



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:32 am GMT

PDB ID : 3ABK
Title : Bovine heart cytochrome c oxidase at the NO-bound fully reduced state (50K)
Authors : Ohta, K.; Muramoto, K.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.;
Tsukihara, T.
Deposited on : 2009-12-16
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

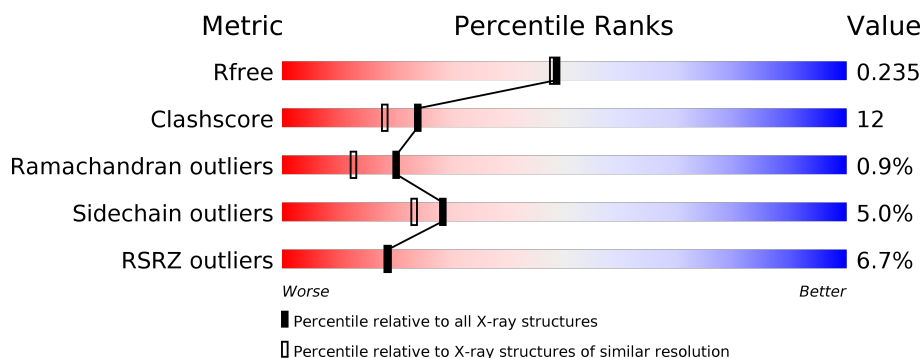
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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} | 100719 | 6609 (2.00-2.00) |
| Clashscore | 112137 | 7775 (2.00-2.00) |
| Ramachandran outliers | 110173 | 7679 (2.00-2.00) |
| Sidechain outliers | 110143 | 7678 (2.00-2.00) |
| RSRZ outliers | 101464 | 6696 (2.00-2.00) |

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 514 | <div> <div>2%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div> |
| 1 | N | 514 | <div> <div>4%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div> |
| 2 | B | 227 | <div> <div></div> <div> <div></div> <div>77%</div> <div>20%</div> <div>••</div> </div> </div> |
| 2 | O | 227 | <div> <div>2%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>5%</div> </div> </div> |
| 3 | C | 261 | <div> <div>%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>•••</div> </div> </div> |
| 3 | P | 261 | <div> <div>5%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>••</div> </div> </div> |

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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 | 515 | X | - | - | - |
| 14 | HEA | A | 516 | X | - | - | - |
| 14 | HEA | N | 515 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14 | HEA | N | 516 | X | - | - | - |
| 17 | MG | A | 518 | - | - | - | X |
| 17 | MG | N | 518 | - | - | - | X |
| 19 | PGV | A | 524 | - | - | - | X |
| 19 | PGV | C | 268 | - | - | - | X |
| 19 | PGV | N | 1524 | - | - | - | X |
| 19 | PGV | U | 1268 | - | - | - | X |
| 21 | TGL | B | 521 | - | - | - | X |
| 21 | TGL | D | 523 | - | - | - | X |
| 21 | TGL | L | 522 | - | - | - | X |
| 21 | TGL | N | 1523 | - | - | - | X |
| 21 | TGL | O | 1521 | - | - | - | X |
| 21 | TGL | Y | 1522 | - | - | - | X |
| 22 | PSC | B | 229 | - | - | - | X |
| 22 | PSC | R | 1229 | - | - | - | X |
| 23 | CHD | C | 271 | X | - | - | - |
| 23 | CHD | J | 60 | X | - | - | X |
| 23 | CHD | P | 1271 | X | - | - | X |
| 23 | CHD | P | 1525 | X | - | - | - |
| 23 | CHD | W | 1059 | X | - | - | X |
| 25 | PEK | G | 1263 | - | - | - | X |
| 25 | PEK | T | 263 | - | - | - | X |
| 26 | CDL | C | 270 | - | - | - | X |
| 26 | CDL | G | 269 | - | - | X | X |
| 26 | CDL | P | 1270 | - | - | X | X |
| 26 | CDL | T | 1269 | - | - | X | X |
| 27 | DMU | C | 272 | X | - | - | X |
| 27 | DMU | M | 526 | X | - | - | - |
| 27 | DMU | P | 272 | X | - | - | X |
| 27 | DMU | Z | 1526 | X | - | - | - |

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32382 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 | 5 | 0 |
| | | | 4060 | 2712 | 628 | 684 | 36 | | | |
| 1 | N | 514 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 4060 | 2712 | 628 | 684 | 36 | | | |

- 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 | 0 | 0 |
| | | | 1824 | 1185 | 281 | 340 | 18 | | | |
| 2 | O | 227 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1185 | 281 | 340 | 18 | | | |

- 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 | 0 | 0 |
| | | | 2110 | 1412 | 336 | 350 | 12 | | | |
| 3 | P | 259 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2110 | 1412 | 336 | 350 | 12 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | D | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1195 | 777 | 196 | 218 | 4 | | | |
| 4 | Q | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1195 | 777 | 196 | 218 | 4 | | | |

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

| 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 | 0 | 0 |
| | | | 852 | 544 | 144 | 162 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 748 | 464 | 134 | 145 | 5 | | | |
| 6 | S | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 748 | 464 | 134 | 145 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|--------|---------|---------|-------|
| 7 | G | 84 | Total 675 | C 431 | N 129 | O 113 | P 1 | S 1 | 0 | 0 | 0 |
| 7 | T | 84 | Total 675 | C 431 | N 129 | O 113 | P 1 | S 1 | 0 | 0 | 0 |

- 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 polypeptide 7A1.

| 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 | 0 | 0 |
| | | | 460 | 297 | 78 | 82 | 3 | | | |

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

| 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 | 0 | 0 |
| | | | 384 | 250 | 65 | 67 | 2 | | | |

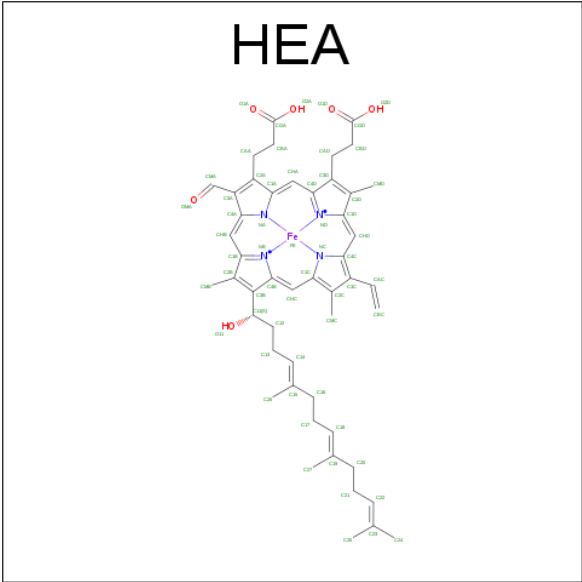
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

| 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 | 0 | 0 |
| | | | 380 | 254 | 64 | 60 | 2 | | | |

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

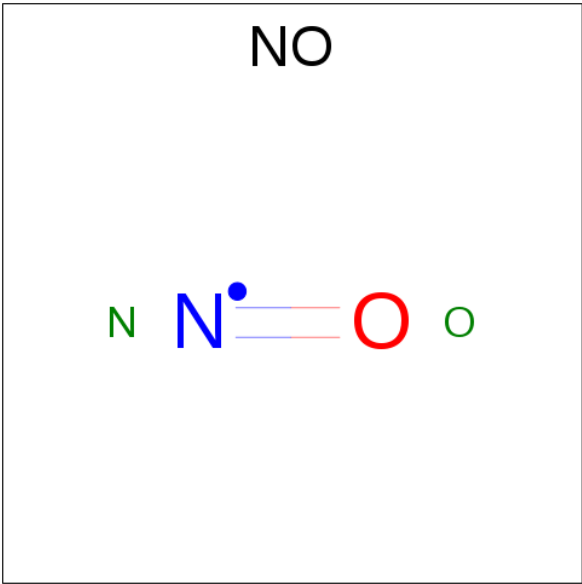
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 13 | M | 43 | Total | C | N | O | 0 | 0 | 0 |
| | | | 335 | 223 | 53 | 59 | | | |
| 13 | Z | 43 | Total | C | N | O | 0 | 0 | 0 |
| | | | 335 | 223 | 53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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 15 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 15 | A | 1 | Total N O 2 1 1 | 0 | 0 |
| 15 | N | 1 | Total N O 2 1 1 | 0 | 0 |

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

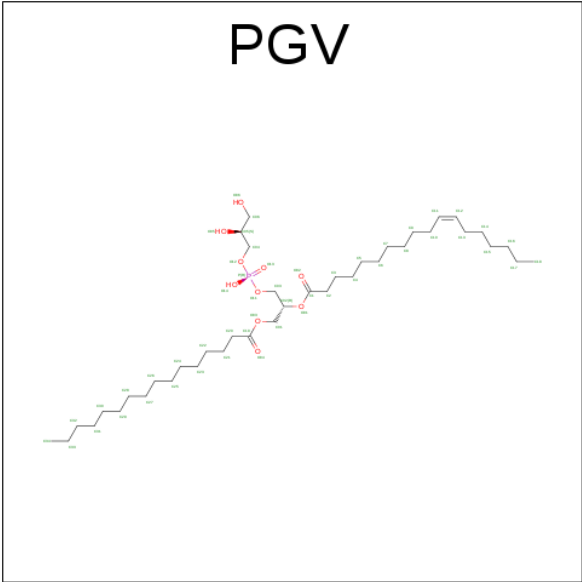
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 17 | A | 1 | Total Mg 1 1 | 0 | 0 |
| 17 | N | 1 | Total Mg 1 1 | 0 | 0 |

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

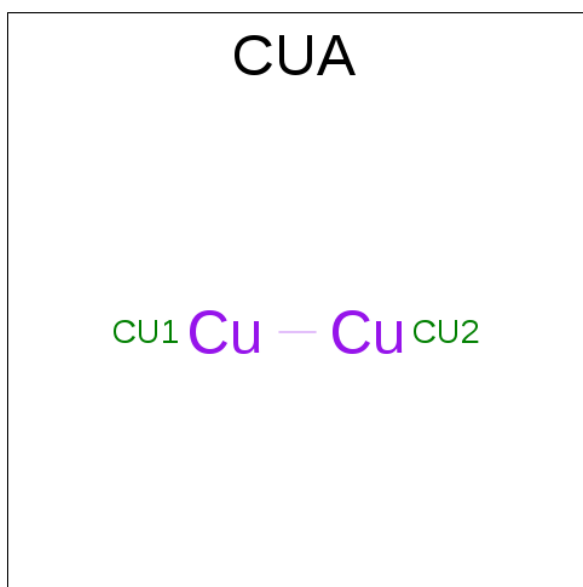
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 18 | A | 1 | Total Na 1 1 | 0 | 0 |
| 18 | N | 1 | Total Na 1 1 | 0 | 0 |

- 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: C₄₀H₇₇O₁₀P).



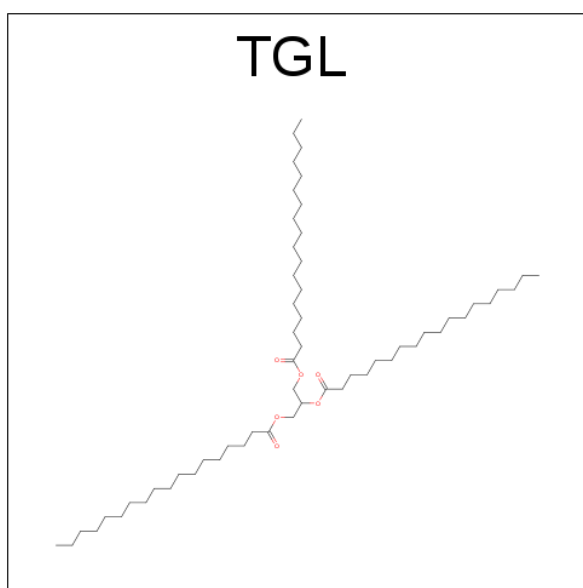
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | C | 1 | Total |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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 20 | B | 1 | Total | Cu | 0 | 0 |
| | | | 2 | 2 | | |
| 20 | O | 1 | Total | Cu | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



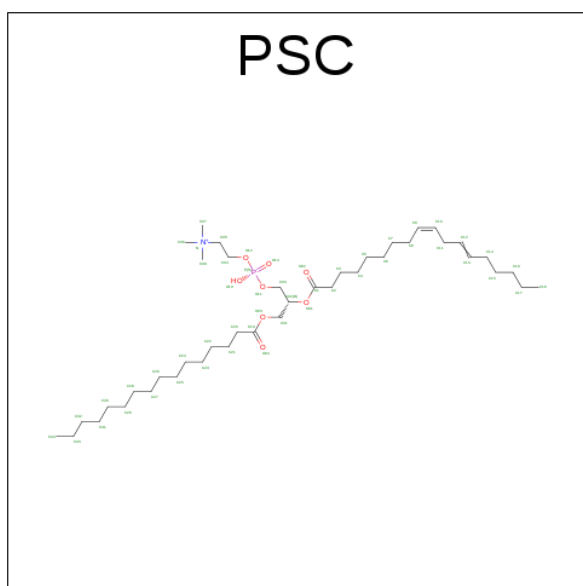
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21 | B | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 21 | D | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |

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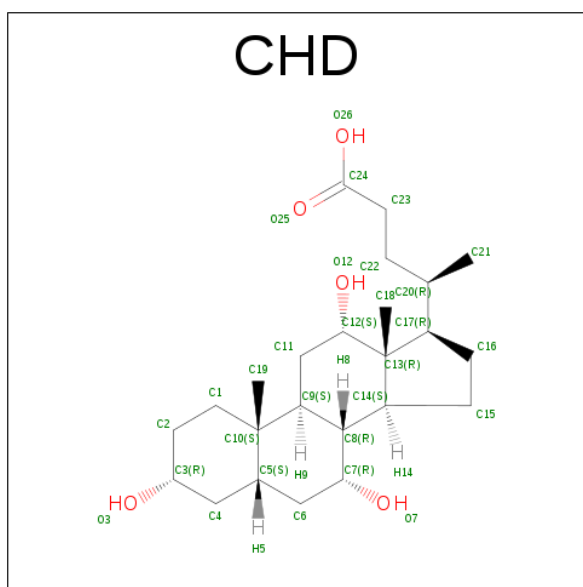
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21 | L | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 21 | N | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 21 | O | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 21 | Y | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |

- Molecule 22 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 |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 22 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |
| 22 | R | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).

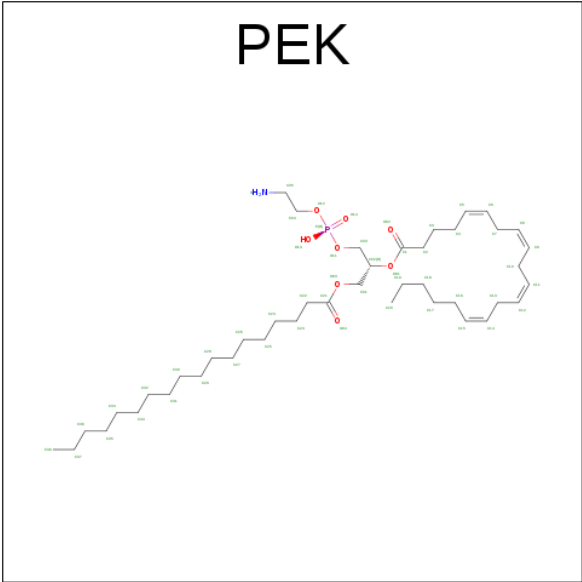


| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 23 | B | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | C | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | C | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | J | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | O | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | P | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | P | 1 | Total C O 29 24 5 | 0 | 0 |
| 23 | W | 1 | Total C O 29 24 5 | 0 | 0 |

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

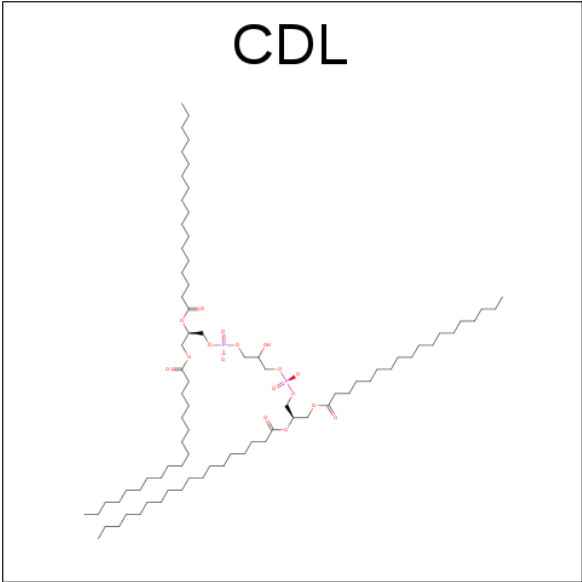
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 24 | P | 1 | Total X 1 1 | 0 | 0 |
| 24 | C | 1 | Total X 1 1 | 0 | 0 |

- Molecule 25 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: C₄₃H₇₈NO₈P).



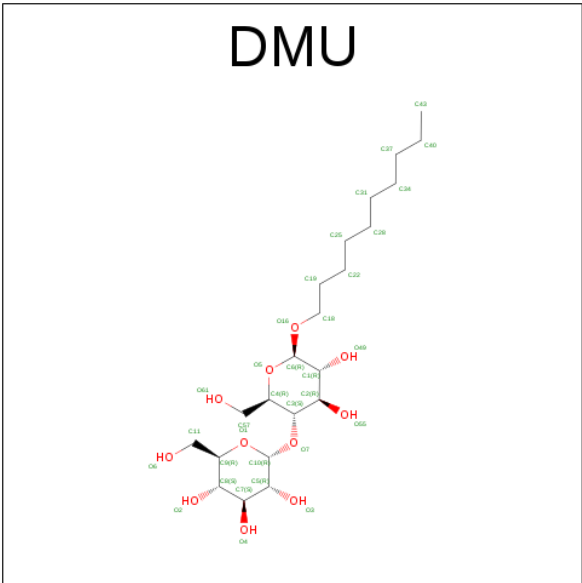
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 25 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 25 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 25 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 25 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 25 | T | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 25 | T | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 26 | C | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 26 | G | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 26 | P | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 26 | T | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |

- Molecule 27 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 27 | C | 1 | Total C O 33 22 11 | 0 | 0 |
| 27 | M | 1 | Total C O 33 22 11 | 0 | 0 |
| 27 | P | 1 | Total C O 33 22 11 | 0 | 0 |
| 27 | Z | 1 | Total C O 33 22 11 | 0 | 0 |

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 28 | S | 1 | Total Zn 1 1 | 0 | 0 |
| 28 | F | 1 | Total Zn 1 1 | 0 | 0 |

- Molecule 29 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 29 | A | 217 | Total O 217 217 | 0 | 0 |
| 29 | B | 127 | Total O 127 127 | 0 | 0 |
| 29 | C | 93 | Total O 93 93 | 0 | 0 |
| 29 | D | 86 | Total O 86 86 | 0 | 0 |
| 29 | E | 52 | Total O 52 52 | 0 | 0 |
| 29 | F | 72 | Total O 72 72 | 0 | 0 |
| 29 | G | 42 | Total O 42 42 | 0 | 0 |
| 29 | H | 46 | Total O 46 46 | 0 | 0 |
| 29 | I | 31 | Total O 31 31 | 0 | 0 |
| 29 | J | 28 | Total O 28 28 | 0 | 0 |
| 29 | K | 27 | Total O 27 27 | 0 | 0 |
| 29 | L | 16 | Total O 16 16 | 0 | 0 |

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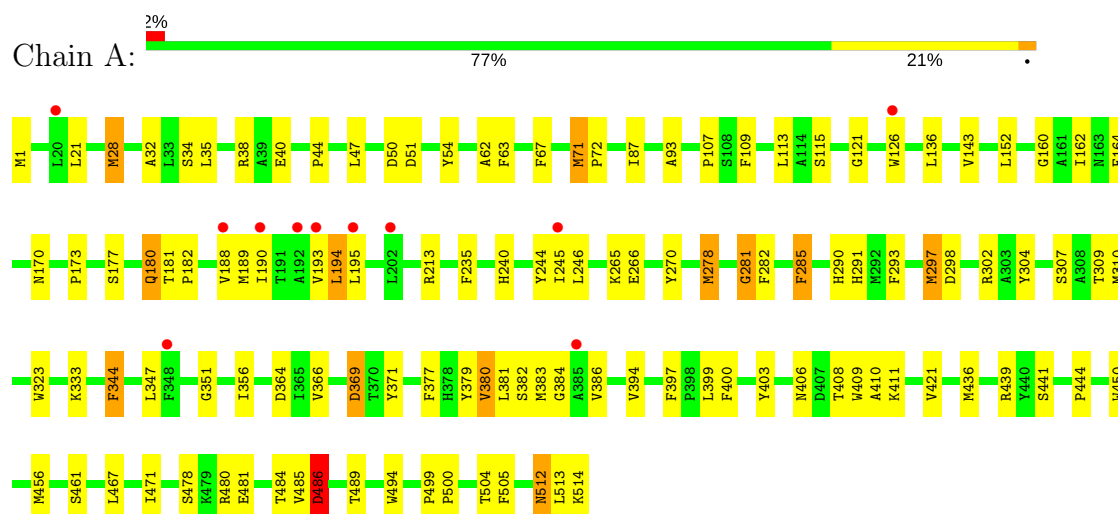
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 29 | M | 20 | Total 20 | O 20 | 0 | 0 |
| 29 | N | 207 | Total 207 | O 207 | 0 | 0 |
| 29 | O | 105 | Total 105 | O 105 | 0 | 0 |
| 29 | P | 96 | Total 96 | O 96 | 0 | 0 |
| 29 | Q | 57 | Total 57 | O 57 | 0 | 0 |
| 29 | R | 35 | Total 35 | O 35 | 0 | 0 |
| 29 | S | 63 | Total 63 | O 63 | 0 | 0 |
| 29 | T | 44 | Total 44 | O 44 | 0 | 0 |
| 29 | U | 43 | Total 43 | O 43 | 0 | 0 |
| 29 | V | 20 | Total 20 | O 20 | 0 | 0 |
| 29 | W | 17 | Total 17 | O 17 | 0 | 0 |
| 29 | X | 13 | Total 13 | O 13 | 0 | 0 |
| 29 | Y | 12 | Total 12 | O 12 | 0 | 0 |
| 29 | Z | 11 | Total 11 | O 11 | 0 | 0 |

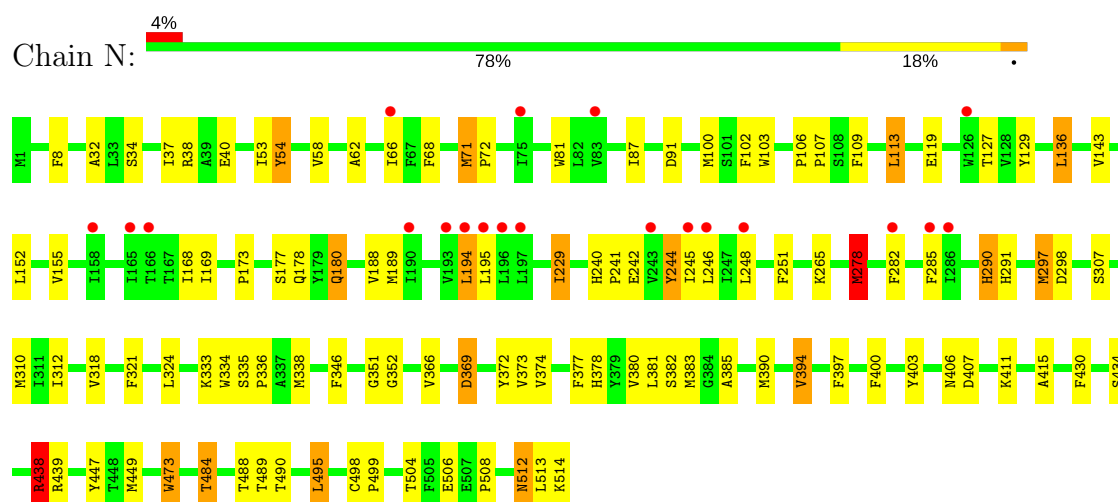
3 Residue-property plots

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.

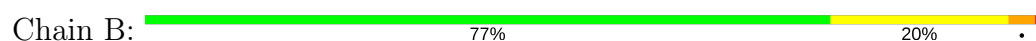
• Molecule 1: Cytochrome c oxidase subunit 1

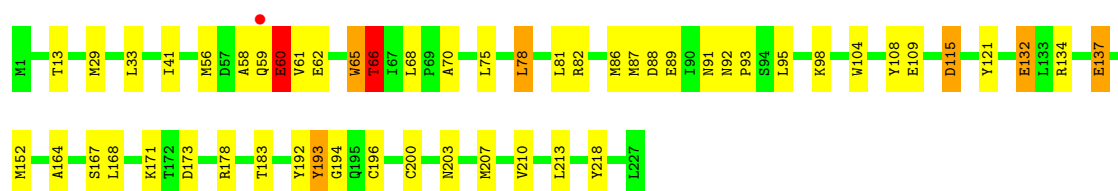


• Molecule 1: Cytochrome c oxidase subunit 1

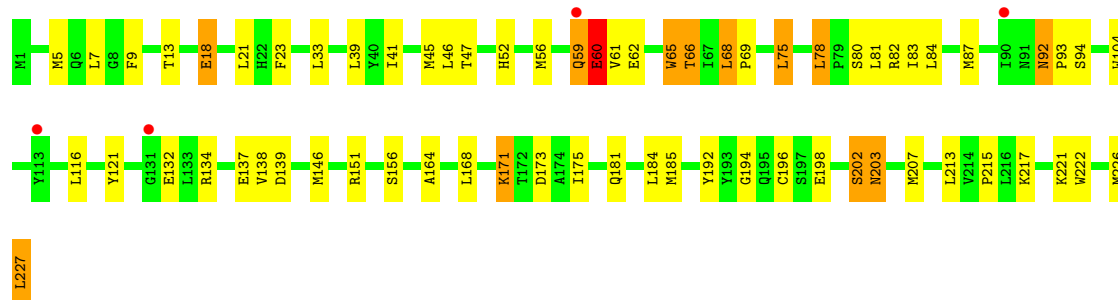


• Molecule 2: Cytochrome c oxidase subunit 2

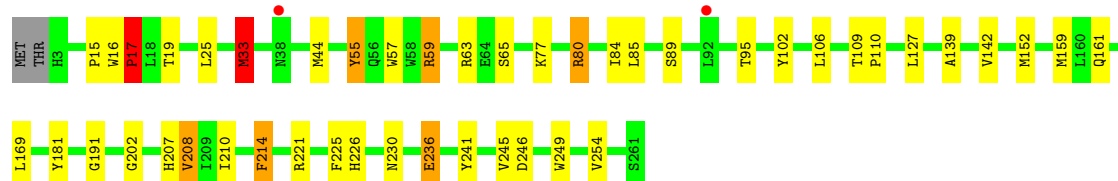
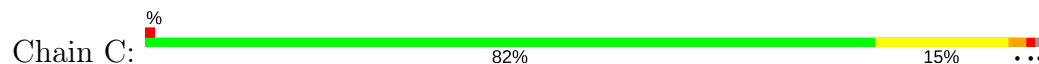




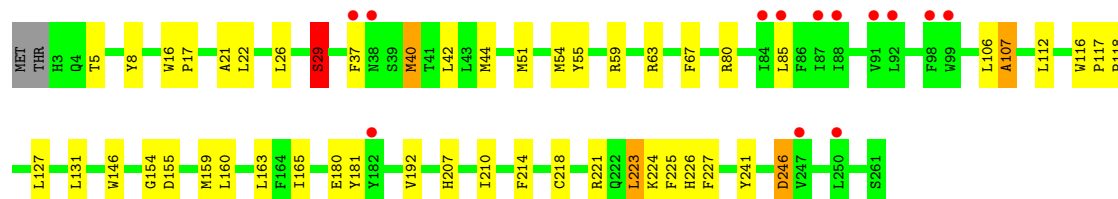
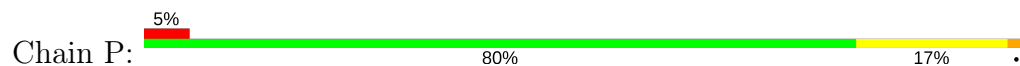
• Molecule 2: Cytochrome c oxidase subunit 2



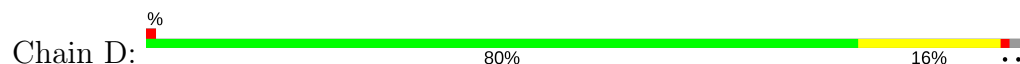
• Molecule 3: Cytochrome c oxidase subunit 3



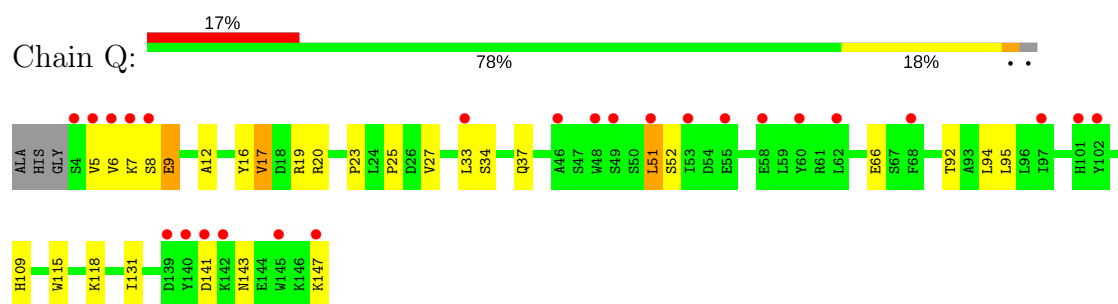
• Molecule 3: Cytochrome c oxidase subunit 3



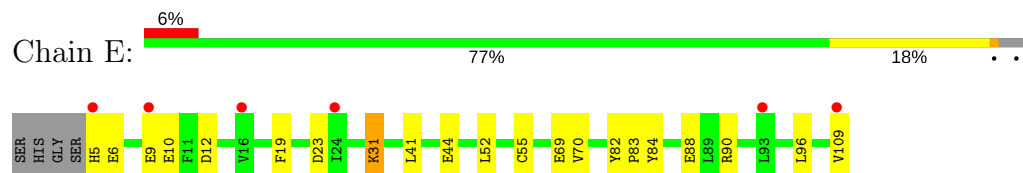
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



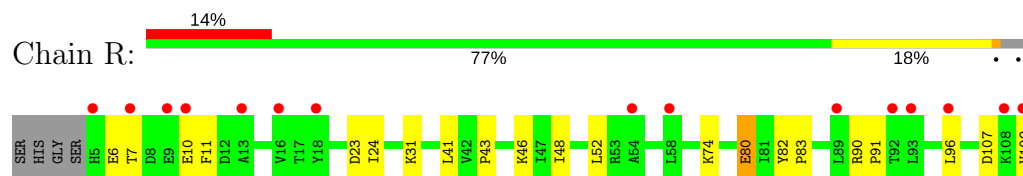
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



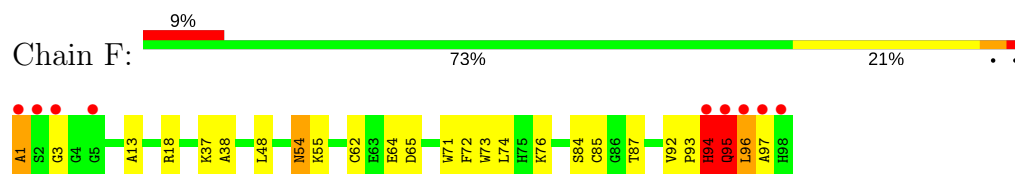
- Molecule 5: Cytochrome c oxidase subunit 5A



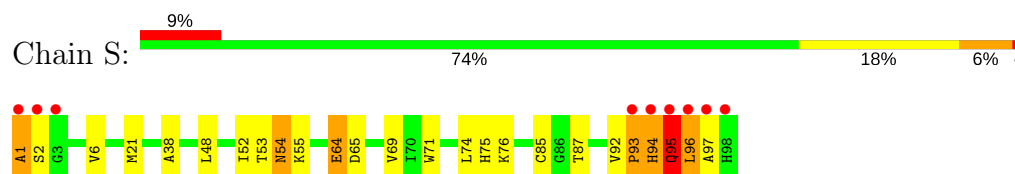
- Molecule 5: Cytochrome c oxidase subunit 5A



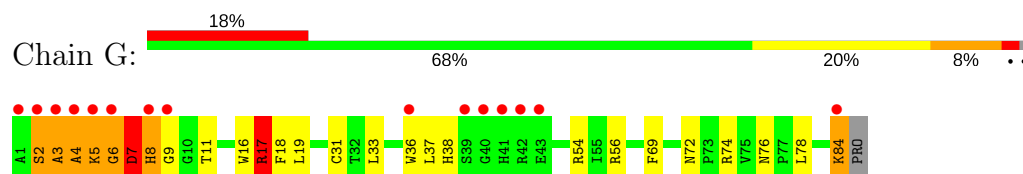
- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B

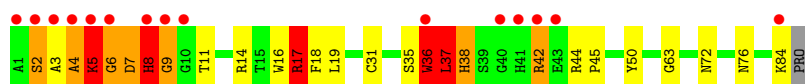


- Molecule 7: Cytochrome c oxidase subunit 6A2

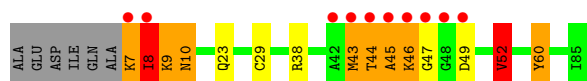
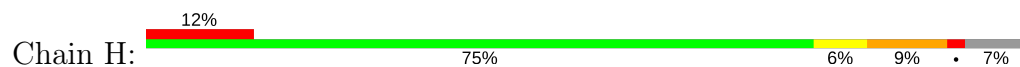


- Molecule 7: Cytochrome c oxidase subunit 6A2





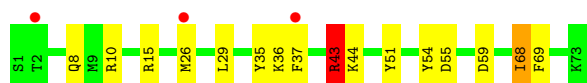
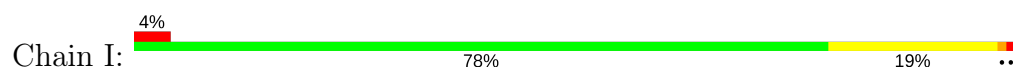
- Molecule 8: Cytochrome c oxidase subunit 6B1



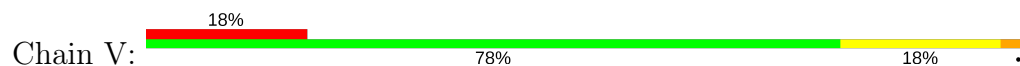
- Molecule 8: Cytochrome c oxidase subunit 6B1



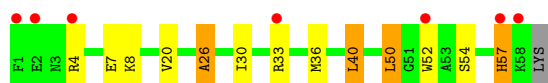
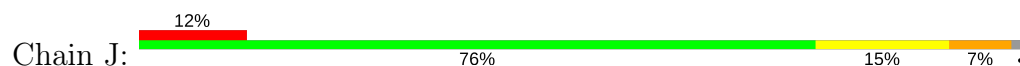
- Molecule 9: Cytochrome c oxidase subunit 6C



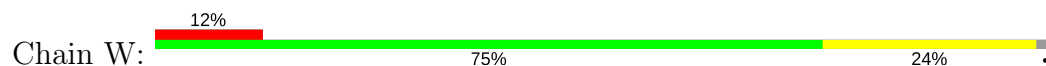
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 10: Cytochrome c oxidase polypeptide 7A1

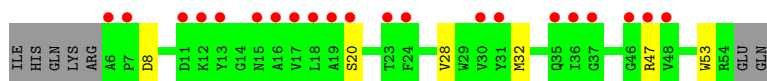
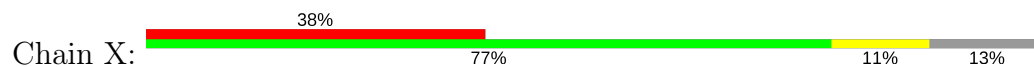


- Molecule 11: Cytochrome c oxidase subunit 7B





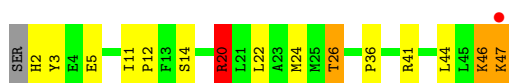
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



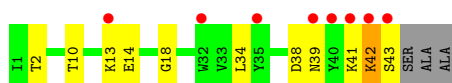
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 182.25Å 207.94Å 178.00Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 2.00 75.57 – 2.00 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (40.00-2.00) 98.7 (75.57-2.00) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.08 (at 2.00Å) | Xtriage |
| Refinement program | REFMAC 5.3 | Depositor |
| R, R_{free} | 0.183 , 0.219 0.201 , 0.235 | Depositor DCC |
| R_{free} test set | 22073 reflections (5.23%) | DCC |
| Wilson B-factor (Å ²) | 33.0 | Xtriage |
| Anisotropy | 0.521 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.38 , 69.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Estimated twinning fraction | 0.014 for l,-k,h | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 32382 | wwPDB-VP |
| Average B, all atoms (Å ²) | 43.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PEK, ZN, CHD, HEA, SAC, CDL, PSC, NO, MG, TGL, PGV, TPO, UNX, CUA, NA, FME, 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 | 1.64 | 40/4189 (1.0%) | 1.27 | 19/5722 (0.3%) |
| 1 | N | 1.46 | 26/4189 (0.6%) | 1.20 | 22/5722 (0.4%) |
| 2 | B | 1.54 | 15/1860 (0.8%) | 1.32 | 11/2534 (0.4%) |
| 2 | O | 1.32 | 7/1860 (0.4%) | 1.14 | 9/2534 (0.4%) |
| 3 | C | 1.43 | 15/2197 (0.7%) | 1.13 | 10/3005 (0.3%) |
| 3 | P | 1.36 | 9/2197 (0.4%) | 1.16 | 11/3005 (0.4%) |
| 4 | D | 1.33 | 2/1229 (0.2%) | 1.11 | 5/1658 (0.3%) |
| 4 | Q | 1.24 | 5/1229 (0.4%) | 1.04 | 5/1658 (0.3%) |
| 5 | E | 1.32 | 4/871 (0.5%) | 0.98 | 0/1182 |
| 5 | R | 1.15 | 0/871 | 0.98 | 1/1182 (0.1%) |
| 6 | F | 1.44 | 6/765 (0.8%) | 1.23 | 1/1038 (0.1%) |
| 6 | S | 1.33 | 3/765 (0.4%) | 1.17 | 1/1038 (0.1%) |
| 7 | G | 1.38 | 3/690 (0.4%) | 1.28 | 7/937 (0.7%) |
| 7 | T | 1.36 | 3/690 (0.4%) | 1.21 | 6/937 (0.6%) |
| 8 | H | 1.34 | 0/682 | 1.12 | 2/921 (0.2%) |
| 8 | U | 1.16 | 0/682 | 0.97 | 0/921 |
| 9 | I | 1.32 | 3/605 (0.5%) | 1.20 | 5/802 (0.6%) |
| 9 | V | 1.22 | 1/605 (0.2%) | 0.97 | 1/802 (0.1%) |
| 10 | J | 1.26 | 2/471 (0.4%) | 1.09 | 2/636 (0.3%) |
| 10 | W | 1.25 | 0/471 | 1.10 | 2/636 (0.3%) |
| 11 | K | 1.36 | 0/398 | 1.19 | 4/546 (0.7%) |
| 11 | X | 1.11 | 0/398 | 0.95 | 1/546 (0.2%) |
| 12 | L | 1.42 | 2/393 (0.5%) | 1.09 | 0/526 |
| 12 | Y | 1.35 | 1/393 (0.3%) | 1.00 | 1/526 (0.2%) |
| 13 | M | 1.41 | 1/345 (0.3%) | 1.23 | 2/470 (0.4%) |
| 13 | Z | 1.17 | 0/345 | 0.99 | 0/470 |
| All | All | 1.41 | 148/29390 (0.5%) | 1.16 | 128/39954 (0.3%) |

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 |
|-----|-------|---------------------|---------------------|
| 5 | E | 0 | 1 |
| 6 | F | 0 | 1 |
| 6 | S | 0 | 2 |
| 12 | Y | 0 | 1 |
| All | All | 0 | 5 |

