



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:50 PM GMT

PDB ID : 1V54
Title : Bovine heart cytochrome c oxidase at the fully oxidized state
Authors : Tsukihara, T.; Shimokata, K.; Katayama, Y.; Shimada, H.; Muramoto, K.; Aoyama, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yao, M.; Ishimura, Y.; Yoshikawa, S.
Deposited on : 2003-11-21
Resolution : 1.80 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

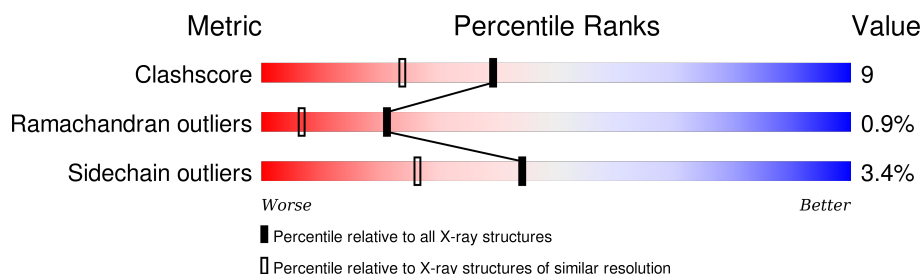
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 5383 (1.80-1.80) |
| Ramachandran outliers | 100387 | 5320 (1.80-1.80) |
| Sidechain outliers | 100360 | 5319 (1.80-1.80) |









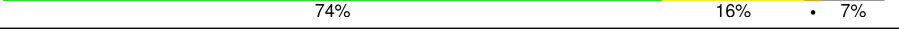


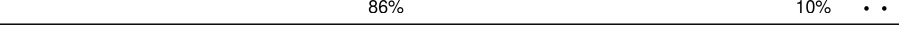
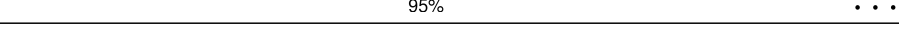
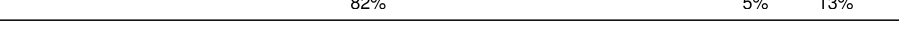


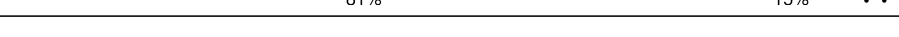

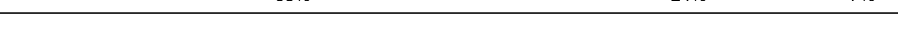
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 514 | 87% 12% . |
| 1 | N | 514 | 84% 16% . |
| 2 | B | 227 | 81% 16% . |
| 2 | O | 227 | 74% 23% . |
| 3 | C | 261 | 91% 8% . |
| 3 | P | 261 | 89% 9% .. |
| 4 | D | 147 | 87% 11% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 17 | HEA | A | 515 | X | - | - | - |
| 17 | HEA | A | 516 | X | - | - | - |
| 17 | HEA | N | 515 | X | - | - | - |
| 17 | HEA | N | 516 | X | - | - | - |
| 18 | TGL | L | 3522 | - | - | X | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 21 | CHD | C | 3271 | X | - | - | - |
| 21 | CHD | J | 3060 | X | - | - | - |
| 21 | CHD | P | 4271 | X | - | - | - |
| 21 | CHD | W | 4060 | X | - | - | - |
| 25 | PSC | O | 4230 | - | - | X | - |
| 27 | DMU | M | 3526 | X | - | - | - |
| 27 | DMU | Z | 4526 | X | - | - | - |

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32636 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 polypeptide I.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4027 | 2691 | 623 | 678 | 35 | | | |
| 1 | N | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4027 | 2691 | 623 | 678 | 35 | | | |

- Molecule 2 is a protein called Cytochrome c oxidase polypeptide II.

| 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 polypeptide III.

| 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 IV 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 polypeptide Va.

| 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 polypeptide Vb.

| 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 polypeptide VIa-heart.

