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

May 16, 2020 – 07:09 pm BST

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|---|---|---|
| PDB ID | : | 5B1A |
| Title | : | Bovine heart cytochrome c oxidase in the fully oxidized state at 1.5 angstrom resolution |
| Authors | : | Yano, N.; Muramoto, K.; Shimada, A.; Takemura, S.; Baba, J.; Fujisawa, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S. |
| Deposited on | : | 2015-12-01 |
| Resolution | : | 1.50 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.

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The following versions of software and data (see references (1)) were used in the production of this report:

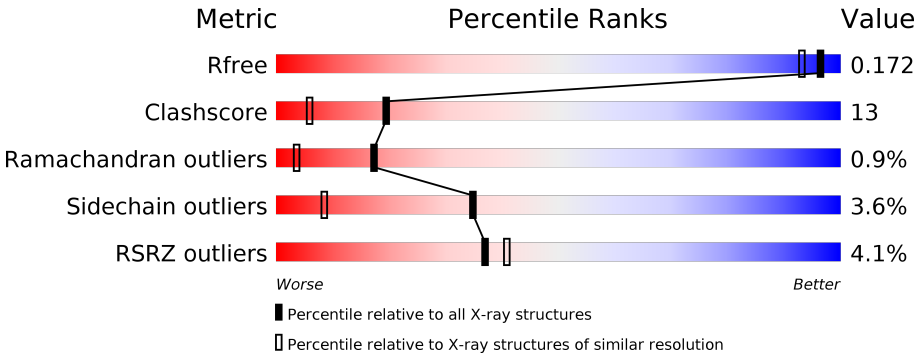
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

# 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 1.50 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2936 (1.50-1.50) |
| Clashscore | 141614 | 3144 (1.50-1.50) |
| Ramachandran outliers | 138981 | 3066 (1.50-1.50) |
| Sidechain outliers | 138945 | 3064 (1.50-1.50) |
| RSRZ outliers | 127900 | 2884 (1.50-1.50) |

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 on 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 | A | 514 | 73% 22% • |
| 1 | N | 514 | 73% 24% • |
| 2 | B | 227 | 2% 65% 29% • • |
| 2 | O | 227 | 2% 69% 26% • • |
| 3 | C | 261 | 72% 25% • • |
| 3 | P | 261 | % 71% 22% 6% • |

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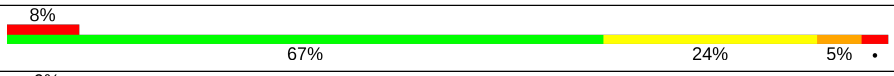
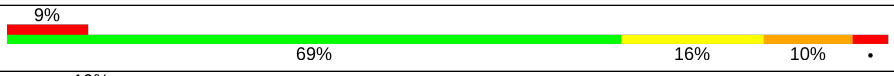
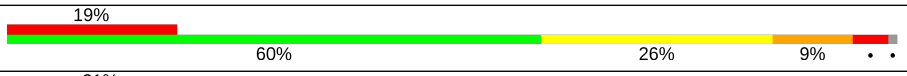
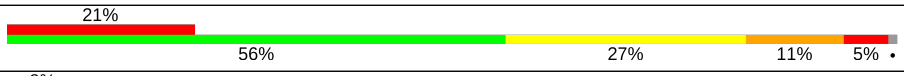
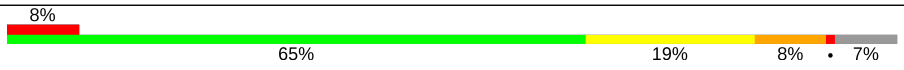
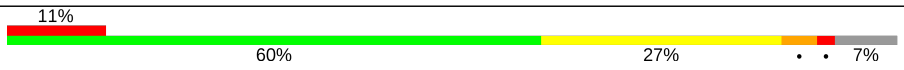
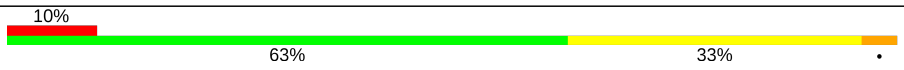
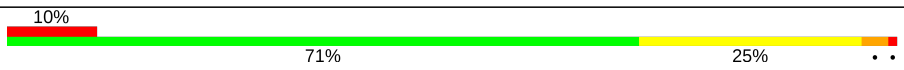
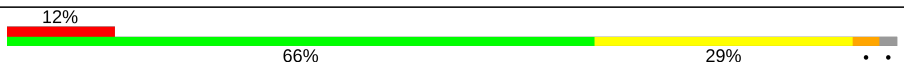
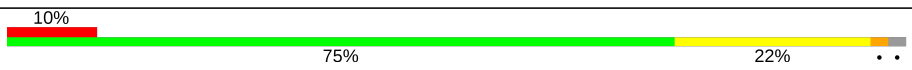
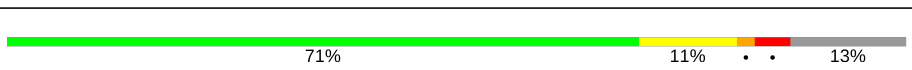
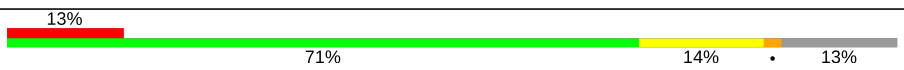
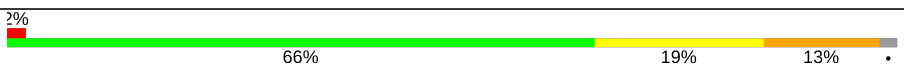
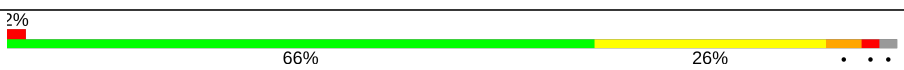
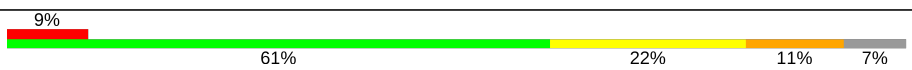
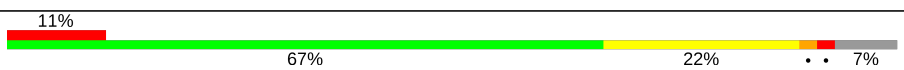
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | D | 147 |   |
| 4 | Q | 147 |   |
| 5 | E | 109 |   |
| 5 | R | 109 |   |
| 6 | F | 98 |   |
| 6 | S | 98 |   |
| 7 | G | 85 |   |
| 7 | T | 85 |   |
| 8 | H | 85 |   |
| 8 | U | 85 |   |
| 9 | I | 73 |   |
| 9 | V | 73 |   |
| 10 | J | 59 |   |
| 10 | W | 59 |   |
| 11 | K | 56 |   |
| 11 | X | 56 |   |
| 12 | L | 47 |   |
| 12 | Y | 47 |   |
| 13 | M | 46 |   |
| 13 | Z | 46 |   |

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 |
|---|---|---|---|---|---|---|---|
| 14 | HEA | A | 601 | X | - | - | - |
| 14 | HEA | A | 602 | X | - | - | - |
| 14 | HEA | N | 601 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 14 | HEA | N | 602 | X | - | - | - |
| 2 | FME | B | 1 | - | X | X | - |
| 20 | TGL | D | 201 | - | - | X | - |
| 20 | TGL | Y | 101 | - | X | X | - |
| 22 | CHD | J | 102 | - | - | - | X |
| 22 | CHD | W | 101 | - | - | - | X |
| 25 | CDL | C | 303 | - | - | X | - |
| 25 | CDL | G | 102 | - | - | X | - |
| 25 | CDL | P | 304 | - | - | X | - |
| 25 | CDL | T | 103 | - | - | X | - |
| 9 | SAC | V | 1 | - | X | - | - |

# 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 35054 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 Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 514 | Total | C | N | O | S | 0 | 18 | 0 |
| | | | 4168 | 2778 | 645 | 704 | 41 | | | |
| 1 | N | 514 | Total | C | N | O | S | 0 | 16 | 0 |
| | | | 4154 | 2771 | 643 | 699 | 41 | | | |

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 227 | Total | C | N | O | S | 0 | 9 | 0 |
| | | | 1899 | 1234 | 292 | 353 | 20 | | | |
| 2 | O | 227 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 1870 | 1215 | 288 | 347 | 20 | | | |

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 259 | Total | C | N | O | S | 0 | 9 | 0 |
| | | | 2185 | 1457 | 349 | 363 | 16 | | | |
| 3 | P | 259 | Total | C | N | O | S | 0 | 9 | 0 |
| | | | 2185 | 1457 | 349 | 363 | 16 | | | |

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 144 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 1242 | 809 | 206 | 223 | 4 | | | |
| 4 | Q | 144 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 1224 | 797 | 202 | 221 | 4 | | | |

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | E | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 852 | 544 | 144 | 162 | 2 | | | |
| 5 | R | 105 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 863 | 550 | 148 | 163 | 2 | | | |

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 98 | Total | C | N | O | S | 0 | 4 | 0 |
| | | | 778 | 481 | 139 | 152 | 6 | | | |
| 6 | S | 98 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 763 | 473 | 136 | 148 | 6 | | | |

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 84 | Total | C | N | O | P | S | 0 | 1 | 0 |
| | | | 686 | 440 | 130 | 114 | 1 | 1 | | | |
| 7 | T | 84 | Total | C | N | O | P | S | 0 | 1 | 0 |
| | | | 686 | 440 | 130 | 114 | 1 | 1 | | | |

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 417 | 121 | 119 | 5 | | | |
| 8 | U | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 417 | 121 | 119 | 5 | | | |

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 601 | 390 | 107 | 100 | 4 | | | |
| 9 | V | 73 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 601 | 390 | 107 | 100 | 4 | | | |

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 460 | 297 | 78 | 82 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | W | 58 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 469 | 302 | 79 | 85 | 3 | | | |

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 384 | 250 | 65 | 67 | 2 | | | |
| 11 | X | 49 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 391 | 255 | 66 | 68 | 2 | | | |

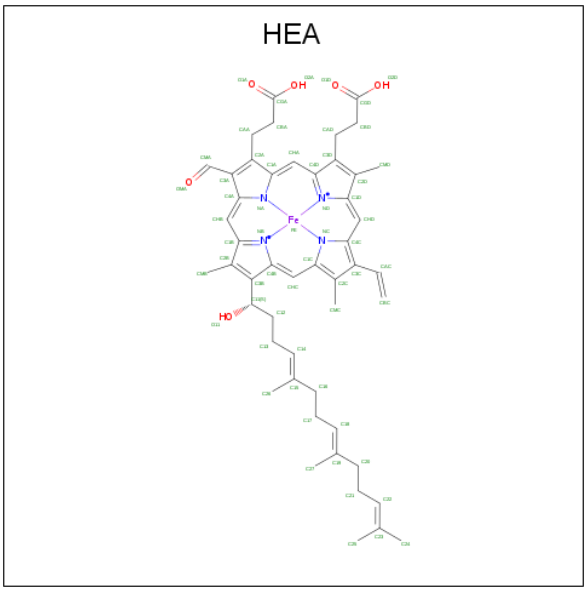
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 380 | 254 | 64 | 60 | 2 | | | |
| 12 | Y | 46 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 388 | 259 | 65 | 61 | 3 | | | |

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | M | 43 | Total | C | N | O | 0 | 0 | 0 |
| | | | 335 | 223 | 53 | 59 | | | |
| 13 | Z | 43 | Total | C | N | O | 0 | 0 | 0 |
| | | | 335 | 223 | 53 | 59 | | | |

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 14 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |
| 14 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |
| 14 | N | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |
| 14 | N | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 15 | A | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 15 | N | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |

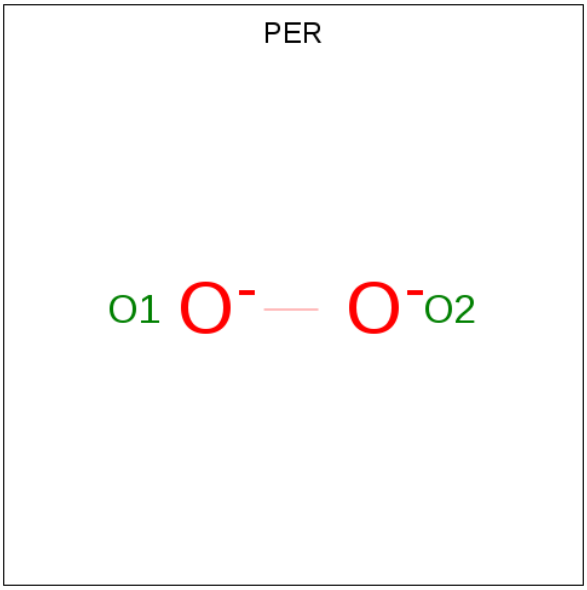
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 16 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 16 | N | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

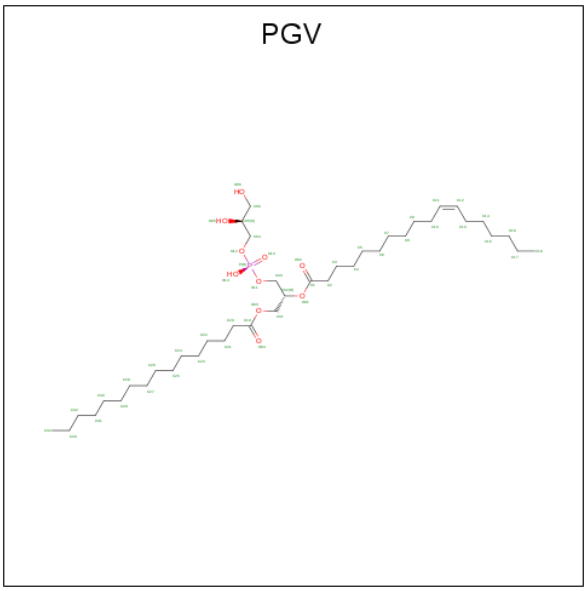
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 17 | A | 1 | Total Na<br>1 1 | 0 | 0 |
| 17 | N | 1 | Total Na<br>1 1 | 0 | 0 |

- Molecule 18 is PEROXIDE ION (three-letter code: PER) (formula: $O_2$).



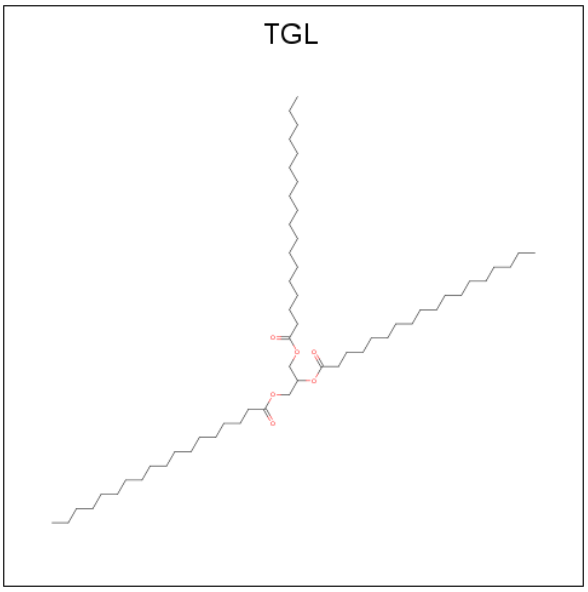

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 18 | A | 1 | Total O<br>2 2 | 0 | 0 |
| 18 | N | 1 | Total O<br>2 2 | 0 | 0 |

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



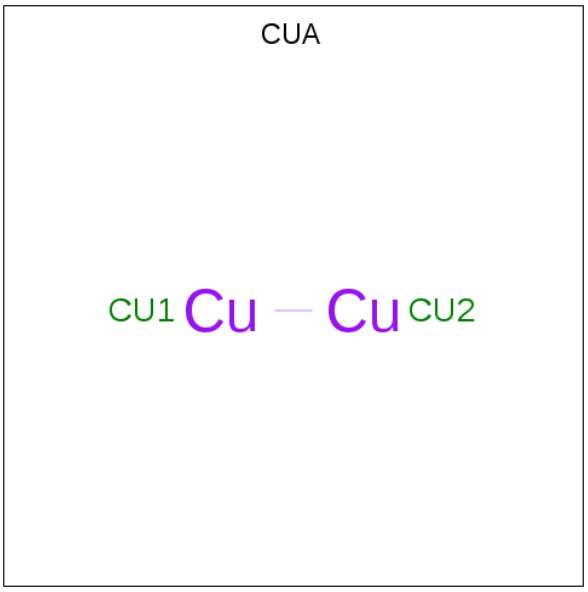

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 19 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | C | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | C | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | N | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | P | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | P | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | Q | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



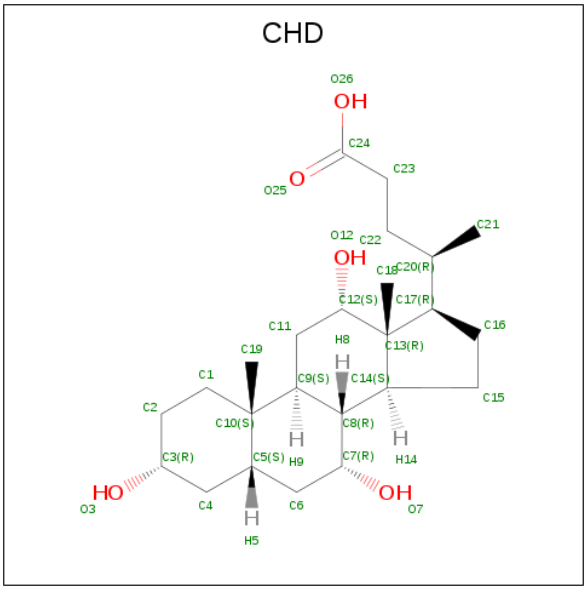

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 20 | B | 1 | Total C O<br>63 57 6 | 0 | 0 |
| 20 | D | 1 | Total C O<br>63 57 6 | 0 | 0 |
| 20 | L | 1 | Total C O<br>63 57 6 | 0 | 0 |
| 20 | N | 1 | Total C O<br>63 57 6 | 0 | 0 |
| 20 | Q | 1 | Total C O<br>63 57 6 | 0 | 0 |
| 20 | Y | 1 | Total C O<br>63 57 6 | 0 | 0 |

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: $Cu_2$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 21 | B | 1 | Total Cu<br>2 2 | 0 | 0 |
| 21 | O | 1 | Total Cu<br>2 2 | 0 | 0 |

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 22 | B | 1 | Total C O<br>29 24 5 | 0 | 0 |
| 22 | C | 1 | Total C O<br>29 24 5 | 0 | 0 |

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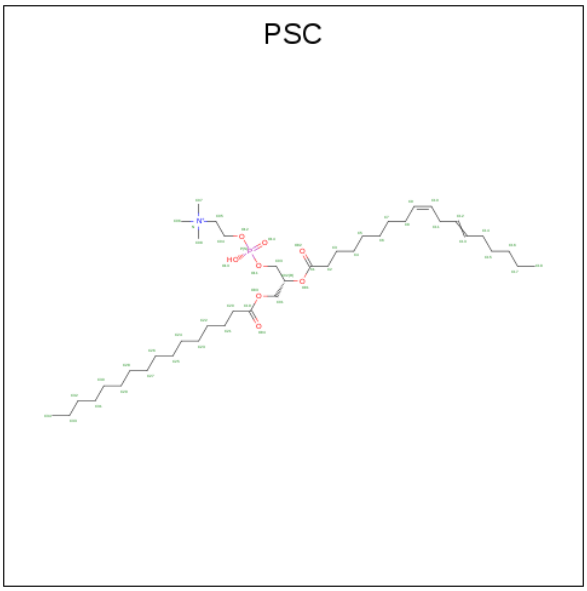
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 22 | C | 1 | Total C O<br>29 24 5 | 0 | 0 |
| 22 | J | 1 | Total C O<br>29 24 5 | 0 | 0 |
| 22 | O | 1 | Total C O<br>29 24 5 | 0 | 0 |
| 22 | P | 1 | Total C O<br>29 24 5 | 0 | 0 |
| 22 | P | 1 | Total C O<br>29 24 5 | 0 | 0 |
| 22 | W | 1 | Total C O<br>29 24 5 | 0 | 0 |

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).

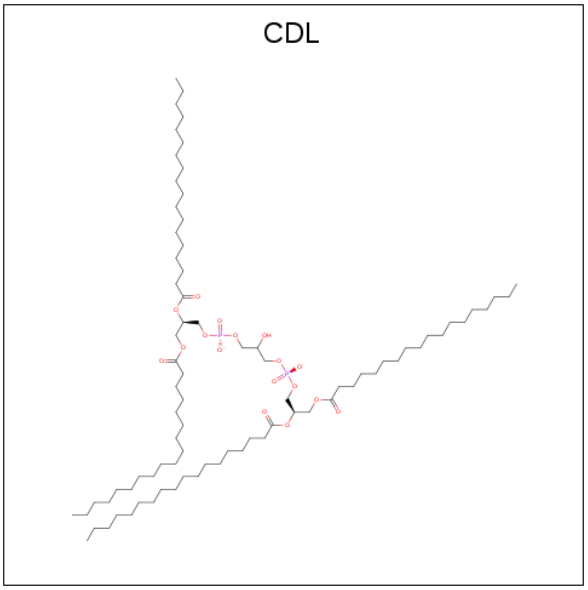



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 23 | B | 1 | Total C N O P<br>52 42 1 8 1 | 0 | 0 |
| 23 | O | 1 | Total C N O P<br>52 42 1 8 1 | 0 | 0 |

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

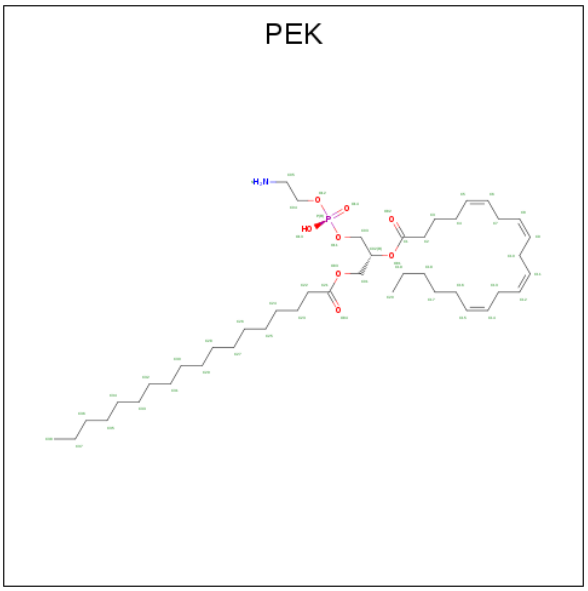
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 24 | P | 1 | Total X<br>1 1 | 0 | 0 |
| 24 | C | 1 | Total X<br>1 1 | 0 | 0 |

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 25 | C | 1 | Total C O P<br>100 81 17 2 | 0 | 0 |
| 25 | G | 1 | Total C O P<br>100 81 17 2 | 0 | 0 |
| 25 | P | 1 | Total C O P<br>100 81 17 2 | 0 | 0 |
| 25 | T | 1 | Total C O P<br>100 81 17 2 | 0 | 0 |

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).

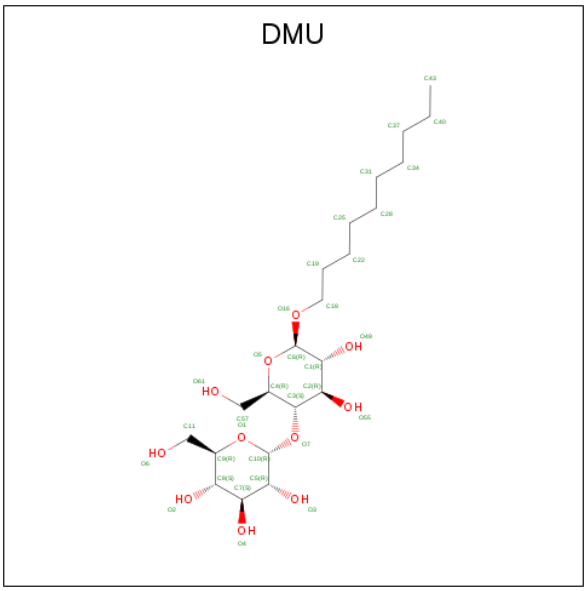



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 26 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 26 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 26 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 26 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 26 | T | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 26 | T | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 27 | S | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 27 | F | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 28 | J | 1 | Total C O<br>33 22 11 | 0 | 0 |
| 28 | M | 1 | Total C O<br>33 22 11 | 0 | 0 |
| 28 | P | 1 | Total C O<br>33 22 11 | 0 | 0 |
| 28 | Z | 1 | Total C O<br>33 22 11 | 0 | 0 |

- Molecule 29 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 29 | A | 297 | Total O<br>297 297 | 0 | 0 |
| 29 | B | 273 | Total O<br>274 274 | 0 | 1 |
| 29 | C | 176 | Total O<br>176 176 | 0 | 0 |
| 29 | D | 266 | Total O<br>266 266 | 0 | 0 |
| 29 | E | 178 | Total O<br>178 178 | 0 | 0 |
| 29 | F | 199 | Total O<br>199 199 | 0 | 0 |
| 29 | G | 100 | Total O<br>100 100 | 0 | 0 |
| 29 | H | 122 | Total O<br>122 122 | 0 | 0 |

*Continued on next page...*

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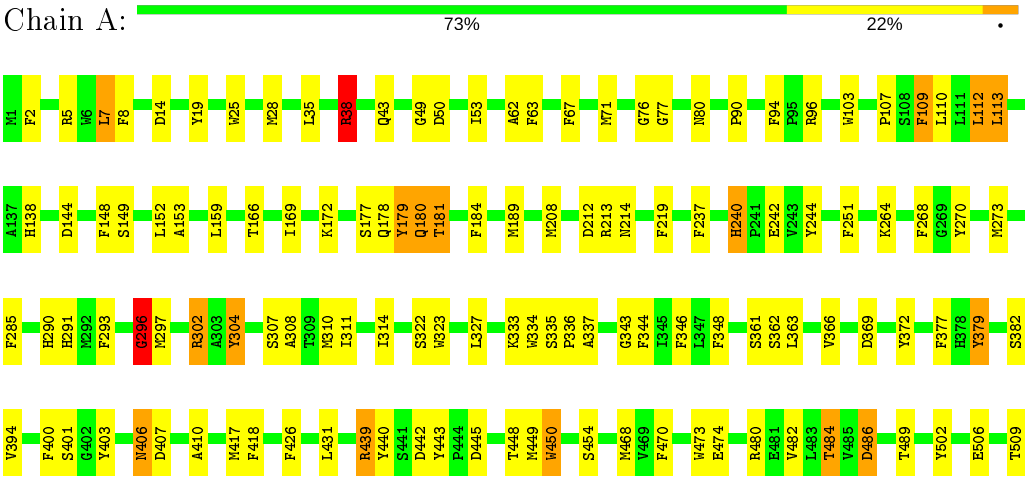
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 29 | I | 88 | Total O<br>88 88 | 0 | 0 |
| 29 | J | 63 | Total O<br>63 63 | 0 | 0 |
| 29 | K | 69 | Total O<br>69 69 | 0 | 0 |
| 29 | L | 48 | Total O<br>48 48 | 0 | 0 |
| 29 | M | 47 | Total O<br>47 47 | 0 | 0 |
| 29 | N | 290 | Total O<br>290 290 | 0 | 0 |
| 29 | O | 242 | Total O<br>243 243 | 0 | 1 |
| 29 | P | 173 | Total O<br>173 173 | 0 | 0 |
| 29 | Q | 164 | Total O<br>164 164 | 0 | 0 |
| 29 | R | 151 | Total O<br>151 151 | 0 | 0 |
| 29 | S | 186 | Total O<br>186 186 | 0 | 0 |
| 29 | T | 94 | Total O<br>94 94 | 0 | 0 |
| 29 | U | 110 | Total O<br>110 110 | 0 | 0 |
| 29 | V | 71 | Total O<br>71 71 | 0 | 0 |
| 29 | W | 58 | Total O<br>58 58 | 0 | 0 |
| 29 | X | 57 | Total O<br>57 57 | 0 | 0 |
| 29 | Y | 40 | Total O<br>40 40 | 0 | 0 |
| 29 | Z | 37 | Total O<br>37 37 | 0 | 0 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

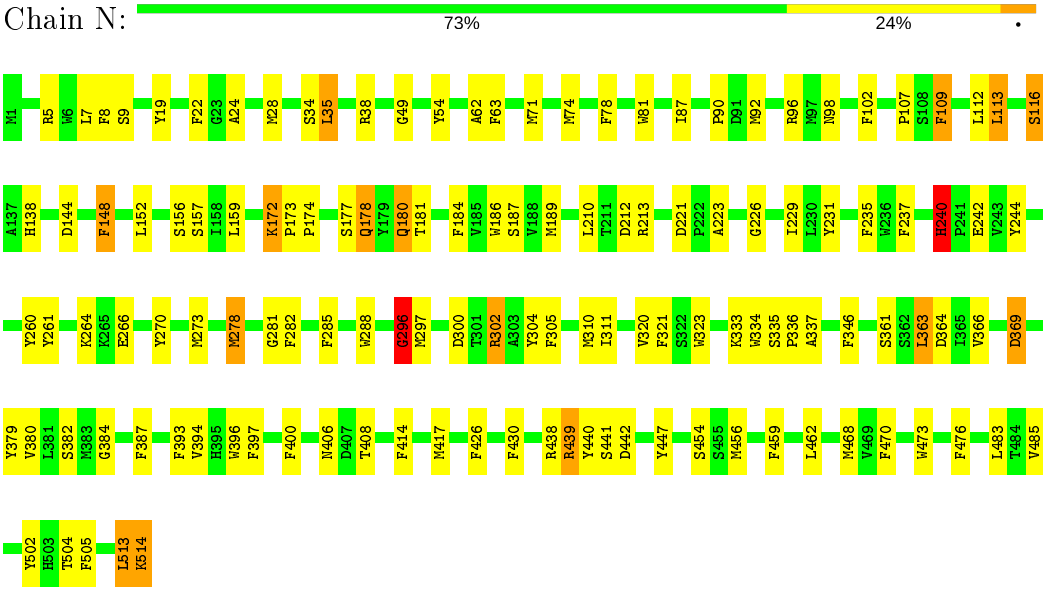
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



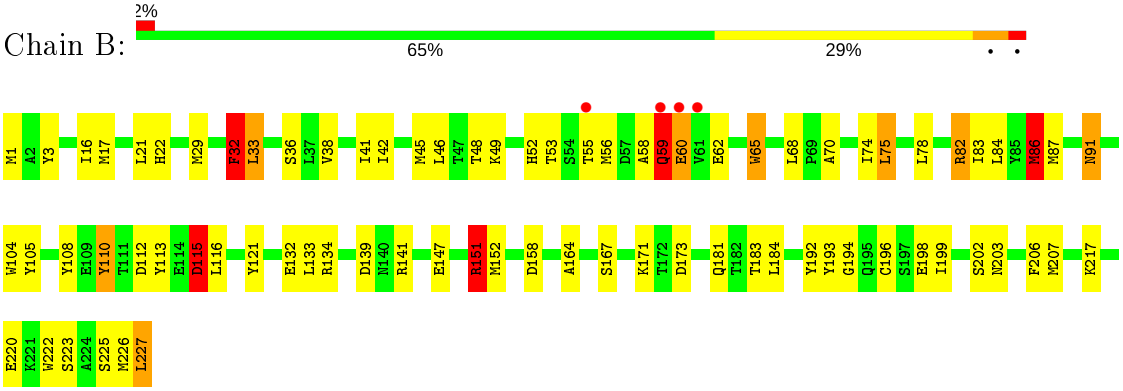

- Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



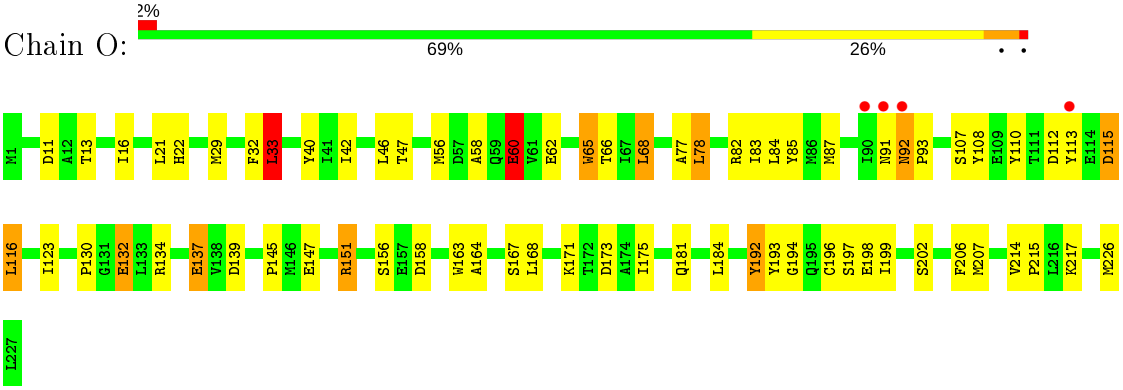

- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



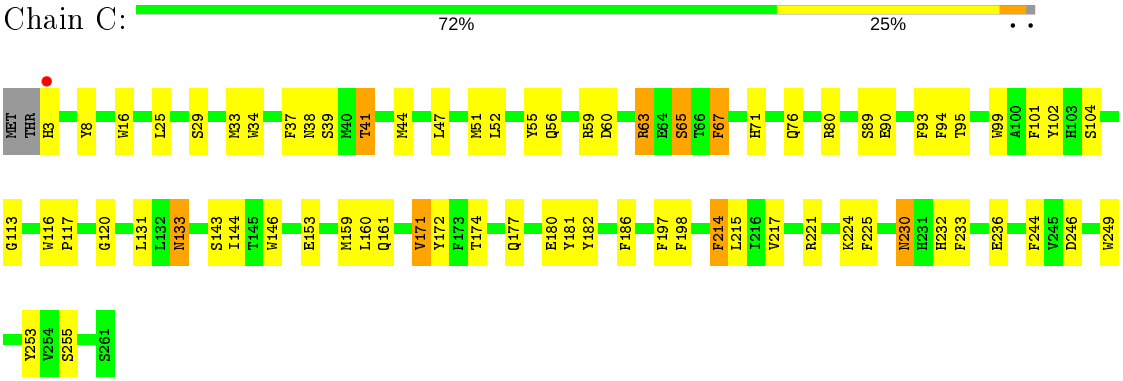

- Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



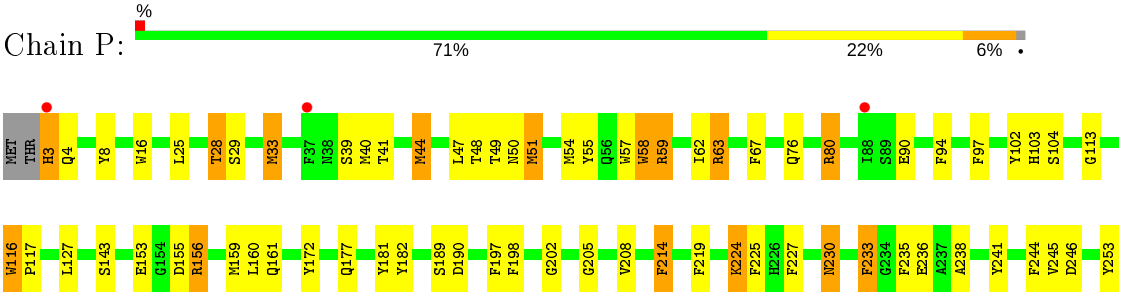

- Molecule 3: Cytochrome c oxidase subunit 3

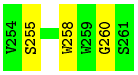
Chain C:




- Molecule 3: Cytochrome c oxidase subunit 3

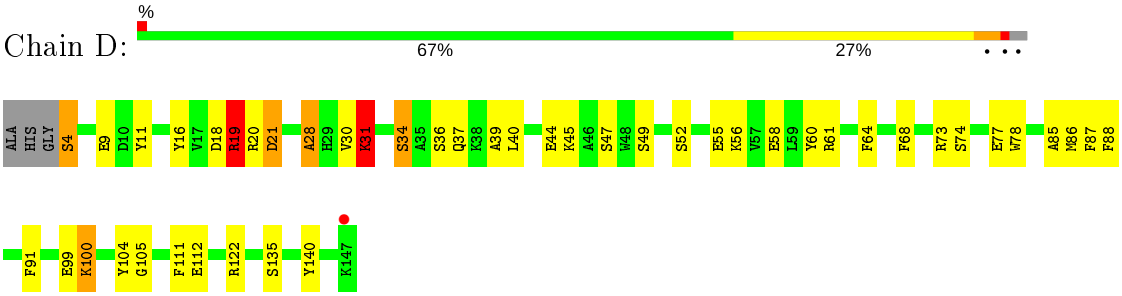
Chain P:





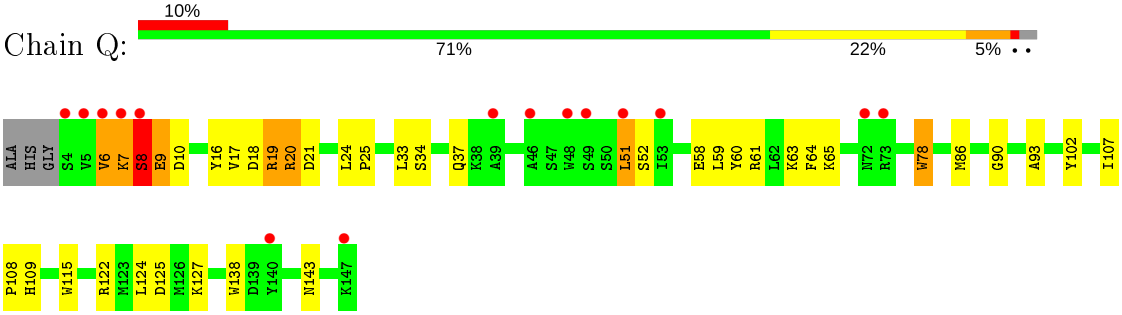

• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



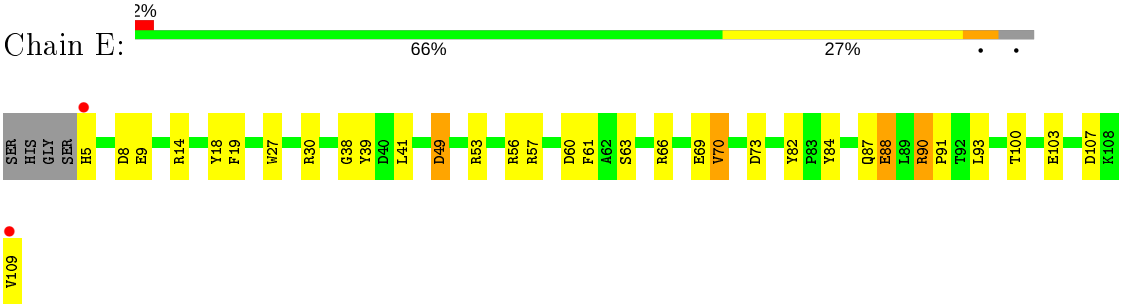

• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q:



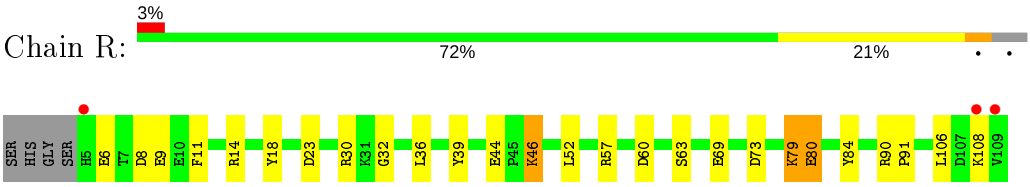

• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



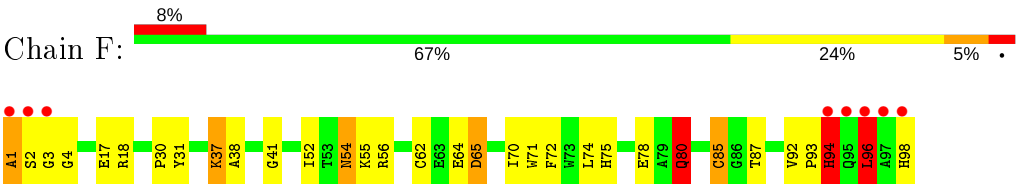

• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



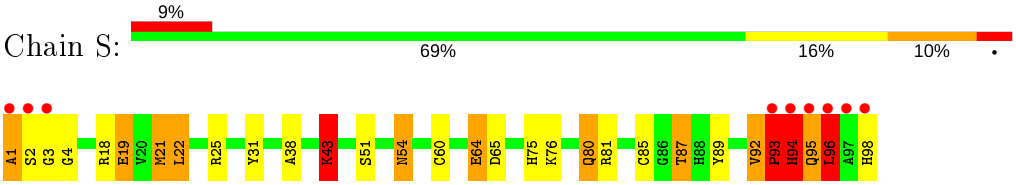

• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



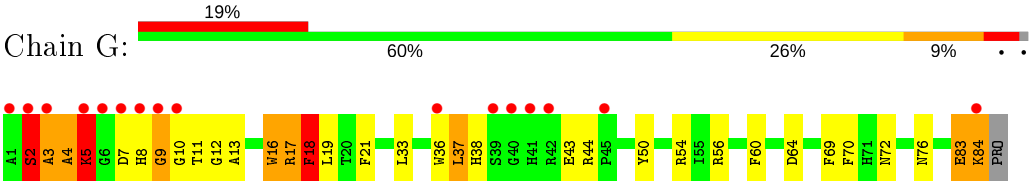
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



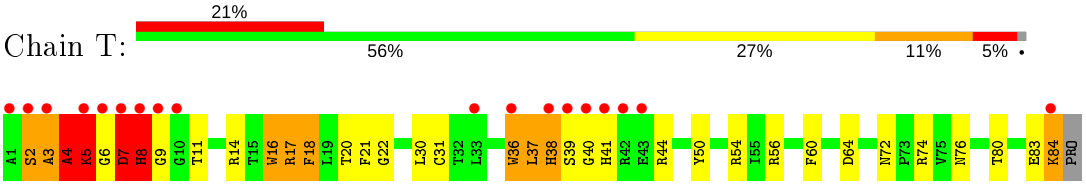

• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



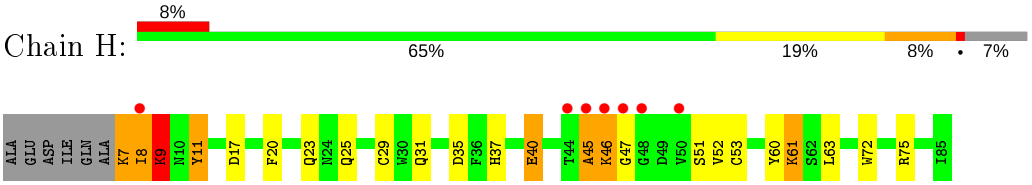

• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



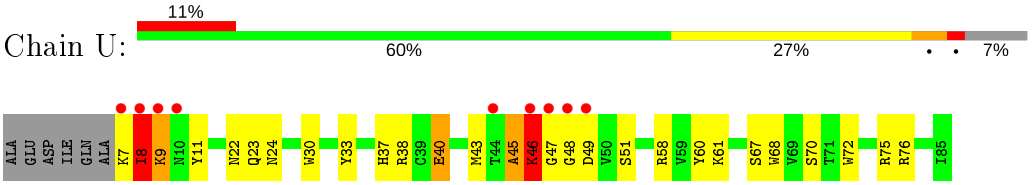

• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



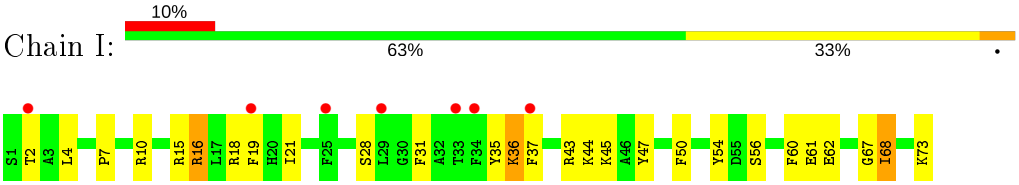

• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



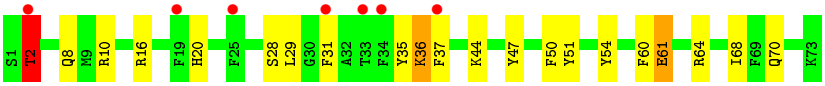

• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:

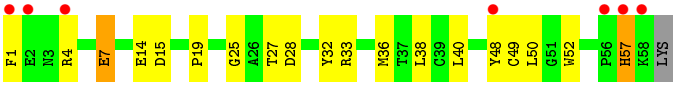



• Molecule 9: Cytochrome c oxidase subunit 6C

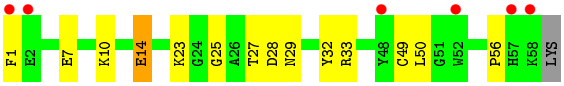
Chain V:




• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

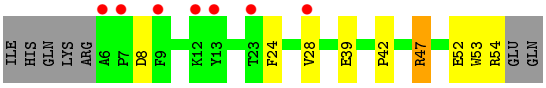

• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial


• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



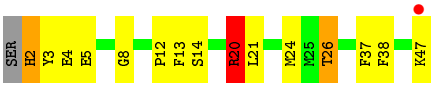
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

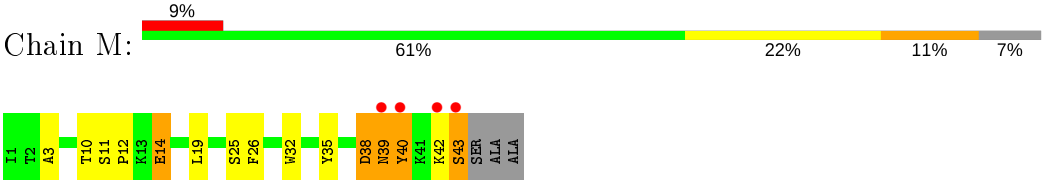


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

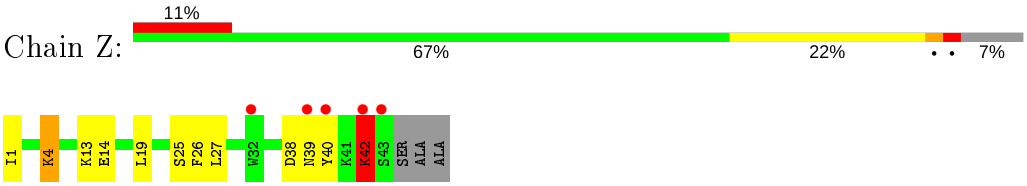

• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:




- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain Z:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 181.94Å 204.40Å 177.90Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 1.50<br>89.10 – 1.40 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.3 (40.00-1.50)<br>98.2 (89.10-1.40) | Depositor<br>EDS |
| $R_{merge}$ | 0.11 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.86 (at 1.40Å) | Xtriage |
| Refinement program | REFMAC 5.8.0103 | Depositor |
| R, $R_{free}$ | 0.149 , 0.172<br>0.149 , 0.172 | Depositor<br>DCC |
| $R_{free}$ test set | 63174 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 20.6 | Xtriage |
| Anisotropy | 0.642 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 66.8 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.51$, $< L^2 > = 0.35$ | Xtriage |
| Estimated twinning fraction | 0.001 for l,-k,h | Xtriage |
| $F_o$,$F_c$ correlation | 0.98 | EDS |
| Total number of atoms | 35054 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 37.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, PER, PGV, TPO, UNX, CUA, NA, FME, TGL, CU, DMU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 1.84 | 54/4297 (1.3%) | 1.89 | 89/5864 (1.5%) |
| 1 | N | 1.85 | 57/4283 (1.3%) | 1.76 | 84/5845 (1.4%) |
| 2 | B | 1.94 | 37/1937 (1.9%) | 1.80 | 32/2637 (1.2%) |
| 2 | O | 1.82 | 30/1908 (1.6%) | 1.57 | 23/2597 (0.9%) |
| 3 | C | 1.91 | 41/2272 (1.8%) | 1.79 | 46/3102 (1.5%) |
| 3 | P | 1.91 | 37/2272 (1.6%) | 1.77 | 52/3102 (1.7%) |
| 4 | D | 2.05 | 31/1277 (2.4%) | 1.87 | 40/1720 (2.3%) |
| 4 | Q | 1.67 | 17/1259 (1.4%) | 1.88 | 23/1698 (1.4%) |
| 5 | E | 2.01 | 24/871 (2.8%) | 2.45 | 41/1182 (3.5%) |
| 5 | R | 1.89 | 18/882 (2.0%) | 1.60 | 14/1196 (1.2%) |
| 6 | F | 1.96 | 16/795 (2.0%) | 1.65 | 7/1079 (0.6%) |
| 6 | S | 1.89 | 17/780 (2.2%) | 1.69 | 14/1058 (1.3%) |
| 7 | G | 2.03 | 15/702 (2.1%) | 1.87 | 19/953 (2.0%) |
| 7 | T | 1.95 | 14/702 (2.0%) | 1.59 | 9/953 (0.9%) |
| 8 | H | 1.77 | 7/682 (1.0%) | 1.52 | 9/921 (1.0%) |
| 8 | U | 1.74 | 10/682 (1.5%) | 1.36 | 5/921 (0.5%) |
| 9 | I | 1.96 | 13/605 (2.1%) | 1.73 | 13/802 (1.6%) |
| 9 | V | 1.70 | 7/605 (1.2%) | 1.85 | 9/802 (1.1%) |
| 10 | J | 1.80 | 6/471 (1.3%) | 1.54 | 4/636 (0.6%) |
| 10 | W | 1.65 | 4/480 (0.8%) | 1.36 | 2/648 (0.3%) |
| 11 | K | 2.09 | 14/398 (3.5%) | 1.91 | 7/546 (1.3%) |
| 11 | X | 1.63 | 7/405 (1.7%) | 1.47 | 5/556 (0.9%) |
| 12 | L | 2.01 | 6/393 (1.5%) | 1.76 | 11/526 (2.1%) |
| 12 | Y | 1.97 | 11/401 (2.7%) | 1.52 | 3/536 (0.6%) |
| 13 | M | 1.80 | 6/345 (1.7%) | 1.68 | 5/470 (1.1%) |
| 13 | Z | 1.70 | 4/345 (1.2%) | 1.43 | 3/470 (0.6%) |
| All | All | 1.87 | 503/30049 (1.7%) | 1.77 | 569/40820 (1.4%) |

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 | A | 0 | 4 |
| 1 | N | 0 | 3 |
| 2 | B | 0 | 3 |
| 3 | C | 0 | 1 |
| 4 | Q | 0 | 1 |
| 5 | E | 0 | 2 |
| 6 | F | 0 | 1 |
| 6 | S | 0 | 2 |
| 7 | G | 0 | 1 |
| 7 | T | 0 | 1 |
| 10 | J | 0 | 1 |
| 11 | K | 0 | 1 |
| 13 | M | 0 | 1 |
| All | All | 0 | 22 |

All (503) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | O | 65 | TRP | CB-CG | -17.96 | 1.18 | 1.50 |
| 2 | B | 65 | TRP | CB-CG | -17.06 | 1.19 | 1.50 |
| 4 | D | 58 | GLU | CD-OE1 | 15.90 | 1.43 | 1.25 |
| 11 | K | 47 | ARG | CZ-NH2 | 14.60 | 1.52 | 1.33 |
| 7 | T | 36 | TRP | CB-CG | 13.34 | 1.74 | 1.50 |
| 2 | O | 60 | GLU | CD-OE1 | 12.69 | 1.39 | 1.25 |
| 11 | X | 54 | ARG | CZ-NH2 | 12.54 | 1.49 | 1.33 |
| 5 | R | 90 | ARG | NE-CZ | 12.50 | 1.49 | 1.33 |
| 7 | G | 36 | TRP | CB-CG | 11.64 | 1.71 | 1.50 |
| 2 | O | 167 | SER | CB-OG | -11.38 | 1.27 | 1.42 |
| 3 | P | 224 | LYS | CE-NZ | 11.24 | 1.77 | 1.49 |
| 11 | K | 54 | ARG | NE-CZ | 11.17 | 1.47 | 1.33 |
| 4 | D | 44 | GLU | CD-OE1 | 10.96 | 1.37 | 1.25 |
| 12 | L | 26 | THR | CB-CG2 | -10.21 | 1.18 | 1.52 |
| 12 | L | 5 | GLU | CD-OE2 | -10.04 | 1.14 | 1.25 |
| 2 | B | 115 | ASP | CB-CG | 9.99 | 1.72 | 1.51 |
| 6 | F | 1 | ALA | C-O | 9.89 | 1.42 | 1.23 |
| 5 | R | 46 | LYS | CE-NZ | 9.87 | 1.73 | 1.49 |
| 7 | T | 17 | ARG | CZ-NH2 | 9.84 | 1.45 | 1.33 |
| 1 | N | 242 | GLU | CD-OE1 | 9.65 | 1.36 | 1.25 |
| 8 | H | 40 | GLU | CD-OE2 | 9.63 | 1.36 | 1.25 |
| 3 | P | 104 | SER | CB-OG | 9.56 | 1.54 | 1.42 |
| 3 | C | 172 | TYR | CG-CD1 | 9.45 | 1.51 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | V | 8 | GLN | CG-CD | -9.33 | 1.29 | 1.51 |
| 13 | Z | 40 | TYR | CE1-CZ | 9.31 | 1.50 | 1.38 |
| 8 | U | 40 | GLU | CD-OE2 | 9.23 | 1.35 | 1.25 |
| 12 | Y | 4 | GLU | CD-OE1 | 9.23 | 1.35 | 1.25 |
| 9 | I | 61 | GLU | CD-OE1 | -9.21 | 1.15 | 1.25 |
| 3 | C | 90 | GLU | CD-OE1 | 9.20 | 1.35 | 1.25 |
| 5 | E | 39 | TYR | CG-CD2 | -9.10 | 1.27 | 1.39 |
| 3 | C | 104 | SER | CB-OG | 9.10 | 1.54 | 1.42 |
| 1 | A | 96 | ARG | CZ-NH1 | 8.97 | 1.44 | 1.33 |
| 2 | B | 132 | GLU | CD-OE2 | 8.96 | 1.35 | 1.25 |
| 6 | S | 1 | ALA | C-O | 8.84 | 1.40 | 1.23 |
| 3 | C | 63 | ARG | CZ-NH2 | 8.79 | 1.44 | 1.33 |
| 2 | O | 60 | GLU | CD-OE2 | 8.76 | 1.35 | 1.25 |
| 5 | R | 84 | TYR | CG-CD1 | 8.70 | 1.50 | 1.39 |
| 1 | N | 278[A] | MET | SD-CE | -8.67 | 1.29 | 1.77 |
| 1 | N | 278[B] | MET | SD-CE | -8.67 | 1.29 | 1.77 |
| 3 | P | 172 | TYR | CG-CD1 | 8.67 | 1.50 | 1.39 |
| 11 | X | 52 | GLU | CD-OE1 | 8.67 | 1.35 | 1.25 |
| 6 | F | 4 | GLY | N-CA | 8.66 | 1.59 | 1.46 |
| 12 | L | 29 | PHE | CD2-CE2 | -8.45 | 1.22 | 1.39 |
| 3 | P | 102 | TYR | CG-CD1 | -8.36 | 1.28 | 1.39 |
| 6 | S | 4 | GLY | N-CA | 8.36 | 1.58 | 1.46 |
| 7 | T | 80 | THR | C-O | -8.33 | 1.07 | 1.23 |
| 3 | P | 182 | TYR | CD2-CE2 | -8.29 | 1.26 | 1.39 |
| 4 | Q | 20 | ARG | CD-NE | -8.26 | 1.32 | 1.46 |
| 9 | I | 28 | SER | CB-OG | 8.26 | 1.52 | 1.42 |
| 7 | G | 16 | TRP | CZ3-CH2 | 8.18 | 1.53 | 1.40 |
| 1 | A | 382 | SER | CA-CB | 8.15 | 1.65 | 1.52 |
| 1 | N | 382 | SER | CB-OG | -8.13 | 1.31 | 1.42 |
| 2 | O | 147 | GLU | CD-OE1 | -8.12 | 1.16 | 1.25 |
| 2 | O | 132 | GLU | CD-OE2 | 8.08 | 1.34 | 1.25 |
| 2 | B | 223 | SER | CA-CB | 8.03 | 1.65 | 1.52 |
| 2 | O | 197 | SER | CB-OG | 8.03 | 1.52 | 1.42 |
| 10 | J | 48 | TYR | CG-CD2 | 8.01 | 1.49 | 1.39 |
| 4 | D | 60 | TYR | CE1-CZ | 7.98 | 1.49 | 1.38 |
| 5 | E | 9 | GLU | CG-CD | 7.97 | 1.64 | 1.51 |
| 4 | D | 77 | GLU | CD-OE1 | 7.96 | 1.34 | 1.25 |
| 4 | Q | 20 | ARG | CZ-NH2 | -7.96 | 1.22 | 1.33 |
| 2 | O | 65 | TRP | CE3-CZ3 | 7.93 | 1.51 | 1.38 |
| 3 | P | 153 | GLU | CG-CD | 7.92 | 1.63 | 1.51 |
| 11 | K | 31 | TYR | CE1-CZ | 7.89 | 1.48 | 1.38 |
| 4 | Q | 6 | VAL | C-O | 7.88 | 1.38 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 244 | PHE | CD1-CE1 | 7.88 | 1.55 | 1.39 |
| 6 | F | 56 | ARG | CZ-NH1 | 7.88 | 1.43 | 1.33 |
| 3 | P | 76 | GLN | CB-CG | -7.80 | 1.31 | 1.52 |
| 6 | S | 18 | ARG | CZ-NH1 | 7.78 | 1.43 | 1.33 |
| 9 | I | 62 | GLU | CD-OE1 | 7.76 | 1.34 | 1.25 |
| 1 | N | 439 | ARG | CZ-NH1 | 7.75 | 1.43 | 1.33 |
| 4 | D | 135 | SER | CA-CB | 7.73 | 1.64 | 1.52 |
| 6 | F | 17 | GLU | CD-OE1 | 7.68 | 1.34 | 1.25 |
| 13 | M | 40 | TYR | CE1-CZ | 7.67 | 1.48 | 1.38 |
| 1 | A | 19 | TYR | CG-CD2 | 7.62 | 1.49 | 1.39 |
| 1 | A | 514 | LYS | N-CA | 7.57 | 1.61 | 1.46 |
| 9 | V | 47 | TYR | CE1-CZ | 7.56 | 1.48 | 1.38 |
| 1 | N | 441 | SER | CA-CB | 7.54 | 1.64 | 1.52 |
| 13 | M | 14 | GLU | CD-OE2 | 7.53 | 1.33 | 1.25 |
| 5 | E | 90 | ARG | CZ-NH1 | 7.51 | 1.42 | 1.33 |
| 11 | K | 39 | GLU | CG-CD | -7.51 | 1.40 | 1.51 |
| 5 | E | 103 | GLU | CD-OE2 | 7.46 | 1.33 | 1.25 |
| 7 | T | 21 | PHE | CG-CD1 | -7.44 | 1.27 | 1.38 |
| 2 | B | 59 | GLN | CD-OE1 | 7.41 | 1.40 | 1.24 |
| 2 | B | 36 | SER | CB-OG | 7.40 | 1.51 | 1.42 |
| 3 | C | 253 | TYR | CG-CD2 | -7.35 | 1.29 | 1.39 |
| 11 | K | 47 | ARG | CD-NE | 7.34 | 1.58 | 1.46 |
| 5 | R | 32 | GLY | N-CA | 7.32 | 1.57 | 1.46 |
| 1 | A | 189 | MET | CG-SD | -7.32 | 1.62 | 1.81 |
| 2 | B | 59 | GLN | CG-CD | 7.31 | 1.67 | 1.51 |
| 3 | C | 230 | ASN | CB-CG | -7.30 | 1.34 | 1.51 |
| 1 | N | 323 | TRP | CZ3-CH2 | 7.29 | 1.51 | 1.40 |
| 2 | O | 198 | GLU | CD-OE2 | -7.28 | 1.17 | 1.25 |
| 3 | C | 182 | TYR | CZ-OH | -7.26 | 1.25 | 1.37 |
| 2 | O | 60 | GLU | CG-CD | 7.20 | 1.62 | 1.51 |
| 1 | A | 322 | SER | CA-CB | 7.19 | 1.63 | 1.52 |
| 10 | J | 25 | GLY | N-CA | 7.18 | 1.56 | 1.46 |
| 5 | E | 9 | GLU | CD-OE2 | 7.17 | 1.33 | 1.25 |
| 9 | I | 60 | PHE | CG-CD2 | 7.17 | 1.49 | 1.38 |
| 9 | I | 4 | LEU | CA-CB | 7.14 | 1.70 | 1.53 |
| 1 | N | 226 | GLY | N-CA | 7.13 | 1.56 | 1.46 |
| 6 | S | 92 | VAL | C-O | -7.13 | 1.09 | 1.23 |
| 1 | A | 401 | SER | CA-CB | 7.12 | 1.63 | 1.52 |
| 4 | D | 100[A] | LYS | CE-NZ | 7.11 | 1.66 | 1.49 |
| 4 | D | 100[B] | LYS | CE-NZ | 7.11 | 1.66 | 1.49 |
| 3 | C | 102 | TYR | CG-CD1 | -7.11 | 1.29 | 1.39 |
| 2 | B | 113 | TYR | CG-CD2 | 7.09 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | C | 16 | TRP | CE3-CZ3 | 7.07 | 1.50 | 1.38 |
| 4 | D | 47 | SER | CA-CB | 7.07 | 1.63 | 1.52 |
| 1 | N | 470 | PHE | CE2-CZ | 7.03 | 1.50 | 1.37 |
| 2 | O | 65 | TRP | CD2-CE3 | 7.01 | 1.50 | 1.40 |
| 3 | C | 65 | SER | CA-CB | 6.99 | 1.63 | 1.52 |
| 5 | E | 56 | ARG | CZ-NH2 | 6.99 | 1.42 | 1.33 |
| 3 | C | 94 | PHE | CG-CD2 | 6.99 | 1.49 | 1.38 |
| 6 | F | 18 | ARG | CZ-NH2 | 6.99 | 1.42 | 1.33 |
| 7 | G | 17 | ARG | CZ-NH2 | 6.98 | 1.42 | 1.33 |
| 4 | D | 61 | ARG | CZ-NH2 | 6.97 | 1.42 | 1.33 |
| 5 | E | 9 | GLU | CA-CB | 6.94 | 1.69 | 1.53 |
| 3 | P | 182 | TYR | CE1-CZ | 6.92 | 1.47 | 1.38 |
| 5 | R | 39 | TYR | CG-CD2 | -6.91 | 1.30 | 1.39 |
| 3 | C | 113 | GLY | N-CA | 6.91 | 1.56 | 1.46 |
| 1 | A | 242 | GLU | CD-OE1 | 6.88 | 1.33 | 1.25 |
| 3 | C | 29 | SER | CB-OG | -6.86 | 1.33 | 1.42 |
| 1 | A | 49 | GLY | C-O | 6.86 | 1.34 | 1.23 |
| 7 | G | 83 | GLU | CD-OE1 | 6.86 | 1.33 | 1.25 |
| 3 | P | 258 | TRP | CG-CD1 | 6.84 | 1.46 | 1.36 |
| 1 | A | 149 | SER | CB-OG | 6.83 | 1.51 | 1.42 |
| 1 | N | 335 | SER | CB-OG | 6.83 | 1.51 | 1.42 |
| 1 | N | 49 | GLY | C-O | 6.83 | 1.34 | 1.23 |
| 1 | N | 514 | LYS | N-CA | 6.82 | 1.59 | 1.46 |
| 5 | E | 109 | VAL | N-CA | 6.82 | 1.59 | 1.46 |
| 12 | L | 14 | SER | CB-OG | 6.77 | 1.51 | 1.42 |
| 2 | B | 167 | SER | CB-OG | -6.76 | 1.33 | 1.42 |
| 2 | O | 193 | TYR | CG-CD1 | 6.75 | 1.48 | 1.39 |
| 5 | E | 84 | TYR | CG-CD1 | 6.74 | 1.48 | 1.39 |
| 12 | Y | 5 | GLU | CD-OE2 | -6.74 | 1.18 | 1.25 |
| 1 | A | 450 | TRP | CE3-CZ3 | 6.71 | 1.49 | 1.38 |
| 1 | A | 480 | ARG | CZ-NH2 | 6.69 | 1.41 | 1.33 |
| 2 | B | 82 | ARG | CZ-NH1 | 6.69 | 1.41 | 1.33 |
| 10 | W | 25 | GLY | N-CA | 6.69 | 1.56 | 1.46 |
| 3 | C | 8 | TYR | CG-CD2 | 6.69 | 1.47 | 1.39 |
| 12 | Y | 26 | THR | CB-CG2 | -6.67 | 1.30 | 1.52 |
| 6 | S | 89 | TYR | CE1-CZ | 6.64 | 1.47 | 1.38 |
| 13 | M | 40 | TYR | CG-CD1 | 6.62 | 1.47 | 1.39 |
| 1 | N | 270 | TYR | CE1-CZ | 6.62 | 1.47 | 1.38 |
| 11 | K | 47 | ARG | CG-CD | 6.60 | 1.68 | 1.51 |
| 1 | N | 281 | GLY | N-CA | 6.60 | 1.55 | 1.46 |
| 5 | R | 39 | TYR | CE2-CZ | -6.59 | 1.29 | 1.38 |
| 1 | N | 514 | LYS | CA-CB | 6.54 | 1.68 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | G | 12 | GLY | CA-C | 6.54 | 1.62 | 1.51 |
| 6 | S | 93 | PRO | CA-CB | 6.54 | 1.66 | 1.53 |
| 1 | N | 502 | TYR | CG-CD2 | 6.54 | 1.47 | 1.39 |
| 2 | B | 223 | SER | CB-OG | -6.53 | 1.33 | 1.42 |
| 5 | E | 73 | ASP | CB-CG | 6.52 | 1.65 | 1.51 |
| 7 | G | 5 | LYS | CA-CB | 6.50 | 1.68 | 1.53 |
| 5 | E | 38 | GLY | N-CA | 6.49 | 1.55 | 1.46 |
| 11 | K | 17 | VAL | N-CA | 6.49 | 1.59 | 1.46 |
| 1 | A | 382 | SER | CB-OG | -6.46 | 1.33 | 1.42 |
| 3 | P | 233 | PHE | CD2-CE2 | 6.45 | 1.52 | 1.39 |
| 5 | E | 84 | TYR | CE1-CZ | -6.44 | 1.30 | 1.38 |
| 2 | B | 108 | TYR | CE2-CZ | 6.43 | 1.47 | 1.38 |
| 8 | U | 33 | TYR | CG-CD1 | 6.42 | 1.47 | 1.39 |
| 3 | P | 143 | SER | CA-CB | 6.42 | 1.62 | 1.52 |
| 11 | K | 39 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 8 | H | 72 | TRP | CD2-CE2 | 6.41 | 1.49 | 1.41 |
| 12 | Y | 4 | GLU | CG-CD | 6.41 | 1.61 | 1.51 |
| 4 | D | 88 | PHE | CE2-CZ | 6.39 | 1.49 | 1.37 |
| 3 | C | 143 | SER | CA-CB | 6.38 | 1.62 | 1.52 |
| 2 | B | 65 | TRP | CD2-CE3 | 6.38 | 1.50 | 1.40 |
| 11 | K | 39 | GLU | CB-CG | 6.38 | 1.64 | 1.52 |
| 7 | G | 56 | ARG | CZ-NH1 | 6.37 | 1.41 | 1.33 |
| 6 | F | 3 | GLY | CA-C | 6.36 | 1.62 | 1.51 |
| 4 | D | 52 | SER | CB-OG | 6.34 | 1.50 | 1.42 |
| 1 | N | 264 | LYS | CD-CE | 6.33 | 1.67 | 1.51 |
| 1 | N | 187 | SER | CA-CB | 6.33 | 1.62 | 1.52 |
| 6 | S | 19 | GLU | CD-OE1 | 6.33 | 1.32 | 1.25 |
| 2 | B | 65 | TRP | CD2-CE2 | 6.32 | 1.49 | 1.41 |
| 2 | B | 113 | TYR | CB-CG | -6.31 | 1.42 | 1.51 |
| 12 | Y | 5 | GLU | CD-OE1 | -6.31 | 1.18 | 1.25 |
| 2 | O | 123 | ILE | N-CA | 6.28 | 1.58 | 1.46 |
| 7 | T | 17 | ARG | CZ-NH1 | 6.27 | 1.41 | 1.33 |
| 4 | D | 34 | SER | CB-OG | 6.27 | 1.50 | 1.42 |
| 1 | A | 450 | TRP | CG-CD1 | 6.26 | 1.45 | 1.36 |
| 3 | C | 41 | THR | C-O | 6.24 | 1.35 | 1.23 |
| 5 | E | 103 | GLU | CB-CG | 6.22 | 1.64 | 1.52 |
| 7 | G | 21 | PHE | CG-CD1 | -6.22 | 1.29 | 1.38 |
| 5 | R | 80 | GLU | CD-OE1 | 6.21 | 1.32 | 1.25 |
| 9 | I | 56 | SER | CB-OG | 6.18 | 1.50 | 1.42 |
| 4 | Q | 18 | ASP | N-CA | 6.17 | 1.58 | 1.46 |
| 3 | C | 99 | TRP | CE3-CZ3 | 6.17 | 1.49 | 1.38 |
| 3 | C | 120 | GLY | N-CA | 6.17 | 1.55 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 10 | W | 14[A] | GLU | CD-OE1 | -6.17 | 1.18 | 1.25 |
| 10 | W | 14[B] | GLU | CD-OE1 | -6.17 | 1.18 | 1.25 |
| 4 | Q | 64 | PHE | CG-CD2 | 6.16 | 1.48 | 1.38 |
| 3 | P | 116 | TRP | CZ3-CH2 | 6.16 | 1.49 | 1.40 |
| 1 | A | 242 | GLU | CD-OE2 | -6.14 | 1.18 | 1.25 |
| 2 | B | 152 | MET | CB-CG | -6.14 | 1.31 | 1.51 |
| 1 | A | 335 | SER | CB-OG | 6.14 | 1.50 | 1.42 |
| 5 | E | 41 | LEU | C-O | 6.14 | 1.35 | 1.23 |
| 4 | Q | 78 | TRP | CE3-CZ3 | 6.14 | 1.48 | 1.38 |
| 7 | G | 13 | ALA | N-CA | 6.13 | 1.58 | 1.46 |
| 3 | C | 255 | SER | CA-CB | 6.13 | 1.62 | 1.52 |
| 5 | R | 80 | GLU | CG-CD | 6.11 | 1.61 | 1.51 |
| 8 | U | 72 | TRP | CD1-NE1 | 6.11 | 1.48 | 1.38 |
| 5 | R | 84 | TYR | CE1-CZ | -6.11 | 1.30 | 1.38 |
| 1 | N | 116 | SER | CB-OG | 6.11 | 1.50 | 1.42 |
| 2 | O | 115 | ASP | CB-CG | 6.10 | 1.64 | 1.51 |
| 5 | R | 18 | TYR | CG-CD2 | 6.10 | 1.47 | 1.39 |
| 2 | B | 225 | SER | CA-CB | 6.09 | 1.62 | 1.52 |
| 6 | F | 72 | PHE | CD1-CE1 | 6.09 | 1.51 | 1.39 |
| 3 | C | 153 | GLU | CD-OE2 | -6.09 | 1.19 | 1.25 |
| 3 | C | 171 | VAL | CB-CG1 | 6.09 | 1.65 | 1.52 |
| 3 | C | 34 | TRP | CE3-CZ3 | 6.08 | 1.48 | 1.38 |
| 1 | A | 213 | ARG | CZ-NH2 | 6.08 | 1.41 | 1.33 |
| 1 | A | 363 | LEU | CB-CG | -6.08 | 1.34 | 1.52 |
| 3 | C | 249 | TRP | CE3-CZ3 | 6.08 | 1.48 | 1.38 |
| 12 | Y | 2 | HIS | N-CA | 6.07 | 1.58 | 1.46 |
| 1 | N | 96 | ARG | CZ-NH1 | 6.07 | 1.41 | 1.33 |
| 5 | E | 91 | PRO | CA-C | 6.06 | 1.65 | 1.52 |
| 5 | E | 84 | TYR | CE2-CZ | 6.05 | 1.46 | 1.38 |
| 2 | B | 167 | SER | CA-CB | -6.02 | 1.44 | 1.52 |
| 3 | P | 59 | ARG | CZ-NH1 | 6.02 | 1.40 | 1.33 |
| 13 | Z | 40 | TYR | CG-CD2 | 6.01 | 1.47 | 1.39 |
| 7 | T | 14 | ARG | CZ-NH1 | 6.01 | 1.40 | 1.33 |
| 6 | F | 78 | GLU | CD-OE2 | -6.00 | 1.19 | 1.25 |
| 4 | D | 68 | PHE | CG-CD1 | 5.98 | 1.47 | 1.38 |
| 5 | R | 84 | TYR | CE2-CZ | 5.97 | 1.46 | 1.38 |
| 1 | A | 400 | PHE | CD2-CE2 | 5.97 | 1.51 | 1.39 |
| 1 | N | 441 | SER | CB-OG | 5.96 | 1.50 | 1.42 |
| 6 | S | 43 | LYS | CB-CG | 5.96 | 1.68 | 1.52 |
| 6 | F | 2 | SER | N-CA | 5.95 | 1.58 | 1.46 |
| 10 | J | 7 | GLU | CD-OE1 | 5.95 | 1.32 | 1.25 |
| 3 | C | 76 | GLN | CB-CG | -5.95 | 1.36 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | D | 105 | GLY | N-CA | 5.95 | 1.54 | 1.46 |
| 3 | P | 198 | PHE | CG-CD2 | 5.93 | 1.47 | 1.38 |
| 4 | D | 9 | GLU | CG-CD | 5.92 | 1.60 | 1.51 |
| 3 | C | 233 | PHE | CD1-CE1 | 5.92 | 1.51 | 1.39 |
| 5 | E | 19 | PHE | CE1-CZ | 5.92 | 1.48 | 1.37 |
| 6 | F | 62 | CYS | N-CA | 5.92 | 1.58 | 1.46 |
| 6 | S | 3 | GLY | C-O | 5.91 | 1.33 | 1.23 |
| 13 | M | 40 | TYR | CG-CD2 | 5.91 | 1.46 | 1.39 |
| 11 | X | 53 | TRP | CE3-CZ3 | 5.91 | 1.48 | 1.38 |
| 3 | C | 225 | PHE | CG-CD1 | 5.90 | 1.47 | 1.38 |
| 3 | P | 16 | TRP | CG-CD1 | 5.88 | 1.45 | 1.36 |
| 3 | C | 181 | TYR | CE2-CZ | -5.87 | 1.30 | 1.38 |
| 7 | G | 18 | PHE | CG-CD2 | -5.87 | 1.29 | 1.38 |
| 3 | P | 253 | TYR | CZ-OH | 5.86 | 1.47 | 1.37 |
| 2 | O | 163 | TRP | CG-CD1 | 5.85 | 1.45 | 1.36 |
| 1 | N | 19 | TYR | CG-CD2 | 5.85 | 1.46 | 1.39 |
| 11 | X | 47 | ARG | NE-CZ | 5.84 | 1.40 | 1.33 |
| 12 | Y | 38 | PHE | CG-CD1 | 5.83 | 1.47 | 1.38 |
| 1 | A | 214 | ASN | C-O | 5.83 | 1.34 | 1.23 |
| 9 | V | 51 | TYR | CG-CD1 | 5.83 | 1.46 | 1.39 |
| 7 | G | 5 | LYS | CA-C | 5.83 | 1.68 | 1.52 |
| 1 | N | 129 | TYR | CD2-CE2 | 5.83 | 1.48 | 1.39 |
| 1 | A | 281 | GLY | N-CA | 5.81 | 1.54 | 1.46 |
| 2 | B | 222 | TRP | CE3-CZ3 | 5.81 | 1.48 | 1.38 |
| 6 | F | 80 | GLN | CD-OE1 | 5.80 | 1.36 | 1.24 |
| 10 | J | 19 | PRO | CA-CB | 5.79 | 1.65 | 1.53 |
| 2 | B | 55 | THR | C-O | 5.79 | 1.34 | 1.23 |
| 13 | Z | 4 | LYS | N-CA | 5.78 | 1.57 | 1.46 |
| 3 | C | 177 | GLN | CB-CG | -5.78 | 1.36 | 1.52 |
| 10 | J | 14 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | A | 90 | PRO | N-CD | 5.77 | 1.55 | 1.47 |
| 4 | D | 36 | SER | CB-OG | -5.76 | 1.34 | 1.42 |
| 4 | D | 49 | SER | CA-CB | 5.75 | 1.61 | 1.52 |
| 1 | A | 474 | GLU | CD-OE1 | 5.75 | 1.31 | 1.25 |
| 5 | R | 11 | PHE | CG-CD2 | 5.74 | 1.47 | 1.38 |
| 1 | A | 43 | GLN | CG-CD | 5.73 | 1.64 | 1.51 |
| 5 | E | 27 | TRP | CE3-CZ3 | 5.73 | 1.48 | 1.38 |
| 1 | N | 454 | SER | CA-CB | 5.73 | 1.61 | 1.52 |
| 4 | D | 91 | PHE | CG-CD1 | 5.73 | 1.47 | 1.38 |
| 2 | B | 55 | THR | CB-CG2 | 5.73 | 1.71 | 1.52 |
| 11 | K | 54 | ARG | CZ-NH2 | 5.72 | 1.40 | 1.33 |
| 13 | M | 11 | SER | CB-OG | 5.72 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | N | 384 | GLY | N-CA | 5.72 | 1.54 | 1.46 |
| 4 | Q | 125 | ASP | CB-CG | 5.72 | 1.63 | 1.51 |
| 2 | B | 198 | GLU | CB-CG | 5.71 | 1.62 | 1.52 |
| 1 | N | 250 | GLY | CA-C | 5.69 | 1.60 | 1.51 |
| 8 | U | 30 | TRP | CG-CD1 | 5.69 | 1.44 | 1.36 |
| 11 | K | 31 | TYR | CG-CD2 | 5.68 | 1.46 | 1.39 |
| 9 | I | 7 | PRO | CA-C | -5.68 | 1.41 | 1.52 |
| 1 | A | 179 | TYR | CG-CD1 | 5.67 | 1.46 | 1.39 |
| 9 | I | 68 | ILE | CB-CG1 | -5.67 | 1.38 | 1.54 |
| 9 | V | 50 | PHE | CG-CD1 | 5.66 | 1.47 | 1.38 |
| 9 | I | 54 | TYR | CD2-CE2 | 5.65 | 1.47 | 1.39 |
| 7 | G | 3 | ALA | N-CA | 5.64 | 1.57 | 1.46 |
| 2 | O | 21 | LEU | CA-CB | 5.64 | 1.66 | 1.53 |
| 8 | U | 67 | SER | CA-CB | 5.63 | 1.61 | 1.52 |
| 2 | O | 192 | TYR | CE2-CZ | 5.63 | 1.45 | 1.38 |
| 11 | K | 53 | TRP | CE3-CZ3 | 5.63 | 1.48 | 1.38 |
| 1 | A | 448 | THR | C-O | 5.62 | 1.34 | 1.23 |
| 2 | B | 21 | LEU | CA-CB | 5.62 | 1.66 | 1.53 |
| 3 | C | 101 | PHE | CD1-CE1 | 5.62 | 1.50 | 1.39 |
| 5 | R | 9 | GLU | CG-CD | 5.62 | 1.60 | 1.51 |
| 12 | Y | 20 | ARG | CZ-NH1 | 5.62 | 1.40 | 1.33 |
| 7 | T | 83 | GLU | CD-OE1 | 5.61 | 1.31 | 1.25 |
| 6 | S | 89 | TYR | CG-CD2 | 5.61 | 1.46 | 1.39 |
| 2 | O | 110 | TYR | CG-CD2 | 5.61 | 1.46 | 1.39 |
| 12 | Y | 8 | GLY | N-CA | 5.61 | 1.54 | 1.46 |
| 5 | R | 69 | GLU | CB-CG | 5.60 | 1.62 | 1.52 |
| 6 | S | 3 | GLY | CA-C | 5.60 | 1.60 | 1.51 |
| 4 | D | 85 | ALA | C-O | 5.59 | 1.33 | 1.23 |
| 3 | C | 253 | TYR | CE1-CZ | -5.59 | 1.31 | 1.38 |
| 9 | V | 28 | SER | CB-OG | 5.58 | 1.49 | 1.42 |
| 2 | O | 66 | THR | CB-OG1 | 5.58 | 1.54 | 1.43 |
| 2 | O | 107 | SER | CA-CB | 5.57 | 1.61 | 1.52 |
| 2 | B | 82 | ARG | CZ-NH2 | 5.56 | 1.40 | 1.33 |
| 4 | D | 64 | PHE | CA-CB | 5.56 | 1.66 | 1.53 |
| 12 | Y | 3 | TYR | CG-CD1 | 5.56 | 1.46 | 1.39 |
| 4 | D | 58 | GLU | CB-CG | 5.56 | 1.62 | 1.52 |
| 1 | N | 231 | TYR | CE1-CZ | 5.55 | 1.45 | 1.38 |
| 12 | L | 6 | GLY | CA-C | 5.55 | 1.60 | 1.51 |
| 4 | Q | 102 | TYR | CG-CD2 | 5.55 | 1.46 | 1.39 |
| 2 | B | 121 | TYR | CE2-CZ | 5.55 | 1.45 | 1.38 |
| 6 | F | 18 | ARG | CZ-NH1 | 5.55 | 1.40 | 1.33 |
| 1 | N | 382 | SER | CA-CB | 5.55 | 1.61 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | V | 10 | ARG | CZ-NH1 | 5.53 | 1.40 | 1.33 |
| 1 | A | 307 | SER | CB-OG | 5.52 | 1.49 | 1.42 |
| 1 | A | 506 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | A | 77 | GLY | N-CA | 5.51 | 1.54 | 1.46 |
| 3 | C | 172 | TYR | CE2-CZ | 5.51 | 1.45 | 1.38 |
| 5 | E | 69 | GLU | CA-CB | 5.51 | 1.66 | 1.53 |
| 3 | P | 94 | PHE | CE1-CZ | 5.51 | 1.47 | 1.37 |
| 3 | C | 233 | PHE | CD2-CE2 | 5.50 | 1.50 | 1.39 |
| 1 | N | 9 | SER | CB-OG | 5.50 | 1.49 | 1.42 |
| 1 | A | 362[A] | SER | CA-CB | 5.50 | 1.61 | 1.52 |
| 1 | A | 362[B] | SER | CA-CB | 5.50 | 1.61 | 1.52 |
| 11 | X | 39 | GLU | CD-OE1 | 5.50 | 1.31 | 1.25 |
| 1 | A | 410 | ALA | CA-CB | 5.50 | 1.64 | 1.52 |
| 1 | N | 494 | TRP | CE3-CZ3 | 5.50 | 1.47 | 1.38 |
| 3 | P | 102 | TYR | CG-CD2 | 5.50 | 1.46 | 1.39 |
| 1 | A | 184 | PHE | CG-CD1 | 5.49 | 1.47 | 1.38 |
| 1 | A | 333 | LYS | C-O | 5.49 | 1.33 | 1.23 |
| 6 | F | 85 | CYS | C-O | 5.49 | 1.33 | 1.23 |
| 1 | N | 440 | TYR | CE1-CZ | 5.48 | 1.45 | 1.38 |
| 1 | N | 486 | ASP | CG-OD1 | 5.48 | 1.38 | 1.25 |
| 1 | N | 144 | ASP | CB-CG | 5.47 | 1.63 | 1.51 |
| 1 | N | 189 | MET | CG-SD | -5.47 | 1.67 | 1.81 |
| 1 | N | 92 | MET | CB-CG | 5.46 | 1.68 | 1.51 |
| 3 | P | 230 | ASN | CB-CG | -5.46 | 1.38 | 1.51 |
| 2 | B | 110 | TYR | CD1-CE1 | 5.45 | 1.47 | 1.39 |
| 3 | P | 80[A] | ARG | CZ-NH1 | -5.45 | 1.25 | 1.33 |
| 3 | P | 80[B] | ARG | CZ-NH1 | -5.45 | 1.25 | 1.33 |
| 1 | A | 418 | PHE | CD2-CE2 | 5.44 | 1.50 | 1.39 |
| 1 | N | 156 | SER | CB-OG | 5.44 | 1.49 | 1.42 |
| 11 | K | 39 | GLU | CD-OE1 | 5.44 | 1.31 | 1.25 |
| 11 | K | 47 | ARG | NE-CZ | 5.43 | 1.40 | 1.33 |
| 1 | N | 320 | VAL | CB-CG1 | 5.42 | 1.64 | 1.52 |
| 3 | C | 146 | TRP | CE3-CZ3 | 5.42 | 1.47 | 1.38 |
| 3 | C | 198 | PHE | CG-CD2 | 5.42 | 1.46 | 1.38 |
| 5 | R | 63 | SER | CB-OG | 5.42 | 1.49 | 1.42 |
| 2 | B | 220 | GLU | CD-OE1 | -5.41 | 1.19 | 1.25 |
| 7 | T | 56 | ARG | CZ-NH1 | 5.41 | 1.40 | 1.33 |
| 4 | D | 28 | ALA | C-O | 5.41 | 1.33 | 1.23 |
| 1 | N | 305 | PHE | CG-CD2 | 5.41 | 1.46 | 1.38 |
| 2 | B | 60 | GLU | CG-CD | 5.41 | 1.60 | 1.51 |
| 5 | R | 57 | ARG | CZ-NH1 | 5.41 | 1.40 | 1.33 |
| 1 | A | 426 | PHE | CG-CD1 | 5.41 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | U | 76 | ARG | CZ-NH1 | 5.40 | 1.40 | 1.33 |
| 1 | A | 296 | GLY | N-CA | 5.39 | 1.54 | 1.46 |
| 8 | H | 20 | PHE | CG-CD1 | 5.39 | 1.46 | 1.38 |
| 2 | O | 85 | TYR | CG-CD2 | 5.39 | 1.46 | 1.39 |
| 2 | O | 137 | GLU | CD-OE1 | 5.39 | 1.31 | 1.25 |
| 7 | T | 16 | TRP | CD2-CE2 | 5.39 | 1.47 | 1.41 |
| 1 | N | 157 | SER | CB-OG | 5.38 | 1.49 | 1.42 |
| 1 | N | 71 | MET | CG-SD | 5.37 | 1.95 | 1.81 |
| 4 | Q | 90 | GLY | N-CA | 5.37 | 1.54 | 1.46 |
| 2 | O | 202 | SER | CA-CB | 5.37 | 1.61 | 1.52 |
| 1 | N | 502 | TYR | CE1-CZ | 5.36 | 1.45 | 1.38 |
| 3 | P | 153 | GLU | CD-OE1 | -5.36 | 1.19 | 1.25 |
| 5 | E | 88 | GLU | CG-CD | 5.36 | 1.59 | 1.51 |
| 3 | P | 255 | SER | C-O | 5.36 | 1.33 | 1.23 |
| 2 | B | 65 | TRP | CZ2-CH2 | 5.36 | 1.47 | 1.37 |
| 5 | E | 57 | ARG | CZ-NH1 | 5.36 | 1.40 | 1.33 |
| 4 | D | 140 | TYR | CB-CG | 5.35 | 1.59 | 1.51 |
| 3 | P | 198 | PHE | CE2-CZ | 5.35 | 1.47 | 1.37 |
| 3 | C | 89 | SER | CB-OG | 5.34 | 1.49 | 1.42 |
| 12 | L | 5 | GLU | CD-OE1 | -5.34 | 1.19 | 1.25 |
| 13 | M | 26 | PHE | CE1-CZ | 5.34 | 1.47 | 1.37 |
| 4 | Q | 6 | VAL | CA-CB | 5.33 | 1.66 | 1.54 |
| 5 | E | 61 | PHE | CG-CD1 | 5.33 | 1.46 | 1.38 |
| 2 | O | 145 | PRO | C-O | 5.33 | 1.33 | 1.23 |
| 4 | D | 60 | TYR | CG-CD1 | 5.33 | 1.46 | 1.39 |
| 3 | P | 90 | GLU | CD-OE2 | 5.33 | 1.31 | 1.25 |
| 3 | C | 221 | ARG | CZ-NH2 | 5.32 | 1.40 | 1.33 |
| 3 | C | 181 | TYR | CB-CG | 5.32 | 1.59 | 1.51 |
| 6 | S | 3 | GLY | N-CA | 5.32 | 1.54 | 1.46 |
| 6 | F | 31 | TYR | CE1-CZ | 5.31 | 1.45 | 1.38 |
| 8 | U | 70 | SER | CB-OG | -5.31 | 1.35 | 1.42 |
| 3 | P | 182 | TYR | CE2-CZ | 5.31 | 1.45 | 1.38 |
| 5 | R | 30 | ARG | CZ-NH2 | 5.30 | 1.40 | 1.33 |
| 6 | S | 21[A] | MET | C-O | 5.30 | 1.33 | 1.23 |
| 6 | S | 21[B] | MET | C-O | 5.30 | 1.33 | 1.23 |
| 8 | U | 22 | ASN | CG-OD1 | 5.30 | 1.35 | 1.24 |
| 11 | X | 53 | TRP | CB-CG | 5.30 | 1.59 | 1.50 |
| 1 | A | 103 | TRP | CE3-CZ3 | 5.30 | 1.47 | 1.38 |
| 3 | P | 235 | PHE | CD1-CE1 | 5.30 | 1.49 | 1.39 |
| 1 | A | 264 | LYS | CD-CE | 5.29 | 1.64 | 1.51 |
| 6 | S | 60 | CYS | CB-SG | 5.29 | 1.91 | 1.82 |
| 9 | I | 18 | ARG | C-O | 5.28 | 1.33 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 10 | J | 14 | GLU | CD-OE1 | 5.28 | 1.31 | 1.25 |
| 1 | N | 81 | TRP | CG-CD1 | 5.27 | 1.44 | 1.36 |
| 1 | A | 406 | ASN | C-O | 5.27 | 1.33 | 1.23 |
| 2 | O | 156 | SER | CA-CB | 5.26 | 1.60 | 1.52 |
| 7 | T | 5 | LYS | CA-CB | 5.26 | 1.65 | 1.53 |
| 1 | N | 266 | GLU | CD-OE2 | 5.25 | 1.31 | 1.25 |
| 2 | B | 192 | TYR | CD1-CE1 | 5.25 | 1.47 | 1.39 |
| 2 | O | 40 | TYR | CG-CD1 | 5.25 | 1.46 | 1.39 |
| 2 | O | 65 | TRP | CD2-CE2 | 5.25 | 1.47 | 1.41 |
| 7 | T | 4 | ALA | C-O | -5.25 | 1.13 | 1.23 |
| 3 | P | 253 | TYR | CD2-CE2 | 5.25 | 1.47 | 1.39 |
| 1 | N | 184 | PHE | CG-CD1 | 5.24 | 1.46 | 1.38 |
| 4 | D | 111 | PHE | CD1-CE1 | 5.24 | 1.49 | 1.39 |
| 3 | P | 16 | TRP | CE3-CZ3 | 5.24 | 1.47 | 1.38 |
| 1 | N | 235 | PHE | CG-CD2 | 5.23 | 1.46 | 1.38 |
| 4 | Q | 138 | TRP | CE3-CZ3 | 5.23 | 1.47 | 1.38 |
| 1 | A | 5 | ARG | CZ-NH1 | 5.23 | 1.39 | 1.33 |
| 3 | C | 94 | PHE | CE1-CZ | 5.23 | 1.47 | 1.37 |
| 12 | Y | 13 | PHE | CG-CD1 | 5.22 | 1.46 | 1.38 |
| 1 | A | 71 | MET | CG-SD | 5.21 | 1.94 | 1.81 |
| 3 | P | 55 | TYR | CE1-CZ | 5.21 | 1.45 | 1.38 |
| 1 | A | 509 | THR | C-O | 5.21 | 1.33 | 1.23 |
| 5 | E | 87 | GLN | N-CA | 5.21 | 1.56 | 1.46 |
| 1 | A | 443 | TYR | CB-CG | 5.21 | 1.59 | 1.51 |
| 2 | B | 198 | GLU | CD-OE2 | -5.20 | 1.20 | 1.25 |
| 8 | H | 11 | TYR | N-CA | 5.20 | 1.56 | 1.46 |
| 1 | A | 278[A] | MET | SD-CE | -5.20 | 1.48 | 1.77 |
| 1 | A | 278[B] | MET | SD-CE | -5.20 | 1.48 | 1.77 |
| 5 | E | 82 | TYR | CD1-CE1 | 5.20 | 1.47 | 1.39 |
| 4 | D | 87[A] | PHE | CG-CD1 | 5.20 | 1.46 | 1.38 |
| 4 | D | 87[B] | PHE | CG-CD1 | 5.20 | 1.46 | 1.38 |
| 8 | U | 40 | GLU | CD-OE1 | -5.19 | 1.20 | 1.25 |
| 4 | Q | 18 | ASP | CB-CG | -5.18 | 1.40 | 1.51 |
| 1 | A | 343 | GLY | N-CA | 5.17 | 1.53 | 1.46 |
| 1 | A | 482 | VAL | CA-CB | 5.17 | 1.65 | 1.54 |
| 4 | D | 58 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |
| 3 | P | 3 | HIS | C-O | 5.17 | 1.33 | 1.23 |
| 7 | T | 22 | GLY | N-CA | 5.17 | 1.53 | 1.46 |
| 6 | F | 70 | ILE | N-CA | 5.16 | 1.56 | 1.46 |
| 1 | N | 92 | MET | CG-SD | -5.16 | 1.67 | 1.81 |
| 1 | N | 387 | PHE | CE1-CZ | 5.16 | 1.47 | 1.37 |
| 11 | X | 53 | TRP | CG-CD1 | 5.15 | 1.44 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | I | 35 | TYR | CG-CD1 | 5.15 | 1.45 | 1.39 |
| 1 | N | 396 | TRP | CD2-CE2 | 5.14 | 1.47 | 1.41 |
| 3 | P | 113 | GLY | N-CA | 5.14 | 1.53 | 1.46 |
| 8 | U | 68 | TRP | CZ3-CH2 | 5.14 | 1.48 | 1.40 |
| 2 | B | 147 | GLU | CD-OE2 | -5.14 | 1.20 | 1.25 |
| 6 | S | 43 | LYS | CG-CD | 5.14 | 1.70 | 1.52 |
| 2 | B | 220 | GLU | CG-CD | 5.13 | 1.59 | 1.51 |
| 1 | N | 513 | LEU | C-O | 5.13 | 1.33 | 1.23 |
| 9 | I | 47 | TYR | CE1-CZ | 5.13 | 1.45 | 1.38 |
| 2 | B | 38 | VAL | CA-CB | 5.12 | 1.65 | 1.54 |
| 4 | Q | 60 | TYR | CE2-CZ | 5.12 | 1.45 | 1.38 |
| 7 | T | 64 | ASP | CG-OD1 | 5.12 | 1.37 | 1.25 |
| 7 | T | 44 | ARG | CZ-NH2 | 5.12 | 1.39 | 1.33 |
| 1 | A | 403 | TYR | CG-CD2 | -5.12 | 1.32 | 1.39 |
| 4 | D | 40 | LEU | C-O | 5.11 | 1.33 | 1.23 |
| 1 | N | 485 | VAL | CA-CB | 5.11 | 1.65 | 1.54 |
| 4 | D | 11 | TYR | CE1-CZ | -5.10 | 1.31 | 1.38 |
| 1 | A | 38 | ARG | CZ-NH2 | 5.09 | 1.39 | 1.33 |
| 3 | C | 65 | SER | CB-OG | 5.09 | 1.48 | 1.42 |
| 9 | I | 19 | PHE | CG-CD2 | 5.09 | 1.46 | 1.38 |
| 1 | A | 379 | TYR | CZ-OH | 5.08 | 1.46 | 1.37 |
| 3 | P | 260 | GLY | N-CA | 5.08 | 1.53 | 1.46 |
| 1 | N | 476 | PHE | CG-CD2 | 5.08 | 1.46 | 1.38 |
| 3 | P | 244 | PHE | CD1-CE1 | 5.08 | 1.49 | 1.39 |
| 2 | B | 202 | SER | CB-OG | 5.08 | 1.48 | 1.42 |
| 3 | C | 56 | GLN | CB-CG | 5.08 | 1.66 | 1.52 |
| 2 | B | 198 | GLU | CD-OE1 | -5.08 | 1.20 | 1.25 |
| 10 | W | 1 | PHE | N-CA | 5.08 | 1.56 | 1.46 |
| 4 | Q | 25 | PRO | N-CA | 5.07 | 1.55 | 1.47 |
| 1 | N | 90 | PRO | N-CD | 5.07 | 1.54 | 1.47 |
| 7 | G | 69 | PHE | CG-CD2 | 5.07 | 1.46 | 1.38 |
| 8 | H | 75 | ARG | NE-CZ | 5.07 | 1.39 | 1.33 |
| 2 | O | 202 | SER | CB-OG | -5.06 | 1.35 | 1.42 |
| 3 | P | 58 | TRP | CZ3-CH2 | 5.06 | 1.48 | 1.40 |
| 4 | Q | 6 | VAL | C-N | 5.06 | 1.45 | 1.34 |
| 13 | Z | 14 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 2 | B | 147 | GLU | CD-OE1 | -5.05 | 1.20 | 1.25 |
| 1 | A | 144 | ASP | CB-CG | 5.04 | 1.62 | 1.51 |
| 4 | D | 56 | LYS | CE-NZ | 5.04 | 1.61 | 1.49 |
| 1 | N | 261 | TYR | CD1-CE1 | 5.04 | 1.47 | 1.39 |
| 2 | O | 65 | TRP | CG-CD2 | 5.04 | 1.52 | 1.43 |
| 2 | O | 82 | ARG | CZ-NH1 | 5.04 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | N | 244 | TYR | CE1-CZ | 5.04 | 1.45 | 1.38 |
| 1 | A | 94 | PHE | CG-CD2 | 5.04 | 1.46 | 1.38 |
| 3 | P | 189 | SER | CB-OG | 5.03 | 1.48 | 1.42 |
| 9 | V | 54 | TYR | CG-CD2 | 5.03 | 1.45 | 1.39 |
| 1 | A | 502 | TYR | CD1-CE1 | 5.03 | 1.46 | 1.39 |
| 1 | N | 223 | ALA | N-CA | 5.02 | 1.56 | 1.46 |
| 1 | N | 5 | ARG | CZ-NH2 | 5.02 | 1.39 | 1.33 |
| 7 | G | 69 | PHE | C-O | 5.02 | 1.32 | 1.23 |
| 5 | R | 73 | ASP | CG-OD2 | -5.02 | 1.13 | 1.25 |
| 8 | H | 40 | GLU | CG-CD | 5.01 | 1.59 | 1.51 |
| 6 | S | 93 | PRO | CA-C | 5.01 | 1.62 | 1.52 |
| 6 | F | 3 | GLY | N-CA | 5.01 | 1.53 | 1.46 |
| 1 | N | 473 | TRP | CE3-CZ3 | 5.01 | 1.47 | 1.38 |
| 8 | H | 53 | CYS | C-O | 5.00 | 1.32 | 1.23 |
| 3 | P | 227 | PHE | CE1-CZ | 5.00 | 1.46 | 1.37 |
| 4 | Q | 138 | TRP | CD1-NE1 | 5.00 | 1.46 | 1.38 |
| 7 | G | 17 | ARG | CZ-NH1 | 5.00 | 1.39 | 1.33 |
| 4 | Q | 6 | VAL | CA-C | 5.00 | 1.66 | 1.52 |