All (148) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 7 | G | 36 | TRP | CB-CG | 10.56 | 1.69 | 1.50 |
| 7 | T | 36 | TRP | CB-CG | 10.45 | 1.69 | 1.50 |
| 1 | A | 380[A] | VAL | CB-CG1 | -9.14 | 1.33 | 1.52 |
| 1 | A | 380[B] | VAL | CB-CG1 | -9.14 | 1.33 | 1.52 |
| 3 | P | 180 | GLU | CD-OE1 | 8.86 | 1.35 | 1.25 |
| 2 | O | 198 | GLU | C-O | 8.77 | 1.40 | 1.23 |
| 2 | B | 59 | GLN | CG-CD | 8.68 | 1.71 | 1.51 |
| 1 | A | 371 | TYR | CD1-CE1 | 8.39 | 1.51 | 1.39 |
| 1 | N | 54 | TYR | CD1-CE1 | 8.15 | 1.51 | 1.39 |
| 1 | A | 394 | VAL | CB-CG2 | -8.09 | 1.35 | 1.52 |
| 1 | A | 371 | TYR | CD2-CE2 | 8.00 | 1.51 | 1.39 |
| 1 | A | 189 | MET | CG-SD | -7.71 | 1.61 | 1.81 |
| 1 | A | 285 | PHE | CE1-CZ | 7.71 | 1.51 | 1.37 |
| 3 | C | 57 | TRP | CB-CG | 7.58 | 1.63 | 1.50 |
| 2 | B | 200 | CYS | CB-SG | 7.56 | 1.95 | 1.82 |
| 3 | C | 181 | TYR | CD1-CE1 | 7.56 | 1.50 | 1.39 |
| 2 | B | 132 | GLU | CD-OE2 | 7.54 | 1.33 | 1.25 |
| 2 | B | 65 | TRP | CB-CG | -7.53 | 1.36 | 1.50 |
| 3 | P | 218 | CYS | CB-SG | 7.53 | 1.95 | 1.82 |
| 3 | C | 142 | VAL | CB-CG2 | 7.36 | 1.68 | 1.52 |
| 1 | N | 188 | VAL | N-CA | 7.05 | 1.60 | 1.46 |
| 3 | C | 102 | TYR | CE1-CZ | 7.03 | 1.47 | 1.38 |
| 12 | L | 16 | GLU | CG-CD | 7.03 | 1.62 | 1.51 |
| 1 | A | 512 | ASN | CB-CG | -6.93 | 1.35 | 1.51 |
| 5 | E | 9 | GLU | CG-CD | 6.88 | 1.62 | 1.51 |
| 1 | N | 54 | TYR | CD2-CE2 | 6.87 | 1.49 | 1.39 |
| 1 | N | 403 | TYR | CD1-CE1 | 6.80 | 1.49 | 1.39 |
| 2 | B | 60 | GLU | CG-CD | 6.71 | 1.62 | 1.51 |
| 1 | N | 394 | VAL | CB-CG2 | -6.70 | 1.38 | 1.52 |
| 6 | F | 72 | PHE | CE2-CZ | 6.63 | 1.50 | 1.37 |
| 1 | A | 189 | MET | CB-CG | 6.62 | 1.72 | 1.51 |
| 1 | N | 434 | SER | CB-OG | 6.60 | 1.50 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | C | 225 | PHE | CE2-CZ | 6.58 | 1.49 | 1.37 |
| 1 | A | 436 | MET | N-CA | 6.54 | 1.59 | 1.46 |
| 1 | N | 473 | TRP | CE3-CZ3 | 6.51 | 1.49 | 1.38 |
| 1 | A | 113 | LEU | CB-CG | 6.48 | 1.71 | 1.52 |
| 2 | B | 115 | ASP | CB-CG | 6.45 | 1.65 | 1.51 |
| 3 | C | 57 | TRP | CD1-NE1 | 6.43 | 1.48 | 1.38 |
| 2 | B | 218 | TYR | CD1-CE1 | 6.41 | 1.49 | 1.39 |
| 1 | N | 102 | PHE | CD2-CE2 | -6.39 | 1.26 | 1.39 |
| 1 | A | 323 | TRP | CB-CG | 6.34 | 1.61 | 1.50 |
| 3 | P | 181 | TYR | CD1-CE1 | 6.33 | 1.48 | 1.39 |
| 2 | O | 65 | TRP | CB-CG | -6.33 | 1.38 | 1.50 |
| 1 | A | 439 | ARG | C-O | 6.30 | 1.35 | 1.23 |
| 2 | B | 108 | TYR | CD2-CE2 | 6.22 | 1.48 | 1.39 |
| 2 | B | 59 | GLN | CB-CG | 6.17 | 1.69 | 1.52 |
| 2 | O | 192 | TYR | CD1-CE1 | 6.16 | 1.48 | 1.39 |
| 7 | G | 17 | ARG | CD-NE | -6.16 | 1.35 | 1.46 |
| 2 | B | 60 | GLU | CB-CG | 6.13 | 1.63 | 1.52 |
| 4 | Q | 9 | GLU | CB-CG | 6.12 | 1.63 | 1.52 |
| 1 | A | 297 | MET | CB-CG | 6.10 | 1.70 | 1.51 |
| 3 | C | 208 | VAL | CB-CG2 | 6.10 | 1.65 | 1.52 |
| 3 | C | 254 | VAL | CB-CG2 | 6.09 | 1.65 | 1.52 |
| 13 | M | 32 | TRP | CG-CD1 | 6.03 | 1.45 | 1.36 |
| 3 | C | 55 | TYR | CD2-CE2 | 6.02 | 1.48 | 1.39 |
| 10 | J | 20 | VAL | CB-CG1 | 6.02 | 1.65 | 1.52 |
| 1 | N | 397 | PHE | CE2-CZ | 5.99 | 1.48 | 1.37 |
| 2 | B | 167 | SER | CB-OG | -5.97 | 1.34 | 1.42 |
| 1 | A | 270 | TYR | CB-CG | 5.94 | 1.60 | 1.51 |
| 4 | Q | 17 | VAL | CB-CG1 | -5.94 | 1.40 | 1.52 |
| 1 | A | 397 | PHE | CD2-CE2 | 5.84 | 1.50 | 1.39 |
| 9 | I | 69 | PHE | CG-CD2 | 5.84 | 1.47 | 1.38 |
| 1 | N | 438 | ARG | CB-CG | -5.83 | 1.36 | 1.52 |
| 1 | A | 93 | ALA | CA-CB | 5.80 | 1.64 | 1.52 |
| 1 | N | 372 | TYR | CB-CG | 5.79 | 1.60 | 1.51 |
| 3 | C | 214 | PHE | CE2-CZ | 5.78 | 1.48 | 1.37 |
| 1 | N | 297 | MET | SD-CE | 5.75 | 2.10 | 1.77 |
| 1 | A | 164 | PHE | CE1-CZ | 5.73 | 1.48 | 1.37 |
| 2 | O | 221 | LYS | CD-CE | 5.72 | 1.65 | 1.51 |
| 6 | F | 1 | ALA | C-O | 5.71 | 1.34 | 1.23 |
| 1 | A | 293 | PHE | CE2-CZ | 5.67 | 1.48 | 1.37 |
| 1 | N | 113 | LEU | CB-CG | 5.67 | 1.69 | 1.52 |
| 6 | F | 3 | GLY | C-O | 5.66 | 1.32 | 1.23 |
| 1 | N | 244 | TYR | CD2-CE2 | -5.66 | 1.30 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 143 | VAL | CB-CG1 | 5.65 | 1.64 | 1.52 |
| 7 | T | 17 | ARG | CD-NE | -5.62 | 1.36 | 1.46 |
| 3 | P | 16 | TRP | CE3-CZ3 | 5.61 | 1.48 | 1.38 |
| 1 | A | 467 | LEU | N-CA | -5.61 | 1.35 | 1.46 |
| 4 | Q | 115 | TRP | CE3-CZ3 | 5.58 | 1.48 | 1.38 |
| 10 | J | 26 | ALA | CA-CB | 5.58 | 1.64 | 1.52 |
| 2 | O | 18 | GLU | CB-CG | -5.58 | 1.41 | 1.52 |
| 5 | E | 84 | TYR | CG-CD1 | 5.57 | 1.46 | 1.39 |
| 6 | F | 72 | PHE | CE1-CZ | 5.56 | 1.48 | 1.37 |
| 1 | N | 168 | ILE | CB-CG2 | 5.55 | 1.70 | 1.52 |
| 4 | Q | 9 | GLU | CG-CD | 5.55 | 1.60 | 1.51 |
| 1 | N | 415 | ALA | CA-CB | 5.54 | 1.64 | 1.52 |
| 2 | O | 156 | SER | CB-OG | 5.54 | 1.49 | 1.42 |
| 3 | P | 246 | ASP | CG-OD2 | 5.54 | 1.38 | 1.25 |
| 1 | A | 266 | GLU | CB-CG | 5.53 | 1.62 | 1.52 |
| 1 | A | 411 | LYS | CE-NZ | 5.53 | 1.62 | 1.49 |
| 1 | N | 189 | MET | CB-CG | 5.52 | 1.69 | 1.51 |
| 1 | A | 213 | ARG | CG-CD | 5.50 | 1.65 | 1.51 |
| 4 | D | 104 | TYR | CD1-CE1 | 5.50 | 1.47 | 1.39 |
| 3 | P | 8 | TYR | CD1-CE1 | -5.46 | 1.31 | 1.39 |
| 1 | N | 372 | TYR | CD2-CE2 | 5.46 | 1.47 | 1.39 |
| 1 | N | 8 | PHE | CD2-CE2 | 5.45 | 1.50 | 1.39 |
| 1 | A | 281 | GLY | C-O | 5.43 | 1.32 | 1.23 |
| 3 | C | 249 | TRP | CB-CG | 5.42 | 1.60 | 1.50 |
| 12 | L | 5 | GLU | CD-OE2 | -5.42 | 1.19 | 1.25 |
| 12 | Y | 20 | ARG | CG-CD | 5.42 | 1.65 | 1.51 |
| 6 | F | 54 | ASN | CB-CG | 5.42 | 1.63 | 1.51 |
| 2 | B | 193 | TYR | CD1-CE1 | 5.42 | 1.47 | 1.39 |
| 3 | C | 17 | PRO | CG-CD | 5.41 | 1.68 | 1.50 |
| 4 | D | 64 | PHE | CE1-CZ | 5.40 | 1.47 | 1.37 |
| 1 | A | 244 | TYR | CD1-CE1 | 5.40 | 1.47 | 1.39 |
| 6 | F | 73 | TRP | CE3-CZ3 | 5.40 | 1.47 | 1.38 |
| 5 | E | 88 | GLU | CG-CD | 5.37 | 1.60 | 1.51 |
| 1 | A | 379 | TYR | CE2-CZ | 5.36 | 1.45 | 1.38 |
| 2 | B | 137 | GLU | C-O | 5.35 | 1.33 | 1.23 |
| 7 | G | 5 | LYS | CB-CG | 5.33 | 1.67 | 1.52 |
| 3 | C | 89 | SER | CB-OG | 5.32 | 1.49 | 1.42 |
| 3 | C | 139 | ALA | CA-CB | 5.28 | 1.63 | 1.52 |
| 1 | A | 113 | LEU | CG-CD1 | 5.27 | 1.71 | 1.51 |
| 9 | I | 69 | PHE | CE2-CZ | 5.27 | 1.47 | 1.37 |
| 1 | A | 126 | TRP | CG-CD1 | 5.26 | 1.44 | 1.36 |
| 3 | P | 107 | ALA | CA-CB | 5.24 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | Q | 6 | VAL | CA-CB | 5.23 | 1.65 | 1.54 |
| 1 | N | 244 | TYR | CE2-CZ | 5.22 | 1.45 | 1.38 |
| 1 | A | 410 | ALA | CA-CB | 5.22 | 1.63 | 1.52 |
| 1 | A | 160 | GLY | N-CA | 5.22 | 1.53 | 1.46 |
| 1 | A | 304 | TYR | CD2-CE2 | 5.22 | 1.47 | 1.39 |
| 1 | A | 505 | PHE | CG-CD2 | 5.20 | 1.46 | 1.38 |
| 1 | N | 373 | VAL | CB-CG2 | 5.20 | 1.63 | 1.52 |
| 2 | B | 121 | TYR | CE1-CZ | -5.19 | 1.31 | 1.38 |
| 6 | S | 1 | ALA | C-O | 5.19 | 1.33 | 1.23 |
| 1 | N | 81 | TRP | CD1-NE1 | 5.17 | 1.46 | 1.38 |
| 1 | N | 506 | GLU | CB-CG | -5.16 | 1.42 | 1.52 |
| 6 | S | 2 | SER | N-CA | 5.14 | 1.56 | 1.46 |
| 1 | A | 193 | VAL | CA-CB | 5.13 | 1.65 | 1.54 |
| 1 | A | 63 | PHE | CD1-CE1 | 5.12 | 1.49 | 1.39 |
| 1 | N | 447 | TYR | CD2-CE2 | 5.12 | 1.47 | 1.39 |
| 1 | A | 67 | PHE | CE2-CZ | 5.12 | 1.47 | 1.37 |
| 1 | A | 494 | TRP | CZ3-CH2 | 5.12 | 1.48 | 1.40 |
| 3 | C | 236 | GLU | CG-CD | 5.11 | 1.59 | 1.51 |
| 1 | A | 344 | PHE | CD2-CE2 | 5.10 | 1.49 | 1.39 |
| 1 | A | 162 | ILE | CA-CB | 5.10 | 1.66 | 1.54 |
| 1 | N | 143 | VAL | CB-CG2 | 5.10 | 1.63 | 1.52 |
| 7 | T | 50 | TYR | CE1-CZ | 5.09 | 1.45 | 1.38 |
| 5 | E | 19 | PHE | CD1-CE1 | 5.07 | 1.49 | 1.39 |
| 9 | V | 51 | TYR | CD1-CE1 | 5.07 | 1.47 | 1.39 |
| 3 | P | 181 | TYR | CD2-CE2 | 5.07 | 1.47 | 1.39 |
| 1 | A | 235 | PHE | CG-CD1 | 5.05 | 1.46 | 1.38 |
| 9 | I | 15 | ARG | CG-CD | 5.04 | 1.64 | 1.51 |
| 3 | P | 227 | PHE | CE2-CZ | 5.04 | 1.47 | 1.37 |
| 6 | S | 69 | VAL | CA-CB | -5.04 | 1.44 | 1.54 |
| 2 | B | 192 | TYR | CG-CD1 | 5.03 | 1.45 | 1.39 |
| 2 | O | 171 | LYS | CB-CG | 5.01 | 1.66 | 1.52 |
| 1 | N | 447 | TYR | CD1-CE1 | 5.00 | 1.46 | 1.39 |

