 | ALA | 3.7 |
| 5 | A | 362 | LEU | 3.7 |
| 1 | 1 | 47 | CYS | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 57 | LEU | 3.7 |
| 6 | B | 336 | LEU | 3.7 |
| 6 | B | 620 | LEU | 3.7 |
| 5 | A | 66 | SER | 3.7 |
| 6 | B | 658 | ALA | 3.7 |
| 6 | B | 12 | ILE | 3.7 |
| 6 | B | 95 | HIS | 3.7 |
| 6 | B | 587 | ILE | 3.7 |
| 11 | G | 23 | PHE | 3.7 |
| 3 | 3 | 109 | ASP | 3.6 |
| 11 | G | 53 | GLU | 3.6 |
| 11 | G | 22 | VAL | 3.6 |
| 14 | J | 10 | VAL | 3.6 |
| 6 | B | 73 | ASN | 3.6 |
| 3 | 3 | 77 | ILE | 3.6 |
| 6 | B | 338 | LEU | 3.6 |
| 6 | B | 474 | PHE | 3.6 |
| 6 | B | 221 | GLY | 3.6 |
| 6 | B | 667 | TRP | 3.6 |
| 3 | 3 | 198 | PHE | 3.6 |
| 5 | A | 458 | PHE | 3.6 |
| 3 | 3 | 206 | VAL | 3.6 |
| 5 | A | 384 | TYR | 3.6 |
| 6 | B | 239 | SER | 3.6 |
| 16 | L | 33 | ILE | 3.6 |
| 5 | A | 60 | ASP | 3.6 |
| 5 | A | 118 | PRO | 3.6 |
| 10 | F | 146 | ASN | 3.6 |
| 6 | B | 444 | LEU | 3.6 |
| 2 | 2 | 152 | SER | 3.6 |
| 5 | A | 52 | THR | 3.6 |
| 6 | B | 571 | SER | 3.6 |
| 6 | B | 569 | ASP | 3.6 |
| 6 | B | 244 | PHE | 3.5 |
| 6 | B | 178 | HIS | 3.5 |
| 6 | B | 335 | GLY | 3.5 |
| 4 | 4 | 115 | VAL | 3.5 |
| 5 | A | 487 | VAL | 3.5 |
| 3 | 3 | 190 | ALA | 3.5 |
| 11 | G | 46 | ALA | 3.5 |
| 5 | A | 346 | LEU | 3.5 |
| 5 | A | 727 | ILE | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | 3 | 56 | TYR | 3.5 |
| 8 | D | 58 | PHE | 3.5 |
| 5 | A | 374 | GLN | 3.5 |
| 6 | B | 215 | VAL | 3.5 |
| 8 | D | 115 | LYS | 3.5 |
| 3 | 3 | 73 | ILE | 3.5 |
| 10 | F | 108 | ILE | 3.5 |
| 6 | B | 27 | THR | 3.5 |
| 7 | C | 10 | THR | 3.5 |
| 3 | 3 | 207 | GLY | 3.5 |
| 5 | A | 100 | GLY | 3.5 |
| 8 | D | 21 | ASP | 3.5 |
| 15 | K | 68 | HIS | 3.5 |
| 3 | 3 | 78 | LEU | 3.5 |
| 5 | A | 381 | PRO | 3.5 |
| 5 | A | 540 | LEU | 3.5 |
| 6 | B | 448 | THR | 3.5 |
| 5 | A | 551 | VAL | 3.5 |
| 6 | B | 350 | GLN | 3.5 |
| 6 | B | 516 | ASP | 3.5 |
| 6 | B | 575 | ASP | 3.5 |
| 6 | B | 124 | TRP | 3.5 |
| 1 | 1 | 97 | ILE | 3.5 |
| 3 | 3 | 70 | VAL | 3.5 |
| 3 | 3 | 96 | GLY | 3.5 |
| 3 | 3 | 184 | VAL | 3.5 |
| 12 | H | 26 | SER | 3.5 |
| 5 | A | 482 | ILE | 3.5 |
| 5 | A | 704 | ILE | 3.5 |
| 5 | A | 743 | ILE | 3.5 |
| 6 | B | 622 | ASP | 3.5 |
| 5 | A | 539 | PHE | 3.4 |
| 6 | B | 327 | ASN | 3.4 |
| 1 | 1 | 104 | ALA | 3.4 |
| 3 | 3 | 65 | ALA | 3.4 |
| 6 | B | 255 | LEU | 3.4 |
| 6 | B | 408 | LEU | 3.4 |
| 3 | 3 | 121 | MET | 3.4 |
| 3 | 3 | 159 | PRO | 3.4 |
| 5 | A | 89 | ILE | 3.4 |
| 5 | A | 201 | SER | 3.4 |
| 5 | A | 613 | ILE | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 662 | SER | 3.4 |
| 6 | B | 666 | SER | 3.4 |
| 12 | H | 46 | PRO | 3.4 |
| 6 | B | 560 | ASP | 3.4 |
| 5 | A | 562 | PHE | 3.4 |
| 2 | 2 | 50 | VAL | 3.4 |
| 6 | B | 207 | VAL | 3.4 |
| 6 | B | 343 | VAL | 3.4 |
| 3 | 3 | 72 | ALA | 3.4 |
| 6 | B | 432 | HIS | 3.4 |
| 11 | G | 96 | SER | 3.4 |
| 11 | G | 70 | ASP | 3.4 |
| 16 | L | 159 | TYR | 3.4 |
| 16 | L | 91 | LEU | 3.4 |
| 5 | A | 587 | GLY | 3.4 |
| 1 | 1 | 93 | THR | 3.4 |
| 5 | A | 146 | THR | 3.4 |
| 6 | B | 440 | ASN | 3.4 |
| 5 | A | 77 | LYS | 3.4 |
| 10 | F | 11 | SER | 3.4 |
| 5 | A | 203 | LEU | 3.4 |
| 6 | B | 377 | TYR | 3.4 |
| 3 | 3 | 60 | ILE | 3.4 |
| 5 | A | 745 | THR | 3.4 |
| 8 | D | 50 | TRP | 3.4 |
| 6 | B | 568 | CYS | 3.4 |
| 5 | A | 415 | ALA | 3.4 |
| 6 | B | 647 | ALA | 3.4 |
| 6 | B | 237 | PRO | 3.4 |
| 2 | 2 | 78 | SER | 3.3 |
| 3 | 3 | 195 | LEU | 3.3 |
| 6 | B | 438 | VAL | 3.3 |
| 2 | 2 | 132 | GLY | 3.3 |
| 6 | B | 513 | GLY | 3.3 |
| 8 | D | 137 | ILE | 3.3 |
| 6 | B | 439 | HIS | 3.3 |
| 9 | E | 80 | ASN | 3.3 |
| 7 | C | 70 | TRP | 3.3 |
| 11 | G | 11 | SER | 3.3 |
| 3 | 3 | 118 | MET | 3.3 |
| 6 | B | 198 | ALA | 3.3 |
| 10 | F | 94 | ALA | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 9 | E | 36 | VAL | 3.3 |
| 5 | A | 285 | GLY | 3.3 |
| 5 | A | 300 | ALA | 3.3 |
| 6 | B | 479 | SER | 3.3 |
| 6 | B | 701 | SER | 3.3 |
| 1 | 1 | 38 | ARG | 3.3 |
| 4 | 4 | 105 | ARG | 3.3 |
| 6 | B | 333 | GLN | 3.3 |
| 5 | A | 693 | LEU | 3.3 |
| 6 | B | 663 | PHE | 3.3 |
| 8 | D | 20 | LEU | 3.3 |
| 10 | F | 82 | GLU | 3.3 |
| 15 | K | 65 | ALA | 3.3 |
| 5 | A | 567 | ARG | 3.3 |
| 6 | B | 508 | LEU | 3.3 |
| 6 | B | 320 | LYS | 3.3 |
| 4 | 4 | 39 | TRP | 3.3 |
| 6 | B | 211 | ASN | 3.3 |
| 6 | B | 573 | TRP | 3.3 |
| 7 | C | 41 | SER | 3.2 |
| 2 | 2 | 197 | LEU | 3.2 |
| 3 | 3 | 200 | GLN | 3.2 |
| 8 | D | 41 | GLN | 3.2 |
| 6 | B | 297 | ILE | 3.2 |
| 5 | A | 233 | LEU | 3.2 |
| 2 | 2 | 125 | PHE | 3.2 |
| 5 | A | 448 | TRP | 3.2 |
| 11 | G | 47 | GLY | 3.2 |
| 12 | H | 77 | LEU | 3.2 |
| 6 | B | 86 | PRO | 3.2 |
| 1 | 1 | 161 | PHE | 3.2 |
| 10 | F | 150 | VAL | 3.2 |
| 7 | C | 54 | CYS | 3.2 |
| 5 | A | 400 | MET | 3.2 |
| 6 | B | 594 | TRP | 3.2 |
| 5 | A | 568 | LEU | 3.2 |
| 6 | B | 422 | LEU | 3.2 |
| 6 | B | 427 | LEU | 3.2 |
| 8 | D | 22 | PRO | 3.2 |
| 5 | A | 94 | SER | 3.2 |
| 5 | A | 301 | HIS | 3.2 |
| 5 | A | 511 | THR | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | B | 433 | THR | 3.2 |
| 6 | B | 523 | ILE | 3.2 |
| 6 | B | 618 | GLY | 3.2 |
| 5 | A | 395 | LEU | 3.2 |
| 5 | A | 513 | LEU | 3.2 |
| 6 | B | 664 | LEU | 3.2 |
| 6 | B | 437 | TYR | 3.2 |
| 6 | B | 637 | PRO | 3.2 |
| 6 | B | 698 | VAL | 3.2 |
| 8 | D | 130 | VAL | 3.2 |
| 5 | A | 671 | SER | 3.2 |
| 5 | A | 695 | SER | 3.2 |
| 6 | B | 612 | SER | 3.2 |
| 6 | B | 675 | ILE | 3.2 |
| 5 | A | 148 | GLY | 3.1 |
| 6 | B | 181 | GLY | 3.1 |
| 3 | 3 | 125 | GLU | 3.1 |
| 5 | A | 477 | PHE | 3.1 |
| 5 | A | 749 | PHE | 3.1 |
| 2 | 2 | 182 | ILE | 3.1 |
| 9 | E | 28 | ILE | 3.1 |
| 1 | 1 | 164 | GLN | 3.1 |
| 2 | 2 | 82 | ALA | 3.1 |
| 10 | F | 64 | GLY | 3.1 |
| 1 | 1 | 43 | GLU | 3.1 |
| 5 | A | 612 | VAL | 3.1 |
| 6 | B | 519 | VAL | 3.1 |
| 11 | G | 98 | PHE | 3.1 |
| 7 | C | 40 | ALA | 3.1 |
| 5 | A | 387 | THR | 3.1 |
| 6 | B | 373 | THR | 3.1 |
| 6 | B | 223 | GLY | 3.1 |
| 6 | B | 342 | GLY | 3.1 |
| 11 | G | 19 | GLY | 3.1 |
| 16 | L | 30 | SER | 3.1 |
| 6 | B | 625 | TRP | 3.1 |
| 1 | 1 | 147 | GLU | 3.1 |
| 6 | B | 208 | ARG | 3.1 |
| 3 | 3 | 166 | PRO | 3.1 |
| 9 | E | 74 | TYR | 3.1 |
| 4 | 4 | 116 | ASN | 3.1 |
| 5 | A | 737 | HIS | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | B | 723 | ALA | 3.1 |
| 16 | L | 115 | ALA | 3.1 |
| 1 | 1 | 27 | LEU | 3.1 |
| 5 | A | 93 | LEU | 3.1 |
| 16 | L | 40 | LEU | 3.1 |
| 5 | A | 648 | THR | 3.1 |
| 6 | B | 619 | TRP | 3.1 |
| 4 | 4 | 168 | ILE | 3.1 |
| 5 | A | 143 | ILE | 3.1 |
| 5 | A | 707 | ILE | 3.1 |
| 10 | F | 106 | ILE | 3.1 |
| 12 | H | 58 | ILE | 3.1 |
| 5 | A | 67 | HIS | 3.1 |
| 6 | B | 699 | ALA | 3.1 |
| 6 | B | 626 | LEU | 3.1 |
| 9 | E | 84 | LEU | 3.1 |
| 3 | 3 | 82 | GLY | 3.1 |
| 6 | B | 567 | THR | 3.1 |
| 6 | B | 423 | SER | 3.1 |
| 1 | 1 | 117 | ASP | 3.1 |
| 7 | C | 47 | ASP | 3.1 |
| 5 | A | 245 | PRO | 3.1 |
| 6 | B | 163 | PRO | 3.1 |
| 6 | B | 371 | LEU | 3.0 |
| 11 | G | 6 | LEU | 3.0 |
| 5 | A | 636 | HIS | 3.0 |
| 11 | G | 39 | ASN | 3.0 |
| 5 | A | 103 | PHE | 3.0 |
| 10 | F | 65 | SER | 3.0 |
| 5 | A | 125 | PRO | 3.0 |
| 1 | 1 | 177 | LEU | 3.0 |
| 5 | A | 211 | LEU | 3.0 |
| 6 | B | 425 | ALA | 3.0 |
| 6 | B | 538 | ALA | 3.0 |
| 10 | F | 145 | LEU | 3.0 |
| 5 | A | 591 | GLN | 3.0 |
| 8 | D | 99 | GLN | 3.0 |
| 14 | J | 13 | VAL | 3.0 |
| 5 | A | 692 | PHE | 3.0 |
| 5 | A | 510 | SER | 3.0 |
| 6 | B | 5 | ILE | 3.0 |
| 1 | 1 | 19 | PRO | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 243 | PRO | 3.0 |
| 3 | 3 | 197 | TYR | 3.0 |
| 5 | A | 235 | ALA | 3.0 |
| 5 | A | 683 | HIS | 3.0 |
| 6 | B | 241 | ASN | 3.0 |
| 5 | A | 449 | VAL | 3.0 |
| 5 | A | 598 | VAL | 3.0 |
| 3 | 3 | 204 | THR | 3.0 |
| 10 | F | 42 | ILE | 3.0 |
| 13 | I | 5 | PRO | 3.0 |
| 12 | H | 37 | SER | 3.0 |
| 5 | A | 45 | ALA | 3.0 |
| 6 | B | 386 | ALA | 3.0 |
| 6 | B | 623 | TYR | 3.0 |
| 6 | B | 721 | TYR | 3.0 |
| 2 | 2 | 144 | ASP | 3.0 |
| 3 | 3 | 41 | ASP | 3.0 |
| 10 | F | 110 | ASP | 3.0 |
| 1 | 1 | 165 | GLN | 3.0 |
| 6 | B | 128 | GLY | 3.0 |
| 16 | L | 22 | GLY | 3.0 |
| 6 | B | 365 | PHE | 3.0 |
| 3 | 3 | 67 | LEU | 3.0 |
| 8 | D | 19 | GLU | 3.0 |
| 5 | A | 512 | SER | 3.0 |
| 6 | B | 299 | HIS | 3.0 |
| 5 | A | 581 | CYS | 3.0 |
| 5 | A | 614 | PHE | 3.0 |
| 5 | A | 679 | PHE | 3.0 |
| 5 | A | 234 | ASN | 3.0 |
| 5 | A | 360 | ILE | 3.0 |
| 8 | D | 96 | ILE | 3.0 |
| 5 | A | 534 | LEU | 2.9 |
| 3 | 3 | 51 | PRO | 2.9 |
| 3 | 3 | 92 | TRP | 2.9 |
| 17 | N | 85 | TRP | 2.9 |
| 17 | N | 74 | LYS | 2.9 |
| 5 | A | 646 | SER | 2.9 |
| 8 | D | 32 | SER | 2.9 |
| 3 | 3 | 199 | VAL | 2.9 |
| 4 | 4 | 135 | GLY | 2.9 |
| 5 | A | 225 | VAL | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | B | 298 | GLY | 2.9 |
| 6 | B | 389 | HIS | 2.9 |
| 6 | B | 715 | VAL | 2.9 |
| 1 | 1 | 114 | MET | 2.9 |
| 5 | A | 158 | ILE | 2.9 |
| 6 | B | 411 | MET | 2.9 |
| 6 | B | 718 | ILE | 2.9 |
| 8 | D | 144 | ILE | 2.9 |
| 9 | E | 38 | ILE | 2.9 |
| 3 | 3 | 192 | LEU | 2.9 |
| 6 | B | 347 | LEU | 2.9 |
| 6 | B | 610 | ASN | 2.9 |
| 6 | B | 603 | ARG | 2.9 |
| 12 | H | 65 | LEU | 2.9 |
| 6 | B | 451 | LYS | 2.9 |
| 1 | 1 | 34 | ALA | 2.9 |
| 5 | A | 741 | GLY | 2.9 |
| 11 | G | 17 | PHE | 2.9 |
| 8 | D | 116 | ASP | 2.9 |
| 5 | A | 299 | ILE | 2.9 |
| 3 | 3 | 202 | LEU | 2.9 |
| 8 | D | 37 | LEU | 2.9 |
| 5 | A | 297 | THR | 2.9 |
| 2 | 2 | 66 | GLU | 2.9 |
| 5 | A | 424 | PRO | 2.9 |
| 2 | 2 | 148 | TRP | 2.9 |
| 5 | A | 682 | ALA | 2.9 |
| 16 | L | 34 | ALA | 2.9 |
| 5 | A | 716 | VAL | 2.9 |
| 5 | A | 128 | GLY | 2.9 |
| 5 | A | 478 | SER | 2.9 |
| 5 | A | 131 | ILE | 2.9 |
| 5 | A | 755 | ILE | 2.9 |
| 6 | B | 492 | ILE | 2.9 |
| 6 | B | 550 | LYS | 2.9 |
| 3 | 3 | 135 | PRO | 2.9 |
| 5 | A | 497 | ALA | 2.9 |
| 5 | A | 354 | TRP | 2.9 |
| 5 | A | 566 | SER | 2.9 |
| 6 | B | 374 | HIS | 2.9 |
| 6 | B | 578 | LEU | 2.9 |
| 6 | B | 376 | GLN | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | B | 227 | THR | 2.9 |
| 6 | B | 357 | ALA | 2.9 |
| 2 | 2 | 54 | TRP | 2.9 |
| 5 | A | 428 | TYR | 2.9 |
| 5 | A | 758 | GLY | 2.9 |
| 4 | 4 | 109 | ILE | 2.9 |
| 5 | A | 628 | ILE | 2.9 |
| 6 | B | 46 | ILE | 2.9 |
| 15 | K | 61 | LEU | 2.9 |
| 6 | B | 29 | HIS | 2.8 |
| 10 | F | 116 | GLN | 2.8 |
| 6 | B | 324 | ASP | 2.8 |
| 9 | E | 91 | ALA | 2.8 |
| 16 | L | 17 | ASP | 2.8 |
| 6 | B | 224 | PRO | 2.8 |
| 6 | B | 673 | GLU | 2.8 |
| 2 | 2 | 178 | TRP | 2.8 |
| 5 | A | 295 | TRP | 2.8 |
| 6 | B | 689 | ASN | 2.8 |
| 6 | B | 410 | ARG | 2.8 |
| 10 | F | 30 | LYS | 2.8 |
| 3 | 3 | 106 | TYR | 2.8 |
| 16 | L | 14 | LEU | 2.8 |
| 6 | B | 672 | GLN | 2.8 |
| 17 | N | 23 | ALA | 2.8 |
| 2 | 2 | 93 | THR | 2.8 |
| 5 | A | 112 | ASP | 2.8 |
| 6 | B | 636 | THR | 2.8 |
| 6 | B | 113 | VAL | 2.8 |
| 6 | B | 328 | ASN | 2.8 |
| 1 | 1 | 86 | GLY | 2.8 |
| 5 | A | 684 | PHE | 2.8 |
| 6 | B | 546 | LEU | 2.8 |
| 1 | 1 | 168 | TYR | 2.8 |
| 10 | F | 32 | TYR | 2.8 |
| 5 | A | 663 | GLN | 2.8 |
| 2 | 2 | 194 | ALA | 2.8 |
| 5 | A | 594 | ALA | 2.8 |
| 6 | B | 2 | ALA | 2.8 |
| 2 | 2 | 53 | ARG | 2.8 |
| 5 | A | 419 | VAL | 2.8 |
| 5 | A | 425 | THR | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | 3 | 48 | PHE | 2.8 |
| 3 | 3 | 71 | GLY | 2.8 |
| 17 | N | 77 | CYS | 2.8 |
| 5 | A | 543 | HIS | 2.8 |
| 6 | B | 277 | HIS | 2.8 |
| 6 | B | 485 | ALA | 2.8 |
| 6 | B | 684 | ARG | 2.8 |
| 5 | A | 173 | VAL | 2.8 |
| 6 | B | 49 | SER | 2.8 |
| 1 | 1 | 58 | LEU | 2.8 |
| 6 | B | 367 | THR | 2.8 |
| 16 | L | 28 | THR | 2.8 |
| 6 | B | 140 | ILE | 2.8 |
| 6 | B | 282 | PHE | 2.8 |
| 6 | B | 588 | GLY | 2.8 |
| 6 | B | 577 | TYR | 2.8 |
| 2 | 2 | 181 | HIS | 2.8 |
| 5 | A | 546 | ALA | 2.8 |
| 8 | D | 152 | GLN | 2.8 |
| 16 | L | 137 | ALA | 2.8 |
| 6 | B | 686 | PRO | 2.8 |
| 5 | A | 665 | ILE | 2.8 |
| 6 | B | 326 | ILE | 2.8 |
| 6 | B | 384 | THR | 2.8 |
| 6 | B | 418 | ILE | 2.8 |
| 5 | A | 501 | GLY | 2.7 |
| 9 | E | 56 | ASP | 2.7 |
| 6 | B | 524 | ALA | 2.7 |
| 7 | C | 6 | LYS | 2.7 |
| 10 | F | 112 | LYS | 2.7 |
| 16 | L | 70 | LYS | 2.7 |
| 2 | 2 | 200 | PRO | 2.7 |
| 5 | A | 570 | PRO | 2.7 |
| 16 | L | 67 | PRO | 2.7 |
| 6 | B | 225 | LEU | 2.7 |
| 6 | B | 355 | LEU | 2.7 |
| 11 | G | 18 | LEU | 2.7 |
| 6 | B | 144 | PHE | 2.7 |
| 6 | B | 671 | TRP | 2.7 |
| 15 | K | 73 | GLY | 2.7 |
| 6 | B | 80 | ASP | 2.7 |
| 6 | B | 19 | ARG | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 8 | D | 38 | ARG | 2.7 |
| 3 | 3 | 211 | ASN | 2.7 |
| 6 | B | 132 | ASN | 2.7 |
| 17 | N | 56 | LYS | 2.7 |
| 3 | 3 | 115 | VAL | 2.7 |
| 5 | A | 408 | VAL | 2.7 |
| 5 | A | 733 | VAL | 2.7 |
| 12 | H | 43 | PHE | 2.7 |
| 6 | B | 435 | GLY | 2.7 |
| 8 | D | 126 | GLY | 2.7 |
| 8 | D | 89 | ARG | 2.7 |
| 4 | 4 | 110 | LYS | 2.7 |
| 7 | C | 37 | LYS | 2.7 |
| 3 | 3 | 131 | ASP | 2.7 |
| 5 | A | 571 | ASP | 2.7 |
| 1 | 1 | 53 | ALA | 2.7 |
| 8 | D | 40 | ALA | 2.7 |
| 7 | C | 63 | LEU | 2.7 |
| 16 | L | 58 | LEU | 2.7 |
| 2 | 2 | 138 | PRO | 2.7 |
| 6 | B | 112 | PRO | 2.7 |
| 5 | A | 577 | PHE | 2.7 |
| 11 | G | 21 | PHE | 2.7 |
| 5 | A | 626 | GLY | 2.7 |
| 5 | A | 50 | THR | 2.7 |
| 5 | A | 167 | THR | 2.7 |
| 16 | L | 77 | THR | 2.7 |
| 3 | 3 | 107 | TRP | 2.7 |
| 11 | G | 76 | SER | 2.7 |
| 4 | 4 | 118 | ASP | 2.7 |
| 6 | B | 681 | ALA | 2.7 |
| 6 | B | 348 | VAL | 2.7 |
| 6 | B | 434 | LEU | 2.7 |
| 6 | B | 584 | LEU | 2.7 |
| 5 | A | 116 | ILE | 2.7 |
| 6 | B | 87 | ILE | 2.7 |
| 1 | 1 | 30 | GLY | 2.7 |
| 5 | A | 36 | LYS | 2.7 |
| 6 | B | 685 | THR | 2.7 |
| 15 | K | 6 | SER | 2.7 |
| 6 | B | 69 | ALA | 2.7 |
| 6 | B | 445 | ALA | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 15 | K | 27 | ALA | 2.7 |
| 14 | J | 37 | LEU | 2.7 |
| 15 | K | 76 | LEU | 2.7 |
| 6 | B | 521 | HIS | 2.7 |
| 2 | 2 | 96 | ILE | 2.6 |
| 4 | 4 | 166 | PHE | 2.6 |
| 6 | B | 617 | MET | 2.6 |
| 3 | 3 | 149 | GLY | 2.6 |
| 5 | A | 524 | GLY | 2.6 |
| 8 | D | 64 | GLY | 2.6 |
| 2 | 2 | 202 | ALA | 2.6 |
| 5 | A | 75 | SER | 2.6 |
| 6 | B | 525 | LEU | 2.6 |
| 15 | K | 26 | LEU | 2.6 |
| 7 | C | 81 | TYR | 2.6 |
| 6 | B | 375 | HIS | 2.6 |
| 12 | H | 75 | ASP | 2.6 |
| 15 | K | 3 | ILE | 2.6 |
| 1 | 1 | 95 | PRO | 2.6 |
| 3 | 3 | 186 | ASN | 2.6 |
| 4 | 4 | 58 | MET | 2.6 |
| 5 | A | 620 | MET | 2.6 |
| 6 | B | 317 | ARG | 2.6 |
| 6 | B | 564 | ARG | 2.6 |
| 8 | D | 105 | PRO | 2.6 |
| 5 | A | 138 | GLY | 2.6 |
| 1 | 1 | 174 | LEU | 2.6 |
| 2 | 2 | 105 | ALA | 2.6 |
| 3 | 3 | 119 | ALA | 2.6 |
| 5 | A | 529 | LEU | 2.6 |
| 6 | B | 646 | TRP | 2.6 |
| 6 | B | 657 | TRP | 2.6 |
| 16 | L | 82 | ALA | 2.6 |
| 2 | 2 | 52 | SER | 2.6 |
| 5 | A | 622 | SER | 2.6 |
| 7 | C | 8 | TYR | 2.6 |
| 5 | A | 472 | ARG | 2.6 |
| 7 | C | 52 | LYS | 2.6 |
| 5 | A | 251 | ASN | 2.6 |
| 5 | A | 607 | ASN | 2.6 |
| 6 | B | 114 | ASN | 2.6 |
| 5 | A | 293 | GLY | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | B | 537 | GLY | 2.6 |
| 17 | N | 5 | GLU | 2.6 |
| 2 | 2 | 141 | LEU | 2.6 |
| 4 | 4 | 181 | LEU | 2.6 |
| 6 | B | 532 | LEU | 2.6 |
| 12 | H | 57 | LEU | 2.6 |
| 1 | 1 | 106 | ALA | 2.6 |
| 4 | 4 | 131 | VAL | 2.6 |
| 5 | A | 127 | VAL | 2.6 |
| 5 | A | 573 | ALA | 2.6 |
| 5 | A | 639 | ALA | 2.6 |
| 6 | B | 582 | TRP | 2.6 |
| 3 | 3 | 52 | LYS | 2.6 |
| 6 | B | 25 | ILE | 2.6 |
| 8 | D | 106 | SER | 2.6 |
| 12 | H | 20 | GLN | 2.6 |
| 4 | 4 | 147 | LEU | 2.6 |
| 5 | A | 81 | ALA | 2.6 |
| 6 | B | 120 | VAL | 2.6 |
| 6 | B | 417 | ALA | 2.6 |
| 6 | B | 442 | VAL | 2.6 |
| 10 | F | 107 | ALA | 2.6 |
| 5 | A | 747 | TRP | 2.6 |
| 15 | K | 60 | THR | 2.6 |
| 3 | 3 | 194 | ILE | 2.6 |
| 6 | B | 632 | ILE | 2.6 |
| 5 | A | 31 | PHE | 2.6 |
| 5 | A | 338 | PHE | 2.6 |
| 6 | B | 31 | PHE | 2.6 |
| 9 | E | 44 | TYR | 2.6 |
| 6 | B | 420 | SER | 2.6 |
| 1 | 1 | 136 | ASP | 2.6 |
| 5 | A | 350 | LEU | 2.6 |
| 6 | B | 643 | LEU | 2.6 |
| 12 | H | 53 | LEU | 2.6 |
| 3 | 3 | 69 | ALA | 2.6 |
| 5 | A | 735 | VAL | 2.6 |
| 6 | B | 732 | LYS | 2.6 |
| 5 | A | 736 | THR | 2.6 |
| 8 | D | 24 | THR | 2.6 |
| 5 | A | 364 | MET | 2.5 |
| 13 | I | 25 | PHE | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 224 | HIS | 2.5 |
| 5 | A | 382 | TYR | 2.5 |
| 6 | B | 43 | TYR | 2.5 |
| 6 | B | 303 | TYR | 2.5 |
| 4 | 4 | 88 | SER | 2.5 |
| 6 | B | 473 | GLY | 2.5 |
| 8 | D | 87 | GLY | 2.5 |
| 13 | I | 7 | LEU | 2.5 |
| 2 | 2 | 97 | VAL | 2.5 |
| 2 | 2 | 165 | LYS | 2.5 |
| 4 | 4 | 156 | ASN | 2.5 |
| 6 | B | 585 | ASN | 2.5 |
| 6 | B | 281 | ALA | 2.5 |
| 2 | 2 | 79 | TRP | 2.5 |
| 16 | L | 136 | TRP | 2.5 |
| 17 | N | 69 | CYS | 2.5 |
| 2 | 2 | 41 | LEU | 2.5 |
| 5 | A | 85 | GLN | 2.5 |
| 5 | A | 517 | GLY | 2.5 |
| 5 | A | 696 | GLY | 2.5 |
| 8 | D | 36 | LEU | 2.5 |
| 2 | 2 | 108 | ARG | 2.5 |
| 3 | 3 | 203 | VAL | 2.5 |
| 8 | D | 109 | VAL | 2.5 |
| 11 | G | 64 | VAL | 2.5 |
| 3 | 3 | 172 | ASP | 2.5 |
| 6 | B | 397 | ASP | 2.5 |
| 13 | I | 22 | ALA | 2.5 |
| 14 | J | 35 | ASP | 2.5 |
| 5 | A | 649 | ILE | 2.5 |
| 7 | C | 12 | ILE | 2.5 |
| 2 | 2 | 89 | THR | 2.5 |
| 6 | B | 383 | MET | 2.5 |
| 3 | 3 | 93 | PHE | 2.5 |
| 6 | B | 360 | PHE | 2.5 |
| 5 | A | 545 | HIS | 2.5 |
| 6 | B | 412 | LEU | 2.5 |
| 10 | F | 109 | ARG | 2.5 |
| 5 | A | 457 | SER | 2.5 |
| 5 | A | 565 | SER | 2.5 |
| 3 | 3 | 59 | ILE | 2.5 |
| 9 | E | 58 | ASP | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 113 | PRO | 2.5 |
| 3 | 3 | 180 | LYS | 2.5 |
| 5 | A | 347 | TYR | 2.5 |
| 11 | G | 50 | ARG | 2.5 |
| 4 | 4 | 79 | GLY | 2.5 |
| 5 | A | 660 | GLN | 2.5 |
| 3 | 3 | 110 | SER | 2.5 |
| 6 | B | 171 | ALA | 2.5 |
| 5 | A | 150 | PHE | 2.5 |
| 6 | B | 591 | THR | 2.5 |
| 11 | G | 57 | LEU | 2.5 |
| 5 | A | 615 | HIS | 2.5 |
| 5 | A | 738 | TYR | 2.5 |
| 8 | D | 46 | TYR | 2.5 |
| 12 | H | 61 | GLY | 2.5 |
| 4 | 4 | 92 | VAL | 2.5 |
| 15 | K | 66 | VAL | 2.5 |
| 6 | B | 608 | GLN | 2.5 |
| 9 | E | 75 | ALA | 2.4 |
| 5 | A | 569 | ILE | 2.4 |
| 6 | B | 304 | ILE | 2.4 |
| 7 | C | 34 | CYS | 2.4 |
| 12 | H | 30 | SER | 2.4 |
| 5 | A | 196 | PHE | 2.4 |
| 4 | 4 | 122 | LYS | 2.4 |
| 5 | A | 198 | ASP | 2.4 |
| 6 | B | 77 | TRP | 2.4 |
| 6 | B | 230 | TRP | 2.4 |
| 6 | B | 216 | LEU | 2.4 |
| 16 | L | 74 | LEU | 2.4 |
| 6 | B | 697 | PRO | 2.4 |
| 6 | B | 136 | TYR | 2.4 |
| 6 | B | 68 | VAL | 2.4 |
| 11 | G | 13 | GLY | 2.4 |
| 5 | A | 231 | GLN | 2.4 |
| 10 | F | 3 | ALA | 2.4 |
| 6 | B | 458 | ILE | 2.4 |
| 6 | B | 628 | SER | 2.4 |
| 10 | F | 74 | SER | 2.4 |
| 16 | L | 149 | SER | 2.4 |
| 4 | 4 | 138 | PHE | 2.4 |
| 6 | B | 7 | ARG | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | 4 | 141 | LEU | 2.4 |
| 6 | B | 518 | LEU | 2.4 |
| 10 | F | 125 | LEU | 2.4 |
| 5 | A | 604 | TRP | 2.4 |
| 2 | 2 | 122 | ASP | 2.4 |
| 8 | D | 62 | THR | 2.4 |
| 6 | B | 703 | VAL | 2.4 |
| 16 | L | 102 | TYR | 2.4 |
| 6 | B | 378 | ILE | 2.4 |
| 7 | C | 16 | GLN | 2.4 |
| 6 | B | 583 | MET | 2.4 |
| 4 | 4 | 130 | GLU | 2.4 |
| 5 | A | 367 | SER | 2.4 |
| 13 | I | 6 | SER | 2.4 |
| 1 | 1 | 162 | CYS | 2.4 |
| 6 | B | 289 | LEU | 2.4 |
| 16 | L | 63 | LEU | 2.4 |
| 3 | 3 | 208 | PRO | 2.4 |
| 6 | B | 549 | ASP | 2.4 |
| 10 | F | 151 | ASP | 2.4 |
| 3 | 3 | 158 | TYR | 2.4 |
| 5 | A | 730 | GLY | 2.4 |
| 6 | B | 233 | TYR | 2.4 |
| 6 | B | 259 | GLY | 2.4 |
| 6 | B | 712 | HIS | 2.4 |
| 5 | A | 609 | ILE | 2.4 |
| 6 | B | 500 | ALA | 2.4 |
| 6 | B | 722 | ALA | 2.4 |
| 8 | D | 48 | ILE | 2.4 |
| 12 | H | 36 | GLN | 2.4 |
| 8 | D | 100 | PHE | 2.4 |
| 6 | B | 678 | LEU | 2.4 |
| 11 | G | 16 | LEU | 2.4 |
| 6 | B | 166 | SER | 2.4 |
| 2 | 2 | 142 | TRP | 2.4 |
| 5 | A | 491 | TRP | 2.4 |
| 6 | B | 680 | TRP | 2.4 |
| 1 | 1 | 54 | VAL | 2.4 |
| 6 | B | 586 | THR | 2.4 |
| 8 | D | 114 | PRO | 2.4 |
| 17 | N | 47 | THR | 2.4 |
| 5 | A | 63 | ASP | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 95 | GLY | 2.4 |
| 5 | A | 170 | GLY | 2.4 |
| 5 | A | 315 | HIS | 2.4 |
| 6 | B | 153 | GLY | 2.4 |
| 6 | B | 641 | ASN | 2.4 |
| 11 | G | 48 | ASP | 2.4 |
| 1 | 1 | 50 | ALA | 2.4 |
| 4 | 4 | 120 | ILE | 2.4 |
| 5 | A | 88 | ILE | 2.4 |
| 6 | B | 254 | ILE | 2.4 |
| 6 | B | 370 | ALA | 2.4 |
| 17 | N | 30 | ALA | 2.4 |
| 1 | 1 | 146 | LYS | 2.4 |
| 1 | 1 | 152 | ARG | 2.4 |
| 5 | A | 202 | MET | 2.4 |
| 6 | B | 14 | GLN | 2.4 |
| 5 | A | 79 | PHE | 2.4 |
| 6 | B | 650 | PHE | 2.4 |
| 5 | A | 657 | LEU | 2.4 |
| 8 | D | 77 | LEU | 2.4 |
| 11 | G | 29 | GLU | 2.4 |
| 6 | B | 186 | SER | 2.4 |
| 1 | 1 | 91 | TRP | 2.4 |
| 4 | 4 | 63 | VAL | 2.4 |
| 7 | C | 25 | VAL | 2.4 |
| 7 | C | 67 | VAL | 2.4 |
| 10 | F | 63 | CYS | 2.4 |
| 5 | A | 559 | GLY | 2.3 |
| 6 | B | 390 | GLY | 2.3 |
| 5 | A | 105 | ASN | 2.3 |
| 5 | A | 429 | ASN | 2.3 |
| 3 | 3 | 128 | ARG | 2.3 |
| 5 | A | 563 | ALA | 2.3 |
| 5 | A | 578 | ARG | 2.3 |
| 6 | B | 206 | TYR | 2.3 |
| 6 | B | 705 | ALA | 2.3 |
| 6 | B | 540 | ASP | 2.3 |
| 6 | B | 555 | TYR | 2.3 |
| 10 | F | 104 | TYR | 2.3 |
| 16 | L | 83 | ALA | 2.3 |
| 5 | A | 98 | PHE | 2.3 |
| 6 | B | 98 | GLN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 10 | F | 138 | VAL | 2.3 |
| 13 | I | 12 | VAL | 2.3 |
| 4 | 4 | 145 | PRO | 2.3 |
| 5 | A | 595 | TRP | 2.3 |
| 5 | A | 726 | SER | 2.3 |
| 6 | B | 424 | TRP | 2.3 |
| 6 | B | 507 | SER | 2.3 |
| 6 | B | 613 | SER | 2.3 |
| 9 | E | 45 | TRP | 2.3 |
| 9 | E | 59 | PRO | 2.3 |
| 2 | 2 | 133 | THR | 2.3 |
| 4 | 4 | 173 | THR | 2.3 |
| 5 | A | 619 | LYS | 2.3 |
| 6 | B | 604 | GLY | 2.3 |
| 6 | B | 395 | ILE | 2.3 |
| 5 | A | 375 | HIS | 2.3 |
| 6 | B | 177 | HIS | 2.3 |
| 6 | B | 65 | LEU | 2.3 |
| 8 | D | 128 | GLN | 2.3 |
| 14 | J | 39 | PHE | 2.3 |
| 16 | L | 19 | PHE | 2.3 |
| 9 | E | 42 | GLU | 2.3 |
| 7 | C | 35 | LYS | 2.3 |
| 1 | 1 | 48 | ARG | 2.3 |
| 5 | A | 531 | PRO | 2.3 |
| 5 | A | 442 | ILE | 2.3 |
| 5 | A | 444 | SER | 2.3 |
| 5 | A | 637 | ILE | 2.3 |
| 6 | B | 184 | GLY | 2.3 |
| 6 | B | 602 | TRP | 2.3 |
| 1 | 1 | 83 | THR | 2.3 |
| 2 | 2 | 92 | THR | 2.3 |
| 5 | A | 480 | THR | 2.3 |
| 6 | B | 247 | THR | 2.3 |
| 7 | C | 80 | ALA | 2.3 |
| 11 | G | 41 | MET | 2.3 |
| 17 | N | 33 | TYR | 2.3 |
| 2 | 2 | 169 | LEU | 2.3 |
| 5 | A | 447 | ASN | 2.3 |
| 6 | B | 710 | LEU | 2.3 |
| 9 | E | 76 | ASN | 2.3 |
| 12 | H | 71 | ASN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 14 | J | 8 | LEU | 2.3 |
| 10 | F | 83 | PHE | 2.3 |
| 1 | 1 | 129 | ASP | 2.3 |
| 5 | A | 237 | VAL | 2.3 |
| 2 | 2 | 77 | PRO | 2.3 |
| 4 | 4 | 127 | PRO | 2.3 |
| 5 | A | 451 | ILE | 2.3 |
| 4 | 4 | 144 | ALA | 2.3 |
| 5 | A | 109 | TRP | 2.3 |
| 6 | B | 119 | GLY | 2.3 |
| 10 | F | 95 | GLY | 2.3 |
| 5 | A | 226 | SER | 2.3 |
| 5 | A | 436 | LEU | 2.3 |
| 5 | A | 550 | HIS | 2.3 |
| 5 | A | 672 | LEU | 2.3 |
| 6 | B | 54 | LEU | 2.3 |
| 6 | B | 593 | TYR | 2.3 |
| 12 | H | 39 | PHE | 2.3 |
| 6 | B | 15 | ASP | 2.3 |
| 6 | B | 122 | GLN | 2.3 |
| 7 | C | 61 | ASP | 2.3 |
| 7 | C | 18 | VAL | 2.3 |
| 6 | B | 286 | ILE | 2.3 |
| 6 | B | 382 | ILE | 2.3 |
| 6 | B | 400 | PRO | 2.3 |
| 10 | F | 119 | ILE | 2.3 |
| 6 | B | 380 | GLY | 2.3 |
| 6 | B | 653 | GLY | 2.3 |
| 6 | B | 123 | TRP | 2.3 |
| 5 | A | 282 | THR | 2.3 |
| 6 | B | 157 | LEU | 2.3 |
| 6 | B | 624 | LEU | 2.3 |
| 2 | 2 | 51 | HIS | 2.3 |
| 5 | A | 187 | HIS | 2.3 |
| 6 | B | 381 | PHE | 2.3 |
| 17 | N | 45 | ASN | 2.3 |
| 5 | A | 596 | ASP | 2.3 |
| 6 | B | 165 | VAL | 2.3 |
| 10 | F | 118 | GLU | 2.2 |
| 10 | F | 143 | GLU | 2.2 |
| 12 | H | 12 | GLU | 2.2 |
| 8 | D | 28 | ILE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1 | 124 | PRO | 2.2 |
| 5 | A | 265 | GLY | 2.2 |
| 5 | A | 535 | GLY | 2.2 |
| 5 | A | 580 | PRO | 2.2 |
| 5 | A | 181 | ALA | 2.2 |
| 5 | A | 698 | GLY | 2.2 |
| 15 | K | 77 | GLY | 2.2 |
| 1 | 1 | 52 | LEU | 2.2 |
| 1 | 1 | 156 | LEU | 2.2 |
| 6 | B | 315 | LEU | 2.2 |
| 6 | B | 616 | LEU | 2.2 |
| 8 | D | 156 | LEU | 2.2 |
| 10 | F | 71 | LEU | 2.2 |
| 14 | J | 14 | LEU | 2.2 |
| 17 | N | 65 | LEU | 2.2 |
| 4 | 4 | 65 | THR | 2.2 |
| 5 | A | 39 | HIS | 2.2 |
| 5 | A | 280 | PHE | 2.2 |
| 5 | A | 656 | PHE | 2.2 |
| 5 | A | 694 | PHE | 2.2 |
| 6 | B | 262 | HIS | 2.2 |
| 16 | L | 152 | THR | 2.2 |
| 1 | 1 | 134 | SER | 2.2 |
| 5 | A | 394 | SER | 2.2 |
| 6 | B | 340 | SER | 2.2 |
| 6 | B | 544 | SER | 2.2 |
| 16 | L | 125 | LYS | 2.2 |
| 2 | 2 | 174 | VAL | 2.2 |
| 6 | B | 44 | GLN | 2.2 |
| 6 | B | 635 | ILE | 2.2 |
| 4 | 4 | 85 | ALA | 2.2 |
| 5 | A | 35 | ALA | 2.2 |
| 5 | A | 441 | ALA | 2.2 |
| 5 | A | 516 | GLY | 2.2 |
| 6 | B | 391 | PRO | 2.2 |
| 14 | J | 23 | ALA | 2.2 |
| 4 | 4 | 50 | TRP | 2.2 |
| 4 | 4 | 106 | TRP | 2.2 |
| 6 | B | 720 | THR | 2.2 |
| 8 | D | 149 | THR | 2.2 |
| 10 | F | 56 | TYR | 2.2 |
| 5 | A | 664 | VAL | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 11 | G | 71 | VAL | 2.2 |
| 4 | 4 | 67 | ILE | 2.2 |
| 17 | N | 49 | CYS | 2.2 |
| 1 | 1 | 181 | LEU | 2.2 |
| 2 | 2 | 210 | PRO | 2.2 |
| 5 | A | 453 | LEU | 2.2 |
| 6 | B | 388 | ALA | 2.2 |
| 6 | B | 498 | LEU | 2.2 |
| 8 | D | 88 | THR | 2.2 |
| 16 | L | 7 | THR | 2.2 |
| 5 | A | 317 | TYR | 2.2 |
| 2 | 2 | 135 | VAL | 2.2 |
| 5 | A | 634 | VAL | 2.2 |
| 10 | F | 100 | VAL | 2.2 |
| 17 | N | 2 | VAL | 2.2 |
| 5 | A | 275 | SER | 2.2 |
| 5 | A | 359 | SER | 2.2 |
| 14 | J | 15 | SER | 2.2 |
| 5 | A | 555 | ILE | 2.2 |
| 6 | B | 463 | ILE | 2.2 |
| 6 | B | 450 | GLU | 2.2 |
| 10 | F | 18 | GLU | 2.2 |
| 16 | L | 76 | ASN | 2.2 |
| 5 | A | 172 | LEU | 2.2 |
| 5 | A | 703 | LEU | 2.2 |
| 6 | B | 547 | MET | 2.2 |
| 3 | 3 | 62 | GLY | 2.2 |
| 3 | 3 | 151 | GLY | 2.2 |
| 4 | 4 | 68 | GLY | 2.2 |
| 6 | B | 287 | GLY | 2.2 |
| 6 | B | 447 | GLY | 2.2 |
| 14 | J | 11 | ALA | 2.2 |
| 4 | 4 | 75 | TRP | 2.2 |
| 5 | A | 218 | TRP | 2.2 |
| 6 | B | 22 | TRP | 2.2 |
| 4 | 4 | 146 | THR | 2.2 |
| 5 | A | 99 | HIS | 2.2 |
| 6 | B | 421 | HIS | 2.2 |
| 7 | C | 5 | VAL | 2.2 |
| 4 | 4 | 169 | GLN | 2.2 |
| 5 | A | 30 | SER | 2.2 |
| 5 | A | 215 | SER | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 8 | D | 56 | GLN | 2.2 |
| 9 | E | 77 | ILE | 2.2 |
| 16 | L | 97 | MET | 2.2 |
| 5 | A | 528 | ALA | 2.2 |
| 3 | 3 | 75 | PRO | 2.2 |
| 3 | 3 | 160 | GLY | 2.2 |
| 4 | 4 | 140 | PRO | 2.2 |
| 6 | B | 598 | HIS | 2.2 |
| 15 | K | 49 | THR | 2.1 |
| 6 | B | 398 | TYR | 2.1 |
| 1 | 1 | 81 | GLN | 2.1 |
| 5 | A | 164 | LEU | 2.1 |
| 5 | A | 556 | LEU | 2.1 |
| 6 | B | 687 | LEU | 2.1 |
| 6 | B | 704 | GLN | 2.1 |
| 11 | G | 14 | LEU | 2.1 |
| 3 | 3 | 137 | SER | 2.1 |
| 3 | 3 | 148 | LYS | 2.1 |
| 5 | A | 537 | ALA | 2.1 |
| 7 | C | 76 | SER | 2.1 |
| 16 | L | 29 | SER | 2.1 |
| 6 | B | 503 | GLU | 2.1 |
| 7 | C | 72 | GLU | 2.1 |
| 3 | 3 | 187 | GLY | 2.1 |
| 5 | A | 182 | GLY | 2.1 |
| 1 | 1 | 150 | ASN | 2.1 |
| 2 | 2 | 166 | ASN | 2.1 |
| 5 | A | 289 | PRO | 2.1 |
| 6 | B | 313 | GLY | 2.1 |
| 16 | L | 72 | GLY | 2.1 |
| 16 | L | 75 | ARG | 2.1 |
| 5 | A | 180 | PHE | 2.1 |
| 8 | D | 155 | ASP | 2.1 |
| 5 | A | 183 | TRP | 2.1 |
| 5 | A | 611 | VAL | 2.1 |
| 2 | 2 | 186 | THR | 2.1 |
| 17 | N | 24 | THR | 2.1 |
| 6 | B | 472 | TYR | 2.1 |
| 6 | B | 285 | LEU | 2.1 |
| 7 | C | 69 | LEU | 2.1 |
| 10 | F | 61 | LEU | 2.1 |
| 6 | B | 452 | GLN | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | 1 | 167 | ALA | 2.1 |
| 5 | A | 674 | ALA | 2.1 |
| 6 | B | 572 | ALA | 2.1 |
| 6 | B | 714 | SER | 2.1 |
| 7 | C | 3 | HIS | 2.1 |
| 5 | A | 627 | THR | 2.1 |
| 7 | C | 15 | THR | 2.1 |
| 10 | F | 5 | LEU | 2.1 |
| 12 | H | 66 | THR | 2.1 |
| 5 | A | 675 | TYR | 2.1 |
| 8 | D | 127 | ARG | 2.1 |
| 1 | 1 | 178 | ALA | 2.1 |
| 5 | A | 414 | ALA | 2.1 |
| 6 | B | 369 | ALA | 2.1 |
| 3 | 3 | 152 | GLY | 2.1 |
| 5 | A | 588 | GLY | 2.1 |
| 10 | F | 137 | PRO | 2.1 |
| 6 | B | 502 | ASN | 2.1 |
| 1 | 1 | 145 | VAL | 2.1 |
| 6 | B | 606 | VAL | 2.1 |
| 5 | A | 91 | LEU | 2.1 |
| 5 | A | 714 | LEU | 2.1 |
| 6 | B | 129 | LEU | 2.1 |
| 5 | A | 635 | THR | 2.1 |
| 6 | B | 125 | TYR | 2.1 |
| 6 | B | 659 | THR | 2.1 |
| 6 | B | 13 | ALA | 2.1 |
| 16 | L | 117 | ALA | 2.1 |
| 5 | A | 129 | GLN | 2.1 |
| 5 | A | 632 | GLY | 2.1 |
| 3 | 3 | 164 | PHE | 2.1 |
| 6 | B | 557 | PHE | 2.1 |
| 4 | 4 | 66 | SER | 2.1 |
| 6 | B | 396 | ARG | 2.1 |
| 6 | B | 655 | LEU | 2.1 |
| 6 | B | 693 | TRP | 2.1 |
| 11 | G | 10 | LEU | 2.1 |
| 2 | 2 | 196 | HIS | 2.1 |
| 2 | 2 | 90 | ASP | 2.1 |
| 4 | 4 | 100 | TYR | 2.1 |
| 6 | B | 105 | THR | 2.1 |
| 5 | A | 732 | ALA | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 621 | GLN | 2.1 |
| 8 | D | 107 | GLY | 2.1 |
| 10 | F | 13 | GLN | 2.1 |
| 4 | 4 | 64 | PHE | 2.1 |
| 5 | A | 380 | PRO | 2.1 |
| 5 | A | 722 | PRO | 2.1 |
| 6 | B | 652 | PHE | 2.1 |
| 16 | L | 31 | PRO | 2.1 |
| 1 | 1 | 159 | VAL | 2.0 |
| 5 | A | 560 | VAL | 2.0 |
| 6 | B | 536 | LYS | 2.0 |
| 6 | B | 149 | SER | 2.0 |
| 4 | 4 | 38 | ARG | 2.0 |
| 4 | 4 | 96 | ILE | 2.0 |
| 5 | A | 439 | ARG | 2.0 |
| 6 | B | 419 | ILE | 2.0 |
| 11 | G | 77 | ILE | 2.0 |
| 16 | L | 86 | LEU | 2.0 |
| 1 | 1 | 74 | TRP | 2.0 |
| 5 | A | 465 | ASP | 2.0 |
| 6 | B | 291 | TYR | 2.0 |
| 15 | K | 35 | THR | 2.0 |
| 17 | N | 12 | THR | 2.0 |
| 7 | C | 48 | CYS | 2.0 |
| 5 | A | 342 | GLY | 2.0 |
| 6 | B | 661 | PHE | 2.0 |
| 10 | F | 131 | PHE | 2.0 |
| 1 | 1 | 37 | GLU | 2.0 |
| 10 | F | 9 | LYS | 2.0 |
| 5 | A | 446 | LEU | 2.0 |
| 10 | F | 105 | LEU | 2.0 |
| 5 | A | 407 | ILE | 2.0 |
| 6 | B | 453 | ILE | 2.0 |
| 8 | D | 67 | ILE | 2.0 |
| 10 | F | 72 | ILE | 2.0 |
| 14 | J | 9 | SER | 2.0 |
| 5 | A | 605 | MET | 2.0 |
| 6 | B | 589 | TRP | 2.0 |
| 6 | B | 662 | MET | 2.0 |
| 9 | E | 61 | THR | 2.0 |
| 16 | L | 25 | THR | 2.0 |
| 5 | A | 144 | GLN | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | A | 240 | LYS | 2.0 |
| 6 | B | 219 | PRO | 2.0 |
| 11 | G | 27 | GLN | 2.0 |
| 14 | J | 12 | PRO | 2.0 |
| 5 | A | 523 | VAL | 2.0 |
| 5 | A | 624 | VAL | 2.0 |
| 6 | B | 84 | VAL | 2.0 |
| 6 | B | 570 | ILE | 2.0 |
| 6 | B | 665 | ILE | 2.0 |

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

## 6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 19 | GLC | M | 1 | 11/12 | - | - | 2,44,60,60 | 0 |
| 19 | FRU | M | 2 | 12/12 | - | - | 9,35,60,60 | 0 |
| 19 | GLC | O | 1 | 10/12 | - | - | 4,38,60,60 | 0 |
| 19 | FRU | O | 2 | 12/12 | - | - | 2,28,60,60 | 0 |
| 19 | GLC | P | 1 | 11/12 | - | - | 2,13,57,60 | 0 |
| 19 | FRU | P | 2 | 12/12 | - | - | 2,36,60,60 | 0 |
| 19 | GLC | Q | 1 | 11/12 | - | - | 2,27,60,60 | 0 |
| 19 | FRU | Q | 2 | 12/12 | - | - | 2,28,60,60 | 0 |
| 19 | GLC | Y | 1 | 11/12 | 0.64 | 0.15 | 2,34,60,60 | 0 |
| 19 | GLC | S | 1 | 11/12 | 0.67 | 0.15 | 2,19,60,60 | 0 |
| 19 | FRU | S | 2 | 12/12 | 0.73 | 0.12 | 2,32,60,60 | 0 |
| 19 | FRU | T | 2 | 12/12 | 0.74 | 0.18 | 6,39,60,60 | 0 |
| 19 | GLC | W | 1 | 11/12 | 0.76 | 0.19 | 9,40,60,60 | 0 |
| 19 | GLC | T | 1 | 11/12 | 0.78 | 0.14 | 13,47,60,60 | 0 |
| 19 | FRU | Y | 2 | 12/12 | 0.78 | 0.15 | 2,30,60,60 | 0 |
| 19 | GLC | X | 1 | 10/12 | 0.80 | 0.12 | 6,52,60,60 | 0 |
| 19 | FRU | U | 2 | 12/12 | 0.81 | 0.12 | 2,34,60,60 | 0 |
| 19 | GLC | V | 1 | 11/12 | 0.81 | 0.12 | 2,57,60,60 | 0 |
| 19 | FRU | W | 2 | 12/12 | 0.82 | 0.13 | 17,37,60,60 | 0 |

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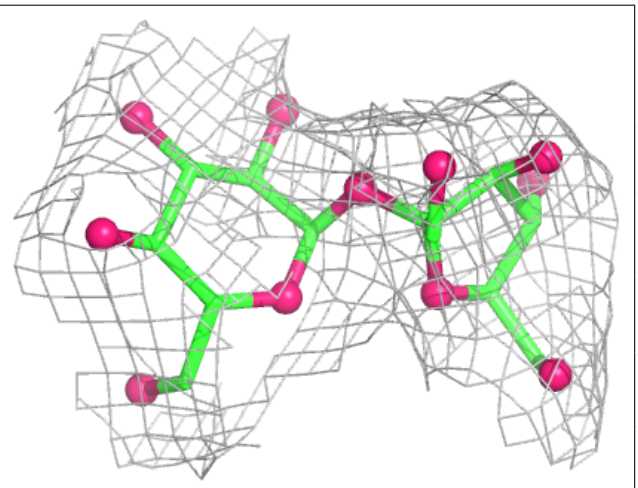
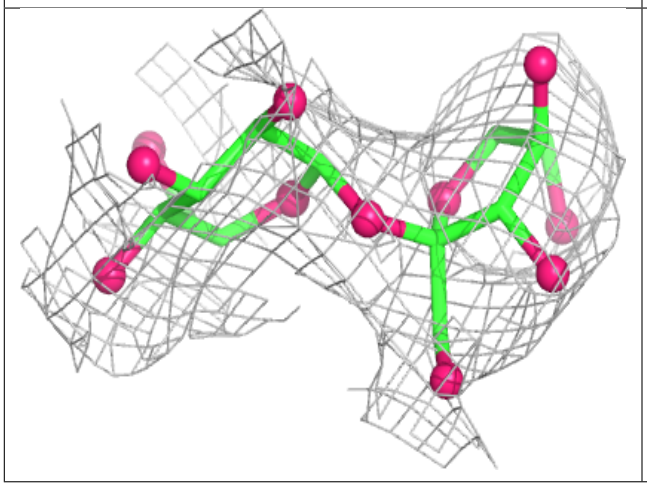
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 19 | FRU | X | 2 | 12/12 | 0.83 | 0.13 | 11,32,60,60 | 0 |
| 19 | GLC | U | 1 | 11/12 | 0.85 | 0.13 | 2,60,60,60 | 0 |
| 19 | GLC | Z | 1 | 11/12 | 0.85 | 0.10 | 4,31,60,60 | 0 |
| 19 | FRU | V | 2 | 12/12 | 0.87 | 0.10 | 2,33,60,60 | 0 |
| 19 | FRU | Z | 2 | 12/12 | 0.87 | 0.10 | 3,43,60,60 | 0 |
| 19 | GLC | a | 1 | 11/12 | - | - | 2,23,50,54 | 0 |
| 19 | FRU | a | 2 | 12/12 | - | - | 6,32,60,60 | 0 |

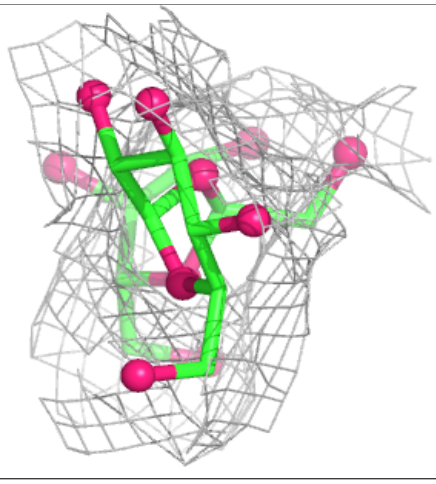
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain M:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

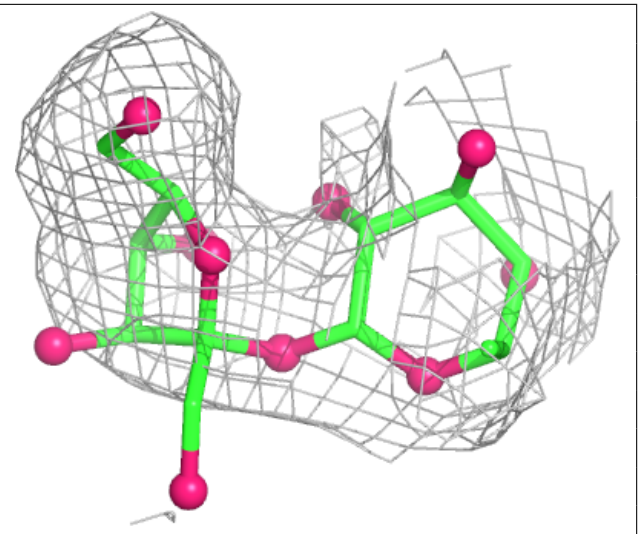


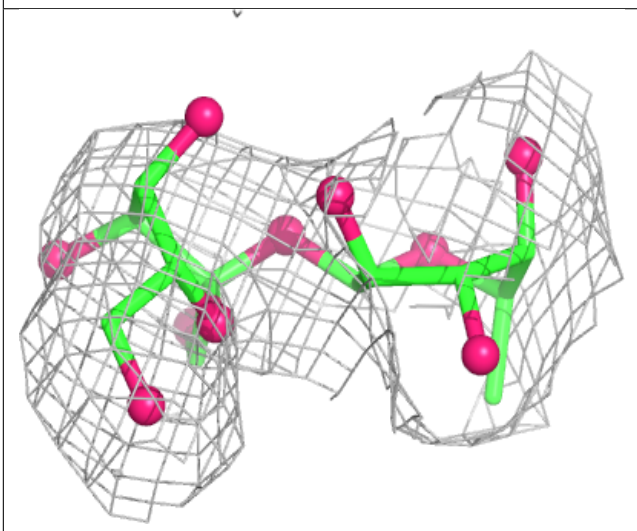


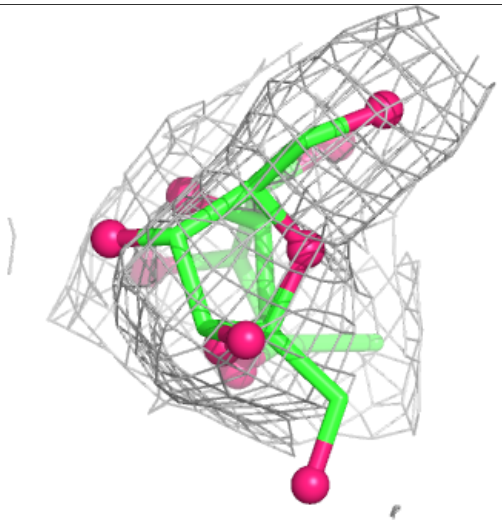


**Electron density around Chain O:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

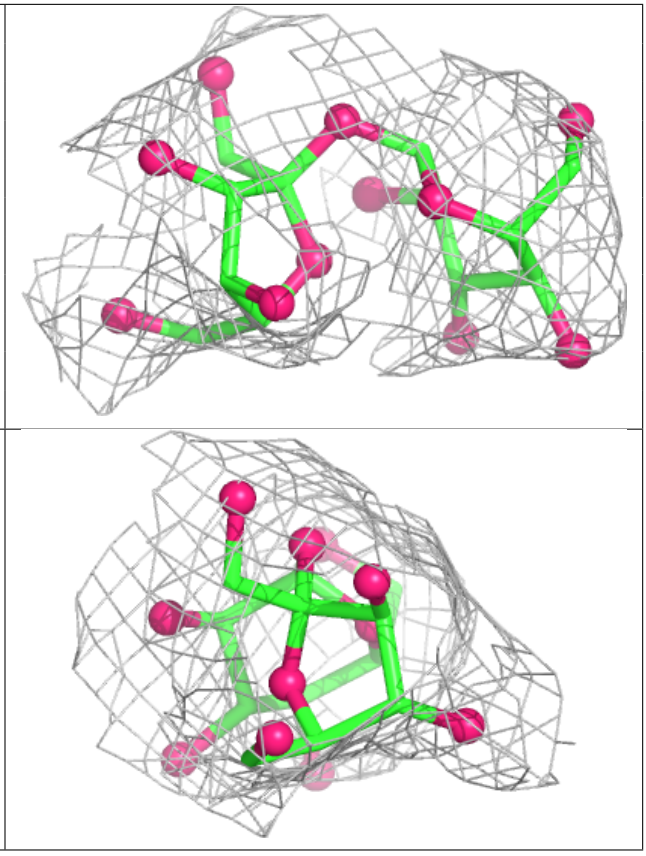






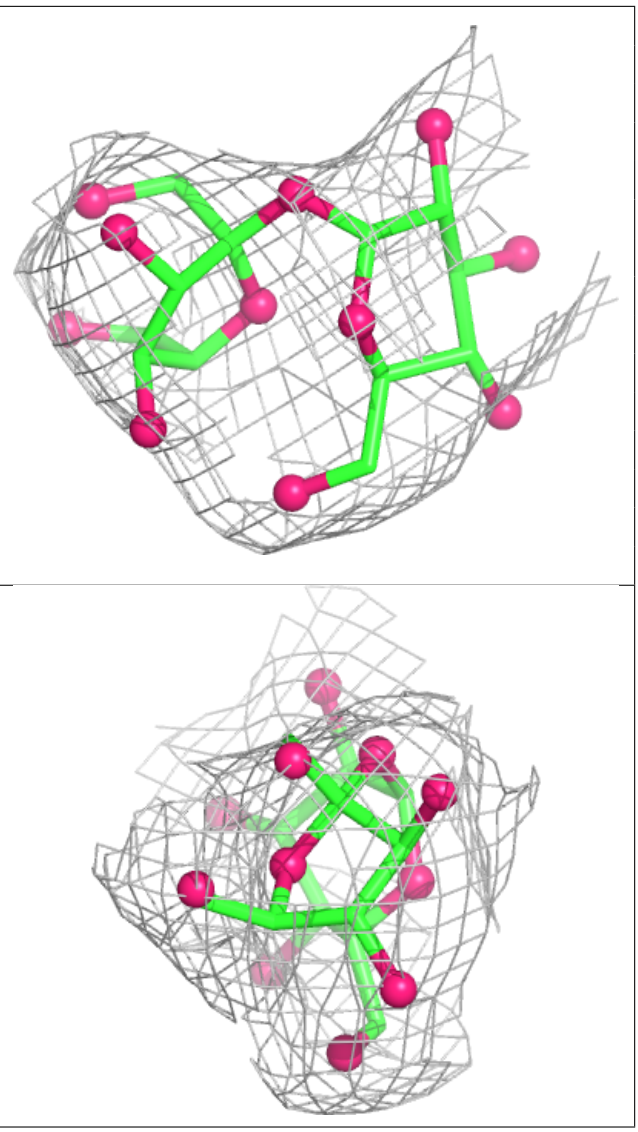
**Electron density around Chain P:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



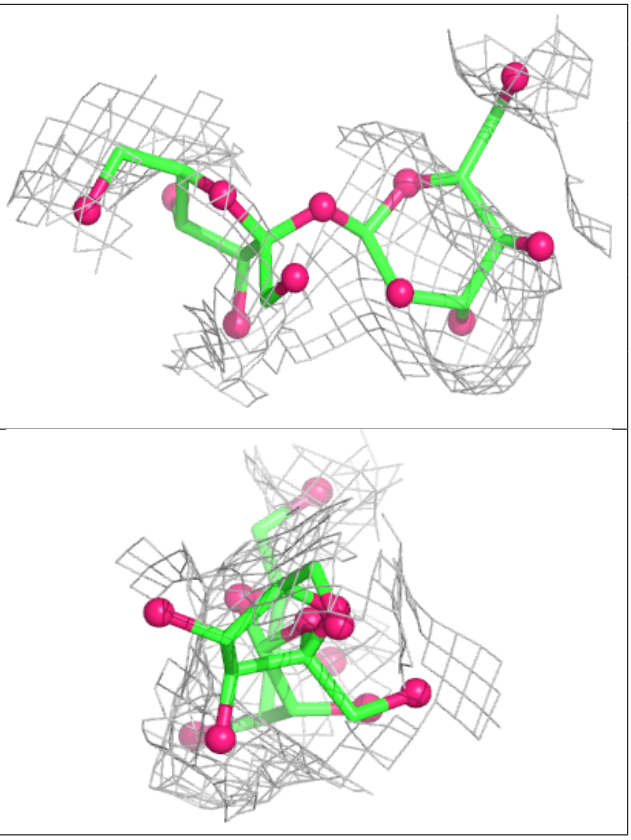
**Electron density around Chain Q:**

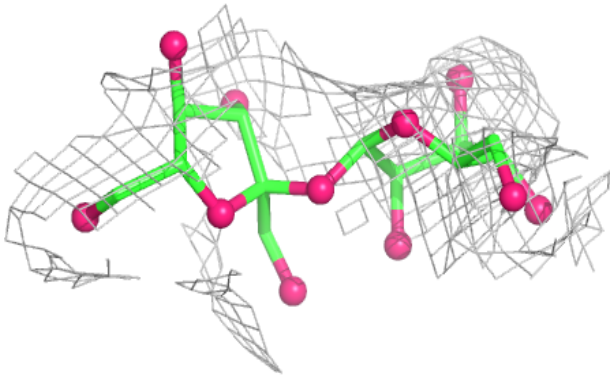
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