All (569) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | E | 90 | ARG | NE-CZ-NH1 | 35.49 | 138.05 | 120.30 |
| 4 | Q | 20 | ARG | NE-CZ-NH1 | 32.93 | 136.77 | 120.30 |
| 4 | Q | 20 | ARG | NE-CZ-NH2 | -31.64 | 104.48 | 120.30 |
| 5 | E | 90 | ARG | NE-CZ-NH2 | -24.93 | 107.83 | 120.30 |
| 9 | V | 10 | ARG | NE-CZ-NH2 | -21.32 | 109.64 | 120.30 |
| 9 | V | 10 | ARG | NE-CZ-NH1 | 21.08 | 130.84 | 120.30 |
| 11 | K | 47 | ARG | NE-CZ-NH1 | -19.70 | 110.45 | 120.30 |
| 2 | B | 151 | ARG | NE-CZ-NH1 | 18.72 | 129.66 | 120.30 |
| 1 | A | 213 | ARG | NE-CZ-NH2 | -17.11 | 111.75 | 120.30 |
| 1 | N | 189 | MET | CG-SD-CE | -16.98 | 73.03 | 100.20 |
| 1 | A | 38 | ARG | NE-CZ-NH1 | 16.94 | 128.77 | 120.30 |
| 1 | A | 38 | ARG | NE-CZ-NH2 | -15.95 | 112.32 | 120.30 |
| 2 | B | 151 | ARG | NE-CZ-NH2 | -14.92 | 112.84 | 120.30 |
| 11 | K | 54 | ARG | NE-CZ-NH1 | -14.87 | 112.87 | 120.30 |
| 11 | K | 47 | ARG | NE-CZ-NH2 | 14.80 | 127.70 | 120.30 |
| 3 | C | 181 | TYR | CB-CG-CD2 | -14.70 | 112.18 | 121.00 |
| 11 | X | 54 | ARG | NE-CZ-NH1 | -14.52 | 113.04 | 120.30 |
| 1 | A | 189 | MET | CG-SD-CE | -14.16 | 77.54 | 100.20 |
| 3 | P | 153 | GLU | OE1-CD-OE2 | 14.02 | 140.12 | 123.30 |
| 4 | D | 20 | ARG | NE-CZ-NH1 | -13.88 | 113.36 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 82 | ARG | NE-CZ-NH2 | -13.82 | 113.39 | 120.30 |
| 7 | G | 64 | ASP | CB-CG-OD2 | -13.77 | 105.91 | 118.30 |
| 5 | E | 56 | ARG | NE-CZ-NH1 | 13.70 | 127.15 | 120.30 |
| 2 | B | 134 | ARG | NE-CZ-NH2 | -13.46 | 113.57 | 120.30 |
| 1 | A | 8 | PHE | CB-CG-CD2 | -13.38 | 111.43 | 120.80 |
| 1 | A | 129 | TYR | CB-CG-CD1 | -13.09 | 113.15 | 121.00 |
| 3 | C | 63 | ARG | NE-CZ-NH2 | -12.99 | 113.81 | 120.30 |
| 2 | O | 82 | ARG | NE-CZ-NH2 | -12.95 | 113.83 | 120.30 |
| 12 | L | 20 | ARG | NE-CZ-NH2 | -12.94 | 113.83 | 120.30 |
| 5 | E | 66 | ARG | NE-CZ-NH2 | -12.77 | 113.91 | 120.30 |
| 1 | N | 144 | ASP | CB-CG-OD1 | -12.54 | 107.02 | 118.30 |
| 5 | E | 56 | ARG | NE-CZ-NH2 | -12.19 | 114.20 | 120.30 |
| 1 | N | 71 | MET | CG-SD-CE | -11.76 | 81.38 | 100.20 |
| 3 | P | 156 | ARG | NE-CZ-NH1 | 11.57 | 126.08 | 120.30 |
| 2 | B | 115 | ASP | CB-CG-OD1 | 11.25 | 128.43 | 118.30 |
| 4 | Q | 122 | ARG | NE-CZ-NH2 | -11.12 | 114.74 | 120.30 |
| 1 | N | 440 | TYR | CB-CG-CD1 | -11.11 | 114.33 | 121.00 |
| 7 | G | 56 | ARG | NE-CZ-NH2 | 11.09 | 125.84 | 120.30 |
| 1 | A | 14 | ASP | CB-CG-OD1 | -11.01 | 108.39 | 118.30 |
| 1 | N | 302[A] | ARG | NE-CZ-NH1 | 10.84 | 125.72 | 120.30 |
| 1 | N | 302[B] | ARG | NE-CZ-NH1 | 10.84 | 125.72 | 120.30 |
| 5 | E | 70 | VAL | CA-CB-CG1 | -10.57 | 95.04 | 110.90 |
| 5 | E | 84 | TYR | CZ-CE2-CD2 | -10.52 | 110.33 | 119.80 |
| 11 | K | 47 | ARG | CG-CD-NE | 10.50 | 133.85 | 111.80 |
| 1 | A | 8 | PHE | CB-CG-CD1 | 10.47 | 128.13 | 120.80 |
| 10 | J | 28 | ASP | CB-CG-OD2 | -10.40 | 108.94 | 118.30 |
| 9 | V | 8 | GLN | CB-CA-C | 10.31 | 131.02 | 110.40 |
| 9 | V | 8 | GLN | CB-CG-CD | -10.28 | 84.88 | 111.60 |
| 1 | A | 400 | PHE | CB-CG-CD2 | -10.23 | 113.64 | 120.80 |
| 1 | N | 372 | TYR | CB-CG-CD1 | -10.15 | 114.91 | 121.00 |
| 5 | E | 73 | ASP | CB-CG-OD2 | -10.12 | 109.19 | 118.30 |
| 1 | N | 486 | ASP | CB-CG-OD1 | 10.11 | 127.40 | 118.30 |
| 3 | P | 253 | TYR | CB-CG-CD2 | -10.09 | 114.94 | 121.00 |
| 5 | E | 90 | ARG | CD-NE-CZ | 10.05 | 137.68 | 123.60 |
| 5 | E | 61 | PHE | CB-CG-CD1 | -9.99 | 113.81 | 120.80 |
| 1 | N | 8 | PHE | CB-CG-CD2 | -9.95 | 113.84 | 120.80 |
| 6 | S | 43 | LYS | CB-CG-CD | 9.91 | 137.38 | 111.60 |
| 9 | I | 10 | ARG | NE-CZ-NH1 | 9.84 | 125.22 | 120.30 |
| 3 | C | 181 | TYR | CZ-CE2-CD2 | -9.79 | 110.99 | 119.80 |
| 11 | X | 54 | ARG | NE-CZ-NH2 | 9.66 | 125.13 | 120.30 |
| 1 | A | 71 | MET | CG-SD-CE | -9.62 | 84.82 | 100.20 |
| 10 | W | 28 | ASP | CB-CG-OD2 | -9.61 | 109.65 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 366 | VAL | CG1-CB-CG2 | -9.52 | 95.66 | 110.90 |
| 9 | I | 10 | ARG | NE-CZ-NH2 | -9.50 | 115.55 | 120.30 |
| 1 | N | 400 | PHE | CB-CG-CD2 | -9.46 | 114.17 | 120.80 |
| 4 | D | 58 | GLU | OE1-CD-OE2 | 9.35 | 134.52 | 123.30 |
| 5 | E | 49 | ASP | CB-CG-OD2 | 9.33 | 126.69 | 118.30 |
| 3 | C | 181 | TYR | CD1-CE1-CZ | -9.22 | 111.50 | 119.80 |
| 1 | N | 251 | PHE | CB-CG-CD1 | -9.21 | 114.35 | 120.80 |
| 1 | A | 372 | TYR | CB-CG-CD1 | -9.20 | 115.48 | 121.00 |
| 3 | C | 181 | TYR | CE1-CZ-CE2 | 9.15 | 134.45 | 119.80 |
| 5 | R | 90 | ARG | NE-CZ-NH1 | -9.09 | 115.76 | 120.30 |
| 1 | A | 442 | ASP | CB-CG-OD1 | -9.06 | 110.15 | 118.30 |
| 1 | A | 442 | ASP | CB-CG-OD2 | 9.05 | 126.44 | 118.30 |
| 4 | D | 58 | GLU | CG-CD-OE2 | -9.00 | 100.31 | 118.30 |
| 1 | A | 387 | PHE | CB-CG-CD1 | -8.97 | 114.52 | 120.80 |
| 2 | O | 134 | ARG | NE-CZ-NH2 | -8.90 | 115.85 | 120.30 |
| 5 | E | 84 | TYR | CG-CD1-CE1 | -8.89 | 114.19 | 121.30 |
| 2 | O | 33 | LEU | CB-CG-CD1 | 8.87 | 126.07 | 111.00 |
| 1 | N | 270 | TYR | CB-CG-CD2 | -8.81 | 115.71 | 121.00 |
| 2 | O | 21 | LEU | CB-CG-CD1 | -8.78 | 96.08 | 111.00 |
| 5 | E | 53 | ARG | NE-CZ-NH1 | 8.72 | 124.66 | 120.30 |
| 1 | N | 414 | PHE | CB-CG-CD1 | -8.72 | 114.70 | 120.80 |
| 11 | X | 47 | ARG | NE-CZ-NH1 | 8.71 | 124.65 | 120.30 |
| 3 | C | 63 | ARG | NE-CZ-NH1 | 8.69 | 124.65 | 120.30 |
| 3 | C | 244 | PHE | CD1-CE1-CZ | -8.68 | 109.69 | 120.10 |
| 1 | A | 439 | ARG | NE-CZ-NH1 | 8.67 | 124.64 | 120.30 |
| 3 | P | 233 | PHE | CB-CG-CD2 | -8.66 | 114.74 | 120.80 |
| 7 | T | 60 | PHE | CB-CG-CD2 | -8.60 | 114.78 | 120.80 |
| 2 | B | 3 | TYR | CB-CG-CD2 | -8.57 | 115.86 | 121.00 |
| 9 | V | 68 | ILE | CB-CG1-CD1 | -8.57 | 89.91 | 113.90 |
| 5 | E | 14 | ARG | NE-CZ-NH1 | 8.56 | 124.58 | 120.30 |
| 1 | A | 302[A] | ARG | NE-CZ-NH1 | 8.52 | 124.56 | 120.30 |
| 1 | A | 302[B] | ARG | NE-CZ-NH1 | 8.52 | 124.56 | 120.30 |
| 3 | C | 233 | PHE | CB-CG-CD2 | -8.50 | 114.85 | 120.80 |
| 5 | R | 8 | ASP | CB-CG-OD2 | -8.50 | 110.65 | 118.30 |
| 7 | T | 60 | PHE | CB-CG-CD1 | 8.48 | 126.74 | 120.80 |
| 4 | Q | 61 | ARG | NE-CZ-NH1 | 8.47 | 124.53 | 120.30 |
| 3 | P | 155 | ASP | CB-CG-OD1 | 8.41 | 125.87 | 118.30 |
| 2 | B | 206 | PHE | CB-CG-CD1 | -8.33 | 114.97 | 120.80 |
| 3 | C | 172 | TYR | CG-CD2-CE2 | 8.32 | 127.96 | 121.30 |
| 7 | G | 5 | LYS | CB-CA-C | 8.30 | 127.00 | 110.40 |
| 4 | D | 19[A] | ARG | CG-CD-NE | 8.28 | 129.18 | 111.80 |
| 4 | D | 19[B] | ARG | CG-CD-NE | 8.28 | 129.18 | 111.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | P | 156 | ARG | NE-CZ-NH2 | -8.22 | 116.19 | 120.30 |
| 5 | R | 30 | ARG | NE-CZ-NH1 | 8.18 | 124.39 | 120.30 |
| 3 | P | 214 | PHE | CB-CG-CD2 | -8.17 | 115.08 | 120.80 |
| 1 | A | 366 | VAL | CG1-CB-CG2 | -8.10 | 97.94 | 110.90 |
| 5 | R | 30 | ARG | NE-CZ-NH2 | -8.08 | 116.26 | 120.30 |
| 2 | B | 75 | LEU | CB-CG-CD2 | -8.08 | 97.27 | 111.00 |
| 1 | A | 450 | TRP | CB-CG-CD1 | -8.04 | 116.54 | 127.00 |
| 1 | N | 363 | LEU | CB-CG-CD2 | 8.00 | 124.61 | 111.00 |
| 1 | A | 440 | TYR | CB-CG-CD1 | -7.96 | 116.22 | 121.00 |
| 3 | C | 153 | GLU | OE1-CD-OE2 | 7.96 | 132.85 | 123.30 |
| 1 | N | 430 | PHE | CB-CG-CD2 | -7.95 | 115.23 | 120.80 |
| 2 | B | 134 | ARG | NE-CZ-NH1 | 7.95 | 124.27 | 120.30 |
| 2 | B | 141 | ARG | NE-CZ-NH2 | -7.93 | 116.34 | 120.30 |
| 3 | P | 33[A] | MET | CG-SD-CE | 7.91 | 112.86 | 100.20 |
| 3 | P | 33[B] | MET | CG-SD-CE | 7.91 | 112.86 | 100.20 |
| 2 | B | 105 | TYR | CD1-CE1-CZ | -7.88 | 112.71 | 119.80 |
| 1 | A | 7 | LEU | CB-CG-CD1 | 7.84 | 124.32 | 111.00 |
| 1 | A | 470 | PHE | CB-CG-CD2 | -7.76 | 115.37 | 120.80 |
| 3 | P | 197 | PHE | CB-CG-CD1 | -7.71 | 115.40 | 120.80 |
| 6 | F | 1 | ALA | C-N-CA | 7.68 | 140.91 | 121.70 |
| 3 | C | 186 | PHE | CG-CD1-CE1 | -7.66 | 112.38 | 120.80 |
| 2 | O | 151 | ARG | NE-CZ-NH2 | -7.66 | 116.47 | 120.30 |
| 7 | G | 56 | ARG | NH1-CZ-NH2 | -7.64 | 111.00 | 119.40 |
| 12 | L | 20 | ARG | NE-CZ-NH1 | 7.63 | 124.11 | 120.30 |
| 3 | P | 63 | ARG | NE-CZ-NH1 | 7.63 | 124.11 | 120.30 |
| 3 | C | 244 | PHE | CB-CG-CD1 | -7.62 | 115.47 | 120.80 |
| 3 | C | 67 | PHE | CB-CG-CD1 | -7.60 | 115.48 | 120.80 |
| 12 | Y | 20 | ARG | NE-CZ-NH1 | 7.59 | 124.09 | 120.30 |
| 7 | G | 60 | PHE | CB-CG-CD2 | -7.58 | 115.50 | 120.80 |
| 1 | N | 439 | ARG | NE-CZ-NH1 | 7.53 | 124.06 | 120.30 |
| 5 | E | 57 | ARG | NE-CZ-NH1 | -7.52 | 116.54 | 120.30 |
| 2 | O | 11 | ASP | CB-CG-OD2 | 7.51 | 125.06 | 118.30 |
| 5 | E | 100 | THR | CA-CB-CG2 | -7.51 | 101.89 | 112.40 |
| 1 | N | 231 | TYR | CB-CG-CD1 | -7.42 | 116.55 | 121.00 |
| 4 | Q | 127 | LYS | CD-CE-NZ | 7.42 | 128.78 | 111.70 |
| 3 | P | 90 | GLU | OE1-CD-OE2 | 7.41 | 132.19 | 123.30 |
| 3 | P | 244 | PHE | CD1-CE1-CZ | -7.40 | 111.22 | 120.10 |
| 1 | N | 129 | TYR | CB-CG-CD1 | -7.40 | 116.56 | 121.00 |
| 4 | D | 111 | PHE | CB-CG-CD1 | -7.39 | 115.62 | 120.80 |
| 5 | E | 66 | ARG | NE-CZ-NH1 | 7.38 | 123.99 | 120.30 |
| 1 | N | 442 | ASP | CB-CG-OD2 | 7.38 | 124.94 | 118.30 |
| 1 | N | 129 | TYR | CG-CD2-CE2 | -7.36 | 115.41 | 121.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 8 | PHE | CB-CG-CD1 | 7.33 | 125.93 | 120.80 |
| 1 | N | 486 | ASP | CB-CG-OD2 | -7.32 | 111.71 | 118.30 |
| 7 | G | 19 | LEU | CB-CG-CD1 | -7.24 | 98.69 | 111.00 |
| 4 | D | 20 | ARG | NE-CZ-NH2 | 7.23 | 123.92 | 120.30 |
| 9 | I | 54 | TYR | CB-CG-CD1 | -7.22 | 116.67 | 121.00 |
| 2 | O | 173 | ASP | CB-CG-OD1 | 7.22 | 124.80 | 118.30 |
| 1 | N | 212 | ASP | CB-CG-OD2 | 7.21 | 124.79 | 118.30 |
| 4 | Q | 19[A] | ARG | NE-CZ-NH2 | -7.21 | 116.70 | 120.30 |
| 4 | Q | 19[B] | ARG | NE-CZ-NH2 | -7.21 | 116.70 | 120.30 |
| 1 | A | 270 | TYR | CB-CG-CD2 | -7.20 | 116.68 | 121.00 |
| 1 | A | 35 | LEU | CB-CG-CD2 | 7.19 | 123.23 | 111.00 |
| 3 | P | 219 | PHE | CB-CG-CD2 | -7.17 | 115.78 | 120.80 |
| 9 | I | 43 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 3 | P | 8 | TYR | CZ-CE2-CD2 | -7.14 | 113.37 | 119.80 |
| 4 | D | 122 | ARG | NE-CZ-NH2 | -7.13 | 116.74 | 120.30 |
| 11 | K | 51 | LYS | CD-CE-NZ | -7.12 | 95.32 | 111.70 |
| 10 | J | 4 | ARG | NE-CZ-NH1 | 7.10 | 123.85 | 120.30 |
| 5 | E | 82 | TYR | CB-CG-CD2 | -7.09 | 116.75 | 121.00 |
| 3 | P | 181 | TYR | CB-CG-CD2 | -7.06 | 116.77 | 121.00 |
| 5 | R | 23 | ASP | CB-CG-OD2 | 7.05 | 124.65 | 118.30 |
| 1 | N | 513 | LEU | C-N-CA | -7.05 | 104.08 | 121.70 |
| 4 | Q | 8 | SER | N-CA-C | 7.04 | 130.02 | 111.00 |
| 3 | P | 198 | PHE | CB-CG-CD2 | -7.03 | 115.88 | 120.80 |
| 2 | O | 206 | PHE | CB-CG-CD1 | -7.00 | 115.90 | 120.80 |
| 2 | O | 147 | GLU | OE1-CD-OE2 | -6.99 | 114.91 | 123.30 |
| 1 | A | 251 | PHE | CB-CG-CD1 | -6.99 | 115.91 | 120.80 |
| 9 | I | 61 | GLU | OE1-CD-OE2 | -6.99 | 114.92 | 123.30 |
| 3 | P | 102 | TYR | CB-CG-CD2 | -6.97 | 116.82 | 121.00 |
| 4 | Q | 19[A] | ARG | CB-CG-CD | 6.97 | 129.73 | 111.60 |
| 4 | Q | 19[B] | ARG | CB-CG-CD | 6.97 | 129.73 | 111.60 |
| 7 | G | 50 | TYR | CG-CD2-CE2 | -6.96 | 115.73 | 121.30 |
| 4 | Q | 6 | VAL | CB-CA-C | 6.96 | 124.62 | 111.40 |
| 3 | C | 233 | PHE | CD1-CG-CD2 | 6.96 | 127.34 | 118.30 |
| 6 | S | 25 | ARG | NE-CZ-NH1 | 6.96 | 123.78 | 120.30 |
| 13 | M | 38 | ASP | CB-CG-OD2 | -6.94 | 112.05 | 118.30 |
| 2 | O | 134 | ARG | NE-CZ-NH1 | 6.91 | 123.76 | 120.30 |
| 5 | E | 103 | GLU | OE1-CD-OE2 | -6.89 | 115.03 | 123.30 |
| 1 | N | 213 | ARG | NE-CZ-NH2 | -6.89 | 116.86 | 120.30 |
| 1 | N | 63 | PHE | CB-CG-CD2 | -6.88 | 115.98 | 120.80 |
| 1 | A | 270 | TYR | CD1-CE1-CZ | -6.86 | 113.63 | 119.80 |
| 2 | O | 108 | TYR | CZ-CE2-CD2 | -6.85 | 113.63 | 119.80 |
| 1 | A | 377 | PHE | CB-CG-CD2 | -6.85 | 116.01 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | P | 253 | TYR | CZ-CE2-CD2 | -6.85 | 113.64 | 119.80 |
| 5 | R | 69 | GLU | OE1-CD-OE2 | 6.84 | 131.51 | 123.30 |
| 4 | D | 4 | SER | N-CA-C | 6.83 | 129.44 | 111.00 |
| 5 | E | 103 | GLU | O-C-N | 6.83 | 133.62 | 122.70 |
| 3 | C | 146 | TRP | CD1-CG-CD2 | -6.81 | 100.85 | 106.30 |
| 1 | A | 5 | ARG | NE-CZ-NH1 | -6.79 | 116.91 | 120.30 |
| 8 | H | 63 | LEU | CB-CG-CD1 | -6.78 | 99.48 | 111.00 |
| 3 | P | 214 | PHE | CB-CG-CD1 | 6.77 | 125.54 | 120.80 |
| 6 | F | 1 | ALA | O-C-N | 6.76 | 133.52 | 122.70 |
| 2 | O | 65 | TRP | CB-CA-C | 6.76 | 123.93 | 110.40 |
| 2 | B | 133 | LEU | CB-CG-CD1 | -6.74 | 99.54 | 111.00 |
| 1 | A | 109 | PHE | CB-CG-CD1 | -6.74 | 116.08 | 120.80 |
| 3 | P | 97 | PHE | CB-CG-CD2 | -6.74 | 116.08 | 120.80 |
| 6 | S | 25 | ARG | NE-CZ-NH2 | -6.73 | 116.94 | 120.30 |
| 1 | A | 484 | THR | CA-CB-CG2 | -6.72 | 102.99 | 112.40 |
| 3 | C | 94 | PHE | CB-CG-CD2 | -6.71 | 116.10 | 120.80 |
| 5 | R | 60 | ASP | CB-CG-OD2 | 6.68 | 124.31 | 118.30 |
| 5 | E | 90 | ARG | CB-CG-CD | 6.68 | 128.96 | 111.60 |
| 7 | G | 18 | PHE | CB-CG-CD1 | -6.67 | 116.13 | 120.80 |
| 3 | C | 101 | PHE | CG-CD1-CE1 | -6.67 | 113.46 | 120.80 |
| 4 | D | 34 | SER | O-C-N | -6.67 | 112.03 | 122.70 |
| 8 | H | 52 | VAL | CB-CA-C | -6.67 | 98.73 | 111.40 |
| 1 | N | 7 | LEU | CB-CG-CD1 | 6.65 | 122.31 | 111.00 |
| 6 | F | 96 | LEU | CA-CB-CG | 6.64 | 130.58 | 115.30 |
| 7 | T | 7 | ASP | N-CA-C | 6.64 | 128.92 | 111.00 |
| 1 | N | 74 | MET | CA-CB-CG | -6.63 | 102.02 | 113.30 |
| 9 | I | 15 | ARG | NE-CZ-NH2 | -6.63 | 116.99 | 120.30 |
| 4 | D | 112 | GLU | OE1-CD-OE2 | -6.62 | 115.35 | 123.30 |
| 7 | T | 44 | ARG | NE-CZ-NH1 | 6.60 | 123.60 | 120.30 |
| 1 | N | 296 | GLY | O-C-N | -6.59 | 112.16 | 122.70 |
| 3 | P | 241 | TYR | CB-CG-CD1 | -6.59 | 117.05 | 121.00 |
| 1 | A | 129 | TYR | CD1-CG-CD2 | 6.57 | 125.13 | 117.90 |
| 9 | I | 50 | PHE | CB-CG-CD1 | -6.57 | 116.20 | 120.80 |
| 1 | N | 505 | PHE | CB-CG-CD2 | -6.56 | 116.21 | 120.80 |
| 1 | N | 438 | ARG | NE-CZ-NH2 | -6.53 | 117.03 | 120.30 |
| 5 | E | 8 | ASP | CB-CG-OD2 | -6.53 | 112.42 | 118.30 |
| 2 | O | 151 | ARG | NE-CZ-NH1 | 6.53 | 123.57 | 120.30 |
| 4 | Q | 124 | LEU | CB-CG-CD2 | 6.52 | 122.09 | 111.00 |
| 1 | A | 63 | PHE | CB-CG-CD2 | -6.52 | 116.24 | 120.80 |
| 1 | A | 240 | HIS | CA-CB-CG | -6.51 | 102.53 | 113.60 |
| 5 | E | 60 | ASP | CB-CG-OD1 | -6.50 | 112.45 | 118.30 |
| 6 | S | 92 | VAL | C-N-CD | 6.48 | 142.01 | 128.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 346 | PHE | CB-CG-CD2 | -6.48 | 116.27 | 120.80 |
| 3 | C | 90 | GLU | OE1-CD-OE2 | 6.47 | 131.07 | 123.30 |
| 1 | A | 50 | ASP | CB-CG-OD2 | 6.46 | 124.12 | 118.30 |
| 9 | I | 4 | LEU | CB-CG-CD1 | -6.46 | 100.02 | 111.00 |
| 4 | Q | 16 | TYR | CB-CG-CD1 | -6.45 | 117.13 | 121.00 |
| 4 | D | 74 | SER | CA-CB-OG | -6.45 | 93.80 | 111.20 |
| 13 | M | 35 | TYR | CG-CD2-CE2 | -6.44 | 116.15 | 121.30 |
| 3 | C | 146 | TRP | CD1-NE1-CE2 | -6.43 | 103.21 | 109.00 |
| 4 | D | 61 | ARG | NE-CZ-NH1 | 6.43 | 123.52 | 120.30 |
| 1 | A | 480 | ARG | NE-CZ-NH1 | 6.43 | 123.52 | 120.30 |
| 3 | C | 52 | LEU | CB-CG-CD1 | -6.43 | 100.07 | 111.00 |
| 1 | N | 38 | ARG | NE-CZ-NH1 | 6.42 | 123.51 | 120.30 |
| 1 | N | 144 | ASP | OD1-CG-OD2 | 6.41 | 135.47 | 123.30 |
| 1 | N | 393 | PHE | CB-CG-CD2 | -6.39 | 116.33 | 120.80 |
| 4 | Q | 51 | LEU | CB-CG-CD1 | 6.38 | 121.84 | 111.00 |
| 11 | X | 47 | ARG | CD-NE-CZ | 6.37 | 132.51 | 123.60 |
| 1 | N | 136[A] | LEU | CB-CG-CD2 | -6.36 | 100.19 | 111.00 |
| 1 | N | 136[B] | LEU | CB-CG-CD2 | -6.36 | 100.19 | 111.00 |
| 2 | O | 132 | GLU | CG-CD-OE1 | -6.35 | 105.61 | 118.30 |
| 3 | P | 233 | PHE | CZ-CE2-CD2 | -6.34 | 112.49 | 120.10 |
| 1 | A | 344 | PHE | CB-CG-CD2 | -6.34 | 116.36 | 120.80 |
| 4 | D | 99 | GLU | OE1-CD-OE2 | -6.34 | 115.69 | 123.30 |
| 7 | T | 20 | THR | CA-CB-CG2 | -6.33 | 103.54 | 112.40 |
| 5 | E | 84 | TYR | CB-CG-CD1 | -6.30 | 117.22 | 121.00 |
| 1 | N | 364 | ASP | CB-CG-OD2 | -6.30 | 112.63 | 118.30 |
| 1 | N | 35 | LEU | CB-CG-CD1 | -6.29 | 100.31 | 111.00 |
| 2 | O | 132 | GLU | CG-CD-OE2 | 6.29 | 130.88 | 118.30 |
| 8 | H | 61 | LYS | CD-CE-NZ | 6.28 | 126.15 | 111.70 |
| 8 | H | 17 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | A | 285 | PHE | CB-CG-CD2 | -6.26 | 116.42 | 120.80 |
| 12 | Y | 37 | PHE | CB-CG-CD2 | -6.25 | 116.43 | 120.80 |
| 5 | E | 49 | ASP | OD1-CG-OD2 | -6.25 | 111.43 | 123.30 |
| 2 | B | 158 | ASP | CB-CG-OD2 | -6.24 | 112.69 | 118.30 |
| 6 | S | 96 | LEU | CB-CG-CD2 | 6.24 | 121.60 | 111.00 |
| 9 | I | 47 | TYR | CB-CG-CD2 | -6.23 | 117.26 | 121.00 |
| 1 | N | 235 | PHE | CB-CG-CD2 | -6.23 | 116.44 | 120.80 |
| 4 | D | 91 | PHE | CB-CG-CD2 | -6.22 | 116.45 | 120.80 |
| 1 | A | 251 | PHE | CB-CG-CD2 | 6.21 | 125.15 | 120.80 |
| 8 | U | 75 | ARG | NE-CZ-NH2 | -6.19 | 117.20 | 120.30 |
| 1 | A | 67 | PHE | CB-CG-CD1 | -6.19 | 116.47 | 120.80 |
| 1 | N | 260 | TYR | CB-CG-CD2 | -6.17 | 117.30 | 121.00 |
| 12 | L | 29 | PHE | CB-CG-CD2 | 6.16 | 125.11 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 148 | PHE | CB-CG-CD2 | -6.16 | 116.49 | 120.80 |
| 6 | S | 1 | ALA | C-N-CA | 6.15 | 137.07 | 121.70 |
| 1 | N | 387 | PHE | CB-CG-CD1 | -6.13 | 116.51 | 120.80 |
| 1 | A | 213 | ARG | NE-CZ-NH1 | 6.13 | 123.36 | 120.30 |
| 1 | A | 372 | TYR | CG-CD1-CE1 | -6.12 | 116.41 | 121.30 |
| 1 | N | 213 | ARG | NE-CZ-NH1 | 6.12 | 123.36 | 120.30 |
| 1 | N | 113[A] | LEU | CB-CG-CD1 | 6.12 | 121.40 | 111.00 |
| 1 | N | 113[B] | LEU | CB-CG-CD1 | 6.12 | 121.40 | 111.00 |
| 13 | M | 10 | THR | CA-CB-CG2 | -6.11 | 103.84 | 112.40 |
| 3 | C | 214 | PHE | CB-CG-CD1 | 6.09 | 125.07 | 120.80 |
| 6 | S | 94 | HIS | N-CA-C | 6.09 | 127.45 | 111.00 |
| 3 | P | 63 | ARG | NE-CZ-NH2 | -6.07 | 117.26 | 120.30 |
| 1 | N | 240 | HIS | CA-CB-CG | -6.07 | 103.28 | 113.60 |
| 2 | O | 112 | ASP | CB-CG-OD1 | 6.06 | 123.75 | 118.30 |
| 10 | J | 38 | LEU | CB-CG-CD1 | -6.05 | 100.71 | 111.00 |
| 6 | S | 96 | LEU | CB-CG-CD1 | -6.04 | 100.73 | 111.00 |
| 3 | C | 181 | TYR | CD1-CG-CD2 | 6.04 | 124.54 | 117.90 |
| 5 | E | 82 | TYR | CD1-CE1-CZ | -6.03 | 114.38 | 119.80 |
| 1 | N | 476 | PHE | CB-CG-CD1 | -6.03 | 116.58 | 120.80 |
| 3 | C | 233 | PHE | CB-CG-CD1 | -6.02 | 116.58 | 120.80 |
| 4 | Q | 18 | ASP | CB-CG-OD2 | 6.02 | 123.72 | 118.30 |
| 1 | A | 2 | PHE | CB-CG-CD1 | -6.01 | 116.59 | 120.80 |
| 5 | E | 70 | VAL | CB-CA-C | 6.00 | 122.80 | 111.40 |
| 7 | G | 3 | ALA | N-CA-C | 6.00 | 127.19 | 111.00 |
| 5 | R | 36 | LEU | CB-CG-CD2 | -6.00 | 100.81 | 111.00 |
| 3 | C | 59 | ARG | NE-CZ-NH1 | -5.99 | 117.31 | 120.30 |
| 1 | N | 253 | MET | CA-CB-CG | -5.98 | 103.13 | 113.30 |
| 3 | C | 102 | TYR | CB-CG-CD2 | -5.98 | 117.41 | 121.00 |
| 12 | L | 45 | LEU | CB-CG-CD1 | -5.97 | 100.85 | 111.00 |
| 1 | A | 513 | LEU | C-N-CA | -5.96 | 106.79 | 121.70 |
| 4 | Q | 20 | ARG | CD-NE-CZ | 5.96 | 131.94 | 123.60 |
| 1 | A | 152 | LEU | CB-CG-CD2 | 5.94 | 121.10 | 111.00 |
| 12 | L | 46 | LYS | CB-CG-CD | -5.94 | 96.17 | 111.60 |
| 2 | B | 65 | TRP | CB-CA-C | 5.93 | 122.25 | 110.40 |
| 6 | F | 3 | GLY | C-N-CA | 5.93 | 134.74 | 122.30 |
| 1 | A | 327 | LEU | CB-CG-CD1 | -5.91 | 100.95 | 111.00 |
| 2 | B | 45 | MET | CG-SD-CE | 5.91 | 109.66 | 100.20 |
| 2 | B | 184 | LEU | N-CA-CB | -5.90 | 98.60 | 110.40 |
| 6 | S | 1 | ALA | O-C-N | 5.89 | 132.13 | 122.70 |
| 3 | C | 197 | PHE | CB-CG-CD1 | -5.88 | 116.68 | 120.80 |
| 1 | A | 450 | TRP | CG-CD1-NE1 | -5.88 | 104.22 | 110.10 |
| 5 | E | 70 | VAL | CA-CB-CG2 | -5.87 | 102.09 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | R | 18 | TYR | CB-CG-CD1 | -5.87 | 117.48 | 121.00 |
| 4 | D | 21 | ASP | CB-CG-OD2 | 5.87 | 123.58 | 118.30 |
| 1 | N | 251 | PHE | CB-CG-CD2 | 5.86 | 124.91 | 120.80 |
| 5 | E | 61 | PHE | CB-CG-CD2 | 5.86 | 124.90 | 120.80 |
| 1 | A | 372 | TYR | CD1-CG-CD2 | 5.85 | 124.34 | 117.90 |
| 3 | P | 8 | TYR | CB-CG-CD2 | -5.85 | 117.49 | 121.00 |
| 11 | K | 47 | ARG | CB-CG-CD | 5.84 | 126.78 | 111.60 |
| 5 | R | 52 | LEU | CB-CG-CD2 | 5.83 | 120.92 | 111.00 |
| 3 | P | 233 | PHE | CD1-CG-CD2 | 5.82 | 125.86 | 118.30 |
| 4 | Q | 63 | LYS | CD-CE-NZ | -5.82 | 98.32 | 111.70 |
| 1 | A | 486[A] | ASP | CB-CG-OD1 | -5.82 | 113.07 | 118.30 |
| 1 | A | 486[B] | ASP | CB-CG-OD1 | -5.82 | 113.07 | 118.30 |
| 12 | L | 29 | PHE | CG-CD2-CE2 | 5.82 | 127.20 | 120.80 |
| 7 | G | 19 | LEU | CA-CB-CG | -5.81 | 101.93 | 115.30 |
| 4 | D | 31[A] | LYS | C-N-CA | -5.81 | 107.17 | 121.70 |
| 4 | D | 31[B] | LYS | C-N-CA | -5.81 | 107.17 | 121.70 |
| 9 | V | 10 | ARG | CG-CD-NE | -5.81 | 99.60 | 111.80 |
| 1 | A | 270 | TYR | CG-CD2-CE2 | -5.81 | 116.65 | 121.30 |
| 3 | C | 214 | PHE | CB-CG-CD2 | -5.81 | 116.73 | 120.80 |
| 1 | A | 112 | LEU | CD1-CG-CD2 | -5.79 | 93.12 | 110.50 |
| 2 | O | 158 | ASP | CB-CG-OD1 | 5.79 | 123.51 | 118.30 |
| 3 | P | 80[A] | ARG | CD-NE-CZ | -5.78 | 115.50 | 123.60 |
| 3 | P | 80[B] | ARG | CD-NE-CZ | -5.78 | 115.50 | 123.60 |
| 12 | L | 9 | LYS | CD-CE-NZ | -5.78 | 98.42 | 111.70 |
| 5 | E | 19 | PHE | CB-CG-CD2 | -5.77 | 116.76 | 120.80 |
| 12 | L | 37 | PHE | CB-CG-CD1 | -5.76 | 116.76 | 120.80 |
| 1 | N | 152 | LEU | CD1-CG-CD2 | 5.76 | 127.79 | 110.50 |
| 2 | B | 82 | ARG | NH1-CZ-NH2 | 5.75 | 125.73 | 119.40 |
| 3 | C | 172 | TYR | CG-CD1-CE1 | -5.75 | 116.70 | 121.30 |
| 6 | S | 22 | LEU | CB-CG-CD1 | 5.75 | 120.78 | 111.00 |
| 1 | A | 136[A] | LEU | CB-CG-CD2 | -5.75 | 101.22 | 111.00 |
| 1 | A | 136[B] | LEU | CB-CG-CD2 | -5.75 | 101.22 | 111.00 |
| 2 | B | 32[A] | PHE | O-C-N | 5.75 | 131.90 | 122.70 |
| 2 | B | 32[B] | PHE | O-C-N | 5.75 | 131.90 | 122.70 |
| 1 | N | 397 | PHE | CB-CG-CD2 | -5.74 | 116.78 | 120.80 |
| 1 | A | 407 | ASP | CB-CG-OD2 | 5.74 | 123.46 | 118.30 |
| 1 | N | 237 | PHE | CB-CG-CD2 | -5.74 | 116.79 | 120.80 |
| 3 | C | 93 | PHE | CG-CD1-CE1 | 5.73 | 127.10 | 120.80 |
| 1 | N | 109 | PHE | CB-CG-CD2 | 5.73 | 124.81 | 120.80 |
| 6 | F | 3 | GLY | N-CA-C | -5.72 | 98.80 | 113.10 |
| 3 | C | 16 | TRP | NE1-CE2-CD2 | 5.71 | 113.00 | 107.30 |
| 1 | A | 304 | TYR | CB-CG-CD2 | -5.69 | 117.58 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | P | 233 | PHE | CG-CD1-CE1 | -5.69 | 114.54 | 120.80 |
| 13 | M | 26 | PHE | CB-CG-CD2 | -5.68 | 116.82 | 120.80 |
| 7 | T | 18 | PHE | CB-CG-CD1 | -5.68 | 116.82 | 120.80 |
| 8 | H | 75 | ARG | NE-CZ-NH2 | -5.68 | 117.46 | 120.30 |
| 9 | I | 16 | ARG | NE-CZ-NH2 | -5.68 | 117.46 | 120.30 |
| 4 | D | 74 | SER | N-CA-CB | -5.67 | 101.99 | 110.50 |
| 12 | L | 26 | THR | CA-CB-OG1 | -5.67 | 97.09 | 109.00 |
| 3 | P | 57 | TRP | CD1-CG-CD2 | 5.67 | 110.84 | 106.30 |
| 5 | E | 19 | PHE | CD1-CE1-CZ | -5.66 | 113.30 | 120.10 |
| 8 | H | 9 | LYS | CD-CE-NZ | 5.66 | 124.73 | 111.70 |
| 7 | G | 18 | PHE | CB-CG-CD2 | 5.66 | 124.76 | 120.80 |
| 5 | E | 90 | ARG | NH1-CZ-NH2 | -5.66 | 113.17 | 119.40 |
| 3 | C | 146 | TRP | CG-CD1-NE1 | 5.66 | 115.76 | 110.10 |
| 2 | B | 112 | ASP | CB-CG-OD2 | 5.65 | 123.39 | 118.30 |
| 4 | D | 91 | PHE | CG-CD2-CE2 | -5.65 | 114.59 | 120.80 |
| 11 | K | 54 | ARG | CA-C-O | 5.65 | 131.96 | 120.10 |
| 13 | M | 3 | ALA | O-C-N | 5.65 | 131.74 | 122.70 |
| 1 | A | 403 | TYR | CZ-CE2-CD2 | -5.65 | 114.72 | 119.80 |
| 8 | H | 25 | GLN | CA-C-O | 5.64 | 131.95 | 120.10 |
| 1 | A | 449 | MET | CA-CB-CG | -5.64 | 103.72 | 113.30 |
| 3 | P | 253 | TYR | CD1-CE1-CZ | -5.64 | 114.73 | 119.80 |
| 6 | S | 3 | GLY | N-CA-C | -5.61 | 99.08 | 113.10 |
| 1 | A | 237 | PHE | CD1-CG-CD2 | 5.59 | 125.57 | 118.30 |
| 4 | Q | 86 | MET | CG-SD-CE | -5.59 | 91.26 | 100.20 |
| 5 | E | 61 | PHE | CG-CD1-CE1 | -5.58 | 114.66 | 120.80 |
| 9 | V | 68 | ILE | CA-CB-CG2 | 5.58 | 122.06 | 110.90 |
| 4 | D | 122 | ARG | NE-CZ-NH1 | 5.57 | 123.09 | 120.30 |
| 2 | O | 108 | TYR | CG-CD1-CE1 | -5.57 | 116.84 | 121.30 |
| 1 | N | 96 | ARG | NE-CZ-NH1 | 5.57 | 123.09 | 120.30 |
| 4 | D | 64 | PHE | CB-CG-CD1 | -5.57 | 116.90 | 120.80 |
| 8 | H | 35 | ASP | CB-CG-OD1 | -5.57 | 113.29 | 118.30 |
| 4 | D | 39 | ALA | O-C-N | 5.56 | 131.60 | 122.70 |
| 1 | N | 78 | PHE | CB-CG-CD2 | -5.56 | 116.91 | 120.80 |
| 3 | P | 253 | TYR | CD1-CG-CD2 | 5.56 | 124.02 | 117.90 |
| 1 | A | 113[A] | LEU | O-C-N | -5.56 | 113.80 | 122.70 |
| 1 | A | 113[B] | LEU | O-C-N | -5.56 | 113.80 | 122.70 |
| 3 | C | 146 | TRP | CG-CD2-CE3 | -5.56 | 128.90 | 133.90 |
| 3 | P | 236 | GLU | CA-CB-CG | -5.56 | 101.17 | 113.40 |
| 3 | C | 16 | TRP | CD1-NE1-CE2 | -5.56 | 104.00 | 109.00 |
| 5 | E | 30 | ARG | NE-CZ-NH2 | -5.56 | 117.52 | 120.30 |
| 1 | A | 148 | PHE | CB-CG-CD2 | -5.54 | 116.92 | 120.80 |
| 9 | I | 47 | TYR | CB-CG-CD1 | 5.54 | 124.32 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | S | 92 | VAL | CB-CA-C | 5.54 | 121.92 | 111.40 |
| 1 | A | 310 | MET | CA-CB-CG | -5.54 | 103.89 | 113.30 |
| 1 | N | 456 | MET | CA-CB-CG | -5.52 | 103.91 | 113.30 |
| 5 | R | 106 | LEU | CB-CG-CD2 | -5.51 | 101.63 | 111.00 |
| 1 | A | 348 | PHE | CB-CG-CD2 | -5.50 | 116.95 | 120.80 |
| 7 | G | 56 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | A | 212 | ASP | CB-CG-OD2 | 5.50 | 123.25 | 118.30 |
| 4 | D | 16 | TYR | CB-CG-CD2 | -5.50 | 117.70 | 121.00 |
| 4 | D | 55 | GLU | OE1-CD-OE2 | -5.49 | 116.72 | 123.30 |
| 8 | H | 35 | ASP | CB-CG-OD2 | 5.49 | 123.24 | 118.30 |
| 1 | A | 110 | LEU | CB-CG-CD2 | -5.48 | 101.68 | 111.00 |
| 1 | N | 379 | TYR | CB-CG-CD2 | -5.48 | 117.71 | 121.00 |
| 2 | O | 139 | ASP | CB-CG-OD2 | 5.47 | 123.23 | 118.30 |
| 1 | A | 390 | MET | CG-SD-CE | 5.47 | 108.95 | 100.20 |
| 2 | B | 59 | GLN | N-CA-CB | 5.47 | 120.44 | 110.60 |
| 2 | O | 116 | LEU | CB-CG-CD2 | -5.46 | 101.72 | 111.00 |
| 7 | T | 8 | HIS | N-CA-C | 5.46 | 125.74 | 111.00 |
| 8 | U | 38 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 7 | G | 44 | ARG | CB-CG-CD | -5.46 | 97.42 | 111.60 |
| 1 | N | 98 | ASN | N-CA-CB | -5.45 | 100.78 | 110.60 |
| 1 | A | 296 | GLY | O-C-N | -5.45 | 113.98 | 122.70 |
| 9 | V | 29 | LEU | CB-CG-CD1 | 5.45 | 120.26 | 111.00 |
| 5 | R | 84 | TYR | CG-CD1-CE1 | -5.44 | 116.95 | 121.30 |
| 1 | N | 310 | MET | CG-SD-CE | -5.44 | 91.50 | 100.20 |
| 1 | N | 159 | LEU | CB-CG-CD1 | -5.43 | 101.76 | 111.00 |
| 7 | T | 5 | LYS | CB-CA-C | 5.42 | 121.23 | 110.40 |
| 3 | C | 95 | THR | OG1-CB-CG2 | -5.42 | 97.54 | 110.00 |
| 4 | Q | 6 | VAL | CA-CB-CG1 | 5.42 | 119.03 | 110.90 |
| 1 | A | 159 | LEU | CB-CG-CD1 | -5.42 | 101.79 | 111.00 |
| 1 | N | 430 | PHE | CD1-CG-CD2 | 5.41 | 125.33 | 118.30 |
| 12 | L | 20 | ARG | CG-CD-NE | -5.40 | 100.47 | 111.80 |
| 1 | N | 212 | ASP | CB-CG-OD1 | -5.40 | 113.44 | 118.30 |
| 1 | N | 96 | ARG | N-CA-CB | -5.39 | 100.89 | 110.60 |
| 4 | D | 16 | TYR | CG-CD2-CE2 | -5.38 | 117.00 | 121.30 |
| 4 | D | 86 | MET | CA-CB-CG | -5.38 | 104.16 | 113.30 |
| 7 | G | 16 | TRP | O-C-N | 5.38 | 131.30 | 122.70 |
| 9 | I | 45 | LYS | CD-CE-NZ | -5.37 | 99.36 | 111.70 |
| 1 | N | 102 | PHE | CB-CG-CD1 | -5.36 | 117.05 | 120.80 |
| 1 | A | 445 | ASP | CB-CG-OD1 | -5.35 | 113.48 | 118.30 |
| 3 | C | 233 | PHE | CG-CD2-CE2 | -5.35 | 114.92 | 120.80 |
| 1 | N | 221 | ASP | CB-CG-OD2 | -5.35 | 113.48 | 118.30 |
| 11 | X | 47 | ARG | NH1-CZ-NH2 | -5.34 | 113.52 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 103 | TRP | CD1-CG-CD2 | 5.34 | 110.57 | 106.30 |
| 4 | Q | 125 | ASP | CB-CG-OD1 | -5.34 | 113.49 | 118.30 |
| 3 | C | 233 | PHE | CG-CD1-CE1 | -5.33 | 114.94 | 120.80 |
| 5 | E | 8 | ASP | CB-CG-OD1 | 5.32 | 123.09 | 118.30 |
| 7 | G | 16 | TRP | CD1-CG-CD2 | 5.32 | 110.56 | 106.30 |
| 1 | A | 237 | PHE | CB-CG-CD1 | -5.32 | 117.08 | 120.80 |
| 1 | N | 253 | MET | CG-SD-CE | -5.31 | 91.70 | 100.20 |
| 12 | Y | 21 | LEU | CB-CG-CD2 | -5.31 | 101.97 | 111.00 |
| 3 | P | 51[A] | MET | CA-CB-CG | -5.31 | 104.27 | 113.30 |
| 3 | P | 51[B] | MET | CA-CB-CG | -5.31 | 104.27 | 113.30 |
| 4 | D | 18 | ASP | CB-CG-OD1 | 5.30 | 123.07 | 118.30 |
| 6 | S | 81 | ARG | NE-CZ-NH2 | -5.30 | 117.65 | 120.30 |
| 5 | E | 107 | ASP | CB-CG-OD2 | 5.29 | 123.06 | 118.30 |
| 1 | A | 372 | TYR | CZ-CE2-CD2 | -5.28 | 115.04 | 119.80 |
| 3 | P | 244 | PHE | CG-CD2-CE2 | -5.28 | 114.99 | 120.80 |
| 1 | A | 237 | PHE | CB-CG-CD2 | -5.27 | 117.11 | 120.80 |
| 1 | N | 172 | LYS | CD-CE-NZ | -5.27 | 99.57 | 111.70 |
| 1 | N | 210 | LEU | CB-CG-CD2 | -5.27 | 102.04 | 111.00 |
| 1 | N | 288 | TRP | CD1-NE1-CE2 | -5.27 | 104.25 | 109.00 |
| 1 | A | 363 | LEU | CB-CG-CD1 | 5.27 | 119.96 | 111.00 |
| 2 | B | 139 | ASP | CB-CG-OD2 | 5.26 | 123.04 | 118.30 |
| 4 | D | 31[A] | LYS | CD-CE-NZ | -5.26 | 99.59 | 111.70 |
| 4 | D | 31[B] | LYS | CD-CE-NZ | -5.26 | 99.59 | 111.70 |
| 6 | S | 64 | GLU | CA-C-N | -5.26 | 105.62 | 117.20 |
| 8 | U | 76 | ARG | NE-CZ-NH2 | -5.26 | 117.67 | 120.30 |
| 1 | A | 473 | TRP | CD1-CG-CD2 | 5.26 | 110.51 | 106.30 |
| 2 | B | 32[A] | PHE | CB-CG-CD1 | -5.26 | 117.12 | 120.80 |
| 2 | B | 32[B] | PHE | CB-CG-CD1 | -5.26 | 117.12 | 120.80 |
| 7 | G | 17 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 4 | D | 31[A] | LYS | CA-CB-CG | 5.26 | 124.96 | 113.40 |
| 4 | D | 31[B] | LYS | CA-CB-CG | 5.26 | 124.96 | 113.40 |
| 3 | P | 28 | THR | CA-CB-CG2 | -5.25 | 105.05 | 112.40 |
| 9 | V | 10 | ARG | CD-NE-CZ | 5.25 | 130.95 | 123.60 |
| 3 | C | 76 | GLN | CB-CG-CD | 5.25 | 125.25 | 111.60 |
| 1 | N | 495 | LEU | CB-CG-CD1 | 5.25 | 119.92 | 111.00 |
| 3 | P | 16 | TRP | CG-CD1-NE1 | -5.24 | 104.86 | 110.10 |
| 2 | B | 86 | MET | CG-SD-CE | 5.24 | 108.58 | 100.20 |
| 3 | P | 227 | PHE | CB-CG-CD1 | -5.24 | 117.13 | 120.80 |
| 2 | B | 65 | TRP | CA-CB-CG | 5.24 | 123.65 | 113.70 |
| 2 | B | 91 | ASN | N-CA-C | 5.24 | 125.14 | 111.00 |
| 1 | A | 445 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 1 | A | 502 | TYR | CB-CG-CD2 | -5.23 | 117.86 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | E | 63 | SER | O-C-N | 5.23 | 131.07 | 122.70 |
| 5 | R | 44 | GLU | OE1-CD-OE2 | -5.23 | 117.02 | 123.30 |
| 1 | A | 129 | TYR | CG-CD2-CE2 | -5.23 | 117.12 | 121.30 |
| 1 | N | 54 | TYR | CG-CD2-CE2 | -5.23 | 117.12 | 121.30 |
| 2 | O | 184 | LEU | N-CA-CB | -5.23 | 99.95 | 110.40 |
| 1 | N | 514 | LYS | CA-C-O | -5.22 | 109.14 | 120.10 |
| 1 | N | 447 | TYR | CB-CG-CD1 | 5.22 | 124.13 | 121.00 |
| 3 | C | 197 | PHE | CG-CD1-CE1 | -5.20 | 115.08 | 120.80 |
| 3 | P | 253 | TYR | CE1-CZ-CE2 | 5.20 | 128.12 | 119.80 |
| 3 | C | 80[A] | ARG | NE-CZ-NH1 | -5.19 | 117.70 | 120.30 |
| 3 | C | 80[B] | ARG | NE-CZ-NH1 | -5.19 | 117.70 | 120.30 |
| 3 | C | 215 | LEU | CB-CG-CD1 | -5.19 | 102.18 | 111.00 |
| 1 | A | 244 | TYR | CB-CG-CD2 | -5.18 | 117.89 | 121.00 |
| 4 | D | 16 | TYR | CE1-CZ-CE2 | 5.17 | 128.08 | 119.80 |
| 1 | N | 156 | SER | N-CA-CB | -5.17 | 102.74 | 110.50 |
| 1 | A | 366 | VAL | CA-CB-CG2 | -5.17 | 103.14 | 110.90 |
| 2 | B | 141 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 3 | P | 182 | TYR | CZ-CE2-CD2 | 5.16 | 124.45 | 119.80 |
| 5 | R | 23 | ASP | CB-CG-OD1 | -5.16 | 113.66 | 118.30 |
| 3 | C | 8 | TYR | CZ-CE2-CD2 | -5.15 | 115.16 | 119.80 |
| 3 | C | 41 | THR | CA-CB-CG2 | -5.14 | 105.20 | 112.40 |
| 6 | F | 94 | HIS | C-N-CA | 5.14 | 134.56 | 121.70 |
| 1 | N | 270 | TYR | CD1-CE1-CZ | -5.14 | 115.17 | 119.80 |
| 3 | C | 244 | PHE | CE1-CZ-CE2 | 5.14 | 129.25 | 120.00 |
| 5 | E | 73 | ASP | OD1-CG-OD2 | 5.14 | 133.06 | 123.30 |
| 1 | A | 454 | SER | N-CA-CB | -5.14 | 102.80 | 110.50 |
| 7 | G | 2 | SER | CA-CB-OG | 5.14 | 125.07 | 111.20 |
| 1 | N | 346 | PHE | CG-CD2-CE2 | -5.14 | 115.15 | 120.80 |
| 4 | D | 45 | LYS | CG-CD-CE | 5.13 | 127.30 | 111.90 |
| 1 | N | 35 | LEU | CA-CB-CG | -5.13 | 103.49 | 115.30 |
| 1 | A | 323 | TRP | CD1-NE1-CE2 | -5.13 | 104.38 | 109.00 |
| 13 | Z | 27 | LEU | CB-CG-CD2 | 5.13 | 119.72 | 111.00 |
| 2 | B | 227 | LEU | CB-CG-CD2 | -5.13 | 102.28 | 111.00 |
| 6 | F | 65 | ASP | CB-CG-OD1 | -5.13 | 113.69 | 118.30 |
| 3 | P | 190 | ASP | CB-CG-OD2 | -5.12 | 113.69 | 118.30 |
| 4 | D | 104 | TYR | CG-CD2-CE2 | -5.12 | 117.21 | 121.30 |
| 1 | N | 285 | PHE | CB-CG-CD2 | -5.11 | 117.22 | 120.80 |
| 7 | G | 64 | ASP | OD1-CG-OD2 | 5.11 | 133.01 | 123.30 |
| 4 | Q | 16 | TYR | CE1-CZ-CE2 | 5.11 | 127.98 | 119.80 |
| 4 | D | 61 | ARG | NE-CZ-NH2 | -5.11 | 117.75 | 120.30 |
| 1 | A | 153 | ALA | N-CA-CB | -5.10 | 102.96 | 110.10 |
| 1 | A | 166 | THR | CA-CB-CG2 | -5.10 | 105.26 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | P | 225 | PHE | CB-CG-CD1 | -5.09 | 117.23 | 120.80 |
| 2 | B | 133 | LEU | CB-CG-CD2 | -5.09 | 102.35 | 111.00 |
| 7 | T | 50 | TYR | CB-CG-CD2 | -5.09 | 117.95 | 121.00 |
| 4 | D | 73 | ARG | CB-CG-CD | -5.09 | 98.37 | 111.60 |
| 1 | N | 54 | TYR | CD1-CE1-CZ | -5.09 | 115.22 | 119.80 |
| 8 | U | 8 | ILE | CB-CA-C | 5.09 | 121.77 | 111.60 |
| 3 | C | 60 | ASP | CB-CG-OD2 | -5.08 | 113.72 | 118.30 |
| 4 | D | 30 | VAL | O-C-N | -5.08 | 114.58 | 122.70 |
| 10 | W | 23 | LYS | CD-CE-NZ | -5.07 | 100.03 | 111.70 |
| 5 | E | 103 | GLU | CG-CD-OE1 | 5.07 | 128.43 | 118.30 |
| 1 | N | 189 | MET | CB-CG-SD | -5.06 | 97.21 | 112.40 |
| 2 | O | 214 | VAL | CG1-CB-CG2 | 5.06 | 119.00 | 110.90 |
| 4 | D | 19[A] | ARG | CD-NE-CZ | 5.06 | 130.69 | 123.60 |
| 4 | D | 19[B] | ARG | CD-NE-CZ | 5.06 | 130.69 | 123.60 |
| 5 | E | 93 | LEU | CB-CG-CD1 | -5.06 | 102.40 | 111.00 |
| 5 | E | 18 | TYR | N-CA-CB | -5.06 | 101.50 | 110.60 |
| 9 | I | 35 | TYR | CB-CG-CD2 | -5.05 | 117.97 | 121.00 |
| 3 | P | 44[A] | MET | CG-SD-CE | 5.05 | 108.28 | 100.20 |
| 3 | P | 44[B] | MET | CG-SD-CE | 5.05 | 108.28 | 100.20 |
| 3 | P | 181 | TYR | CD1-CE1-CZ | -5.05 | 115.25 | 119.80 |
| 1 | A | 379 | TYR | CZ-CE2-CD2 | -5.05 | 115.26 | 119.80 |
| 4 | Q | 59 | LEU | CB-CG-CD2 | -5.05 | 102.42 | 111.00 |
| 3 | C | 236 | GLU | CA-CB-CG | -5.04 | 102.31 | 113.40 |
| 13 | Z | 1 | ILE | CG1-CB-CG2 | -5.04 | 100.31 | 111.40 |
| 3 | P | 49 | THR | CA-CB-CG2 | -5.04 | 105.34 | 112.40 |
| 13 | Z | 26 | PHE | CB-CG-CD2 | -5.04 | 117.27 | 120.80 |
| 8 | U | 46 | LYS | CB-CA-C | 5.04 | 120.47 | 110.40 |
| 1 | A | 450 | TRP | CB-CG-CD2 | 5.03 | 133.14 | 126.60 |
| 10 | J | 15 | ASP | CB-CG-OD2 | 5.03 | 122.83 | 118.30 |
| 1 | N | 300 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 3 | P | 244 | PHE | CB-CG-CD1 | -5.03 | 117.28 | 120.80 |
| 4 | Q | 24 | LEU | CB-CG-CD1 | -5.03 | 102.45 | 111.00 |
| 1 | A | 237 | PHE | CG-CD1-CE1 | -5.03 | 115.27 | 120.80 |
| 2 | O | 68 | LEU | CB-CG-CD1 | 5.02 | 119.54 | 111.00 |
| 7 | G | 2 | SER | C-N-CA | 5.02 | 134.25 | 121.70 |
| 3 | P | 80[A] | ARG | NE-CZ-NH1 | -5.02 | 117.79 | 120.30 |
| 3 | P | 80[B] | ARG | NE-CZ-NH1 | -5.02 | 117.79 | 120.30 |
| 1 | A | 181 | THR | OG1-CB-CG2 | -5.02 | 98.46 | 110.00 |
| 1 | N | 346 | PHE | CD1-CE1-CZ | -5.01 | 114.08 | 120.10 |
| 2 | B | 173 | ASP | CB-CG-OD1 | 5.01 | 122.81 | 118.30 |
| 12 | L | 14 | SER | N-CA-CB | -5.01 | 102.98 | 110.50 |
| 2 | B | 151 | ARG | CD-NE-CZ | -5.01 | 116.59 | 123.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 369 | ASP | CB-CG-OD2 | -5.00 | 113.80 | 118.30 |
| 3 | P | 238 | ALA | N-CA-CB | -5.00 | 103.09 | 110.10 |
| 3 | P | 181 | TYR | CE1-CZ-CE2 | 5.00 | 127.80 | 119.80 |

There are no chirality outliers.

All (22) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 296 | GLY | Mainchain |
| 1 | A | 304 | TYR | Sidechain |
| 1 | A | 379 | TYR | Sidechain |
| 1 | A | 38 | ARG | Sidechain |
| 2 | B | 110 | TYR | Sidechain |
| 2 | B | 151 | ARG | Sidechain |
| 2 | B | 68 | LEU | Mainchain |
| 3 | C | 133 | ASN | Sidechain |
| 5 | E | 49 | ASP | Sidechain |
| 5 | E | 88 | GLU | Sidechain |
| 6 | F | 93 | PRO | Peptide |
| 7 | G | 18 | PHE | Sidechain |
| 10 | J | 57 | HIS | Peptide |
| 11 | K | 39 | GLU | Mainchain |
| 13 | M | 14 | GLU | Sidechain |
| 1 | N | 240 | HIS | Sidechain |
| 1 | N | 296 | GLY | Mainchain |
| 1 | N | 304 | TYR | Sidechain |
| 4 | Q | 8 | SER | Peptide |
| 6 | S | 92 | VAL | Mainchain |
| 6 | S | 93 | PRO | Peptide |
| 7 | T | 40 | GLY | 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 | A | 4168 | 0 | 4137 | 74 | 0 |
| 1 | N | 4154 | 0 | 4129 | 81 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | B | 1899 | 0 | 1898 | 65 | 0 |
| 2 | O | 1870 | 0 | 1868 | 40 | 0 |
| 3 | C | 2185 | 0 | 2097 | 38 | 0 |
| 3 | P | 2185 | 0 | 2097 | 51 | 0 |
| 4 | D | 1242 | 0 | 1235 | 19 | 0 |
| 4 | Q | 1224 | 0 | 1211 | 25 | 0 |
| 5 | E | 852 | 0 | 845 | 1 | 0 |
| 5 | R | 863 | 0 | 857 | 8 | 2 |
| 6 | F | 778 | 0 | 754 | 27 | 0 |
| 6 | S | 763 | 0 | 742 | 42 | 0 |
| 7 | G | 686 | 0 | 651 | 42 | 0 |
| 7 | T | 686 | 0 | 651 | 45 | 0 |
| 8 | H | 662 | 0 | 623 | 24 | 0 |
| 8 | U | 662 | 0 | 623 | 15 | 0 |
| 9 | I | 601 | 0 | 613 | 17 | 2 |
| 9 | V | 601 | 0 | 613 | 13 | 0 |
| 10 | J | 460 | 0 | 459 | 13 | 0 |
| 10 | W | 469 | 0 | 464 | 9 | 0 |
| 11 | K | 384 | 0 | 366 | 6 | 0 |
| 11 | X | 391 | 0 | 374 | 4 | 0 |
| 12 | L | 380 | 0 | 380 | 19 | 0 |
| 12 | Y | 388 | 0 | 388 | 29 | 0 |
| 13 | M | 335 | 0 | 352 | 7 | 0 |
| 13 | Z | 335 | 0 | 352 | 5 | 0 |
| 14 | A | 120 | 0 | 107 | 10 | 0 |
| 14 | N | 120 | 0 | 107 | 11 | 0 |
| 15 | A | 1 | 0 | 0 | 0 | 0 |
| 15 | N | 1 | 0 | 0 | 0 | 0 |
| 16 | A | 1 | 0 | 0 | 0 | 0 |
| 16 | N | 1 | 0 | 0 | 0 | 0 |
| 17 | A | 1 | 0 | 0 | 0 | 0 |
| 17 | N | 1 | 0 | 0 | 0 | 0 |
| 18 | A | 2 | 0 | 0 | 1 | 0 |
| 18 | N | 2 | 0 | 0 | 1 | 0 |
| 19 | A | 102 | 0 | 152 | 11 | 0 |
| 19 | C | 102 | 0 | 152 | 8 | 0 |
| 19 | N | 51 | 0 | 76 | 1 | 0 |
| 19 | P | 102 | 0 | 152 | 9 | 0 |
| 19 | Q | 51 | 0 | 76 | 11 | 0 |
| 20 | B | 63 | 0 | 109 | 3 | 0 |
| 20 | D | 63 | 0 | 106 | 21 | 0 |
| 20 | L | 63 | 0 | 110 | 19 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 20 | N | 63 | 0 | 110 | 6 | 0 |
| 20 | Q | 63 | 0 | 110 | 15 | 0 |
| 20 | Y | 63 | 0 | 110 | 23 | 0 |
| 21 | B | 2 | 0 | 0 | 0 | 0 |
| 21 | O | 2 | 0 | 0 | 0 | 0 |
| 22 | B | 29 | 0 | 39 | 0 | 0 |
| 22 | C | 58 | 0 | 77 | 3 | 0 |
| 22 | J | 29 | 0 | 37 | 6 | 0 |
| 22 | O | 29 | 0 | 39 | 0 | 0 |
| 22 | P | 58 | 0 | 77 | 7 | 0 |
| 22 | W | 29 | 0 | 38 | 6 | 0 |
| 23 | B | 52 | 0 | 80 | 13 | 0 |
| 23 | O | 52 | 0 | 80 | 19 | 0 |
| 24 | C | 1 | 0 | 0 | 0 | 0 |
| 24 | P | 1 | 0 | 0 | 0 | 0 |
| 25 | C | 100 | 0 | 154 | 26 | 0 |
| 25 | G | 100 | 0 | 156 | 37 | 0 |
| 25 | P | 100 | 0 | 156 | 24 | 0 |
| 25 | T | 100 | 0 | 156 | 28 | 0 |
| 26 | C | 53 | 0 | 77 | 13 | 0 |
| 26 | G | 106 | 0 | 154 | 16 | 0 |
| 26 | P | 53 | 0 | 77 | 16 | 0 |
| 26 | T | 106 | 0 | 154 | 18 | 0 |
| 27 | F | 1 | 0 | 0 | 0 | 0 |
| 27 | S | 1 | 0 | 0 | 0 | 0 |
| 28 | J | 33 | 0 | 42 | 5 | 0 |
| 28 | M | 33 | 0 | 42 | 0 | 0 |
| 28 | P | 33 | 0 | 42 | 10 | 0 |
| 28 | Z | 33 | 0 | 42 | 0 | 0 |
| 29 | A | 297 | 0 | 0 | 17 | 0 |
| 29 | B | 274 | 0 | 0 | 13 | 0 |
| 29 | C | 176 | 0 | 0 | 8 | 0 |
| 29 | D | 266 | 0 | 0 | 5 | 0 |
| 29 | E | 178 | 0 | 0 | 2 | 0 |
| 29 | F | 199 | 0 | 0 | 9 | 0 |
| 29 | G | 100 | 0 | 0 | 7 | 0 |
| 29 | H | 122 | 0 | 0 | 8 | 0 |
| 29 | I | 88 | 0 | 0 | 2 | 0 |
| 29 | J | 63 | 0 | 0 | 2 | 0 |
| 29 | K | 69 | 0 | 0 | 4 | 0 |
| 29 | L | 48 | 0 | 0 | 2 | 0 |
| 29 | M | 47 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 29 | N | 290 | 0 | 0 | 12 | 0 |
| 29 | O | 243 | 0 | 0 | 4 | 0 |
| 29 | P | 173 | 0 | 0 | 8 | 0 |
| 29 | Q | 164 | 0 | 0 | 8 | 0 |
| 29 | R | 151 | 0 | 0 | 4 | 0 |
| 29 | S | 186 | 0 | 0 | 9 | 0 |
| 29 | T | 94 | 0 | 0 | 3 | 0 |
| 29 | U | 110 | 0 | 0 | 5 | 0 |
| 29 | V | 71 | 0 | 0 | 2 | 0 |
| 29 | W | 58 | 0 | 0 | 1 | 0 |
| 29 | X | 57 | 0 | 0 | 1 | 0 |
| 29 | Y | 40 | 0 | 0 | 3 | 0 |
| 29 | Z | 37 | 0 | 0 | 0 | 0 |
| All | All | 35054 | 0 | 31975 | 816 | 2 |

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 13.