All (128) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 7 | G | 17 | ARG | NE-CZ-NH2 | -14.38 | 113.11 | 120.30 |
| 1 | A | 71 | MET | CG-SD-CE | -14.02 | 77.77 | 100.20 |
| 7 | G | 17 | ARG | NE-CZ-NH1 | 12.88 | 126.74 | 120.30 |
| 3 | P | 246 | ASP | CB-CG-OD1 | -12.27 | 107.26 | 118.30 |
| 1 | N | 278 | MET | CG-SD-CE | -11.92 | 81.12 | 100.20 |
| 1 | N | 71 | MET | CG-SD-CE | -11.66 | 81.54 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3 | P | 221 | ARG | NE-CZ-NH1 | -10.62 | 114.99 | 120.30 |
| 1 | A | 136 | LEU | CB-CG-CD1 | -10.11 | 93.81 | 111.00 |
| 1 | N | 310 | MET | CG-SD-CE | -9.35 | 85.24 | 100.20 |
| 9 | I | 43 | ARG | NE-CZ-NH2 | 9.15 | 124.88 | 120.30 |
| 7 | T | 17 | ARG | NE-CZ-NH2 | -9.12 | 115.74 | 120.30 |
| 7 | T | 17 | ARG | NE-CZ-NH1 | 8.68 | 124.64 | 120.30 |
| 1 | N | 298 | ASP | CB-CG-OD1 | -8.56 | 110.59 | 118.30 |
| 4 | D | 20 | ARG | NE-CZ-NH2 | -8.41 | 116.09 | 120.30 |
| 1 | N | 298 | ASP | CB-CG-OD2 | 8.40 | 125.86 | 118.30 |
| 8 | H | 38 | ARG | NE-CZ-NH1 | -8.36 | 116.12 | 120.30 |
| 1 | A | 298 | ASP | CB-CG-OD2 | 8.29 | 125.76 | 118.30 |
| 1 | N | 113 | LEU | CB-CG-CD2 | 8.07 | 124.71 | 111.00 |
| 2 | B | 173 | ASP | CB-CG-OD1 | 7.96 | 125.47 | 118.30 |
| 2 | B | 65 | TRP | CB-CA-C | 7.75 | 125.90 | 110.40 |
| 4 | D | 51 | LEU | CA-CB-CG | 7.67 | 132.94 | 115.30 |
| 2 | B | 178 | ARG | NE-CZ-NH1 | -7.64 | 116.48 | 120.30 |
| 4 | Q | 20 | ARG | NE-CZ-NH1 | 7.64 | 124.12 | 120.30 |
| 1 | A | 278 | MET | CG-SD-CE | -7.51 | 88.19 | 100.20 |
| 9 | I | 68 | ILE | CG1-CB-CG2 | 7.30 | 127.45 | 111.40 |
| 4 | Q | 17 | VAL | CB-CA-C | -7.20 | 97.72 | 111.40 |
| 1 | A | 512 | ASN | CB-CA-C | -7.16 | 96.09 | 110.40 |
| 4 | D | 19 | ARG | NE-CZ-NH1 | -7.06 | 116.77 | 120.30 |
| 1 | A | 486 | ASP | CB-CG-OD2 | -7.04 | 111.97 | 118.30 |
| 3 | P | 29 | SER | CB-CA-C | -6.96 | 96.88 | 110.10 |
| 2 | B | 152 | MET | CG-SD-CE | 6.95 | 111.31 | 100.20 |
| 13 | M | 34 | LEU | CB-CG-CD1 | 6.86 | 122.66 | 111.00 |
| 1 | N | 136 | LEU | CA-CB-CG | 6.83 | 131.01 | 115.30 |
| 1 | A | 302 | ARG | NE-CZ-NH2 | -6.81 | 116.89 | 120.30 |
| 3 | P | 80 | ARG | CG-CD-NE | -6.79 | 97.55 | 111.80 |
| 1 | A | 366 | VAL | CG1-CB-CG2 | -6.78 | 100.06 | 110.90 |
| 1 | A | 189 | MET | CG-SD-CE | -6.77 | 89.37 | 100.20 |
| 1 | N | 438 | ARG | NE-CZ-NH1 | -6.76 | 116.92 | 120.30 |
| 8 | H | 52 | VAL | CB-CA-C | -6.75 | 98.57 | 111.40 |
| 1 | A | 369 | ASP | CB-CG-OD1 | 6.75 | 124.37 | 118.30 |
| 1 | A | 439 | ARG | NE-CZ-NH1 | -6.72 | 116.94 | 120.30 |
| 2 | O | 139 | ASP | CB-CG-OD2 | 6.70 | 124.33 | 118.30 |
| 1 | A | 456 | MET | CG-SD-CE | -6.65 | 89.56 | 100.20 |
| 10 | W | 44 | LEU | CB-CG-CD1 | -6.60 | 99.78 | 111.00 |
| 11 | K | 47 | ARG | NE-CZ-NH1 | -6.59 | 117.01 | 120.30 |
| 6 | S | 21 | MET | CG-SD-CE | 6.57 | 110.72 | 100.20 |
| 1 | N | 136 | LEU | CB-CG-CD2 | -6.50 | 99.95 | 111.00 |
| 4 | Q | 20 | ARG | NE-CZ-NH2 | -6.48 | 117.06 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | N | 91 | ASP | CB-CG-OD1 | 6.40 | 124.06 | 118.30 |
| 2 | B | 134 | ARG | NE-CZ-NH2 | -6.34 | 117.13 | 120.30 |
| 1 | N | 244 | TYR | CG-CD2-CE2 | 6.29 | 126.33 | 121.30 |
| 1 | A | 35 | LEU | CB-CG-CD1 | -6.26 | 100.35 | 111.00 |
| 3 | C | 152 | MET | CG-SD-CE | 6.24 | 110.18 | 100.20 |
| 1 | A | 113 | LEU | CB-CG-CD2 | 6.24 | 121.60 | 111.00 |
| 2 | O | 184 | LEU | CA-CB-CG | 6.22 | 129.60 | 115.30 |
| 4 | D | 20 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 4 | Q | 51 | LEU | CA-CB-CG | 6.18 | 129.52 | 115.30 |
| 9 | I | 55 | ASP | CB-CG-OD1 | 6.18 | 123.86 | 118.30 |
| 2 | O | 185 | MET | CG-SD-CE | 6.17 | 110.08 | 100.20 |
| 2 | B | 82 | ARG | CG-CD-NE | -6.16 | 98.87 | 111.80 |
| 11 | K | 54 | ARG | NE-CZ-NH2 | -6.15 | 117.22 | 120.30 |
| 2 | B | 95 | LEU | CB-CG-CD1 | 6.13 | 121.42 | 111.00 |
| 1 | N | 244 | TYR | CZ-CE2-CD2 | -6.11 | 114.30 | 119.80 |
| 1 | A | 188 | VAL | CG1-CB-CG2 | -6.03 | 101.26 | 110.90 |
| 3 | P | 163 | LEU | CB-CG-CD2 | -6.02 | 100.76 | 111.00 |
| 2 | B | 88 | ASP | CB-CG-OD2 | 6.02 | 123.72 | 118.30 |
| 3 | P | 221 | ARG | NE-CZ-NH2 | 6.01 | 123.31 | 120.30 |
| 7 | G | 78 | LEU | CB-CG-CD1 | -6.00 | 100.80 | 111.00 |
| 1 | A | 194 | LEU | CB-CG-CD1 | 5.97 | 121.16 | 111.00 |
| 1 | N | 189 | MET | CA-CB-CG | -5.95 | 103.18 | 113.30 |
| 3 | C | 59 | ARG | NE-CZ-NH1 | -5.95 | 117.33 | 120.30 |
| 10 | J | 40 | LEU | CB-CG-CD2 | 5.94 | 121.10 | 111.00 |
| 3 | P | 180 | GLU | OE1-CD-OE2 | 5.89 | 130.36 | 123.30 |
| 2 | O | 173 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 |
| 6 | F | 95 | GLN | N-CA-C | 5.87 | 126.85 | 111.00 |
| 1 | N | 438 | ARG | CG-CD-NE | -5.81 | 99.61 | 111.80 |
| 1 | A | 189 | MET | CA-CB-CG | -5.80 | 103.43 | 113.30 |
| 3 | C | 80 | ARG | CG-CD-NE | -5.76 | 99.71 | 111.80 |
| 1 | N | 38 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |
| 11 | X | 32 | MET | CG-SD-CE | 5.68 | 109.30 | 100.20 |
| 7 | T | 44 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 7 | G | 56 | ARG | NE-CZ-NH2 | -5.65 | 117.47 | 120.30 |
| 13 | M | 27 | LEU | CB-CG-CD1 | -5.63 | 101.44 | 111.00 |
| 2 | O | 202 | SER | CB-CA-C | -5.62 | 99.42 | 110.10 |
| 3 | P | 192 | VAL | CG1-CB-CG2 | 5.62 | 119.89 | 110.90 |
| 7 | G | 19 | LEU | CB-CG-CD2 | -5.62 | 101.45 | 111.00 |
| 1 | N | 369 | ASP | CB-CG-OD2 | 5.62 | 123.36 | 118.30 |
| 1 | N | 438 | ARG | CB-CA-C | -5.61 | 99.19 | 110.40 |
| 7 | T | 14 | ARG | NE-CZ-NH1 | -5.60 | 117.50 | 120.30 |
| 9 | I | 15 | ARG | NE-CZ-NH2 | 5.59 | 123.09 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 9 | I | 43 | ARG | NE-CZ-NH1 | -5.59 | 117.50 | 120.30 |
| 12 | Y | 41 | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 1 | N | 366 | VAL | CG1-CB-CG2 | -5.49 | 102.11 | 110.90 |
| 3 | C | 221 | ARG | NE-CZ-NH1 | -5.48 | 117.56 | 120.30 |
| 1 | A | 28 | MET | CG-SD-CE | 5.47 | 108.96 | 100.20 |
| 2 | O | 134 | ARG | NE-CZ-NH1 | -5.47 | 117.56 | 120.30 |
| 2 | O | 92 | ASN | CB-CA-C | 5.47 | 121.34 | 110.40 |
| 10 | J | 57 | HIS | CB-CA-C | 5.46 | 121.31 | 110.40 |
| 2 | B | 87 | MET | CA-CB-CG | 5.46 | 122.57 | 113.30 |
| 7 | T | 17 | ARG | CB-CG-CD | -5.43 | 97.47 | 111.60 |
| 1 | N | 438 | ARG | N-CA-CB | -5.39 | 100.89 | 110.60 |
| 4 | D | 137 | LYS | CD-CE-NZ | -5.35 | 99.40 | 111.70 |
| 2 | O | 75 | LEU | CB-CG-CD1 | 5.34 | 120.07 | 111.00 |
| 1 | N | 113 | LEU | CB-CG-CD1 | 5.33 | 120.06 | 111.00 |
| 3 | P | 155 | ASP | CB-CG-OD1 | 5.33 | 123.09 | 118.30 |
| 3 | C | 33 | MET | CG-SD-CE | 5.32 | 108.72 | 100.20 |
| 3 | C | 169 | LEU | CB-CG-CD2 | -5.31 | 101.97 | 111.00 |
| 2 | O | 82 | ARG | NE-CZ-NH2 | -5.28 | 117.66 | 120.30 |
| 7 | G | 7 | ASP | N-CA-C | 5.27 | 125.24 | 111.00 |
| 3 | P | 223 | LEU | CB-CG-CD1 | -5.22 | 102.12 | 111.00 |
| 2 | B | 66 | THR | OG1-CB-CG2 | 5.22 | 122.01 | 110.00 |
| 4 | Q | 19 | ARG | NE-CZ-NH1 | -5.22 | 117.69 | 120.30 |
| 5 | R | 96 | LEU | CA-CB-CG | 5.21 | 127.29 | 115.30 |
| 3 | C | 33 | MET | CB-CG-SD | 5.18 | 127.93 | 112.40 |
| 3 | C | 44 | MET | CG-SD-CE | 5.18 | 108.48 | 100.20 |
| 7 | G | 17 | ARG | CB-CG-CD | -5.17 | 98.16 | 111.60 |
| 1 | A | 152 | LEU | CA-CB-CG | 5.13 | 127.11 | 115.30 |
| 3 | C | 102 | TYR | CB-CG-CD2 | -5.12 | 117.92 | 121.00 |
| 11 | K | 39 | GLU | OE1-CD-OE2 | -5.12 | 117.15 | 123.30 |
| 1 | N | 229 | ILE | CG1-CB-CG2 | -5.12 | 100.13 | 111.40 |
| 7 | T | 19 | LEU | CB-CG-CD2 | -5.12 | 102.30 | 111.00 |
| 2 | B | 213 | LEU | CB-CG-CD1 | -5.10 | 102.32 | 111.00 |
| 3 | C | 85 | LEU | CA-CB-CG | -5.10 | 103.56 | 115.30 |
| 3 | P | 40 | MET | CB-CG-SD | -5.10 | 97.10 | 112.40 |
| 9 | V | 64 | ARG | NE-CZ-NH1 | 5.09 | 122.85 | 120.30 |
| 11 | K | 47 | ARG | CG-CD-NE | -5.09 | 101.12 | 111.80 |
| 1 | N | 194 | LEU | CB-CG-CD1 | 5.07 | 119.61 | 111.00 |
| 10 | W | 44 | LEU | CB-CG-CD2 | 5.02 | 119.54 | 111.00 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 5 | E | 5 | HIS | Peptide |
| 6 | F | 93 | PRO | Peptide |
| 6 | S | 93 | PRO | Peptide |
| 6 | S | 95 | GLN | Peptide |
| 12 | Y | 46 | LYS | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4060 | 0 | 4037 | 74 | 0 |
| 1 | N | 4060 | 0 | 4037 | 86 | 0 |
| 2 | B | 1824 | 0 | 1833 | 25 | 0 |
| 2 | O | 1824 | 0 | 1833 | 50 | 0 |
| 3 | C | 2110 | 0 | 2027 | 24 | 0 |
| 3 | P | 2110 | 0 | 2027 | 35 | 0 |
| 4 | D | 1195 | 0 | 1183 | 19 | 0 |
| 4 | Q | 1195 | 0 | 1183 | 20 | 0 |
| 5 | E | 852 | 0 | 845 | 10 | 0 |
| 5 | R | 852 | 0 | 845 | 19 | 0 |
| 6 | F | 748 | 0 | 728 | 22 | 0 |
| 6 | S | 748 | 0 | 728 | 40 | 0 |
| 7 | G | 675 | 0 | 643 | 45 | 0 |
| 7 | T | 675 | 0 | 643 | 43 | 0 |
| 8 | H | 662 | 0 | 623 | 19 | 0 |
| 8 | U | 662 | 0 | 623 | 20 | 0 |
| 9 | I | 601 | 0 | 613 | 8 | 0 |
| 9 | V | 601 | 0 | 613 | 9 | 0 |
| 10 | J | 460 | 0 | 459 | 13 | 0 |
| 10 | W | 460 | 0 | 459 | 12 | 0 |
| 11 | K | 384 | 0 | 366 | 2 | 0 |
| 11 | X | 384 | 0 | 366 | 4 | 0 |
| 12 | L | 380 | 0 | 380 | 16 | 0 |
| 12 | Y | 380 | 0 | 380 | 20 | 0 |
| 13 | M | 335 | 0 | 352 | 13 | 0 |
| 13 | Z | 335 | 0 | 352 | 6 | 0 |
| 14 | A | 120 | 0 | 108 | 16 | 0 |
| 14 | N | 120 | 0 | 108 | 9 | 0 |
| 15 | A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 15 | N | 2 | 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 | 1 | 0 | 0 | 0 | 0 |
| 18 | N | 1 | 0 | 0 | 0 | 0 |
| 19 | A | 102 | 0 | 152 | 16 | 0 |
| 19 | C | 102 | 0 | 152 | 10 | 0 |
| 19 | N | 102 | 0 | 152 | 7 | 0 |
| 19 | P | 51 | 0 | 76 | 3 | 0 |
| 19 | U | 51 | 0 | 76 | 4 | 0 |
| 20 | B | 2 | 0 | 0 | 0 | 0 |
| 20 | O | 2 | 0 | 0 | 0 | 0 |
| 21 | B | 63 | 0 | 110 | 4 | 0 |
| 21 | D | 63 | 0 | 110 | 10 | 0 |
| 21 | L | 63 | 0 | 110 | 15 | 0 |
| 21 | N | 63 | 0 | 110 | 14 | 0 |
| 21 | O | 63 | 0 | 110 | 5 | 0 |
| 21 | Y | 63 | 0 | 110 | 20 | 0 |
| 22 | B | 52 | 0 | 80 | 20 | 0 |
| 22 | R | 52 | 0 | 80 | 20 | 0 |
| 23 | B | 29 | 0 | 37 | 4 | 0 |
| 23 | C | 58 | 0 | 71 | 4 | 0 |
| 23 | J | 29 | 0 | 36 | 8 | 0 |
| 23 | O | 29 | 0 | 37 | 3 | 0 |
| 23 | P | 58 | 0 | 72 | 5 | 0 |
| 23 | W | 29 | 0 | 35 | 3 | 0 |
| 24 | C | 1 | 0 | 0 | 0 | 0 |
| 24 | P | 1 | 0 | 0 | 0 | 0 |
| 25 | C | 106 | 0 | 154 | 22 | 0 |
| 25 | G | 53 | 0 | 77 | 19 | 0 |
| 25 | P | 53 | 0 | 77 | 6 | 0 |
| 25 | T | 106 | 0 | 154 | 34 | 0 |
| 26 | C | 100 | 0 | 156 | 20 | 0 |
| 26 | G | 100 | 0 | 156 | 33 | 0 |
| 26 | P | 100 | 0 | 156 | 27 | 0 |
| 26 | T | 100 | 0 | 156 | 30 | 0 |
| 27 | C | 33 | 0 | 39 | 4 | 0 |
| 27 | M | 33 | 0 | 39 | 0 | 0 |
| 27 | P | 33 | 0 | 38 | 1 | 0 |
| 27 | Z | 33 | 0 | 38 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28 | F | 1 | 0 | 0 | 0 | 0 |
| 28 | S | 1 | 0 | 0 | 0 | 0 |
| 29 | A | 217 | 0 | 0 | 5 | 0 |
| 29 | B | 127 | 0 | 0 | 3 | 0 |
| 29 | C | 93 | 0 | 0 | 4 | 0 |
| 29 | D | 86 | 0 | 0 | 6 | 0 |
| 29 | E | 52 | 0 | 0 | 0 | 0 |
| 29 | F | 72 | 0 | 0 | 3 | 0 |
| 29 | G | 42 | 0 | 0 | 7 | 0 |
| 29 | H | 46 | 0 | 0 | 1 | 0 |
| 29 | I | 31 | 0 | 0 | 3 | 0 |
| 29 | J | 28 | 0 | 0 | 4 | 0 |
| 29 | K | 27 | 0 | 0 | 2 | 0 |
| 29 | L | 16 | 0 | 0 | 1 | 0 |
| 29 | M | 20 | 0 | 0 | 0 | 0 |
| 29 | N | 207 | 0 | 0 | 6 | 0 |
| 29 | O | 105 | 0 | 0 | 2 | 0 |
| 29 | P | 96 | 0 | 0 | 3 | 0 |
| 29 | Q | 57 | 0 | 0 | 4 | 0 |
| 29 | R | 35 | 0 | 0 | 1 | 0 |
| 29 | S | 63 | 0 | 0 | 5 | 0 |
| 29 | T | 44 | 0 | 0 | 5 | 0 |
| 29 | U | 43 | 0 | 0 | 5 | 0 |
| 29 | V | 20 | 0 | 0 | 0 | 0 |
| 29 | W | 17 | 0 | 0 | 2 | 0 |
| 29 | X | 13 | 0 | 0 | 0 | 0 |
| 29 | Y | 12 | 0 | 0 | 1 | 0 |
| 29 | Z | 11 | 0 | 0 | 1 | 0 |
| All | All | 32382 | 0 | 31350 | 777 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (777) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:T:1265:PEK:H383 | 26:T:1269:CDL:C27 | 1.34 | 1.51 |
| 1:N:297:MET:CE | 1:N:297:MET:SD | 2.10 | 1.40 |
| 25:T:1265:PEK:C38 | 26:T:1269:CDL:H273 | 1.51 | 1.36 |
| 10:W:2:GLU:HB2 | 10:W:4:ARG:NH1 | 1.50 | 1.26 |
| 25:T:1265:PEK:C38 | 26:T:1269:CDL:C27 | 2.12 | 1.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G:5:LYS:HD2 | 25:G:1263:PEK:C37 | 1.73 | 1.18 |
| 19:A:524:PGV:H311 | 13:M:19:LEU:HD23 | 1.24 | 1.16 |
| 19:U:1268:PGV:H032 | 29:U:4495:HOH:O | 1.43 | 1.14 |
| 25:C:264:PEK:H162 | 25:C:264:PEK:H101 | 1.17 | 1.14 |
| 7:G:5:LYS:CD | 25:G:1263:PEK:H371 | 1.78 | 1.13 |
| 26:C:270:CDL:HB22 | 10:J:8:LYS:NZ | 1.62 | 1.13 |
| 29:B:2562:HOH:O | 21:D:523:TGL:HC61 | 1.50 | 1.11 |
| 26:C:270:CDL:HB22 | 10:J:8:LYS:HZ2 | 1.09 | 1.10 |
| 7:G:84:LYS:HD2 | 7:G:84:LYS:H | 1.03 | 1.10 |
| 12:L:20:ARG:NH2 | 21:L:522:TGL:HC32 | 1.64 | 1.10 |
| 25:T:1265:PEK:H383 | 26:T:1269:CDL:H271 | 1.23 | 1.10 |
| 26:G:269:CDL:H561 | 26:G:269:CDL:H762 | 1.33 | 1.09 |
| 8:H:52:VAL:HG12 | 8:U:46:LYS:HB2 | 1.17 | 1.09 |
| 21:N:1523:TGL:HC21 | 21:N:1523:TGL:HG11 | 1.31 | 1.08 |
| 7:G:5:LYS:HD2 | 25:G:1263:PEK:H371 | 1.26 | 1.06 |
| 26:G:269:CDL:H222 | 26:G:269:CDL:H522 | 1.39 | 1.04 |
| 1:N:513:LEU:O | 1:N:514:LYS:HB2 | 1.55 | 1.04 |
| 7:G:5:LYS:CG | 25:G:1263:PEK:H371 | 1.88 | 1.03 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:N | 2.26 | 1.03 |
| 26:C:270:CDL:H212 | 26:C:270:CDL:H631 | 1.05 | 1.02 |
| 1:A:513:LEU:O | 1:A:514:LYS:HB2 | 1.60 | 1.02 |
| 8:U:9:LYS:HG3 | 8:U:10:ASN:H | 1.21 | 1.01 |
| 2:O:59:GLN:O | 2:O:59:GLN:HG3 | 1.59 | 0.98 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:H | 1.80 | 0.98 |
| 22:R:1229:PSC:C34 | 22:R:1229:PSC:H142 | 1.94 | 0.98 |
| 19:N:1524:PGV:H012 | 19:N:1524:PGV:H221 | 1.45 | 0.97 |
| 7:G:84:LYS:N | 7:G:84:LYS:HD2 | 1.78 | 0.95 |
| 19:N:1524:PGV:H221 | 19:N:1524:PGV:C01 | 1.96 | 0.94 |
| 26:P:1270:CDL:HB21 | 26:P:1270:CDL:CB3 | 1.98 | 0.94 |
| 10:W:2:GLU:HB2 | 10:W:4:ARG:HH12 | 1.32 | 0.94 |
| 22:B:229:PSC:O01 | 22:B:229:PSC:H212 | 1.67 | 0.94 |
| 19:C:267:PGV:H181 | 26:C:270:CDL:H652 | 1.48 | 0.93 |
| 7:G:2:SER:OG | 25:G:1263:PEK:H291 | 1.66 | 0.93 |
| 6:F:94:HIS:HB3 | 6:F:95:GLN:OE1 | 1.68 | 0.93 |
| 7:G:72:ASN:H | 7:G:76:ASN:HD22 | 0.99 | 0.93 |
| 26:P:1270:CDL:HB21 | 26:P:1270:CDL:HB32 | 1.49 | 0.93 |
| 25:T:1265:PEK:H383 | 26:T:1269:CDL:H273 | 1.00 | 0.92 |
| 6:F:85:CYS:SG | 6:F:87:THR:HG23 | 2.09 | 0.92 |
| 26:G:269:CDL:HA21 | 26:G:269:CDL:H112 | 1.52 | 0.92 |
| 25:T:1265:PEK:H381 | 26:T:1269:CDL:H273 | 1.48 | 0.92 |
| 10:W:2:GLU:HB2 | 10:W:4:ARG:HH11 | 1.35 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:B:229:PSC:H072 | 9:I:10:ARG:HH21 | 1.32 | 0.91 |
| 6:S:85:CYS:SG | 6:S:87:THR:HG23 | 2.10 | 0.91 |
| 26:T:1269:CDL:H241 | 26:T:1269:CDL:H531 | 1.53 | 0.90 |
| 25:P:1264:PEK:H32 | 25:P:1264:PEK:H71 | 1.55 | 0.89 |
| 3:P:29:SER:HB2 | 3:P:42:LEU:HD13 | 1.53 | 0.89 |
| 25:T:1265:PEK:H71 | 29:T:4407:HOH:O | 1.73 | 0.89 |
| 8:H:9:LYS:O | 8:H:10:ASN:HB2 | 1.71 | 0.88 |
| 7:T:7:ASP:O | 7:T:8:HIS:HB2 | 1.73 | 0.88 |
| 1:A:513:LEU:O | 1:A:514:LYS:CB | 2.22 | 0.87 |
| 7:G:84:LYS:H | 7:G:84:LYS:CD | 1.87 | 0.87 |
| 1:A:282:PHE:HA | 7:T:4:ALA:CB | 2.04 | 0.87 |
| 26:C:270:CDL:H212 | 26:C:270:CDL:C63 | 1.99 | 0.87 |
| 12:L:20:ARG:HH22 | 21:L:522:TGL:HC32 | 1.38 | 0.87 |
| 1:N:513:LEU:O | 1:N:514:LYS:CB | 2.23 | 0.86 |
| 7:G:2:SER:OG | 25:G:1263:PEK:C29 | 2.22 | 0.86 |
| 7:G:11:TPO:HG22 | 7:G:16:TRP:HE1 | 1.41 | 0.86 |
| 12:Y:20:ARG:HH21 | 21:Y:1522:TGL:HC32 | 1.39 | 0.86 |
| 19:A:524:PGV:H011 | 19:A:524:PGV:H22 | 1.59 | 0.85 |
| 3:C:63:ARG:HH21 | 26:C:270:CDL:HA21 | 1.38 | 0.85 |
| 2:B:81:LEU:HD12 | 26:T:1269:CDL:H351 | 1.57 | 0.85 |
| 7:G:2:SER:O | 25:G:1263:PEK:H331 | 1.77 | 0.84 |
| 9:I:44:LYS:HE2 | 29:I:4717:HOH:O | 1.77 | 0.84 |
| 8:H:52:VAL:HG12 | 8:U:46:LYS:CB | 2.06 | 0.83 |
| 19:A:524:PGV:H311 | 13:M:19:LEU:CD2 | 2.09 | 0.83 |
| 21:D:523:TGL:HG32 | 29:D:4105:HOH:O | 1.76 | 0.83 |
| 6:F:97:ALA:CB | 29:F:4782:HOH:O | 2.26 | 0.83 |
| 7:G:5:LYS:HG3 | 25:G:1263:PEK:H371 | 1.60 | 0.82 |
| 7:G:3:ALA:HB1 | 25:G:1263:PEK:H383 | 1.61 | 0.82 |
| 7:G:4:ALA:HB3 | 1:N:282:PHE:HA | 1.60 | 0.82 |
| 12:Y:20:ARG:HH21 | 21:Y:1522:TGL:CC3 | 1.93 | 0.82 |
| 3:C:246:ASP:HB2 | 29:C:4124:HOH:O | 1.81 | 0.81 |
| 7:G:72:ASN:H | 7:G:76:ASN:ND2 | 1.78 | 0.81 |
| 8:U:9:LYS:HG3 | 8:U:10:ASN:N | 1.94 | 0.81 |
| 6:S:76:LYS:HE2 | 29:S:4790:HOH:O | 1.80 | 0.81 |
| 7:T:2:SER:OG | 25:T:263:PEK:H301 | 1.79 | 0.81 |
| 5:R:7:THR:OG1 | 5:R:10:GLU:HG3 | 1.80 | 0.81 |
| 1:N:351:GLY:HA3 | 1:N:380[A]:VAL:HG13 | 1.62 | 0.81 |
| 22:B:229:PSC:C07 | 9:I:10:ARG:HH21 | 1.93 | 0.81 |
| 4:D:45:LYS:HB3 | 29:D:4504:HOH:O | 1.81 | 0.81 |
| 1:N:229:ILE:HD11 | 2:O:175:ILE:HD13 | 1.63 | 0.80 |
| 22:B:229:PSC:H142 | 22:B:229:PSC:H343 | 1.62 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:U:45:ALA:O | 8:U:47:GLY:N | 2.14 | 0.80 |
| 6:S:94:HIS:HD2 | 6:S:95:GLN:N | 1.80 | 0.80 |
| 26:C:270:CDL:C21 | 26:C:270:CDL:H631 | 2.01 | 0.80 |
| 21:N:1523:TGL:HC21 | 21:N:1523:TGL:CG1 | 2.12 | 0.80 |
| 25:C:264:PEK:H162 | 25:C:264:PEK:C10 | 2.07 | 0.79 |
| 26:T:1269:CDL:H111 | 26:T:1269:CDL:CA2 | 2.11 | 0.79 |
| 3:P:5:THR:HG22 | 6:S:96:LEU:HD13 | 1.61 | 0.79 |
| 3:P:67:PHE:HE1 | 26:P:1270:CDL:H1 | 1.48 | 0.79 |
| 19:N:1524:PGV:H321 | 19:N:1524:PGV:H151 | 1.64 | 0.79 |
| 7:G:31:CYS:SG | 26:G:269:CDL:H532 | 2.22 | 0.78 |
| 8:H:43:MET:HE3 | 8:H:49:ASP:H | 1.47 | 0.78 |
| 1:A:481:GLU:HB2 | 13:M:4:LYS:HE2 | 1.63 | 0.78 |
| 22:R:1229:PSC:H142 | 22:R:1229:PSC:H343 | 1.63 | 0.78 |
| 12:L:20:ARG:HH21 | 21:L:522:TGL:HC32 | 1.48 | 0.78 |
| 8:U:9:LYS:O | 8:U:10:ASN:HB2 | 1.82 | 0.77 |
| 10:W:33:ARG:HG2 | 23:W:1059:CHD:H152 | 1.66 | 0.77 |
| 6:F:97:ALA:HB3 | 29:F:4782:HOH:O | 1.84 | 0.77 |
| 6:S:94:HIS:HD2 | 6:S:95:GLN:CA | 1.97 | 0.77 |
| 3:P:107:ALA:HB2 | 19:U:1268:PGV:H031 | 1.66 | 0.77 |
| 1:N:514:LYS:HA | 6:S:38:ALA:HB3 | 1.67 | 0.77 |
| 1:A:351:GLY:HA3 | 1:A:380[A]:VAL:HG13 | 1.67 | 0.76 |
| 5:R:90:ARG:HB3 | 5:R:91:PRO:HD3 | 1.65 | 0.76 |
| 21:Y:1522:TGL:CA9 | 21:Y:1522:TGL:H231 | 2.14 | 0.76 |
| 7:T:72:ASN:H | 7:T:76:ASN:HD22 | 1.33 | 0.76 |
| 25:C:264:PEK:H101 | 25:C:264:PEK:C16 | 2.08 | 0.76 |
| 2:O:227:LEU:OXT | 2:O:227:LEU:HD13 | 1.86 | 0.76 |
| 1:N:334:TRP:CH2 | 2:O:46:LEU:HD13 | 2.21 | 0.75 |
| 26:G:269:CDL:H372 | 2:O:78:LEU:CD1 | 2.16 | 0.75 |
| 22:B:229:PSC:O02 | 22:B:229:PSC:H032 | 1.85 | 0.75 |
| 1:A:484:THR:HB | 13:M:2:THR:OG1 | 1.87 | 0.75 |
| 22:B:229:PSC:H142 | 22:B:229:PSC:C34 | 2.17 | 0.75 |
| 4:Q:34:SER:H | 4:Q:37:GLN:NE2 | 1.84 | 0.74 |
| 6:F:1:ALA:HB3 | 6:S:65:ASP:OD1 | 1.87 | 0.74 |
| 4:D:20:ARG:HG3 | 29:D:4132:HOH:O | 1.86 | 0.74 |
| 2:B:56:MET:HA | 22:B:229:PSC:H201 | 1.68 | 0.74 |
| 19:A:521:PGV:H183 | 25:C:264:PEK:H332 | 1.68 | 0.74 |
| 26:T:1269:CDL:H111 | 26:T:1269:CDL:HA22 | 1.67 | 0.74 |
| 22:R:1229:PSC:H22 | 22:R:1229:PSC:H221 | 1.70 | 0.74 |
| 7:G:5:LYS:HD2 | 25:G:1263:PEK:H372 | 1.69 | 0.73 |
| 2:B:70:ALA:HB1 | 26:T:1269:CDL:H451 | 1.70 | 0.73 |
| 26:G:269:CDL:C22 | 26:G:269:CDL:H522 | 2.18 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:S:95:GLN:CG | 29:S:4728:HOH:O | 2.36 | 0.73 |
| 19:C:267:PGV:C18 | 26:C:270:CDL:H652 | 2.18 | 0.72 |
| 8:H:43:MET:HE3 | 8:H:49:ASP:N | 2.04 | 0.72 |
| 21:N:1523:TGL:HA81 | 21:N:1523:TGL:H231 | 1.71 | 0.72 |
| 19:C:268:PGV:H061 | 29:C:4333:HOH:O | 1.89 | 0.72 |
| 3:C:95:THR:HG21 | 19:C:268:PGV:H282 | 1.71 | 0.72 |
| 26:G:269:CDL:H171 | 29:G:4479:HOH:O | 1.90 | 0.71 |
| 7:G:72:ASN:N | 7:G:76:ASN:HD22 | 1.83 | 0.71 |
| 22:R:1229:PSC:H343 | 22:R:1229:PSC:C14 | 2.20 | 0.71 |
| 9:V:61:GLU:HG3 | 9:V:65:LYS:NZ | 2.06 | 0.71 |
| 12:Y:20:ARG:NH2 | 21:Y:1522:TGL:HC32 | 2.05 | 0.71 |
| 6:S:52:ILE:O | 6:S:94:HIS:ND1 | 2.25 | 0.70 |
| 12:Y:20:ARG:NH2 | 21:Y:1522:TGL:CC3 | 2.54 | 0.70 |
| 26:C:270:CDL:HA22 | 29:J:4496:HOH:O | 1.92 | 0.70 |
| 3:P:67:PHE:CE1 | 26:P:1270:CDL:H1 | 2.27 | 0.70 |
| 7:G:3:ALA:CB | 25:G:1263:PEK:H383 | 2.22 | 0.69 |
| 25:C:265:PEK:H041 | 7:G:17:ARG:HH22 | 1.57 | 0.69 |
| 19:N:1524:PGV:H012 | 19:N:1524:PGV:C22 | 2.22 | 0.69 |
| 1:N:351:GLY:CA | 1:N:380[A]:VAL:HG13 | 2.21 | 0.69 |
| 6:S:94:HIS:HD2 | 6:S:95:GLN:HA | 1.57 | 0.69 |
| 12:Y:12:PRO:HB2 | 21:Y:1522:TGL:HG11 | 1.72 | 0.69 |
| 22:B:229:PSC:H041 | 5:E:41:LEU:HD23 | 1.73 | 0.69 |
| 21:B:521:TGL:H252 | 21:B:521:TGL:HA91 | 1.75 | 0.69 |
| 7:T:3:ALA:CB | 25:T:263:PEK:H383 | 2.22 | 0.69 |
| 21:D:523:TGL:H242 | 21:D:523:TGL:HA91 | 1.74 | 0.69 |
| 25:P:1264:PEK:HN2 | 7:T:76:ASN:HD21 | 1.39 | 0.68 |
| 1:A:282:PHE:HA | 7:T:4:ALA:HB3 | 1.75 | 0.68 |
| 10:J:26:ALA:O | 10:J:30:ILE:HD12 | 1.94 | 0.68 |
| 10:J:4:ARG:HD3 | 10:J:7:GLU:OE2 | 1.94 | 0.68 |
| 7:T:2:SER:O | 25:T:263:PEK:H331 | 1.93 | 0.68 |
| 7:G:5:LYS:HB3 | 1:N:278:MET:SD | 2.34 | 0.68 |
| 7:T:45:PRO:HD2 | 29:T:3099:HOH:O | 1.94 | 0.68 |
| 26:C:270:CDL:H222 | 26:C:270:CDL:H661 | 1.76 | 0.68 |
| 14:N:515:HEA:HMC1 | 14:N:515:HEA:HBC1 | 1.76 | 0.67 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:CA | 2.73 | 0.67 |
| 14:A:515:HEA:HMC1 | 14:A:515:HEA:HBC1 | 1.75 | 0.67 |
| 21:N:1523:TGL:HG11 | 21:N:1523:TGL:CC2 | 2.18 | 0.67 |
| 7:T:37:LEU:HD21 | 26:T:1269:CDL:H361 | 1.76 | 0.67 |
| 7:G:7:ASP:O | 7:G:9:GLY:N | 2.22 | 0.67 |
| 1:N:378:HIS:HA | 1:N:382[A]:SER:OG | 1.93 | 0.67 |
| 26:T:1269:CDL:OB4 | 26:T:1269:CDL:H1 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:C:268:PGV:H102 | 29:C:4697:HOH:O | 1.94 | 0.67 |
| 1:N:290:HIS:CD2 | 1:N:291:HIS:CD2 | 2.82 | 0.67 |
| 1:N:351:GLY:C | 1:N:380[A]:VAL:CG1 | 2.62 | 0.66 |
| 29:A:4171:HOH:O | 22:B:229:PSC:H32 | 1.96 | 0.66 |
| 2:O:52:HIS:CE1 | 22:R:1229:PSC:H202 | 2.31 | 0.66 |
| 21:Y:1522:TGL:OC1 | 21:Y:1522:TGL:HC51 | 1.96 | 0.66 |
| 2:B:183:THR:CG2 | 29:B:4424:HOH:O | 2.43 | 0.66 |
| 25:C:265:PEK:H371 | 26:G:269:CDL:C27 | 2.26 | 0.66 |
| 2:O:227:LEU:HB2 | 29:O:4695:HOH:O | 1.96 | 0.66 |
| 10:J:33:ARG:HG2 | 23:J:60:CHD:C15 | 2.25 | 0.66 |
| 1:A:282:PHE:HA | 7:T:4:ALA:HB1 | 1.76 | 0.66 |
| 1:N:265:LYS:HB2 | 1:N:490:THR:HG21 | 1.77 | 0.66 |
| 25:C:265:PEK:H042 | 6:F:1:ALA:H1 | 1.61 | 0.66 |
| 22:B:229:PSC:H31 | 22:B:229:PSC:H221 | 1.78 | 0.66 |
| 8:H:9:LYS:O | 8:H:10:ASN:CB | 2.43 | 0.65 |
| 29:N:4633:HOH:O | 2:O:87:MET:SD | 2.53 | 0.65 |
| 26:G:269:CDL:H752 | 1:N:282:PHE:HZ | 1.62 | 0.65 |
| 3:P:160:LEU:HD13 | 23:P:1271:CHD:H181 | 1.79 | 0.65 |
| 26:T:1269:CDL:H111 | 26:T:1269:CDL:HA21 | 1.78 | 0.65 |
| 6:S:94:HIS:CG | 6:S:95:GLN:H | 2.12 | 0.65 |
| 6:F:87:THR:HG21 | 29:F:4730:HOH:O | 1.97 | 0.65 |
| 19:P:1267:PGV:H181 | 26:P:1270:CDL:H651 | 1.79 | 0.65 |
| 4:D:86:MET:CE | 29:K:4243:HOH:O | 2.44 | 0.64 |
| 12:L:11:ILE:CG2 | 21:L:522:TGL:H272 | 2.27 | 0.64 |
| 1:N:407:ASP:O | 1:N:411:LYS:HG3 | 1.97 | 0.64 |
| 12:Y:47:LYS:OXT | 12:Y:47:LYS:HE2 | 1.97 | 0.64 |
| 25:C:265:PEK:H222 | 25:C:265:PEK:H6 | 1.80 | 0.64 |
| 26:T:1269:CDL:H241 | 26:T:1269:CDL:C53 | 2.27 | 0.64 |
| 7:T:7:ASP:CG | 7:T:8:HIS:N | 2.51 | 0.64 |
| 1:A:51:ASP:OD1 | 1:A:441:SER:OG | 2.12 | 0.64 |
| 12:Y:22:LEU:O | 12:Y:26:THR:HB | 1.96 | 0.64 |
| 4:Q:94:LEU:HD23 | 11:X:28:VAL:HG21 | 1.79 | 0.64 |
| 1:N:406:ASN:HD21 | 19:N:1524:PGV:H21 | 1.63 | 0.63 |
| 1:N:87:ILE:O | 1:N:173:PRO:HD3 | 1.99 | 0.63 |
| 8:H:43:MET:CE | 8:H:49:ASP:H | 2.11 | 0.63 |
| 1:N:113:LEU:HD12 | 21:Y:1522:TGL:C13 | 2.28 | 0.63 |
| 8:H:46:LYS:HE2 | 8:U:8:ILE:CG2 | 2.27 | 0.63 |
| 2:O:59:GLN:C | 2:O:60:GLU:HG3 | 2.19 | 0.63 |
| 25:C:264:PEK:HN2 | 7:G:76:ASN:HD21 | 1.46 | 0.63 |
| 6:F:64:GLU:O | 6:F:65:ASP:HB2 | 1.97 | 0.63 |
| 4:Q:92:THR:O | 4:Q:95:LEU:HB2 | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 10:W:2:GLU:HG2 | 29:W:4564:HOH:O | 1.98 | 0.63 |
| 4:D:78:TRP:HB3 | 21:D:523:TGL:HB22 | 1.81 | 0.62 |
| 10:J:33:ARG:HG2 | 23:J:60:CHD:H151 | 1.80 | 0.62 |
| 1:A:485:VAL:HG22 | 13:M:1:ILE:HG13 | 1.82 | 0.62 |
| 25:P:1264:PEK:H12 | 25:P:1264:PEK:H242 | 1.80 | 0.62 |
| 6:S:94:HIS:CG | 6:S:95:GLN:N | 2.66 | 0.62 |
| 12:Y:2:HIS:CG | 12:Y:3:TYR:H | 2.17 | 0.62 |
| 2:B:196:CYS:HB2 | 2:B:207:MET:HG3 | 1.82 | 0.62 |
| 13:M:10:THR:HA | 13:M:14:GLU:OE2 | 2.00 | 0.62 |
| 26:P:1270:CDL:HB22 | 26:P:1270:CDL:PA1 | 2.40 | 0.62 |
| 22:R:1229:PSC:H071 | 9:V:10:ARG:HE | 1.65 | 0.62 |
| 26:G:269:CDL:H351 | 2:O:78:LEU:HD12 | 1.80 | 0.61 |
| 3:P:29:SER:CB | 3:P:42:LEU:HD13 | 2.28 | 0.61 |
| 1:A:32:ALA:HB3 | 12:L:36:PRO:HG2 | 1.83 | 0.61 |
| 1:N:488:THR:HB | 1:N:495:LEU:HD13 | 1.82 | 0.61 |
| 23:P:1271:CHD:C16 | 23:P:1271:CHD:H232 | 2.31 | 0.61 |
| 14:A:516:HEA:HMC1 | 14:A:516:HEA:HBC1 | 1.81 | 0.61 |
| 12:Y:20:ARG:NH2 | 12:Y:24:MET:HG3 | 2.15 | 0.61 |
| 1:N:351:GLY:C | 1:N:380[A]:VAL:HG13 | 2.21 | 0.61 |
| 26:T:1269:CDL:H751 | 26:T:1269:CDL:H582 | 1.83 | 0.61 |
| 1:A:514:LYS:NZ | 29:A:2645:HOH:O | 2.34 | 0.61 |
| 19:A:524:PGV:H221 | 19:A:524:PGV:H012 | 1.82 | 0.61 |
| 3:C:63:ARG:NH2 | 26:C:270:CDL:HA21 | 2.15 | 0.61 |
| 2:O:62:GLU:O | 2:O:66:THR:HB | 2.01 | 0.61 |
| 3:C:33:MET:HE3 | 29:J:4237:HOH:O | 2.01 | 0.60 |
| 10:W:2:GLU:CB | 10:W:4:ARG:HH12 | 2.10 | 0.60 |
| 26:G:269:CDL:H362 | 2:O:81:LEU:HD12 | 1.83 | 0.60 |
| 8:U:48:GLY:HA2 | 29:U:4792:HOH:O | 2.00 | 0.60 |
| 1:N:113:LEU:HD12 | 21:Y:1522:TGL:C14 | 2.31 | 0.60 |
| 1:N:484:THR:HB | 13:Z:2:THR:OG1 | 2.02 | 0.60 |
| 4:Q:66:GLU:HG2 | 29:Q:4646:HOH:O | 2.02 | 0.60 |
| 7:G:2:SER:OG | 25:G:1263:PEK:H292 | 2.00 | 0.60 |
| 2:O:66:THR:HG21 | 23:O:229:CHD:H3 | 1.84 | 0.60 |
| 6:F:1:ALA:CB | 6:S:65:ASP:OD1 | 2.49 | 0.60 |
| 12:L:2:HIS:CG | 12:L:3:TYR:H | 2.19 | 0.59 |
| 1:A:351:GLY:C | 1:A:380[A]:VAL:CG1 | 2.70 | 0.59 |
| 7:G:6:GLY:O | 25:G:1263:PEK:H311 | 2.03 | 0.59 |
| 29:A:2527:HOH:O | 12:L:7:PRO:HG3 | 2.03 | 0.59 |
| 1:A:351:GLY:CA | 1:A:380[A]:VAL:HG13 | 2.33 | 0.59 |
| 3:P:210:ILE:HG12 | 19:P:1267:PGV:H132 | 1.85 | 0.59 |
| 21:B:521:TGL:C28 | 21:B:521:TGL:H101 | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:215:PRO:HD3 | 9:V:60:PHE:CD2 | 2.38 | 0.58 |
| 2:O:56:MET:HA | 22:R:1229:PSC:H201 | 1.83 | 0.58 |
| 3:C:80:ARG:NH1 | 3:C:236:GLU:OE2 | 2.34 | 0.58 |
| 1:N:177:SER:H | 1:N:180:GLN:NE2 | 2.00 | 0.58 |
| 1:N:377:PHE:O | 1:N:381[A]:LEU:HB3 | 2.03 | 0.58 |
| 25:G:1263:PEK:H221 | 25:G:1263:PEK:HN1 | 1.68 | 0.58 |
| 21:N:1523:TGL:H231 | 21:N:1523:TGL:CA9 | 2.33 | 0.58 |
| 1:A:107:PRO:HB3 | 3:C:25:LEU:HB2 | 1.84 | 0.58 |
| 1:N:113:LEU:CD1 | 21:Y:1522:TGL:H292 | 2.33 | 0.58 |
| 21:N:1523:TGL:HC61 | 29:O:3562:HOH:O | 2.03 | 0.58 |
| 4:Q:109:HIS:HD2 | 29:Q:3122:HOH:O | 1.86 | 0.58 |
| 26:C:270:CDL:O1 | 26:C:270:CDL:OA3 | 2.11 | 0.58 |
| 1:N:377:PHE:O | 1:N:381[B]:LEU:HB2 | 2.04 | 0.58 |
| 2:O:59:GLN:O | 2:O:59:GLN:CG | 2.40 | 0.58 |
| 1:A:400:PHE:HB3 | 21:L:522:TGL:H283 | 1.86 | 0.58 |
| 19:A:524:PGV:H142 | 19:A:524:PGV:C30 | 2.34 | 0.58 |
| 23:O:229:CHD:H212 | 23:O:229:CHD:H12 | 1.85 | 0.58 |
| 23:C:525:CHD:H152 | 19:C:268:PGV:H11 | 1.86 | 0.58 |
| 3:C:55:TYR:CE1 | 26:C:270:CDL:H512 | 2.38 | 0.58 |
| 2:O:23:PHE:CZ | 2:O:80:SER:HB2 | 2.39 | 0.58 |
| 9:V:10:ARG:HG3 | 9:V:10:ARG:HH11 | 1.68 | 0.58 |
| 9:V:61:GLU:HG3 | 9:V:65:LYS:HZ1 | 1.69 | 0.58 |
| 1:N:113:LEU:HD13 | 21:Y:1522:TGL:H292 | 1.85 | 0.57 |
| 25:C:265:PEK:H371 | 26:G:269:CDL:H273 | 1.86 | 0.57 |
| 26:C:270:CDL:CB2 | 10:J:8:LYS:HZ2 | 2.01 | 0.57 |
| 1:N:194:LEU:HD22 | 1:N:285:PHE:HE2 | 1.69 | 0.57 |
| 21:B:521:TGL:HC21 | 29:I:2606:HOH:O | 2.04 | 0.57 |
| 25:C:265:PEK:H042 | 6:F:1:ALA:N | 2.20 | 0.57 |
| 1:N:400:PHE:HB3 | 21:Y:1522:TGL:H283 | 1.87 | 0.57 |
| 1:A:514:LYS:HA | 6:F:38:ALA:HB3 | 1.87 | 0.57 |
| 1:N:449:MET:SD | 2:O:5:MET:HG2 | 2.44 | 0.57 |
| 25:T:1265:PEK:C37 | 26:T:1269:CDL:C27 | 2.82 | 0.57 |
| 2:B:132:GLU:HB3 | 2:B:137:GLU:HG3 | 1.86 | 0.57 |
| 9:V:2:THR:HG22 | 9:V:3:ALA:H | 1.69 | 0.57 |
| 7:G:7:ASP:HB3 | 29:N:4167:HOH:O | 2.02 | 0.57 |
| 8:H:45:ALA:O | 8:H:47:GLY:N | 2.37 | 0.57 |
| 3:P:223:LEU:HD21 | 23:P:1271:CHD:H183 | 1.87 | 0.57 |
| 1:N:514:LYS:HA | 6:S:38:ALA:CB | 2.35 | 0.56 |
| 26:C:270:CDL:HB22 | 10:J:8:LYS:HZ1 | 1.65 | 0.56 |
| 1:A:307:SER:HB3 | 26:T:1269:CDL:H171 | 1.86 | 0.56 |
| 22:R:1229:PSC:H011 | 22:R:1229:PSC:C2 | 2.35 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G:11:TPO:CG2 | 7:G:11:TPO:O | 2.53 | 0.56 |
| 29:N:4604:HOH:O | 11:X:8:ASP:HB2 | 2.05 | 0.56 |
| 2:O:13:THR:HB | 2:O:168:LEU:HD23 | 1.88 | 0.56 |
| 21:O:1521:TGL:H241 | 21:O:1521:TGL:H201 | 1.87 | 0.56 |
| 19:C:268:PGV:C06 | 29:C:4333:HOH:O | 2.52 | 0.56 |
| 2:O:52:HIS:HE1 | 22:R:1229:PSC:H202 | 1.68 | 0.56 |
| 6:S:64:GLU:O | 6:S:65:ASP:HB2 | 2.05 | 0.56 |
| 19:A:524:PGV:H312 | 13:M:16:ALA:HA | 1.88 | 0.56 |
| 2:O:146:MET:HA | 2:O:213:LEU:HD12 | 1.88 | 0.56 |
| 9:V:52:ARG:CZ | 9:V:52:ARG:HB2 | 2.36 | 0.55 |
| 23:P:1271:CHD:H232 | 23:P:1271:CHD:H162 | 1.87 | 0.55 |
| 7:T:35:SER:HB3 | 7:T:36:TRP:CE3 | 2.42 | 0.55 |
| 6:S:54:ASN:HD22 | 6:S:54:ASN:C | 2.09 | 0.55 |
| 7:T:5:LYS:CG | 25:T:263:PEK:H371 | 2.36 | 0.55 |
| 7:G:2:SER:HG | 25:G:1263:PEK:H291 | 1.71 | 0.55 |
| 12:L:14:SER:H | 21:L:522:TGL:HC31 | 1.72 | 0.55 |
| 25:P:1264:PEK:C3 | 25:P:1264:PEK:H71 | 2.26 | 0.55 |
| 22:B:229:PSC:H42 | 29:I:2588:HOH:O | 2.07 | 0.55 |
| 2:O:84:LEU:HA | 2:O:87:MET:CE | 2.36 | 0.55 |
| 3:P:40:MET:O | 3:P:44:MET:HG2 | 2.07 | 0.55 |
| 6:S:92:VAL:HG23 | 6:S:92:VAL:O | 2.06 | 0.55 |
| 1:A:382[A]:SER:O | 1:A:386:VAL:HB | 2.06 | 0.55 |
| 26:G:269:CDL:C11 | 26:G:269:CDL:HA21 | 2.33 | 0.55 |
| 2:O:164:ALA:O | 2:O:194:GLY:HA3 | 2.07 | 0.55 |
| 21:D:523:TGL:HG31 | 21:D:523:TGL:OA1 | 2.07 | 0.55 |
| 14:A:516:HEA:HMC1 | 14:A:516:HEA:CBC | 2.37 | 0.55 |
| 21:N:1523:TGL:CA8 | 21:N:1523:TGL:H231 | 2.36 | 0.55 |
| 25:T:1265:PEK:C38 | 26:T:1269:CDL:H271 | 2.11 | 0.55 |
| 4:D:34:SER:O | 4:D:38:LYS:HG3 | 2.07 | 0.54 |
| 7:G:7:ASP:CB | 29:N:4167:HOH:O | 2.55 | 0.54 |
| 8:H:23:GLN:HG3 | 29:H:4128:HOH:O | 2.07 | 0.54 |
| 5:R:48:ILE:O | 5:R:52:LEU:HG | 2.07 | 0.54 |
| 19:U:1268:PGV:C03 | 29:U:4495:HOH:O | 2.22 | 0.54 |
| 6:S:1:ALA:N | 25:T:1265:PEK:H041 | 2.22 | 0.54 |
| 7:T:5:LYS:HG3 | 25:T:263:PEK:H371 | 1.90 | 0.54 |
| 4:Q:33:LEU:HA | 4:Q:37:GLN:NE2 | 2.22 | 0.54 |
| 6:S:95:GLN:HG2 | 29:S:4728:HOH:O | 2.05 | 0.54 |
| 23:W:1059:CHD:H41 | 29:W:4647:HOH:O | 2.07 | 0.54 |
| 1:A:381[A]:LEU:HB2 | 14:A:516:HEA:CAC | 2.38 | 0.54 |
| 6:S:95:GLN:HG3 | 29:S:4728:HOH:O | 2.03 | 0.54 |
| 7:T:31:CYS:SG | 26:T:1269:CDL:H532 | 2.48 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:104:TRP:CG | 2:B:203:ASN:HB2 | 2.43 | 0.54 |
| 7:T:7:ASP:O | 7:T:8:HIS:CB | 2.53 | 0.54 |
| 2:B:29:MET:HB2 | 9:I:35:TYR:CE2 | 2.43 | 0.53 |
| 3:C:59:ARG:HA | 26:C:270:CDL:H522 | 1.90 | 0.53 |
| 9:V:1:SAC:OAC | 9:V:1:SAC:HB3 | 2.09 | 0.53 |
| 21:D:523:TGL:CG3 | 29:D:4105:HOH:O | 2.42 | 0.53 |
| 2:O:104:TRP:CD2 | 2:O:203:ASN:HB2 | 2.44 | 0.53 |
| 26:P:1270:CDL:H352 | 26:P:1270:CDL:H162 | 1.90 | 0.53 |
| 3:P:51:MET:HB3 | 26:P:1270:CDL:H392 | 1.90 | 0.53 |
| 1:N:297:MET:CE | 1:N:297:MET:HB2 | 2.39 | 0.53 |
| 26:T:1269:CDL:C11 | 26:T:1269:CDL:HA22 | 2.36 | 0.53 |
| 8:U:43:MET:HE3 | 8:U:49:ASP:N | 2.23 | 0.53 |
| 7:T:8:HIS:O | 7:T:9:GLY:C | 2.46 | 0.53 |
| 4:Q:118:LYS:HB3 | 11:X:53:TRP:HB3 | 1.91 | 0.53 |
| 19:N:1524:PGV:H011 | 19:N:1524:PGV:H221 | 1.85 | 0.53 |
| 21:N:1523:TGL:HA92 | 21:N:1523:TGL:H231 | 1.91 | 0.53 |
| 3:C:106:LEU:HD13 | 19:C:268:PGV:H22 | 1.90 | 0.53 |
| 4:D:121:LYS:HD3 | 11:K:52:GLU:HA | 1.91 | 0.53 |
| 1:A:47:LEU:O | 13:M:41:LYS:HE3 | 2.09 | 0.53 |
| 7:T:42:ARG:HB2 | 29:T:4747:HOH:O | 2.09 | 0.53 |
| 2:B:58:ALA:O | 2:B:62:GLU:HG3 | 2.09 | 0.53 |
| 25:C:265:PEK:C37 | 26:G:269:CDL:C27 | 2.86 | 0.53 |
| 12:L:20:ARG:HH12 | 21:L:522:TGL:HC61 | 1.74 | 0.53 |
| 6:S:1:ALA:N | 25:T:1265:PEK:C04 | 2.72 | 0.53 |
| 22:B:229:PSC:C07 | 9:I:10:ARG:NH2 | 2.69 | 0.52 |
| 26:G:269:CDL:H471 | 29:G:4791:HOH:O | 2.08 | 0.52 |
| 4:Q:34:SER:H | 4:Q:37:GLN:HE21 | 1.56 | 0.52 |
| 1:A:28:MET:HE2 | 14:A:515:HEA:H271 | 1.92 | 0.52 |
| 19:A:524:PGV:C22 | 19:A:524:PGV:H012 | 2.39 | 0.52 |
| 2:B:183:THR:HG23 | 29:B:4424:HOH:O | 2.04 | 0.52 |
| 1:N:352:GLY:N | 1:N:380[A]:VAL:CG1 | 2.72 | 0.52 |
| 1:A:87:ILE:O | 1:A:173:PRO:HD3 | 2.10 | 0.52 |
| 8:H:45:ALA:C | 8:H:47:GLY:H | 2.12 | 0.52 |
| 7:T:11:TPO:HG22 | 7:T:16:TRP:HE1 | 1.74 | 0.52 |
| 2:B:89:GLU:O | 2:B:91:ASN:ND2 | 2.42 | 0.52 |
| 7:G:11:TPO:CG2 | 7:G:16:TRP:HE1 | 2.19 | 0.52 |
| 26:C:270:CDL:PA1 | 26:C:270:CDL:HB21 | 2.50 | 0.52 |
| 5:E:52:LEU:O | 5:E:55:CYS:HB2 | 2.09 | 0.52 |
| 2:O:222:TRP:O | 2:O:226:MET:HB2 | 2.10 | 0.52 |
| 6:F:55:LYS:HA | 6:F:74:LEU:O | 2.10 | 0.52 |
| 2:O:104:TRP:CG | 2:O:203:ASN:HB2 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 19:A:524:PGV:H142 | 19:A:524:PGV:H301 | 1.90 | 0.52 |
| 8:U:9:LYS:CG | 8:U:10:ASN:H | 2.09 | 0.52 |
| 2:O:84:LEU:HA | 2:O:87:MET:HE3 | 1.92 | 0.51 |
| 25:C:264:PEK:H71 | 25:C:264:PEK:H32 | 1.93 | 0.51 |
| 4:D:61:ARG:HD2 | 29:D:2674:HOH:O | 2.10 | 0.51 |
| 29:L:4557:HOH:O | 13:M:32:TRP:HH2 | 1.94 | 0.51 |
| 6:S:76:LYS:HG3 | 6:S:93:PRO:HG2 | 1.92 | 0.51 |
| 6:S:94:HIS:O | 6:S:95:GLN:HB2 | 2.09 | 0.51 |
| 5:R:23:ASP:O | 5:R:24:ILE:C | 2.49 | 0.51 |
| 6:S:95:GLN:O | 6:S:97:ALA:N | 2.43 | 0.51 |
| 7:G:3:ALA:HB3 | 25:G:1263:PEK:H362 | 1.91 | 0.51 |
| 1:N:290:HIS:HD2 | 1:N:291:HIS:CD2 | 2.26 | 0.51 |
| 1:A:290:HIS:CD2 | 1:A:291:HIS:CD2 | 2.98 | 0.51 |
| 12:L:20:ARG:HH22 | 21:L:522:TGL:CC3 | 2.19 | 0.51 |
| 1:N:106:PRO:HB2 | 1:N:107:PRO:HD3 | 1.92 | 0.51 |
| 8:H:7:LYS:O | 8:H:8:ILE:HG22 | 2.10 | 0.51 |
| 1:N:381[A]:LEU:O | 1:N:385:ALA:HB3 | 2.11 | 0.51 |
| 6:S:55:LYS:HA | 6:S:74:LEU:O | 2.11 | 0.51 |
| 3:P:131:LEU:HD21 | 26:T:1269:CDL:HB61 | 1.91 | 0.51 |
| 1:A:177:SER:H | 1:A:180:GLN:NE2 | 2.08 | 0.51 |
| 2:B:62:GLU:O | 2:B:66:THR:HB | 2.11 | 0.51 |
| 3:P:59:ARG:HA | 26:P:1270:CDL:H522 | 1.93 | 0.51 |
| 7:T:38:HIS:NE2 | 26:T:1269:CDL:HA21 | 2.26 | 0.51 |
| 8:U:43:MET:HG3 | 8:U:49:ASP:O | 2.11 | 0.51 |
| 8:H:46:LYS:HE2 | 8:U:8:ILE:HG21 | 1.92 | 0.51 |
| 26:P:1270:CDL:OB7 | 26:P:1270:CDL:H112 | 2.10 | 0.51 |
| 25:C:265:PEK:C04 | 6:F:1:ALA:N | 2.74 | 0.51 |
| 7:T:17:ARG:NH1 | 25:T:1265:PEK:O13 | 2.43 | 0.51 |
| 5:E:31:LYS:HE3 | 6:F:84:SER:O | 2.12 | 0.50 |
| 2:O:83:ILE:O | 2:O:87:MET:HG3 | 2.11 | 0.50 |
| 25:G:1263:PEK:H281 | 3:P:85:LEU:HD21 | 1.93 | 0.50 |
| 1:A:351:GLY:HA3 | 1:A:380[A]:VAL:CG1 | 2.39 | 0.50 |
| 26:G:269:CDL:C37 | 2:O:78:LEU:CD1 | 2.88 | 0.50 |
| 3:C:65:SER:HB2 | 19:C:267:PGV:H041 | 1.94 | 0.50 |
| 7:T:5:LYS:HG3 | 25:T:263:PEK:H383 | 1.93 | 0.50 |
| 26:G:269:CDL:CA2 | 26:G:269:CDL:H112 | 2.33 | 0.50 |
| 8:U:27:ARG:HG2 | 29:U:4672:HOH:O | 2.12 | 0.50 |
| 1:A:377:PHE:O | 1:A:381[A]:LEU:HB3 | 2.11 | 0.50 |
| 1:N:381[A]:LEU:HD13 | 14:N:516:HEA:HBC2 | 1.94 | 0.50 |
| 6:S:1:ALA:H1 | 25:T:1265:PEK:C04 | 2.24 | 0.50 |
| 9:V:61:GLU:HG3 | 9:V:65:LYS:HZ2 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:78:LEU:HD12 | 26:T:1269:CDL:H352 | 1.93 | 0.50 |
| 12:Y:2:HIS:N | 29:Y:4665:HOH:O | 2.44 | 0.50 |
| 7:T:8:HIS:O | 7:T:9:GLY:O | 2.30 | 0.49 |
| 12:Y:14:SER:H | 21:Y:1522:TGL:HC31 | 1.77 | 0.49 |
| 3:P:59:ARG:HG3 | 26:P:1270:CDL:H511 | 1.93 | 0.49 |
| 1:A:347:LEU:HD22 | 1:A:383[B]:MET:SD | 2.51 | 0.49 |
| 2:B:68:LEU:HB3 | 22:B:229:PSC:H182 | 1.92 | 0.49 |
| 7:G:5:LYS:HB2 | 25:G:1263:PEK:H351 | 1.95 | 0.49 |
| 10:J:36:MET:HG2 | 23:J:60:CHD:H221 | 1.95 | 0.49 |
| 21:N:1523:TGL:HG32 | 21:N:1523:TGL:OB1 | 2.11 | 0.49 |
| 1:N:177:SER:H | 1:N:180:GLN:HE21 | 1.60 | 0.49 |
| 26:G:269:CDL:H182 | 1:N:307:SER:CB | 2.42 | 0.49 |
| 8:H:7:LYS:O | 8:H:8:ILE:HB | 2.12 | 0.49 |
| 1:A:21:LEU:CD2 | 21:L:522:TGL:HA81 | 2.43 | 0.49 |
| 7:T:5:LYS:HG3 | 25:T:263:PEK:C37 | 2.42 | 0.49 |
| 10:W:3:ASN:C | 10:W:3:ASN:OD1 | 2.51 | 0.49 |
| 1:A:115:SER:O | 1:A:121:GLY:HA2 | 2.12 | 0.49 |
| 6:F:54:ASN:OD1 | 6:F:76:LYS:HD2 | 2.12 | 0.49 |
| 1:N:489:THR:HA | 6:S:71:TRP:O | 2.12 | 0.49 |
| 29:N:4743:HOH:O | 23:W:1059:CHD:H212 | 2.12 | 0.49 |
| 1:A:489:THR:HA | 6:F:71:TRP:O | 2.12 | 0.49 |
| 1:N:71:MET:HE3 | 1:N:195:LEU:HD21 | 1.94 | 0.49 |
| 1:A:194:LEU:HD22 | 1:A:285:PHE:HE2 | 1.77 | 0.49 |
| 3:C:191:GLY:HA3 | 29:G:2132:HOH:O | 2.13 | 0.49 |
| 12:Y:20:ARG:NH2 | 21:Y:1522:TGL:HC31 | 2.25 | 0.49 |
| 1:A:310:MET:HE2 | 1:A:356:ILE:HG23 | 1.95 | 0.49 |
| 7:G:17:ARG:HD2 | 29:G:2446:HOH:O | 2.12 | 0.49 |
| 3:C:84:ILE:HD13 | 25:T:263:PEK:H241 | 1.95 | 0.49 |
| 3:C:210:ILE:HG21 | 19:C:267:PGV:H282 | 1.95 | 0.49 |
| 4:D:86:MET:HE2 | 29:K:4243:HOH:O | 2.10 | 0.49 |
| 25:C:265:PEK:C36 | 26:G:269:CDL:H271 | 2.42 | 0.49 |
| 4:D:60:TYR:OH | 5:E:69:GLU:OE1 | 2.22 | 0.48 |
| 21:N:1523:TGL:HC81 | 2:O:47:THR:HA | 1.95 | 0.48 |
| 5:R:41:LEU:HD22 | 22:R:1229:PSC:H072 | 1.95 | 0.48 |
| 1:N:53:ILE:HD12 | 12:Y:44:LEU:HD23 | 1.95 | 0.48 |
| 1:A:310:MET:CE | 1:A:356:ILE:HG23 | 2.43 | 0.48 |
| 1:A:383[A]:MET:O | 1:A:384[A]:GLY:C | 2.48 | 0.48 |
| 1:N:381[A]:LEU:HB2 | 14:N:516:HEA:CAC | 2.43 | 0.48 |
| 7:T:5:LYS:HG3 | 25:T:263:PEK:C38 | 2.42 | 0.48 |
| 7:T:72:ASN:H | 7:T:76:ASN:ND2 | 2.06 | 0.48 |
| 7:G:11:TPO:HG23 | 7:G:11:TPO:O | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:Y:1522:TGL:OC1 | 21:Y:1522:TGL:CC5 | 2.61 | 0.48 |
| 1:A:478:SER:O | 13:M:6:ALA:HB1 | 2.13 | 0.48 |
| 22:B:229:PSC:H041 | 5:E:41:LEU:CD2 | 2.41 | 0.48 |
| 4:Q:23:PRO:O | 4:Q:25:PRO:HD3 | 2.13 | 0.48 |
| 23:C:271:CHD:H12A | 23:C:271:CHD:H112 | 1.61 | 0.48 |
| 19:A:524:PGV:H011 | 19:A:524:PGV:C2 | 2.38 | 0.48 |
| 7:G:17:ARG:CD | 29:G:2446:HOH:O | 2.60 | 0.48 |
| 27:C:272:DMU:H1 | 7:G:69:PHE:HZ | 1.79 | 0.48 |
| 1:N:248:LEU:O | 1:N:251:PHE:HB2 | 2.13 | 0.48 |
| 7:G:4:ALA:CB | 1:N:282:PHE:HA | 2.39 | 0.48 |
| 7:T:38:HIS:HE1 | 26:T:1269:CDL:OA7 | 1.95 | 0.48 |
| 1:A:281:GLY:O | 7:T:4:ALA:HB1 | 2.14 | 0.48 |
| 1:A:409:TRP:HB3 | 1:A:471:ILE:HG12 | 1.95 | 0.48 |
| 14:N:516:HEA:HBC1 | 14:N:516:HEA:HMC1 | 1.96 | 0.48 |
| 5:R:41:LEU:HD23 | 22:R:1229:PSC:H041 | 1.95 | 0.48 |
| 26:G:269:CDL:H762 | 26:G:269:CDL:C56 | 2.25 | 0.48 |
| 1:N:390:MET:O | 1:N:394:VAL:HG13 | 2.13 | 0.48 |
| 1:N:155:VAL:CG2 | 25:P:1264:PEK:H382 | 2.44 | 0.48 |
| 4:Q:12:ALA:O | 6:S:75:HIS:NE2 | 2.46 | 0.48 |
| 1:A:406:ASN:HD21 | 19:A:524:PGV:H21 | 1.78 | 0.47 |
| 25:C:265:PEK:H362 | 26:G:269:CDL:C27 | 2.44 | 0.47 |
| 7:G:5:LYS:HG3 | 25:G:1263:PEK:C37 | 2.40 | 0.47 |
| 3:P:22:LEU:O | 3:P:26:LEU:HG | 2.14 | 0.47 |
| 1:A:28:MET:CE | 14:A:515:HEA:H271 | 2.45 | 0.47 |
| 21:O:1521:TGL:HA82 | 21:O:1521:TGL:H301 | 1.96 | 0.47 |
| 3:P:112:LEU:HD13 | 3:P:118:PRO:HG3 | 1.97 | 0.47 |
| 6:F:62:CYS:HB3 | 6:F:85:CYS:HB3 | 1.96 | 0.47 |
| 1:N:498:CYS:HA | 1:N:499:PRO:HA | 1.74 | 0.47 |
| 2:B:41:ILE:HD13 | 22:B:229:PSC:H342 | 1.97 | 0.47 |
| 1:N:242:GLU:HA | 1:N:245:ILE:HD12 | 1.97 | 0.47 |
| 14:N:515:HEA:HHC | 14:N:515:HEA:H11 | 1.63 | 0.47 |
| 3:P:63:ARG:HE | 26:P:1270:CDL:CA2 | 2.28 | 0.47 |
| 7:T:17:ARG:HD2 | 29:T:3446:HOH:O | 2.13 | 0.47 |
| 27:C:272:DMU:O1 | 27:C:272:DMU:H29 | 2.15 | 0.47 |
| 8:U:45:ALA:C | 8:U:47:GLY:H | 2.13 | 0.47 |
| 2:B:13:THR:HB | 2:B:168:LEU:HD23 | 1.97 | 0.47 |
| 25:C:265:PEK:C36 | 26:G:269:CDL:C27 | 2.93 | 0.47 |
| 10:J:40:LEU:HD12 | 23:J:60:CHD:H183 | 1.97 | 0.47 |
| 26:C:270:CDL:HA4 | 26:C:270:CDL:H131 | 1.97 | 0.47 |
| 4:D:109:HIS:HD2 | 29:D:2122:HOH:O | 1.97 | 0.47 |
| 1:N:240:HIS:O | 1:N:241:PRO:C | 2.51 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 22:R:1229:PSC:O01 | 22:R:1229:PSC:H212 | 2.15 | 0.47 |
| 1:N:321:PHE:CD2 | 22:R:1229:PSC:H341 | 2.49 | 0.47 |
| 7:T:6:GLY:O | 7:T:7:ASP:O | 2.32 | 0.47 |
| 21:B:521:TGL:H211 | 21:B:521:TGL:H241 | 1.59 | 0.47 |
| 8:H:43:MET:O | 8:H:44:THR:C | 2.53 | 0.47 |
| 10:J:52:TRP:O | 10:J:57:HIS:HE1 | 1.98 | 0.47 |
| 21:Y:1522:TGL:CC4 | 21:Y:1522:TGL:OC1 | 2.63 | 0.47 |
| 2:B:196:CYS:CB | 2:B:207:MET:HG3 | 2.45 | 0.47 |
| 26:T:1269:CDL:H732 | 26:T:1269:CDL:H541 | 1.97 | 0.47 |
| 10:W:36:MET:HG3 | 10:W:40:LEU:HD12 | 1.97 | 0.47 |
| 7:G:38:HIS:CE1 | 26:G:269:CDL:H111 | 2.50 | 0.46 |
| 1:N:62:ALA:HB1 | 14:N:515:HEA:HMD3 | 1.96 | 0.46 |
| 21:Y:1522:TGL:H231 | 21:Y:1522:TGL:HA92 | 1.92 | 0.46 |
| 1:A:380[A]:VAL:HG23 | 1:A:381[A]:LEU:N | 2.30 | 0.46 |
| 1:A:383[B]:MET:HG2 | 1:A:421:VAL:HG21 | 1.95 | 0.46 |
| 5:E:6:GLU:HB2 | 5:E:10:GLU:OE1 | 2.15 | 0.46 |
| 25:C:265:PEK:H362 | 26:G:269:CDL:H272 | 1.97 | 0.46 |
| 1:N:430:PHE:HE1 | 21:O:1521:TGL:HB21 | 1.79 | 0.46 |
| 2:O:196:CYS:HB2 | 2:O:207:MET:HG3 | 1.97 | 0.46 |
| 23:O:229:CHD:H112 | 23:O:229:CHD:H12A | 1.67 | 0.46 |
| 12:Y:47:LYS:HE3 | 13:Z:42:LYS:NZ | 2.30 | 0.46 |
| 26:P:1270:CDL:H152 | 26:P:1270:CDL:H202 | 1.97 | 0.46 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:HA | 2.44 | 0.46 |
| 1:A:309:THR:CG2 | 14:A:516:HEA:HMB2 | 2.45 | 0.46 |
| 2:B:66:THR:HG21 | 23:B:1085:CHD:H42 | 1.97 | 0.46 |
| 26:C:270:CDL:C13 | 26:C:270:CDL:HA4 | 2.45 | 0.46 |
| 27:C:272:DMU:H1 | 7:G:69:PHE:CZ | 2.51 | 0.46 |
| 5:E:82:TYR:HB3 | 5:E:83:PRO:HD3 | 1.98 | 0.46 |
| 8:U:78:GLU:O | 8:U:78:GLU:HG2 | 2.15 | 0.46 |
| 10:W:4:ARG:HD2 | 10:W:7:GLU:OE2 | 2.16 | 0.46 |
| 12:Y:2:HIS:NE2 | 12:Y:5:GLU:OE1 | 2.48 | 0.46 |
| 5:E:23:ASP:N | 5:E:23:ASP:OD2 | 2.49 | 0.46 |
| 2:O:65:TRP:O | 2:O:69:PRO:HG2 | 2.15 | 0.46 |
| 3:P:54:MET:HE3 | 26:P:1270:CDL:H601 | 1.97 | 0.46 |
| 4:Q:33:LEU:HA | 4:Q:37:GLN:HE21 | 1.78 | 0.46 |
| 2:O:9:PHE:HB2 | 2:O:21:LEU:CD2 | 2.46 | 0.46 |
| 19:P:1267:PGV:C18 | 26:P:1270:CDL:H651 | 2.46 | 0.46 |
| 3:P:55:TYR:OH | 26:P:1270:CDL:H121 | 2.15 | 0.46 |
| 2:B:92:ASN:HA | 2:B:93:PRO:HD2 | 1.87 | 0.46 |
| 5:E:12:ASP:OD1 | 5:E:44:GLU:HG3 | 2.16 | 0.46 |
| 3:P:116:TRP:HA | 3:P:117:PRO:C | 2.36 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:Y:46:LYS:O | 12:Y:47:LYS:HB2 | 2.15 | 0.46 |
| 1:N:346:PHE:CE2 | 21:O:1521:TGL:H271 | 2.50 | 0.46 |
| 7:T:2:SER:O | 25:T:263:PEK:C33 | 2.62 | 0.46 |
| 1:N:32:ALA:HB3 | 12:Y:36:PRO:HG2 | 1.98 | 0.46 |
| 1:A:309:THR:HG22 | 14:A:516:HEA:HMB2 | 1.99 | 0.45 |
| 26:P:1270:CDL:H181 | 26:P:1270:CDL:H632 | 1.97 | 0.45 |
| 4:Q:94:LEU:CD2 | 11:X:28:VAL:HG21 | 2.46 | 0.45 |
| 1:A:382[A]:SER:HB3 | 14:A:515:HEA:HMC2 | 1.98 | 0.45 |
| 1:A:399:LEU:O | 1:A:499:PRO:HA | 2.17 | 0.45 |
| 4:D:34:SER:H | 4:D:37:GLN:NE2 | 2.14 | 0.45 |
| 23:J:60:CHD:H12A | 23:J:60:CHD:H112 | 1.54 | 0.45 |
| 2:O:226:MET:O | 2:O:227:LEU:C | 2.55 | 0.45 |
| 4:Q:131:ILE:N | 4:Q:131:ILE:HD12 | 2.32 | 0.45 |
| 5:R:23:ASP:N | 5:R:23:ASP:OD2 | 2.34 | 0.45 |
| 1:A:170:ASN:OD1 | 3:C:77:LYS:HD2 | 2.17 | 0.45 |
| 5:R:11:PHE:CG | 22:R:1229:PSC:H073 | 2.51 | 0.45 |
| 1:A:40:GLU:HG2 | 1:A:54:TYR:CD2 | 2.52 | 0.45 |
| 14:A:516:HEA:HHA | 14:A:516:HEA:HAD2 | 1.79 | 0.45 |
| 25:C:265:PEK:C37 | 26:G:269:CDL:H271 | 2.45 | 0.45 |
| 5:R:31:LYS:O | 5:R:31:LYS:HD2 | 2.16 | 0.45 |
| 1:A:240:HIS:C | 1:A:240:HIS:CD2 | 2.89 | 0.45 |
| 7:G:84:LYS:NZ | 29:G:4536:HOH:O | 2.48 | 0.45 |
| 7:T:3:ALA:O | 7:T:4:ALA:HB2 | 2.16 | 0.45 |
| 3:C:226:HIS:CE1 | 26:C:270:CDL:HB31 | 2.52 | 0.45 |
| 4:D:48:TRP:HA | 4:D:51:LEU:HD22 | 1.98 | 0.45 |
| 29:P:4419:HOH:O | 25:T:1265:PEK:H41 | 2.17 | 0.45 |
| 7:T:17:ARG:CD | 29:T:3446:HOH:O | 2.65 | 0.45 |
| 1:A:71:MET:N | 1:A:72:PRO:CD | 2.80 | 0.45 |
| 26:G:269:CDL:C47 | 29:G:4791:HOH:O | 2.64 | 0.45 |
| 1:N:513:LEU:HD23 | 1:N:513:LEU:HA | 1.79 | 0.45 |
| 5:R:43:PRO:HB2 | 5:R:48:ILE:HD11 | 1.99 | 0.45 |
| 1:A:461:SER:HB2 | 29:A:2700:HOH:O | 2.16 | 0.45 |
| 2:B:66:THR:HG21 | 23:B:1085:CHD:H3 | 1.97 | 0.45 |
| 4:D:34:SER:H | 4:D:37:GLN:HE21 | 1.65 | 0.45 |
| 21:L:522:TGL:H202 | 21:L:522:TGL:H231 | 1.27 | 0.45 |
| 26:P:1270:CDL:H652 | 26:P:1270:CDL:H612 | 1.98 | 0.45 |
| 3:P:51:MET:HG3 | 26:P:1270:CDL:H672 | 1.99 | 0.45 |
| 25:T:1265:PEK:H6 | 25:T:1265:PEK:H222 | 1.99 | 0.45 |
| 1:A:50:ASP:OD1 | 1:A:50:ASP:C | 2.54 | 0.45 |
| 3:P:55:TYR:CE1 | 26:P:1270:CDL:H161 | 2.51 | 0.45 |
| 3:P:63:ARG:HE | 26:P:1270:CDL:HA21 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:G:3:ALA:O | 7:G:4:ALA:HB2 | 2.16 | 0.44 |
| 13:Z:39:ASN:O | 13:Z:43:SER:OG | 2.27 | 0.44 |
| 1:N:100:MET:N | 3:P:17:PRO:HB3 | 2.32 | 0.44 |
| 2:O:121:TYR:O | 2:O:138:VAL:HA | 2.17 | 0.44 |
| 2:O:132:GLU:HB3 | 2:O:137:GLU:HG3 | 2.00 | 0.44 |
| 19:A:524:PGV:H152 | 4:D:87:PHE:CZ | 2.53 | 0.44 |
| 2:O:7:LEU:HD12 | 21:O:1521:TGL:HC31 | 1.98 | 0.44 |
| 7:T:5:LYS:HB2 | 25:T:263:PEK:H362 | 1.98 | 0.44 |
| 13:Z:10:THR:HA | 13:Z:14:GLU:OE2 | 2.18 | 0.44 |
| 1:N:113:LEU:HD12 | 21:Y:1522:TGL:H131 | 1.98 | 0.44 |
| 26:P:1270:CDL:H432 | 26:P:1270:CDL:H362 | 1.99 | 0.44 |
| 3:C:208:VAL:HG22 | 3:C:245:VAL:CG1 | 2.47 | 0.44 |
| 8:H:7:LYS:O | 8:H:8:ILE:CB | 2.65 | 0.44 |
| 3:C:16:TRP:N | 3:C:17:PRO:CD | 2.80 | 0.44 |
| 1:A:351:GLY:C | 1:A:380[A]:VAL:HG13 | 2.38 | 0.44 |
| 2:B:56:MET:CA | 22:B:229:PSC:H201 | 2.42 | 0.44 |
| 23:C:271:CHD:H232 | 23:C:271:CHD:H162 | 1.98 | 0.44 |
| 12:L:2:HIS:CG | 12:L:3:TYR:N | 2.85 | 0.44 |
| 21:N:1523:TGL:H181 | 2:O:47:THR:HB | 2.00 | 0.44 |
| 26:P:1270:CDL:HB32 | 26:P:1270:CDL:CB2 | 2.36 | 0.44 |
| 5:R:80:GLU:CD | 5:R:80:GLU:H | 2.21 | 0.44 |
| 1:A:377:PHE:CD1 | 14:A:516:HEA:HAD1 | 2.52 | 0.44 |
| 22:B:229:PSC:C02 | 22:B:229:PSC:H212 | 2.46 | 0.44 |
| 8:H:49:ASP:O | 8:H:52:VAL:HG22 | 2.18 | 0.44 |
| 9:I:54:TYR:OH | 9:I:59:ASP:OD1 | 2.27 | 0.44 |
| 3:P:37:PHE:HD1 | 29:P:4771:HOH:O | 2.00 | 0.44 |
| 1:A:486:ASP:HB2 | 29:A:2142:HOH:O | 2.18 | 0.44 |
| 1:A:62:ALA:HB2 | 14:A:515:HEA:HBD1 | 1.99 | 0.44 |
| 3:C:15:PRO:O | 3:C:19:THR:HG23 | 2.18 | 0.44 |
| 26:G:269:CDL:CA2 | 26:G:269:CDL:C11 | 2.95 | 0.44 |
| 1:N:378:HIS:O | 1:N:382[A]:SER:HB2 | 2.18 | 0.44 |
| 19:A:524:PGV:H12 | 4:D:87:PHE:CD2 | 2.53 | 0.43 |
| 9:I:43:ARG:HD3 | 9:I:43:ARG:HH11 | 1.62 | 0.43 |
| 11:K:6:ALA:HA | 11:K:7:PRO:HD2 | 1.78 | 0.43 |
| 4:Q:12:ALA:CB | 6:S:55:LYS:HE3 | 2.48 | 0.43 |
| 22:B:229:PSC:H062 | 22:B:229:PSC:H042 | 1.75 | 0.43 |
| 3:C:33:MET:CE | 29:J:4237:HOH:O | 2.61 | 0.43 |
| 26:G:269:CDL:H182 | 1:N:307:SER:HB2 | 2.00 | 0.43 |
| 25:P:1264:PEK:H32 | 25:P:1264:PEK:C7 | 2.38 | 0.43 |
| 1:A:181:THR:HA | 1:A:182:PRO:HD3 | 1.78 | 0.43 |
| 1:A:34:SER:HB2 | 14:A:515:HEA:C2B | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:A:521:PGV:C18 | 25:C:264:PEK:H332 | 2.42 | 0.43 |
| 27:C:272:DMU:H29 | 27:C:272:DMU:C10 | 2.47 | 0.43 |
| 21:N:1523:TGL:H222 | 2:O:39:LEU:CD1 | 2.48 | 0.43 |
| 1:N:514:LYS:H | 6:S:38:ALA:H | 1.67 | 0.43 |
| 3:P:224:LYS:O | 3:P:225:PHE:HB2 | 2.18 | 0.43 |
| 1:A:408:THR:HB | 19:A:524:PGV:H32 | 2.01 | 0.43 |
| 3:C:109:THR:HB | 3:C:110:PRO:CD | 2.48 | 0.43 |
| 21:L:522:TGL:HC22 | 21:L:522:TGL:HC62 | 1.99 | 0.43 |
| 3:P:165:ILE:HG12 | 25:T:1265:PEK:H102 | 2.01 | 0.43 |
| 5:R:107:ASP:N | 5:R:107:ASP:OD2 | 2.45 | 0.43 |
| 8:U:49:ASP:O | 8:U:52:VAL:HG13 | 2.18 | 0.43 |
| 6:F:65:ASP:OD1 | 6:S:1:ALA:HB3 | 2.18 | 0.43 |
| 8:H:60:TYR:C | 8:H:60:TYR:CD1 | 2.91 | 0.43 |
| 1:N:512:ASN:HB2 | 29:N:4003:HOH:O | 2.18 | 0.43 |
| 1:N:40:GLU:HG2 | 1:N:54:TYR:CD2 | 2.53 | 0.43 |
| 21:Y:1522:TGL:C23 | 21:Y:1522:TGL:HA92 | 2.49 | 0.43 |
| 1:A:450:TRP:CE3 | 1:A:450:TRP:HA | 2.54 | 0.43 |
| 12:L:46:LYS:O | 12:L:47:LYS:HB2 | 2.18 | 0.43 |
| 26:P:1270:CDL:H222 | 26:P:1270:CDL:H191 | 1.77 | 0.43 |
| 12:Y:2:HIS:CG | 12:Y:3:TYR:N | 2.85 | 0.43 |
| 1:N:473:TRP:CZ3 | 13:Z:18:GLY:HA3 | 2.53 | 0.43 |
| 6:F:13:ALA:O | 6:F:18:ARG:HD2 | 2.19 | 0.43 |
| 9:I:51:TYR:HA | 9:I:54:TYR:HB2 | 2.00 | 0.43 |
| 1:N:312:ILE:HG22 | 1:N:312:ILE:O | 2.17 | 0.43 |
| 2:O:41:ILE:O | 2:O:45:MET:HG2 | 2.19 | 0.43 |
| 2:O:92:ASN:HA | 2:O:93:PRO:HD2 | 1.76 | 0.43 |
| 27:P:272:DMU:H34 | 7:T:63:GLY:HA2 | 2.00 | 0.43 |
| 8:U:60:TYR:CD1 | 8:U:60:TYR:C | 2.92 | 0.43 |
| 1:A:500:PRO:HB2 | 1:A:504:THR:HG21 | 2.00 | 0.43 |
| 26:G:269:CDL:H241 | 26:G:269:CDL:H531 | 1.99 | 0.43 |
| 5:R:41:LEU:CD2 | 22:R:1229:PSC:H041 | 2.48 | 0.43 |
| 5:R:74:LYS:HD2 | 5:R:74:LYS:HA | 1.85 | 0.43 |
| 6:S:1:ALA:H2 | 25:T:1265:PEK:H041 | 1.83 | 0.43 |
| 6:S:1:ALA:N | 25:T:1265:PEK:H042 | 2.33 | 0.43 |
| 1:A:344:PHE:CD2 | 1:A:384[B]:GLY:O | 2.72 | 0.43 |
| 23:B:1085:CHD:H212 | 23:B:1085:CHD:H12 | 2.00 | 0.43 |
| 21:D:523:TGL:OG1 | 21:D:523:TGL:HB31 | 2.18 | 0.43 |
| 1:A:21:LEU:HD23 | 21:L:522:TGL:HA81 | 2.00 | 0.43 |
| 12:Y:11:ILE:CG2 | 21:Y:1522:TGL:H272 | 2.48 | 0.43 |
| 23:B:1085:CHD:H12A | 23:B:1085:CHD:H112 | 1.69 | 0.42 |
| 1:N:382[A]:SER:O | 1:N:383[A]:MET:C | 2.58 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:Q:109:HIS:CD2 | 29:Q:3122:HOH:O | 2.68 | 0.42 |
| 1:A:71:MET:HB2 | 1:A:72:PRO:HD3 | 2.01 | 0.42 |
| 23:J:60:CHD:H211 | 23:J:60:CHD:H232 | 1.74 | 0.42 |
| 2:O:68:LEU:HA | 2:O:68:LEU:HD12 | 1.73 | 0.42 |
| 4:Q:33:LEU:HD22 | 4:Q:37:GLN:HB3 | 2.01 | 0.42 |
| 22:R:1229:PSC:H042 | 29:R:3664:HOH:O | 2.19 | 0.42 |
| 5:R:11:PHE:CD1 | 22:R:1229:PSC:H073 | 2.54 | 0.42 |
| 1:A:246:LEU:HD13 | 1:A:381[A]:LEU:HD11 | 2.01 | 0.42 |
| 2:B:78:LEU:CD1 | 26:T:1269:CDL:H352 | 2.50 | 0.42 |
| 3:C:109:THR:HB | 3:C:110:PRO:HD2 | 1.99 | 0.42 |
| 3:C:202:GLY:HA3 | 25:C:264:PEK:H21 | 2.01 | 0.42 |
| 2:O:202:SER:HB3 | 2:O:203:ASN:HD22 | 1.84 | 0.42 |
| 4:Q:7:LYS:HB3 | 4:Q:8:SER:H | 1.68 | 0.42 |
| 5:R:80:GLU:N | 5:R:80:GLU:CD | 2.73 | 0.42 |
| 26:T:1269:CDL:H581 | 26:T:1269:CDL:H552 | 1.94 | 0.42 |
| 10:W:57:HIS:O | 10:W:58:LYS:HB2 | 2.18 | 0.42 |
| 1:A:382[B]:SER:OG | 14:A:515:HEA:H121 | 2.20 | 0.42 |
| 1:N:438:ARG:O | 1:N:439:ARG:HB2 | 2.19 | 0.42 |
| 2:O:52:HIS:HE1 | 22:R:1229:PSC:H02 | 1.84 | 0.42 |
| 26:P:1270:CDL:CB2 | 26:P:1270:CDL:CB3 | 2.85 | 0.42 |
| 7:T:3:ALA:O | 7:T:4:ALA:CB | 2.67 | 0.42 |
| 12:L:20:ARG:HH22 | 21:L:522:TGL:CC5 | 2.33 | 0.42 |
| 3:P:106:LEU:HD13 | 19:U:1268:PGV:H21 | 2.01 | 0.42 |
| 7:G:3:ALA:O | 7:G:4:ALA:CB | 2.67 | 0.42 |
| 1:N:335:SER:HB2 | 1:N:336:PRO:HD2 | 2.00 | 0.42 |
| 1:N:62:ALA:HB2 | 14:N:515:HEA:HBD1 | 2.02 | 0.42 |
| 5:R:90:ARG:HB3 | 5:R:91:PRO:CD | 2.43 | 0.42 |
| 2:B:193:TYR:CD1 | 2:B:210:VAL:HG22 | 2.55 | 0.42 |
| 21:D:523:TGL:HA91 | 21:D:523:TGL:C24 | 2.47 | 0.42 |
| 1:A:1:FME:CE | 12:L:3:TYR:HE1 | 2.33 | 0.42 |
| 13:M:13:LYS:HD2 | 13:M:13:LYS:C | 2.40 | 0.42 |
| 4:D:101:HIS:CD2 | 4:D:102:TYR:CE2 | 3.08 | 0.42 |
| 1:N:127:THR:HB | 1:N:129:TYR:CE2 | 2.55 | 0.42 |
| 1:N:514:LYS:HE2 | 29:S:3514:HOH:O | 2.18 | 0.42 |
| 14:N:515:HEA:HMC1 | 14:N:515:HEA:CBC | 2.46 | 0.42 |
| 6:F:92:VAL:O | 6:F:92:VAL:HG23 | 2.18 | 0.41 |
| 26:G:269:CDL:OA7 | 26:G:269:CDL:H311 | 2.20 | 0.41 |
| 7:G:9:GLY:HA3 | 1:N:178:GLN:HE21 | 1.85 | 0.41 |
| 10:J:50:LEU:HD22 | 10:J:54:SER:OG | 2.20 | 0.41 |
| 1:N:229:ILE:HD11 | 2:O:175:ILE:CD1 | 2.42 | 0.41 |
| 13:Z:41:LYS:NZ | 29:Z:3672:HOH:O | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:A:364:ASP:OD2 | 14:A:516:HEA:O1A | 2.38 | 0.41 |
| 5:R:82:TYR:HB3 | 5:R:83:PRO:HD3 | 2.02 | 0.41 |
| 21:D:523:TGL:HB71 | 21:D:523:TGL:HA52 | 2.01 | 0.41 |
| 12:L:24:MET:SD | 21:L:522:TGL:H161 | 2.60 | 0.41 |
| 6:S:54:ASN:ND2 | 6:S:54:ASN:C | 2.73 | 0.41 |
| 29:P:4425:HOH:O | 7:T:11:TPO:CG2 | 2.68 | 0.41 |
| 7:T:7:ASP:CG | 7:T:8:HIS:H | 2.24 | 0.41 |
| 1:N:119:GLU:O | 12:Y:46:LYS:HE2 | 2.21 | 0.41 |
| 1:N:377:PHE:HA | 1:N:380[B]:VAL:HG22 | 2.02 | 0.41 |
| 8:U:84:LYS:HA | 29:U:3538:HOH:O | 2.21 | 0.41 |
| 10:W:31:LEU:HA | 10:W:31:LEU:HD12 | 1.88 | 0.41 |
| 1:A:177:SER:H | 1:A:180:GLN:HE21 | 1.68 | 0.41 |
| 23:C:525:CHD:H112 | 23:C:525:CHD:H12A | 1.81 | 0.41 |
| 4:D:39:ALA:O | 4:D:42:GLU:HB2 | 2.21 | 0.41 |
| 26:G:269:CDL:C24 | 26:G:269:CDL:H542 | 2.51 | 0.41 |
| 26:G:269:CDL:H571 | 26:G:269:CDL:H782 | 2.01 | 0.41 |
| 26:G:269:CDL:H821 | 26:G:269:CDL:H791 | 1.50 | 0.41 |
| 1:A:382[A]:SER:HB3 | 14:A:515:HEA:C2C | 2.50 | 0.41 |
| 12:L:20:ARG:HH22 | 21:L:522:TGL:CC6 | 2.33 | 0.41 |
| 13:M:17:ILE:HD13 | 13:M:17:ILE:HG21 | 1.87 | 0.41 |
| 22:B:229:PSC:H242 | 22:B:229:PSC:H271 | 1.01 | 0.41 |
| 8:H:46:LYS:HE2 | 8:U:8:ILE:HG22 | 1.99 | 0.41 |
| 3:P:207:HIS:CD2 | 3:P:241:TYR:OH | 2.74 | 0.41 |
| 4:Q:52:SER:HB2 | 29:Q:4686:HOH:O | 2.19 | 0.41 |
| 7:T:3:ALA:HB1 | 25:T:263:PEK:H383 | 2.00 | 0.41 |
| 8:U:50:VAL:O | 8:U:51:SER:C | 2.57 | 0.41 |
| 10:W:55:PHE:HA | 10:W:56:PRO:HD3 | 1.83 | 0.41 |
| 1:A:195:LEU:HD23 | 1:A:245:ILE:HD13 | 2.02 | 0.41 |
| 1:N:334:TRP:CE3 | 21:N:1523:TGL:HA31 | 2.56 | 0.41 |
| 1:N:318:VAL:HG22 | 2:O:65:TRP:HD1 | 1.85 | 0.41 |
| 1:N:324:LEU:HD13 | 2:O:41:ILE:CG2 | 2.51 | 0.41 |
| 5:R:90:ARG:CB | 5:R:91:PRO:HD3 | 2.44 | 0.41 |
| 6:F:92:VAL:O | 6:F:92:VAL:CG2 | 2.69 | 0.41 |
| 21:N:1523:TGL:OB1 | 21:N:1523:TGL:CG3 | 2.68 | 0.41 |
| 22:R:1229:PSC:H063 | 22:R:1229:PSC:H042 | 1.76 | 0.41 |
| 3:P:154:GLY:HA2 | 6:S:6:VAL:HB | 2.02 | 0.41 |
| 1:A:190:ILE:CD1 | 1:A:278:MET:HG2 | 2.51 | 0.41 |
| 19:A:524:PGV:C21 | 19:A:524:PGV:H012 | 2.51 | 0.41 |
| 23:J:60:CHD:H161 | 29:J:4539:HOH:O | 2.21 | 0.41 |
| 1:N:66:ILE:HG23 | 1:N:246:LEU:HD21 | 2.03 | 0.41 |
| 2:O:151:ARG:HD3 | 2:O:181:GLN:HE21 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:514:LYS:HG3 | 6:F:38:ALA:HB2 | 2.02 | 0.41 |
| 2:O:226:MET:O | 2:O:227:LEU:O | 2.38 | 0.41 |
| 26:P:1270:CDL:HB21 | 26:P:1270:CDL:CB4 | 2.51 | 0.41 |
| 1:N:103:TRP:O | 3:P:21:ALA:HB1 | 2.21 | 0.41 |
| 6:S:1:ALA:H1 | 25:T:1265:PEK:H042 | 1.86 | 0.41 |
| 25:T:1265:PEK:H311 | 25:T:1265:PEK:H282 | 1.84 | 0.41 |
| 7:T:3:ALA:CB | 25:T:263:PEK:C38 | 2.95 | 0.41 |
| 25:C:264:PEK:C7 | 25:C:264:PEK:H32 | 2.51 | 0.40 |
| 22:R:1229:PSC:C02 | 22:R:1229:PSC:H212 | 2.51 | 0.40 |
| 26:T:1269:CDL:OA7 | 26:T:1269:CDL:H342 | 2.21 | 0.40 |
| 22:B:229:PSC:H341 | 22:B:229:PSC:H142 | 2.00 | 0.40 |
| 10:J:33:ARG:HG2 | 23:J:60:CHD:H152 | 2.01 | 0.40 |
| 19:N:1524:PGV:H22 | 19:N:1524:PGV:C01 | 2.52 | 0.40 |
| 3:P:226:HIS:CE1 | 26:P:1270:CDL:HB31 | 2.57 | 0.40 |
| 3:P:146:TRP:CZ2 | 7:T:17:ARG:HG3 | 2.56 | 0.40 |
| 7:T:3:ALA:HB3 | 25:T:263:PEK:H383 | 2.01 | 0.40 |
| 4:D:92:THR:O | 4:D:95:LEU:HB2 | 2.21 | 0.40 |
| 1:N:374:VAL:HG13 | 1:N:378:HIS:CE1 | 2.56 | 0.40 |
| 1:N:37:ILE:HD11 | 1:N:58:VAL:HA | 2.03 | 0.40 |
| 1:N:68:PHE:HA | 1:N:72:PRO:HG2 | 2.03 | 0.40 |
| 2:O:116:LEU:HD13 | 2:O:226:MET:HG3 | 2.03 | 0.40 |
| 2:B:98:LYS:HB2 | 2:B:109:GLU:HB2 | 2.02 | 0.40 |
| 2:B:164:ALA:O | 2:B:194:GLY:HA3 | 2.21 | 0.40 |
| 21:D:523:TGL:H231 | 21:D:523:TGL:CA9 | 2.51 | 0.40 |
| 1:N:34:SER:HB2 | 14:N:515:HEA:C2B | 2.51 | 0.40 |
| 23:P:1271:CHD:H12A | 23:P:1271:CHD:H112 | 1.54 | 0.40 |
| 4:Q:16:TYR:HB2 | 4:Q:27:VAL:HG23 | 2.04 | 0.40 |
| 1:A:403:TYR:HA | 1:A:480:ARG:O | 2.21 | 0.40 |
| 3:C:207:HIS:HD2 | 3:C:241:TYR:OH | 2.05 | 0.40 |
| 4:D:48:TRP:HB2 | 5:E:96:LEU:O | 2.21 | 0.40 |
| 13:M:37:LEU:HD23 | 13:M:37:LEU:HA | 1.93 | 0.40 |
| 1:N:240:HIS:CE1 | 1:N:244:TYR:OH | 2.74 | 0.40 |
| 4:Q:131:ILE:HD12 | 4:Q:131:ILE:H | 1.85 | 0.40 |
| 3:P:131:LEU:CD2 | 26:T:1269:CDL:HB61 | 2.51 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 517/514 (101%) | 502 (97%) | 15 (3%) | 0 | 100 | 100 |
| 1 | N | 517/514 (101%) | 495 (96%) | 22 (4%) | 0 | 100 | 100 |
| 2 | B | 225/227 (99%) | 217 (96%) | 7 (3%) | 1 (0%) | 38 | 33 |
| 2 | O | 225/227 (99%) | 219 (97%) | 5 (2%) | 1 (0%) | 38 | 33 |
| 3 | C | 257/261 (98%) | 251 (98%) | 6 (2%) | 0 | 100 | 100 |
| 3 | P | 257/261 (98%) | 250 (97%) | 7 (3%) | 0 | 100 | 100 |
| 4 | D | 142/147 (97%) | 138 (97%) | 4 (3%) | 0 | 100 | 100 |
| 4 | Q | 142/147 (97%) | 134 (94%) | 8 (6%) | 0 | 100 | 100 |
| 5 | E | 103/109 (94%) | 101 (98%) | 2 (2%) | 0 | 100 | 100 |
| 5 | R | 103/109 (94%) | 100 (97%) | 2 (2%) | 1 (1%) | 18 | 10 |
| 6 | F | 96/98 (98%) | 90 (94%) | 3 (3%) | 3 (3%) | 5 | 1 |
| 6 | S | 96/98 (98%) | 88 (92%) | 5 (5%) | 3 (3%) | 5 | 1 |
| 7 | G | 81/85 (95%) | 68 (84%) | 7 (9%) | 6 (7%) | 1 | 0 |
| 7 | T | 81/85 (95%) | 67 (83%) | 6 (7%) | 8 (10%) | 1 | 0 |
| 8 | H | 77/85 (91%) | 68 (88%) | 3 (4%) | 6 (8%) | 1 | 0 |
| 8 | U | 77/85 (91%) | 68 (88%) | 5 (6%) | 4 (5%) | 2 | 0 |
| 9 | I | 71/73 (97%) | 68 (96%) | 3 (4%) | 0 | 100 | 100 |
| 9 | V | 71/73 (97%) | 67 (94%) | 4 (6%) | 0 | 100 | 100 |
| 10 | J | 56/59 (95%) | 56 (100%) | 0 | 0 | 100 | 100 |
| 10 | W | 56/59 (95%) | 56 (100%) | 0 | 0 | 100 | 100 |
| 11 | K | 47/56 (84%) | 44 (94%) | 3 (6%) | 0 | 100 | 100 |
| 11 | X | 47/56 (84%) | 45 (96%) | 2 (4%) | 0 | 100 | 100 |
| 12 | L | 44/47 (94%) | 42 (96%) | 2 (4%) | 0 | 100 | 100 |
| 12 | Y | 44/47 (94%) | 42 (96%) | 2 (4%) | 0 | 100 | 100 |
| 13 | M | 41/46 (89%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 13 | Z | 41/46 (89%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |
| All | All | 3514/3614 (97%) | 3356 (96%) | 125 (4%) | 33 (1%) | 20 | 12 |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 94 | HIS |
| 6 | F | 95 | GLN |
| 7 | G | 4 | ALA |
| 7 | G | 7 | ASP |
| 7 | G | 8 | HIS |
| 8 | H | 8 | ILE |
| 8 | H | 44 | THR |
| 8 | H | 46 | LYS |
| 2 | O | 60 | GLU |
| 5 | R | 6 | GLU |
| 6 | S | 94 | HIS |
| 6 | S | 95 | GLN |
| 6 | S | 96 | LEU |
| 7 | T | 4 | ALA |
| 7 | T | 7 | ASP |
| 7 | T | 8 | HIS |
| 7 | T | 37 | LEU |
| 7 | T | 38 | HIS |
| 8 | U | 10 | ASN |
| 8 | U | 45 | ALA |
| 8 | U | 46 | LYS |
| 7 | G | 3 | ALA |
| 7 | G | 37 | LEU |
| 7 | T | 9 | GLY |
| 8 | U | 8 | ILE |
| 2 | B | 60 | GLU |
| 6 | F | 96 | LEU |
| 8 | H | 10 | ASN |
| 8 | H | 43 | MET |
| 7 | T | 5 | LYS |
| 7 | G | 6 | GLY |
| 8 | H | 45 | ALA |
| 7 | T | 6 | GLY |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 430/426 (101%) | 419 (97%) | 11 (3%) | 51 | 52 |
| 1 | N | 430/426 (101%) | 414 (96%) | 16 (4%) | 39 | 36 |
| 2 | B | 210/210 (100%) | 200 (95%) | 10 (5%) | 30 | 25 |
| 2 | O | 210/210 (100%) | 196 (93%) | 14 (7%) | 19 | 13 |
| 3 | C | 224/226 (99%) | 217 (97%) | 7 (3%) | 45 | 44 |
| 3 | P | 224/226 (99%) | 219 (98%) | 5 (2%) | 57 | 60 |
| 4 | D | 128/129 (99%) | 124 (97%) | 4 (3%) | 45 | 44 |
| 4 | Q | 128/129 (99%) | 121 (94%) | 7 (6%) | 25 | 20 |
| 5 | E | 92/95 (97%) | 88 (96%) | 4 (4%) | 33 | 29 |
| 5 | R | 92/95 (97%) | 89 (97%) | 3 (3%) | 43 | 41 |
| 6 | F | 81/81 (100%) | 76 (94%) | 5 (6%) | 21 | 16 |
| 6 | S | 81/81 (100%) | 77 (95%) | 4 (5%) | 29 | 24 |
| 7 | G | 67/68 (98%) | 59 (88%) | 8 (12%) | 6 | 3 |
| 7 | T | 67/68 (98%) | 58 (87%) | 9 (13%) | 4 | 2 |
| 8 | H | 71/75 (95%) | 65 (92%) | 6 (8%) | 12 | 7 |
| 8 | U | 71/75 (95%) | 66 (93%) | 5 (7%) | 18 | 12 |
| 9 | I | 57/57 (100%) | 50 (88%) | 7 (12%) | 5 | 3 |
| 9 | V | 57/57 (100%) | 48 (84%) | 9 (16%) | 3 | 1 |
| 10 | J | 49/50 (98%) | 48 (98%) | 1 (2%) | 60 | 64 |
| 10 | W | 49/50 (98%) | 48 (98%) | 1 (2%) | 60 | 64 |
| 11 | K | 39/46 (85%) | 36 (92%) | 3 (8%) | 15 | 9 |
| 11 | X | 39/46 (85%) | 37 (95%) | 2 (5%) | 28 | 22 |
| 12 | L | 39/40 (98%) | 38 (97%) | 1 (3%) | 51 | 52 |
| 12 | Y | 39/40 (98%) | 36 (92%) | 3 (8%) | 15 | 9 |
| 13 | M | 37/38 (97%) | 33 (89%) | 4 (11%) | 7 | 4 |
| 13 | Z | 37/38 (97%) | 33 (89%) | 4 (11%) | 7 | 4 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| All | All | 3048/3082 (99%) | 2895 (95%) | 153 (5%) | 28 | 23 |