**Electron density around Chain S:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

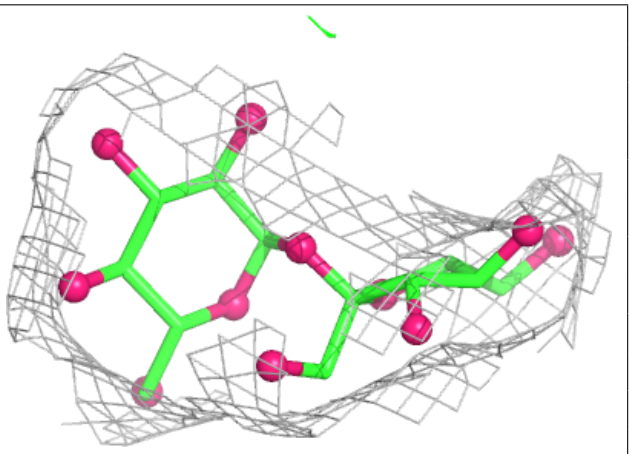


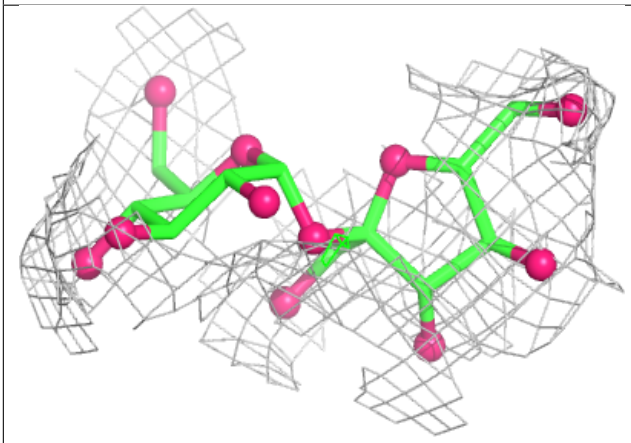


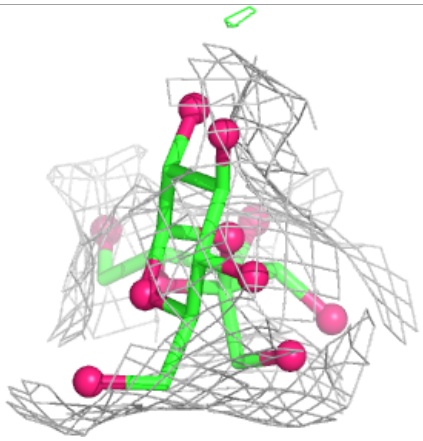


**Electron density around Chain T:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

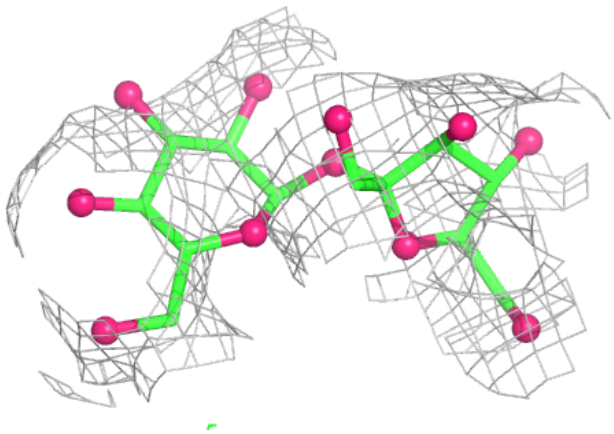


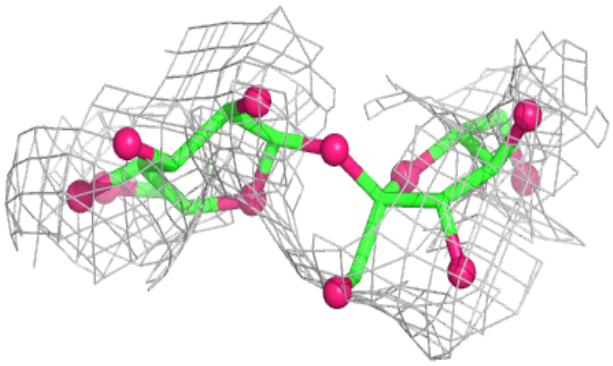


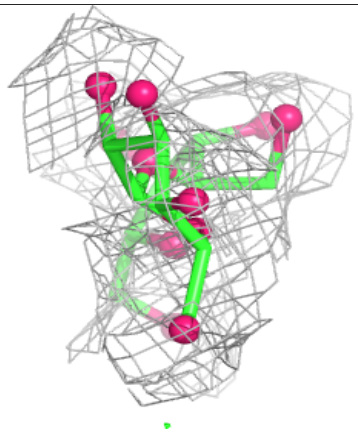


**Electron density around Chain U:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

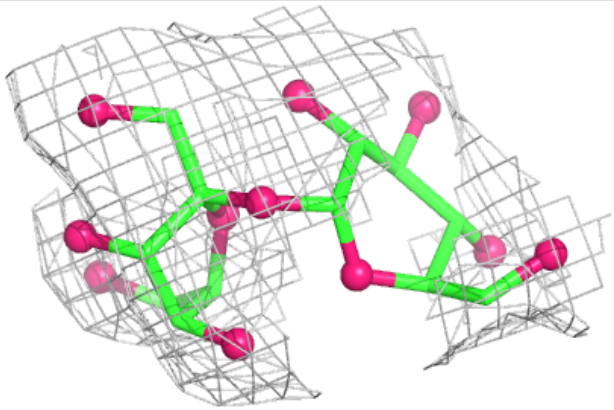


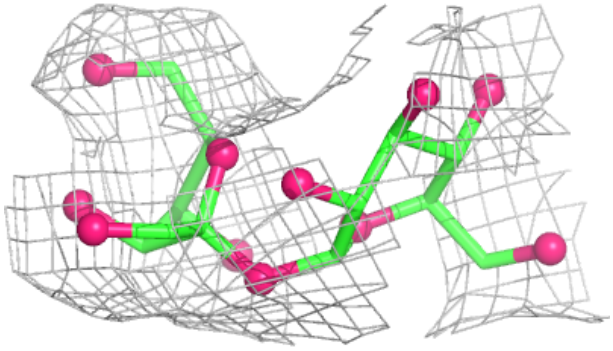


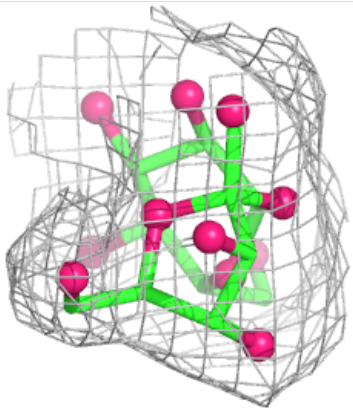


**Electron density around Chain V:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

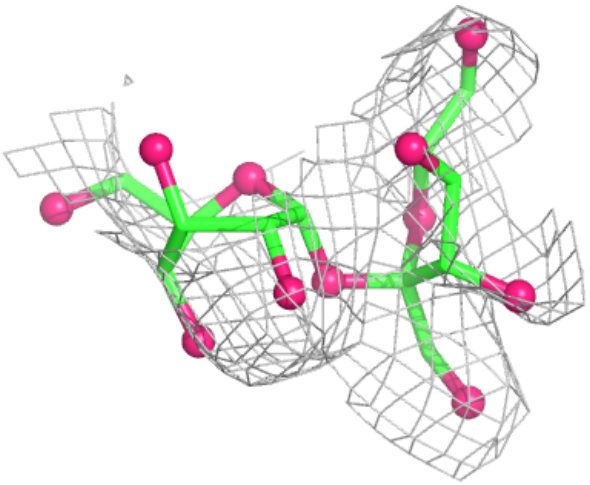


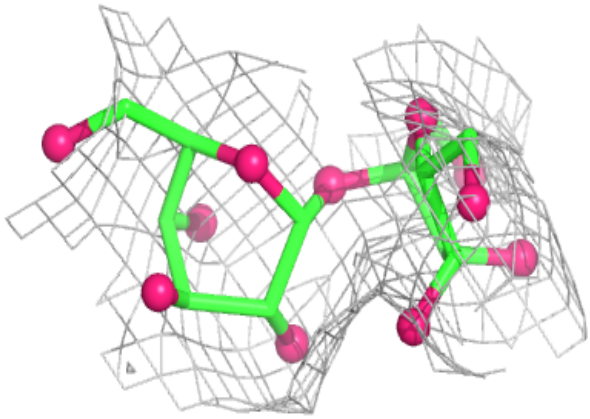


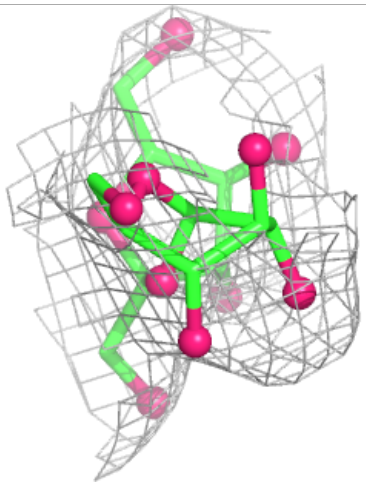


**Electron density around Chain W:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

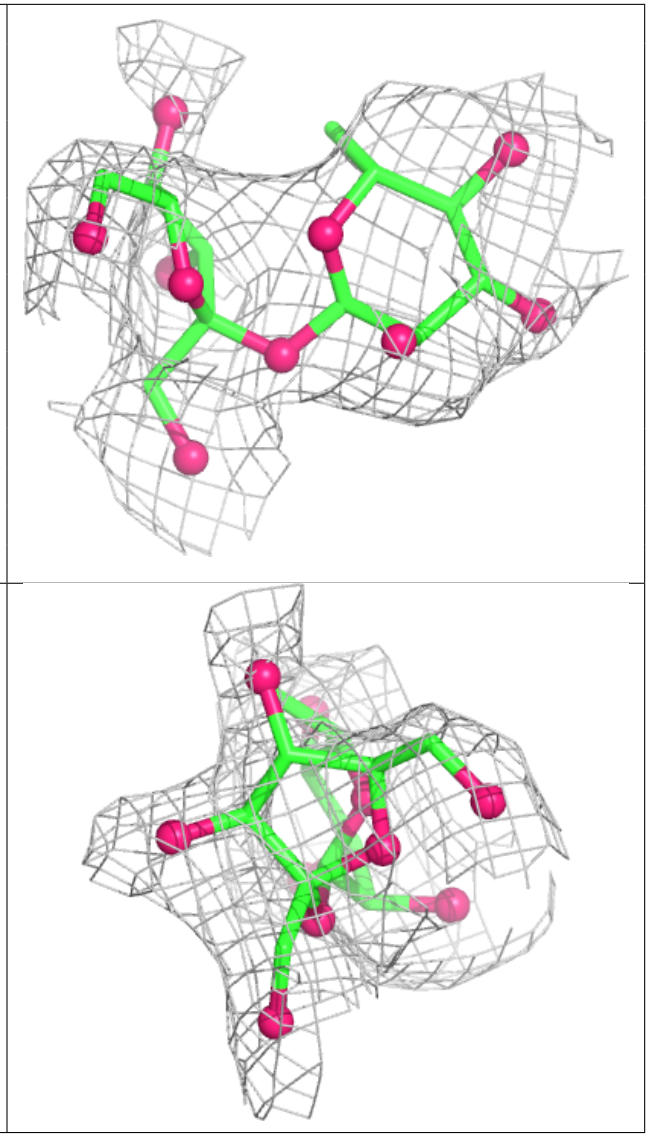






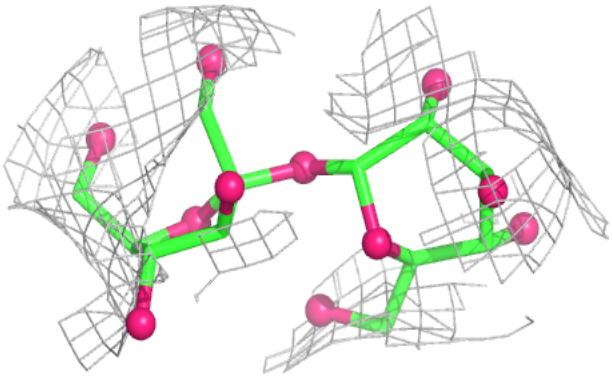
**Electron density around Chain X:**

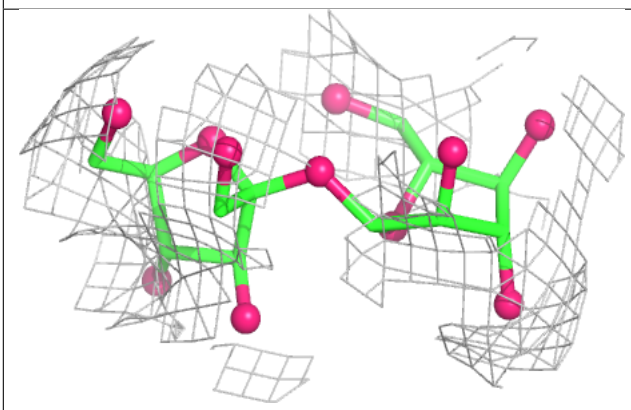
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

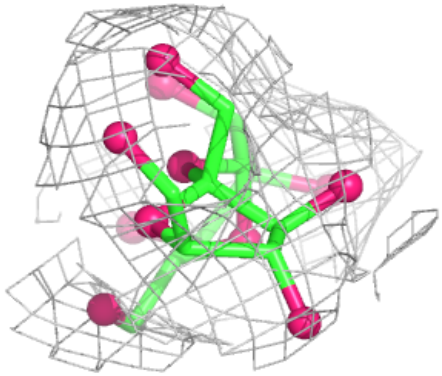


**Electron density around Chain Y:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

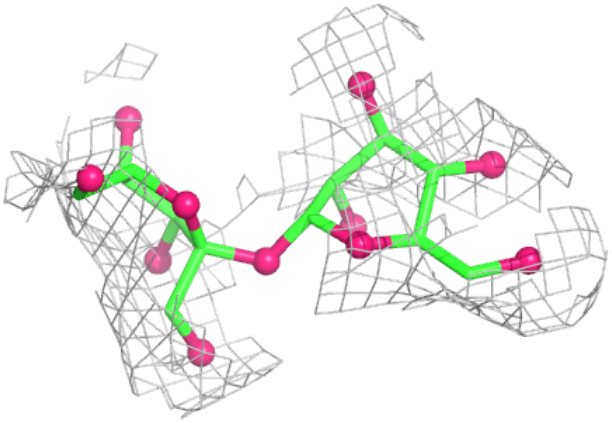


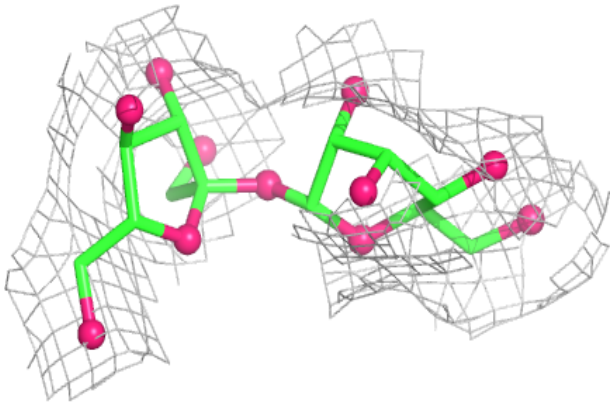


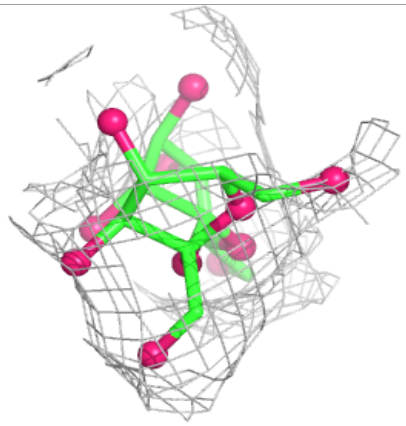


**Electron density around Chain Z:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

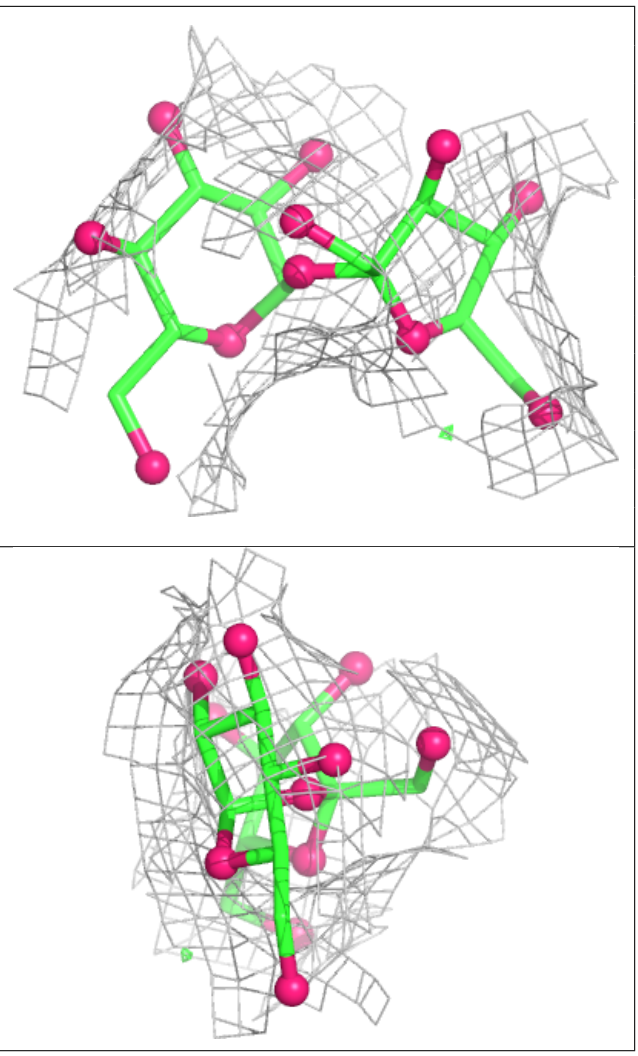






**Electron density around Chain a:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 21 | LMU | A | 852 | 35/35 | 0.50 | 0.21 | 2,39,60,60 | 0 |
| 20 | CLA | 4 | 307 | 25/65 | 0.54 | 0.23 | 2,39,60,60 | 0 |
| 22 | BCR | 2 | 317 | 40/40 | 0.54 | 0.29 | 2,32,60,60 | 0 |
| 20 | CLA | B | 816 | 60/65 | 0.57 | 0.23 | 2,40,60,60 | 0 |
| 20 | CLA | H | 102 | 55/65 | 0.57 | 0.21 | 2,49,60,60 | 0 |
| 22 | BCR | A | 843 | 40/40 | 0.57 | 0.30 | 2,45,60,60 | 0 |
| 22 | BCR | I | 103 | 40/40 | 0.59 | 0.22 | 2,38,60,60 | 0 |
| 20 | CLA | G | 105 | 51/65 | 0.60 | 0.17 | 2,44,60,60 | 0 |
| 20 | CLA | 1 | 211 | 51/65 | 0.60 | 0.18 | 2,42,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 20 | CLA | 3 | 313 | 50/65 | 0.60 | 0.17 | 2,56,60,60 | 0 |
| 20 | CLA | B | 835 | 45/65 | 0.61 | 0.18 | 12,37,60,60 | 0 |
| 21 | LMU | 2 | 320 | 35/35 | 0.61 | 0.17 | 2,40,60,60 | 0 |
| 20 | CLA | A | 802 | 25/65 | 0.61 | 0.17 | 2,42,60,60 | 0 |
| 21 | LMU | A | 853 | 35/35 | 0.62 | 0.19 | 2,45,60,60 | 0 |
| 20 | CLA | 3 | 311 | 65/65 | 0.62 | 0.21 | 2,46,60,60 | 0 |
| 21 | LMU | 4 | 320 | 35/35 | 0.62 | 0.18 | 2,43,60,60 | 0 |
| 20 | CLA | 4 | 304 | 55/65 | 0.62 | 0.20 | 4,39,60,60 | 0 |
| 20 | CLA | 3 | 305 | 25/65 | 0.63 | 0.21 | 17,42,60,60 | 0 |
| 21 | LMU | 1 | 217 | 35/35 | 0.63 | 0.16 | 2,44,60,60 | 0 |
| 20 | CLA | 4 | 314 | 25/65 | 0.63 | 0.21 | 2,35,60,60 | 0 |
| 20 | CLA | F | 206 | 41/65 | 0.64 | 0.21 | 2,41,60,60 | 0 |
| 20 | CLA | 4 | 317 | 52/65 | 0.64 | 0.19 | 2,34,60,60 | 0 |
| 21 | LMU | E | 101 | 35/35 | 0.64 | 0.20 | 2,30,60,60 | 0 |
| 20 | CLA | 3 | 317 | 36/65 | 0.65 | 0.23 | 2,51,60,60 | 0 |
| 20 | CLA | B | 836 | 51/65 | 0.65 | 0.18 | 2,45,60,60 | 0 |
| 21 | LMU | R | 101 | 35/35 | 0.65 | 0.16 | 2,45,60,60 | 0 |
| 20 | CLA | 4 | 303 | 65/65 | 0.65 | 0.24 | 2,32,60,60 | 0 |
| 20 | CLA | B | 817 | 46/65 | 0.65 | 0.25 | 2,28,60,60 | 0 |
| 20 | CLA | H | 101 | 55/65 | 0.65 | 0.16 | 2,47,60,60 | 0 |
| 21 | LMU | H | 106 | 35/35 | 0.66 | 0.18 | 2,41,60,60 | 0 |
| 21 | LMU | K | 106 | 35/35 | 0.66 | 0.16 | 2,38,60,60 | 0 |
| 20 | CLA | K | 103 | 50/65 | 0.66 | 0.18 | 2,60,60,60 | 0 |
| 20 | CLA | 3 | 309 | 25/65 | 0.66 | 0.19 | 2,47,60,60 | 0 |
| 21 | LMU | 2 | 313 | 35/35 | 0.66 | 0.18 | 2,21,60,60 | 0 |
| 20 | CLA | A | 840 | 55/65 | 0.66 | 0.24 | 2,44,60,60 | 0 |
| 20 | CLA | 3 | 312 | 25/65 | 0.67 | 0.17 | 2,30,60,60 | 0 |
| 21 | LMU | G | 103 | 35/35 | 0.67 | 0.16 | 2,51,60,60 | 0 |
| 20 | CLA | 1 | 205 | 36/65 | 0.67 | 0.19 | 2,52,60,60 | 0 |
| 21 | LMU | 3 | 318 | 35/35 | 0.67 | 0.17 | 2,44,60,60 | 0 |
| 21 | LMU | L | 205 | 35/35 | 0.68 | 0.16 | 2,31,60,60 | 0 |
| 20 | CLA | 4 | 308 | 25/65 | 0.68 | 0.20 | 2,29,60,60 | 0 |
| 20 | CLA | H | 109 | 55/65 | 0.68 | 0.18 | 2,33,60,60 | 0 |
| 20 | CLA | 3 | 310 | 65/65 | 0.68 | 0.18 | 2,26,60,60 | 0 |
| 21 | LMU | 2 | 321 | 35/35 | 0.68 | 0.17 | 2,40,60,60 | 0 |
| 20 | CLA | 3 | 303 | 36/65 | 0.69 | 0.17 | 2,53,60,60 | 0 |
| 20 | CLA | K | 101 | 46/65 | 0.69 | 0.16 | 2,51,60,60 | 0 |
| 21 | LMU | R | 102 | 35/35 | 0.69 | 0.16 | 2,38,60,60 | 0 |
| 21 | LMU | R | 103 | 35/35 | 0.69 | 0.17 | 2,35,60,60 | 0 |
| 21 | LMU | H | 103 | 35/35 | 0.69 | 0.15 | 2,15,60,60 | 0 |
| 20 | CLA | 1 | 215 | 51/65 | 0.69 | 0.16 | 2,51,60,60 | 0 |
| 22 | BCR | G | 104 | 40/40 | 0.69 | 0.28 | 2,33,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 20 | CLA | L | 204 | 55/65 | 0.69 | 0.20 | 2,44,60,60 | 0 |
| 21 | LMU | A | 848 | 35/35 | 0.70 | 0.17 | 2,45,60,60 | 0 |
| 21 | LMU | A | 854 | 35/35 | 0.70 | 0.17 | 2,32,60,60 | 0 |
| 21 | LMU | B | 804 | 35/35 | 0.70 | 0.16 | 2,34,60,60 | 0 |
| 20 | CLA | 4 | 301 | 55/65 | 0.70 | 0.23 | 2,33,60,60 | 0 |
| 22 | BCR | L | 209 | 40/40 | 0.70 | 0.30 | 2,18,60,60 | 0 |
| 20 | CLA | A | 811 | 65/65 | 0.71 | 0.20 | 2,15,60,60 | 0 |
| 20 | CLA | A | 819 | 58/65 | 0.71 | 0.22 | 2,20,60,60 | 0 |
| 20 | CLA | A | 820 | 51/65 | 0.71 | 0.18 | 2,44,60,60 | 0 |
| 21 | LMU | C | 101 | 35/35 | 0.71 | 0.14 | 2,35,60,60 | 0 |
| 20 | CLA | 2 | 307 | 65/65 | 0.71 | 0.15 | 2,24,60,60 | 0 |
| 20 | CLA | 3 | 306 | 25/65 | 0.71 | 0.16 | 2,56,60,60 | 0 |
| 22 | BCR | A | 844 | 40/40 | 0.71 | 0.26 | 2,34,60,60 | 0 |
| 20 | CLA | 2 | 311 | 50/65 | 0.71 | 0.25 | 2,25,60,60 | 0 |
| 20 | CLA | A | 801 | 46/65 | 0.71 | 0.15 | 2,43,60,60 | 0 |
| 20 | CLA | 2 | 305 | 50/65 | 0.71 | 0.21 | 2,48,60,60 | 0 |
| 20 | CLA | 2 | 301 | 25/65 | 0.72 | 0.17 | 2,48,60,60 | 0 |
| 20 | CLA | 1 | 207 | 51/65 | 0.72 | 0.16 | 2,36,60,60 | 0 |
| 20 | CLA | 4 | 305 | 50/65 | 0.72 | 0.19 | 2,21,60,60 | 0 |
| 20 | CLA | K | 104 | 56/65 | 0.72 | 0.17 | 2,36,60,60 | 0 |
| 20 | CLA | 1 | 209 | 25/65 | 0.73 | 0.16 | 11,37,60,60 | 0 |
| 20 | CLA | R | 107 | 57/65 | 0.73 | 0.19 | 2,38,60,60 | 0 |
| 20 | CLA | A | 821 | 42/65 | 0.73 | 0.21 | 2,46,60,60 | 0 |
| 20 | CLA | 3 | 307 | 42/65 | 0.73 | 0.16 | 2,53,60,60 | 0 |
| 21 | LMU | K | 107 | 35/35 | 0.73 | 0.14 | 2,38,60,60 | 0 |
| 21 | LMU | A | 846 | 35/35 | 0.73 | 0.17 | 2,26,60,60 | 0 |
| 21 | LMU | L | 210 | 35/35 | 0.73 | 0.16 | 2,22,60,60 | 0 |
| 21 | LMU | 2 | 319 | 35/35 | 0.73 | 0.14 | 2,29,60,60 | 0 |
| 20 | CLA | 4 | 318 | 47/65 | 0.74 | 0.17 | 2,37,60,60 | 0 |
| 20 | CLA | R | 108 | 65/65 | 0.74 | 0.16 | 2,35,60,60 | 0 |
| 20 | CLA | 2 | 312 | 61/65 | 0.74 | 0.15 | 2,34,60,60 | 0 |
| 21 | LMU | R | 104 | 35/35 | 0.74 | 0.14 | 2,36,60,60 | 0 |
| 20 | CLA | 3 | 302 | 25/65 | 0.74 | 0.18 | 15,54,60,60 | 0 |
| 21 | LMU | K | 105 | 35/35 | 0.74 | 0.15 | 2,37,60,60 | 0 |
| 20 | CLA | 1 | 206 | 61/65 | 0.74 | 0.16 | 2,35,60,60 | 0 |
| 20 | CLA | 1 | 201 | 46/65 | 0.74 | 0.17 | 2,56,60,60 | 0 |
| 20 | CLA | 4 | 315 | 46/65 | 0.74 | 0.15 | 2,45,60,60 | 0 |
| 20 | CLA | 2 | 302 | 51/65 | 0.74 | 0.17 | 2,33,60,60 | 0 |
| 20 | CLA | B | 842 | 36/65 | 0.75 | 0.17 | 2,52,60,60 | 0 |
| 21 | LMU | R | 106 | 35/35 | 0.75 | 0.15 | 2,27,60,60 | 0 |
| 20 | CLA | L | 202 | 55/65 | 0.75 | 0.15 | 2,46,60,60 | 0 |
| 20 | CLA | 1 | 210 | 36/65 | 0.75 | 0.19 | 2,35,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 20 | CLA | J | 101 | 48/65 | 0.75 | 0.17 | 2,34,60,60 | 0 |
| 21 | LMU | H | 104 | 35/35 | 0.75 | 0.14 | 2,16,60,60 | 0 |
| 20 | CLA | A | 841 | 25/65 | 0.75 | 0.16 | 2,43,60,60 | 0 |
| 20 | CLA | A | 810 | 45/65 | 0.75 | 0.17 | 2,38,60,60 | 0 |
| 21 | LMU | R | 105 | 35/35 | 0.76 | 0.13 | 2,35,60,60 | 0 |
| 21 | LMU | F | 202 | 34/35 | 0.76 | 0.15 | 2,23,60,60 | 0 |
| 20 | CLA | 3 | 316 | 25/65 | 0.76 | 0.14 | 2,42,60,60 | 0 |
| 20 | CLA | A | 814 | 25/65 | 0.76 | 0.18 | 2,31,60,60 | 0 |
| 20 | CLA | 1 | 214 | 25/65 | 0.76 | 0.15 | 5,42,60,60 | 0 |
| 22 | BCR | B | 845 | 40/40 | 0.76 | 0.22 | 2,21,60,60 | 0 |
| 21 | LMU | B | 849 | 25/35 | 0.76 | 0.14 | 2,36,60,60 | 0 |
| 20 | CLA | K | 102 | 50/65 | 0.76 | 0.16 | 2,28,60,60 | 0 |
| 20 | CLA | 1 | 203 | 47/65 | 0.76 | 0.16 | 2,17,60,60 | 0 |
| 26 | UNL | H | 107 | 23/- | 0.76 | 0.14 | 2,31,60,60 | 0 |
| 20 | CLA | A | 839 | 59/65 | 0.77 | 0.16 | 2,30,60,60 | 0 |
| 21 | LMU | G | 102 | 35/35 | 0.77 | 0.16 | 2,33,60,60 | 0 |
| 21 | LMU | 4 | 316 | 35/35 | 0.77 | 0.14 | 2,37,60,60 | 0 |
| 20 | CLA | 4 | 302 | 36/65 | 0.77 | 0.24 | 2,26,60,60 | 0 |
| 20 | CLA | 2 | 306 | 25/65 | 0.77 | 0.17 | 2,57,60,60 | 0 |
| 20 | CLA | 1 | 208 | 25/65 | 0.78 | 0.17 | 2,31,60,60 | 0 |
| 20 | CLA | 2 | 310 | 50/65 | 0.78 | 0.19 | 2,18,60,60 | 0 |
| 20 | CLA | B | 813 | 55/65 | 0.78 | 0.22 | 2,28,60,60 | 0 |
| 21 | LMU | G | 101 | 35/35 | 0.78 | 0.15 | 2,34,60,60 | 0 |
| 21 | LMU | L | 206 | 35/35 | 0.78 | 0.15 | 2,23,60,60 | 0 |
| 20 | CLA | 3 | 314 | 65/65 | 0.78 | 0.15 | 2,33,60,60 | 0 |
| 20 | CLA | L | 201 | 60/65 | 0.78 | 0.22 | 2,18,60,60 | 0 |
| 20 | CLA | A | 829 | 50/65 | 0.78 | 0.19 | 2,32,60,60 | 0 |
| 22 | BCR | J | 102 | 40/40 | 0.78 | 0.24 | 2,31,60,60 | 0 |
| 20 | CLA | A | 833 | 45/65 | 0.78 | 0.18 | 2,37,60,60 | 0 |
| 25 | LMG | B | 848 | 49/55 | 0.78 | 0.27 | 2,20,60,60 | 0 |
| 20 | CLA | A | 817 | 52/65 | 0.78 | 0.23 | 2,33,60,60 | 0 |
| 20 | CLA | 3 | 301 | 36/65 | 0.79 | 0.16 | 2,34,60,60 | 0 |
| 20 | CLA | B | 812 | 54/65 | 0.79 | 0.19 | 2,17,60,60 | 0 |
| 22 | BCR | A | 845 | 40/40 | 0.79 | 0.25 | 2,5,44,60 | 0 |
| 20 | CLA | A | 823 | 58/65 | 0.79 | 0.23 | 2,18,60,60 | 0 |
| 20 | CLA | B | 815 | 60/65 | 0.79 | 0.21 | 2,19,60,60 | 0 |
| 20 | CLA | A | 815 | 50/65 | 0.79 | 0.17 | 2,21,60,60 | 0 |
| 20 | CLA | 1 | 212 | 25/65 | 0.79 | 0.18 | 2,42,60,60 | 0 |
| 20 | CLA | 1 | 213 | 51/65 | 0.79 | 0.19 | 2,39,60,60 | 0 |
| 20 | CLA | J | 103 | 61/65 | 0.79 | 0.16 | 2,19,60,60 | 0 |
| 20 | CLA | 4 | 310 | 50/65 | 0.79 | 0.16 | 2,20,60,60 | 0 |
| 20 | CLA | B | 822 | 46/65 | 0.80 | 0.20 | 2,34,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 21 | LMU | 4 | 321 | 35/35 | 0.80 | 0.13 | 2,21,55,60 | 0 |
| 22 | BCR | B | 844 | 40/40 | 0.80 | 0.21 | 2,5,60,60 | 0 |
| 20 | CLA | 3 | 315 | 25/65 | 0.80 | 0.14 | 2,47,60,60 | 0 |
| 20 | CLA | 2 | 309 | 25/65 | 0.80 | 0.14 | 2,34,60,60 | 0 |
| 20 | CLA | 4 | 306 | 52/65 | 0.81 | 0.14 | 2,26,60,60 | 0 |
| 20 | CLA | L | 208 | 50/65 | 0.81 | 0.17 | 2,18,60,60 | 0 |
| 20 | CLA | B | 823 | 55/65 | 0.81 | 0.18 | 2,30,60,60 | 0 |
| 20 | CLA | B | 834 | 45/65 | 0.81 | 0.19 | 2,16,60,60 | 0 |
| 20 | CLA | 1 | 204 | 46/65 | 0.81 | 0.16 | 2,35,60,60 | 0 |
| 21 | LMU | 1 | 218 | 35/35 | 0.81 | 0.15 | 2,46,60,60 | 0 |
| 20 | CLA | A | 812 | 54/65 | 0.81 | 0.16 | 2,28,60,60 | 0 |
| 20 | CLA | H | 110 | 50/65 | 0.81 | 0.17 | 2,27,60,60 | 0 |
| 20 | CLA | A | 807 | 46/65 | 0.81 | 0.19 | 2,20,60,60 | 0 |
| 20 | CLA | A | 834 | 46/65 | 0.82 | 0.21 | 2,20,60,60 | 0 |
| 20 | CLA | A | 804 | 55/65 | 0.82 | 0.19 | 2,11,60,60 | 0 |
| 20 | CLA | B | 837 | 60/65 | 0.82 | 0.22 | 2,2,60,60 | 0 |
| 21 | LMU | R | 109 | 35/35 | 0.82 | 0.14 | 2,21,60,60 | 0 |
| 21 | LMU | A | 847 | 35/35 | 0.82 | 0.14 | 2,27,60,60 | 0 |
| 20 | CLA | A | 824 | 59/65 | 0.82 | 0.19 | 2,25,60,60 | 0 |
| 20 | CLA | A | 825 | 65/65 | 0.82 | 0.19 | 2,16,60,60 | 0 |
| 20 | CLA | F | 207 | 53/65 | 0.82 | 0.14 | 2,22,60,60 | 0 |
| 21 | LMU | 2 | 318 | 35/35 | 0.82 | 0.12 | 2,25,60,60 | 0 |
| 20 | CLA | A | 805 | 54/65 | 0.82 | 0.20 | 2,10,60,60 | 0 |
| 22 | BCR | B | 847 | 40/40 | 0.82 | 0.23 | 2,10,60,60 | 0 |
| 21 | LMU | B | 805 | 35/35 | 0.82 | 0.16 | 2,37,60,60 | 0 |
| 20 | CLA | B | 825 | 54/65 | 0.82 | 0.24 | 2,15,60,60 | 0 |
| 20 | CLA | B | 826 | 58/65 | 0.82 | 0.23 | 2,13,60,60 | 0 |
| 21 | LMU | D | 201 | 35/35 | 0.82 | 0.12 | 2,12,50,57 | 0 |
| 20 | CLA | L | 203 | 65/65 | 0.82 | 0.23 | 2,22,60,60 | 0 |
| 20 | CLA | 2 | 314 | 50/65 | 0.82 | 0.13 | 2,33,60,60 | 0 |
| 20 | CLA | B | 807 | 45/65 | 0.83 | 0.19 | 2,14,56,60 | 0 |
| 20 | CLA | B | 808 | 61/65 | 0.83 | 0.18 | 2,9,48,60 | 0 |
| 20 | CLA | 2 | 303 | 58/65 | 0.83 | 0.13 | 2,22,60,60 | 0 |
| 20 | CLA | L | 207 | 47/65 | 0.83 | 0.18 | 2,13,45,60 | 0 |
| 21 | LMU | A | 855 | 35/35 | 0.83 | 0.14 | 2,29,60,60 | 0 |
| 20 | CLA | F | 201 | 50/65 | 0.83 | 0.15 | 2,7,51,60 | 0 |
| 20 | CLA | 2 | 304 | 25/65 | 0.83 | 0.14 | 2,27,60,60 | 0 |
| 20 | CLA | A | 813 | 50/65 | 0.83 | 0.20 | 2,29,60,60 | 0 |
| 21 | LMU | 1 | 216 | 35/35 | 0.83 | 0.12 | 2,11,50,60 | 0 |
| 20 | CLA | 4 | 309 | 25/65 | 0.83 | 0.17 | 2,40,60,60 | 0 |
| 20 | CLA | 3 | 308 | 25/65 | 0.83 | 0.15 | 2,37,60,60 | 0 |
| 20 | CLA | B | 820 | 61/65 | 0.83 | 0.19 | 2,16,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 20 | CLA | B | 821 | 50/65 | 0.83 | 0.20 | 2,37,60,60 | 0 |
| 20 | CLA | A | 816 | 54/65 | 0.83 | 0.16 | 2,31,60,60 | 0 |
| 20 | CLA | I | 102 | 60/65 | 0.83 | 0.15 | 2,18,60,60 | 0 |
| 20 | CLA | 2 | 315 | 25/65 | 0.83 | 0.16 | 2,36,60,60 | 0 |
| 20 | CLA | A | 818 | 60/65 | 0.83 | 0.20 | 2,11,52,60 | 0 |
| 22 | BCR | I | 101 | 39/40 | 0.83 | 0.22 | 2,8,60,60 | 0 |
| 20 | CLA | 3 | 304 | 25/65 | 0.83 | 0.14 | 2,28,60,60 | 0 |
| 20 | CLA | B | 827 | 65/65 | 0.83 | 0.21 | 2,15,60,60 | 0 |
| 20 | CLA | B | 832 | 59/65 | 0.83 | 0.21 | 2,6,60,60 | 0 |
| 20 | CLA | 2 | 316 | 65/65 | 0.83 | 0.16 | 2,15,60,60 | 0 |
| 20 | CLA | B | 806 | 65/65 | 0.83 | 0.23 | 2,11,60,60 | 0 |
| 20 | CLA | A | 806 | 56/65 | 0.84 | 0.18 | 2,2,54,60 | 0 |
| 21 | LMU | 3 | 319 | 35/35 | 0.84 | 0.10 | 2,28,59,60 | 0 |
| 20 | CLA | 4 | 313 | 36/65 | 0.84 | 0.16 | 2,21,60,60 | 0 |
| 20 | CLA | A | 828 | 65/65 | 0.84 | 0.21 | 2,12,60,60 | 0 |
| 20 | CLA | A | 851 | 65/65 | 0.84 | 0.22 | 2,2,60,60 | 0 |
| 22 | BCR | B | 846 | 40/40 | 0.84 | 0.23 | 2,11,60,60 | 0 |
| 20 | CLA | A | 803 | 46/65 | 0.84 | 0.14 | 2,14,49,60 | 0 |
| 20 | CLA | A | 832 | 50/65 | 0.84 | 0.18 | 2,18,56,60 | 0 |
| 20 | CLA | 1 | 202 | 41/65 | 0.84 | 0.15 | 2,41,60,60 | 0 |
| 20 | CLA | 4 | 312 | 25/65 | 0.84 | 0.15 | 2,2,26,32 | 0 |
| 20 | CLA | A | 835 | 65/65 | 0.84 | 0.19 | 2,6,60,60 | 0 |
| 20 | CLA | B | 814 | 65/65 | 0.84 | 0.19 | 2,13,60,60 | 0 |
| 23 | PQN | B | 843 | 33/33 | 0.84 | 0.22 | 2,2,46,51 | 0 |
| 20 | CLA | H | 108 | 58/65 | 0.84 | 0.20 | 2,15,60,60 | 0 |
| 20 | CLA | A | 837 | 51/65 | 0.84 | 0.24 | 2,12,60,60 | 0 |
| 20 | CLA | B | 803 | 65/65 | 0.85 | 0.22 | 2,14,56,60 | 0 |
| 20 | CLA | B | 838 | 65/65 | 0.85 | 0.18 | 2,7,60,60 | 0 |
| 20 | CLA | B | 840 | 65/65 | 0.85 | 0.22 | 2,11,60,60 | 0 |
| 20 | CLA | B | 824 | 65/65 | 0.85 | 0.18 | 2,17,60,60 | 0 |
| 20 | CLA | B | 833 | 50/65 | 0.85 | 0.24 | 2,11,53,60 | 0 |
| 20 | CLA | B | 811 | 25/65 | 0.86 | 0.17 | 2,2,60,60 | 0 |
| 20 | CLA | A | 850 | 65/65 | 0.86 | 0.21 | 2,4,48,60 | 0 |
| 20 | CLA | B | 810 | 60/65 | 0.86 | 0.21 | 2,2,60,60 | 0 |
| 22 | BCR | F | 203 | 40/40 | 0.86 | 0.21 | 2,2,60,60 | 0 |
| 20 | CLA | B | 829 | 65/65 | 0.86 | 0.18 | 2,11,46,60 | 0 |
| 21 | LMU | 4 | 319 | 34/35 | 0.86 | 0.12 | 2,22,60,60 | 0 |
| 21 | LMU | H | 105 | 35/35 | 0.87 | 0.11 | 2,31,60,60 | 0 |
| 22 | BCR | B | 801 | 40/40 | 0.87 | 0.20 | 2,4,50,60 | 0 |
| 20 | CLA | A | 838 | 65/65 | 0.87 | 0.19 | 2,8,60,60 | 0 |
| 20 | CLA | A | 826 | 65/65 | 0.87 | 0.21 | 2,2,50,60 | 0 |
| 20 | CLA | 4 | 311 | 25/65 | 0.87 | 0.23 | 2,15,60,60 | 0 |

*Continued on next page...*

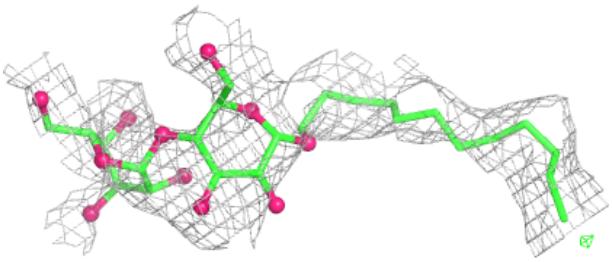
*Continued from previous page...*

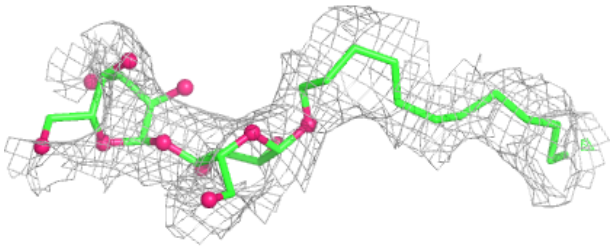
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 23 | PQN | A | 842 | 33/33 | 0.87 | 0.23 | 2,4,59,60 | 0 |
| 20 | CLA | F | 205 | 36/65 | 0.87 | 0.17 | 2,17,60,60 | 0 |
| 20 | CLA | B | 818 | 53/65 | 0.87 | 0.17 | 2,14,60,60 | 0 |
| 22 | BCR | F | 204 | 40/40 | 0.87 | 0.17 | 2,6,60,60 | 0 |
| 20 | CLA | 2 | 308 | 25/65 | 0.88 | 0.14 | 2,12,60,60 | 0 |
| 20 | CLA | B | 839 | 47/65 | 0.88 | 0.14 | 2,5,55,60 | 0 |
| 20 | CLA | A | 827 | 55/65 | 0.88 | 0.20 | 2,12,60,60 | 0 |
| 20 | CLA | B | 841 | 65/65 | 0.88 | 0.20 | 2,2,55,60 | 0 |
| 20 | CLA | A | 830 | 65/65 | 0.88 | 0.17 | 2,9,59,60 | 0 |
| 20 | CLA | A | 831 | 65/65 | 0.88 | 0.17 | 2,14,60,60 | 0 |
| 20 | CLA | A | 836 | 47/65 | 0.88 | 0.16 | 2,8,50,60 | 0 |
| 20 | CLA | B | 831 | 50/65 | 0.89 | 0.14 | 2,12,60,60 | 0 |
| 20 | CLA | A | 822 | 50/65 | 0.89 | 0.21 | 2,7,60,60 | 0 |
| 20 | CLA | B | 850 | 65/65 | 0.89 | 0.22 | 2,2,55,60 | 0 |
| 20 | CLA | A | 808 | 60/65 | 0.90 | 0.20 | 2,10,60,60 | 0 |
| 20 | CLA | B | 830 | 65/65 | 0.90 | 0.20 | 2,6,53,60 | 0 |
| 20 | CLA | A | 809 | 52/65 | 0.90 | 0.18 | 2,10,60,60 | 0 |
| 20 | CLA | B | 809 | 65/65 | 0.90 | 0.20 | 2,2,53,60 | 0 |
| 20 | CLA | B | 819 | 41/65 | 0.90 | 0.14 | 2,5,40,60 | 0 |
| 20 | CLA | B | 828 | 65/65 | 0.90 | 0.18 | 2,10,56,60 | 0 |
| 20 | CLA | A | 849 | 65/65 | 0.91 | 0.22 | 2,2,48,60 | 0 |
| 20 | CLA | B | 802 | 54/65 | 0.91 | 0.18 | 2,6,45,60 | 0 |
| 24 | SF4 | C | 103 | 8/8 | 0.98 | 0.05 | 12,19,20,24 | 0 |
| 24 | SF4 | A | 856 | 8/8 | 0.98 | 0.05 | 23,24,24,25 | 0 |
| 24 | SF4 | C | 102 | 8/8 | 0.98 | 0.06 | 18,22,26,32 | 0 |

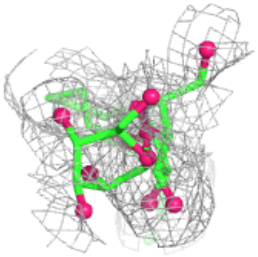
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around LMU A 852:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

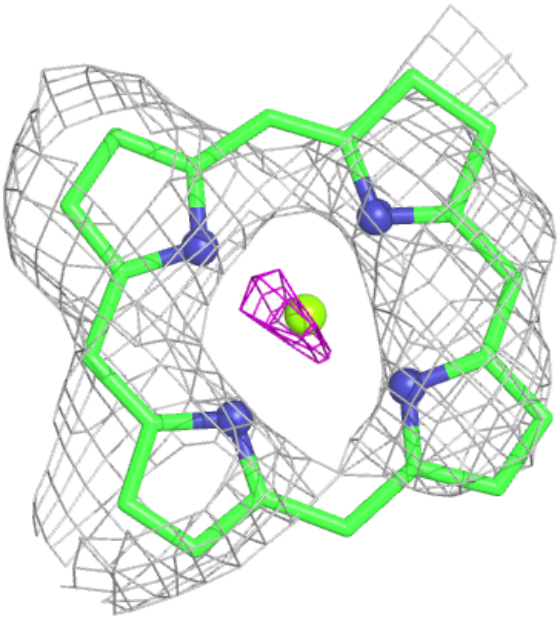


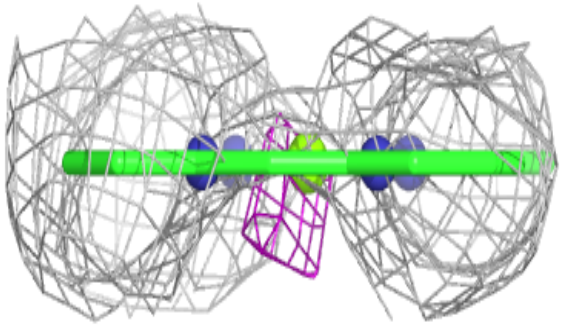


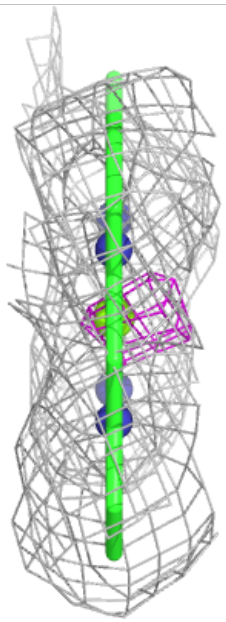


**Electron density around CLA 4 307:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

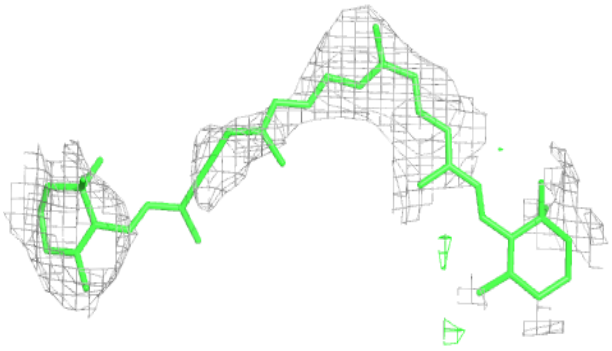


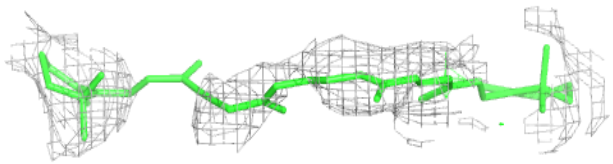


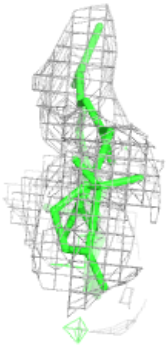


**Electron density around BCR 2 317:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

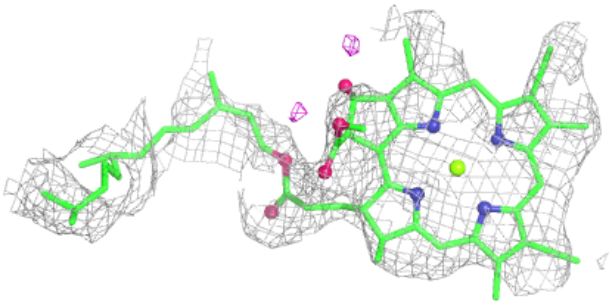


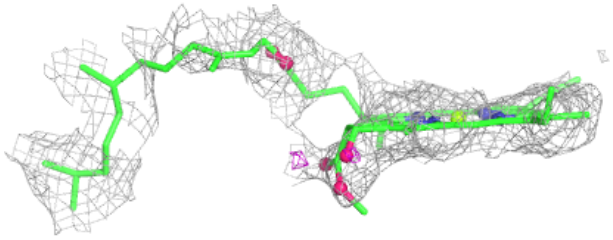


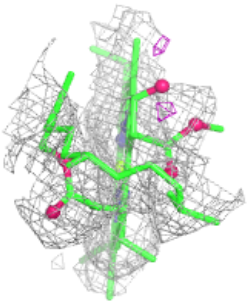


**Electron density around CLA B 816:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

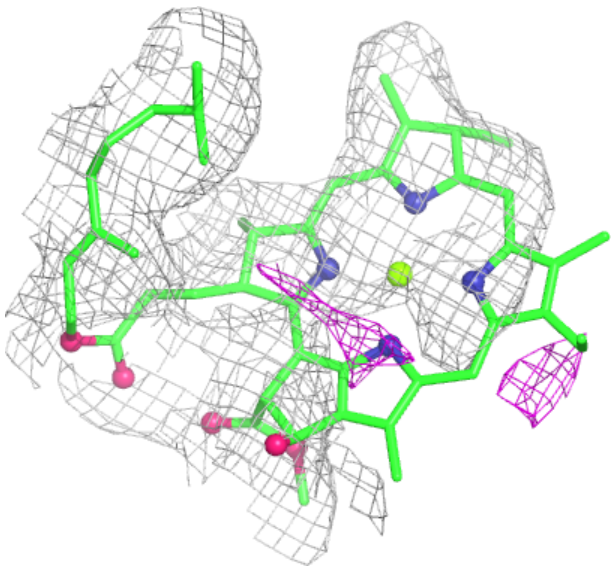


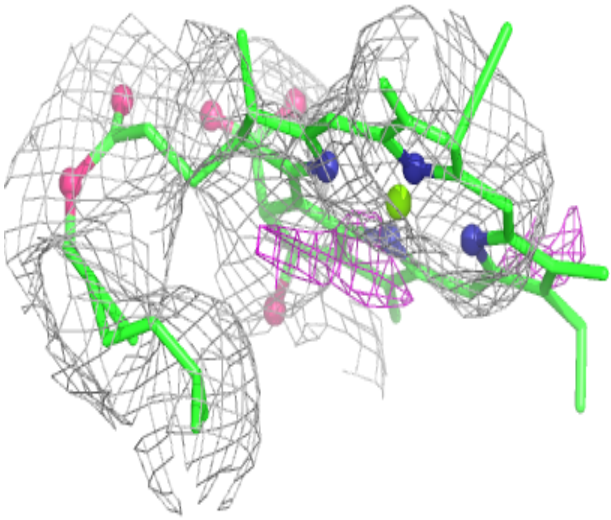




**Electron density around CLA H 102:**

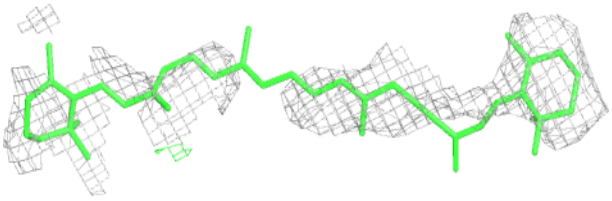
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

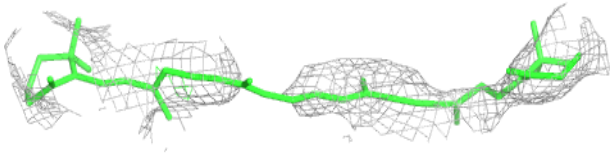


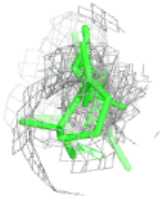


**Electron density around BCR A 843:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

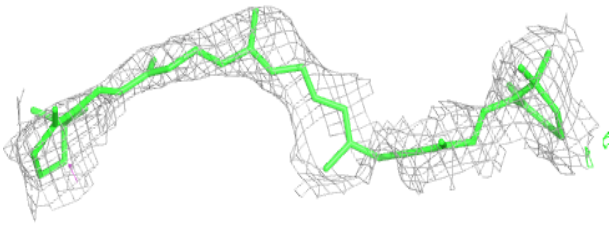


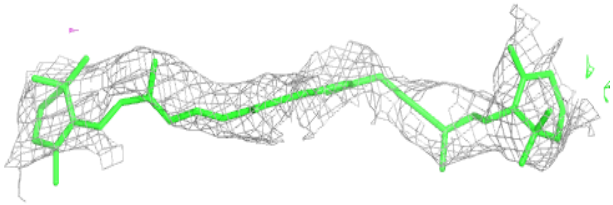


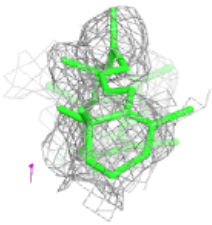


**Electron density around BCR I 103:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

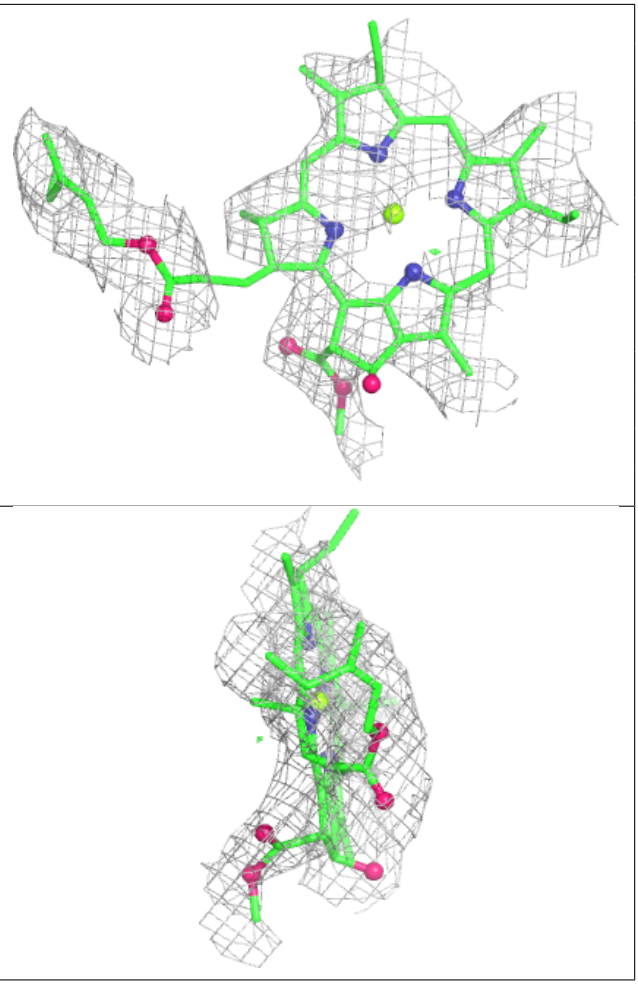






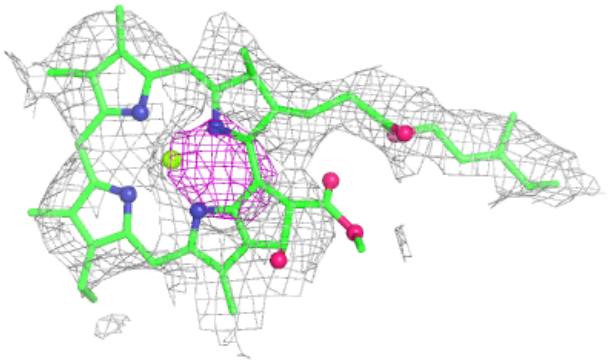
**Electron density around CLA G 105:**

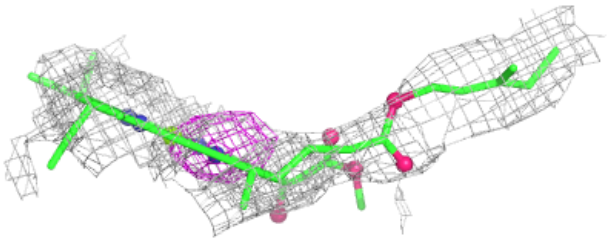
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

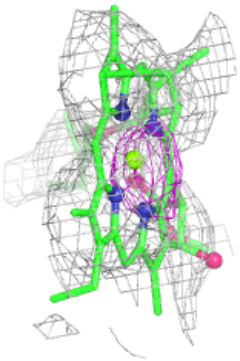


**Electron density around CLA 1 211:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

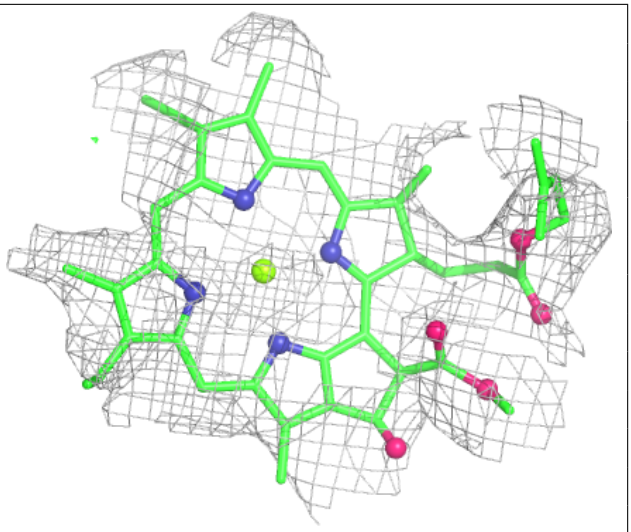


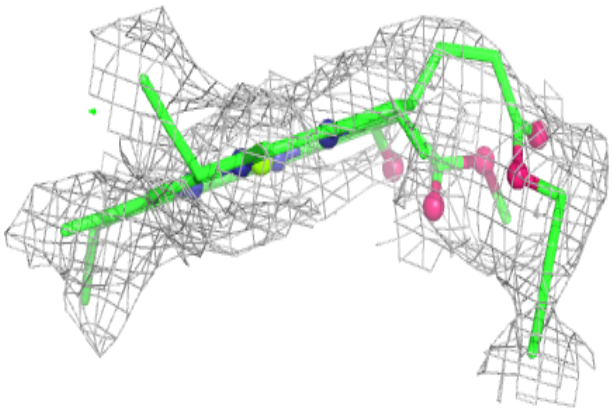




**Electron density around CLA 3 313:**

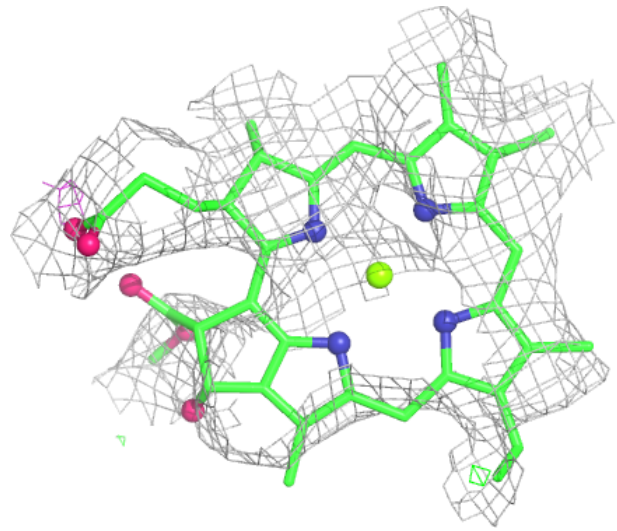
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

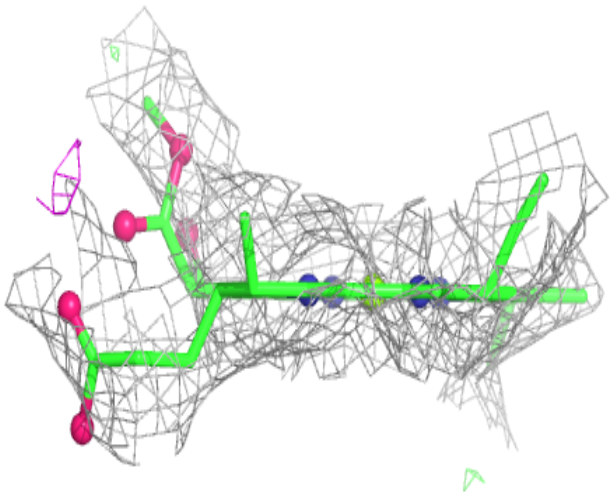


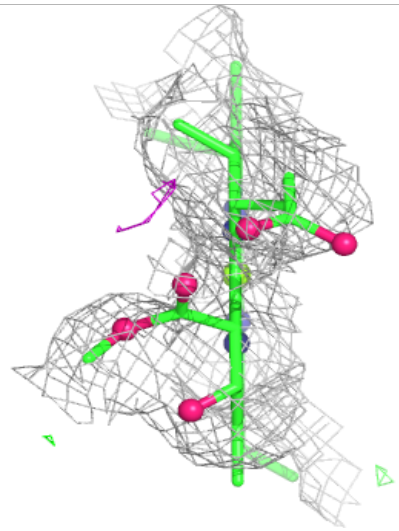


**Electron density around CLA B 835:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

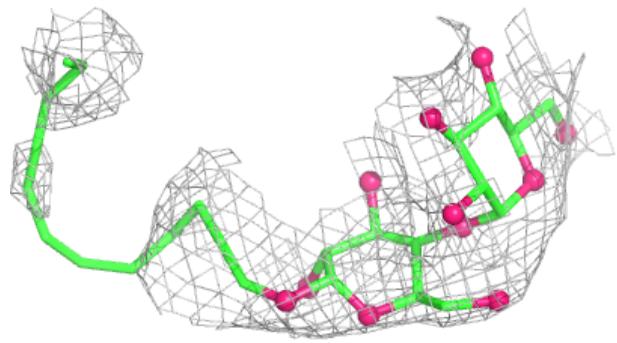


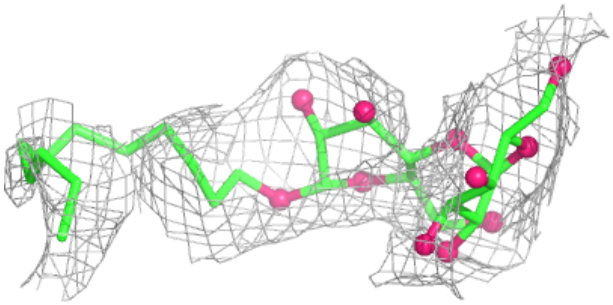


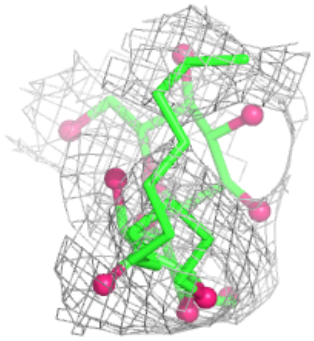


**Electron density around LMU 2 320:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

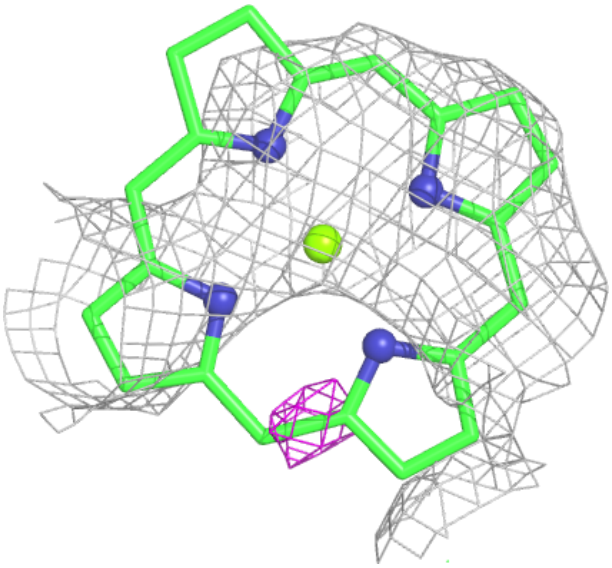


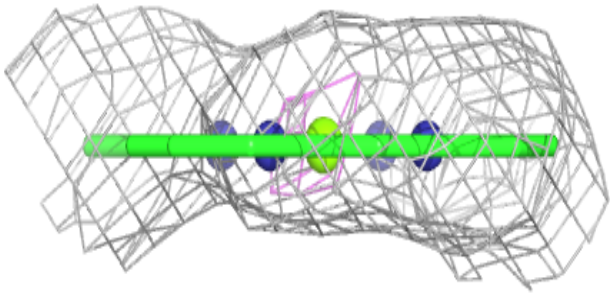


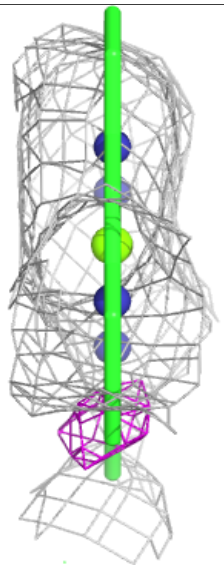


**Electron density around CLA A 802:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

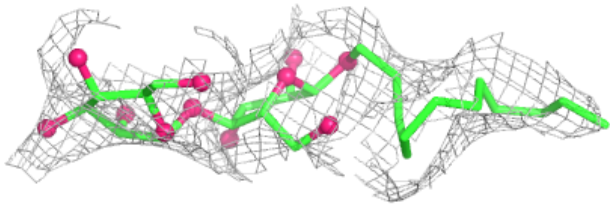


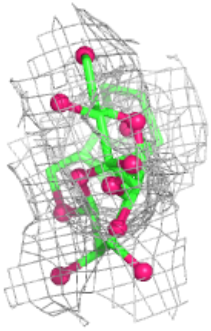




**Electron density around LMU A 853:**

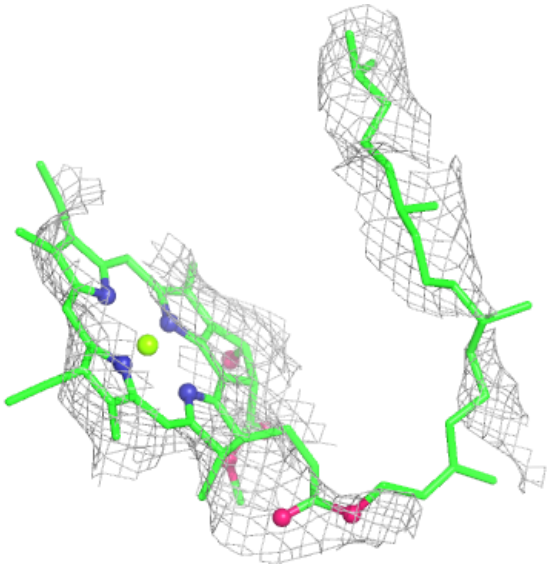
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