All (816) 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) |
|---|---|---|---|
| 19:C:302:PGV:C21 | 19:C:302:PGV:C22 | 1.77 | 1.62 |
| 26:T:101:PEK:C2 | 26:T:101:PEK:C3 | 1.76 | 1.56 |
| 2:B:1:FME:CN | 2:B:1:FME:N | 1.70 | 1.53 |
| 3:P:224:LYS:NZ | 3:P:224:LYS:CE | 1.77 | 1.47 |
| 20:D:201:TGL:OG2 | 20:D:201:TGL:CB1 | 1.63 | 1.47 |
| 1:N:302[B]:ARG:NH1 | 1:N:361:SER:CB | 1.76 | 1.47 |
| 1:N:302[B]:ARG:HH12 | 1:N:361:SER:CB | 1.27 | 1.45 |
| 5:R:46:LYS:CE | 5:R:46:LYS:NZ | 1.73 | 1.45 |
| 12:Y:20:ARG:HH22 | 12:Y:24[B]:MET:CE | 1.36 | 1.37 |
| 12:Y:20:ARG:NH2 | 20:Y:101:TGL:HC32 | 1.35 | 1.37 |
| 2:B:22[B]:HIS:CE1 | 9:I:44:LYS:HE3 | 1.65 | 1.31 |
| 12:L:20:ARG:NH2 | 20:L:101:TGL:HC32 | 1.43 | 1.31 |
| 26:C:306:PEK:H383 | 25:G:102:CDL:C27 | 1.62 | 1.26 |
| 2:O:22[B]:HIS:CE1 | 9:V:44:LYS:HE2 | 1.70 | 1.25 |
| 18:A:606:PER:O1 | 18:A:606:PER:O2 | 1.55 | 1.24 |
| 2:B:115:ASP:HB3 | 29:B:601:HOH:O | 1.34 | 1.23 |
| 1:N:302[B]:ARG:NH1 | 1:N:361:SER:HB2 | 0.92 | 1.22 |
| 6:S:76:LYS:CE | 6:S:93:PRO:HG2 | 1.68 | 1.22 |
| 18:N:606:PER:O1 | 18:N:606:PER:O2 | 1.55 | 1.21 |
| 4:D:100[B]:LYS:HE2 | 29:D:401:HOH:O | 1.40 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:Y:20:ARG:NH2 | 12:Y:24[B]:MET:CE | 2.07 | 1.17 |
| 12:L:9:LYS:HE3 | 29:L:224:HOH:O | 1.42 | 1.15 |
| 7:G:5:LYS:HG3 | 26:G:103:PEK:H371 | 1.28 | 1.15 |
| 2:B:1:FME:O1 | 2:B:1:FME:N | 1.80 | 1.14 |
| 29:P:436:HOH:O | 6:S:1:ALA:HB2 | 1.45 | 1.14 |
| 23:O:303:PSC:H12 | 23:O:303:PSC:C34 | 1.77 | 1.13 |
| 6:S:85:CYS:SG | 6:S:87[A]:THR:HG23 | 1.88 | 1.13 |
| 20:Q:202:TGL:H362 | 9:V:20:HIS:HE1 | 1.12 | 1.12 |
| 11:K:54:ARG:HD2 | 29:K:141:HOH:O | 1.45 | 1.12 |
| 8:H:9:LYS:HA | 8:H:9:LYS:CE | 1.79 | 1.11 |
| 26:C:306:PEK:H383 | 25:G:102:CDL:H273 | 1.13 | 1.11 |
| 26:P:308:PEK:H383 | 25:T:103:CDL:H273 | 1.21 | 1.10 |
| 26:P:308:PEK:C38 | 25:T:103:CDL:H273 | 1.82 | 1.09 |
| 7:G:84:LYS:HD2 | 7:G:84:LYS:H | 1.11 | 1.09 |
| 1:A:136[B]:LEU:HD11 | 29:A:988:HOH:O | 1.52 | 1.09 |
| 20:D:201:TGL:CB2 | 20:D:201:TGL:OG2 | 2.01 | 1.08 |
| 8:H:9:LYS:HA | 8:H:9:LYS:HE2 | 1.33 | 1.08 |
| 1:A:486[B]:ASP:OD2 | 4:D:19[B]:ARG:HD2 | 1.52 | 1.08 |
| 12:Y:20:ARG:HH22 | 12:Y:24[B]:MET:HE1 | 0.90 | 1.07 |
| 6:S:19:GLU:HG2 | 29:S:314:HOH:O | 1.54 | 1.07 |
| 1:A:513:LEU:O | 1:A:514:LYS:HB2 | 1.54 | 1.06 |
| 26:T:102:PEK:H361 | 25:T:103:CDL:H872 | 1.32 | 1.06 |
| 1:N:513:LEU:O | 1:N:514:LYS:HB2 | 1.52 | 1.06 |
| 23:O:303:PSC:H12 | 23:O:303:PSC:H342 | 1.34 | 1.06 |
| 6:S:76:LYS:HE2 | 6:S:93:PRO:HG2 | 1.11 | 1.05 |
| 12:Y:20:ARG:NH2 | 12:Y:24[B]:MET:HE1 | 1.69 | 1.05 |
| 26:C:306:PEK:C38 | 25:G:102:CDL:C27 | 2.33 | 1.05 |
| 19:Q:201:PGV:H011 | 19:Q:201:PGV:C2 | 1.84 | 1.05 |
| 2:B:22[B]:HIS:CE1 | 9:I:44:LYS:CE | 2.40 | 1.04 |
| 12:Y:24[B]:MET:SD | 20:Y:101:TGL:HC21 | 1.97 | 1.04 |
| 12:L:14:SER:H | 20:L:101:TGL:HC31 | 1.17 | 1.04 |
| 1:N:417[A]:MET:HE2 | 29:N:880:HOH:O | 1.56 | 1.04 |
| 4:Q:9:GLU:HB3 | 29:Q:427:HOH:O | 1.54 | 1.03 |
| 20:Y:101:TGL:OC1 | 20:Y:101:TGL:HC41 | 1.21 | 1.03 |
| 1:A:282:PHE:HA | 7:T:4:ALA:HB3 | 1.41 | 1.03 |
| 12:Y:20:ARG:HH21 | 20:Y:101:TGL:CC3 | 1.72 | 1.02 |
| 19:A:608:PGV:H311 | 13:M:19:LEU:HD23 | 1.41 | 1.02 |
| 1:N:513:LEU:O | 1:N:514:LYS:CB | 2.04 | 1.02 |
| 1:N:483:LEU:HD13 | 4:Q:6:VAL:HB | 1.39 | 1.02 |
| 4:Q:65:LYS:HE3 | 29:Q:421:HOH:O | 1.55 | 1.02 |
| 12:Y:20:ARG:NH2 | 20:Y:101:TGL:CC3 | 2.23 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:90:ARG:HD2 | 29:E:311:HOH:O | 1.58 | 1.01 |
| 26:P:308:PEK:C38 | 25:T:103:CDL:C27 | 2.39 | 1.01 |
| 1:N:302[B]:ARG:HH11 | 1:N:361:SER:HB2 | 1.19 | 1.01 |
| 20:Q:202:TGL:H362 | 9:V:20:HIS:CE1 | 1.97 | 0.99 |
| 7:G:11:TPO:HG22 | 7:G:16:TRP:HE1 | 1.28 | 0.98 |
| 7:G:5:LYS:HB2 | 26:G:103:PEK:H351 | 1.45 | 0.98 |
| 29:A:964:HOH:O | 20:D:201:TGL:HC31 | 1.62 | 0.98 |
| 1:N:486:ASP:OD2 | 4:Q:19[B]:ARG:HD2 | 1.64 | 0.97 |
| 2:B:49:LYS:HE2 | 29:B:609:HOH:O | 1.65 | 0.97 |
| 12:Y:14:SER:H | 20:Y:101:TGL:HC31 | 1.31 | 0.95 |
| 6:F:1:ALA:HB3 | 6:S:65:ASP:OD1 | 1.67 | 0.95 |
| 1:A:178[B]:GLN:NE2 | 29:A:701:HOH:O | 1.97 | 0.95 |
| 25:G:102:CDL:H541 | 25:G:102:CDL:C24 | 1.96 | 0.94 |
| 26:C:306:PEK:C38 | 25:G:102:CDL:H273 | 1.93 | 0.94 |
| 26:P:308:PEK:H382 | 25:T:103:CDL:C27 | 1.98 | 0.94 |
| 7:G:4:ALA:CB | 1:N:282:PHE:HA | 1.98 | 0.94 |
| 23:O:303:PSC:H342 | 23:O:303:PSC:C12 | 1.96 | 0.94 |
| 26:P:308:PEK:H051 | 29:P:476:HOH:O | 1.67 | 0.93 |
| 6:S:76:LYS:HE2 | 6:S:93:PRO:CG | 1.99 | 0.93 |
| 3:C:67:PHE:HE1 | 25:C:303:CDL:H1 | 1.35 | 0.92 |
| 12:L:20:ARG:HH22 | 20:L:101:TGL:CC3 | 1.81 | 0.92 |
| 2:O:22[B]:HIS:HE1 | 9:V:44:LYS:HE2 | 1.27 | 0.92 |
| 1:N:178[B]:GLN:HG3 | 1:N:186:TRP:CZ2 | 2.04 | 0.92 |
| 25:T:103:CDL:H541 | 25:T:103:CDL:H242 | 1.48 | 0.92 |
| 2:B:56:MET:HA | 23:B:304:PSC:H201 | 1.51 | 0.91 |
| 2:B:22[B]:HIS:HE1 | 9:I:44:LYS:HE3 | 1.11 | 0.91 |
| 3:C:180[B]:GLU:HG2 | 29:C:422:HOH:O | 1.70 | 0.91 |
| 19:Q:201:PGV:H011 | 19:Q:201:PGV:H22 | 1.51 | 0.91 |
| 3:C:51[B]:MET:HE2 | 25:C:303:CDL:H391 | 1.53 | 0.90 |
| 23:O:303:PSC:H71 | 29:V:170:HOH:O | 1.69 | 0.90 |
| 3:C:224:LYS:CD | 25:C:303:CDL:HB31 | 2.00 | 0.90 |
| 2:B:1:FME:CN | 2:B:1:FME:CA | 2.49 | 0.90 |
| 1:A:282:PHE:HA | 7:T:4:ALA:CB | 2.01 | 0.89 |
| 8:U:9:LYS:HG2 | 29:U:187:HOH:O | 1.71 | 0.89 |
| 1:A:486[B]:ASP:OD2 | 4:D:19[B]:ARG:CD | 2.20 | 0.89 |
| 7:G:72:ASN:H | 7:G:76:ASN:HD22 | 1.17 | 0.89 |
| 19:A:607:PGV:H343 | 26:G:101:PEK:H382 | 1.55 | 0.88 |
| 12:L:20:ARG:HH22 | 20:L:101:TGL:HC32 | 1.12 | 0.88 |
| 1:A:417[B]:MET:CE | 29:A:816:HOH:O | 2.21 | 0.88 |
| 12:Y:20:ARG:NH2 | 12:Y:24[B]:MET:SD | 2.47 | 0.88 |
| 23:B:304:PSC:H212 | 23:B:304:PSC:H02 | 1.54 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:156:ARG:HE | 22:P:305:CHD:H232 | 1.38 | 0.88 |
| 3:P:67:PHE:HE1 | 25:P:304:CDL:H1 | 1.39 | 0.87 |
| 4:D:19[A]:ARG:NH2 | 4:D:21:ASP:OD1 | 2.07 | 0.87 |
| 20:Y:101:TGL:OC1 | 20:Y:101:TGL:CC4 | 2.17 | 0.87 |
| 12:L:20:ARG:NH2 | 20:L:101:TGL:CC3 | 2.34 | 0.86 |
| 4:Q:6:VAL:HG12 | 4:Q:10:ASP:OD2 | 1.74 | 0.86 |
| 7:T:72:ASN:H | 7:T:76:ASN:HD22 | 1.19 | 0.86 |
| 4:Q:9:GLU:HA | 4:Q:9:GLU:OE2 | 1.76 | 0.86 |
| 2:B:22[B]:HIS:HE1 | 9:I:44:LYS:CE | 1.79 | 0.85 |
| 25:G:102:CDL:H212 | 1:N:311[A]:ILE:CD1 | 2.07 | 0.85 |
| 23:O:303:PSC:H12 | 23:O:303:PSC:H343 | 1.58 | 0.85 |
| 6:S:75:HIS:H | 6:S:80:GLN:HE22 | 1.21 | 0.85 |
| 1:A:178[B]:GLN:HG3 | 7:T:7:ASP:OD2 | 1.77 | 0.85 |
| 10:J:49:CYS:HB3 | 28:J:101:DMU:H9 | 1.58 | 0.84 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:H | 1.93 | 0.84 |
| 1:N:136[B]:LEU:HD11 | 29:N:976:HOH:O | 1.77 | 0.84 |
| 7:G:84:LYS:H | 7:G:84:LYS:CD | 1.89 | 0.84 |
| 2:O:29[B]:MET:SD | 2:O:33:LEU:HD22 | 2.18 | 0.83 |
| 7:G:4:ALA:HB1 | 1:N:282:PHE:HA | 1.59 | 0.83 |
| 1:N:417[A]:MET:CE | 29:N:880:HOH:O | 2.19 | 0.83 |
| 6:F:75:HIS:H | 6:F:80:GLN:HE22 | 1.26 | 0.83 |
| 1:N:514:LYS:HA | 6:S:38:ALA:HB3 | 1.61 | 0.83 |
| 1:N:321:PHE:CD2 | 23:O:303:PSC:H341 | 2.12 | 0.83 |
| 1:A:513:LEU:O | 1:A:514:LYS:CB | 2.27 | 0.82 |
| 3:C:224:LYS:HE3 | 25:C:303:CDL:HB31 | 1.61 | 0.82 |
| 12:Y:24[B]:MET:HG2 | 20:Y:101:TGL:HA22 | 1.61 | 0.82 |
| 25:G:102:CDL:H352 | 2:O:78:LEU:HD12 | 1.59 | 0.82 |
| 19:Q:201:PGV:H011 | 19:Q:201:PGV:H21 | 1.61 | 0.82 |
| 1:N:28:MET:CE | 14:N:601:HEA:H271 | 2.10 | 0.81 |
| 25:G:102:CDL:H241 | 25:G:102:CDL:H541 | 1.61 | 0.81 |
| 20:D:201:TGL:CB1 | 20:D:201:TGL:CG2 | 2.57 | 0.81 |
| 26:P:308:PEK:H383 | 25:T:103:CDL:C27 | 2.04 | 0.81 |
| 7:T:30:LEU:HD21 | 25:T:103:CDL:H471 | 1.61 | 0.81 |
| 19:Q:201:PGV:H311 | 13:Z:19:LEU:HD23 | 1.63 | 0.81 |
| 6:F:85:CYS:SG | 6:F:87[A]:THR:HG23 | 2.21 | 0.81 |
| 6:S:94:HIS:HA | 29:S:318:HOH:O | 1.81 | 0.81 |
| 12:L:20:ARG:HH21 | 20:L:101:TGL:HC32 | 1.42 | 0.81 |
| 3:P:63:ARG:HE | 25:P:304:CDL:CA2 | 1.93 | 0.80 |
| 8:H:9:LYS:CA | 8:H:9:LYS:CE | 2.53 | 0.80 |
| 3:C:161[A]:GLN:HE22 | 26:C:306:PEK:C2 | 1.95 | 0.80 |
| 2:B:16[B]:ILE:HG23 | 29:B:523:HOH:O | 1.80 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:T:103:CDL:H511 | 25:T:103:CDL:H181 | 1.61 | 0.79 |
| 7:G:37:LEU:HD21 | 25:G:102:CDL:H361 | 1.65 | 0.79 |
| 6:F:54[A]:ASN:H | 6:F:54[A]:ASN:HD22 | 1.29 | 0.79 |
| 20:Q:202:TGL:H352 | 9:V:16:ARG:HE | 1.46 | 0.79 |
| 26:P:308:PEK:H382 | 25:T:103:CDL:H272 | 1.64 | 0.79 |
| 4:Q:19[A]:ARG:HG2 | 4:Q:21:ASP:OD1 | 1.81 | 0.79 |
| 3:P:160:LEU:HD13 | 22:P:305:CHD:H181 | 1.65 | 0.79 |
| 12:Y:20:ARG:HH21 | 20:Y:101:TGL:HC32 | 0.89 | 0.79 |
| 3:C:67:PHE:CE1 | 25:C:303:CDL:H1 | 2.18 | 0.78 |
| 12:Y:24[B]:MET:SD | 20:Y:101:TGL:CC2 | 2.72 | 0.78 |
| 2:B:87[B]:MET:HE2 | 29:B:417:HOH:O | 1.80 | 0.78 |
| 3:C:224:LYS:CE | 25:C:303:CDL:HB31 | 2.11 | 0.78 |
| 3:P:156:ARG:HE | 22:P:305:CHD:C23 | 1.96 | 0.78 |
| 3:C:63:ARG:HE | 25:C:303:CDL:CA2 | 1.96 | 0.78 |
| 8:H:9:LYS:CA | 8:H:9:LYS:HE2 | 2.13 | 0.78 |
| 1:A:178[B]:GLN:H | 1:A:178[B]:GLN:CD | 1.87 | 0.78 |
| 2:B:82:ARG:HD2 | 29:B:403:HOH:O | 1.82 | 0.78 |
| 26:P:308:PEK:N | 26:P:308:PEK:O02 | 2.16 | 0.78 |
| 26:C:306:PEK:H383 | 25:G:102:CDL:H271 | 1.63 | 0.77 |
| 7:T:36:TRP:HE3 | 7:T:39:SER:HB3 | 1.47 | 0.77 |
| 3:C:63:ARG:HE | 25:C:303:CDL:HA21 | 1.48 | 0.77 |
| 26:T:101:PEK:C3 | 26:T:101:PEK:C1 | 2.62 | 0.77 |
| 1:N:28:MET:CE | 14:N:601:HEA:C27 | 2.63 | 0.77 |
| 4:D:34:SER:H | 4:D:37:GLN:HE21 | 1.33 | 0.77 |
| 19:C:302:PGV:H221 | 19:C:302:PGV:C21 | 2.12 | 0.77 |
| 25:G:102:CDL:H332 | 29:O:488:HOH:O | 1.85 | 0.77 |
| 25:G:102:CDL:OA7 | 25:G:102:CDL:H342 | 1.84 | 0.77 |
| 3:P:67:PHE:CE1 | 25:P:304:CDL:H1 | 2.20 | 0.77 |
| 20:N:608:TGL:H281 | 20:N:608:TGL:HB91 | 1.68 | 0.76 |
| 19:P:303:PGV:H172 | 25:P:304:CDL:H642 | 1.65 | 0.76 |
| 23:O:303:PSC:C12 | 23:O:303:PSC:C34 | 2.59 | 0.76 |
| 4:D:78:TRP:CA | 20:D:201:TGL:HB21 | 2.15 | 0.75 |
| 6:S:43:LYS:H | 6:S:43:LYS:HD2 | 1.52 | 0.75 |
| 2:B:74:ILE:O | 2:B:78:LEU:HD13 | 1.85 | 0.75 |
| 12:L:20:ARG:HH22 | 20:L:101:TGL:HC52 | 1.52 | 0.75 |
| 1:A:53:ILE:HG13 | 29:A:980:HOH:O | 1.87 | 0.75 |
| 2:B:56:MET:HG2 | 23:B:304:PSC:H211 | 1.68 | 0.75 |
| 20:L:101:TGL:H312 | 20:L:101:TGL:H362 | 1.67 | 0.75 |
| 20:N:608:TGL:H281 | 20:N:608:TGL:CB9 | 2.17 | 0.75 |
| 14:A:602:HEA:HBC1 | 14:A:602:HEA:HMC1 | 1.69 | 0.75 |
| 1:N:297[B]:MET:SD | 1:N:302[B]:ARG:HG3 | 2.27 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:514:LYS:HA | 6:F:38:ALA:HB3 | 1.69 | 0.74 |
| 2:B:53:THR:HG21 | 29:D:305:HOH:O | 1.88 | 0.74 |
| 26:P:308:PEK:H041 | 7:T:17:ARG:HH22 | 1.52 | 0.74 |
| 3:C:224:LYS:HD2 | 25:C:303:CDL:HB31 | 1.68 | 0.74 |
| 1:N:406:ASN:HD21 | 19:Q:201:PGV:H21 | 1.52 | 0.73 |
| 3:C:161[A]:GLN:HE22 | 26:C:306:PEK:H22 | 1.50 | 0.73 |
| 25:C:303:CDL:H522 | 25:C:303:CDL:OB9 | 1.88 | 0.73 |
| 3:C:33[B]:MET:HG2 | 3:C:39:SER:O | 1.88 | 0.73 |
| 25:T:103:CDL:H762 | 25:T:103:CDL:H562 | 1.69 | 0.73 |
| 6:S:43:LYS:CD | 6:S:43:LYS:H | 2.00 | 0.73 |
| 25:G:102:CDL:H212 | 1:N:311[A]:ILE:HD12 | 1.69 | 0.73 |
| 3:P:33[A]:MET:HB2 | 28:P:306:DMU:H8 | 1.70 | 0.73 |
| 25:G:102:CDL:H201 | 25:G:102:CDL:H522 | 1.71 | 0.73 |
| 7:G:76:ASN:HD21 | 26:G:101:PEK:HN2 | 1.37 | 0.72 |
| 23:O:303:PSC:H02 | 23:O:303:PSC:H212 | 1.71 | 0.72 |
| 1:N:28:MET:HE1 | 14:N:601:HEA:H271 | 1.70 | 0.72 |
| 3:P:156:ARG:NE | 22:P:305:CHD:H232 | 2.05 | 0.72 |
| 7:T:11:TPO:HG22 | 7:T:16:TRP:HE1 | 1.55 | 0.72 |
| 3:P:33[A]:MET:HB2 | 28:P:306:DMU:C19 | 2.20 | 0.71 |
| 19:A:607:PGV:H183 | 26:G:101:PEK:H322 | 1.71 | 0.71 |
| 12:L:20:ARG:HH22 | 20:L:101:TGL:CC5 | 2.03 | 0.71 |
| 7:T:30:LEU:CD2 | 25:T:103:CDL:H471 | 2.20 | 0.70 |
| 2:B:49:LYS:HD3 | 20:D:201:TGL:HC71 | 1.73 | 0.70 |
| 7:T:36:TRP:CE3 | 7:T:39:SER:HB3 | 2.26 | 0.70 |
| 8:U:45:ALA:O | 8:U:47:GLY:N | 2.25 | 0.70 |
| 1:N:302[B]:ARG:HH12 | 1:N:361:SER:CA | 2.04 | 0.70 |
| 3:P:63:ARG:HE | 25:P:304:CDL:HA22 | 1.54 | 0.70 |
| 1:A:112:LEU:HG | 29:A:937:HOH:O | 1.90 | 0.70 |
| 14:N:601:HEA:HMC1 | 14:N:601:HEA:HBC1 | 1.74 | 0.70 |
| 2:O:22[B]:HIS:CE1 | 9:V:44:LYS:CE | 2.63 | 0.70 |
| 1:N:178[B]:GLN:CG | 1:N:186:TRP:CZ2 | 2.73 | 0.70 |
| 4:Q:6:VAL:CG1 | 4:Q:10:ASP:OD2 | 2.40 | 0.70 |
| 12:Y:14:SER:N | 20:Y:101:TGL:HC31 | 2.06 | 0.70 |
| 4:D:31[A]:LYS:CG | 29:D:301:HOH:O | 2.40 | 0.70 |
| 25:G:102:CDL:H241 | 25:G:102:CDL:C54 | 2.21 | 0.70 |
| 20:Q:202:TGL:CA9 | 20:Q:202:TGL:H231 | 2.21 | 0.70 |
| 19:C:302:PGV:H222 | 19:C:302:PGV:C21 | 2.12 | 0.70 |
| 2:B:29[B]:MET:SD | 2:B:33:LEU:HD22 | 2.32 | 0.69 |
| 1:A:406:ASN:HD21 | 19:A:608:PGV:H22 | 1.56 | 0.69 |
| 10:J:33:ARG:HG2 | 22:J:102:CHD:H152 | 1.75 | 0.69 |
| 1:A:28:MET:CE | 14:A:601:HEA:C27 | 2.71 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O:56:MET:HG2 | 23:O:303:PSC:H211 | 1.75 | 0.69 |
| 3:P:127:LEU:HD13 | 25:T:103:CDL:OB3 | 1.92 | 0.69 |
| 7:T:76:ASN:HD21 | 26:T:101:PEK:HN2 | 1.36 | 0.69 |
| 11:K:47:ARG:HD3 | 29:K:160:HOH:O | 1.91 | 0.69 |
| 1:A:177:SER:H | 1:A:180:GLN:HE21 | 1.40 | 0.69 |
| 19:P:301:PGV:H32 | 29:P:523:HOH:O | 1.91 | 0.69 |
| 6:S:94:HIS:HD2 | 6:S:95:GLN:O | 1.76 | 0.68 |
| 25:T:103:CDL:H511 | 25:T:103:CDL:C18 | 2.23 | 0.68 |
| 26:P:308:PEK:H042 | 6:S:1:ALA:N | 2.08 | 0.68 |
| 6:F:92:VAL:HG21 | 29:F:387:HOH:O | 1.94 | 0.68 |
| 1:N:178[B]:GLN:HG3 | 1:N:186:TRP:CE2 | 2.29 | 0.67 |
| 3:P:63:ARG:HE | 25:P:304:CDL:HA21 | 1.59 | 0.67 |
| 10:W:10:LYS:O | 10:W:14[B]:GLU:HG3 | 1.94 | 0.67 |
| 7:T:38:HIS:HD2 | 29:T:210:HOH:O | 1.76 | 0.67 |
| 25:P:304:CDL:OB9 | 25:P:304:CDL:H522 | 1.94 | 0.67 |
| 1:A:484:THR:HG22 | 29:A:972:HOH:O | 1.94 | 0.67 |
| 8:U:48:GLY:HA2 | 29:U:176:HOH:O | 1.94 | 0.67 |
| 14:N:602:HEA:HBC1 | 14:N:602:HEA:HMC1 | 1.77 | 0.67 |
| 8:U:43:MET:HE3 | 8:U:49:ASP:N | 2.09 | 0.67 |
| 1:N:302[B]:ARG:NH1 | 1:N:361:SER:OG | 2.28 | 0.67 |
| 2:O:60:GLU:CD | 2:O:60:GLU:H | 1.97 | 0.67 |
| 19:P:303:PGV:H172 | 25:P:304:CDL:C64 | 2.25 | 0.67 |
| 1:A:273:MET:HE2 | 29:A:888:HOH:O | 1.94 | 0.66 |
| 7:G:72:ASN:H | 7:G:76:ASN:ND2 | 1.93 | 0.66 |
| 25:P:304:CDL:HB21 | 25:P:304:CDL:OB6 | 1.95 | 0.66 |
| 7:T:5:LYS:HG3 | 26:T:102:PEK:H351 | 1.76 | 0.66 |
| 2:B:33:LEU:HD13 | 9:I:31:PHE:CD1 | 2.30 | 0.66 |
| 7:G:11:TPO:HG21 | 29:G:280:HOH:O | 1.96 | 0.66 |
| 8:H:23:GLN:HG3 | 29:H:166:HOH:O | 1.95 | 0.66 |
| 10:W:33:ARG:HG2 | 22:W:101:CHD:H182 | 1.76 | 0.66 |
| 12:L:14:SER:N | 20:L:101:TGL:HC31 | 2.01 | 0.66 |
| 6:S:43:LYS:HE2 | 29:S:342:HOH:O | 1.95 | 0.66 |
| 3:P:4:GLN:N | 29:P:401:HOH:O | 2.29 | 0.66 |
| 7:T:37:LEU:HD23 | 25:T:103:CDL:H361 | 1.77 | 0.66 |
| 29:C:541:HOH:O | 10:J:1:PHE:HE2 | 1.79 | 0.65 |
| 23:O:303:PSC:C02 | 23:O:303:PSC:H212 | 2.26 | 0.65 |
| 4:Q:78:TRP:N | 20:Q:202:TGL:HB21 | 2.11 | 0.65 |
| 4:D:31[A]:LYS:HG2 | 29:D:301:HOH:O | 1.95 | 0.65 |
| 7:G:3:ALA:HB3 | 26:G:103:PEK:H362 | 1.79 | 0.65 |
| 2:O:29[B]:MET:SD | 2:O:33:LEU:CD2 | 2.84 | 0.65 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:N | 2.64 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:28:MET:HE2 | 14:N:601:HEA:H273 | 1.78 | 0.65 |
| 26:T:102:PEK:C36 | 25:T:103:CDL:H872 | 2.20 | 0.65 |
| 12:Y:20:ARG:CZ | 12:Y:24[B]:MET:CE | 2.75 | 0.65 |
| 7:G:3:ALA:CB | 26:G:103:PEK:H383 | 2.27 | 0.64 |
| 29:N:703:HOH:O | 4:Q:6:VAL:HG11 | 1.97 | 0.64 |
| 10:J:32:TYR:OH | 22:J:102:CHD:H213 | 1.97 | 0.64 |
| 5:R:46:LYS:CD | 5:R:46:LYS:NZ | 2.56 | 0.64 |
| 6:F:41:GLY:HA3 | 6:F:87[B]:THR:HG22 | 1.80 | 0.64 |
| 7:G:5:LYS:CG | 26:G:103:PEK:H371 | 2.17 | 0.64 |
| 23:O:303:PSC:H322 | 23:O:303:PSC:C28 | 2.27 | 0.64 |
| 1:A:468:MET:HG3 | 29:A:957:HOH:O | 1.97 | 0.64 |
| 1:N:302[B]:ARG:HH11 | 1:N:361:SER:CB | 1.87 | 0.64 |
| 5:R:80:GLU:CD | 5:R:80:GLU:H | 2.00 | 0.64 |
| 4:D:28:ALA:H | 4:D:31[B]:LYS:NZ | 1.95 | 0.63 |
| 8:H:47:GLY:HA2 | 29:H:180:HOH:O | 1.97 | 0.63 |
| 1:N:177:SER:H | 1:N:180:GLN:HE21 | 1.46 | 0.63 |
| 1:N:297[B]:MET:HB3 | 1:N:302[B]:ARG:HD2 | 1.79 | 0.63 |
| 2:O:22[B]:HIS:HE1 | 9:V:44:LYS:CE | 2.06 | 0.63 |
| 19:A:608:PGV:H061 | 19:A:608:PGV:O11 | 1.99 | 0.63 |
| 7:G:3:ALA:HB1 | 26:G:103:PEK:H383 | 1.79 | 0.63 |
| 7:T:84:LYS:H | 7:T:84:LYS:NZ | 1.96 | 0.63 |
| 2:B:83:ILE:O | 2:B:87[A]:MET:HG3 | 1.99 | 0.62 |
| 13:M:39:ASN:O | 13:M:43:SER:HB3 | 1.99 | 0.62 |
| 7:T:72:ASN:H | 7:T:76:ASN:ND2 | 1.94 | 0.62 |
| 2:B:1:FME:HCN | 2:B:193:TYR:H | 1.64 | 0.62 |
| 3:C:51[B]:MET:CE | 25:C:303:CDL:H391 | 2.29 | 0.62 |
| 6:S:22:LEU:HD12 | 29:S:329:HOH:O | 1.99 | 0.62 |
| 20:Q:202:TGL:HA92 | 20:Q:202:TGL:H231 | 1.81 | 0.62 |
| 13:Z:42:LYS:HG3 | 13:Z:42:LYS:O | 1.99 | 0.62 |
| 1:A:28:MET:HE2 | 14:A:601:HEA:H273 | 1.81 | 0.62 |
| 2:O:92:ASN:HB3 | 29:U:128:HOH:O | 1.99 | 0.62 |
| 7:T:11:TPO:O | 7:T:11:TPO:CG2 | 2.48 | 0.62 |
| 20:D:201:TGL:CG3 | 20:D:201:TGL:CB1 | 2.77 | 0.62 |
| 25:G:102:CDL:H541 | 25:G:102:CDL:H242 | 1.80 | 0.62 |
| 20:N:608:TGL:HB91 | 20:N:608:TGL:C28 | 2.30 | 0.61 |
| 1:A:417[B]:MET:HE2 | 29:A:816:HOH:O | 1.92 | 0.61 |
| 26:P:308:PEK:H042 | 6:S:1:ALA:H1 | 1.64 | 0.61 |
| 6:S:94:HIS:CG | 6:S:95:GLN:H | 2.14 | 0.61 |
| 1:A:334:TRP:CH2 | 2:B:46:LEU:HD13 | 2.35 | 0.61 |
| 2:O:47:THR:HB | 20:Q:202:TGL:H181 | 1.81 | 0.61 |
| 2:B:32[B]:PHE:CD2 | 9:I:31:PHE:CZ | 2.89 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:Q:78:TRP:HB3 | 20:Q:202:TGL:HB22 | 1.83 | 0.61 |
| 6:S:43:LYS:HD3 | 29:S:251:HOH:O | 1.99 | 0.61 |
| 20:Y:101:TGL:HG31 | 29:Y:221:HOH:O | 2.00 | 0.61 |
| 7:T:84:LYS:H | 7:T:84:LYS:HZ3 | 1.48 | 0.61 |
| 23:B:304:PSC:H212 | 23:B:304:PSC:C02 | 2.28 | 0.61 |
| 1:A:278[B]:MET:HE3 | 7:T:5:LYS:HB3 | 1.83 | 0.60 |
| 20:D:201:TGL:HG12 | 20:D:201:TGL:HC32 | 1.82 | 0.60 |
| 5:R:46:LYS:NZ | 29:R:202:HOH:O | 2.34 | 0.60 |
| 6:S:76:LYS:NZ | 6:S:93:PRO:HG2 | 2.15 | 0.60 |
| 2:B:183[A]:THR:HG22 | 29:B:462:HOH:O | 2.00 | 0.60 |
| 26:G:101:PEK:C12 | 26:G:101:PEK:H161 | 2.30 | 0.60 |
| 14:A:601:HEA:HBC1 | 14:A:601:HEA:HMC1 | 1.83 | 0.60 |
| 19:A:608:PGV:H311 | 13:M:19:LEU:CD2 | 2.26 | 0.60 |
| 7:T:3:ALA:O | 7:T:4:ALA:HB2 | 2.02 | 0.60 |
| 19:C:302:PGV:H161 | 19:C:302:PGV:H12 | 1.84 | 0.60 |
| 6:F:94:HIS:CE1 | 29:F:203:HOH:O | 2.53 | 0.60 |
| 1:N:468:MET:HG3 | 29:N:943:HOH:O | 2.00 | 0.60 |
| 3:P:50:ASN:HD22 | 3:P:51[A]:MET:HE2 | 1.65 | 0.60 |
| 1:N:28:MET:HE2 | 14:N:601:HEA:C27 | 2.27 | 0.60 |
| 20:D:201:TGL:HA91 | 20:D:201:TGL:H231 | 1.84 | 0.60 |
| 1:A:278[B]:MET:CE | 7:T:5:LYS:HB3 | 2.31 | 0.60 |
| 6:S:19:GLU:OE1 | 6:S:31:TYR:OH | 2.17 | 0.60 |
| 7:T:38:HIS:CD2 | 29:T:210:HOH:O | 2.50 | 0.60 |
| 8:U:43:MET:CE | 8:U:49:ASP:H | 2.15 | 0.59 |
| 1:A:514:LYS:HD2 | 29:F:252:HOH:O | 2.02 | 0.59 |
| 2:B:52:HIS:HE1 | 23:B:304:PSC:H212 | 1.66 | 0.59 |
| 6:F:54[A]:ASN:H | 6:F:54[A]:ASN:ND2 | 1.99 | 0.59 |
| 1:N:334:TRP:CH2 | 2:O:46:LEU:HD13 | 2.37 | 0.59 |
| 3:P:224:LYS:CD | 25:P:304:CDL:HB32 | 2.32 | 0.59 |
| 6:S:43:LYS:CE | 29:S:342:HOH:O | 2.48 | 0.59 |
| 3:C:161[A]:GLN:HE22 | 26:C:306:PEK:H21 | 1.66 | 0.59 |
| 4:D:78:TRP:HA | 20:D:201:TGL:HB21 | 1.84 | 0.59 |
| 26:C:306:PEK:H382 | 25:G:102:CDL:C27 | 2.29 | 0.59 |
| 3:C:224:LYS:CD | 25:C:303:CDL:CB3 | 2.77 | 0.58 |
| 6:F:54[A]:ASN:N | 6:F:54[A]:ASN:HD22 | 2.00 | 0.58 |
| 2:B:52:HIS:CE1 | 23:B:304:PSC:H211 | 2.38 | 0.58 |
| 6:F:30:PRO:O | 6:F:96:LEU:HD11 | 2.02 | 0.58 |
| 29:C:541:HOH:O | 10:J:1:PHE:CE2 | 2.52 | 0.58 |
| 25:G:102:CDL:HA21 | 25:G:102:CDL:H111 | 1.86 | 0.58 |
| 20:Y:101:TGL:CG3 | 29:Y:221:HOH:O | 2.52 | 0.58 |
| 23:O:303:PSC:H012 | 23:O:303:PSC:P | 2.43 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:T:31:CYS:SG | 25:T:103:CDL:H532 | 2.43 | 0.58 |
| 8:U:43:MET:HE3 | 8:U:49:ASP:H | 1.68 | 0.58 |
| 12:Y:24[B]:MET:CG | 20:Y:101:TGL:HA22 | 2.32 | 0.58 |
| 1:N:273:MET:HE2 | 29:N:749:HOH:O | 2.03 | 0.58 |
| 4:D:78:TRP:N | 20:D:201:TGL:HB21 | 2.17 | 0.58 |
| 12:L:2:HIS:CG | 12:L:3:TYR:H | 2.21 | 0.58 |
| 12:Y:20:ARG:NH2 | 12:Y:24[B]:MET:HE2 | 2.14 | 0.58 |
| 1:A:113[B]:LEU:HD11 | 1:A:117[B]:MET:SD | 2.43 | 0.58 |
| 7:G:4:ALA:HB1 | 1:N:282:PHE:CA | 2.32 | 0.58 |
| 1:N:302[B]:ARG:HH11 | 1:N:302[B]:ARG:HG2 | 1.66 | 0.58 |
| 3:C:55:TYR:CE1 | 25:C:303:CDL:H532 | 2.38 | 0.58 |
| 7:G:84:LYS:N | 7:G:84:LYS:HD2 | 1.97 | 0.58 |
| 1:A:302[B]:ARG:NE | 1:A:361[B]:SER:OG | 2.35 | 0.58 |
| 7:G:4:ALA:HB3 | 1:N:282:PHE:HA | 1.81 | 0.58 |
| 7:T:2:SER:OG | 26:T:102:PEK:H302 | 2.04 | 0.58 |
| 6:F:87[A]:THR:HG21 | 29:F:324:HOH:O | 2.03 | 0.57 |
| 10:J:50:LEU:HB2 | 28:J:101:DMU:H20 | 1.86 | 0.57 |
| 2:B:70:ALA:HB1 | 25:T:103:CDL:H461 | 1.86 | 0.57 |
| 19:P:301:PGV:H062 | 8:U:24:ASN:HB3 | 1.86 | 0.57 |
| 2:B:1:FME:CN | 2:B:1:FME:HA | 2.35 | 0.57 |
| 2:O:42:ILE:HG21 | 20:Q:202:TGL:H232 | 1.86 | 0.57 |
| 19:A:607:PGV:C18 | 26:G:101:PEK:H322 | 2.34 | 0.57 |
| 25:G:102:CDL:HA31 | 29:G:267:HOH:O | 2.04 | 0.57 |
| 1:N:35:LEU:HD11 | 1:N:462:LEU:HB2 | 1.87 | 0.57 |
| 3:P:51[A]:MET:HE1 | 3:P:54[A]:MET:HE1 | 1.87 | 0.57 |
| 1:A:281:GLY:C | 7:T:4:ALA:HB1 | 2.25 | 0.57 |
| 7:G:9:GLY:HA3 | 29:N:797:HOH:O | 2.05 | 0.57 |
| 3:C:224:LYS:HE3 | 25:C:303:CDL:CB3 | 2.32 | 0.57 |
| 20:Y:101:TGL:HC42 | 29:Y:225:HOH:O | 2.04 | 0.56 |
| 1:A:177:SER:H | 1:A:180:GLN:NE2 | 2.03 | 0.56 |
| 12:L:46:LYS:HA | 29:L:217:HOH:O | 2.04 | 0.56 |
| 1:N:116:SER:HB3 | 29:N:931:HOH:O | 2.05 | 0.56 |
| 3:C:63:ARG:HE | 25:C:303:CDL:HA22 | 1.69 | 0.56 |
| 6:F:94:HIS:HE1 | 29:F:203:HOH:O | 1.85 | 0.56 |
| 1:A:302[B]:ARG:NE | 2:B:84:LEU:HD11 | 2.20 | 0.56 |
| 3:C:174:THR:HG21 | 25:C:303:CDL:H861 | 1.88 | 0.56 |
| 1:N:177:SER:H | 1:N:180:GLN:NE2 | 2.04 | 0.56 |
| 2:B:52:HIS:HE1 | 23:B:304:PSC:C21 | 2.18 | 0.56 |
| 6:F:54[B]:ASN:ND2 | 29:F:203:HOH:O | 2.39 | 0.56 |
| 20:N:608:TGL:H281 | 20:N:608:TGL:HB92 | 1.88 | 0.56 |
| 1:N:136[B]:LEU:CD1 | 29:N:976:HOH:O | 2.47 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:B:304:PSC:H032 | 29:E:275:HOH:O | 2.05 | 0.56 |
| 25:G:102:CDL:H182 | 25:G:102:CDL:H511 | 1.87 | 0.56 |
| 26:T:101:PEK:C2 | 26:T:101:PEK:H32 | 2.19 | 0.55 |
| 2:B:29[B]:MET:SD | 2:B:33:LEU:CD2 | 2.93 | 0.55 |
| 4:D:34:SER:H | 4:D:37:GLN:NE2 | 2.03 | 0.55 |
| 8:H:8:ILE:HG22 | 8:H:8:ILE:O | 2.06 | 0.55 |
| 1:A:311[B]:ILE:HG13 | 1:A:314:ILE:HD12 | 1.87 | 0.55 |
| 10:J:27:THR:HG22 | 29:J:205:HOH:O | 2.06 | 0.55 |
| 2:O:132:GLU:HB3 | 2:O:137:GLU:HG3 | 1.88 | 0.55 |
| 2:B:49:LYS:HD3 | 20:D:201:TGL:CC7 | 2.36 | 0.55 |
| 4:D:100[B]:LYS:CE | 29:D:401:HOH:O | 2.18 | 0.55 |
| 1:A:282:PHE:CA | 7:T:4:ALA:HB3 | 2.24 | 0.55 |
| 6:S:94:HIS:N | 29:S:204:HOH:O | 2.38 | 0.55 |
| 12:Y:20:ARG:NH1 | 12:Y:24[B]:MET:HE2 | 2.22 | 0.55 |
| 1:A:172:LYS:NZ | 1:A:178[A]:GLN:HE22 | 2.05 | 0.55 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:O | 2.59 | 0.55 |
| 23:B:304:PSC:H21 | 23:B:304:PSC:H011 | 1.88 | 0.55 |
| 3:P:246:ASP:HB2 | 29:P:522:HOH:O | 2.06 | 0.54 |
| 8:U:9:LYS:HA | 29:U:129:HOH:O | 2.07 | 0.54 |
| 7:T:5:LYS:HB2 | 26:T:102:PEK:H331 | 1.88 | 0.54 |
| 25:G:102:CDL:H632 | 29:G:258:HOH:O | 2.07 | 0.54 |
| 19:P:303:PGV:H182 | 25:P:304:CDL:H662 | 1.89 | 0.54 |
| 7:T:5:LYS:HG3 | 26:T:102:PEK:H371 | 1.88 | 0.54 |
| 2:B:83:ILE:O | 2:B:87[B]:MET:HB2 | 2.07 | 0.54 |
| 2:B:227:LEU:HD21 | 29:B:548:HOH:O | 2.06 | 0.54 |
| 23:O:303:PSC:H22 | 23:O:303:PSC:H201 | 1.89 | 0.54 |
| 19:N:607:PGV:H61 | 3:P:54[A]:MET:HG2 | 1.89 | 0.54 |
| 2:B:217:LYS:HD3 | 29:B:615:HOH:O | 2.08 | 0.54 |
| 19:C:302:PGV:H211 | 19:C:302:PGV:C22 | 2.17 | 0.54 |
| 1:A:28:MET:CE | 14:A:601:HEA:H271 | 2.35 | 0.54 |
| 2:O:58:ALA:O | 2:O:62:GLU:HG3 | 2.08 | 0.54 |
| 4:Q:17[A]:VAL:CG1 | 29:Q:419:HOH:O | 2.56 | 0.54 |
| 25:C:303:CDL:H672 | 25:C:303:CDL:H811 | 1.89 | 0.53 |
| 3:P:29:SER:HB2 | 28:P:306:DMU:H21 | 1.90 | 0.53 |
| 2:B:16[A]:ILE:HD12 | 2:B:87[A]:MET:HG2 | 1.89 | 0.53 |
| 2:B:52:HIS:CE1 | 23:B:304:PSC:C21 | 2.91 | 0.53 |
| 4:Q:19[B]:ARG:NH2 | 29:Q:302:HOH:O | 2.39 | 0.53 |
| 1:N:172:LYS:NZ | 1:N:178[A]:GLN:HE22 | 2.06 | 0.53 |
| 1:N:459:PHE:HE2 | 29:Q:311:HOH:O | 1.92 | 0.53 |
| 12:Y:20:ARG:CZ | 12:Y:24[B]:MET:HE2 | 2.38 | 0.53 |
| 26:T:101:PEK:H31 | 26:T:101:PEK:C1 | 2.36 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:334:TRP:CZ3 | 20:D:201:TGL:HA52 | 2.43 | 0.53 |
| 20:B:301:TGL:HC22 | 29:I:173:HOH:O | 2.08 | 0.53 |
| 6:F:41:GLY:HA3 | 6:F:87[B]:THR:CG2 | 2.38 | 0.53 |
| 25:P:304:CDL:OB9 | 25:P:304:CDL:HB4 | 2.09 | 0.53 |
| 2:B:183[A]:THR:HG23 | 29:B:622:HOH:O | 2.08 | 0.53 |
| 3:P:161[A]:GLN:HE22 | 26:P:308:PEK:H21 | 1.74 | 0.53 |
| 19:Q:201:PGV:C01 | 19:Q:201:PGV:C2 | 2.67 | 0.53 |
| 6:S:76:LYS:CE | 6:S:93:PRO:CG | 2.62 | 0.53 |
| 6:F:1:ALA:HA | 7:G:17:ARG:NH1 | 2.24 | 0.53 |
| 7:G:2:SER:OG | 26:G:103:PEK:C29 | 2.56 | 0.53 |
| 2:O:87[B]:MET:HE2 | 29:O:411:HOH:O | 2.09 | 0.53 |
| 1:A:514:LYS:HE2 | 29:F:223:HOH:O | 2.09 | 0.53 |
| 3:C:246:ASP:HB2 | 29:C:531:HOH:O | 2.09 | 0.53 |
| 3:C:171:VAL:HG22 | 25:C:303:CDL:H851 | 1.90 | 0.53 |
| 3:C:51[B]:MET:HE2 | 25:C:303:CDL:C39 | 2.34 | 0.53 |
| 25:G:102:CDL:H761 | 1:N:282:PHE:HZ | 1.74 | 0.53 |
| 19:Q:201:PGV:H162 | 19:Q:201:PGV:H321 | 1.91 | 0.53 |
| 1:A:25:TRP:CE3 | 20:L:101:TGL:HB92 | 2.44 | 0.53 |
| 23:O:303:PSC:H22 | 23:O:303:PSC:H231 | 1.91 | 0.53 |
| 19:P:303:PGV:H11 | 19:P:303:PGV:C15 | 2.40 | 0.52 |
| 2:B:41[B]:ILE:HD11 | 9:I:21:ILE:HD13 | 1.90 | 0.52 |
| 3:P:33[A]:MET:HB2 | 28:P:306:DMU:H9 | 1.91 | 0.52 |
| 4:Q:93:ALA:HB3 | 11:X:28[B]:VAL:HG12 | 1.91 | 0.52 |
| 7:T:2:SER:OG | 26:T:102:PEK:H291 | 2.09 | 0.52 |
| 9:I:67:GLY:HA3 | 11:K:54:ARG:HD3 | 1.91 | 0.52 |
| 25:G:102:CDL:H611 | 25:G:102:CDL:H652 | 1.92 | 0.52 |
| 28:P:306:DMU:H11 | 10:W:49:CYS:HB3 | 1.91 | 0.52 |
| 2:B:22[B]:HIS:CE1 | 9:I:44:LYS:HE2 | 2.41 | 0.52 |
| 25:C:303:CDL:OB6 | 25:C:303:CDL:HB22 | 2.10 | 0.52 |
| 20:B:301:TGL:HC21 | 29:B:589:HOH:O | 2.10 | 0.52 |
| 3:P:80[A]:ARG:HG2 | 3:P:233:PHE:CE2 | 2.45 | 0.52 |
| 12:Y:20:ARG:NH1 | 12:Y:24[B]:MET:CE | 2.73 | 0.52 |
| 25:G:102:CDL:C18 | 25:G:102:CDL:H511 | 2.40 | 0.52 |
| 6:F:1:ALA:CB | 6:S:65:ASP:OD1 | 2.50 | 0.52 |
| 8:U:9:LYS:HG3 | 8:U:11:TYR:H | 1.76 | 0.52 |
| 1:A:486[A]:ASP:OD1 | 4:D:19[A]:ARG:HD2 | 2.10 | 0.51 |
| 8:U:7:LYS:O | 8:U:8:ILE:HB | 2.10 | 0.51 |
| 19:Q:201:PGV:H301 | 19:Q:201:PGV:H142 | 1.92 | 0.51 |
| 1:A:281:GLY:O | 7:T:4:ALA:HB1 | 2.10 | 0.51 |
| 12:L:20:ARG:HH22 | 20:L:101:TGL:CC4 | 2.22 | 0.51 |
| 7:G:5:LYS:CB | 26:G:103:PEK:H351 | 2.31 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:9:LYS:HD3 | 8:H:11:TYR:H | 1.75 | 0.51 |
| 4:D:100[B]:LYS:HD2 | 4:D:100[B]:LYS:O | 2.10 | 0.51 |
| 5:R:14[B]:ARG:HG2 | 29:R:228:HOH:O | 2.11 | 0.51 |
| 12:Y:24[B]:MET:SD | 20:Y:101:TGL:CC3 | 2.99 | 0.51 |
| 20:Y:101:TGL:OA1 | 20:Y:101:TGL:H162 | 2.11 | 0.51 |
| 20:L:101:TGL:H292 | 20:L:101:TGL:H102 | 1.92 | 0.51 |
| 7:G:11:TPO:CG2 | 7:G:16:TRP:HE1 | 2.12 | 0.51 |
| 19:Q:201:PGV:H22 | 19:Q:201:PGV:C01 | 2.32 | 0.51 |
| 10:W:33:ARG:HG2 | 22:W:101:CHD:C18 | 2.39 | 0.51 |
| 1:A:28:MET:CE | 14:A:601:HEA:H273 | 2.38 | 0.51 |
| 2:O:113:TYR:HD1 | 8:U:58:ARG:HH22 | 1.59 | 0.51 |
| 1:N:112:LEU:HD23 | 1:N:112:LEU:C | 2.32 | 0.50 |
| 12:Y:26:THR:HG23 | 13:Z:25:SER:CB | 2.41 | 0.50 |
| 3:P:40:MET:O | 3:P:44[B]:MET:HG3 | 2.10 | 0.50 |
| 7:T:5:LYS:HB2 | 26:T:102:PEK:H351 | 1.94 | 0.50 |
| 1:A:514:LYS:HA | 6:F:38:ALA:CB | 2.39 | 0.50 |
| 7:G:5:LYS:HB3 | 1:N:278[B]:MET:HE3 | 1.93 | 0.50 |
| 29:O:571:HOH:O | 20:Q:202:TGL:HC61 | 2.12 | 0.50 |
| 4:Q:33:LEU:HD22 | 4:Q:37:GLN:HB3 | 1.94 | 0.50 |
| 12:Y:20:ARG:HH12 | 12:Y:24[B]:MET:CE | 2.23 | 0.50 |
| 2:O:113:TYR:HD1 | 8:U:58:ARG:NH2 | 2.10 | 0.50 |
| 2:O:196:CYS:HB2 | 2:O:207:MET:HG3 | 1.93 | 0.50 |
| 3:P:54[A]:MET:HB3 | 3:P:58:TRP:CZ3 | 2.46 | 0.50 |
| 4:Q:7:LYS:N | 4:Q:10:ASP:OD2 | 2.44 | 0.50 |
| 10:W:32:TYR:OH | 22:W:101:CHD:H213 | 2.11 | 0.50 |
| 12:Y:20:ARG:NH2 | 12:Y:24[A]:MET:HG3 | 2.27 | 0.50 |
| 23:O:303:PSC:C2 | 23:O:303:PSC:H201 | 2.42 | 0.50 |
| 1:A:28:MET:HE1 | 14:A:601:HEA:H271 | 1.94 | 0.50 |
| 1:N:296:GLY:HA2 | 8:U:23:GLN:OE1 | 2.11 | 0.50 |
| 6:S:54:ASN:HD22 | 6:S:54:ASN:C | 2.15 | 0.50 |
| 12:Y:24[B]:MET:HG2 | 20:Y:101:TGL:CA2 | 2.39 | 0.50 |
| 12:L:26:THR:HG23 | 13:M:25:SER:HB3 | 1.92 | 0.50 |
| 4:Q:34:SER:H | 4:Q:37:GLN:NE2 | 2.10 | 0.50 |
| 6:S:64:GLU:O | 6:S:65:ASP:HB2 | 2.11 | 0.50 |
| 19:P:303:PGV:H11 | 19:P:303:PGV:H151 | 1.94 | 0.49 |
| 7:G:37:LEU:HD21 | 25:G:102:CDL:C36 | 2.37 | 0.49 |
| 2:O:116:LEU:HD13 | 2:O:226:MET:HG2 | 1.94 | 0.49 |
| 4:Q:78:TRP:CA | 20:Q:202:TGL:HB21 | 2.43 | 0.49 |
| 20:N:608:TGL:C28 | 20:N:608:TGL:CB9 | 2.86 | 0.49 |
| 20:D:201:TGL:H342 | 9:I:16:ARG:HH21 | 1.76 | 0.49 |
| 1:A:28:MET:HE1 | 14:A:601:HEA:C27 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:11:TPO:HG22 | 7:G:16:TRP:NE1 | 2.12 | 0.49 |
| 20:L:101:TGL:H362 | 20:L:101:TGL:C31 | 2.39 | 0.49 |
| 25:P:304:CDL:H392 | 25:P:304:CDL:H271 | 1.95 | 0.49 |
| 6:S:85:CYS:SG | 6:S:87[A]:THR:CG2 | 2.82 | 0.49 |
| 1:A:107:PRO:HB3 | 3:C:25:LEU:HB2 | 1.95 | 0.49 |
| 11:X:42:PRO:O | 11:X:47:ARG:NH2 | 2.45 | 0.49 |
| 2:B:16[B]:ILE:HG13 | 2:B:17:MET:N | 2.27 | 0.49 |
| 1:N:178[B]:GLN:HA | 1:N:181:THR:HG23 | 1.95 | 0.49 |
| 22:P:307:CHD:H12 | 22:P:307:CHD:H212 | 1.95 | 0.48 |
| 2:B:41[A]:ILE:HD13 | 23:B:304:PSC:H342 | 1.94 | 0.48 |
| 8:H:8:ILE:O | 8:H:9:LYS:HE2 | 2.13 | 0.48 |
| 8:H:9:LYS:N | 8:H:9:LYS:HE2 | 2.28 | 0.48 |
| 12:L:47:LYS:NZ | 12:L:47:LYS:HB3 | 2.28 | 0.48 |
| 3:P:33[B]:MET:CE | 28:P:306:DMU:H6 | 2.43 | 0.48 |
| 3:P:59:ARG:HA | 25:P:304:CDL:H512 | 1.94 | 0.48 |
| 3:P:33[B]:MET:HA | 28:P:306:DMU:H9 | 1.96 | 0.48 |
| 12:Y:20:ARG:CZ | 12:Y:24[B]:MET:HE1 | 2.40 | 0.48 |
| 6:S:1:ALA:HA | 7:T:17:ARG:NH1 | 2.29 | 0.48 |
| 2:B:86:MET:HE1 | 29:B:403:HOH:O | 2.13 | 0.48 |
| 19:C:302:PGV:H212 | 19:C:302:PGV:C22 | 2.17 | 0.48 |
| 7:G:70[B]:PHE:HB2 | 26:G:101:PEK:H041 | 1.94 | 0.48 |
| 8:H:9:LYS:CE | 29:H:103:HOH:O | 2.60 | 0.48 |
| 2:B:196:CYS:HB2 | 2:B:207:MET:HG3 | 1.94 | 0.48 |
| 10:W:56:PRO:HG3 | 12:Y:47:LYS:HE2 | 1.96 | 0.48 |
| 4:D:78:TRP:HB3 | 20:D:201:TGL:CB2 | 2.44 | 0.48 |
| 2:O:29[A]:MET:HB2 | 9:V:35:TYR:CE2 | 2.49 | 0.48 |
| 20:D:201:TGL:CB3 | 20:D:201:TGL:OG2 | 2.61 | 0.48 |
| 25:G:102:CDL:C33 | 29:O:488:HOH:O | 2.50 | 0.48 |
| 1:A:486[B]:ASP:OD2 | 4:D:19[B]:ARG:HD3 | 2.12 | 0.48 |
| 8:H:45:ALA:O | 8:H:47:GLY:N | 2.47 | 0.48 |
| 6:F:64:GLU:O | 6:F:65:ASP:HB2 | 2.15 | 0.47 |
| 2:O:83:ILE:O | 2:O:87[A]:MET:HG3 | 2.13 | 0.47 |
| 6:S:94:HIS:HD2 | 6:S:95:GLN:N | 2.10 | 0.47 |
| 8:H:37:HIS:HE1 | 29:H:111:HOH:O | 1.96 | 0.47 |
| 3:P:33[A]:MET:CB | 28:P:306:DMU:H9 | 2.44 | 0.47 |
| 7:T:8:HIS:O | 7:T:9:GLY:C | 2.51 | 0.47 |
| 3:P:3:HIS:C | 29:P:401:HOH:O | 2.52 | 0.47 |
| 1:N:408:THR:HB | 19:Q:201:PGV:H51 | 1.96 | 0.47 |
| 4:Q:52:SER:HB2 | 29:Q:316:HOH:O | 2.12 | 0.47 |
| 22:C:305:CHD:H212 | 22:C:305:CHD:H12 | 1.95 | 0.47 |
| 20:Q:202:TGL:HA91 | 20:Q:202:TGL:H231 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:3:HIS:N | 29:C:406:HOH:O | 2.46 | 0.47 |
| 1:N:22:PHE:HA | 20:Y:101:TGL:HB61 | 1.95 | 0.47 |
| 5:R:79:LYS:HD2 | 5:R:79:LYS:HA | 1.71 | 0.47 |
| 2:B:1:FME:CN | 2:B:193:TYR:H | 2.27 | 0.47 |
| 2:B:41[B]:ILE:HD11 | 9:I:21:ILE:CD1 | 2.44 | 0.47 |
| 26:C:306:PEK:H382 | 25:G:102:CDL:H272 | 1.97 | 0.47 |
| 1:N:337:ALA:HB2 | 1:N:394[A]:VAL:HG23 | 1.96 | 0.47 |
| 3:P:62:ILE:HD12 | 25:P:304:CDL:H511 | 1.97 | 0.47 |
| 1:N:113[A]:LEU:HD12 | 20:Y:101:TGL:C13 | 2.44 | 0.47 |
| 1:N:513:LEU:O | 1:N:514:LYS:CG | 2.63 | 0.47 |
| 25:P:304:CDL:H411 | 25:P:304:CDL:H452 | 1.96 | 0.47 |
| 11:K:47:ARG:HG2 | 11:K:48:VAL:HG23 | 1.95 | 0.47 |
| 19:A:608:PGV:H231 | 13:M:12:PRO:HG3 | 1.97 | 0.47 |
| 7:G:5:LYS:HB3 | 1:N:278[B]:MET:CE | 2.44 | 0.47 |
| 2:O:60:GLU:CD | 2:O:60:GLU:N | 2.68 | 0.47 |
| 3:P:205:GLY:HA3 | 26:T:101:PEK:H181 | 1.95 | 0.47 |
| 25:P:304:CDL:H242 | 25:P:304:CDL:H652 | 1.96 | 0.47 |
| 20:Y:101:TGL:HC52 | 20:Y:101:TGL:HC22 | 1.45 | 0.47 |
| 3:C:47:LEU:O | 3:C:51[A]:MET:HG2 | 2.15 | 0.47 |
| 6:F:87[A]:THR:HG21 | 29:F:223:HOH:O | 2.14 | 0.47 |
| 25:G:102:CDL:H201 | 25:G:102:CDL:C52 | 2.42 | 0.47 |
| 10:J:40:LEU:HD12 | 22:J:102:CHD:O12 | 2.15 | 0.47 |
| 1:A:513:LEU:HD23 | 1:A:513:LEU:HA | 1.82 | 0.47 |
| 19:A:607:PGV:H343 | 26:G:101:PEK:C38 | 2.36 | 0.47 |
| 2:B:58:ALA:O | 2:B:62:GLU:HG3 | 2.15 | 0.47 |
| 1:A:240:HIS:C | 1:A:240:HIS:CD2 | 2.88 | 0.46 |
| 25:G:102:CDL:C44 | 1:N:311[B]:ILE:HG22 | 2.45 | 0.46 |
| 8:H:9:LYS:CA | 8:H:9:LYS:HE3 | 2.42 | 0.46 |
| 25:T:103:CDL:H561 | 25:T:103:CDL:H592 | 1.52 | 0.46 |
| 1:A:308:ALA:O | 1:A:311[B]:ILE:HG22 | 2.16 | 0.46 |
| 2:B:104:TRP:CG | 2:B:203:ASN:HB2 | 2.50 | 0.46 |
| 2:B:42:ILE:HG21 | 20:D:201:TGL:H232 | 1.97 | 0.46 |
| 3:P:224:LYS:CE | 25:P:304:CDL:HB32 | 2.45 | 0.46 |
| 23:B:304:PSC:H221 | 23:B:304:PSC:H251 | 1.36 | 0.46 |
| 4:D:78:TRP:CB | 20:D:201:TGL:HB21 | 2.45 | 0.46 |
| 1:N:112:LEU:HG | 29:N:921:HOH:O | 2.15 | 0.46 |
| 6:S:2:SER:HB2 | 29:S:309:HOH:O | 2.16 | 0.46 |
| 25:T:103:CDL:H142 | 25:T:103:CDL:H362 | 1.98 | 0.46 |
| 1:A:282:PHE:CA | 7:T:4:ALA:CB | 2.85 | 0.46 |
| 9:I:73:LYS:HD3 | 9:I:73:LYS:HA | 1.54 | 0.46 |
| 11:K:39:GLU:HB3 | 29:K:112:HOH:O | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:P:156:ARG:HE | 22:P:305:CHD:C24 | 2.28 | 0.46 |
| 7:G:84:LYS:NZ | 29:G:203:HOH:O | 2.49 | 0.46 |
| 1:N:229:ILE:HD11 | 2:O:175:ILE:HD13 | 1.98 | 0.46 |
| 1:N:148:PHE:HB3 | 3:P:28:THR:HB | 1.98 | 0.46 |
| 3:P:3:HIS:HD2 | 29:P:534:HOH:O | 1.97 | 0.46 |
| 7:G:3:ALA:O | 7:G:4:ALA:CB | 2.64 | 0.46 |
| 8:H:7:LYS:HG3 | 8:H:8:ILE:HD12 | 1.97 | 0.46 |
| 1:A:136[B]:LEU:CD1 | 29:A:988:HOH:O | 2.33 | 0.46 |
| 10:J:36:MET:HB3 | 22:J:102:CHD:H183 | 1.97 | 0.46 |
| 1:N:34:SER:HB2 | 14:N:601:HEA:C2B | 2.46 | 0.46 |
| 2:O:116:LEU:HD13 | 2:O:226:MET:CG | 2.46 | 0.46 |
| 19:A:608:PGV:P | 19:A:608:PGV:H061 | 2.55 | 0.46 |
| 3:C:133:ASN:ND2 | 29:C:402:HOH:O | 2.39 | 0.46 |
| 3:P:103:HIS:HA | 19:P:301:PGV:H012 | 1.98 | 0.46 |
| 19:P:303:PGV:C18 | 25:P:304:CDL:H662 | 2.46 | 0.46 |
| 12:Y:12:PRO:HB2 | 20:Y:101:TGL:HG2 | 1.97 | 0.46 |
| 3:C:160:LEU:HD13 | 22:C:304:CHD:H181 | 1.96 | 0.45 |
| 3:P:208:VAL:HG22 | 3:P:245:VAL:CG1 | 2.46 | 0.45 |
| 1:A:337:ALA:HB2 | 1:A:394[A]:VAL:HG23 | 1.98 | 0.45 |
| 29:A:703:HOH:O | 6:F:37:LYS:HE2 | 2.17 | 0.45 |
| 7:G:33:LEU:O | 7:G:37:LEU:HB2 | 2.15 | 0.45 |
| 3:P:33[B]:MET:HG2 | 3:P:39:SER:O | 2.14 | 0.45 |
| 7:T:3:ALA:O | 7:T:4:ALA:CB | 2.63 | 0.45 |
| 9:V:61:GLU:OE1 | 9:V:64:ARG:NE | 2.46 | 0.45 |
| 10:J:49:CYS:HB3 | 28:J:101:DMU:C19 | 2.40 | 0.45 |
| 1:A:290:HIS:CD2 | 1:A:291:HIS:CD2 | 3.04 | 0.45 |
| 1:A:297[A]:MET:HG2 | 29:A:933:HOH:O | 2.15 | 0.45 |
| 3:C:41:THR:HA | 3:C:44[B]:MET:HE2 | 1.98 | 0.45 |
| 7:T:31:CYS:SG | 25:T:103:CDL:H551 | 2.56 | 0.45 |
| 1:N:240:HIS:CD2 | 1:N:240:HIS:C | 2.90 | 0.45 |
| 25:C:303:CDL:OB6 | 25:C:303:CDL:CB2 | 2.65 | 0.45 |
| 4:D:78:TRP:HB3 | 20:D:201:TGL:HB21 | 1.98 | 0.45 |
| 1:N:136[B]:LEU:HD11 | 29:T:280:HOH:O | 2.16 | 0.45 |
| 3:P:116:TRP:HA | 3:P:117:PRO:C | 2.37 | 0.45 |
| 8:H:31:GLN:NE2 | 29:H:101:HOH:O | 2.37 | 0.45 |
| 20:L:101:TGL:H222 | 20:L:101:TGL:HA91 | 1.63 | 0.45 |
| 26:C:306:PEK:H331 | 26:C:306:PEK:H362 | 1.72 | 0.45 |
| 6:F:87[B]:THR:HG21 | 29:F:304:HOH:O | 2.16 | 0.45 |
| 8:H:9:LYS:HD3 | 8:H:11:TYR:HB2 | 1.98 | 0.45 |
| 2:O:32[B]:PHE:CD2 | 9:V:31:PHE:CZ | 3.05 | 0.45 |
| 2:B:22[B]:HIS:CE1 | 29:B:461:HOH:O | 2.69 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:C:304:CHD:H231 | 22:C:304:CHD:H162 | 1.98 | 0.45 |
| 2:B:116:LEU:HD11 | 2:B:226:MET:HB3 | 1.99 | 0.45 |
| 12:L:20:ARG:NH2 | 20:L:101:TGL:HC52 | 2.27 | 0.45 |
| 3:P:33[A]:MET:CB | 28:P:306:DMU:C19 | 2.94 | 0.45 |
| 5:R:108:LYS:NZ | 29:R:203:HOH:O | 2.48 | 0.44 |
| 1:A:178[B]:GLN:HG2 | 1:A:179:TYR:CE2 | 2.52 | 0.44 |
| 2:O:92:ASN:HA | 2:O:93:PRO:HD2 | 1.72 | 0.44 |
| 25:T:103:CDL:H612 | 25:T:103:CDL:H672 | 1.99 | 0.44 |
| 9:V:36:LYS:NZ | 9:V:36:LYS:HB2 | 2.32 | 0.44 |
| 2:B:78:LEU:CD1 | 2:B:78:LEU:N | 2.81 | 0.44 |
| 8:H:37:HIS:HD2 | 8:H:40:GLU:OE2 | 2.00 | 0.44 |
| 3:P:47:LEU:O | 3:P:51[A]:MET:HG2 | 2.18 | 0.44 |
| 26:T:101:PEK:H203 | 26:T:101:PEK:H171 | 1.71 | 0.44 |
| 7:G:2:SER:OG | 26:G:103:PEK:H292 | 2.17 | 0.44 |
| 10:J:7:GLU:HG3 | 29:J:238:HOH:O | 2.16 | 0.44 |
| 20:L:101:TGL:H312 | 20:L:101:TGL:C36 | 2.43 | 0.44 |
| 1:N:336:PRO:HB2 | 1:N:394[B]:VAL:HG11 | 2.00 | 0.44 |
| 1:N:483:LEU:HD21 | 13:Z:4:LYS:HE3 | 1.99 | 0.44 |
| 10:J:52:TRP:O | 10:J:57:HIS:HE1 | 2.00 | 0.44 |
| 1:N:178[B]:GLN:HG3 | 1:N:178[B]:GLN:O | 2.18 | 0.44 |
| 3:P:80[A]:ARG:HH11 | 3:P:80[A]:ARG:HD3 | 1.49 | 0.44 |
| 6:S:21[B]:MET:HE2 | 6:S:21[B]:MET:HB2 | 1.64 | 0.44 |
| 25:T:103:CDL:H382 | 25:T:103:CDL:H161 | 1.98 | 0.44 |
| 7:T:37:LEU:HD12 | 7:T:37:LEU:HA | 1.89 | 0.44 |
| 23:O:303:PSC:H242 | 23:O:303:PSC:H272 | 1.66 | 0.44 |
| 25:P:304:CDL:H132 | 25:P:304:CDL:OA6 | 2.17 | 0.44 |
| 7:T:38:HIS:CE1 | 25:T:103:CDL:H122 | 2.52 | 0.44 |
| 12:Y:26:THR:HG23 | 13:Z:25:SER:HB3 | 1.99 | 0.44 |
| 1:A:28:MET:HE2 | 14:A:601:HEA:C27 | 2.41 | 0.44 |
| 7:G:38:HIS:CD2 | 29:G:209:HOH:O | 2.71 | 0.44 |
| 7:G:84:LYS:N | 7:G:84:LYS:CD | 2.69 | 0.44 |
| 26:P:308:PEK:C04 | 6:S:1:ALA:N | 2.78 | 0.44 |
| 7:T:11:TPO:O | 7:T:11:TPO:HG22 | 2.18 | 0.44 |
| 2:B:164:ALA:O | 2:B:194:GLY:HA3 | 2.18 | 0.44 |
| 20:B:301:TGL:H252 | 20:B:301:TGL:H221 | 1.76 | 0.44 |
| 29:A:703:HOH:O | 6:F:37:LYS:HG3 | 2.17 | 0.44 |
| 25:P:304:CDL:H261 | 25:P:304:CDL:H672 | 1.99 | 0.44 |
| 3:P:41:THR:HA | 3:P:44[B]:MET:HE2 | 2.00 | 0.44 |
| 5:R:6:GLU:HA | 29:R:308:HOH:O | 2.17 | 0.44 |
| 11:K:6:ALA:N | 29:K:103:HOH:O | 2.51 | 0.44 |
| 26:P:308:PEK:H042 | 6:S:1:ALA:H2 | 1.80 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:Q:6:VAL:HG13 | 29:Q:446:HOH:O | 2.18 | 0.44 |
| 1:A:302[B]:ARG:NH1 | 29:A:705:HOH:O | 2.51 | 0.43 |
| 2:B:32[B]:PHE:CE2 | 9:I:31:PHE:CZ | 3.06 | 0.43 |
| 20:Y:101:TGL:H283 | 20:Y:101:TGL:H252 | 1.53 | 0.43 |
| 25:C:303:CDL:H671 | 25:C:303:CDL:H641 | 1.87 | 0.43 |
| 8:H:9:LYS:NZ | 29:H:103:HOH:O | 2.45 | 0.43 |
| 7:G:5:LYS:HA | 1:N:278[B]:MET:HE3 | 2.00 | 0.43 |
| 3:C:55:TYR:CD1 | 25:C:303:CDL:H532 | 2.54 | 0.43 |
| 19:C:302:PGV:H172 | 25:C:303:CDL:C65 | 2.48 | 0.43 |
| 12:L:26:THR:HG23 | 13:M:25:SER:CB | 2.47 | 0.43 |
| 1:N:514:LYS:HG2 | 6:S:38:ALA:CB | 2.48 | 0.43 |
| 14:N:601:HEA:HHC | 14:N:601:HEA:H122 | 2.01 | 0.43 |
| 2:O:215:PRO:HD3 | 9:V:60:PHE:CD2 | 2.53 | 0.43 |
| 7:T:8:HIS:CD2 | 7:T:8:HIS:O | 2.71 | 0.43 |
| 1:A:334:TRP:HB2 | 20:D:201:TGL:HG11 | 2.00 | 0.43 |
| 2:B:41[B]:ILE:HA | 2:B:41[B]:ILE:HD13 | 1.72 | 0.43 |
| 7:G:83:GLU:OE2 | 29:G:201:HOH:O | 2.21 | 0.43 |
| 8:H:8:ILE:C | 8:H:9:LYS:HE2 | 2.38 | 0.43 |
| 10:J:32:TYR:CE2 | 22:J:102:CHD:H213 | 2.54 | 0.43 |
| 1:N:426:PHE:HZ | 20:N:608:TGL:HA42 | 1.83 | 0.43 |
| 2:O:151:ARG:HD3 | 2:O:181:GLN:HE21 | 1.84 | 0.43 |
| 26:P:308:PEK:C1 | 29:P:441:HOH:O | 2.67 | 0.43 |
| 6:S:87[A]:THR:HG21 | 29:S:266:HOH:O | 2.19 | 0.43 |
| 7:T:5:LYS:CG | 26:T:102:PEK:H351 | 2.46 | 0.43 |
| 1:A:62:ALA:HB2 | 14:A:601:HEA:HBD1 | 2.00 | 0.43 |
| 7:G:10:GLY:HA3 | 29:G:272:HOH:O | 2.19 | 0.43 |
| 1:N:377:PHE:HA | 1:N:380:VAL:HG22 | 2.00 | 0.43 |
| 1:N:514:LYS:NZ | 29:N:704:HOH:O | 2.50 | 0.43 |
| 23:O:303:PSC:H322 | 23:O:303:PSC:H281 | 1.99 | 0.43 |
| 3:P:63:ARG:NE | 25:P:304:CDL:HA22 | 2.29 | 0.43 |
| 29:C:401:HOH:O | 6:F:52:ILE:HD11 | 2.18 | 0.43 |
| 25:G:102:CDL:H441 | 1:N:311[B]:ILE:HG22 | 2.01 | 0.43 |
| 4:Q:17[B]:VAL:HG22 | 4:Q:19[B]:ARG:HG3 | 2.00 | 0.43 |
| 1:A:112:LEU:HD23 | 1:A:112:LEU:C | 2.38 | 0.43 |
| 9:I:36:LYS:HZ2 | 9:I:36:LYS:HB2 | 1.84 | 0.43 |
| 25:G:102:CDL:H401 | 2:O:77:ALA:CB | 2.48 | 0.43 |
| 10:W:27:THR:HG22 | 29:W:208:HOH:O | 2.18 | 0.43 |
| 29:A:763:HOH:O | 12:L:7:PRO:HG3 | 2.19 | 0.43 |
| 1:N:24:ALA:HB2 | 14:N:601:HEA:H253 | 2.01 | 0.43 |
| 23:O:303:PSC:H292 | 23:O:303:PSC:H262 | 1.04 | 0.43 |
| 20:Q:202:TGL:CA9 | 20:Q:202:TGL:C23 | 2.95 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:T:103:CDL:H631 | 25:T:103:CDL:H661 | 1.77 | 0.43 |
| 2:B:41[A]:ILE:O | 2:B:42:ILE:C | 2.56 | 0.42 |
| 7:G:5:LYS:HD3 | 1:N:278[B]:MET:HE3 | 2.00 | 0.42 |
| 23:O:303:PSC:H291 | 23:O:303:PSC:H261 | 0.86 | 0.42 |
| 1:A:431:LEU:HD21 | 1:A:450:TRP:HB2 | 2.01 | 0.42 |
| 1:A:76:GLY:O | 1:A:80:ASN:HB2 | 2.20 | 0.42 |
| 26:C:306:PEK:C38 | 25:G:102:CDL:H271 | 2.30 | 0.42 |
| 7:G:3:ALA:O | 7:G:4:ALA:HB2 | 2.19 | 0.42 |
| 6:S:51:SER:O | 6:S:93:PRO:HA | 2.19 | 0.42 |
| 22:W:101:CHD:H111 | 22:W:101:CHD:H12A | 1.90 | 0.42 |
| 12:L:25:MET:HG2 | 20:L:101:TGL:HA62 | 2.01 | 0.42 |
| 19:Q:201:PGV:H22 | 19:Q:201:PGV:H202 | 2.01 | 0.42 |
| 25:T:103:CDL:H541 | 25:T:103:CDL:C24 | 2.34 | 0.42 |
| 3:C:37:PHE:CG | 28:J:101:DMU:H6 | 2.54 | 0.42 |
| 2:B:16[A]:ILE:HD11 | 2:B:86:MET:HG2 | 2.00 | 0.42 |
| 3:C:33[A]:MET:HB2 | 28:J:101:DMU:C22 | 2.49 | 0.42 |
| 1:N:302[B]:ARG:HG2 | 1:N:302[B]:ARG:NH1 | 2.35 | 0.42 |
| 2:O:116:LEU:CD1 | 2:O:226:MET:HG2 | 2.50 | 0.42 |
| 2:B:151:ARG:HD3 | 2:B:181:GLN:HE21 | 1.85 | 0.42 |
| 9:I:73:LYS:HD3 | 29:I:125:HOH:O | 2.18 | 0.42 |
| 1:N:87:ILE:O | 1:N:173:PRO:HD3 | 2.20 | 0.42 |
| 25:T:103:CDL:HA21 | 25:T:103:CDL:H111 | 2.02 | 0.42 |
| 1:A:169:ILE:HA | 1:A:169:ILE:HD13 | 1.87 | 0.42 |
| 19:A:608:PGV:O06 | 29:A:702:HOH:O | 2.18 | 0.42 |
| 19:C:307:PGV:H72 | 19:C:307:PGV:H42 | 1.77 | 0.42 |
| 3:P:177:GLN:HA | 3:P:177:GLN:OE1 | 2.20 | 0.42 |
| 10:W:32:TYR:CE2 | 22:W:101:CHD:H213 | 2.55 | 0.42 |
| 1:A:172:LYS:HD2 | 1:A:181:THR:HG22 | 2.01 | 0.41 |
| 3:C:144[B]:ILE:HA | 3:C:144[B]:ILE:HD12 | 1.93 | 0.41 |
| 1:N:62:ALA:HB2 | 14:N:601:HEA:HBD1 | 2.01 | 0.41 |
| 20:Q:202:TGL:HG31 | 20:Q:202:TGL:HC21 | 1.55 | 0.41 |
| 3:C:217:VAL:HG22 | 25:C:303:CDL:H732 | 2.02 | 0.41 |
| 20:D:201:TGL:HB92 | 20:D:201:TGL:H132 | 2.02 | 0.41 |
| 7:G:5:LYS:CB | 1:N:278[B]:MET:HE3 | 2.50 | 0.41 |
| 1:A:336:PRO:HB2 | 1:A:394[B]:VAL:HG11 | 2.02 | 0.41 |
| 1:A:489:THR:HA | 6:F:71:TRP:O | 2.20 | 0.41 |
| 2:O:16:ILE:HD12 | 2:O:87[A]:MET:HG2 | 2.03 | 0.41 |
| 3:P:33[B]:MET:HE3 | 28:P:306:DMU:H6 | 2.02 | 0.41 |
| 2:O:130:PRO:HA | 4:Q:115:TRP:CZ3 | 2.55 | 0.41 |
| 2:B:56:MET:HA | 23:B:304:PSC:C20 | 2.37 | 0.41 |
| 9:I:68:ILE:HD13 | 9:I:68:ILE:HG21 | 1.71 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:G:102:CDL:H371 | 2:O:78:LEU:CD1 | 2.51 | 0.41 |
| 3:C:116:TRP:HA | 3:C:117:PRO:C | 2.40 | 0.41 |
| 25:G:102:CDL:H201 | 25:G:102:CDL:H511 | 2.03 | 0.41 |
| 1:N:439:ARG:HD3 | 2:O:199:ILE:HB | 2.03 | 0.41 |
| 25:T:103:CDL:H581 | 25:T:103:CDL:H782 | 2.03 | 0.41 |
| 3:C:65:SER:HB3 | 3:C:71:HIS:CE1 | 2.56 | 0.41 |
| 6:F:55:LYS:HA | 6:F:74:LEU:O | 2.20 | 0.41 |
| 1:N:333:LYS:CD | 29:N:988:HOH:O | 2.68 | 0.41 |
| 25:G:102:CDL:H541 | 25:G:102:CDL:C23 | 2.47 | 0.41 |
| 8:H:8:ILE:CG2 | 8:H:8:ILE:O | 2.69 | 0.41 |
| 13:M:32:TRP:CZ3 | 13:M:40:TYR:OH | 2.74 | 0.41 |
| 1:N:107:PRO:HB3 | 3:P:25:LEU:HB2 | 2.01 | 0.41 |
| 1:N:361:SER:OG | 2:O:84:LEU:HD13 | 2.20 | 0.41 |
| 7:T:38:HIS:ND1 | 7:T:38:HIS:N | 2.69 | 0.41 |
| 2:B:1:FME:HCN | 2:B:193:TYR:HB2 | 2.02 | 0.41 |
| 1:A:268:PHE:CZ | 2:B:58:ALA:HA | 2.55 | 0.41 |
| 3:C:131:LEU:CD2 | 25:G:102:CDL:HB61 | 2.51 | 0.41 |
| 22:J:102:CHD:H193 | 22:J:102:CHD:H111 | 1.60 | 0.41 |
| 2:O:164:ALA:O | 2:O:194:GLY:HA3 | 2.21 | 0.41 |
| 22:P:305:CHD:H222 | 22:P:305:CHD:H162 | 1.50 | 0.41 |
| 11:X:24:PHE:O | 11:X:28[A]:VAL:HG12 | 2.21 | 0.41 |
| 11:X:8:ASP:HB2 | 29:X:111:HOH:O | 2.20 | 0.41 |
| 4:Q:107:ILE:HB | 4:Q:108:PRO:CD | 2.51 | 0.41 |
| 7:T:41:HIS:HB3 | 7:T:74:ARG:NH1 | 2.36 | 0.41 |
| 8:U:37:HIS:HD2 | 8:U:40:GLU:OE2 | 2.04 | 0.41 |
| 29:H:145:HOH:O | 8:U:46:LYS:HD3 | 2.19 | 0.41 |
| 8:H:46:LYS:HD2 | 29:U:155:HOH:O | 2.20 | 0.41 |
| 6:F:54[A]:ASN:N | 6:F:54[A]:ASN:ND2 | 2.65 | 0.41 |
| 25:G:102:CDL:C24 | 25:G:102:CDL:C54 | 2.80 | 0.41 |
| 2:O:13:THR:HG21 | 2:O:192:TYR:CZ | 2.55 | 0.41 |
| 2:O:84:LEU:HA | 2:O:87[A]:MET:HE2 | 2.03 | 0.41 |
| 3:P:50:ASN:HD22 | 3:P:51[A]:MET:CE | 2.33 | 0.41 |
| 4:Q:109:HIS:HD2 | 29:Q:401:HOH:O | 2.03 | 0.41 |
| 9:V:2:THR:HG22 | 29:V:137:HOH:O | 2.19 | 0.41 |
| 2:B:48:THR:HB | 9:I:16:ARG:CZ | 2.51 | 0.40 |
| 20:L:101:TGL:HB62 | 20:L:101:TGL:HB31 | 1.80 | 0.40 |
| 3:P:202:GLY:HA3 | 26:T:101:PEK:H21 | 2.03 | 0.40 |
| 1:A:172:LYS:HZ2 | 1:A:178[A]:GLN:HE22 | 1.69 | 0.40 |
| 1:A:439:ARG:HD3 | 2:B:199:ILE:HB | 2.03 | 0.40 |
| 8:H:46:LYS:HG2 | 29:H:171:HOH:O | 2.20 | 0.40 |
| 3:P:48:THR:HG23 | 25:P:304:CDL:H401 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:S:94:HIS:CG | 6:S:95:GLN:N | 2.84 | 0.40 |
| 1:A:208[B]:MET:HB3 | 1:A:219:PHE:CD1 | 2.57 | 0.40 |
| 1:A:293:PHE:CE1 | 1:A:361[B]:SER:HB2 | 2.57 | 0.40 |
| 1:A:361[A]:SER:OG | 2:B:84:LEU:HD13 | 2.21 | 0.40 |
| 2:O:13:THR:HB | 2:O:168:LEU:HD23 | 2.03 | 0.40 |
| 4:Q:78:TRP:CB | 20:Q:202:TGL:HB22 | 2.50 | 0.40 |
| 1:A:296:GLY:HA2 | 8:H:23:GLN:OE1 | 2.22 | 0.40 |
| 25:P:304:CDL:H631 | 25:P:304:CDL:H222 | 2.02 | 0.40 |
| 7:T:5:LYS:CB | 26:T:102:PEK:H351 | 2.51 | 0.40 |
| 2:B:59:GLN:HG2 | 29:B:468:HOH:O | 2.20 | 0.40 |
| 25:C:303:CDL:H201 | 25:C:303:CDL:H621 | 2.03 | 0.40 |
| 3:C:38:ASN:HA | 29:C:450:HOH:O | 2.21 | 0.40 |
| 26:C:306:PEK:H041 | 7:G:17:ARG:HH22 | 1.87 | 0.40 |
| 26:P:308:PEK:C04 | 6:S:1:ALA:H2 | 2.33 | 0.40 |
| 1:A:278[B]:MET:HE1 | 7:T:5:LYS:HB3 | 2.02 | 0.40 |
| 22:W:101:CHD:H212 | 22:W:101:CHD:H162 | 1.82 | 0.40 |
| 10:W:29:ASN:H | 10:W:29:ASN:HD22 | 1.69 | 0.40 |

All (2) 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) |
|---|---|---|---|
| 9:I:2:THR:CB | 5:R:80:GLU:OE1[3_647] | 2.00 | 0.20 |
| 9:I:2:THR:CG2 | 5:R:80:GLU:OE1[3_647] | 2.19 | 0.01 |

## 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 | A | 530/514 (103%) | 515 (97%) | 15 (3%) | 0 | 100 | 100 |
| 1 | N | 528/514 (103%) | 511 (97%) | 17 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 2 | B | 234/227 (103%) | 230 (98%) | 4 (2%) | 0 | 100 100 |
| 2 | O | 230/227 (101%) | 225 (98%) | 4 (2%) | 1 (0%) | 34 13 |
| 3 | C | 266/261 (102%) | 261 (98%) | 4 (2%) | 1 (0%) | 34 13 |
| 3 | P | 266/261 (102%) | 261 (98%) | 5 (2%) | 0 | 100 100 |
| 4 | D | 147/147 (100%) | 143 (97%) | 4 (3%) | 0 | 100 100 |
| 4 | Q | 145/147 (99%) | 139 (96%) | 5 (3%) | 1 (1%) | 22 6 |
| 5 | E | 103/109 (94%) | 102 (99%) | 1 (1%) | 0 | 100 100 |
| 5 | R | 104/109 (95%) | 104 (100%) | 0 | 0 | 100 100 |
| 6 | F | 100/98 (102%) | 95 (95%) | 3 (3%) | 2 (2%) | 7 1 |
| 6 | S | 98/98 (100%) | 92 (94%) | 2 (2%) | 4 (4%) | 3 0 |
| 7 | G | 82/85 (96%) | 68 (83%) | 8 (10%) | 6 (7%) | 1 0 |
| 7 | T | 82/85 (96%) | 71 (87%) | 5 (6%) | 6 (7%) | 1 0 |
| 8 | H | 77/85 (91%) | 68 (88%) | 6 (8%) | 3 (4%) | 3 0 |
| 8 | U | 77/85 (91%) | 68 (88%) | 5 (6%) | 4 (5%) | 2 0 |
| 9 | I | 71/73 (97%) | 71 (100%) | 0 | 0 | 100 100 |
| 9 | V | 71/73 (97%) | 69 (97%) | 1 (1%) | 1 (1%) | 11 1 |
| 10 | J | 56/59 (95%) | 56 (100%) | 0 | 0 | 100 100 |
| 10 | W | 57/59 (97%) | 57 (100%) | 0 | 0 | 100 100 |
| 11 | K | 47/56 (84%) | 45 (96%) | 2 (4%) | 0 | 100 100 |
| 11 | X | 48/56 (86%) | 46 (96%) | 2 (4%) | 0 | 100 100 |
| 12 | L | 44/47 (94%) | 42 (96%) | 2 (4%) | 0 | 100 100 |
| 12 | Y | 45/47 (96%) | 43 (96%) | 2 (4%) | 0 | 100 100 |
| 13 | M | 41/46 (89%) | 39 (95%) | 2 (5%) | 0 | 100 100 |
| 13 | Z | 41/46 (89%) | 39 (95%) | 1 (2%) | 1 (2%) | 6 0 |
| All | All | 3590/3614 (99%) | 3460 (96%) | 100 (3%) | 30 (1%) | 17 5 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | F | 94 | HIS |
| 6 | F | 96 | LEU |
| 7 | G | 4 | ALA |
| 7 | G | 5 | LYS |
| 7 | G | 8 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | H | 8 | ILE |
| 8 | H | 45 | ALA |
| 4 | Q | 8 | SER |
| 6 | S | 94 | HIS |
| 6 | S | 95 | GLN |
| 7 | T | 3 | ALA |
| 7 | T | 4 | ALA |
| 7 | T | 5 | LYS |
| 7 | T | 7 | ASP |
| 7 | T | 8 | HIS |
| 8 | U | 8 | ILE |
| 8 | U | 45 | ALA |
| 8 | U | 46 | LYS |
| 8 | H | 46 | LYS |
| 6 | S | 96 | LEU |
| 9 | V | 2 | THR |
| 13 | Z | 42 | LYS |
| 7 | G | 37 | LEU |
| 7 | G | 7 | ASP |
| 8 | U | 51 | SER |
| 3 | C | 232 | HIS |
| 2 | O | 92 | ASN |
| 7 | T | 6 | GLY |
| 6 | S | 93 | PRO |
| 7 | G | 9 | GLY |

### 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 | A | 444/426 (104%) | 438 (99%) | 6 (1%) | 67 42 |
| 1 | N | 442/426 (104%) | 432 (98%) | 10 (2%) | 50 20 |
| 2 | B | 219/210 (104%) | 208 (95%) | 11 (5%) | 24 4 |
| 2 | O | 215/210 (102%) | 206 (96%) | 9 (4%) | 30 6 |
| 3 | C | 233/226 (103%) | 230 (99%) | 3 (1%) | 69 44 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 3 | P | 233/226 (103%) | 230 (99%) | 3 (1%) | 69 44 |
| 4 | D | 133/129 (103%) | 128 (96%) | 5 (4%) | 33 7 |
| 4 | Q | 131/129 (102%) | 124 (95%) | 7 (5%) | 22 3 |
| 5 | E | 92/95 (97%) | 90 (98%) | 2 (2%) | 52 22 |
| 5 | R | 93/95 (98%) | 91 (98%) | 2 (2%) | 52 22 |
| 6 | F | 85/81 (105%) | 79 (93%) | 6 (7%) | 14 1 |
| 6 | S | 83/81 (102%) | 75 (90%) | 8 (10%) | 8 0 |
| 7 | G | 68/68 (100%) | 63 (93%) | 5 (7%) | 13 1 |
| 7 | T | 68/68 (100%) | 61 (90%) | 7 (10%) | 7 0 |
| 8 | H | 71/75 (95%) | 65 (92%) | 6 (8%) | 10 1 |
| 8 | U | 71/75 (95%) | 67 (94%) | 4 (6%) | 21 3 |
| 9 | I | 57/57 (100%) | 55 (96%) | 2 (4%) | 36 9 |
| 9 | V | 57/57 (100%) | 52 (91%) | 5 (9%) | 10 0 |
| 10 | J | 49/50 (98%) | 49 (100%) | 0 | 100 100 |
| 10 | W | 50/50 (100%) | 48 (96%) | 2 (4%) | 31 6 |
| 11 | K | 39/46 (85%) | 38 (97%) | 1 (3%) | 46 16 |
| 11 | X | 40/46 (87%) | 40 (100%) | 0 | 100 100 |
| 12 | L | 39/40 (98%) | 38 (97%) | 1 (3%) | 46 16 |
| 12 | Y | 40/40 (100%) | 38 (95%) | 2 (5%) | 24 4 |
| 13 | M | 37/38 (97%) | 33 (89%) | 4 (11%) | 6 0 |
| 13 | Z | 37/38 (97%) | 33 (89%) | 4 (11%) | 6 0 |
| All | All | 3126/3082 (101%) | 3011 (96%) | 115 (4%) | 35 8 |

All (115) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 7 | LEU |
| 1 | A | 38 | ARG |
| 1 | A | 109 | PHE |
| 1 | A | 138 | HIS |
| 1 | A | 180 | GLN |
| 1 | A | 369 | ASP |
| 2 | B | 32[A] | PHE |
| 2 | B | 32[B] | PHE |
| 2 | B | 33 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 59 | GLN |
| 2 | B | 60 | GLU |
| 2 | B | 65 | TRP |
| 2 | B | 75 | LEU |
| 2 | B | 86 | MET |
| 2 | B | 91 | ASN |
| 2 | B | 115 | ASP |
| 2 | B | 171 | LYS |
| 3 | C | 159 | MET |
| 3 | C | 214 | PHE |
| 3 | C | 230 | ASN |
| 4 | D | 4 | SER |
| 4 | D | 19[A] | ARG |
| 4 | D | 19[B] | ARG |
| 4 | D | 31[A] | LYS |
| 4 | D | 31[B] | LYS |
| 5 | E | 5 | HIS |
| 5 | E | 70 | VAL |
| 6 | F | 37 | LYS |
| 6 | F | 54[A] | ASN |
| 6 | F | 54[B] | ASN |
| 6 | F | 80 | GLN |
| 6 | F | 94 | HIS |
| 6 | F | 98 | HIS |
| 7 | G | 2 | SER |
| 7 | G | 18 | PHE |
| 7 | G | 43 | GLU |
| 7 | G | 54 | ARG |
| 7 | G | 84 | LYS |
| 8 | H | 7 | LYS |
| 8 | H | 9 | LYS |
| 8 | H | 29 | CYS |
| 8 | H | 51 | SER |
| 8 | H | 60 | TYR |
| 8 | H | 61 | LYS |
| 9 | I | 36 | LYS |
| 9 | I | 37 | PHE |
| 11 | K | 47 | ARG |
| 12 | L | 47 | LYS |
| 13 | M | 38 | ASP |
| 13 | M | 39 | ASN |
| 13 | M | 42 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | M | 43 | SER |
| 1 | N | 109 | PHE |
| 1 | N | 138 | HIS |
| 1 | N | 174 | PRO |
| 1 | N | 178[A] | GLN |
| 1 | N | 178[B] | GLN |
| 1 | N | 180 | GLN |
| 1 | N | 363 | LEU |
| 1 | N | 369 | ASP |
| 1 | N | 495 | LEU |
| 1 | N | 504 | THR |
| 2 | O | 33 | LEU |
| 2 | O | 60 | GLU |
| 2 | O | 65 | TRP |
| 2 | O | 68 | LEU |
| 2 | O | 78 | LEU |
| 2 | O | 91 | ASN |
| 2 | O | 115 | ASP |
| 2 | O | 171 | LYS |
| 2 | O | 217 | LYS |
| 3 | P | 159 | MET |
| 3 | P | 214 | PHE |
| 3 | P | 230 | ASN |
| 4 | Q | 7 | LYS |
| 4 | Q | 8 | SER |
| 4 | Q | 9 | GLU |
| 4 | Q | 20 | ARG |
| 4 | Q | 51 | LEU |
| 4 | Q | 58 | GLU |
| 4 | Q | 143 | ASN |
| 5 | R | 79 | LYS |
| 5 | R | 91 | PRO |
| 6 | S | 43 | LYS |
| 6 | S | 54 | ASN |
| 6 | S | 80 | GLN |
| 6 | S | 87[A] | THR |
| 6 | S | 87[B] | THR |
| 6 | S | 94 | HIS |
| 6 | S | 96 | LEU |
| 6 | S | 98 | HIS |
| 7 | T | 2 | SER |
| 7 | T | 7 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | T | 18 | PHE |
| 7 | T | 37 | LEU |
| 7 | T | 38 | HIS |
| 7 | T | 54 | ARG |
| 7 | T | 84 | LYS |
| 8 | U | 8 | ILE |
| 8 | U | 9 | LYS |
| 8 | U | 60 | TYR |
| 8 | U | 61 | LYS |
| 9 | V | 2 | THR |
| 9 | V | 36 | LYS |
| 9 | V | 37 | PHE |
| 9 | V | 61 | GLU |
| 9 | V | 70 | GLN |
| 10 | W | 7 | GLU |
| 10 | W | 50 | LEU |
| 12 | Y | 2 | HIS |
| 12 | Y | 20 | ARG |
| 13 | Z | 13 | LYS |
| 13 | Z | 38 | ASP |
| 13 | Z | 39 | ASN |
| 13 | Z | 42 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 180 | GLN |
| 2 | B | 10 | GLN |
| 2 | B | 52 | HIS |
| 2 | B | 59 | GLN |
| 2 | B | 181 | GLN |
| 2 | B | 195 | GLN |
| 3 | C | 3 | HIS |
| 3 | C | 68 | GLN |
| 3 | C | 76 | GLN |
| 4 | D | 37 | GLN |
| 4 | D | 109 | HIS |
| 4 | D | 143 | ASN |
| 5 | E | 94 | ASN |
| 6 | F | 80 | GLN |
| 7 | G | 76 | ASN |
| 8 | H | 31 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | H | 37 | HIS |
| 10 | J | 29 | ASN |
| 10 | J | 57 | HIS |
| 1 | N | 180 | GLN |
| 2 | O | 10 | GLN |
| 2 | O | 91 | ASN |
| 2 | O | 181 | GLN |
| 2 | O | 195 | GLN |
| 3 | P | 50 | ASN |
| 3 | P | 68 | GLN |
| 4 | Q | 37 | GLN |
| 4 | Q | 101 | HIS |
| 5 | R | 94 | ASN |
| 6 | S | 54 | ASN |
| 6 | S | 80 | GLN |
| 6 | S | 94 | HIS |
| 7 | T | 8 | HIS |
| 7 | T | 76 | ASN |
| 8 | U | 31 | GLN |
| 8 | U | 37 | HIS |
| 9 | V | 20 | HIS |
| 10 | W | 29 | ASN |
| 10 | W | 57 | HIS |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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 | $\#\|Z\|>2$ |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | FME | O | 1 | 2 | 8,9,10 | 1.93 | 4 (50%) | 7,9,11 | 2.34 | 3 (42%) |
| 7 | TPO | G | 11 | 7 | 8,10,11 | 2.10 | 4 (50%) | 10,14,16 | 1.99 | 2 (20%) |
| 1 | FME | A | 1 | 1 | 8,9,10 | 1.69 | 2 (25%) | 7,9,11 | 1.64 | 3 (42%) |
| 2 | FME | B | 1 | 2 | 8,9,10 | 5.84 | 6 (75%) | 7,9,11 | 8.82 | 4 (57%) |
| 9 | SAC | I | 1 | 9 | 7,8,9 | 2.70 | 3 (42%) | 8,9,11 | 1.44 | 1 (12%) |
| 1 | FME | N | 1 | 1 | 8,9,10 | 1.31 | 1 (12%) | 7,9,11 | 1.73 | 2 (28%) |
| 9 | SAC | V | 1 | 9 | 7,8,9 | 2.32 | 2 (28%) | 8,9,11 | 3.04 | 4 (50%) |
| 7 | TPO | T | 11 | 7 | 8,10,11 | 1.69 | 2 (25%) | 10,14,16 | 1.24 | 1 (10%) |

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 |
|---|---|---|---|---|---|---|---|
| 2 | FME | O | 1 | 2 | - | 0/7/9/11 | - |
| 7 | TPO | G | 11 | 7 | - | 5/9/11/13 | - |
| 1 | FME | A | 1 | 1 | - | 3/7/9/11 | - |
| 2 | FME | B | 1 | 2 | - | 1/7/9/11 | - |
| 9 | SAC | I | 1 | 9 | - | 1/7/8/10 | - |
| 1 | FME | N | 1 | 1 | - | 4/7/9/11 | - |
| 9 | SAC | V | 1 | 9 | - | 4/7/8/10 | - |
| 7 | TPO | T | 11 | 7 | - | 4/9/11/13 | - |

All (24) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 1 | FME | CN-N | 11.15 | 1.71 | 1.33 |
| 2 | B | 1 | FME | O1-CN | -8.94 | 0.95 | 1.22 |
| 9 | I | 1 | SAC | OAC-C1A | 5.36 | 1.35 | 1.23 |
| 9 | V | 1 | SAC | OAC-C1A | 4.57 | 1.33 | 1.23 |
| 2 | B | 1 | FME | CB-CA | 4.52 | 1.61 | 1.53 |
| 2 | B | 1 | FME | CG-SD | -4.20 | 1.59 | 1.81 |
| 9 | V | 1 | SAC | CA-N | 3.84 | 1.51 | 1.46 |
| 2 | B | 1 | FME | CA-N | 3.75 | 1.51 | 1.46 |
| 2 | B | 1 | FME | CB-CG | 3.68 | 1.65 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1 | FME | CA-N | 3.41 | 1.51 | 1.46 |
| 7 | G | 11 | TPO | P-O1P | 3.38 | 1.61 | 1.50 |
| 9 | I | 1 | SAC | CA-N | 3.32 | 1.51 | 1.46 |
| 2 | O | 1 | FME | CG-SD | -3.03 | 1.65 | 1.81 |
| 7 | T | 11 | TPO | P-O1P | 2.97 | 1.60 | 1.50 |
| 2 | O | 1 | FME | CB-CA | 2.87 | 1.58 | 1.53 |
| 1 | A | 1 | FME | O-C | 2.85 | 1.31 | 1.19 |
| 7 | G | 11 | TPO | CG2-CB | 2.60 | 1.57 | 1.51 |
| 9 | I | 1 | SAC | O-C | 2.33 | 1.29 | 1.19 |
| 2 | O | 1 | FME | CN-N | 2.24 | 1.40 | 1.33 |
| 2 | O | 1 | FME | CB-CG | 2.22 | 1.60 | 1.51 |
| 1 | N | 1 | FME | CB-CG | 2.17 | 1.59 | 1.51 |
| 7 | G | 11 | TPO | P-OG1 | 2.14 | 1.63 | 1.59 |
| 7 | T | 11 | TPO | P-OG1 | 2.08 | 1.63 | 1.59 |
| 7 | G | 11 | TPO | P-O2P | 2.02 | 1.62 | 1.54 |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 1 | FME | O1-CN-N | -17.24 | 79.86 | 125.27 |
| 2 | B | 1 | FME | CA-N-CN | -13.95 | 101.37 | 122.82 |
| 2 | B | 1 | FME | CG-CB-CA | -5.63 | 97.31 | 112.95 |
| 7 | G | 11 | TPO | CG2-CB-CA | 5.16 | 123.35 | 113.16 |
| 9 | V | 1 | SAC | C-CA-N | -5.02 | 100.67 | 109.73 |
| 2 | O | 1 | FME | CG-CB-CA | -4.32 | 100.96 | 112.95 |
| 2 | B | 1 | FME | C-CA-N | 4.25 | 117.40 | 109.73 |
| 9 | V | 1 | SAC | C2A-C1A-N | 3.90 | 122.70 | 116.10 |
| 9 | V | 1 | SAC | CA-N-C1A | 3.83 | 130.21 | 123.15 |
| 9 | I | 1 | SAC | CB-CA-N | 3.14 | 117.60 | 110.55 |
| 1 | N | 1 | FME | CE-SD-CG | 3.13 | 111.16 | 100.40 |
| 9 | V | 1 | SAC | OAC-C1A-N | -3.10 | 116.26 | 121.95 |
| 2 | O | 1 | FME | C-CA-N | -3.02 | 104.28 | 109.73 |
| 7 | T | 11 | TPO | O3P-P-OG1 | 2.99 | 119.39 | 105.99 |
| 1 | N | 1 | FME | O-C-CA | -2.68 | 117.75 | 124.78 |
| 7 | G | 11 | TPO | O-C-CA | -2.68 | 117.75 | 124.78 |
| 2 | O | 1 | FME | CA-N-CN | -2.62 | 118.79 | 122.82 |
| 1 | A | 1 | FME | O-C-CA | -2.60 | 117.97 | 124.78 |
| 1 | A | 1 | FME | CE-SD-CG | 2.07 | 107.50 | 100.40 |
| 1 | A | 1 | FME | O1-CN-N | -2.03 | 119.92 | 125.27 |

There are no chirality outliers.