All (153) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 38 | ARG |
| 1 | A | 44 | PRO |
| 1 | A | 109 | PHE |
| 1 | A | 180 | GLN |
| 1 | A | 265 | LYS |
| 1 | A | 297 | MET |
| 1 | A | 333 | LYS |
| 1 | A | 369 | ASP |
| 1 | A | 444 | PRO |
| 1 | A | 486 | ASP |
| 1 | A | 512 | ASN |
| 2 | B | 33 | LEU |
| 2 | B | 60 | GLU |
| 2 | B | 61 | VAL |
| 2 | B | 65 | TRP |
| 2 | B | 66 | THR |
| 2 | B | 75 | LEU |
| 2 | B | 78 | LEU |
| 2 | B | 86 | MET |
| 2 | B | 115 | ASP |
| 2 | B | 171 | LYS |
| 3 | C | 17 | PRO |
| 3 | C | 33 | MET |
| 3 | C | 127 | LEU |
| 3 | C | 159 | MET |
| 3 | C | 161 | GLN |
| 3 | C | 214 | PHE |
| 3 | C | 230 | ASN |
| 4 | D | 4 | SER |
| 4 | D | 20 | ARG |
| 4 | D | 31 | LYS |
| 4 | D | 51 | LEU |
| 5 | E | 31 | LYS |
| 5 | E | 70 | VAL |
| 5 | E | 90 | ARG |
| 5 | E | 109 | VAL |
| 6 | F | 37 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 48 | LEU |
| 6 | F | 94 | HIS |
| 6 | F | 95 | GLN |
| 6 | F | 96 | LEU |
| 7 | G | 2 | SER |
| 7 | G | 8 | HIS |
| 7 | G | 17 | ARG |
| 7 | G | 18 | PHE |
| 7 | G | 33 | LEU |
| 7 | G | 54 | ARG |
| 7 | G | 74 | ARG |
| 7 | G | 84 | LYS |
| 8 | H | 7 | LYS |
| 8 | H | 8 | ILE |
| 8 | H | 9 | LYS |
| 8 | H | 29 | CYS |
| 8 | H | 52 | VAL |
| 8 | H | 60 | TYR |
| 9 | I | 8 | GLN |
| 9 | I | 26 | MET |
| 9 | I | 29 | LEU |
| 9 | I | 36 | LYS |
| 9 | I | 37 | PHE |
| 9 | I | 43 | ARG |
| 9 | I | 68 | ILE |
| 10 | J | 50 | LEU |
| 11 | K | 20 | SER |
| 11 | K | 47 | ARG |
| 11 | K | 54 | ARG |
| 12 | L | 47 | LYS |
| 13 | M | 34 | LEU |
| 13 | M | 38 | ASP |
| 13 | M | 39 | ASN |
| 13 | M | 42 | LYS |
| 1 | N | 109 | PHE |
| 1 | N | 136 | LEU |
| 1 | N | 152 | LEU |
| 1 | N | 169 | ILE |
| 1 | N | 180 | GLN |
| 1 | N | 278 | MET |
| 1 | N | 290 | HIS |
| 1 | N | 333 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 338 | MET |
| 1 | N | 369 | ASP |
| 1 | N | 438 | ARG |
| 1 | N | 484 | THR |
| 1 | N | 495 | LEU |
| 1 | N | 504 | THR |
| 1 | N | 508 | PRO |
| 1 | N | 512 | ASN |
| 2 | O | 18 | GLU |
| 2 | O | 33 | LEU |
| 2 | O | 59 | GLN |
| 2 | O | 60 | GLU |
| 2 | O | 61 | VAL |
| 2 | O | 66 | THR |
| 2 | O | 68 | LEU |
| 2 | O | 75 | LEU |
| 2 | O | 78 | LEU |
| 2 | O | 94 | SER |
| 2 | O | 171 | LYS |
| 2 | O | 203 | ASN |
| 2 | O | 217 | LYS |
| 2 | O | 227 | LEU |
| 3 | P | 29 | SER |
| 3 | P | 127 | LEU |
| 3 | P | 159 | MET |
| 3 | P | 214 | PHE |
| 3 | P | 246 | ASP |
| 4 | Q | 5 | VAL |
| 4 | Q | 9 | GLU |
| 4 | Q | 17 | VAL |
| 4 | Q | 51 | LEU |
| 4 | Q | 141 | ASP |
| 4 | Q | 143 | ASN |
| 4 | Q | 147 | LYS |
| 5 | R | 46 | LYS |
| 5 | R | 80 | GLU |
| 5 | R | 109 | VAL |
| 6 | S | 48 | LEU |
| 6 | S | 53 | THR |
| 6 | S | 54 | ASN |
| 6 | S | 64 | GLU |
| 7 | T | 2 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | T | 5 | LYS |
| 7 | T | 8 | HIS |
| 7 | T | 17 | ARG |
| 7 | T | 18 | PHE |
| 7 | T | 36 | TRP |
| 7 | T | 37 | LEU |
| 7 | T | 42 | ARG |
| 7 | T | 84 | LYS |
| 8 | U | 7 | LYS |
| 8 | U | 9 | LYS |
| 8 | U | 52 | VAL |
| 8 | U | 60 | TYR |
| 8 | U | 84 | LYS |
| 9 | V | 2 | THR |
| 9 | V | 18 | ARG |
| 9 | V | 26 | MET |
| 9 | V | 29 | LEU |
| 9 | V | 37 | PHE |
| 9 | V | 61 | GLU |
| 9 | V | 65 | LYS |
| 9 | V | 70 | GLN |
| 9 | V | 73 | LYS |
| 10 | W | 50 | LEU |
| 11 | X | 20 | SER |
| 11 | X | 47 | ARG |
| 12 | Y | 20 | ARG |
| 12 | Y | 26 | THR |
| 12 | Y | 47 | LYS |
| 13 | Z | 13 | LYS |
| 13 | Z | 34 | LEU |
| 13 | Z | 38 | ASP |
| 13 | Z | 42 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 80 | ASN |
| 1 | A | 98 | ASN |
| 1 | A | 178 | GLN |
| 1 | A | 180 | GLN |
| 1 | A | 512 | ASN |
| 2 | B | 10 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 91 | ASN |
| 2 | B | 181 | GLN |
| 2 | B | 195 | GLN |
| 3 | C | 3 | HIS |
| 3 | C | 68 | GLN |
| 3 | C | 70 | HIS |
| 3 | C | 207 | HIS |
| 4 | D | 29 | HIS |
| 4 | D | 32 | ASN |
| 4 | D | 37 | GLN |
| 4 | D | 101 | HIS |
| 4 | D | 109 | HIS |
| 5 | E | 78 | HIS |
| 5 | E | 94 | ASN |
| 7 | G | 76 | ASN |
| 8 | H | 23 | GLN |
| 9 | I | 8 | GLN |
| 10 | J | 29 | ASN |
| 10 | J | 57 | HIS |
| 1 | N | 80 | ASN |
| 1 | N | 98 | ASN |
| 1 | N | 178 | GLN |
| 1 | N | 180 | GLN |
| 1 | N | 328 | HIS |
| 1 | N | 512 | ASN |
| 2 | O | 10 | GLN |
| 2 | O | 22 | HIS |
| 2 | O | 52 | HIS |
| 2 | O | 91 | ASN |
| 2 | O | 181 | GLN |
| 2 | O | 195 | GLN |
| 2 | O | 203 | ASN |
| 3 | P | 50 | ASN |
| 3 | P | 68 | GLN |
| 3 | P | 70 | HIS |
| 3 | P | 207 | HIS |
| 4 | Q | 37 | GLN |
| 4 | Q | 109 | HIS |
| 5 | R | 94 | ASN |
| 6 | S | 54 | ASN |
| 6 | S | 94 | HIS |
| 6 | S | 95 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | S | 98 | HIS |
| 7 | T | 8 | HIS |
| 7 | T | 76 | ASN |
| 8 | U | 12 | GLN |
| 9 | V | 8 | GLN |
| 13 | Z | 36 | 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 | $\# Z > 2$ |
| 1 | FME | A | 1 | 1 | 9,9,10 | 1.05 | 1 (11%) | 7,9,11 | 5.42 | 3 (42%) |
| 2 | FME | B | 1 | 2 | 9,9,10 | 2.05 | 3 (33%) | 7,9,11 | 8.13 | 4 (57%) |
| 7 | TPO | G | 11 | 7 | 9,10,11 | 2.76 | 5 (55%) | 10,14,16 | 1.43 | 2 (20%) |
| 9 | SAC | I | 1 | 9 | 8,8,9 | 2.50 | 2 (25%) | 6,9,11 | 1.80 | 1 (16%) |
| 1 | FME | N | 1 | 1 | 9,9,10 | 0.67 | 0 | 7,9,11 | 6.37 | 3 (42%) |
| 2 | FME | O | 1 | 2 | 9,9,10 | 1.33 | 2 (22%) | 7,9,11 | 5.22 | 3 (42%) |
| 7 | TPO | T | 11 | 7 | 9,10,11 | 3.40 | 4 (44%) | 10,14,16 | 1.75 | 3 (30%) |
| 9 | SAC | V | 1 | 9 | 8,8,9 | 3.35 | 3 (37%) | 6,9,11 | 1.29 | 1 (16%) |