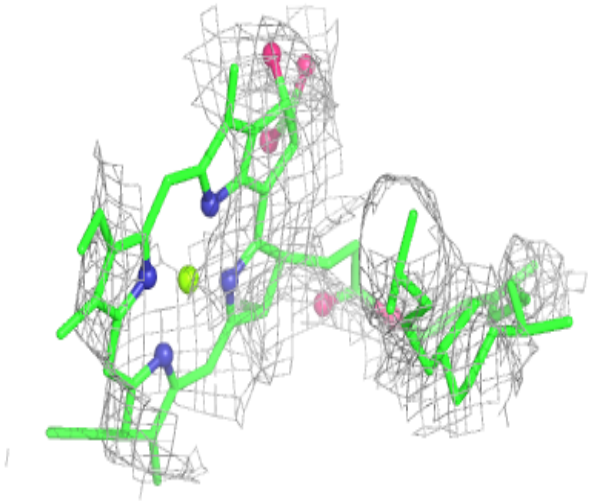


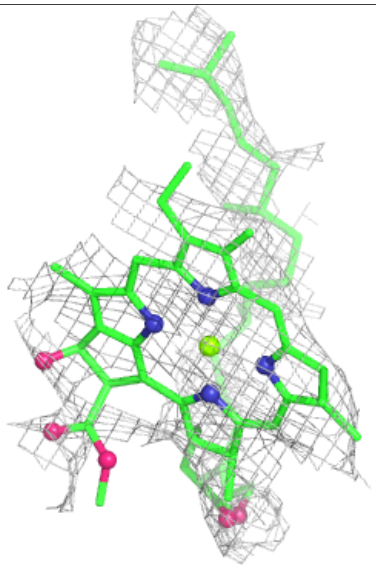


**Electron density around CLA 3 311:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

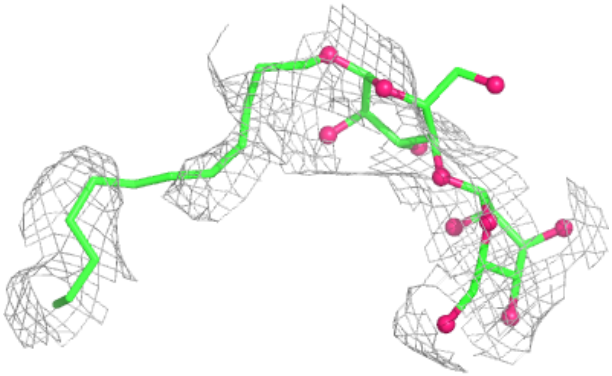


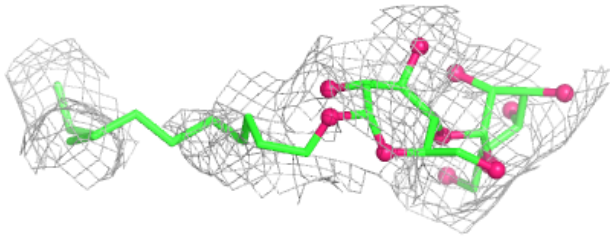




**Electron density around LMU 4 320:**

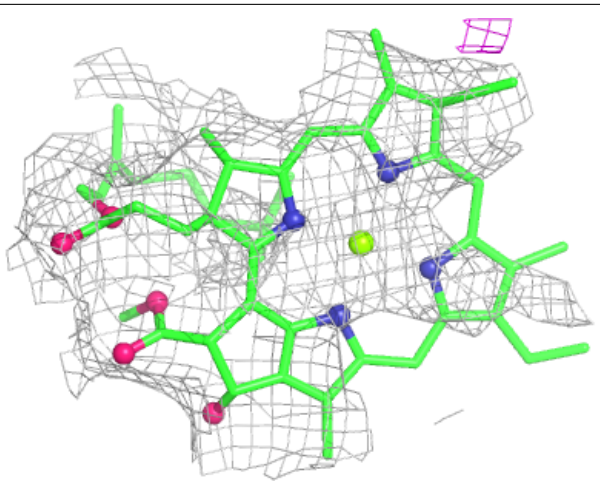
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

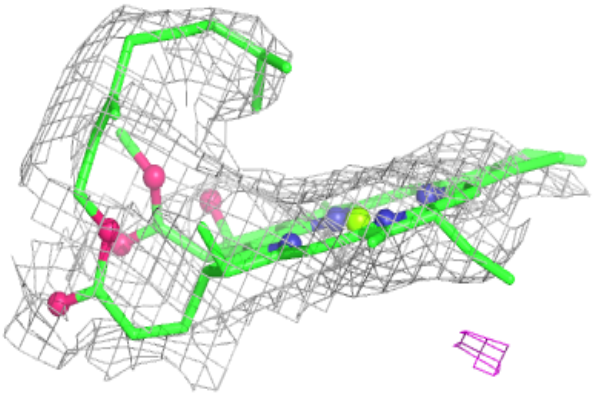


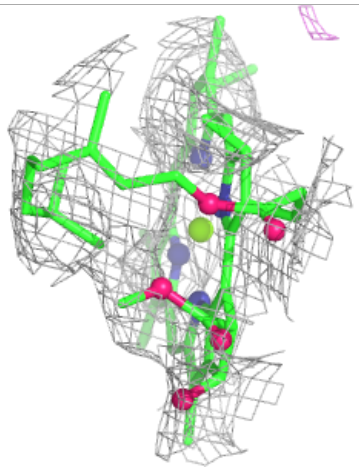


**Electron density around CLA 4 304:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

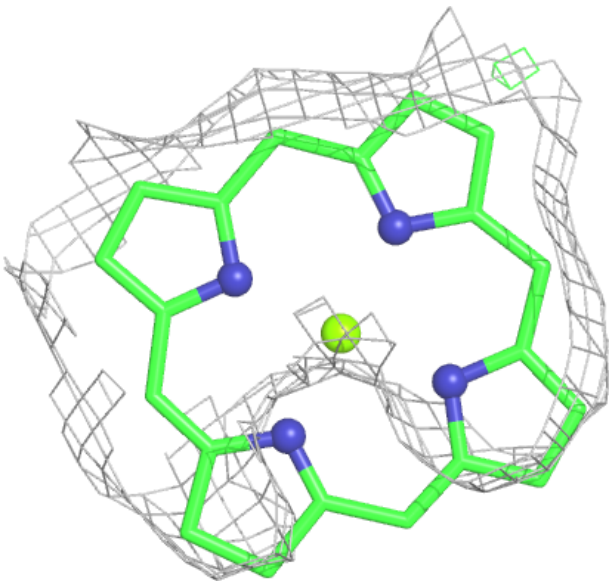


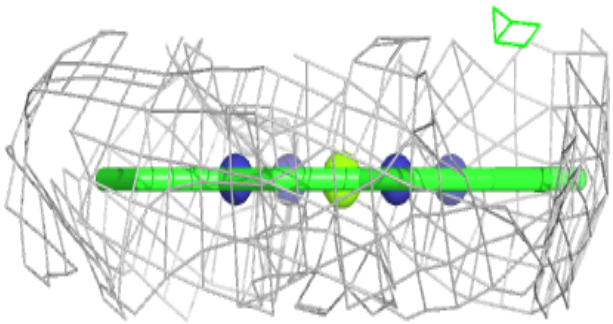


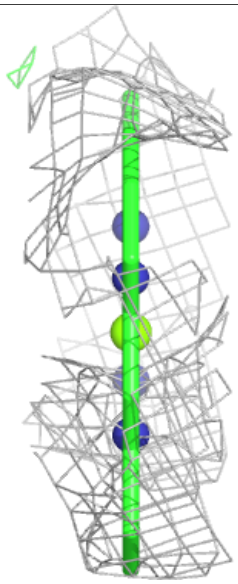


**Electron density around CLA 3 305:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

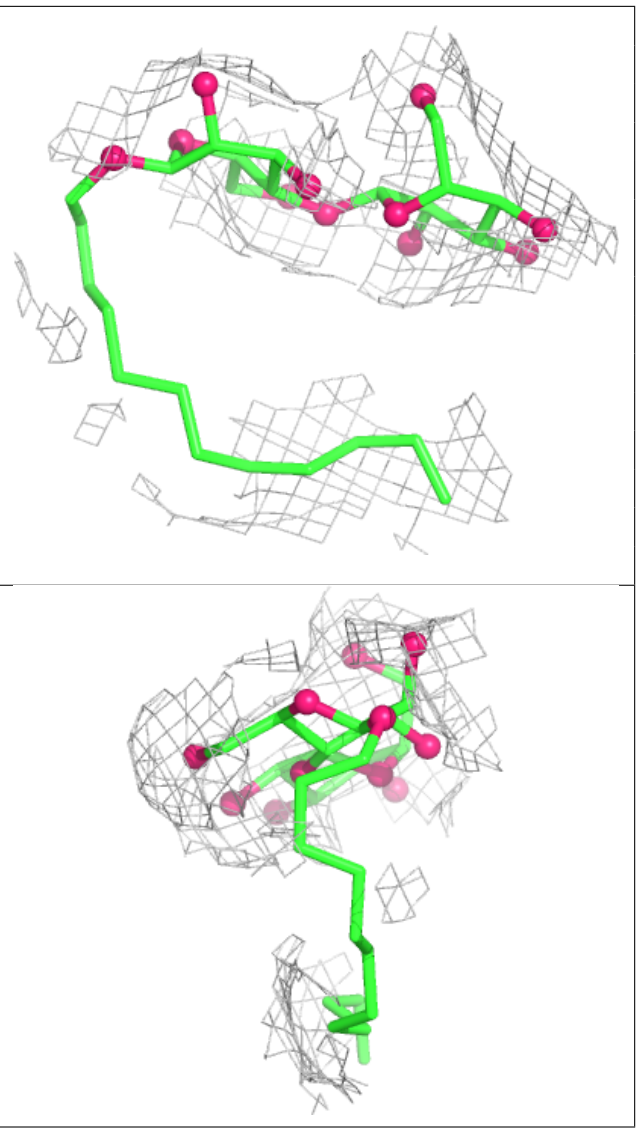






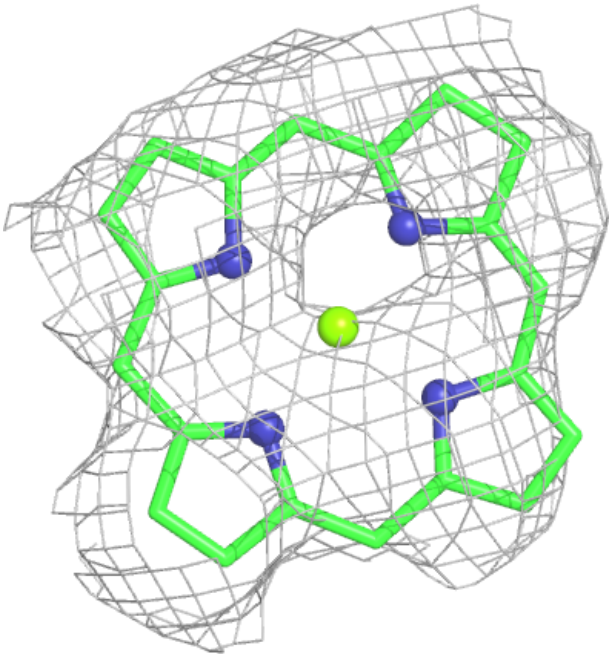
**Electron density around LMU 1 217:**

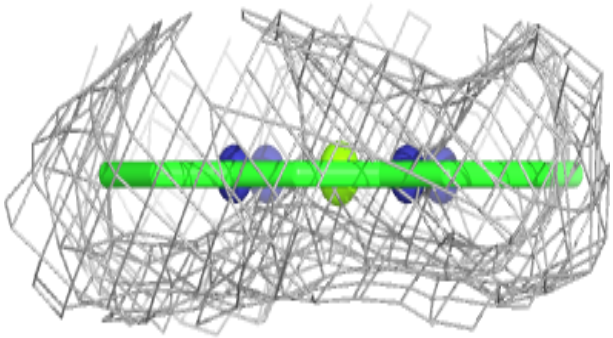
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

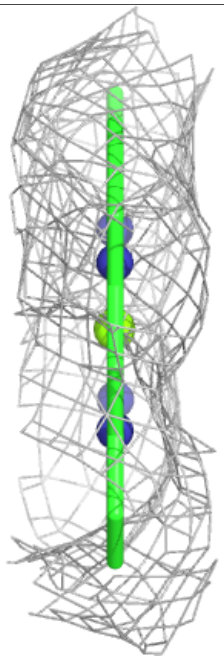


**Electron density around CLA 4 314:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

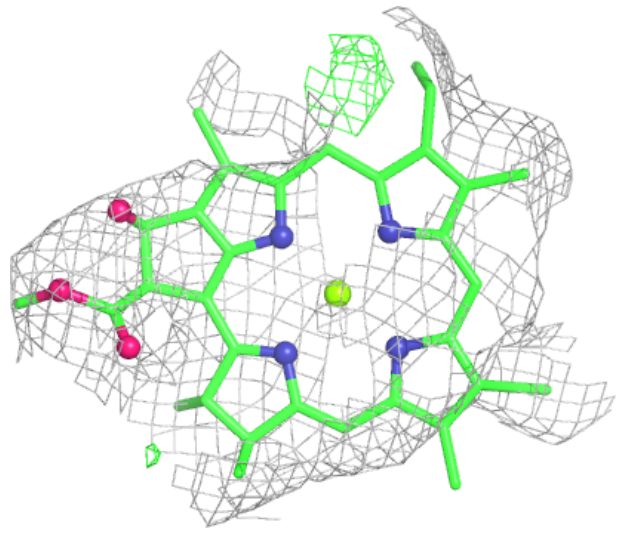


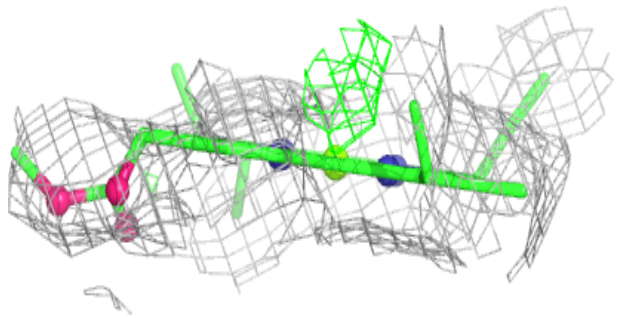


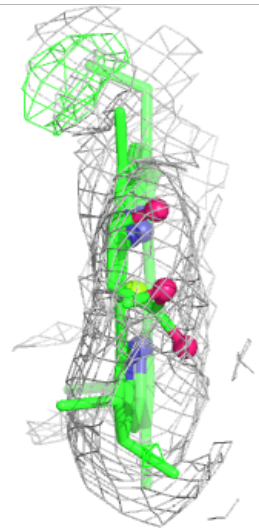


**Electron density around CLA F 206:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

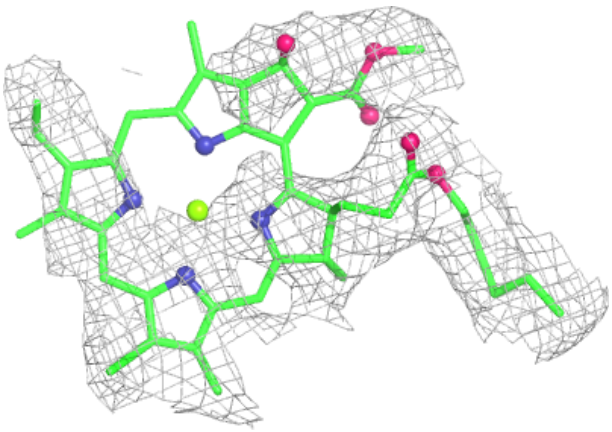


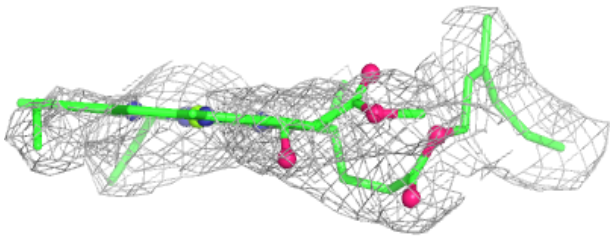


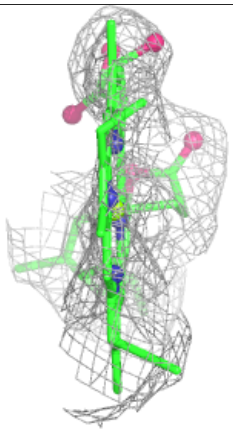


**Electron density around CLA 4 317:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

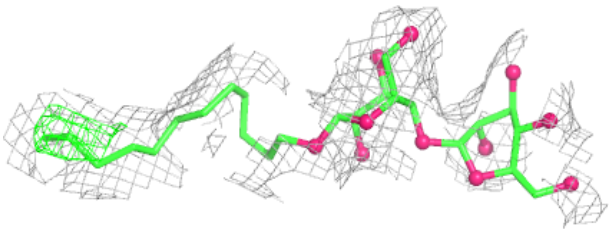


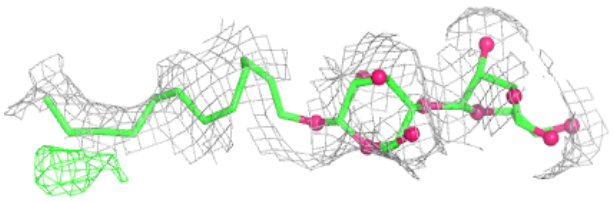


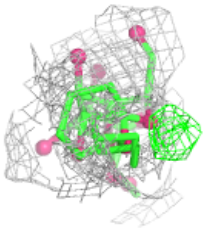


**Electron density around LMU E 101:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

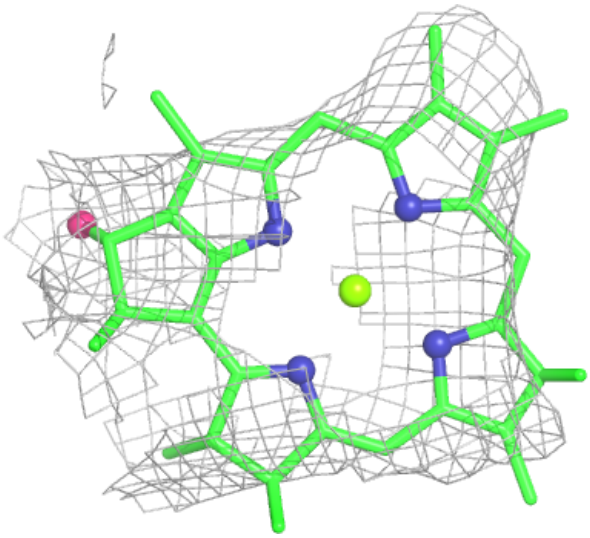


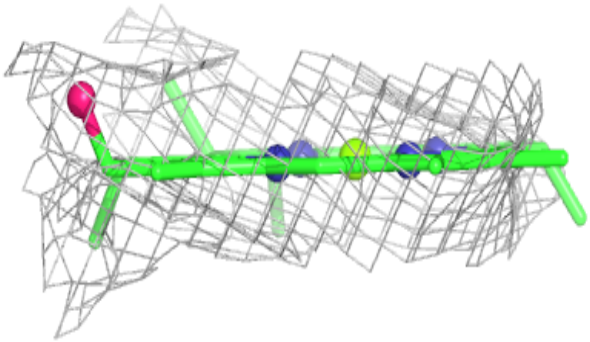


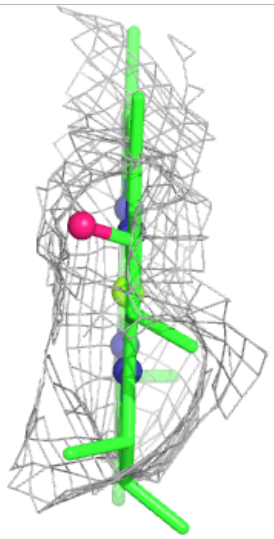


**Electron density around CLA 3 317:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

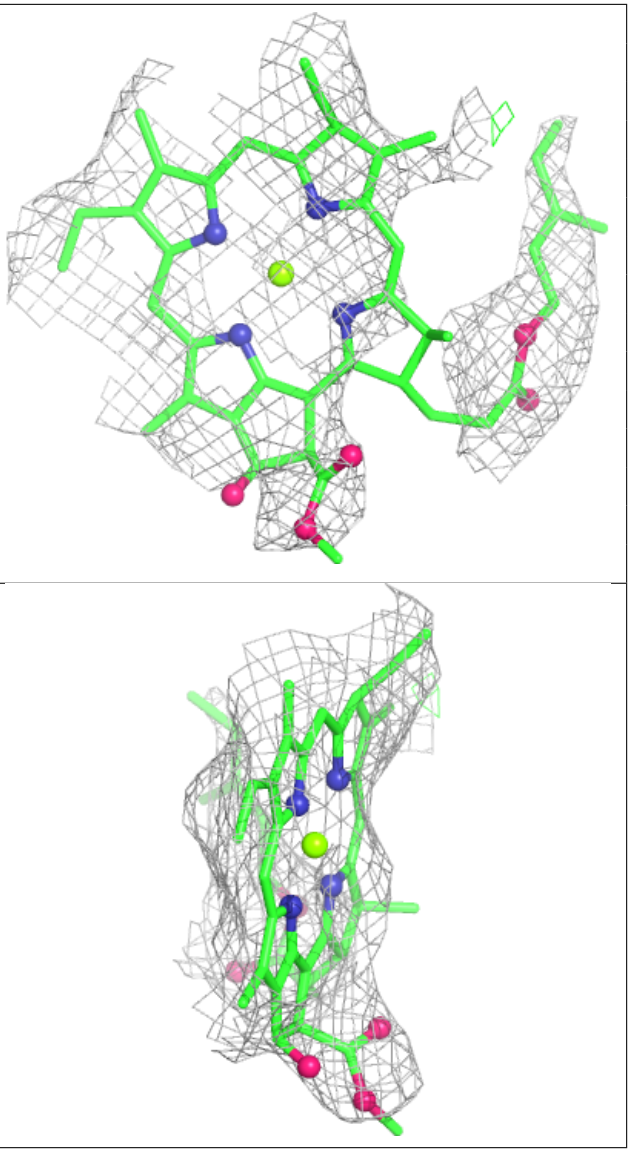






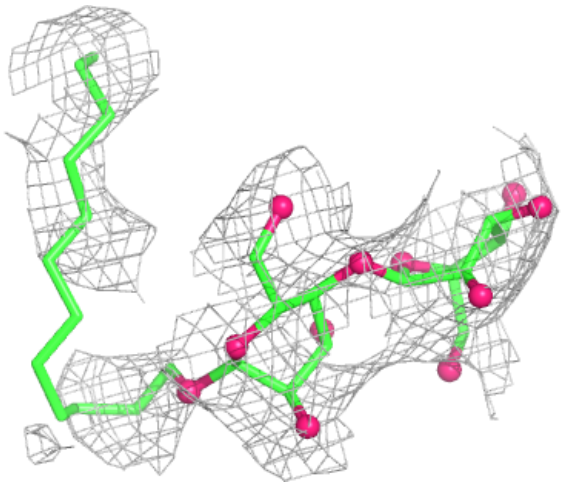
**Electron density around CLA B 836:**

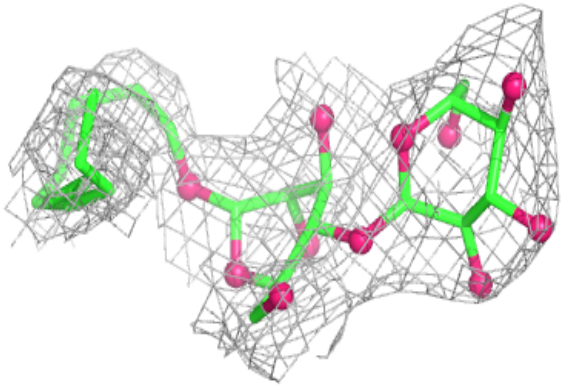
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

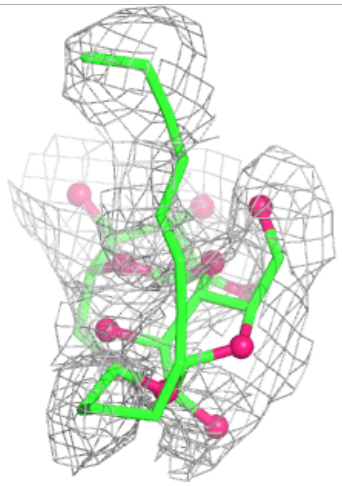


**Electron density around LMU R 101:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

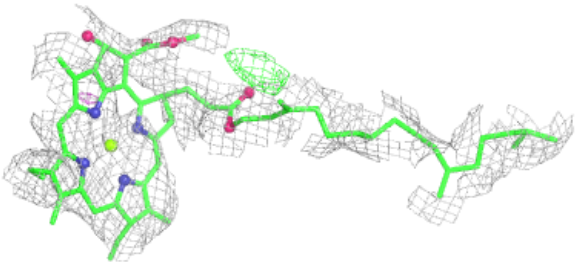


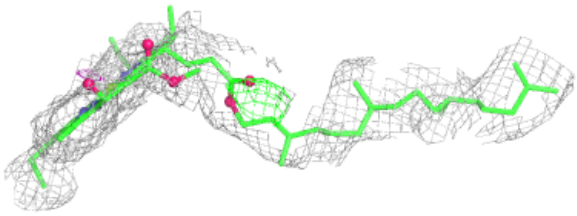


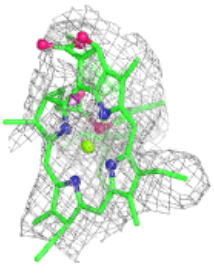


**Electron density around CLA 4 303:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

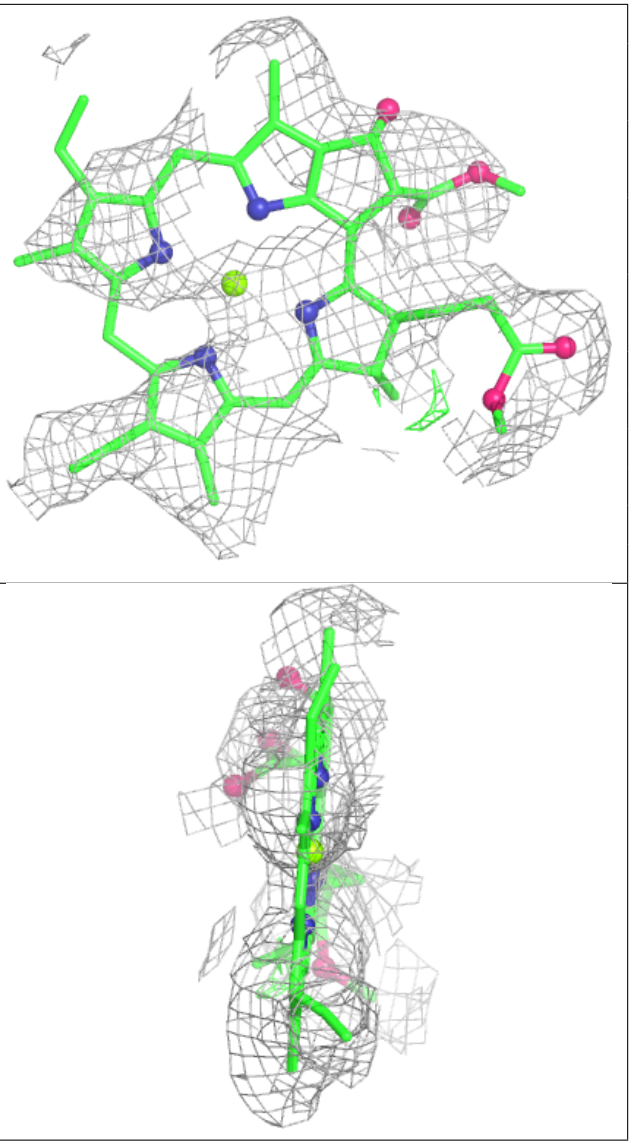






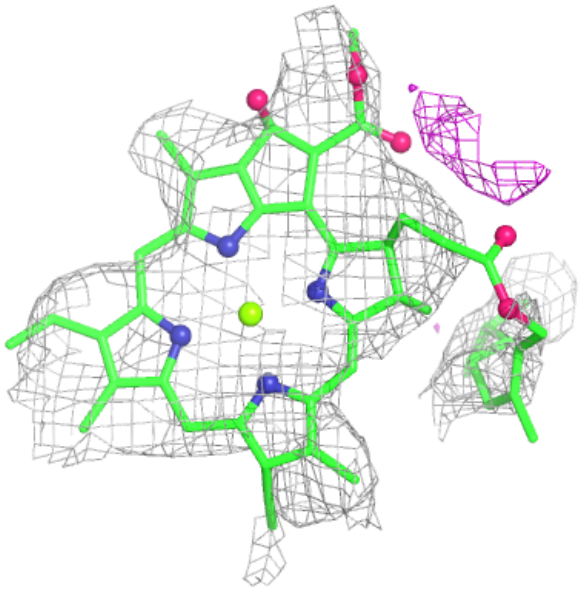
**Electron density around CLA B 817:**

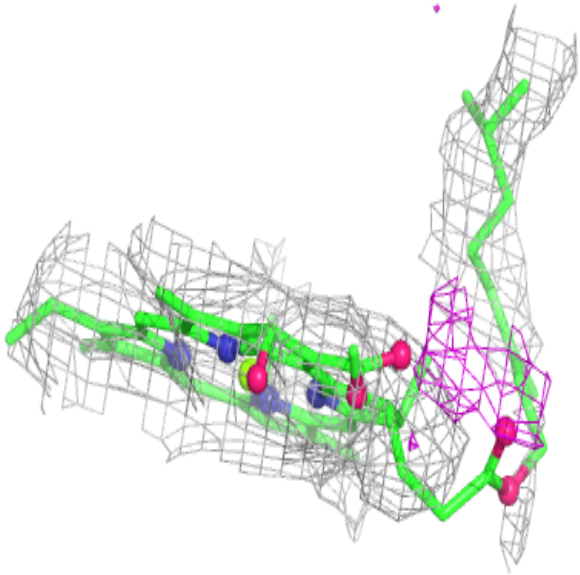
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

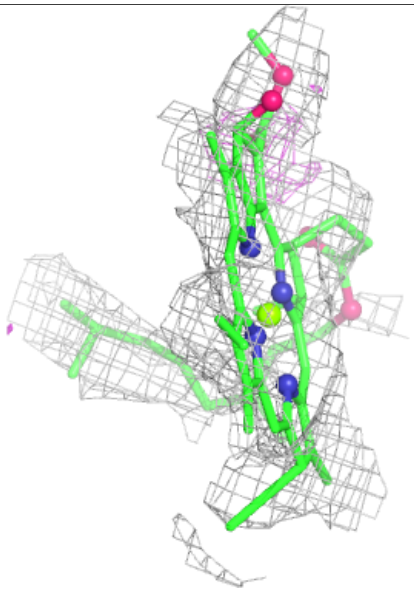


**Electron density around CLA H 101:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

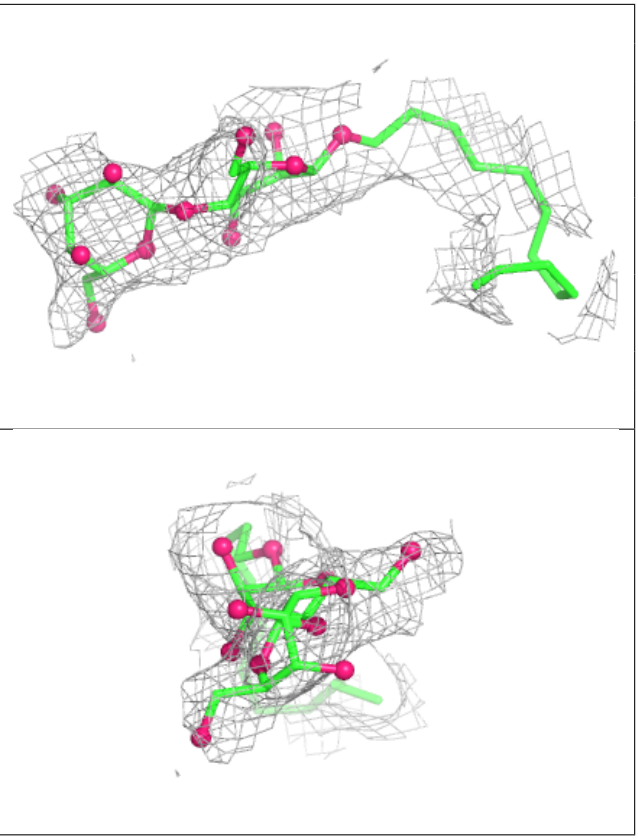






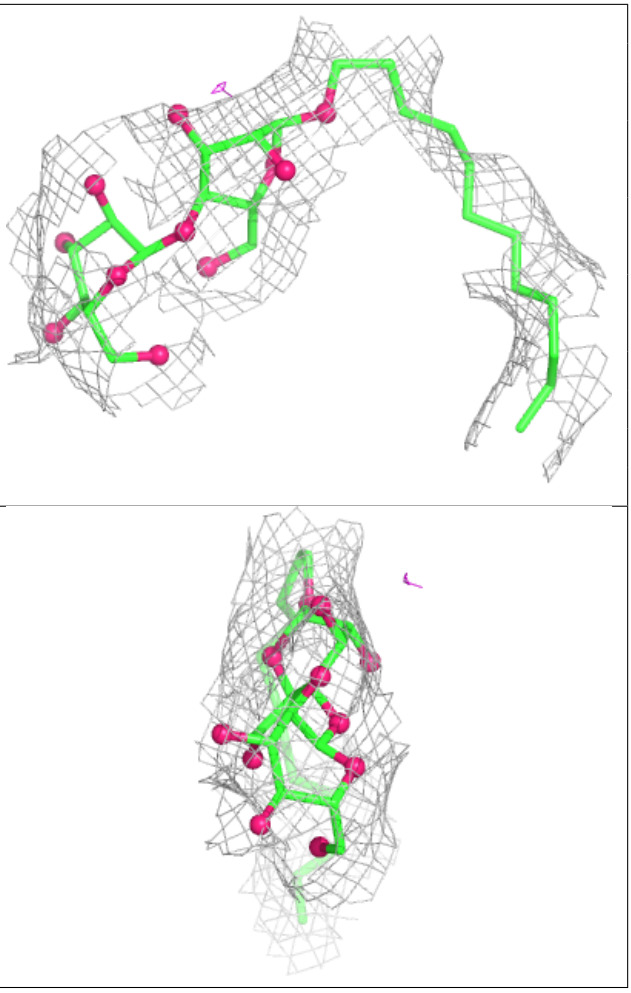
**Electron density around LMU H 106:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



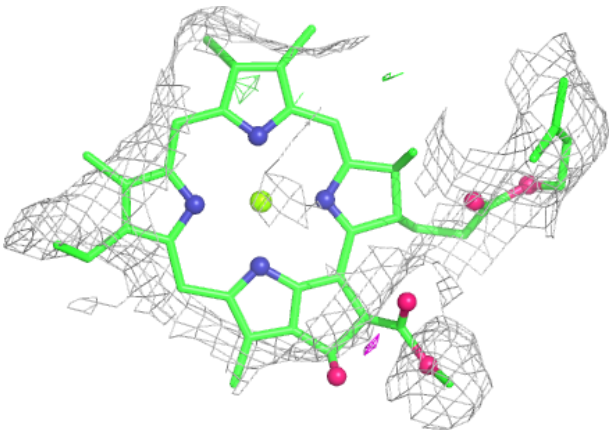
**Electron density around LMU K 106:**

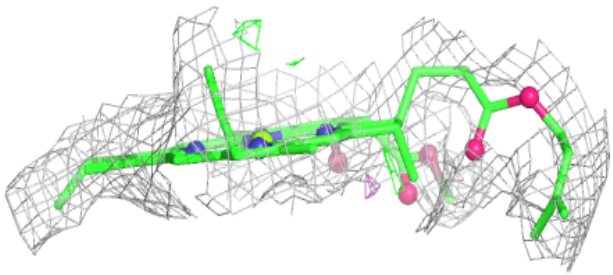
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

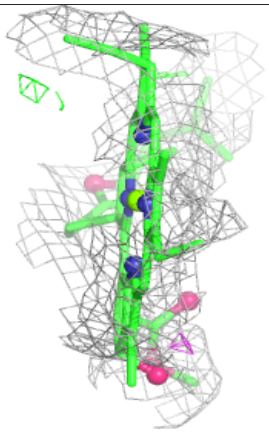


**Electron density around CLA K 103:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

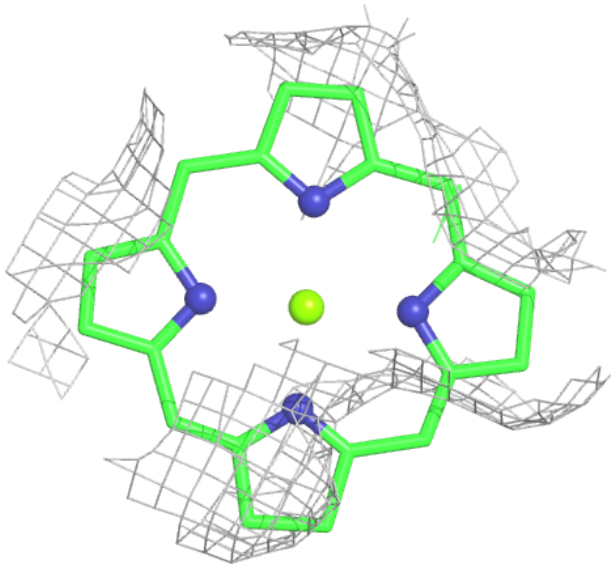


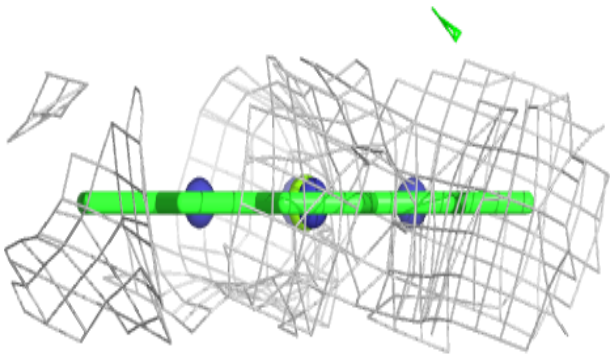


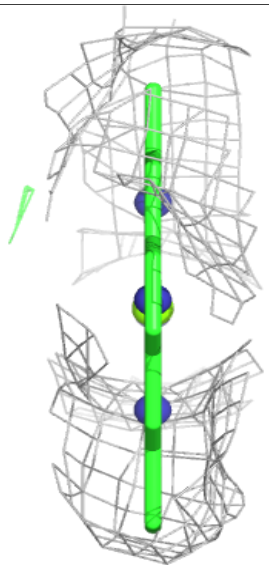


**Electron density around CLA 3 309:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

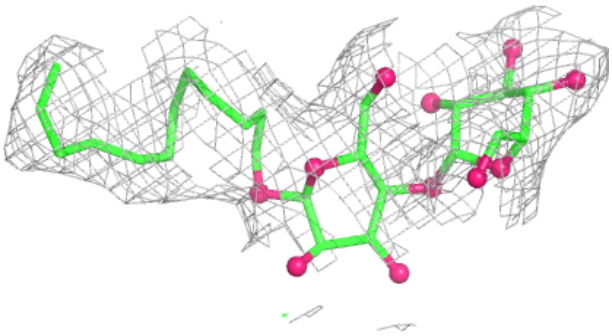


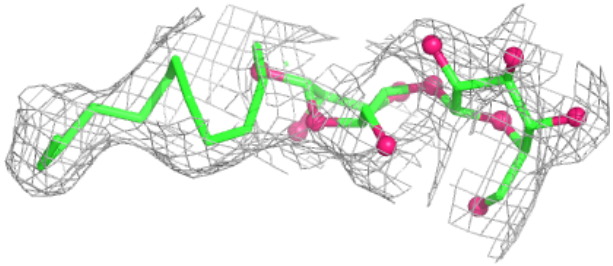


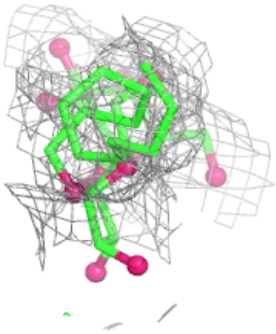


**Electron density around LMU 2 313:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

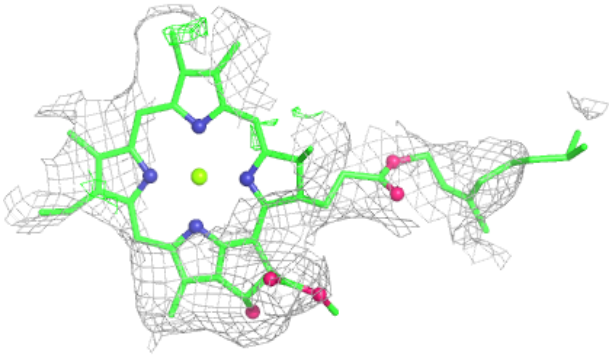


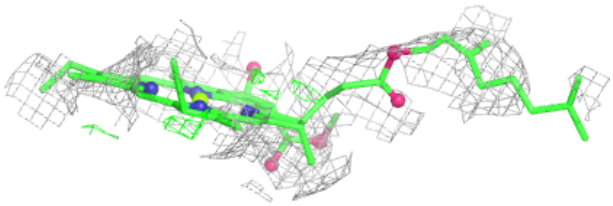


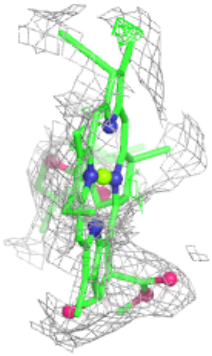


**Electron density around CLA A 840:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

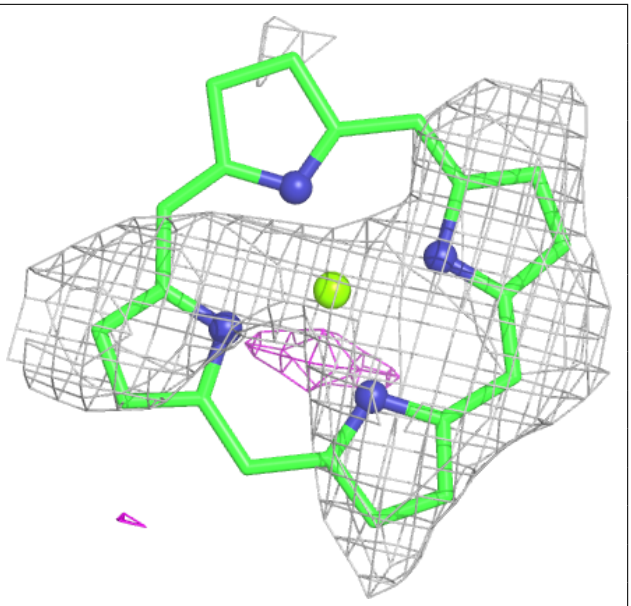


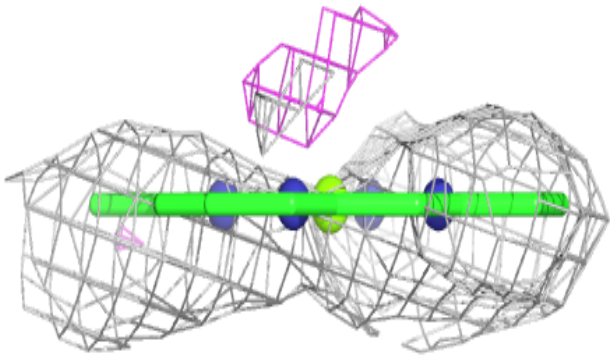


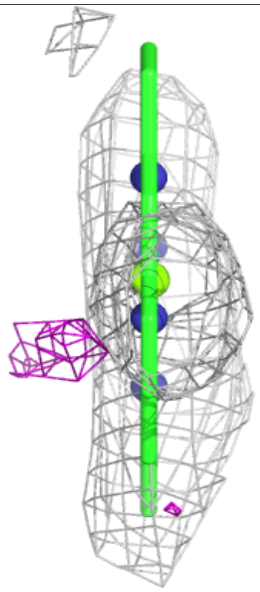


**Electron density around CLA 3 312:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

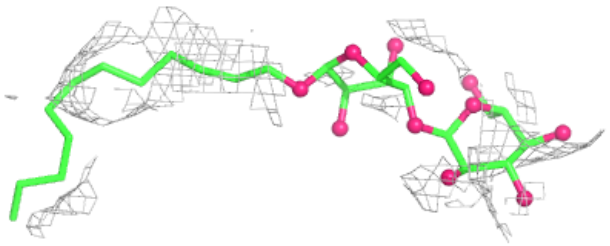


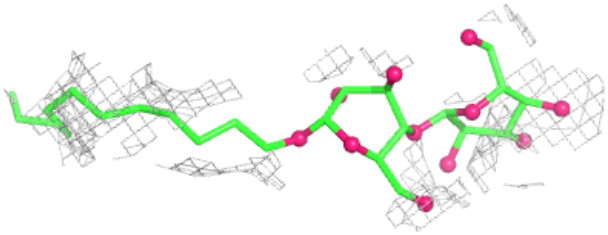


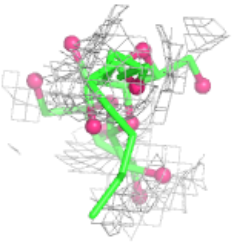


**Electron density around LMU G 103:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

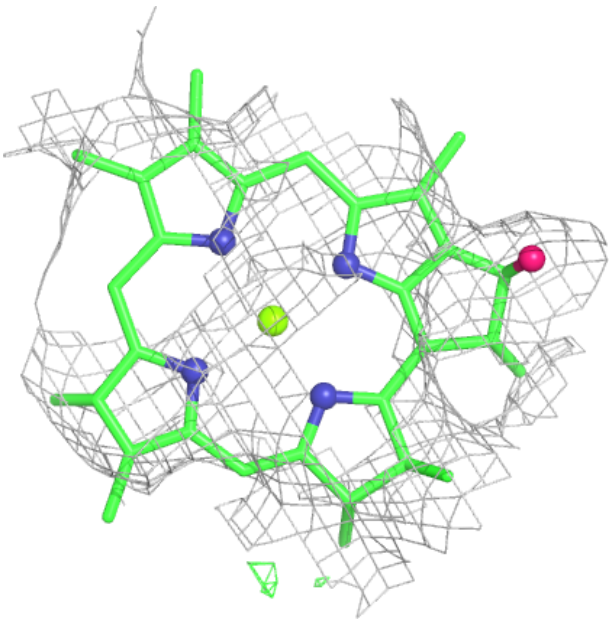


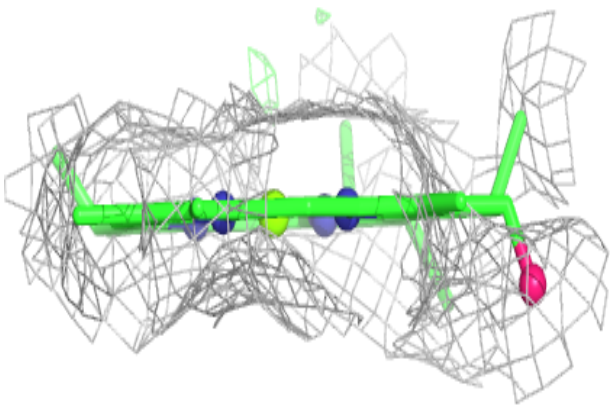


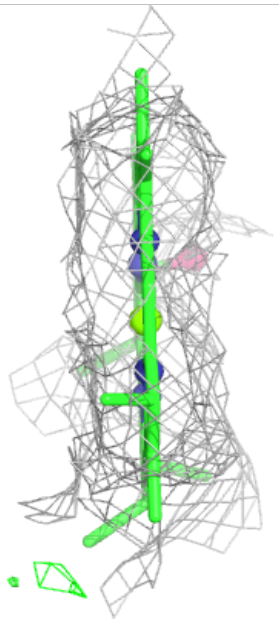


**Electron density around CLA 1 205:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

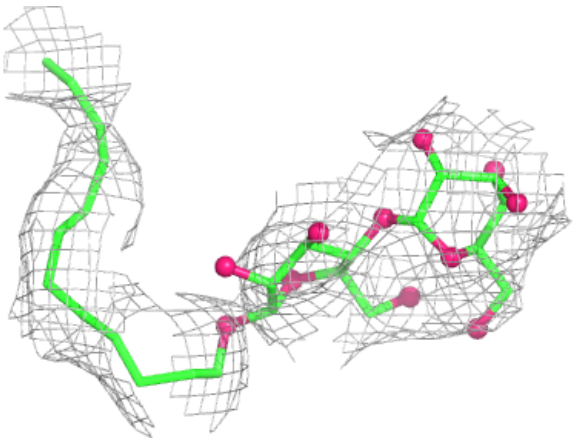


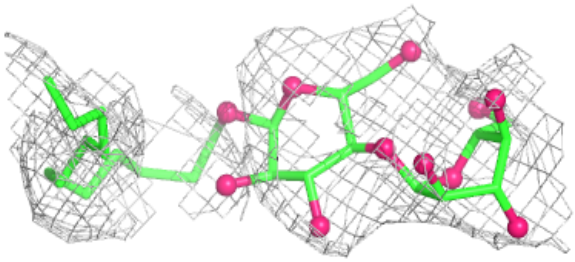


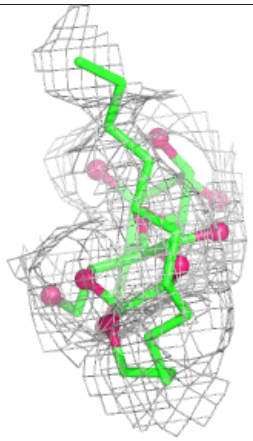


**Electron density around LMU 3 318:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

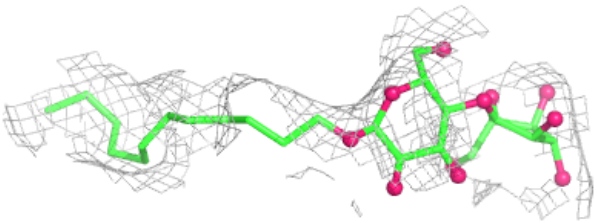


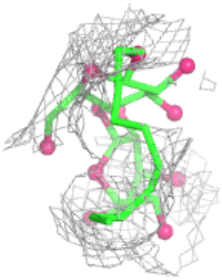




**Electron density around LMU L 205:**

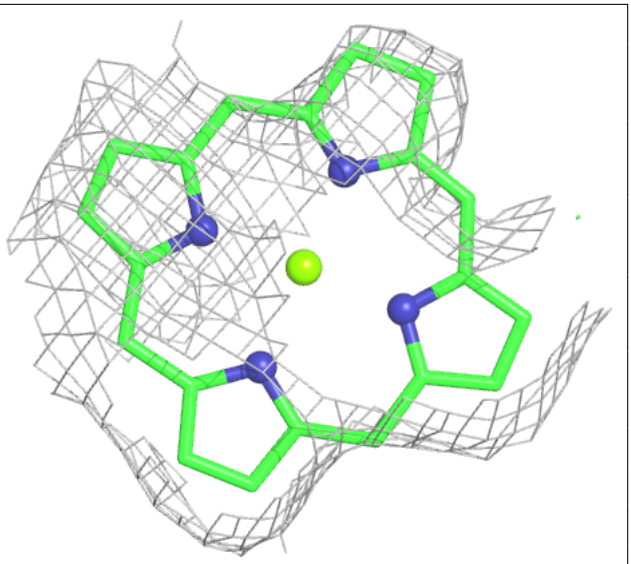
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

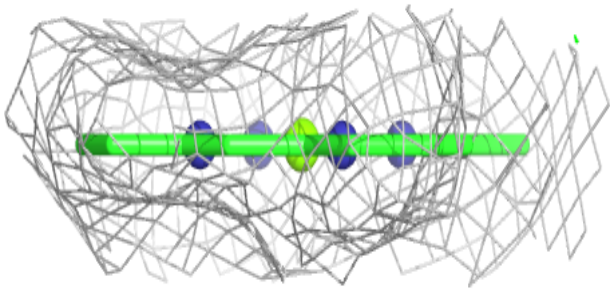


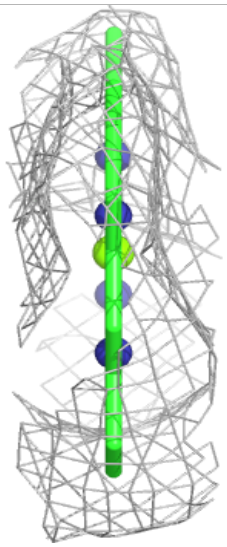


**Electron density around CLA 4 308:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

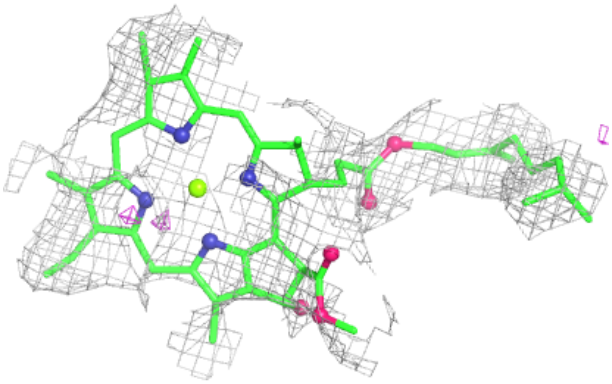


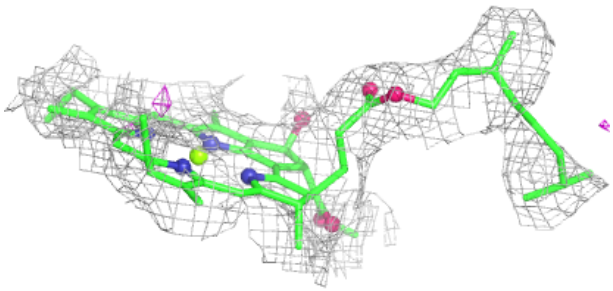




**Electron density around CLA H 109:**

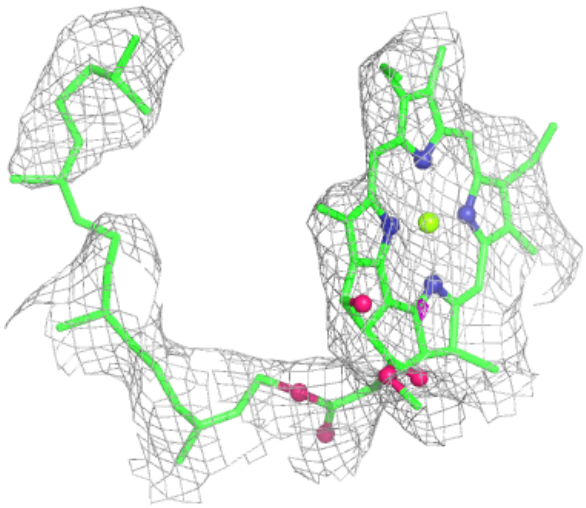
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

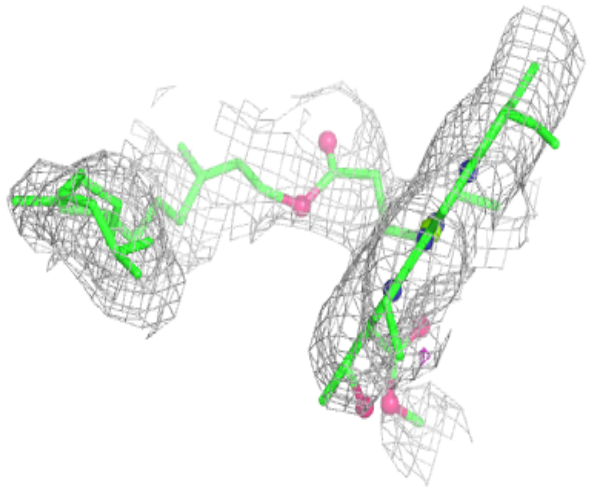


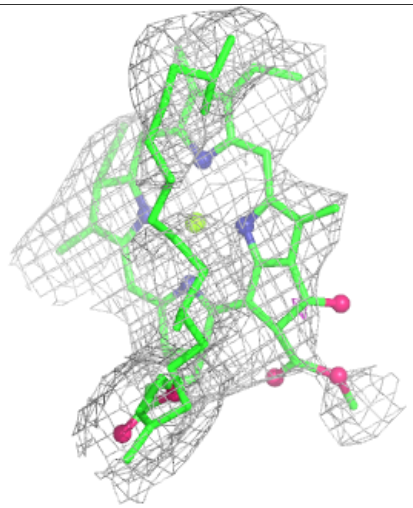


**Electron density around CLA 3 310:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

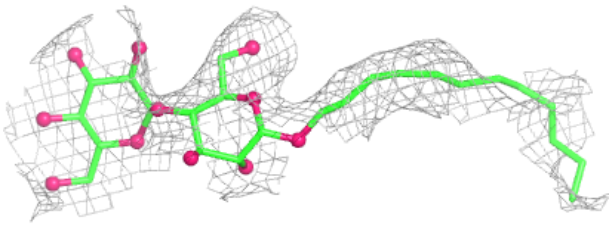


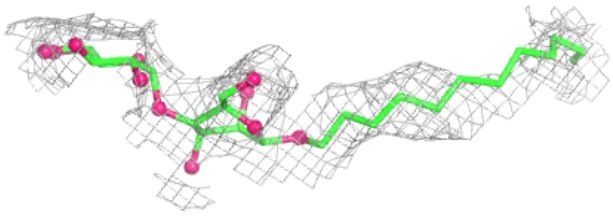


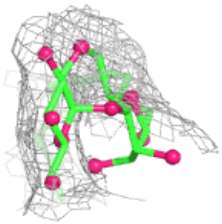


**Electron density around LMU 2 321:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

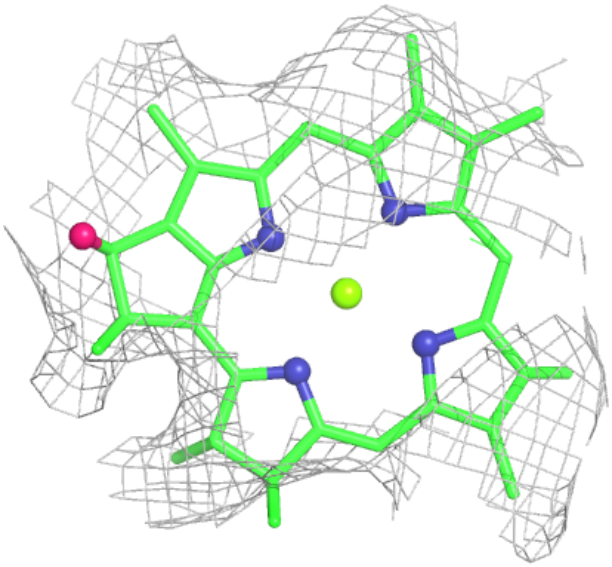


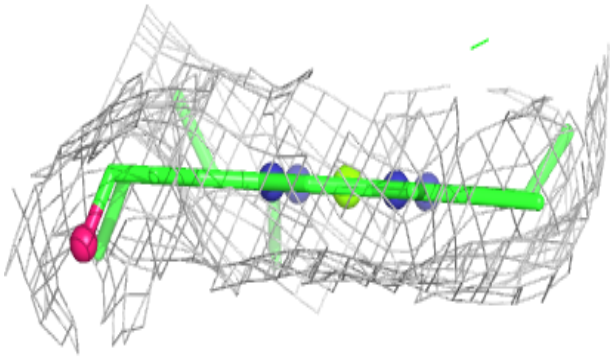


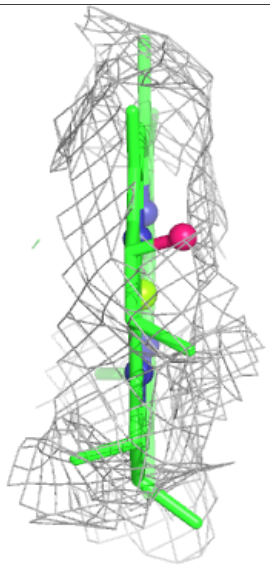


**Electron density around CLA 3 303:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

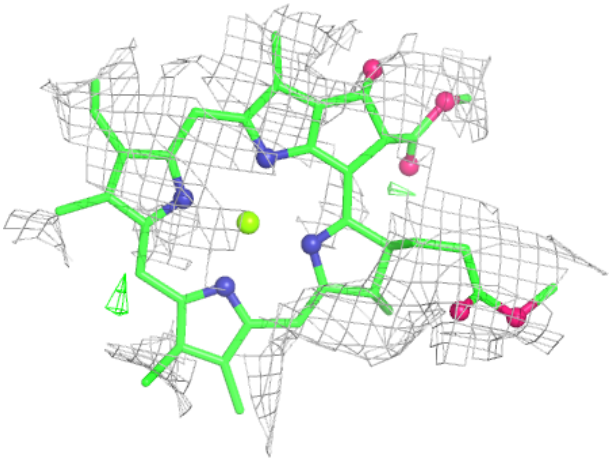


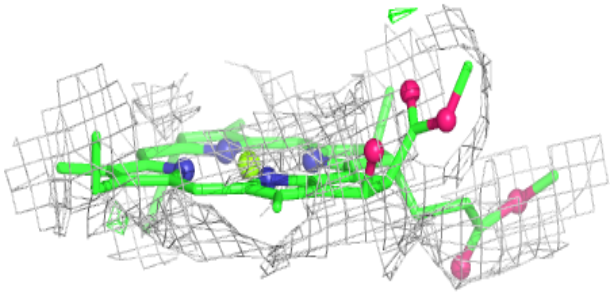


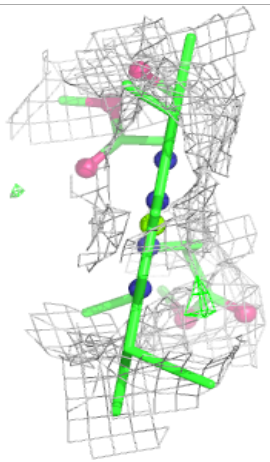


**Electron density around CLA K 101:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

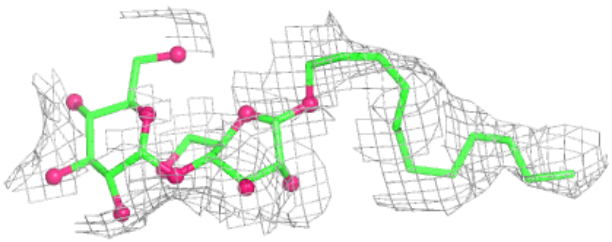


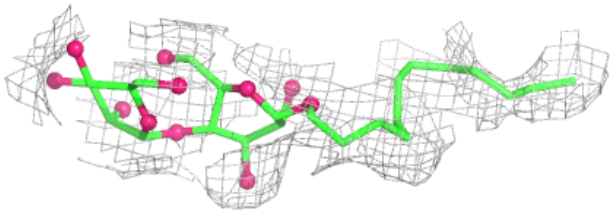


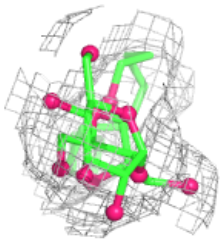


**Electron density around LMU R 102:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

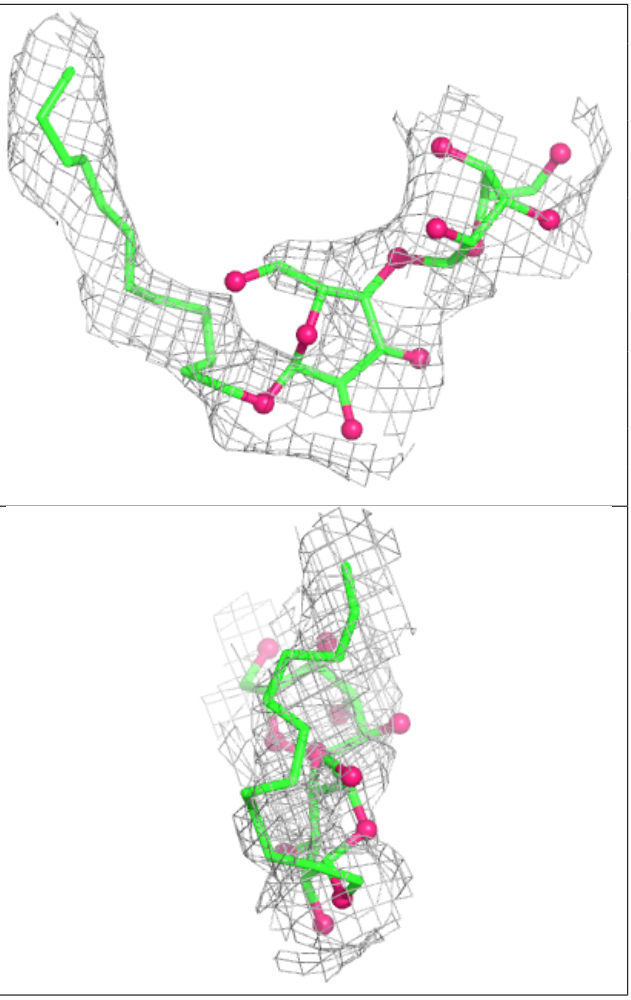






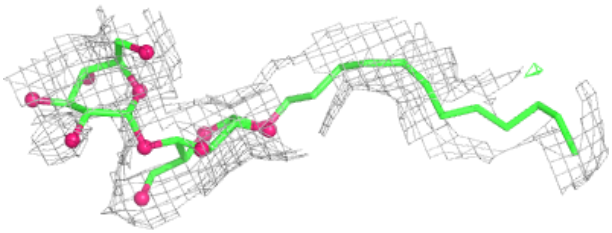
**Electron density around LMU R 103:**

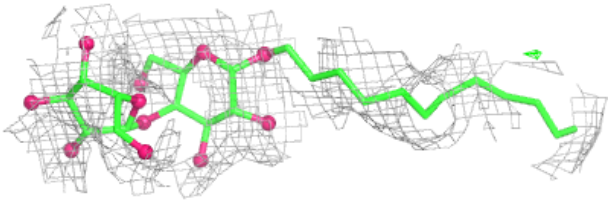
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