All (22) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 7 | G | 11 | TPO | N-CA-CB-CG2 |
| 7 | G | 11 | TPO | N-CA-CB-OG1 |
| 7 | G | 11 | TPO | C-CA-CB-CG2 |
| 1 | A | 1 | FME | N-CA-CB-CG |
| 2 | B | 1 | FME | O1-CN-N-CA |
| 1 | N | 1 | FME | N-CA-CB-CG |
| 1 | N | 1 | FME | C-CA-CB-CG |
| 9 | V | 1 | SAC | C-CA-CB-OG |
| 7 | T | 11 | TPO | N-CA-CB-CG2 |
| 7 | T | 11 | TPO | N-CA-CB-OG1 |
| 7 | T | 11 | TPO | C-CA-CB-CG2 |
| 7 | T | 11 | TPO | CB-OG1-P-O2P |
| 1 | N | 1 | FME | CA-CB-CG-SD |
| 9 | V | 1 | SAC | C2A-C1A-N-CA |
| 9 | V | 1 | SAC | OAC-C1A-N-CA |
| 9 | V | 1 | SAC | N-CA-CB-OG |
| 9 | I | 1 | SAC | N-CA-CB-OG |
| 7 | G | 11 | TPO | CB-OG1-P-O2P |
| 1 | A | 1 | FME | CA-CB-CG-SD |
| 1 | N | 1 | FME | CB-CG-SD-CE |
| 1 | A | 1 | FME | C-CA-CB-CG |
| 7 | G | 11 | TPO | O-C-CA-CB |

There are no ring outliers.

3 monomers are involved in 14 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 7 | G | 11 | TPO | 4 | 0 |
| 2 | B | 1 | FME | 7 | 0 |
| 7 | T | 11 | TPO | 3 | 0 |

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 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 | $\#\|Z\| > 2$ |
| 21 | CUA | B | 302 | 2 | 0,1,1 | 0.00 | - | - | | |
| 26 | PEK | C | 306 | - | 52,52,52 | 1.61 | 5 (9%) | 55,57,57 | 2.21 | 18 (32%) |
| 19 | PGV | A | 607 | - | 50,50,50 | 1.49 | 9 (18%) | 53,56,56 | 1.54 | 11 (20%) |
| 14 | HEA | A | 602 | 1,18 | 44,67,67 | 1.78 | 8 (18%) | 37,103,103 | 2.30 | 14 (37%) |
| 20 | TGL | D | 201 | - | 62,62,62 | 2.77 | 11 (17%) | 65,65,65 | 3.36 | 24 (36%) |
| 14 | HEA | N | 601 | 1 | 44,67,67 | 2.43 | 14 (31%) | 37,103,103 | 3.23 | 13 (35%) |
| 14 | HEA | A | 601 | 1 | 44,67,67 | 2.49 | 15 (34%) | 37,103,103 | 2.92 | 16 (43%) |
| 19 | PGV | C | 302 | - | 50,50,50 | 1.41 | 5 (10%) | 53,56,56 | 2.06 | 5 (9%) |
| 20 | TGL | L | 101 | - | 62,62,62 | 2.10 | 13 (20%) | 65,65,65 | 2.84 | 27 (41%) |
| 28 | DMU | Z | 101 | - | 34,34,34 | 1.26 | 5 (14%) | 45,45,45 | 1.84 | 12 (26%) |
| 26 | PEK | G | 101 | - | 52,52,52 | 1.20 | 5 (9%) | 55,57,57 | 1.66 | 12 (21%) |
| 26 | PEK | G | 103 | - | 52,52,52 | 1.29 | 3 (5%) | 55,57,57 | 1.64 | 11 (20%) |
| 20 | TGL | B | 301 | - | 62,62,62 | 1.71 | 8 (12%) | 65,65,65 | 2.82 | 21 (32%) |
| 19 | PGV | Q | 201 | - | 50,50,50 | 1.31 | 3 (6%) | 53,56,56 | 1.74 | 10 (18%) |
| 18 | PER | A | 606 | 15,14 | 0,1,1 | 0.00 | - | - | | |
| 23 | PSC | O | 303 | - | 51,51,51 | 1.45 | 3 (5%) | 57,59,59 | 1.73 | 11 (19%) |
| 22 | CHD | B | 303 | - | 29,32,32 | 2.79 | 17 (58%) | 48,51,51 | 2.69 | 22 (45%) |
| 22 | CHD | C | 304 | - | 29,32,32 | 1.50 | 5 (17%) | 48,51,51 | 3.97 | 28 (58%) |
| 22 | CHD | O | 302 | - | 29,32,32 | 2.50 | 10 (34%) | 48,51,51 | 2.49 | 20 (41%) |
| 19 | PGV | A | 608 | - | 50,50,50 | 1.97 | 6 (12%) | 53,56,56 | 2.43 | 14 (26%) |
| 26 | PEK | T | 101 | - | 52,52,52 | 1.60 | 4 (7%) | 55,57,57 | 2.28 | 10 (18%) |
| 22 | CHD | J | 102 | - | 29,32,32 | 1.86 | 8 (27%) | 48,51,51 | 4.75 | 33 (68%) |
| 19 | PGV | P | 303 | - | 50,50,50 | 1.06 | 3 (6%) | 53,56,56 | 1.51 | 13 (24%) |
| 22 | CHD | C | 305 | - | 29,32,32 | 2.48 | 13 (44%) | 48,51,51 | 2.93 | 20 (41%) |
| 28 | DMU | M | 101 | - | 34,34,34 | 1.49 | 5 (14%) | 45,45,45 | 2.24 | 16 (35%) |
| 21 | CUA | O | 301 | 2 | 0,1,1 | 0.00 | - | - | | |
| 26 | PEK | T | 102 | - | 52,52,52 | 1.30 | 2 (3%) | 55,57,57 | 1.55 | 8 (14%) |
| 25 | CDL | C | 303 | - | 99,99,99 | 1.82 | 20 (20%) | 105,111,111 | 2.30 | 34 (32%) |
| 14 | HEA | N | 602 | 1,18 | 44,67,67 | 1.66 | 9 (20%) | 37,103,103 | 2.68 | 17 (45%) |
| 19 | PGV | N | 607 | - | 50,50,50 | 1.47 | 7 (14%) | 53,56,56 | 1.50 | 11 (20%) |
| 19 | PGV | P | 301 | - | 50,50,50 | 1.11 | 2 (4%) | 53,56,56 | 1.68 | 10 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 20 | TGL | N | 608 | - | 62,62,62 | 1.44 | 8 (12%) | 65,65,65 | 2.18 | 14 (21%) |
| 25 | CDL | P | 304 | - | 99,99,99 | 2.05 | 22 (22%) | 105,111,111 | 2.17 | 35 (33%) |
| 18 | PER | N | 606 | 15,14 | 0,1,1 | 0.00 | - | - | | |
| 22 | CHD | W | 101 | - | 29,32,32 | 1.98 | 10 (34%) | 48,51,51 | 4.66 | 29 (60%) |
| 25 | CDL | T | 103 | - | 99,99,99 | 1.53 | 12 (12%) | 105,111,111 | 1.67 | 18 (17%) |
| 26 | PEK | P | 308 | - | 52,52,52 | 1.68 | 6 (11%) | 55,57,57 | 1.92 | 14 (25%) |
| 20 | TGL | Y | 101 | - | 62,62,62 | 2.05 | 11 (17%) | 65,65,65 | 3.06 | 27 (41%) |
| 23 | PSC | B | 304 | - | 51,51,51 | 1.32 | 3 (5%) | 57,59,59 | 1.77 | 12 (21%) |
| 28 | DMU | J | 101 | - | 34,34,34 | 1.00 | 1 (2%) | 45,45,45 | 1.48 | 6 (13%) |
| 19 | PGV | C | 307 | - | 50,50,50 | 1.29 | 4 (8%) | 53,56,56 | 1.60 | 8 (15%) |
| 28 | DMU | P | 306 | - | 34,34,34 | 0.87 | 1 (2%) | 45,45,45 | 1.80 | 9 (20%) |
| 22 | CHD | P | 307 | - | 29,32,32 | 1.92 | 10 (34%) | 48,51,51 | 2.66 | 19 (39%) |
| 25 | CDL | G | 102 | - | 99,99,99 | 1.49 | 13 (13%) | 105,111,111 | 1.82 | 22 (20%) |
| 22 | CHD | P | 305 | - | 29,32,32 | 1.41 | 5 (17%) | 48,51,51 | 3.60 | 28 (58%) |
| 20 | TGL | Q | 202 | - | 62,62,62 | 2.36 | 11 (17%) | 65,65,65 | 2.77 | 14 (21%) |

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 |
|---|---|---|---|---|---|---|---|
| 26 | PEK | C | 306 | - | - | 34/56/56/56 | - |
| 19 | PGV | A | 607 | - | - | 8/55/55/55 | - |
| 28 | DMU | P | 306 | - | - | 6/19/59/59 | 0/2/2/2 |
| 20 | TGL | D | 201 | - | - | 33/65/65/65 | - |
| 14 | HEA | N | 601 | 1 | 2/2/7/16 | 3/24/76/76 | - |
| 14 | HEA | A | 601 | 1 | 3/3/7/16 | 2/24/76/76 | - |
| 19 | PGV | C | 302 | - | - | 14/55/55/55 | - |
| 20 | TGL | L | 101 | - | - | 34/65/65/65 | - |
| 28 | DMU | Z | 101 | - | - | 5/19/59/59 | 0/2/2/2 |
| 26 | PEK | G | 101 | - | - | 16/56/56/56 | - |
| 26 | PEK | G | 103 | - | - | 22/56/56/56 | - |
| 20 | TGL | B | 301 | - | - | 31/65/65/65 | - |
| 19 | PGV | Q | 201 | - | - | 31/55/55/55 | - |
| 20 | TGL | Q | 202 | - | - | 36/65/65/65 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 23 | PSC | O | 303 | - | - | 27/55/55/55 | - |
| 22 | CHD | B | 303 | - | - | 0/7/74/74 | 0/4/4/4 |
| 22 | CHD | C | 304 | - | - | 6/7/74/74 | 0/4/4/4 |
| 14 | HEA | A | 602 | 1,18 | 3/3/7/16 | 1/24/76/76 | - |
| 19 | PGV | A | 608 | - | - | 34/55/55/55 | - |
| 26 | PEK | T | 101 | - | - | 21/56/56/56 | - |
| 22 | CHD | J | 102 | - | - | 5/7/74/74 | 0/4/4/4 |
| 19 | PGV | P | 303 | - | - | 10/55/55/55 | - |
| 22 | CHD | C | 305 | - | - | 0/7/74/74 | 0/4/4/4 |
| 28 | DMU | M | 101 | - | - | 5/19/59/59 | 0/2/2/2 |
| 22 | CHD | W | 101 | - | - | 7/7/74/74 | 0/4/4/4 |
| 25 | CDL | C | 303 | - | - | 57/110/110/110 | - |
| 14 | HEA | N | 602 | 1,18 | 3/3/7/16 | 0/24/76/76 | - |
| 19 | PGV | N | 607 | - | - | 9/55/55/55 | - |
| 19 | PGV | P | 301 | - | - | 30/55/55/55 | - |
| 20 | TGL | N | 608 | - | - | 43/65/65/65 | - |
| 25 | CDL | P | 304 | - | - | 62/110/110/110 | - |
| 26 | PEK | T | 102 | - | - | 28/56/56/56 | - |
| 22 | CHD | O | 302 | - | - | 0/7/74/74 | 0/4/4/4 |
| 25 | CDL | T | 103 | - | - | 62/110/110/110 | - |
| 26 | PEK | P | 308 | - | - | 22/56/56/56 | - |
| 20 | TGL | Y | 101 | - | - | 41/65/65/65 | - |
| 23 | PSC | B | 304 | - | - | 31/55/55/55 | - |
| 28 | DMU | J | 101 | - | - | 6/19/59/59 | 0/2/2/2 |
| 19 | PGV | C | 307 | - | - | 33/55/55/55 | - |
| 22 | CHD | P | 307 | - | - | 1/7/74/74 | 0/4/4/4 |
| 25 | CDL | G | 102 | - | - | 59/110/110/110 | - |
| 22 | CHD | P | 305 | - | - | 5/7/74/74 | 0/4/4/4 |

All (335) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | D | 201 | TGL | OB1-CB1 | 12.98 | 1.61 | 1.22 |
| 20 | Q | 202 | TGL | OB1-CB1 | 11.24 | 1.55 | 1.22 |
| 20 | D | 201 | TGL | OG2-CB1 | 10.44 | 1.63 | 1.34 |
| 20 | Q | 202 | TGL | OG2-CB1 | 9.46 | 1.60 | 1.34 |
| 14 | A | 601 | HEA | C18-C19 | -8.37 | 1.12 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | L | 101 | TGL | OG2-CB1 | 8.31 | 1.57 | 1.34 |
| 20 | Y | 101 | TGL | OG2-CB1 | 7.74 | 1.56 | 1.34 |
| 19 | A | 608 | PGV | O02-C1 | 7.55 | 1.44 | 1.22 |
| 20 | B | 301 | TGL | OG1-CA1 | 7.27 | 1.54 | 1.33 |
| 25 | P | 304 | CDL | OB8-CB7 | 7.06 | 1.54 | 1.33 |
| 20 | Y | 101 | TGL | OG3-CC1 | 7.02 | 1.53 | 1.33 |
| 26 | P | 308 | PEK | O01-C1 | 7.01 | 1.54 | 1.34 |
| 19 | A | 608 | PGV | O03-C19 | 6.99 | 1.53 | 1.33 |
| 25 | P | 304 | CDL | PB2-OB3 | 6.75 | 1.74 | 1.50 |
| 26 | T | 101 | PEK | C3-C2 | 6.53 | 1.76 | 1.52 |
| 20 | D | 201 | TGL | OC1-CC1 | 6.49 | 1.41 | 1.22 |
| 26 | C | 306 | PEK | O01-C1 | 6.39 | 1.52 | 1.34 |
| 14 | N | 601 | HEA | C18-C19 | -6.29 | 1.17 | 1.33 |
| 14 | A | 601 | HEA | C16-C17 | -6.26 | 1.32 | 1.53 |
| 23 | O | 303 | PSC | O01-C1 | 6.22 | 1.51 | 1.34 |
| 25 | C | 303 | CDL | PB2-OB3 | 6.21 | 1.72 | 1.50 |
| 20 | Y | 101 | TGL | OG1-CA1 | 6.20 | 1.51 | 1.33 |
| 26 | P | 308 | PEK | O03-C21 | 6.20 | 1.51 | 1.33 |
| 26 | C | 306 | PEK | O03-C21 | 6.17 | 1.51 | 1.33 |
| 20 | B | 301 | TGL | OC1-CC1 | -6.16 | 1.04 | 1.22 |
| 14 | N | 601 | HEA | C3B-C11 | -6.13 | 1.48 | 1.52 |
| 25 | C | 303 | CDL | OB8-CB7 | 6.13 | 1.51 | 1.33 |
| 26 | G | 103 | PEK | O01-C1 | 6.06 | 1.51 | 1.34 |
| 25 | P | 304 | CDL | OA8-CA7 | 6.02 | 1.50 | 1.33 |
| 19 | Q | 201 | PGV | O03-C19 | 5.89 | 1.50 | 1.33 |
| 20 | L | 101 | TGL | OG3-CC1 | 5.87 | 1.50 | 1.33 |
| 25 | T | 103 | CDL | OB8-CB7 | 5.81 | 1.50 | 1.33 |
| 25 | P | 304 | CDL | OA6-CA5 | 5.78 | 1.50 | 1.34 |
| 25 | C | 303 | CDL | OA8-CA7 | 5.76 | 1.50 | 1.33 |
| 26 | T | 101 | PEK | C2-C1 | 5.74 | 1.67 | 1.50 |
| 20 | D | 201 | TGL | OG1-CA1 | 5.71 | 1.50 | 1.33 |
| 23 | B | 304 | PSC | O01-C1 | 5.71 | 1.50 | 1.34 |
| 25 | T | 103 | CDL | OA6-CA5 | 5.66 | 1.50 | 1.34 |
| 26 | T | 102 | PEK | O01-C1 | 5.64 | 1.50 | 1.34 |
| 25 | P | 304 | CDL | O1-C1 | 5.59 | 1.60 | 1.43 |
| 22 | O | 302 | CHD | C10-C5 | -5.56 | 1.46 | 1.55 |
| 20 | N | 608 | TGL | OG1-CA1 | 5.50 | 1.49 | 1.33 |
| 26 | G | 103 | PEK | O03-C21 | 5.46 | 1.49 | 1.33 |
| 20 | L | 101 | TGL | OG1-CA1 | 5.44 | 1.49 | 1.33 |
| 25 | G | 102 | CDL | OB6-CB5 | 5.42 | 1.49 | 1.34 |
| 25 | G | 102 | CDL | OB8-CB7 | 5.38 | 1.49 | 1.33 |
| 26 | T | 102 | PEK | O03-C21 | 5.35 | 1.49 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | G | 102 | CDL | OA6-CA5 | 5.28 | 1.49 | 1.34 |
| 25 | T | 103 | CDL | OB6-CB5 | 5.27 | 1.49 | 1.34 |
| 25 | C | 303 | CDL | OA6-CA5 | 5.20 | 1.49 | 1.34 |
| 22 | C | 305 | CHD | C22-C20 | 5.19 | 1.67 | 1.54 |
| 22 | O | 302 | CHD | C19-C10 | 5.19 | 1.63 | 1.54 |
| 22 | B | 303 | CHD | C13-C14 | -5.14 | 1.46 | 1.55 |
| 20 | Q | 202 | TGL | OG3-CC1 | 5.10 | 1.48 | 1.33 |
| 22 | B | 303 | CHD | C19-C10 | 5.10 | 1.63 | 1.54 |
| 20 | Q | 202 | TGL | OG1-CA1 | 5.06 | 1.48 | 1.33 |
| 14 | N | 601 | HEA | O11-C11 | 5.00 | 1.54 | 1.42 |
| 22 | O | 302 | CHD | C15-C14 | 4.93 | 1.64 | 1.54 |
| 14 | A | 602 | HEA | C18-C19 | 4.91 | 1.44 | 1.33 |
| 19 | C | 307 | PGV | O01-C1 | 4.85 | 1.48 | 1.34 |
| 14 | A | 602 | HEA | C3C-C2C | -4.85 | 1.33 | 1.40 |
| 19 | A | 608 | PGV | P-O13 | 4.82 | 1.68 | 1.50 |
| 25 | T | 103 | CDL | OA8-CA7 | 4.80 | 1.47 | 1.33 |
| 22 | P | 307 | CHD | C11-C12 | 4.79 | 1.61 | 1.53 |
| 19 | Q | 201 | PGV | O01-C1 | 4.75 | 1.47 | 1.34 |
| 25 | C | 303 | CDL | O1-C1 | 4.69 | 1.57 | 1.43 |
| 25 | P | 304 | CDL | CB2-C1 | 4.65 | 1.67 | 1.51 |
| 25 | G | 102 | CDL | OA8-CA7 | 4.58 | 1.46 | 1.33 |
| 19 | C | 302 | PGV | C22-C21 | 4.57 | 1.77 | 1.51 |
| 19 | P | 301 | PGV | O03-C19 | 4.55 | 1.46 | 1.33 |
| 20 | D | 201 | TGL | CC2-CC1 | 4.53 | 1.63 | 1.50 |
| 22 | J | 102 | CHD | C20-C17 | 4.51 | 1.62 | 1.54 |
| 22 | B | 303 | CHD | C4-C3 | 4.49 | 1.60 | 1.51 |
| 23 | B | 304 | PSC | O03-C19 | 4.42 | 1.46 | 1.33 |
| 14 | N | 601 | HEA | C16-C17 | -4.38 | 1.39 | 1.53 |
| 20 | D | 201 | TGL | OG3-CC1 | 4.36 | 1.46 | 1.33 |
| 19 | P | 301 | PGV | O01-C1 | 4.35 | 1.46 | 1.34 |
| 25 | P | 304 | CDL | OB8-CB6 | 4.32 | 1.55 | 1.45 |
| 20 | N | 608 | TGL | OG3-CC1 | 4.31 | 1.45 | 1.33 |
| 14 | N | 601 | HEA | C1C-NC | 4.29 | 1.45 | 1.36 |
| 25 | C | 303 | CDL | CB2-C1 | 4.26 | 1.66 | 1.51 |
| 22 | W | 101 | CHD | C13-C17 | 4.23 | 1.62 | 1.55 |
| 19 | A | 607 | PGV | C01-C02 | 4.23 | 1.63 | 1.50 |
| 19 | C | 302 | PGV | C20-C19 | 4.22 | 1.63 | 1.50 |
| 14 | A | 602 | HEA | C3B-C11 | 4.22 | 1.56 | 1.52 |
| 20 | B | 301 | TGL | OG3-CC1 | 4.18 | 1.45 | 1.33 |
| 22 | B | 303 | CHD | C16-C17 | 4.16 | 1.63 | 1.54 |
| 23 | O | 303 | PSC | O03-C19 | 4.16 | 1.45 | 1.33 |
| 14 | N | 601 | HEA | C3C-C2C | -4.14 | 1.34 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | O | 302 | CHD | C16-C17 | 4.10 | 1.62 | 1.54 |
| 20 | D | 201 | TGL | C10-CB9 | -4.08 | 1.28 | 1.51 |
| 23 | O | 303 | PSC | C13-C12 | 4.07 | 1.55 | 1.31 |
| 25 | C | 303 | CDL | C79-C78 | -4.05 | 1.28 | 1.51 |
| 19 | C | 307 | PGV | O03-C19 | 4.05 | 1.45 | 1.33 |
| 22 | B | 303 | CHD | C4-C5 | 4.03 | 1.60 | 1.53 |
| 28 | J | 101 | DMU | O16-C6 | 4.03 | 1.47 | 1.40 |
| 22 | B | 303 | CHD | C15-C14 | 4.02 | 1.62 | 1.54 |
| 25 | P | 304 | CDL | OB6-CB5 | 3.98 | 1.45 | 1.34 |
| 14 | A | 601 | HEA | C3C-C2C | -3.97 | 1.34 | 1.40 |
| 22 | C | 305 | CHD | C11-C12 | 3.96 | 1.59 | 1.53 |
| 23 | B | 304 | PSC | C13-C12 | 3.92 | 1.54 | 1.31 |
| 19 | N | 607 | PGV | C01-C02 | 3.90 | 1.62 | 1.50 |
| 22 | C | 305 | CHD | C4-C3 | 3.88 | 1.59 | 1.51 |
| 14 | A | 601 | HEA | C14-C15 | -3.87 | 1.23 | 1.33 |
| 22 | B | 303 | CHD | O7-C7 | 3.84 | 1.51 | 1.43 |
| 20 | B | 301 | TGL | CB2-CB1 | -3.83 | 1.39 | 1.50 |
| 14 | N | 601 | HEA | CMC-C2C | 3.81 | 1.59 | 1.51 |
| 22 | W | 101 | CHD | C13-C12 | 3.81 | 1.60 | 1.54 |
| 19 | A | 608 | PGV | P-O12 | 3.79 | 1.74 | 1.59 |
| 22 | C | 305 | CHD | C6-C5 | 3.78 | 1.59 | 1.53 |
| 22 | O | 302 | CHD | C6-C7 | 3.78 | 1.59 | 1.52 |
| 19 | A | 608 | PGV | O01-C1 | 3.74 | 1.44 | 1.34 |
| 14 | N | 602 | HEA | C3B-C11 | -3.73 | 1.50 | 1.52 |
| 20 | L | 101 | TGL | CC2-CC1 | 3.72 | 1.61 | 1.50 |
| 14 | A | 601 | HEA | C16-C15 | 3.71 | 1.59 | 1.51 |
| 25 | T | 103 | CDL | C42-C41 | -3.70 | 1.30 | 1.51 |
| 20 | N | 608 | TGL | OG2-CB1 | 3.69 | 1.44 | 1.34 |
| 28 | M | 101 | DMU | O7-C3 | 3.67 | 1.53 | 1.43 |
| 28 | P | 306 | DMU | O16-C6 | 3.60 | 1.46 | 1.40 |
| 14 | A | 601 | HEA | C3A-C2A | -3.58 | 1.35 | 1.40 |
| 22 | B | 303 | CHD | C10-C5 | -3.56 | 1.49 | 1.55 |
| 14 | A | 601 | HEA | CAD-C3D | 3.52 | 1.57 | 1.52 |
| 14 | N | 601 | HEA | C16-C15 | 3.52 | 1.58 | 1.51 |
| 20 | L | 101 | TGL | C20-CA9 | -3.52 | 1.31 | 1.51 |
| 22 | W | 101 | CHD | C8-C14 | 3.51 | 1.60 | 1.53 |
| 14 | N | 602 | HEA | C4D-ND | 3.49 | 1.43 | 1.36 |
| 22 | C | 305 | CHD | C16-C17 | 3.48 | 1.61 | 1.54 |
| 22 | J | 102 | CHD | C8-C14 | 3.48 | 1.60 | 1.53 |
| 25 | P | 304 | CDL | C79-C78 | -3.46 | 1.32 | 1.51 |
| 25 | P | 304 | CDL | OB2-CB2 | 3.46 | 1.58 | 1.44 |
| 25 | P | 304 | CDL | C59-C58 | -3.45 | 1.32 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | P | 307 | CHD | C22-C20 | 3.44 | 1.63 | 1.54 |
| 22 | P | 307 | CHD | C6-C7 | 3.41 | 1.58 | 1.52 |
| 22 | B | 303 | CHD | C6-C7 | 3.39 | 1.58 | 1.52 |
| 14 | N | 601 | HEA | CMB-C2B | 3.39 | 1.58 | 1.51 |
| 20 | L | 101 | TGL | C10-CB9 | -3.36 | 1.32 | 1.51 |
| 25 | G | 102 | CDL | C59-C58 | -3.36 | 1.32 | 1.51 |
| 19 | N | 607 | PGV | O01-C02 | -3.36 | 1.38 | 1.46 |
| 20 | L | 101 | TGL | CB2-CB1 | 3.35 | 1.60 | 1.50 |
| 22 | B | 303 | CHD | C6-C5 | 3.35 | 1.59 | 1.53 |
| 22 | C | 305 | CHD | O12-C12 | 3.33 | 1.49 | 1.43 |
| 14 | A | 602 | HEA | C24-C23 | 3.31 | 1.59 | 1.50 |
| 26 | T | 101 | PEK | O11-C03 | 3.31 | 1.57 | 1.44 |
| 25 | P | 304 | CDL | PB2-OB2 | 3.31 | 1.72 | 1.59 |
| 14 | N | 602 | HEA | C14-C15 | 3.30 | 1.40 | 1.33 |
| 14 | N | 602 | HEA | C20-C19 | 3.30 | 1.58 | 1.51 |
| 25 | C | 303 | CDL | PB2-OB2 | 3.29 | 1.72 | 1.59 |
| 22 | B | 303 | CHD | C18-C13 | 3.29 | 1.59 | 1.54 |
| 20 | Q | 202 | TGL | C10-CB9 | -3.28 | 1.33 | 1.51 |
| 26 | G | 101 | PEK | C23-C22 | -3.27 | 1.40 | 1.52 |
| 25 | G | 102 | CDL | C62-C61 | -3.27 | 1.33 | 1.51 |
| 22 | P | 305 | CHD | C11-C9 | 3.24 | 1.59 | 1.53 |
| 25 | T | 103 | CDL | C62-C61 | -3.23 | 1.33 | 1.51 |
| 20 | Y | 101 | TGL | C20-CA9 | -3.22 | 1.33 | 1.51 |
| 22 | W | 101 | CHD | C20-C17 | 3.21 | 1.60 | 1.54 |
| 22 | C | 305 | CHD | C13-C17 | 3.20 | 1.61 | 1.55 |
| 22 | C | 304 | CHD | C8-C9 | 3.20 | 1.60 | 1.53 |
| 19 | N | 607 | PGV | O03-C01 | 3.18 | 1.52 | 1.45 |
| 22 | C | 305 | CHD | C2-C3 | 3.17 | 1.59 | 1.51 |
| 19 | N | 607 | PGV | C3-C2 | 3.17 | 1.63 | 1.52 |
| 20 | L | 101 | TGL | OG2-CG2 | 3.16 | 1.54 | 1.46 |
| 20 | N | 608 | TGL | OC1-CC1 | -3.14 | 1.13 | 1.22 |
| 22 | W | 101 | CHD | C8-C9 | 3.13 | 1.60 | 1.53 |
| 22 | J | 102 | CHD | C13-C17 | 3.13 | 1.60 | 1.55 |
| 20 | L | 101 | TGL | CG3-CG2 | 3.12 | 1.60 | 1.50 |
| 20 | Q | 202 | TGL | OC1-CC1 | 3.12 | 1.31 | 1.22 |
| 25 | P | 304 | CDL | C19-C18 | -3.12 | 1.34 | 1.51 |
| 22 | J | 102 | CHD | C8-C9 | 3.10 | 1.59 | 1.53 |
| 25 | P | 304 | CDL | C62-C61 | -3.10 | 1.34 | 1.51 |
| 25 | T | 103 | CDL | C22-C21 | -3.09 | 1.34 | 1.51 |
| 22 | P | 307 | CHD | C16-C15 | 3.09 | 1.62 | 1.54 |
| 25 | C | 303 | CDL | OB6-CB5 | 3.08 | 1.43 | 1.34 |
| 19 | C | 302 | PGV | C21-C20 | 3.07 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | G | 102 | CDL | C82-C81 | -3.07 | 1.34 | 1.51 |
| 14 | N | 602 | HEA | O11-C11 | 3.06 | 1.49 | 1.42 |
| 22 | C | 305 | CHD | C16-C15 | 3.06 | 1.62 | 1.54 |
| 22 | P | 305 | CHD | C8-C9 | 3.06 | 1.59 | 1.53 |
| 14 | N | 601 | HEA | C1B-NB | 3.06 | 1.42 | 1.36 |
| 26 | P | 308 | PEK | P-O11 | 3.04 | 1.71 | 1.59 |
| 25 | P | 304 | CDL | C22-C21 | -3.04 | 1.34 | 1.51 |
| 22 | O | 302 | CHD | C4-C3 | 3.03 | 1.57 | 1.51 |
| 20 | Y | 101 | TGL | C10-CB9 | -3.03 | 1.34 | 1.51 |
| 14 | A | 601 | HEA | C3B-C2B | -3.02 | 1.31 | 1.41 |
| 14 | A | 601 | HEA | C22-C23 | 3.02 | 1.41 | 1.32 |
| 25 | C | 303 | CDL | C82-C81 | -3.01 | 1.34 | 1.51 |
| 25 | T | 103 | CDL | C59-C58 | -3.00 | 1.34 | 1.51 |
| 22 | C | 304 | CHD | C10-C5 | 2.99 | 1.60 | 1.55 |
| 22 | O | 302 | CHD | C13-C12 | 2.99 | 1.59 | 1.54 |
| 22 | O | 302 | CHD | C8-C9 | 2.98 | 1.59 | 1.53 |
| 25 | C | 303 | CDL | C59-C58 | -2.97 | 1.34 | 1.51 |
| 26 | C | 306 | PEK | C22-C21 | 2.97 | 1.59 | 1.50 |
| 25 | C | 303 | CDL | C62-C61 | -2.95 | 1.35 | 1.51 |
| 22 | C | 304 | CHD | C8-C14 | 2.95 | 1.59 | 1.53 |
| 26 | P | 308 | PEK | C22-C21 | 2.94 | 1.59 | 1.50 |
| 25 | P | 304 | CDL | PA1-OA5 | 2.93 | 1.71 | 1.59 |
| 22 | W | 101 | CHD | C13-C14 | 2.93 | 1.60 | 1.55 |
| 20 | N | 608 | TGL | C20-CA9 | -2.91 | 1.35 | 1.51 |
| 25 | T | 103 | CDL | C19-C18 | -2.91 | 1.35 | 1.51 |
| 22 | J | 102 | CHD | C8-C7 | 2.90 | 1.58 | 1.53 |
| 20 | L | 101 | TGL | OB1-CB1 | 2.89 | 1.31 | 1.22 |
| 20 | Y | 101 | TGL | CG3-CG2 | 2.88 | 1.59 | 1.50 |
| 19 | P | 303 | PGV | C20-C19 | 2.88 | 1.59 | 1.50 |
| 28 | Z | 101 | DMU | O55-C2 | 2.87 | 1.49 | 1.43 |
| 14 | A | 601 | HEA | C3B-C11 | -2.87 | 1.50 | 1.52 |
| 26 | C | 306 | PEK | P-O11 | 2.86 | 1.70 | 1.59 |
| 22 | B | 303 | CHD | C8-C7 | -2.86 | 1.48 | 1.53 |
| 14 | A | 601 | HEA | C12-C13 | 2.85 | 1.62 | 1.53 |
| 25 | T | 103 | CDL | C39-C38 | -2.85 | 1.35 | 1.51 |
| 25 | C | 303 | CDL | C19-C18 | -2.85 | 1.35 | 1.51 |
| 19 | N | 607 | PGV | O01-C1 | 2.84 | 1.42 | 1.34 |
| 19 | A | 607 | PGV | C3-C2 | 2.84 | 1.62 | 1.52 |
| 20 | B | 301 | TGL | C20-CA9 | -2.83 | 1.35 | 1.51 |
| 20 | N | 608 | TGL | C10-CB9 | -2.83 | 1.35 | 1.51 |
| 20 | D | 201 | TGL | C15-CC9 | -2.80 | 1.35 | 1.51 |
| 20 | Y | 101 | TGL | CC3-CC2 | 2.80 | 1.62 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | N | 607 | PGV | C03-C02 | 2.80 | 1.59 | 1.50 |
| 25 | P | 304 | CDL | C39-C38 | -2.79 | 1.35 | 1.51 |
| 22 | C | 305 | CHD | C10-C9 | 2.79 | 1.61 | 1.56 |
| 25 | C | 303 | CDL | OB8-CB6 | 2.79 | 1.51 | 1.45 |
| 14 | N | 601 | HEA | C12-C13 | 2.78 | 1.62 | 1.53 |
| 26 | G | 101 | PEK | O01-C02 | 2.78 | 1.53 | 1.46 |
| 14 | A | 602 | HEA | C12-C13 | 2.77 | 1.62 | 1.53 |
| 20 | D | 201 | TGL | C20-CA9 | -2.76 | 1.36 | 1.51 |
| 22 | P | 307 | CHD | C16-C17 | 2.76 | 1.60 | 1.54 |
| 14 | N | 602 | HEA | C12-C13 | 2.76 | 1.62 | 1.53 |
| 25 | G | 102 | CDL | C39-C38 | -2.75 | 1.36 | 1.51 |
| 26 | T | 101 | PEK | C23-C22 | -2.74 | 1.42 | 1.52 |
| 28 | M | 101 | DMU | C2-C1 | 2.73 | 1.59 | 1.52 |
| 20 | Q | 202 | TGL | C20-CA9 | -2.72 | 1.36 | 1.51 |
| 25 | G | 102 | CDL | C19-C18 | -2.71 | 1.36 | 1.51 |
| 25 | C | 303 | CDL | OB2-CB2 | 2.71 | 1.55 | 1.44 |
| 25 | C | 303 | CDL | C22-C21 | -2.71 | 1.36 | 1.51 |
| 22 | W | 101 | CHD | C8-C7 | 2.71 | 1.58 | 1.53 |
| 22 | P | 307 | CHD | C6-C5 | 2.71 | 1.58 | 1.53 |
| 14 | A | 601 | HEA | CMB-C2B | 2.71 | 1.57 | 1.51 |
| 28 | M | 101 | DMU | O5-C4 | 2.70 | 1.50 | 1.44 |
| 20 | N | 608 | TGL | C15-CC9 | -2.68 | 1.36 | 1.51 |
| 26 | G | 101 | PEK | O11-C03 | 2.68 | 1.55 | 1.44 |
| 25 | P | 304 | CDL | C82-C81 | -2.68 | 1.36 | 1.51 |
| 22 | C | 305 | CHD | C8-C7 | 2.66 | 1.58 | 1.53 |
| 22 | C | 305 | CHD | C13-C12 | -2.65 | 1.50 | 1.54 |
| 19 | A | 607 | PGV | O03-C01 | 2.63 | 1.51 | 1.45 |
| 20 | D | 201 | TGL | CG3-CG2 | 2.63 | 1.58 | 1.50 |
| 22 | B | 303 | CHD | C21-C20 | 2.63 | 1.59 | 1.53 |
| 22 | C | 305 | CHD | C11-C9 | 2.62 | 1.58 | 1.53 |
| 25 | C | 303 | CDL | PA1-OA5 | 2.61 | 1.69 | 1.59 |
| 14 | N | 602 | HEA | CMB-C2B | 2.61 | 1.57 | 1.51 |
| 19 | P | 303 | PGV | P-O14 | -2.61 | 1.43 | 1.55 |
| 22 | W | 101 | CHD | C11-C9 | 2.59 | 1.58 | 1.53 |
| 22 | P | 307 | CHD | C11-C9 | 2.58 | 1.58 | 1.53 |
| 20 | Y | 101 | TGL | C15-CC9 | -2.58 | 1.37 | 1.51 |
| 20 | Y | 101 | TGL | OG2-CG2 | 2.57 | 1.53 | 1.46 |
| 14 | A | 602 | HEA | CAD-C3D | -2.56 | 1.48 | 1.52 |
| 28 | M | 101 | DMU | O16-C6 | 2.54 | 1.44 | 1.40 |
| 14 | N | 602 | HEA | C13-C14 | 2.53 | 1.58 | 1.50 |
| 22 | B | 303 | CHD | C10-C9 | -2.52 | 1.51 | 1.56 |
| 20 | Y | 101 | TGL | CB2-CB1 | 2.52 | 1.58 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | T | 103 | CDL | C82-C81 | -2.52 | 1.37 | 1.51 |
| 28 | Z | 101 | DMU | O7-C3 | 2.52 | 1.50 | 1.43 |
| 25 | C | 303 | CDL | C39-C38 | -2.52 | 1.37 | 1.51 |
| 25 | G | 102 | CDL | C79-C78 | -2.51 | 1.37 | 1.51 |
| 25 | C | 303 | CDL | C42-C41 | -2.51 | 1.37 | 1.51 |
| 22 | P | 305 | CHD | C10-C5 | 2.48 | 1.59 | 1.55 |
| 20 | Y | 101 | TGL | CC2-CC1 | 2.48 | 1.58 | 1.50 |
| 25 | P | 304 | CDL | C42-C41 | -2.46 | 1.37 | 1.51 |
| 22 | O | 302 | CHD | C13-C14 | -2.46 | 1.51 | 1.55 |
| 22 | P | 307 | CHD | C2-C3 | 2.44 | 1.57 | 1.51 |
| 19 | A | 607 | PGV | O01-C1 | 2.43 | 1.41 | 1.34 |
| 25 | G | 102 | CDL | C42-C41 | -2.43 | 1.37 | 1.51 |
| 20 | Q | 202 | TGL | C15-CC9 | -2.42 | 1.38 | 1.51 |
| 25 | P | 304 | CDL | OA2-CA2 | -2.41 | 1.35 | 1.44 |
| 20 | B | 301 | TGL | C10-CB9 | -2.41 | 1.38 | 1.51 |
| 14 | A | 601 | HEA | C4C-CHD | 2.40 | 1.47 | 1.41 |
| 22 | B | 303 | CHD | C8-C9 | 2.40 | 1.58 | 1.53 |
| 14 | N | 601 | HEA | C14-C15 | -2.39 | 1.27 | 1.33 |
| 14 | N | 602 | HEA | C1C-NC | 2.39 | 1.41 | 1.36 |
| 20 | L | 101 | TGL | C15-CC9 | -2.39 | 1.38 | 1.51 |
| 20 | Q | 202 | TGL | CB3-CB2 | 2.39 | 1.61 | 1.52 |
| 26 | C | 306 | PEK | O04-C21 | 2.38 | 1.29 | 1.22 |
| 20 | L | 101 | TGL | CG1-CG2 | 2.37 | 1.58 | 1.50 |
| 14 | N | 601 | HEA | CMD-C2D | 2.37 | 1.57 | 1.51 |
| 28 | Z | 101 | DMU | O16-C6 | 2.37 | 1.44 | 1.40 |
| 22 | J | 102 | CHD | C13-C12 | 2.37 | 1.58 | 1.54 |
| 19 | C | 302 | PGV | O06-C06 | 2.35 | 1.52 | 1.42 |
| 19 | C | 307 | PGV | P-O11 | 2.35 | 1.68 | 1.59 |
| 19 | A | 607 | PGV | C29-C28 | 2.31 | 1.64 | 1.51 |
| 26 | P | 308 | PEK | P-O12 | 2.31 | 1.68 | 1.59 |
| 20 | L | 101 | TGL | CA6-CA5 | -2.31 | 1.38 | 1.51 |
| 19 | A | 608 | PGV | C3-C2 | -2.29 | 1.43 | 1.52 |
| 25 | C | 303 | CDL | CA2-C1 | 2.29 | 1.59 | 1.51 |
| 14 | A | 602 | HEA | CMC-C2C | 2.28 | 1.56 | 1.51 |
| 28 | Z | 101 | DMU | O1-C10 | 2.28 | 1.47 | 1.41 |
| 20 | B | 301 | TGL | C15-CC9 | -2.28 | 1.38 | 1.51 |
| 25 | G | 102 | CDL | C22-C21 | -2.28 | 1.38 | 1.51 |
| 14 | A | 601 | HEA | CAA-C2A | 2.27 | 1.56 | 1.52 |
| 22 | O | 302 | CHD | C4-C5 | 2.27 | 1.57 | 1.53 |
| 22 | B | 303 | CHD | O3-C3 | 2.27 | 1.50 | 1.43 |
| 28 | M | 101 | DMU | C3-C4 | 2.26 | 1.58 | 1.52 |
| 25 | P | 304 | CDL | C31-CA7 | 2.26 | 1.57 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | A | 607 | PGV | C8-C7 | 2.26 | 1.64 | 1.51 |
| 25 | T | 103 | CDL | C79-C78 | -2.26 | 1.38 | 1.51 |
| 19 | Q | 201 | PGV | C3-C2 | -2.25 | 1.43 | 1.52 |
| 19 | N | 607 | PGV | C8-C7 | 2.25 | 1.64 | 1.51 |
| 22 | P | 305 | CHD | C8-C14 | 2.24 | 1.58 | 1.53 |
| 20 | B | 301 | TGL | CG1-CG2 | 2.24 | 1.57 | 1.50 |
| 25 | G | 102 | CDL | CB6-CB4 | 2.23 | 1.57 | 1.50 |
| 22 | W | 101 | CHD | C16-C17 | 2.22 | 1.59 | 1.54 |
| 26 | P | 308 | PEK | C03-C02 | 2.21 | 1.57 | 1.50 |
| 20 | N | 608 | TGL | CG1-CG2 | 2.20 | 1.57 | 1.50 |
| 19 | A | 607 | PGV | C04-C05 | 2.20 | 1.58 | 1.51 |
| 14 | A | 601 | HEA | CMC-C2C | 2.19 | 1.56 | 1.51 |
| 19 | A | 607 | PGV | O06-C06 | 2.19 | 1.51 | 1.42 |
| 22 | J | 102 | CHD | C6-C7 | 2.17 | 1.56 | 1.52 |
| 26 | G | 101 | PEK | C38-C37 | 2.14 | 1.67 | 1.49 |
| 22 | P | 305 | CHD | C13-C14 | 2.13 | 1.59 | 1.55 |
| 22 | B | 303 | CHD | C1-C10 | 2.12 | 1.57 | 1.54 |
| 19 | A | 607 | PGV | C25-C24 | 2.12 | 1.63 | 1.51 |
| 14 | A | 602 | HEA | C21-C22 | 2.11 | 1.57 | 1.50 |
| 28 | Z | 101 | DMU | O3-C5 | 2.11 | 1.47 | 1.43 |
| 22 | J | 102 | CHD | C6-C5 | 2.09 | 1.57 | 1.53 |
| 20 | Q | 202 | TGL | CC2-CC1 | 2.09 | 1.56 | 1.50 |
| 19 | C | 307 | PGV | C21-C20 | -2.08 | 1.44 | 1.52 |
| 25 | P | 304 | CDL | C11-CA5 | 2.08 | 1.56 | 1.50 |
| 26 | G | 103 | PEK | C01-C02 | 2.08 | 1.57 | 1.50 |
| 22 | C | 304 | CHD | C20-C17 | 2.08 | 1.58 | 1.54 |
| 22 | C | 304 | CHD | C11-C9 | 2.07 | 1.57 | 1.53 |
| 14 | N | 601 | HEA | C3B-C2B | -2.06 | 1.34 | 1.41 |
| 22 | P | 307 | CHD | C13-C17 | 2.05 | 1.59 | 1.55 |
| 22 | W | 101 | CHD | C6-C7 | 2.04 | 1.56 | 1.52 |
| 19 | C | 302 | PGV | O01-C02 | -2.04 | 1.41 | 1.46 |
| 22 | P | 307 | CHD | C8-C14 | 2.04 | 1.57 | 1.53 |
| 19 | P | 303 | PGV | C01-C02 | 2.03 | 1.56 | 1.50 |
| 20 | D | 201 | TGL | CB2-CB1 | 2.03 | 1.56 | 1.50 |
| 20 | Q | 202 | TGL | CC3-CC2 | 2.02 | 1.59 | 1.52 |
| 26 | G | 101 | PEK | P-O12 | -2.00 | 1.51 | 1.59 |

All (716) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | W | 101 | CHD | C17-C13-C12 | 17.08 | 133.26 | 117.67 |
| 20 | D | 201 | TGL | OG2-CB1-CB2 | -15.65 | 77.78 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | W | 101 | CHD | C18-C13-C12 | -13.78 | 95.04 | 109.07 |
| 22 | J | 102 | CHD | C17-C13-C12 | 13.68 | 130.16 | 117.67 |
| 20 | D | 201 | TGL | OG2-CB1-OB1 | 13.55 | 156.45 | 123.70 |
| 26 | T | 101 | PEK | C2-C3-C4 | 13.21 | 136.78 | 113.23 |
| 20 | Q | 202 | TGL | OG2-CB1-CB2 | -12.51 | 84.54 | 111.50 |
| 20 | Q | 202 | TGL | OG2-CB1-OB1 | 11.29 | 150.99 | 123.70 |
| 14 | N | 601 | HEA | C17-C18-C19 | 10.46 | 152.85 | 127.66 |
| 22 | P | 305 | CHD | C18-C13-C12 | -10.04 | 98.84 | 109.07 |
| 22 | J | 102 | CHD | C14-C8-C7 | 10.01 | 125.09 | 111.81 |
| 25 | C | 303 | CDL | C52-C51-CB5 | -9.90 | 77.62 | 113.62 |
| 20 | Y | 101 | TGL | CC4-CC3-CC2 | -9.74 | 78.17 | 113.19 |
| 22 | J | 102 | CHD | C15-C14-C8 | 9.67 | 131.85 | 118.33 |
| 22 | J | 102 | CHD | C13-C17-C20 | 9.58 | 130.94 | 119.50 |
| 20 | L | 101 | TGL | CC4-CC3-CC2 | -9.48 | 79.13 | 113.19 |
| 22 | W | 101 | CHD | C13-C17-C20 | 9.28 | 130.57 | 119.50 |
| 20 | B | 301 | TGL | OG2-CB1-CB2 | 9.24 | 131.43 | 111.50 |
| 22 | C | 304 | CHD | C18-C13-C12 | -9.23 | 99.66 | 109.07 |
| 20 | Y | 101 | TGL | OG2-CB1-CB2 | 8.94 | 130.76 | 111.50 |
| 22 | J | 102 | CHD | C10-C9-C8 | 8.70 | 121.16 | 111.82 |
| 25 | P | 304 | CDL | C52-C51-CB5 | -8.59 | 82.38 | 113.62 |
| 20 | L | 101 | TGL | CG2-OG2-CB1 | 8.35 | 138.36 | 117.79 |
| 19 | C | 302 | PGV | C23-C22-C21 | 8.33 | 156.69 | 114.42 |
| 14 | A | 601 | HEA | C17-C18-C19 | 8.29 | 147.62 | 127.66 |
| 19 | C | 302 | PGV | C22-C21-C20 | 8.18 | 142.59 | 113.19 |
| 20 | Y | 101 | TGL | CG2-OG2-CB1 | 8.03 | 137.57 | 117.79 |
| 20 | B | 301 | TGL | CG3-OG3-CC1 | 7.99 | 146.69 | 117.12 |
| 14 | N | 601 | HEA | C27-C19-C18 | -7.84 | 103.56 | 123.68 |
| 22 | P | 305 | CHD | C6-C7-C8 | 7.71 | 119.71 | 111.48 |
| 22 | C | 304 | CHD | C22-C23-C24 | -7.61 | 97.24 | 113.59 |
| 20 | B | 301 | TGL | OG2-CG2-CG3 | 7.58 | 135.85 | 108.40 |
| 26 | C | 306 | PEK | C36-C35-C34 | -7.51 | 76.28 | 114.42 |
| 22 | C | 305 | CHD | C23-C22-C20 | -7.51 | 104.61 | 114.72 |
| 14 | A | 601 | HEA | C20-C19-C18 | 7.50 | 136.29 | 121.12 |
| 22 | C | 305 | CHD | C22-C23-C24 | -7.46 | 97.56 | 113.59 |
| 23 | O | 303 | PSC | O01-C1-C2 | 7.44 | 127.53 | 111.50 |
| 22 | C | 304 | CHD | C6-C7-C8 | 7.35 | 119.33 | 111.48 |
| 22 | C | 304 | CHD | C16-C17-C20 | 7.31 | 123.47 | 112.15 |
| 22 | W | 101 | CHD | O12-C12-C13 | 7.24 | 123.27 | 111.03 |
| 19 | A | 608 | PGV | C3-C2-C1 | 7.22 | 139.87 | 113.62 |
| 25 | G | 102 | CDL | OA6-CA5-C11 | 7.10 | 126.81 | 111.50 |
| 14 | N | 602 | HEA | C4B-C3B-C2B | 7.08 | 111.82 | 106.87 |
| 14 | N | 601 | HEA | C27-C19-C20 | 7.07 | 127.16 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | C | 305 | CHD | C17-C13-C12 | -6.98 | 111.30 | 117.67 |
| 22 | W | 101 | CHD | C14-C8-C7 | 6.98 | 121.06 | 111.81 |
| 28 | M | 101 | DMU | C28-C25-C22 | -6.95 | 79.15 | 114.42 |
| 22 | P | 305 | CHD | C6-C5-C10 | 6.94 | 120.02 | 112.66 |
| 22 | P | 307 | CHD | C6-C7-C8 | -6.94 | 104.08 | 111.48 |
| 26 | G | 103 | PEK | O01-C1-C2 | 6.89 | 126.35 | 111.50 |
| 22 | P | 305 | CHD | C4-C3-C2 | 6.82 | 118.69 | 110.55 |
| 19 | A | 608 | PGV | O01-C1-C2 | -6.81 | 96.82 | 111.50 |
| 20 | Q | 202 | TGL | CB3-CB2-CB1 | 6.74 | 138.13 | 113.62 |
| 20 | L | 101 | TGL | OG3-CC1-CC2 | 6.68 | 132.86 | 111.91 |
| 22 | C | 304 | CHD | C14-C13-C12 | 6.67 | 113.61 | 107.40 |
| 20 | Y | 101 | TGL | C26-C25-C24 | -6.64 | 80.72 | 114.42 |
| 14 | N | 602 | HEA | CAD-CBD-CGD | -6.64 | 101.53 | 112.67 |
| 25 | G | 102 | CDL | OB6-CB5-C51 | 6.56 | 125.65 | 111.50 |
| 22 | W | 101 | CHD | C17-C13-C14 | -6.56 | 93.48 | 100.09 |
| 22 | B | 303 | CHD | C11-C12-C13 | -6.54 | 104.53 | 111.24 |
| 22 | C | 304 | CHD | C6-C5-C4 | -6.53 | 103.68 | 111.19 |
| 22 | J | 102 | CHD | C18-C13-C12 | -6.50 | 102.45 | 109.07 |
| 22 | W | 101 | CHD | C11-C12-C13 | 6.49 | 117.91 | 111.24 |
| 22 | J | 102 | CHD | C11-C12-C13 | 6.49 | 117.91 | 111.24 |
| 22 | C | 304 | CHD | C6-C5-C10 | 6.46 | 119.52 | 112.66 |
| 22 | C | 304 | CHD | C15-C14-C8 | 6.43 | 127.33 | 118.33 |
| 26 | T | 102 | PEK | O01-C1-C2 | 6.42 | 125.34 | 111.50 |
| 22 | C | 304 | CHD | C10-C9-C8 | 6.42 | 118.71 | 111.82 |
| 19 | P | 301 | PGV | O03-C19-C20 | 6.39 | 131.96 | 111.91 |
| 23 | B | 304 | PSC | O01-C1-C2 | 6.38 | 125.26 | 111.50 |
| 22 | J | 102 | CHD | C5-C6-C7 | 6.37 | 121.49 | 114.46 |
| 20 | N | 608 | TGL | CG2-OG2-CB1 | 6.36 | 133.44 | 117.79 |
| 22 | P | 307 | CHD | C22-C23-C24 | -6.32 | 100.00 | 113.59 |
| 14 | A | 602 | HEA | C13-C12-C11 | -6.31 | 104.87 | 114.35 |
| 22 | C | 305 | CHD | C6-C7-C8 | -6.29 | 104.77 | 111.48 |
| 22 | P | 307 | CHD | C23-C22-C20 | -6.25 | 106.30 | 114.72 |
| 14 | N | 601 | HEA | CMB-C2B-C1B | -6.17 | 118.98 | 128.46 |
| 20 | D | 201 | TGL | CB3-CB2-CB1 | 6.15 | 136.00 | 113.62 |
| 20 | B | 301 | TGL | OG1-CA1-CA2 | 6.03 | 130.84 | 111.91 |
| 19 | C | 307 | PGV | O03-C19-C20 | 6.03 | 130.82 | 111.91 |
| 22 | J | 102 | CHD | C6-C5-C10 | 6.02 | 119.05 | 112.66 |
| 22 | C | 304 | CHD | C4-C5-C10 | 5.98 | 119.00 | 112.66 |
| 25 | P | 304 | CDL | OB8-CB7-C71 | 5.94 | 130.54 | 111.91 |
| 22 | P | 305 | CHD | O7-C7-C6 | -5.92 | 95.25 | 109.94 |
| 19 | A | 608 | PGV | O01-C1-O02 | 5.92 | 138.00 | 123.70 |
| 25 | P | 304 | CDL | OA6-CA5-C11 | 5.87 | 124.15 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | C | 304 | CHD | O7-C7-C6 | -5.85 | 95.42 | 109.94 |
| 25 | C | 303 | CDL | OA6-CA5-C11 | 5.83 | 124.06 | 111.50 |
| 20 | N | 608 | TGL | OG2-CG2-CG3 | 5.81 | 129.44 | 108.40 |
| 22 | C | 304 | CHD | C19-C10-C1 | -5.79 | 98.93 | 108.26 |
| 20 | Q | 202 | TGL | CG3-CG2-CG1 | -5.77 | 98.15 | 111.79 |
| 19 | A | 608 | PGV | C02-O01-C1 | 5.74 | 131.93 | 117.79 |
| 20 | B | 301 | TGL | OG3-CG3-CG2 | -5.72 | 91.79 | 108.43 |
| 25 | T | 103 | CDL | OA6-CA5-C11 | 5.72 | 123.83 | 111.50 |
| 20 | Y | 101 | TGL | CB3-CB2-CB1 | 5.66 | 134.20 | 113.62 |
| 25 | C | 303 | CDL | OB8-CB7-C71 | 5.64 | 129.62 | 111.91 |
| 20 | N | 608 | TGL | CG3-OG3-CC1 | 5.64 | 138.02 | 117.12 |
| 20 | Y | 101 | TGL | OG3-CC1-CC2 | 5.55 | 129.34 | 111.91 |
| 20 | D | 201 | TGL | OC1-CC1-CC2 | 5.50 | 145.21 | 123.73 |
| 25 | P | 304 | CDL | CA4-OA6-CA5 | 5.48 | 131.29 | 117.79 |
| 20 | N | 608 | TGL | OG1-CA1-CA2 | 5.46 | 129.03 | 111.91 |
| 22 | P | 307 | CHD | C21-C20-C22 | -5.45 | 101.81 | 110.36 |
| 22 | C | 305 | CHD | C18-C13-C12 | 5.44 | 114.61 | 109.07 |
| 22 | B | 303 | CHD | C5-C4-C3 | -5.41 | 104.81 | 112.76 |
| 22 | C | 304 | CHD | C16-C17-C13 | 5.40 | 108.85 | 103.55 |
| 22 | P | 307 | CHD | C17-C13-C12 | -5.38 | 112.75 | 117.67 |
| 25 | T | 103 | CDL | OB6-CB5-C51 | 5.37 | 123.07 | 111.50 |
| 26 | P | 308 | PEK | O03-C21-C22 | 5.36 | 128.74 | 111.91 |
| 22 | P | 305 | CHD | C15-C14-C13 | 5.28 | 108.74 | 103.55 |
| 22 | B | 303 | CHD | C19-C10-C1 | -5.26 | 99.79 | 108.26 |
| 22 | O | 302 | CHD | C5-C4-C3 | -5.23 | 105.08 | 112.76 |
| 22 | J | 102 | CHD | C9-C8-C7 | 5.20 | 118.10 | 111.88 |
| 28 | M | 101 | DMU | O5-C4-C3 | -5.20 | 98.79 | 109.75 |
| 14 | A | 601 | HEA | CMB-C2B-C1B | -5.16 | 120.53 | 128.46 |
| 26 | C | 306 | PEK | O03-C21-O04 | -5.16 | 110.58 | 123.59 |
| 20 | L | 101 | TGL | OG2-CB1-CB2 | 5.12 | 122.53 | 111.50 |
| 14 | A | 601 | HEA | C27-C19-C18 | -5.04 | 110.76 | 123.68 |
| 22 | P | 305 | CHD | C6-C5-C4 | -5.03 | 105.39 | 111.19 |
| 20 | D | 201 | TGL | C21-C20-CA9 | 5.03 | 139.94 | 114.42 |
| 14 | N | 601 | HEA | CMB-C2B-C3B | 5.00 | 134.48 | 124.69 |
| 14 | A | 602 | HEA | CAD-CBD-CGD | -4.98 | 104.32 | 112.67 |
| 22 | P | 305 | CHD | C10-C9-C8 | 4.97 | 117.16 | 111.82 |
| 22 | W | 101 | CHD | C4-C5-C10 | 4.96 | 117.93 | 112.66 |
| 22 | O | 302 | CHD | C6-C5-C4 | -4.94 | 105.50 | 111.19 |
| 20 | L | 101 | TGL | C22-C21-C20 | -4.93 | 89.39 | 114.42 |
| 14 | N | 602 | HEA | C13-C12-C11 | -4.93 | 106.94 | 114.35 |
| 22 | O | 302 | CHD | C2-C1-C10 | -4.92 | 104.34 | 112.78 |
| 19 | C | 302 | PGV | C30-C29-C28 | -4.86 | 89.77 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | O | 302 | CHD | C15-C14-C8 | -4.85 | 111.55 | 118.33 |
| 22 | W | 101 | CHD | C23-C22-C20 | 4.85 | 121.25 | 114.72 |
| 20 | Y | 101 | TGL | OG3-CG3-CG2 | 4.81 | 122.43 | 108.43 |
| 20 | B | 301 | TGL | OG3-CC1-CC2 | 4.80 | 126.98 | 111.91 |
| 20 | D | 201 | TGL | CG1-OG1-CA1 | 4.79 | 134.88 | 117.12 |
| 26 | C | 306 | PEK | O01-C1-C2 | 4.78 | 121.80 | 111.50 |
| 20 | N | 608 | TGL | OG2-CB1-CB2 | 4.78 | 121.79 | 111.50 |
| 14 | A | 601 | HEA | CMB-C2B-C3B | 4.77 | 134.03 | 124.69 |
| 22 | P | 305 | CHD | C16-C17-C13 | 4.76 | 108.23 | 103.55 |
| 20 | L | 101 | TGL | OG3-CC1-OC1 | -4.74 | 111.62 | 123.59 |
| 20 | L | 101 | TGL | OG1-CG1-CG2 | 4.73 | 122.21 | 108.43 |
| 22 | O | 302 | CHD | C19-C10-C1 | -4.73 | 100.64 | 108.26 |
| 22 | P | 305 | CHD | C14-C8-C9 | -4.72 | 103.24 | 109.71 |
| 22 | P | 307 | CHD | C22-C20-C17 | -4.71 | 100.55 | 110.28 |
| 23 | O | 303 | PSC | C28-C27-C26 | -4.69 | 90.61 | 114.42 |
| 20 | B | 301 | TGL | CB3-CB2-CB1 | -4.68 | 96.59 | 113.62 |
| 22 | C | 304 | CHD | C17-C13-C14 | -4.68 | 95.37 | 100.09 |
| 22 | J | 102 | CHD | C1-C10-C9 | -4.68 | 104.00 | 111.35 |
| 22 | C | 304 | CHD | C5-C6-C7 | 4.67 | 119.61 | 114.46 |
| 20 | B | 301 | TGL | CG2-OG2-CB1 | 4.61 | 129.15 | 117.79 |
| 28 | Z | 101 | DMU | C28-C25-C22 | -4.60 | 91.06 | 114.42 |
| 25 | C | 303 | CDL | C53-C52-C51 | -4.59 | 96.69 | 113.19 |
| 19 | Q | 201 | PGV | C5-C4-C3 | -4.58 | 91.17 | 114.42 |
| 22 | W | 101 | CHD | C15-C14-C8 | 4.58 | 124.73 | 118.33 |
| 20 | N | 608 | TGL | OG1-CA1-OA1 | -4.57 | 112.06 | 123.59 |
| 22 | B | 303 | CHD | C15-C14-C13 | 4.55 | 108.02 | 103.55 |
| 22 | J | 102 | CHD | C23-C22-C20 | 4.54 | 120.84 | 114.72 |
| 22 | P | 305 | CHD | C4-C5-C10 | 4.53 | 117.47 | 112.66 |
| 26 | P | 308 | PEK | C02-O01-C1 | 4.52 | 128.93 | 117.79 |
| 25 | C | 303 | CDL | OB6-CB5-C51 | 4.52 | 121.25 | 111.50 |
| 22 | J | 102 | CHD | O12-C12-C13 | 4.52 | 118.67 | 111.03 |
| 20 | D | 201 | TGL | CB5-CB4-CB3 | 4.52 | 137.35 | 114.42 |
| 20 | B | 301 | TGL | CB4-CB3-CB2 | -4.51 | 96.99 | 113.19 |
| 26 | P | 308 | PEK | O03-C21-O04 | -4.50 | 112.25 | 123.59 |
| 20 | L | 101 | TGL | CB3-CB2-CB1 | 4.48 | 129.92 | 113.62 |
| 22 | J | 102 | CHD | C2-C1-C10 | 4.47 | 120.45 | 112.78 |
| 26 | C | 306 | PEK | C24-C23-C22 | 4.47 | 129.26 | 113.19 |
| 25 | C | 303 | CDL | C76-C75-C74 | -4.46 | 91.79 | 114.42 |
| 22 | B | 303 | CHD | O3-C3-C4 | -4.43 | 101.03 | 109.85 |
| 25 | T | 103 | CDL | CA4-OA6-CA5 | 4.42 | 128.67 | 117.79 |
| 20 | D | 201 | TGL | OG3-CC1-OC1 | -4.41 | 112.46 | 123.59 |
| 22 | P | 307 | CHD | C1-C10-C5 | 4.39 | 114.26 | 107.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | C | 303 | CDL | OB5-PB2-OB3 | 4.37 | 126.15 | 109.07 |
| 19 | C | 307 | PGV | O03-C01-C02 | 4.37 | 121.16 | 108.43 |
| 22 | J | 102 | CHD | C6-C5-C4 | -4.37 | 106.16 | 111.19 |
| 25 | C | 303 | CDL | CB6-CB4-CB3 | -4.36 | 101.46 | 111.79 |
| 22 | B | 303 | CHD | C2-C1-C10 | -4.35 | 105.31 | 112.78 |
| 22 | W | 101 | CHD | C10-C9-C8 | 4.35 | 116.49 | 111.82 |
| 22 | J | 102 | CHD | C9-C10-C5 | 4.34 | 114.68 | 108.58 |
| 22 | J | 102 | CHD | C14-C13-C12 | -4.33 | 103.37 | 107.40 |
| 22 | B | 303 | CHD | C6-C5-C4 | -4.33 | 106.20 | 111.19 |
| 22 | O | 302 | CHD | C17-C13-C14 | 4.31 | 104.44 | 100.09 |
| 22 | J | 102 | CHD | C5-C4-C3 | 4.30 | 119.07 | 112.76 |
| 25 | T | 103 | CDL | OB8-CB6-CB4 | 4.28 | 120.88 | 108.43 |
| 28 | J | 101 | DMU | O16-C6-C1 | 4.28 | 114.98 | 108.30 |
| 19 | C | 302 | PGV | C28-C27-C26 | -4.27 | 92.74 | 114.42 |
| 20 | N | 608 | TGL | CB3-CB2-CB1 | 4.27 | 129.15 | 113.62 |
| 14 | N | 602 | HEA | CAA-CBA-CGA | -4.27 | 105.51 | 112.67 |
| 22 | J | 102 | CHD | C1-C2-C3 | 4.25 | 115.93 | 110.47 |
| 26 | G | 101 | PEK | C24-C23-C22 | -4.24 | 97.93 | 113.19 |
| 26 | G | 101 | PEK | O04-C21-C22 | 4.24 | 140.28 | 123.73 |
| 22 | J | 102 | CHD | C4-C3-C2 | 4.22 | 115.60 | 110.55 |
| 22 | J | 102 | CHD | C17-C13-C14 | -4.21 | 95.85 | 100.09 |
| 22 | B | 303 | CHD | C15-C14-C8 | -4.20 | 112.46 | 118.33 |
| 20 | B | 301 | TGL | OG3-CC1-OC1 | -4.20 | 113.00 | 123.59 |
| 20 | Y | 101 | TGL | CA4-CA3-CA2 | -4.19 | 98.13 | 113.19 |
| 28 | P | 306 | DMU | O1-C10-C5 | -4.17 | 101.52 | 110.35 |
| 20 | Y | 101 | TGL | CA8-CA7-CA6 | -4.16 | 93.33 | 114.42 |
| 26 | C | 306 | PEK | C02-O01-C1 | 4.15 | 128.01 | 117.79 |
| 22 | P | 307 | CHD | C14-C8-C7 | -4.13 | 106.33 | 111.81 |
| 26 | P | 308 | PEK | C24-C23-C22 | 4.13 | 128.02 | 113.19 |
| 22 | C | 305 | CHD | C22-C20-C17 | -4.12 | 101.77 | 110.28 |
| 19 | A | 608 | PGV | O03-C19-C20 | 4.12 | 124.83 | 111.91 |
| 25 | C | 303 | CDL | OB8-CB6-CB4 | -4.11 | 96.47 | 108.43 |
| 20 | Y | 101 | TGL | CG3-OG3-CC1 | 4.10 | 132.31 | 117.12 |
| 28 | M | 101 | DMU | C18-O16-C6 | -4.09 | 107.05 | 113.84 |
| 22 | W | 101 | CHD | C4-C3-C2 | 4.09 | 115.43 | 110.55 |
| 14 | A | 602 | HEA | C27-C19-C20 | 4.08 | 122.14 | 115.27 |
| 22 | C | 305 | CHD | C16-C17-C13 | -4.07 | 99.56 | 103.55 |
| 22 | C | 305 | CHD | C11-C9-C10 | -4.07 | 109.53 | 113.73 |
| 25 | T | 103 | CDL | OA8-CA7-C31 | 4.06 | 124.64 | 111.91 |
| 28 | M | 101 | DMU | O5-C6-O16 | -4.05 | 100.38 | 109.97 |
| 14 | A | 602 | HEA | C20-C19-C18 | -4.04 | 112.94 | 121.12 |
| 20 | L | 101 | TGL | C20-CA9-CA8 | -4.04 | 93.93 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 26 | C | 306 | PEK | C03-C02-C01 | -4.03 | 102.25 | 111.79 |
| 22 | W | 101 | CHD | C5-C4-C3 | 4.02 | 118.66 | 112.76 |
| 23 | B | 304 | PSC | C32-C31-C30 | -4.01 | 94.07 | 114.42 |
| 22 | B | 303 | CHD | C9-C11-C12 | 4.01 | 119.59 | 114.30 |
| 25 | G | 102 | CDL | OA6-CA5-OA7 | -4.00 | 114.03 | 123.70 |
| 20 | L | 101 | TGL | CA4-CA3-CA2 | -4.00 | 98.80 | 113.19 |
| 14 | N | 602 | HEA | C1B-C2B-C3B | -3.99 | 104.22 | 107.00 |
| 22 | J | 102 | CHD | C1-C10-C5 | 3.98 | 113.65 | 107.77 |
| 19 | Q | 201 | PGV | C8-C7-C6 | -3.97 | 94.25 | 114.42 |
| 14 | N | 601 | HEA | C20-C19-C18 | 3.97 | 129.15 | 121.12 |
| 22 | W | 101 | CHD | C11-C9-C10 | 3.96 | 117.81 | 113.73 |
| 25 | G | 102 | CDL | OB8-CB6-CB4 | 3.95 | 119.94 | 108.43 |
| 28 | Z | 101 | DMU | O55-C2-C1 | -3.94 | 101.25 | 110.35 |
| 19 | Q | 201 | PGV | C3-C2-C1 | -3.93 | 99.31 | 113.62 |
| 22 | W | 101 | CHD | C22-C20-C17 | 3.93 | 118.40 | 110.28 |
| 22 | O | 302 | CHD | C16-C17-C13 | -3.91 | 99.71 | 103.55 |
| 26 | P | 308 | PEK | O01-C1-C2 | 3.91 | 119.94 | 111.50 |
| 22 | P | 305 | CHD | C19-C10-C9 | -3.91 | 105.80 | 111.18 |
| 20 | N | 608 | TGL | OG2-CB1-OB1 | -3.90 | 114.28 | 123.70 |
| 22 | J | 102 | CHD | C9-C11-C12 | -3.89 | 109.16 | 114.30 |
| 20 | Q | 202 | TGL | OG3-CC1-OC1 | -3.88 | 113.81 | 123.59 |
| 25 | G | 102 | CDL | OA8-CA7-C31 | 3.86 | 124.03 | 111.91 |
| 25 | C | 303 | CDL | C77-C76-C75 | -3.86 | 94.82 | 114.42 |
| 22 | J | 102 | CHD | C22-C20-C17 | 3.86 | 118.26 | 110.28 |
| 19 | Q | 201 | PGV | O01-C02-C01 | 3.86 | 122.37 | 108.40 |
| 28 | P | 306 | DMU | O1-C9-C8 | 3.86 | 116.69 | 109.69 |
| 22 | C | 305 | CHD | C14-C8-C7 | -3.85 | 106.70 | 111.81 |
| 20 | B | 301 | TGL | CB5-CB4-CB3 | -3.82 | 95.03 | 114.42 |
| 26 | T | 101 | PEK | C3-C2-C1 | -3.80 | 99.78 | 113.62 |
| 20 | L | 101 | TGL | CG3-OG3-CC1 | 3.80 | 131.20 | 117.12 |
| 19 | P | 301 | PGV | O04-C19-C20 | -3.79 | 108.94 | 123.73 |
| 25 | P | 304 | CDL | OA4-PA1-OA3 | 3.79 | 130.96 | 112.24 |
| 25 | C | 303 | CDL | C73-C72-C71 | -3.77 | 99.65 | 113.19 |
| 20 | Y | 101 | TGL | OG1-CA1-CA2 | 3.77 | 123.73 | 111.91 |
| 19 | A | 607 | PGV | C34-C33-C32 | -3.75 | 84.93 | 113.42 |
| 20 | L | 101 | TGL | C24-C23-C22 | -3.73 | 95.47 | 114.42 |
| 19 | A | 608 | PGV | O01-C02-C01 | 3.71 | 121.84 | 108.40 |
| 28 | P | 306 | DMU | O7-C10-C5 | 3.70 | 117.69 | 108.10 |
| 20 | B | 301 | TGL | OG2-CB1-OB1 | -3.70 | 114.76 | 123.70 |
| 26 | T | 102 | PEK | C2-C3-C4 | 3.69 | 119.81 | 113.23 |
| 22 | P | 305 | CHD | C19-C10-C1 | -3.69 | 102.31 | 108.26 |
| 25 | C | 303 | CDL | OB4-PB2-OB5 | -3.69 | 90.60 | 107.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | A | 608 | PGV | C23-C22-C21 | -3.68 | 95.75 | 114.42 |
| 19 | Q | 201 | PGV | C01-O03-C19 | 3.67 | 130.72 | 117.12 |
| 25 | G | 102 | CDL | OA8-CA7-OA9 | -3.67 | 114.34 | 123.59 |
| 19 | A | 608 | PGV | C01-O03-C19 | 3.66 | 130.69 | 117.12 |
| 26 | C | 306 | PEK | O03-C21-C22 | 3.65 | 123.37 | 111.91 |
| 26 | G | 103 | PEK | O03-C01-C02 | 3.64 | 119.02 | 108.43 |
| 25 | P | 304 | CDL | O1-C1-CB2 | 3.64 | 122.31 | 109.56 |
| 28 | M | 101 | DMU | C31-C28-C25 | -3.63 | 95.98 | 114.42 |
| 25 | C | 303 | CDL | OB6-CB5-OB7 | -3.63 | 114.92 | 123.70 |
| 22 | P | 305 | CHD | C14-C13-C12 | 3.63 | 110.78 | 107.40 |
| 20 | D | 201 | TGL | CG3-OG3-CC1 | 3.62 | 130.54 | 117.12 |
| 22 | B | 303 | CHD | O12-C12-C13 | -3.61 | 104.92 | 111.03 |
| 28 | Z | 101 | DMU | C6-C1-C2 | -3.60 | 102.49 | 110.00 |
| 20 | Y | 101 | TGL | CB5-CB4-CB3 | -3.60 | 96.17 | 114.42 |
| 20 | L | 101 | TGL | OG2-CG2-CG3 | 3.59 | 121.40 | 108.40 |
| 26 | C | 306 | PEK | C26-C25-C24 | 3.59 | 132.63 | 114.42 |
| 25 | C | 303 | CDL | C39-C38-C37 | 3.58 | 132.61 | 114.42 |
| 23 | B | 304 | PSC | C28-C27-C26 | -3.58 | 96.27 | 114.42 |
| 25 | P | 304 | CDL | C54-C53-C52 | 3.57 | 132.57 | 114.42 |
| 19 | Q | 201 | PGV | O01-C1-C2 | 3.57 | 119.20 | 111.50 |
| 20 | Y | 101 | TGL | CG1-OG1-CA1 | 3.57 | 130.34 | 117.12 |
| 22 | J | 102 | CHD | C14-C8-C9 | -3.57 | 104.82 | 109.71 |
| 22 | P | 305 | CHD | O3-C3-C4 | -3.57 | 102.75 | 109.85 |
| 14 | A | 601 | HEA | CAA-CBA-CGA | -3.55 | 106.71 | 112.67 |
| 14 | N | 602 | HEA | CBA-CAA-C2A | -3.55 | 105.94 | 112.48 |
| 22 | O | 302 | CHD | O3-C3-C4 | -3.54 | 102.81 | 109.85 |
| 20 | L | 101 | TGL | C26-C25-C24 | -3.54 | 96.47 | 114.42 |
| 22 | J | 102 | CHD | C6-C7-C8 | 3.53 | 115.24 | 111.48 |
| 22 | B | 303 | CHD | C14-C13-C12 | 3.52 | 110.68 | 107.40 |
| 26 | P | 308 | PEK | C36-C35-C34 | -3.52 | 96.55 | 114.42 |
| 22 | W | 101 | CHD | C1-C10-C5 | 3.52 | 112.97 | 107.77 |
| 14 | A | 601 | HEA | C13-C12-C11 | -3.50 | 109.09 | 114.35 |
| 28 | P | 306 | DMU | O3-C5-C10 | 3.50 | 118.54 | 110.05 |
| 28 | Z | 101 | DMU | C18-O16-C6 | -3.49 | 108.05 | 113.84 |
| 28 | Z | 101 | DMU | O49-C1-C6 | -3.46 | 101.63 | 110.05 |
| 14 | N | 601 | HEA | CAA-CBA-CGA | -3.45 | 106.88 | 112.67 |
| 20 | L | 101 | TGL | CA5-CA4-CA3 | -3.45 | 96.89 | 114.42 |
| 26 | P | 308 | PEK | C35-C34-C33 | 3.45 | 131.91 | 114.42 |
| 22 | C | 305 | CHD | C15-C14-C8 | -3.43 | 113.53 | 118.33 |
| 19 | P | 301 | PGV | C03-C02-C01 | -3.43 | 103.66 | 111.79 |
| 20 | B | 301 | TGL | OA1-CA1-CA2 | -3.43 | 110.35 | 123.73 |
| 25 | C | 303 | CDL | OB6-CB4-CB3 | -3.43 | 95.99 | 108.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | G | 102 | CDL | CA4-OA6-CA5 | 3.42 | 126.20 | 117.79 |
| 19 | A | 607 | PGV | C30-C29-C28 | 3.41 | 131.76 | 114.42 |
| 20 | Y | 101 | TGL | OB1-CB1-CB2 | -3.41 | 110.44 | 123.73 |
| 28 | P | 306 | DMU | O6-C11-C9 | -3.41 | 99.61 | 111.29 |
| 19 | N | 607 | PGV | O02-C1-C2 | 3.40 | 137.01 | 123.73 |
| 25 | G | 102 | CDL | C80-C79-C78 | 3.39 | 131.62 | 114.42 |
| 22 | O | 302 | CHD | C14-C8-C9 | -3.38 | 105.07 | 109.71 |
| 22 | W | 101 | CHD | C21-C20-C22 | 3.38 | 115.66 | 110.36 |
| 23 | B | 304 | PSC | C08-N-C07 | -3.37 | 100.31 | 108.97 |
| 28 | P | 306 | DMU | O16-C6-C1 | 3.37 | 113.56 | 108.30 |
| 20 | D | 201 | TGL | CA4-CA3-CA2 | 3.37 | 125.29 | 113.19 |
| 14 | A | 602 | HEA | C4B-C3B-C2B | 3.34 | 109.20 | 106.87 |
| 22 | P | 305 | CHD | C15-C14-C8 | 3.34 | 123.00 | 118.33 |
| 14 | A | 602 | HEA | C16-C15-C14 | -3.33 | 114.39 | 121.12 |
| 19 | P | 301 | PGV | C02-O01-C1 | 3.32 | 125.97 | 117.79 |
| 25 | P | 304 | CDL | OB2-PB2-OB3 | 3.31 | 122.00 | 109.07 |
| 25 | P | 304 | CDL | CB4-OB6-CB5 | -3.30 | 109.67 | 117.79 |
| 28 | Z | 101 | DMU | O5-C6-O16 | -3.30 | 102.17 | 109.97 |
| 22 | O | 302 | CHD | O7-C7-C8 | 3.29 | 116.77 | 109.43 |
| 23 | B | 304 | PSC | C29-C28-C27 | -3.29 | 97.74 | 114.42 |
| 19 | P | 303 | PGV | C27-C26-C25 | -3.28 | 97.78 | 114.42 |
| 22 | C | 305 | CHD | C9-C11-C12 | -3.27 | 109.98 | 114.30 |
| 19 | A | 608 | PGV | O04-C19-C20 | -3.27 | 110.96 | 123.73 |
| 28 | M | 101 | DMU | C22-C19-C18 | -3.27 | 99.01 | 113.49 |
| 22 | O | 302 | CHD | C14-C13-C12 | -3.26 | 104.36 | 107.40 |
| 14 | A | 601 | HEA | CMC-C2C-C1C | -3.26 | 123.45 | 128.46 |
| 22 | P | 305 | CHD | C5-C6-C7 | 3.25 | 118.05 | 114.46 |
| 22 | C | 304 | CHD | C4-C3-C2 | 3.25 | 114.43 | 110.55 |
| 20 | Q | 202 | TGL | C16-C15-CC9 | 3.25 | 130.91 | 114.42 |
| 22 | P | 305 | CHD | C21-C20-C22 | 3.24 | 115.44 | 110.36 |
| 25 | P | 304 | CDL | C78-C77-C76 | -3.22 | 98.07 | 114.42 |
| 22 | W | 101 | CHD | C13-C14-C8 | 3.22 | 118.85 | 114.74 |
| 22 | P | 305 | CHD | O12-C12-C13 | 3.21 | 116.46 | 111.03 |
| 14 | N | 602 | HEA | C26-C15-C16 | 3.20 | 120.66 | 115.27 |
| 25 | T | 103 | CDL | CB6-OB8-CB7 | 3.19 | 128.94 | 117.12 |
| 26 | P | 308 | PEK | C27-C26-C25 | 3.19 | 130.62 | 114.42 |
| 19 | P | 303 | PGV | C03-C02-C01 | -3.19 | 104.25 | 111.79 |
| 22 | P | 307 | CHD | C11-C12-C13 | -3.18 | 107.97 | 111.24 |
| 22 | B | 303 | CHD | C6-C7-C8 | 3.18 | 114.88 | 111.48 |
| 22 | P | 307 | CHD | O7-C7-C8 | 3.18 | 116.54 | 109.43 |
| 23 | O | 303 | PSC | C29-C28-C27 | -3.18 | 98.30 | 114.42 |
| 20 | Q | 202 | TGL | C21-C20-CA9 | 3.16 | 130.48 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | N | 601 | HEA | OMA-CMA-C3A | -3.16 | 118.02 | 124.91 |
| 22 | B | 303 | CHD | C5-C6-C7 | -3.16 | 110.97 | 114.46 |
| 25 | C | 303 | CDL | CA6-OA8-CA7 | 3.16 | 128.82 | 117.12 |
| 28 | J | 101 | DMU | C28-C25-C22 | 3.15 | 130.40 | 114.42 |
| 25 | G | 102 | CDL | C40-C39-C38 | 3.15 | 130.40 | 114.42 |
| 22 | P | 305 | CHD | C17-C13-C12 | 3.14 | 120.54 | 117.67 |
| 20 | B | 301 | TGL | C15-CC9-CC8 | 3.14 | 130.38 | 114.42 |
| 19 | A | 608 | PGV | O14-P-O11 | -3.14 | 93.15 | 107.75 |
| 25 | T | 103 | CDL | CA6-CA4-CA3 | -3.14 | 104.36 | 111.79 |
| 25 | G | 102 | CDL | CB6-OB8-CB7 | 3.13 | 128.73 | 117.12 |
| 19 | A | 608 | PGV | C27-C26-C25 | -3.13 | 98.56 | 114.42 |
| 25 | C | 303 | CDL | C42-C41-C40 | 3.12 | 130.28 | 114.42 |
| 25 | P | 304 | CDL | C32-C31-CA7 | 3.12 | 124.96 | 113.62 |
| 20 | D | 201 | TGL | OG3-CC1-CC2 | -3.12 | 102.12 | 111.91 |
| 26 | T | 102 | PEK | O03-C21-C22 | 3.12 | 121.69 | 111.91 |
| 20 | D | 201 | TGL | C14-C13-C12 | 3.12 | 130.25 | 114.42 |
| 25 | P | 304 | CDL | OA6-CA4-CA3 | 3.11 | 119.65 | 108.40 |
| 26 | G | 103 | PEK | C01-O03-C21 | 3.11 | 128.62 | 117.12 |
| 25 | T | 103 | CDL | C83-C82-C81 | 3.10 | 130.18 | 114.42 |
| 19 | Q | 201 | PGV | C4-C3-C2 | 3.10 | 124.34 | 113.19 |
| 23 | B | 304 | PSC | C31-C30-C29 | 3.09 | 130.13 | 114.42 |
| 26 | G | 101 | PEK | C30-C29-C28 | 3.09 | 130.13 | 114.42 |
| 25 | P | 304 | CDL | CA6-OA8-CA7 | 3.09 | 128.55 | 117.12 |
| 19 | C | 307 | PGV | O03-C19-O04 | -3.08 | 115.81 | 123.59 |
| 22 | W | 101 | CHD | O7-C7-C8 | 3.08 | 116.31 | 109.43 |
| 25 | P | 304 | CDL | OB8-CB7-OB9 | -3.08 | 115.82 | 123.59 |
| 25 | C | 303 | CDL | OB9-CB7-C71 | -3.08 | 111.72 | 123.73 |
| 20 | N | 608 | TGL | OG1-CG1-CG2 | 3.07 | 117.37 | 108.43 |
| 22 | C | 305 | CHD | C1-C10-C5 | 3.06 | 112.30 | 107.77 |
| 14 | N | 601 | HEA | C20-C21-C22 | 3.06 | 121.95 | 111.88 |
| 22 | C | 304 | CHD | C18-C13-C17 | 3.06 | 116.00 | 111.21 |
| 19 | P | 301 | PGV | O01-C1-C2 | 3.05 | 118.07 | 111.50 |
| 28 | M | 101 | DMU | O16-C6-C1 | -3.05 | 103.54 | 108.30 |
| 20 | L | 101 | TGL | C12-C11-C10 | -3.04 | 99.00 | 114.42 |
| 22 | P | 305 | CHD | C18-C13-C14 | 3.04 | 115.96 | 111.21 |
| 23 | B | 304 | PSC | C22-C21-C20 | 3.04 | 124.11 | 113.19 |
| 23 | B | 304 | PSC | C27-C26-C25 | -3.03 | 99.02 | 114.42 |
| 14 | N | 602 | HEA | C3C-C4C-NC | 3.03 | 113.12 | 109.21 |
| 22 | P | 305 | CHD | C1-C10-C5 | 3.03 | 112.24 | 107.77 |
| 23 | O | 303 | PSC | O01-C02-C03 | 3.02 | 119.33 | 108.40 |
| 20 | N | 608 | TGL | C11-C10-CB9 | 3.02 | 129.74 | 114.42 |
| 26 | G | 101 | PEK | O03-C21-C22 | -3.01 | 102.45 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | W | 101 | CHD | C19-C10-C1 | -3.01 | 103.41 | 108.26 |
| 20 | D | 201 | TGL | OG1-CA1-CA2 | 3.01 | 121.36 | 111.91 |
| 25 | G | 102 | CDL | C23-C22-C21 | 3.01 | 129.70 | 114.42 |
| 14 | N | 601 | HEA | C3C-C4C-NC | 3.01 | 113.10 | 109.21 |
| 22 | P | 307 | CHD | C13-C17-C20 | -3.01 | 115.91 | 119.50 |
| 25 | C | 303 | CDL | OA8-CA7-C31 | 3.00 | 121.33 | 111.91 |
| 25 | P | 304 | CDL | C72-C71-CB7 | 3.00 | 124.52 | 113.62 |
| 25 | P | 304 | CDL | C73-C72-C71 | -3.00 | 102.42 | 113.19 |
| 26 | P | 308 | PEK | O03-C01-C02 | 2.99 | 117.14 | 108.43 |
| 14 | A | 601 | HEA | CBA-CAA-C2A | -2.99 | 106.98 | 112.48 |
| 26 | T | 101 | PEK | O03-C21-C22 | 2.98 | 121.27 | 111.91 |
| 22 | C | 305 | CHD | C14-C8-C9 | -2.98 | 105.62 | 109.71 |
| 25 | P | 304 | CDL | OB6-CB4-CB3 | -2.98 | 97.63 | 108.40 |
| 20 | L | 101 | TGL | CC3-CC2-CC1 | 2.97 | 124.42 | 113.62 |
| 14 | A | 601 | HEA | C20-C21-C22 | -2.97 | 102.12 | 111.88 |
| 19 | P | 301 | PGV | C21-C20-C19 | -2.97 | 102.82 | 113.62 |
| 22 | B | 303 | CHD | C11-C9-C8 | -2.96 | 106.55 | 110.88 |
| 28 | Z | 101 | DMU | O16-C6-C1 | -2.95 | 103.70 | 108.30 |
| 23 | O | 303 | PSC | O01-C1-O02 | -2.95 | 116.58 | 123.70 |
| 20 | Q | 202 | TGL | OC1-CC1-CC2 | 2.94 | 135.21 | 123.73 |
| 22 | J | 102 | CHD | C4-C5-C10 | 2.94 | 115.78 | 112.66 |
| 14 | A | 601 | HEA | C27-C19-C20 | -2.94 | 110.33 | 115.27 |
| 20 | Y | 101 | TGL | C23-C22-C21 | -2.93 | 99.54 | 114.42 |
| 26 | T | 101 | PEK | O02-C1-C2 | 2.91 | 135.10 | 123.73 |
| 14 | N | 602 | HEA | C16-C15-C14 | -2.91 | 115.22 | 121.12 |
| 14 | N | 602 | HEA | C12-C13-C14 | -2.91 | 104.56 | 112.23 |
| 22 | J | 102 | CHD | C13-C14-C8 | -2.90 | 111.03 | 114.74 |
| 25 | P | 304 | CDL | C39-C38-C37 | 2.90 | 129.13 | 114.42 |
| 22 | B | 303 | CHD | O3-C3-C2 | 2.89 | 117.52 | 110.16 |
| 23 | O | 303 | PSC | C27-C26-C25 | -2.89 | 99.77 | 114.42 |
| 26 | G | 103 | PEK | C02-O01-C1 | 2.89 | 124.90 | 117.79 |
| 20 | L | 101 | TGL | C13-C12-C11 | 2.89 | 129.07 | 114.42 |
| 14 | N | 602 | HEA | CBD-CAD-C3D | -2.88 | 107.18 | 112.49 |
| 22 | O | 302 | CHD | C1-C10-C5 | 2.87 | 112.01 | 107.77 |
| 19 | Q | 201 | PGV | O03-C19-C20 | 2.87 | 120.91 | 111.91 |
| 22 | C | 305 | CHD | C1-C2-C3 | -2.86 | 106.79 | 110.47 |
| 20 | Y | 101 | TGL | CC3-CC2-CC1 | 2.86 | 124.02 | 113.62 |
| 22 | B | 303 | CHD | C1-C10-C9 | 2.86 | 115.85 | 111.35 |
| 20 | B | 301 | TGL | OG1-CG1-CG2 | 2.86 | 116.75 | 108.43 |
| 22 | P | 305 | CHD | C13-C14-C8 | 2.85 | 118.38 | 114.74 |
| 26 | T | 102 | PEK | O01-C1-O02 | -2.85 | 116.80 | 123.70 |
| 23 | B | 304 | PSC | O01-C1-O02 | -2.85 | 116.82 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | C | 303 | CDL | C75-C74-C73 | -2.85 | 99.98 | 114.42 |
| 25 | P | 304 | CDL | OA8-CA6-CA4 | 2.84 | 116.71 | 108.43 |
| 19 | A | 607 | PGV | C27-C26-C25 | 2.84 | 128.84 | 114.42 |
| 25 | C | 303 | CDL | OB4-PB2-OB2 | -2.84 | 94.58 | 107.75 |
| 19 | A | 607 | PGV | C31-C30-C29 | -2.83 | 100.04 | 114.42 |
| 25 | G | 102 | CDL | C19-C18-C17 | 2.83 | 128.81 | 114.42 |
| 26 | G | 103 | PEK | C14-C13-C12 | 2.83 | 125.97 | 112.02 |
| 22 | C | 304 | CHD | O7-C7-C8 | 2.83 | 115.76 | 109.43 |
| 20 | Y | 101 | TGL | OG2-CG2-CG3 | 2.83 | 118.64 | 108.40 |
| 22 | J | 102 | CHD | O7-C7-C8 | 2.82 | 115.73 | 109.43 |
| 25 | T | 103 | CDL | C76-C75-C74 | 2.82 | 128.72 | 114.42 |
| 20 | Q | 202 | TGL | CB5-CB4-CB3 | 2.81 | 128.72 | 114.42 |
| 20 | B | 301 | TGL | CB6-CB5-CB4 | -2.81 | 100.14 | 114.42 |
| 20 | N | 608 | TGL | C15-CC9-CC8 | 2.81 | 128.67 | 114.42 |
| 19 | N | 607 | PGV | C3-C2-C1 | -2.80 | 103.42 | 113.62 |
| 19 | N | 607 | PGV | O01-C1-C2 | -2.80 | 105.46 | 111.50 |
| 22 | P | 305 | CHD | C1-C2-C3 | 2.79 | 114.05 | 110.47 |
| 26 | C | 306 | PEK | C33-C32-C31 | -2.79 | 100.28 | 114.42 |
| 25 | P | 304 | CDL | OA8-CA7-C31 | 2.78 | 120.62 | 111.91 |
| 22 | C | 304 | CHD | C9-C11-C12 | -2.78 | 110.64 | 114.30 |
| 19 | N | 607 | PGV | C14-C13-C12 | -2.78 | 96.53 | 112.43 |
| 22 | C | 305 | CHD | C19-C10-C1 | -2.77 | 103.80 | 108.26 |
| 25 | T | 103 | CDL | C72-C71-CB7 | 2.77 | 123.69 | 113.62 |
| 20 | D | 201 | TGL | CG2-OG2-CB1 | -2.77 | 110.98 | 117.79 |
| 25 | P | 304 | CDL | C42-C41-C40 | 2.77 | 128.47 | 114.42 |
| 20 | N | 608 | TGL | OG3-CC1-OC1 | -2.77 | 116.61 | 123.59 |
| 28 | M | 101 | DMU | O49-C1-C2 | -2.76 | 103.96 | 110.35 |
| 25 | G | 102 | CDL | C72-C71-CB7 | 2.76 | 123.66 | 113.62 |
| 22 | W | 101 | CHD | C6-C7-C8 | 2.75 | 114.42 | 111.48 |
| 25 | C | 303 | CDL | CA4-OA6-CA5 | 2.75 | 124.57 | 117.79 |
| 22 | C | 304 | CHD | C14-C8-C7 | 2.75 | 115.46 | 111.81 |
| 28 | M | 101 | DMU | O1-C9-C8 | -2.75 | 104.70 | 109.69 |
| 14 | A | 601 | HEA | CMD-C2D-C3D | 2.75 | 130.13 | 124.94 |
| 25 | G | 102 | CDL | C43-C42-C41 | -2.75 | 100.46 | 114.42 |
| 26 | T | 101 | PEK | O01-C1-C2 | -2.75 | 105.58 | 111.50 |
| 22 | C | 304 | CHD | C1-C10-C5 | 2.74 | 111.82 | 107.77 |
| 28 | M | 101 | DMU | O7-C3-C4 | -2.73 | 101.97 | 109.45 |
| 14 | N | 601 | HEA | C25-C23-C22 | -2.73 | 114.77 | 122.65 |
| 26 | G | 101 | PEK | C02-O01-C1 | -2.72 | 111.09 | 117.79 |
| 20 | B | 301 | TGL | OB1-CB1-CB2 | -2.72 | 113.13 | 123.73 |
| 28 | M | 101 | DMU | C6-C1-C2 | -2.71 | 104.34 | 110.00 |
| 25 | C | 303 | CDL | PA1-OA2-CA2 | 2.71 | 137.59 | 121.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | C | 307 | PGV | O04-C19-C20 | -2.71 | 113.15 | 123.73 |
| 19 | N | 607 | PGV | O03-C19-O04 | -2.71 | 116.76 | 123.59 |
| 23 | O | 303 | PSC | C02-O01-C1 | 2.71 | 124.45 | 117.79 |
| 22 | P | 305 | CHD | C11-C9-C8 | 2.70 | 114.84 | 110.88 |
| 22 | P | 307 | CHD | C16-C17-C20 | -2.70 | 107.97 | 112.15 |
| 22 | P | 307 | CHD | C10-C9-C8 | -2.70 | 108.92 | 111.82 |
| 20 | B | 301 | TGL | CB8-CB7-CB6 | -2.69 | 100.76 | 114.42 |
| 22 | O | 302 | CHD | C18-C13-C12 | -2.69 | 106.33 | 109.07 |
| 22 | P | 305 | CHD | C2-C1-C10 | 2.69 | 117.39 | 112.78 |
| 19 | P | 303 | PGV | C24-C23-C22 | -2.69 | 100.77 | 114.42 |
| 28 | P | 306 | DMU | O16-C18-C19 | 2.68 | 118.97 | 109.56 |
| 20 | Q | 202 | TGL | C10-CB9-CB8 | 2.68 | 128.03 | 114.42 |
| 25 | G | 102 | CDL | C83-C82-C81 | 2.68 | 128.03 | 114.42 |
| 26 | T | 101 | PEK | C24-C23-C22 | -2.67 | 103.59 | 113.19 |
| 26 | T | 102 | PEK | O03-C01-C02 | 2.66 | 116.19 | 108.43 |
| 26 | T | 101 | PEK | C25-C24-C23 | 2.65 | 127.89 | 114.42 |
| 22 | C | 305 | CHD | C11-C9-C8 | 2.65 | 114.76 | 110.88 |
| 25 | T | 103 | CDL | OA6-CA5-OA7 | -2.65 | 117.30 | 123.70 |
| 19 | Q | 201 | PGV | C32-C31-C30 | 2.65 | 127.86 | 114.42 |
| 20 | Y | 101 | TGL | OC1-CC1-CC2 | -2.65 | 113.41 | 123.73 |
| 22 | J | 102 | CHD | C21-C20-C22 | 2.63 | 114.49 | 110.36 |
| 20 | Y | 101 | TGL | CA7-CA6-CA5 | -2.63 | 101.08 | 114.42 |
| 25 | T | 103 | CDL | CB2-C1-CA2 | -2.63 | 105.06 | 112.79 |
| 22 | P | 307 | CHD | C16-C17-C13 | -2.63 | 100.98 | 103.55 |
| 22 | W | 101 | CHD | C19-C10-C5 | -2.62 | 105.91 | 110.36 |
| 20 | L | 101 | TGL | OG1-CA1-CA2 | 2.62 | 120.14 | 111.91 |
| 20 | L | 101 | TGL | OB1-CB1-CB2 | -2.62 | 113.50 | 123.73 |
| 22 | B | 303 | CHD | C4-C3-C2 | 2.62 | 113.68 | 110.55 |
| 22 | W | 101 | CHD | C15-C14-C13 | 2.62 | 106.12 | 103.55 |
| 28 | Z | 101 | DMU | O61-C57-C4 | -2.62 | 102.32 | 111.29 |
| 20 | Q | 202 | TGL | OG3-CG3-CG2 | -2.61 | 100.82 | 108.43 |
| 19 | P | 303 | PGV | C21-C20-C19 | -2.61 | 104.12 | 113.62 |
| 19 | Q | 201 | PGV | C7-C6-C5 | 2.61 | 127.69 | 114.42 |
| 25 | C | 303 | CDL | OA8-CA6-CA4 | 2.61 | 116.03 | 108.43 |
| 19 | N | 607 | PGV | O01-C1-O02 | -2.61 | 117.40 | 123.70 |
| 19 | A | 607 | PGV | O01-C1-O02 | -2.61 | 117.40 | 123.70 |
| 25 | G | 102 | CDL | C84-C83-C82 | 2.60 | 127.63 | 114.42 |
| 19 | C | 302 | PGV | C15-C14-C13 | 2.60 | 125.12 | 113.79 |
| 14 | A | 602 | HEA | C12-C13-C14 | -2.60 | 105.38 | 112.23 |
| 25 | G | 102 | CDL | C44-C43-C42 | 2.59 | 127.58 | 114.42 |
| 25 | P | 304 | CDL | OB9-CB7-C71 | -2.59 | 113.64 | 123.73 |
| 28 | M | 101 | DMU | O2-C8-C9 | -2.59 | 102.88 | 109.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | P | 304 | CDL | C83-C82-C81 | 2.58 | 127.54 | 114.42 |
| 26 | C | 306 | PEK | C29-C28-C27 | 2.57 | 127.48 | 114.42 |
| 19 | A | 608 | PGV | C8-C9-C10 | -2.57 | 102.60 | 113.79 |
| 19 | P | 303 | PGV | C32-C31-C30 | 2.56 | 127.42 | 114.42 |
| 26 | T | 102 | PEK | C02-O01-C1 | 2.56 | 124.08 | 117.79 |
| 14 | A | 602 | HEA | C3C-C4C-NC | 2.55 | 112.51 | 109.21 |
| 20 | B | 301 | TGL | C14-C13-C12 | -2.55 | 101.45 | 114.42 |
| 20 | D | 201 | TGL | C20-CA9-CA8 | 2.55 | 127.39 | 114.42 |
| 26 | G | 101 | PEK | O03-C21-O04 | -2.55 | 117.15 | 123.59 |
| 14 | N | 602 | HEA | C25-C23-C24 | 2.55 | 120.24 | 114.60 |
| 19 | A | 608 | PGV | O12-P-O13 | 2.55 | 119.03 | 109.07 |
| 25 | G | 102 | CDL | C79-C78-C77 | 2.54 | 127.31 | 114.42 |
| 22 | P | 305 | CHD | C9-C10-C5 | 2.54 | 112.14 | 108.58 |
| 25 | P | 304 | CDL | CB6-CB4-CB3 | 2.53 | 117.78 | 111.79 |
| 20 | Y | 101 | TGL | CC7-CC6-CC5 | 2.53 | 127.25 | 114.42 |
| 22 | C | 304 | CHD | C15-C14-C13 | 2.53 | 106.03 | 103.55 |
| 20 | Y | 101 | TGL | OG3-CC1-OC1 | -2.52 | 117.22 | 123.59 |
| 19 | C | 307 | PGV | O01-C1-C2 | 2.51 | 116.92 | 111.50 |
| 26 | P | 308 | PEK | C26-C25-C24 | 2.51 | 127.19 | 114.42 |
| 22 | B | 303 | CHD | C16-C15-C14 | -2.51 | 100.15 | 105.13 |
| 26 | G | 103 | PEK | O02-C1-C2 | -2.51 | 113.94 | 123.73 |
| 26 | G | 101 | PEK | O01-C02-C01 | -2.51 | 99.31 | 108.40 |
| 14 | A | 602 | HEA | C13-C14-C15 | -2.51 | 121.62 | 127.66 |
| 25 | T | 103 | CDL | C19-C18-C17 | 2.51 | 127.15 | 114.42 |
| 25 | P | 304 | CDL | C82-C81-C80 | 2.50 | 127.12 | 114.42 |
| 19 | P | 303 | PGV | O03-C01-C02 | -2.50 | 101.16 | 108.43 |
| 14 | A | 601 | HEA | C1B-C2B-C3B | -2.49 | 105.26 | 107.00 |
| 22 | O | 302 | CHD | C1-C10-C9 | 2.49 | 115.27 | 111.35 |
| 28 | P | 306 | DMU | C1-C2-C3 | 2.48 | 115.35 | 109.68 |
| 26 | T | 101 | PEK | O01-C1-O02 | -2.48 | 117.71 | 123.70 |
| 26 | P | 308 | PEK | C29-C28-C27 | 2.48 | 127.01 | 114.42 |
| 19 | P | 303 | PGV | C15-C14-C13 | 2.48 | 124.58 | 113.79 |
| 25 | P | 304 | CDL | OA8-CA7-OA9 | -2.47 | 117.36 | 123.59 |
| 22 | C | 305 | CHD | O3-C3-C2 | -2.46 | 103.90 | 110.16 |
| 25 | C | 303 | CDL | C57-C56-C55 | 2.46 | 126.91 | 114.42 |
| 22 | P | 307 | CHD | C4-C5-C10 | -2.45 | 110.05 | 112.66 |
| 19 | P | 303 | PGV | O03-C19-C20 | -2.45 | 104.21 | 111.91 |
| 25 | P | 304 | CDL | C56-C55-C54 | 2.45 | 126.85 | 114.42 |
| 26 | C | 306 | PEK | O03-C01-C02 | 2.45 | 115.56 | 108.43 |
| 26 | C | 306 | PEK | O12-P-O14 | -2.45 | 99.51 | 109.07 |
| 26 | T | 102 | PEK | C01-O03-C21 | 2.45 | 126.18 | 117.12 |
| 26 | G | 103 | PEK | C24-C23-C22 | -2.45 | 104.40 | 113.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | B | 303 | CHD | C18-C13-C12 | -2.44 | 106.58 | 109.07 |
| 22 | C | 305 | CHD | C4-C5-C10 | -2.43 | 110.08 | 112.66 |
| 25 | P | 304 | CDL | C76-C75-C74 | -2.43 | 102.09 | 114.42 |
| 19 | A | 607 | PGV | O02-C1-C2 | 2.43 | 133.21 | 123.73 |
| 20 | D | 201 | TGL | C12-C11-C10 | -2.42 | 102.14 | 114.42 |
| 28 | Z | 101 | DMU | O5-C4-C57 | 2.42 | 112.45 | 106.44 |
| 25 | P | 304 | CDL | CA6-CA4-CA3 | -2.42 | 106.07 | 111.79 |
| 19 | A | 607 | PGV | C4-C3-C2 | -2.41 | 104.52 | 113.19 |
| 22 | O | 302 | CHD | C4-C3-C2 | 2.41 | 113.43 | 110.55 |
| 22 | C | 304 | CHD | C21-C20-C22 | -2.41 | 106.59 | 110.36 |
| 14 | N | 601 | HEA | CMC-C2C-C1C | -2.41 | 124.77 | 128.46 |
| 25 | T | 103 | CDL | OB7-CB5-C51 | -2.41 | 114.35 | 123.73 |
| 23 | O | 303 | PSC | C21-C20-C19 | -2.40 | 104.88 | 113.62 |
| 22 | C | 304 | CHD | C19-C10-C9 | -2.40 | 107.88 | 111.18 |
| 22 | W | 101 | CHD | C9-C8-C7 | -2.40 | 109.01 | 111.88 |
| 28 | Z | 101 | DMU | O49-C1-C2 | -2.39 | 104.82 | 110.35 |
| 14 | A | 602 | HEA | CBA-CAA-C2A | -2.39 | 108.08 | 112.48 |
| 20 | Y | 101 | TGL | C22-C21-C20 | -2.39 | 102.30 | 114.42 |
| 25 | C | 303 | CDL | C58-C57-C56 | 2.39 | 126.54 | 114.42 |
| 19 | C | 307 | PGV | P-O11-C03 | 2.39 | 135.67 | 121.68 |
| 25 | C | 303 | CDL | C87-C86-C85 | 2.38 | 131.51 | 113.42 |
| 25 | T | 103 | CDL | C23-C22-C21 | 2.38 | 126.52 | 114.42 |
| 26 | P | 308 | PEK | C3-C2-C1 | 2.38 | 122.28 | 113.62 |
| 22 | O | 302 | CHD | C16-C15-C14 | -2.38 | 100.42 | 105.13 |
| 22 | B | 303 | CHD | C9-C8-C7 | -2.38 | 109.03 | 111.88 |
| 20 | L | 101 | TGL | C15-CC9-CC8 | 2.37 | 126.47 | 114.42 |
| 14 | A | 602 | HEA | C21-C20-C19 | 2.37 | 120.78 | 112.98 |
| 26 | P | 308 | PEK | P-O11-C03 | 2.37 | 135.58 | 121.68 |
| 26 | G | 103 | PEK | C2-C3-C4 | -2.37 | 109.00 | 113.23 |
| 20 | Y | 101 | TGL | C15-CC9-CC8 | 2.37 | 126.44 | 114.42 |
| 23 | B | 304 | PSC | C07-N-C06 | 2.36 | 115.05 | 108.97 |
| 20 | Q | 202 | TGL | C15-CC9-CC8 | 2.36 | 126.39 | 114.42 |
| 26 | G | 101 | PEK | C03-C02-C01 | 2.36 | 117.36 | 111.79 |
| 26 | G | 101 | PEK | C38-C37-C36 | 2.35 | 131.26 | 113.42 |
| 26 | C | 306 | PEK | C34-C33-C32 | 2.35 | 126.35 | 114.42 |
| 20 | D | 201 | TGL | CC3-CC2-CC1 | -2.35 | 105.08 | 113.62 |
| 26 | G | 103 | PEK | C11-C10-C9 | 2.35 | 123.58 | 112.02 |
| 22 | W | 101 | CHD | C11-C9-C8 | 2.34 | 114.31 | 110.88 |
| 19 | P | 301 | PGV | P-O11-C03 | 2.34 | 135.40 | 121.68 |
| 25 | C | 303 | CDL | C22-C21-C20 | 2.34 | 126.30 | 114.42 |
| 28 | J | 101 | DMU | C18-O16-C6 | -2.33 | 109.97 | 113.84 |
| 20 | D | 201 | TGL | C16-C15-CC9 | 2.33 | 126.26 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | L | 101 | TGL | CC6-CC5-CC4 | 2.33 | 126.26 | 114.42 |
| 25 | T | 103 | CDL | OA6-CA4-CA6 | 2.33 | 116.83 | 108.40 |
| 26 | C | 306 | PEK | O02-C1-C2 | -2.33 | 114.66 | 123.73 |
| 28 | P | 306 | DMU | O5-C6-O16 | 2.32 | 115.46 | 109.97 |
| 25 | C | 303 | CDL | OB2-PB2-OB3 | 2.32 | 118.12 | 109.07 |
| 28 | M | 101 | DMU | O4-C7-C5 | -2.31 | 105.00 | 110.35 |
| 28 | J | 101 | DMU | O1-C10-C5 | -2.31 | 105.46 | 110.35 |
| 22 | C | 304 | CHD | O3-C3-C4 | -2.31 | 105.26 | 109.85 |
| 14 | A | 602 | HEA | O11-C11-C3B | -2.30 | 105.36 | 112.00 |
| 22 | O | 302 | CHD | C13-C17-C20 | -2.30 | 116.75 | 119.50 |
| 14 | A | 602 | HEA | CMC-C2C-C3C | 2.30 | 128.98 | 124.68 |
| 19 | P | 303 | PGV | C26-C25-C24 | 2.30 | 126.10 | 114.42 |
| 22 | W | 101 | CHD | C16-C17-C13 | 2.30 | 105.81 | 103.55 |
| 26 | G | 103 | PEK | O03-C21-C22 | 2.29 | 119.11 | 111.91 |
| 19 | A | 607 | PGV | C32-C31-C30 | 2.29 | 126.05 | 114.42 |
| 20 | Y | 101 | TGL | OG2-CB1-OB1 | -2.28 | 118.19 | 123.70 |
| 22 | P | 307 | CHD | C18-C13-C12 | 2.28 | 111.39 | 109.07 |
| 28 | Z | 101 | DMU | O3-C5-C7 | 2.28 | 115.62 | 110.35 |
| 22 | O | 302 | CHD | C17-C13-C12 | -2.27 | 115.59 | 117.67 |
| 20 | D | 201 | TGL | OG1-CA1-OA1 | -2.27 | 117.86 | 123.59 |
| 25 | G | 102 | CDL | C22-C21-C20 | 2.27 | 125.96 | 114.42 |
| 19 | N | 607 | PGV | C03-C02-C01 | -2.27 | 106.42 | 111.79 |
| 26 | C | 306 | PEK | C3-C2-C1 | 2.27 | 121.87 | 113.62 |
| 14 | A | 602 | HEA | CMC-C2C-C1C | -2.27 | 124.98 | 128.46 |
| 28 | J | 101 | DMU | O16-C18-C19 | 2.27 | 117.51 | 109.56 |
| 14 | A | 601 | HEA | CBD-CAD-C3D | -2.26 | 108.32 | 112.49 |
| 22 | C | 305 | CHD | C16-C15-C14 | -2.26 | 100.66 | 105.13 |
| 19 | C | 307 | PGV | C25-C24-C23 | 2.26 | 125.88 | 114.42 |
| 23 | O | 303 | PSC | C08-N-C06 | -2.25 | 103.19 | 108.97 |
| 20 | D | 201 | TGL | C11-C10-CB9 | 2.24 | 125.82 | 114.42 |
| 14 | N | 602 | HEA | C21-C20-C19 | 2.24 | 120.36 | 112.98 |
| 20 | Y | 101 | TGL | C30-C29-C14 | 2.24 | 125.82 | 114.42 |
| 20 | D | 201 | TGL | CB7-CB6-CB5 | -2.24 | 103.05 | 114.42 |
| 19 | P | 301 | PGV | C24-C23-C22 | 2.24 | 125.79 | 114.42 |
| 22 | C | 304 | CHD | C18-C13-C14 | 2.23 | 114.70 | 111.21 |
| 28 | M | 101 | DMU | C25-C22-C19 | -2.22 | 103.13 | 114.42 |
| 26 | T | 101 | PEK | O11-P-O14 | -2.22 | 100.40 | 109.07 |
| 14 | A | 601 | HEA | C3C-C4C-NC | 2.22 | 112.08 | 109.21 |
| 20 | L | 101 | TGL | C25-C24-C23 | -2.22 | 103.16 | 114.42 |
| 23 | B | 304 | PSC | C26-C25-C24 | -2.21 | 103.19 | 114.42 |
| 25 | P | 304 | CDL | C63-C62-C61 | 2.21 | 125.66 | 114.42 |
| 19 | A | 607 | PGV | O01-C02-C01 | -2.21 | 100.41 | 108.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | C | 303 | CDL | CA6-CA4-CA3 | -2.21 | 106.57 | 111.79 |
| 22 | P | 307 | CHD | C19-C10-C1 | -2.20 | 104.71 | 108.26 |
| 20 | Q | 202 | TGL | CG2-OG2-CB1 | 2.20 | 123.22 | 117.79 |
| 22 | C | 305 | CHD | C2-C1-C10 | 2.20 | 116.56 | 112.78 |
| 19 | P | 301 | PGV | C15-C14-C13 | 2.20 | 123.38 | 113.79 |
| 25 | T | 103 | CDL | OA9-CA7-C31 | -2.20 | 115.15 | 123.73 |
| 14 | A | 601 | HEA | CAD-CBD-CGD | -2.20 | 108.98 | 112.67 |
| 22 | W | 101 | CHD | C18-C13-C14 | 2.20 | 114.65 | 111.21 |
| 14 | N | 602 | HEA | CAD-C3D-C2D | 2.20 | 133.56 | 127.25 |
| 19 | N | 607 | PGV | O03-C19-C20 | 2.19 | 118.79 | 111.91 |
| 22 | C | 304 | CHD | C22-C20-C17 | 2.19 | 114.82 | 110.28 |
| 19 | A | 607 | PGV | C01-O03-C19 | -2.19 | 109.00 | 117.12 |
| 26 | C | 306 | PEK | O13-P-O11 | 2.19 | 117.91 | 107.75 |
| 20 | Y | 101 | TGL | CB8-CB7-CB6 | -2.18 | 103.33 | 114.42 |
| 19 | P | 303 | PGV | C33-C32-C31 | 2.18 | 135.59 | 115.30 |
| 25 | G | 102 | CDL | OB7-CB5-C51 | -2.18 | 115.22 | 123.73 |
| 19 | P | 303 | PGV | C10-C11-C12 | -2.18 | 107.98 | 124.73 |
| 22 | O | 302 | CHD | C19-C10-C9 | -2.18 | 108.18 | 111.18 |
| 28 | Z | 101 | DMU | C11-C9-C8 | 2.18 | 118.11 | 113.00 |
| 26 | C | 306 | PEK | P-O11-C03 | 2.18 | 134.47 | 121.68 |
| 19 | C | 307 | PGV | C26-C25-C24 | 2.18 | 125.50 | 114.42 |
| 26 | P | 308 | PEK | C01-O03-C21 | 2.18 | 125.20 | 117.12 |
| 19 | A | 607 | PGV | C5-C4-C3 | -2.18 | 103.36 | 114.42 |
| 20 | B | 301 | TGL | C27-C26-C25 | -2.18 | 95.07 | 115.30 |
| 20 | L | 101 | TGL | CC7-CC6-CC5 | 2.17 | 125.44 | 114.42 |
| 20 | B | 301 | TGL | CG3-CG2-CG1 | -2.17 | 106.66 | 111.79 |
| 19 | P | 303 | PGV | C9-C10-C11 | 2.17 | 124.85 | 112.43 |
| 25 | G | 102 | CDL | C39-C38-C37 | 2.16 | 125.40 | 114.42 |
| 25 | P | 304 | CDL | OA6-CA5-OA7 | -2.16 | 118.48 | 123.70 |
| 26 | G | 101 | PEK | C25-C24-C23 | -2.16 | 103.47 | 114.42 |
| 19 | A | 608 | PGV | C10-C11-C12 | -2.16 | 108.17 | 124.73 |
| 25 | P | 304 | CDL | PA1-OA2-CA2 | 2.16 | 134.32 | 121.68 |
| 22 | P | 305 | CHD | C11-C12-C13 | -2.15 | 109.03 | 111.24 |
| 25 | C | 303 | CDL | OA4-PA1-OA3 | 2.15 | 122.86 | 112.24 |
| 26 | T | 101 | PEK | C3-C4-C5 | 2.15 | 124.73 | 112.43 |
| 20 | L | 101 | TGL | OG3-CG3-CG2 | 2.15 | 114.68 | 108.43 |
| 19 | N | 607 | PGV | C18-C17-C16 | -2.14 | 97.19 | 113.42 |
| 26 | G | 101 | PEK | C11-C10-C9 | 2.13 | 122.53 | 112.02 |
| 14 | N | 602 | HEA | C13-C14-C15 | -2.12 | 122.54 | 127.66 |
| 25 | C | 303 | CDL | C59-C58-C57 | 2.12 | 125.19 | 114.42 |
| 22 | W | 101 | CHD | C6-C5-C4 | -2.11 | 108.76 | 111.19 |
| 25 | G | 102 | CDL | C61-C60-C59 | -2.11 | 103.71 | 114.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | D | 201 | TGL | C22-C21-C20 | 2.11 | 125.14 | 114.42 |
| 20 | L | 101 | TGL | OC1-CC1-CC2 | -2.11 | 115.51 | 123.73 |
| 20 | D | 201 | TGL | OG3-CG3-CG2 | -2.10 | 102.32 | 108.43 |
| 26 | C | 306 | PEK | C31-C30-C29 | 2.10 | 125.07 | 114.42 |
| 25 | P | 304 | CDL | C43-C42-C41 | 2.09 | 125.05 | 114.42 |
| 22 | P | 307 | CHD | C14-C8-C9 | -2.09 | 106.84 | 109.71 |
| 22 | J | 102 | CHD | C15-C14-C13 | 2.09 | 105.60 | 103.55 |
| 25 | T | 103 | CDL | C22-C21-C20 | 2.09 | 125.02 | 114.42 |
| 19 | N | 607 | PGV | C32-C31-C30 | -2.08 | 103.86 | 114.42 |
| 22 | B | 303 | CHD | C18-C13-C17 | -2.08 | 107.96 | 111.21 |
| 22 | O | 302 | CHD | O12-C12-C13 | -2.08 | 107.52 | 111.03 |
| 26 | T | 102 | PEK | C11-C10-C9 | 2.07 | 122.23 | 112.02 |
| 22 | J | 102 | CHD | C18-C13-C17 | 2.07 | 114.45 | 111.21 |
| 28 | J | 101 | DMU | O1-C9-C8 | 2.06 | 113.44 | 109.69 |
| 23 | O | 303 | PSC | C04-C05-N | 2.06 | 122.66 | 115.78 |
| 20 | Q | 202 | TGL | CG1-OG1-CA1 | 2.06 | 124.74 | 117.12 |
| 20 | N | 608 | TGL | C20-CA9-CA8 | 2.06 | 124.88 | 114.42 |
| 26 | G | 103 | PEK | O01-C02-C01 | 2.06 | 115.85 | 108.40 |
| 19 | P | 301 | PGV | C25-C24-C23 | 2.06 | 124.87 | 114.42 |
| 14 | N | 602 | HEA | C25-C23-C22 | -2.05 | 116.71 | 122.65 |
| 25 | P | 304 | CDL | C19-C18-C17 | 2.05 | 124.85 | 114.42 |
| 14 | N | 601 | HEA | C21-C20-C19 | -2.04 | 106.27 | 112.98 |
| 23 | B | 304 | PSC | C16-C15-C14 | 2.04 | 122.67 | 113.79 |
| 28 | M | 101 | DMU | O4-C7-C8 | 2.04 | 115.06 | 110.35 |
| 20 | N | 608 | TGL | C30-C29-C14 | 2.04 | 124.77 | 114.42 |
| 19 | P | 303 | PGV | C22-C21-C20 | -2.04 | 105.87 | 113.19 |
| 28 | M | 101 | DMU | O3-C5-C10 | -2.04 | 105.10 | 110.05 |
| 20 | D | 201 | TGL | CC6-CC5-CC4 | -2.03 | 104.10 | 114.42 |
| 22 | W | 101 | CHD | C14-C8-C9 | 2.03 | 112.50 | 109.71 |
| 22 | C | 304 | CHD | C19-C10-C5 | 2.03 | 113.81 | 110.36 |
| 14 | N | 602 | HEA | C3A-C4A-NA | 2.03 | 114.78 | 110.94 |
| 25 | P | 304 | CDL | OA5-PA1-OA3 | -2.03 | 101.14 | 109.07 |
| 26 | G | 101 | PEK | C32-C31-C30 | -2.02 | 104.16 | 114.42 |
| 22 | J | 102 | CHD | C21-C20-C17 | 2.01 | 116.01 | 112.92 |
| 23 | O | 303 | PSC | O02-C1-C2 | -2.01 | 115.89 | 123.73 |
| 20 | Y | 101 | TGL | CG3-CG2-CG1 | -2.01 | 107.03 | 111.79 |
| 25 | C | 303 | CDL | O1-C1-CB2 | 2.01 | 116.59 | 109.56 |
| 22 | B | 303 | CHD | O7-C7-C8 | 2.01 | 113.91 | 109.43 |
| 22 | P | 307 | CHD | C15-C14-C8 | -2.01 | 115.53 | 118.33 |
| 19 | N | 607 | PGV | C4-C3-C2 | -2.00 | 105.98 | 113.19 |
| 20 | L | 101 | TGL | C16-C15-CC9 | 2.00 | 124.58 | 114.42 |
| 25 | C | 303 | CDL | C45-C44-C43 | 2.00 | 124.58 | 114.42 |