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 |
|-----|------|-------|-----|------|---------|-----------|---------|
| 1 | FME | A | 1 | 1 | - | 1/6/9/11 | 0/0/0/0 |
| 2 | FME | B | 1 | 2 | - | 1/6/9/11 | 0/0/0/0 |
| 7 | TPO | G | 11 | 7 | - | 0/8/11/13 | 0/0/0/0 |
| 9 | SAC | I | 1 | 9 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | FME | N | 1 | 1 | - | 1/6/9/11 | 0/0/0/0 |
| 2 | FME | O | 1 | 2 | - | 1/6/9/11 | 0/0/0/0 |
| 7 | TPO | T | 11 | 7 | - | 0/8/11/13 | 0/0/0/0 |
| 9 | SAC | V | 1 | 9 | - | 1/6/8/10 | 0/0/0/0 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 1 | FME | O1-CN | -4.58 | 1.08 | 1.22 |
| 2 | B | 1 | FME | CG-SD | -2.26 | 1.68 | 1.81 |
| 2 | O | 1 | FME | CA-C | -2.22 | 1.47 | 1.50 |
| 2 | O | 1 | FME | O1-CN | -2.21 | 1.15 | 1.22 |
| 7 | G | 11 | TPO | CG2-CB | 2.03 | 1.56 | 1.51 |
| 7 | T | 11 | TPO | P-O3P | 2.13 | 1.63 | 1.54 |
| 7 | G | 11 | TPO | CA-C | 2.32 | 1.53 | 1.50 |
| 7 | G | 11 | TPO | P-O2P | 2.35 | 1.64 | 1.54 |
| 1 | A | 1 | FME | CA-C | 2.49 | 1.53 | 1.50 |
| 2 | B | 1 | FME | CA-N | 2.68 | 1.50 | 1.46 |
| 7 | T | 11 | TPO | P-O1P | 3.38 | 1.62 | 1.50 |
| 9 | V | 1 | SAC | CA-C | 3.57 | 1.54 | 1.50 |
| 7 | G | 11 | TPO | P-O1P | 3.89 | 1.64 | 1.50 |
| 9 | I | 1 | SAC | CA-N | 4.07 | 1.52 | 1.46 |
| 9 | I | 1 | SAC | OAC-C1A | 5.12 | 1.35 | 1.23 |
| 7 | T | 11 | TPO | CA-C | 5.28 | 1.57 | 1.50 |
| 9 | V | 1 | SAC | OAC-C1A | 5.57 | 1.36 | 1.23 |
| 7 | G | 11 | TPO | P-OG1 | 5.66 | 1.69 | 1.59 |
| 9 | V | 1 | SAC | CA-N | 6.20 | 1.55 | 1.46 |
| 7 | T | 11 | TPO | P-OG1 | 6.97 | 1.71 | 1.59 |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 2 | B | 1 | FME | CA-N-CN | -20.70 | 90.98 | 122.82 |
| 1 | N | 1 | FME | CA-N-CN | -15.77 | 98.57 | 122.82 |
| 1 | A | 1 | FME | CA-N-CN | -13.36 | 102.27 | 122.82 |
| 2 | O | 1 | FME | CA-N-CN | -13.30 | 102.36 | 122.82 |
| 2 | B | 1 | FME | CG-CB-CA | -3.96 | 101.51 | 112.97 |
| 9 | I | 1 | SAC | OG-CB-CA | -3.23 | 102.83 | 111.02 |
| 2 | B | 1 | FME | CB-CG-SD | -2.79 | 99.92 | 113.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 7 | G | 11 | TPO | O-C-CA | -2.75 | 118.74 | 125.15 |
| 2 | B | 1 | FME | O-C-CA | -2.72 | 118.80 | 125.15 |
| 7 | T | 11 | TPO | O-C-CA | -2.63 | 119.03 | 125.15 |
| 9 | V | 1 | SAC | O-C-CA | -2.48 | 119.37 | 125.15 |
| 7 | T | 11 | TPO | C-CA-N | -2.46 | 104.90 | 109.86 |
| 1 | A | 1 | FME | O-C-CA | -2.40 | 119.55 | 125.15 |
| 1 | N | 1 | FME | O-C-CA | -2.30 | 119.78 | 125.15 |
| 2 | O | 1 | FME | O-C-CA | -2.13 | 120.18 | 125.15 |
| 2 | O | 1 | FME | CG-CB-CA | -2.05 | 107.04 | 112.97 |
| 7 | G | 11 | TPO | O2P-P-OG1 | 2.50 | 117.36 | 106.00 |
| 7 | T | 11 | TPO | O3P-P-OG1 | 3.27 | 120.87 | 106.00 |
| 1 | A | 1 | FME | CE-SD-CG | 4.42 | 116.22 | 100.35 |
| 1 | N | 1 | FME | CB-CA-C | 5.06 | 120.00 | 111.65 |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 9 | V | 1 | SAC | CB-CA-N-C1A |
| 2 | B | 1 | FME | O1-CN-N-CA |
| 2 | O | 1 | FME | O1-CN-N-CA |
| 1 | A | 1 | FME | O1-CN-N-CA |
| 1 | N | 1 | FME | O1-CN-N-CA |

There are no ring outliers.

4 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 1 | FME | 1 | 0 |
| 7 | G | 11 | TPO | 4 | 0 |
| 7 | T | 11 | TPO | 2 | 0 |
| 9 | V | 1 | SAC | 1 | 0 |

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - 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 |
| 14 | HEA | A | 515 | 1 | 44,67,67 | 1.49 | 10 (22%) | 37,103,103 | 2.05 | 12 (32%) |
| 14 | HEA | A | 516 | 1 | 44,67,67 | 1.39 | 7 (15%) | 37,103,103 | 2.21 | 11 (29%) |
| 15 | NO | A | 520 | 16 | 0,1,1 | 0.00 | - | 0,0,0 | 0.00 | - |
| 19 | PGV | A | 521 | - | 50,50,50 | 1.26 | 6 (12%) | 51,56,56 | 1.79 | 14 (27%) |
| 19 | PGV | A | 524 | - | 50,50,50 | 1.34 | 4 (8%) | 51,56,56 | 1.73 | 10 (19%) |
| 23 | CHD | B | 1085 | - | 29,32,32 | 1.85 | 5 (17%) | 47,51,51 | 5.73 | 34 (72%) |
| 20 | CUA | B | 228 | 2 | 0,1,1 | 0.00 | - | 0,0,0 | 0.00 | - |
| 22 | PSC | B | 229 | - | 51,51,51 | 1.20 | 3 (5%) | 56,59,59 | 1.41 | 9 (16%) |
| 21 | TGL | B | 521 | - | 62,62,62 | 1.29 | 6 (9%) | 65,65,65 | 1.98 | 13 (20%) |
| 25 | PEK | C | 264 | - | 52,52,52 | 0.93 | 2 (3%) | 54,57,57 | 1.87 | 16 (29%) |
| 25 | PEK | C | 265 | - | 52,52,52 | 1.59 | 6 (11%) | 54,57,57 | 1.67 | 7 (12%) |
| 19 | PGV | C | 267 | - | 50,50,50 | 0.87 | 3 (6%) | 51,56,56 | 1.38 | 8 (15%) |
| 19 | PGV | C | 268 | - | 50,50,50 | 1.39 | 4 (8%) | 51,56,56 | 1.67 | 6 (11%) |
| 26 | CDL | C | 270 | - | 99,99,99 | 1.47 | 13 (13%) | 101,111,111 | 1.50 | 16 (15%) |
| 23 | CHD | C | 271 | - | 29,32,32 | 0.73 | 0 | 47,51,51 | 5.02 | 32 (68%) |
| 27 | DMU | C | 272 | - | 34,34,34 | 1.51 | 4 (11%) | 45,45,45 | 3.54 | 26 (57%) |
| 23 | CHD | C | 525 | - | 29,32,32 | 1.57 | 6 (20%) | 47,51,51 | 5.56 | 37 (78%) |
| 21 | TGL | D | 523 | - | 62,62,62 | 1.59 | 8 (12%) | 65,65,65 | 1.57 | 15 (23%) |
| 25 | PEK | G | 1263 | - | 52,52,52 | 1.33 | 4 (7%) | 54,57,57 | 1.51 | 7 (12%) |
| 26 | CDL | G | 269 | - | 99,99,99 | 1.42 | 12 (12%) | 101,111,111 | 1.58 | 20 (19%) |
| 23 | CHD | J | 60 | - | 29,32,32 | 0.96 | 0 | 47,51,51 | 5.35 | 35 (74%) |
| 21 | TGL | L | 522 | - | 62,62,62 | 1.56 | 8 (12%) | 65,65,65 | 2.15 | 16 (24%) |
| 27 | DMU | M | 526 | - | 34,34,34 | 1.13 | 4 (11%) | 45,45,45 | 3.55 | 27 (60%) |
| 19 | PGV | N | 1266 | - | 50,50,50 | 0.97 | 2 (4%) | 51,56,56 | 1.59 | 10 (19%) |
| 21 | TGL | N | 1523 | - | 62,62,62 | 1.39 | 7 (11%) | 65,65,65 | 1.47 | 10 (15%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 19 | PGV | N | 1524 | - | 50,50,50 | 1.09 | 2 (4%) | 51,56,56 | 1.36 | 6 (11%) |
| 14 | HEA | N | 515 | 1 | 44,67,67 | 1.14 | 4 (9%) | 37,103,103 | 1.84 | 9 (24%) |
| 14 | HEA | N | 516 | 1,15 | 44,67,67 | 1.24 | 7 (15%) | 37,103,103 | 2.43 | 14 (37%) |
| 15 | NO | N | 520 | 14,16 | 0,1,1 | 0.00 | - | 0,0,0 | 0.00 | - |
| 21 | TGL | O | 1521 | - | 62,62,62 | 1.35 | 6 (9%) | 65,65,65 | 1.66 | 11 (16%) |
| 20 | CUA | O | 228 | 2 | 0,1,1 | 0.00 | - | 0,0,0 | 0.00 | - |
| 23 | CHD | O | 229 | - | 29,32,32 | 1.64 | 5 (17%) | 47,51,51 | 5.71 | 32 (68%) |
| 25 | PEK | P | 1264 | - | 52,52,52 | 0.92 | 3 (5%) | 54,57,57 | 1.84 | 15 (27%) |
| 19 | PGV | P | 1267 | - | 50,50,50 | 0.92 | 3 (6%) | 51,56,56 | 1.56 | 8 (15%) |
| 26 | CDL | P | 1270 | - | 99,99,99 | 1.44 | 12 (12%) | 101,111,111 | 1.76 | 22 (21%) |
| 23 | CHD | P | 1271 | - | 29,32,32 | 0.80 | 1 (3%) | 47,51,51 | 5.12 | 33 (70%) |
| 23 | CHD | P | 1525 | - | 29,32,32 | 1.68 | 7 (24%) | 47,51,51 | 5.59 | 38 (80%) |
| 27 | DMU | P | 272 | - | 34,34,34 | 1.67 | 6 (17%) | 45,45,45 | 3.51 | 26 (57%) |
| 22 | PSC | R | 1229 | - | 51,51,51 | 1.34 | 3 (5%) | 56,59,59 | 1.36 | 4 (7%) |
| 25 | PEK | T | 1265 | - | 52,52,52 | 1.41 | 6 (11%) | 54,57,57 | 1.58 | 7 (12%) |
| 26 | CDL | T | 1269 | - | 99,99,99 | 1.41 | 13 (13%) | 101,111,111 | 1.58 | 17 (16%) |
| 25 | PEK | T | 263 | - | 52,52,52 | 1.46 | 5 (9%) | 54,57,57 | 1.41 | 7 (12%) |
| 19 | PGV | U | 1268 | - | 50,50,50 | 1.55 | 2 (4%) | 51,56,56 | 1.94 | 9 (17%) |
| 23 | CHD | W | 1059 | - | 29,32,32 | 1.25 | 3 (10%) | 47,51,51 | 5.44 | 33 (70%) |
| 21 | TGL | Y | 1522 | - | 62,62,62 | 1.68 | 10 (16%) | 65,65,65 | 2.27 | 17 (26%) |
| 27 | DMU | Z | 1526 | - | 34,34,34 | 1.12 | 2 (5%) | 45,45,45 | 3.32 | 27 (60%) |

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 |
|-----|------|-------|------|------|----------|------------|---------|
| 14 | HEA | A | 515 | 1 | 3/3/7/16 | 0/24/76/76 | 0/0/8/8 |
| 14 | HEA | A | 516 | 1 | 3/3/7/16 | 0/24/76/76 | 0/0/8/8 |
| 15 | NO | A | 520 | 16 | - | 0/0/0/0 | 0/0/0/0 |
| 19 | PGV | A | 521 | - | - | 0/55/55/55 | 0/0/0/0 |
| 19 | PGV | A | 524 | - | - | 0/55/55/55 | 0/0/0/0 |
| 23 | CHD | B | 1085 | - | - | 0/7/74/74 | 0/4/4/4 |
| 20 | CUA | B | 228 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 22 | PSC | B | 229 | - | - | 0/55/55/55 | 0/0/0/0 |
| 21 | TGL | B | 521 | - | - | 0/65/65/65 | 0/0/0/0 |
| 25 | PEK | C | 264 | - | - | 0/56/56/56 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|-----------|---------------|---------|
| 25 | PEK | C | 265 | - | - | 0/56/56/56 | 0/0/0/0 |
| 19 | PGV | C | 267 | - | - | 0/55/55/55 | 0/0/0/0 |
| 19 | PGV | C | 268 | - | - | 0/55/55/55 | 0/0/0/0 |
| 26 | CDL | C | 270 | - | - | 0/110/110/110 | 0/0/0/0 |
| 23 | CHD | C | 271 | - | 1/1/12/12 | 0/7/74/74 | 0/4/4/4 |
| 27 | DMU | C | 272 | - | 6/6/10/10 | 0/19/59/59 | 0/2/2/2 |
| 23 | CHD | C | 525 | - | - | 0/7/74/74 | 0/4/4/4 |
| 21 | TGL | D | 523 | - | - | 0/65/65/65 | 0/0/0/0 |
| 25 | PEK | G | 1263 | - | - | 0/56/56/56 | 0/0/0/0 |
| 26 | CDL | G | 269 | - | - | 0/110/110/110 | 0/0/0/0 |
| 23 | CHD | J | 60 | - | 2/2/12/12 | 0/7/74/74 | 0/4/4/4 |
| 21 | TGL | L | 522 | - | - | 0/65/65/65 | 0/0/0/0 |
| 27 | DMU | M | 526 | - | 4/4/10/10 | 0/19/59/59 | 0/2/2/2 |
| 19 | PGV | N | 1266 | - | - | 0/55/55/55 | 0/0/0/0 |
| 21 | TGL | N | 1523 | - | - | 0/65/65/65 | 0/0/0/0 |
| 19 | PGV | N | 1524 | - | - | 1/55/55/55 | 0/0/0/0 |
| 14 | HEA | N | 515 | 1 | 3/3/7/16 | 0/24/76/76 | 0/0/8/8 |
| 14 | HEA | N | 516 | 1,15 | 3/3/7/16 | 0/24/76/76 | 0/0/8/8 |
| 15 | NO | N | 520 | 14,16 | - | 0/0/0/0 | 0/0/0/0 |
| 21 | TGL | O | 1521 | - | - | 0/65/65/65 | 0/0/0/0 |
| 20 | CUA | O | 228 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 23 | CHD | O | 229 | - | - | 0/7/74/74 | 0/4/4/4 |
| 25 | PEK | P | 1264 | - | - | 0/56/56/56 | 0/0/0/0 |
| 19 | PGV | P | 1267 | - | - | 0/55/55/55 | 0/0/0/0 |
| 26 | CDL | P | 1270 | - | - | 2/110/110/110 | 0/0/0/0 |
| 23 | CHD | P | 1271 | - | 1/1/12/12 | 0/7/74/74 | 0/4/4/4 |
| 23 | CHD | P | 1525 | - | 1/1/12/12 | 0/7/74/74 | 0/4/4/4 |
| 27 | DMU | P | 272 | - | 6/6/10/10 | 0/19/59/59 | 0/2/2/2 |
| 22 | PSC | R | 1229 | - | - | 0/55/55/55 | 0/0/0/0 |
| 25 | PEK | T | 1265 | - | - | 0/56/56/56 | 0/0/0/0 |
| 26 | CDL | T | 1269 | - | - | 3/110/110/110 | 0/0/0/0 |
| 25 | PEK | T | 263 | - | - | 0/56/56/56 | 0/0/0/0 |
| 19 | PGV | U | 1268 | - | - | 0/55/55/55 | 0/0/0/0 |
| 23 | CHD | W | 1059 | - | 1/1/12/12 | 0/7/74/74 | 0/4/4/4 |
| 21 | TGL | Y | 1522 | - | - | 2/65/65/65 | 0/0/0/0 |
| 27 | DMU | Z | 1526 | - | 5/5/10/10 | 0/19/59/59 | 0/2/2/2 |