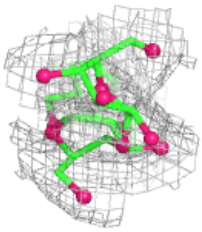


**Electron density around LMU H 103:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

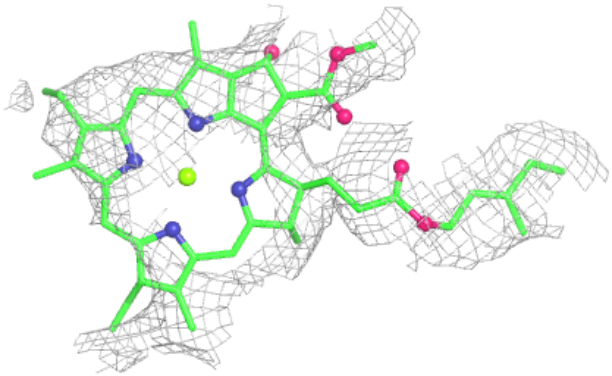


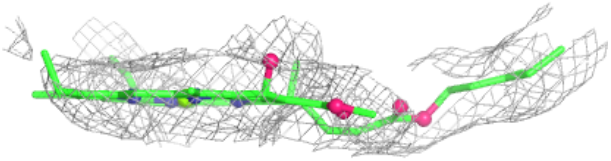


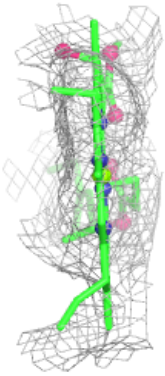


**Electron density around CLA 1 215:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

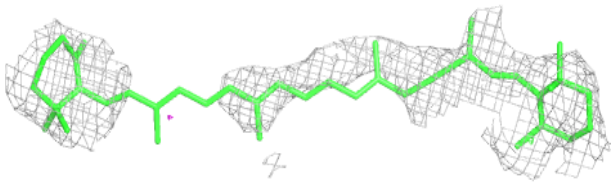


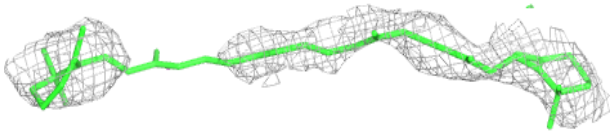


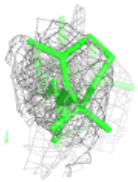


**Electron density around BCR G 104:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

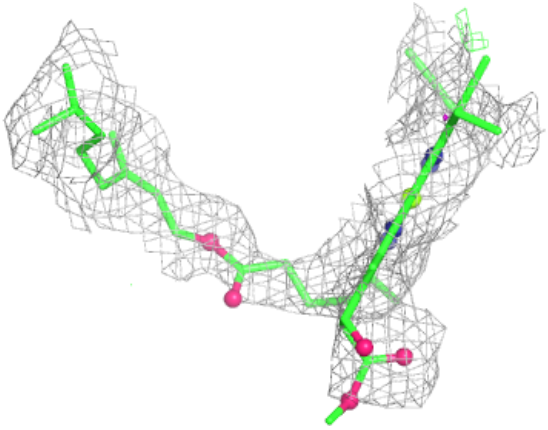


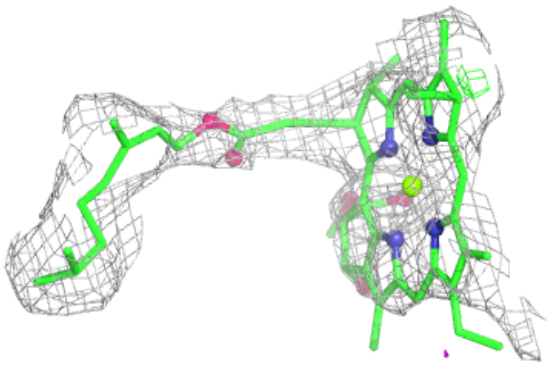


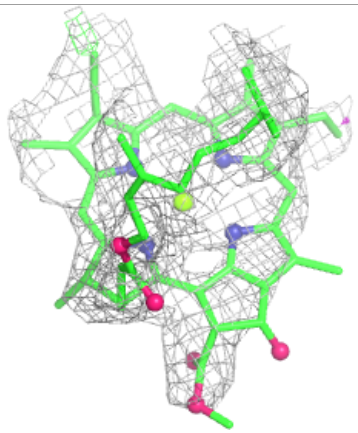


**Electron density around CLA L 204:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

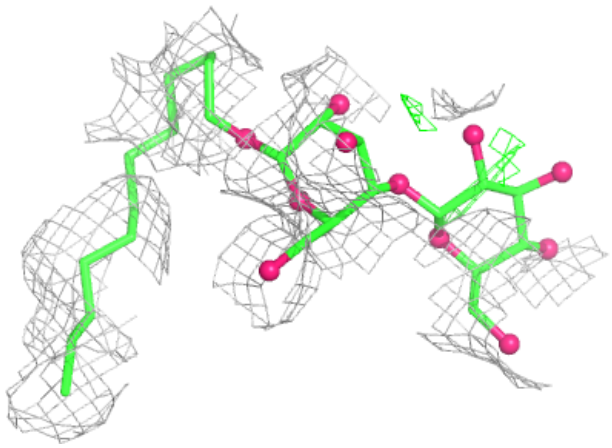


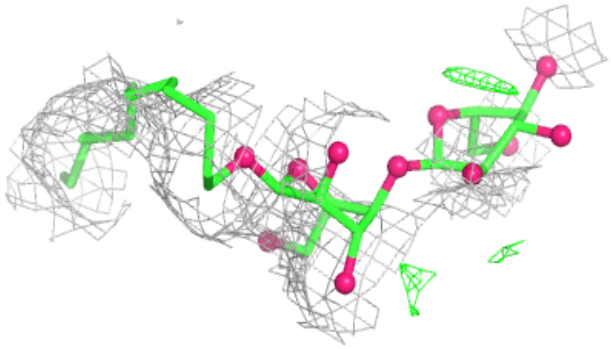




**Electron density around LMU A 848:**

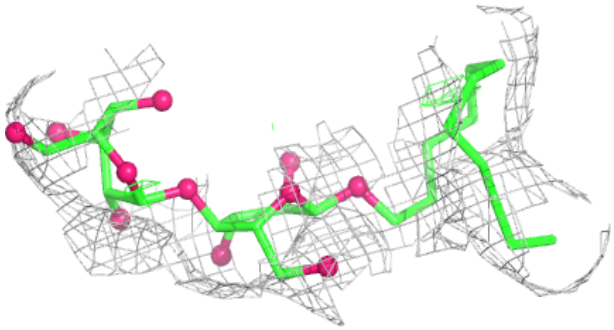
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

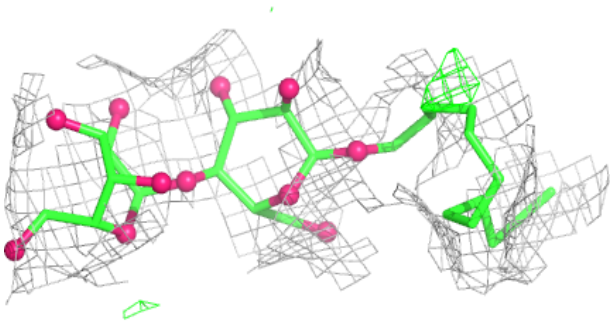


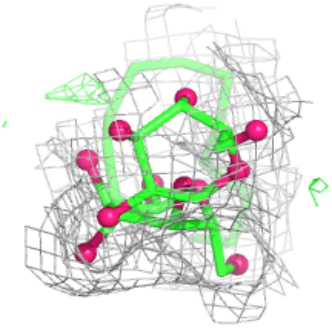


**Electron density around LMU A 854:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

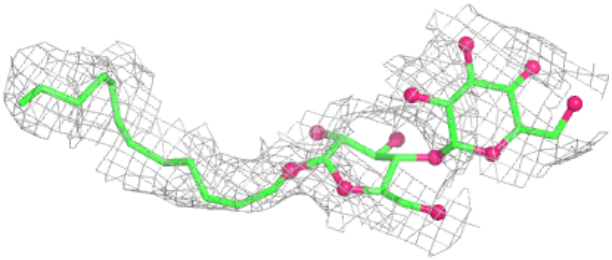


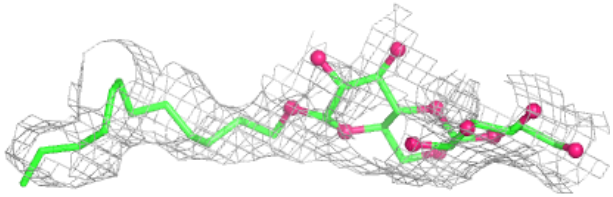


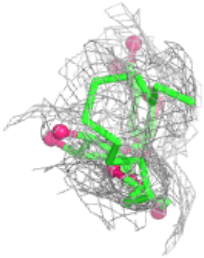


**Electron density around LMU B 804:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

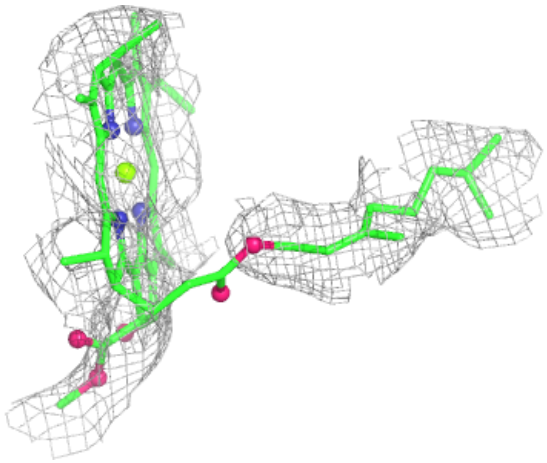


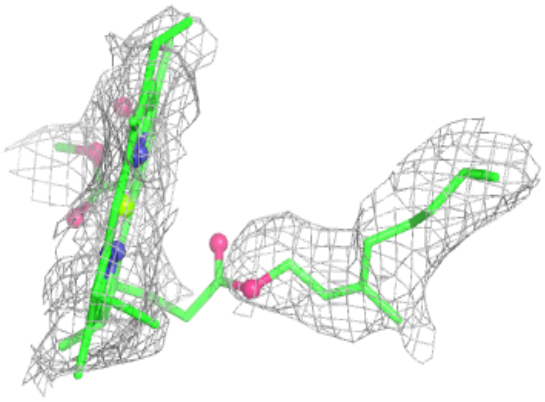


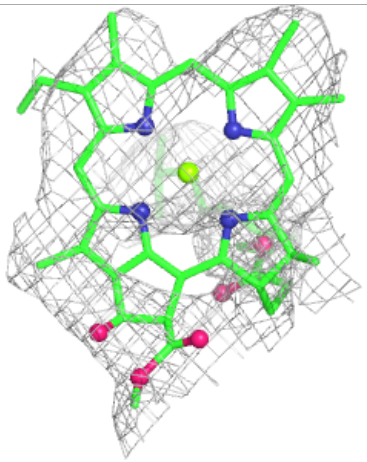


**Electron density around CLA 4 301:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

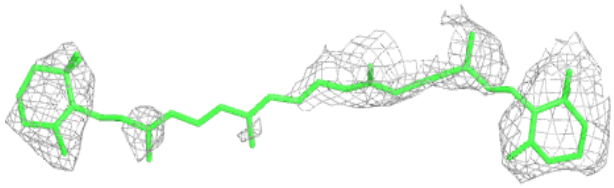


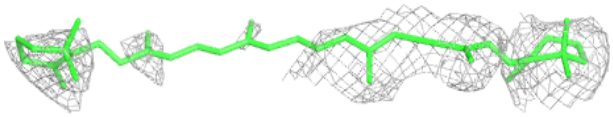


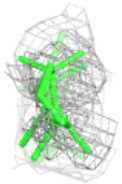


**Electron density around BCR L 209:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

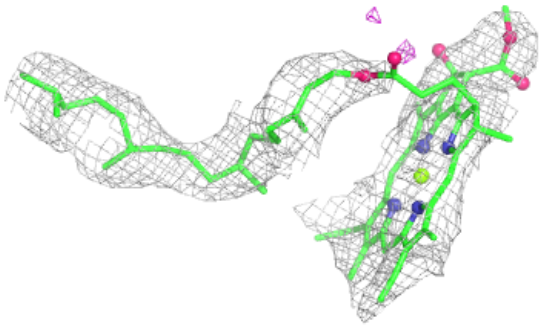


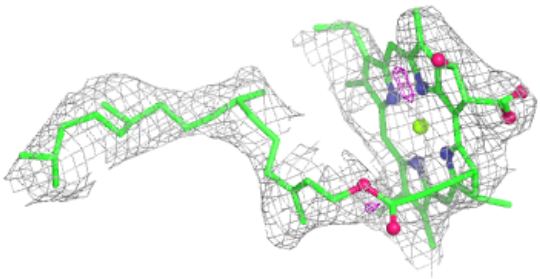


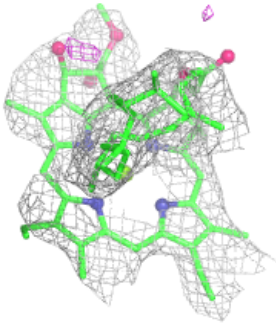


**Electron density around CLA A 811:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

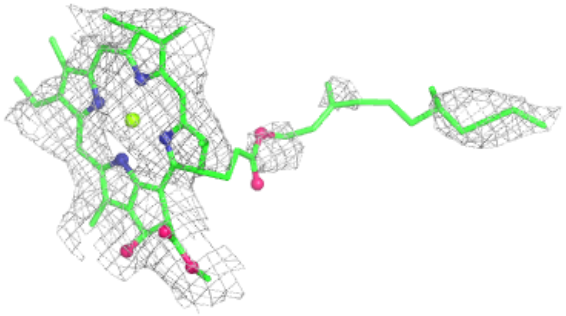


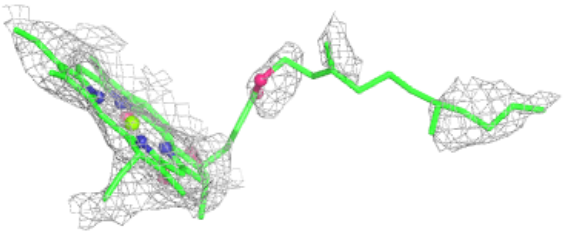


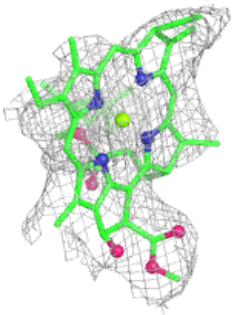


**Electron density around CLA A 819:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

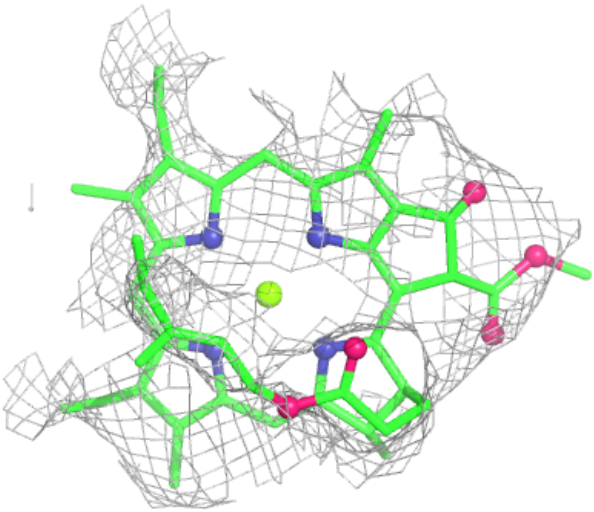


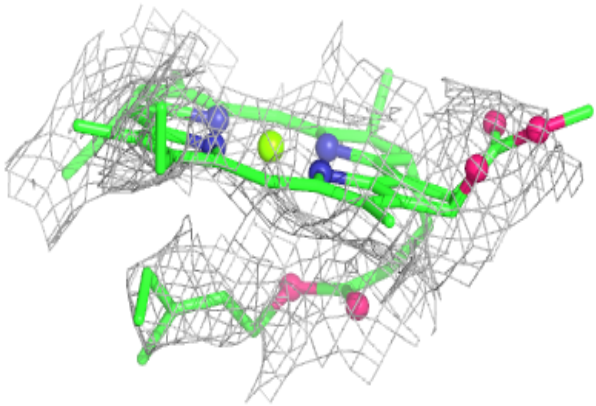


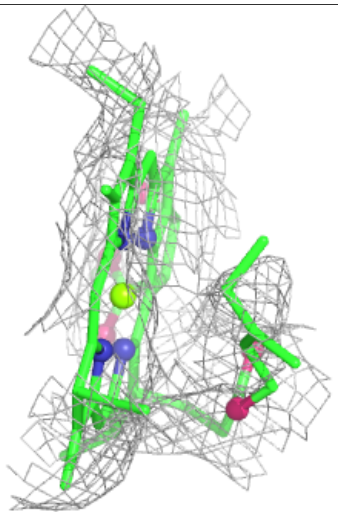


**Electron density around CLA A 820:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

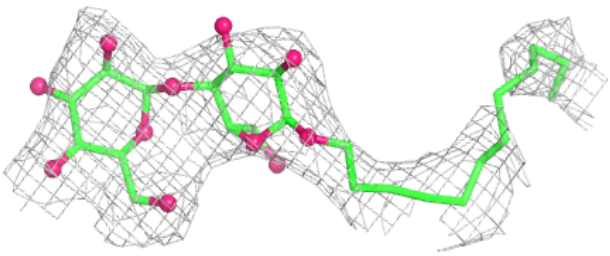


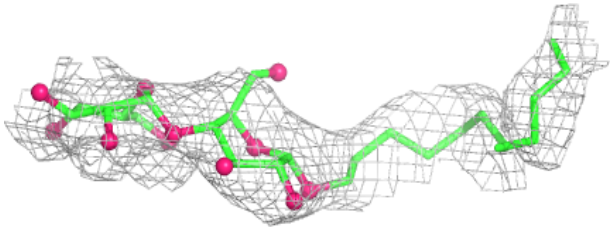


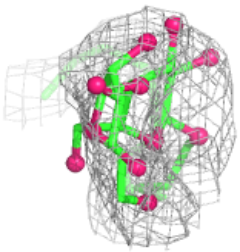


**Electron density around LMU C 101:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

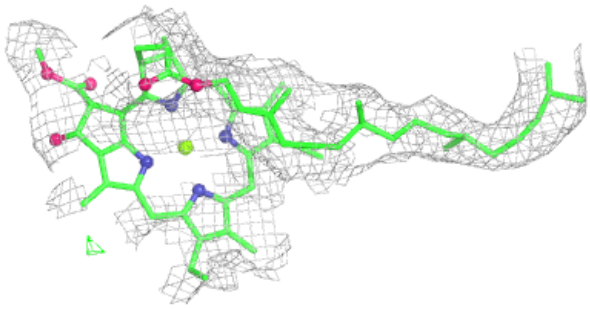


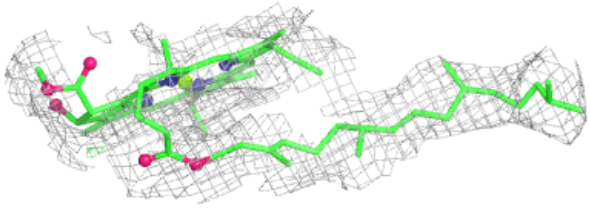


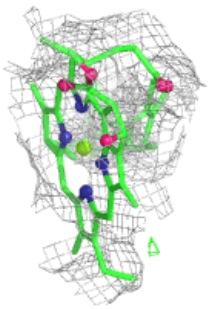


**Electron density around CLA 2 307:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

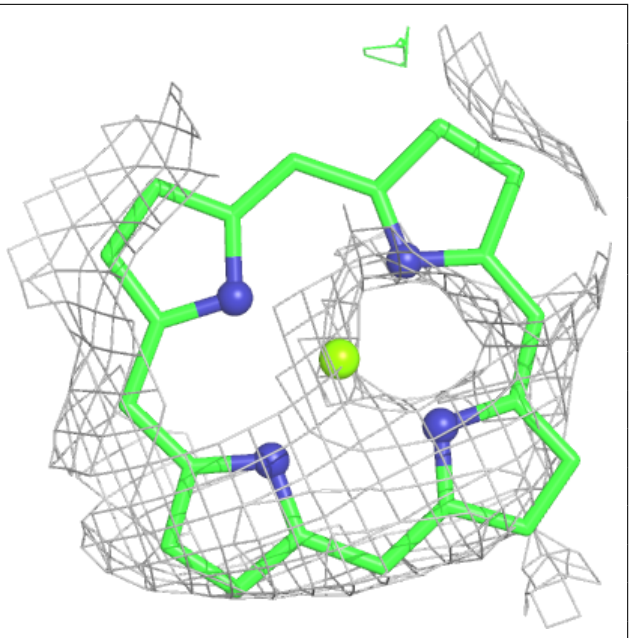


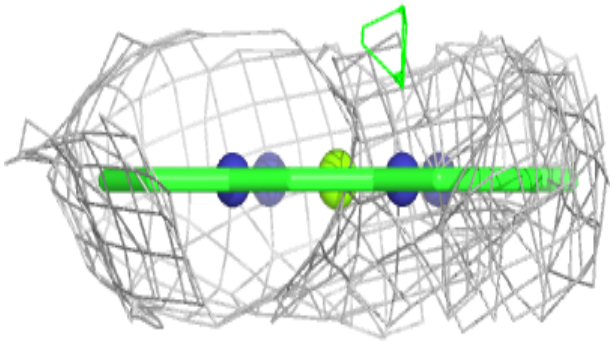


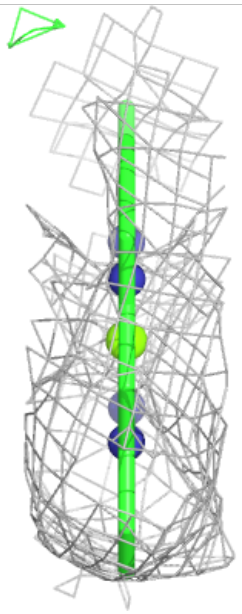


**Electron density around CLA 3 306:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

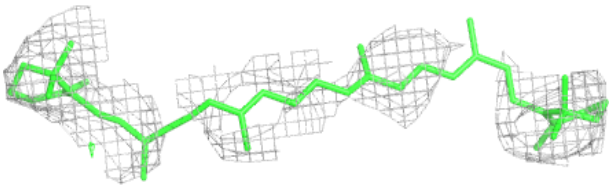


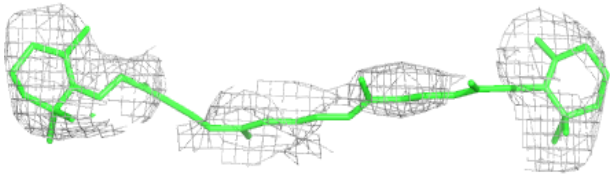


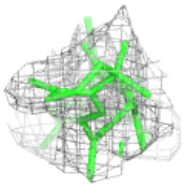


**Electron density around BCR A 844:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

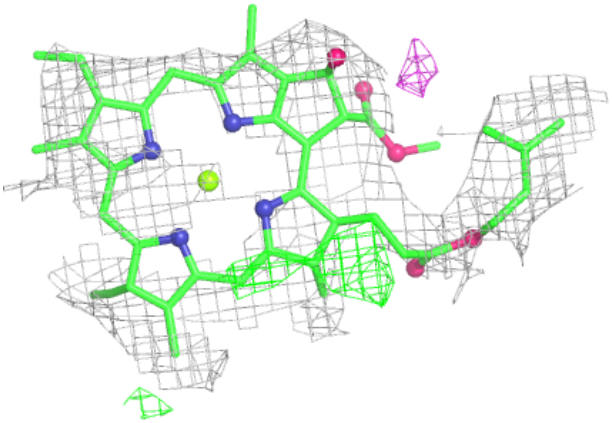


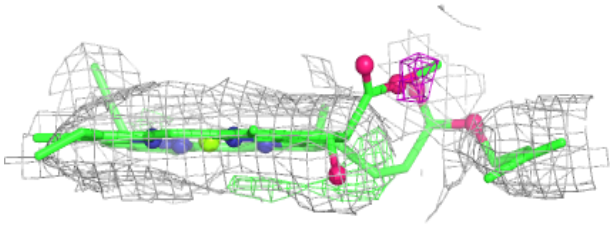


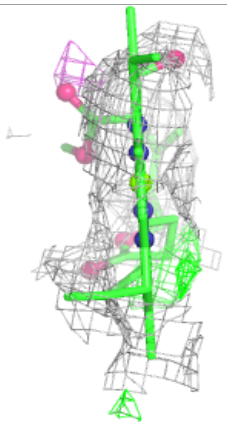


**Electron density around CLA 2 311:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

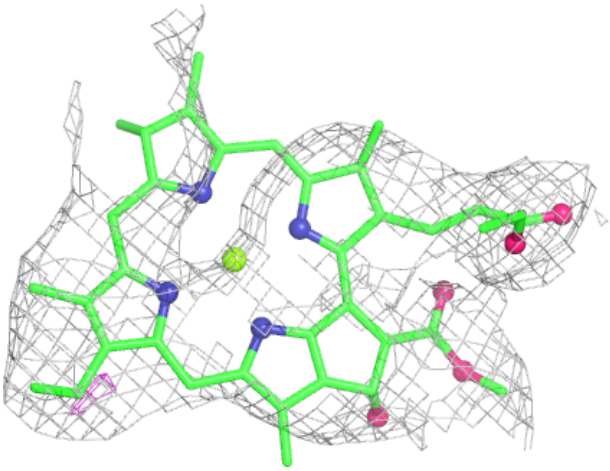


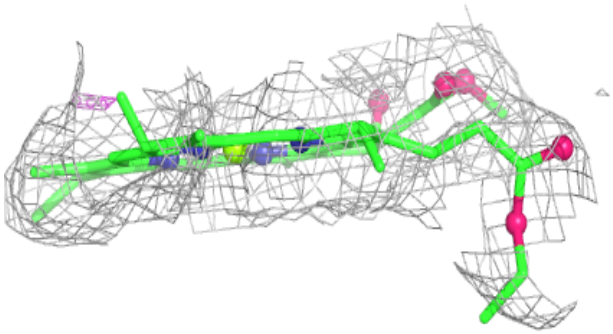


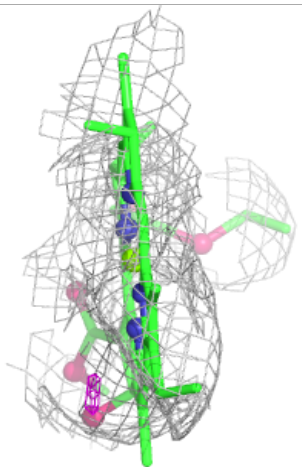


**Electron density around CLA A 801:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

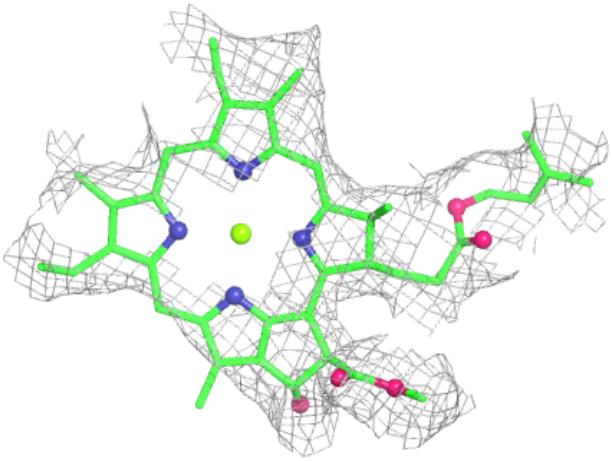


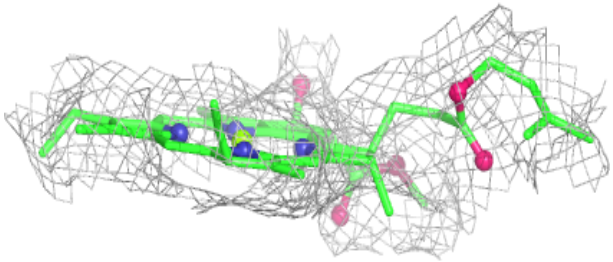


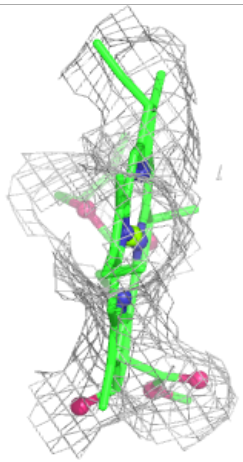


**Electron density around CLA 2 305:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

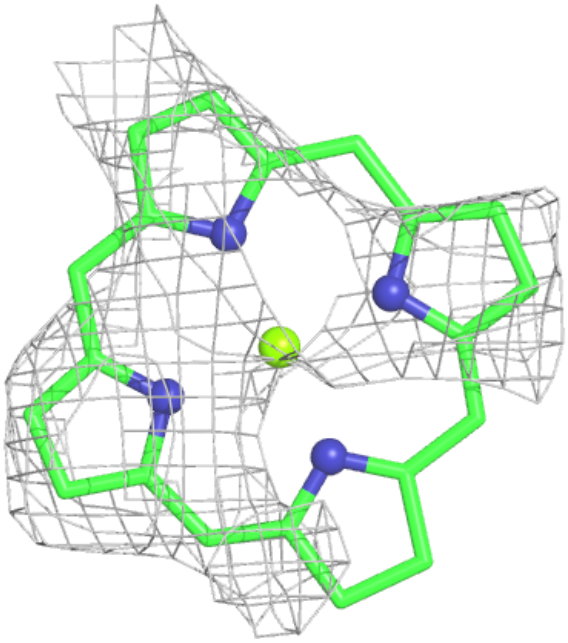


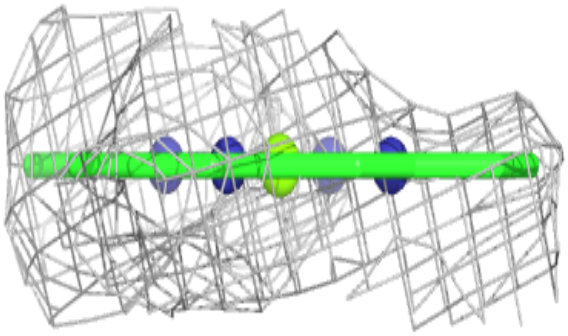


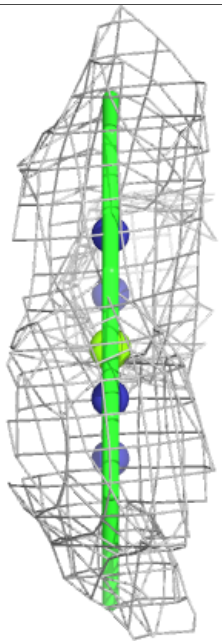


**Electron density around CLA 2 301:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

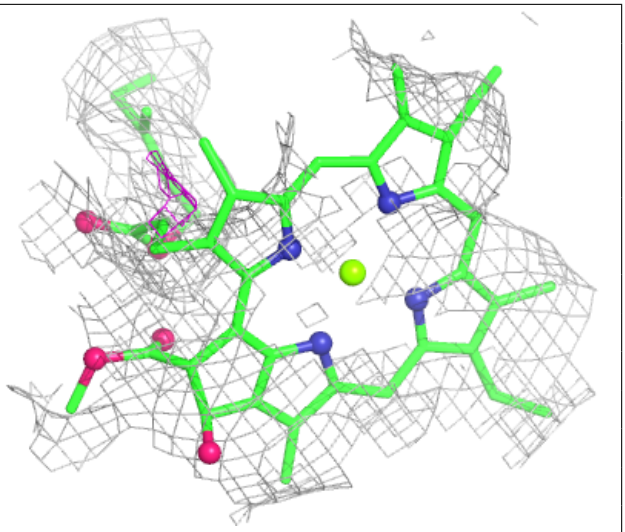


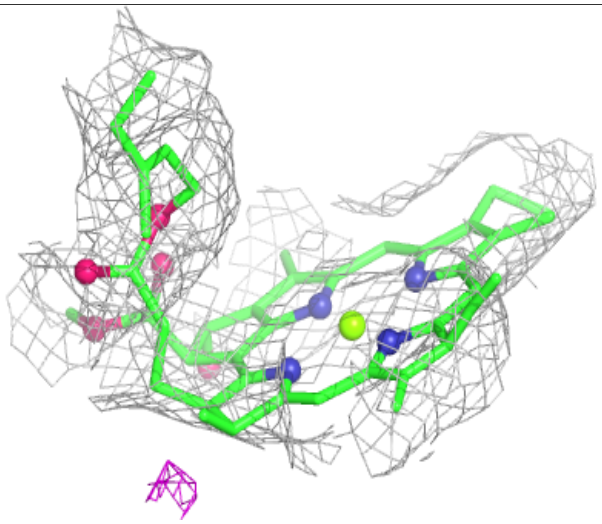




**Electron density around CLA 1 207:**

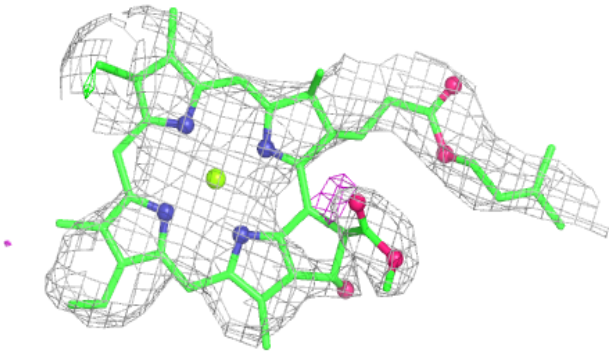
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

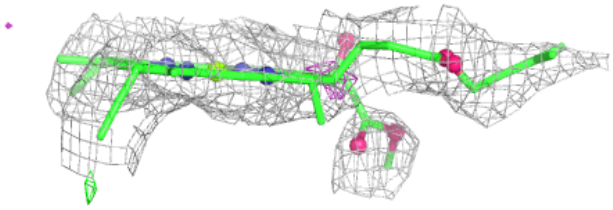


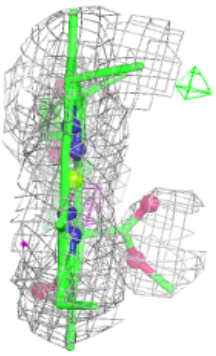


**Electron density around CLA 4 305:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

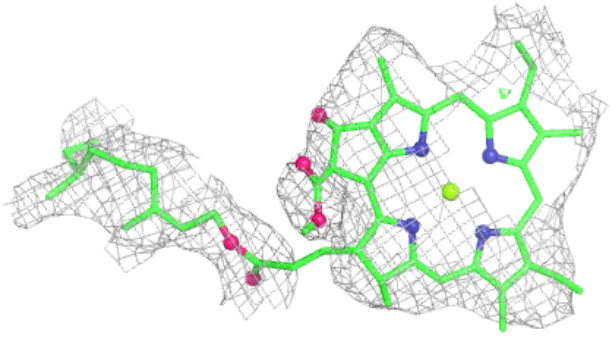


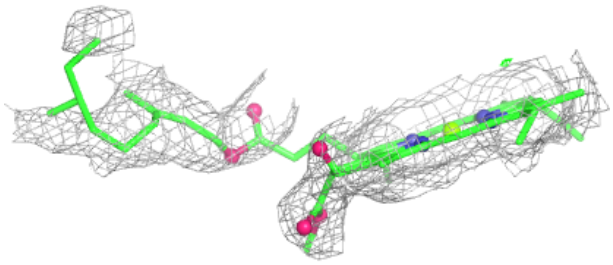


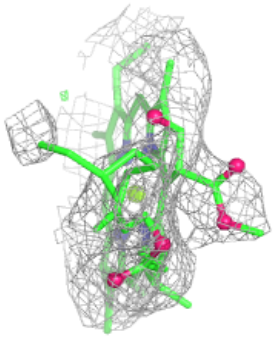


**Electron density around CLA K 104:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

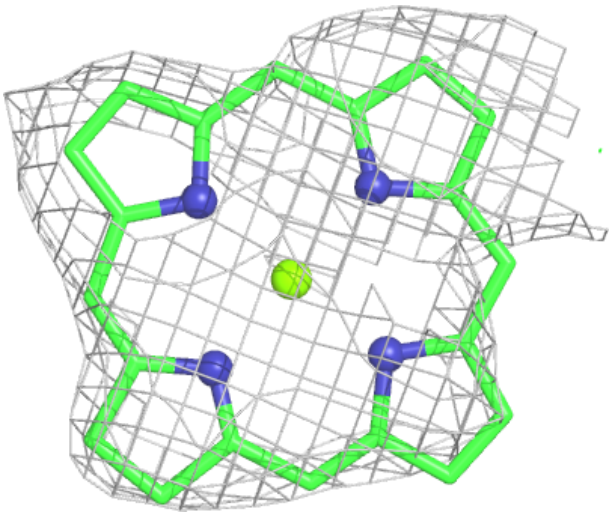


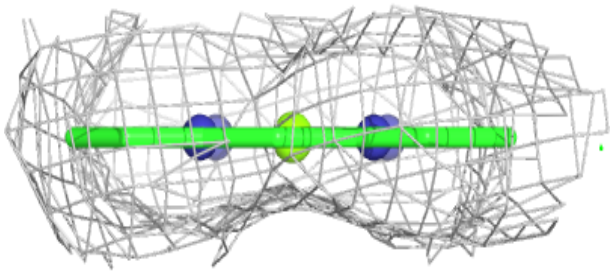


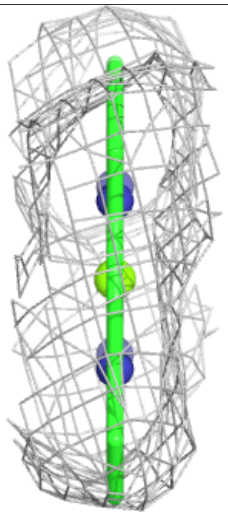


**Electron density around CLA 1 209:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

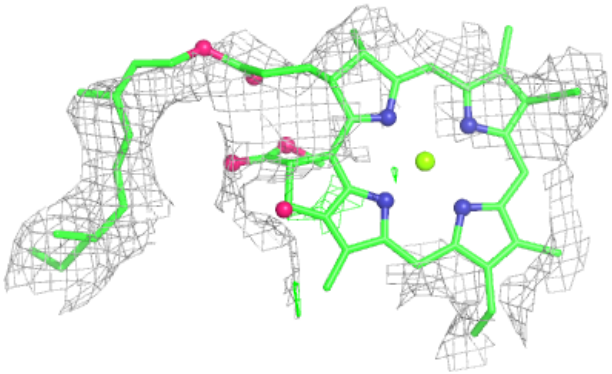


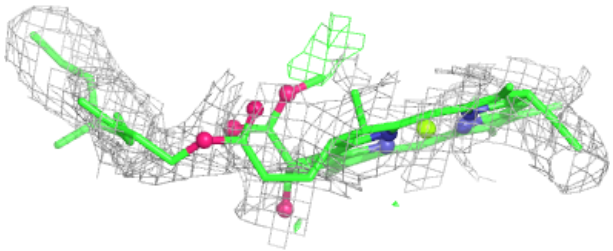




**Electron density around CLA R 107:**

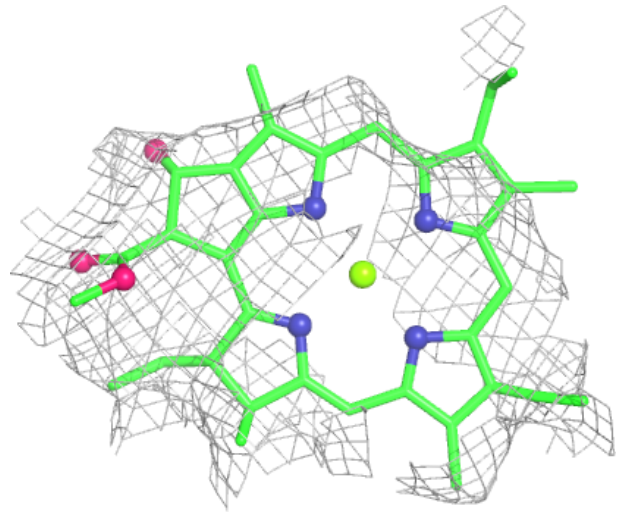
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

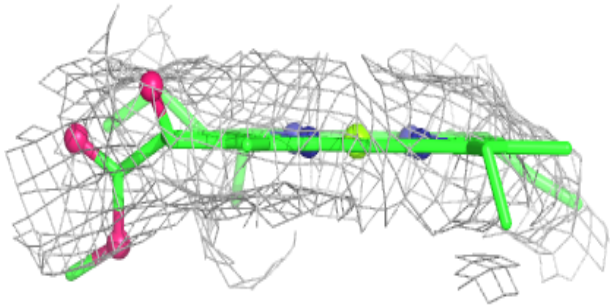


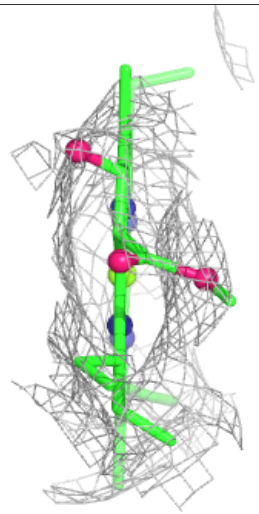


**Electron density around CLA A 821:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

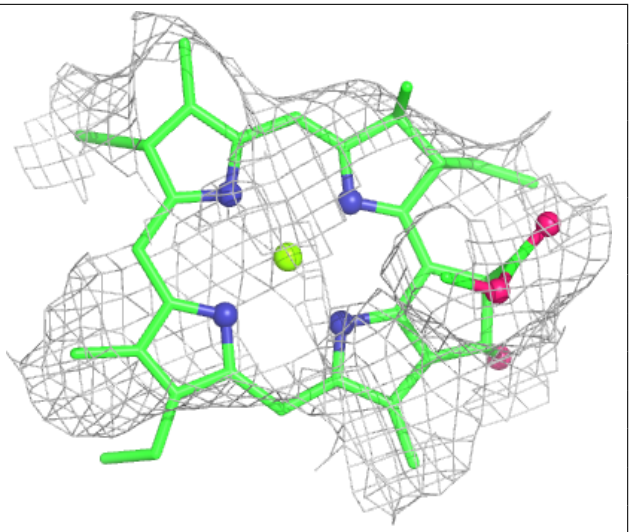


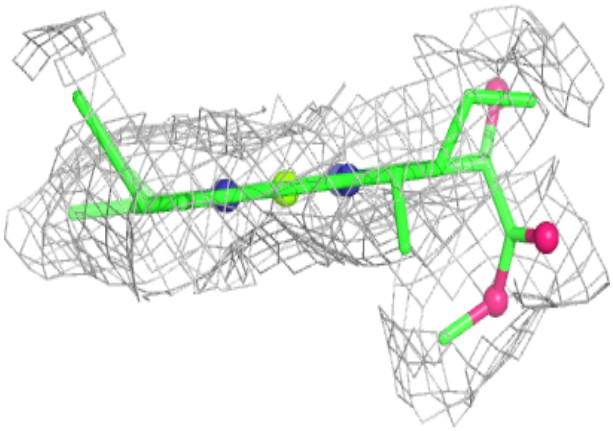


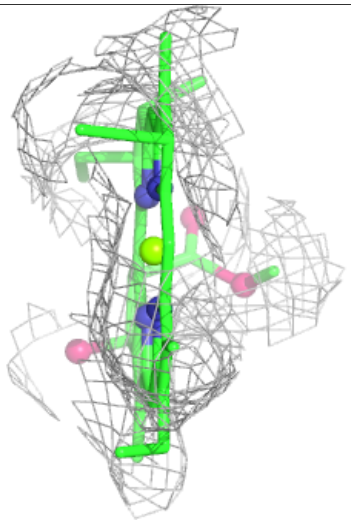


**Electron density around CLA 3 307:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

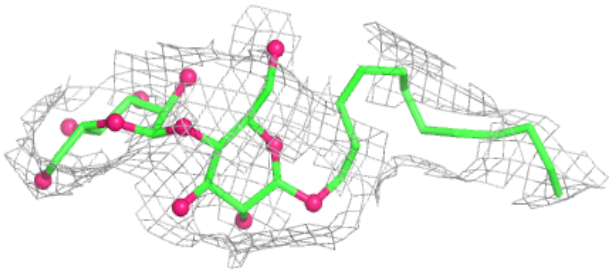


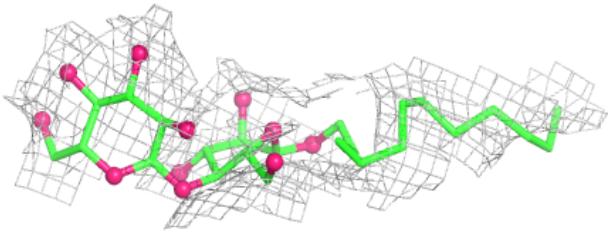


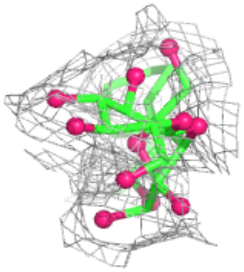


**Electron density around LMU K 107:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

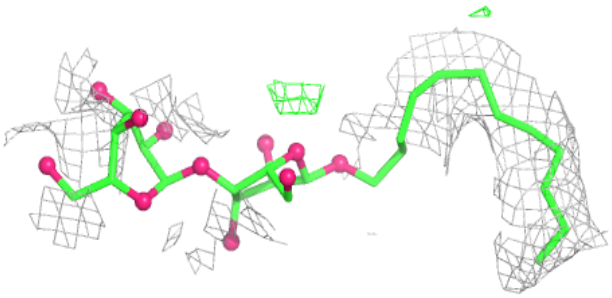


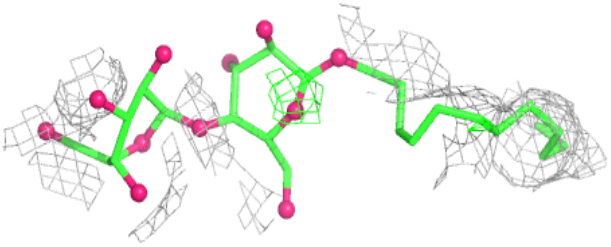


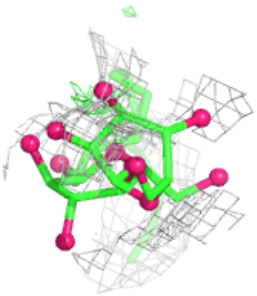


**Electron density around LMU A 846:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

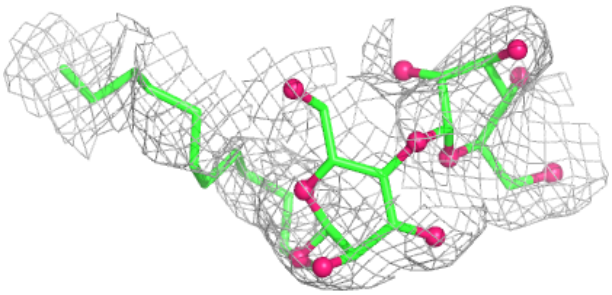


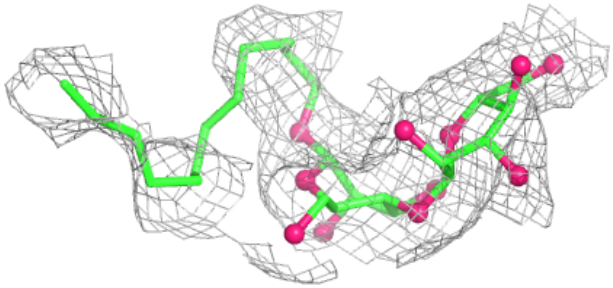


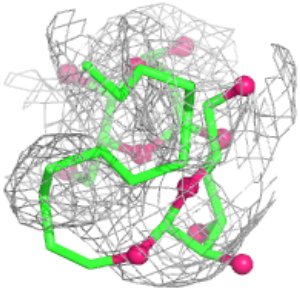


**Electron density around LMU L 210:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

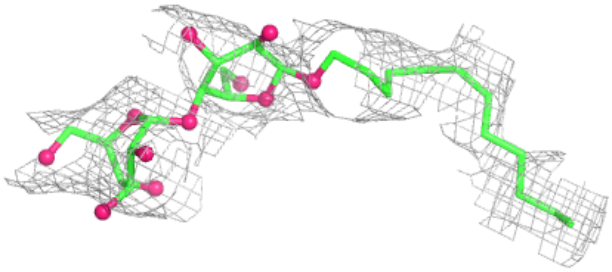


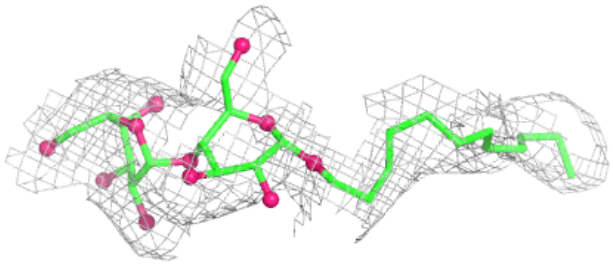


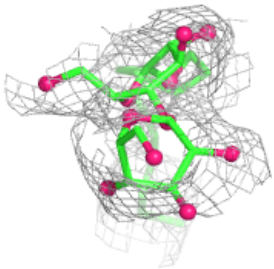


**Electron density around LMU 2 319:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

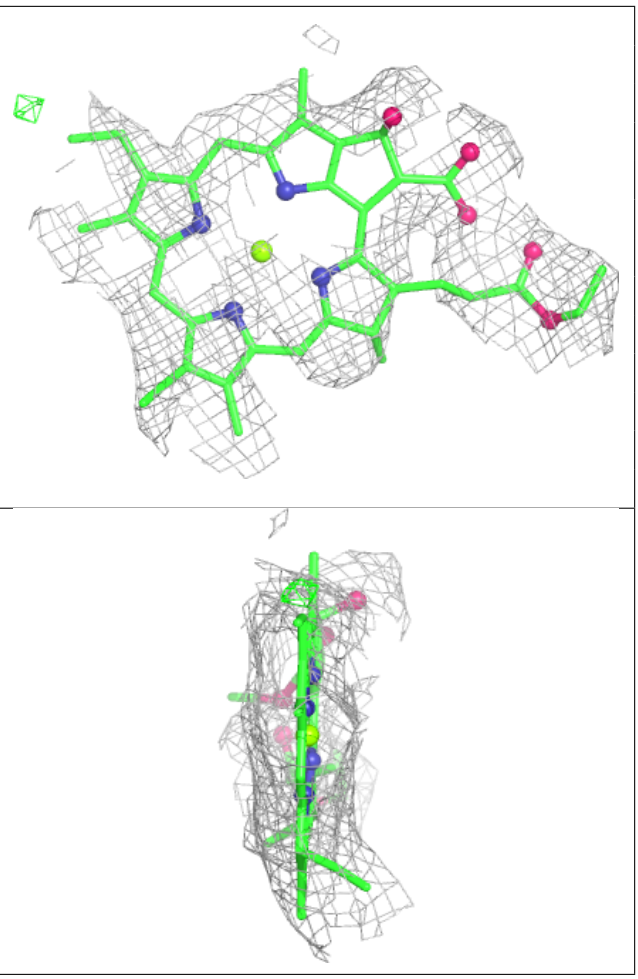






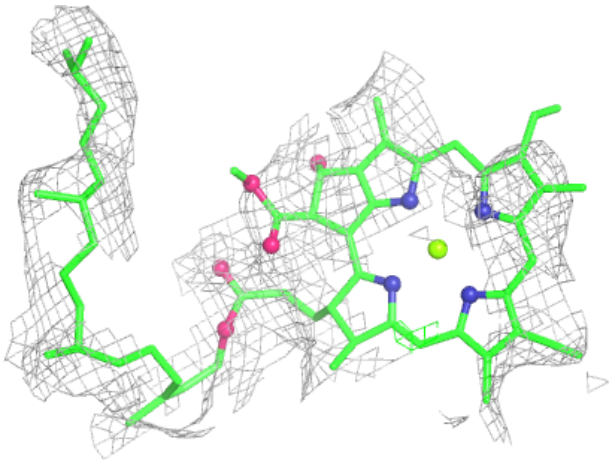
**Electron density around CLA 4 318:**

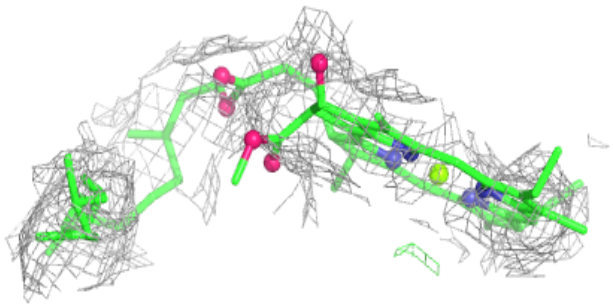
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

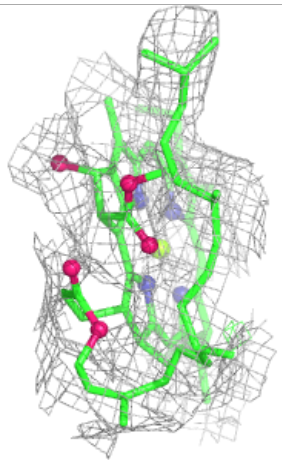


**Electron density around CLA R 108:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

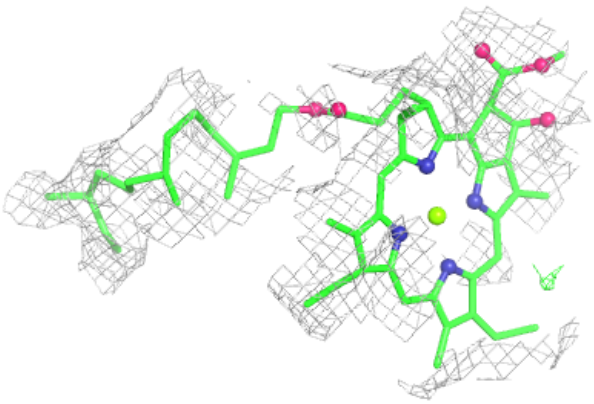


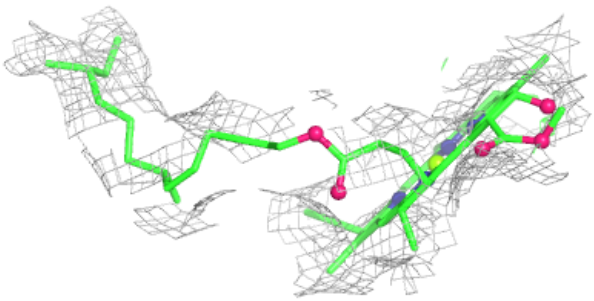


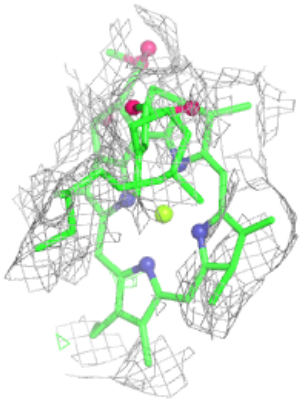


**Electron density around CLA 2 312:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

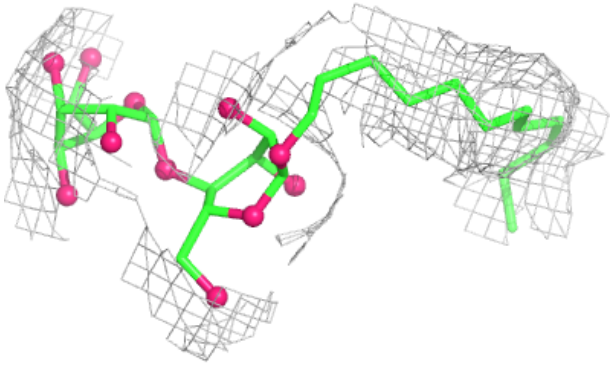


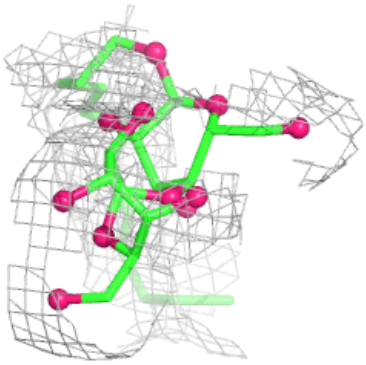




**Electron density around LMU R 104:**

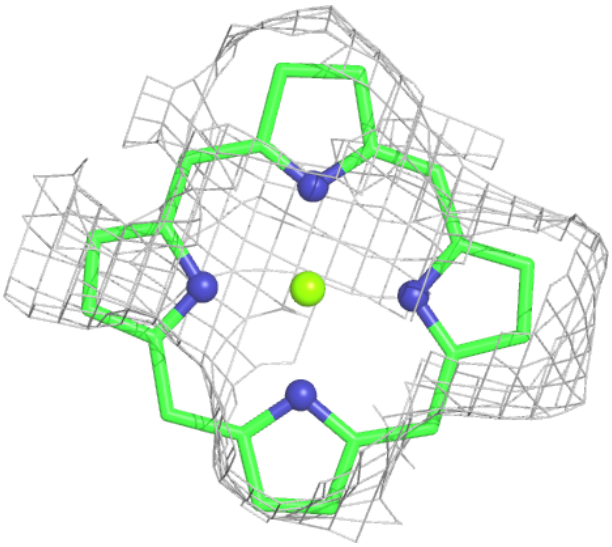
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

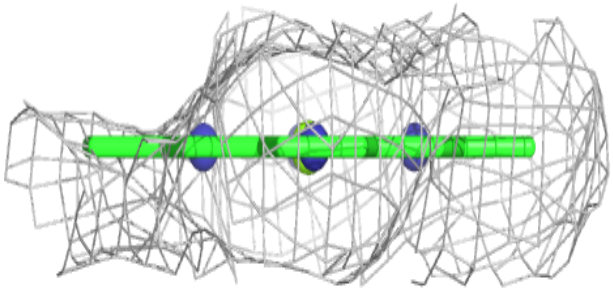


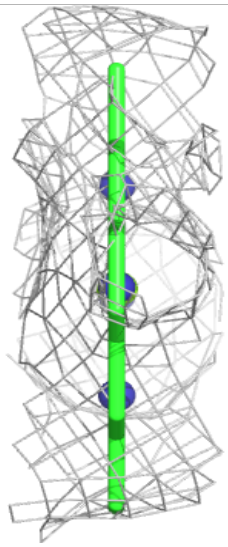


**Electron density around CLA 3 302:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

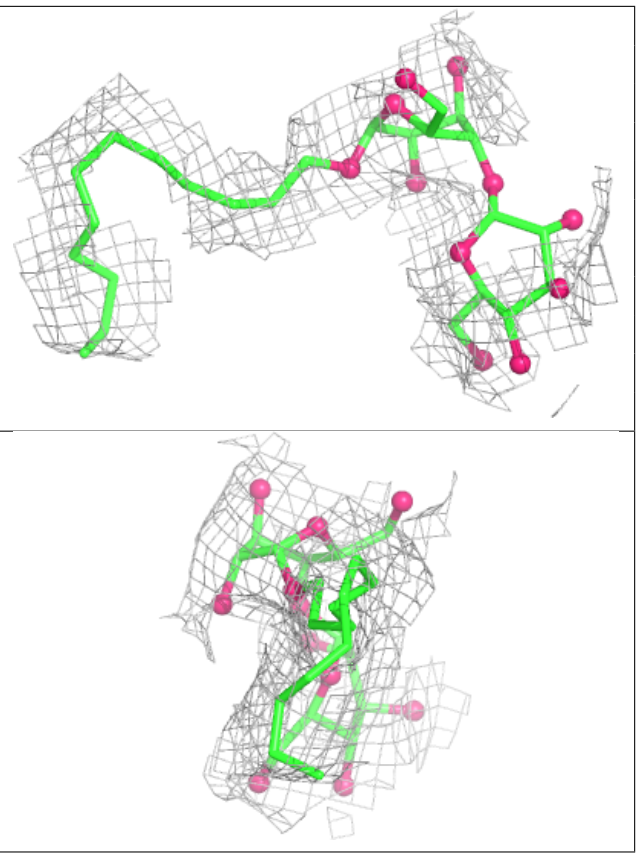


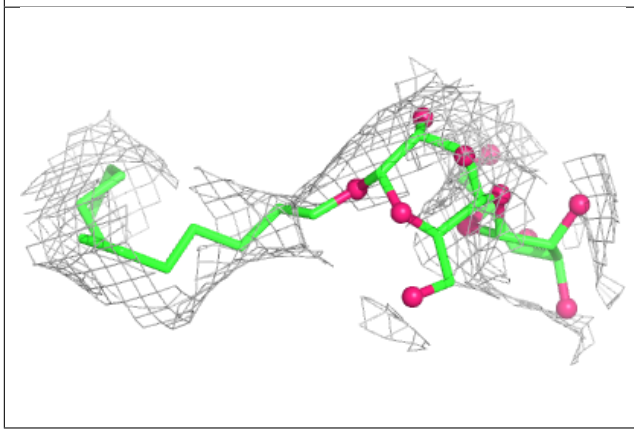




**Electron density around LMU K 105:**

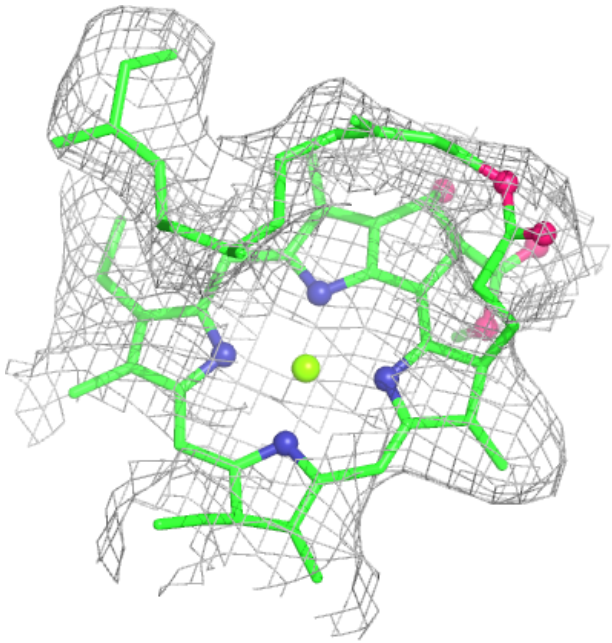
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