All (11) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 14 | A | 602 | HEA | ND |
| 14 | A | 602 | HEA | NA |
| 14 | A | 602 | HEA | NB |
| 14 | N | 601 | HEA | ND |
| 14 | N | 601 | HEA | NB |
| 14 | A | 601 | HEA | ND |
| 14 | A | 601 | HEA | NA |
| 14 | A | 601 | HEA | NB |
| 14 | N | 602 | HEA | ND |
| 14 | N | 602 | HEA | NA |
| 14 | N | 602 | HEA | NB |

All (880) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | G | 103 | PEK | C03-O11-P-O14 |
| 26 | G | 103 | PEK | O12-C04-C05-N |
| 26 | G | 103 | PEK | C2-C1-O01-C02 |
| 26 | G | 103 | PEK | C11-C12-C13-C14 |
| 25 | T | 103 | CDL | CA2-C1-CB2-OB2 |
| 25 | T | 103 | CDL | OA7-CA5-OA6-CA4 |
| 25 | T | 103 | CDL | OA9-CA7-OA8-CA6 |
| 25 | T | 103 | CDL | C31-CA7-OA8-CA6 |
| 25 | T | 103 | CDL | C1-CB2-OB2-PB2 |
| 25 | T | 103 | CDL | CB2-OB2-PB2-OB5 |
| 25 | T | 103 | CDL | CB3-OB5-PB2-OB3 |
| 25 | T | 103 | CDL | CB3-OB5-PB2-OB4 |
| 19 | Q | 201 | PGV | C04-O12-P-O14 |
| 19 | Q | 201 | PGV | C02-C03-O11-P |
| 19 | Q | 201 | PGV | C04-C05-C06-O06 |
| 19 | Q | 201 | PGV | O02-C1-O01-C02 |
| 19 | Q | 201 | PGV | C2-C1-O01-C02 |
| 23 | O | 303 | PSC | C03-O11-P-O13 |
| 23 | O | 303 | PSC | C03-O11-P-O14 |
| 23 | O | 303 | PSC | C2-C1-O01-C02 |
| 23 | O | 303 | PSC | C11-C12-C13-C14 |
| 19 | A | 608 | PGV | C03-O11-P-O13 |
| 19 | A | 608 | PGV | C03-O11-P-O14 |
| 19 | A | 608 | PGV | C04-O12-P-O13 |
| 19 | A | 608 | PGV | C04-O12-P-O14 |
| 19 | A | 608 | PGV | O02-C1-O01-C02 |
| 19 | A | 608 | PGV | C2-C1-O01-C02 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | T | 101 | PEK | C11-C12-C13-C14 |
| 26 | T | 101 | PEK | C12-C13-C14-C15 |
| 28 | P | 306 | DMU | C1-C6-O16-C18 |
| 28 | P | 306 | DMU | O5-C6-O16-C18 |
| 22 | J | 102 | CHD | C13-C17-C20-C22 |
| 22 | J | 102 | CHD | C16-C17-C20-C21 |
| 26 | T | 102 | PEK | C04-O12-P-O14 |
| 26 | T | 102 | PEK | O12-C04-C05-N |
| 26 | C | 306 | PEK | C04-O12-P-O14 |
| 26 | C | 306 | PEK | C2-C1-O01-C02 |
| 26 | C | 306 | PEK | C6-C7-C8-C9 |
| 26 | C | 306 | PEK | C9-C10-C11-C12 |
| 26 | C | 306 | PEK | C11-C12-C13-C14 |
| 25 | C | 303 | CDL | CA3-OA5-PA1-OA3 |
| 25 | C | 303 | CDL | C11-CA5-OA6-CA4 |
| 25 | C | 303 | CDL | CB2-OB2-PB2-OB4 |
| 25 | C | 303 | CDL | C51-CB5-OB6-CB4 |
| 19 | P | 301 | PGV | C02-C03-O11-P |
| 19 | P | 301 | PGV | C12-C13-C14-C15 |
| 25 | P | 304 | CDL | CB2-C1-CA2-OA2 |
| 25 | P | 304 | CDL | CA2-OA2-PA1-OA4 |
| 25 | P | 304 | CDL | CA3-OA5-PA1-OA3 |
| 25 | P | 304 | CDL | CB2-OB2-PB2-OB3 |
| 25 | P | 304 | CDL | CB2-OB2-PB2-OB4 |
| 25 | P | 304 | CDL | CB2-OB2-PB2-OB5 |
| 25 | P | 304 | CDL | CB3-OB5-PB2-OB3 |
| 25 | P | 304 | CDL | CB3-OB5-PB2-OB4 |
| 25 | P | 304 | CDL | C51-CB5-OB6-CB4 |
| 22 | W | 101 | CHD | C13-C17-C20-C22 |
| 22 | W | 101 | CHD | C20-C22-C23-C24 |
| 23 | B | 304 | PSC | C03-O11-P-O14 |
| 23 | B | 304 | PSC | O12-C04-C05-N |
| 23 | B | 304 | PSC | C2-C1-O01-C02 |
| 26 | P | 308 | PEK | O02-C1-O01-C02 |
| 26 | P | 308 | PEK | C2-C1-O01-C02 |
| 20 | Y | 101 | TGL | CB2-CB1-OG2-CG2 |
| 19 | C | 307 | PGV | C03-O11-P-O13 |
| 19 | C | 307 | PGV | C04-O12-P-O11 |
| 19 | C | 307 | PGV | C02-C03-O11-P |
| 25 | G | 102 | CDL | CA2-OA2-PA1-OA3 |
| 25 | G | 102 | CDL | CA2-OA2-PA1-OA4 |
| 25 | G | 102 | CDL | CA2-OA2-PA1-OA5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | G | 102 | CDL | OA7-CA5-OA6-CA4 |
| 25 | G | 102 | CDL | C1-CB2-OB2-PB2 |
| 25 | G | 102 | CDL | CB2-OB2-PB2-OB4 |
| 25 | G | 102 | CDL | CB3-OB5-PB2-OB2 |
| 25 | G | 102 | CDL | CB3-OB5-PB2-OB3 |
| 25 | G | 102 | CDL | CB3-OB5-PB2-OB4 |
| 20 | Q | 202 | TGL | CC2-CC1-OG3-CG3 |
| 20 | Q | 202 | TGL | OC1-CC1-OG3-CG3 |
| 20 | D | 201 | TGL | OC1-CC1-OG3-CG3 |
| 19 | Q | 201 | PGV | O04-C19-O03-C01 |
| 19 | A | 608 | PGV | O04-C19-O03-C01 |
| 20 | Y | 101 | TGL | OA1-CA1-OG1-CG1 |
| 19 | Q | 201 | PGV | C20-C19-O03-C01 |
| 23 | O | 303 | PSC | C20-C19-O03-C01 |
| 19 | A | 608 | PGV | C20-C19-O03-C01 |
| 23 | O | 303 | PSC | O04-C19-O03-C01 |
| 25 | G | 102 | CDL | OA9-CA7-OA8-CA6 |
| 22 | J | 102 | CHD | C13-C17-C20-C21 |
| 22 | W | 101 | CHD | C13-C17-C20-C21 |
| 20 | L | 101 | TGL | OB1-CB1-OG2-CG2 |
| 26 | T | 102 | PEK | O02-C1-O01-C02 |
| 26 | C | 306 | PEK | O02-C1-O01-C02 |
| 25 | C | 303 | CDL | OA7-CA5-OA6-CA4 |
| 25 | C | 303 | CDL | OB7-CB5-OB6-CB4 |
| 19 | P | 301 | PGV | O02-C1-O01-C02 |
| 23 | B | 304 | PSC | O02-C1-O01-C02 |
| 20 | Y | 101 | TGL | OB1-CB1-OG2-CG2 |
| 20 | D | 201 | TGL | CC2-CC1-OG3-CG3 |
| 20 | Y | 101 | TGL | CA2-CA1-OG1-CG1 |
| 26 | T | 102 | PEK | C2-C1-O01-C02 |
| 19 | P | 301 | PGV | C2-C1-O01-C02 |
| 25 | G | 102 | CDL | C11-CA5-OA6-CA4 |
| 22 | C | 304 | CHD | C13-C17-C20-C21 |
| 22 | J | 102 | CHD | C16-C17-C20-C22 |
| 22 | C | 304 | CHD | C13-C17-C20-C22 |
| 22 | P | 305 | CHD | C13-C17-C20-C22 |
| 23 | B | 304 | PSC | C20-C21-C22-C23 |
| 23 | B | 304 | PSC | C20-C19-O03-C01 |
| 25 | G | 102 | CDL | C31-CA7-OA8-CA6 |
| 19 | A | 608 | PGV | C10-C11-C12-C13 |
| 26 | T | 101 | PEK | C7-C8-C9-C10 |
| 19 | C | 307 | PGV | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | G | 103 | PEK | O02-C1-O01-C02 |
| 23 | O | 303 | PSC | O02-C1-O01-C02 |
| 23 | B | 304 | PSC | O04-C19-O03-C01 |
| 22 | P | 305 | CHD | C16-C17-C20-C22 |
| 25 | T | 103 | CDL | O1-C1-CB2-OB2 |
| 19 | P | 301 | PGV | O12-C04-C05-O05 |
| 25 | G | 102 | CDL | O1-C1-CA2-OA2 |
| 23 | B | 304 | PSC | C22-C23-C24-C25 |
| 25 | T | 103 | CDL | C11-CA5-OA6-CA4 |
| 20 | B | 301 | TGL | CA1-CA2-CA3-CA4 |
| 26 | P | 308 | PEK | C33-C34-C35-C36 |
| 20 | D | 201 | TGL | CA9-C20-C21-C22 |
| 25 | T | 103 | CDL | C79-C80-C81-C82 |
| 23 | O | 303 | PSC | C26-C27-C28-C29 |
| 25 | C | 303 | CDL | C76-C77-C78-C79 |
| 20 | Y | 101 | TGL | CC5-CC6-CC7-CC8 |
| 28 | P | 306 | DMU | O6-C11-C9-O1 |
| 22 | P | 305 | CHD | C16-C17-C20-C21 |
| 19 | P | 303 | PGV | C12-C13-C14-C15 |
| 25 | P | 304 | CDL | CA5-C11-C12-C13 |
| 19 | C | 307 | PGV | C20-C21-C22-C23 |
| 20 | B | 301 | TGL | OB1-CB1-OG2-CG2 |
| 23 | O | 303 | PSC | C20-C21-C22-C23 |
| 25 | C | 303 | CDL | CA4-CA3-OA5-PA1 |
| 23 | O | 303 | PSC | C24-C25-C26-C27 |
| 20 | D | 201 | TGL | C20-C21-C22-C23 |
| 22 | W | 101 | CHD | C16-C17-C20-C21 |
| 25 | T | 103 | CDL | C56-C57-C58-C59 |
| 20 | L | 101 | TGL | CC1-CC2-CC3-CC4 |
| 19 | A | 608 | PGV | O12-C04-C05-C06 |
| 25 | C | 303 | CDL | CB2-C1-CA2-OA2 |
| 25 | G | 102 | CDL | CB2-C1-CA2-OA2 |
| 25 | P | 304 | CDL | OB7-CB5-OB6-CB4 |
| 20 | L | 101 | TGL | CA2-CA1-OG1-CG1 |
| 20 | B | 301 | TGL | CA2-CA1-OG1-CG1 |
| 25 | T | 103 | CDL | C63-C64-C65-C66 |
| 28 | P | 306 | DMU | O6-C11-C9-C8 |
| 19 | A | 608 | PGV | O12-C04-C05-O05 |
| 25 | P | 304 | CDL | O1-C1-CA2-OA2 |
| 25 | P | 304 | CDL | O1-C1-CB2-OB2 |
| 19 | C | 307 | PGV | O12-C04-C05-O05 |
| 19 | C | 307 | PGV | C1-C2-C3-C4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | Q | 202 | TGL | OG1-CG1-CG2-OG2 |
| 19 | P | 303 | PGV | C30-C31-C32-C33 |
| 20 | Y | 101 | TGL | CA9-C20-C21-C22 |
| 20 | Q | 202 | TGL | CA9-C20-C21-C22 |
| 20 | B | 301 | TGL | CA9-C20-C21-C22 |
| 26 | G | 103 | PEK | C21-C22-C23-C24 |
| 22 | W | 101 | CHD | C17-C20-C22-C23 |
| 20 | N | 608 | TGL | CC7-CC8-CC9-C15 |
| 19 | A | 608 | PGV | C1-C2-C3-C4 |
| 23 | B | 304 | PSC | C1-C2-C3-C4 |
| 22 | C | 304 | CHD | C16-C17-C20-C21 |
| 26 | P | 308 | PEK | C2-C3-C4-C5 |
| 26 | T | 101 | PEK | C1-C2-C3-C4 |
| 19 | Q | 201 | PGV | C19-C20-C21-C22 |
| 19 | P | 301 | PGV | C1-C2-C3-C4 |
| 20 | B | 301 | TGL | OA1-CA1-OG1-CG1 |
| 25 | T | 103 | CDL | C73-C74-C75-C76 |
| 20 | L | 101 | TGL | OA1-CA1-OG1-CG1 |
| 14 | N | 601 | HEA | C19-C20-C21-C22 |
| 14 | A | 601 | HEA | C15-C16-C17-C18 |
| 20 | N | 608 | TGL | C22-C23-C24-C25 |
| 25 | C | 303 | CDL | O1-C1-CA2-OA2 |
| 25 | G | 102 | CDL | O1-C1-CB2-OB2 |
| 20 | L | 101 | TGL | CB3-CB4-CB5-CB6 |
| 22 | W | 101 | CHD | C16-C17-C20-C22 |
| 26 | C | 306 | PEK | C1-C2-C3-C4 |
| 26 | T | 101 | PEK | C13-C14-C15-C16 |
| 26 | C | 306 | PEK | C4-C5-C6-C7 |
| 26 | P | 308 | PEK | C10-C11-C12-C13 |
| 25 | T | 103 | CDL | CB3-OB5-PB2-OB2 |
| 19 | Q | 201 | PGV | C03-O11-P-O12 |
| 19 | Q | 201 | PGV | C04-O12-P-O11 |
| 23 | O | 303 | PSC | C03-O11-P-O12 |
| 19 | A | 608 | PGV | C03-O11-P-O12 |
| 19 | A | 608 | PGV | C04-O12-P-O11 |
| 25 | C | 303 | CDL | CB2-OB2-PB2-OB5 |
| 25 | C | 303 | CDL | CB3-OB5-PB2-OB2 |
| 25 | P | 304 | CDL | CA2-OA2-PA1-OA5 |
| 25 | P | 304 | CDL | CB3-OB5-PB2-OB2 |
| 23 | B | 304 | PSC | C03-O11-P-O12 |
| 26 | P | 308 | PEK | C04-O12-P-O11 |
| 25 | G | 102 | CDL | CB2-OB2-PB2-OB5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | T | 103 | CDL | CB5-C51-C52-C53 |
| 20 | Q | 202 | TGL | CB9-C10-C11-C12 |
| 20 | Q | 202 | TGL | CB1-CB2-CB3-CB4 |
| 19 | C | 307 | PGV | O12-C04-C05-C06 |
| 25 | G | 102 | CDL | CA2-C1-CB2-OB2 |
| 20 | N | 608 | TGL | OB1-CB1-OG2-CG2 |
| 26 | T | 101 | PEK | C2-C3-C4-C5 |
| 20 | N | 608 | TGL | CB4-CB5-CB6-CB7 |
| 25 | C | 303 | CDL | C12-C13-C14-C15 |
| 19 | P | 301 | PGV | C22-C23-C24-C25 |
| 25 | G | 102 | CDL | C23-C24-C25-C26 |
| 20 | L | 101 | TGL | CB2-CB1-OG2-CG2 |
| 20 | B | 301 | TGL | CB2-CB1-OG2-CG2 |
| 14 | A | 601 | HEA | C16-C17-C18-C19 |
| 19 | C | 302 | PGV | C14-C15-C16-C17 |
| 20 | L | 101 | TGL | CC6-CC7-CC8-CC9 |
| 20 | N | 608 | TGL | C13-C14-C29-C30 |
| 20 | B | 301 | TGL | CA5-CA6-CA7-CA8 |
| 25 | T | 103 | CDL | C18-C19-C20-C21 |
| 20 | Y | 101 | TGL | C23-C24-C25-C26 |
| 19 | C | 307 | PGV | C3-C4-C5-C6 |
| 19 | C | 307 | PGV | C22-C23-C24-C25 |
| 20 | Q | 202 | TGL | CC9-C15-C16-C17 |
| 20 | N | 608 | TGL | CA3-CA4-CA5-CA6 |
| 26 | G | 101 | PEK | C26-C27-C28-C29 |
| 19 | A | 608 | PGV | C23-C24-C25-C26 |
| 26 | T | 101 | PEK | C30-C31-C32-C33 |
| 26 | T | 102 | PEK | C28-C29-C30-C31 |
| 25 | C | 303 | CDL | C72-C73-C74-C75 |
| 25 | P | 304 | CDL | C38-C39-C40-C41 |
| 20 | Y | 101 | TGL | C10-C11-C12-C13 |
| 25 | G | 102 | CDL | C19-C20-C21-C22 |
| 25 | G | 102 | CDL | C59-C60-C61-C62 |
| 26 | G | 103 | PEK | C01-C02-O01-C1 |
| 19 | Q | 201 | PGV | C01-C02-O01-C1 |
| 23 | O | 303 | PSC | C01-C02-O01-C1 |
| 19 | A | 608 | PGV | C03-C02-O01-C1 |
| 20 | Q | 202 | TGL | CG3-CG2-OG2-CB1 |
| 19 | A | 608 | PGV | C19-C20-C21-C22 |
| 20 | D | 201 | TGL | CC9-C15-C16-C17 |
| 28 | M | 101 | DMU | C19-C22-C25-C28 |
| 25 | G | 102 | CDL | C82-C83-C84-C85 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | G | 102 | CDL | CB4-CB3-OB5-PB2 |
| 26 | T | 101 | PEK | C10-C11-C12-C13 |
| 26 | T | 102 | PEK | C13-C14-C15-C16 |
| 26 | P | 308 | PEK | C4-C5-C6-C7 |
| 20 | N | 608 | TGL | CA2-CA3-CA4-CA5 |
| 19 | C | 307 | PGV | C28-C29-C30-C31 |
| 20 | L | 101 | TGL | CB6-CB7-CB8-CB9 |
| 20 | L | 101 | TGL | C17-C18-C19-C33 |
| 20 | B | 301 | TGL | C11-C12-C13-C14 |
| 25 | T | 103 | CDL | C72-C73-C74-C75 |
| 19 | P | 303 | PGV | C7-C8-C9-C10 |
| 19 | P | 301 | PGV | C5-C6-C7-C8 |
| 19 | P | 301 | PGV | C23-C24-C25-C26 |
| 25 | G | 102 | CDL | C35-C36-C37-C38 |
| 20 | Q | 202 | TGL | C11-C10-CB9-CB8 |
| 20 | Q | 202 | TGL | C19-C33-C34-C35 |
| 19 | C | 302 | PGV | C7-C8-C9-C10 |
| 28 | Z | 101 | DMU | C22-C25-C28-C31 |
| 19 | A | 608 | PGV | C22-C23-C24-C25 |
| 25 | P | 304 | CDL | C36-C37-C38-C39 |
| 19 | C | 307 | PGV | C30-C31-C32-C33 |
| 25 | G | 102 | CDL | C72-C73-C74-C75 |
| 20 | B | 301 | TGL | CB4-CB5-CB6-CB7 |
| 23 | O | 303 | PSC | C5-C6-C7-C8 |
| 25 | C | 303 | CDL | C63-C64-C65-C66 |
| 19 | N | 607 | PGV | C14-C15-C16-C17 |
| 19 | P | 301 | PGV | C24-C25-C26-C27 |
| 20 | Y | 101 | TGL | CA3-CA4-CA5-CA6 |
| 19 | P | 301 | PGV | C19-C20-C21-C22 |
| 20 | D | 201 | TGL | CA3-CA4-CA5-CA6 |
| 20 | D | 201 | TGL | C14-C29-C30-C31 |
| 20 | B | 301 | TGL | CC4-CC5-CC6-CC7 |
| 25 | T | 103 | CDL | C71-C72-C73-C74 |
| 19 | P | 303 | PGV | C24-C25-C26-C27 |
| 20 | Y | 101 | TGL | CC6-CC7-CC8-CC9 |
| 20 | Y | 101 | TGL | C18-C19-C33-C34 |
| 25 | G | 102 | CDL | C38-C39-C40-C41 |
| 25 | G | 102 | CDL | C76-C77-C78-C79 |
| 20 | Q | 202 | TGL | C23-C24-C25-C26 |
| 20 | N | 608 | TGL | CA4-CA5-CA6-CA7 |
| 20 | N | 608 | TGL | CB6-CB7-CB8-CB9 |
| 20 | N | 608 | TGL | C19-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | T | 103 | CDL | C21-C22-C23-C24 |
| 19 | P | 301 | PGV | C04-C05-C06-O06 |
| 20 | L | 101 | TGL | CB4-CB5-CB6-CB7 |
| 25 | T | 103 | CDL | C31-C32-C33-C34 |
| 25 | C | 303 | CDL | C39-C40-C41-C42 |
| 19 | P | 301 | PGV | C4-C5-C6-C7 |
| 25 | P | 304 | CDL | C35-C36-C37-C38 |
| 25 | P | 304 | CDL | C60-C61-C62-C63 |
| 25 | G | 102 | CDL | C54-C55-C56-C57 |
| 19 | A | 608 | PGV | C12-C13-C14-C15 |
| 20 | D | 201 | TGL | C16-C17-C18-C19 |
| 20 | L | 101 | TGL | CA5-CA6-CA7-CA8 |
| 25 | T | 103 | CDL | C39-C40-C41-C42 |
| 23 | O | 303 | PSC | C3-C4-C5-C6 |
| 23 | O | 303 | PSC | C4-C5-C6-C7 |
| 26 | T | 101 | PEK | C26-C27-C28-C29 |
| 25 | C | 303 | CDL | C71-C72-C73-C74 |
| 19 | N | 607 | PGV | C23-C24-C25-C26 |
| 25 | P | 304 | CDL | C73-C74-C75-C76 |
| 25 | P | 304 | CDL | C79-C80-C81-C82 |
| 25 | G | 102 | CDL | C41-C42-C43-C44 |
| 20 | Q | 202 | TGL | CB5-CB6-CB7-CB8 |
| 25 | P | 304 | CDL | C59-C60-C61-C62 |
| 20 | Y | 101 | TGL | CA6-CA7-CA8-CA9 |
| 20 | Y | 101 | TGL | CC9-C15-C16-C17 |
| 20 | D | 201 | TGL | CA7-CA8-CA9-C20 |
| 20 | D | 201 | TGL | CB2-CB3-CB4-CB5 |
| 20 | L | 101 | TGL | C11-C12-C13-C14 |
| 28 | Z | 101 | DMU | C25-C28-C31-C34 |
| 19 | P | 301 | PGV | C13-C14-C15-C16 |
| 25 | P | 304 | CDL | C40-C41-C42-C43 |
| 20 | Q | 202 | TGL | CA5-CA6-CA7-CA8 |
| 19 | C | 302 | PGV | C23-C24-C25-C26 |
| 26 | G | 101 | PEK | C34-C35-C36-C37 |
| 23 | B | 304 | PSC | C24-C25-C26-C27 |
| 25 | C | 303 | CDL | C31-CA7-OA8-CA6 |
| 20 | N | 608 | TGL | C12-C13-C14-C29 |
| 20 | N | 608 | TGL | CA9-C20-C21-C22 |
| 25 | G | 102 | CDL | C20-C21-C22-C23 |
| 20 | N | 608 | TGL | CC5-CC6-CC7-CC8 |
| 25 | T | 103 | CDL | C23-C24-C25-C26 |
| 26 | G | 101 | PEK | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | C | 303 | CDL | C23-C24-C25-C26 |
| 25 | C | 303 | CDL | C31-C32-C33-C34 |
| 19 | P | 301 | PGV | C6-C7-C8-C9 |
| 23 | B | 304 | PSC | C27-C28-C29-C30 |
| 20 | N | 608 | TGL | OC1-CC1-OG3-CG3 |
| 25 | T | 103 | CDL | C13-C14-C15-C16 |
| 19 | Q | 201 | PGV | C4-C5-C6-C7 |
| 25 | P | 304 | CDL | C20-C21-C22-C23 |
| 25 | P | 304 | CDL | CA3-CA4-CA6-OA8 |
| 26 | G | 101 | PEK | C10-C11-C12-C13 |
| 23 | B | 304 | PSC | C11-C12-C13-C14 |
| 19 | A | 607 | PGV | C28-C29-C30-C31 |
| 20 | N | 608 | TGL | CB7-CB8-CB9-C10 |
| 26 | G | 101 | PEK | C23-C24-C25-C26 |
| 25 | G | 102 | CDL | C33-C34-C35-C36 |
| 19 | C | 302 | PGV | C27-C28-C29-C30 |
| 20 | N | 608 | TGL | CB2-CB1-OG2-CG2 |
| 19 | C | 307 | PGV | C2-C1-O01-C02 |
| 19 | Q | 201 | PGV | O05-C05-C06-O06 |
| 20 | N | 608 | TGL | CB5-CB6-CB7-CB8 |
| 26 | T | 102 | PEK | C25-C26-C27-C28 |
| 19 | N | 607 | PGV | C29-C30-C31-C32 |
| 19 | C | 307 | PGV | C23-C24-C25-C26 |
| 20 | Q | 202 | TGL | C17-C18-C19-C33 |
| 25 | C | 303 | CDL | OA9-CA7-OA8-CA6 |
| 25 | P | 304 | CDL | C16-C17-C18-C19 |
| 19 | P | 301 | PGV | C30-C31-C32-C33 |
| 25 | P | 304 | CDL | C43-C44-C45-C46 |
| 20 | L | 101 | TGL | C21-C20-CA9-CA8 |
| 25 | T | 103 | CDL | C61-C62-C63-C64 |
| 19 | Q | 201 | PGV | C14-C15-C16-C17 |
| 26 | G | 101 | PEK | C25-C26-C27-C28 |
| 19 | C | 307 | PGV | O02-C1-O01-C02 |
| 20 | D | 201 | TGL | C11-C12-C13-C14 |
| 28 | M | 101 | DMU | C22-C25-C28-C31 |
| 20 | B | 301 | TGL | C17-C18-C19-C33 |
| 19 | Q | 201 | PGV | C2-C3-C4-C5 |
| 25 | P | 304 | CDL | C74-C75-C76-C77 |
| 20 | Y | 101 | TGL | C16-C15-CC9-CC8 |
| 20 | D | 201 | TGL | CB9-C10-C11-C12 |
| 25 | G | 102 | CDL | C16-C17-C18-C19 |
| 20 | B | 301 | TGL | CC7-CC8-CC9-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 28 | J | 101 | DMU | C19-C22-C25-C28 |
| 20 | N | 608 | TGL | CC2-CC1-OG3-CG3 |
| 20 | N | 608 | TGL | C21-C20-CA9-CA8 |
| 25 | T | 103 | CDL | C75-C76-C77-C78 |
| 25 | T | 103 | CDL | C81-C82-C83-C84 |
| 19 | Q | 201 | PGV | C29-C30-C31-C32 |
| 26 | T | 102 | PEK | C33-C34-C35-C36 |
| 23 | B | 304 | PSC | C30-C31-C32-C33 |
| 20 | Q | 202 | TGL | CB2-CB3-CB4-CB5 |
| 25 | P | 304 | CDL | C31-C32-C33-C34 |
| 26 | G | 101 | PEK | C7-C8-C9-C10 |
| 26 | G | 103 | PEK | C25-C26-C27-C28 |
| 20 | Y | 101 | TGL | C25-C26-C27-C28 |
| 23 | O | 303 | PSC | C6-C7-C8-C9 |
| 26 | G | 101 | PEK | C15-C16-C17-C18 |
| 26 | T | 102 | PEK | C2-C3-C4-C5 |
| 26 | C | 306 | PEK | C2-C3-C4-C5 |
| 20 | N | 608 | TGL | CA2-CA1-OG1-CG1 |
| 19 | C | 307 | PGV | C20-C19-O03-C01 |
| 25 | G | 102 | CDL | C71-CB7-OB8-CB6 |
| 20 | N | 608 | TGL | C11-C10-CB9-CB8 |
| 25 | C | 303 | CDL | C18-C19-C20-C21 |
| 25 | T | 103 | CDL | C83-C84-C85-C86 |
| 25 | G | 102 | CDL | C17-C18-C19-C20 |
| 20 | D | 201 | TGL | CC6-CC7-CC8-CC9 |
| 25 | G | 102 | CDL | C13-C14-C15-C16 |
| 25 | G | 102 | CDL | C14-C15-C16-C17 |
| 25 | G | 102 | CDL | C22-C23-C24-C25 |
| 25 | G | 102 | CDL | C56-C57-C58-C59 |
| 26 | G | 101 | PEK | C16-C17-C18-C19 |
| 26 | C | 306 | PEK | C24-C25-C26-C27 |
| 25 | P | 304 | CDL | C58-C59-C60-C61 |
| 20 | L | 101 | TGL | C18-C19-C33-C34 |
| 19 | A | 608 | PGV | C7-C8-C9-C10 |
| 26 | P | 308 | PEK | C28-C29-C30-C31 |
| 20 | D | 201 | TGL | CA2-CA3-CA4-CA5 |
| 20 | N | 608 | TGL | CC4-CC5-CC6-CC7 |
| 26 | T | 102 | PEK | O01-C02-C03-O11 |
| 19 | C | 307 | PGV | O01-C02-C03-O11 |
| 19 | A | 608 | PGV | C20-C21-C22-C23 |
| 25 | C | 303 | CDL | C64-C65-C66-C67 |
| 28 | P | 306 | DMU | O16-C18-C19-C22 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | P | 308 | PEK | C32-C33-C34-C35 |
| 20 | Y | 101 | TGL | CB7-CB8-CB9-C10 |
| 26 | C | 306 | PEK | C25-C26-C27-C28 |
| 20 | D | 201 | TGL | OG1-CG1-CG2-OG2 |
| 25 | T | 103 | CDL | OB6-CB4-CB6-OB8 |
| 25 | P | 304 | CDL | C57-C58-C59-C60 |
| 20 | Q | 202 | TGL | CC5-CC6-CC7-CC8 |
| 28 | Z | 101 | DMU | C19-C22-C25-C28 |
| 25 | T | 103 | CDL | C15-C16-C17-C18 |
| 26 | T | 102 | PEK | C32-C33-C34-C35 |
| 25 | P | 304 | CDL | C72-C73-C74-C75 |
| 20 | Y | 101 | TGL | CB9-C10-C11-C12 |
| 19 | P | 301 | PGV | C11-C10-C9-C8 |
| 20 | B | 301 | TGL | CB5-CB6-CB7-CB8 |
| 20 | B | 301 | TGL | C12-C13-C14-C29 |
| 20 | B | 301 | TGL | C16-C17-C18-C19 |
| 25 | P | 304 | CDL | C37-C38-C39-C40 |
| 20 | D | 201 | TGL | C17-C18-C19-C33 |
| 22 | P | 305 | CHD | C20-C22-C23-C24 |
| 20 | L | 101 | TGL | CB2-CB3-CB4-CB5 |
| 25 | C | 303 | CDL | C53-C54-C55-C56 |
| 25 | P | 304 | CDL | C12-C13-C14-C15 |
| 20 | N | 608 | TGL | C11-C12-C13-C14 |
| 25 | P | 304 | CDL | C80-C81-C82-C83 |
| 20 | Y | 101 | TGL | CA2-CA3-CA4-CA5 |
| 26 | G | 103 | PEK | C03-O11-P-O12 |
| 19 | C | 307 | PGV | C03-O11-P-O12 |
| 20 | Y | 101 | TGL | CC4-CC5-CC6-CC7 |
| 19 | A | 608 | PGV | C05-C04-O12-P |
| 25 | P | 304 | CDL | C78-C79-C80-C81 |
| 19 | Q | 201 | PGV | C01-C02-C03-O11 |
| 19 | A | 608 | PGV | C01-C02-C03-O11 |
| 25 | C | 303 | CDL | OA5-CA3-CA4-CA6 |
| 25 | P | 304 | CDL | OA5-CA3-CA4-CA6 |
| 19 | C | 307 | PGV | C01-C02-C03-O11 |
| 23 | B | 304 | PSC | C26-C27-C28-C29 |
| 20 | D | 201 | TGL | C23-C24-C25-C26 |
| 25 | P | 304 | CDL | C23-C24-C25-C26 |
| 20 | Y | 101 | TGL | C13-C14-C29-C30 |
| 20 | Q | 202 | TGL | CA6-CA7-CA8-CA9 |
| 20 | Y | 101 | TGL | C22-C23-C24-C25 |
| 20 | Y | 101 | TGL | C11-C10-CB9-CB8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | Q | 202 | TGL | CC2-CC3-CC4-CC5 |
| 25 | G | 102 | CDL | C58-C59-C60-C61 |
| 25 | T | 103 | CDL | CB3-CB4-CB6-OB8 |
| 19 | Q | 201 | PGV | O03-C01-C02-C03 |
| 23 | O | 303 | PSC | O03-C01-C02-C03 |
| 25 | G | 102 | CDL | CA3-CA4-CA6-OA8 |
| 20 | Q | 202 | TGL | CG1-CG2-CG3-OG3 |
| 26 | T | 102 | PEK | C10-C11-C12-C13 |
| 25 | T | 103 | CDL | C64-C65-C66-C67 |
| 28 | J | 101 | DMU | C34-C37-C40-C43 |
| 20 | N | 608 | TGL | OA1-CA1-OG1-CG1 |
| 20 | B | 301 | TGL | OC1-CC1-OG3-CG3 |
| 20 | N | 608 | TGL | CC6-CC7-CC8-CC9 |
| 20 | B | 301 | TGL | C21-C20-CA9-CA8 |
| 19 | P | 301 | PGV | C15-C16-C17-C18 |
| 25 | C | 303 | CDL | C24-C25-C26-C27 |
| 20 | N | 608 | TGL | CA1-CA2-CA3-CA4 |
| 19 | A | 607 | PGV | C31-C32-C33-C34 |
| 25 | T | 103 | CDL | C17-C18-C19-C20 |
| 20 | B | 301 | TGL | C29-C30-C31-C32 |
| 25 | C | 303 | CDL | C43-C44-C45-C46 |
| 25 | T | 103 | CDL | C22-C23-C24-C25 |
| 20 | Q | 202 | TGL | C29-C30-C31-C32 |
| 19 | A | 608 | PGV | C11-C10-C9-C8 |
| 20 | L | 101 | TGL | CC3-CC4-CC5-CC6 |
| 19 | A | 608 | PGV | C31-C32-C33-C34 |
| 19 | C | 302 | PGV | C15-C16-C17-C18 |
| 19 | Q | 201 | PGV | C31-C32-C33-C34 |
| 20 | Y | 101 | TGL | CB3-CB4-CB5-CB6 |
| 20 | Y | 101 | TGL | CC3-CC4-CC5-CC6 |
| 20 | D | 201 | TGL | CG3-CG2-OG2-CB1 |
| 25 | P | 304 | CDL | CA3-CA4-OA6-CA5 |
| 23 | B | 304 | PSC | C01-C02-O01-C1 |
| 25 | P | 304 | CDL | OA7-CA5-OA6-CA4 |
| 25 | C | 303 | CDL | C14-C15-C16-C17 |
| 20 | B | 301 | TGL | CC2-CC1-OG3-CG3 |
| 19 | Q | 201 | PGV | C10-C11-C12-C13 |
| 26 | T | 101 | PEK | C4-C5-C6-C7 |
| 26 | C | 306 | PEK | C7-C8-C9-C10 |
| 25 | G | 102 | CDL | CA5-C11-C12-C13 |
| 23 | O | 303 | PSC | C2-C3-C4-C5 |
| 26 | P | 308 | PEK | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | P | 305 | CHD | C13-C17-C20-C21 |
| 25 | C | 303 | CDL | C61-C62-C63-C64 |
| 25 | G | 102 | CDL | C11-C12-C13-C14 |
| 28 | P | 306 | DMU | C22-C25-C28-C31 |
| 20 | N | 608 | TGL | OG1-CG1-CG2-OG2 |
| 20 | N | 608 | TGL | CB9-C10-C11-C12 |
| 26 | G | 101 | PEK | C35-C36-C37-C38 |
| 25 | G | 102 | CDL | C77-C78-C79-C80 |
| 25 | G | 102 | CDL | OB9-CB7-OB8-CB6 |
| 25 | T | 103 | CDL | C36-C37-C38-C39 |
| 25 | G | 102 | CDL | C12-C13-C14-C15 |
| 20 | L | 101 | TGL | CC2-CC3-CC4-CC5 |
| 26 | C | 306 | PEK | C35-C36-C37-C38 |
| 19 | P | 301 | PGV | O12-C04-C05-C06 |
| 19 | C | 307 | PGV | C21-C22-C23-C24 |
| 25 | G | 102 | CDL | C79-C80-C81-C82 |
| 19 | C | 302 | PGV | C10-C11-C12-C13 |
| 19 | Q | 201 | PGV | C27-C28-C29-C30 |
| 25 | C | 303 | CDL | C73-C74-C75-C76 |
| 20 | Q | 202 | TGL | CB4-CB5-CB6-CB7 |
| 19 | A | 607 | PGV | C30-C31-C32-C33 |
| 20 | D | 201 | TGL | CC5-CC6-CC7-CC8 |
| 26 | T | 102 | PEK | C01-C02-C03-O11 |
| 20 | D | 201 | TGL | C22-C23-C24-C25 |
| 25 | T | 103 | CDL | C12-C13-C14-C15 |
| 19 | N | 607 | PGV | C13-C14-C15-C16 |
| 19 | C | 307 | PGV | C25-C26-C27-C28 |
| 26 | G | 103 | PEK | C23-C24-C25-C26 |
| 23 | B | 304 | PSC | C14-C15-C16-C17 |
| 14 | N | 601 | HEA | C16-C17-C18-C19 |
| 20 | D | 201 | TGL | C13-C14-C29-C30 |
| 23 | O | 303 | PSC | C02-C03-O11-P |
| 25 | P | 304 | CDL | CA4-CA3-OA5-PA1 |
| 19 | P | 303 | PGV | C28-C29-C30-C31 |
| 26 | C | 306 | PEK | C32-C33-C34-C35 |
| 23 | B | 304 | PSC | C2-C3-C4-C5 |
| 26 | G | 103 | PEK | C30-C31-C32-C33 |
| 20 | B | 301 | TGL | OG1-CG1-CG2-CG3 |
| 25 | T | 103 | CDL | CA3-CA4-CA6-OA8 |
| 19 | A | 608 | PGV | O03-C01-C02-C03 |
| 25 | C | 303 | CDL | CB3-CB4-CB6-OB8 |
| 23 | B | 304 | PSC | O03-C01-C02-C03 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | Q | 202 | TGL | C15-C16-C17-C18 |
| 26 | G | 103 | PEK | C10-C11-C12-C13 |
| 23 | O | 303 | PSC | C11-C10-C9-C8 |
| 19 | P | 301 | PGV | C10-C11-C12-C13 |
| 26 | P | 308 | PEK | C7-C8-C9-C10 |
| 20 | D | 201 | TGL | CB4-CB5-CB6-CB7 |
| 25 | T | 103 | CDL | C55-C56-C57-C58 |
| 23 | B | 304 | PSC | C29-C30-C31-C32 |
| 28 | J | 101 | DMU | C28-C31-C34-C37 |
| 28 | J | 101 | DMU | C18-C19-C22-C25 |
| 20 | L | 101 | TGL | CC4-CC5-CC6-CC7 |
| 25 | T | 103 | CDL | C11-C12-C13-C14 |
| 25 | T | 103 | CDL | C43-C44-C45-C46 |
| 20 | Y | 101 | TGL | C11-C12-C13-C14 |
| 26 | G | 103 | PEK | C11-C10-C9-C8 |
| 26 | G | 103 | PEK | C9-C10-C11-C12 |
| 26 | G | 103 | PEK | C12-C13-C14-C15 |
| 23 | O | 303 | PSC | C9-C10-C11-C12 |
| 23 | O | 303 | PSC | C10-C11-C12-C13 |
| 26 | G | 101 | PEK | C9-C10-C11-C12 |
| 26 | T | 101 | PEK | C11-C10-C9-C8 |
| 26 | T | 102 | PEK | C11-C10-C9-C8 |
| 26 | T | 102 | PEK | C9-C10-C11-C12 |
| 26 | T | 102 | PEK | C12-C13-C14-C15 |
| 26 | C | 306 | PEK | C5-C6-C7-C8 |
| 26 | C | 306 | PEK | C11-C10-C9-C8 |
| 23 | B | 304 | PSC | C9-C10-C11-C12 |
| 26 | P | 308 | PEK | C5-C6-C7-C8 |
| 26 | P | 308 | PEK | C6-C7-C8-C9 |
| 25 | G | 102 | CDL | CB5-C51-C52-C53 |
| 23 | B | 304 | PSC | C3-C4-C5-C6 |
| 25 | T | 103 | CDL | C84-C85-C86-C87 |
| 25 | T | 103 | CDL | OA5-CA3-CA4-OA6 |
| 19 | Q | 201 | PGV | O01-C02-C03-O11 |
| 25 | C | 303 | CDL | OA5-CA3-CA4-OA6 |
| 25 | P | 304 | CDL | OA5-CA3-CA4-OA6 |
| 25 | P | 304 | CDL | OB5-CB3-CB4-OB6 |
| 25 | C | 303 | CDL | CB7-C71-C72-C73 |
| 19 | Q | 201 | PGV | C5-C6-C7-C8 |
| 20 | N | 608 | TGL | C20-C21-C22-C23 |
| 19 | A | 608 | PGV | C15-C16-C17-C18 |
| 20 | L | 101 | TGL | OG2-CG2-CG3-OG3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | G | 103 | PEK | O03-C01-C02-O01 |
| 20 | B | 301 | TGL | OG1-CG1-CG2-OG2 |
| 25 | T | 103 | CDL | OA6-CA4-CA6-OA8 |
| 26 | T | 102 | PEK | O03-C01-C02-O01 |
| 19 | C | 307 | PGV | O03-C01-C02-O01 |
| 20 | Q | 202 | TGL | C25-C26-C27-C28 |
| 14 | N | 601 | HEA | C15-C16-C17-C18 |
| 26 | C | 306 | PEK | C29-C30-C31-C32 |
| 22 | J | 102 | CHD | C17-C20-C22-C23 |
| 25 | T | 103 | CDL | C52-C53-C54-C55 |
| 20 | Q | 202 | TGL | C20-C21-C22-C23 |
| 20 | D | 201 | TGL | CC3-CC4-CC5-CC6 |
| 26 | T | 101 | PEK | C34-C35-C36-C37 |
| 19 | P | 303 | PGV | C02-C03-O11-P |
| 26 | C | 306 | PEK | C02-C03-O11-P |
| 26 | P | 308 | PEK | C02-C03-O11-P |
| 20 | D | 201 | TGL | CC7-CC8-CC9-C15 |
| 28 | M | 101 | DMU | C25-C28-C31-C34 |
| 19 | P | 301 | PGV | C31-C32-C33-C34 |
| 25 | G | 102 | CDL | C71-C72-C73-C74 |
| 19 | A | 608 | PGV | C11-C12-C13-C14 |
| 25 | T | 103 | CDL | C14-C15-C16-C17 |
| 25 | P | 304 | CDL | C84-C85-C86-C87 |
| 25 | P | 304 | CDL | C11-CA5-OA6-CA4 |
| 25 | C | 303 | CDL | C84-C85-C86-C87 |
| 19 | P | 303 | PGV | C22-C23-C24-C25 |
| 26 | C | 306 | PEK | C01-C02-C03-O11 |
| 19 | Q | 201 | PGV | C7-C8-C9-C10 |
| 20 | L | 101 | TGL | C13-C14-C29-C30 |
| 20 | B | 301 | TGL | C24-C25-C26-C27 |
| 23 | B | 304 | PSC | C23-C24-C25-C26 |
| 25 | C | 303 | CDL | C58-C59-C60-C61 |
| 20 | L | 101 | TGL | C12-C13-C14-C29 |
| 19 | C | 307 | PGV | O04-C19-O03-C01 |
| 19 | P | 301 | PGV | C29-C30-C31-C32 |
| 19 | C | 302 | PGV | C24-C25-C26-C27 |
| 20 | L | 101 | TGL | C10-C11-C12-C13 |
| 26 | C | 306 | PEK | C22-C21-O03-C01 |
| 25 | T | 103 | CDL | C54-C55-C56-C57 |
| 25 | T | 103 | CDL | C60-C61-C62-C63 |
| 26 | G | 101 | PEK | C22-C23-C24-C25 |
| 19 | C | 302 | PGV | C02-C03-O11-P |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | L | 101 | TGL | CG1-CG2-CG3-OG3 |
| 20 | N | 608 | TGL | OG1-CG1-CG2-CG3 |
| 25 | T | 103 | CDL | CB4-CB3-OB5-PB2 |
| 19 | C | 307 | PGV | O03-C01-C02-C03 |
| 20 | Q | 202 | TGL | OG1-CG1-CG2-CG3 |
| 26 | G | 103 | PEK | C3-C4-C5-C6 |
| 25 | G | 102 | CDL | OB7-CB5-OB6-CB4 |
| 25 | C | 303 | CDL | C77-C78-C79-C80 |
| 25 | P | 304 | CDL | C11-C12-C13-C14 |
| 26 | C | 306 | PEK | O04-C21-O03-C01 |
| 19 | Q | 201 | PGV | O03-C01-C02-O01 |
| 23 | O | 303 | PSC | O03-C01-C02-O01 |
| 20 | Y | 101 | TGL | OG2-CG2-CG3-OG3 |
| 20 | B | 301 | TGL | C18-C19-C33-C34 |
| 25 | T | 103 | CDL | C16-C17-C18-C19 |
| 25 | P | 304 | CDL | CB4-CB6-OB8-CB7 |
| 19 | C | 302 | PGV | C20-C21-C22-C23 |
| 25 | P | 304 | CDL | C63-C64-C65-C66 |
| 25 | G | 102 | CDL | C64-C65-C66-C67 |
| 20 | D | 201 | TGL | CB5-CB6-CB7-CB8 |
| 19 | P | 303 | PGV | C15-C16-C17-C18 |
| 20 | B | 301 | TGL | CA4-CA5-CA6-CA7 |
| 26 | C | 306 | PEK | C10-C11-C12-C13 |
| 22 | C | 304 | CHD | C16-C17-C20-C22 |
| 26 | T | 101 | PEK | C17-C18-C19-C20 |
| 26 | C | 306 | PEK | C26-C27-C28-C29 |
| 14 | A | 602 | HEA | O11-C11-C12-C13 |
| 25 | G | 102 | CDL | C51-CB5-OB6-CB4 |
| 23 | B | 304 | PSC | C15-C16-C17-C18 |
| 20 | N | 608 | TGL | C10-C11-C12-C13 |
| 23 | B | 304 | PSC | C13-C14-C15-C16 |
| 26 | T | 102 | PEK | C04-O12-P-O11 |
| 26 | C | 306 | PEK | C04-O12-P-O11 |
| 25 | P | 304 | CDL | CA3-OA5-PA1-OA2 |
| 23 | B | 304 | PSC | C04-O12-P-O11 |
| 28 | Z | 101 | DMU | C34-C37-C40-C43 |
| 25 | P | 304 | CDL | C44-C45-C46-C47 |
| 20 | Q | 202 | TGL | C16-C17-C18-C19 |
| 25 | T | 103 | CDL | CA4-CA3-OA5-PA1 |
| 19 | A | 608 | PGV | C02-C03-O11-P |
| 26 | C | 306 | PEK | C23-C24-C25-C26 |
| 19 | Q | 201 | PGV | C03-O11-P-O13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 19 | Q | 201 | PGV | C04-O12-P-O13 |
| 26 | T | 102 | PEK | C04-O12-P-O13 |
| 25 | C | 303 | CDL | CB2-OB2-PB2-OB3 |
| 23 | B | 304 | PSC | C03-O11-P-O13 |
| 26 | P | 308 | PEK | C04-O12-P-O14 |
| 19 | C | 307 | PGV | C04-O12-P-O14 |
| 20 | Y | 101 | TGL | CB2-CB3-CB4-CB5 |
| 25 | T | 103 | CDL | C62-C63-C64-C65 |
| 26 | G | 101 | PEK | O12-C04-C05-N |
| 20 | Y | 101 | TGL | C24-C25-C26-C27 |
| 20 | L | 101 | TGL | C20-C21-C22-C23 |
| 20 | Y | 101 | TGL | C33-C34-C35-C36 |
| 19 | C | 307 | PGV | C24-C25-C26-C27 |
| 26 | T | 102 | PEK | C7-C8-C9-C10 |
| 19 | Q | 201 | PGV | C21-C22-C23-C24 |
| 23 | B | 304 | PSC | C05-C04-O12-P |
| 20 | L | 101 | TGL | OG1-CA1-CA2-CA3 |
| 20 | Y | 101 | TGL | C15-C16-C17-C18 |
| 25 | T | 103 | CDL | CA7-C31-C32-C33 |
| 20 | Q | 202 | TGL | CA3-CA4-CA5-CA6 |
| 19 | A | 608 | PGV | O01-C02-C03-O11 |
| 26 | C | 306 | PEK | O01-C02-C03-O11 |
| 25 | C | 303 | CDL | C44-C45-C46-C47 |
| 19 | N | 607 | PGV | C31-C32-C33-C34 |
| 28 | M | 101 | DMU | C18-C19-C22-C25 |
| 20 | N | 608 | TGL | C29-C30-C31-C32 |
| 20 | N | 608 | TGL | CA5-CA6-CA7-CA8 |
| 20 | D | 201 | TGL | C24-C25-C26-C27 |
| 19 | C | 307 | PGV | C27-C28-C29-C30 |
| 25 | G | 102 | CDL | C31-C32-C33-C34 |
| 20 | D | 201 | TGL | OG1-CG1-CG2-CG3 |
| 26 | G | 103 | PEK | O03-C01-C02-C03 |
| 23 | O | 303 | PSC | O12-C04-C05-N |
| 26 | T | 102 | PEK | O03-C01-C02-C03 |
| 20 | Q | 202 | TGL | CC3-CC4-CC5-CC6 |
| 23 | B | 304 | PSC | O03-C01-C02-O01 |
| 20 | Q | 202 | TGL | OG2-CG2-CG3-OG3 |
| 20 | D | 201 | TGL | C18-C19-C33-C34 |
| 25 | T | 103 | CDL | C82-C83-C84-C85 |
| 25 | C | 303 | CDL | C17-C18-C19-C20 |
| 20 | Q | 202 | TGL | CA4-CA5-CA6-CA7 |
| 28 | Z | 101 | DMU | C28-C31-C34-C37 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | C | 303 | CDL | C20-C21-C22-C23 |
| 25 | T | 103 | CDL | C58-C59-C60-C61 |
| 25 | C | 303 | CDL | C19-C20-C21-C22 |
| 26 | C | 306 | PEK | C28-C29-C30-C31 |
| 25 | C | 303 | CDL | C51-C52-C53-C54 |
| 20 | Y | 101 | TGL | OG1-CA1-CA2-CA3 |
| 26 | P | 308 | PEK | O04-C21-O03-C01 |
| 20 | Y | 101 | TGL | OG2-CB1-CB2-CB3 |
| 25 | T | 103 | CDL | C35-C36-C37-C38 |
| 19 | C | 307 | PGV | C15-C16-C17-C18 |
| 20 | D | 201 | TGL | OB1-CB1-OG2-CG2 |
| 19 | A | 608 | PGV | C14-C15-C16-C17 |
| 25 | C | 303 | CDL | C22-C23-C24-C25 |
| 25 | P | 304 | CDL | C18-C19-C20-C21 |
| 25 | C | 303 | CDL | C78-C79-C80-C81 |
| 19 | P | 301 | PGV | C21-C22-C23-C24 |
| 23 | O | 303 | PSC | C28-C29-C30-C31 |
| 25 | G | 102 | CDL | C37-C38-C39-C40 |
| 25 | P | 304 | CDL | C22-C23-C24-C25 |
| 26 | G | 101 | PEK | C17-C18-C19-C20 |
| 26 | P | 308 | PEK | C3-C4-C5-C6 |
| 25 | P | 304 | CDL | OA6-CA4-CA6-OA8 |
| 25 | G | 102 | CDL | OA6-CA4-CA6-OA8 |
| 23 | O | 303 | PSC | C04-O12-P-O11 |
| 25 | C | 303 | CDL | CA2-OA2-PA1-OA5 |
| 25 | C | 303 | CDL | CA3-OA5-PA1-OA2 |
| 19 | P | 301 | PGV | C03-O11-P-O12 |
| 19 | P | 301 | PGV | C04-O12-P-O11 |
| 25 | G | 102 | CDL | CA3-OA5-PA1-OA2 |
| 28 | J | 101 | DMU | O1-C10-O7-C3 |
| 20 | N | 608 | TGL | C14-C29-C30-C31 |
| 20 | D | 201 | TGL | C21-C20-CA9-CA8 |
| 25 | P | 304 | CDL | CB3-CB4-CB6-OB8 |
| 20 | Y | 101 | TGL | CG1-CG2-CG3-OG3 |
| 20 | L | 101 | TGL | CB5-CB6-CB7-CB8 |
| 19 | C | 307 | PGV | C13-C14-C15-C16 |
| 22 | W | 101 | CHD | C21-C20-C22-C23 |
| 19 | C | 302 | PGV | C12-C13-C14-C15 |
| 19 | P | 303 | PGV | C05-C04-O12-P |
| 25 | C | 303 | CDL | C13-C14-C15-C16 |
| 25 | C | 303 | CDL | OB9-CB7-OB8-CB6 |
| 25 | P | 304 | CDL | CA2-C1-CB2-OB2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | Q | 202 | TGL | OG2-CB1-CB2-CB3 |
| 26 | P | 308 | PEK | C22-C21-O03-C01 |
| 22 | C | 304 | CHD | C21-C20-C22-C23 |
| 25 | P | 304 | CDL | C53-C54-C55-C56 |
| 26 | G | 103 | PEK | C13-C14-C15-C16 |
| 26 | T | 101 | PEK | O03-C21-C22-C23 |
| 20 | B | 301 | TGL | CA2-CA3-CA4-CA5 |
| 22 | P | 307 | CHD | C16-C17-C20-C22 |
| 19 | A | 608 | PGV | C13-C14-C15-C16 |
| 28 | M | 101 | DMU | C28-C31-C34-C37 |
| 19 | Q | 201 | PGV | C15-C16-C17-C18 |
| 20 | L | 101 | TGL | C11-C10-CB9-CB8 |
| 26 | G | 103 | PEK | C27-C28-C29-C30 |
| 20 | N | 608 | TGL | C33-C34-C35-C36 |
| 20 | N | 608 | TGL | CB3-CB4-CB5-CB6 |
| 20 | N | 608 | TGL | C21-C22-C23-C24 |
| 19 | C | 302 | PGV | C05-C04-O12-P |
| 26 | G | 103 | PEK | C29-C30-C31-C32 |
| 26 | P | 308 | PEK | C22-C23-C24-C25 |
| 20 | Y | 101 | TGL | C16-C17-C18-C19 |
| 20 | L | 101 | TGL | C24-C25-C26-C27 |
| 25 | T | 103 | CDL | C59-C60-C61-C62 |
| 20 | L | 101 | TGL | C23-C24-C25-C26 |
| 25 | P | 304 | CDL | C81-C82-C83-C84 |
| 25 | C | 303 | CDL | O1-C1-CB2-OB2 |
| 20 | D | 201 | TGL | CC4-CC5-CC6-CC7 |
| 25 | C | 303 | CDL | CA7-C31-C32-C33 |
| 20 | N | 608 | TGL | CA7-CA8-CA9-C20 |
| 26 | T | 101 | PEK | O02-C1-O01-C02 |
| 23 | O | 303 | PSC | C12-C13-C14-C15 |
| 25 | T | 103 | CDL | C19-C20-C21-C22 |
| 26 | T | 102 | PEK | C11-C12-C13-C14 |
| 26 | P | 308 | PEK | C11-C10-C9-C8 |
| 26 | P | 308 | PEK | C9-C10-C11-C12 |
| 20 | N | 608 | TGL | CB2-CB3-CB4-CB5 |
| 20 | L | 101 | TGL | CA4-CA5-CA6-CA7 |
| 25 | P | 304 | CDL | C1-CA2-OA2-PA1 |
| 19 | P | 301 | PGV | O01-C02-C03-O11 |
| 26 | G | 101 | PEK | C13-C14-C15-C16 |
| 26 | T | 101 | PEK | C35-C36-C37-C38 |
| 25 | T | 103 | CDL | OA5-CA3-CA4-CA6 |
| 19 | P | 301 | PGV | C01-C02-C03-O11 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 19 | C | 302 | PGV | C11-C12-C13-C14 |
| 20 | B | 301 | TGL | C16-C15-CC9-CC8 |
| 25 | T | 103 | CDL | C80-C81-C82-C83 |
| 20 | Y | 101 | TGL | CC1-CC2-CC3-CC4 |
| 26 | G | 101 | PEK | C27-C28-C29-C30 |
| 19 | P | 303 | PGV | C31-C32-C33-C34 |
| 25 | G | 102 | CDL | CA7-C31-C32-C33 |
| 20 | D | 201 | TGL | C19-C33-C34-C35 |
| 26 | C | 306 | PEK | C13-C14-C15-C16 |
| 25 | T | 103 | CDL | C24-C25-C26-C27 |
| 25 | C | 303 | CDL | C60-C61-C62-C63 |
| 25 | C | 303 | CDL | C71-CB7-OB8-CB6 |
| 19 | Q | 201 | PGV | C28-C29-C30-C31 |
| 26 | T | 102 | PEK | C3-C4-C5-C6 |
| 19 | C | 302 | PGV | C13-C14-C15-C16 |
| 19 | C | 307 | PGV | C31-C32-C33-C34 |
| 19 | A | 607 | PGV | C26-C27-C28-C29 |
| 26 | C | 306 | PEK | C33-C34-C35-C36 |
| 19 | P | 301 | PGV | C25-C26-C27-C28 |
| 25 | P | 304 | CDL | C21-C22-C23-C24 |
| 25 | G | 102 | CDL | C62-C63-C64-C65 |
| 19 | A | 608 | PGV | C9-C10-C11-C12 |
| 22 | C | 304 | CHD | C17-C20-C22-C23 |
| 20 | Y | 101 | TGL | CB4-CB5-CB6-CB7 |
| 19 | C | 307 | PGV | O05-C05-C06-O06 |
| 20 | Y | 101 | TGL | OB1-CB1-CB2-CB3 |
| 20 | B | 301 | TGL | C11-C10-CB9-CB8 |
| 20 | Q | 202 | TGL | OG3-CC1-CC2-CC3 |
| 20 | D | 201 | TGL | C10-C11-C12-C13 |
| 19 | C | 307 | PGV | C4-C5-C6-C7 |
| 25 | T | 103 | CDL | C40-C41-C42-C43 |
| 25 | P | 304 | CDL | C62-C63-C64-C65 |
| 26 | T | 102 | PEK | O03-C21-C22-C23 |
| 23 | B | 304 | PSC | C25-C26-C27-C28 |
| 20 | Y | 101 | TGL | C21-C22-C23-C24 |
| 26 | C | 306 | PEK | C3-C4-C5-C6 |
| 19 | P | 301 | PGV | C11-C12-C13-C14 |
| 20 | Y | 101 | TGL | C17-C18-C19-C33 |
| 25 | P | 304 | CDL | C71-C72-C73-C74 |
| 20 | N | 608 | TGL | CB1-CB2-CB3-CB4 |
| 19 | C | 302 | PGV | C28-C29-C30-C31 |
| 19 | A | 607 | PGV | O03-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | C | 306 | PEK | O01-C1-C2-C3 |
| 19 | A | 607 | PGV | C11-C12-C13-C14 |
| 19 | A | 607 | PGV | C11-C10-C9-C8 |
| 20 | Y | 101 | TGL | C12-C13-C14-C29 |
| 26 | T | 101 | PEK | O01-C1-C2-C3 |
| 20 | L | 101 | TGL | CA6-CA7-CA8-CA9 |
| 25 | G | 102 | CDL | C61-C62-C63-C64 |
| 26 | P | 308 | PEK | C29-C30-C31-C32 |
| 20 | Q | 202 | TGL | CC4-CC5-CC6-CC7 |
| 20 | Y | 101 | TGL | C29-C30-C31-C32 |
| 20 | B | 301 | TGL | OG1-CA1-CA2-CA3 |
| 19 | Q | 201 | PGV | C20-C21-C22-C23 |
| 20 | B | 301 | TGL | OG3-CC1-CC2-CC3 |
| 20 | Q | 202 | TGL | CB6-CB7-CB8-CB9 |
| 19 | P | 301 | PGV | O05-C05-C06-O06 |
| 26 | T | 102 | PEK | C26-C27-C28-C29 |
| 20 | L | 101 | TGL | CC9-C15-C16-C17 |
| 25 | C | 303 | CDL | C21-C22-C23-C24 |
| 19 | N | 607 | PGV | C12-C13-C14-C15 |
| 26 | T | 102 | PEK | O04-C21-C22-C23 |
| 26 | T | 101 | PEK | C23-C24-C25-C26 |
| 26 | C | 306 | PEK | O02-C1-C2-C3 |
| 25 | C | 303 | CDL | C62-C63-C64-C65 |
| 19 | N | 607 | PGV | C11-C12-C13-C14 |
| 20 | B | 301 | TGL | OA1-CA1-CA2-CA3 |
| 20 | Q | 202 | TGL | OC1-CC1-CC2-CC3 |
| 25 | C | 303 | CDL | C74-C75-C76-C77 |
| 20 | L | 101 | TGL | OG1-CG1-CG2-CG3 |
| 20 | N | 608 | TGL | CG1-CG2-CG3-OG3 |
| 19 | N | 607 | PGV | O03-C19-C20-C21 |
| 19 | A | 607 | PGV | C27-C28-C29-C30 |
| 25 | P | 304 | CDL | C82-C83-C84-C85 |
| 26 | G | 103 | PEK | C03-O11-P-O13 |
| 25 | T | 103 | CDL | CA3-OA5-PA1-OA3 |
| 26 | T | 102 | PEK | C03-O11-P-O14 |
| 26 | C | 306 | PEK | C03-O11-P-O13 |
| 19 | C | 307 | PGV | C03-O11-P-O14 |
| 25 | G | 102 | CDL | CA3-OA5-PA1-OA3 |
| 20 | N | 608 | TGL | C18-C19-C33-C34 |
| 25 | G | 102 | CDL | C18-C19-C20-C21 |
| 26 | T | 101 | PEK | O12-C04-C05-N |
| 25 | C | 303 | CDL | C59-C60-C61-C62 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 20 | L | 101 | TGL | OG2-CB1-CB2-CB3 |
| 25 | C | 303 | CDL | C11-C12-C13-C14 |
| 23 | B | 304 | PSC | C12-C13-C14-C15 |
| 19 | A | 608 | PGV | C24-C25-C26-C27 |
| 20 | Q | 202 | TGL | CC6-CC7-CC8-CC9 |
| 20 | N | 608 | TGL | CA6-CA7-CA8-CA9 |
| 19 | N | 607 | PGV | C24-C25-C26-C27 |
| 26 | C | 306 | PEK | C27-C28-C29-C30 |
| 26 | T | 102 | PEK | C21-C22-C23-C24 |
| 20 | B | 301 | TGL | OC1-CC1-CC2-CC3 |
| 26 | T | 101 | PEK | O02-C1-C2-C3 |
| 28 | J | 101 | DMU | C22-C25-C28-C31 |
| 26 | T | 101 | PEK | C3-C4-C5-C6 |

There are no ring outliers.