All (224) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23 | B | 1085 | CHD | C10-C5 | -4.70 | 1.47 | 1.55 |
| 23 | P | 1525 | CHD | C13-C12 | -4.54 | 1.47 | 1.54 |
| 23 | O | 229 | CHD | C13-C14 | -3.98 | 1.48 | 1.55 |
| 21 | L | 522 | TGL | C20-CA9 | -3.52 | 1.31 | 1.51 |
| 27 | Z | 1526 | DMU | C3-C4 | -3.48 | 1.43 | 1.52 |
| 23 | B | 1085 | CHD | C13-C14 | -3.47 | 1.49 | 1.55 |
| 26 | G | 269 | CDL | C59-C58 | -3.40 | 1.32 | 1.51 |
| 21 | Y | 1522 | TGL | C20-CA9 | -3.34 | 1.32 | 1.51 |
| 26 | C | 270 | CDL | C59-C58 | -3.24 | 1.33 | 1.51 |
| 23 | O | 229 | CHD | C10-C5 | -3.18 | 1.50 | 1.55 |
| 26 | T | 1269 | CDL | C62-C61 | -3.12 | 1.33 | 1.51 |
| 21 | O | 1521 | TGL | C10-CB9 | -3.12 | 1.33 | 1.51 |
| 21 | O | 1521 | TGL | C20-CA9 | -3.12 | 1.33 | 1.51 |
| 26 | P | 1270 | CDL | C59-C58 | -3.09 | 1.33 | 1.51 |
| 21 | B | 521 | TGL | C10-CB9 | -3.09 | 1.33 | 1.51 |
| 27 | M | 526 | DMU | C3-C4 | -3.09 | 1.44 | 1.52 |
| 14 | A | 515 | HEA | C1D-ND | -3.08 | 1.33 | 1.36 |
| 26 | T | 1269 | CDL | C59-C58 | -3.05 | 1.34 | 1.51 |
| 26 | C | 270 | CDL | C79-C78 | -3.01 | 1.34 | 1.51 |
| 26 | G | 269 | CDL | C42-C41 | -2.98 | 1.34 | 1.51 |
| 26 | P | 1270 | CDL | C22-C21 | -2.96 | 1.34 | 1.51 |
| 26 | G | 269 | CDL | C62-C61 | -2.94 | 1.34 | 1.51 |
| 26 | T | 1269 | CDL | C79-C78 | -2.94 | 1.34 | 1.51 |
| 26 | P | 1270 | CDL | C19-C18 | -2.93 | 1.34 | 1.51 |
| 21 | L | 522 | TGL | C10-CB9 | -2.92 | 1.34 | 1.51 |
| 21 | N | 1523 | TGL | C10-CB9 | -2.90 | 1.35 | 1.51 |
| 26 | C | 270 | CDL | C39-C38 | -2.89 | 1.35 | 1.51 |
| 26 | C | 270 | CDL | C62-C61 | -2.88 | 1.35 | 1.51 |
| 21 | N | 1523 | TGL | C20-CA9 | -2.88 | 1.35 | 1.51 |
| 21 | Y | 1522 | TGL | C10-CB9 | -2.86 | 1.35 | 1.51 |
| 23 | P | 1525 | CHD | C6-C5 | -2.85 | 1.48 | 1.53 |
| 26 | C | 270 | CDL | C82-C81 | -2.85 | 1.35 | 1.51 |
| 26 | P | 1270 | CDL | C82-C81 | -2.84 | 1.35 | 1.51 |
| 26 | G | 269 | CDL | C39-C38 | -2.83 | 1.35 | 1.51 |
| 26 | P | 1270 | CDL | C39-C38 | -2.82 | 1.35 | 1.51 |
| 26 | G | 269 | CDL | C22-C21 | -2.81 | 1.35 | 1.51 |
| 26 | T | 1269 | CDL | C82-C81 | -2.81 | 1.35 | 1.51 |
| 26 | G | 269 | CDL | C19-C18 | -2.79 | 1.35 | 1.51 |
| 26 | C | 270 | CDL | C22-C21 | -2.79 | 1.35 | 1.51 |
| 26 | G | 269 | CDL | C79-C78 | -2.78 | 1.35 | 1.51 |
| 21 | D | 523 | TGL | C15-CC9 | -2.78 | 1.35 | 1.51 |
| 26 | P | 1270 | CDL | C62-C61 | -2.77 | 1.35 | 1.51 |
| 26 | T | 1269 | CDL | C42-C41 | -2.77 | 1.35 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14 | A | 516 | HEA | C3C-C2C | -2.75 | 1.36 | 1.40 |
| 21 | N | 1523 | TGL | C15-CC9 | -2.75 | 1.35 | 1.51 |
| 26 | T | 1269 | CDL | C39-C38 | -2.71 | 1.36 | 1.51 |
| 23 | O | 229 | CHD | C6-C7 | -2.67 | 1.48 | 1.52 |
| 26 | T | 1269 | CDL | C19-C18 | -2.65 | 1.36 | 1.51 |
| 26 | C | 270 | CDL | C19-C18 | -2.64 | 1.36 | 1.51 |
| 21 | D | 523 | TGL | C20-CA9 | -2.62 | 1.36 | 1.51 |
| 26 | T | 1269 | CDL | C22-C21 | -2.61 | 1.36 | 1.51 |
| 21 | B | 521 | TGL | C20-CA9 | -2.60 | 1.36 | 1.51 |
| 23 | O | 229 | CHD | C1-C2 | -2.57 | 1.47 | 1.53 |
| 26 | P | 1270 | CDL | C79-C78 | -2.56 | 1.37 | 1.51 |
| 21 | O | 1521 | TGL | C15-CC9 | -2.55 | 1.37 | 1.51 |
| 26 | P | 1270 | CDL | C42-C41 | -2.54 | 1.37 | 1.51 |
| 26 | C | 270 | CDL | C42-C41 | -2.52 | 1.37 | 1.51 |
| 21 | L | 522 | TGL | C15-CC9 | -2.48 | 1.37 | 1.51 |
| 21 | Y | 1522 | TGL | C15-CC9 | -2.48 | 1.37 | 1.51 |
| 23 | C | 525 | CHD | C13-C12 | -2.47 | 1.50 | 1.54 |
| 26 | G | 269 | CDL | C82-C81 | -2.47 | 1.37 | 1.51 |
| 14 | N | 516 | HEA | C4B-NB | -2.46 | 1.33 | 1.36 |
| 27 | M | 526 | DMU | C6-C1 | -2.41 | 1.45 | 1.52 |
| 23 | P | 1525 | CHD | C10-C5 | -2.35 | 1.51 | 1.55 |
| 21 | D | 523 | TGL | C10-CB9 | -2.33 | 1.38 | 1.51 |
| 14 | A | 515 | HEA | C4A-NA | -2.32 | 1.34 | 1.36 |
| 19 | A | 521 | PGV | P-O14 | -2.30 | 1.43 | 1.55 |
| 14 | A | 515 | HEA | C3A-C2A | -2.30 | 1.37 | 1.40 |
| 23 | B | 1085 | CHD | C8-C7 | -2.28 | 1.49 | 1.53 |
| 19 | A | 521 | PGV | O01-C02 | -2.28 | 1.40 | 1.46 |
| 21 | B | 521 | TGL | C15-CC9 | -2.26 | 1.38 | 1.51 |
| 27 | M | 526 | DMU | O49-C1 | -2.23 | 1.37 | 1.43 |
| 14 | N | 516 | HEA | C4A-NA | -2.23 | 1.34 | 1.36 |
| 19 | C | 268 | PGV | O04-C19 | -2.23 | 1.15 | 1.22 |
| 23 | C | 525 | CHD | C1-C2 | -2.20 | 1.48 | 1.53 |
| 23 | C | 525 | CHD | C1-C10 | -2.12 | 1.50 | 1.54 |
| 14 | A | 516 | HEA | C3A-C2A | -2.11 | 1.37 | 1.40 |
| 23 | P | 1525 | CHD | C13-C14 | -2.11 | 1.51 | 1.55 |
| 23 | P | 1525 | CHD | C6-C7 | -2.09 | 1.49 | 1.52 |
| 27 | C | 272 | DMU | C3-C4 | -2.05 | 1.47 | 1.52 |
| 14 | A | 515 | HEA | CMD-C2D | -2.04 | 1.47 | 1.51 |
| 27 | P | 272 | DMU | C3-C4 | -2.02 | 1.47 | 1.52 |
| 27 | M | 526 | DMU | C8-C9 | -2.01 | 1.48 | 1.53 |
| 19 | C | 267 | PGV | O01-C1 | 2.00 | 1.40 | 1.34 |
| 25 | T | 263 | PEK | O12-C04 | 2.01 | 1.53 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 21 | D | 523 | TGL | CB2-CB1 | 2.02 | 1.56 | 1.50 |
| 25 | T | 263 | PEK | C03-C02 | 2.02 | 1.56 | 1.50 |
| 21 | N | 1523 | TGL | OB1-CB1 | 2.03 | 1.28 | 1.22 |
| 25 | T | 1265 | PEK | C22-C21 | 2.03 | 1.56 | 1.50 |
| 25 | G | 1263 | PEK | P-O11 | 2.04 | 1.67 | 1.59 |
| 19 | P | 1267 | PGV | C03-C02 | 2.06 | 1.56 | 1.50 |
| 25 | C | 264 | PEK | C2-C1 | 2.08 | 1.56 | 1.50 |
| 25 | P | 1264 | PEK | C2-C1 | 2.10 | 1.56 | 1.50 |
| 14 | N | 515 | HEA | OMA-CMA | 2.11 | 1.28 | 1.21 |
| 25 | G | 1263 | PEK | C03-C02 | 2.11 | 1.56 | 1.50 |
| 23 | P | 1525 | CHD | C16-C17 | 2.11 | 1.58 | 1.54 |
| 26 | T | 1269 | CDL | CA3-CA4 | 2.13 | 1.56 | 1.50 |
| 14 | A | 516 | HEA | C1B-CHB | 2.13 | 1.45 | 1.40 |
| 14 | N | 515 | HEA | C1C-CHC | 2.14 | 1.45 | 1.40 |
| 19 | A | 524 | PGV | C01-C02 | 2.15 | 1.56 | 1.50 |
| 21 | L | 522 | TGL | CG1-CG2 | 2.15 | 1.56 | 1.50 |
| 21 | Y | 1522 | TGL | CB2-CB1 | 2.18 | 1.57 | 1.50 |
| 19 | A | 524 | PGV | C20-C19 | 2.19 | 1.57 | 1.50 |
| 14 | N | 516 | HEA | OMA-CMA | 2.23 | 1.29 | 1.21 |
| 25 | T | 1265 | PEK | C03-C02 | 2.23 | 1.57 | 1.50 |
| 14 | A | 515 | HEA | C4D-CHA | 2.27 | 1.46 | 1.40 |
| 14 | A | 515 | HEA | C4B-NB | 2.30 | 1.39 | 1.36 |
| 25 | C | 265 | PEK | C22-C21 | 2.30 | 1.57 | 1.50 |
| 14 | A | 516 | HEA | C20-C19 | 2.31 | 1.56 | 1.51 |
| 14 | A | 515 | HEA | CMC-C2C | 2.32 | 1.56 | 1.51 |
| 14 | N | 516 | HEA | CAD-C3D | 2.34 | 1.56 | 1.52 |
| 27 | P | 272 | DMU | O7-C10 | 2.34 | 1.47 | 1.41 |
| 14 | A | 515 | HEA | C12-C13 | 2.36 | 1.61 | 1.53 |
| 21 | L | 522 | TGL | CC2-CC1 | 2.38 | 1.57 | 1.50 |
| 27 | P | 272 | DMU | O5-C4 | 2.38 | 1.50 | 1.44 |
| 27 | P | 272 | DMU | O1-C10 | 2.42 | 1.47 | 1.41 |
| 14 | A | 515 | HEA | C1B-CHB | 2.42 | 1.46 | 1.40 |
| 23 | C | 525 | CHD | C4-C3 | 2.43 | 1.56 | 1.51 |
| 14 | N | 515 | HEA | C4C-CHD | 2.43 | 1.46 | 1.40 |
| 14 | A | 516 | HEA | CAD-C3D | 2.44 | 1.56 | 1.52 |
| 27 | C | 272 | DMU | O1-C10 | 2.45 | 1.47 | 1.41 |
| 14 | N | 516 | HEA | C1D-ND | 2.45 | 1.39 | 1.36 |
| 25 | P | 1264 | PEK | O03-C21 | 2.47 | 1.40 | 1.33 |
| 14 | A | 516 | HEA | C3C-CAC | 2.49 | 1.52 | 1.47 |
| 19 | C | 267 | PGV | C03-C02 | 2.50 | 1.57 | 1.50 |
| 23 | W | 1059 | CHD | C13-C17 | 2.51 | 1.60 | 1.55 |
| 19 | C | 267 | PGV | O03-C19 | 2.59 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 23 | P | 1525 | CHD | C11-C9 | 2.64 | 1.58 | 1.53 |
| 14 | N | 516 | HEA | C4C-CHD | 2.64 | 1.47 | 1.40 |
| 19 | P | 1267 | PGV | O03-C19 | 2.68 | 1.41 | 1.33 |
| 25 | T | 1265 | PEK | P-O11 | 2.69 | 1.70 | 1.59 |
| 19 | A | 521 | PGV | C01-C02 | 2.71 | 1.58 | 1.50 |
| 23 | B | 1085 | CHD | C11-C12 | 2.71 | 1.58 | 1.53 |
| 14 | N | 516 | HEA | C1C-CHC | 2.75 | 1.47 | 1.40 |
| 21 | Y | 1522 | TGL | OG2-CG2 | 2.76 | 1.53 | 1.46 |
| 19 | P | 1267 | PGV | O01-C1 | 2.81 | 1.42 | 1.34 |
| 27 | C | 272 | DMU | O5-C6 | 2.84 | 1.48 | 1.41 |
| 21 | Y | 1522 | TGL | CG3-CG2 | 2.86 | 1.58 | 1.50 |
| 25 | T | 1265 | PEK | P-O12 | 2.86 | 1.71 | 1.59 |
| 27 | P | 272 | DMU | O5-C6 | 2.86 | 1.48 | 1.41 |
| 23 | P | 1271 | CHD | C20-C17 | 2.88 | 1.59 | 1.54 |
| 21 | Y | 1522 | TGL | CG1-CG2 | 2.94 | 1.59 | 1.50 |
| 23 | W | 1059 | CHD | C11-C9 | 2.95 | 1.58 | 1.53 |
| 25 | C | 265 | PEK | P-O11 | 2.96 | 1.71 | 1.59 |
| 14 | A | 515 | HEA | C1C-CHC | 3.07 | 1.48 | 1.40 |
| 25 | C | 265 | PEK | P-O12 | 3.10 | 1.72 | 1.59 |
| 14 | N | 515 | HEA | C4D-CHA | 3.13 | 1.48 | 1.40 |
| 19 | A | 521 | PGV | C03-C02 | 3.17 | 1.59 | 1.50 |
| 27 | Z | 1526 | DMU | O16-C6 | 3.24 | 1.45 | 1.40 |
| 19 | C | 268 | PGV | P-O11 | 3.26 | 1.73 | 1.59 |
| 14 | A | 516 | HEA | CMD-C2D | 3.29 | 1.58 | 1.51 |
| 25 | P | 1264 | PEK | O01-C1 | 3.30 | 1.43 | 1.34 |
| 19 | N | 1266 | PGV | O03-C19 | 3.31 | 1.43 | 1.33 |
| 19 | N | 1524 | PGV | O01-C1 | 3.35 | 1.44 | 1.34 |
| 25 | C | 264 | PEK | O01-C1 | 3.38 | 1.44 | 1.34 |
| 26 | C | 270 | CDL | C18-C17 | 3.39 | 1.70 | 1.51 |
| 21 | B | 521 | TGL | OG3-CC1 | 3.41 | 1.43 | 1.33 |
| 23 | C | 525 | CHD | C18-C13 | 3.42 | 1.60 | 1.54 |
| 19 | N | 1266 | PGV | O01-C1 | 3.55 | 1.44 | 1.34 |
| 23 | C | 525 | CHD | O12-C12 | 3.59 | 1.49 | 1.43 |
| 25 | C | 265 | PEK | O03-C01 | 3.70 | 1.53 | 1.45 |
| 22 | B | 229 | PSC | C13-C12 | 3.72 | 1.52 | 1.31 |
| 21 | L | 522 | TGL | OG3-CC1 | 3.79 | 1.44 | 1.33 |
| 21 | Y | 1522 | TGL | OG1-CA1 | 3.92 | 1.44 | 1.33 |
| 21 | O | 1521 | TGL | OG3-CC1 | 3.98 | 1.45 | 1.33 |
| 23 | W | 1059 | CHD | C20-C17 | 4.00 | 1.61 | 1.54 |
| 26 | G | 269 | CDL | OB8-CB7 | 4.01 | 1.45 | 1.33 |
| 19 | A | 521 | PGV | O03-C19 | 4.11 | 1.45 | 1.33 |
| 23 | O | 229 | CHD | C18-C13 | 4.15 | 1.61 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 19 | A | 521 | PGV | O01-C1 | 4.19 | 1.46 | 1.34 |
| 19 | C | 268 | PGV | O03-C19 | 4.19 | 1.45 | 1.33 |
| 22 | R | 1229 | PSC | O03-C19 | 4.19 | 1.45 | 1.33 |
| 21 | N | 1523 | TGL | OG3-CC1 | 4.24 | 1.45 | 1.33 |
| 22 | R | 1229 | PSC | C13-C12 | 4.24 | 1.55 | 1.31 |
| 26 | C | 270 | CDL | OA6-CA5 | 4.25 | 1.46 | 1.34 |
| 19 | A | 524 | PGV | O01-C1 | 4.29 | 1.46 | 1.34 |
| 22 | B | 229 | PSC | O01-C1 | 4.36 | 1.46 | 1.34 |
| 26 | C | 270 | CDL | OB6-CB5 | 4.42 | 1.47 | 1.34 |
| 26 | T | 1269 | CDL | OA8-CA7 | 4.42 | 1.46 | 1.33 |
| 25 | T | 263 | PEK | O01-C1 | 4.57 | 1.47 | 1.34 |
| 22 | B | 229 | PSC | O03-C19 | 4.58 | 1.46 | 1.33 |
| 21 | B | 521 | TGL | OG2-CB1 | 4.58 | 1.47 | 1.34 |
| 26 | T | 1269 | CDL | OB8-CB7 | 4.64 | 1.47 | 1.33 |
| 21 | D | 523 | TGL | OG3-CC1 | 4.69 | 1.47 | 1.33 |
| 26 | T | 1269 | CDL | OB6-CB5 | 4.70 | 1.47 | 1.34 |
| 21 | N | 1523 | TGL | OG1-CA1 | 4.72 | 1.47 | 1.33 |
| 26 | P | 1270 | CDL | OB6-CB5 | 4.81 | 1.48 | 1.34 |
| 21 | O | 1521 | TGL | OG2-CB1 | 4.81 | 1.48 | 1.34 |
| 21 | L | 522 | TGL | OG1-CA1 | 4.82 | 1.47 | 1.33 |
| 26 | G | 269 | CDL | OA8-CA7 | 4.91 | 1.47 | 1.33 |
| 21 | B | 521 | TGL | OG1-CA1 | 4.92 | 1.47 | 1.33 |
| 26 | P | 1270 | CDL | OB8-CB7 | 4.96 | 1.47 | 1.33 |
| 26 | G | 269 | CDL | OB6-CB5 | 4.97 | 1.48 | 1.34 |
| 26 | C | 270 | CDL | OB8-CB7 | 5.01 | 1.48 | 1.33 |
| 19 | U | 1268 | PGV | O03-C19 | 5.11 | 1.48 | 1.33 |
| 19 | N | 1524 | PGV | O03-C19 | 5.15 | 1.48 | 1.33 |
| 21 | D | 523 | TGL | OB1-CB1 | 5.16 | 1.38 | 1.22 |
| 21 | Y | 1522 | TGL | OG3-CC1 | 5.18 | 1.48 | 1.33 |
| 21 | O | 1521 | TGL | OG1-CA1 | 5.21 | 1.48 | 1.33 |
| 26 | P | 1270 | CDL | OA8-CA7 | 5.27 | 1.48 | 1.33 |
| 21 | N | 1523 | TGL | OG2-CB1 | 5.27 | 1.49 | 1.34 |
| 25 | T | 263 | PEK | C05-C04 | 5.28 | 1.71 | 1.50 |
| 21 | D | 523 | TGL | OG2-CB1 | 5.31 | 1.49 | 1.34 |
| 21 | D | 523 | TGL | OG1-CA1 | 5.33 | 1.49 | 1.33 |
| 25 | T | 263 | PEK | O03-C21 | 5.37 | 1.49 | 1.33 |
| 25 | G | 1263 | PEK | O01-C1 | 5.39 | 1.49 | 1.34 |
| 22 | R | 1229 | PSC | O01-C1 | 5.42 | 1.50 | 1.34 |
| 26 | T | 1269 | CDL | OA6-CA5 | 5.43 | 1.50 | 1.34 |
| 25 | T | 1265 | PEK | O03-C21 | 5.46 | 1.49 | 1.33 |
| 26 | G | 269 | CDL | OA6-CA5 | 5.48 | 1.50 | 1.34 |
| 26 | P | 1270 | CDL | OA6-CA5 | 5.49 | 1.50 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 25 | G | 1263 | PEK | O03-C21 | 5.51 | 1.49 | 1.33 |
| 19 | A | 524 | PGV | O03-C19 | 5.55 | 1.49 | 1.33 |
| 25 | T | 1265 | PEK | O01-C1 | 5.57 | 1.50 | 1.34 |
| 26 | C | 270 | CDL | OA8-CA7 | 5.57 | 1.49 | 1.33 |
| 25 | C | 265 | PEK | O01-C1 | 5.64 | 1.50 | 1.34 |
| 23 | B | 1085 | CHD | C18-C13 | 5.72 | 1.63 | 1.54 |
| 27 | C | 272 | DMU | O16-C6 | 5.87 | 1.50 | 1.40 |
| 19 | C | 268 | PGV | O01-C1 | 6.39 | 1.52 | 1.34 |
| 25 | C | 265 | PEK | O03-C21 | 6.40 | 1.52 | 1.33 |
| 27 | P | 272 | DMU | O16-C6 | 6.83 | 1.52 | 1.40 |
| 21 | L | 522 | TGL | OG2-CB1 | 7.05 | 1.54 | 1.34 |
| 19 | U | 1268 | PGV | O01-C1 | 7.06 | 1.54 | 1.34 |
| 21 | Y | 1522 | TGL | OG2-CB1 | 7.66 | 1.56 | 1.34 |