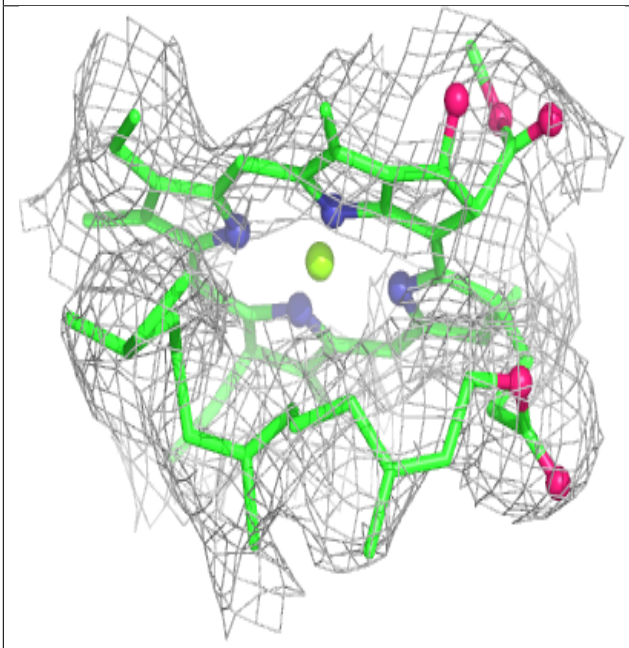


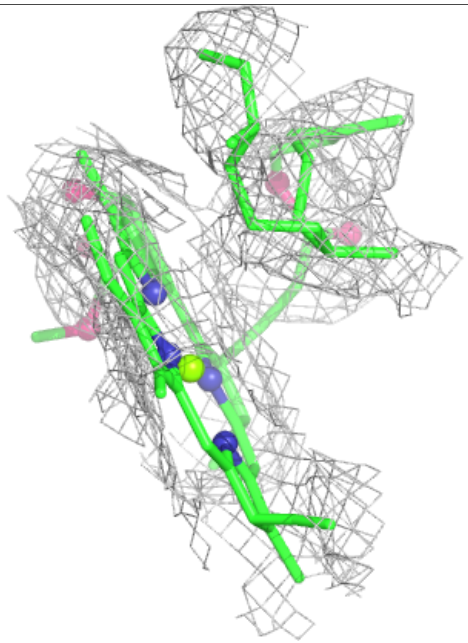


**Electron density around CLA 1 206:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

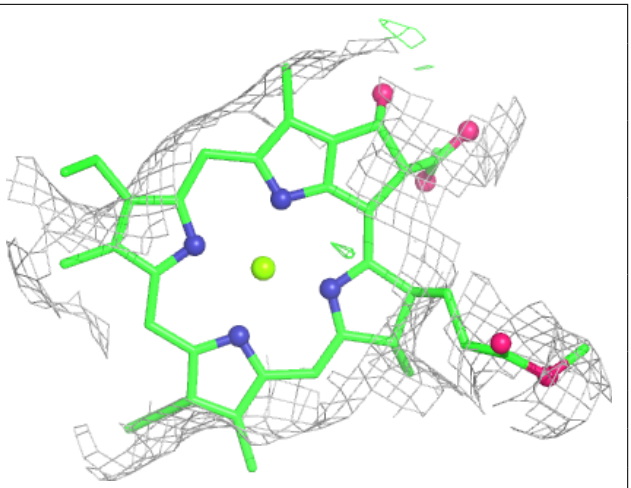


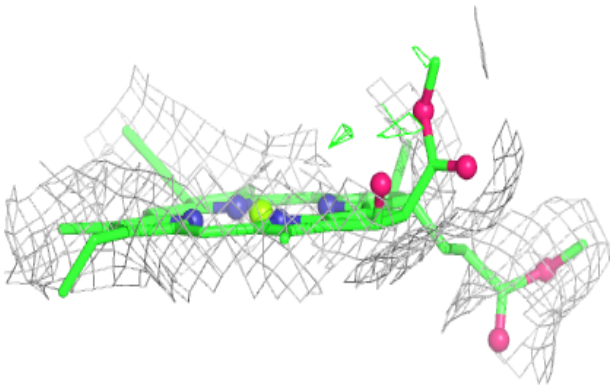


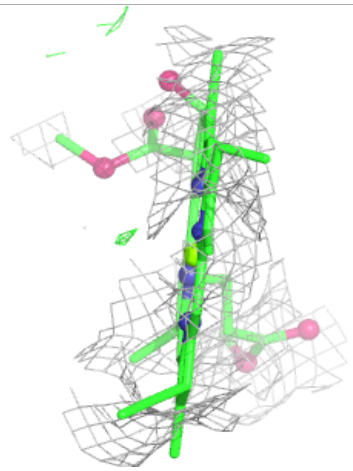


**Electron density around CLA 1 201:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

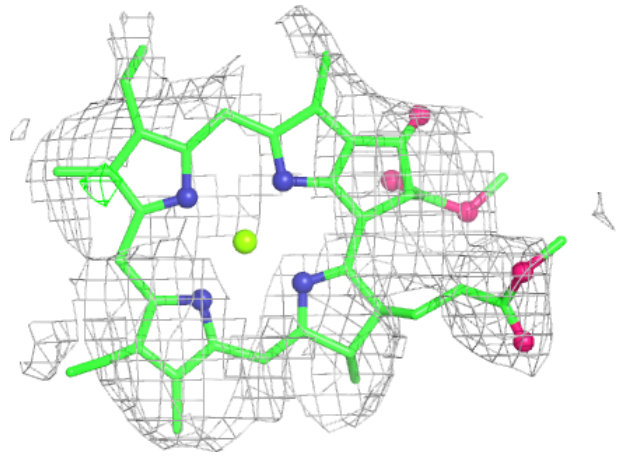


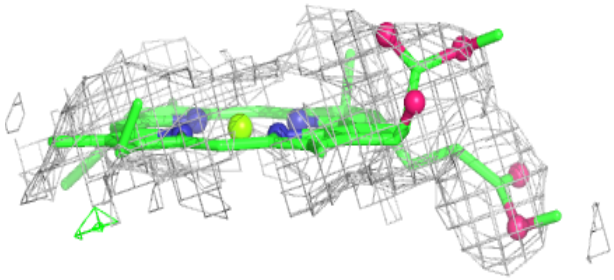


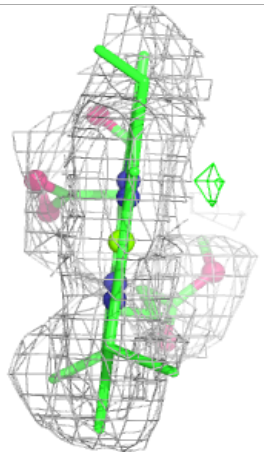


**Electron density around CLA 4 315:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

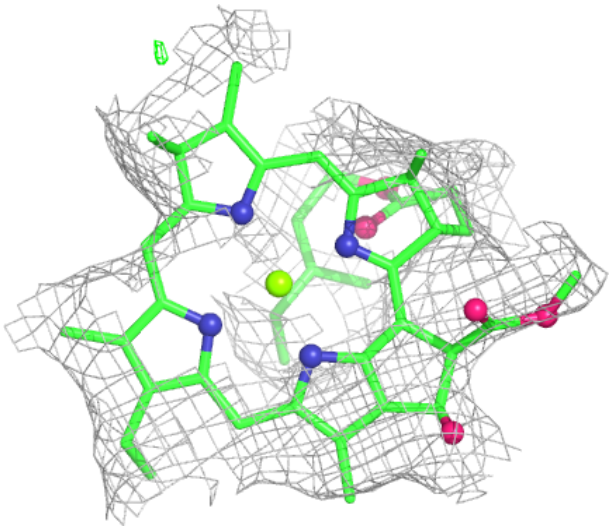


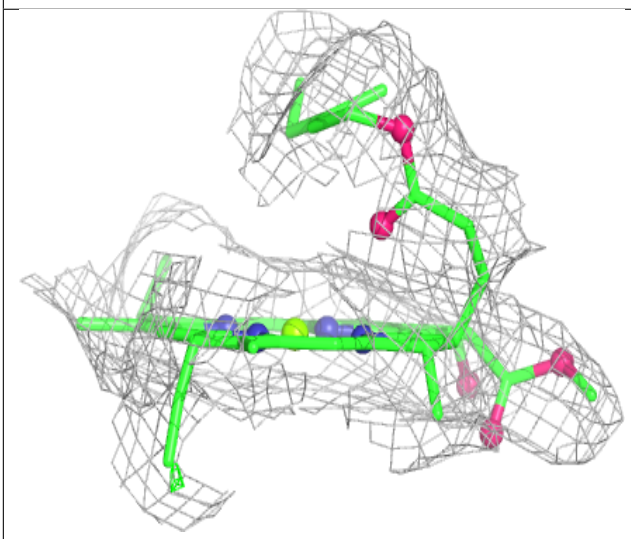


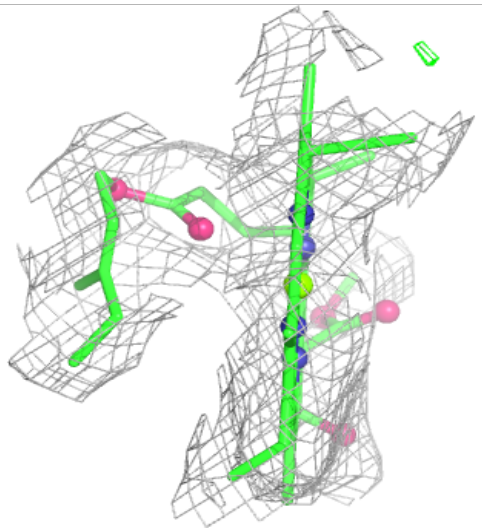


**Electron density around CLA 2 302:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

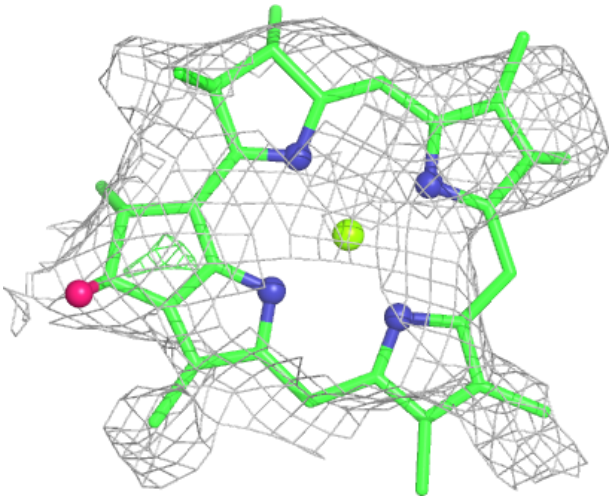


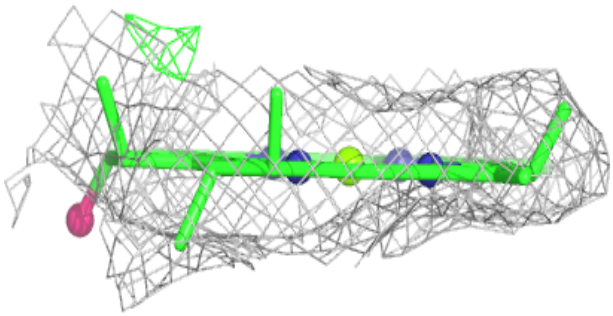


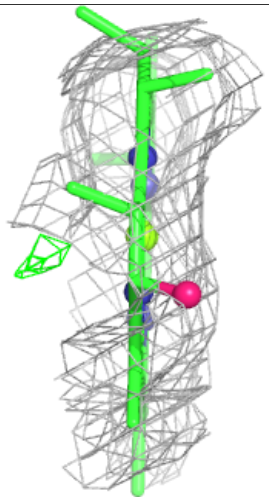


**Electron density around CLA B 842:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

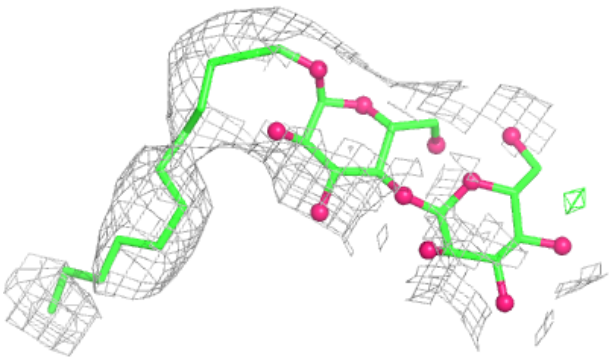


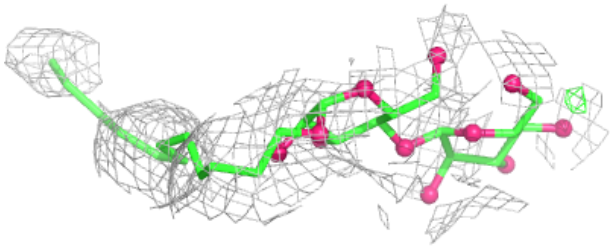


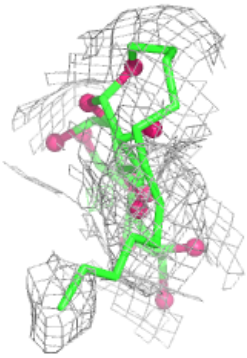


**Electron density around LMU R 106:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

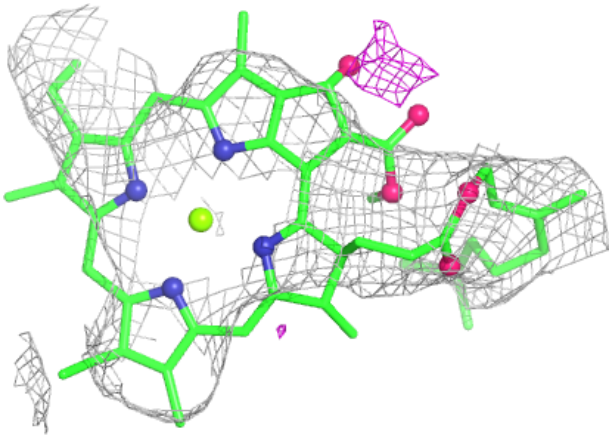


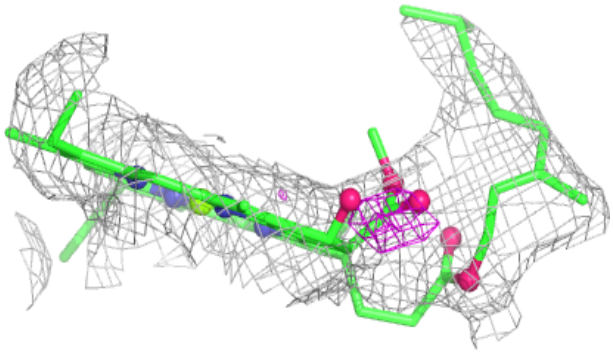


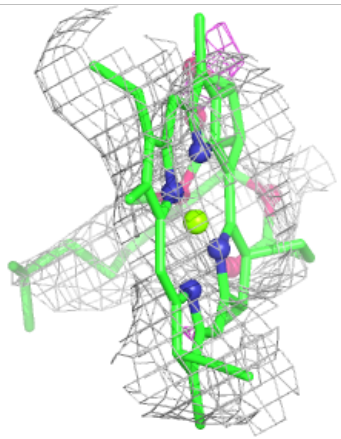


**Electron density around CLA L 202:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

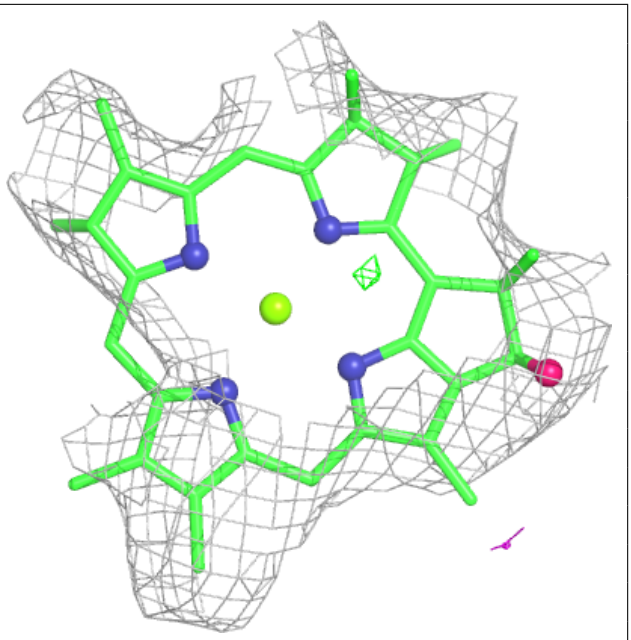


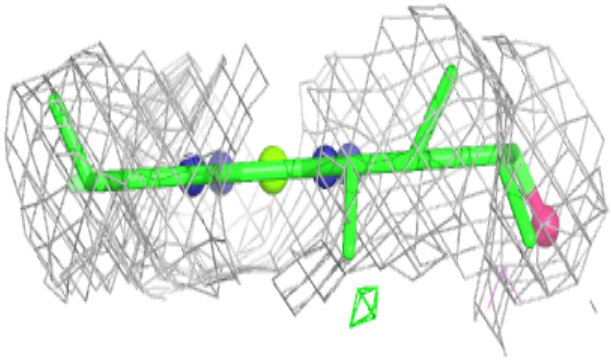


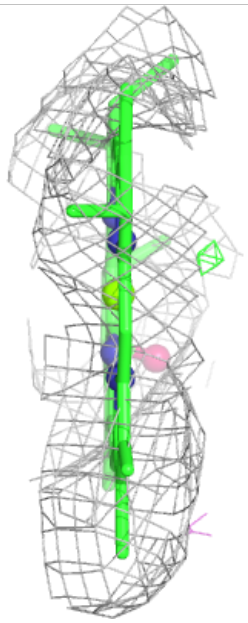


**Electron density around CLA 1 210:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

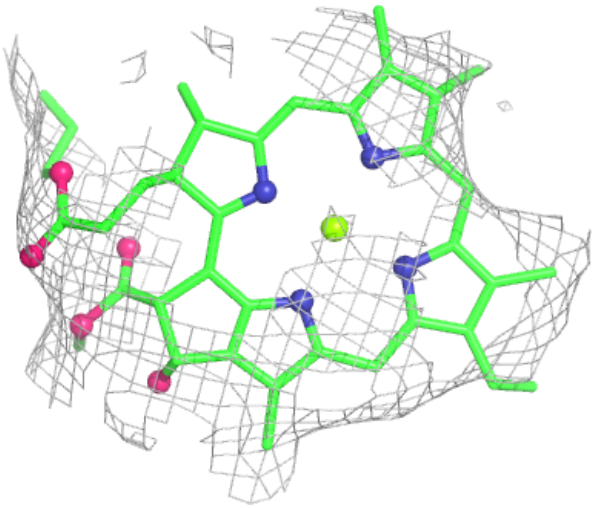


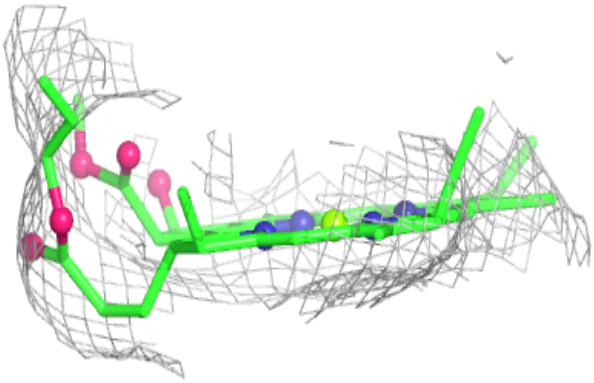




**Electron density around CLA J 101:**

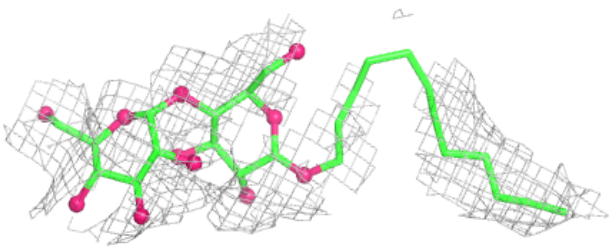
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

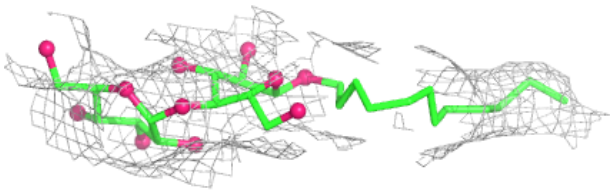


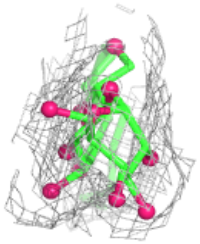


**Electron density around LMU H 104:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

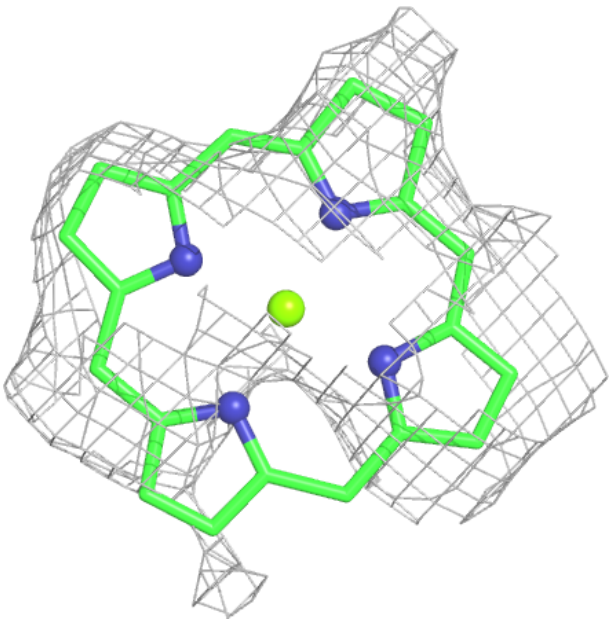


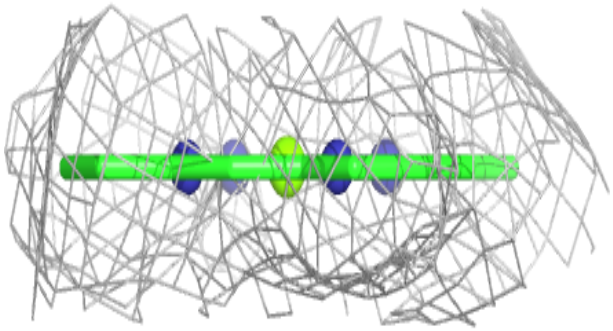


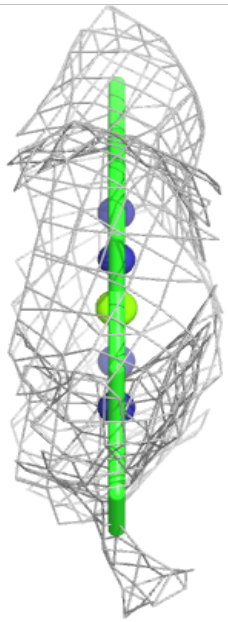


**Electron density around CLA A 841:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

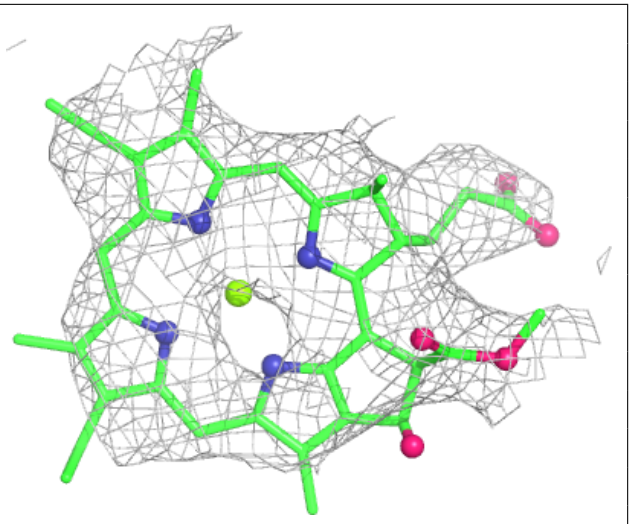


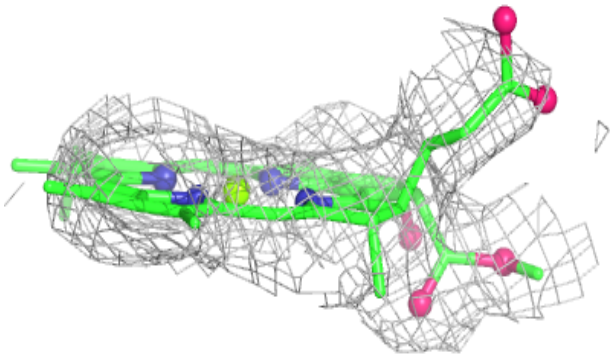


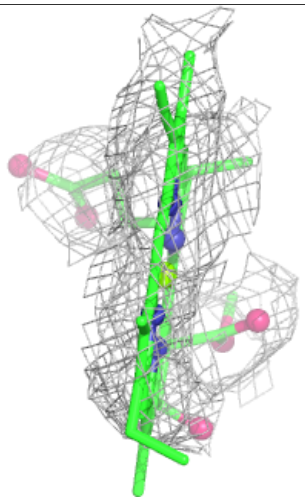


**Electron density around CLA A 810:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

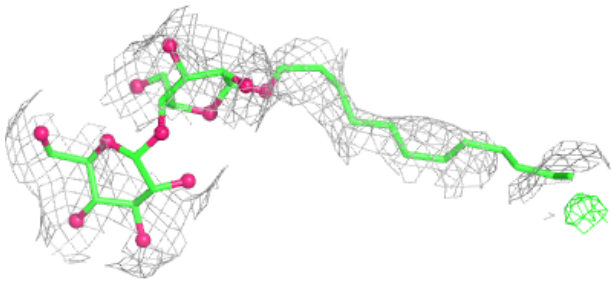


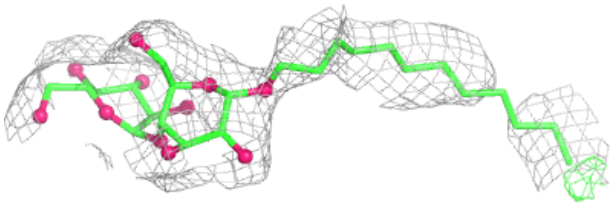


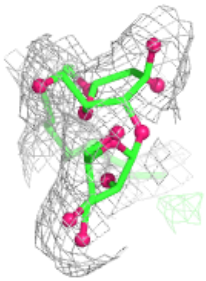


**Electron density around LMU R 105:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

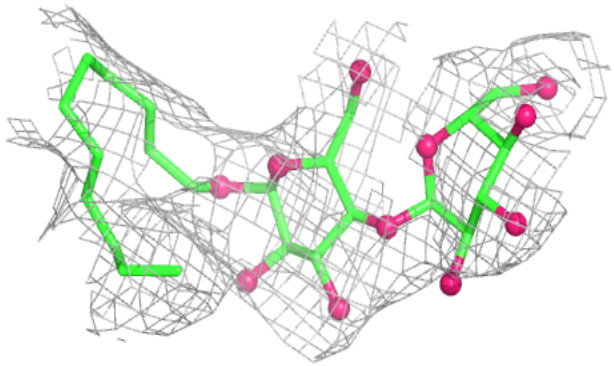


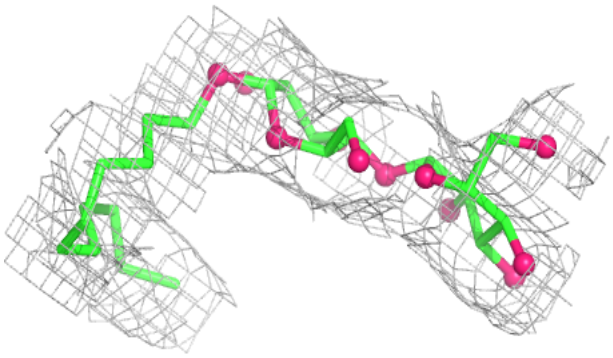


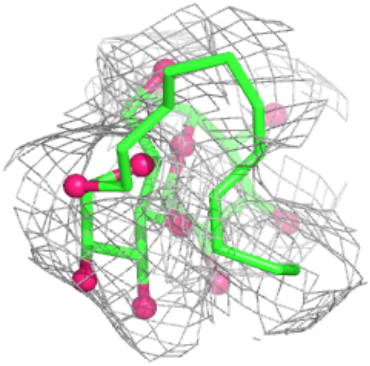


**Electron density around LMU F 202:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

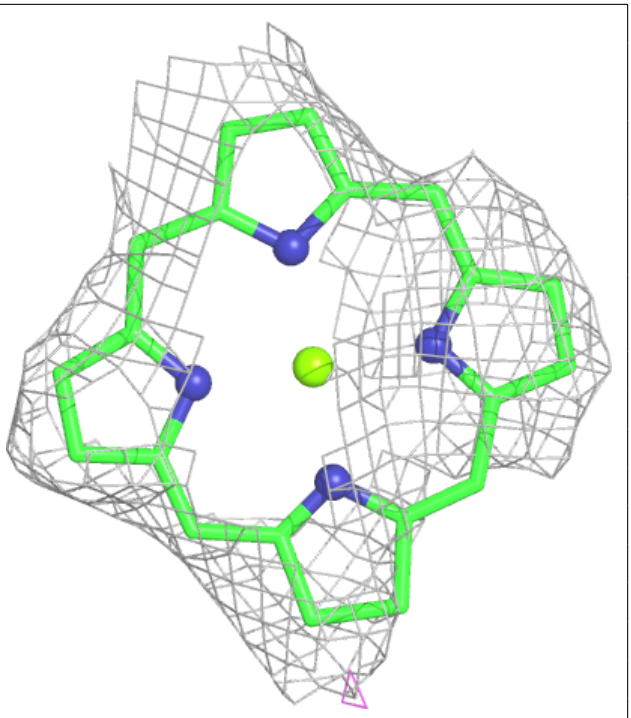


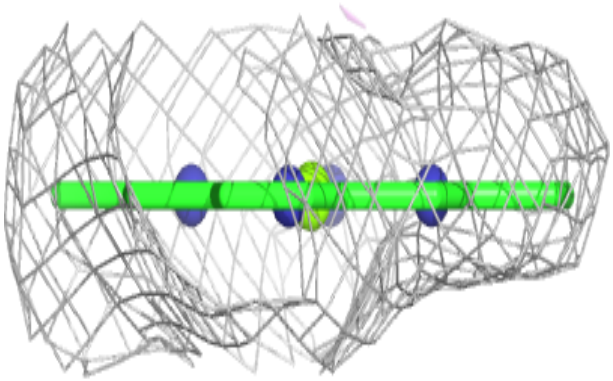


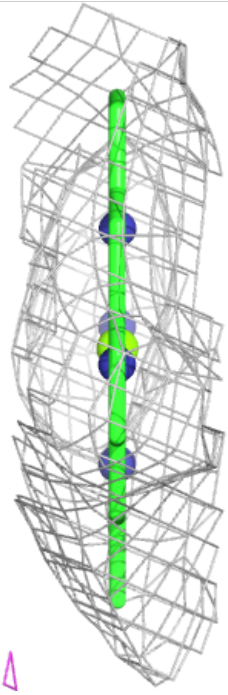


**Electron density around CLA 3 316:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

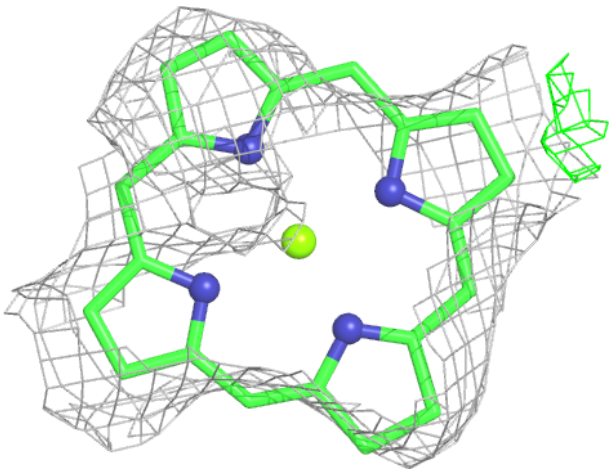


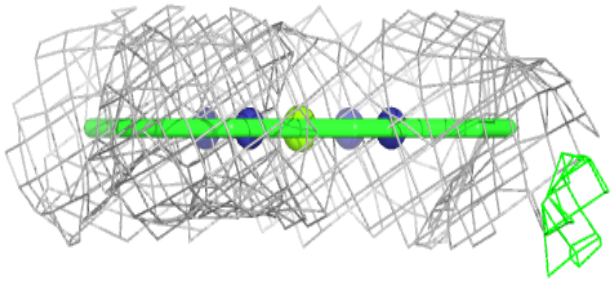


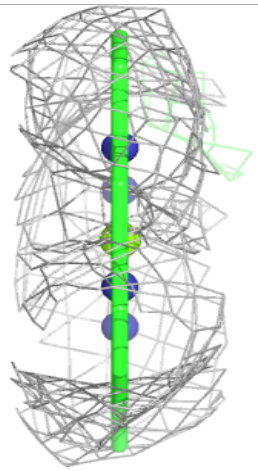


**Electron density around CLA A 814:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

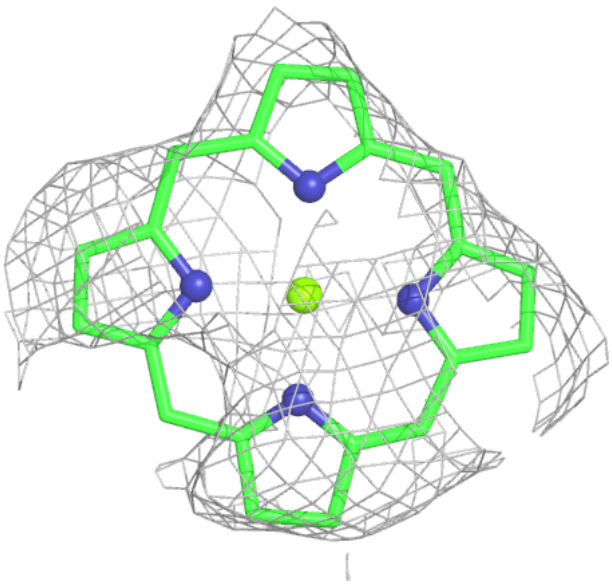


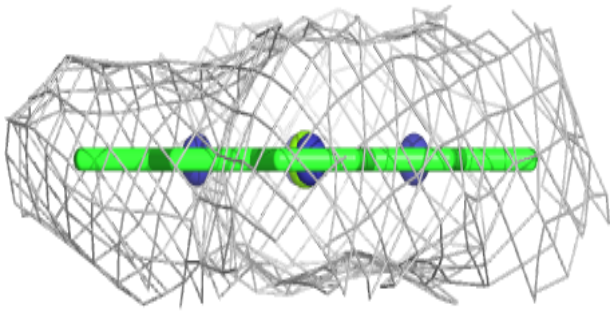


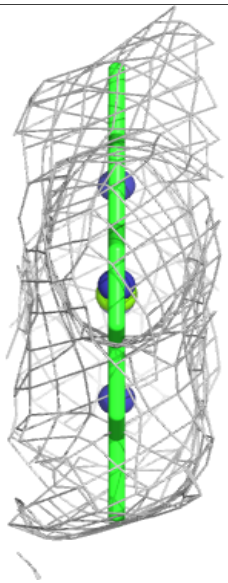


**Electron density around CLA 1 214:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

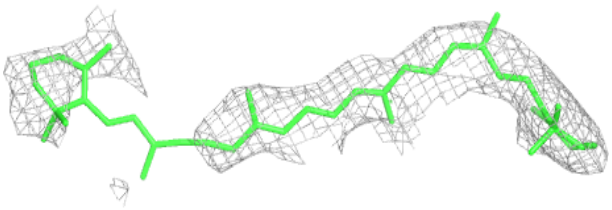


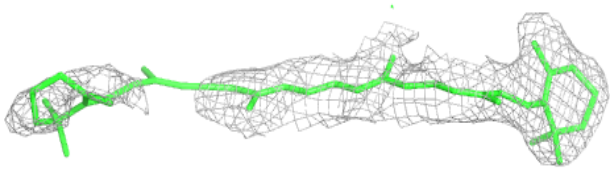


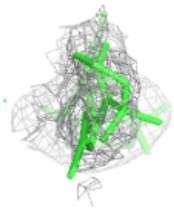


**Electron density around BCR B 845:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

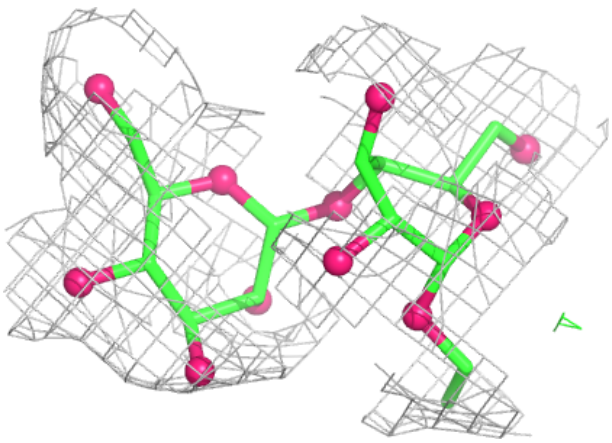


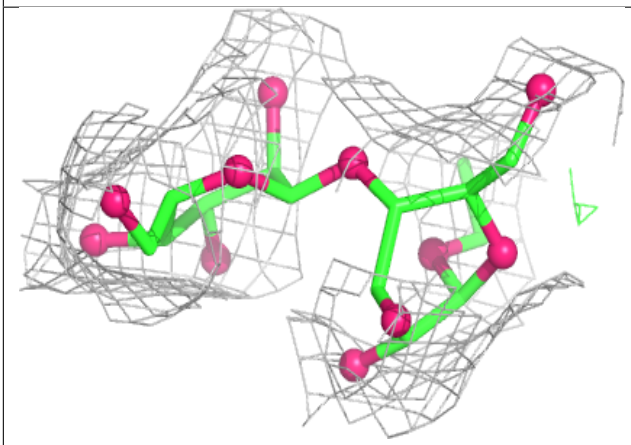


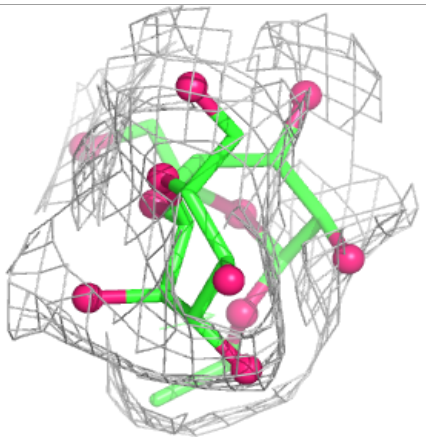


**Electron density around LMU B 849:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

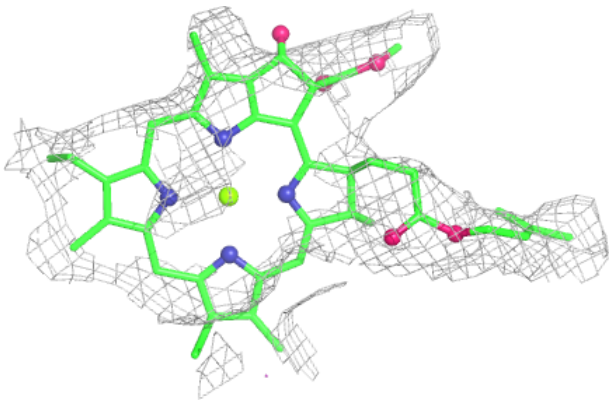


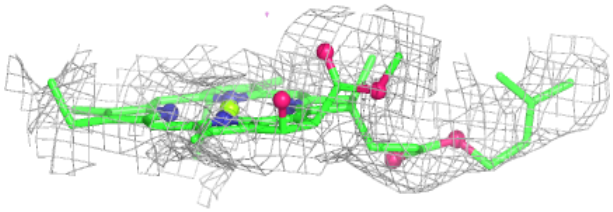


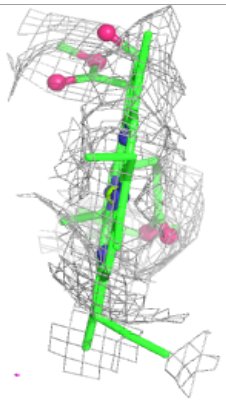


**Electron density around CLA K 102:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

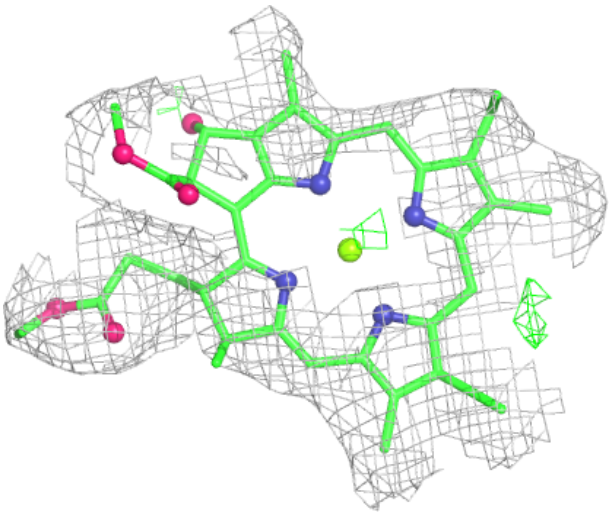


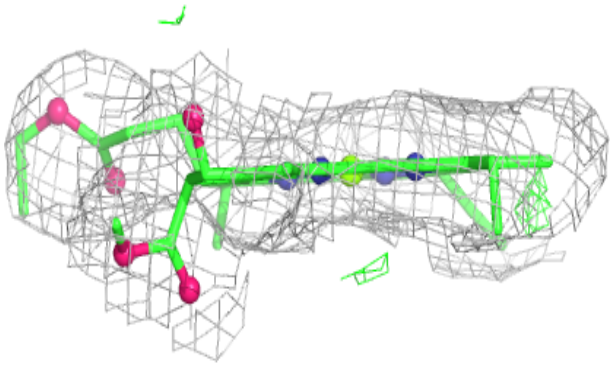


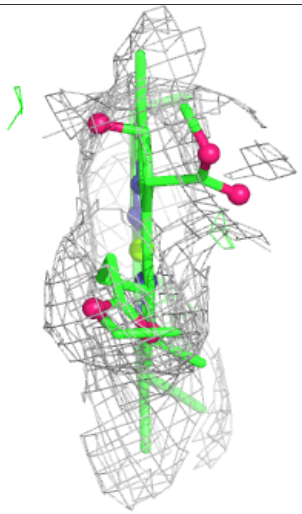


**Electron density around CLA 1 203:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

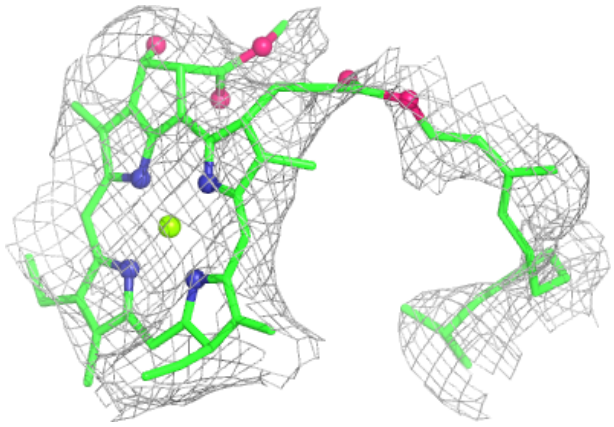


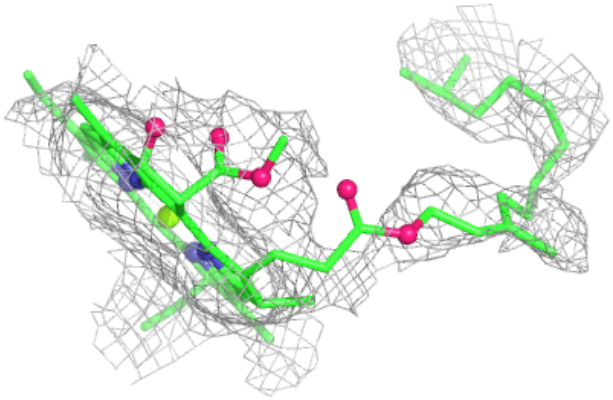


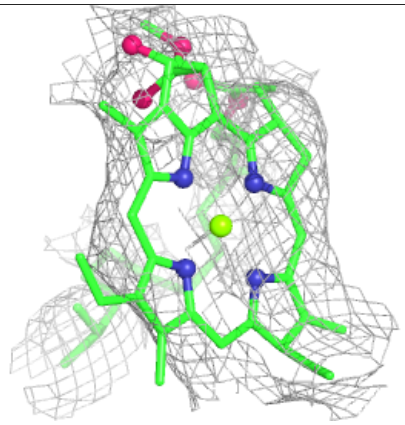


**Electron density around CLA A 839:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

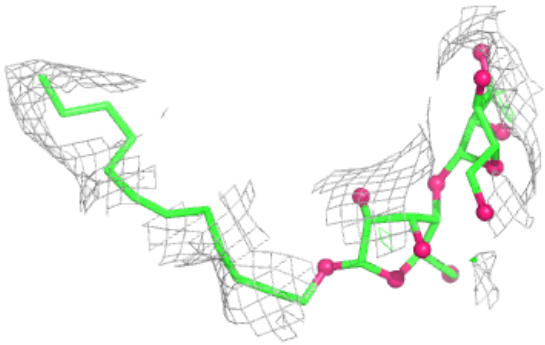


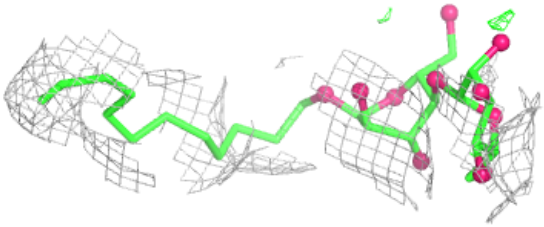


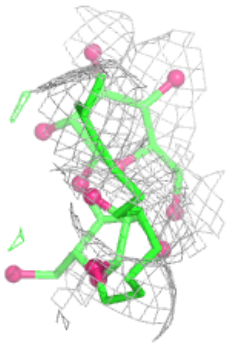


**Electron density around LMU G 102:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

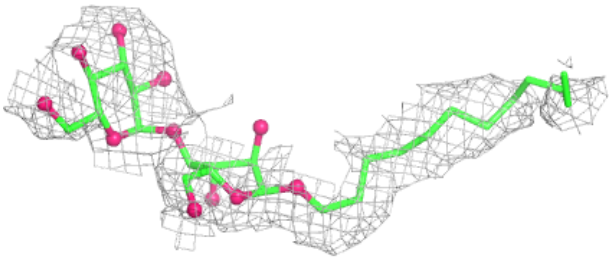


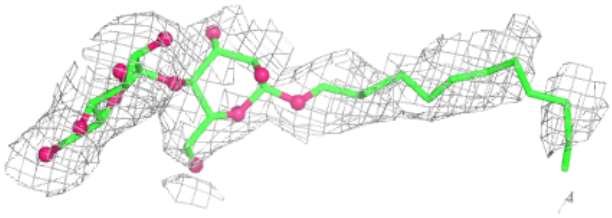


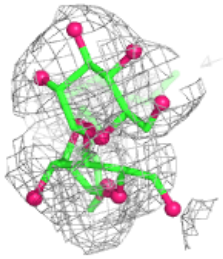


**Electron density around LMU 4 316:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

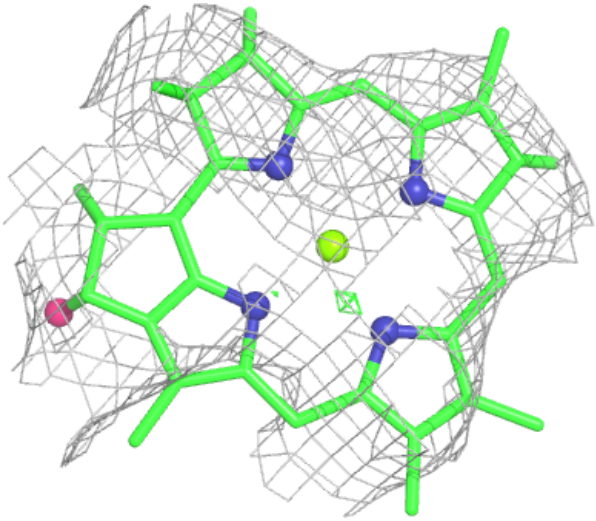


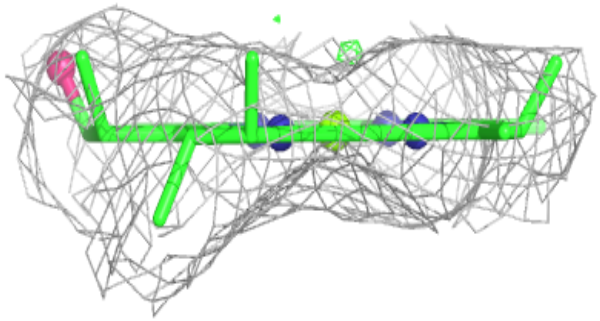


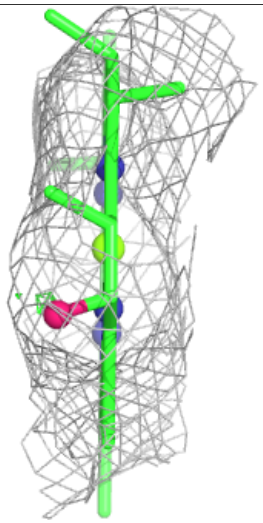


**Electron density around CLA 4 302:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

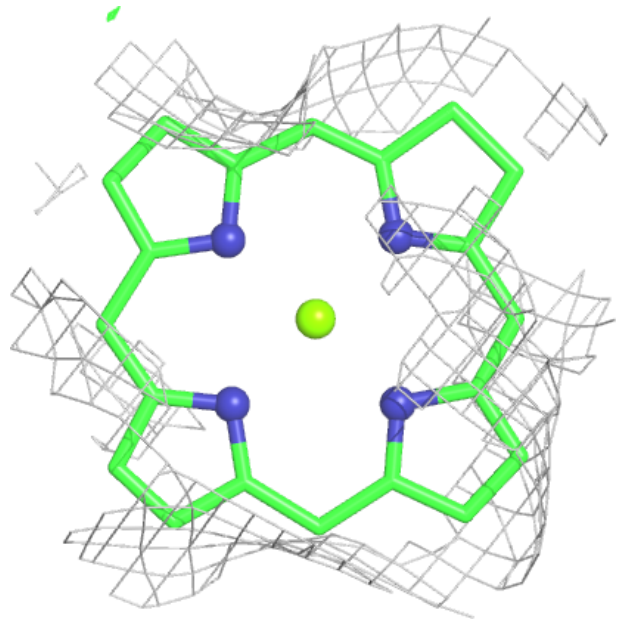


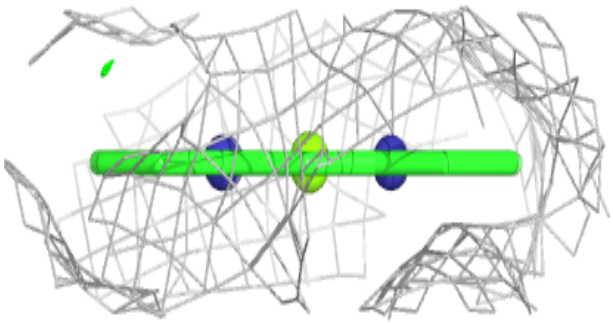


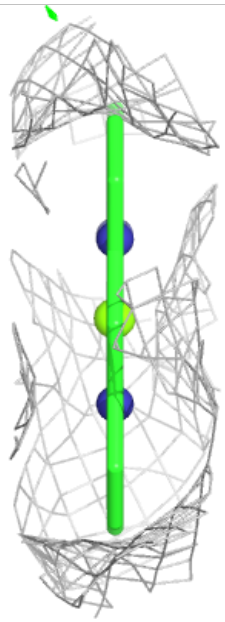


**Electron density around CLA 2 306:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

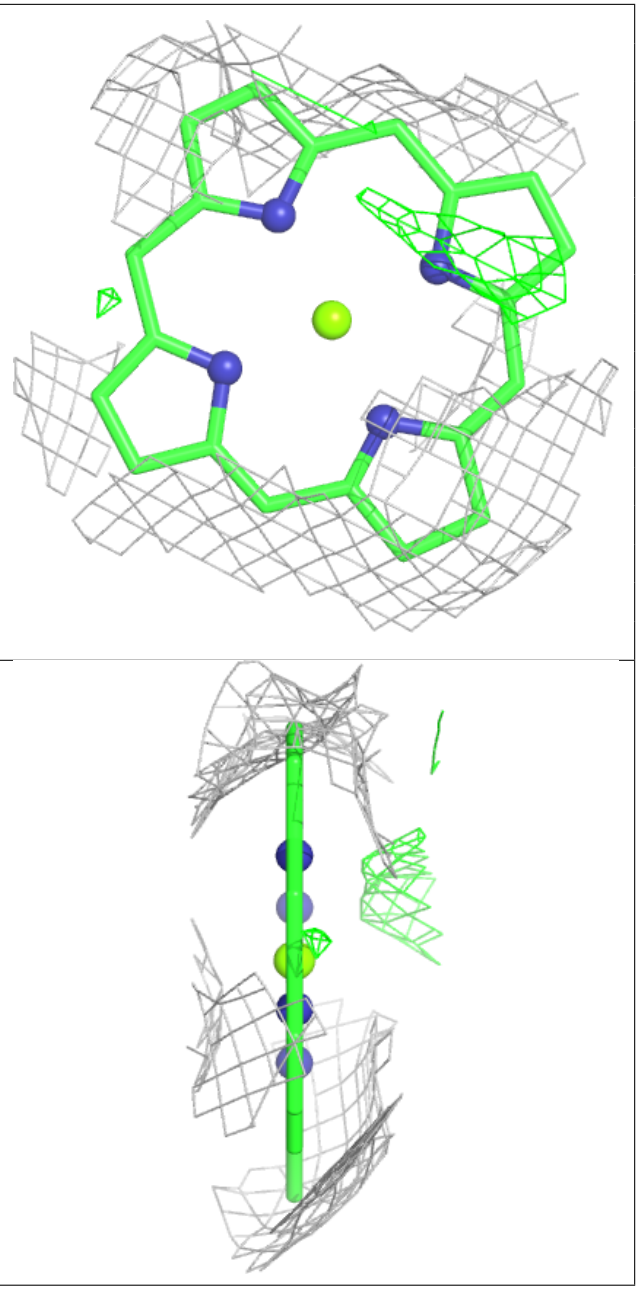






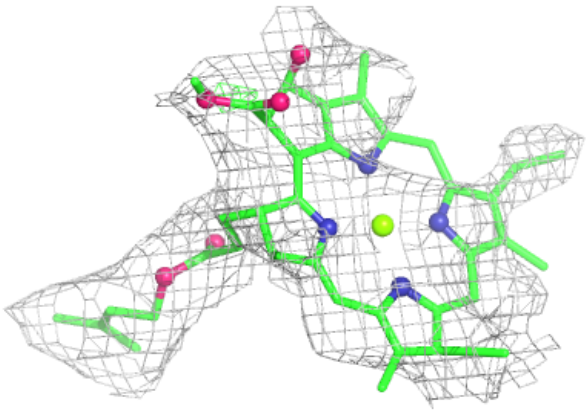
**Electron density around CLA 1 208:**

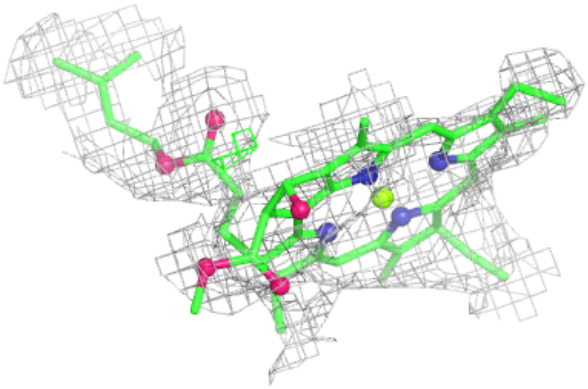
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

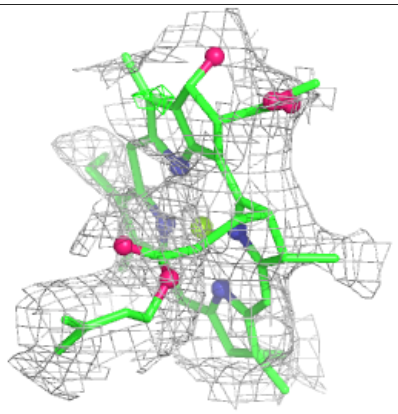


**Electron density around CLA 2 310:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

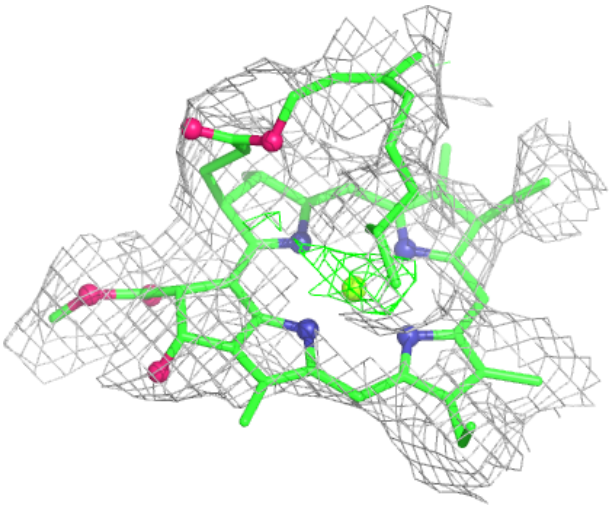


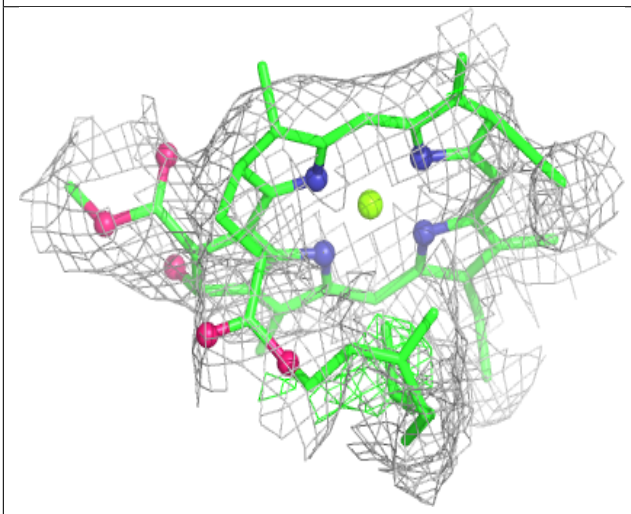


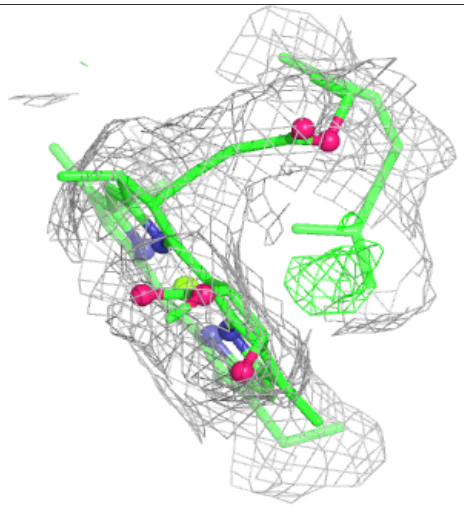


**Electron density around CLA B 813:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

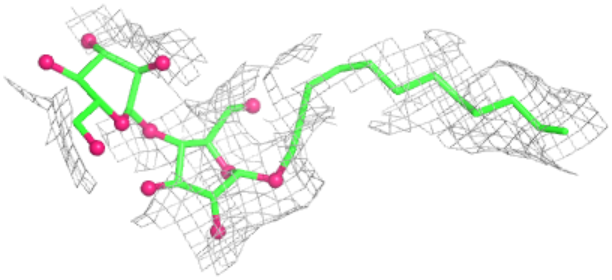


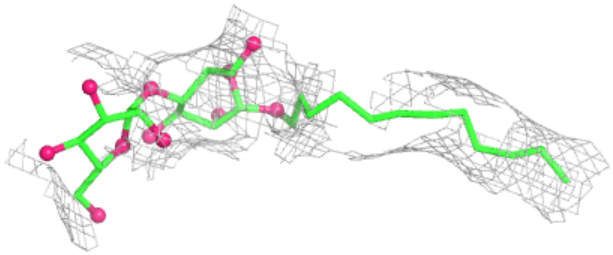




**Electron density around LMU G 101:**

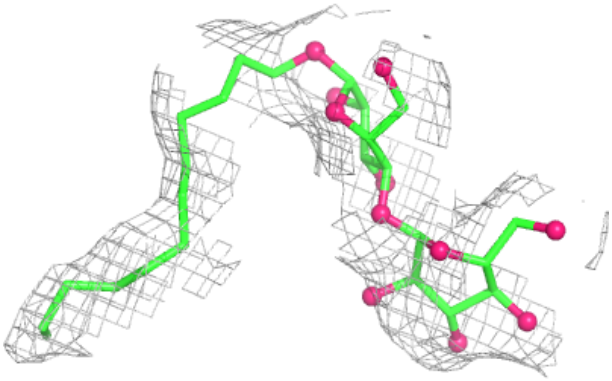
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

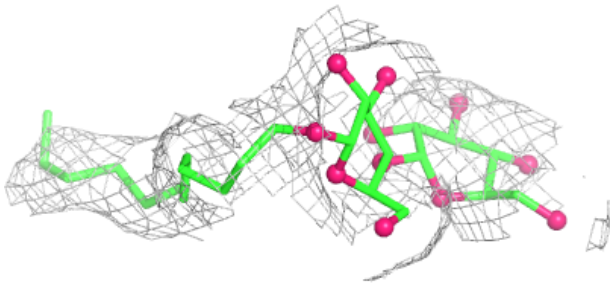




**Electron density around LMU L 206:**

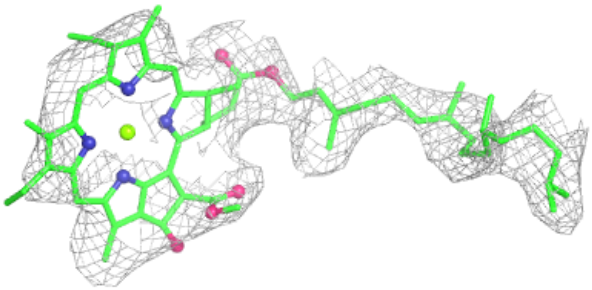
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

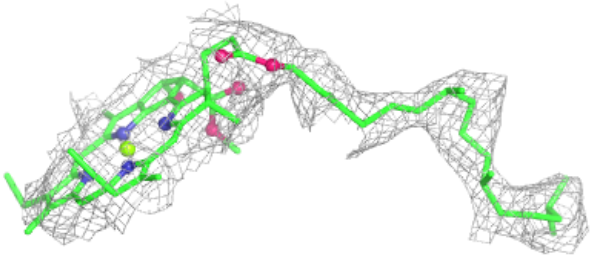


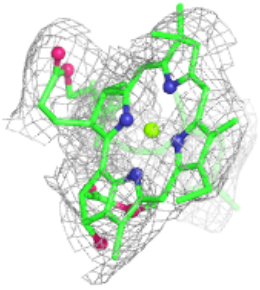


**Electron density around CLA 3 314:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

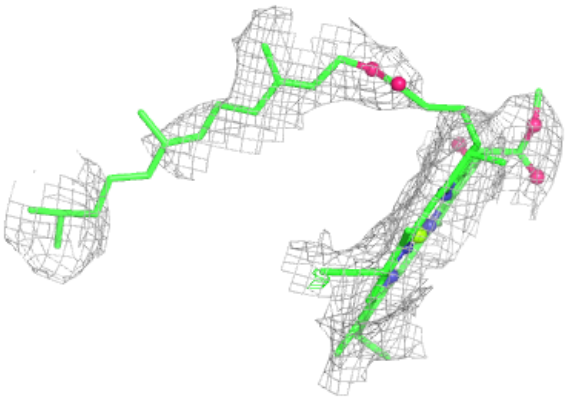


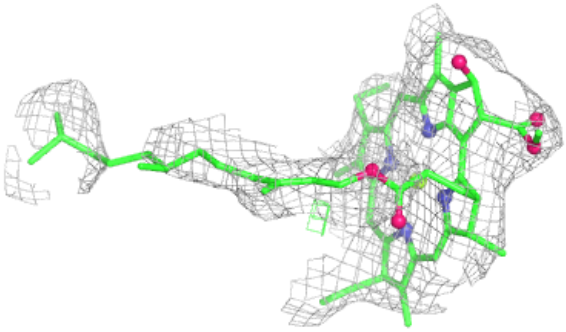


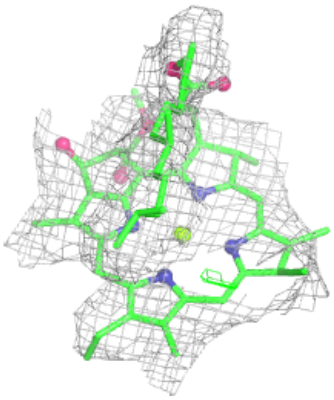


**Electron density around CLA L 201:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

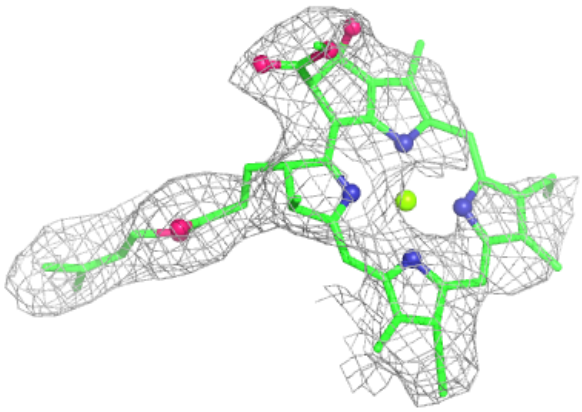


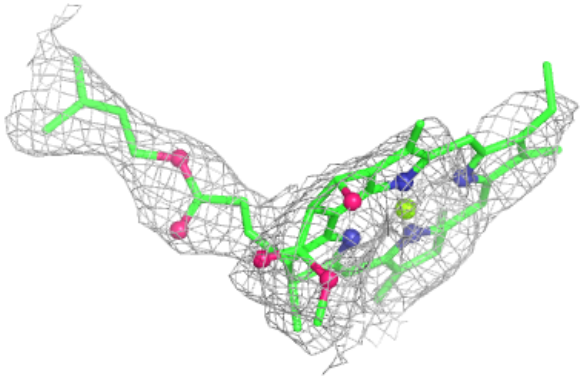


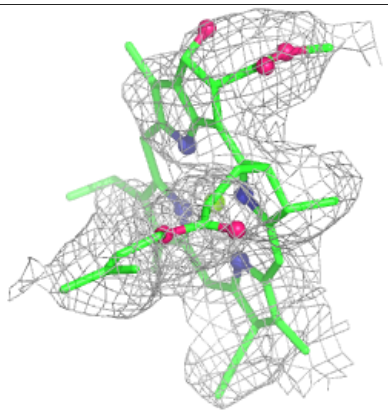


**Electron density around CLA A 829:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

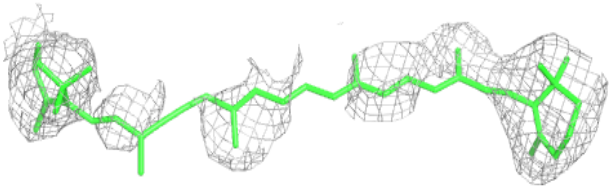


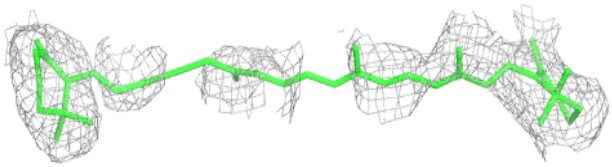


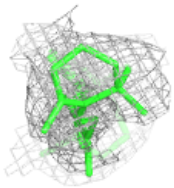


**Electron density around BCR J 102:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

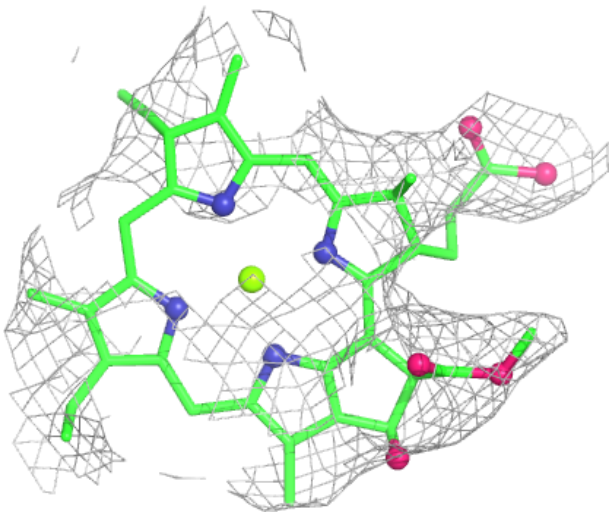


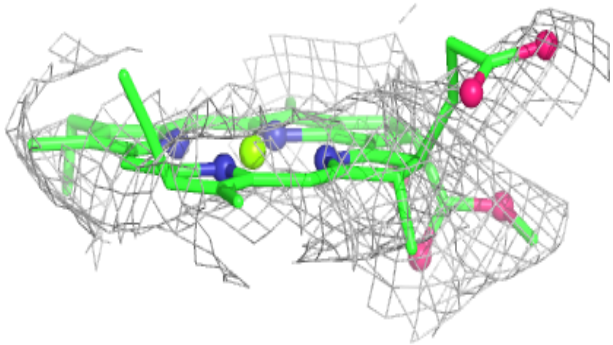


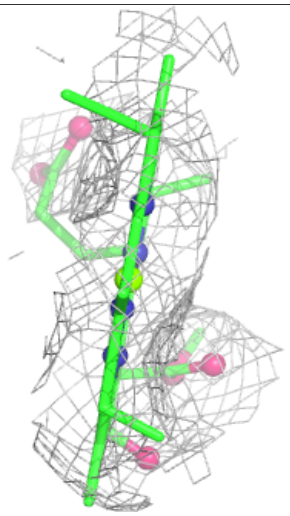


**Electron density around CLA A 833:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

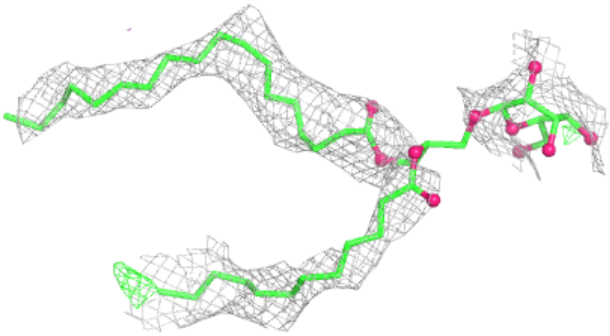


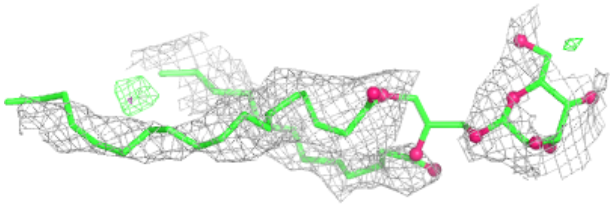




**Electron density around LMG B 848:**

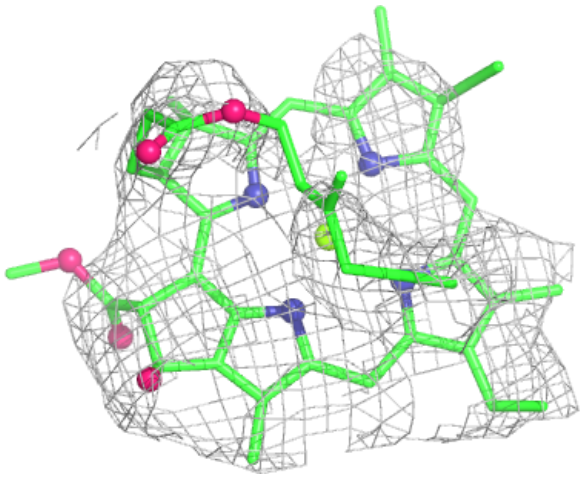
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

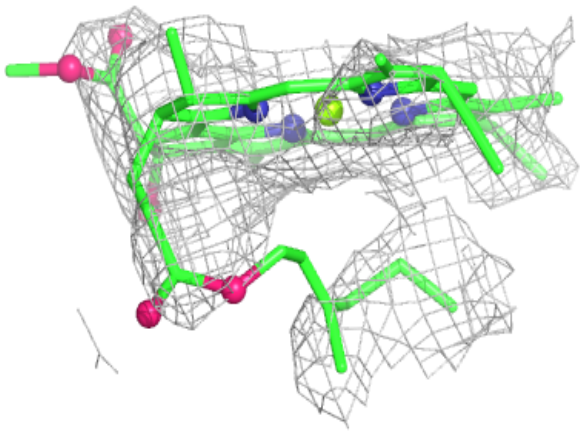




**Electron density around CLA A 817:**

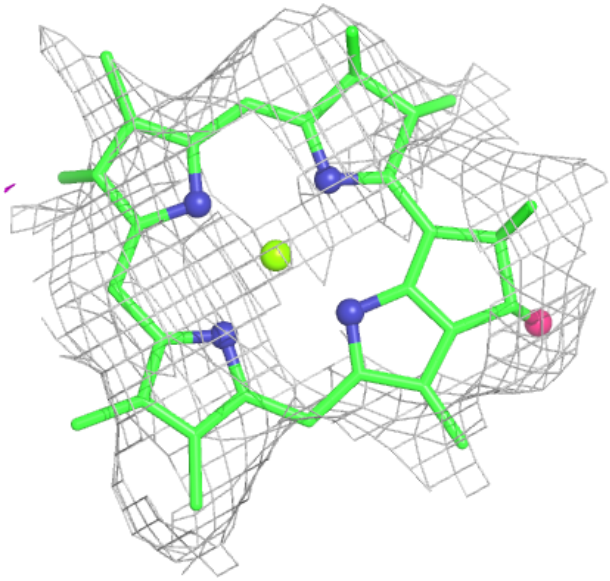
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