40 monomers are involved in 372 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 26 | C | 306 | PEK | 13 | 0 |
| 19 | A | 607 | PGV | 4 | 0 |
| 14 | A | 602 | HEA | 1 | 0 |
| 20 | D | 201 | TGL | 21 | 0 |
| 14 | N | 601 | HEA | 10 | 0 |
| 14 | A | 601 | HEA | 9 | 0 |
| 19 | C | 302 | PGV | 7 | 0 |
| 20 | L | 101 | TGL | 19 | 0 |
| 26 | G | 101 | PEK | 7 | 0 |
| 26 | G | 103 | PEK | 9 | 0 |
| 20 | B | 301 | TGL | 3 | 0 |
| 19 | Q | 201 | PGV | 11 | 0 |
| 18 | A | 606 | PER | 1 | 0 |
| 23 | O | 303 | PSC | 19 | 0 |
| 22 | C | 304 | CHD | 2 | 0 |
| 19 | A | 608 | PGV | 7 | 0 |
| 26 | T | 101 | PEK | 8 | 0 |
| 22 | J | 102 | CHD | 6 | 0 |
| 19 | P | 303 | PGV | 6 | 0 |
| 22 | C | 305 | CHD | 1 | 0 |
| 26 | T | 102 | PEK | 10 | 0 |
| 25 | C | 303 | CDL | 26 | 0 |
| 14 | N | 602 | HEA | 1 | 0 |
| 19 | N | 607 | PGV | 1 | 0 |

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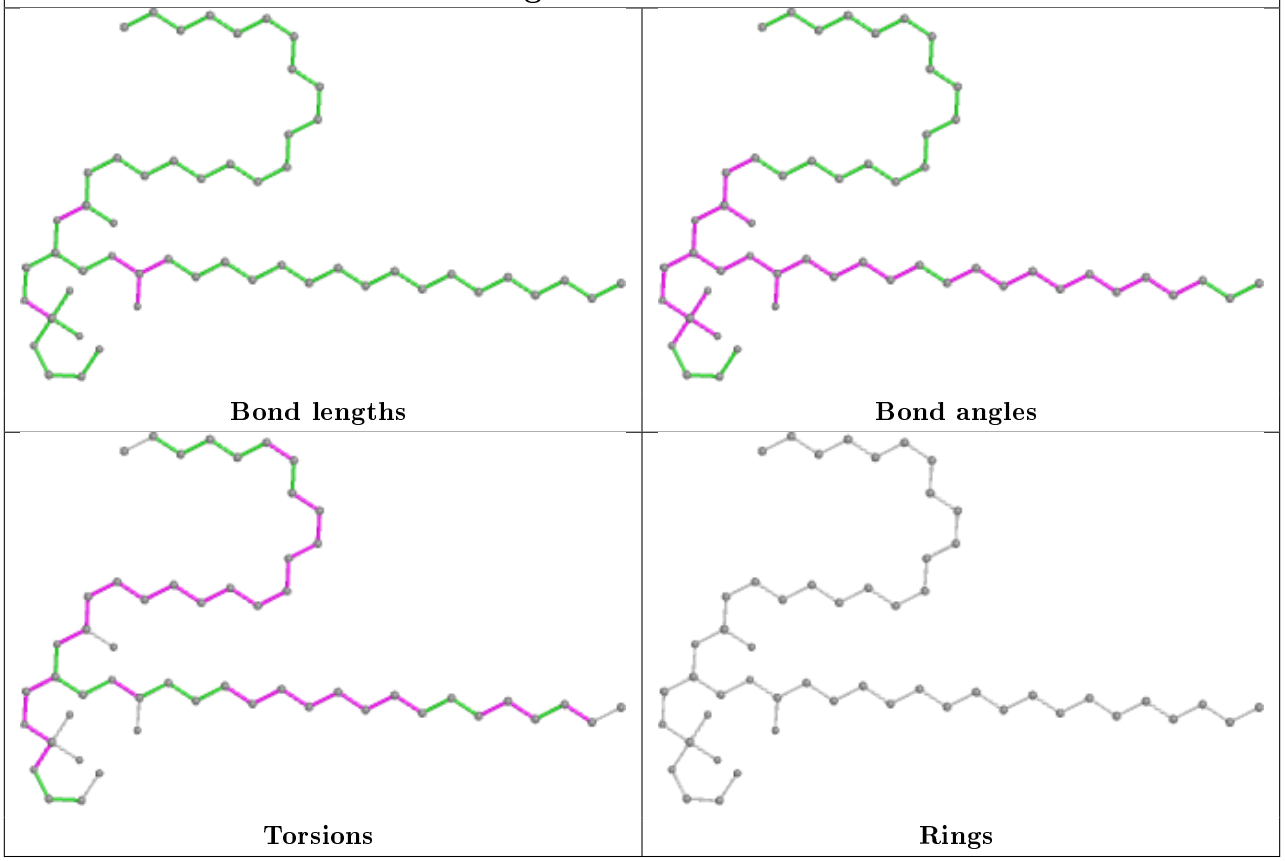
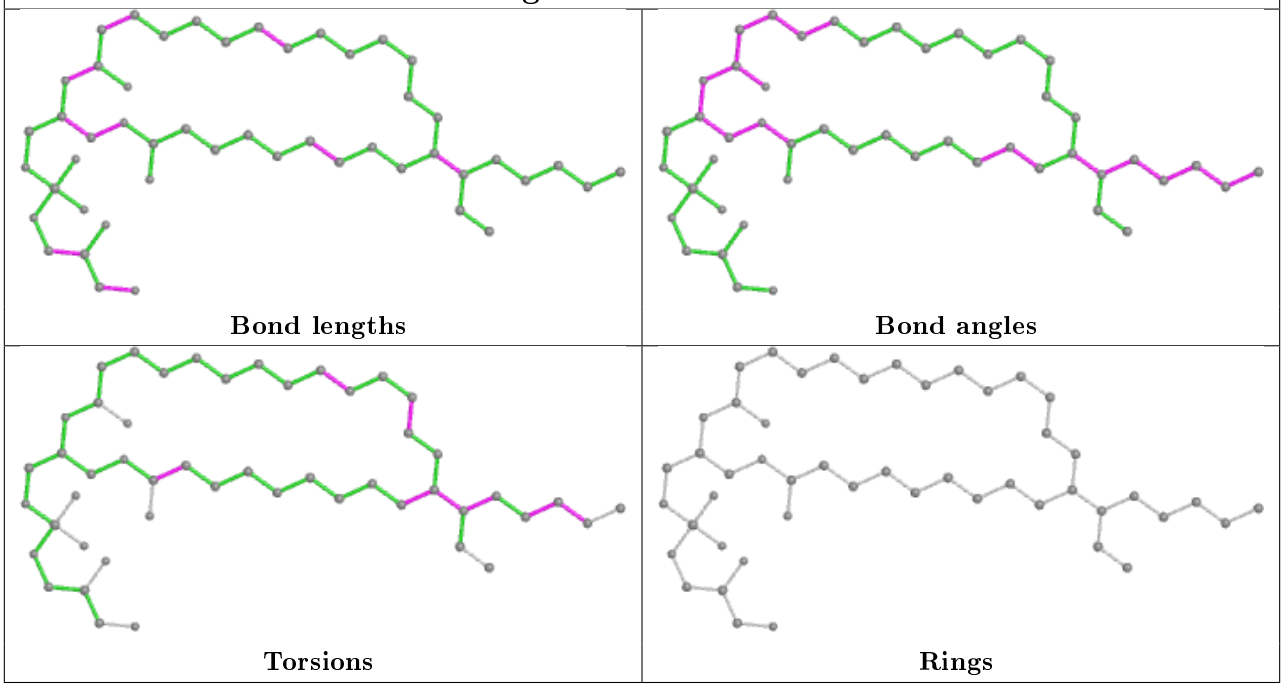
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 19 | P | 301 | PGV | 3 | 0 |
| 20 | N | 608 | TGL | 6 | 0 |
| 25 | P | 304 | CDL | 24 | 0 |
| 18 | N | 606 | PER | 1 | 0 |
| 22 | W | 101 | CHD | 6 | 0 |
| 25 | T | 103 | CDL | 28 | 0 |
| 26 | P | 308 | PEK | 16 | 0 |
| 20 | Y | 101 | TGL | 23 | 0 |
| 23 | B | 304 | PSC | 13 | 0 |
| 28 | J | 101 | DMU | 5 | 0 |
| 19 | C | 307 | PGV | 1 | 0 |
| 28 | P | 306 | DMU | 10 | 0 |
| 22 | P | 307 | CHD | 1 | 0 |
| 25 | G | 102 | CDL | 37 | 0 |
| 22 | P | 305 | CHD | 6 | 0 |
| 20 | Q | 202 | TGL | 15 | 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.

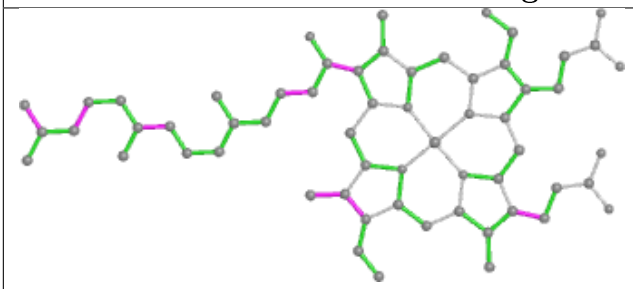
### Ligand PEK C 306



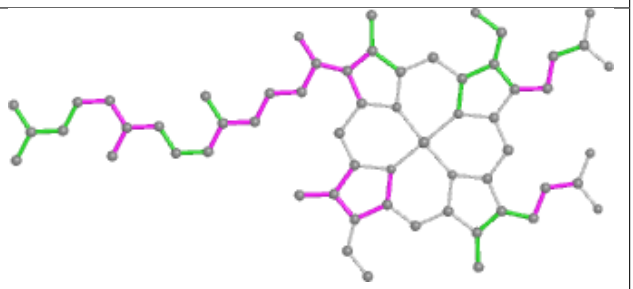

### Ligand PGV A 607



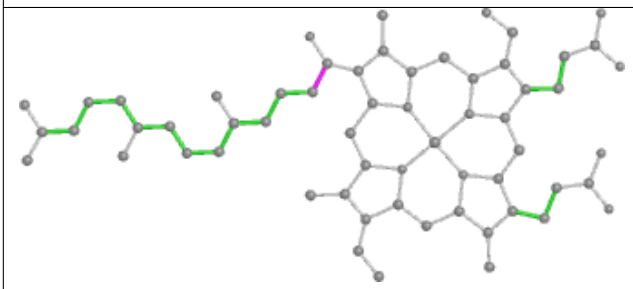
**Ligand HEA A 602**



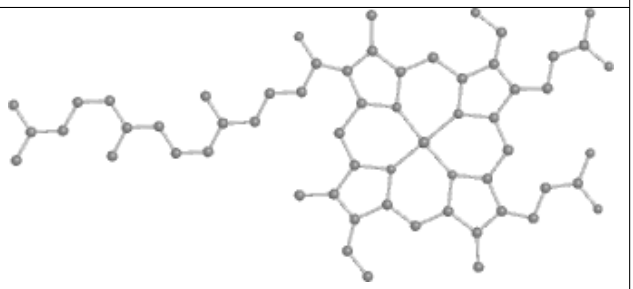
Bond lengths



Bond angles

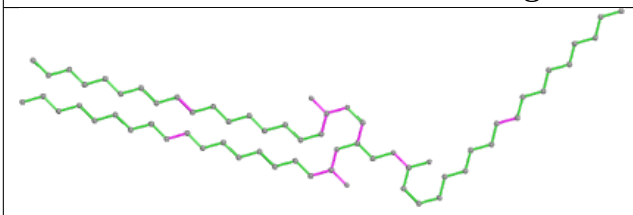


Torsions

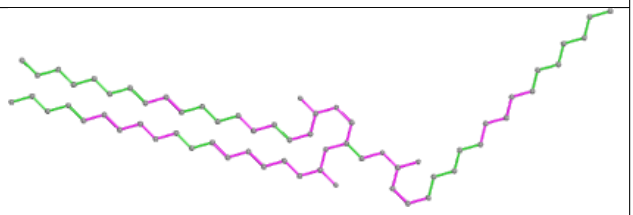


Rings

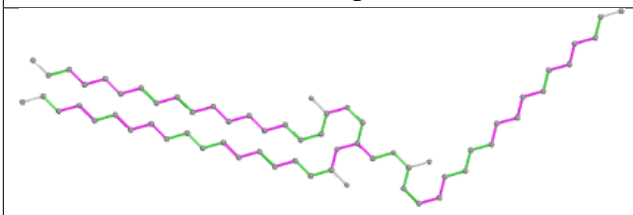
**Ligand TGL D 201**



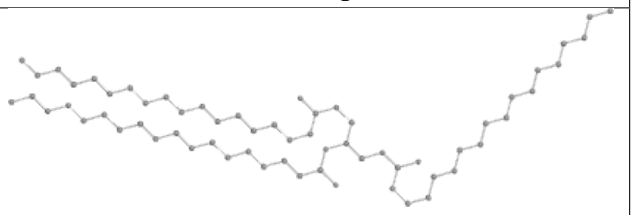
Bond lengths



Bond angles

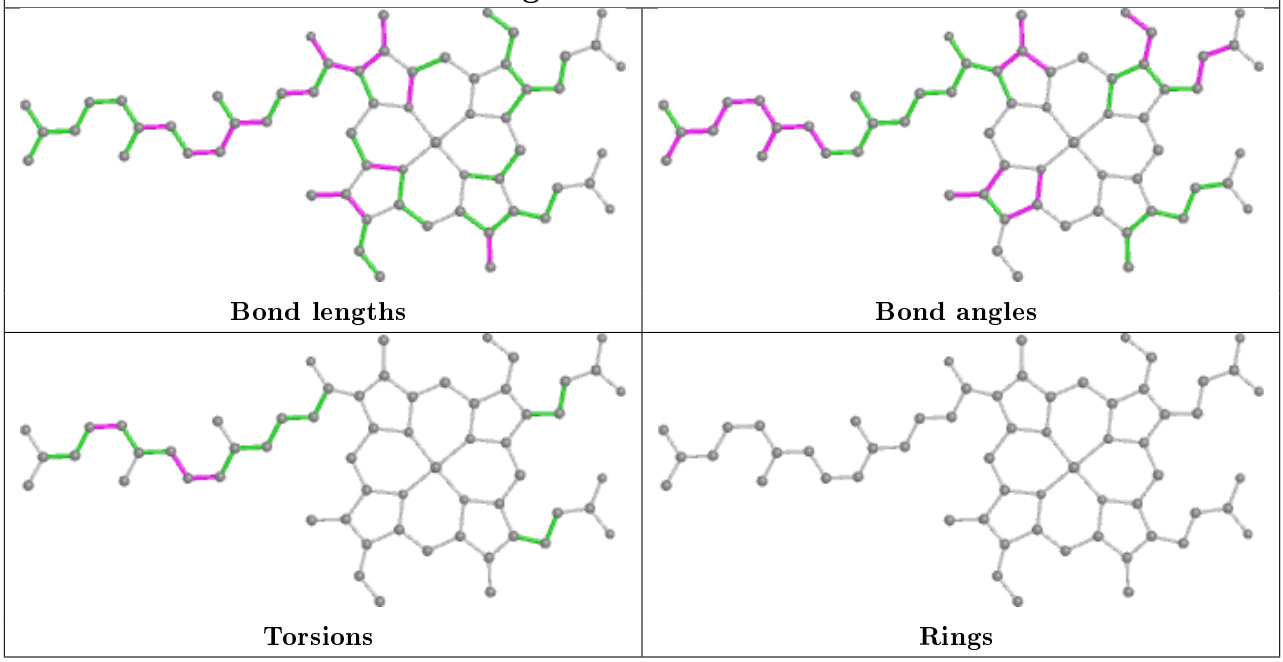


Torsions

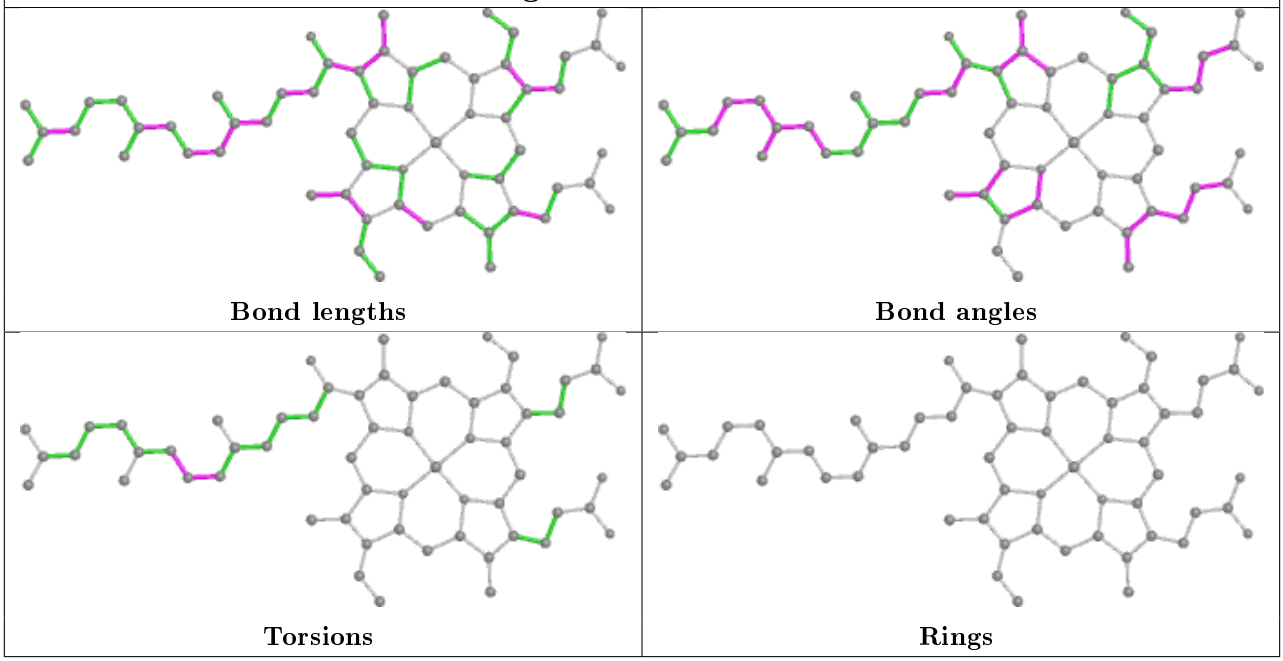


Rings

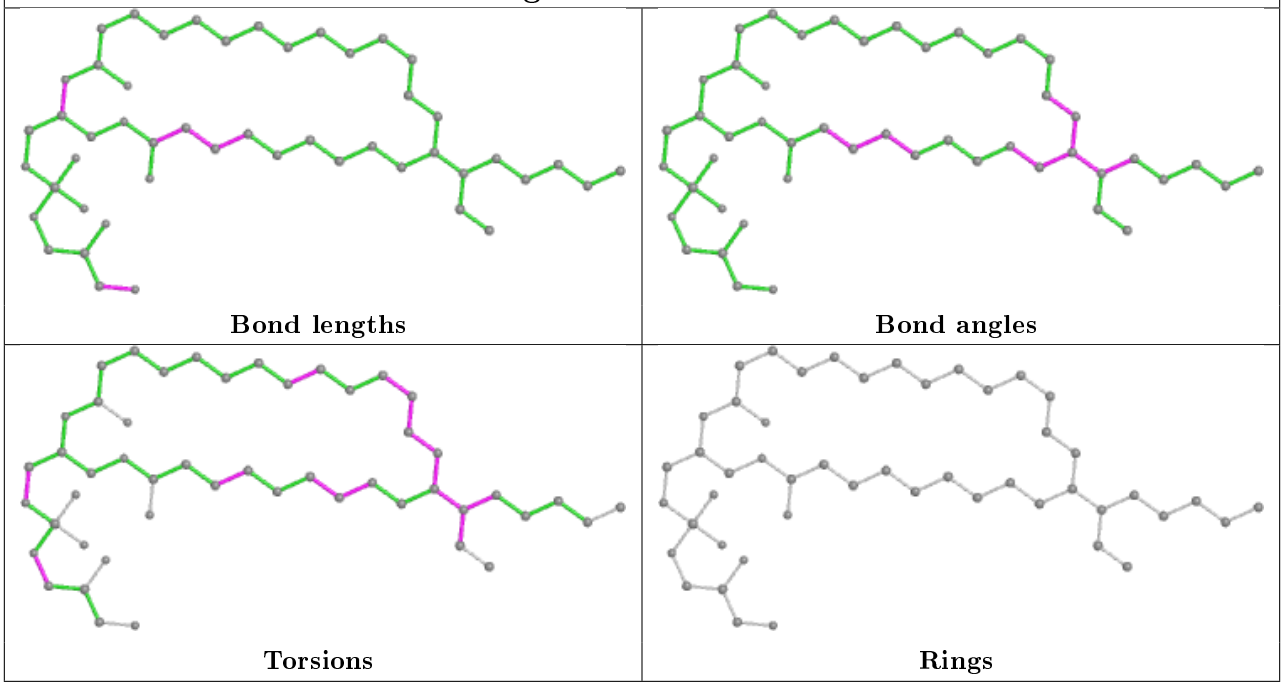
**Ligand HEA N 601**



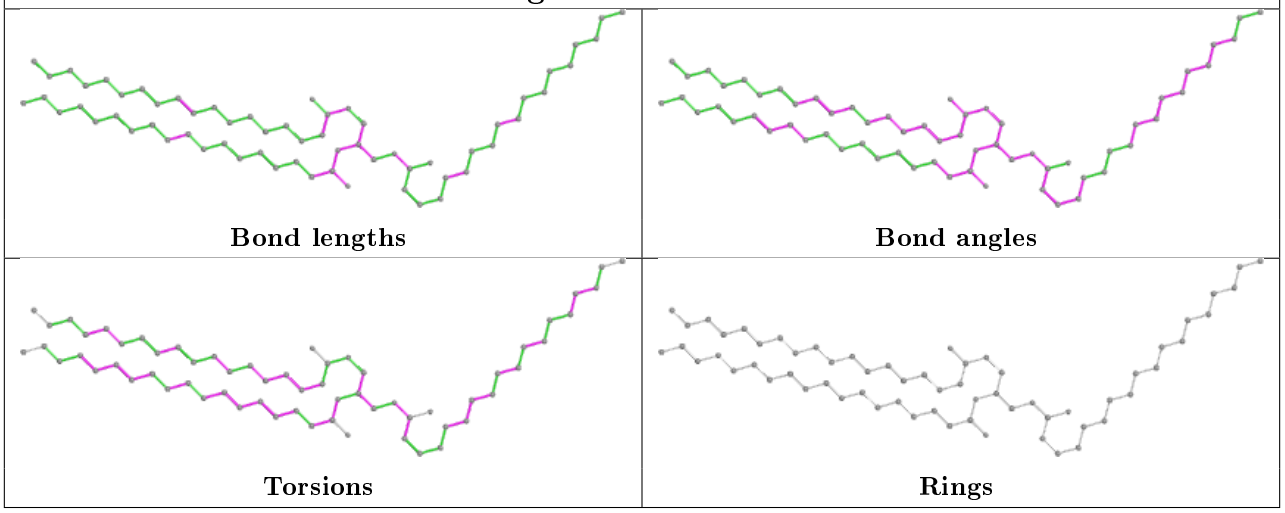

**Ligand HEA A 601**



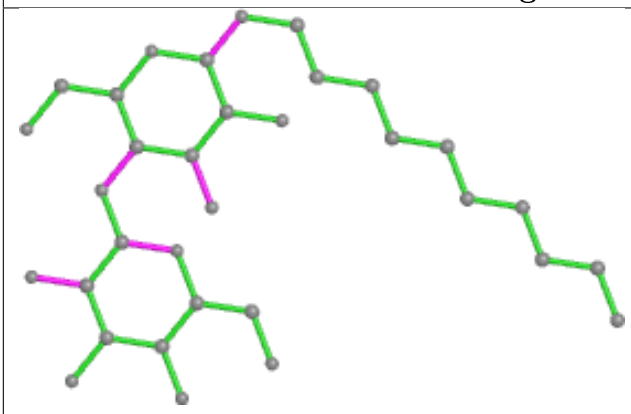
**Ligand PGV C 302**



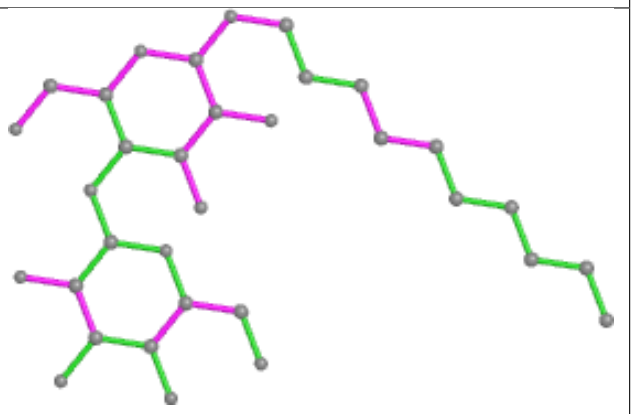

**Ligand TGL L 101**



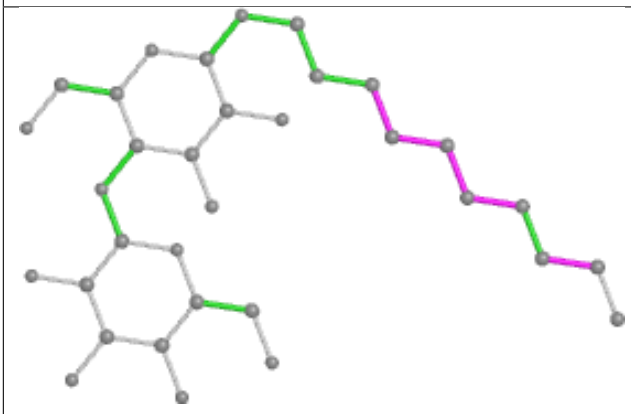
**Ligand DMU Z 101**



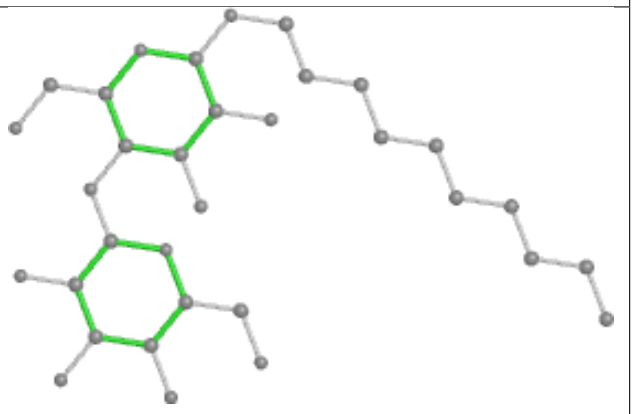
Bond lengths



Bond angles

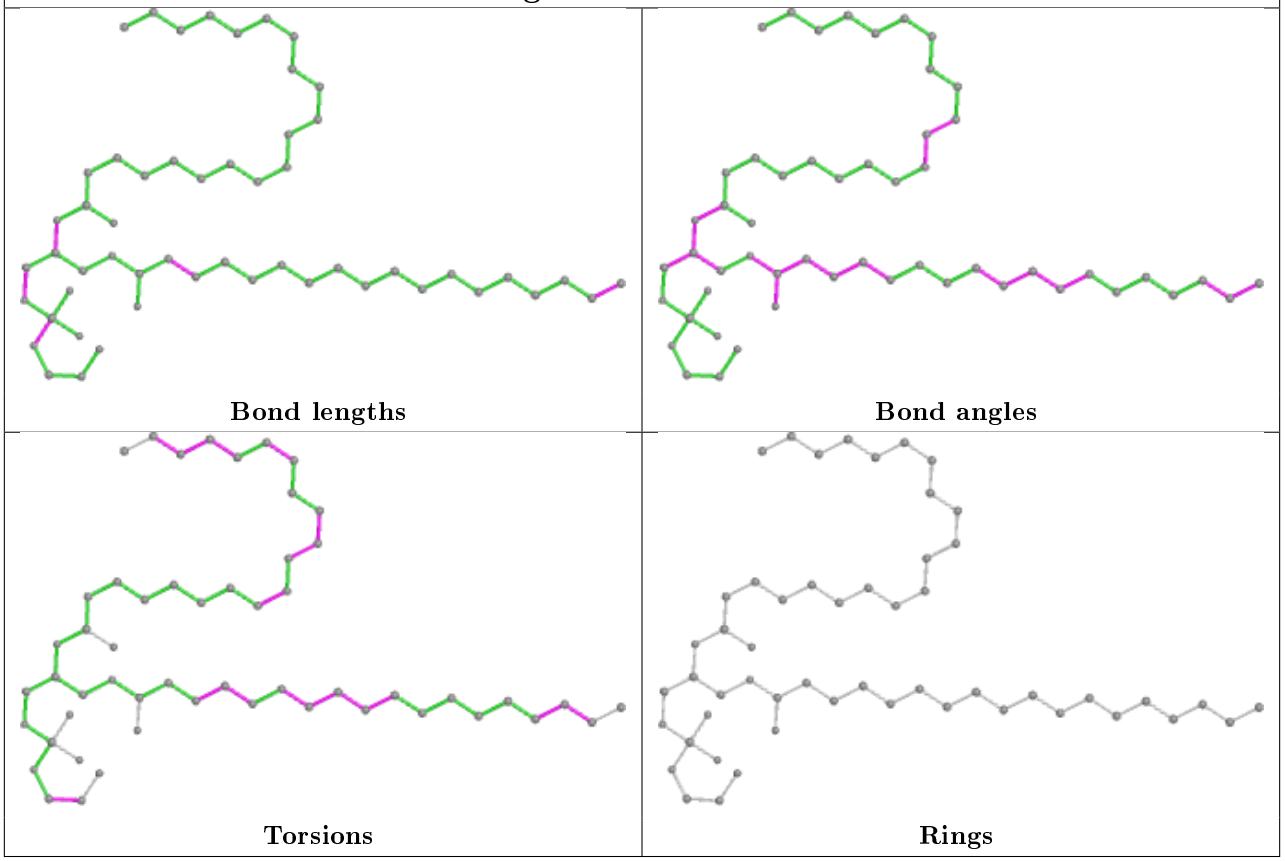


Torsions

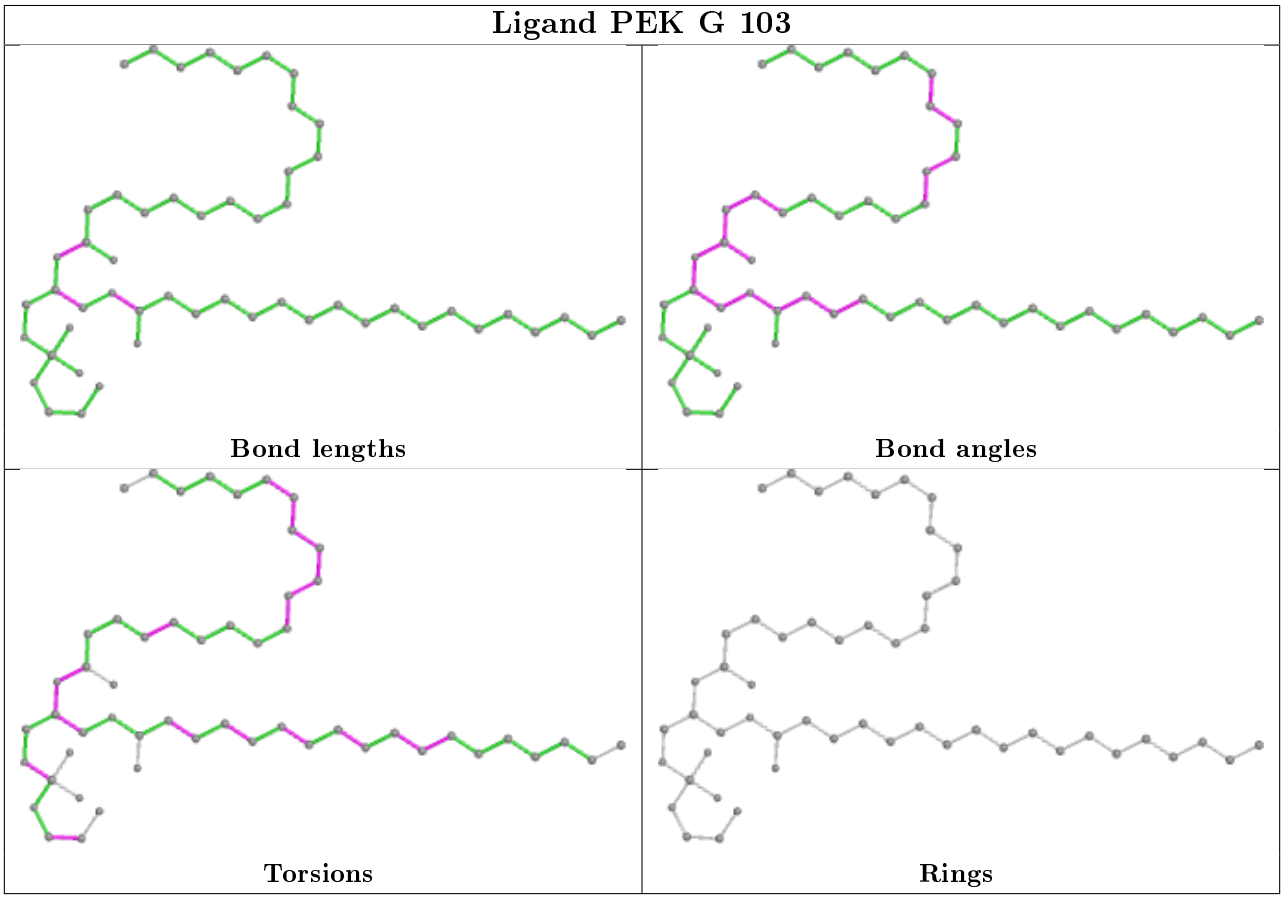


Rings

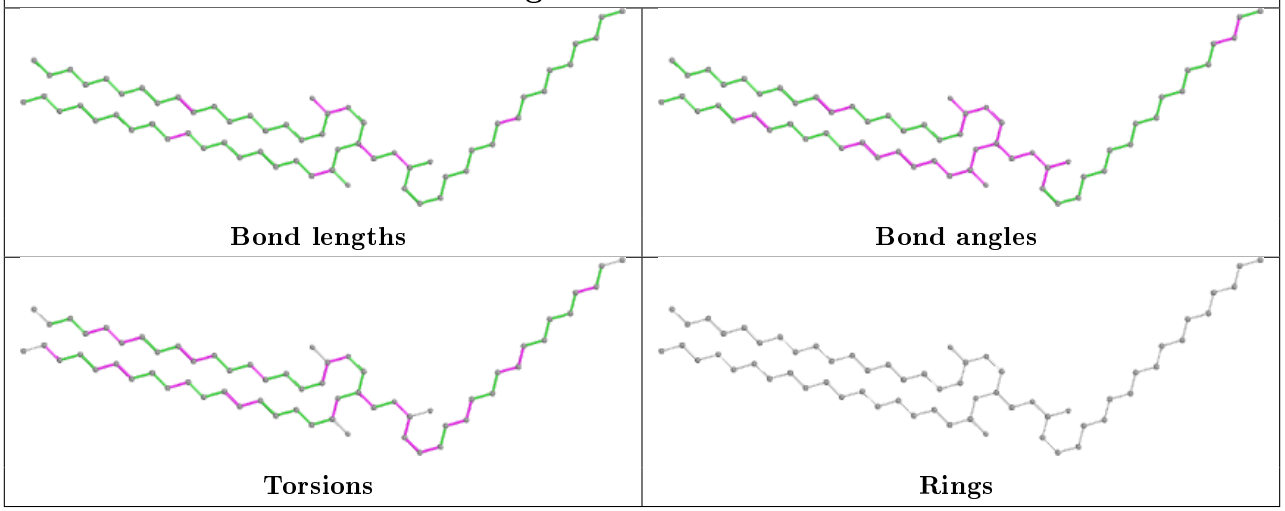
## Ligand PEK G 101



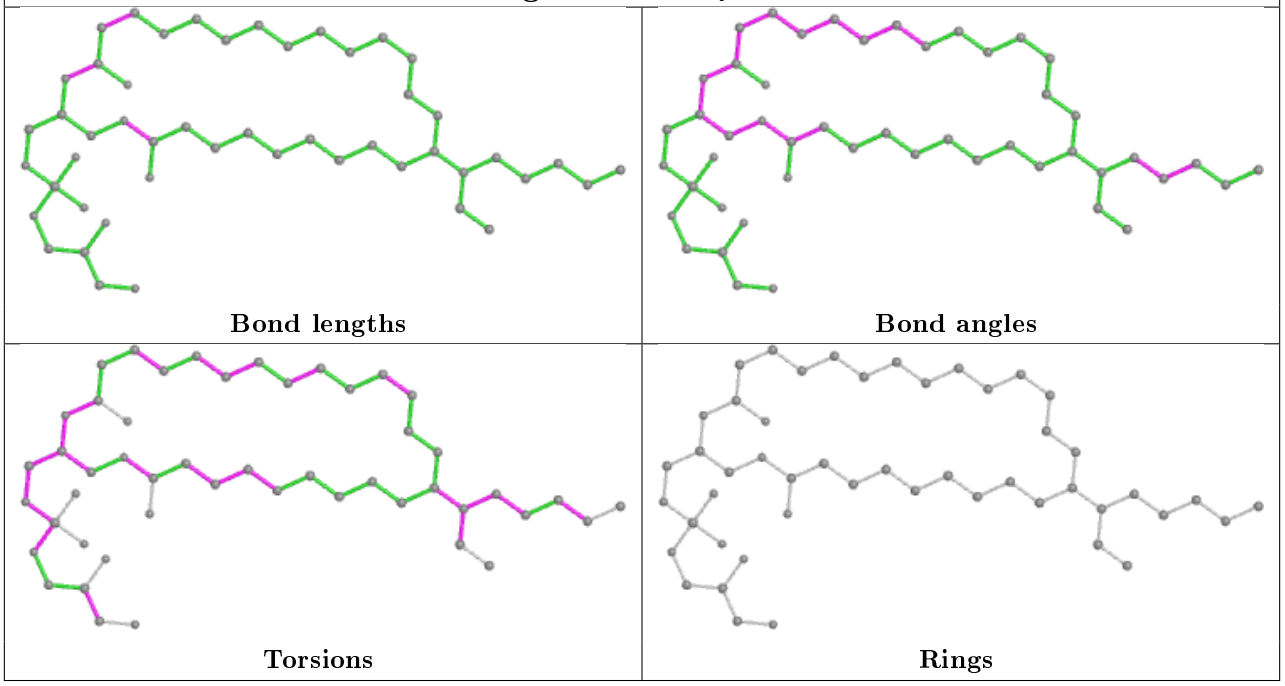

## Ligand PEK G 103



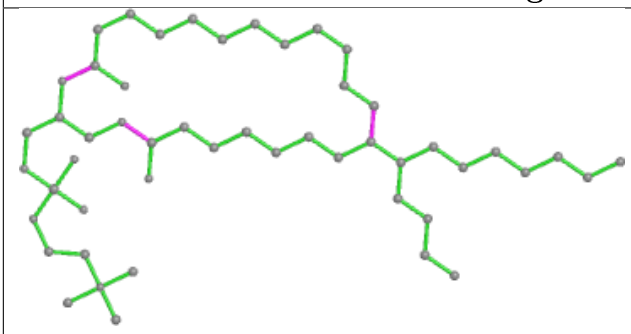
## Ligand TGL B 301



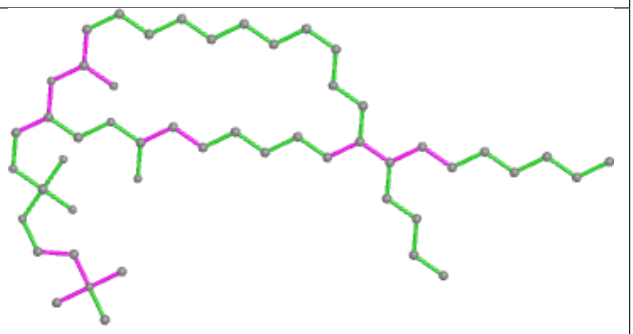

## Ligand PGV Q 201



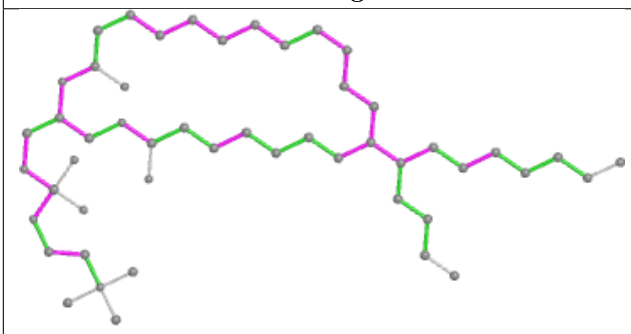
## Ligand PSC O 303



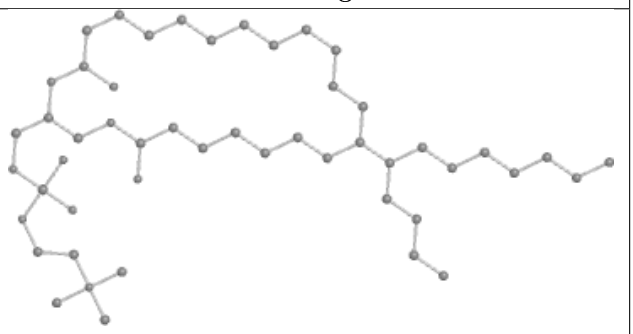
Bond lengths



Bond angles

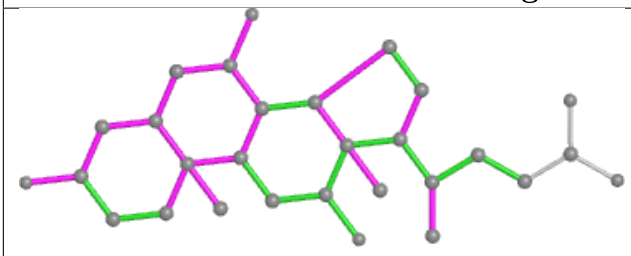


Torsions

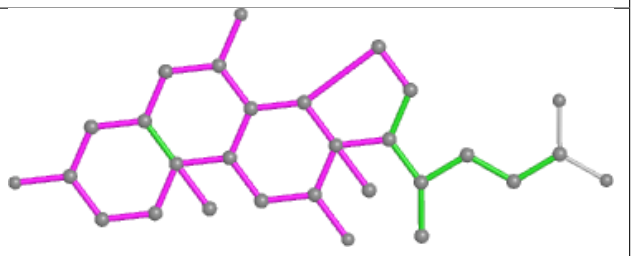


Rings

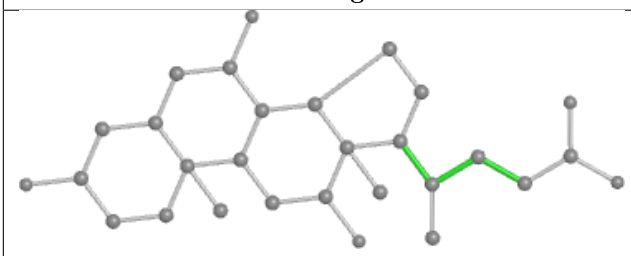
## Ligand CHD B 303



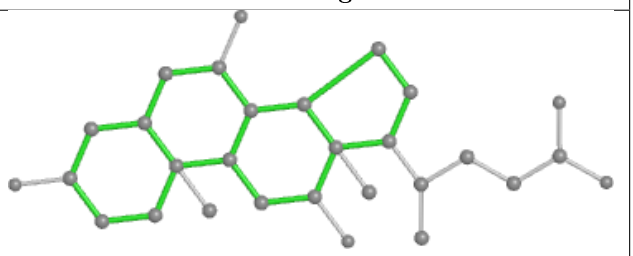
Bond lengths



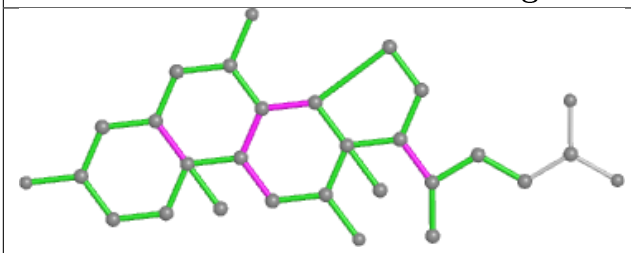
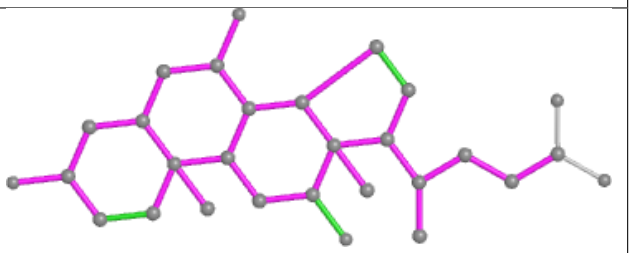
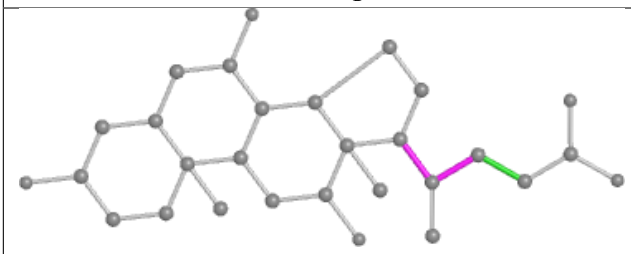
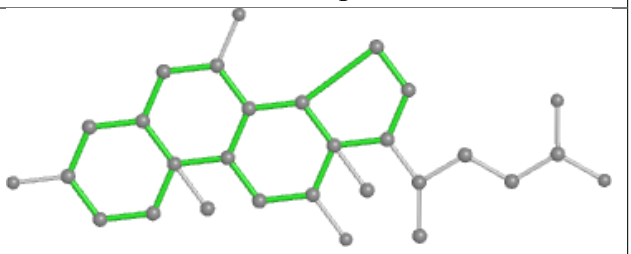
Bond angles

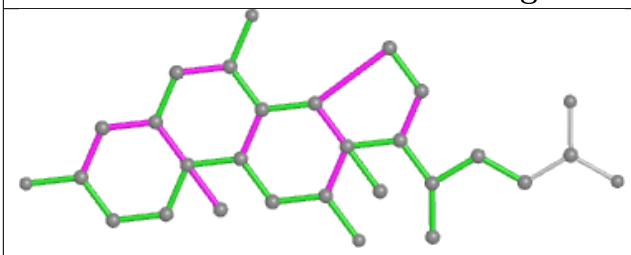
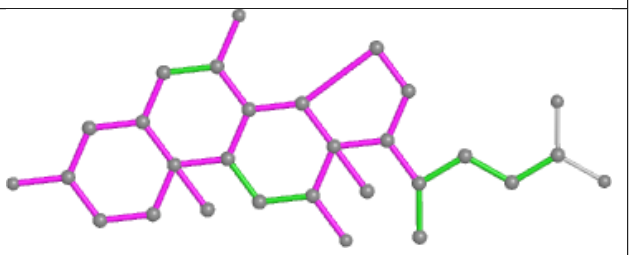
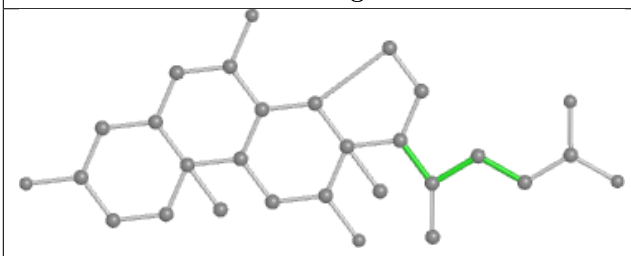
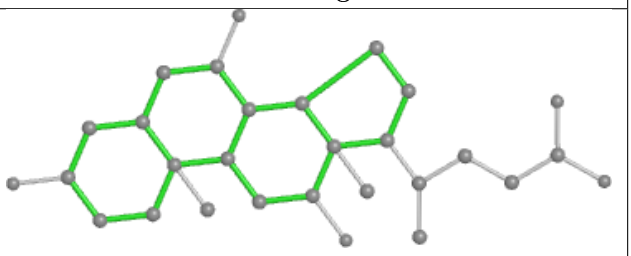


Torsions

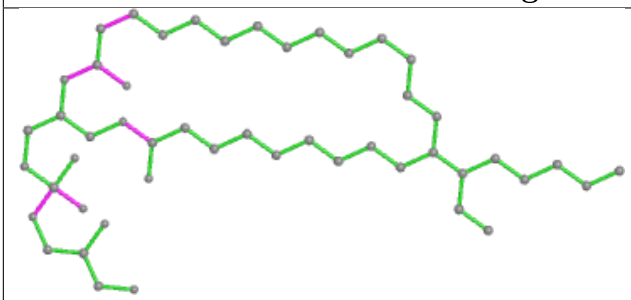


Rings

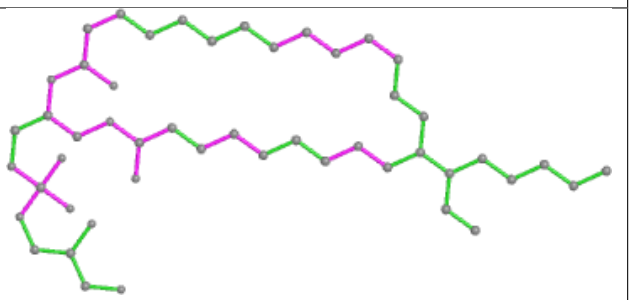
| Ligand CHD C 304 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CHD O 302 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

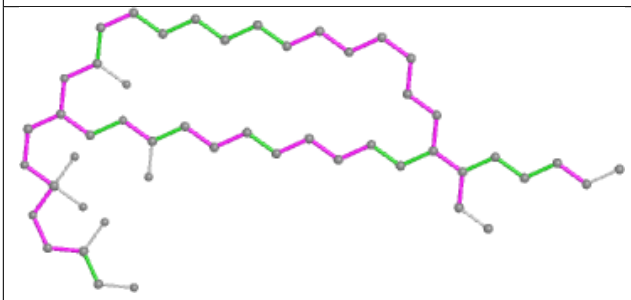
### Ligand PGV A 608



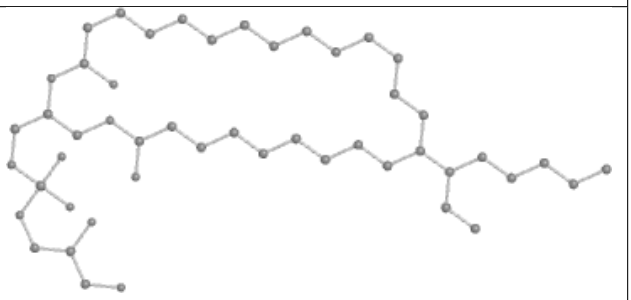
Bond lengths



Bond angles

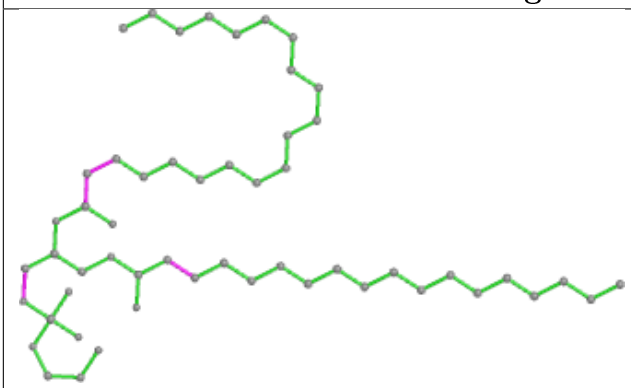


Torsions

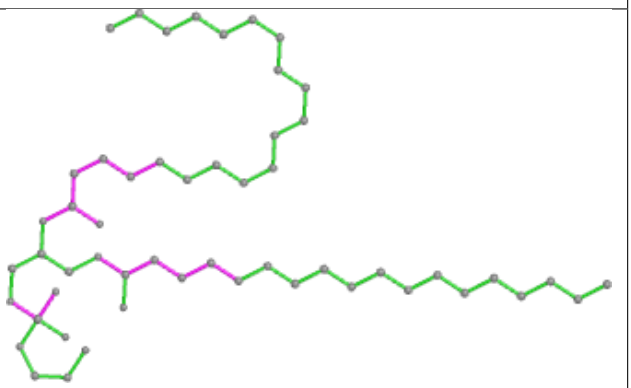


Rings

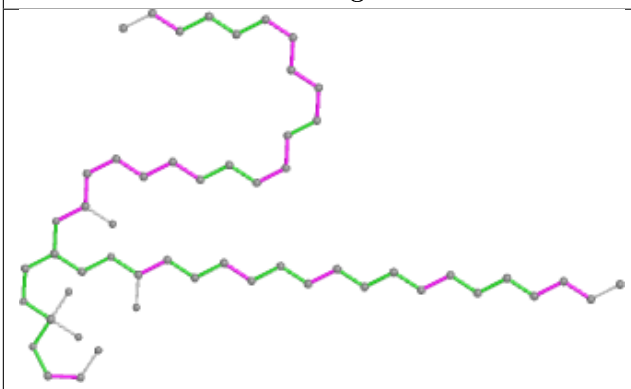
### Ligand PEK T 101



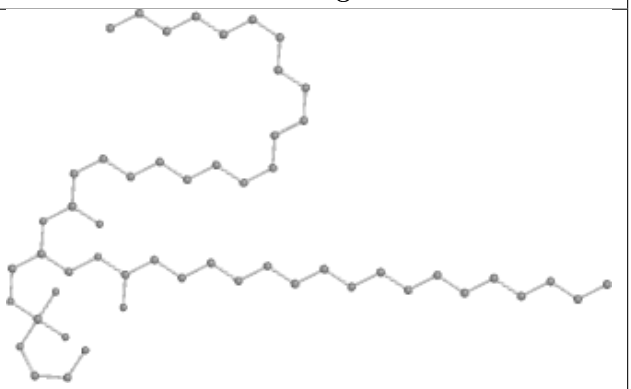
Bond lengths



Bond angles

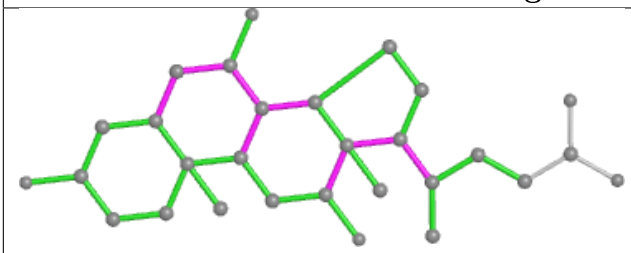


Torsions



Rings

## Ligand CHD J 102



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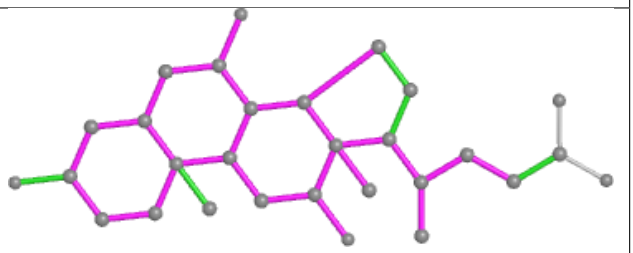
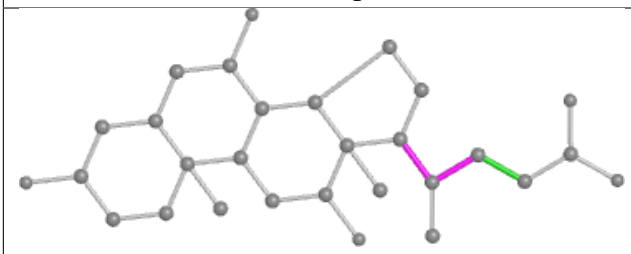
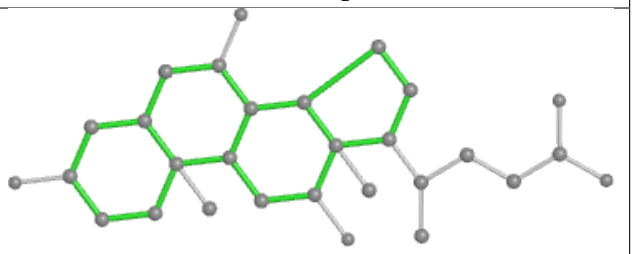