All (726) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 23 | O | 229 | CHD | C18-C13-C12 | -13.92 | 94.92 | 109.08 |
| 23 | P | 1525 | CHD | C18-C13-C12 | -12.00 | 96.87 | 109.08 |
| 23 | B | 1085 | CHD | C18-C13-C12 | -11.18 | 97.70 | 109.08 |
| 23 | C | 525 | CHD | C23-C22-C20 | -10.23 | 100.94 | 114.72 |
| 23 | W | 1059 | CHD | C6-C5-C4 | -9.82 | 99.98 | 111.13 |
| 23 | O | 229 | CHD | C19-C10-C9 | -8.83 | 98.53 | 111.16 |
| 23 | P | 1271 | CHD | C18-C13-C12 | -8.83 | 100.09 | 109.08 |
| 23 | C | 525 | CHD | C19-C10-C9 | -8.76 | 98.63 | 111.16 |
| 23 | P | 1525 | CHD | C19-C10-C9 | -8.51 | 98.98 | 111.16 |
| 23 | J | 60 | CHD | C18-C13-C12 | -8.44 | 100.49 | 109.08 |
| 23 | W | 1059 | CHD | C1-C10-C9 | -8.07 | 98.51 | 111.39 |
| 23 | C | 525 | CHD | C18-C13-C17 | -7.99 | 98.60 | 111.23 |
| 23 | C | 271 | CHD | C18-C13-C12 | -7.67 | 101.27 | 109.08 |
| 23 | B | 1085 | CHD | C19-C10-C9 | -7.50 | 100.44 | 111.16 |
| 21 | L | 522 | TGL | OG3-CC1-OC1 | -7.24 | 105.58 | 123.55 |
| 23 | B | 1085 | CHD | C18-C13-C17 | -7.16 | 99.91 | 111.23 |
| 23 | O | 229 | CHD | O12-C12-C13 | -7.05 | 99.35 | 111.12 |
| 23 | J | 60 | CHD | C6-C5-C4 | -6.42 | 103.84 | 111.13 |
| 23 | B | 1085 | CHD | O12-C12-C13 | -6.41 | 100.43 | 111.12 |
| 23 | O | 229 | CHD | C6-C5-C4 | -6.38 | 103.88 | 111.13 |
| 23 | J | 60 | CHD | C1-C10-C9 | -6.01 | 101.80 | 111.39 |
| 23 | P | 1525 | CHD | C6-C5-C4 | -5.97 | 104.34 | 111.13 |
| 23 | C | 525 | CHD | C18-C13-C12 | -5.92 | 103.06 | 109.08 |
| 23 | B | 1085 | CHD | C6-C5-C4 | -5.82 | 104.52 | 111.13 |
| 23 | C | 525 | CHD | C6-C5-C4 | -5.73 | 104.62 | 111.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | C | 525 | CHD | O12-C12-C13 | -5.67 | 101.66 | 111.12 |
| 23 | B | 1085 | CHD | C4-C5-C10 | -5.58 | 106.56 | 112.66 |
| 14 | N | 515 | HEA | C13-C12-C11 | -5.57 | 106.03 | 114.46 |
| 21 | L | 522 | TGL | CA4-CA3-CA2 | -5.54 | 92.94 | 113.24 |
| 23 | P | 1525 | CHD | O12-C12-C13 | -5.52 | 101.91 | 111.12 |
| 14 | A | 515 | HEA | C13-C12-C11 | -5.22 | 106.56 | 114.46 |
| 23 | O | 229 | CHD | O12-C12-C11 | -5.14 | 98.55 | 109.11 |
| 23 | P | 1525 | CHD | C18-C13-C14 | -5.14 | 103.11 | 111.23 |
| 23 | B | 1085 | CHD | O7-C7-C6 | -5.04 | 97.82 | 110.02 |
| 23 | P | 1271 | CHD | O7-C7-C6 | -5.04 | 97.82 | 110.02 |
| 14 | N | 516 | HEA | C13-C12-C11 | -5.00 | 106.89 | 114.46 |
| 23 | C | 271 | CHD | C19-C10-C9 | -4.94 | 104.09 | 111.16 |
| 23 | O | 229 | CHD | C18-C13-C17 | -4.93 | 103.44 | 111.23 |
| 19 | A | 521 | PGV | C8-C9-C10 | -4.89 | 94.96 | 113.74 |
| 25 | C | 264 | PEK | O01-C1-O02 | -4.86 | 111.55 | 123.68 |
| 23 | O | 229 | CHD | O7-C7-C6 | -4.85 | 98.30 | 110.02 |
| 19 | A | 524 | PGV | C4-C3-C2 | -4.83 | 95.54 | 113.24 |
| 25 | P | 1264 | PEK | O03-C01-C02 | -4.80 | 96.58 | 108.66 |
| 25 | T | 1265 | PEK | O03-C21-O04 | -4.79 | 111.66 | 123.55 |
| 14 | A | 516 | HEA | C20-C19-C18 | -4.77 | 111.34 | 121.10 |
| 23 | C | 525 | CHD | C19-C10-C5 | -4.73 | 102.14 | 110.30 |
| 23 | C | 525 | CHD | O7-C7-C6 | -4.62 | 98.83 | 110.02 |
| 23 | P | 1525 | CHD | O7-C7-C6 | -4.59 | 98.91 | 110.02 |
| 23 | P | 1271 | CHD | C19-C10-C9 | -4.57 | 104.62 | 111.16 |
| 21 | B | 521 | TGL | OG3-CC1-OC1 | -4.56 | 112.23 | 123.55 |
| 23 | P | 1525 | CHD | C1-C10-C9 | -4.52 | 104.17 | 111.39 |
| 19 | P | 1267 | PGV | O12-P-O13 | -4.37 | 91.61 | 109.25 |
| 21 | Y | 1522 | TGL | OG1-CA1-OA1 | -4.36 | 112.71 | 123.55 |
| 27 | M | 526 | DMU | O7-C10-C5 | -4.36 | 98.30 | 108.11 |
| 26 | P | 1270 | CDL | CB4-OB6-CB5 | -4.33 | 107.64 | 117.88 |
| 23 | P | 1271 | CHD | C18-C13-C17 | -4.26 | 104.49 | 111.23 |
| 19 | N | 1266 | PGV | O01-C1-O02 | -4.25 | 113.08 | 123.68 |
| 21 | N | 1523 | TGL | CG3-CG2-CG1 | -4.24 | 102.28 | 111.86 |
| 23 | O | 229 | CHD | C18-C13-C14 | -4.24 | 104.53 | 111.23 |
| 23 | P | 1525 | CHD | C18-C13-C17 | -4.18 | 104.62 | 111.23 |
| 23 | J | 60 | CHD | C19-C10-C5 | -4.17 | 103.12 | 110.30 |
| 14 | N | 516 | HEA | CAD-CBD-CGD | -4.11 | 105.64 | 112.66 |
| 19 | P | 1267 | PGV | O03-C19-O04 | -4.10 | 113.37 | 123.55 |
| 19 | U | 1268 | PGV | O04-C19-C20 | -4.08 | 107.54 | 123.68 |
| 19 | N | 1524 | PGV | C4-C3-C2 | -4.07 | 98.33 | 113.24 |
| 14 | A | 516 | HEA | C4B-C3B-C2B | -4.07 | 104.03 | 106.87 |
| 25 | P | 1264 | PEK | O01-C1-O02 | -4.01 | 113.67 | 123.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19 | A | 524 | PGV | C8-C9-C10 | -4.00 | 98.37 | 113.74 |
| 21 | N | 1523 | TGL | OG3-CC1-OC1 | -3.92 | 113.80 | 123.55 |
| 23 | C | 271 | CHD | C23-C22-C20 | -3.91 | 109.45 | 114.72 |
| 25 | C | 264 | PEK | O03-C01-C02 | -3.91 | 98.83 | 108.66 |
| 25 | C | 265 | PEK | O03-C21-O04 | -3.91 | 113.85 | 123.55 |
| 23 | C | 525 | CHD | O12-C12-C11 | -3.85 | 101.20 | 109.11 |
| 26 | T | 1269 | CDL | CB6-CB4-CB3 | -3.83 | 103.21 | 111.86 |
| 27 | Z | 1526 | DMU | O7-C10-C5 | -3.83 | 99.47 | 108.11 |
| 23 | P | 1525 | CHD | C21-C20-C22 | -3.82 | 104.32 | 110.35 |
| 21 | L | 522 | TGL | CA8-CA7-CA6 | -3.80 | 94.88 | 114.45 |
| 23 | C | 525 | CHD | C18-C13-C14 | -3.77 | 105.27 | 111.23 |
| 14 | A | 515 | HEA | CMB-C2B-C1B | -3.70 | 122.77 | 128.46 |
| 14 | N | 516 | HEA | CAD-C3D-C2D | -3.65 | 118.58 | 129.00 |
| 23 | P | 1271 | CHD | C23-C22-C20 | -3.65 | 109.81 | 114.72 |
| 14 | N | 515 | HEA | C1B-C2B-C3B | -3.62 | 104.47 | 107.00 |
| 23 | C | 271 | CHD | O7-C7-C6 | -3.60 | 101.32 | 110.02 |
| 23 | J | 60 | CHD | O12-C12-C11 | -3.57 | 101.78 | 109.11 |
| 25 | P | 1264 | PEK | C03-C02-C01 | -3.56 | 103.82 | 111.86 |
| 14 | N | 516 | HEA | C13-C14-C15 | -3.56 | 118.75 | 127.68 |
| 23 | C | 525 | CHD | C22-C20-C17 | -3.56 | 102.79 | 110.26 |
| 23 | B | 1085 | CHD | O12-C12-C11 | -3.54 | 101.84 | 109.11 |
| 19 | C | 268 | PGV | O04-C19-C20 | -3.53 | 109.74 | 123.68 |
| 19 | A | 524 | PGV | O03-C19-O04 | -3.48 | 114.90 | 123.55 |
| 14 | N | 516 | HEA | C4B-C3B-C2B | -3.43 | 104.47 | 106.87 |
| 26 | P | 1270 | CDL | C53-C52-C51 | -3.43 | 100.67 | 113.24 |
| 23 | P | 1271 | CHD | O12-C12-C11 | -3.43 | 102.07 | 109.11 |
| 26 | G | 269 | CDL | OB8-CB7-OB9 | -3.40 | 115.10 | 123.55 |
| 21 | O | 1521 | TGL | OG3-CC1-OC1 | -3.38 | 115.17 | 123.55 |
| 25 | P | 1264 | PEK | O01-C02-C01 | -3.34 | 96.31 | 108.44 |
| 25 | C | 264 | PEK | C03-C02-C01 | -3.33 | 104.34 | 111.86 |
| 25 | T | 263 | PEK | O03-C21-O04 | -3.33 | 115.28 | 123.55 |
| 23 | B | 1085 | CHD | C23-C22-C20 | -3.30 | 110.27 | 114.72 |
| 23 | P | 1271 | CHD | C19-C10-C5 | -3.29 | 104.62 | 110.30 |
| 14 | A | 515 | HEA | CAA-CBA-CGA | -3.28 | 107.05 | 112.66 |
| 14 | N | 516 | HEA | C1B-C2B-C3B | -3.27 | 104.72 | 107.00 |
| 22 | B | 229 | PSC | C30-C29-C28 | -3.26 | 97.65 | 114.45 |
| 23 | P | 1525 | CHD | O12-C12-C11 | -3.25 | 102.43 | 109.11 |
| 19 | U | 1268 | PGV | O02-C1-C2 | -3.22 | 110.95 | 123.68 |
| 26 | C | 270 | CDL | OB8-CB7-OB9 | -3.21 | 115.59 | 123.55 |
| 25 | C | 264 | PEK | C3-C2-C1 | -3.19 | 101.95 | 113.58 |
| 14 | A | 516 | HEA | C12-C13-C14 | -3.18 | 103.97 | 112.33 |
| 19 | C | 267 | PGV | O12-P-O13 | -3.17 | 96.46 | 109.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14 | N | 515 | HEA | C21-C20-C19 | -3.17 | 102.22 | 112.93 |
| 23 | C | 271 | CHD | O3-C3-C4 | -3.16 | 103.56 | 109.87 |
| 14 | A | 516 | HEA | CAA-CBA-CGA | -3.16 | 107.27 | 112.66 |
| 26 | P | 1270 | CDL | OA8-CA7-OA9 | -3.16 | 115.72 | 123.55 |
| 19 | A | 521 | PGV | C7-C6-C5 | -3.11 | 98.44 | 114.45 |
| 23 | C | 271 | CHD | C6-C5-C4 | -3.10 | 107.61 | 111.13 |
| 26 | T | 1269 | CDL | OA6-CA5-OA7 | -3.09 | 115.96 | 123.68 |
| 19 | A | 521 | PGV | O01-C1-O02 | -3.06 | 116.05 | 123.68 |
| 25 | C | 264 | PEK | C25-C24-C23 | -3.05 | 98.72 | 114.45 |
| 27 | P | 272 | DMU | O55-C2-C3 | -3.04 | 102.94 | 109.87 |
| 23 | C | 271 | CHD | C19-C10-C1 | -3.03 | 103.26 | 108.24 |
| 19 | A | 521 | PGV | O03-C19-O04 | -2.99 | 116.12 | 123.55 |
| 27 | M | 526 | DMU | O7-C10-O1 | -2.97 | 103.47 | 110.70 |
| 27 | M | 526 | DMU | C25-C28-C31 | -2.96 | 99.21 | 114.45 |
| 23 | O | 229 | CHD | C1-C10-C9 | -2.94 | 106.69 | 111.39 |
| 14 | A | 515 | HEA | C17-C18-C19 | -2.94 | 120.30 | 127.68 |
| 22 | B | 229 | PSC | C32-C31-C30 | -2.90 | 99.49 | 114.45 |
| 23 | W | 1059 | CHD | C18-C13-C14 | -2.90 | 106.64 | 111.23 |
| 26 | P | 1270 | CDL | OA6-CA5-OA7 | -2.90 | 116.45 | 123.68 |
| 23 | C | 271 | CHD | O12-C12-C11 | -2.89 | 103.17 | 109.11 |
| 23 | W | 1059 | CHD | C18-C13-C12 | -2.88 | 106.14 | 109.08 |
| 26 | T | 1269 | CDL | OA8-CA7-OA9 | -2.87 | 116.42 | 123.55 |
| 23 | J | 60 | CHD | C18-C13-C14 | -2.87 | 106.69 | 111.23 |
| 14 | N | 515 | HEA | OMA-CMA-C3A | -2.87 | 118.48 | 125.08 |
| 27 | M | 526 | DMU | O4-C7-C5 | -2.86 | 104.13 | 110.36 |
| 19 | C | 267 | PGV | O03-C19-O04 | -2.85 | 116.48 | 123.55 |
| 21 | D | 523 | TGL | OG1-CA1-OA1 | -2.85 | 116.48 | 123.55 |
| 23 | P | 1525 | CHD | C22-C20-C17 | -2.84 | 104.28 | 110.26 |
| 19 | N | 1266 | PGV | C15-C14-C13 | -2.84 | 102.82 | 113.74 |
| 14 | N | 516 | HEA | C27-C19-C18 | -2.84 | 116.11 | 123.69 |
| 23 | B | 1085 | CHD | C1-C10-C9 | -2.84 | 106.86 | 111.39 |
| 23 | B | 1085 | CHD | C19-C10-C5 | -2.84 | 105.41 | 110.30 |
| 19 | N | 1266 | PGV | C23-C22-C21 | -2.81 | 99.96 | 114.45 |
| 19 | C | 267 | PGV | C30-C29-C28 | -2.80 | 100.01 | 114.45 |
| 21 | L | 522 | TGL | CB4-CB3-CB2 | -2.79 | 103.00 | 113.24 |
| 25 | G | 1263 | PEK | O01-C1-O02 | -2.79 | 116.71 | 123.68 |
| 19 | A | 521 | PGV | C23-C22-C21 | -2.79 | 100.09 | 114.45 |
| 19 | A | 521 | PGV | C15-C14-C13 | -2.78 | 103.06 | 113.74 |
| 14 | A | 516 | HEA | CBA-CAA-C2A | -2.77 | 107.19 | 112.47 |
| 26 | T | 1269 | CDL | OB5-PB2-OB3 | -2.77 | 98.08 | 109.25 |
| 26 | G | 269 | CDL | OB6-CB5-OB7 | -2.75 | 116.81 | 123.68 |
| 23 | J | 60 | CHD | O7-C7-C6 | -2.75 | 103.37 | 110.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | B | 1085 | CHD | C18-C13-C14 | -2.75 | 106.89 | 111.23 |
| 26 | P | 1270 | CDL | OB8-CB7-OB9 | -2.74 | 116.75 | 123.55 |
| 14 | N | 515 | HEA | C13-C14-C15 | -2.73 | 120.81 | 127.68 |
| 21 | L | 522 | TGL | C22-C21-C20 | -2.71 | 100.49 | 114.45 |
| 22 | R | 1229 | PSC | O01-C1-O02 | -2.71 | 116.92 | 123.68 |
| 21 | B | 521 | TGL | OG1-CG1-CG2 | -2.70 | 101.86 | 108.66 |
| 25 | P | 1264 | PEK | O11-P-O14 | -2.70 | 98.36 | 109.25 |
| 14 | A | 516 | HEA | O11-C11-C3B | -2.70 | 104.07 | 111.83 |
| 14 | A | 515 | HEA | CAD-CBD-CGD | -2.69 | 108.06 | 112.66 |
| 14 | A | 515 | HEA | O11-C11-C3B | -2.67 | 104.15 | 111.83 |
| 19 | N | 1524 | PGV | O01-C1-O02 | -2.66 | 117.05 | 123.68 |
| 19 | N | 1524 | PGV | O03-C19-O04 | -2.65 | 116.97 | 123.55 |
| 27 | Z | 1526 | DMU | O7-C10-O1 | -2.65 | 104.26 | 110.70 |
| 21 | Y | 1522 | TGL | OG3-CC1-OC1 | -2.65 | 116.98 | 123.55 |
| 25 | C | 264 | PEK | C32-C31-C30 | -2.64 | 100.85 | 114.45 |
| 21 | D | 523 | TGL | OG2-CB1-CB2 | -2.64 | 106.07 | 111.55 |
| 23 | C | 525 | CHD | C1-C10-C9 | -2.63 | 107.19 | 111.39 |
| 14 | N | 516 | HEA | CMB-C2B-C1B | -2.62 | 124.44 | 128.46 |
| 26 | C | 270 | CDL | C18-C17-C16 | -2.60 | 101.04 | 114.45 |
| 27 | M | 526 | DMU | C22-C19-C18 | -2.57 | 101.94 | 113.48 |
| 21 | L | 522 | TGL | C26-C25-C24 | -2.55 | 101.31 | 114.45 |
| 19 | A | 521 | PGV | C6-C5-C4 | -2.55 | 101.33 | 114.45 |
| 14 | A | 515 | HEA | C26-C15-C14 | -2.54 | 116.90 | 123.69 |
| 14 | A | 515 | HEA | C21-C20-C19 | -2.54 | 104.34 | 112.93 |
| 23 | P | 1271 | CHD | C6-C5-C4 | -2.54 | 108.25 | 111.13 |
| 23 | O | 229 | CHD | C19-C10-C5 | -2.53 | 105.94 | 110.30 |
| 19 | C | 267 | PGV | O03-C01-C02 | -2.52 | 102.32 | 108.66 |
| 25 | T | 1265 | PEK | C2-C3-C4 | -2.50 | 108.82 | 113.29 |
| 19 | C | 268 | PGV | O03-C19-O04 | -2.50 | 117.34 | 123.55 |
| 21 | Y | 1522 | TGL | OB1-CB1-CB2 | -2.50 | 113.80 | 123.68 |
| 26 | C | 270 | CDL | OA6-CA5-OA7 | -2.49 | 117.45 | 123.68 |
| 21 | Y | 1522 | TGL | OG2-CB1-OB1 | -2.49 | 117.48 | 123.68 |
| 23 | C | 271 | CHD | C18-C13-C17 | -2.48 | 107.30 | 111.23 |
| 23 | W | 1059 | CHD | C23-C22-C20 | -2.47 | 111.39 | 114.72 |
| 21 | L | 522 | TGL | CA9-CA8-CA7 | -2.47 | 101.75 | 114.45 |
| 25 | T | 263 | PEK | O01-C1-O02 | -2.46 | 117.55 | 123.68 |
| 19 | P | 1267 | PGV | C03-C02-C01 | -2.43 | 106.39 | 111.86 |
| 21 | O | 1521 | TGL | OG2-CB1-OB1 | -2.40 | 117.69 | 123.68 |
| 23 | W | 1059 | CHD | C19-C10-C1 | -2.40 | 104.30 | 108.24 |
| 21 | D | 523 | TGL | CC4-CC3-CC2 | -2.39 | 104.49 | 113.24 |
| 26 | G | 269 | CDL | CB2-C1-CA2 | -2.39 | 105.57 | 112.73 |
| 19 | P | 1267 | PGV | C7-C6-C5 | -2.37 | 102.23 | 114.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 26 | T | 1269 | CDL | OB8-CB7-OB9 | -2.36 | 117.68 | 123.55 |
| 22 | B | 229 | PSC | C27-C26-C25 | -2.36 | 102.30 | 114.45 |
| 19 | A | 521 | PGV | C01-O03-C19 | -2.36 | 110.05 | 117.13 |
| 22 | B | 229 | PSC | C11-C12-C13 | -2.34 | 111.05 | 124.90 |
| 19 | N | 1266 | PGV | O14-P-O12 | -2.33 | 97.12 | 108.14 |
| 21 | Y | 1522 | TGL | C26-C25-C24 | -2.32 | 102.49 | 114.45 |
| 25 | C | 264 | PEK | C26-C25-C24 | -2.32 | 102.50 | 114.45 |
| 22 | B | 229 | PSC | O01-C1-O02 | -2.31 | 117.91 | 123.68 |
| 26 | C | 270 | CDL | C53-C52-C51 | -2.31 | 104.79 | 113.24 |
| 25 | P | 1264 | PEK | C24-C23-C22 | -2.30 | 104.80 | 113.24 |
| 26 | G | 269 | CDL | OA6-CA5-OA7 | -2.30 | 117.95 | 123.68 |
| 21 | B | 521 | TGL | OB1-CB1-CB2 | -2.29 | 114.62 | 123.68 |
| 21 | N | 1523 | TGL | OG1-CA1-OA1 | -2.29 | 117.86 | 123.55 |
| 19 | A | 524 | PGV | C8-C7-C6 | -2.29 | 102.65 | 114.45 |
| 27 | P | 272 | DMU | O49-C1-C2 | -2.29 | 105.37 | 110.36 |
| 21 | L | 522 | TGL | OB1-CB1-CB2 | -2.29 | 114.63 | 123.68 |
| 19 | N | 1266 | PGV | C6-C5-C4 | -2.29 | 102.66 | 114.45 |
| 23 | W | 1059 | CHD | C19-C10-C5 | -2.29 | 106.36 | 110.30 |
| 26 | G | 269 | CDL | CB6-CB4-CB3 | -2.28 | 106.70 | 111.86 |
| 27 | C | 272 | DMU | O2-C8-C7 | -2.27 | 105.42 | 110.36 |
| 19 | N | 1266 | PGV | O03-C19-O04 | -2.26 | 117.93 | 123.55 |
| 25 | P | 1264 | PEK | C33-C32-C31 | -2.26 | 102.80 | 114.45 |
| 19 | N | 1266 | PGV | O01-C02-C01 | -2.25 | 100.26 | 108.44 |
| 23 | J | 60 | CHD | O12-C12-C13 | -2.24 | 107.39 | 111.12 |
| 25 | C | 264 | PEK | O03-C21-O04 | -2.23 | 118.01 | 123.55 |
| 26 | P | 1270 | CDL | C54-C53-C52 | -2.23 | 102.97 | 114.45 |
| 14 | A | 516 | HEA | C13-C14-C15 | -2.22 | 122.09 | 127.68 |
| 19 | C | 268 | PGV | O02-C1-C2 | -2.22 | 114.90 | 123.68 |
| 26 | P | 1270 | CDL | CA6-CA4-CA3 | -2.21 | 106.88 | 111.86 |
| 26 | P | 1270 | CDL | C56-C55-C54 | -2.21 | 103.08 | 114.45 |
| 25 | C | 265 | PEK | O04-C21-C22 | -2.21 | 114.96 | 123.68 |
| 25 | P | 1264 | PEK | O03-C21-C22 | -2.20 | 105.49 | 111.90 |
| 19 | P | 1267 | PGV | C4-C3-C2 | -2.19 | 105.20 | 113.24 |
| 14 | N | 516 | HEA | C20-C19-C18 | -2.19 | 116.61 | 121.10 |
| 26 | C | 270 | CDL | O1-C1-CA2 | -2.19 | 101.28 | 109.34 |
| 14 | N | 516 | HEA | O11-C11-C3B | -2.18 | 105.56 | 111.83 |
| 23 | C | 525 | CHD | O7-C7-C8 | -2.16 | 104.51 | 109.33 |
| 25 | P | 1264 | PEK | C3-C2-C1 | -2.16 | 105.71 | 113.58 |
| 14 | A | 516 | HEA | OMA-CMA-C3A | -2.15 | 120.12 | 125.08 |
| 25 | C | 264 | PEK | C35-C34-C33 | -2.15 | 103.38 | 114.45 |
| 21 | Y | 1522 | TGL | CG3-CG2-CG1 | -2.13 | 107.04 | 111.86 |
| 23 | P | 1525 | CHD | C4-C5-C10 | -2.13 | 110.33 | 112.66 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | C | 264 | PEK | C24-C23-C22 | -2.12 | 105.48 | 113.24 |
| 23 | P | 1271 | CHD | C1-C10-C9 | -2.11 | 108.03 | 111.39 |
| 26 | C | 270 | CDL | C57-C56-C55 | -2.10 | 103.62 | 114.45 |
| 19 | P | 1267 | PGV | C22-C21-C20 | -2.10 | 105.55 | 113.24 |
| 23 | P | 1525 | CHD | C19-C10-C5 | -2.10 | 106.69 | 110.30 |
| 19 | A | 521 | PGV | C5-C4-C3 | -2.08 | 103.74 | 114.45 |
| 21 | B | 521 | TGL | OG2-CB1-OB1 | -2.08 | 118.49 | 123.68 |
| 25 | T | 1265 | PEK | C35-C34-C33 | -2.07 | 103.80 | 114.45 |
| 23 | C | 271 | CHD | C22-C20-C17 | -2.06 | 105.93 | 110.26 |
| 26 | P | 1270 | CDL | OA7-CA5-C11 | -2.05 | 115.59 | 123.68 |
| 19 | A | 521 | PGV | C25-C24-C23 | -2.05 | 103.91 | 114.45 |
| 26 | P | 1270 | CDL | C55-C54-C53 | -2.04 | 103.92 | 114.45 |
| 27 | Z | 1526 | DMU | O3-C5-C10 | -2.04 | 105.77 | 110.03 |
| 19 | C | 267 | PGV | C21-C20-C19 | -2.03 | 106.18 | 113.58 |
| 23 | W | 1059 | CHD | O7-C7-C6 | -2.03 | 105.12 | 110.02 |
| 25 | P | 1264 | PEK | C35-C34-C33 | -2.02 | 104.03 | 114.45 |
| 27 | C | 272 | DMU | O4-C7-C8 | -2.02 | 105.97 | 110.36 |
| 19 | U | 1268 | PGV | C24-C23-C22 | 2.00 | 124.77 | 114.45 |
| 27 | P | 272 | DMU | O61-C57-C4 | 2.00 | 118.08 | 111.34 |
| 22 | R | 1229 | PSC | C01-O03-C19 | 2.01 | 123.18 | 117.13 |
| 26 | P | 1270 | CDL | C20-C19-C18 | 2.01 | 124.82 | 114.45 |
| 21 | O | 1521 | TGL | OG2-CG2-CG1 | 2.02 | 115.77 | 108.44 |
| 27 | M | 526 | DMU | C57-C4-C3 | 2.02 | 118.74 | 113.24 |
| 26 | T | 1269 | CDL | OB8-CB6-CB4 | 2.03 | 113.77 | 108.66 |
| 26 | T | 1269 | CDL | C83-C82-C81 | 2.04 | 124.96 | 114.45 |
| 26 | G | 269 | CDL | C85-C84-C83 | 2.04 | 124.97 | 114.45 |
| 19 | N | 1266 | PGV | C26-C25-C24 | 2.04 | 124.97 | 114.45 |
| 21 | O | 1521 | TGL | OG2-CG2-CG3 | 2.05 | 115.88 | 108.44 |
| 26 | G | 269 | CDL | OB8-CB6-CB4 | 2.05 | 113.81 | 108.66 |
| 23 | B | 1085 | CHD | C1-C2-C3 | 2.06 | 113.04 | 110.42 |
| 25 | T | 1265 | PEK | C24-C23-C22 | 2.07 | 120.84 | 113.24 |
| 26 | C | 270 | CDL | OB4-PB2-OB3 | 2.08 | 123.04 | 112.28 |
| 22 | B | 229 | PSC | C01-O03-C19 | 2.08 | 123.39 | 117.13 |
| 19 | U | 1268 | PGV | C29-C28-C27 | 2.09 | 125.21 | 114.45 |
| 14 | N | 515 | HEA | CMB-C2B-C3B | 2.11 | 128.98 | 124.92 |
| 26 | C | 270 | CDL | C22-C21-C20 | 2.11 | 125.35 | 114.45 |
| 23 | B | 1085 | CHD | C13-C14-C8 | 2.12 | 117.50 | 114.77 |
| 26 | P | 1270 | CDL | C40-C39-C38 | 2.12 | 125.36 | 114.45 |
| 21 | N | 1523 | TGL | C21-C20-CA9 | 2.12 | 125.36 | 114.45 |
| 25 | C | 264 | PEK | O13-P-O14 | 2.12 | 123.28 | 112.28 |
| 23 | C | 525 | CHD | C2-C1-C10 | 2.13 | 116.50 | 112.80 |
| 27 | Z | 1526 | DMU | O55-C2-C1 | 2.13 | 114.98 | 110.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 19 | C | 267 | PGV | O14-P-O13 | 2.13 | 123.29 | 112.28 |
| 26 | T | 1269 | CDL | CA6-OA8-CA7 | 2.13 | 123.53 | 117.13 |
| 25 | C | 265 | PEK | O13-P-O11 | 2.14 | 118.25 | 108.14 |
| 25 | G | 1263 | PEK | C2-C3-C4 | 2.14 | 117.11 | 113.29 |
| 21 | D | 523 | TGL | C21-C20-CA9 | 2.14 | 125.50 | 114.45 |
| 26 | T | 1269 | CDL | C20-C19-C18 | 2.15 | 125.53 | 114.45 |
| 21 | D | 523 | TGL | CB5-CB4-CB3 | 2.15 | 125.53 | 114.45 |
| 21 | D | 523 | TGL | C13-C12-C11 | 2.16 | 125.56 | 114.45 |
| 26 | G | 269 | CDL | C23-C22-C21 | 2.16 | 125.57 | 114.45 |
| 27 | Z | 1526 | DMU | O61-C57-C4 | 2.16 | 118.61 | 111.34 |
| 21 | Y | 1522 | TGL | C10-CB9-CB8 | 2.16 | 125.58 | 114.45 |
| 26 | T | 1269 | CDL | C39-C38-C37 | 2.17 | 125.66 | 114.45 |
| 21 | D | 523 | TGL | CG3-OG3-CC1 | 2.20 | 123.74 | 117.13 |
| 21 | D | 523 | TGL | C20-CA9-CA8 | 2.21 | 125.83 | 114.45 |
| 26 | C | 270 | CDL | C39-C38-C37 | 2.21 | 125.85 | 114.45 |
| 26 | C | 270 | CDL | C83-C82-C81 | 2.21 | 125.86 | 114.45 |
| 27 | C | 272 | DMU | C11-C9-C8 | 2.22 | 118.19 | 113.00 |
| 25 | T | 263 | PEK | O03-C01-C02 | 2.22 | 114.23 | 108.66 |
| 21 | N | 1523 | TGL | OG2-CG2-CG3 | 2.22 | 116.51 | 108.44 |
| 23 | O | 229 | CHD | C2-C1-C10 | 2.23 | 116.68 | 112.80 |
| 26 | G | 269 | CDL | O1-C1-CB2 | 2.23 | 117.57 | 109.34 |
| 26 | T | 1269 | CDL | CA4-OA6-CA5 | 2.23 | 123.15 | 117.88 |
| 26 | P | 1270 | CDL | OB4-PB2-OB3 | 2.23 | 123.83 | 112.28 |
| 21 | D | 523 | TGL | OG2-CG2-CG3 | 2.24 | 116.58 | 108.44 |
| 23 | J | 60 | CHD | C14-C8-C9 | 2.26 | 112.71 | 109.64 |
| 25 | G | 1263 | PEK | C11-C10-C9 | 2.26 | 119.52 | 111.84 |
| 19 | A | 524 | PGV | C01-O03-C19 | 2.26 | 123.94 | 117.13 |
| 19 | A | 524 | PGV | C02-O01-C1 | 2.27 | 123.23 | 117.88 |
| 14 | N | 515 | HEA | C12-C11-C3B | 2.27 | 118.19 | 112.65 |
| 19 | A | 524 | PGV | O14-P-O13 | 2.28 | 124.09 | 112.28 |
| 21 | N | 1523 | TGL | OG2-CB1-CB2 | 2.30 | 116.33 | 111.55 |
| 27 | P | 272 | DMU | O7-C3-C2 | 2.30 | 112.73 | 107.19 |
| 27 | M | 526 | DMU | O49-C1-C6 | 2.31 | 114.86 | 110.03 |
| 14 | N | 515 | HEA | C3C-C4C-NC | 2.31 | 112.20 | 109.21 |
| 19 | C | 268 | PGV | O01-C02-C03 | 2.32 | 116.86 | 108.44 |
| 21 | Y | 1522 | TGL | C15-CC9-CC8 | 2.32 | 126.39 | 114.45 |
| 26 | P | 1270 | CDL | C42-C41-C40 | 2.32 | 126.42 | 114.45 |
| 14 | N | 516 | HEA | C16-C15-C14 | 2.33 | 125.87 | 121.10 |
| 21 | D | 523 | TGL | CG1-OG1-CA1 | 2.33 | 124.14 | 117.13 |
| 23 | C | 525 | CHD | C9-C11-C12 | 2.33 | 117.39 | 114.32 |
| 19 | U | 1268 | PGV | O01-C02-C01 | 2.34 | 116.94 | 108.44 |
| 26 | C | 270 | CDL | O1-C1-CB2 | 2.34 | 117.97 | 109.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 27 | Z | 1526 | DMU | O16-C18-C19 | 2.35 | 118.07 | 109.68 |
| 27 | C | 272 | DMU | O7-C10-C5 | 2.36 | 113.44 | 108.11 |
| 19 | C | 267 | PGV | O03-C19-C20 | 2.36 | 118.78 | 111.90 |
| 26 | G | 269 | CDL | OA8-CA6-CA4 | 2.37 | 114.62 | 108.66 |
| 26 | G | 269 | CDL | C82-C81-C80 | 2.38 | 126.72 | 114.45 |
| 21 | D | 523 | TGL | C11-C10-CB9 | 2.39 | 126.76 | 114.45 |
| 26 | P | 1270 | CDL | CA6-OA8-CA7 | 2.40 | 124.36 | 117.13 |
| 21 | O | 1521 | TGL | C15-CC9-CC8 | 2.41 | 126.88 | 114.45 |
| 21 | L | 522 | TGL | OG2-CG2-CG1 | 2.41 | 117.21 | 108.44 |
| 22 | B | 229 | PSC | C16-C15-C14 | 2.42 | 123.03 | 113.74 |
| 27 | Z | 1526 | DMU | O7-C3-C4 | 2.42 | 115.29 | 109.34 |
| 26 | T | 1269 | CDL | C82-C81-C80 | 2.42 | 126.93 | 114.45 |
| 21 | L | 522 | TGL | C15-CC9-CC8 | 2.43 | 126.97 | 114.45 |
| 27 | C | 272 | DMU | O55-C2-C3 | 2.44 | 115.43 | 109.87 |
| 19 | U | 1268 | PGV | C01-O03-C19 | 2.45 | 124.50 | 117.13 |
| 26 | G | 269 | CDL | CB6-OB8-CB7 | 2.46 | 124.55 | 117.13 |
| 25 | C | 265 | PEK | C24-C23-C22 | 2.47 | 122.30 | 113.24 |
| 23 | P | 1525 | CHD | C2-C1-C10 | 2.48 | 117.12 | 112.80 |
| 23 | J | 60 | CHD | C9-C8-C7 | 2.49 | 114.85 | 111.92 |
| 25 | C | 265 | PEK | O12-C04-C05 | 2.50 | 118.44 | 109.10 |
| 25 | P | 1264 | PEK | O04-C21-C22 | 2.51 | 133.59 | 123.68 |
| 14 | A | 515 | HEA | C3C-C4C-NC | 2.52 | 112.47 | 109.21 |
| 26 | G | 269 | CDL | OB8-CB7-C71 | 2.52 | 119.25 | 111.90 |
| 27 | Z | 1526 | DMU | C6-C1-C2 | 2.53 | 114.67 | 109.98 |
| 27 | C | 272 | DMU | O16-C18-C19 | 2.53 | 118.70 | 109.68 |
| 26 | P | 1270 | CDL | OB6-CB5-C51 | 2.53 | 116.81 | 111.55 |
| 27 | Z | 1526 | DMU | O5-C6-O16 | 2.54 | 116.05 | 110.02 |
| 27 | Z | 1526 | DMU | O55-C2-C3 | 2.55 | 115.67 | 109.87 |
| 19 | U | 1268 | PGV | C15-C14-C13 | 2.56 | 123.59 | 113.74 |
| 25 | C | 264 | PEK | C14-C13-C12 | 2.58 | 120.60 | 111.84 |
| 21 | B | 521 | TGL | CC3-CC2-CC1 | 2.58 | 123.01 | 113.58 |
| 19 | C | 267 | PGV | O14-P-O12 | 2.58 | 120.35 | 108.14 |
| 26 | G | 269 | CDL | OA6-CA4-CA6 | 2.61 | 117.92 | 108.44 |
| 27 | P | 272 | DMU | C11-C9-C8 | 2.64 | 119.19 | 113.00 |
| 14 | N | 515 | HEA | C26-C15-C16 | 2.65 | 119.89 | 115.29 |
| 19 | A | 521 | PGV | C9-C8-C7 | 2.66 | 128.15 | 114.45 |
| 21 | N | 1523 | TGL | OG1-CA1-CA2 | 2.66 | 119.65 | 111.90 |
| 21 | Y | 1522 | TGL | OG2-CG2-CG3 | 2.68 | 118.18 | 108.44 |
| 26 | P | 1270 | CDL | OA8-CA6-CA4 | 2.69 | 115.43 | 108.66 |
| 26 | T | 1269 | CDL | CB6-OB8-CB7 | 2.69 | 125.24 | 117.13 |
| 26 | G | 269 | CDL | OA8-CA7-C31 | 2.70 | 119.75 | 111.90 |
| 21 | L | 522 | TGL | OG1-CA1-CA2 | 2.71 | 119.78 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 14 | A | 515 | HEA | CMB-C2B-C3B | 2.72 | 130.13 | 124.92 |
| 23 | C | 525 | CHD | C15-C16-C17 | 2.72 | 110.55 | 105.12 |
| 27 | M | 526 | DMU | C11-C9-C8 | 2.72 | 119.37 | 113.00 |
| 23 | P | 1525 | CHD | C1-C2-C3 | 2.73 | 113.89 | 110.42 |
| 14 | N | 516 | HEA | CBD-CAD-C3D | 2.75 | 117.74 | 112.48 |
| 26 | T | 1269 | CDL | C43-C42-C41 | 2.76 | 128.66 | 114.45 |
| 25 | P | 1264 | PEK | C8-C7-C6 | 2.77 | 121.27 | 111.84 |
| 23 | B | 1085 | CHD | C16-C17-C20 | 2.78 | 116.58 | 112.14 |
| 19 | A | 521 | PGV | C8-C7-C6 | 2.78 | 128.77 | 114.45 |
| 23 | P | 1525 | CHD | C13-C14-C8 | 2.80 | 118.38 | 114.77 |
| 26 | P | 1270 | CDL | C79-C78-C77 | 2.81 | 128.95 | 114.45 |
| 27 | Z | 1526 | DMU | O3-C5-C7 | 2.83 | 116.51 | 110.36 |
| 27 | C | 272 | DMU | C10-O1-C9 | 2.84 | 119.06 | 113.72 |
| 27 | M | 526 | DMU | O49-C1-C2 | 2.84 | 116.54 | 110.36 |
| 23 | C | 271 | CHD | C14-C8-C7 | 2.86 | 115.68 | 111.80 |
| 27 | Z | 1526 | DMU | C11-C9-C8 | 2.86 | 119.70 | 113.00 |
| 26 | G | 269 | CDL | C83-C82-C81 | 2.87 | 129.22 | 114.45 |
| 25 | T | 1265 | PEK | O03-C01-C02 | 2.87 | 115.87 | 108.66 |
| 26 | C | 270 | CDL | C42-C41-C40 | 2.88 | 129.31 | 114.45 |
| 26 | C | 270 | CDL | CA6-OA8-CA7 | 2.89 | 125.81 | 117.13 |
| 26 | G | 269 | CDL | C80-C79-C78 | 2.89 | 129.35 | 114.45 |
| 21 | Y | 1522 | TGL | CG3-OG3-CC1 | 2.90 | 125.85 | 117.13 |
| 23 | J | 60 | CHD | C16-C17-C20 | 2.92 | 116.81 | 112.14 |
| 27 | P | 272 | DMU | O7-C10-O1 | 2.93 | 117.80 | 110.70 |
| 27 | M | 526 | DMU | C1-C2-C3 | 2.93 | 115.68 | 109.61 |
| 19 | A | 524 | PGV | O03-C01-C02 | 2.95 | 116.06 | 108.66 |
| 23 | J | 60 | CHD | C11-C9-C10 | 2.95 | 116.87 | 113.74 |
| 25 | C | 264 | PEK | O01-C1-C2 | 2.96 | 117.70 | 111.55 |
| 23 | B | 1085 | CHD | C16-C17-C13 | 2.98 | 106.53 | 103.57 |
| 23 | C | 525 | CHD | C15-C14-C8 | 2.98 | 122.54 | 118.32 |
| 14 | A | 515 | HEA | C16-C17-C18 | 2.99 | 122.22 | 111.97 |
| 27 | P | 272 | DMU | C10-O1-C9 | 3.00 | 119.36 | 113.72 |
| 27 | M | 526 | DMU | C10-C5-C7 | 3.01 | 115.56 | 109.98 |
| 27 | Z | 1526 | DMU | C57-C4-C3 | 3.05 | 121.54 | 113.24 |
| 26 | C | 270 | CDL | OA8-CA7-C31 | 3.05 | 120.78 | 111.90 |
| 23 | B | 1085 | CHD | C11-C9-C10 | 3.06 | 116.98 | 113.74 |
| 14 | N | 516 | HEA | CMB-C2B-C3B | 3.07 | 130.81 | 124.92 |
| 27 | P | 272 | DMU | O16-C18-C19 | 3.07 | 120.64 | 109.68 |
| 27 | P | 272 | DMU | O5-C6-C1 | 3.08 | 116.23 | 110.30 |
| 23 | O | 229 | CHD | C16-C17-C13 | 3.08 | 106.64 | 103.57 |
| 21 | B | 521 | TGL | C15-CC9-CC8 | 3.08 | 130.34 | 114.45 |
| 21 | B | 521 | TGL | CG2-OG2-CB1 | 3.11 | 125.22 | 117.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 23 | O | 229 | CHD | C6-C7-C8 | 3.11 | 114.81 | 111.50 |
| 25 | C | 264 | PEK | C11-C10-C9 | 3.12 | 122.44 | 111.84 |
| 23 | O | 229 | CHD | C11-C9-C10 | 3.17 | 117.10 | 113.74 |
| 23 | P | 1525 | CHD | C16-C17-C13 | 3.18 | 106.73 | 103.57 |
| 23 | C | 525 | CHD | C19-C10-C1 | 3.19 | 113.48 | 108.24 |
| 23 | C | 271 | CHD | C17-C13-C14 | 3.22 | 103.36 | 100.08 |
| 27 | M | 526 | DMU | O55-C2-C1 | 3.22 | 117.36 | 110.36 |
| 21 | D | 523 | TGL | C10-CB9-CB8 | 3.23 | 131.11 | 114.45 |
| 21 | N | 1523 | TGL | CG3-OG3-CC1 | 3.23 | 126.85 | 117.13 |
| 21 | O | 1521 | TGL | CG1-OG1-CA1 | 3.23 | 126.86 | 117.13 |
| 22 | B | 229 | PSC | O03-C19-C20 | 3.24 | 121.31 | 111.90 |
| 23 | C | 525 | CHD | C5-C6-C7 | 3.24 | 118.02 | 114.44 |
| 25 | G | 1263 | PEK | O03-C21-C22 | 3.24 | 121.32 | 111.90 |
| 21 | B | 521 | TGL | CG1-OG1-CA1 | 3.24 | 126.89 | 117.13 |
| 21 | O | 1521 | TGL | CG3-OG3-CC1 | 3.24 | 126.89 | 117.13 |
| 27 | Z | 1526 | DMU | O7-C3-C2 | 3.25 | 115.03 | 107.19 |
| 26 | G | 269 | CDL | CA6-OA8-CA7 | 3.29 | 127.02 | 117.13 |
| 23 | P | 1525 | CHD | C6-C7-C8 | 3.31 | 115.02 | 111.50 |
| 25 | C | 264 | PEK | C01-O03-C21 | 3.31 | 127.09 | 117.13 |
| 23 | B | 1085 | CHD | C14-C8-C7 | 3.31 | 116.29 | 111.80 |
| 19 | A | 524 | PGV | O01-C02-C01 | 3.33 | 120.54 | 108.44 |
| 25 | T | 263 | PEK | C2-C3-C4 | 3.33 | 119.23 | 113.29 |
| 25 | G | 1263 | PEK | C01-O03-C21 | 3.33 | 127.15 | 117.13 |
| 23 | P | 1525 | CHD | C16-C17-C20 | 3.35 | 117.50 | 112.14 |
| 23 | P | 1271 | CHD | C11-C12-C13 | 3.35 | 114.69 | 111.22 |
| 27 | Z | 1526 | DMU | C10-C5-C7 | 3.37 | 116.24 | 109.98 |
| 23 | J | 60 | CHD | C9-C10-C5 | 3.38 | 113.50 | 108.63 |
| 14 | A | 516 | HEA | CBD-CAD-C3D | 3.40 | 118.99 | 112.48 |
| 23 | O | 229 | CHD | C16-C17-C20 | 3.41 | 117.60 | 112.14 |
| 27 | C | 272 | DMU | O7-C3-C4 | 3.44 | 117.81 | 109.34 |
| 22 | R | 1229 | PSC | O03-C19-C20 | 3.45 | 121.94 | 111.90 |
| 19 | N | 1524 | PGV | O01-C1-C2 | 3.46 | 118.73 | 111.55 |
| 21 | L | 522 | TGL | OG1-CG1-CG2 | 3.46 | 117.34 | 108.66 |
| 23 | P | 1525 | CHD | C11-C12-C13 | 3.46 | 114.80 | 111.22 |
| 19 | N | 1524 | PGV | O03-C01-C02 | 3.46 | 117.35 | 108.66 |
| 25 | P | 1264 | PEK | O13-P-O14 | 3.46 | 130.21 | 112.28 |
| 23 | P | 1525 | CHD | C14-C8-C9 | 3.48 | 114.37 | 109.64 |
| 21 | Y | 1522 | TGL | CB3-CB2-CB1 | 3.48 | 126.28 | 113.58 |
| 25 | T | 263 | PEK | O03-C21-C22 | 3.53 | 122.17 | 111.90 |
| 23 | P | 1525 | CHD | C13-C17-C20 | 3.53 | 123.78 | 119.49 |
| 27 | Z | 1526 | DMU | C1-C2-C3 | 3.54 | 116.94 | 109.61 |
| 23 | B | 1085 | CHD | C11-C9-C8 | 3.55 | 115.97 | 110.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 27 | M | 526 | DMU | O3-C5-C7 | 3.56 | 118.09 | 110.36 |
| 25 | T | 263 | PEK | C01-O03-C21 | 3.56 | 127.83 | 117.13 |
| 23 | C | 525 | CHD | C5-C4-C3 | 3.56 | 118.09 | 112.87 |
| 23 | C | 271 | CHD | C21-C20-C17 | 3.57 | 118.53 | 112.95 |
| 27 | C | 272 | DMU | O5-C6-O16 | 3.59 | 118.53 | 110.02 |
| 21 | D | 523 | TGL | OG1-CA1-CA2 | 3.59 | 122.35 | 111.90 |
| 25 | C | 264 | PEK | C2-C3-C4 | 3.59 | 119.70 | 113.29 |
| 21 | B | 521 | TGL | OG1-CA1-CA2 | 3.62 | 122.42 | 111.90 |
| 21 | Y | 1522 | TGL | OG2-CG2-CG1 | 3.62 | 121.61 | 108.44 |
| 25 | P | 1264 | PEK | O01-C1-C2 | 3.65 | 119.13 | 111.55 |
| 23 | B | 1085 | CHD | C9-C11-C12 | 3.66 | 119.15 | 114.32 |
| 19 | A | 521 | PGV | O01-C1-C2 | 3.68 | 119.19 | 111.55 |
| 23 | C | 525 | CHD | C1-C2-C3 | 3.68 | 115.11 | 110.42 |
| 27 | M | 526 | DMU | O5-C4-C3 | 3.69 | 117.30 | 109.75 |
| 19 | N | 1266 | PGV | O01-C1-C2 | 3.70 | 119.24 | 111.55 |
| 23 | P | 1525 | CHD | C21-C20-C17 | 3.71 | 118.75 | 112.95 |
| 23 | P | 1525 | CHD | O3-C3-C4 | 3.72 | 117.30 | 109.87 |
| 27 | C | 272 | DMU | C10-C5-C7 | 3.73 | 116.92 | 109.98 |
| 22 | B | 229 | PSC | O01-C1-C2 | 3.75 | 119.33 | 111.55 |
| 27 | Z | 1526 | DMU | C6-O5-C4 | 3.76 | 120.80 | 113.72 |
| 21 | O | 1521 | TGL | CG2-OG2-CB1 | 3.76 | 126.77 | 117.88 |
| 23 | P | 1271 | CHD | C9-C10-C5 | 3.78 | 114.08 | 108.63 |
| 19 | P | 1267 | PGV | O03-C19-C20 | 3.78 | 122.89 | 111.90 |
| 27 | P | 272 | DMU | C10-C5-C7 | 3.80 | 117.04 | 109.98 |
| 23 | J | 60 | CHD | C4-C5-C10 | 3.82 | 116.83 | 112.66 |
| 23 | O | 229 | CHD | C5-C6-C7 | 3.83 | 118.67 | 114.44 |
| 26 | P | 1270 | CDL | CA4-OA6-CA5 | 3.83 | 126.93 | 117.88 |
| 27 | P | 272 | DMU | C2-C3-C4 | 3.84 | 119.03 | 110.88 |
| 27 | P | 272 | DMU | C7-C8-C9 | 3.84 | 116.99 | 110.22 |
| 23 | W | 1059 | CHD | C9-C11-C12 | 3.85 | 119.40 | 114.32 |
| 23 | P | 1525 | CHD | C17-C13-C14 | 3.86 | 104.01 | 100.08 |
| 25 | G | 1263 | PEK | O03-C01-C02 | 3.86 | 118.36 | 108.66 |
| 23 | C | 271 | CHD | C17-C13-C12 | 3.86 | 121.22 | 117.67 |
| 23 | W | 1059 | CHD | C21-C20-C17 | 3.87 | 119.00 | 112.95 |
| 19 | N | 1266 | PGV | O03-C19-C20 | 3.87 | 123.16 | 111.90 |
| 27 | C | 272 | DMU | O61-C57-C4 | 3.89 | 124.44 | 111.34 |
| 23 | P | 1271 | CHD | C13-C17-C20 | 3.90 | 124.22 | 119.49 |
| 23 | O | 229 | CHD | O3-C3-C4 | 3.90 | 117.67 | 109.87 |
| 25 | T | 1265 | PEK | O01-C1-C2 | 3.91 | 119.68 | 111.55 |
| 23 | C | 271 | CHD | C11-C12-C13 | 3.92 | 115.28 | 111.22 |
| 27 | C | 272 | DMU | O5-C4-C3 | 3.93 | 117.79 | 109.75 |
| 23 | J | 60 | CHD | C11-C9-C8 | 3.96 | 116.56 | 110.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 19 | N | 1524 | PGV | O03-C19-C20 | 3.96 | 123.43 | 111.90 |
| 14 | A | 515 | HEA | C26-C15-C16 | 3.97 | 122.17 | 115.29 |
| 21 | O | 1521 | TGL | OG1-CA1-CA2 | 3.99 | 123.52 | 111.90 |
| 23 | W | 1059 | CHD | C11-C9-C10 | 4.01 | 117.98 | 113.74 |
| 27 | P | 272 | DMU | O7-C3-C4 | 4.01 | 119.21 | 109.34 |
| 23 | P | 1525 | CHD | C5-C6-C7 | 4.03 | 118.90 | 114.44 |
| 27 | M | 526 | DMU | C7-C8-C9 | 4.06 | 117.37 | 110.22 |
| 23 | P | 1525 | CHD | C5-C4-C3 | 4.06 | 118.83 | 112.87 |
| 27 | Z | 1526 | DMU | C7-C8-C9 | 4.06 | 117.37 | 110.22 |
| 19 | P | 1267 | PGV | O14-P-O13 | 4.07 | 133.32 | 112.28 |
| 23 | B | 1085 | CHD | C2-C1-C10 | 4.07 | 119.88 | 112.80 |
| 27 | Z | 1526 | DMU | O16-C6-C1 | 4.07 | 114.87 | 108.23 |
| 23 | C | 525 | CHD | C11-C9-C8 | 4.08 | 116.74 | 110.82 |
| 21 | N | 1523 | TGL | OG1-CG1-CG2 | 4.09 | 118.93 | 108.66 |
| 23 | P | 1271 | CHD | C17-C13-C14 | 4.10 | 104.25 | 100.08 |
| 23 | W | 1059 | CHD | C11-C9-C8 | 4.14 | 116.82 | 110.82 |
| 27 | Z | 1526 | DMU | O5-C4-C3 | 4.14 | 118.23 | 109.75 |
| 27 | C | 272 | DMU | C7-C8-C9 | 4.15 | 117.52 | 110.22 |
| 27 | C | 272 | DMU | C1-C2-C3 | 4.15 | 118.20 | 109.61 |
| 23 | C | 525 | CHD | C6-C7-C8 | 4.15 | 115.91 | 111.50 |
| 21 | L | 522 | TGL | OG2-CB1-CB2 | 4.17 | 120.20 | 111.55 |
| 21 | L | 522 | TGL | CC3-CC2-CC1 | 4.19 | 128.87 | 113.58 |
| 21 | Y | 1522 | TGL | OG3-CC1-CC2 | 4.19 | 124.10 | 111.90 |
| 21 | B | 521 | TGL | OG2-CG2-CG3 | 4.21 | 123.75 | 108.44 |
| 23 | J | 60 | CHD | C22-C20-C17 | 4.24 | 119.16 | 110.26 |
| 23 | P | 1271 | CHD | C21-C20-C17 | 4.25 | 119.60 | 112.95 |
| 27 | M | 526 | DMU | O1-C9-C11 | 4.28 | 116.66 | 106.41 |
| 23 | C | 525 | CHD | C9-C8-C7 | 4.29 | 116.96 | 111.92 |
| 23 | P | 1525 | CHD | C9-C11-C12 | 4.29 | 119.98 | 114.32 |
| 27 | P | 272 | DMU | C6-O5-C4 | 4.32 | 121.85 | 113.72 |
| 23 | W | 1059 | CHD | C22-C20-C17 | 4.32 | 119.34 | 110.26 |
| 27 | P | 272 | DMU | O5-C6-O16 | 4.34 | 120.31 | 110.02 |
| 27 | Z | 1526 | DMU | O1-C9-C11 | 4.37 | 116.87 | 106.41 |
| 25 | T | 263 | PEK | O01-C1-C2 | 4.37 | 120.62 | 111.55 |
| 19 | A | 521 | PGV | O03-C19-C20 | 4.43 | 124.79 | 111.90 |
| 27 | C | 272 | DMU | O5-C6-C1 | 4.44 | 118.85 | 110.30 |
| 21 | D | 523 | TGL | CG2-OG2-CB1 | 4.46 | 128.42 | 117.88 |
| 27 | P | 272 | DMU | C1-C2-C3 | 4.48 | 118.91 | 109.61 |
| 21 | N | 1523 | TGL | OG3-CC1-CC2 | 4.49 | 124.97 | 111.90 |
| 26 | T | 1269 | CDL | OA8-CA7-C31 | 4.50 | 124.98 | 111.90 |
| 27 | M | 526 | DMU | O7-C3-C2 | 4.50 | 118.02 | 107.19 |
| 27 | Z | 1526 | DMU | C8-C7-C5 | 4.51 | 118.80 | 110.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 26 | P | 1270 | CDL | OB8-CB7-C71 | 4.52 | 125.06 | 111.90 |
| 27 | P | 272 | DMU | O1-C9-C11 | 4.55 | 117.30 | 106.41 |
| 23 | C | 271 | CHD | C9-C11-C12 | 4.55 | 120.32 | 114.32 |
| 21 | O | 1521 | TGL | OG3-CC1-CC2 | 4.57 | 125.19 | 111.90 |
| 21 | D | 523 | TGL | CB3-CB2-CB1 | 4.58 | 130.31 | 113.58 |
| 23 | C | 525 | CHD | C11-C9-C10 | 4.59 | 118.60 | 113.74 |
| 25 | P | 1264 | PEK | C2-C3-C4 | 4.65 | 121.59 | 113.29 |
| 26 | P | 1270 | CDL | OA8-CA7-C31 | 4.65 | 125.44 | 111.90 |
| 27 | C | 272 | DMU | C6-C1-C2 | 4.67 | 118.66 | 109.98 |
| 23 | P | 1525 | CHD | C9-C8-C7 | 4.69 | 117.44 | 111.92 |
| 23 | B | 1085 | CHD | C15-C14-C8 | 4.71 | 124.98 | 118.32 |
| 21 | Y | 1522 | TGL | OG1-CA1-CA2 | 4.72 | 125.65 | 111.90 |
| 27 | C | 272 | DMU | O7-C3-C2 | 4.76 | 118.64 | 107.19 |
| 23 | P | 1271 | CHD | C4-C5-C10 | 4.76 | 117.86 | 112.66 |
| 23 | W | 1059 | CHD | C17-C13-C12 | 4.80 | 122.09 | 117.67 |
| 27 | P | 272 | DMU | O7-C10-C5 | 4.81 | 118.94 | 108.11 |
| 23 | J | 60 | CHD | C13-C14-C8 | 4.81 | 120.97 | 114.77 |
| 23 | P | 1525 | CHD | C11-C9-C8 | 4.87 | 117.89 | 110.82 |
| 27 | M | 526 | DMU | C6-C1-C2 | 4.90 | 119.09 | 109.98 |
| 21 | L | 522 | TGL | CG2-OG2-CB1 | 4.93 | 129.53 | 117.88 |
| 27 | M | 526 | DMU | O55-C2-C3 | 4.94 | 121.10 | 109.87 |
| 23 | O | 229 | CHD | C15-C14-C13 | 4.94 | 108.49 | 103.57 |
| 23 | W | 1059 | CHD | C9-C8-C7 | 4.95 | 117.74 | 111.92 |
| 27 | M | 526 | DMU | O16-C6-C1 | 4.99 | 116.37 | 108.23 |
| 23 | C | 525 | CHD | C14-C8-C9 | 5.00 | 116.44 | 109.64 |
| 19 | C | 268 | PGV | O01-C1-C2 | 5.01 | 121.96 | 111.55 |
| 27 | M | 526 | DMU | C8-C7-C5 | 5.03 | 119.72 | 110.84 |
| 21 | B | 521 | TGL | CG3-OG3-CC1 | 5.04 | 132.29 | 117.13 |
| 19 | A | 524 | PGV | O03-C19-C20 | 5.05 | 126.60 | 111.90 |
| 23 | O | 229 | CHD | C17-C13-C14 | 5.07 | 105.24 | 100.08 |
| 27 | C | 272 | DMU | O1-C9-C11 | 5.08 | 118.58 | 106.41 |
| 23 | P | 1271 | CHD | C15-C14-C13 | 5.09 | 108.64 | 103.57 |
| 27 | P | 272 | DMU | C8-C7-C5 | 5.11 | 119.85 | 110.84 |
| 27 | M | 526 | DMU | O5-C6-C1 | 5.11 | 120.16 | 110.30 |
| 27 | M | 526 | DMU | C6-O5-C4 | 5.12 | 123.36 | 113.72 |
| 21 | B | 521 | TGL | OG3-CC1-CC2 | 5.12 | 126.81 | 111.90 |
| 27 | P | 272 | DMU | O16-C6-C1 | 5.16 | 116.65 | 108.23 |
| 26 | C | 270 | CDL | OB8-CB7-C71 | 5.16 | 126.91 | 111.90 |
| 27 | C | 272 | DMU | C8-C7-C5 | 5.18 | 119.98 | 110.84 |
| 26 | T | 1269 | CDL | OB6-CB5-C51 | 5.20 | 122.36 | 111.55 |
| 14 | A | 516 | HEA | C27-C19-C20 | 5.27 | 124.43 | 115.29 |
| 23 | O | 229 | CHD | C4-C3-C2 | 5.28 | 117.11 | 110.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 27 | C | 272 | DMU | C18-O16-C6 | 5.29 | 122.94 | 113.87 |
| 23 | W | 1059 | CHD | C4-C5-C10 | 5.36 | 118.51 | 112.66 |
| 27 | C | 272 | DMU | C2-C3-C4 | 5.36 | 122.25 | 110.88 |
| 23 | C | 271 | CHD | C2-C1-C10 | 5.37 | 122.16 | 112.80 |
| 23 | P | 1271 | CHD | C9-C11-C12 | 5.38 | 121.42 | 114.32 |
| 21 | L | 522 | TGL | OG3-CC1-CC2 | 5.41 | 127.64 | 111.90 |
| 23 | J | 60 | CHD | C15-C14-C8 | 5.46 | 126.05 | 118.32 |
| 25 | C | 265 | PEK | O01-C1-C2 | 5.47 | 122.90 | 111.55 |
| 26 | G | 269 | CDL | OA6-CA5-C11 | 5.52 | 123.01 | 111.55 |
| 23 | C | 525 | CHD | C15-C14-C13 | 5.54 | 109.08 | 103.57 |
| 23 | B | 1085 | CHD | C11-C12-C13 | 5.56 | 116.98 | 111.22 |
| 27 | C | 272 | DMU | C6-O5-C4 | 5.57 | 124.21 | 113.72 |
| 23 | J | 60 | CHD | C2-C1-C10 | 5.58 | 122.52 | 112.80 |
| 23 | P | 1271 | CHD | C5-C6-C7 | 5.60 | 120.63 | 114.44 |
| 21 | Y | 1522 | TGL | CG2-OG2-CB1 | 5.61 | 131.12 | 117.88 |
| 23 | P | 1271 | CHD | C2-C1-C10 | 5.63 | 122.60 | 112.80 |
| 23 | C | 525 | CHD | O3-C3-C4 | 5.67 | 121.18 | 109.87 |
| 23 | J | 60 | CHD | C15-C14-C13 | 5.68 | 109.22 | 103.57 |
| 23 | P | 1525 | CHD | C11-C9-C10 | 5.73 | 119.80 | 113.74 |
| 26 | G | 269 | CDL | OB6-CB5-C51 | 5.73 | 123.46 | 111.55 |
| 27 | Z | 1526 | DMU | O5-C4-C57 | 5.77 | 120.22 | 106.41 |
| 23 | P | 1271 | CHD | C17-C13-C12 | 5.77 | 122.97 | 117.67 |
| 23 | O | 229 | CHD | C11-C9-C8 | 5.77 | 119.19 | 110.82 |
| 23 | W | 1059 | CHD | C1-C10-C5 | 5.79 | 116.76 | 107.79 |
| 23 | W | 1059 | CHD | C14-C13-C12 | 5.79 | 112.88 | 107.39 |
| 23 | W | 1059 | CHD | C6-C5-C10 | 5.93 | 119.13 | 112.66 |
| 27 | M | 526 | DMU | C2-C3-C4 | 5.93 | 123.46 | 110.88 |
| 27 | P | 272 | DMU | O5-C4-C57 | 5.94 | 120.64 | 106.41 |
| 23 | W | 1059 | CHD | C4-C3-C2 | 5.96 | 117.95 | 110.55 |
| 27 | P | 272 | DMU | O5-C4-C3 | 6.00 | 122.02 | 109.75 |
| 26 | C | 270 | CDL | OA6-CA5-C11 | 6.02 | 124.05 | 111.55 |
| 14 | A | 516 | HEA | C3C-C4C-NC | 6.09 | 117.09 | 109.21 |
| 23 | O | 229 | CHD | C5-C4-C3 | 6.09 | 121.81 | 112.87 |
| 22 | R | 1229 | PSC | O01-C1-C2 | 6.12 | 124.26 | 111.55 |
| 23 | O | 229 | CHD | C15-C14-C8 | 6.12 | 126.99 | 118.32 |
| 23 | J | 60 | CHD | C14-C13-C12 | 6.13 | 113.20 | 107.39 |
| 23 | J | 60 | CHD | C1-C2-C3 | 6.13 | 118.24 | 110.42 |
| 23 | B | 1085 | CHD | C17-C13-C14 | 6.14 | 106.34 | 100.08 |
| 23 | O | 229 | CHD | C9-C8-C7 | 6.18 | 119.19 | 111.92 |
| 25 | G | 1263 | PEK | O01-C1-C2 | 6.20 | 124.43 | 111.55 |
| 23 | C | 271 | CHD | C4-C3-C2 | 6.22 | 118.28 | 110.55 |
| 21 | O | 1521 | TGL | OG2-CB1-CB2 | 6.25 | 124.52 | 111.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 23 | C | 271 | CHD | C1-C10-C5 | 6.27 | 117.51 | 107.79 |
| 23 | C | 271 | CHD | C11-C9-C8 | 6.28 | 119.93 | 110.82 |
| 23 | C | 271 | CHD | C4-C5-C10 | 6.31 | 119.55 | 112.66 |
| 23 | W | 1059 | CHD | C9-C10-C5 | 6.32 | 117.75 | 108.63 |
| 25 | T | 1265 | PEK | O03-C21-C22 | 6.37 | 130.44 | 111.90 |
| 23 | J | 60 | CHD | C9-C11-C12 | 6.38 | 122.73 | 114.32 |
| 23 | B | 1085 | CHD | C15-C14-C13 | 6.41 | 109.95 | 103.57 |
| 27 | P | 272 | DMU | C6-C1-C2 | 6.42 | 121.91 | 109.98 |
| 23 | W | 1059 | CHD | C2-C1-C10 | 6.44 | 124.03 | 112.80 |
| 27 | P | 272 | DMU | C18-O16-C6 | 6.46 | 124.95 | 113.87 |
| 23 | B | 1085 | CHD | C14-C8-C9 | 6.47 | 118.44 | 109.64 |
| 23 | C | 525 | CHD | C14-C13-C12 | 6.49 | 113.55 | 107.39 |
| 23 | C | 271 | CHD | C15-C14-C13 | 6.49 | 110.03 | 103.57 |
| 23 | P | 1271 | CHD | C16-C17-C13 | 6.50 | 110.05 | 103.57 |
| 23 | P | 1271 | CHD | C14-C8-C7 | 6.50 | 120.62 | 111.80 |
| 23 | J | 60 | CHD | C5-C4-C3 | 6.52 | 122.44 | 112.87 |
| 23 | J | 60 | CHD | C14-C8-C7 | 6.52 | 120.65 | 111.80 |
| 23 | P | 1271 | CHD | C5-C4-C3 | 6.53 | 122.45 | 112.87 |
| 27 | Z | 1526 | DMU | C2-C3-C4 | 6.53 | 124.74 | 110.88 |
| 23 | P | 1271 | CHD | C4-C3-C2 | 6.58 | 118.72 | 110.55 |
| 23 | C | 271 | CHD | C5-C4-C3 | 6.58 | 122.53 | 112.87 |
| 23 | C | 271 | CHD | C16-C17-C20 | 6.59 | 122.69 | 112.14 |
| 23 | C | 271 | CHD | C6-C7-C8 | 6.61 | 118.53 | 111.50 |
| 25 | C | 265 | PEK | O03-C21-C22 | 6.63 | 131.19 | 111.90 |
| 27 | P | 272 | DMU | O1-C10-C5 | 6.65 | 123.12 | 110.30 |
| 27 | C | 272 | DMU | O1-C10-C5 | 6.69 | 123.21 | 110.30 |
| 26 | T | 1269 | CDL | OA6-CA5-C11 | 6.70 | 125.47 | 111.55 |
| 23 | W | 1059 | CHD | C1-C2-C3 | 6.74 | 119.01 | 110.42 |
| 23 | C | 271 | CHD | C14-C13-C12 | 6.83 | 113.87 | 107.39 |
| 14 | N | 516 | HEA | C27-C19-C20 | 6.84 | 127.16 | 115.29 |
| 27 | C | 272 | DMU | O16-C6-C1 | 6.85 | 119.42 | 108.23 |
| 23 | P | 1271 | CHD | C1-C2-C3 | 6.86 | 119.17 | 110.42 |
| 23 | P | 1271 | CHD | C11-C9-C8 | 6.90 | 120.83 | 110.82 |
| 21 | Y | 1522 | TGL | OG1-CG1-CG2 | 6.98 | 126.18 | 108.66 |
| 23 | O | 229 | CHD | C14-C8-C9 | 7.02 | 119.19 | 109.64 |
| 23 | J | 60 | CHD | C6-C7-C8 | 7.06 | 119.01 | 111.50 |
| 23 | W | 1059 | CHD | C6-C7-C8 | 7.06 | 119.01 | 111.50 |
| 23 | C | 271 | CHD | C1-C2-C3 | 7.08 | 119.44 | 110.42 |
| 19 | U | 1268 | PGV | O01-C1-C2 | 7.15 | 126.40 | 111.55 |
| 23 | P | 1271 | CHD | C16-C17-C20 | 7.16 | 123.60 | 112.14 |
| 19 | C | 268 | PGV | O03-C19-C20 | 7.20 | 132.85 | 111.90 |
| 23 | P | 1271 | CHD | C1-C10-C5 | 7.21 | 118.96 | 107.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 23 | J | 60 | CHD | C11-C12-C13 | 7.22 | 118.70 | 111.22 |
| 23 | P | 1271 | CHD | C15-C14-C8 | 7.25 | 128.58 | 118.32 |
| 27 | Z | 1526 | DMU | O5-C6-C1 | 7.27 | 124.31 | 110.30 |
| 27 | M | 526 | DMU | O5-C4-C57 | 7.30 | 123.89 | 106.41 |
| 19 | U | 1268 | PGV | O03-C19-C20 | 7.31 | 133.16 | 111.90 |
| 21 | B | 521 | TGL | OG2-CB1-CB2 | 7.31 | 126.72 | 111.55 |
| 23 | J | 60 | CHD | C5-C6-C7 | 7.31 | 122.53 | 114.44 |
| 23 | P | 1271 | CHD | C6-C5-C10 | 7.34 | 120.68 | 112.66 |
| 27 | C | 272 | DMU | O1-C9-C8 | 7.34 | 123.18 | 109.66 |
| 23 | W | 1059 | CHD | C5-C4-C3 | 7.36 | 123.67 | 112.87 |
| 27 | Z | 1526 | DMU | O1-C9-C8 | 7.43 | 123.35 | 109.66 |
| 23 | B | 1085 | CHD | C6-C7-C8 | 7.46 | 119.43 | 111.50 |
| 23 | J | 60 | CHD | C6-C5-C10 | 7.47 | 120.81 | 112.66 |
| 27 | P | 272 | DMU | O1-C9-C8 | 7.51 | 123.50 | 109.66 |
| 23 | C | 271 | CHD | C16-C17-C13 | 7.61 | 111.15 | 103.57 |
| 23 | C | 525 | CHD | C17-C13-C14 | 7.63 | 107.85 | 100.08 |
| 23 | J | 60 | CHD | C4-C3-C2 | 7.66 | 120.06 | 110.55 |
| 27 | C | 272 | DMU | O5-C4-C57 | 7.67 | 124.79 | 106.41 |
| 27 | M | 526 | DMU | O1-C9-C8 | 7.71 | 123.87 | 109.66 |
| 23 | O | 229 | CHD | C11-C12-C13 | 7.74 | 119.24 | 111.22 |
| 23 | J | 60 | CHD | C1-C10-C5 | 7.74 | 119.79 | 107.79 |
| 23 | W | 1059 | CHD | C5-C6-C7 | 7.79 | 123.06 | 114.44 |
| 23 | C | 525 | CHD | C13-C17-C20 | 7.81 | 128.97 | 119.49 |
| 23 | J | 60 | CHD | C16-C17-C13 | 7.85 | 111.39 | 103.57 |
| 23 | C | 271 | CHD | C5-C6-C7 | 7.86 | 123.14 | 114.44 |
| 23 | B | 1085 | CHD | C5-C4-C3 | 7.87 | 124.42 | 112.87 |
| 23 | P | 1271 | CHD | C14-C13-C12 | 7.90 | 114.88 | 107.39 |
| 26 | P | 1270 | CDL | OA6-CA5-C11 | 7.90 | 127.95 | 111.55 |
| 27 | M | 526 | DMU | O1-C10-C5 | 7.92 | 125.56 | 110.30 |
| 23 | W | 1059 | CHD | C15-C14-C8 | 7.97 | 129.59 | 118.32 |
| 23 | O | 229 | CHD | C1-C2-C3 | 7.97 | 120.58 | 110.42 |
| 23 | C | 271 | CHD | C6-C5-C10 | 8.00 | 121.40 | 112.66 |
| 23 | O | 229 | CHD | C17-C13-C12 | 8.09 | 125.11 | 117.67 |
| 27 | Z | 1526 | DMU | O1-C10-C5 | 8.11 | 125.93 | 110.30 |
| 23 | C | 271 | CHD | C15-C14-C8 | 8.17 | 129.88 | 118.32 |
| 21 | Y | 1522 | TGL | OG2-CB1-CB2 | 8.27 | 128.72 | 111.55 |
| 23 | C | 525 | CHD | C17-C13-C12 | 8.37 | 125.36 | 117.67 |
| 23 | J | 60 | CHD | C17-C13-C12 | 8.38 | 125.37 | 117.67 |
| 23 | B | 1085 | CHD | C4-C3-C2 | 8.39 | 120.97 | 110.55 |
| 23 | W | 1059 | CHD | C16-C17-C13 | 8.41 | 111.95 | 103.57 |
| 23 | P | 1525 | CHD | C10-C9-C8 | 8.42 | 120.95 | 111.87 |
| 23 | W | 1059 | CHD | C15-C14-C13 | 8.44 | 111.97 | 103.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | W | 1059 | CHD | C11-C12-C13 | 8.51 | 120.03 | 111.22 |
| 23 | P | 1525 | CHD | C15-C14-C13 | 8.54 | 112.07 | 103.57 |
| 23 | O | 229 | CHD | C10-C9-C8 | 8.78 | 121.34 | 111.87 |
| 23 | B | 1085 | CHD | C14-C13-C12 | 8.81 | 115.75 | 107.39 |
| 23 | C | 525 | CHD | C11-C12-C13 | 8.87 | 120.41 | 111.22 |
| 23 | P | 1271 | CHD | C6-C7-C8 | 8.99 | 121.06 | 111.50 |
| 23 | C | 525 | CHD | C4-C3-C2 | 9.30 | 122.10 | 110.55 |
| 23 | C | 525 | CHD | C10-C9-C8 | 9.37 | 121.97 | 111.87 |
| 23 | B | 1085 | CHD | C17-C13-C12 | 9.82 | 126.70 | 117.67 |
| 23 | J | 60 | CHD | C13-C17-C20 | 9.91 | 131.51 | 119.49 |
| 23 | W | 1059 | CHD | C14-C8-C7 | 9.93 | 125.27 | 111.80 |
| 23 | W | 1059 | CHD | C10-C9-C8 | 10.26 | 122.93 | 111.87 |
| 23 | P | 1525 | CHD | C17-C13-C12 | 10.28 | 127.12 | 117.67 |
| 23 | W | 1059 | CHD | C13-C17-C20 | 10.42 | 132.12 | 119.49 |
| 23 | P | 1525 | CHD | C14-C13-C12 | 10.49 | 117.34 | 107.39 |
| 23 | O | 229 | CHD | C1-C10-C5 | 10.69 | 124.36 | 107.79 |
| 23 | P | 1525 | CHD | C4-C3-C2 | 11.11 | 124.35 | 110.55 |
| 23 | B | 1085 | CHD | C10-C9-C8 | 11.33 | 124.08 | 111.87 |
| 23 | C | 525 | CHD | C1-C10-C5 | 11.35 | 125.38 | 107.79 |
| 23 | B | 1085 | CHD | C1-C10-C5 | 11.91 | 126.24 | 107.79 |
| 23 | C | 525 | CHD | C6-C5-C10 | 12.22 | 126.01 | 112.66 |
| 23 | P | 1525 | CHD | C1-C10-C5 | 12.36 | 126.94 | 107.79 |
| 23 | P | 1525 | CHD | C6-C5-C10 | 12.48 | 126.30 | 112.66 |
| 23 | O | 229 | CHD | C6-C5-C10 | 12.55 | 126.37 | 112.66 |
| 23 | P | 1271 | CHD | C10-C9-C8 | 12.63 | 125.48 | 111.87 |
| 23 | O | 229 | CHD | C14-C13-C12 | 12.73 | 119.47 | 107.39 |
| 23 | J | 60 | CHD | C10-C9-C8 | 12.91 | 125.79 | 111.87 |
| 23 | C | 271 | CHD | C10-C9-C8 | 14.55 | 127.55 | 111.87 |
| 23 | B | 1085 | CHD | C6-C5-C10 | 14.88 | 128.91 | 112.66 |