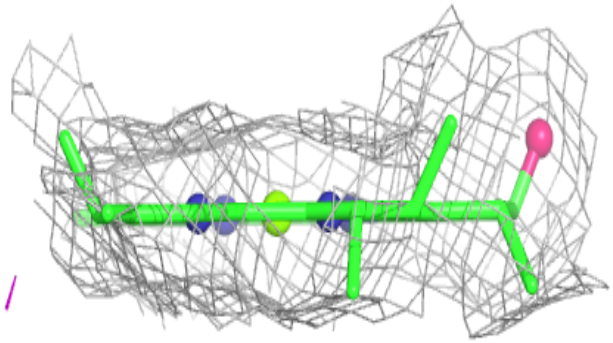


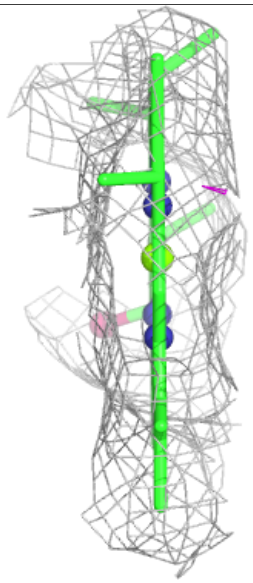


**Electron density around CLA 3 301:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

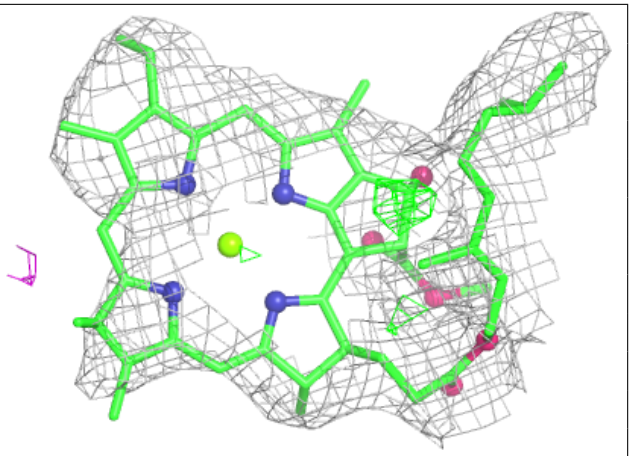


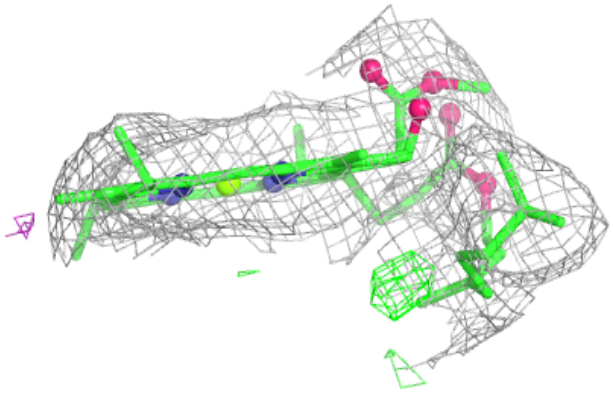


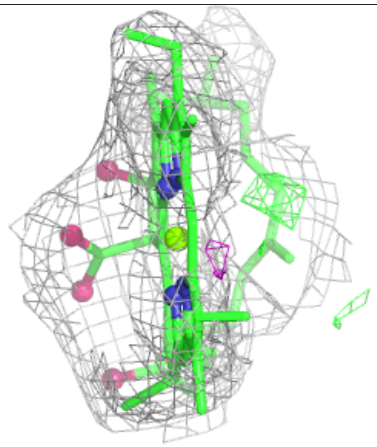


**Electron density around CLA B 812:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

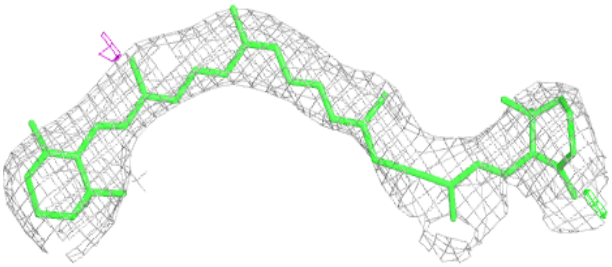


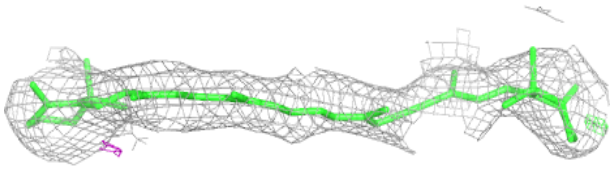


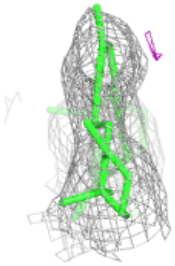


**Electron density around BCR A 845:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

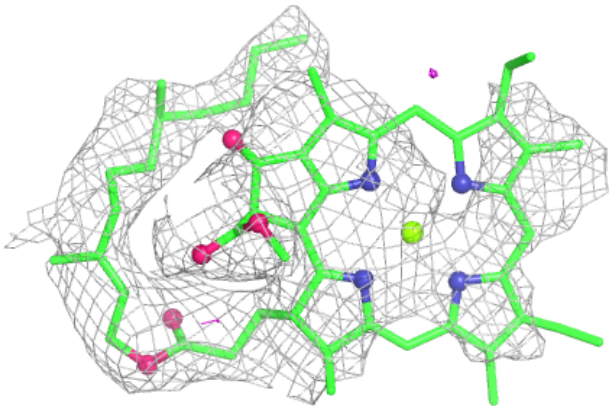


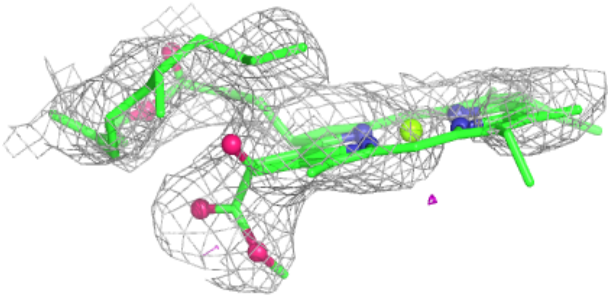


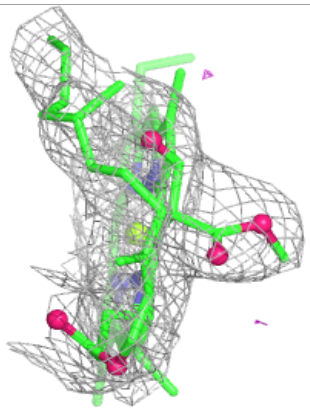


**Electron density around CLA A 823:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

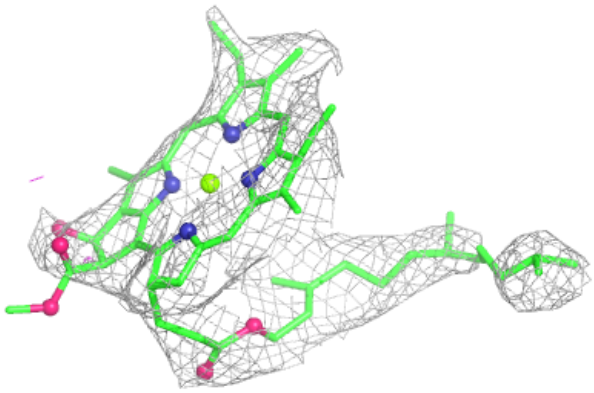


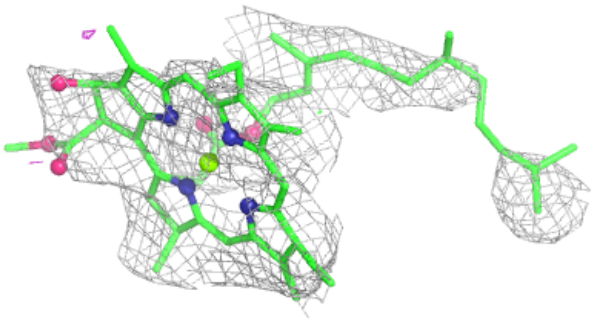


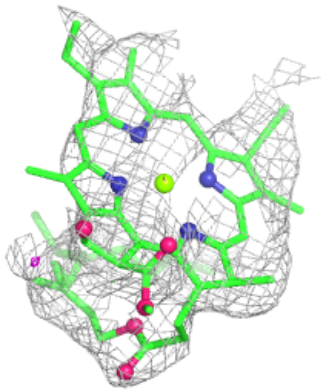


**Electron density around CLA B 815:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

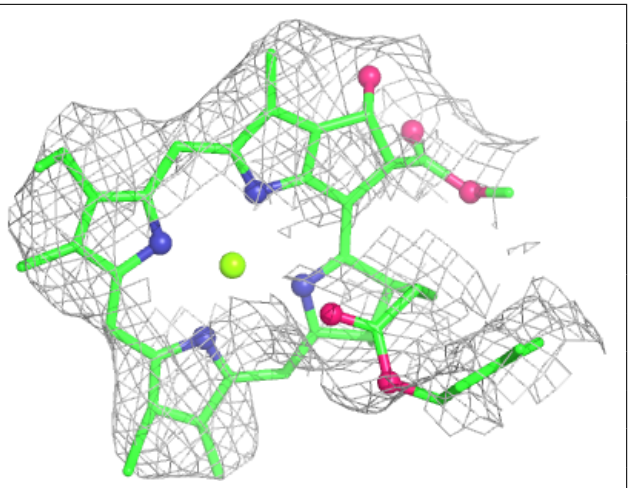


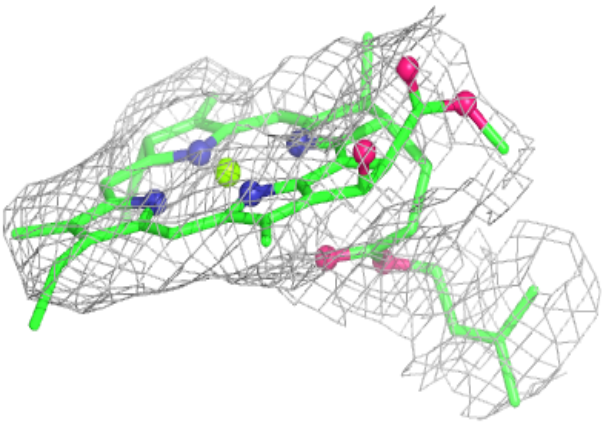


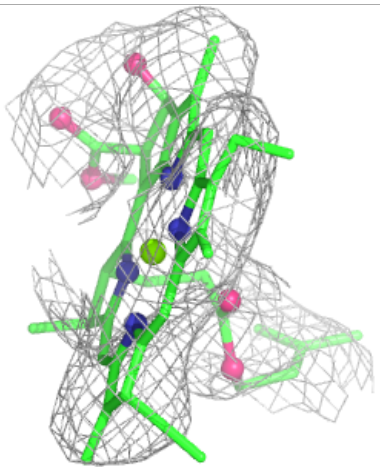


**Electron density around CLA A 815:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

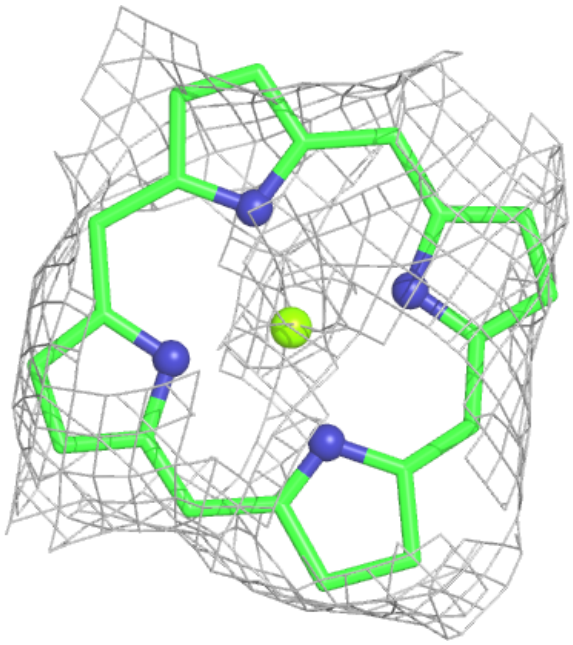


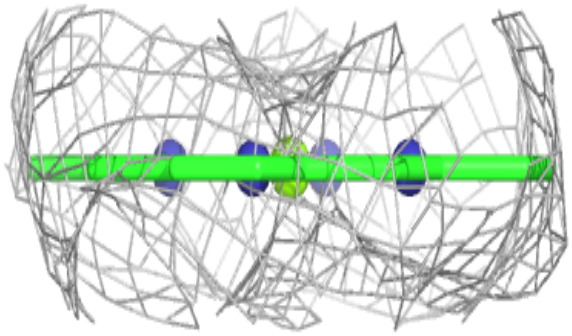


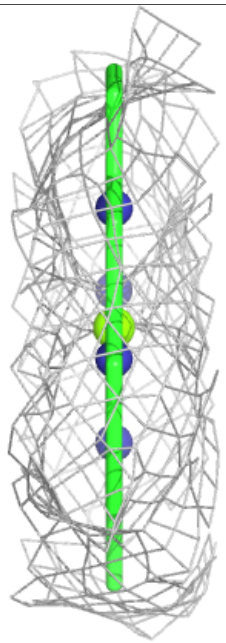


**Electron density around CLA 1 212:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

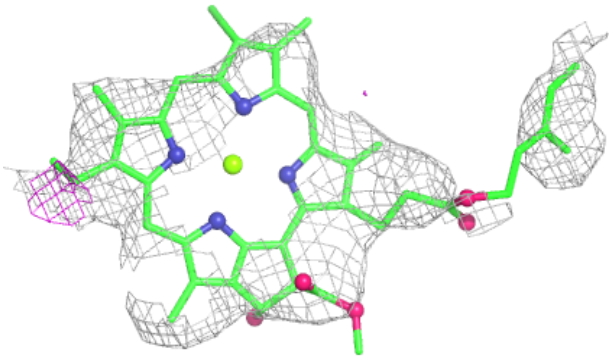


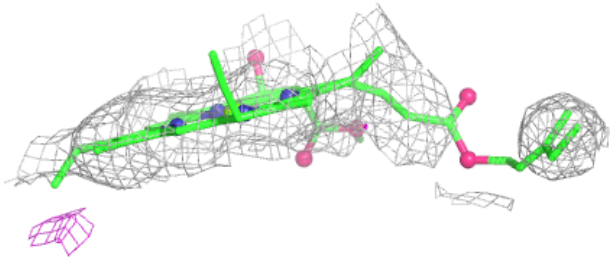


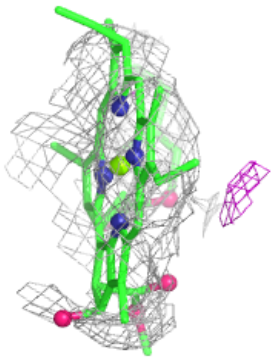


**Electron density around CLA 1 213:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

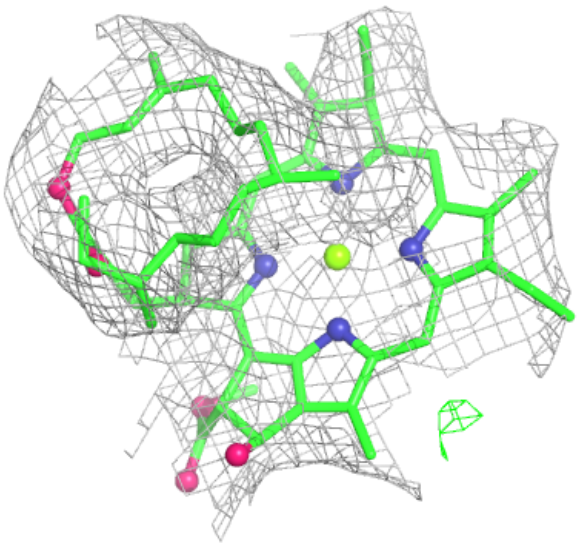


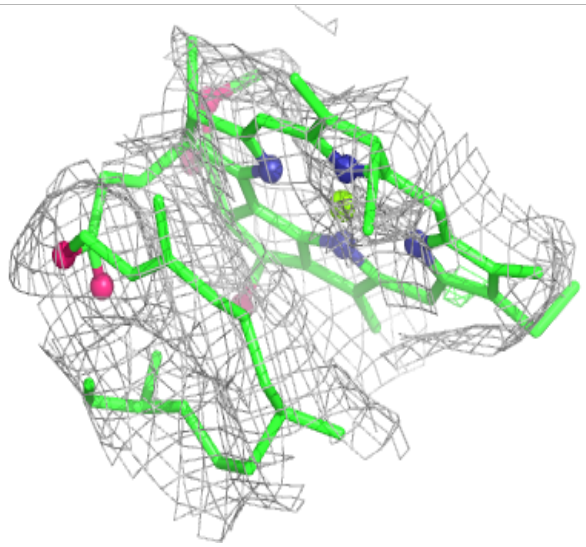




**Electron density around CLA J 103:**

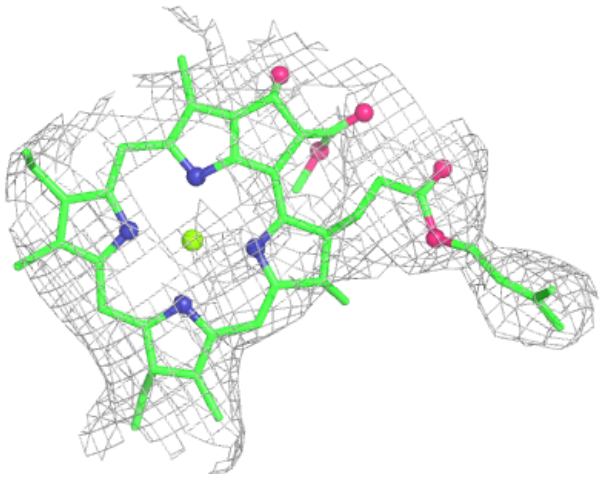
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

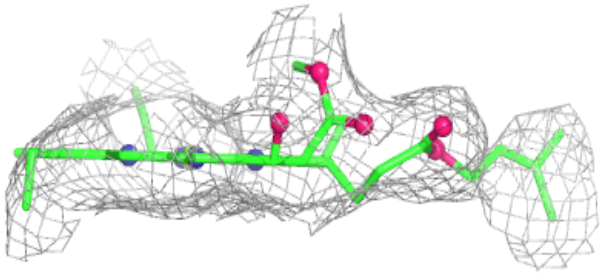


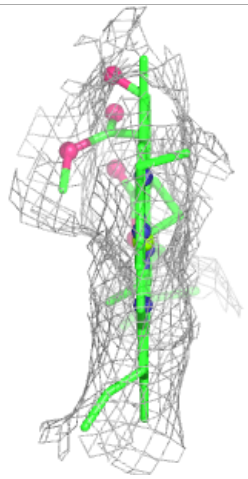


**Electron density around CLA 4 310:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

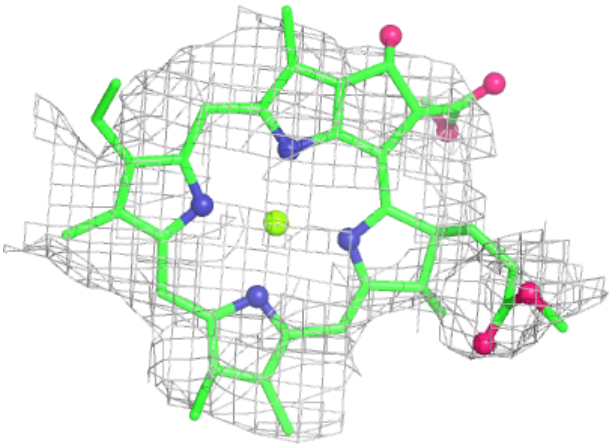


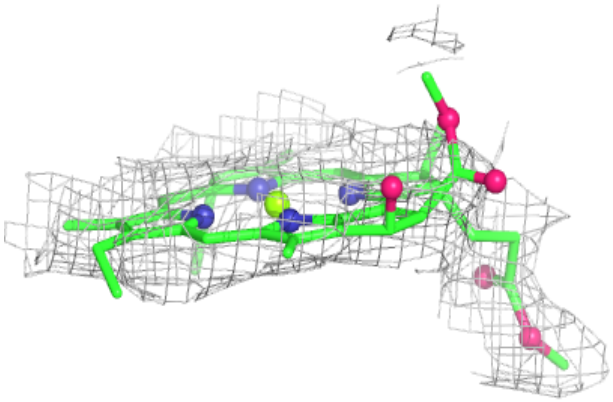




**Electron density around CLA B 822:**

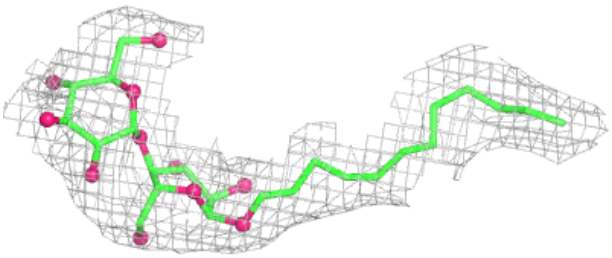
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

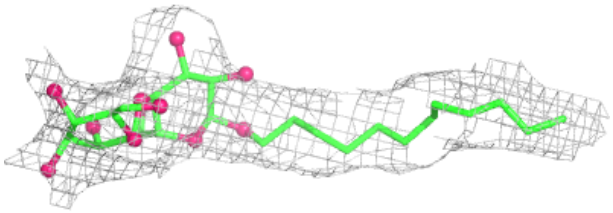


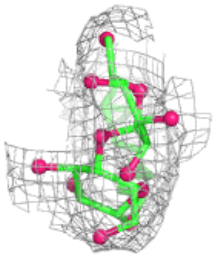


**Electron density around LMU 4 321:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

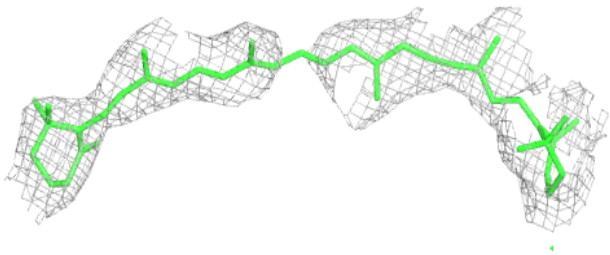


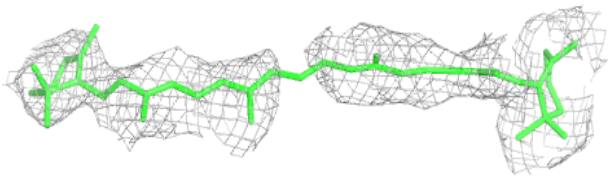


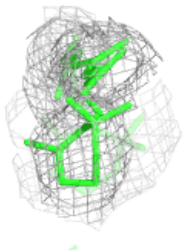


**Electron density around BCR B 844:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

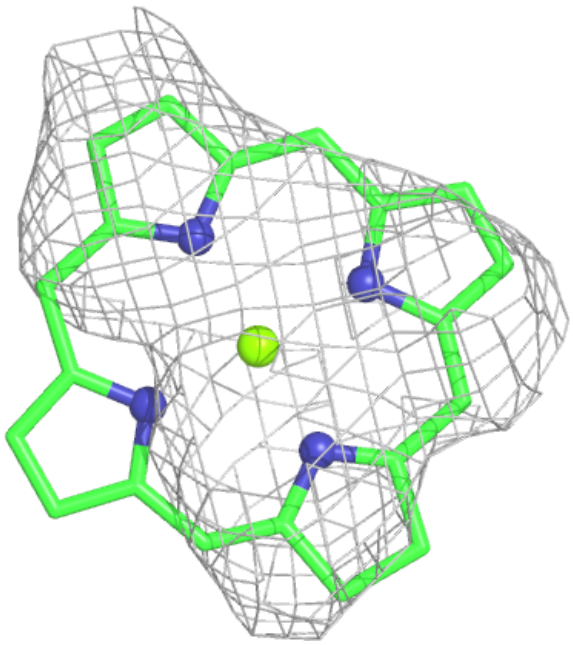


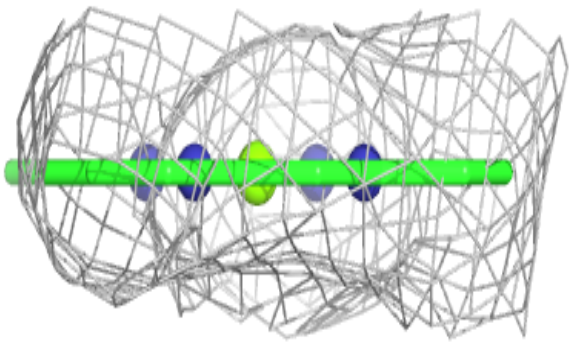


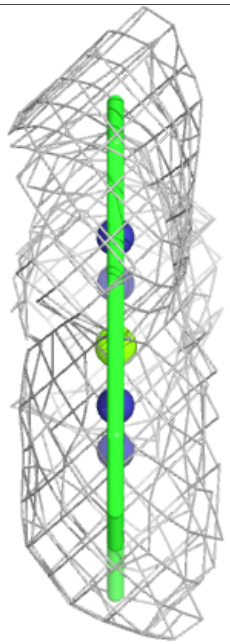


**Electron density around CLA 3 315:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

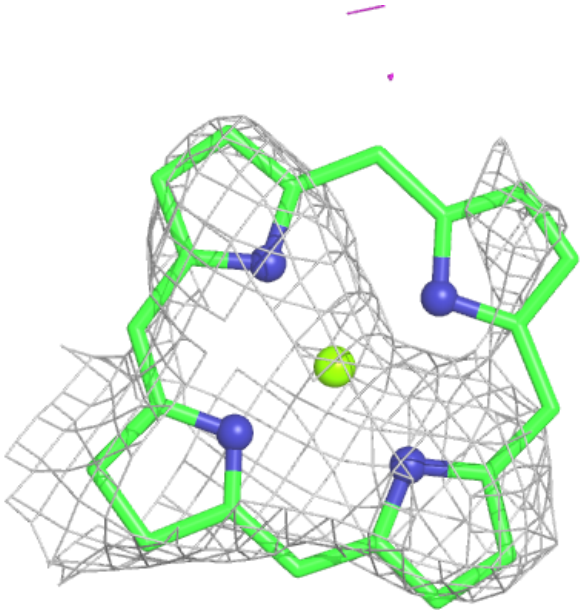


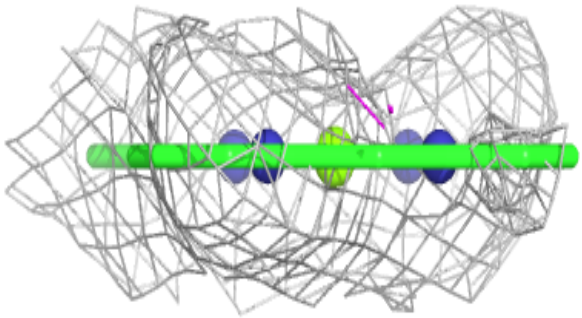


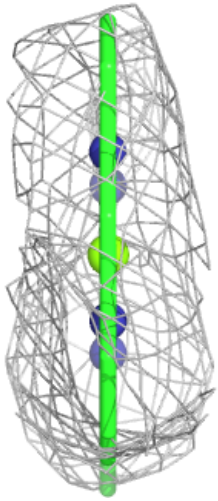


**Electron density around CLA 2 309:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

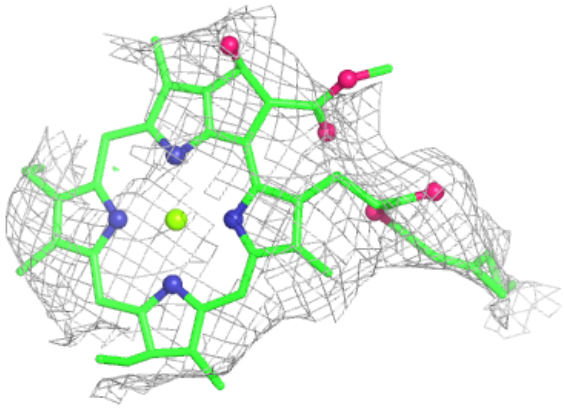


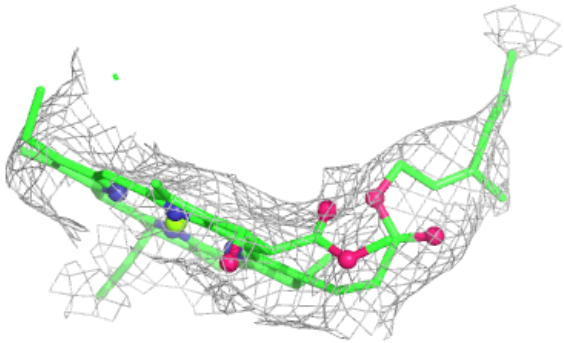




**Electron density around CLA 4 306:**

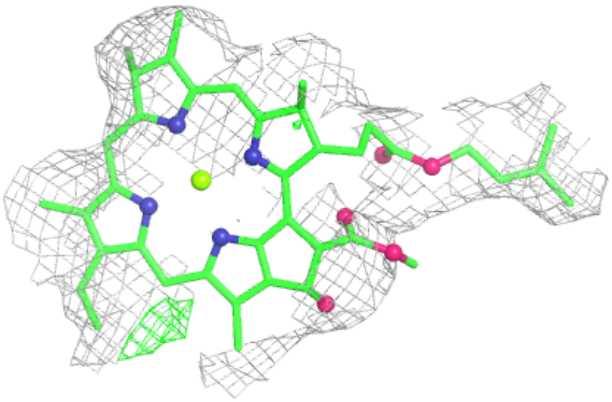
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

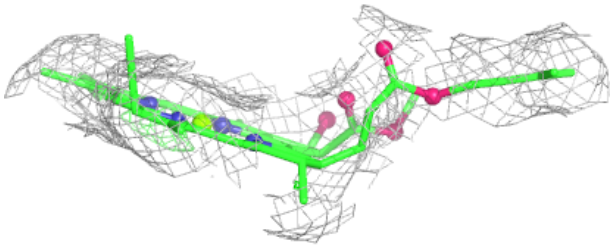




**Electron density around CLA L 208:**

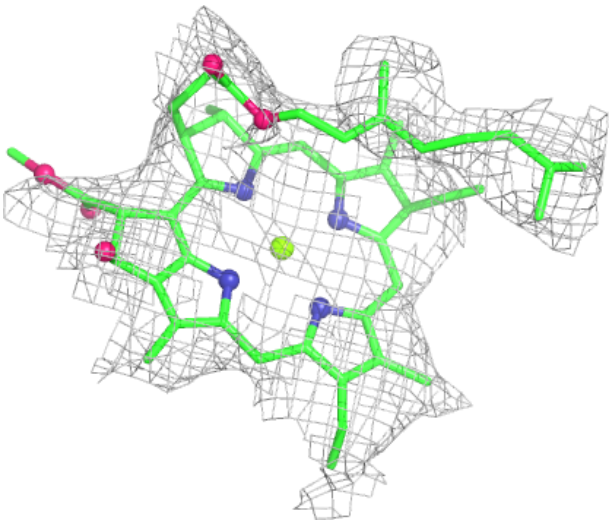
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

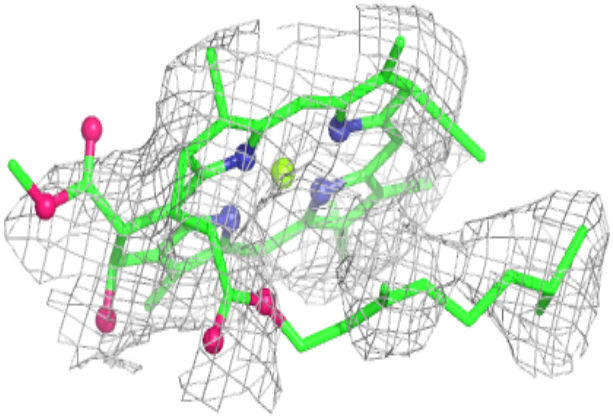




**Electron density around CLA B 823:**

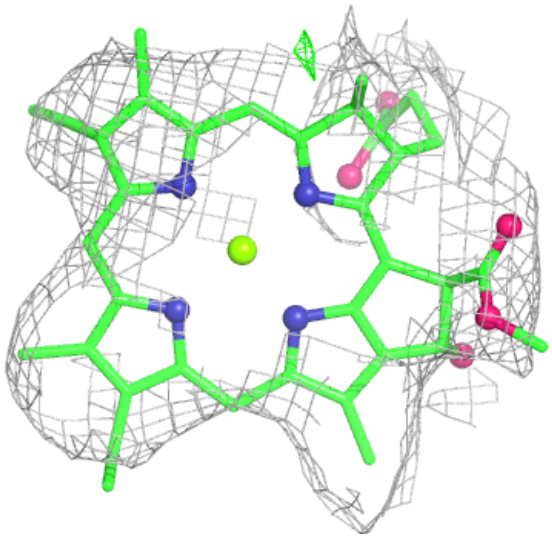
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

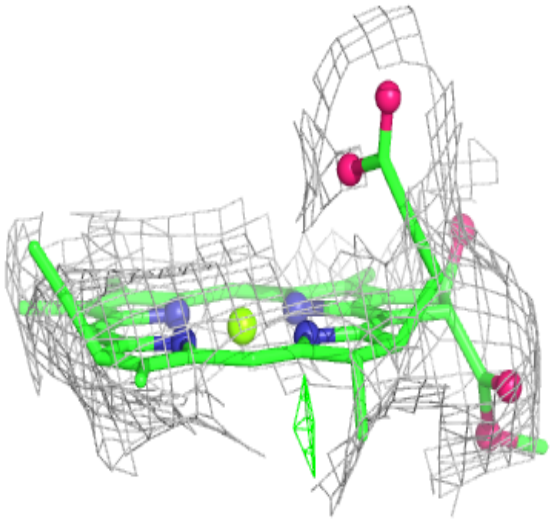




**Electron density around CLA B 834:**

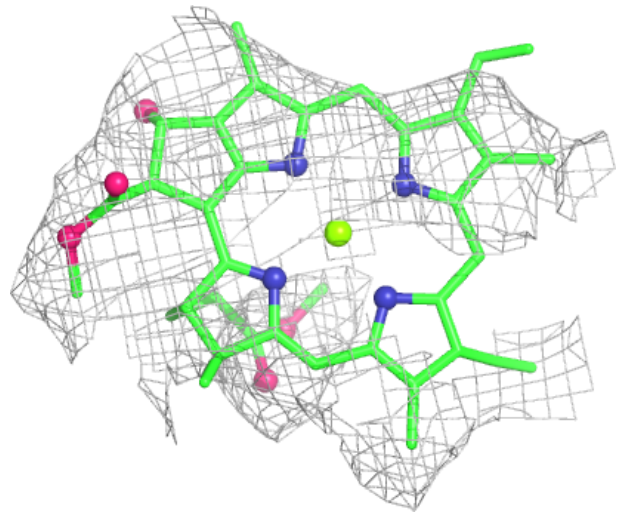
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

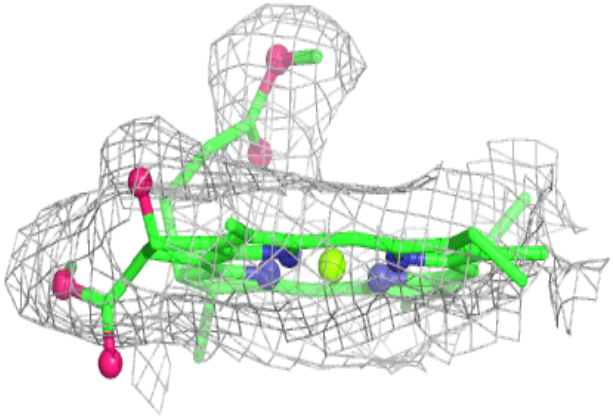




**Electron density around CLA 1 204:**

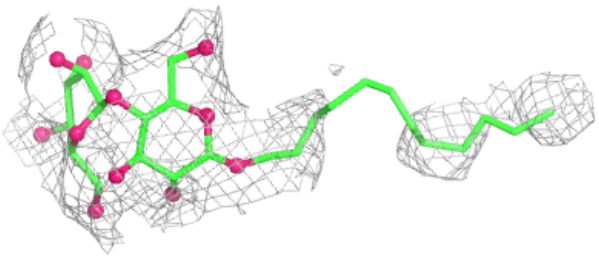
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

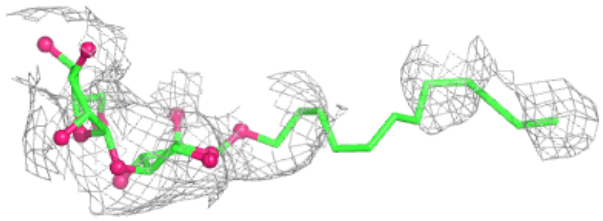


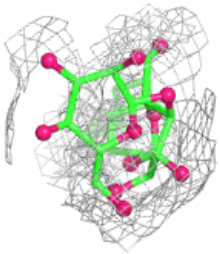


**Electron density around LMU 1 218:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

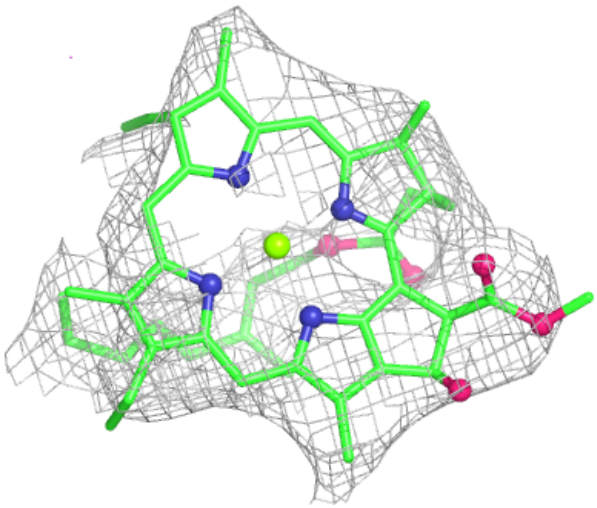


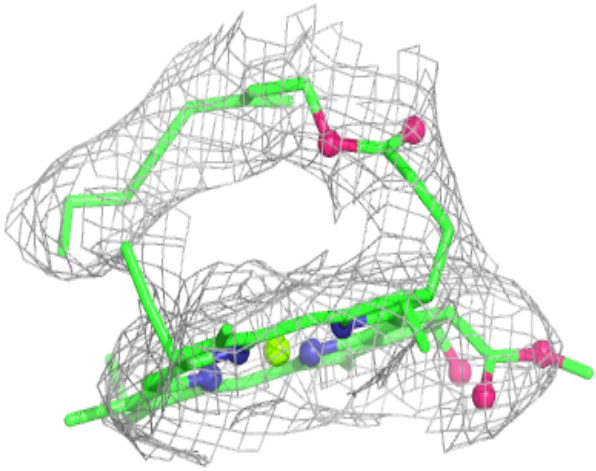


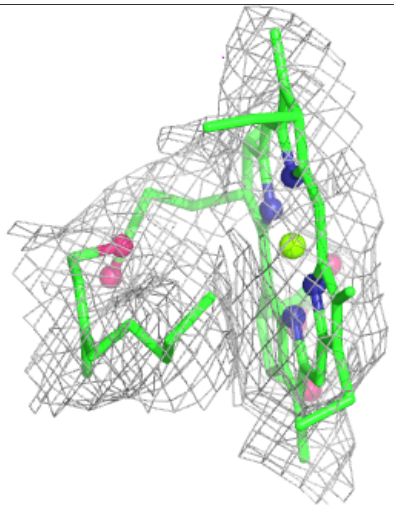


**Electron density around CLA A 812:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

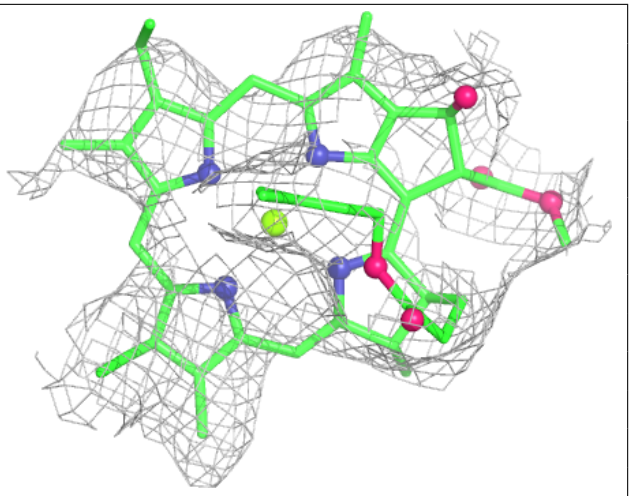


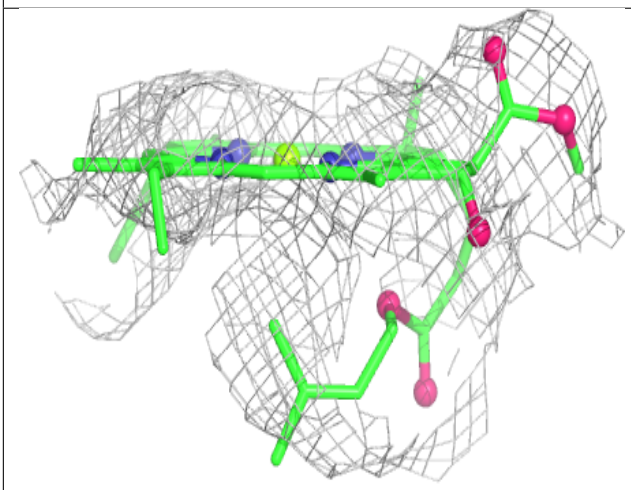


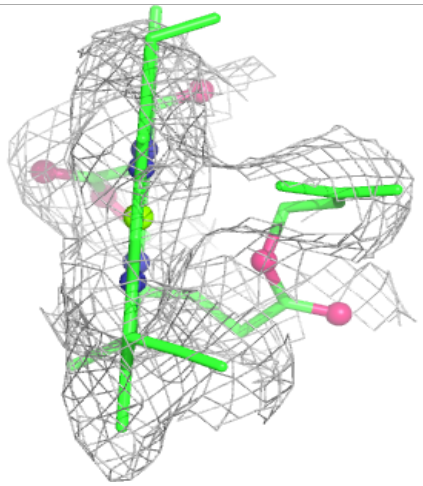


**Electron density around CLA H 110:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

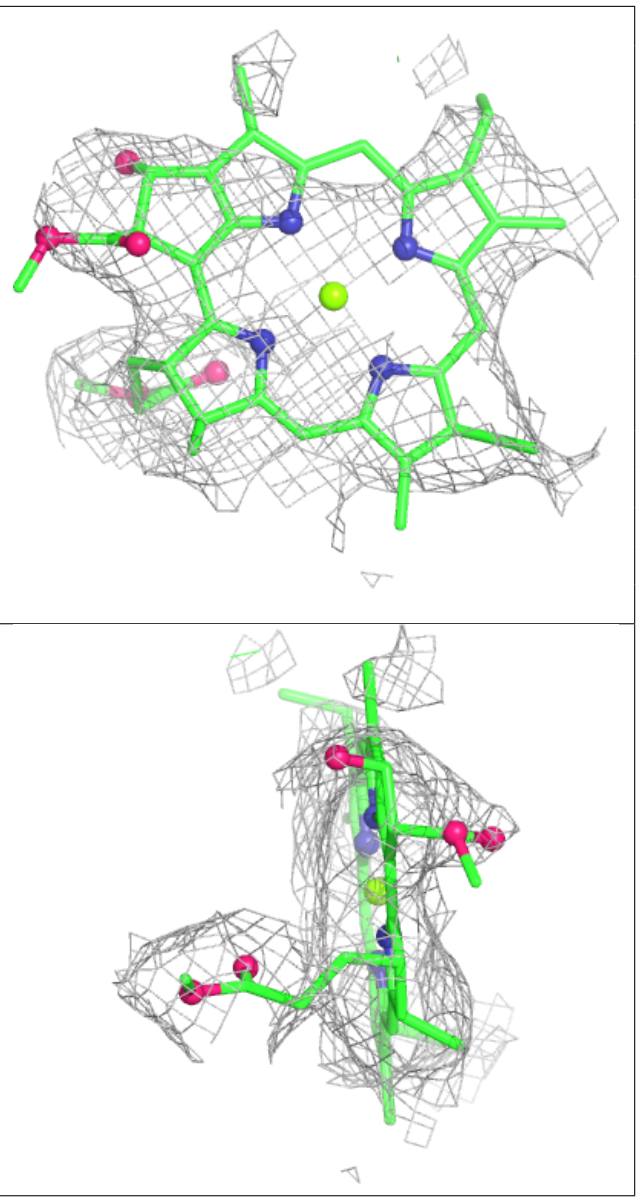






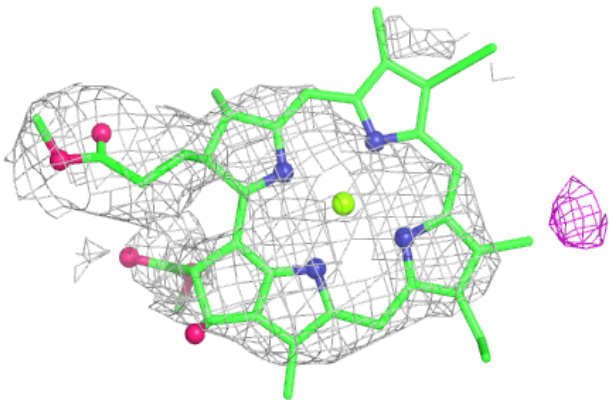
**Electron density around CLA A 807:**

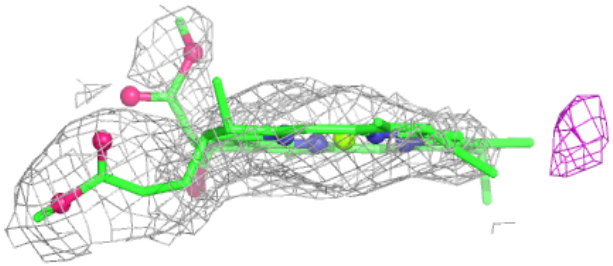
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

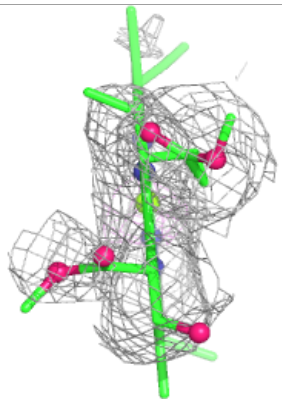


**Electron density around CLA A 834:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

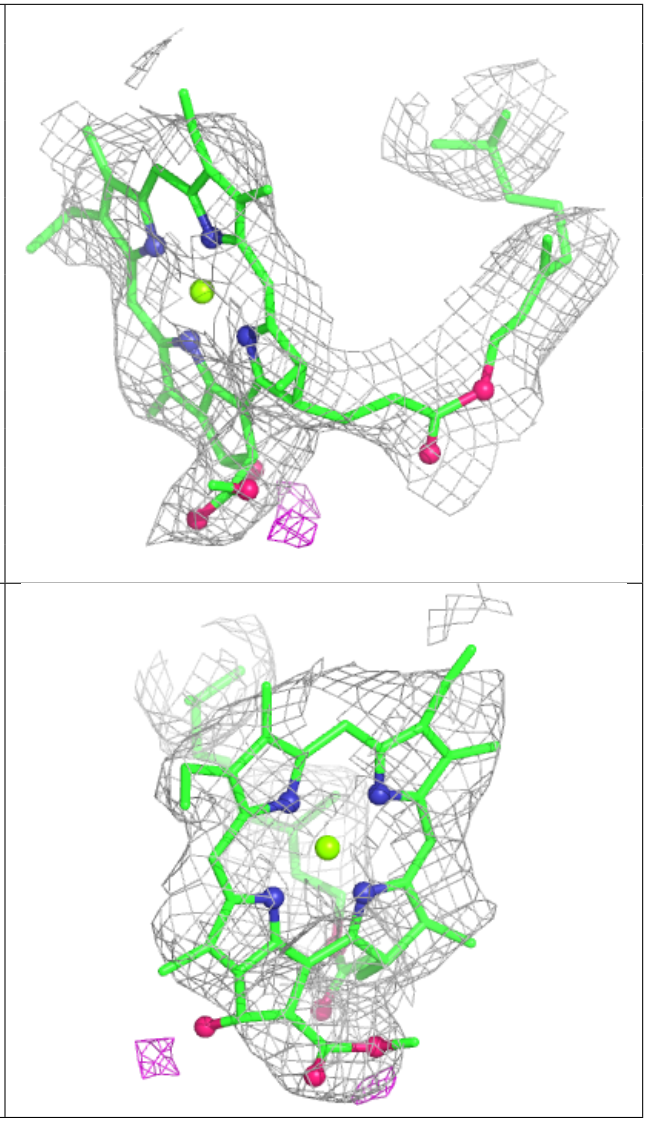






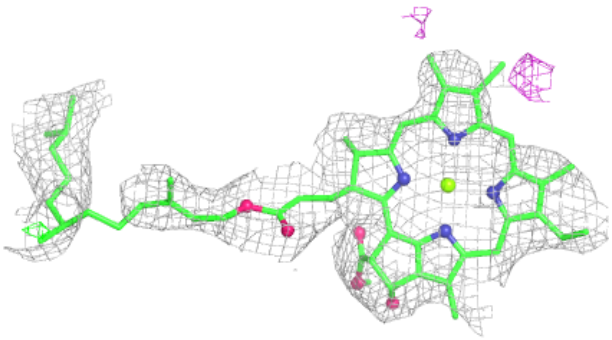
**Electron density around CLA A 804:**

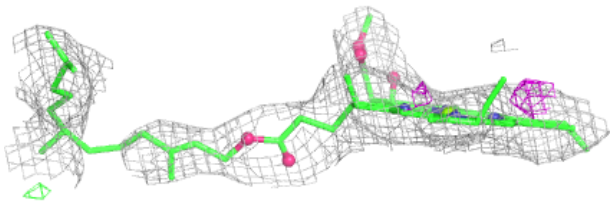
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



**Electron density around CLA B 837:**

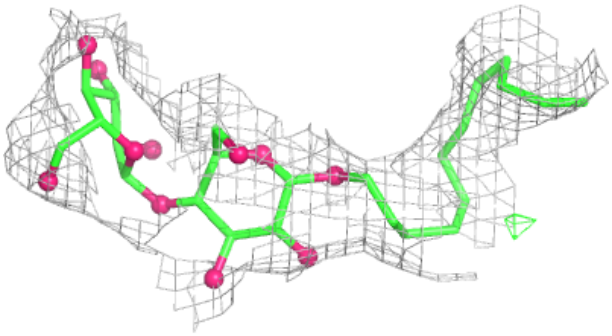
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

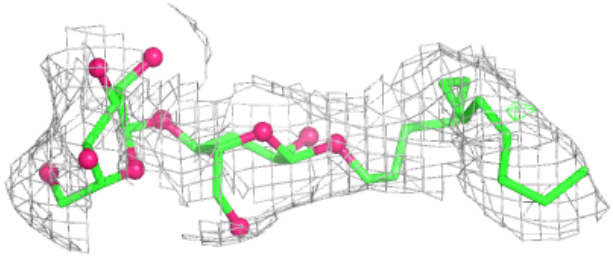


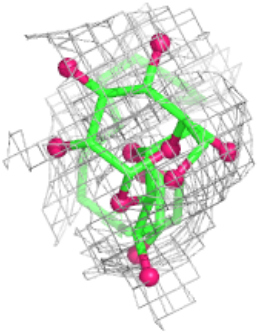


**Electron density around LMU R 109:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

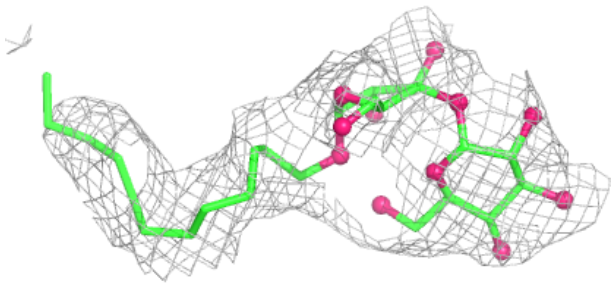


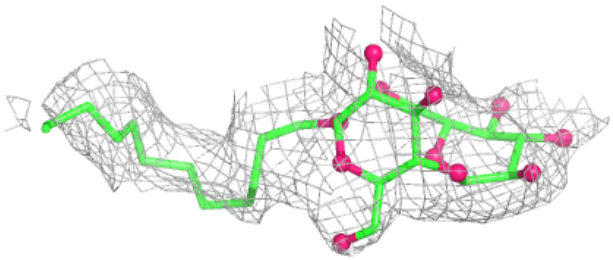


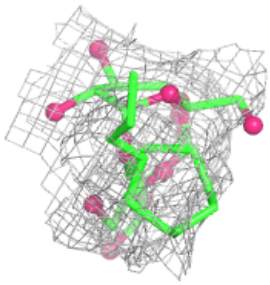


**Electron density around LMU A 847:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

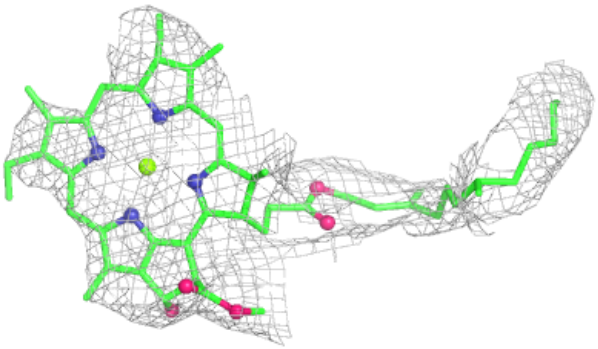


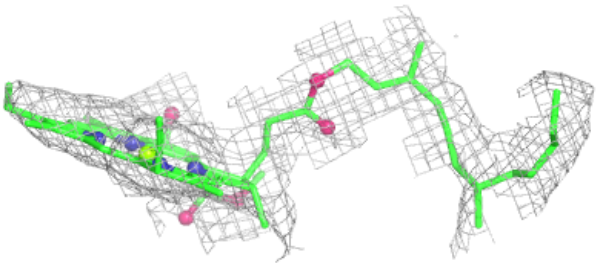


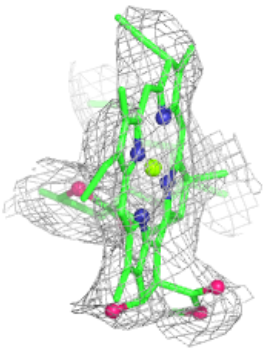


**Electron density around CLA A 824:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

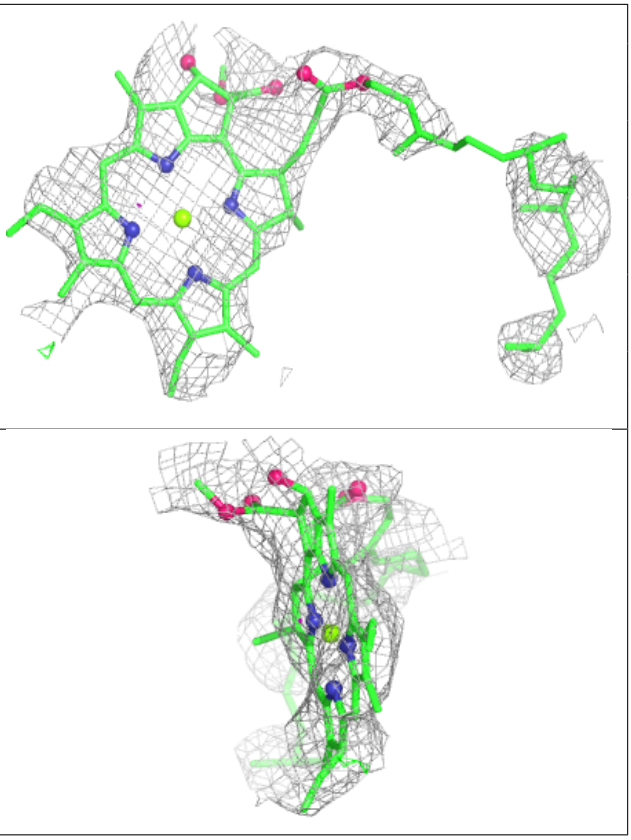






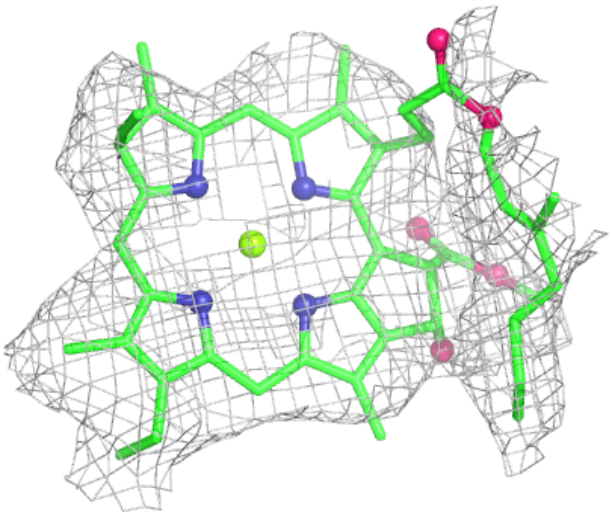
**Electron density around CLA A 825:**

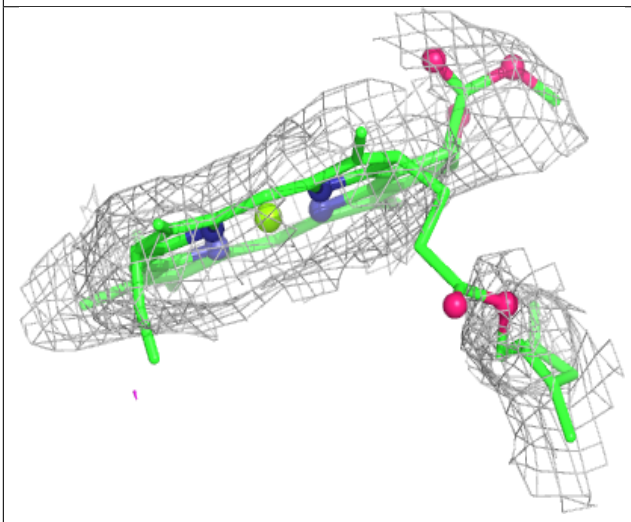
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

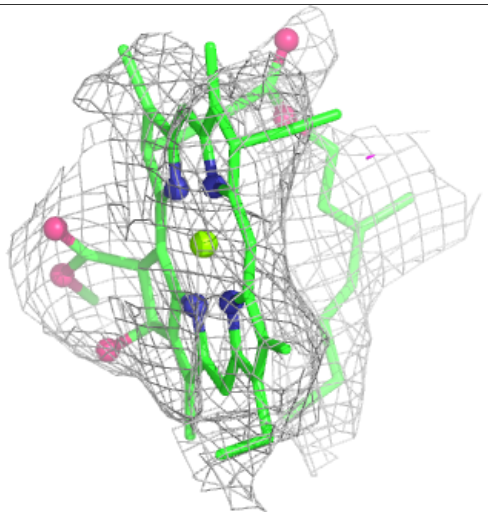


**Electron density around CLA F 207:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

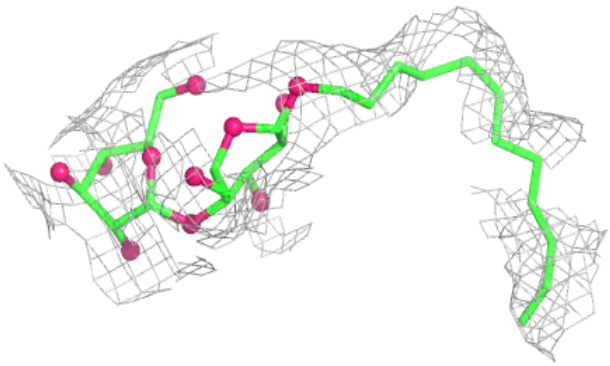


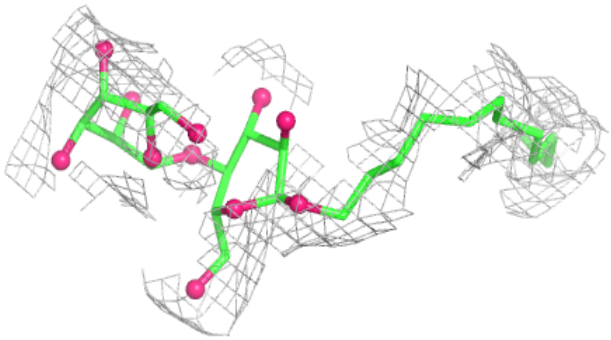


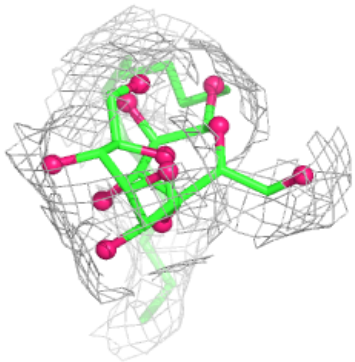


**Electron density around LMU 2 318:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

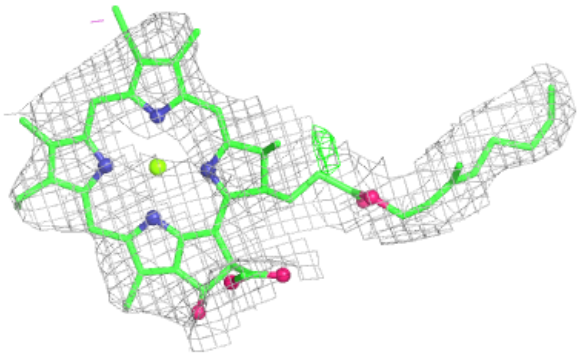


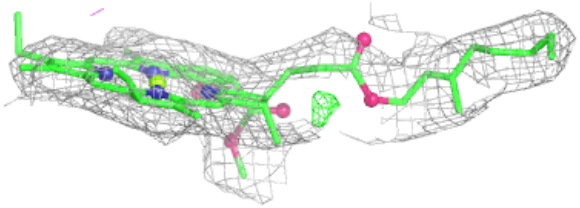


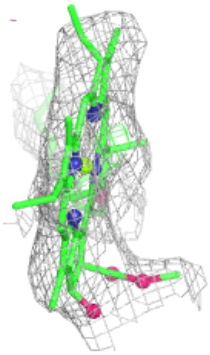


**Electron density around CLA A 805:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

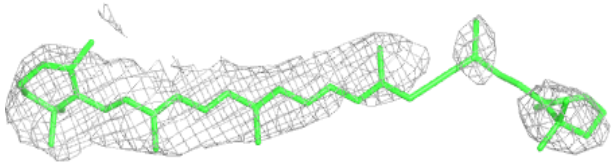


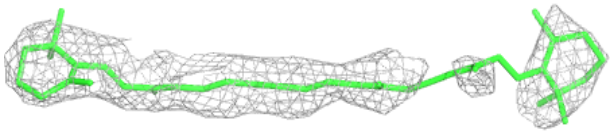


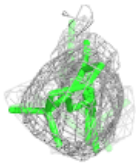


**Electron density around BCR B 847:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

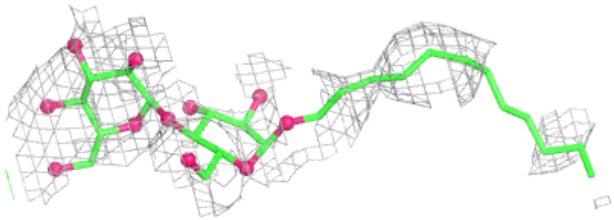


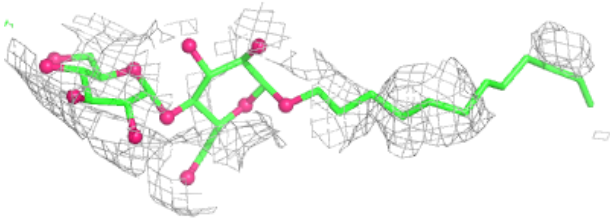


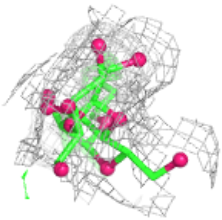


**Electron density around LMU B 805:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

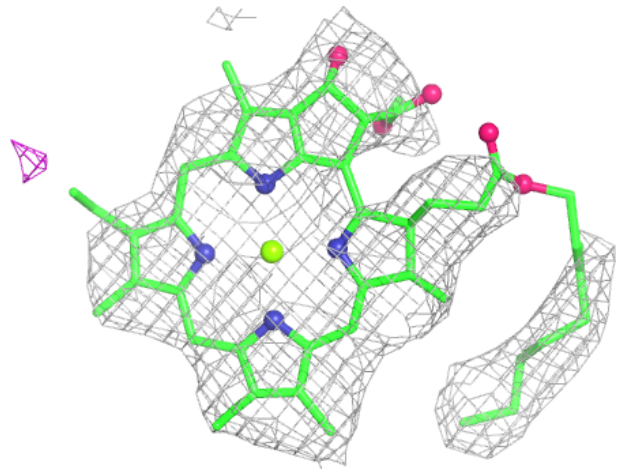


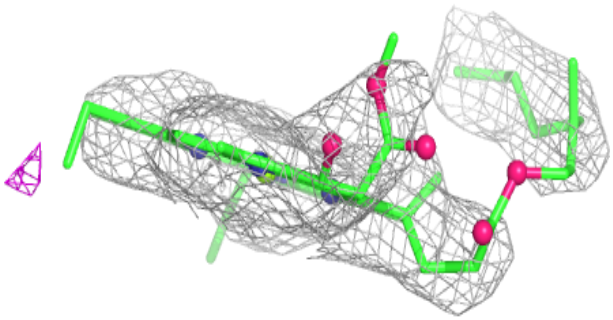


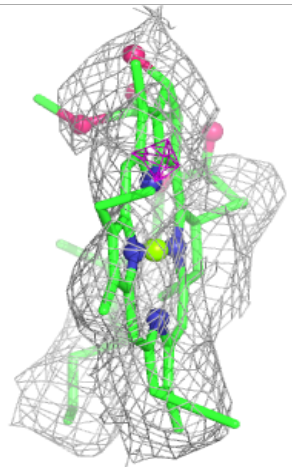


**Electron density around CLA B 825:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

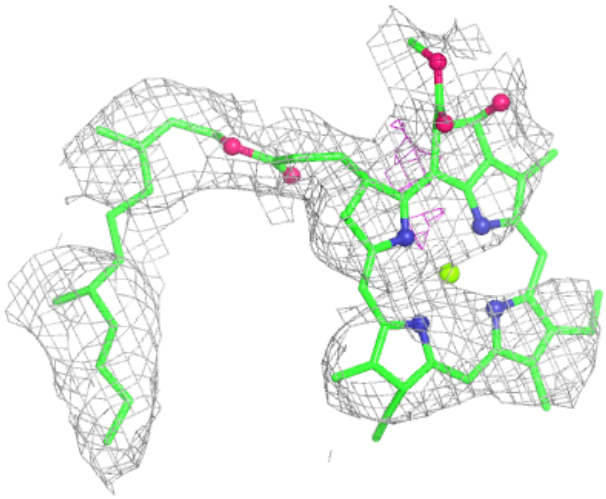


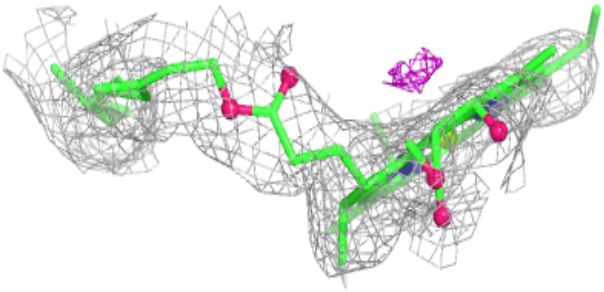




**Electron density around CLA B 826:**

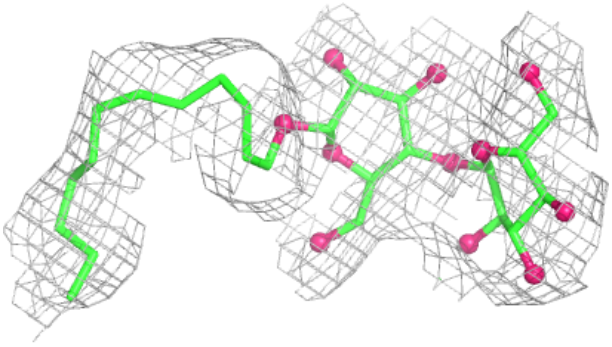
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