Bond angles

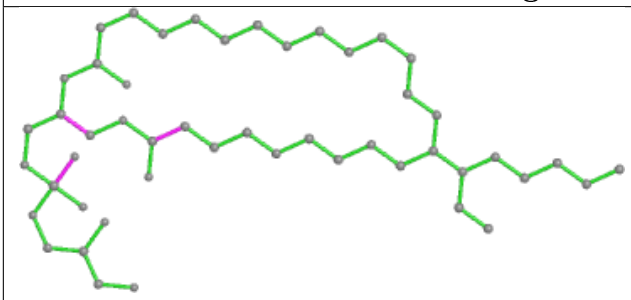


Torsions

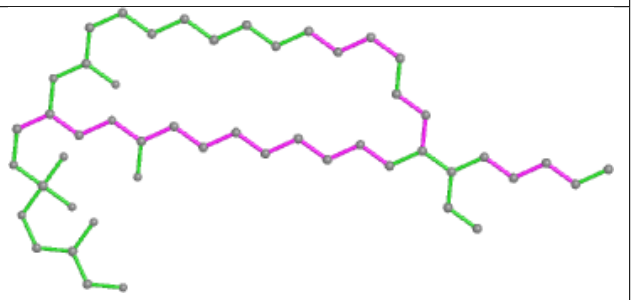


Rings

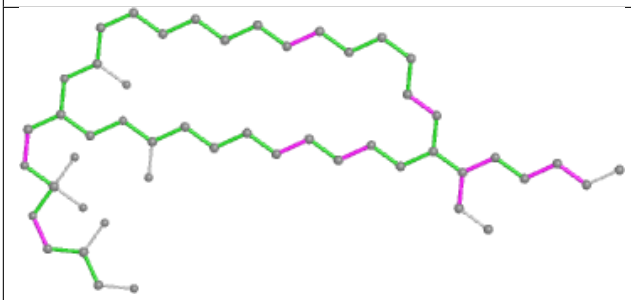
## Ligand PGV P 303



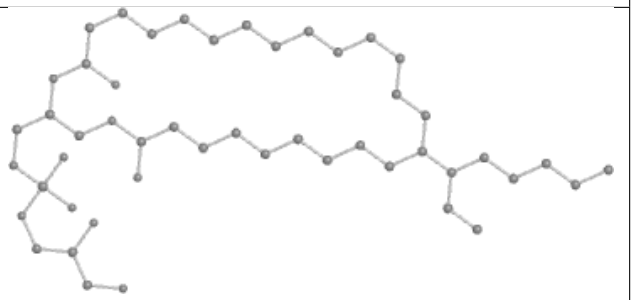
Bond lengths



Bond angles

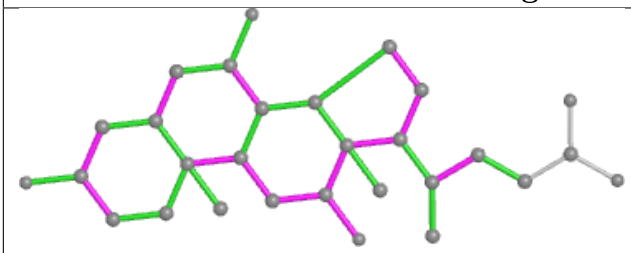


Torsions

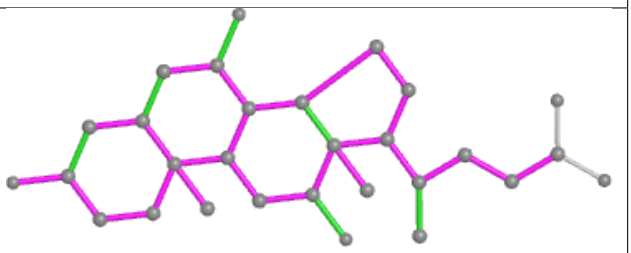


Rings

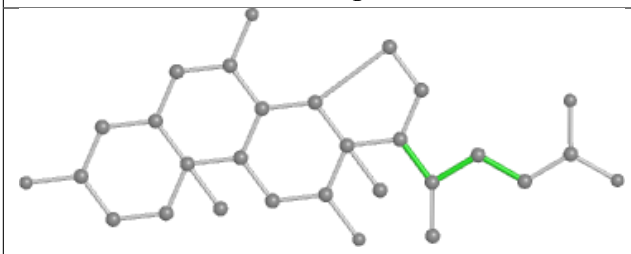
## Ligand CHD C 305



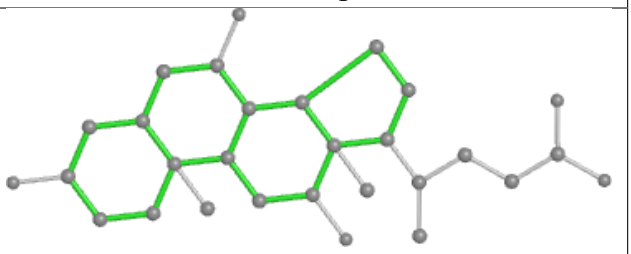
Bond lengths



Bond angles

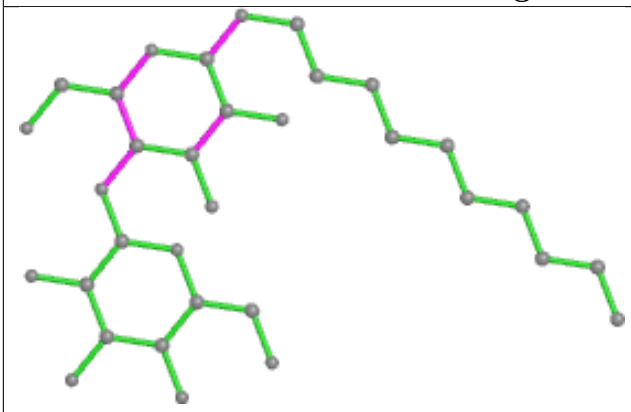


Torsions

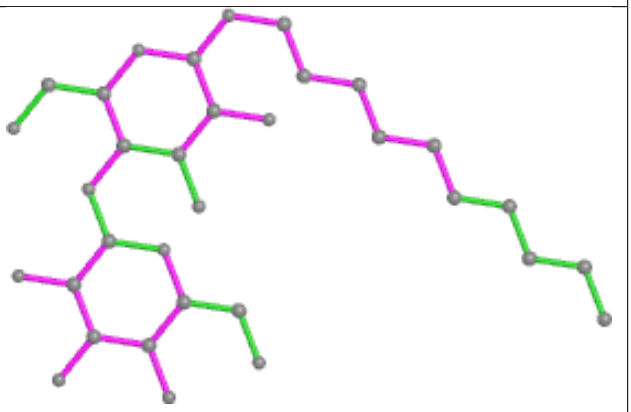


Rings

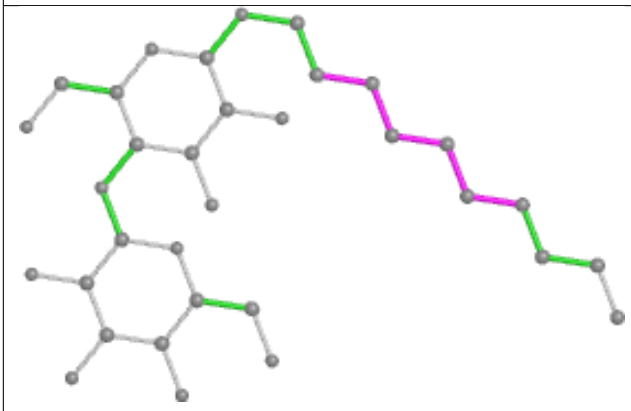
## Ligand DMU M 101



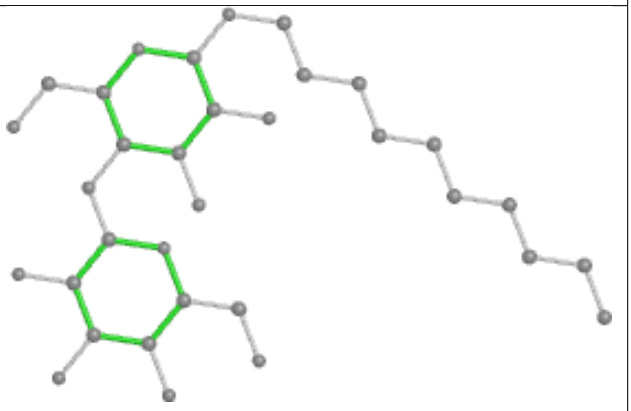
Bond lengths



Bond angles

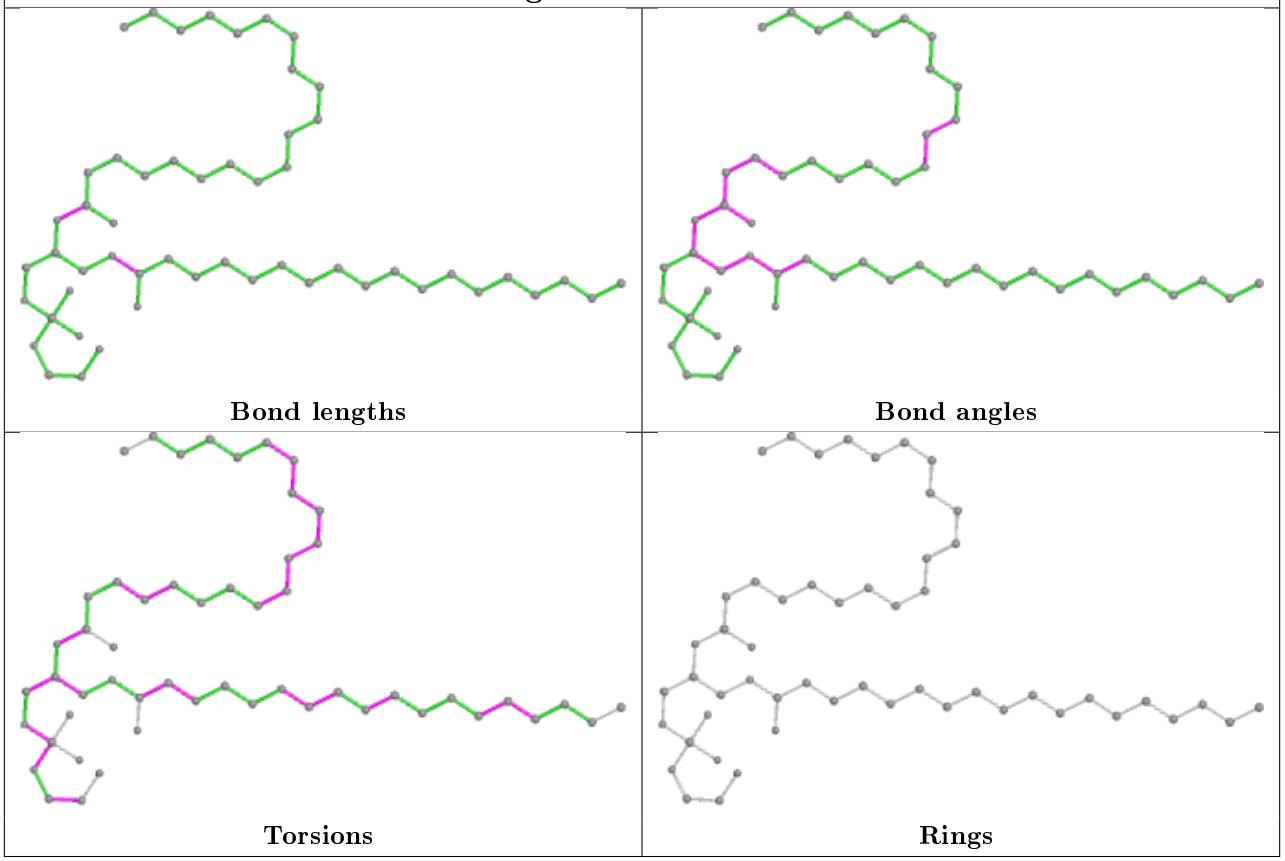


Torsions

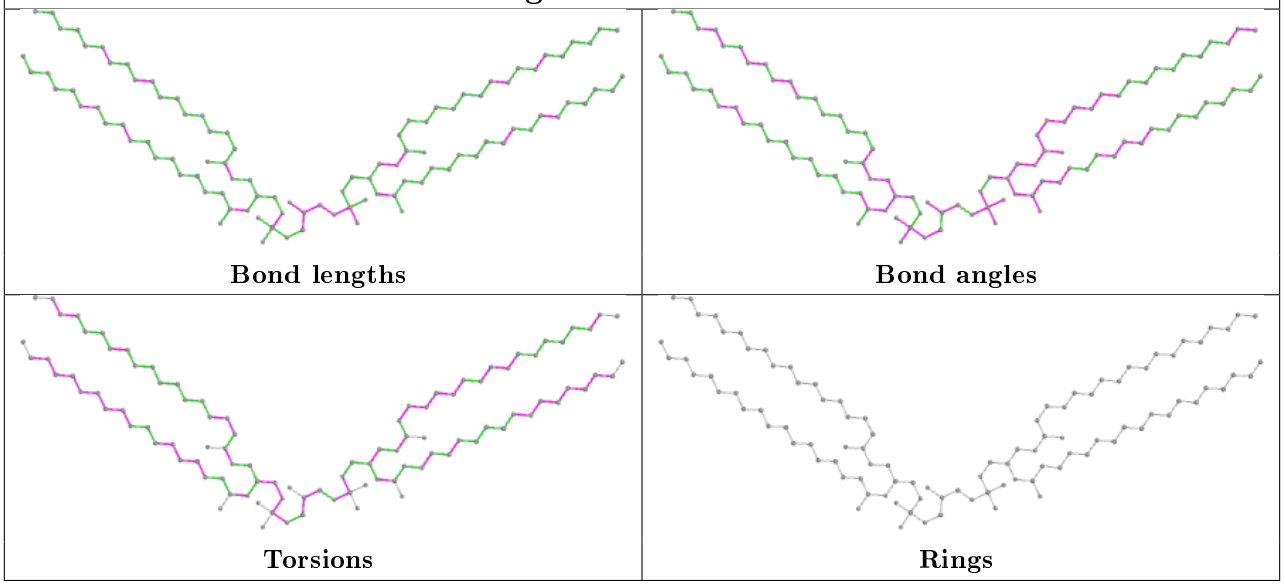


Rings

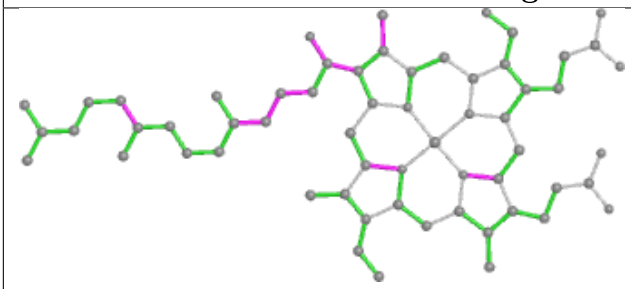
## Ligand PEK T 102



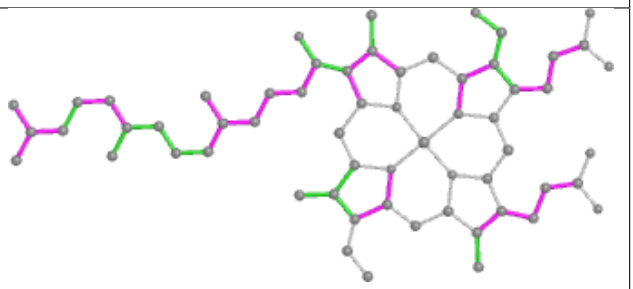

## Ligand CDL C 303



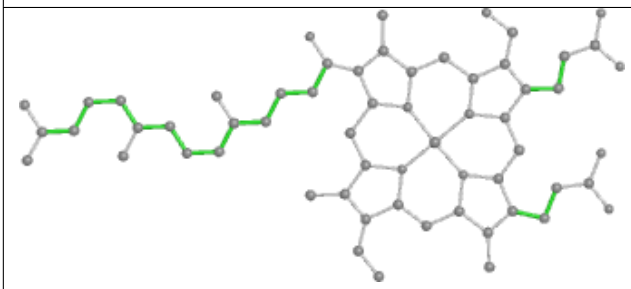
### Ligand HEA N 602



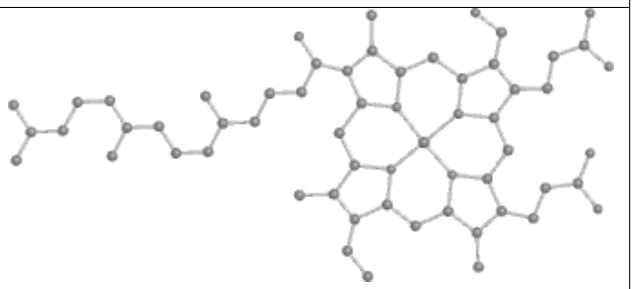
Bond lengths



Bond angles

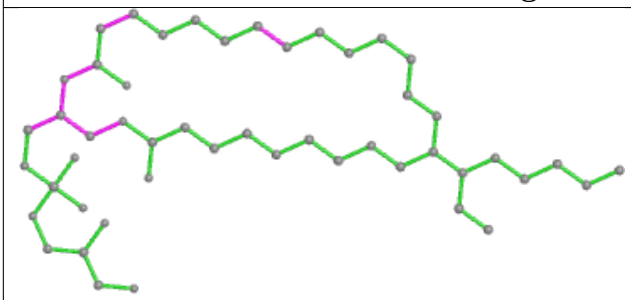


Torsions

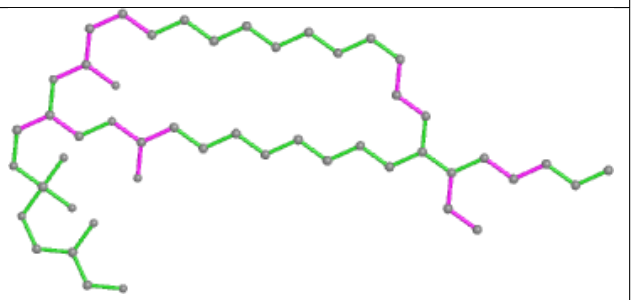


Rings

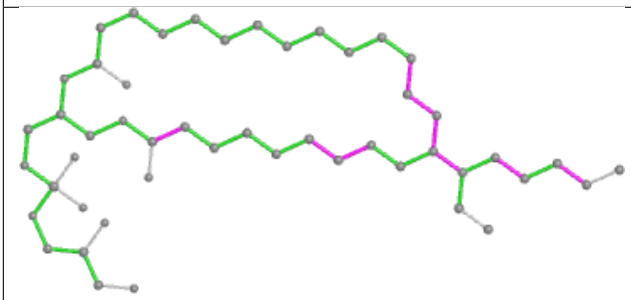
### Ligand PGV N 607



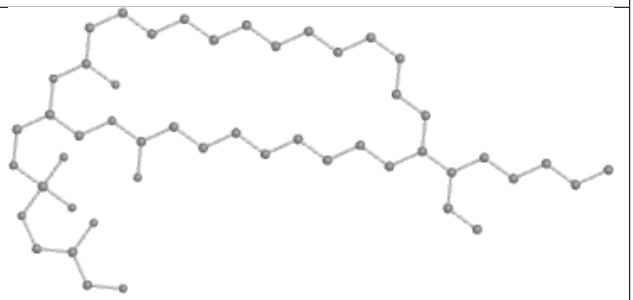
Bond lengths



Bond angles

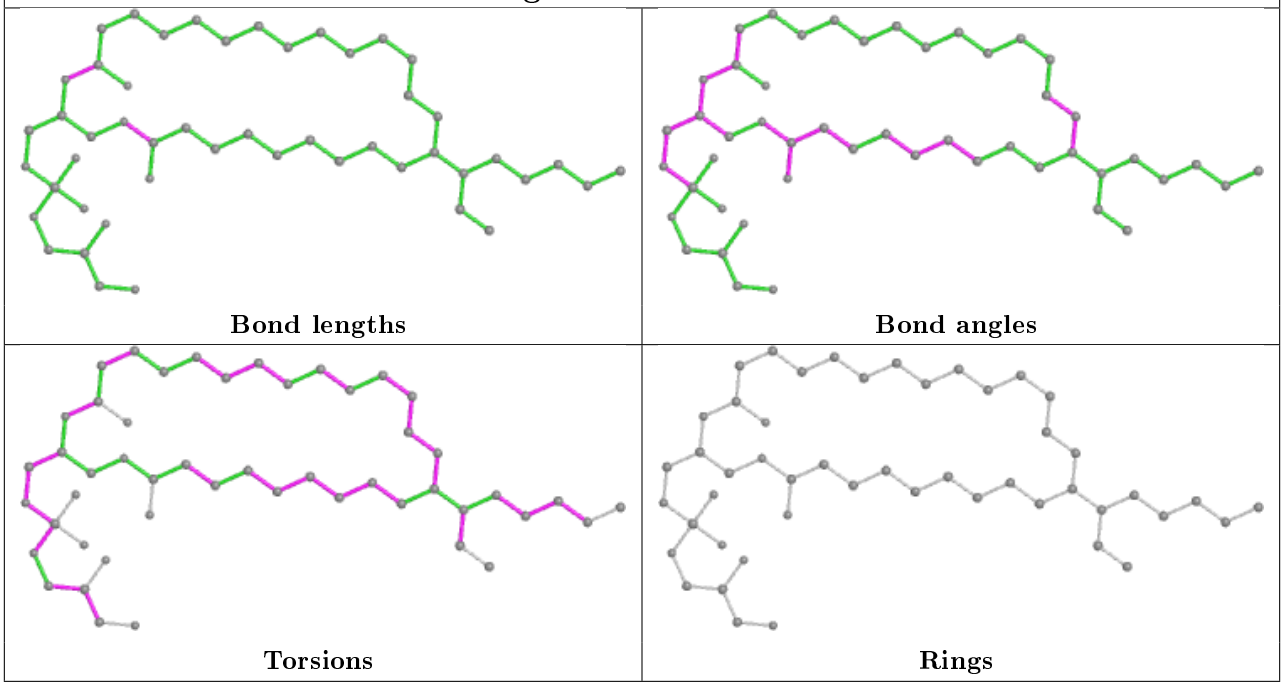


Torsions

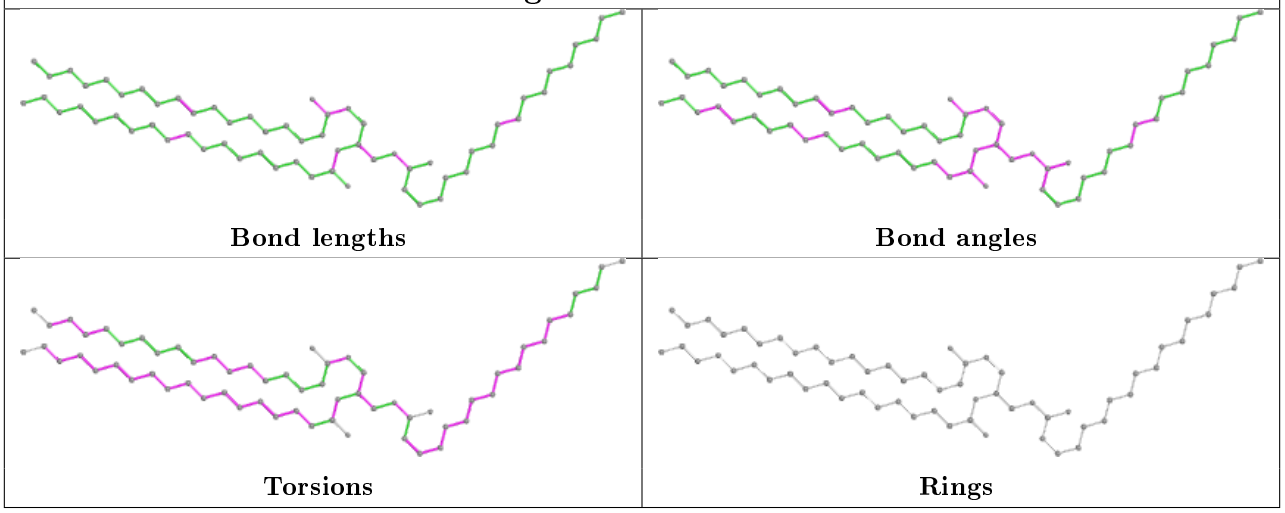


Rings

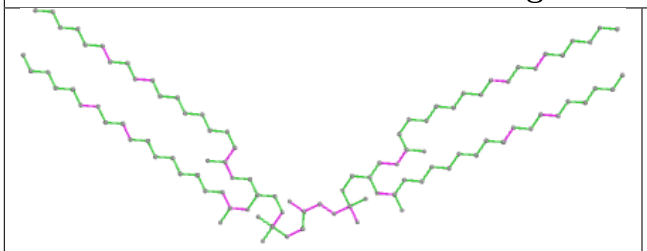
### Ligand PGV P 301



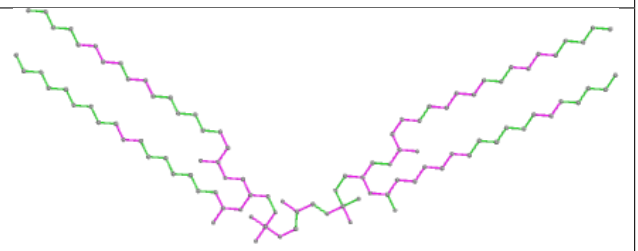

### Ligand TGL N 608



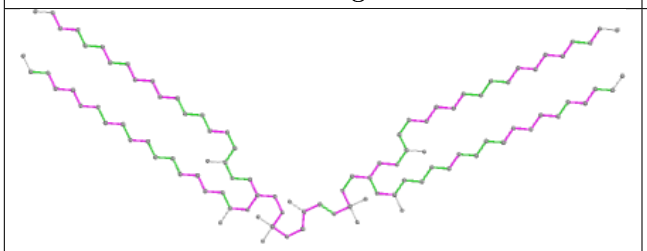
## Ligand CDL P 304



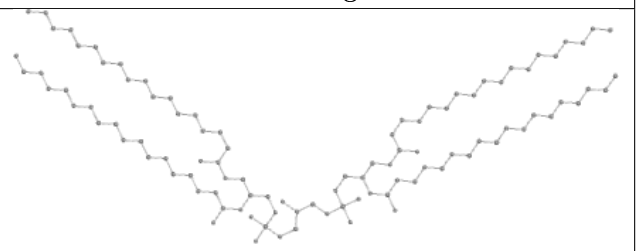
Bond lengths



Bond angles

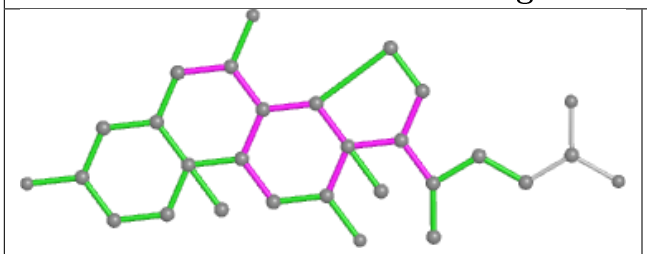


Torsions

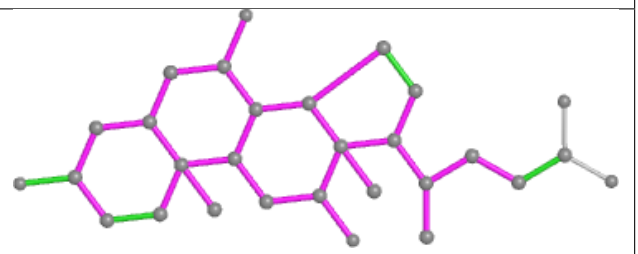


Rings

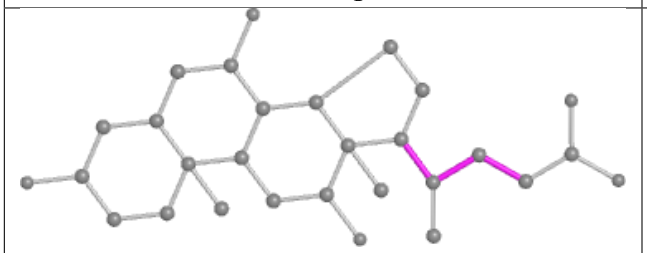
## Ligand CHD W 101



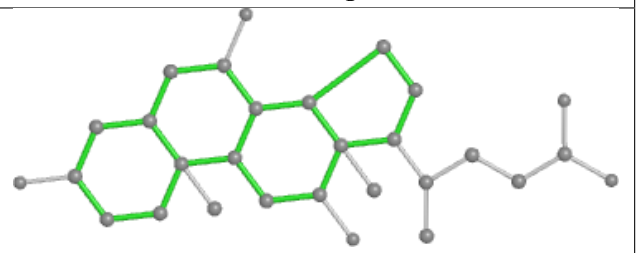
Bond lengths



Bond angles

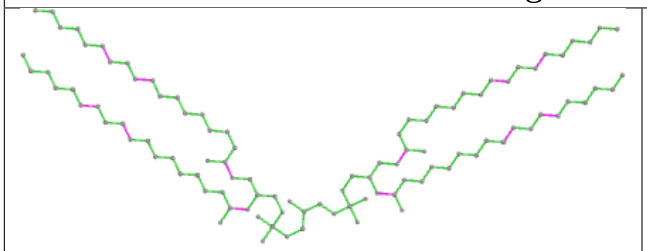


Torsions

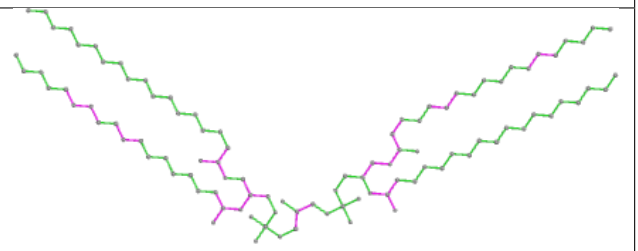


Rings

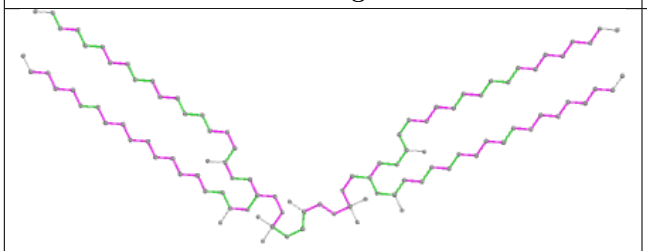
## Ligand CDL T 103



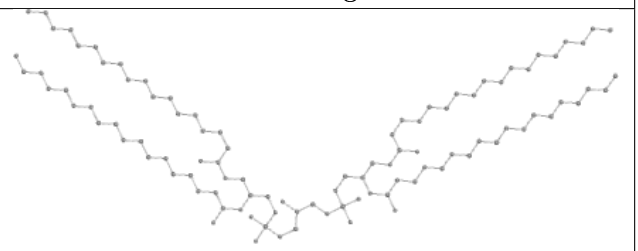
Bond lengths



Bond angles

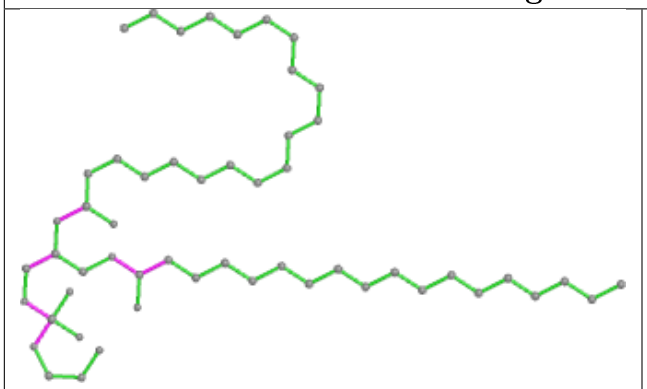


Torsions

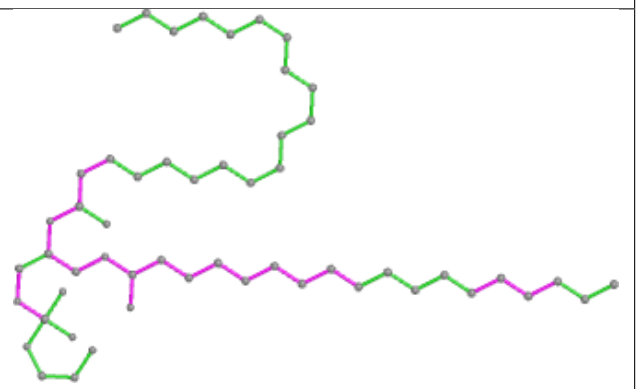


Rings

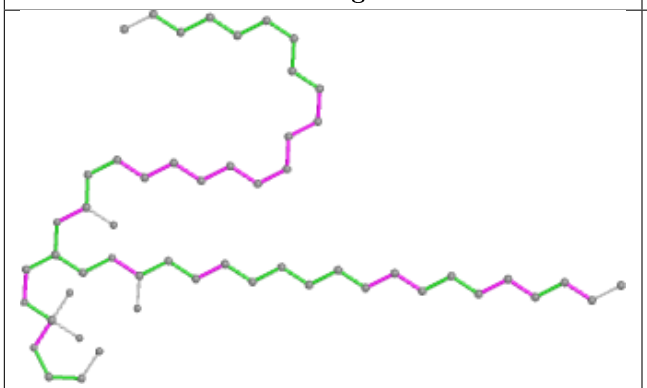
## Ligand PEK P 308



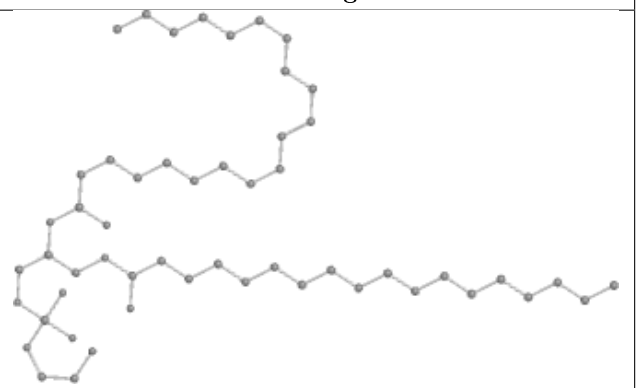
Bond lengths



Bond angles

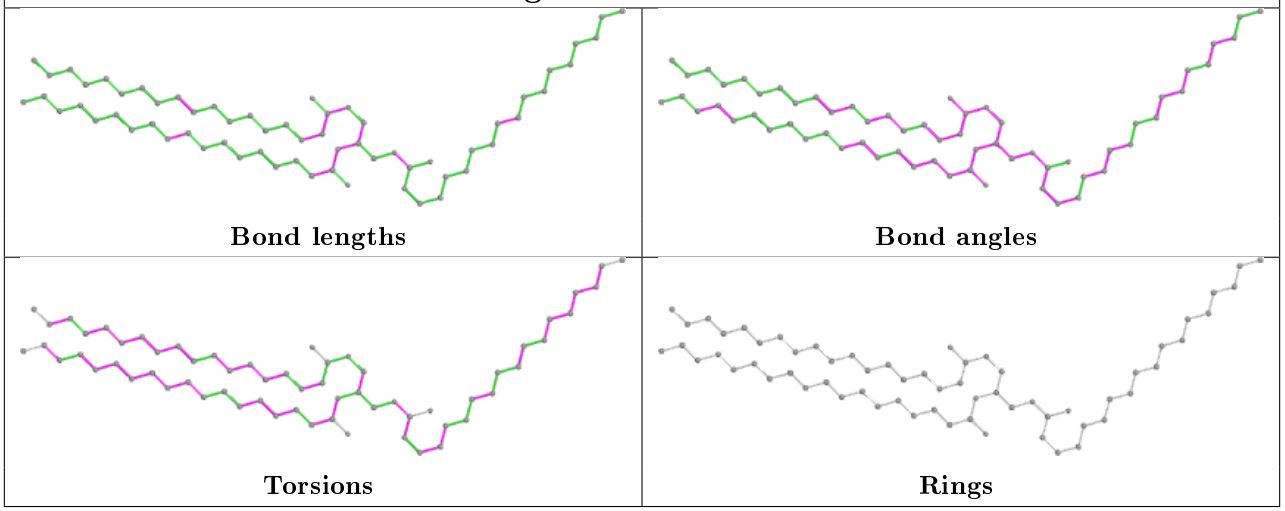


Torsions

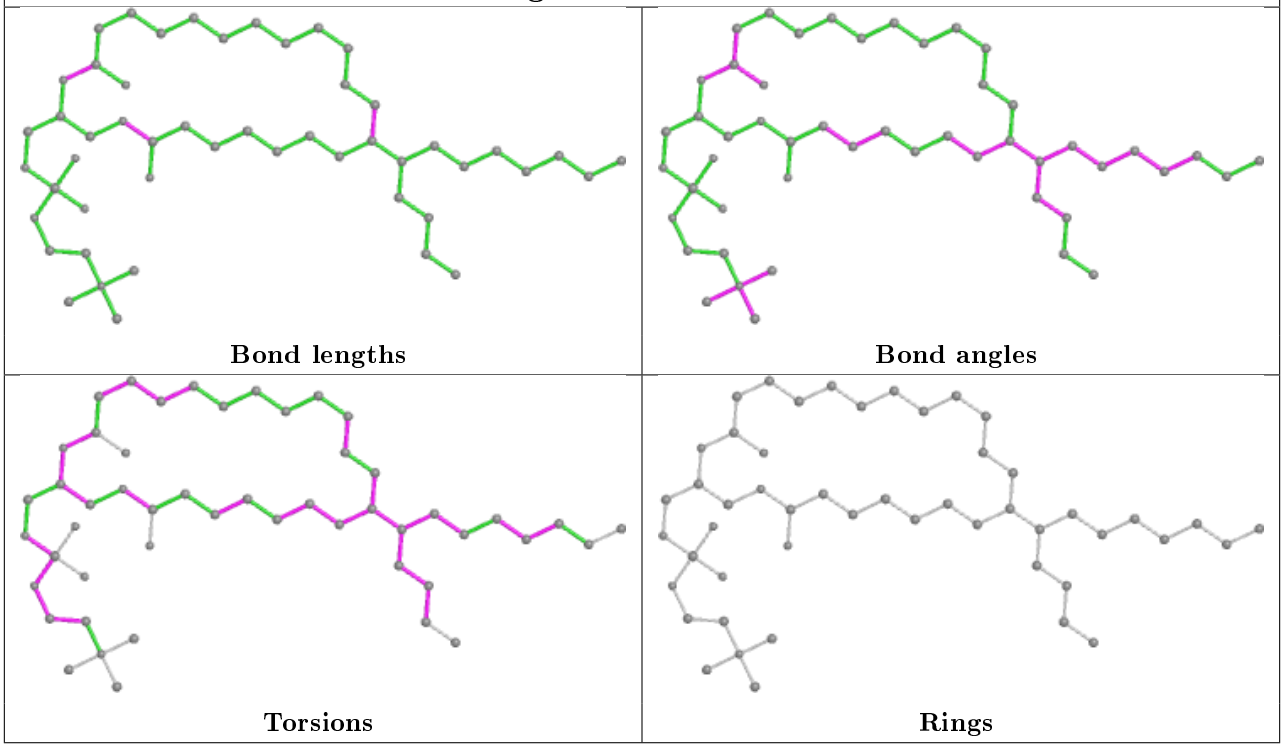


Rings

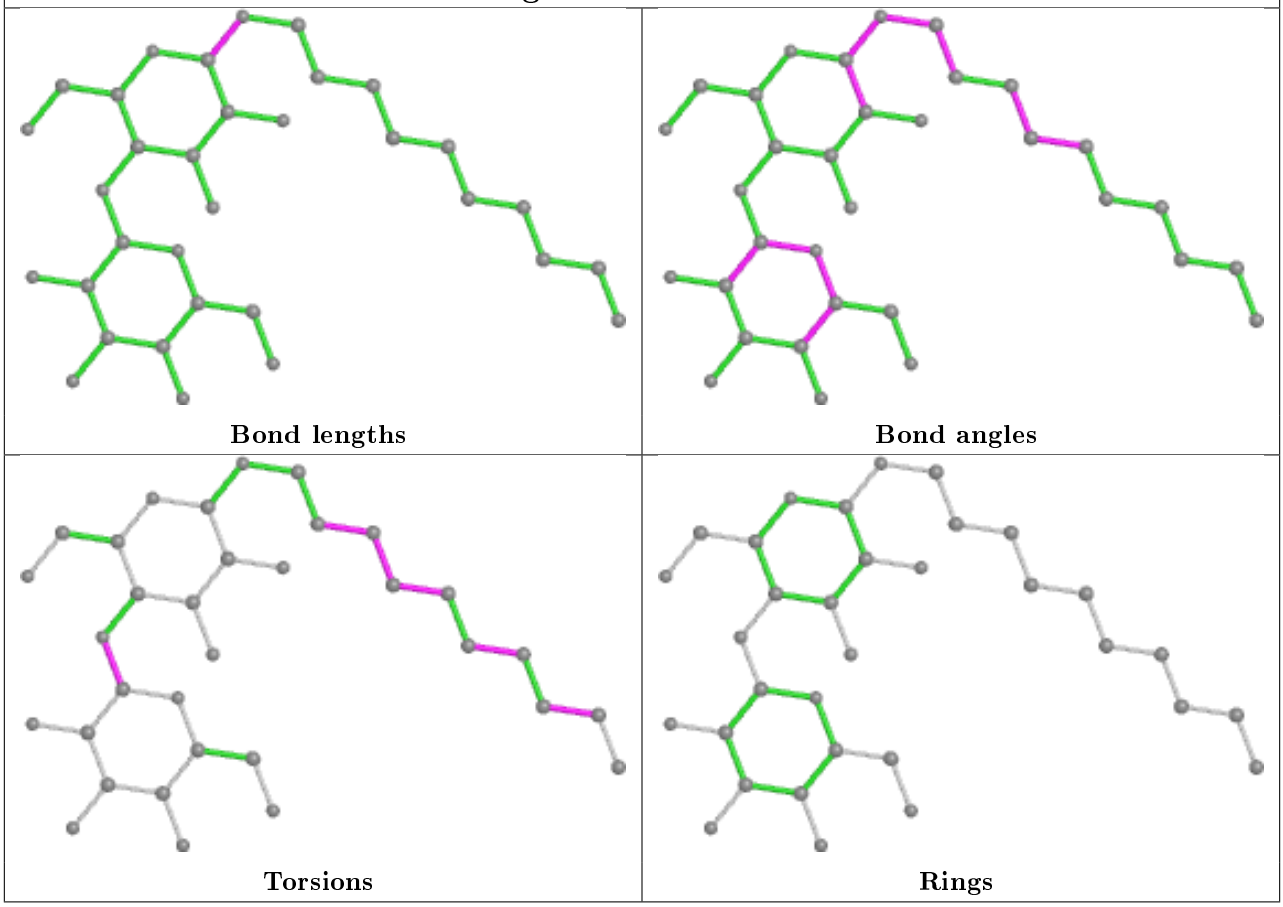
## Ligand TGL Y 101



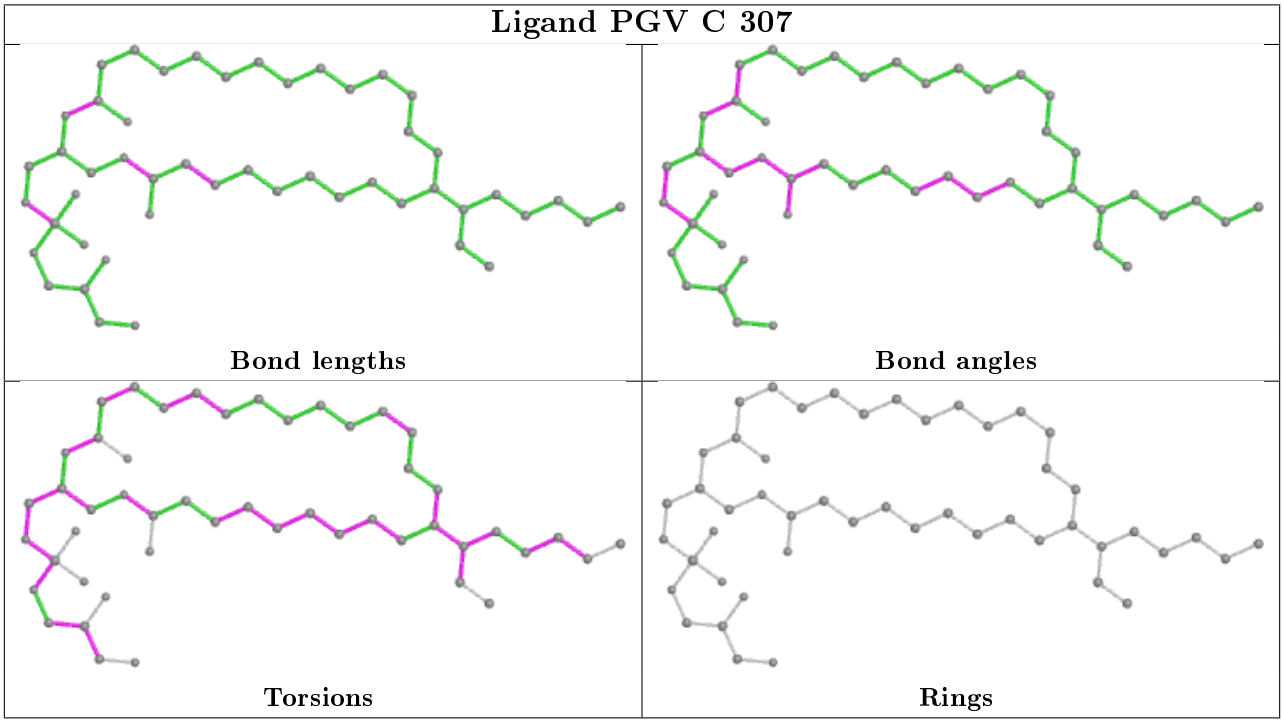

## Ligand PSC B 304



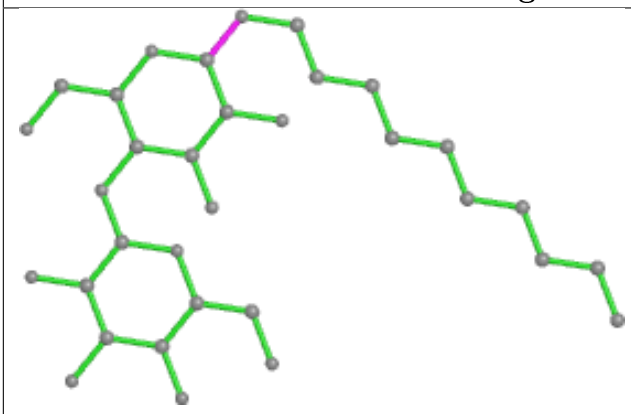
## Ligand DMU J 101



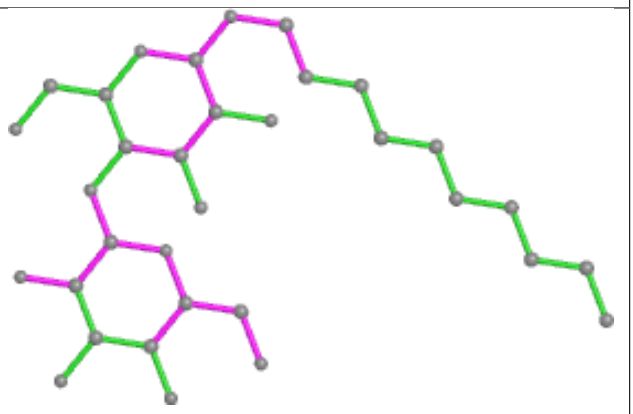

## Ligand PGV C 307



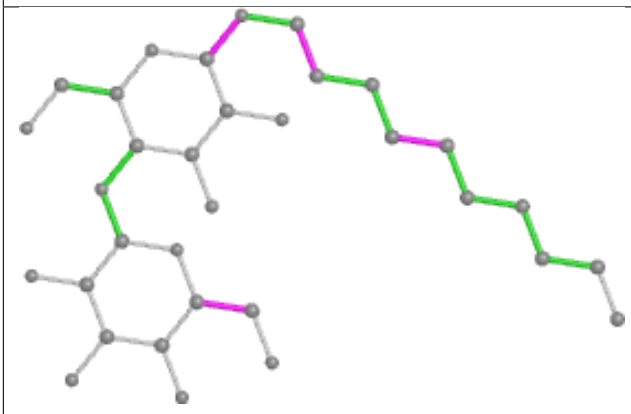
### Ligand DMU P 306



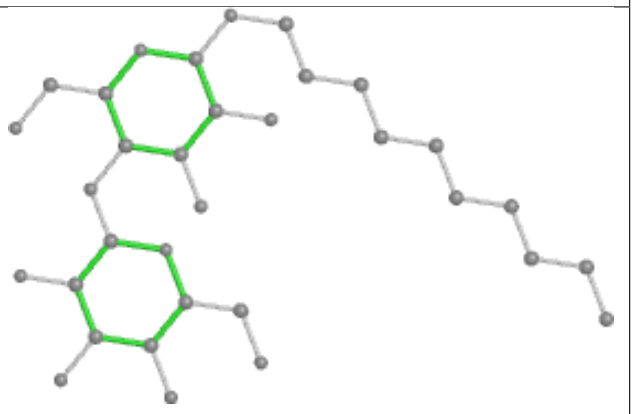
Bond lengths



Bond angles

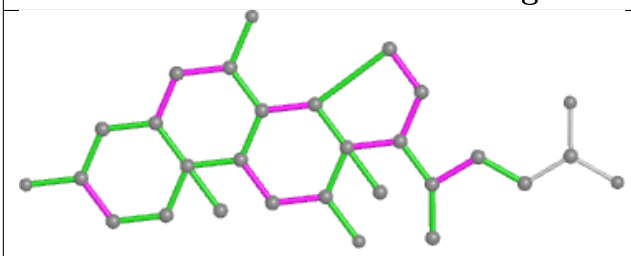


Torsions

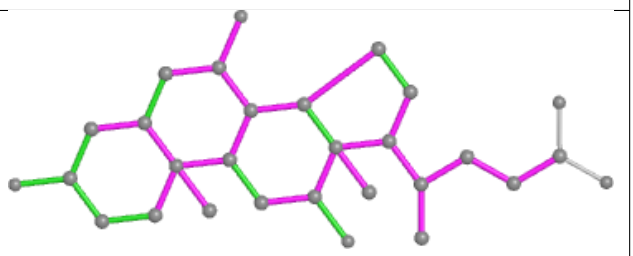


Rings

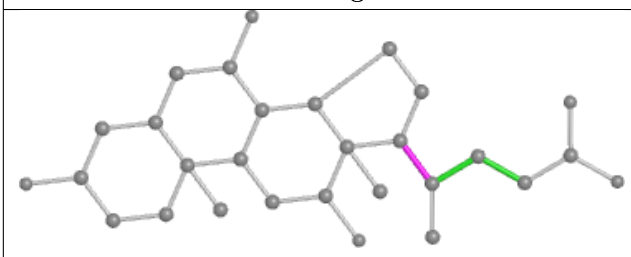
### Ligand CHD P 307



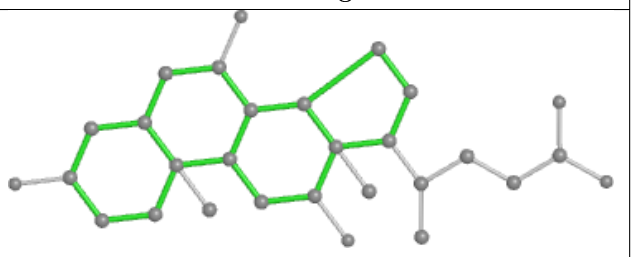
Bond lengths



Bond angles

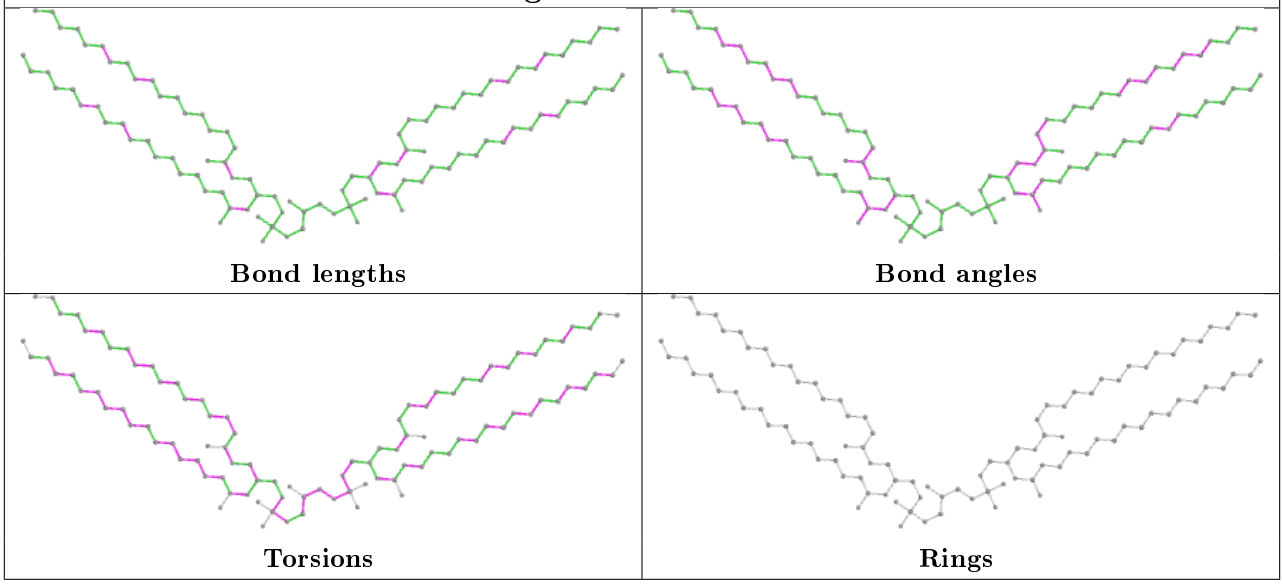


Torsions

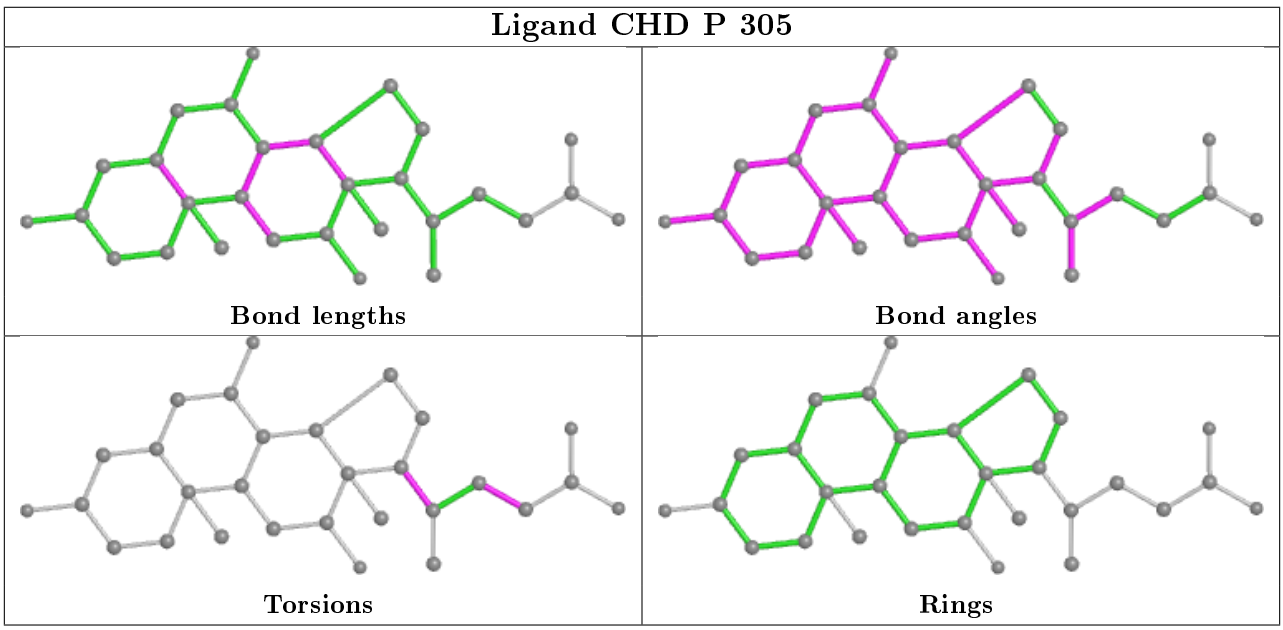


Rings

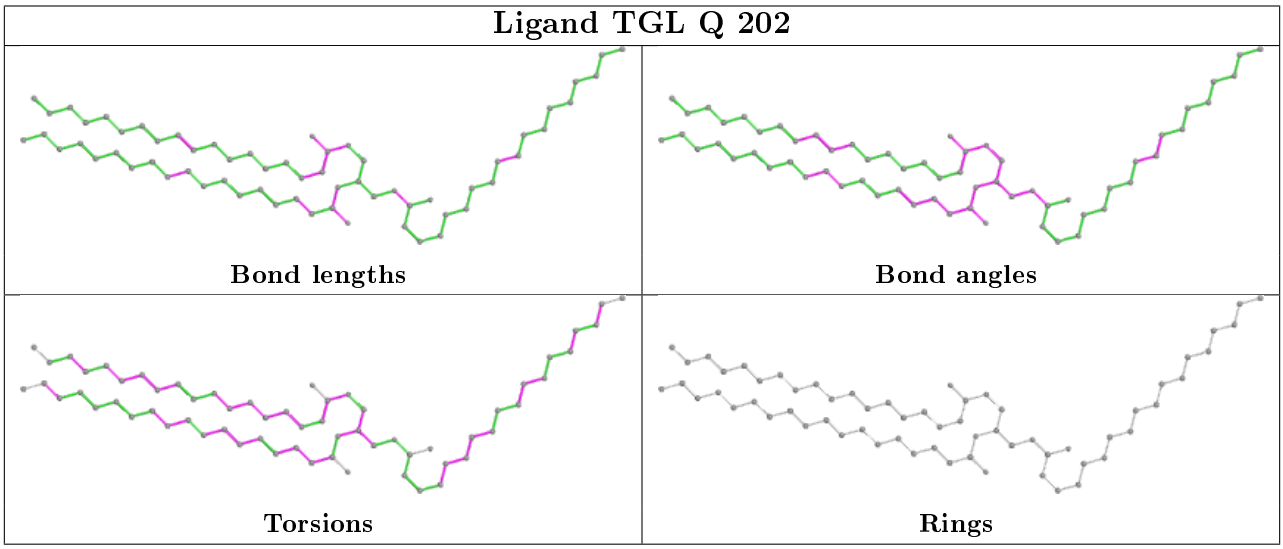
## Ligand CDL G 102




## Ligand CHD P 305




## Ligand TGL Q 202



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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 | A | 513/514 (99%) | -0.46 | 0 100 100 | 17, 21, 29, 68 | 0 |
| 1 | N | 513/514 (99%) | -0.37 | 0 100 100 | 18, 25, 33, 63 | 0 |
| 2 | B | 226/227 (99%) | -0.50 | 4 (1%) 68 73 | 20, 28, 49, 71 | 0 |
| 2 | O | 226/227 (99%) | -0.50 | 4 (1%) 68 73 | 25, 34, 60, 90 | 0 |
| 3 | C | 259/261 (99%) | -0.78 | 1 (0%) 92 94 | 19, 25, 37, 77 | 0 |
| 3 | P | 259/261 (99%) | -0.69 | 3 (1%) 79 82 | 20, 26, 39, 70 | 0 |
| 4 | D | 144/147 (97%) | -0.79 | 1 (0%) 87 90 | 23, 29, 44, 76 | 0 |
| 4 | Q | 144/147 (97%) | 0.57 | 15 (10%) 6 6 | 29, 43, 76, 153 | 0 |
| 5 | E | 105/109 (96%) | -0.62 | 2 (1%) 66 71 | 23, 30, 53, 136 | 0 |
| 5 | R | 105/109 (96%) | -0.12 | 3 (2%) 51 56 | 26, 38, 61, 149 | 0 |
| 6 | F | 98/98 (100%) | 0.06 | 8 (8%) 11 12 | 21, 31, 94, 141 | 0 |
| 6 | S | 98/98 (100%) | 0.07 | 9 (9%) 9 9 | 22, 30, 80, 126 | 0 |
| 7 | G | 83/85 (97%) | 0.59 | 16 (19%) 1 1 | 23, 32, 110, 158 | 0 |
| 7 | T | 83/85 (97%) | 0.56 | 18 (21%) 0 0 | 23, 36, 112, 154 | 0 |
| 8 | H | 79/85 (92%) | -0.18 | 7 (8%) 9 10 | 25, 36, 92, 133 | 0 |
| 8 | U | 79/85 (92%) | -0.21 | 9 (11%) 5 4 | 31, 40, 103, 127 | 0 |
| 9 | I | 72/73 (98%) | 0.27 | 7 (9%) 7 8 | 27, 41, 63, 82 | 0 |
| 9 | V | 72/73 (98%) | 0.55 | 7 (9%) 7 8 | 27, 47, 69, 143 | 0 |
| 10 | J | 58/59 (98%) | 0.33 | 7 (12%) 4 4 | 25, 35, 65, 134 | 0 |
| 10 | W | 58/59 (98%) | 0.04 | 6 (10%) 6 6 | 27, 38, 69, 158 | 0 |
| 11 | K | 49/56 (87%) | -0.54 | 0 100 100 | 28, 35, 49, 58 | 0 |
| 11 | X | 49/56 (87%) | 1.03 | 7 (14%) 2 2 | 36, 47, 68, 81 | 0 |
| 12 | L | 46/47 (97%) | -0.73 | 1 (2%) 62 67 | 22, 27, 53, 95 | 0 |
| 12 | Y | 46/47 (97%) | -0.60 | 1 (2%) 62 67 | 27, 34, 58, 125 | 0 |

*Continued on next page...*

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | M | 43/46 (93%) | -0.24 | 4 (9%) 8 9 | 24, 28, 64, 118 | 0 |
| 13 | Z | 43/46 (93%) | 0.04 | 5 (11%) 4 4 | 31, 38, 79, 145 | 0 |
| All | All | 3550/3614 (98%) | -0.29 | 145 (4%) 37 41 | 17, 29, 61, 158 | 0 |

All (145) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 6 | S | 97 | ALA | 37.3 |
| 4 | Q | 5 | VAL | 33.6 |
| 4 | Q | 6 | VAL | 14.6 |
| 6 | F | 97 | ALA | 13.2 |
| 6 | F | 98 | HIS | 11.6 |
| 5 | R | 109 | VAL | 11.1 |
| 4 | Q | 7 | LYS | 10.4 |
| 10 | J | 1 | PHE | 10.3 |
| 4 | Q | 4 | SER | 10.2 |
| 9 | V | 37 | PHE | 9.5 |
| 6 | F | 96 | LEU | 9.3 |
| 10 | J | 58 | LYS | 9.0 |
| 6 | S | 98 | HIS | 9.0 |
| 7 | G | 1 | ALA | 8.2 |
| 9 | I | 37 | PHE | 7.8 |
| 7 | T | 36 | TRP | 7.8 |
| 13 | Z | 42 | LYS | 7.3 |
| 8 | U | 8 | ILE | 7.3 |
| 8 | U | 7 | LYS | 7.2 |
| 9 | V | 2 | THR | 7.1 |
| 11 | X | 6 | ALA | 7.1 |
| 5 | R | 5 | HIS | 6.8 |
| 6 | F | 1 | ALA | 6.6 |
| 6 | S | 2 | SER | 6.3 |
| 8 | H | 47 | GLY | 6.1 |
| 7 | G | 40 | GLY | 6.1 |
| 10 | W | 58 | LYS | 6.0 |
| 6 | S | 1 | ALA | 6.0 |
| 8 | H | 45 | ALA | 5.9 |
| 7 | T | 8 | HIS | 5.9 |
| 4 | Q | 8 | SER | 5.8 |
| 3 | P | 3 | HIS | 5.8 |
| 6 | S | 96 | LEU | 5.8 |
| 6 | F | 2 | SER | 5.7 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 13 | M | 40 | TYR | 5.6 |
| 11 | X | 7 | PRO | 5.6 |
| 11 | X | 13 | TYR | 5.6 |
| 7 | T | 1 | ALA | 5.6 |
| 4 | Q | 51 | LEU | 5.5 |
| 5 | E | 5 | HIS | 5.5 |
| 10 | W | 1 | PHE | 5.5 |
| 6 | S | 94 | HIS | 5.4 |
| 7 | G | 3 | ALA | 5.3 |
| 8 | H | 44 | THR | 5.3 |
| 7 | T | 3 | ALA | 5.3 |
| 13 | Z | 43 | SER | 5.0 |
| 7 | T | 84 | LYS | 5.0 |
| 9 | I | 25 | PHE | 4.9 |
| 2 | O | 90 | ILE | 4.9 |
| 7 | G | 84 | LYS | 4.9 |
| 13 | M | 42 | LYS | 4.7 |
| 7 | T | 42 | ARG | 4.7 |
| 8 | H | 46 | LYS | 4.7 |
| 7 | G | 36 | TRP | 4.6 |
| 6 | F | 95 | GLN | 4.5 |
| 7 | T | 40 | GLY | 4.5 |
| 7 | T | 10 | GLY | 4.4 |
| 4 | Q | 53 | ILE | 4.4 |
| 13 | M | 43 | SER | 4.3 |
| 4 | Q | 147 | LYS | 4.3 |
| 6 | F | 94 | HIS | 4.3 |
| 9 | V | 34 | PHE | 4.2 |
| 8 | H | 8 | ILE | 4.2 |
| 9 | V | 25 | PHE | 4.2 |
| 7 | G | 2 | SER | 4.2 |
| 7 | T | 2 | SER | 4.1 |
| 12 | Y | 47 | LYS | 4.0 |
| 7 | G | 8 | HIS | 4.0 |
| 10 | W | 57 | HIS | 4.0 |
| 8 | U | 10 | ASN | 4.0 |
| 7 | T | 5 | LYS | 3.9 |
| 5 | E | 109 | VAL | 3.9 |
| 7 | T | 9 | GLY | 3.9 |
| 7 | T | 41 | HIS | 3.8 |
| 7 | G | 7 | ASP | 3.8 |
| 7 | G | 42 | ARG | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 10 | W | 48 | TYR | 3.7 |
| 13 | Z | 40 | TYR | 3.7 |
| 6 | S | 95 | GLN | 3.7 |
| 7 | G | 39 | SER | 3.6 |
| 7 | G | 41 | HIS | 3.6 |
| 8 | U | 48 | GLY | 3.5 |
| 7 | T | 39 | SER | 3.3 |
| 7 | G | 9 | GLY | 3.2 |
| 7 | G | 10 | GLY | 3.1 |
| 4 | Q | 39 | ALA | 3.1 |
| 9 | V | 19 | PHE | 3.1 |
| 9 | V | 31 | PHE | 3.1 |
| 4 | D | 147 | LYS | 3.1 |
| 8 | H | 48 | GLY | 3.1 |
| 9 | I | 29 | LEU | 3.0 |
| 10 | W | 52 | TRP | 3.0 |
| 13 | M | 39 | ASN | 3.0 |
| 7 | G | 6 | GLY | 2.9 |
| 2 | O | 113 | TYR | 2.9 |
| 7 | G | 45 | PRO | 2.9 |
| 7 | G | 5 | LYS | 2.9 |
| 4 | Q | 48 | TRP | 2.9 |
| 13 | Z | 39 | ASN | 2.8 |
| 10 | J | 57 | HIS | 2.8 |
| 2 | B | 55 | THR | 2.8 |
| 8 | U | 49 | ASP | 2.8 |
| 7 | T | 6 | GLY | 2.8 |
| 10 | J | 48 | TYR | 2.8 |
| 7 | T | 7 | ASP | 2.8 |
| 3 | C | 3 | HIS | 2.7 |
| 4 | Q | 140 | TYR | 2.7 |
| 8 | U | 46 | LYS | 2.7 |
| 11 | X | 12 | LYS | 2.7 |
| 2 | B | 59 | GLN | 2.7 |
| 6 | S | 93 | PRO | 2.7 |
| 9 | I | 19 | PHE | 2.7 |
| 7 | T | 33 | LEU | 2.7 |
| 10 | J | 2 | GLU | 2.6 |
| 5 | R | 108 | LYS | 2.6 |
| 4 | Q | 46 | ALA | 2.6 |
| 8 | H | 50 | VAL | 2.6 |
| 9 | I | 2 | THR | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | T | 38 | HIS | 2.5 |
| 11 | X | 28[A] | VAL | 2.5 |
| 2 | O | 91 | ASN | 2.4 |
| 7 | T | 43 | GLU | 2.4 |
| 12 | L | 2 | HIS | 2.4 |
| 8 | U | 47 | GLY | 2.4 |
| 10 | J | 56 | PRO | 2.4 |
| 4 | Q | 72 | ASN | 2.4 |
| 3 | P | 37 | PHE | 2.4 |
| 2 | B | 61 | VAL | 2.3 |
| 9 | I | 33 | THR | 2.3 |
| 2 | B | 60 | GLU | 2.3 |
| 4 | Q | 73 | ARG | 2.3 |
| 6 | F | 3 | GLY | 2.3 |
| 10 | W | 2 | GLU | 2.2 |
| 9 | I | 34 | PHE | 2.2 |
| 8 | U | 9 | LYS | 2.2 |
| 13 | Z | 32 | TRP | 2.2 |
| 9 | V | 33 | THR | 2.1 |
| 11 | X | 23 | THR | 2.1 |
| 11 | X | 9 | PHE | 2.1 |
| 6 | S | 3 | GLY | 2.1 |
| 3 | P | 88 | ILE | 2.1 |
| 2 | O | 92 | ASN | 2.1 |
| 8 | U | 44 | THR | 2.0 |
| 4 | Q | 49 | SER | 2.0 |
| 10 | J | 4 | ARG | 2.0 |

## 6.2 Non-standard residues in protein, DNA, RNA chains (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 |
|---|---|---|---|---|---|---|---|---|
| 7 | TPO | G | 11 | 11/12 | 0.49 | 0.31 | 61,102,165,180 | 0 |
| 9 | SAC | V | 1 | 9/10 | 0.52 | 0.37 | 114,126,154,162 | 0 |
| 7 | TPO | T | 11 | 11/12 | 0.62 | 0.24 | 75,96,179,187 | 0 |
| 9 | SAC | I | 1 | 9/10 | 0.91 | 0.31 | 54,70,75,82 | 0 |
| 2 | FME | O | 1 | 10/11 | 0.97 | 0.06 | 29,34,48,59 | 0 |
| 1 | FME | A | 1 | 10/11 | 0.97 | 0.10 | 31,39,64,89 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | FME | B | 1 | 10/11 | 0.97 | 0.08 | 22,27,48,55 | 0 |
| 1 | FME | N | 1 | 10/11 | 0.98 | 0.09 | 33,40,72,74 | 0 |

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 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 |
|---|---|---|---|---|---|---|---|---|
| 22 | CHD | W | 101 | 29/29 | 0.45 | 0.43 | 59,136,161,164 | 0 |
| 22 | CHD | J | 102 | 29/29 | 0.57 | 0.44 | 57,133,165,172 | 0 |
| 25 | CDL | T | 103 | 100/100 | 0.69 | 0.28 | 50,91,168,202 | 0 |
| 25 | CDL | G | 102 | 100/100 | 0.70 | 0.30 | 51,96,162,187 | 0 |
| 26 | PEK | T | 102 | 53/53 | 0.73 | 0.28 | 44,95,159,176 | 0 |
| 26 | PEK | P | 308 | 53/53 | 0.77 | 0.21 | 38,79,120,144 | 0 |
| 28 | DMU | J | 101 | 33/33 | 0.77 | 0.25 | 44,65,156,176 | 0 |
| 26 | PEK | C | 306 | 53/53 | 0.77 | 0.17 | 34,78,128,158 | 0 |
| 22 | CHD | P | 305 | 29/29 | 0.78 | 0.35 | 47,91,109,111 | 0 |
| 22 | CHD | C | 304 | 29/29 | 0.79 | 0.40 | 46,96,116,118 | 0 |
| 20 | TGL | Q | 202 | 63/63 | 0.79 | 0.17 | 40,62,99,110 | 0 |
| 28 | DMU | P | 306 | 33/33 | 0.80 | 0.21 | 36,105,192,198 | 0 |
| 19 | PGV | C | 307 | 51/51 | 0.81 | 0.25 | 47,85,169,181 | 0 |
| 23 | PSC | B | 304 | 52/52 | 0.81 | 0.24 | 39,107,190,207 | 0 |
| 19 | PGV | P | 301 | 51/51 | 0.81 | 0.21 | 45,85,147,177 | 0 |
| 24 | UNX | P | 302 | 1/1 | 0.81 | 0.39 | 38,38,38,38 | 0 |
| 20 | TGL | Y | 101 | 63/63 | 0.83 | 0.18 | 37,64,106,120 | 0 |
| 26 | PEK | G | 103 | 53/53 | 0.83 | 0.25 | 46,93,150,158 | 0 |
| 23 | PSC | O | 303 | 52/52 | 0.84 | 0.23 | 37,75,191,211 | 0 |
| 20 | TGL | D | 201 | 63/63 | 0.85 | 0.14 | 30,55,90,101 | 0 |
| 25 | CDL | C | 303 | 100/100 | 0.85 | 0.32 | 29,72,127,137 | 0 |
| 28 | DMU | Z | 101 | 33/33 | 0.85 | 0.20 | 41,47,61,63 | 0 |
| 19 | PGV | Q | 201 | 51/51 | 0.85 | 0.26 | 42,79,161,191 | 0 |
| 25 | CDL | P | 304 | 100/100 | 0.86 | 0.27 | 32,78,140,149 | 0 |
| 20 | TGL | N | 608 | 63/63 | 0.86 | 0.20 | 47,76,120,136 | 0 |
| 20 | TGL | L | 101 | 63/63 | 0.87 | 0.17 | 30,58,96,101 | 0 |

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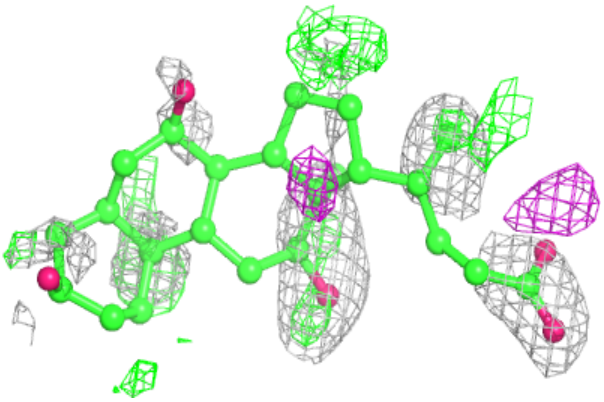
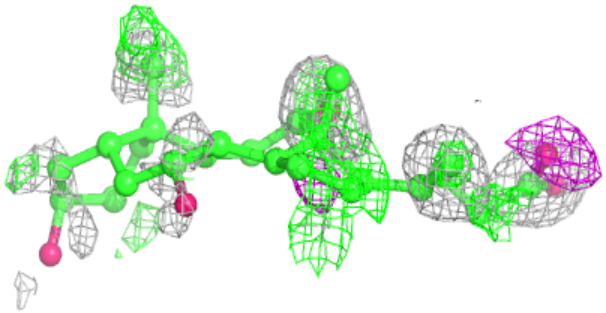
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 19 | PGV | A | 608 | 51/51 | 0.87 | 0.17 | 31,68,107,120 | 0 |
| 24 | UNX | C | 301 | 1/1 | 0.89 | 0.23 | 39,39,39,39 | 0 |
| 20 | TGL | B | 301 | 63/63 | 0.90 | 0.12 | 40,65,90,103 | 0 |
| 28 | DMU | M | 101 | 33/33 | 0.90 | 0.14 | 33,38,51,53 | 0 |
| 22 | CHD | C | 305 | 29/29 | 0.93 | 0.07 | 26,28,31,34 | 0 |
| 22 | CHD | P | 307 | 29/29 | 0.94 | 0.06 | 25,29,32,35 | 0 |
| 22 | CHD | O | 302 | 29/29 | 0.95 | 0.07 | 23,26,29,34 | 0 |
| 22 | CHD | B | 303 | 29/29 | 0.95 | 0.06 | 24,26,29,37 | 0 |
| 18 | PER | N | 606 | 2/2 | 0.96 | 0.18 | 20,20,20,26 | 0 |
| 26 | PEK | T | 101 | 53/53 | 0.97 | 0.08 | 26,42,83,92 | 0 |
| 26 | PEK | G | 101 | 53/53 | 0.97 | 0.08 | 23,40,82,96 | 0 |
| 18 | PER | A | 606 | 2/2 | 0.97 | 0.18 | 17,17,17,22 | 0 |
| 19 | PGV | C | 302 | 51/51 | 0.98 | 0.07 | 22,29,81,98 | 0 |
| 19 | PGV | N | 607 | 51/51 | 0.98 | 0.07 | 22,32,67,68 | 0 |
| 19 | PGV | P | 303 | 51/51 | 0.98 | 0.06 | 21,30,71,79 | 0 |
| 19 | PGV | A | 607 | 51/51 | 0.98 | 0.07 | 20,29,56,65 | 0 |
| 14 | HEA | A | 602 | 60/60 | 0.99 | 0.07 | 17,18,25,30 | 0 |
| 16 | MG | A | 604 | 1/1 | 0.99 | 0.04 | 19,19,19,19 | 0 |
| 14 | HEA | N | 602 | 60/60 | 0.99 | 0.09 | 19,21,28,31 | 0 |
| 14 | HEA | N | 601 | 60/60 | 0.99 | 0.08 | 21,23,43,51 | 0 |
| 14 | HEA | A | 601 | 60/60 | 0.99 | 0.07 | 17,19,37,48 | 0 |
| 16 | MG | N | 604 | 1/1 | 0.99 | 0.08 | 25,25,25,25 | 0 |
| 21 | CUA | O | 301 | 2/2 | 1.00 | 0.07 | 27,27,27,27 | 0 |
| 27 | ZN | S | 101 | 1/1 | 1.00 | 0.04 | 26,26,26,26 | 0 |
| 27 | ZN | F | 101 | 1/1 | 1.00 | 0.04 | 26,26,26,26 | 0 |
| 17 | NA | N | 605 | 1/1 | 1.00 | 0.03 | 30,30,30,30 | 0 |
| 21 | CUA | B | 302 | 2/2 | 1.00 | 0.08 | 21,21,21,21 | 0 |
| 15 | CU | N | 603 | 1/1 | 1.00 | 0.08 | 21,21,21,21 | 0 |
| 17 | NA | A | 605 | 1/1 | 1.00 | 0.02 | 23,23,23,23 | 0 |
| 15 | CU | A | 603 | 1/1 | 1.00 | 0.07 | 19,19,19,19 | 0 |

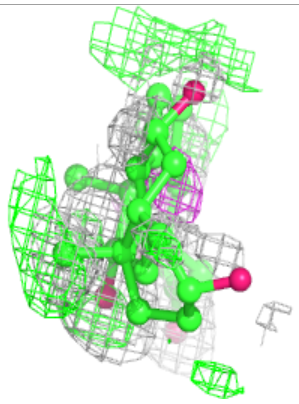
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CHD W 101:**

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

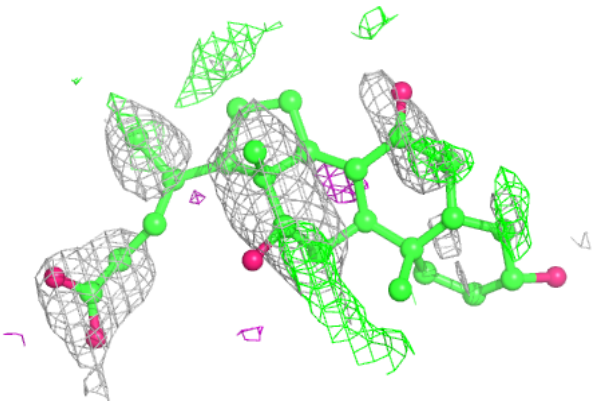


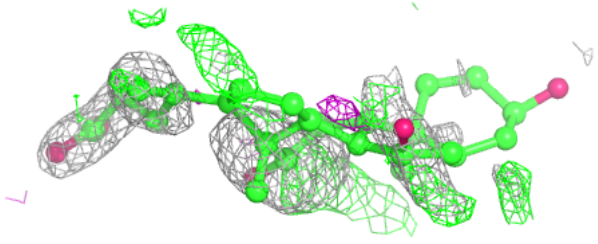


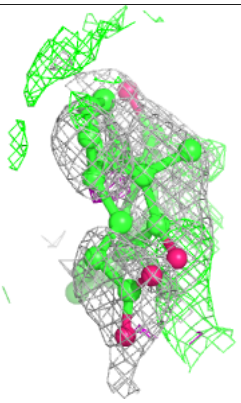


**Electron density around CHD J 102:**

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

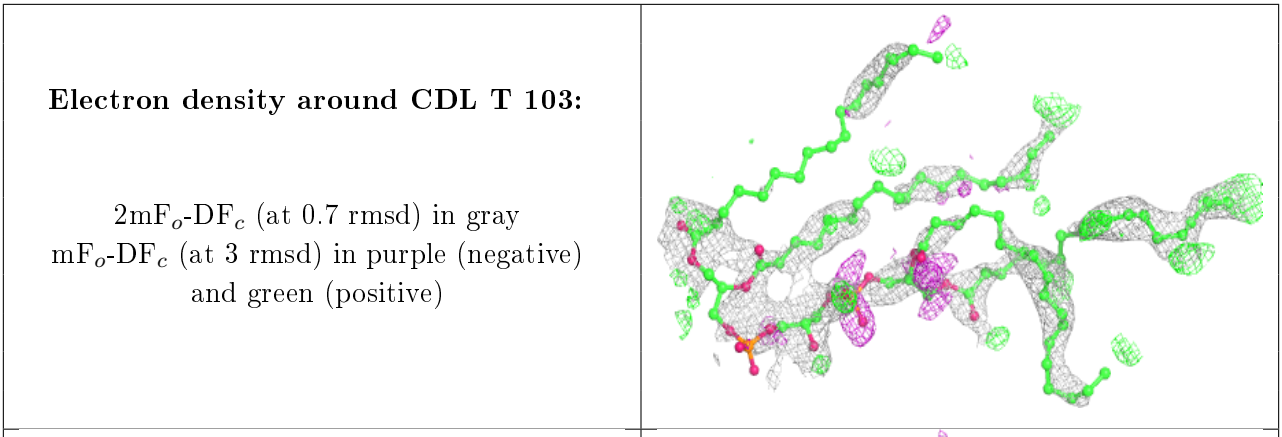






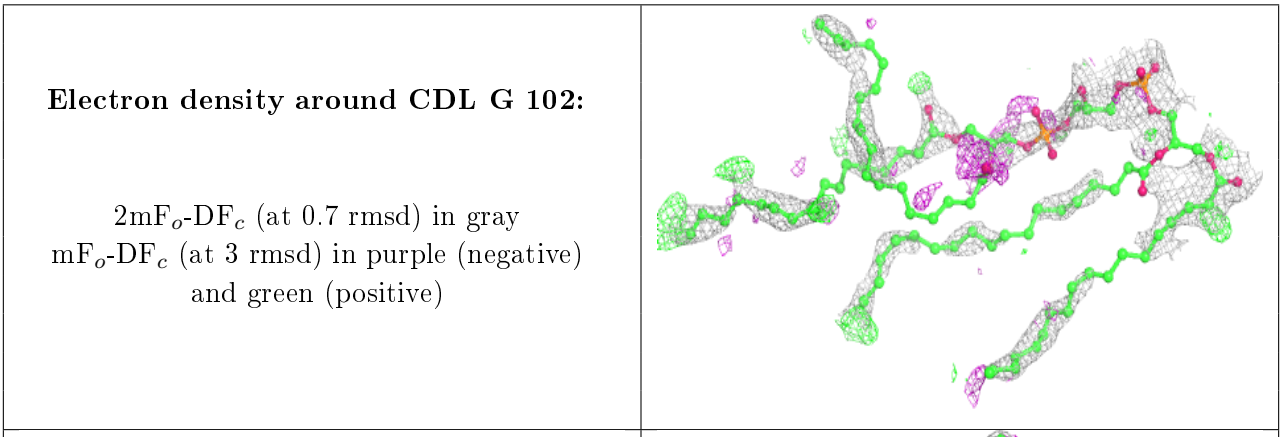
**Electron density around CDL T 103:**

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



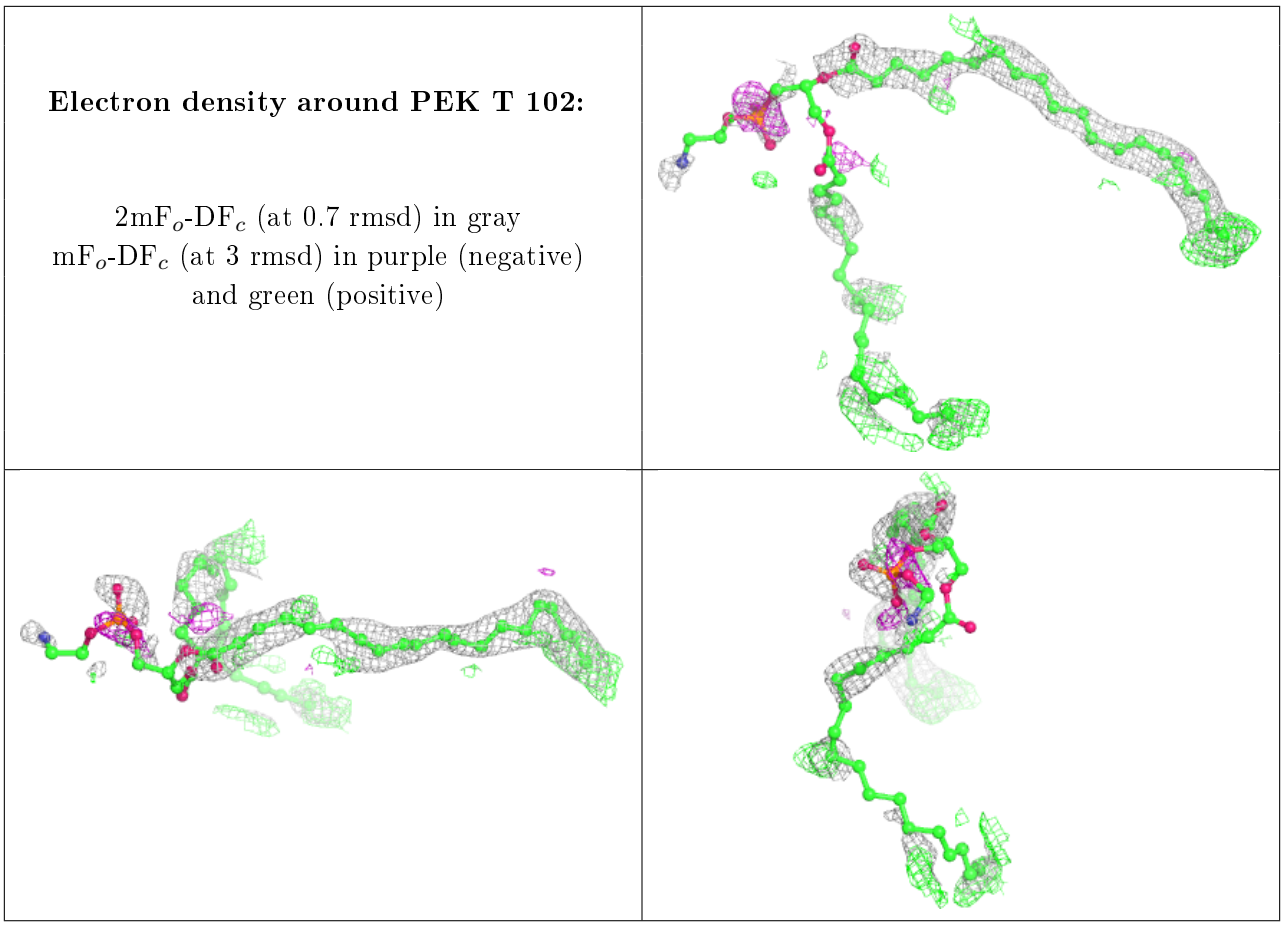
**Electron density around CDL G 102:**

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



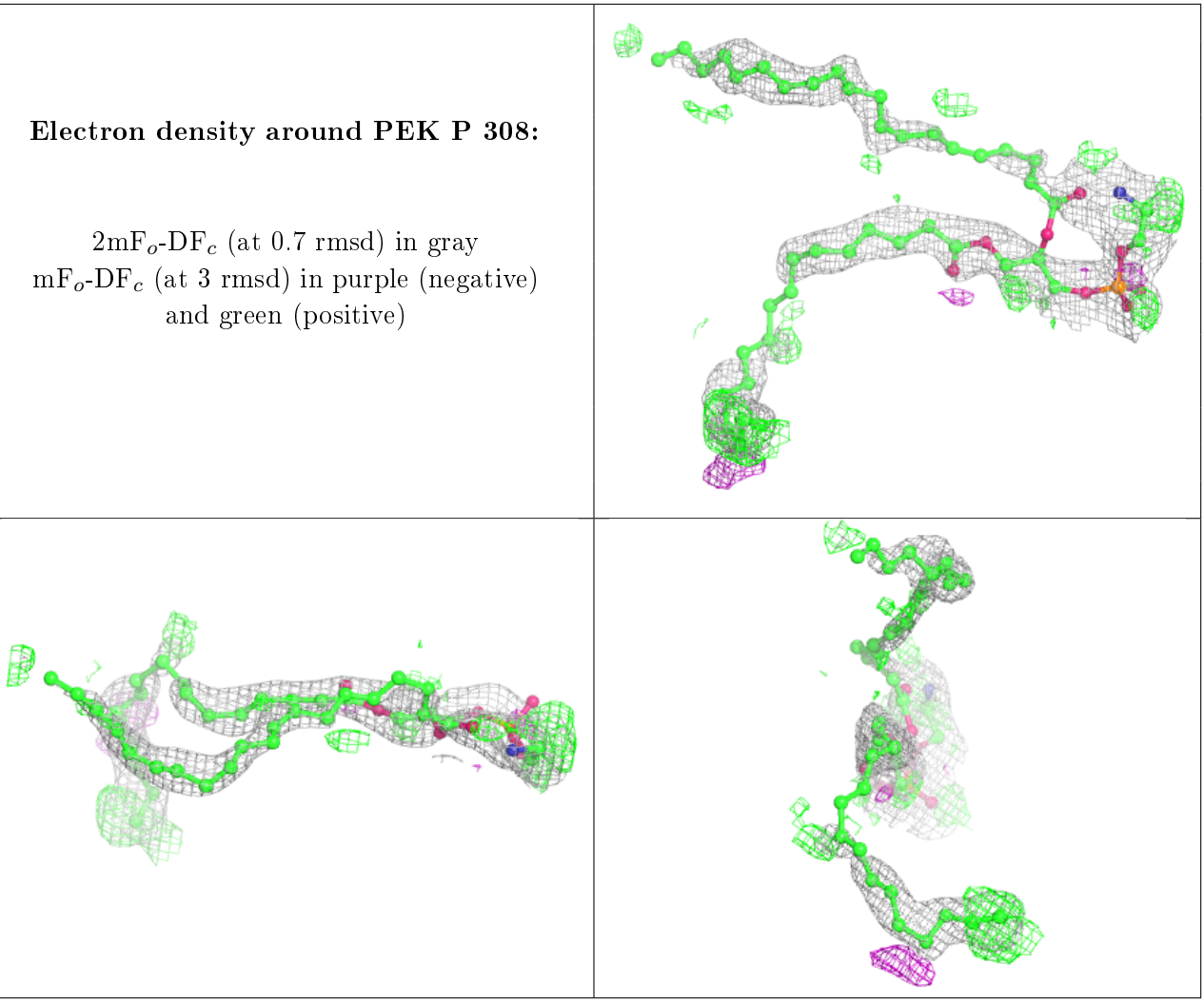
**Electron density around PEK T 102:**

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



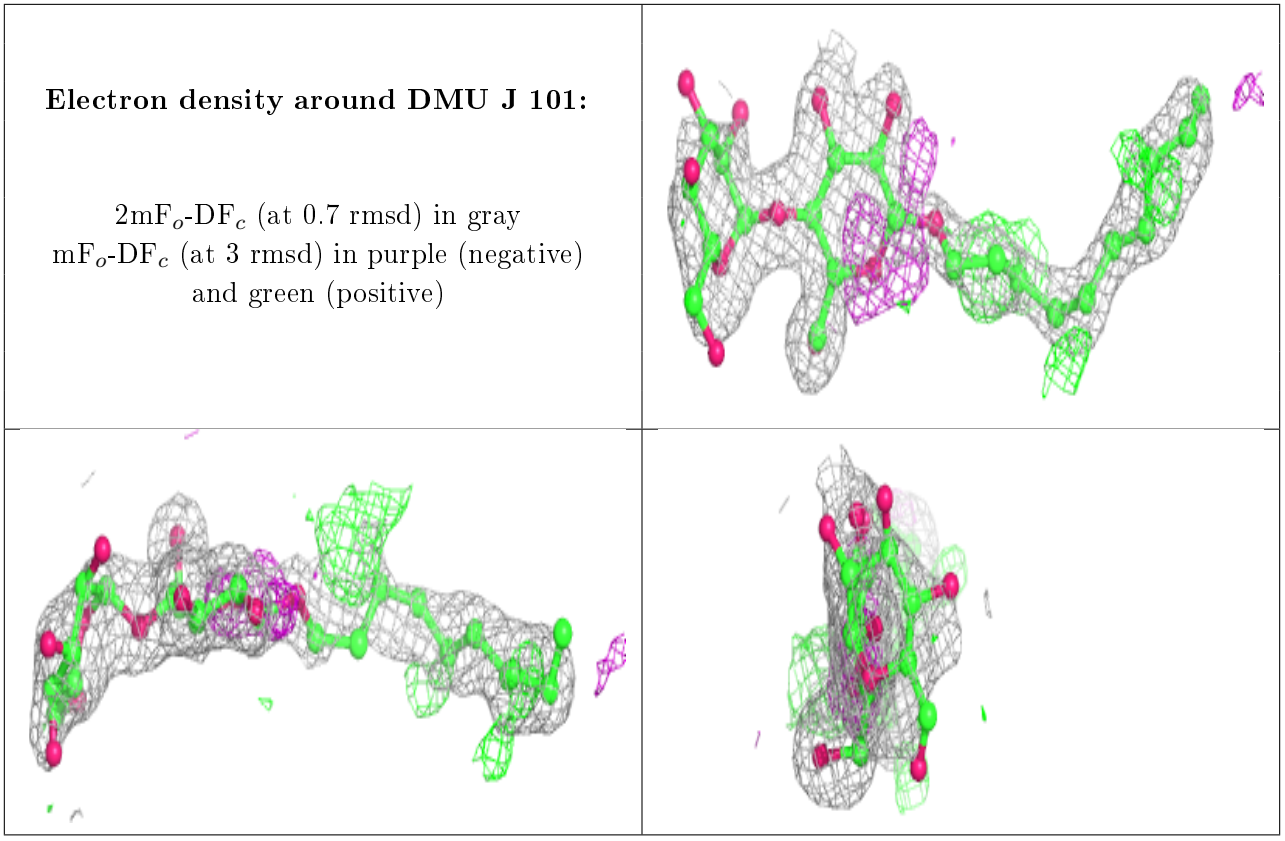
**Electron density around PEK P 308:**

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



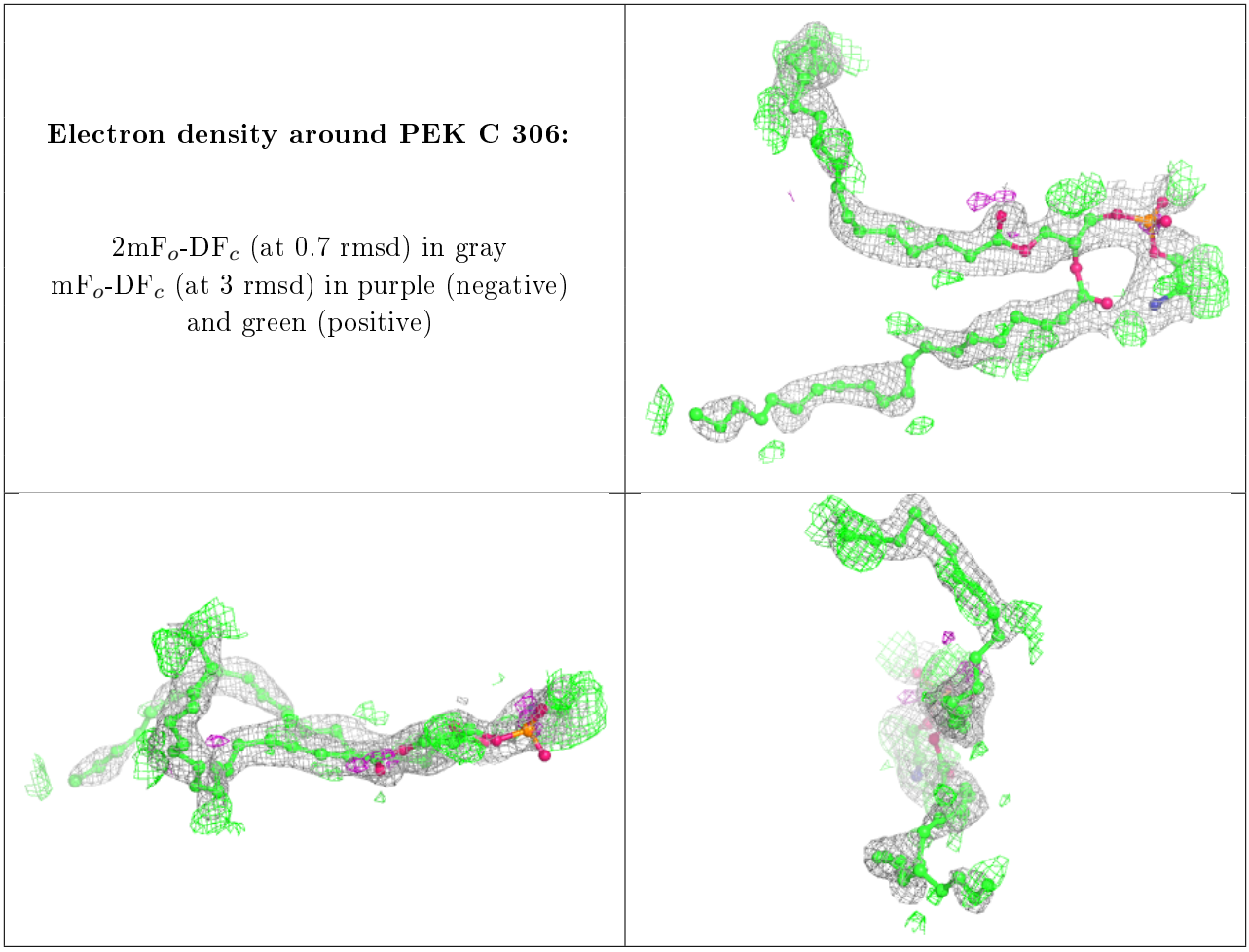
**Electron density around DMU J 101:**

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



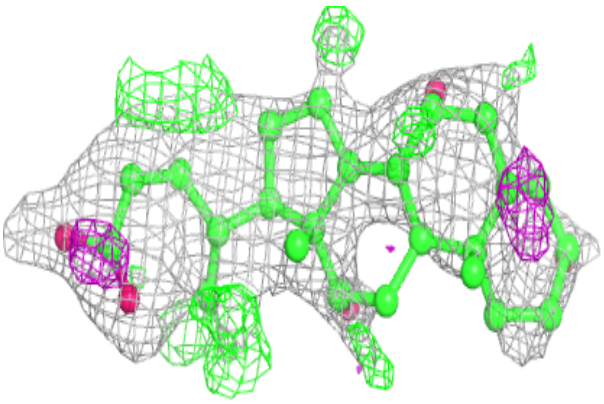
**Electron density around PEK C 306:**

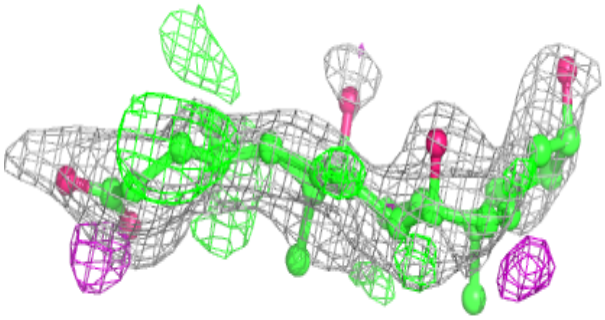
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

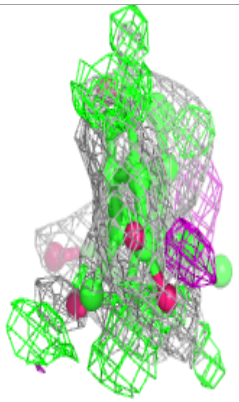


**Electron density around CHD P 305:**

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

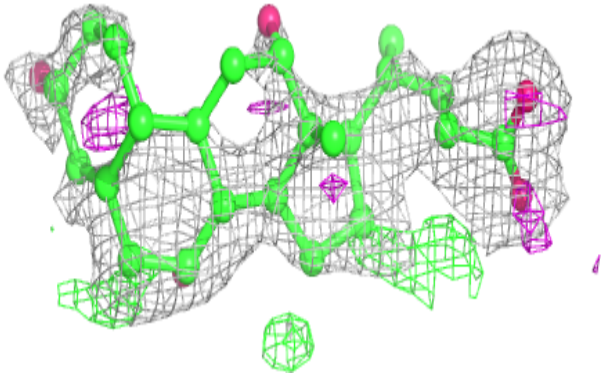


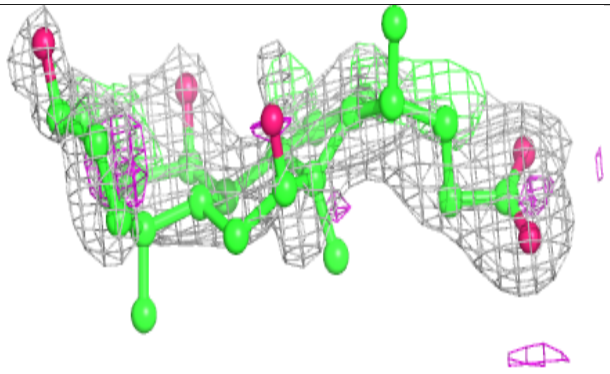


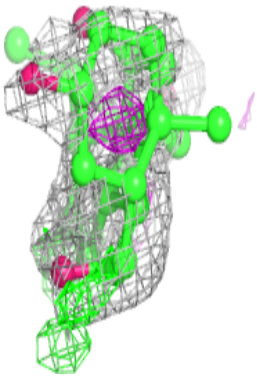


**Electron density around CHD C 304:**

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

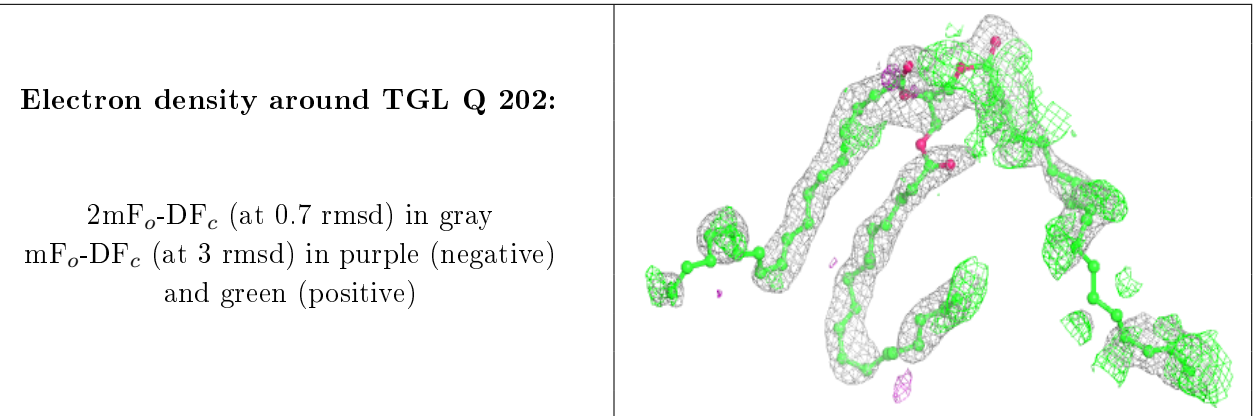


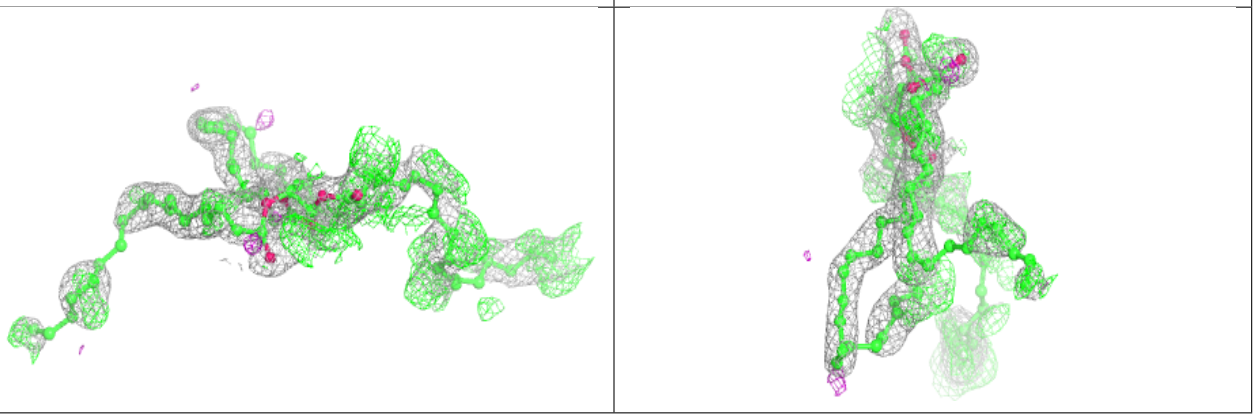




**Electron density around TGL Q 202:**

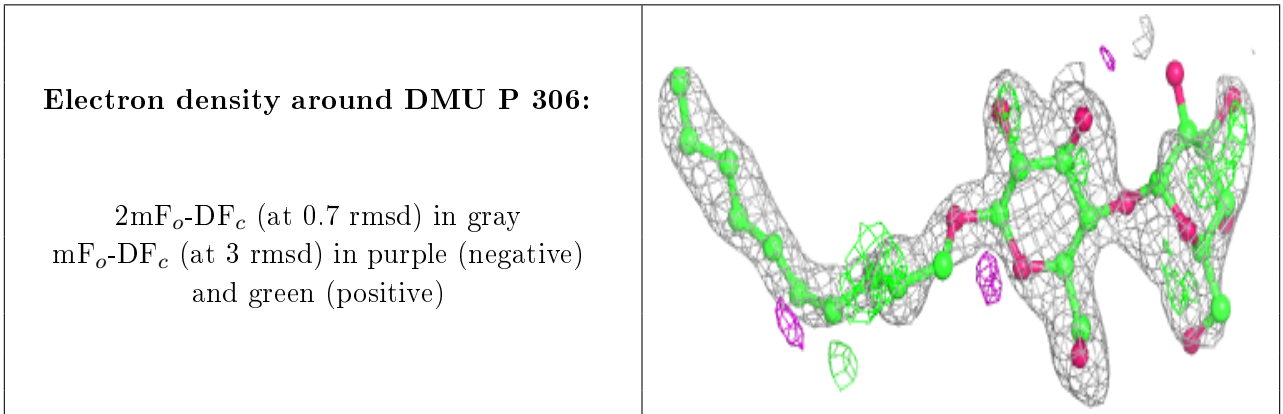
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

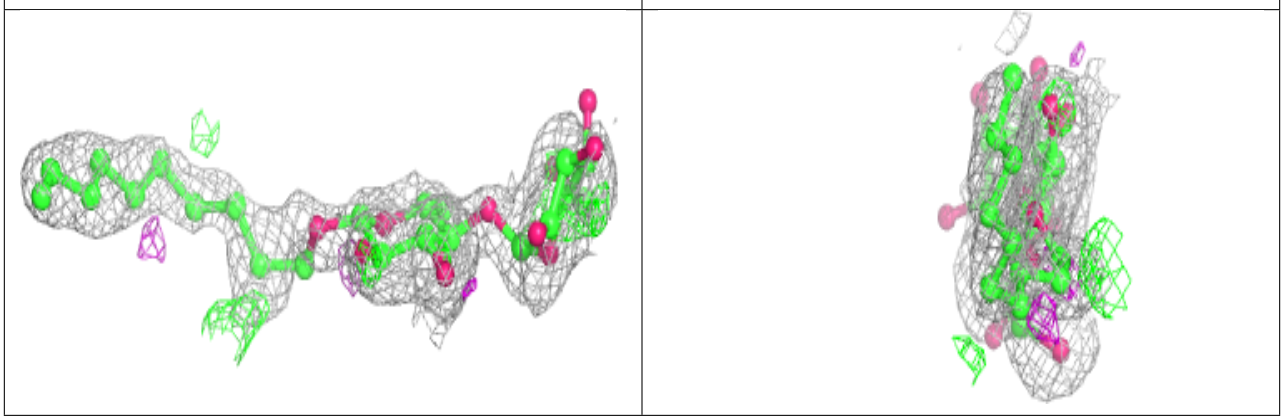




**Electron density around DMU P 306:**

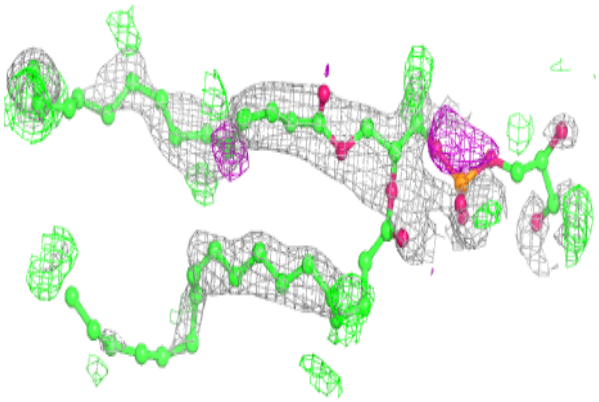
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