All (39) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 14 | N | 515 | HEA | ND |
| 14 | N | 515 | HEA | NA |
| 14 | N | 515 | HEA | NB |
| 27 | Z | 1526 | DMU | C2 |
| 27 | Z | 1526 | DMU | C4 |
| 27 | Z | 1526 | DMU | C9 |
| 27 | Z | 1526 | DMU | C6 |
| 27 | Z | 1526 | DMU | C5 |
| 27 | P | 272 | DMU | C5 |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 27 | P | 272 | DMU | C6 |
| 27 | P | 272 | DMU | C9 |
| 27 | P | 272 | DMU | C4 |
| 27 | P | 272 | DMU | C2 |
| 27 | P | 272 | DMU | C10 |
| 14 | A | 515 | HEA | ND |
| 14 | A | 515 | HEA | NA |
| 14 | A | 515 | HEA | NB |
| 14 | N | 516 | HEA | ND |
| 14 | N | 516 | HEA | NA |
| 14 | N | 516 | HEA | NB |
| 23 | J | 60 | CHD | C17 |
| 23 | J | 60 | CHD | C9 |
| 23 | P | 1271 | CHD | C9 |
| 27 | C | 272 | DMU | C5 |
| 27 | C | 272 | DMU | C6 |
| 27 | C | 272 | DMU | C9 |
| 27 | C | 272 | DMU | C4 |
| 27 | C | 272 | DMU | C2 |
| 27 | C | 272 | DMU | C3 |
| 23 | W | 1059 | CHD | C17 |
| 23 | C | 271 | CHD | C9 |
| 23 | P | 1525 | CHD | C9 |
| 27 | M | 526 | DMU | C2 |
| 27 | M | 526 | DMU | C4 |
| 27 | M | 526 | DMU | C9 |
| 27 | M | 526 | DMU | C5 |
| 14 | A | 516 | HEA | ND |
| 14 | A | 516 | HEA | NA |
| 14 | A | 516 | HEA | NB |

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 21 | Y | 1522 | TGL | CG2-OG2-CB1-OB1 |
| 19 | N | 1524 | PGV | C02-O01-C1-C2 |
| 26 | T | 1269 | CDL | PB2-OB2-CB2-C1 |
| 21 | Y | 1522 | TGL | CG2-OG2-CB1-CB2 |
| 26 | T | 1269 | CDL | CA4-OA6-CA5-OA7 |
| 26 | P | 1270 | CDL | CA4-OA6-CA5-OA7 |
| 26 | T | 1269 | CDL | CA4-OA6-CA5-C11 |
| 26 | P | 1270 | CDL | CA4-OA6-CA5-C11 |

There are no ring outliers.

38 monomers are involved in 373 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14 | A | 515 | HEA | 8 | 0 |
| 14 | A | 516 | HEA | 8 | 0 |
| 19 | A | 521 | PGV | 2 | 0 |
| 19 | A | 524 | PGV | 14 | 0 |
| 23 | B | 1085 | CHD | 4 | 0 |
| 22 | B | 229 | PSC | 20 | 0 |
| 21 | B | 521 | TGL | 4 | 0 |
| 25 | C | 264 | PEK | 9 | 0 |
| 25 | C | 265 | PEK | 13 | 0 |
| 19 | C | 267 | PGV | 4 | 0 |
| 19 | C | 268 | PGV | 6 | 0 |
| 26 | C | 270 | CDL | 20 | 0 |
| 23 | C | 271 | CHD | 2 | 0 |
| 27 | C | 272 | DMU | 4 | 0 |
| 23 | C | 525 | CHD | 2 | 0 |
| 21 | D | 523 | TGL | 10 | 0 |
| 25 | G | 1263 | PEK | 19 | 0 |
| 26 | G | 269 | CDL | 33 | 0 |
| 23 | J | 60 | CHD | 8 | 0 |
| 21 | L | 522 | TGL | 15 | 0 |
| 21 | N | 1523 | TGL | 14 | 0 |
| 19 | N | 1524 | PGV | 7 | 0 |
| 14 | N | 515 | HEA | 6 | 0 |
| 14 | N | 516 | HEA | 3 | 0 |
| 21 | O | 1521 | TGL | 5 | 0 |
| 23 | O | 229 | CHD | 3 | 0 |
| 25 | P | 1264 | PEK | 6 | 0 |
| 19 | P | 1267 | PGV | 3 | 0 |
| 26 | P | 1270 | CDL | 27 | 0 |
| 23 | P | 1271 | CHD | 5 | 0 |
| 27 | P | 272 | DMU | 1 | 0 |
| 22 | R | 1229 | PSC | 20 | 0 |
| 25 | T | 1265 | PEK | 20 | 0 |
| 26 | T | 1269 | CDL | 30 | 0 |
| 25 | T | 263 | PEK | 14 | 0 |
| 19 | U | 1268 | PGV | 4 | 0 |
| 23 | W | 1059 | CHD | 3 | 0 |
| 21 | Y | 1522 | TGL | 20 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th 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%) | 0.30 | 11 (2%) 64 63 | 23, 29, 38, 65 | 0 |
| 1 | N | 513/514 (99%) | 0.23 | 20 (3%) 40 40 | 29, 35, 44, 71 | 0 |
| 2 | B | 226/227 (99%) | -0.25 | 1 (0%) 92 92 | 24, 33, 53, 72 | 0 |
| 2 | O | 226/227 (99%) | -0.14 | 4 (1%) 69 68 | 31, 42, 64, 81 | 0 |
| 3 | C | 259/261 (99%) | -0.17 | 2 (0%) 86 85 | 26, 32, 43, 66 | 0 |
| 3 | P | 259/261 (99%) | 0.05 | 13 (5%) 30 30 | 30, 36, 48, 67 | 0 |
| 4 | D | 144/147 (97%) | -0.18 | 1 (0%) 87 87 | 30, 40, 53, 66 | 0 |
| 4 | Q | 144/147 (97%) | 1.07 | 25 (17%) 2 2 | 39, 50, 71, 105 | 0 |
| 5 | E | 105/109 (96%) | 0.36 | 6 (5%) 24 25 | 33, 40, 64, 97 | 0 |
| 5 | R | 105/109 (96%) | 0.97 | 15 (14%) 3 3 | 36, 46, 70, 97 | 0 |
| 6 | F | 98/98 (100%) | 0.44 | 9 (9%) 10 10 | 30, 41, 80, 117 | 0 |
| 6 | S | 98/98 (100%) | 0.30 | 9 (9%) 10 10 | 34, 46, 80, 113 | 0 |
| 7 | G | 83/85 (97%) | 0.84 | 15 (18%) 1 2 | 29, 38, 90, 106 | 0 |
| 7 | T | 83/85 (97%) | 1.00 | 15 (18%) 1 2 | 32, 41, 91, 106 | 0 |
| 8 | H | 79/85 (92%) | 0.27 | 10 (12%) 4 4 | 29, 41, 81, 101 | 0 |
| 8 | U | 79/85 (92%) | 0.62 | 14 (17%) 2 2 | 37, 47, 85, 106 | 0 |
| 9 | I | 72/73 (98%) | 0.25 | 3 (4%) 37 37 | 31, 46, 65, 70 | 0 |
| 9 | V | 72/73 (98%) | 0.96 | 13 (18%) 1 2 | 36, 52, 67, 77 | 0 |
| 10 | J | 58/59 (98%) | 0.52 | 7 (12%) 5 5 | 32, 41, 66, 95 | 0 |
| 10 | W | 58/59 (98%) | 0.54 | 7 (12%) 5 5 | 36, 45, 67, 97 | 0 |
| 11 | K | 49/56 (87%) | 0.03 | 2 (4%) 38 38 | 31, 39, 54, 64 | 0 |
| 11 | X | 49/56 (87%) | 1.79 | 21 (42%) 0 1 | 42, 50, 66, 78 | 0 |
| 12 | L | 46/47 (97%) | -0.24 | 2 (4%) 36 36 | 29, 34, 51, 77 | 0 |
| 12 | Y | 46/47 (97%) | -0.06 | 1 (2%) 62 61 | 35, 43, 60, 82 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | M | 43/46 (93%) | 0.04 | 4 (9%) 9 9 | 31, 34, 72, 96 | 0 |
| 13 | Z | 43/46 (93%) | 0.74 | 8 (18%) 1 1 | 39, 44, 81, 104 | 0 |
| All | All | 3550/3614 (98%) | 0.27 | 238 (6%) 19 18 | 23, 38, 64, 117 | 0 |

All (238) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | Q | 6 | VAL | 14.9 |
| 6 | F | 1 | ALA | 10.4 |
| 6 | S | 98 | HIS | 9.8 |
| 6 | S | 1 | ALA | 9.6 |
| 6 | S | 97 | ALA | 9.1 |
| 7 | G | 1 | ALA | 8.9 |
| 4 | Q | 4 | SER | 8.6 |
| 6 | F | 97 | ALA | 8.2 |
| 7 | T | 1 | ALA | 7.4 |
| 6 | F | 96 | LEU | 7.2 |
| 6 | S | 2 | SER | 6.5 |
| 5 | R | 109 | VAL | 6.5 |
| 5 | E | 5 | HIS | 6.3 |
| 6 | F | 98 | HIS | 6.3 |
| 13 | Z | 42 | LYS | 6.3 |
| 8 | U | 7 | LYS | 5.9 |
| 4 | Q | 51 | LEU | 5.8 |
| 10 | J | 1 | PHE | 5.6 |
| 6 | S | 94 | HIS | 5.6 |
| 7 | T | 3 | ALA | 5.6 |
| 7 | G | 36 | TRP | 5.5 |
| 7 | T | 36 | TRP | 5.4 |
| 9 | I | 37 | PHE | 5.4 |
| 4 | Q | 48 | TRP | 5.4 |
| 6 | S | 96 | LEU | 5.3 |
| 7 | T | 84 | LYS | 5.2 |
| 8 | U | 8 | ILE | 5.2 |
| 4 | Q | 5 | VAL | 5.1 |
| 13 | Z | 43 | SER | 4.9 |
| 9 | V | 37 | PHE | 4.9 |
| 7 | G | 40 | GLY | 4.9 |
| 11 | X | 7 | PRO | 4.9 |
| 7 | G | 8 | HIS | 4.9 |
| 10 | J | 58 | LYS | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8 | U | 44 | THR | 4.8 |
| 13 | Z | 41 | LYS | 4.8 |
| 9 | V | 2 | THR | 4.7 |
| 7 | G | 2 | SER | 4.7 |
| 7 | T | 42 | ARG | 4.7 |
| 11 | X | 19 | ALA | 4.6 |
| 6 | F | 94 | HIS | 4.6 |
| 8 | H | 48 | GLY | 4.5 |
| 8 | H | 45 | ALA | 4.5 |
| 5 | R | 5 | HIS | 4.5 |
| 13 | M | 43 | SER | 4.4 |
| 13 | M | 42 | LYS | 4.4 |
| 7 | G | 41 | HIS | 4.3 |
| 7 | G | 42 | ARG | 4.3 |
| 2 | O | 113 | TYR | 4.3 |
| 7 | T | 41 | HIS | 4.2 |
| 10 | W | 57 | HIS | 4.2 |
| 7 | T | 5 | LYS | 4.2 |
| 10 | W | 58 | LYS | 4.2 |
| 7 | G | 84 | LYS | 4.1 |
| 4 | Q | 33 | LEU | 4.1 |
| 7 | G | 6 | GLY | 4.1 |
| 4 | Q | 46 | ALA | 4.1 |
| 11 | X | 16 | ALA | 4.0 |
| 2 | O | 90 | ILE | 4.0 |
| 8 | U | 10 | ASN | 4.0 |
| 8 | H | 8 | ILE | 3.9 |
| 10 | W | 55 | PHE | 3.9 |
| 7 | T | 4 | ALA | 3.9 |
| 13 | Z | 40 | TYR | 3.9 |
| 5 | R | 96 | LEU | 3.8 |
| 7 | T | 40 | GLY | 3.8 |
| 4 | Q | 145 | TRP | 3.8 |
| 13 | Z | 35 | TYR | 3.8 |
| 12 | L | 47 | LYS | 3.7 |
| 5 | R | 7 | THR | 3.7 |
| 8 | H | 44 | THR | 3.7 |
| 4 | Q | 49 | SER | 3.7 |
| 6 | F | 2 | SER | 3.7 |
| 10 | J | 57 | HIS | 3.6 |
| 12 | Y | 47 | LYS | 3.6 |
| 13 | Z | 39 | ASN | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 59 | GLN | 3.5 |
| 3 | P | 88 | ILE | 3.5 |
| 7 | T | 10 | GLY | 3.4 |
| 13 | M | 39 | ASN | 3.4 |
| 11 | X | 13 | TYR | 3.4 |
| 8 | U | 49 | ASP | 3.4 |
| 13 | M | 40 | TYR | 3.4 |
| 11 | X | 47 | ARG | 3.4 |
| 5 | R | 108 | LYS | 3.4 |
| 3 | P | 91 | VAL | 3.4 |
| 7 | G | 5 | LYS | 3.3 |
| 11 | X | 24 | PHE | 3.3 |
| 8 | U | 48 | GLY | 3.3 |
| 4 | Q | 102 | TYR | 3.3 |
| 4 | Q | 141 | ASP | 3.3 |
| 7 | G | 3 | ALA | 3.3 |
| 11 | X | 6 | ALA | 3.3 |
| 10 | W | 52 | TRP | 3.3 |
| 8 | U | 52 | VAL | 3.2 |
| 11 | X | 17 | VAL | 3.2 |
| 8 | U | 11 | TYR | 3.2 |
| 7 | T | 8 | HIS | 3.2 |
| 6 | F | 95 | GLN | 3.1 |
| 7 | G | 43 | GLU | 3.1 |
| 11 | X | 46 | GLY | 3.0 |
| 6 | S | 93 | PRO | 3.0 |
| 5 | E | 109 | VAL | 3.0 |
| 9 | V | 36 | LYS | 3.0 |
| 10 | W | 1 | PHE | 3.0 |
| 4 | Q | 7 | LYS | 3.0 |
| 7 | T | 9 | GLY | 3.0 |
| 10 | J | 2 | GLU | 3.0 |
| 8 | U | 9 | LYS | 3.0 |
| 5 | R | 58 | LEU | 3.0 |
| 7 | G | 4 | ALA | 3.0 |
| 1 | N | 193 | VAL | 2.9 |
| 12 | L | 2 | HIS | 2.9 |
| 8 | H | 7 | LYS | 2.9 |
| 10 | J | 52 | TRP | 2.9 |
| 7 | T | 6 | GLY | 2.9 |
| 4 | Q | 139 | ASP | 2.9 |
| 9 | I | 2 | THR | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | P | 37 | PHE | 2.8 |
| 11 | K | 7 | PRO | 2.8 |
| 9 | V | 68 | ILE | 2.8 |
| 9 | V | 3 | ALA | 2.7 |
| 11 | X | 23 | THR | 2.7 |
| 7 | T | 43 | GLU | 2.7 |
| 13 | Z | 32 | TRP | 2.7 |
| 4 | Q | 53 | ILE | 2.7 |
| 7 | G | 39 | SER | 2.7 |
| 4 | Q | 147 | LYS | 2.7 |
| 5 | R | 93 | LEU | 2.7 |
| 9 | V | 7 | PRO | 2.7 |
| 8 | H | 47 | GLY | 2.7 |
| 11 | K | 19 | ALA | 2.7 |
| 11 | X | 18 | LEU | 2.7 |
| 7 | T | 2 | SER | 2.7 |
| 5 | R | 54 | ALA | 2.7 |
| 9 | V | 53 | ASN | 2.7 |
| 4 | Q | 142 | LYS | 2.7 |
| 11 | X | 11 | ASP | 2.6 |
| 1 | N | 195 | LEU | 2.6 |
| 8 | H | 46 | LYS | 2.6 |
| 1 | N | 165 | ILE | 2.6 |
| 1 | N | 190 | ILE | 2.6 |
| 3 | C | 92 | LEU | 2.6 |
| 3 | P | 182 | TYR | 2.6 |
| 10 | W | 2 | GLU | 2.6 |
| 3 | P | 99 | TRP | 2.6 |
| 8 | U | 43 | MET | 2.5 |
| 5 | R | 9 | GLU | 2.5 |
| 4 | Q | 140 | TYR | 2.5 |
| 9 | I | 26 | MET | 2.5 |
| 13 | Z | 13 | LYS | 2.5 |
| 4 | D | 147 | LYS | 2.5 |
| 5 | R | 89 | LEU | 2.5 |
| 11 | X | 20 | SER | 2.5 |
| 3 | P | 84 | ILE | 2.5 |
| 8 | U | 45 | ALA | 2.5 |
| 3 | P | 92 | LEU | 2.4 |
| 3 | P | 38 | ASN | 2.4 |
| 2 | O | 59 | GLN | 2.4 |
| 5 | R | 92 | THR | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | N | 196 | LEU | 2.4 |
| 8 | U | 47 | GLY | 2.4 |
| 1 | N | 245 | ILE | 2.4 |
| 1 | N | 282 | PHE | 2.4 |
| 1 | A | 193 | VAL | 2.4 |
| 10 | J | 4 | ARG | 2.4 |
| 11 | X | 15 | ASN | 2.3 |
| 3 | P | 247 | VAL | 2.3 |
| 4 | Q | 101 | HIS | 2.3 |
| 8 | H | 43 | MET | 2.3 |
| 4 | Q | 60 | TYR | 2.3 |
| 1 | A | 126 | TRP | 2.3 |
| 11 | X | 36 | ILE | 2.3 |
| 8 | U | 42 | ALA | 2.3 |
| 11 | X | 30 | VAL | 2.3 |
| 5 | R | 10 | GLU | 2.3 |
| 1 | N | 126 | TRP | 2.3 |
| 9 | V | 45 | LYS | 2.3 |
| 10 | J | 33 | ARG | 2.3 |
| 10 | W | 4 | ARG | 2.3 |
| 1 | N | 286 | ILE | 2.3 |
| 1 | A | 20 | LEU | 2.2 |
| 1 | N | 246 | LEU | 2.2 |
| 5 | R | 13 | ALA | 2.2 |
| 9 | V | 48 | ALA | 2.2 |
| 11 | X | 12 | LYS | 2.2 |
| 11 | X | 35 | GLN | 2.2 |
| 7 | G | 9 | GLY | 2.2 |
| 1 | N | 66 | ILE | 2.2 |
| 1 | A | 195 | LEU | 2.2 |
| 8 | H | 42 | ALA | 2.2 |
| 3 | P | 250 | LEU | 2.2 |
| 4 | Q | 62 | LEU | 2.2 |
| 1 | N | 285 | PHE | 2.2 |
| 8 | H | 49 | ASP | 2.2 |
| 1 | A | 192 | ALA | 2.2 |
| 2 | O | 131 | GLY | 2.2 |
| 4 | Q | 8 | SER | 2.2 |
| 6 | S | 3 | GLY | 2.2 |
| 4 | Q | 55 | GLU | 2.2 |
| 3 | P | 87 | ILE | 2.2 |
| 4 | Q | 97 | ILE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | P | 85 | LEU | 2.2 |
| 1 | A | 202 | LEU | 2.1 |
| 1 | N | 248 | LEU | 2.1 |
| 1 | N | 83 | VAL | 2.1 |
| 3 | P | 98 | PHE | 2.1 |
| 5 | R | 16 | VAL | 2.1 |
| 11 | X | 48 | VAL | 2.1 |
| 5 | R | 18 | TYR | 2.1 |
| 1 | A | 245 | ILE | 2.1 |
| 8 | U | 46 | LYS | 2.1 |
| 6 | F | 3 | GLY | 2.1 |
| 6 | F | 5 | GLY | 2.1 |
| 1 | N | 158 | ILE | 2.1 |
| 1 | A | 188 | VAL | 2.1 |
| 11 | X | 31 | TYR | 2.1 |
| 1 | N | 166 | THR | 2.1 |
| 9 | V | 33 | THR | 2.1 |
| 6 | S | 95 | GLN | 2.1 |
| 1 | A | 190 | ILE | 2.1 |
| 1 | N | 75 | ILE | 2.1 |
| 1 | N | 197 | LEU | 2.1 |
| 5 | E | 16 | VAL | 2.1 |
| 5 | E | 9 | GLU | 2.1 |
| 1 | N | 194 | LEU | 2.1 |
| 5 | E | 93 | LEU | 2.1 |
| 9 | V | 19 | PHE | 2.1 |
| 9 | V | 65 | LYS | 2.1 |
| 1 | A | 348 | PHE | 2.0 |
| 11 | X | 37 | GLY | 2.0 |
| 3 | C | 38 | ASN | 2.0 |
| 9 | V | 4 | LEU | 2.0 |
| 1 | N | 243 | VAL | 2.0 |
| 4 | Q | 68 | PHE | 2.0 |
| 4 | Q | 58 | GLU | 2.0 |
| 1 | A | 385 | ALA | 2.0 |
| 5 | E | 24 | ILE | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 7 | TPO | T | 11 | 11/12 | 0.61 | 0.28 | - | 75,82,102,103 | 0 |
| 2 | FME | B | 1 | 10/11 | 0.97 | 0.12 | - | 33,33,41,48 | 0 |
| 9 | SAC | I | 1 | 9/10 | 0.67 | 0.28 | - | 73,76,78,80 | 0 |
| 7 | TPO | G | 11 | 11/12 | 0.68 | 0.27 | - | 69,76,102,102 | 0 |
| 9 | SAC | V | 1 | 9/10 | 0.43 | 0.47 | - | 83,84,85,86 | 0 |
| 1 | FME | N | 1 | 10/11 | 0.93 | 0.18 | - | 46,53,78,82 | 0 |
| 1 | FME | A | 1 | 10/11 | 0.91 | 0.18 | - | 44,51,71,75 | 0 |
| 2 | FME | O | 1 | 10/11 | 0.96 | 0.11 | - | 40,42,47,55 | 0 |

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|---------|------|------|-------|----------------------------|-------|
| 27 | DMU | P | 272 | 33/33 | 0.32 | 0.44 | 11.78 | 77,107,124,124 | 0 |
| 27 | DMU | C | 272 | 33/33 | 0.35 | 0.39 | 8.66 | 68,100,115,116 | 0 |
| 23 | CHD | W | 1059 | 29/29 | 0.65 | 0.45 | 7.36 | 101,109,113,115 | 0 |
| 26 | CDL | P | 1270 | 100/100 | 0.74 | 0.30 | 6.28 | 36,94,119,119 | 0 |
| 21 | TGL | Y | 1522 | 63/63 | 0.64 | 0.30 | 5.25 | 51,73,89,92 | 0 |
| 23 | CHD | J | 60 | 29/29 | 0.74 | 0.46 | 4.99 | 99,105,108,110 | 0 |
| 26 | CDL | C | 270 | 100/100 | 0.79 | 0.33 | 4.47 | 41,91,129,130 | 0 |
| 26 | CDL | T | 1269 | 100/100 | 0.65 | 0.30 | 4.29 | 58,86,114,118 | 0 |
| 17 | MG | N | 518 | 1/1 | 0.93 | 0.17 | 4.26 | 34,34,34,34 | 0 |
| 21 | TGL | D | 523 | 63/63 | 0.76 | 0.22 | 3.94 | 48,69,91,91 | 0 |
| 21 | TGL | O | 1521 | 63/63 | 0.80 | 0.21 | 3.92 | 58,80,95,96 | 0 |
| 21 | TGL | L | 522 | 63/63 | 0.76 | 0.26 | 3.88 | 43,66,82,89 | 0 |
| 19 | PGV | A | 524 | 51/51 | 0.76 | 0.23 | 3.66 | 44,72,112,114 | 0 |
| 17 | MG | A | 518 | 1/1 | 0.98 | 0.18 | 3.65 | 23,23,23,23 | 0 |
| 25 | PEK | G | 1263 | 53/53 | 0.62 | 0.51 | 3.52 | 52,103,133,134 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|---------|------|------|-------|----------------------------|-------|
| 19 | PGV | N | 1524 | 51/51 | 0.72 | 0.28 | 3.51 | 54,74,103,105 | 0 |
| 21 | TGL | B | 521 | 63/63 | 0.86 | 0.22 | 3.35 | 53,74,88,90 | 0 |
| 21 | TGL | N | 1523 | 63/63 | 0.72 | 0.24 | 3.04 | 61,79,97,99 | 0 |
| 26 | CDL | G | 269 | 100/100 | 0.58 | 0.31 | 2.80 | 62,86,116,120 | 0 |
| 23 | CHD | P | 1271 | 29/29 | 0.87 | 0.29 | 2.71 | 78,92,94,95 | 0 |
| 25 | PEK | T | 263 | 53/53 | 0.65 | 0.42 | 2.63 | 52,103,125,127 | 0 |
| 22 | PSC | B | 229 | 52/52 | 0.68 | 0.34 | 2.31 | 43,92,139,143 | 0 |
| 22 | PSC | R | 1229 | 52/52 | 0.63 | 0.33 | 2.30 | 48,99,136,139 | 0 |
| 19 | PGV | C | 268 | 51/51 | 0.72 | 0.38 | 2.01 | 53,81,98,102 | 0 |
| 27 | DMU | Z | 1526 | 33/33 | 0.79 | 0.28 | 1.94 | 49,57,70,70 | 0 |
| 19 | PGV | U | 1268 | 51/51 | 0.69 | 0.41 | 1.85 | 60,84,103,105 | 0 |
| 23 | CHD | C | 525 | 29/29 | 0.96 | 0.19 | 1.74 | 26,33,39,41 | 0 |
| 19 | PGV | P | 1267 | 51/51 | 0.93 | 0.17 | 1.45 | 29,40,82,87 | 0 |
| 19 | PGV | N | 1266 | 51/51 | 0.95 | 0.20 | 1.37 | 30,42,65,69 | 0 |
| 20 | CUA | B | 228 | 2/2 | 0.99 | 0.13 | 1.31 | 27,27,27,28 | 0 |
| 23 | CHD | C | 271 | 29/29 | 0.86 | 0.25 | 1.20 | 79,83,85,85 | 0 |
| 25 | PEK | C | 265 | 53/53 | 0.58 | 0.31 | 1.13 | 49,83,106,107 | 0 |
| 27 | DMU | M | 526 | 33/33 | 0.90 | 0.15 | 1.13 | 33,47,65,71 | 0 |
| 19 | PGV | C | 267 | 51/51 | 0.95 | 0.14 | 1.03 | 28,40,73,76 | 0 |
| 25 | PEK | T | 1265 | 53/53 | 0.52 | 0.32 | 1.01 | 49,79,110,118 | 0 |
| 23 | CHD | P | 1525 | 29/29 | 0.96 | 0.18 | 0.97 | 32,37,43,47 | 0 |
| 14 | HEA | N | 516 | 60/60 | 0.98 | 0.18 | 0.88 | 27,33,37,40 | 0 |
| 25 | PEK | C | 264 | 53/53 | 0.94 | 0.14 | 0.73 | 30,46,78,80 | 0 |
| 25 | PEK | P | 1264 | 53/53 | 0.92 | 0.16 | 0.58 | 35,50,86,88 | 0 |
| 19 | PGV | A | 521 | 51/51 | 0.97 | 0.14 | 0.37 | 23,35,63,67 | 0 |
| 14 | HEA | N | 515 | 60/60 | 0.97 | 0.14 | 0.26 | 28,36,45,49 | 0 |
| 18 | NA | N | 519 | 1/1 | 0.94 | 0.11 | 0.19 | 39,39,39,39 | 0 |
| 14 | HEA | A | 516 | 60/60 | 0.99 | 0.17 | 0.12 | 18,26,31,36 | 0 |
| 14 | HEA | A | 515 | 60/60 | 0.98 | 0.15 | -0.17 | 22,28,41,42 | 0 |
| 23 | CHD | O | 229 | 29/29 | 0.97 | 0.10 | -0.45 | 27,32,38,40 | 0 |
| 23 | CHD | B | 1085 | 29/29 | 0.96 | 0.10 | -0.46 | 27,31,36,42 | 0 |
| 15 | NO | N | 520 | 2/2 | 0.95 | 0.14 | -0.61 | 39,39,39,42 | 0 |
| 28 | ZN | S | 99 | 1/1 | 0.99 | 0.08 | -0.81 | 43,43,43,43 | 0 |
| 28 | ZN | F | 99 | 1/1 | 0.99 | 0.08 | -1.08 | 37,37,37,37 | 0 |
| 20 | CUA | O | 228 | 2/2 | 0.97 | 0.09 | -1.16 | 34,34,34,36 | 0 |
| 18 | NA | A | 519 | 1/1 | 0.97 | 0.08 | -1.17 | 32,32,32,32 | 0 |
| 15 | NO | A | 520 | 2/2 | 0.97 | 0.10 | -3.21 | 32,32,32,36 | 0 |
| 24 | UNX | C | 262 | 1/1 | 0.08 | 0.56 | - | 80,80,80,80 | 0 |
| 16 | CU | N | 517 | 1/1 | 0.99 | 0.15 | - | 35,35,35,35 | 0 |
| 16 | CU | A | 517 | 1/1 | 1.00 | 0.15 | - | 29,29,29,29 | 0 |
| 24 | UNX | P | 262 | 1/1 | 0.55 | 0.53 | - | 79,79,79,79 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.