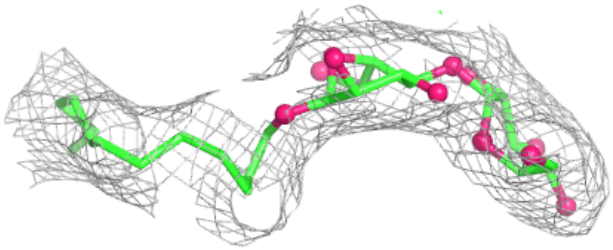


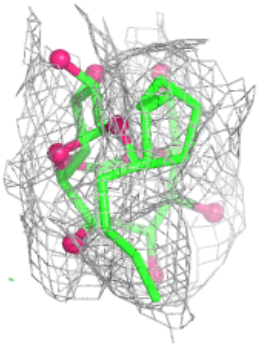


**Electron density around LMU D 201:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

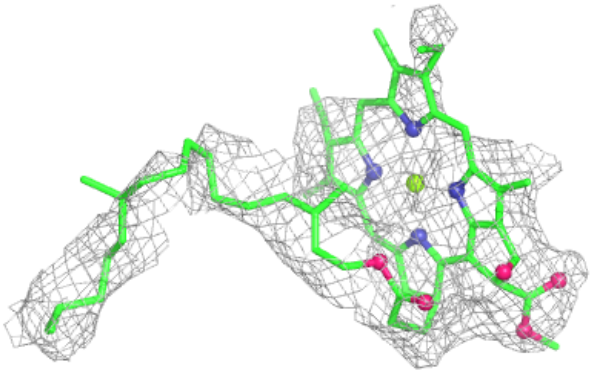


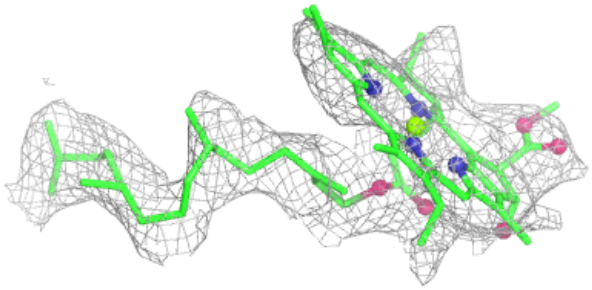


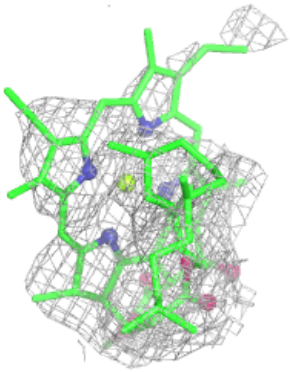


**Electron density around CLA L 203:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

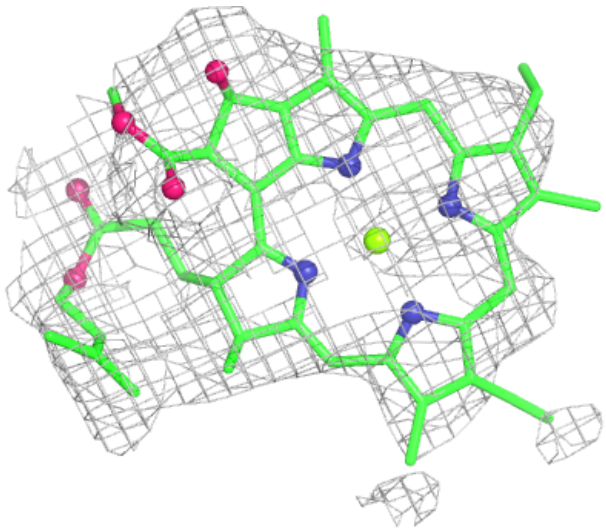


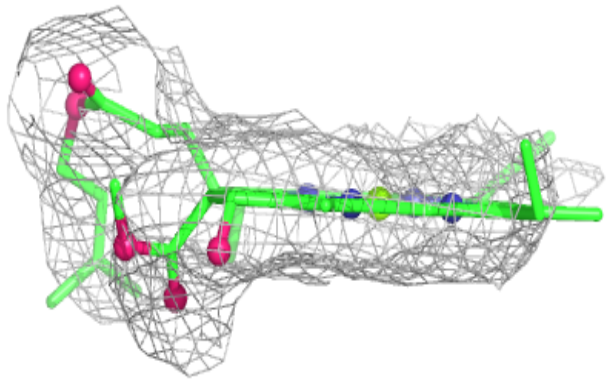


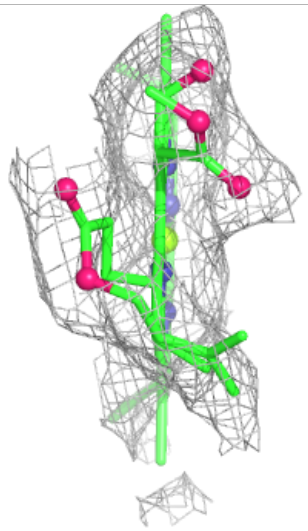


**Electron density around CLA 2 314:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

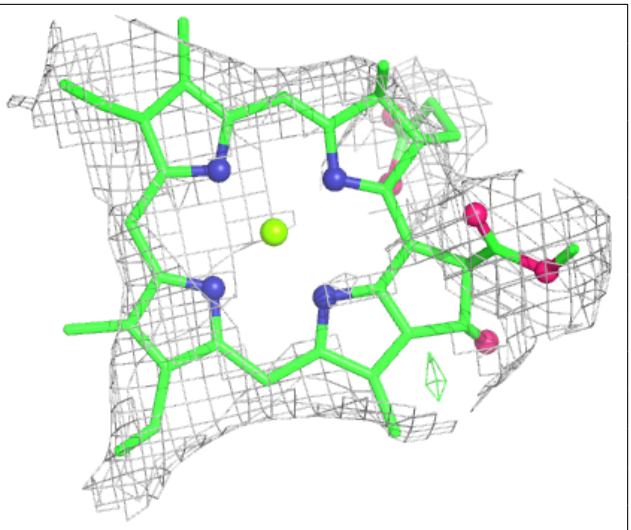






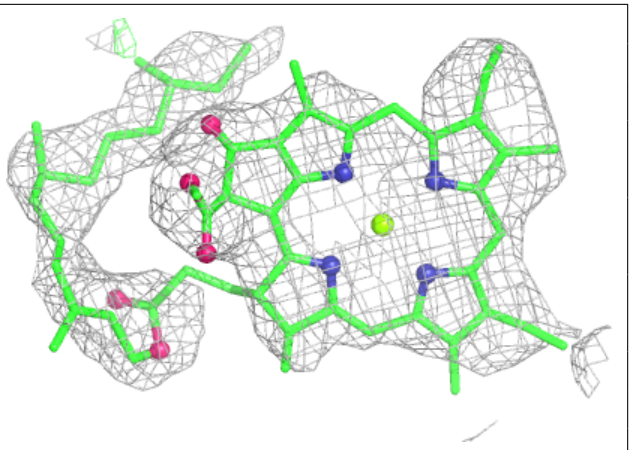
**Electron density around CLA B 807:**

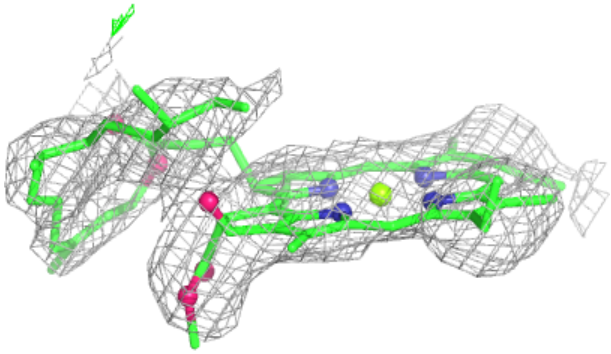
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

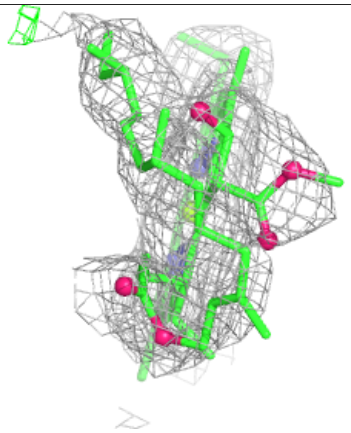


**Electron density around CLA B 808:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

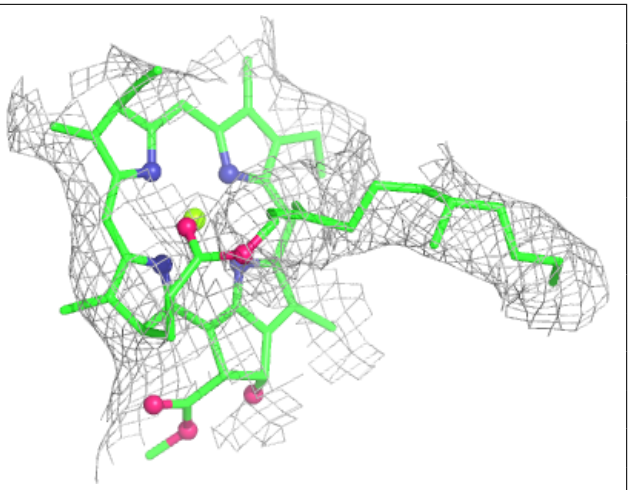


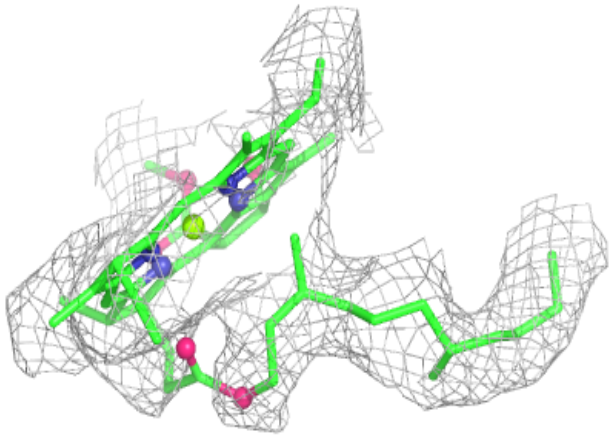


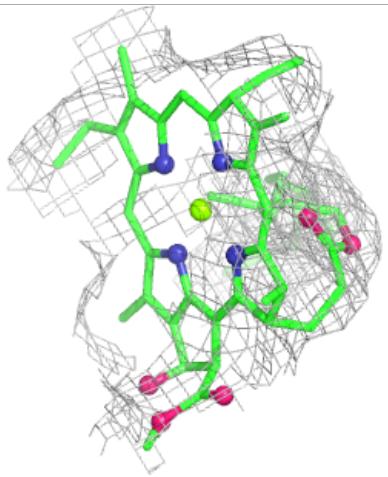


**Electron density around CLA 2 303:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

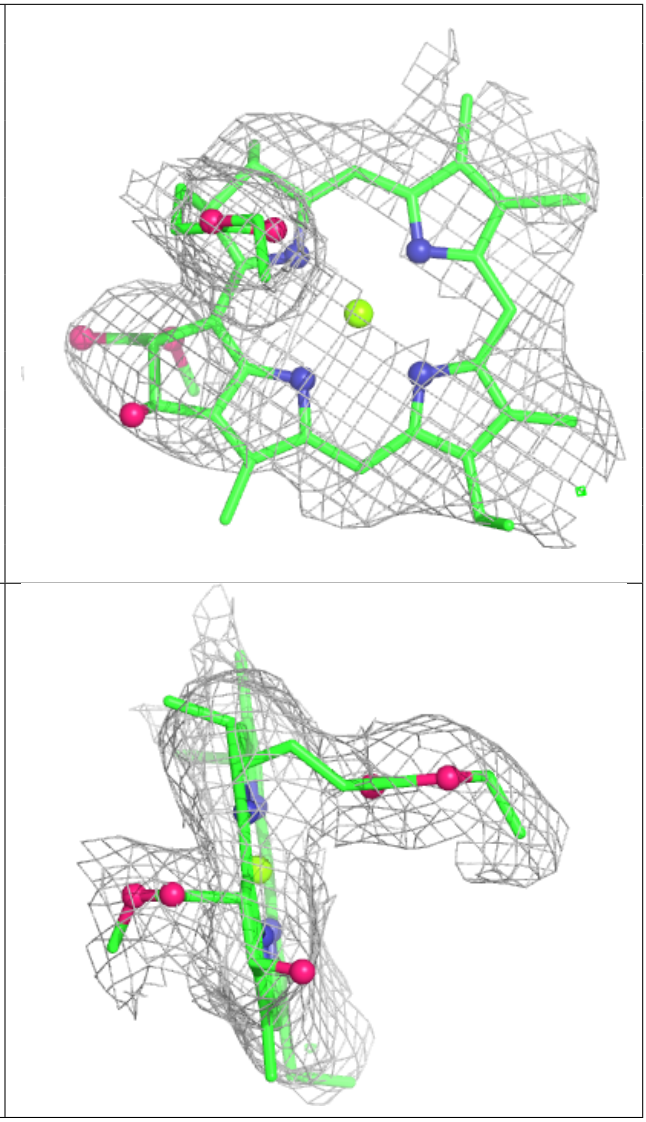






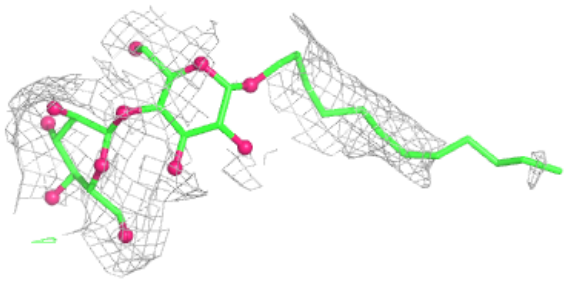
**Electron density around CLA L 207:**

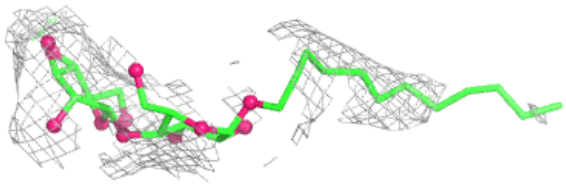
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

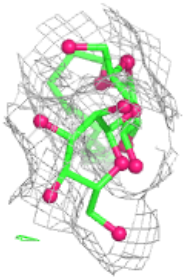


**Electron density around LMU A 855:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

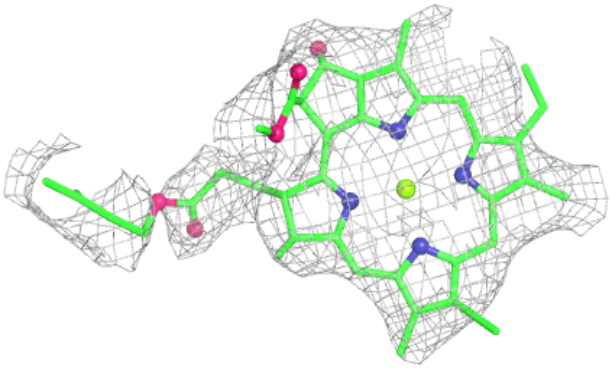


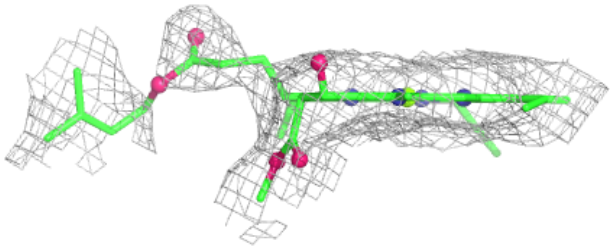




**Electron density around CLA F 201:**

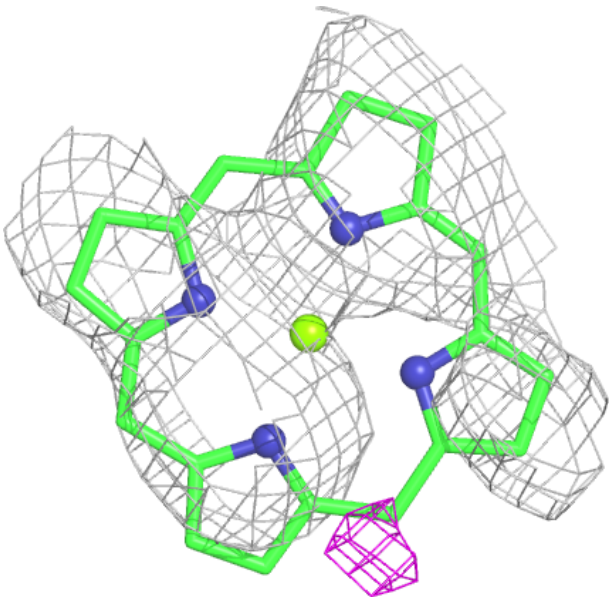
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

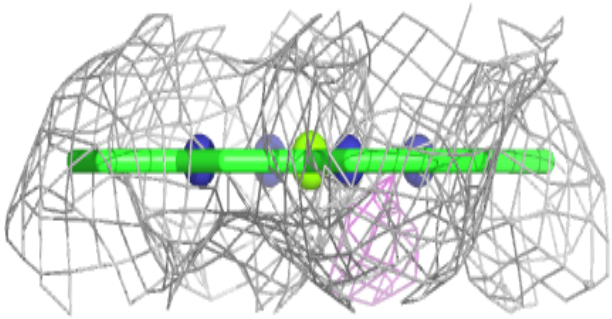


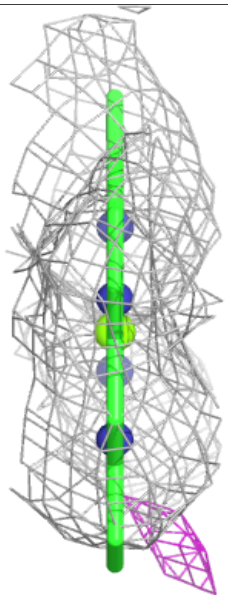


**Electron density around CLA 2 304:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

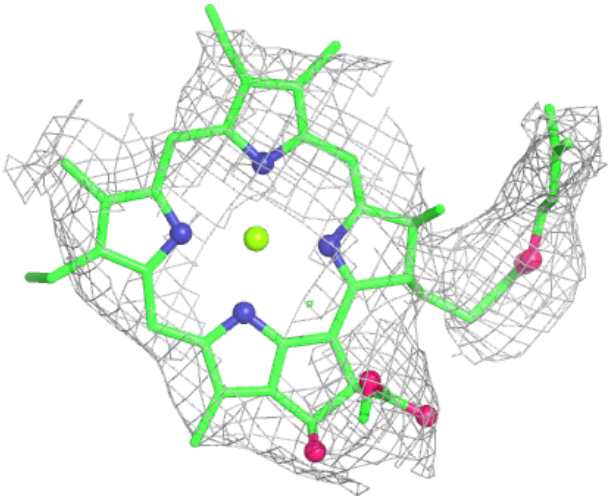


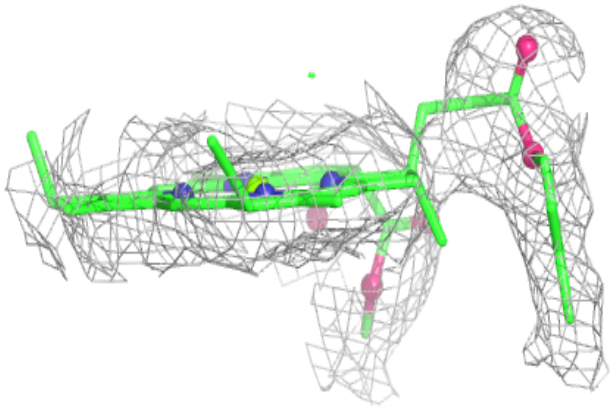


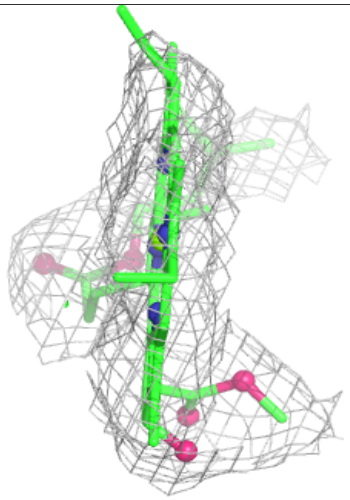


**Electron density around CLA A 813:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

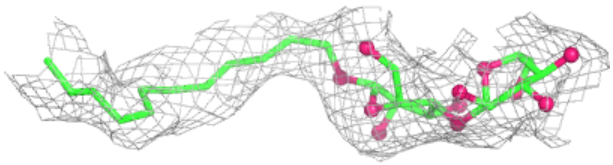


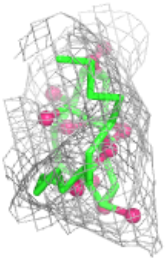




**Electron density around LMU 1 216:**

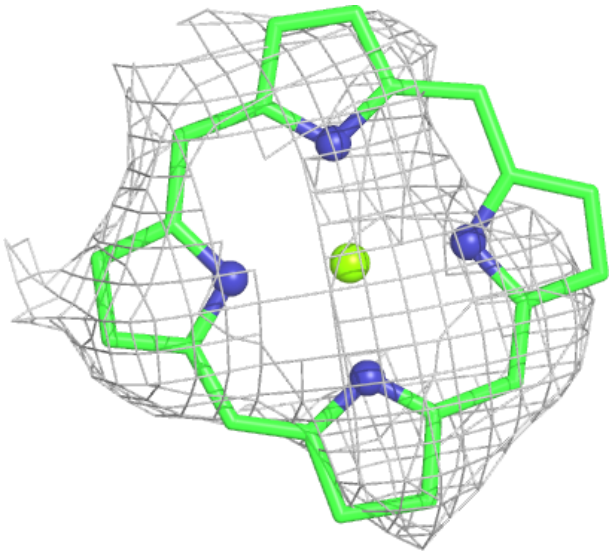
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

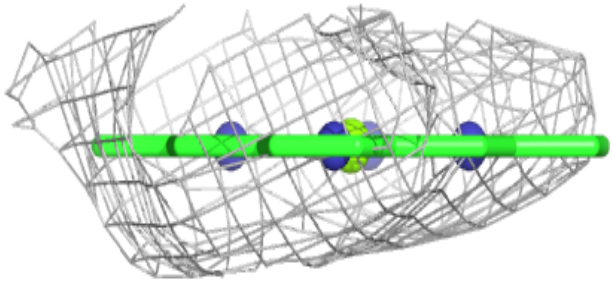


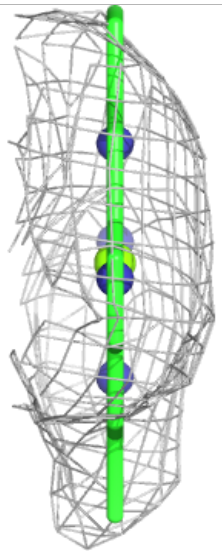


**Electron density around CLA 4 309:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

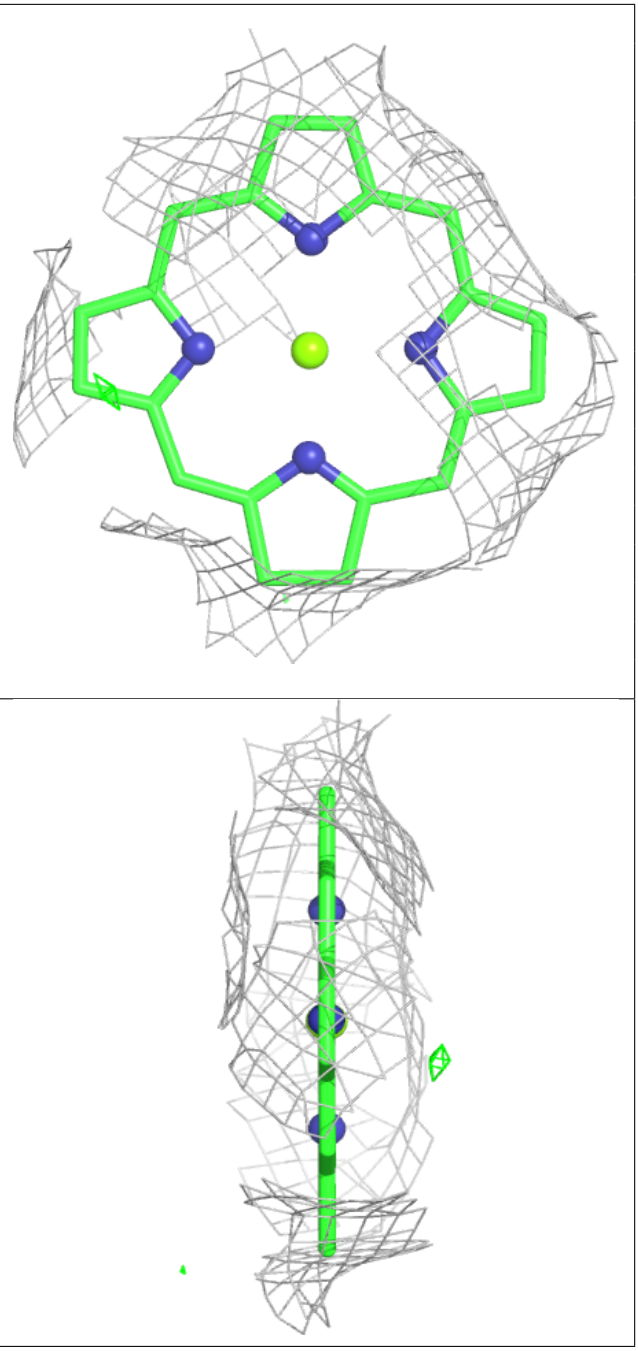






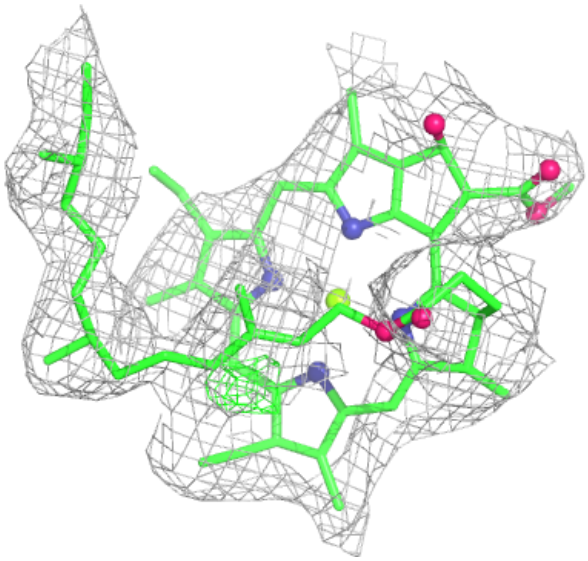
**Electron density around CLA 3 308:**

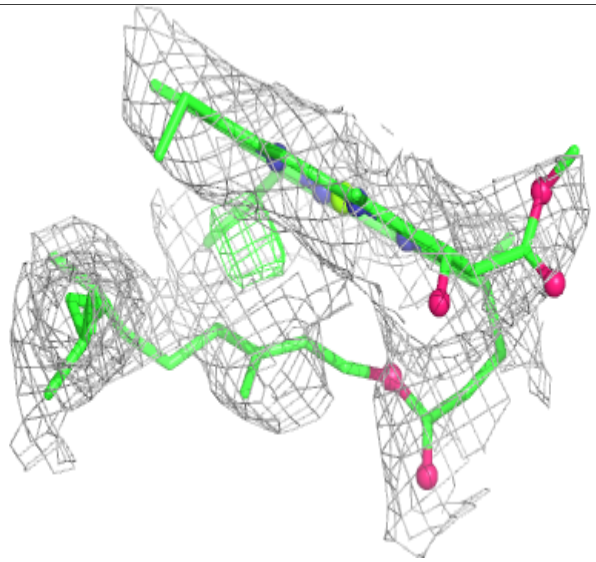
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



**Electron density around CLA B 820:**

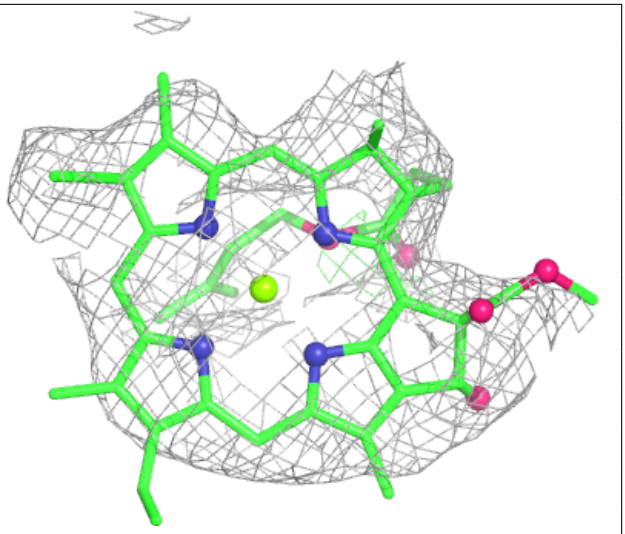
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

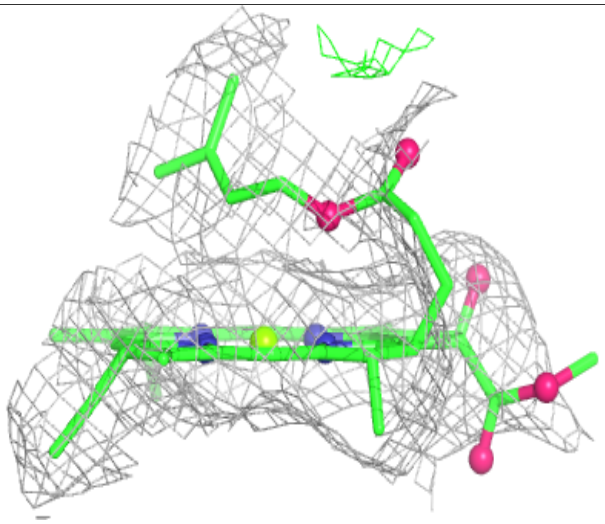


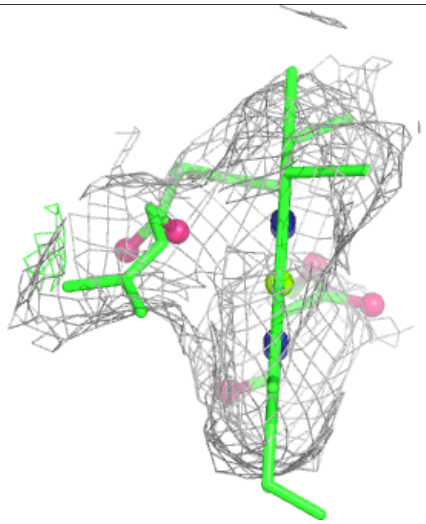


**Electron density around CLA B 821:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

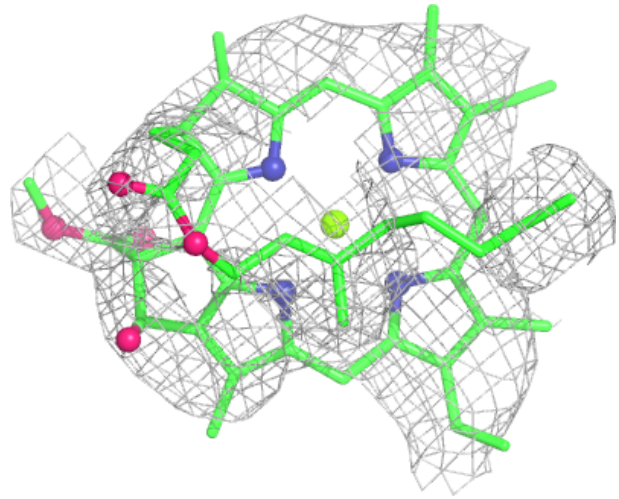


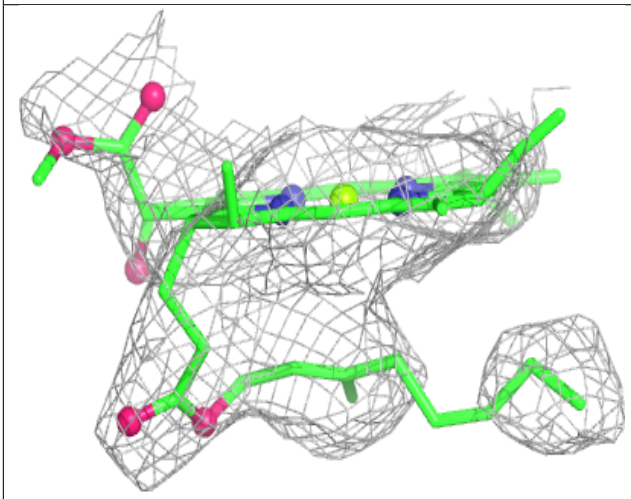


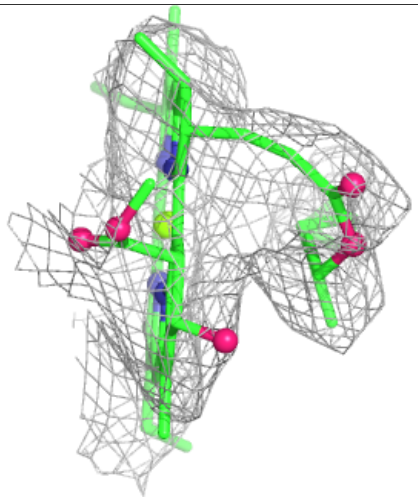


**Electron density around CLA A 816:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

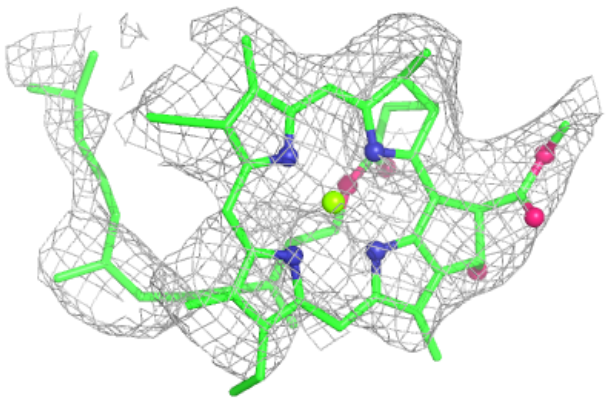


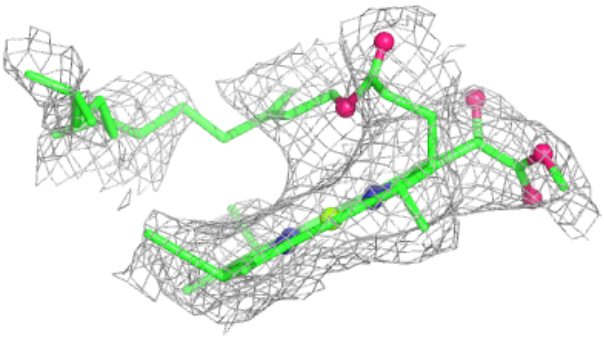


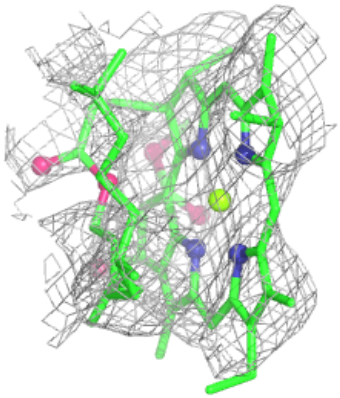


**Electron density around CLA I 102:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

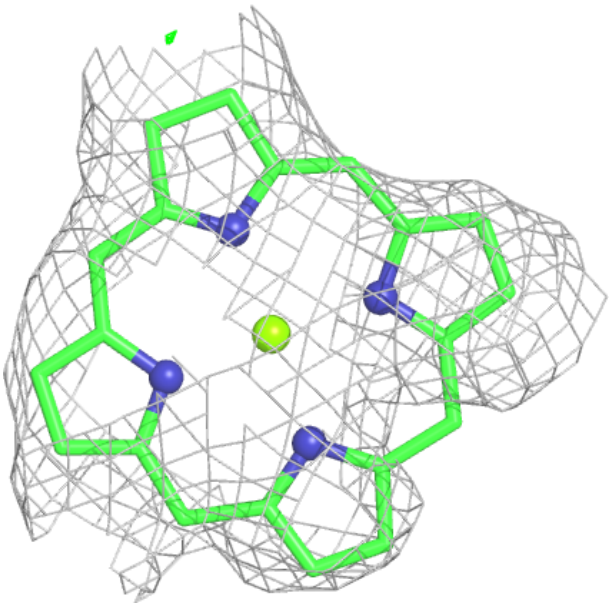


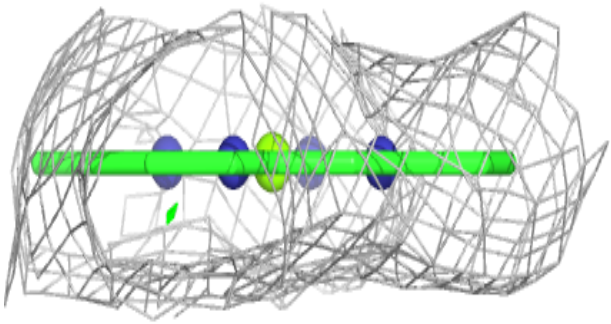


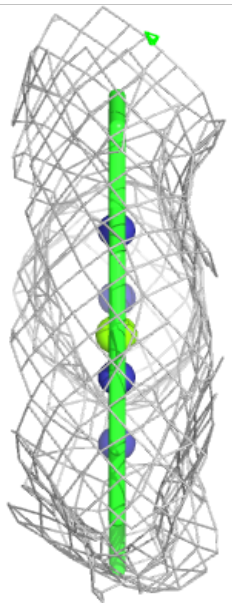


**Electron density around CLA 2 315:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

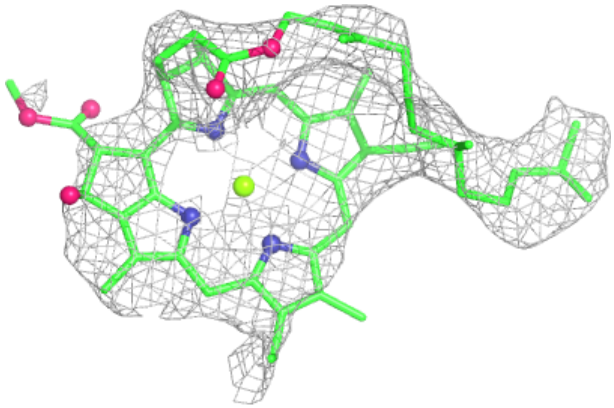


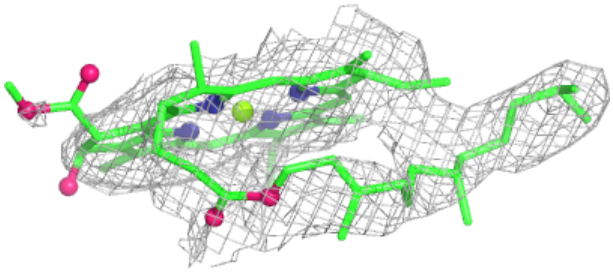


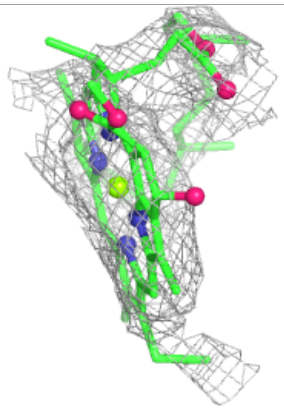


**Electron density around CLA A 818:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

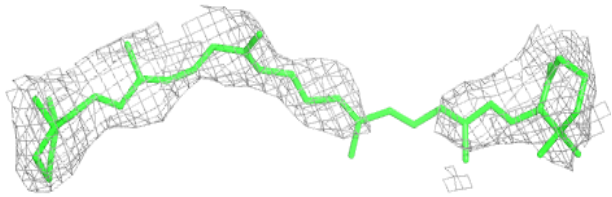


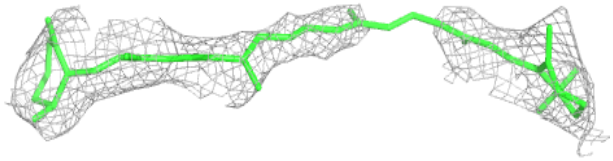


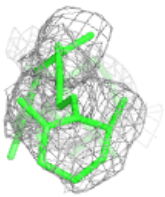


**Electron density around BCR I 101:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

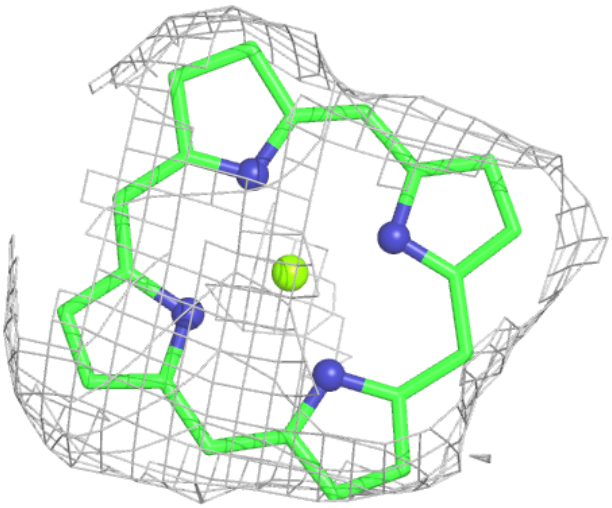


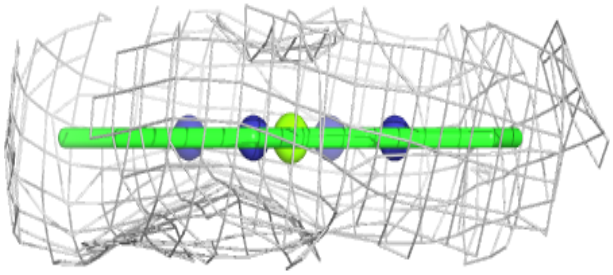


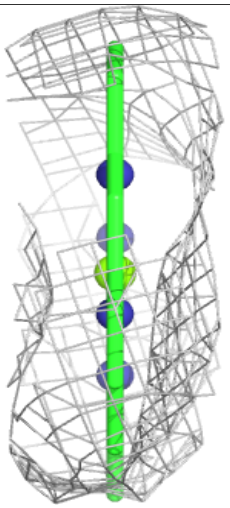


**Electron density around CLA 3 304:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

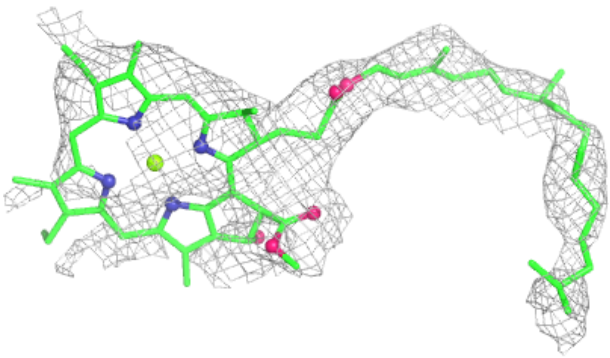


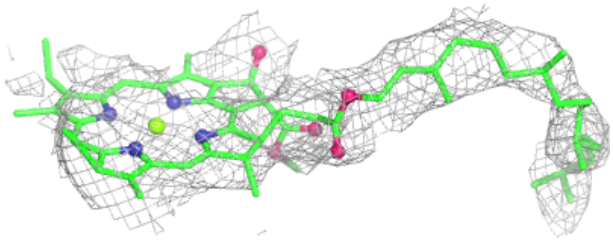


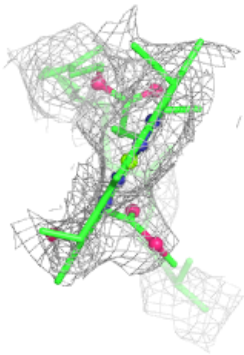


**Electron density around CLA B 827:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

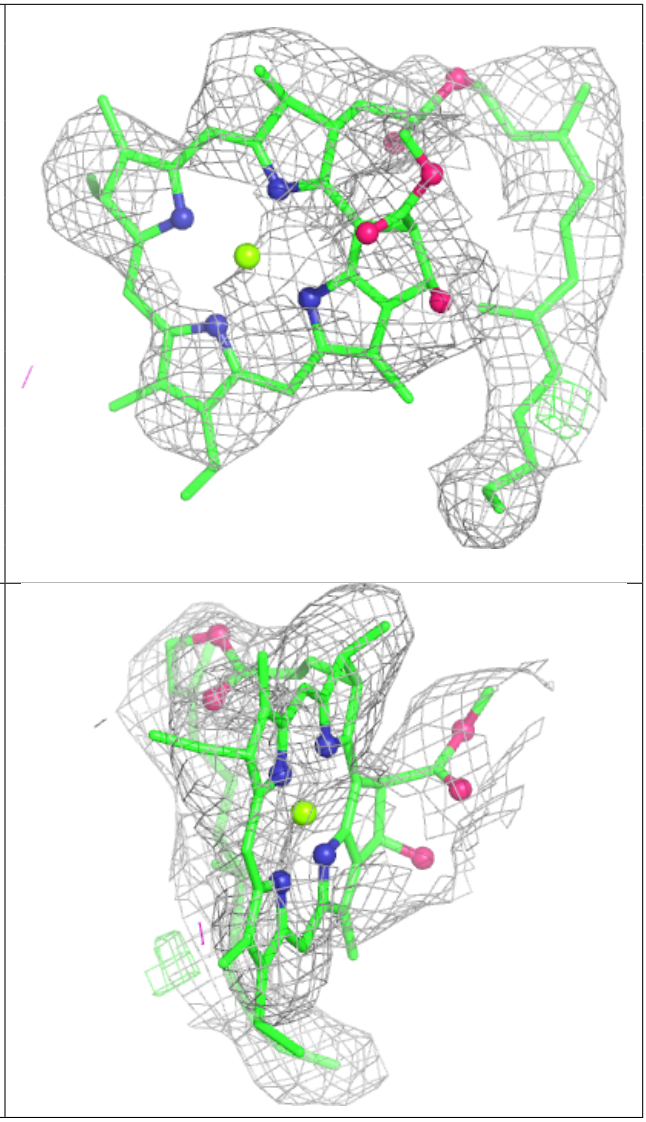






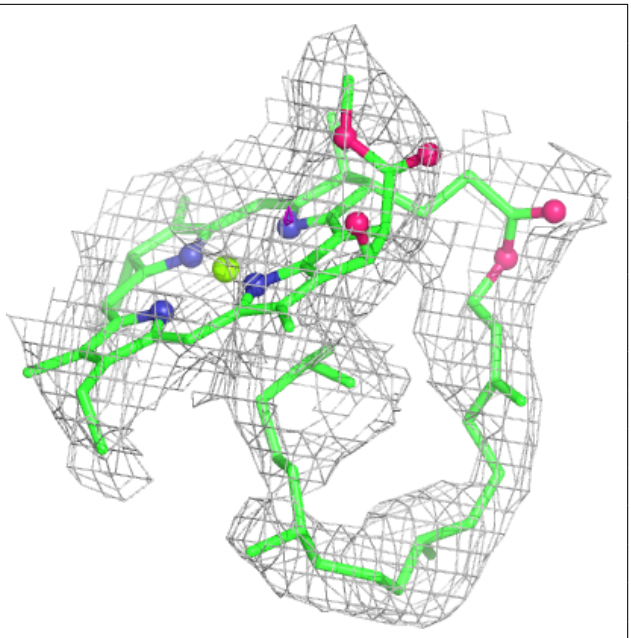
**Electron density around CLA B 832:**

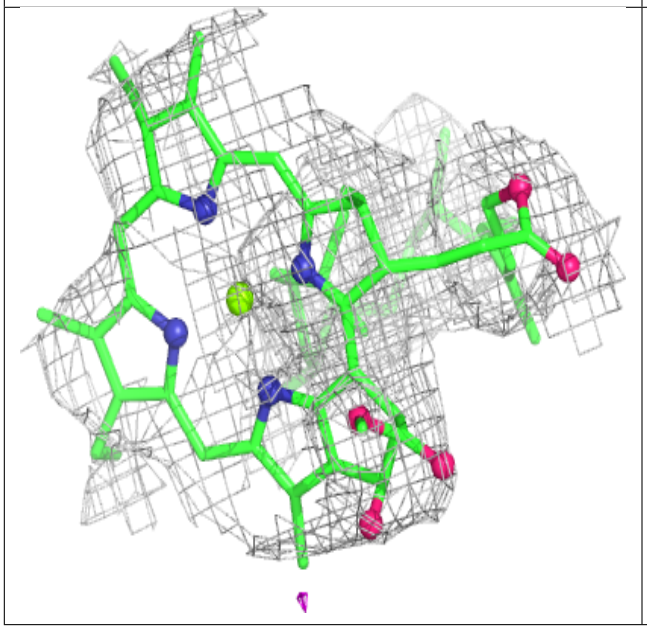
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

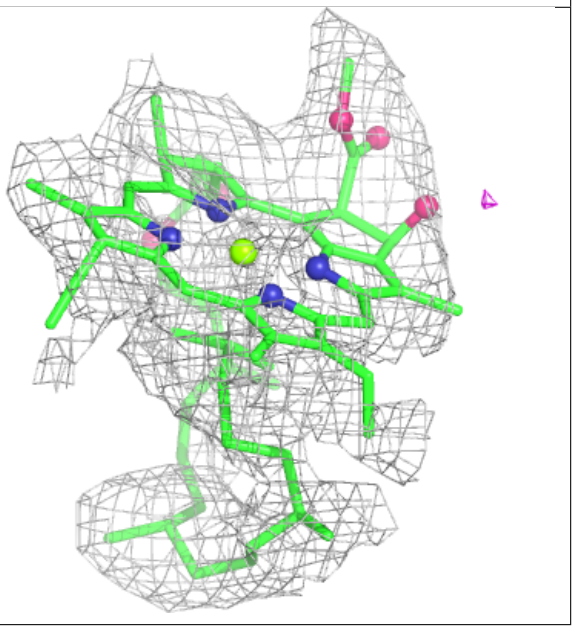


**Electron density around CLA 2 316:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

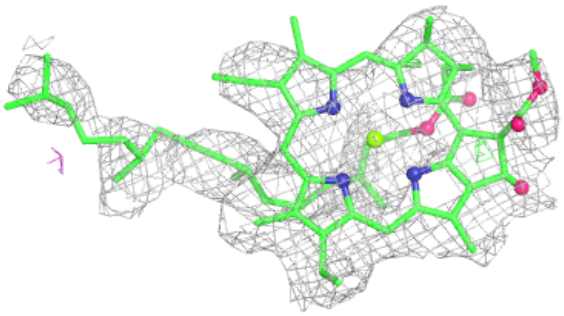


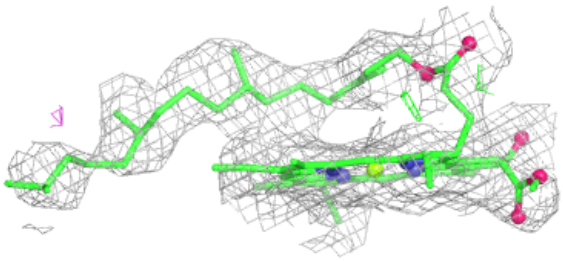


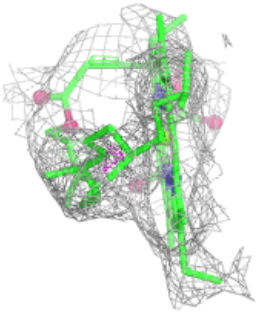


**Electron density around CLA B 806:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

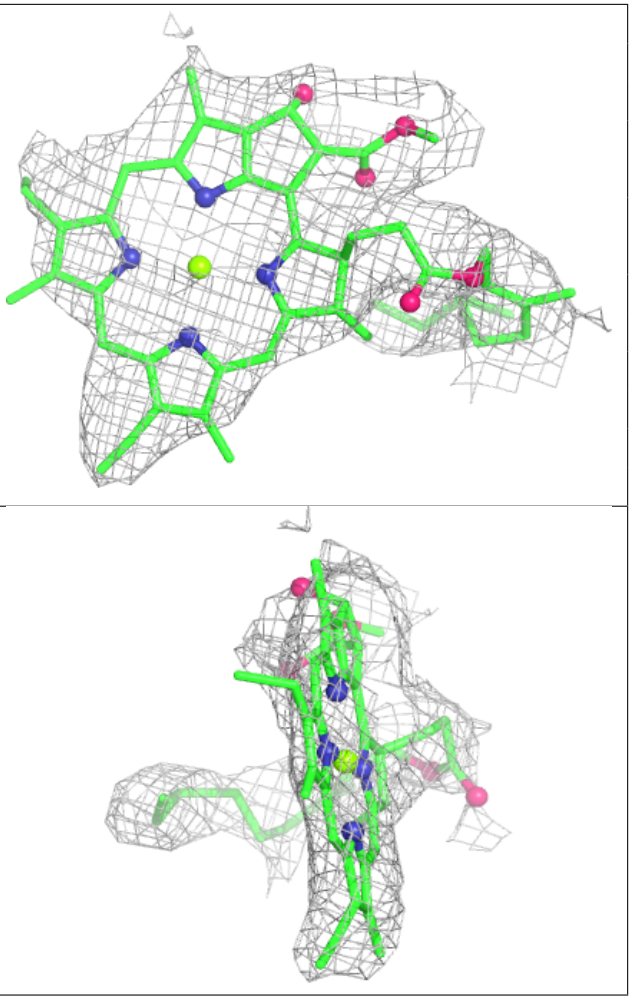






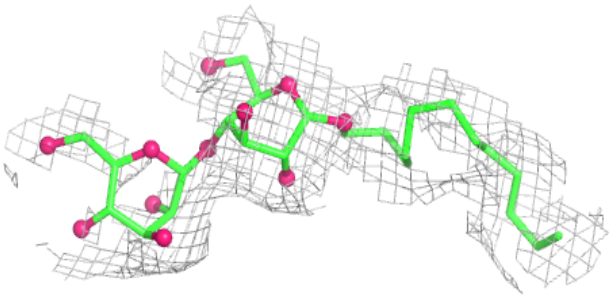
**Electron density around CLA A 806:**

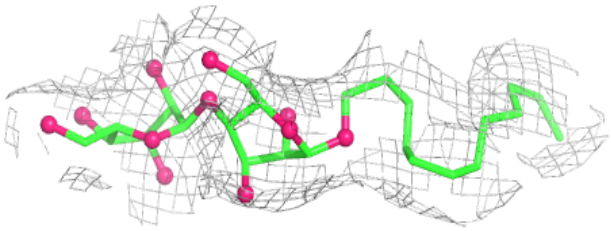
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

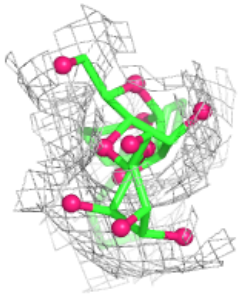


**Electron density around LMU 3 319:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

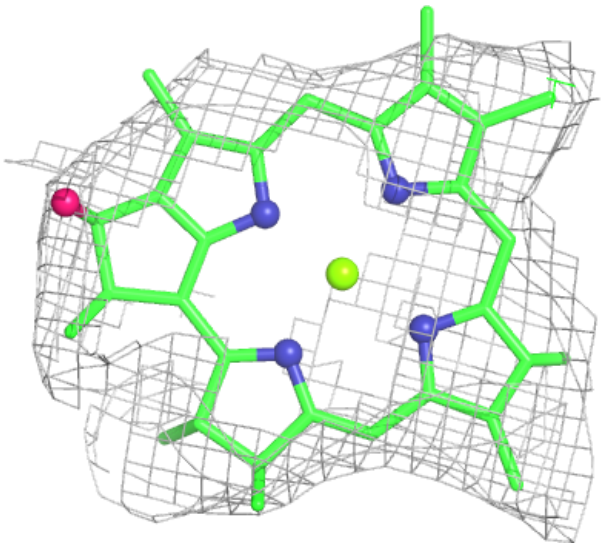


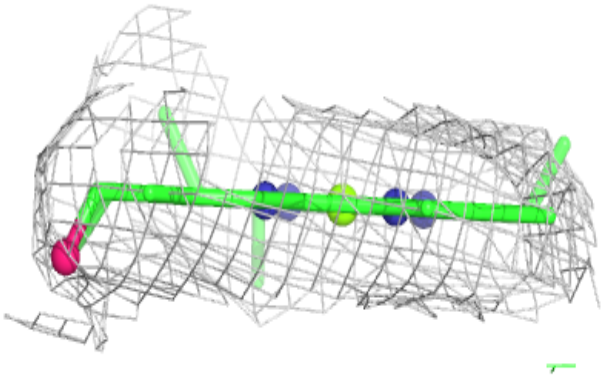


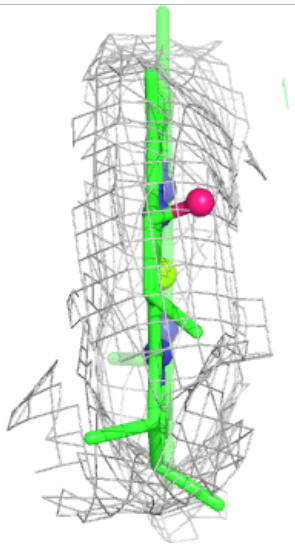


**Electron density around CLA 4 313:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

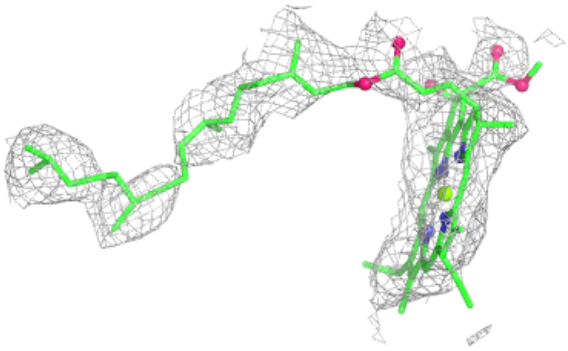


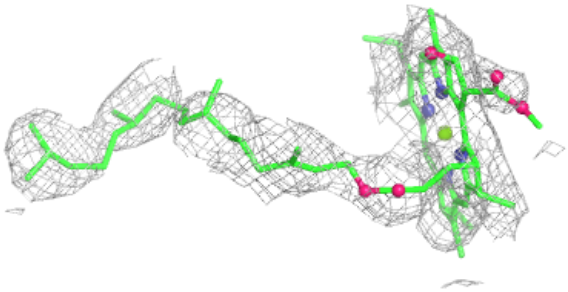


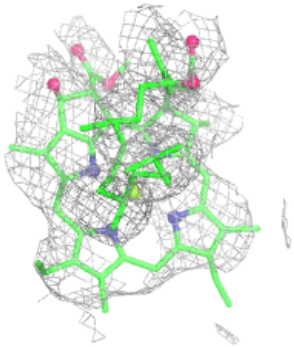


**Electron density around CLA A 828:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

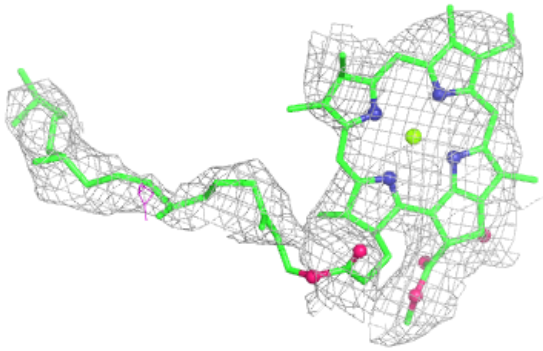


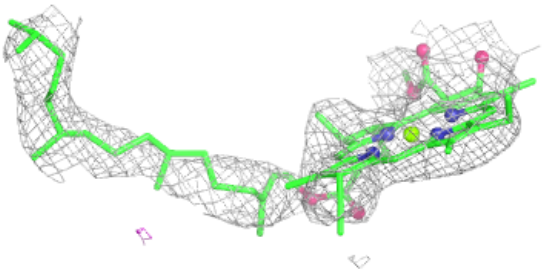




**Electron density around CLA A 851:**

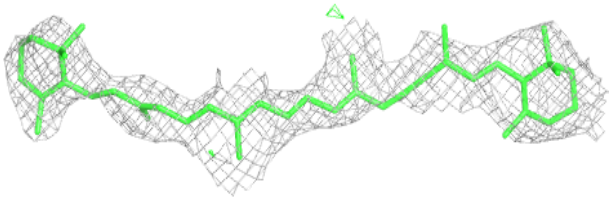
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

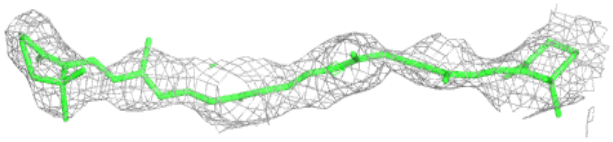


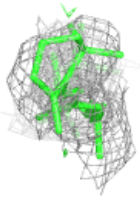


**Electron density around BCR B 846:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

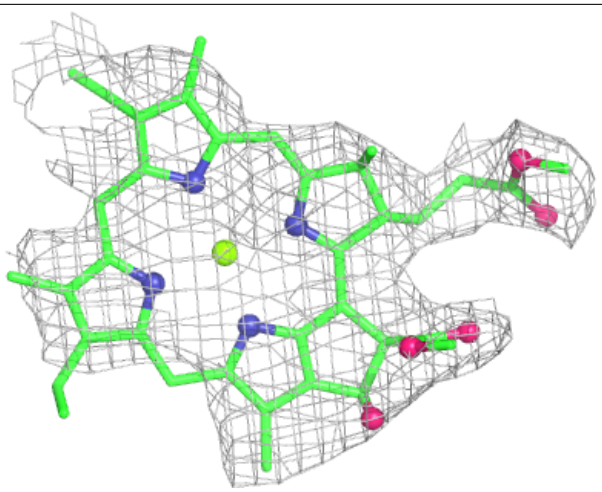


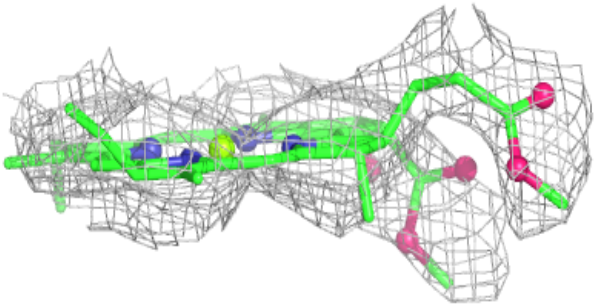


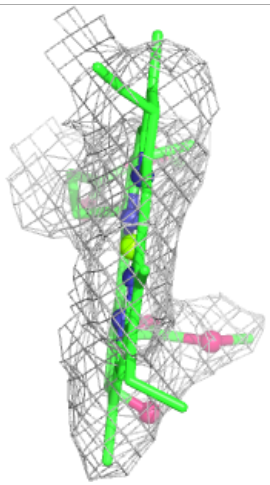


**Electron density around CLA A 803:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

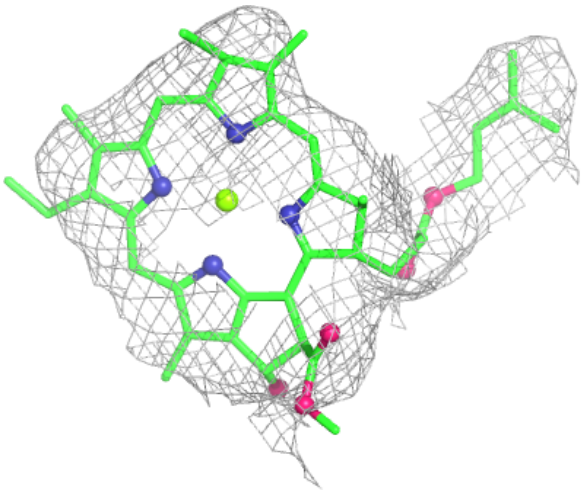


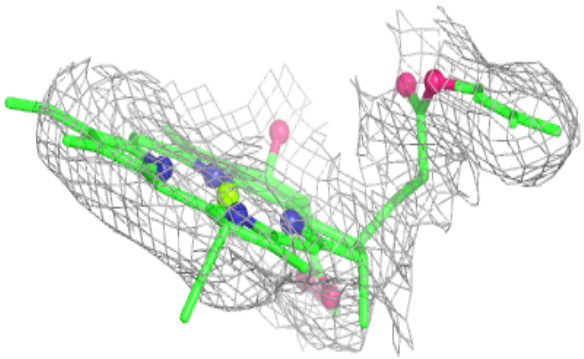




**Electron density around CLA A 832:**

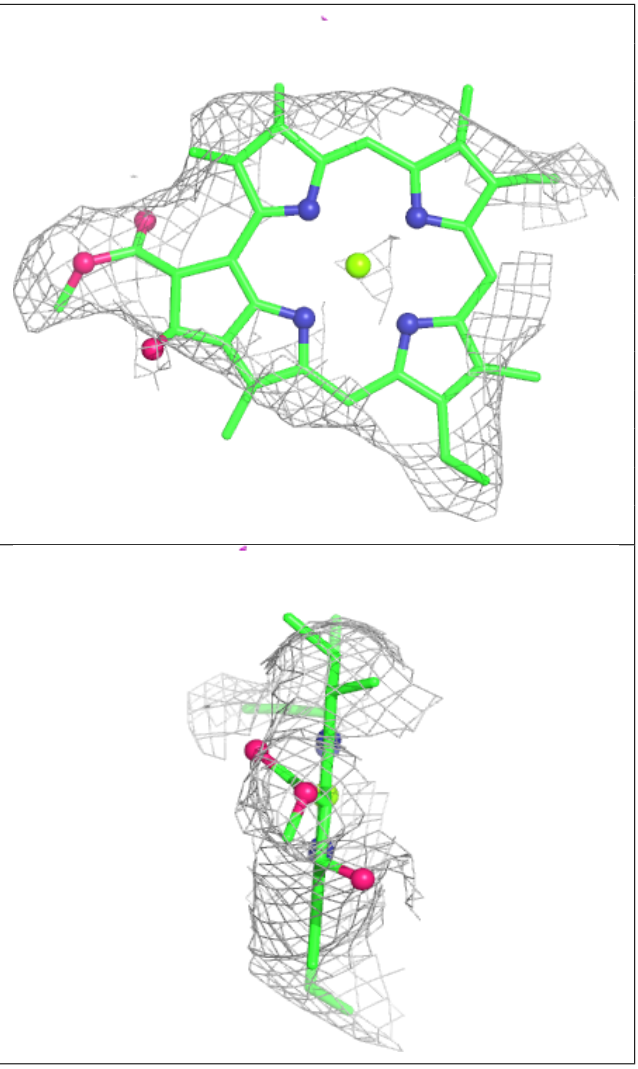
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





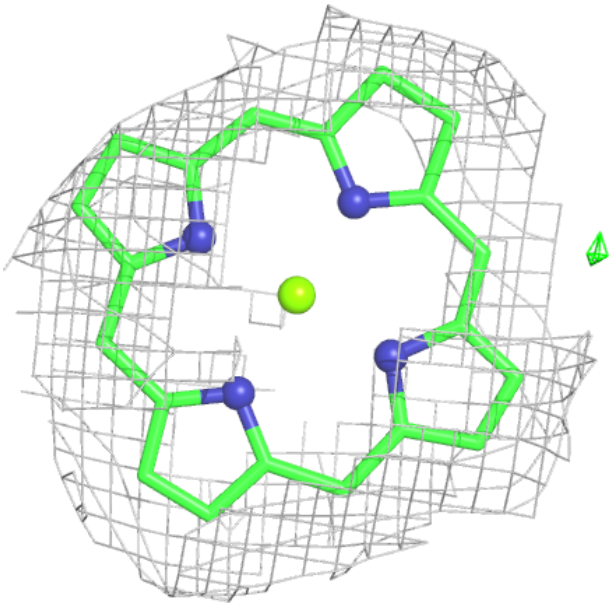
**Electron density around CLA 1 202:**

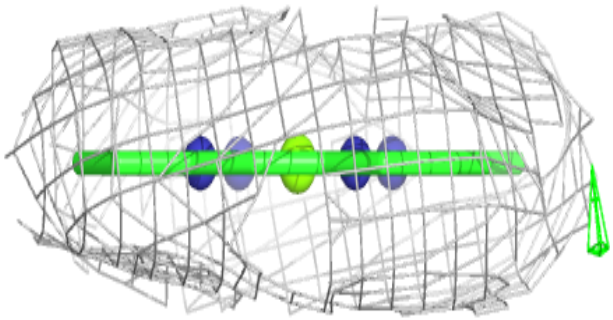
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

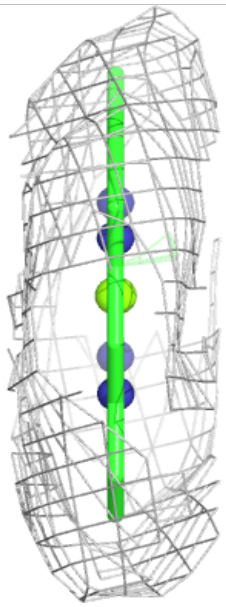


**Electron density around CLA 4 312:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

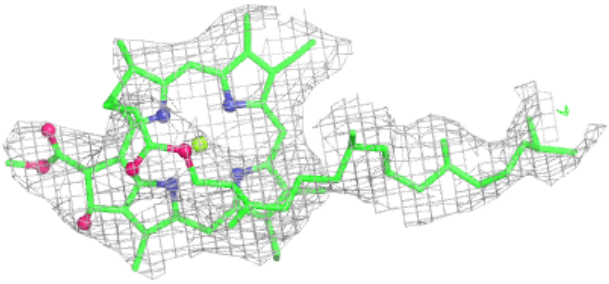


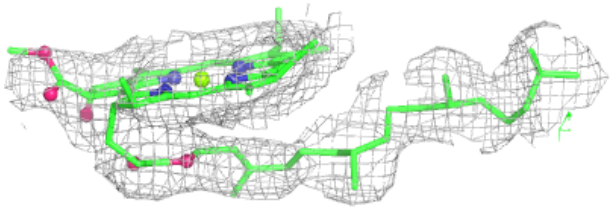


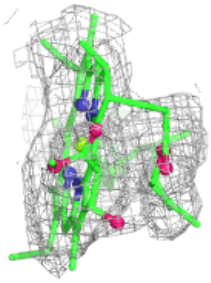


**Electron density around CLA A 835:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

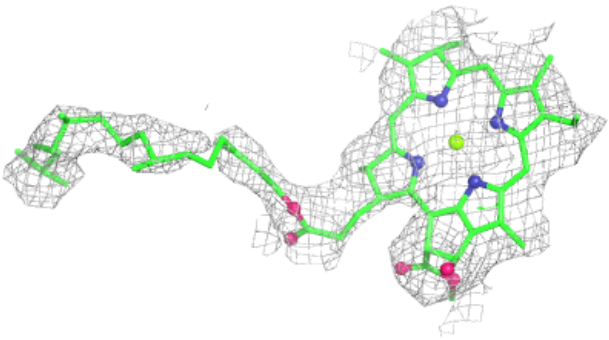


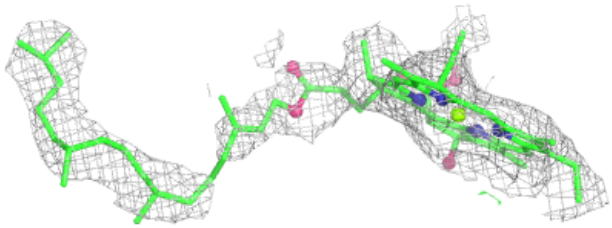




**Electron density around CLA B 814:**

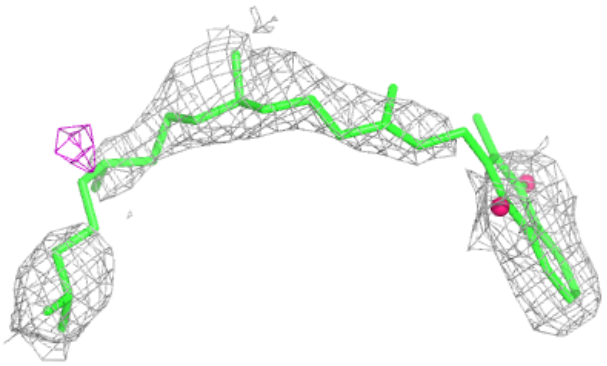
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