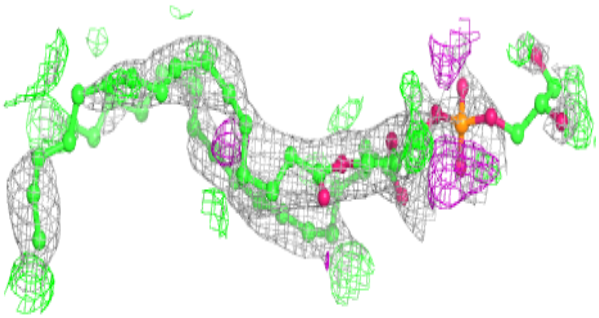


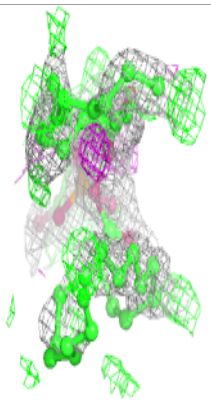


**Electron density around PGV C 307:**

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

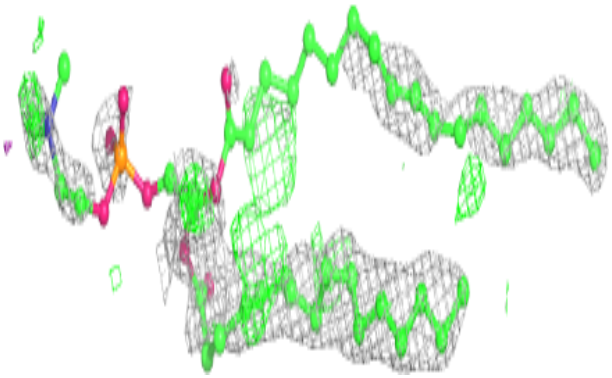


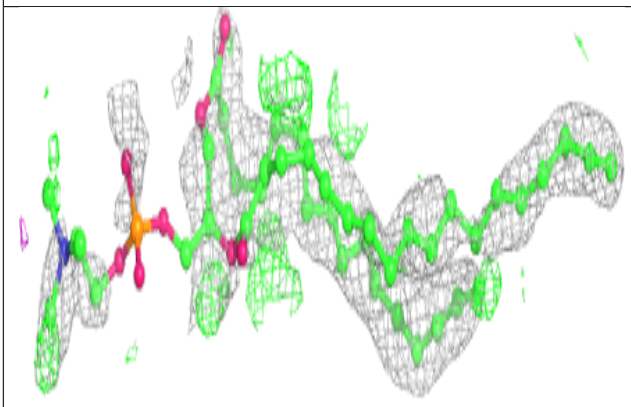


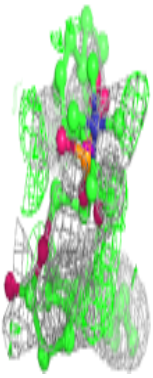


**Electron density around PSC B 304:**

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

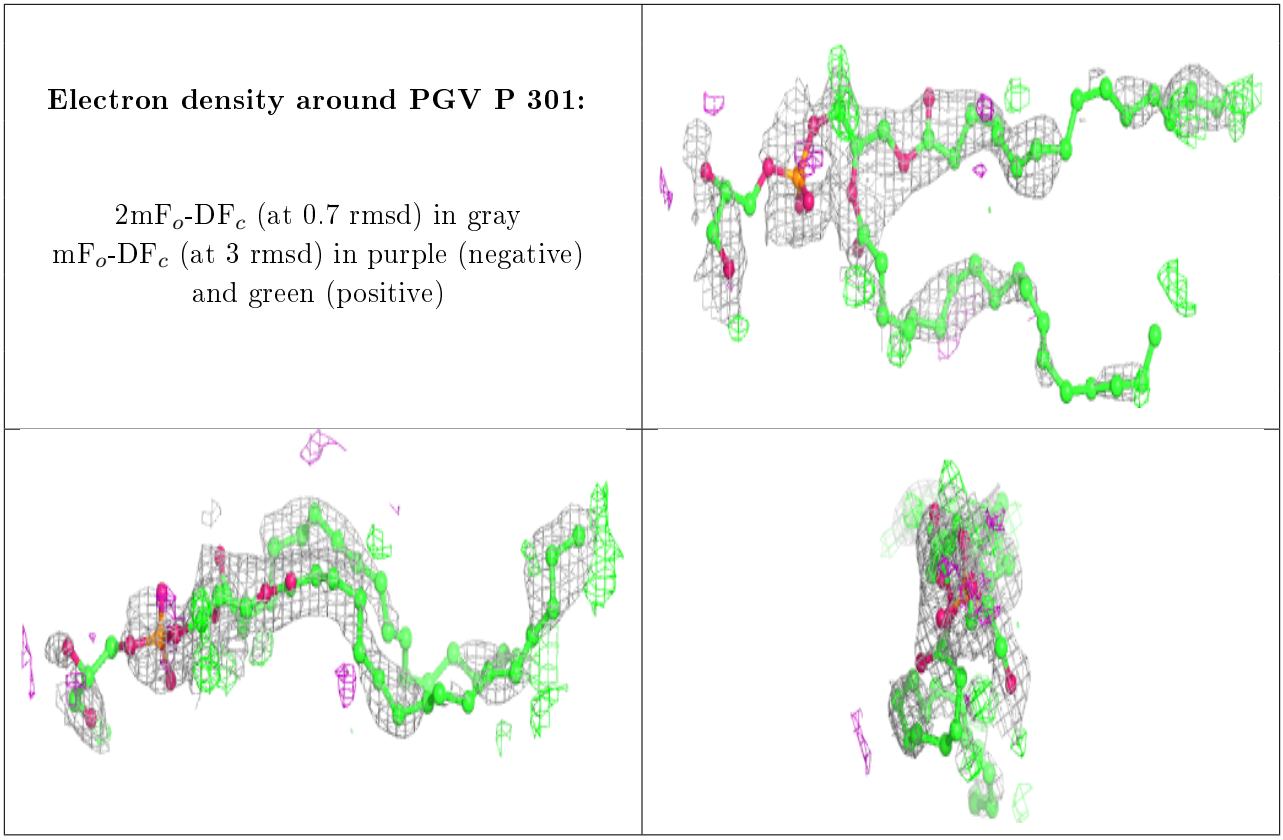






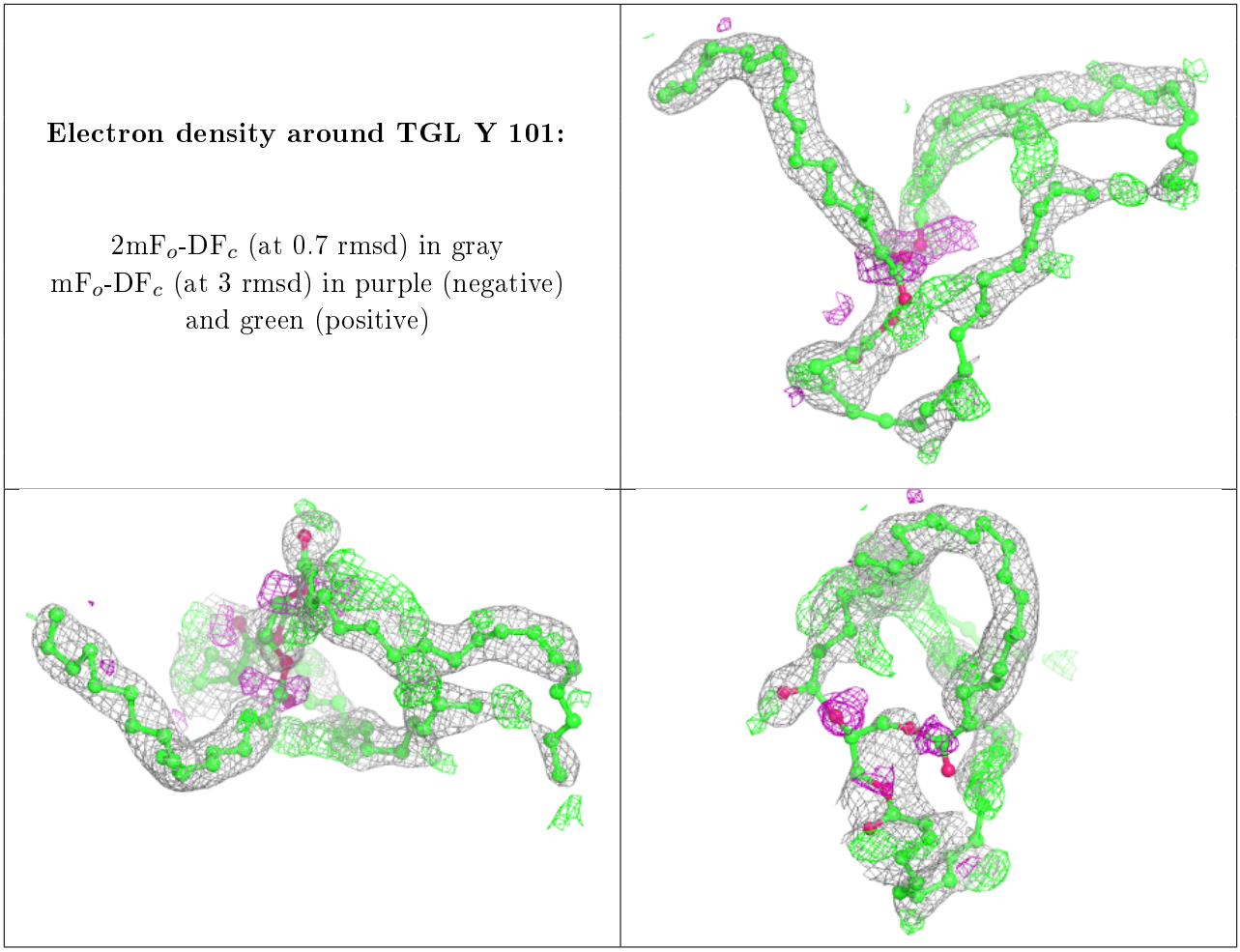
**Electron density around PGV P 301:**

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



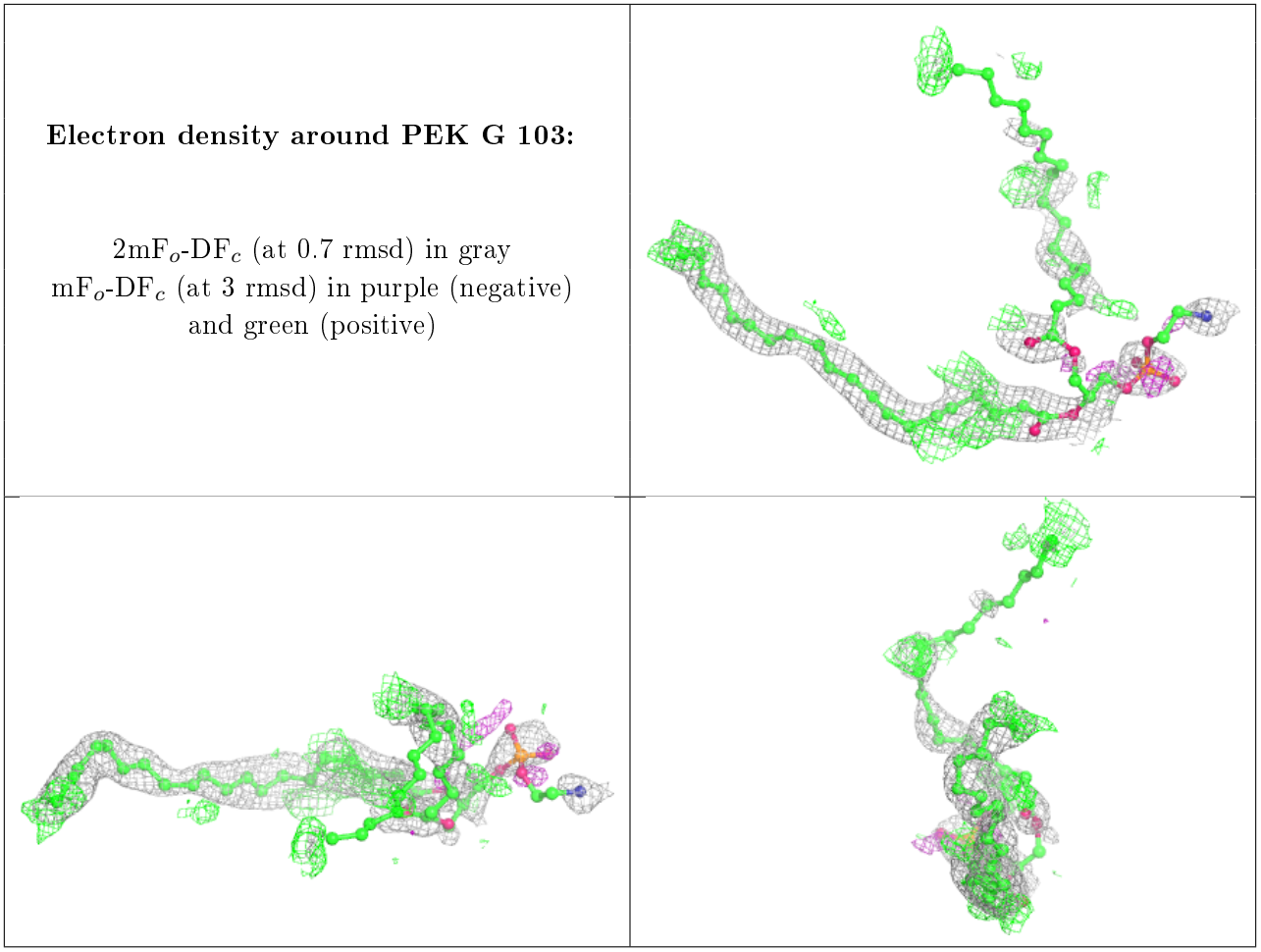
**Electron density around TGL Y 101:**

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



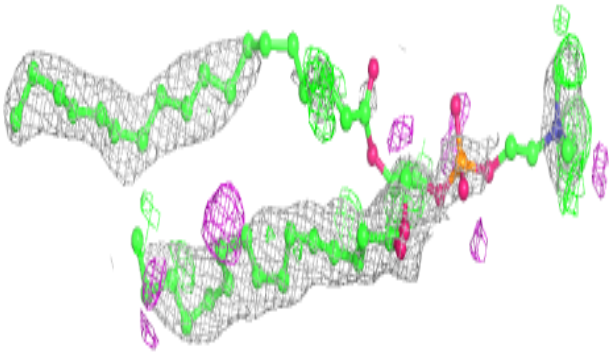
**Electron density around PEK G 103:**

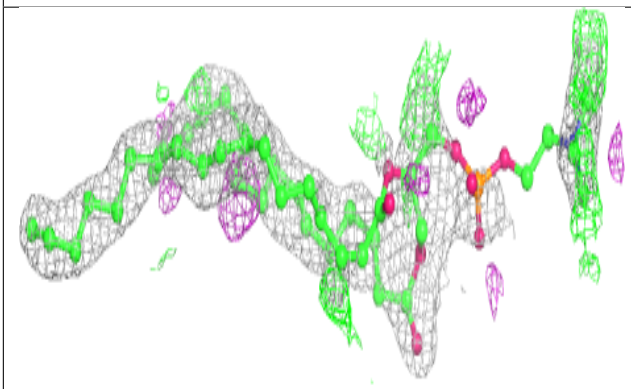
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

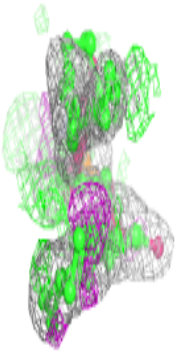


**Electron density around PSC O 303:**

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

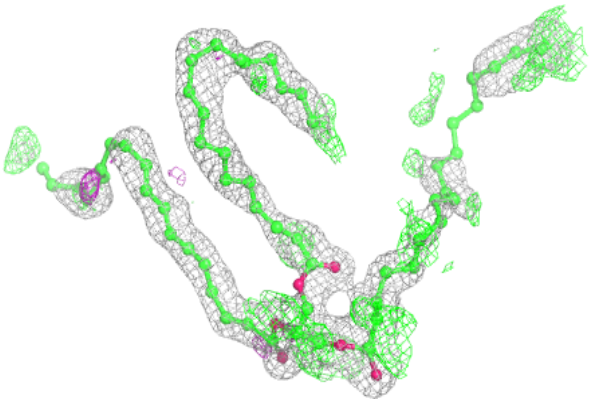


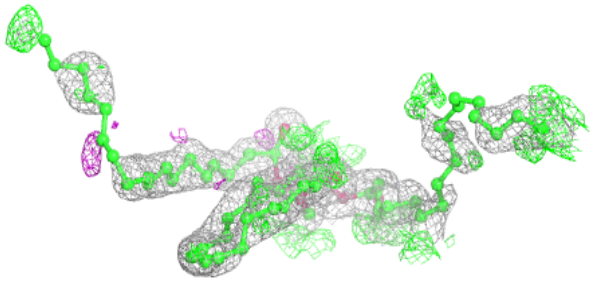


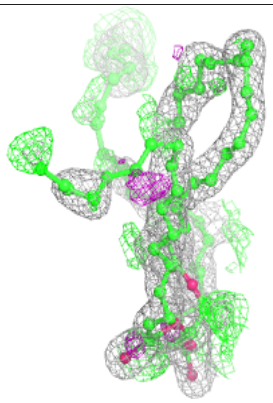


**Electron density around TGL D 201:**

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

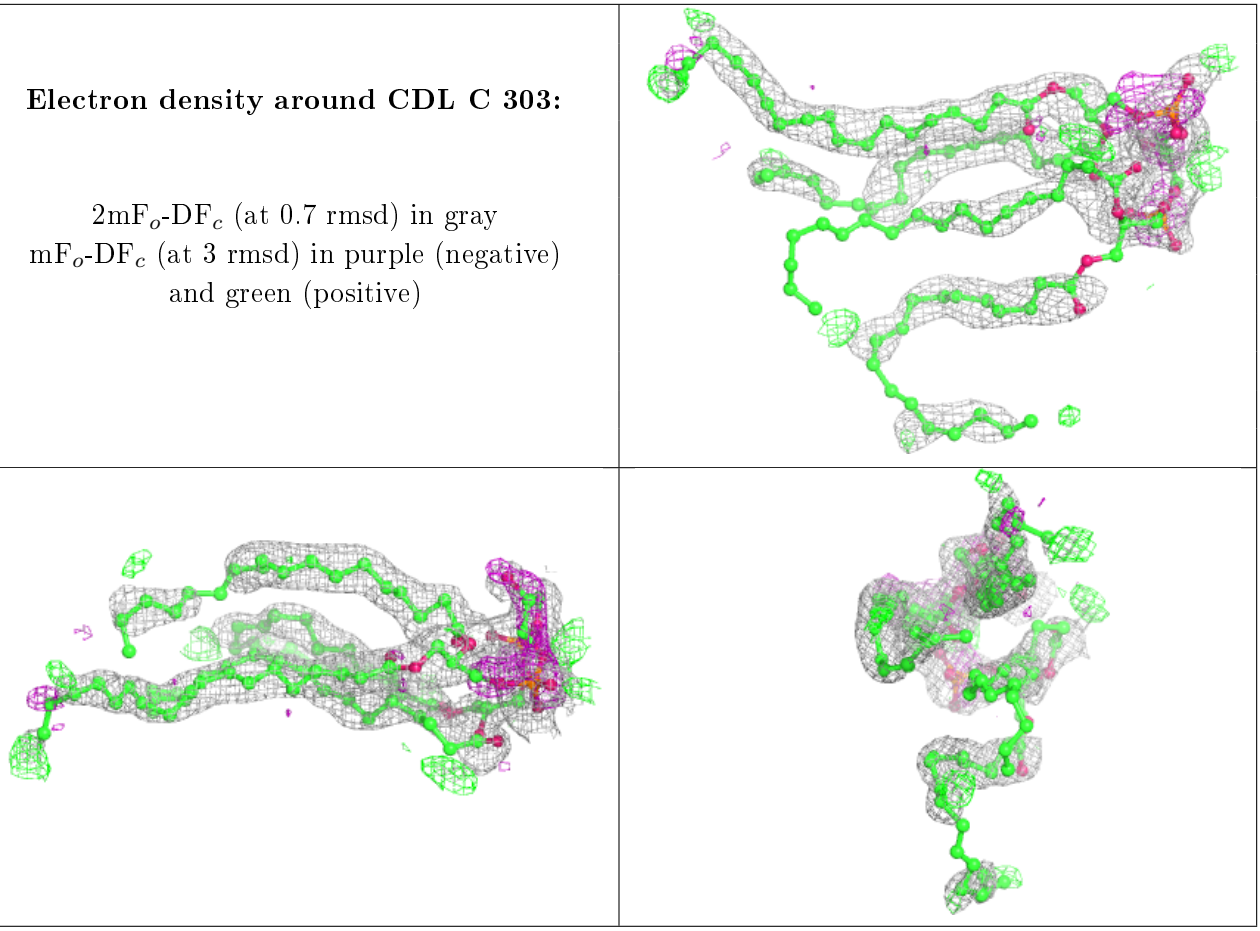






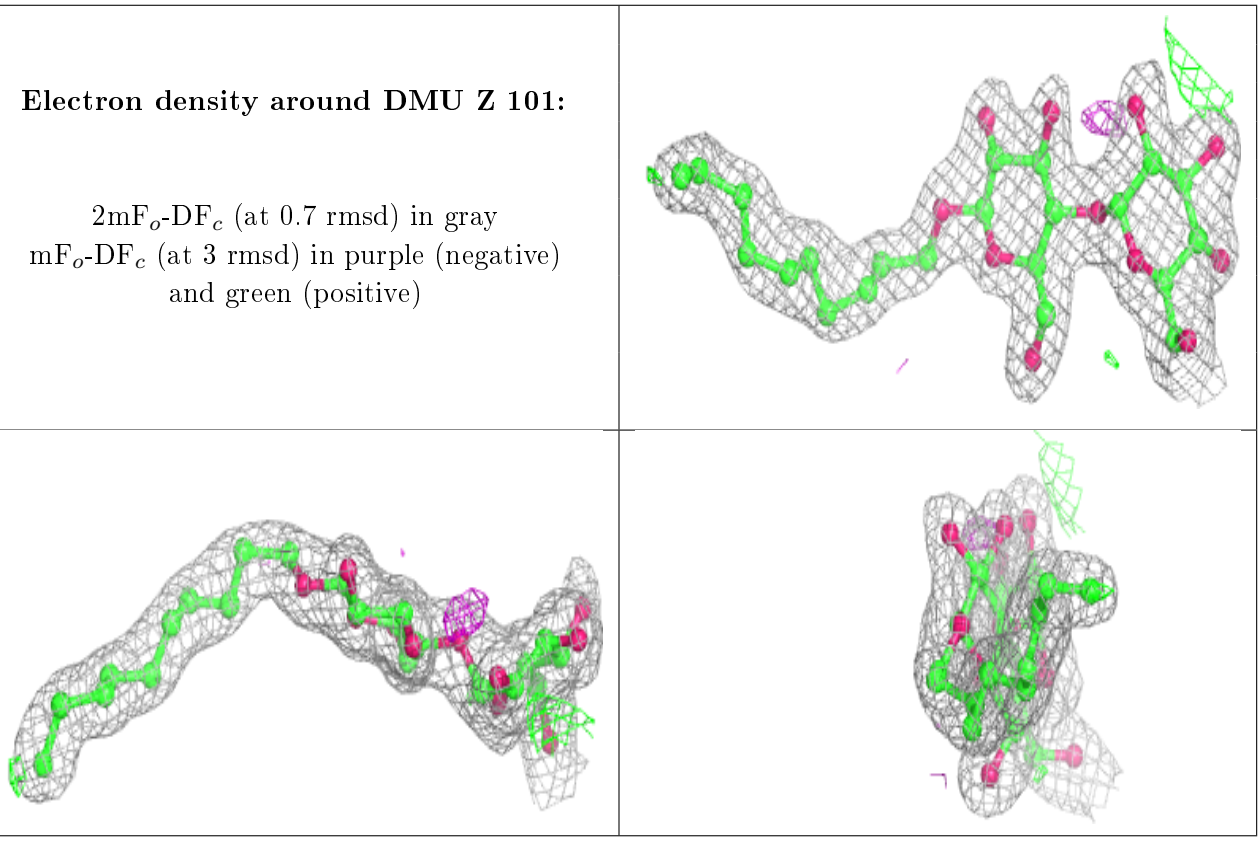
**Electron density around CDL C 303:**

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



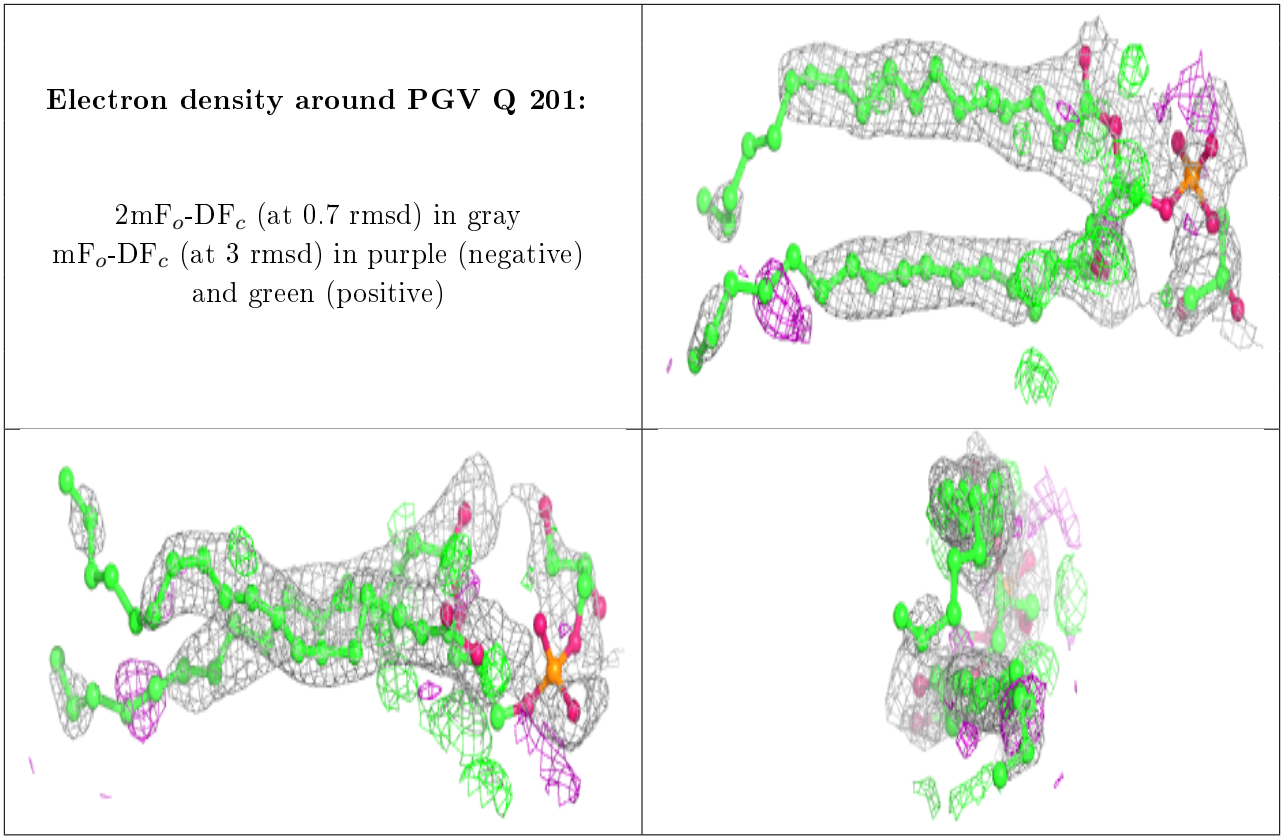
**Electron density around DMU Z 101:**

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



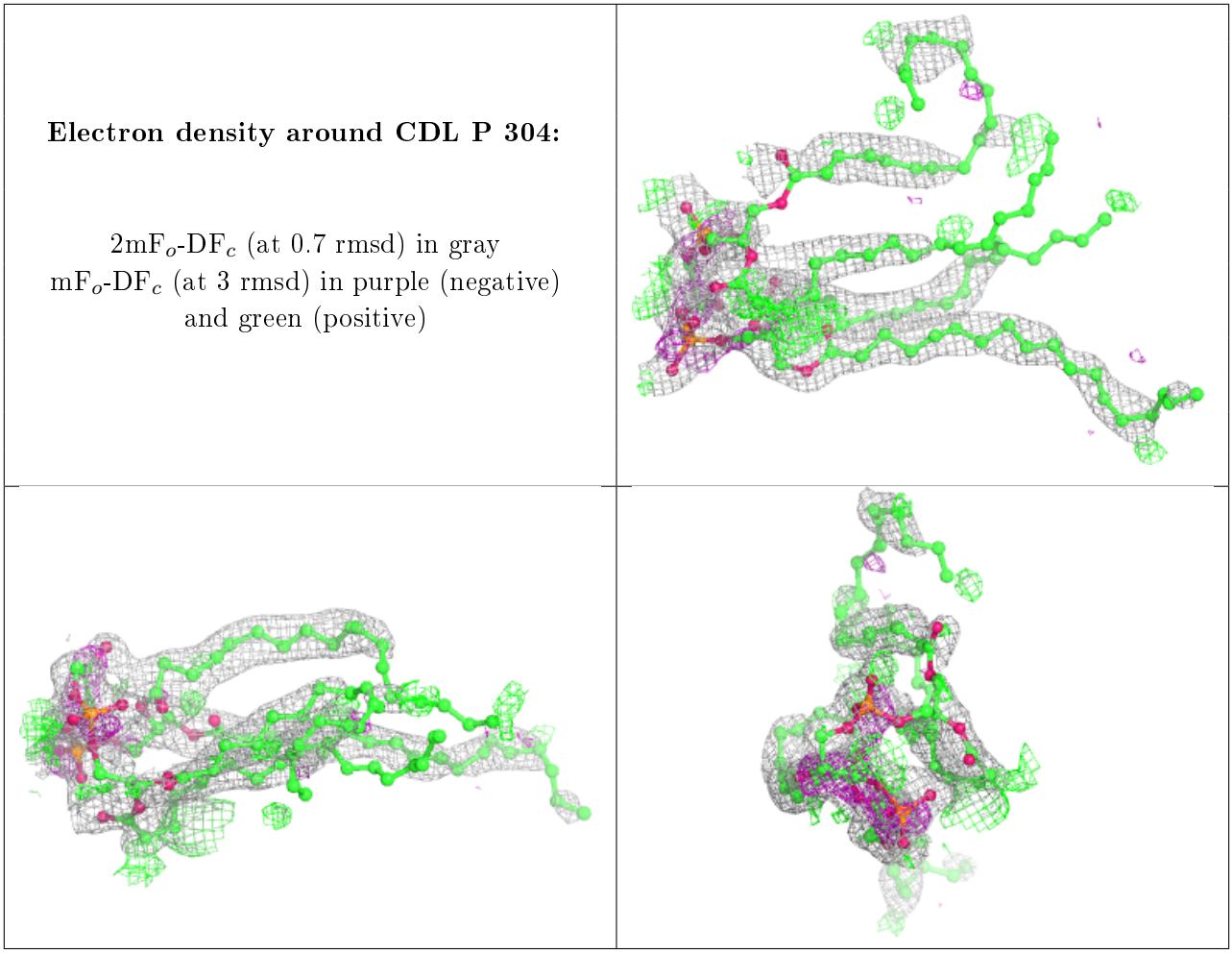
**Electron density around PGV Q 201:**

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



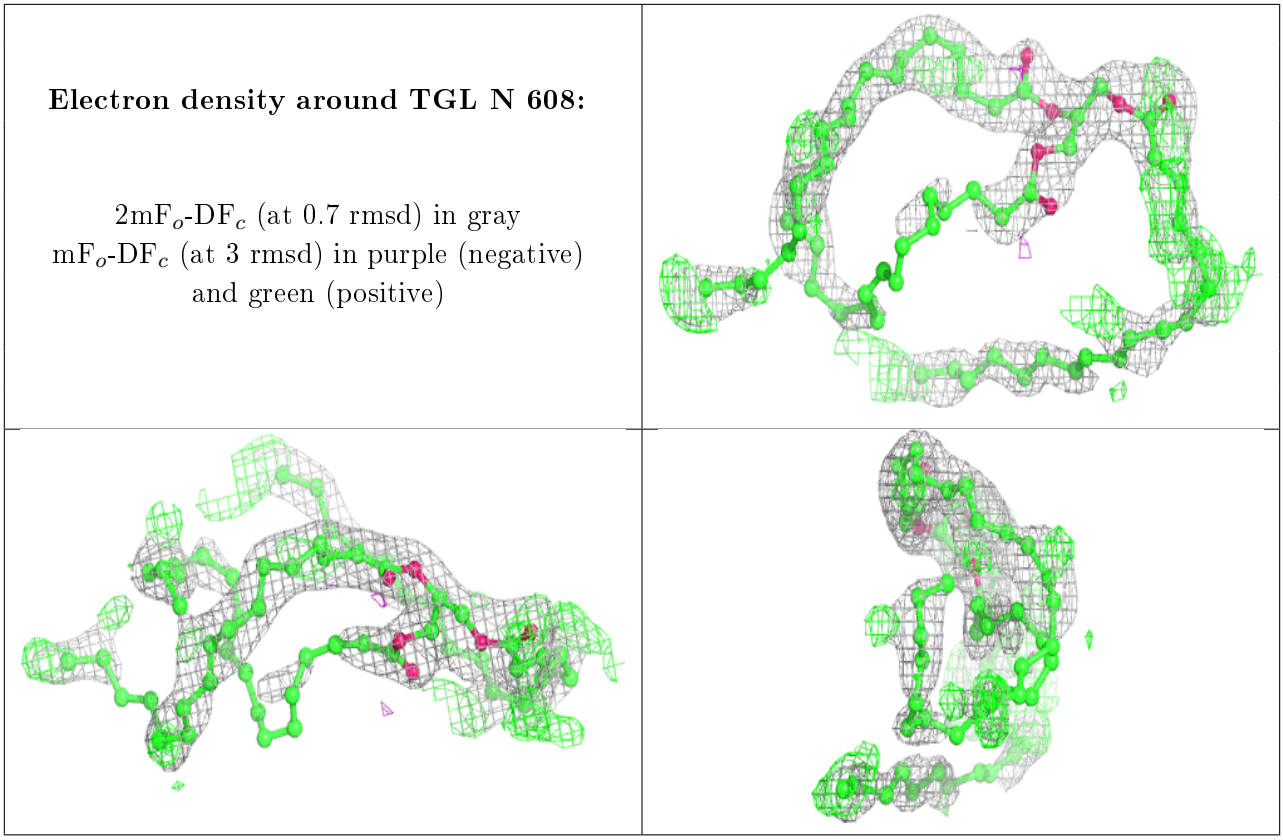
**Electron density around CDL P 304:**

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



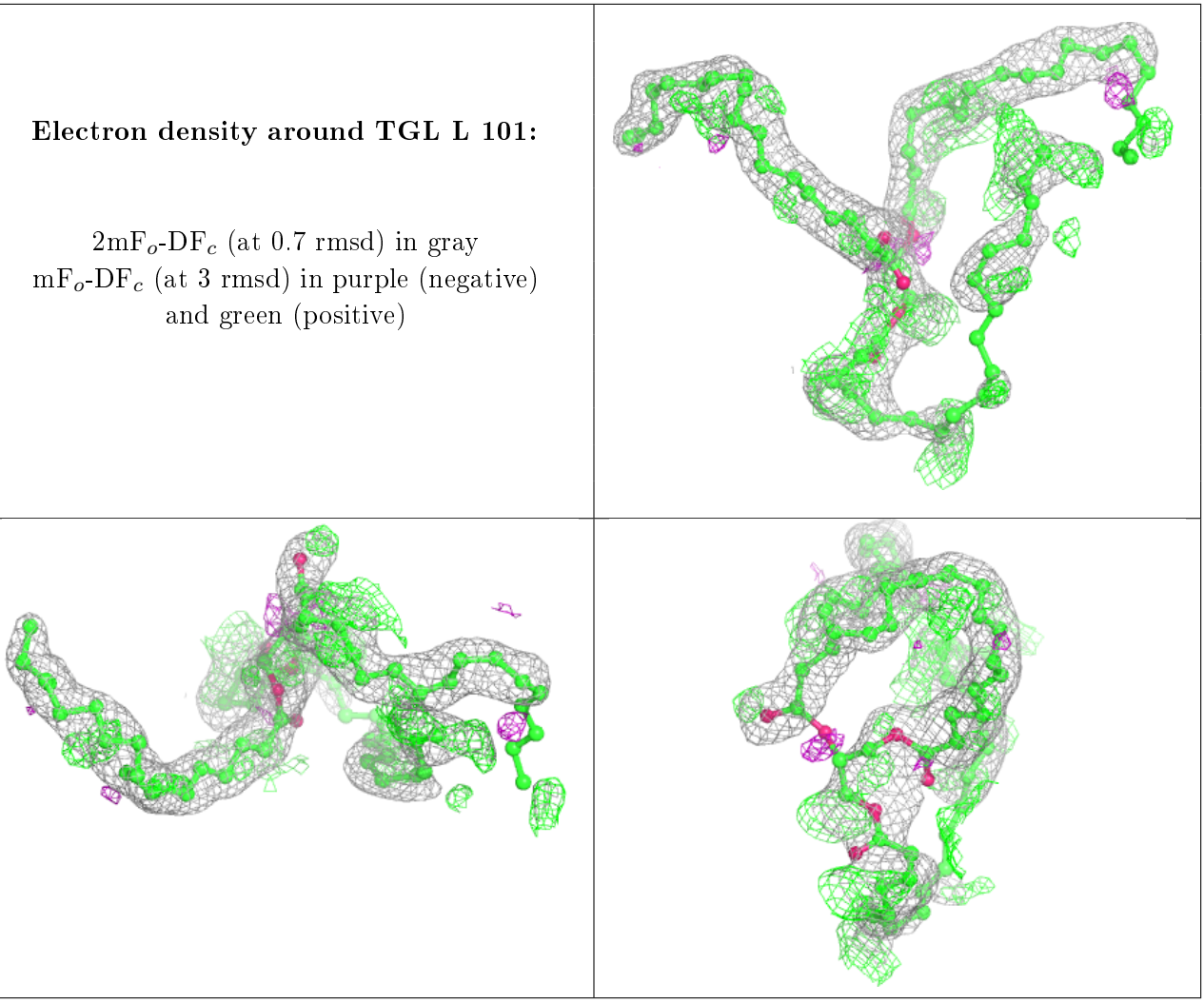
**Electron density around TGL N 608:**

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



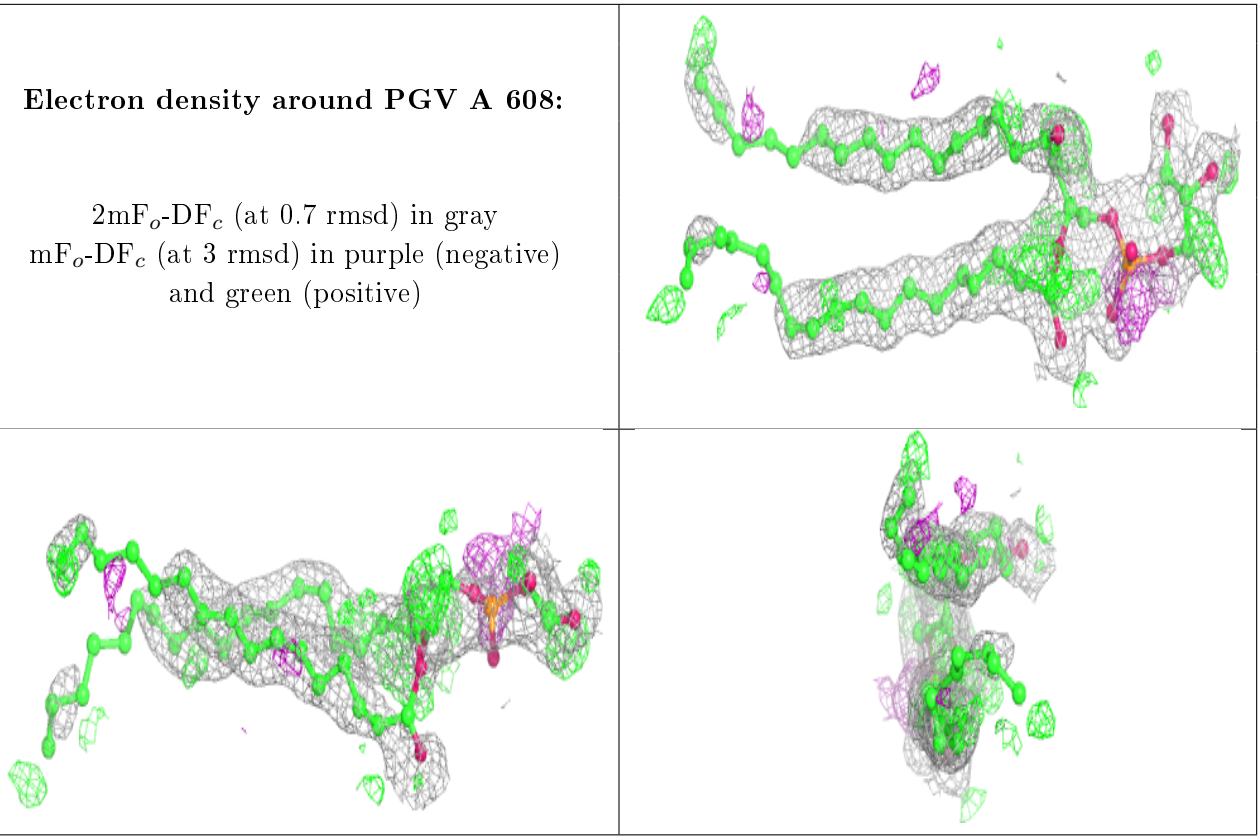
**Electron density around TGL L 101:**

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



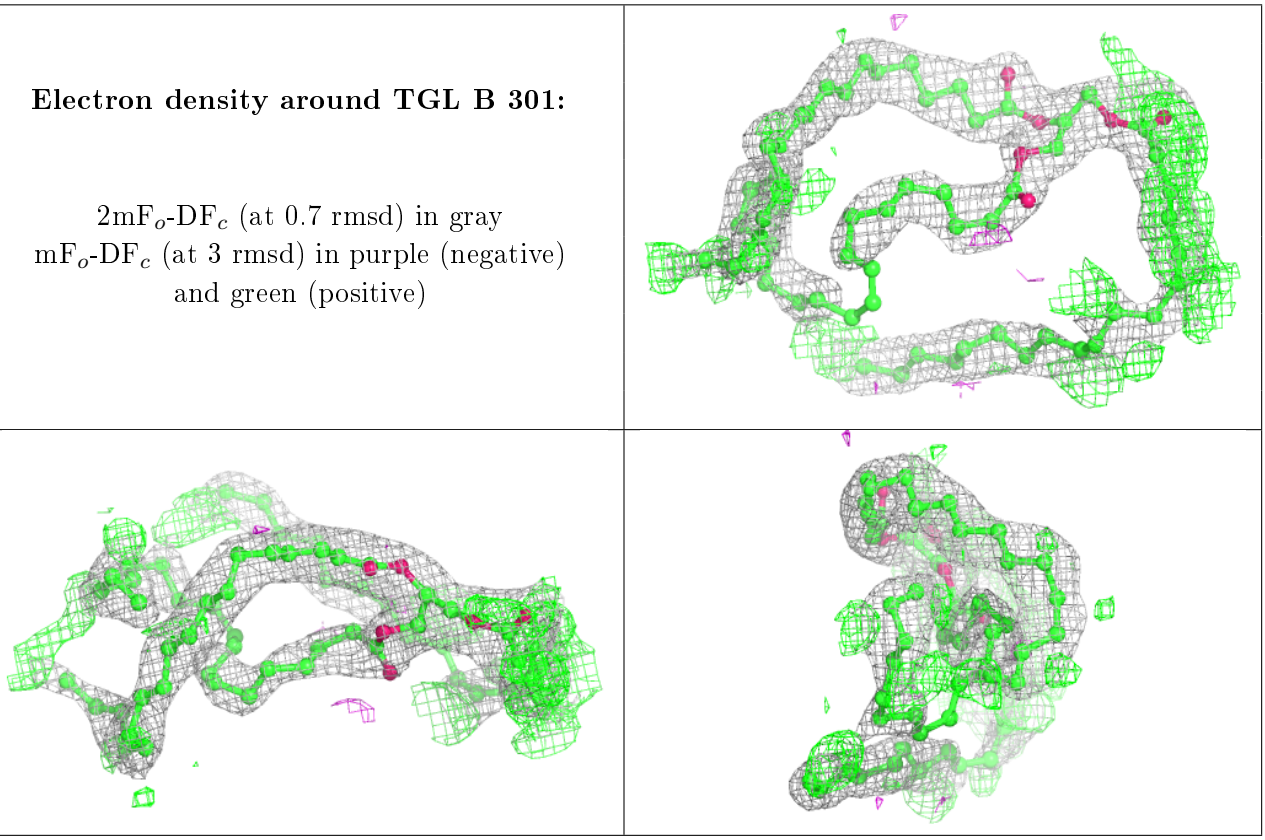
**Electron density around PGV A 608:**

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



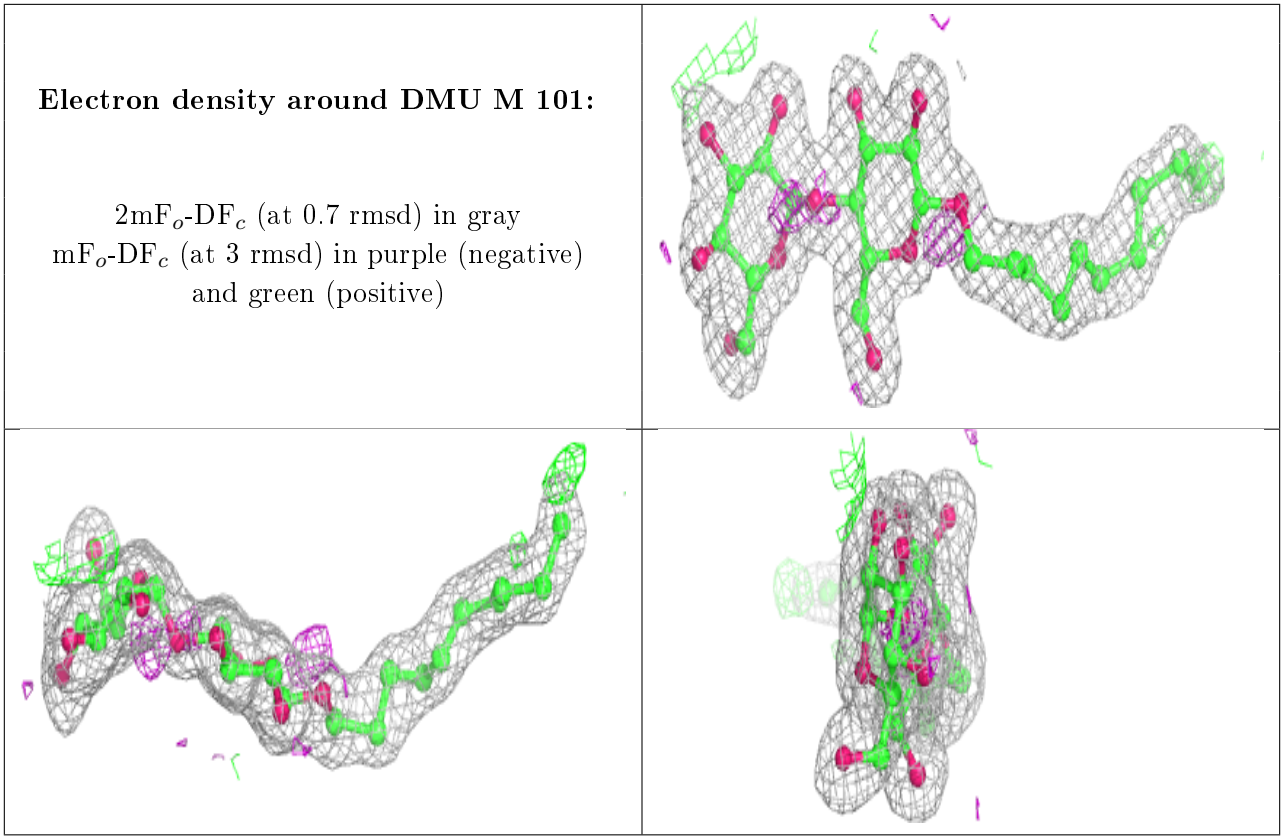
**Electron density around TGL B 301:**

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



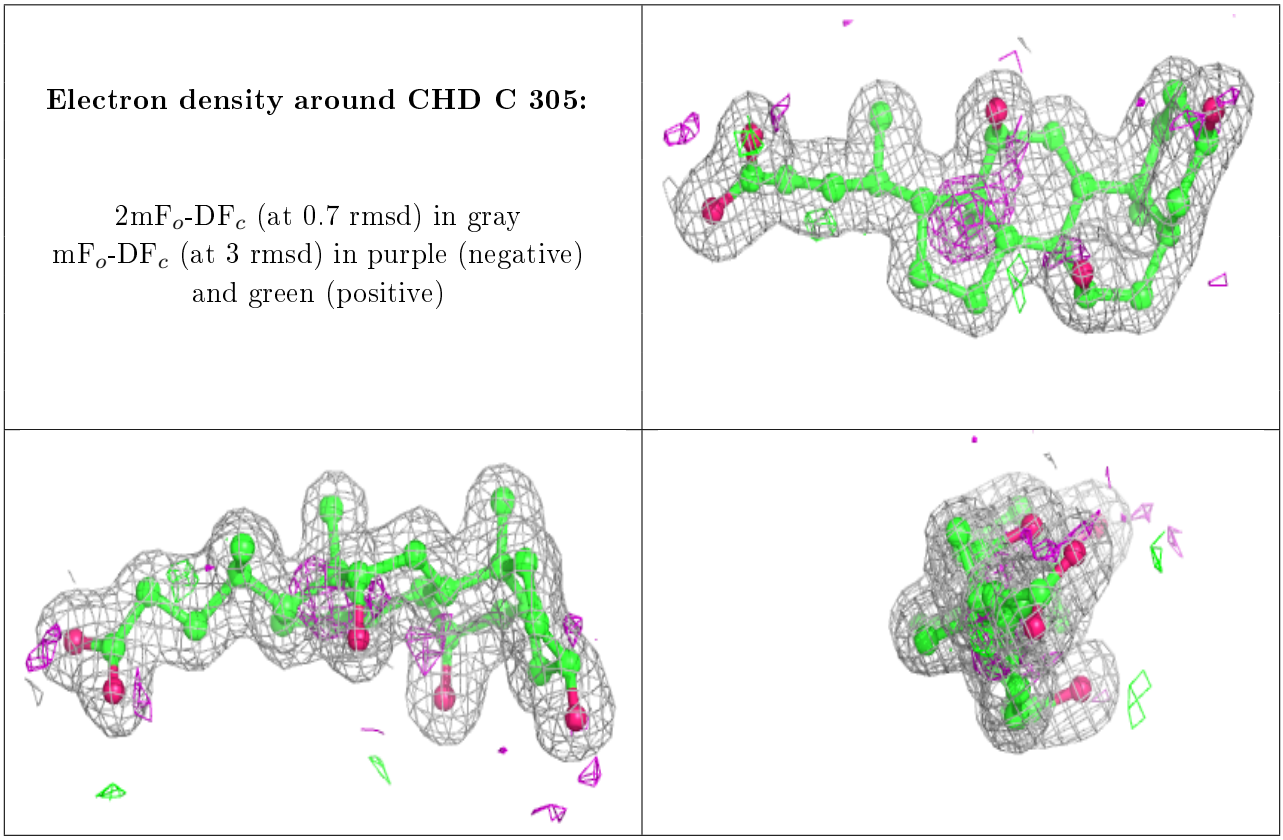
**Electron density around DMU M 101:**

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



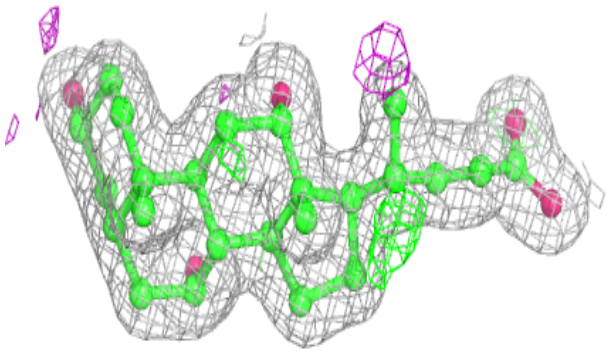
**Electron density around CHD C 305:**

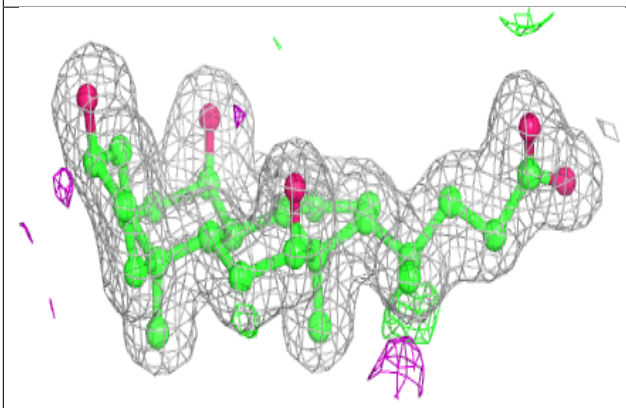
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

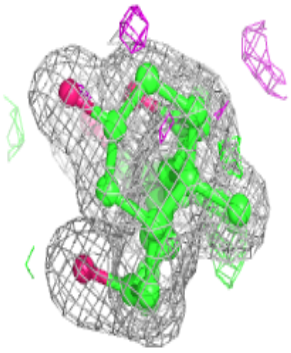


**Electron density around CHD P 307:**

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

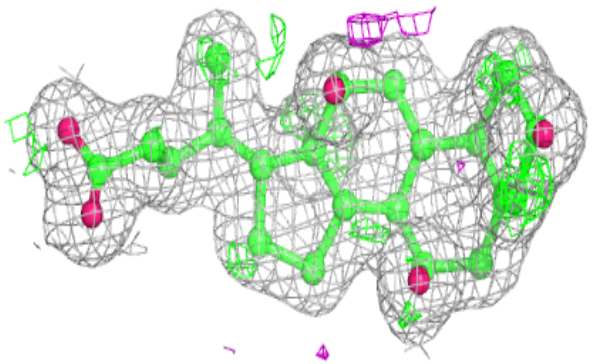


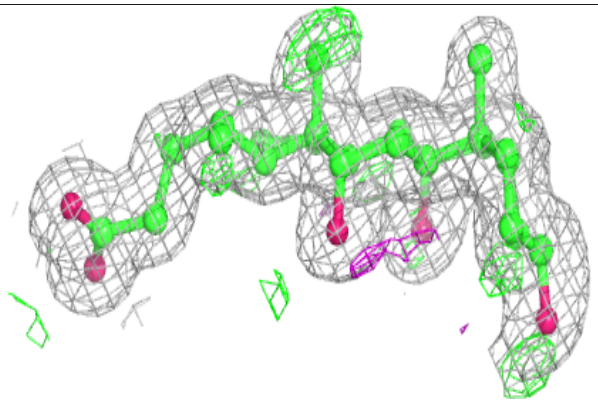


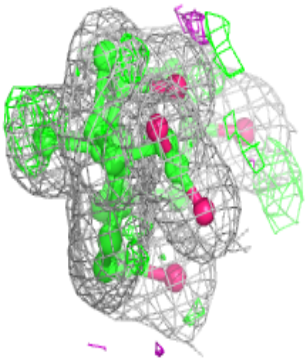


**Electron density around CHD O 302:**

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

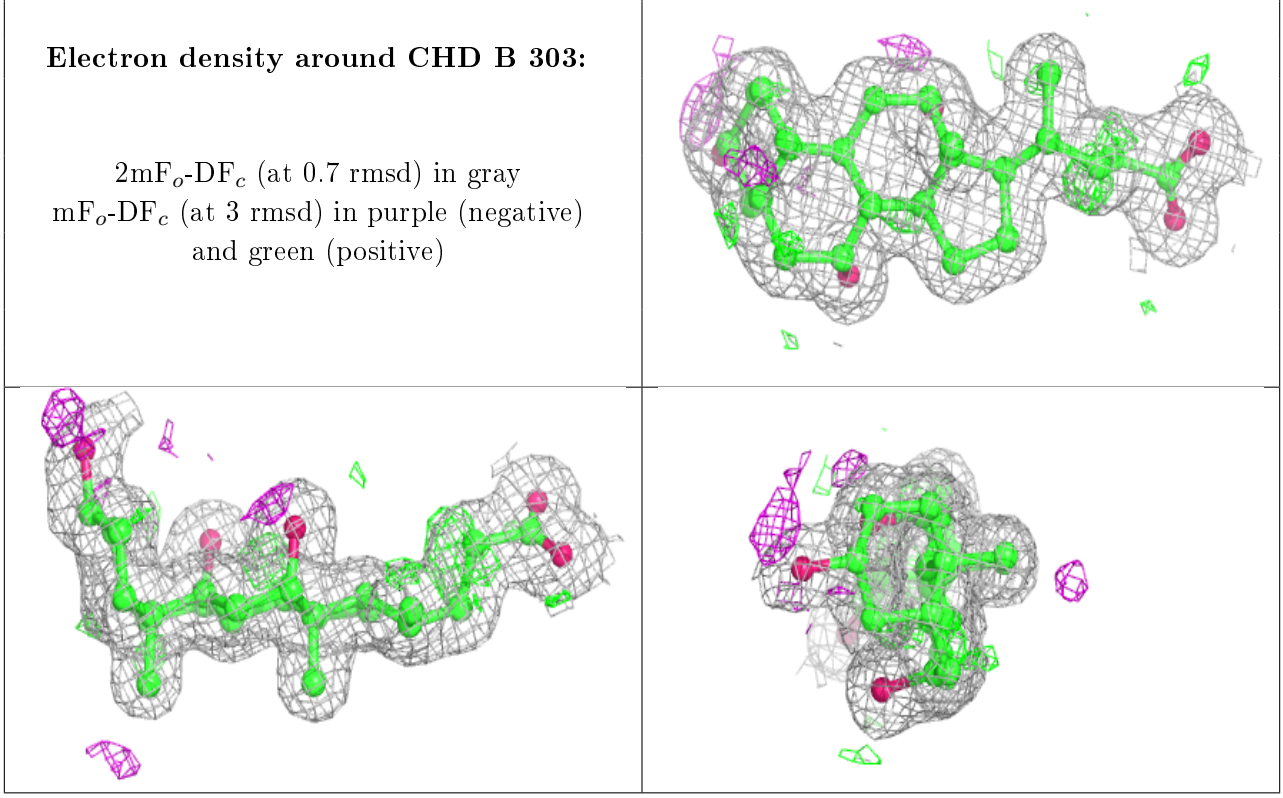






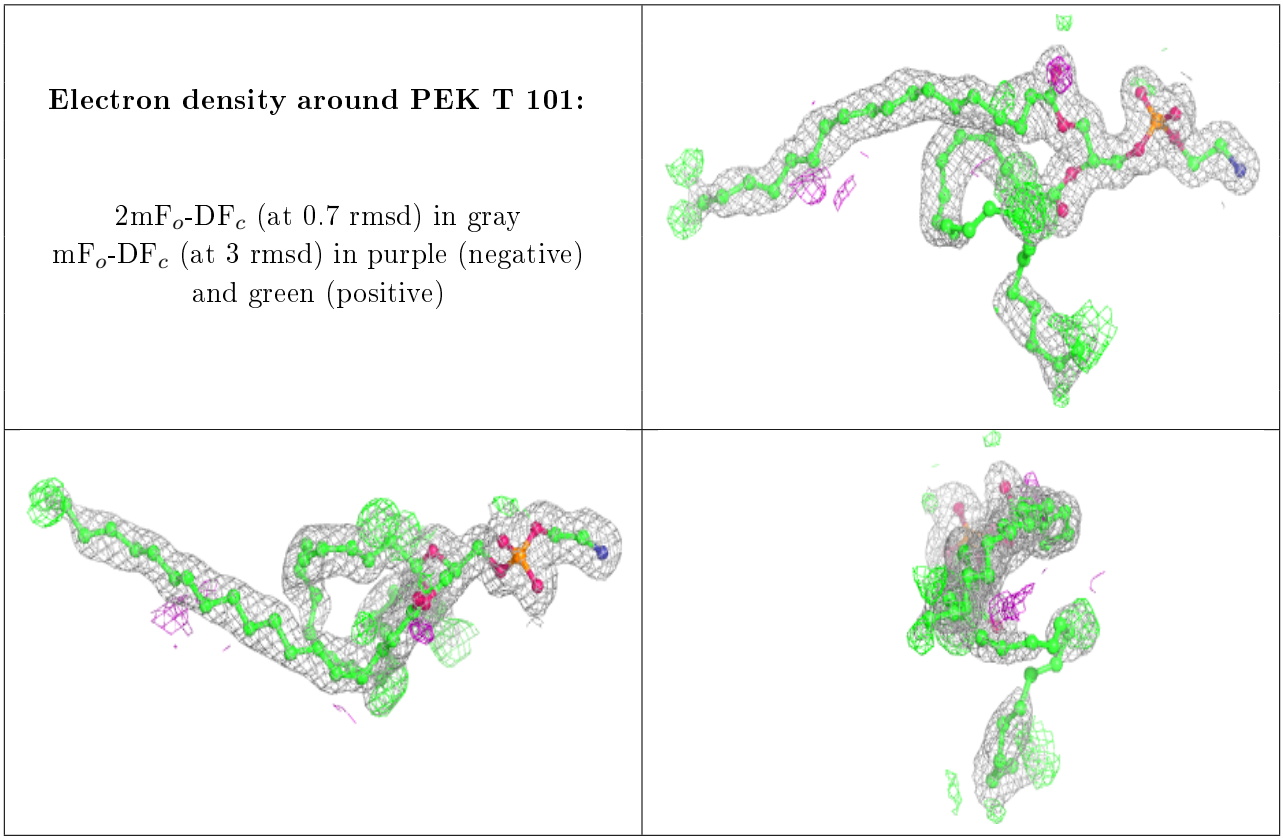
**Electron density around CHD B 303:**

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



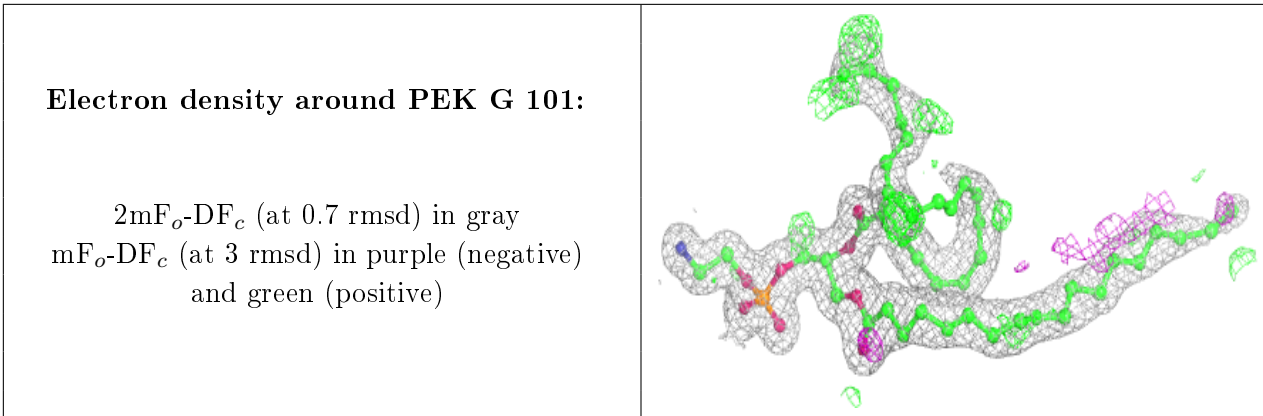
**Electron density around PEK T 101:**

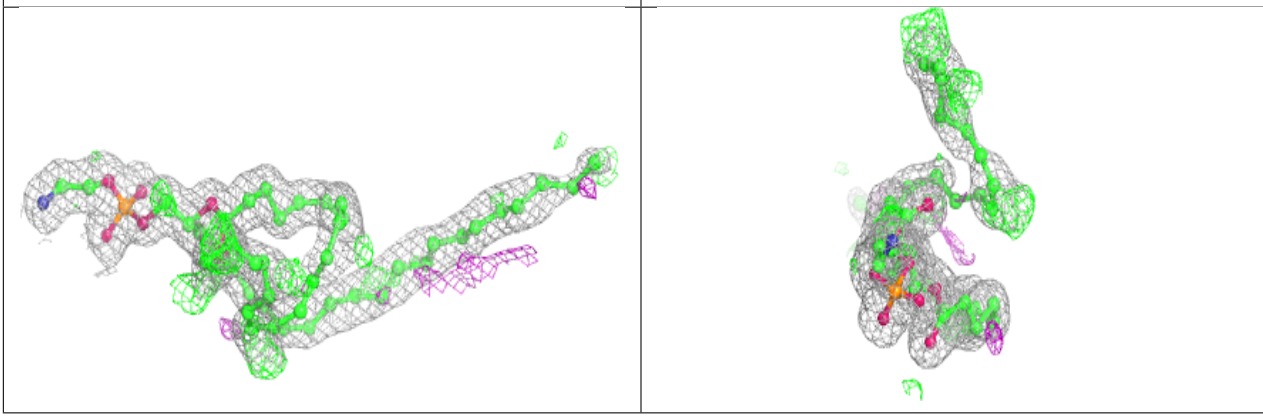
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



**Electron density around PEK G 101:**

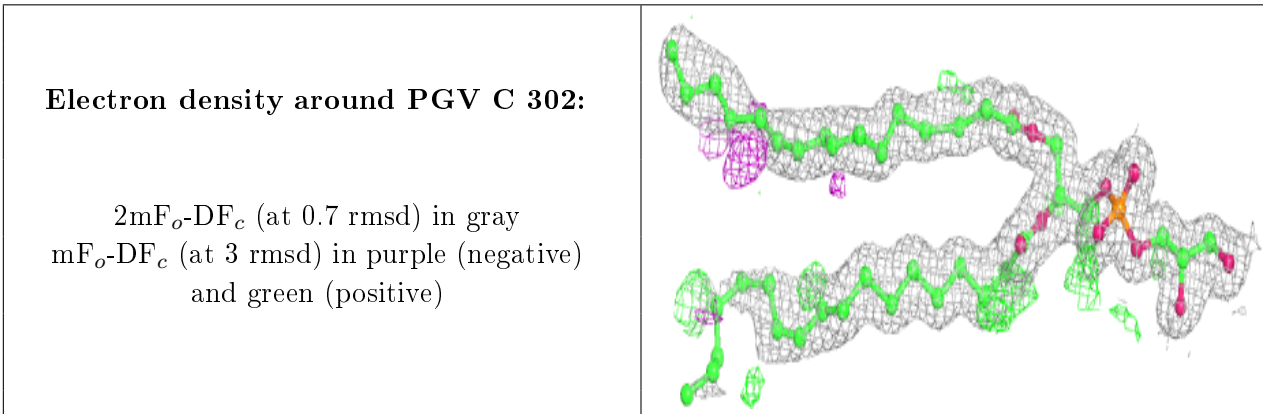
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

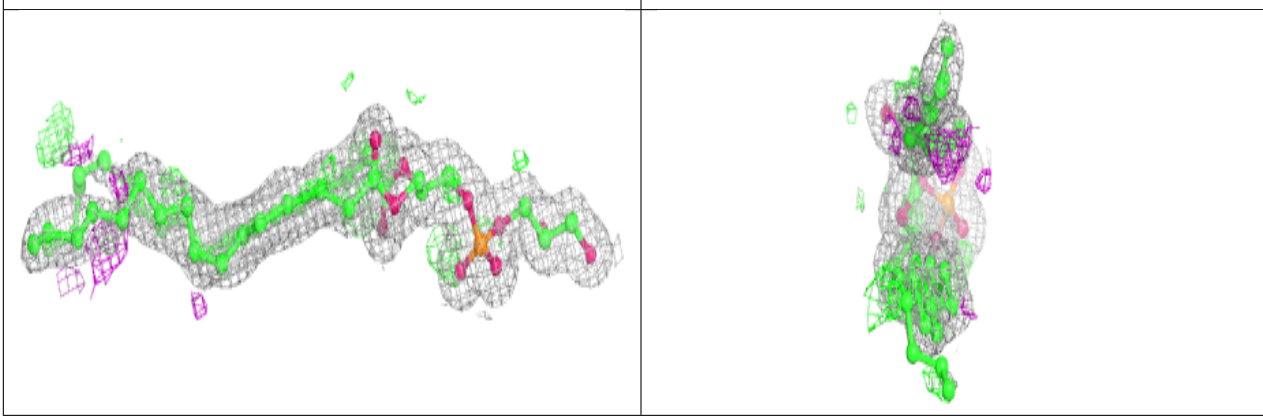




**Electron density around PGV C 302:**

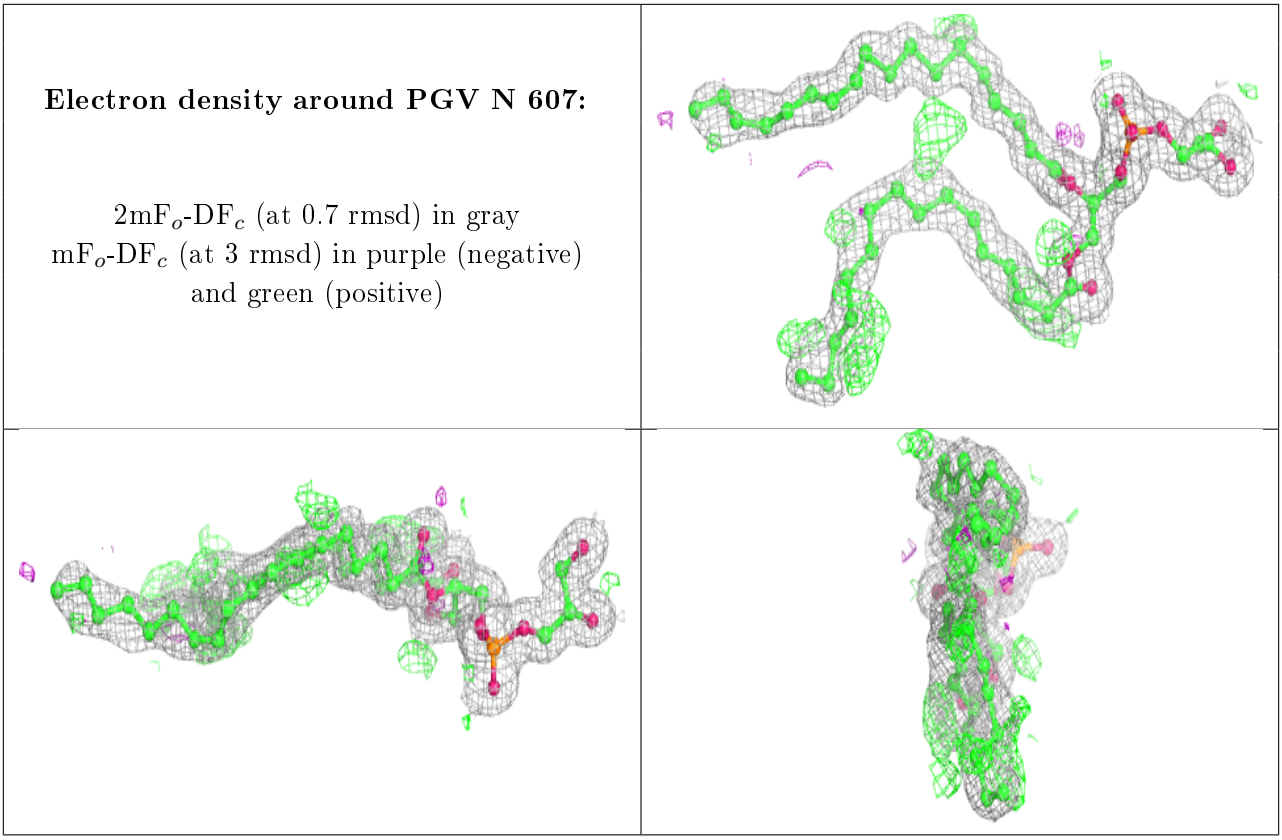
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)





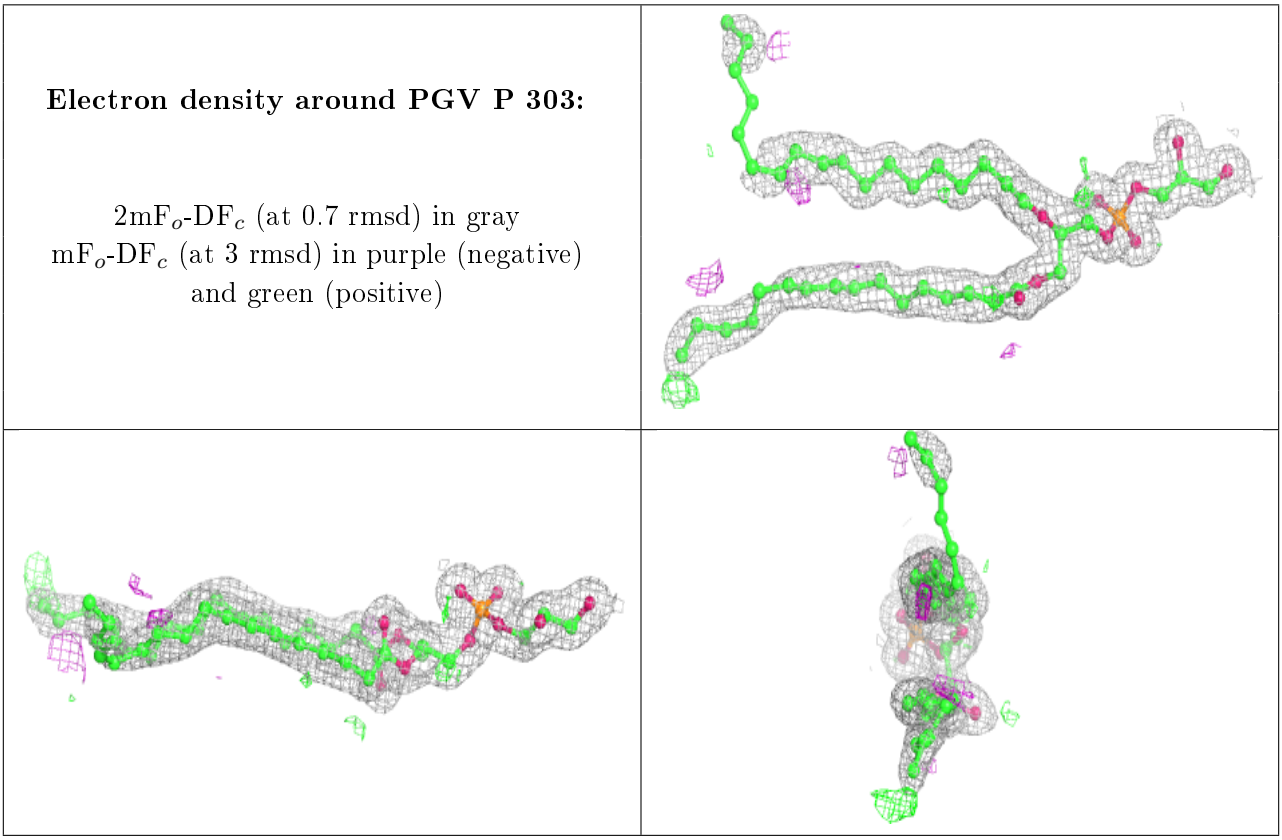
**Electron density around PGV N 607:**

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



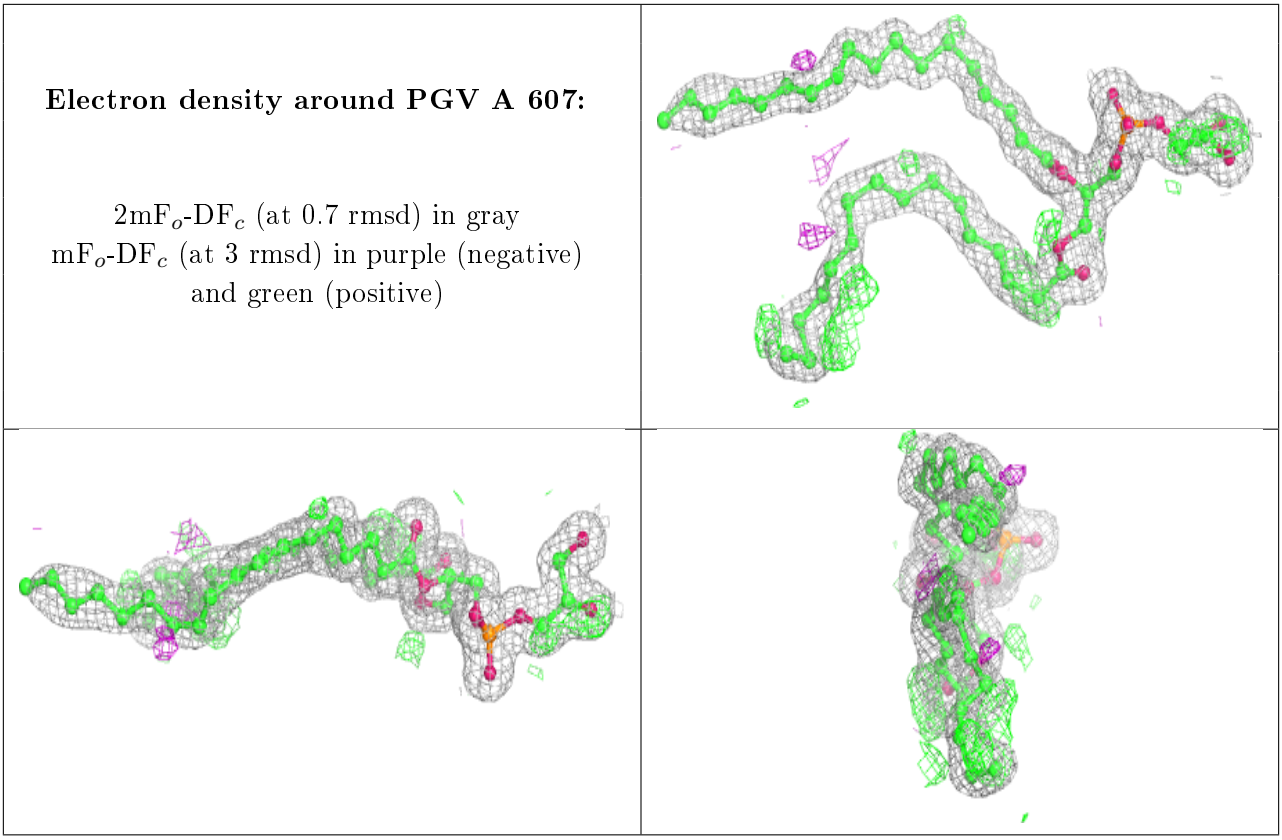
**Electron density around PGV P 303:**

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



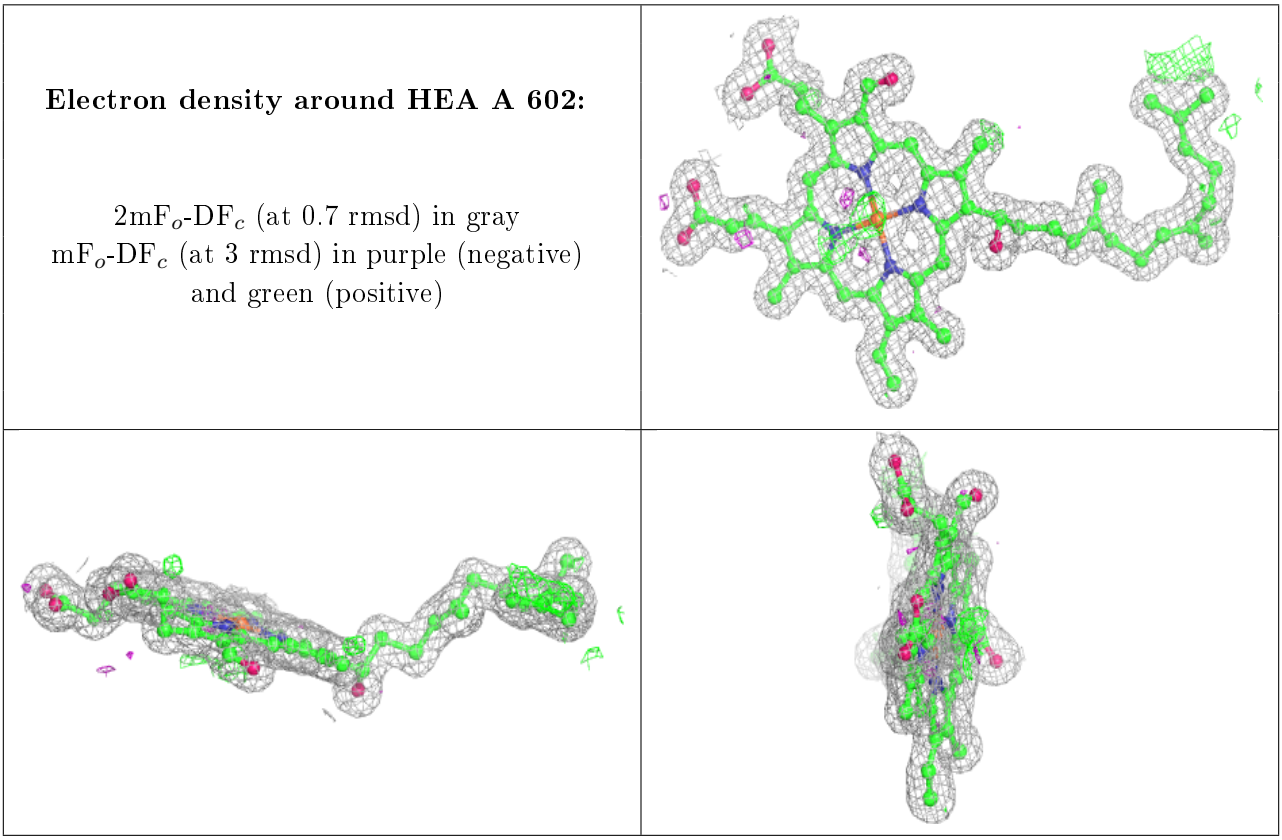
**Electron density around PGV A 607:**

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



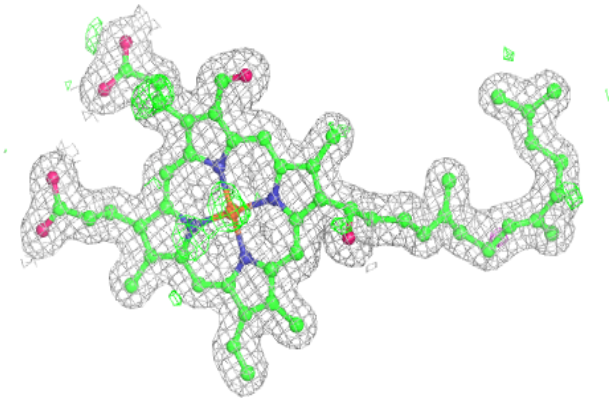
**Electron density around HEA A 602:**

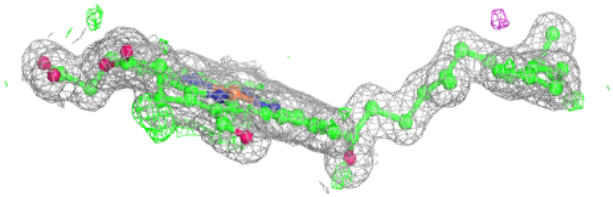
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)

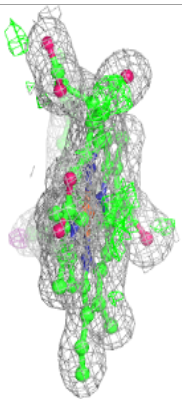


**Electron density around HEA N 602:**

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

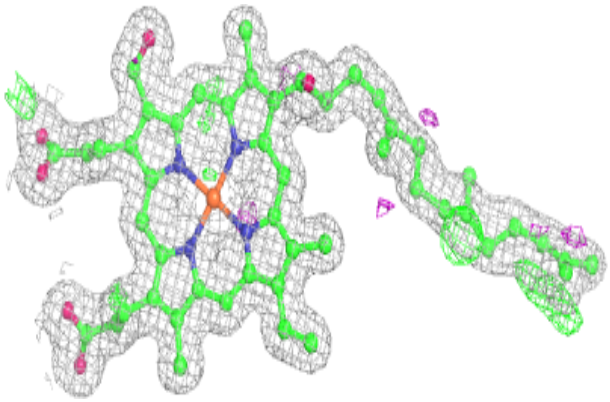


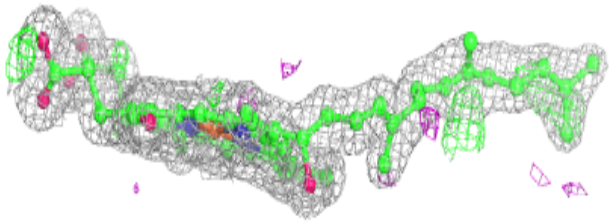


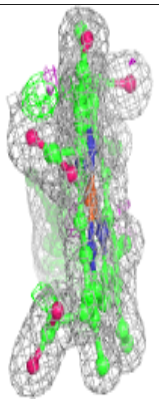


**Electron density around HEA N 601:**

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

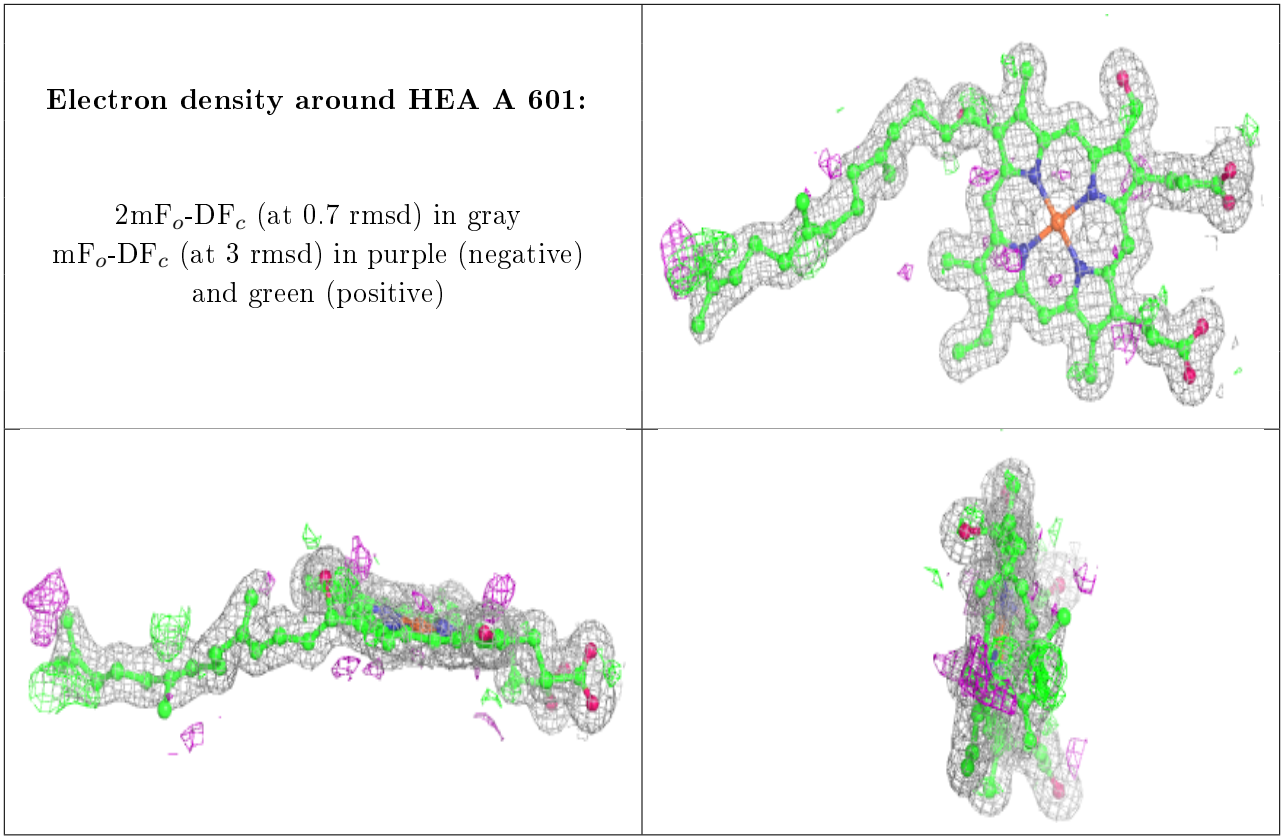






**Electron density around HEA A 601:**

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



## 6.5 Other polymers

There are no such residues in this entry.