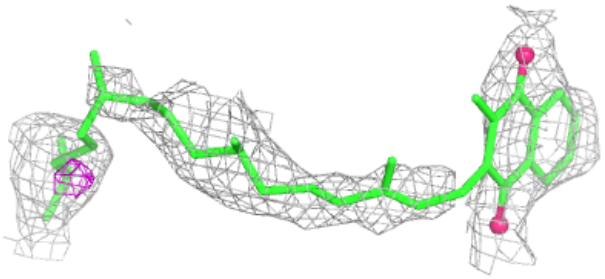


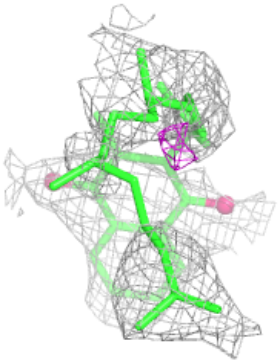


**Electron density around PQN B 843:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

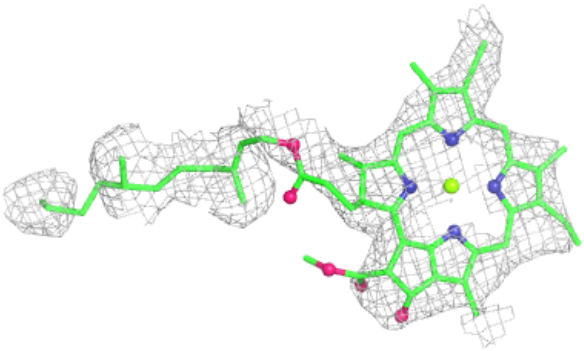


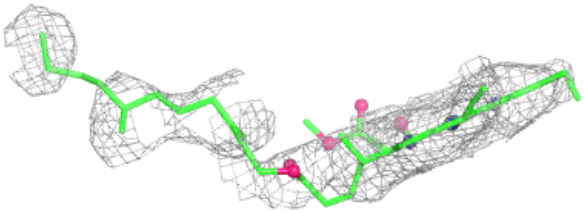


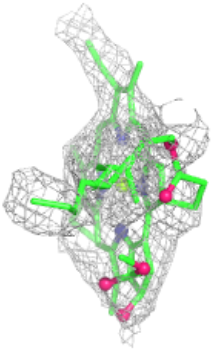


**Electron density around CLA H 108:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

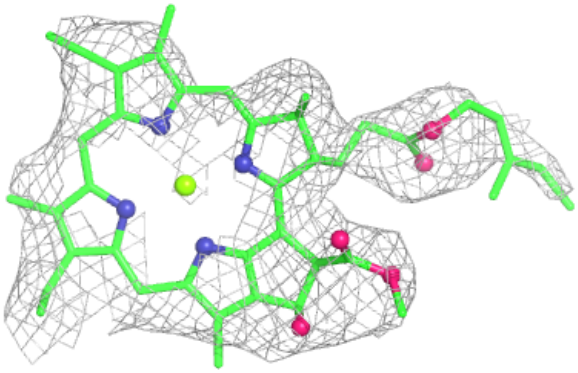


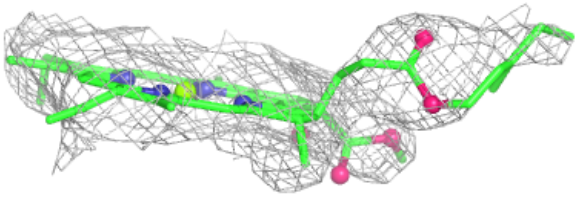


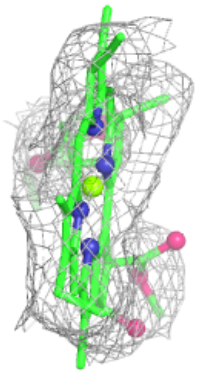


**Electron density around CLA A 837:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

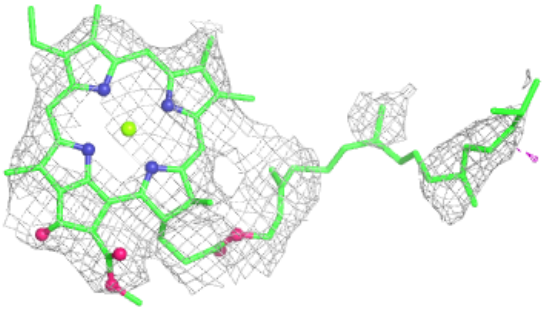


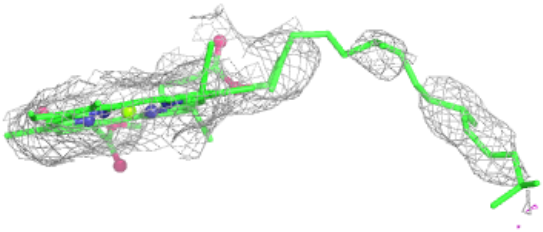


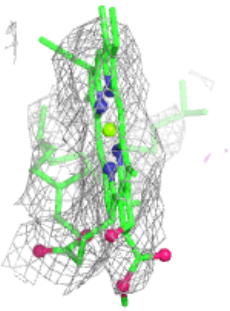


**Electron density around CLA B 803:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

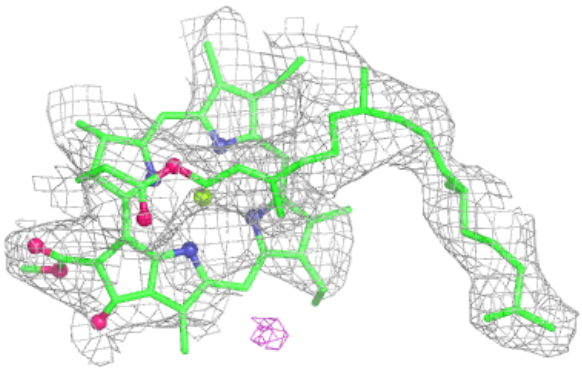


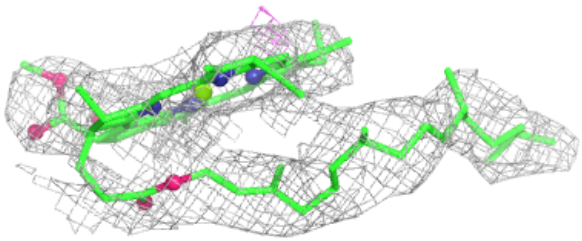


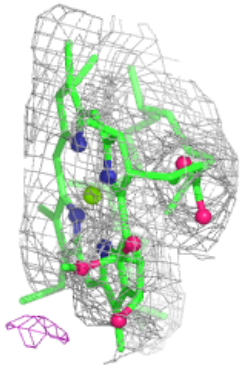


**Electron density around CLA B 838:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

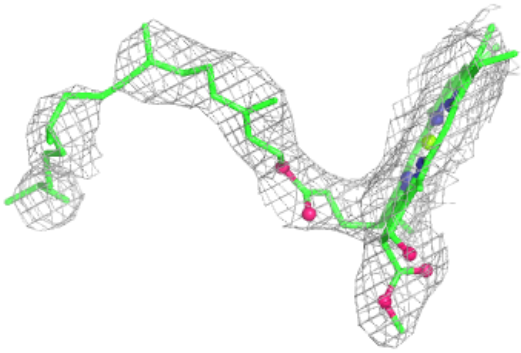


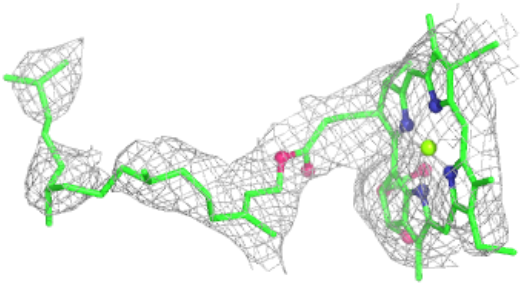


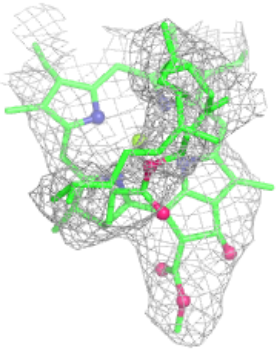


**Electron density around CLA B 840:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

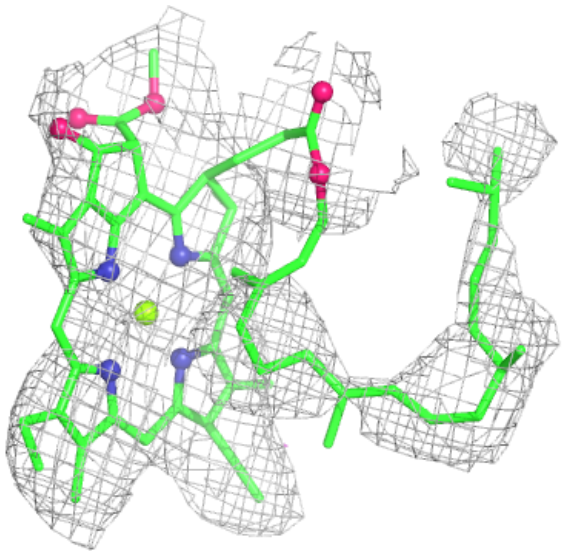


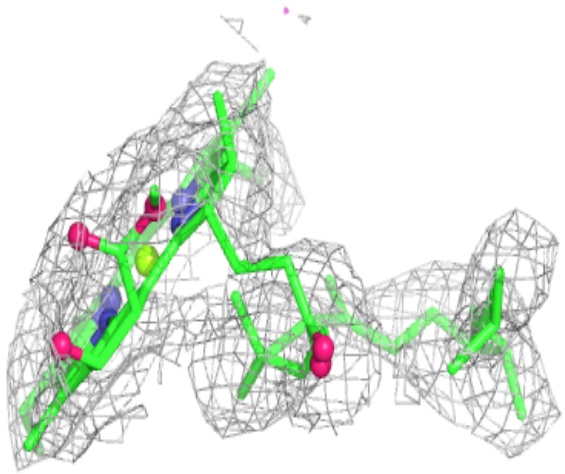


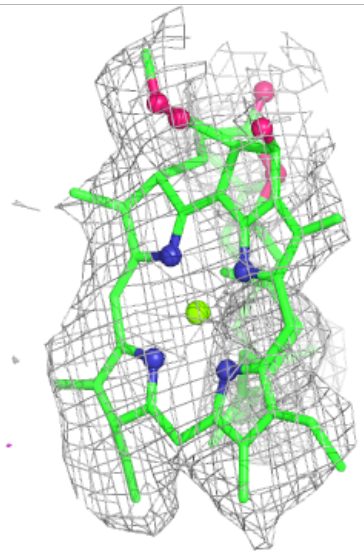


**Electron density around CLA B 824:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

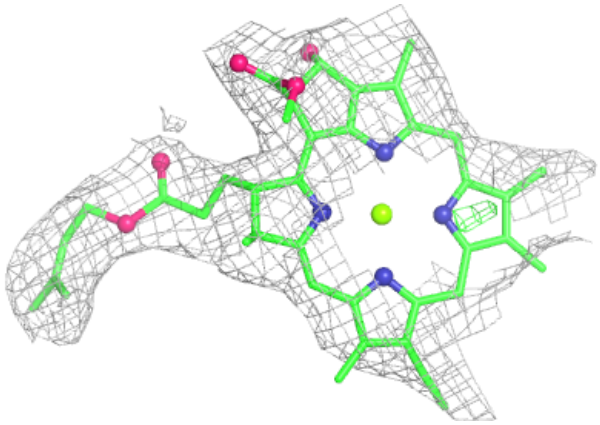


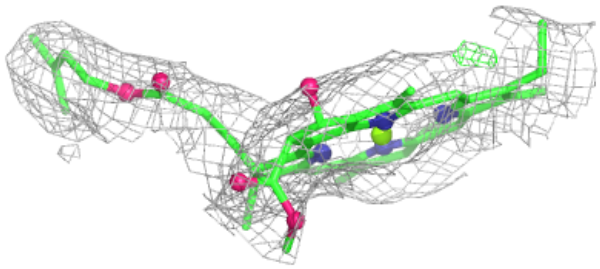


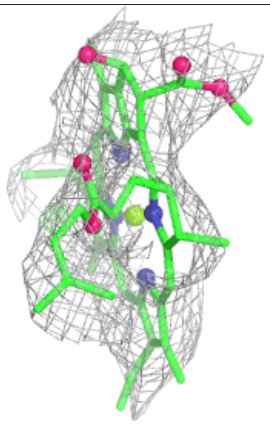


**Electron density around CLA B 833:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

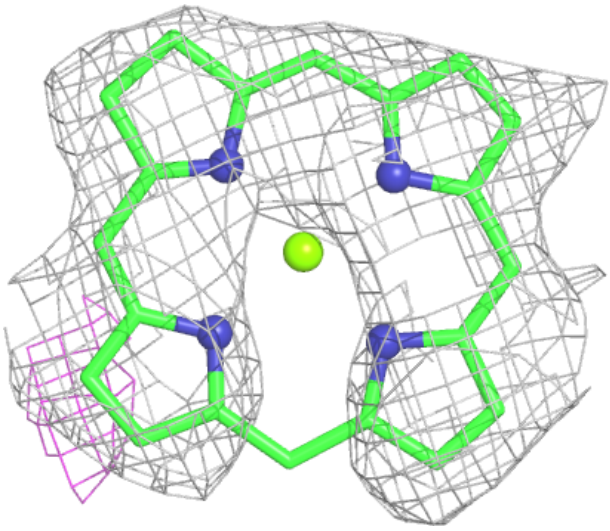


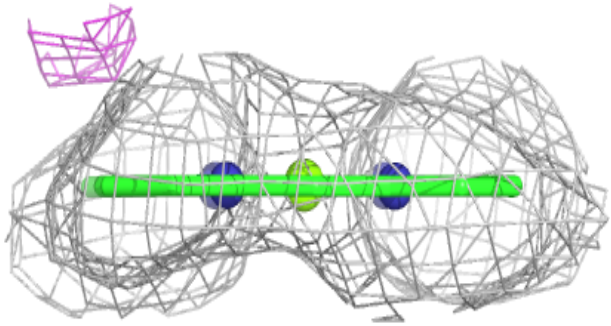


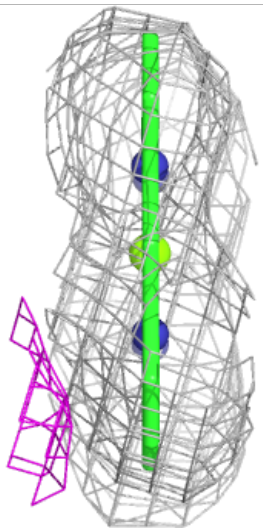


**Electron density around CLA B 811:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

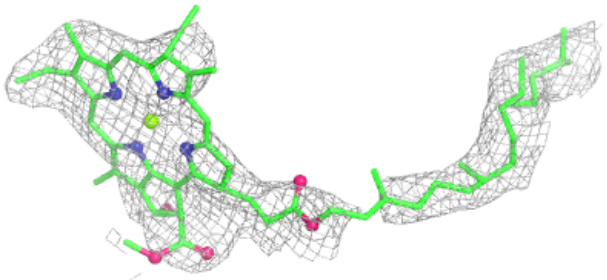


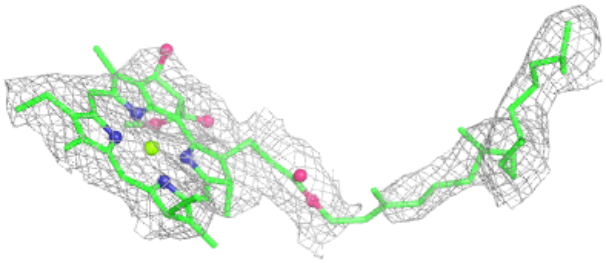


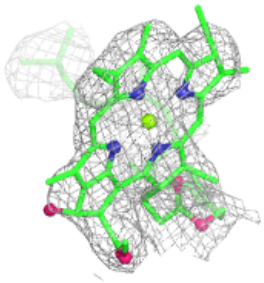


**Electron density around CLA A 850:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

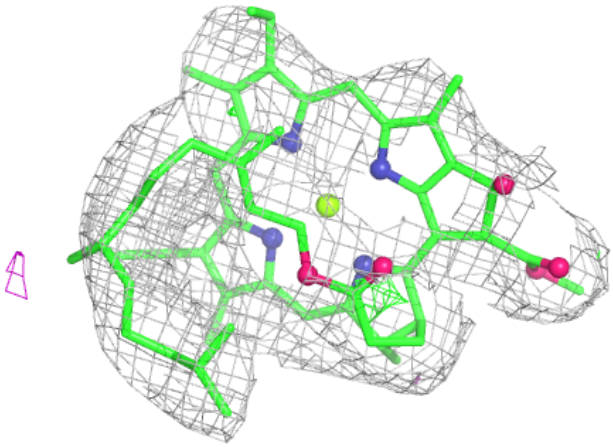


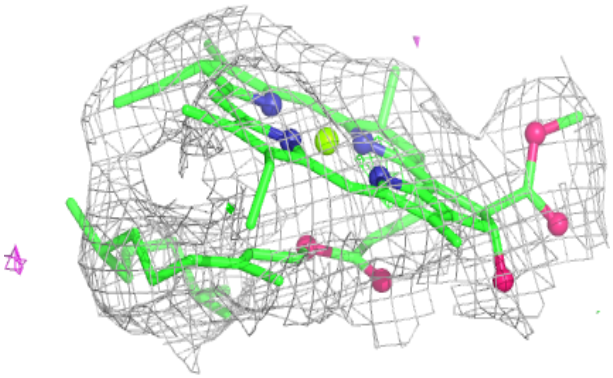




**Electron density around CLA B 810:**

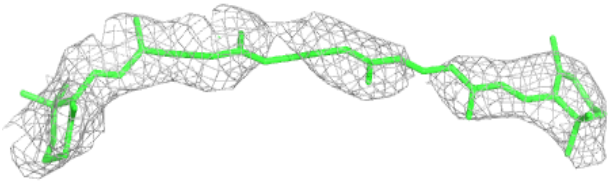
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

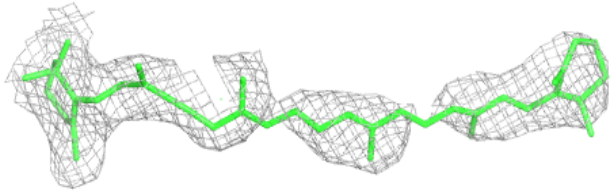


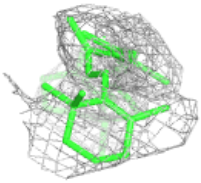


**Electron density around BCR F 203:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

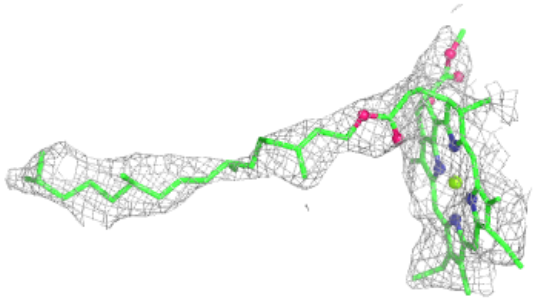


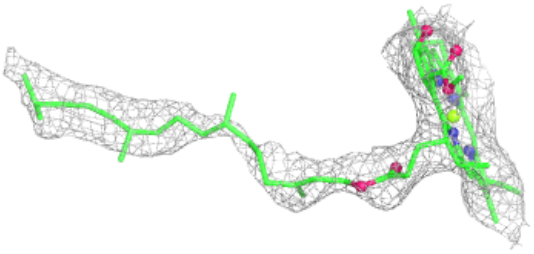


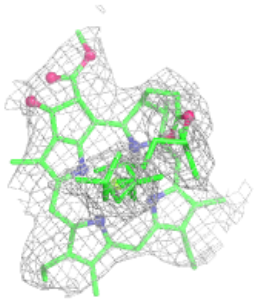


**Electron density around CLA B 829:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

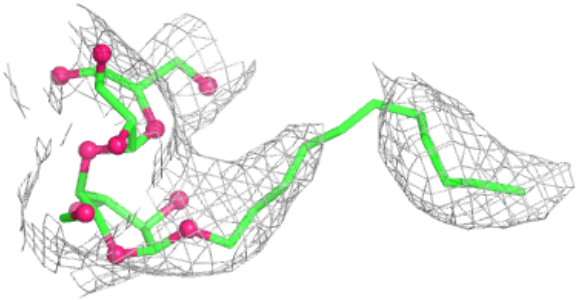


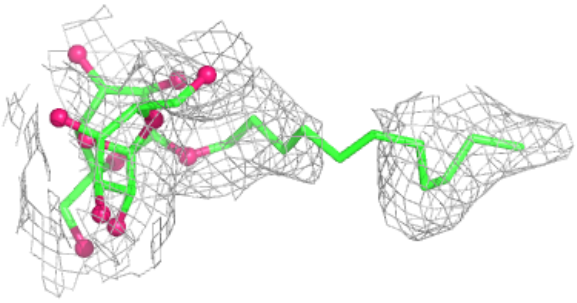


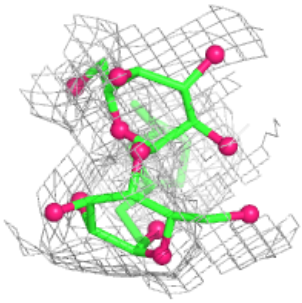


**Electron density around LMU 4 319:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

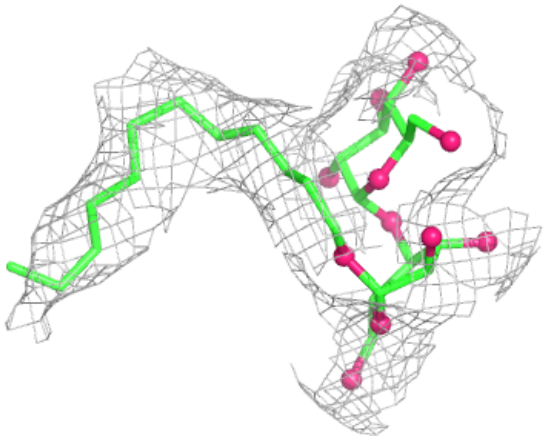


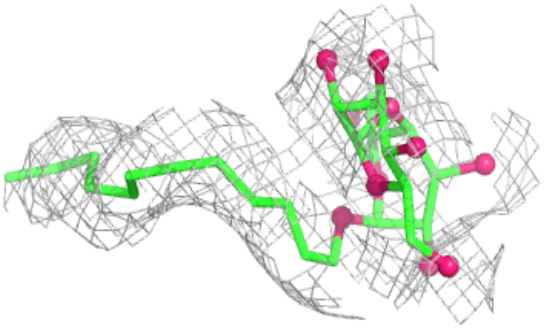


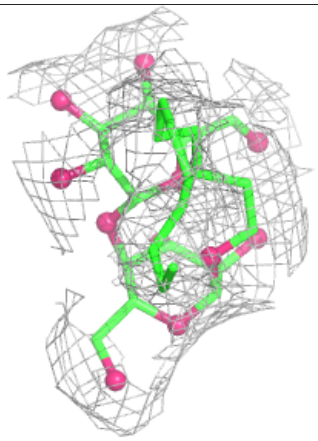


**Electron density around LMU H 105:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

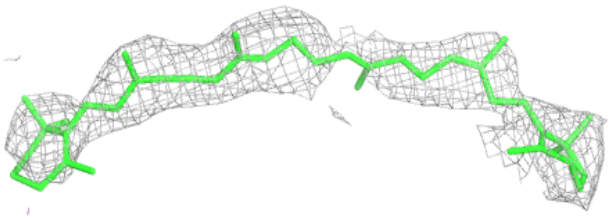


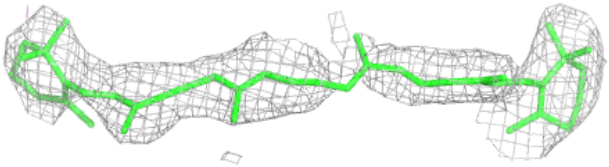


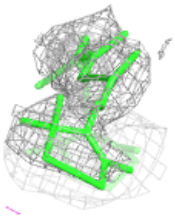


**Electron density around BCR B 801:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

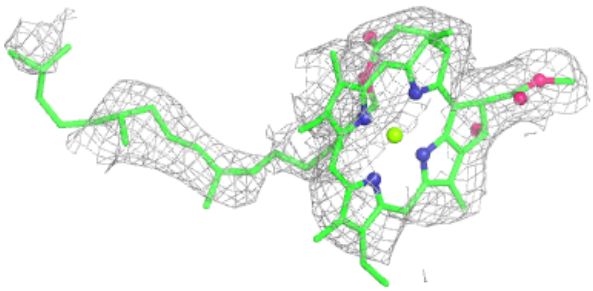


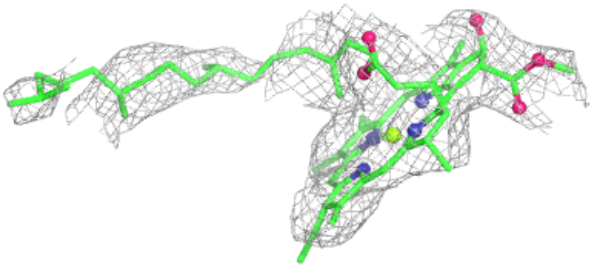


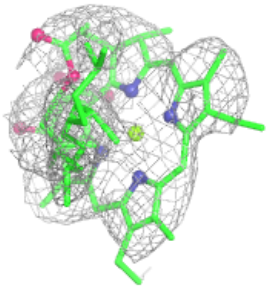


**Electron density around CLA A 838:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

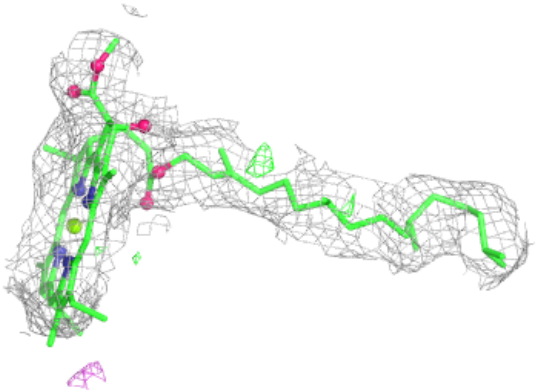


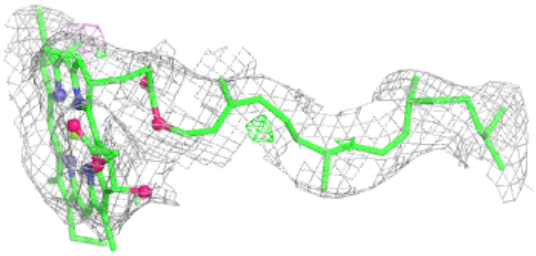


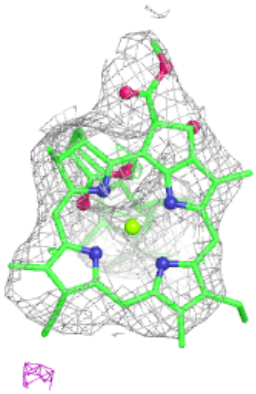


**Electron density around CLA A 826:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

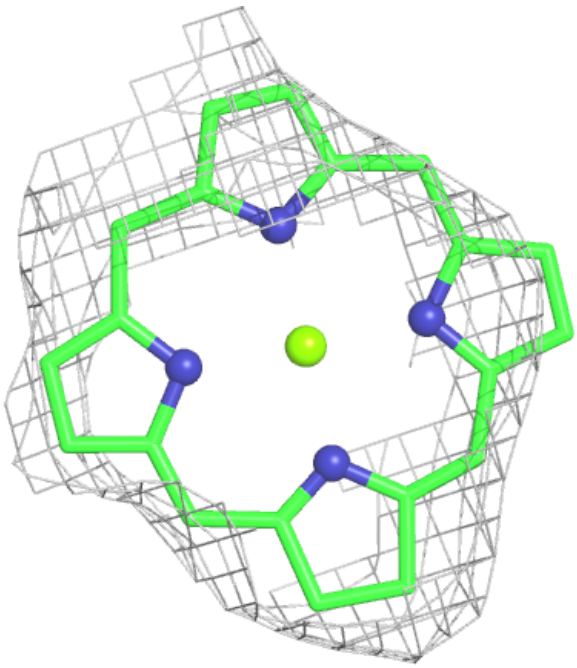


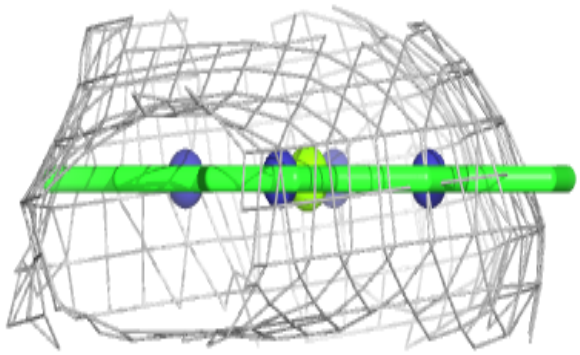


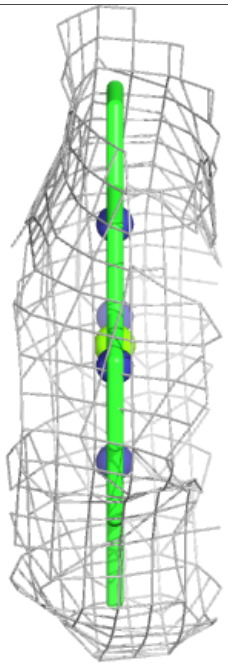


**Electron density around CLA 4 311:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

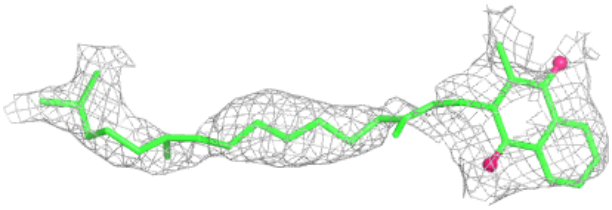


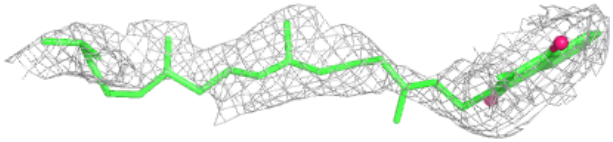


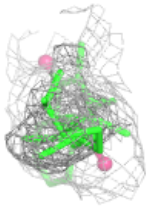


**Electron density around PQN A 842:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

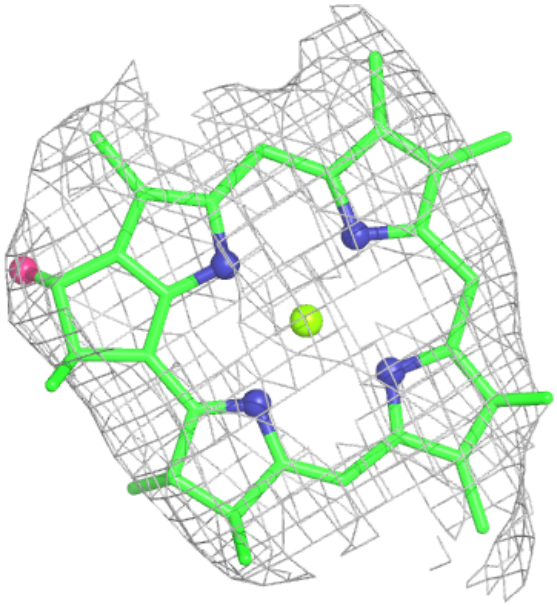


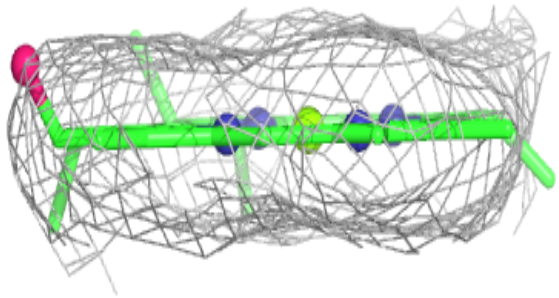


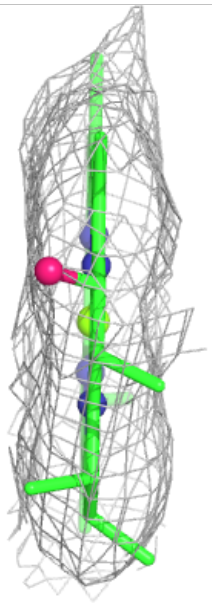


**Electron density around CLA F 205:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

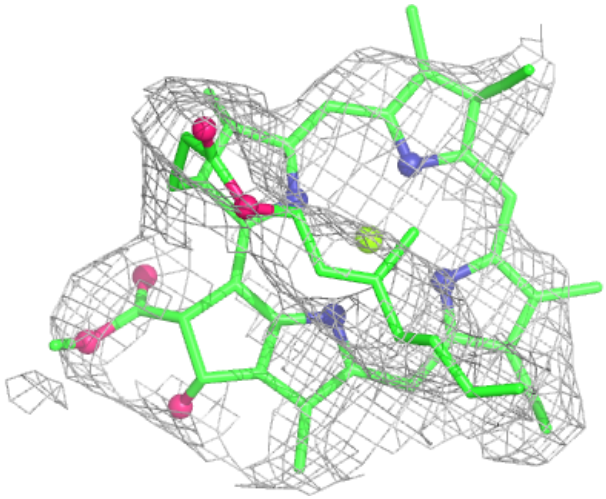


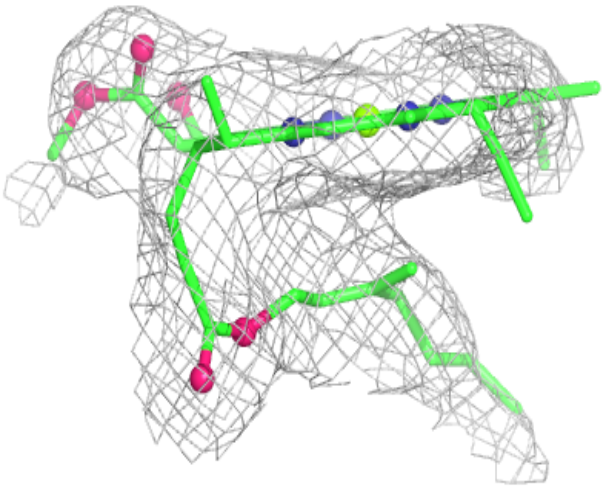


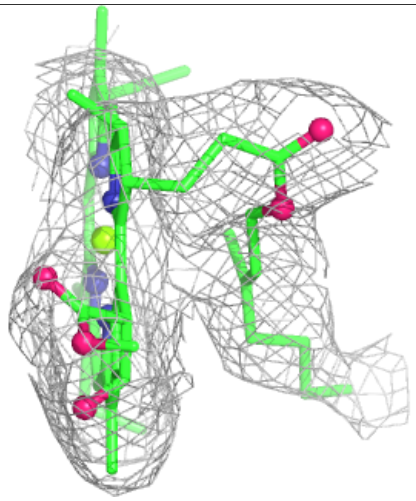


**Electron density around CLA B 818:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

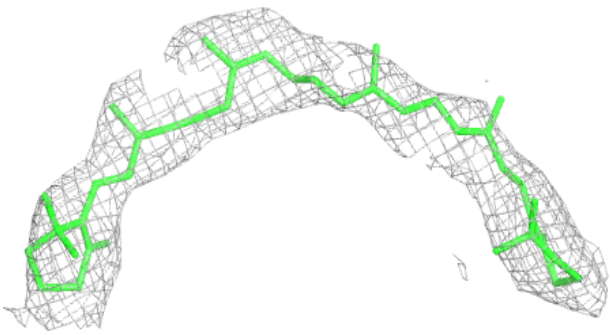


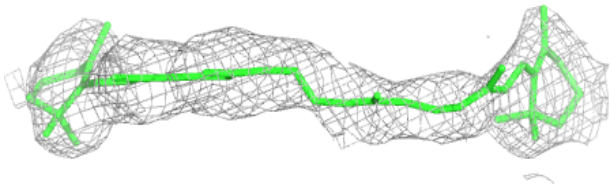


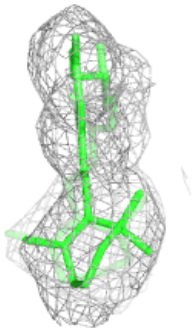


**Electron density around BCR F 204:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

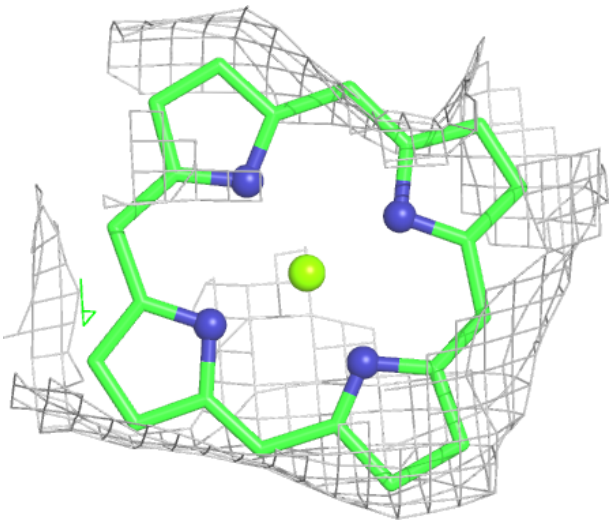


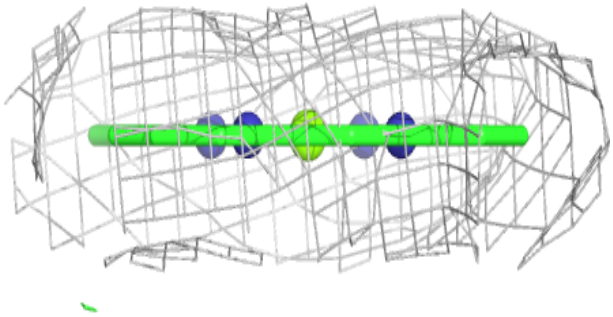


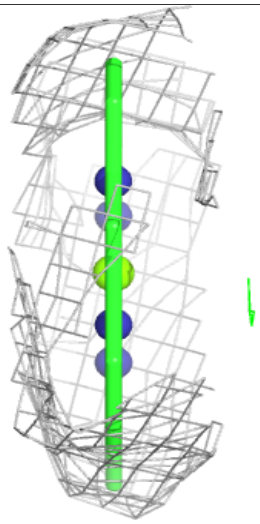


**Electron density around CLA 2 308:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

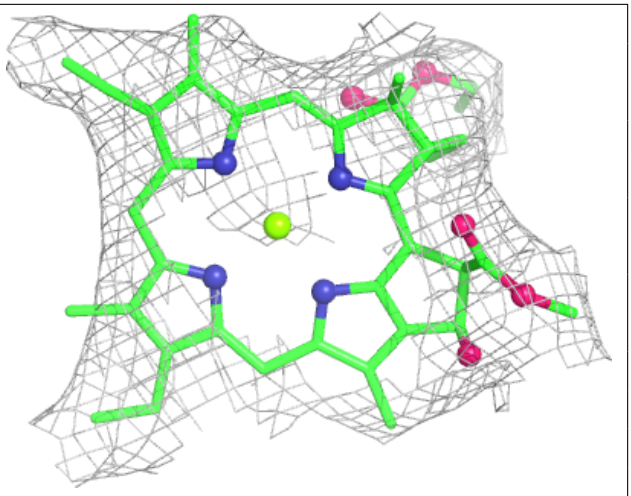


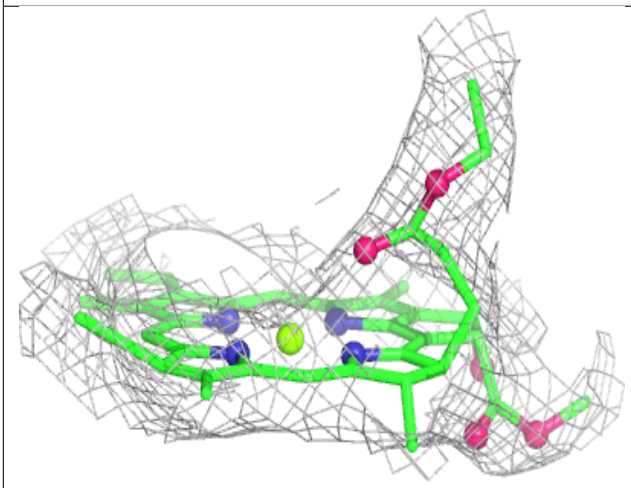


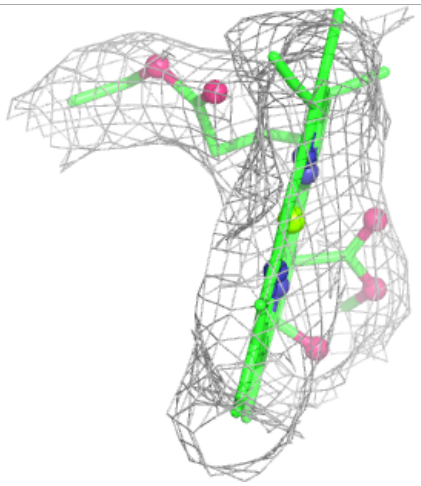


**Electron density around CLA B 839:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

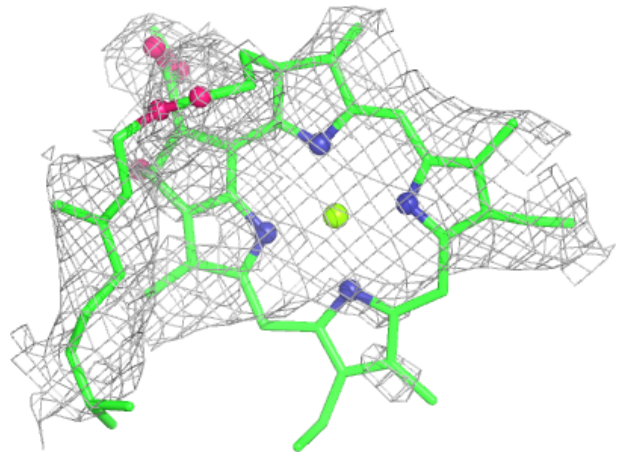


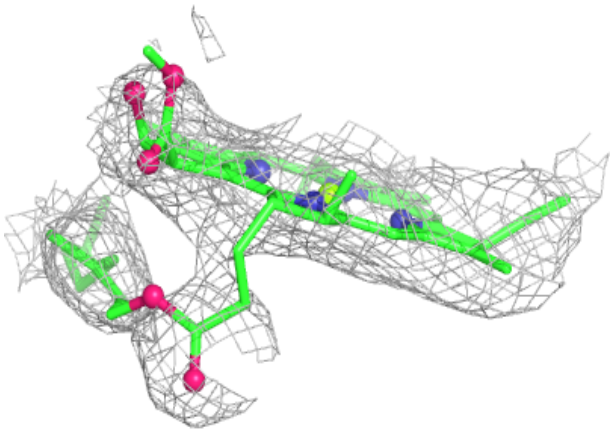


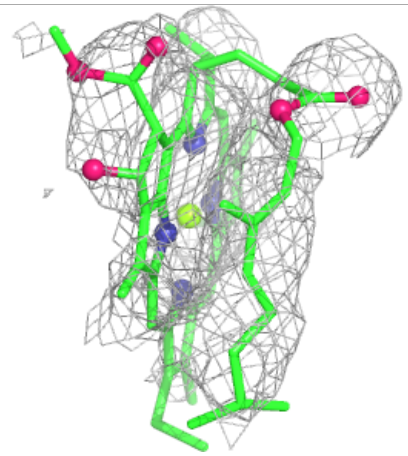


**Electron density around CLA A 827:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

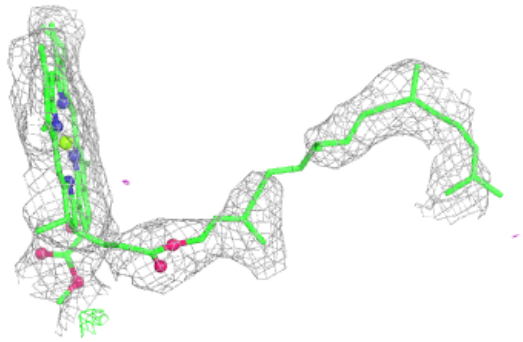


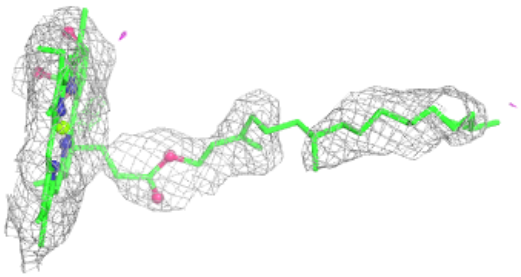


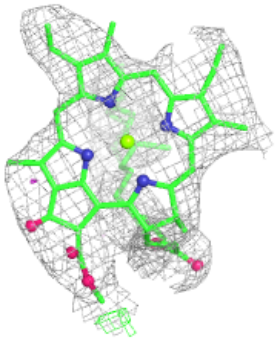


**Electron density around CLA B 841:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

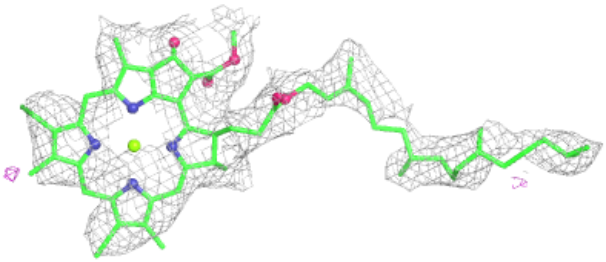


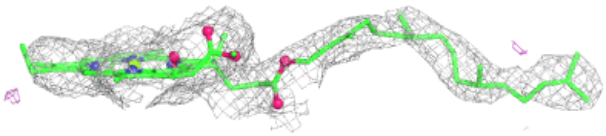




**Electron density around CLA A 830:**

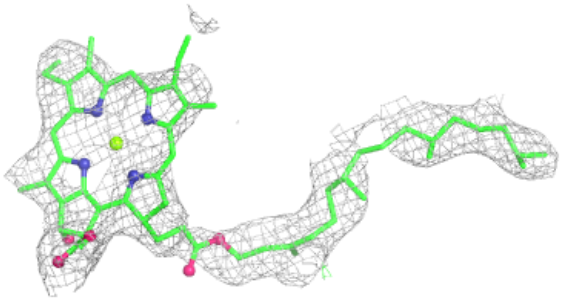
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

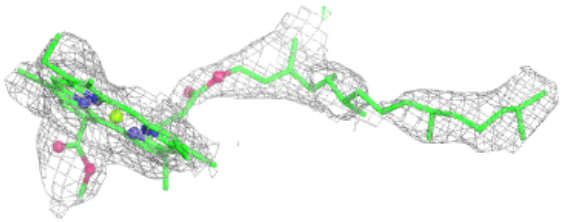


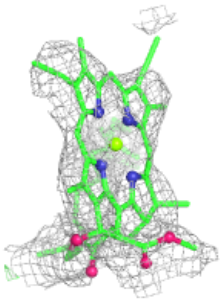


**Electron density around CLA A 831:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

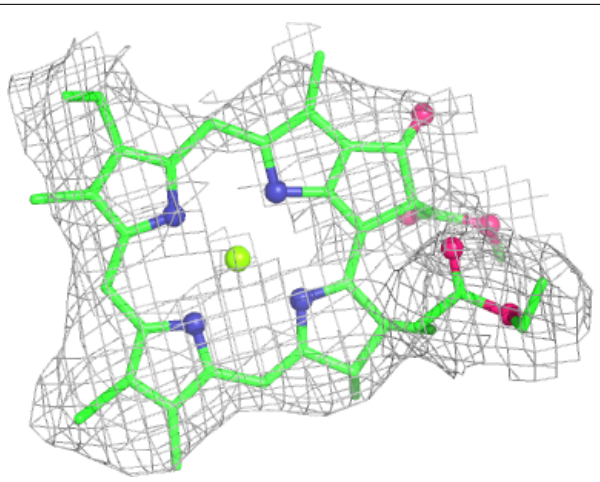


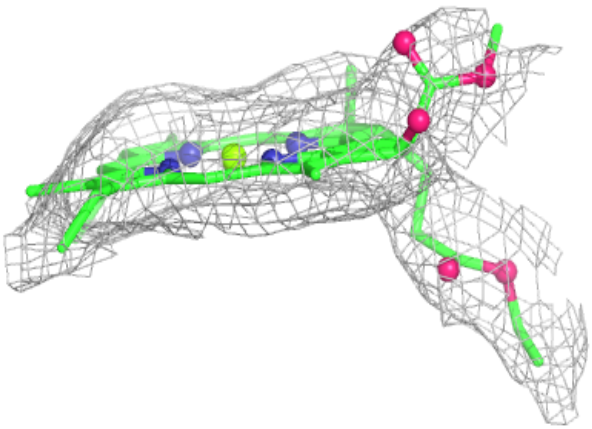


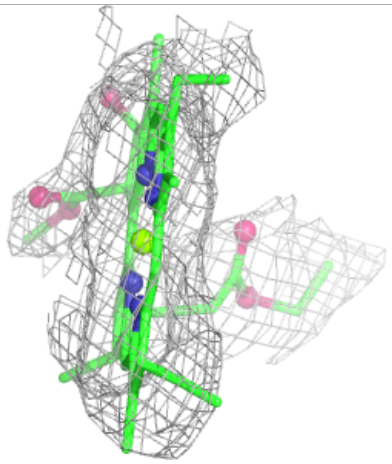


**Electron density around CLA A 836:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

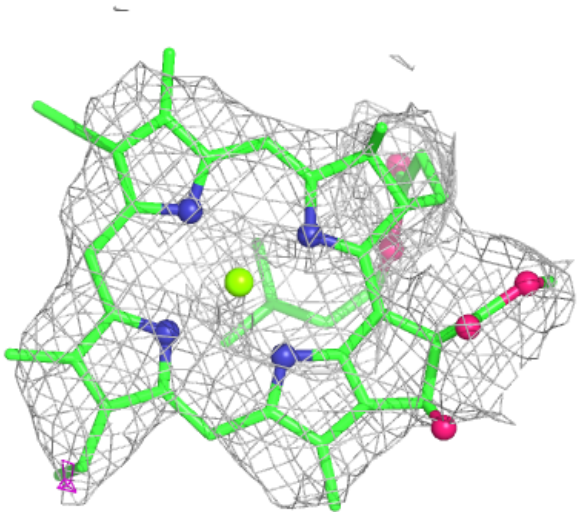


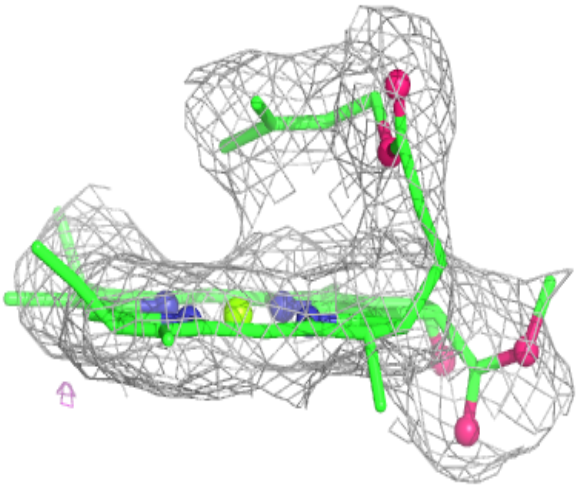


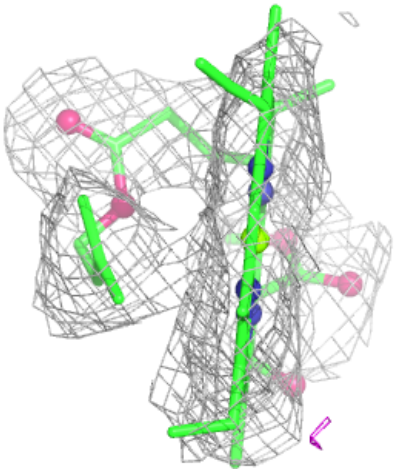


**Electron density around CLA B 831:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

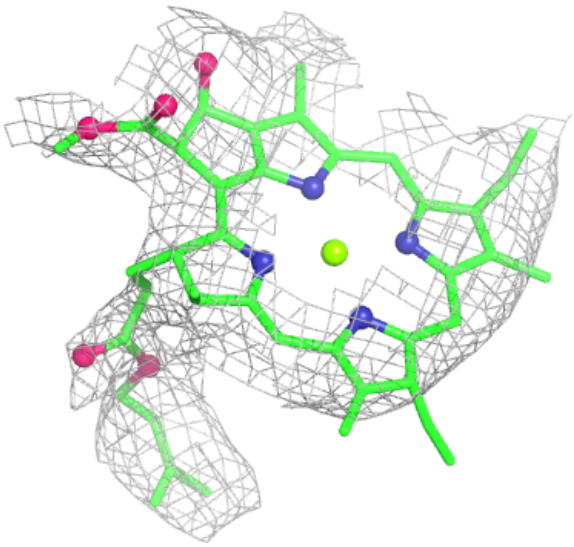


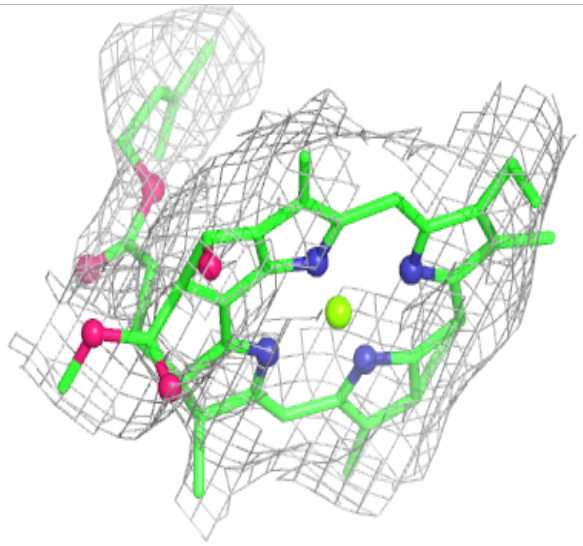


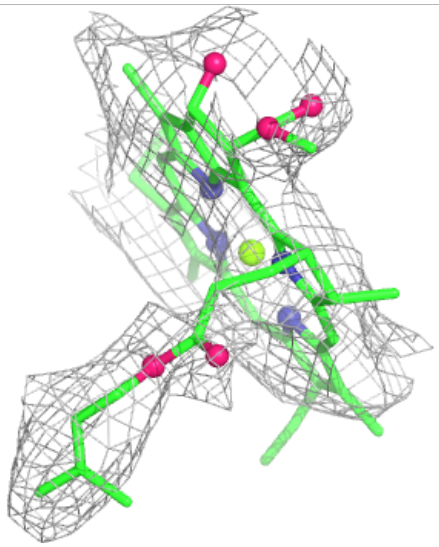


**Electron density around CLA A 822:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

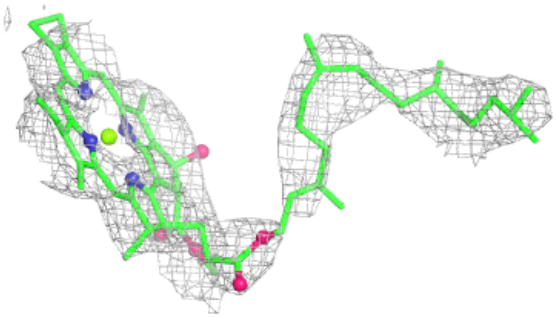


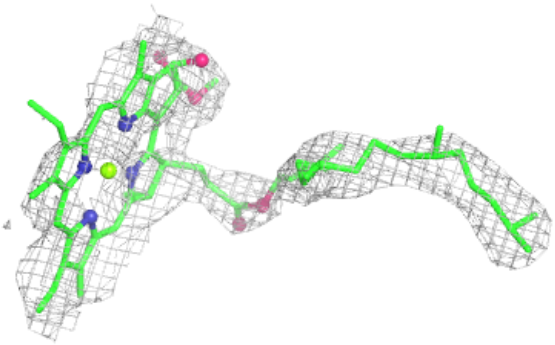


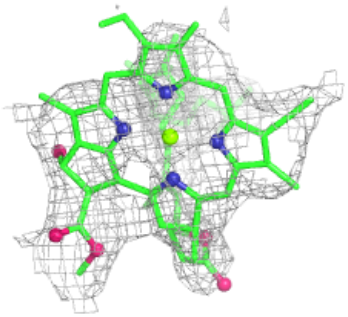


**Electron density around CLA B 850:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

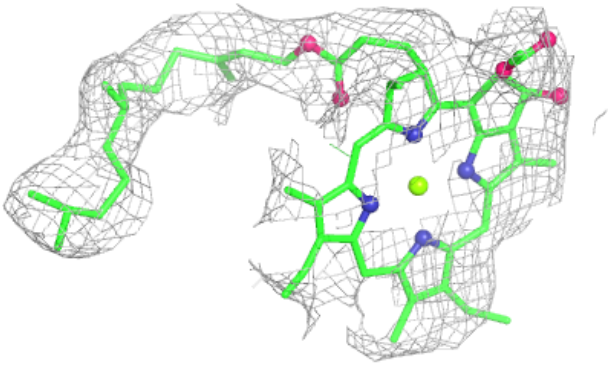


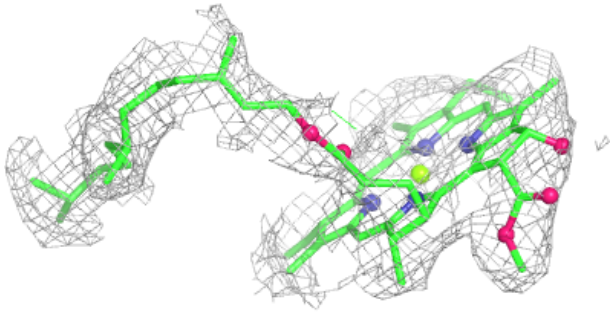


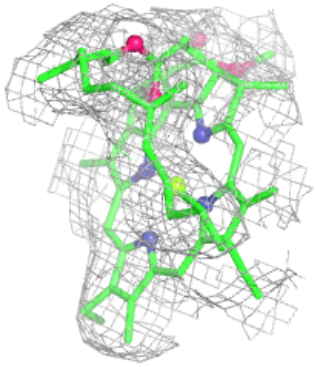


**Electron density around CLA A 808:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

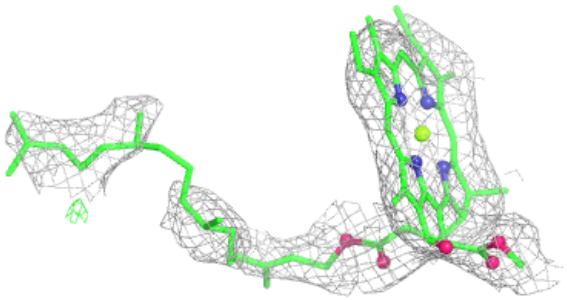


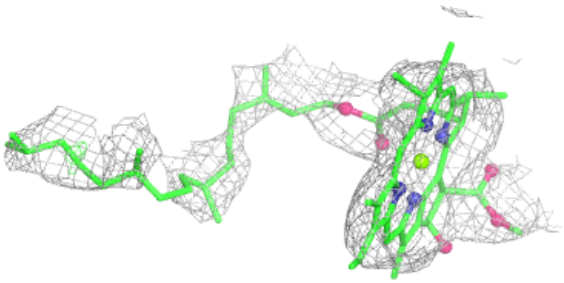


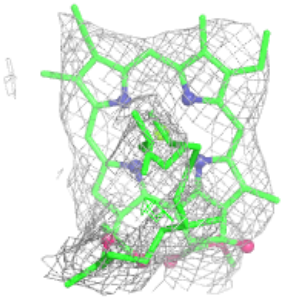


**Electron density around CLA B 830:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

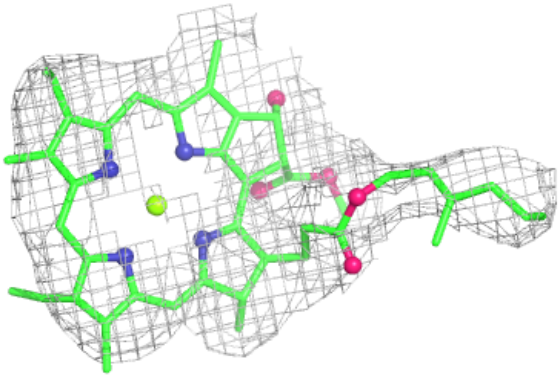






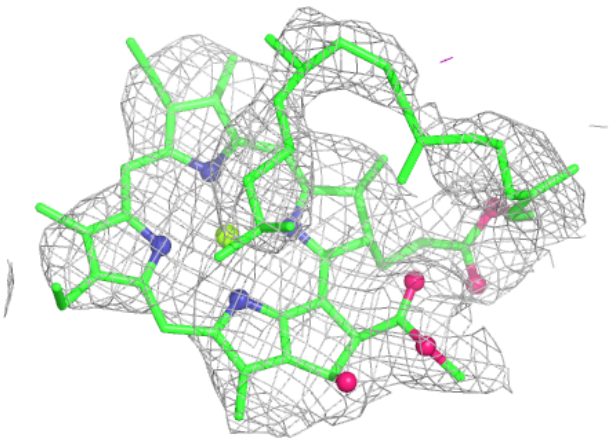
**Electron density around CLA A 809:**

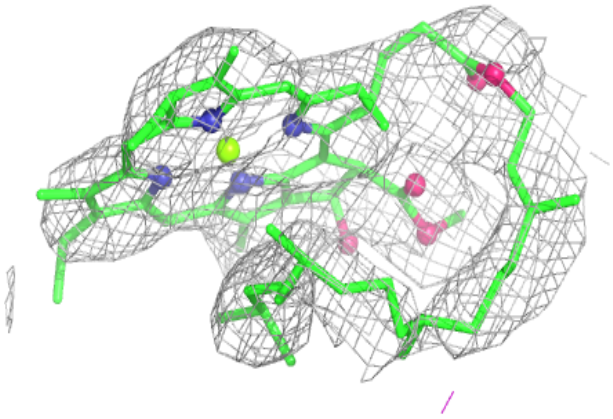
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

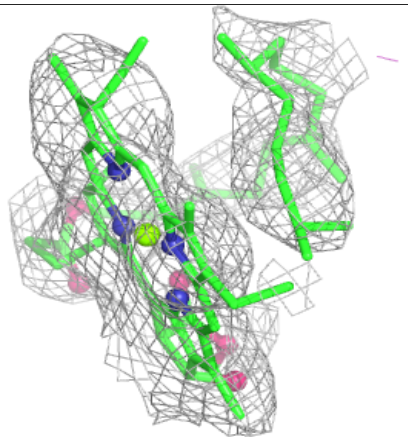


**Electron density around CLA B 809:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

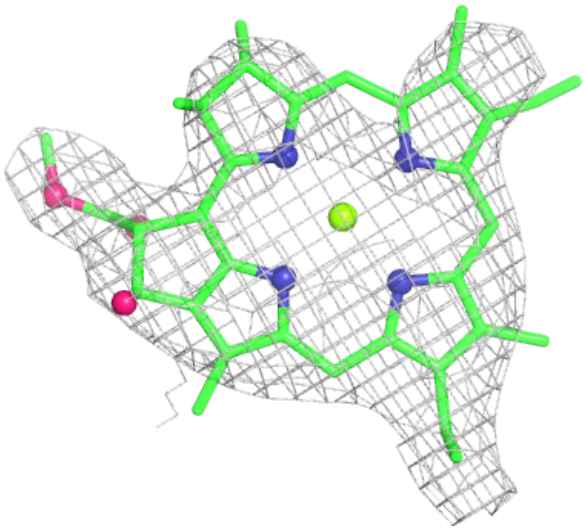


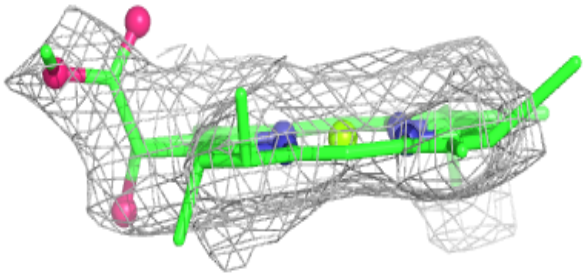


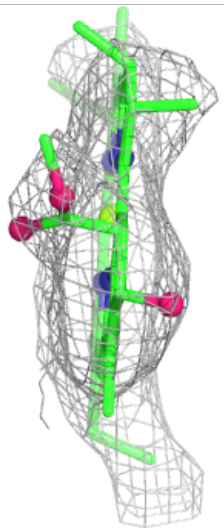


**Electron density around CLA B 819:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

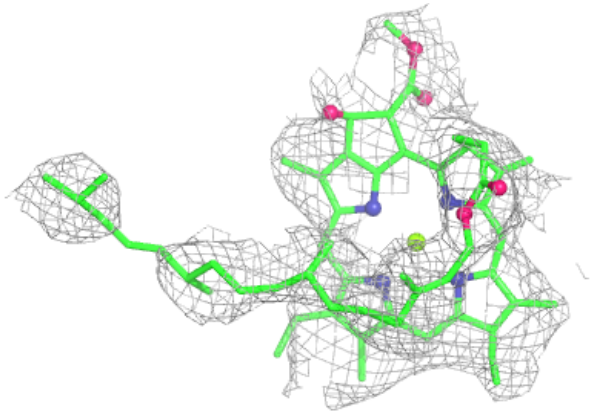


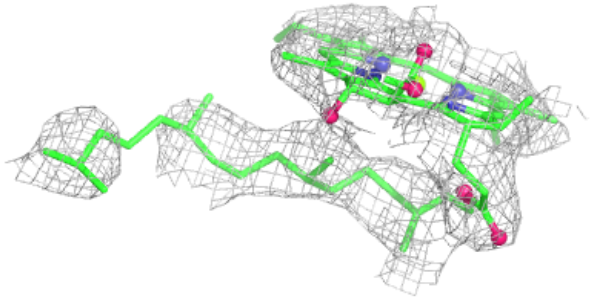




**Electron density around CLA B 828:**

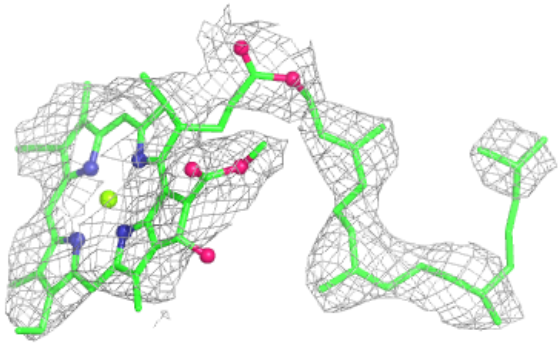
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

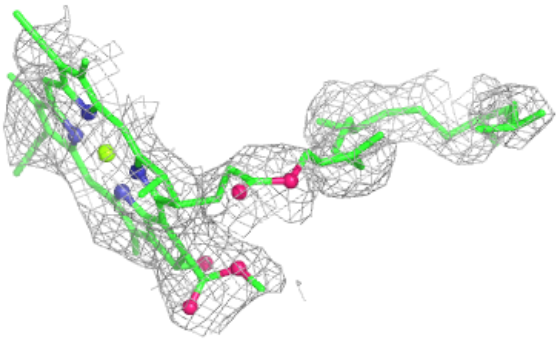


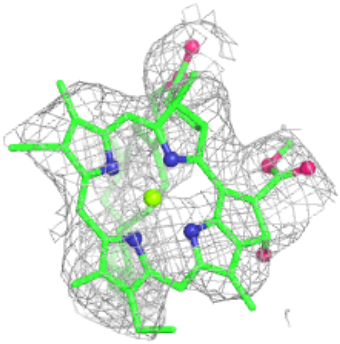


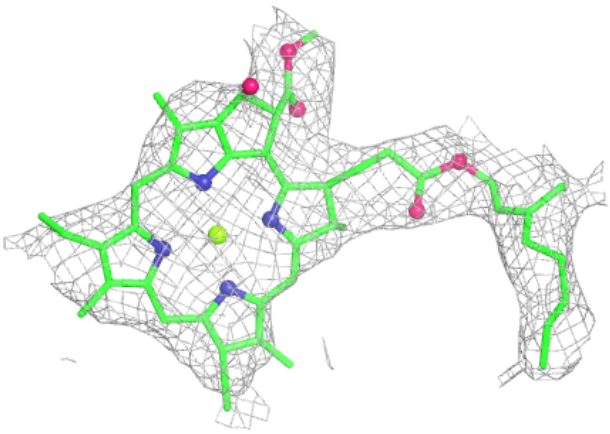
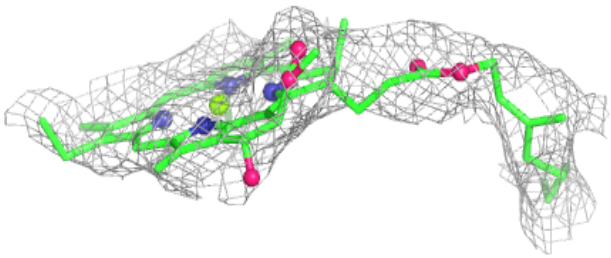
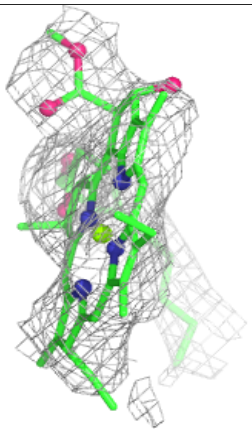
**Electron density around CLA A 849:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)







| | |
|---|---|
| **Electron density around CLA B 802:**<br><br>2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray<br>mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)<br>and green (positive) |  |
|  |  |

## 6.5 Other polymers (i)

There are no such residues in this entry.