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

- Molecule 8 is a protein called Cytochrome c oxidase polypeptide VIb.

| 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 polypeptide VIc.

| 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 VIIa-heart.

| 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 polypeptide VIIb.

| 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 polypeptide VIIc.

| 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 polypeptide VIII-heart.

| 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 COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14 | A | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 14 | N | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |

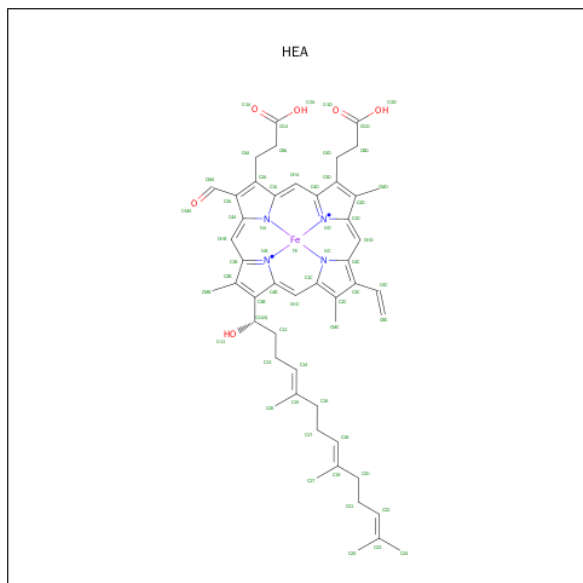
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

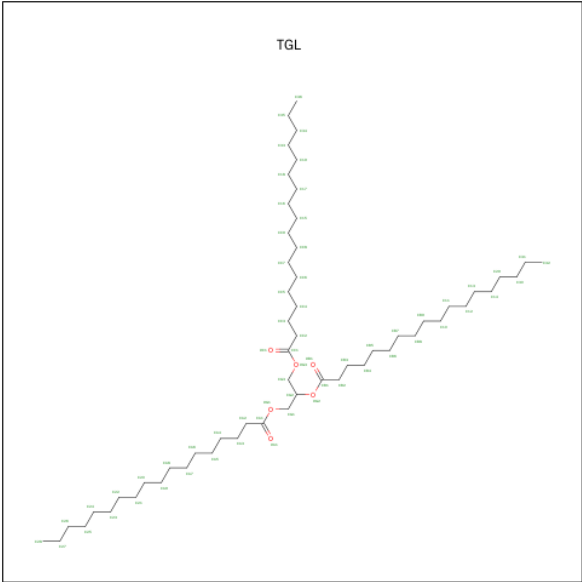
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16 | A | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |
| 16 | N | 1 | Total | Na | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



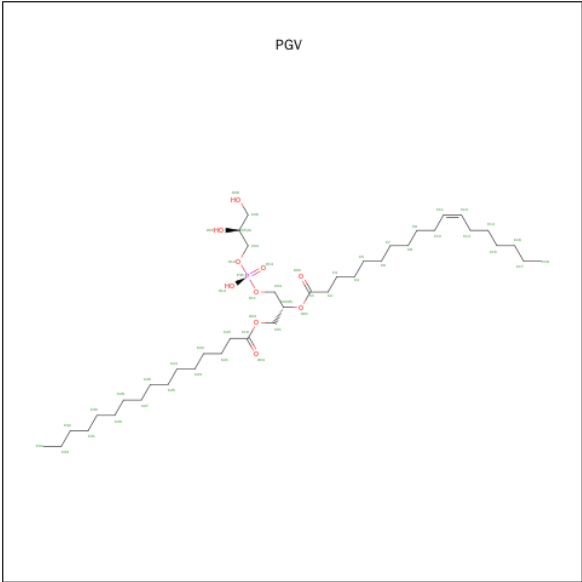
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 17 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |
| 17 | A | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |
| 17 | N | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |
| 17 | N | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | | |

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



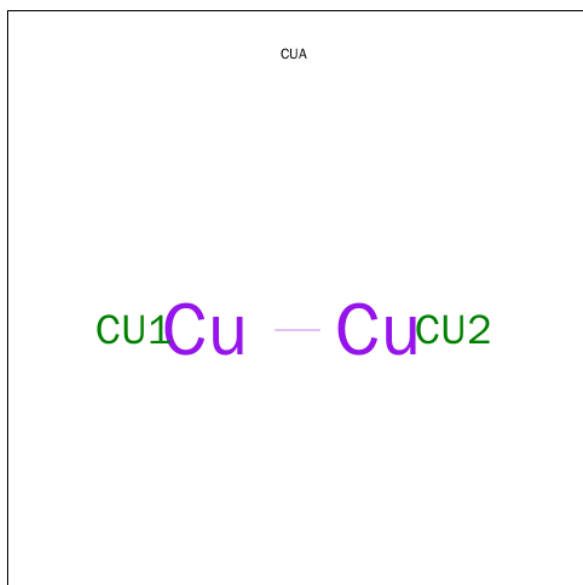
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 18 | A | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 18 | D | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 18 | L | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 18 | N | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 18 | N | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |
| 18 | Q | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 57 | 6 | | |

- 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).



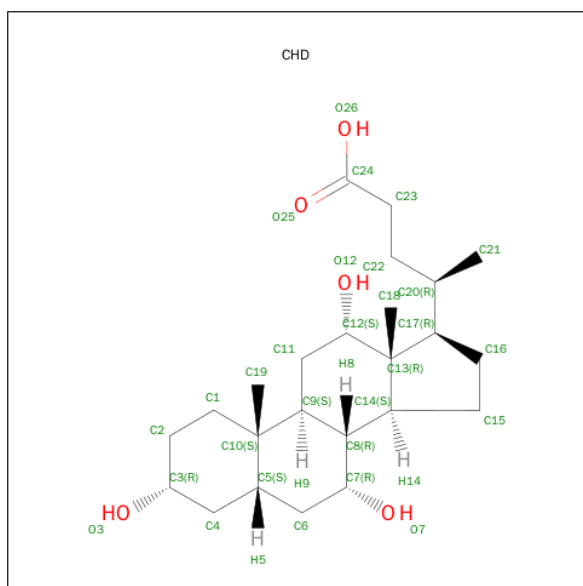
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 19 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 51 | 40 | 10 | 1 | | |
| 19 | C | 1 | Total | 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 | P | 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 CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



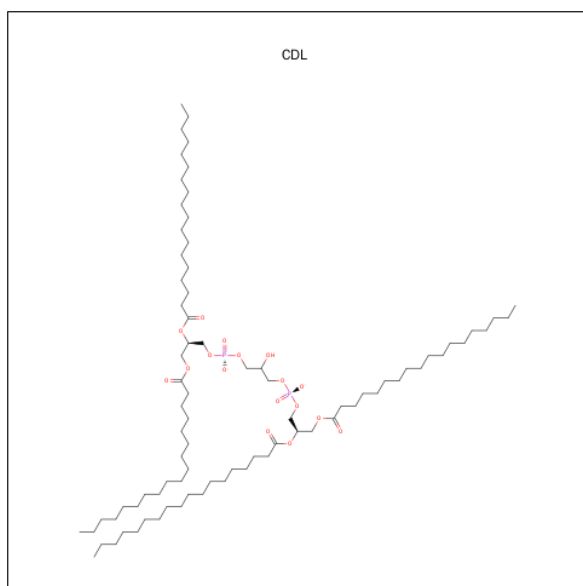
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21 | B | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 21 | C | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21 | C | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 21 | J | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 21 | O | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 21 | P | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 21 | P | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 21 | W | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |

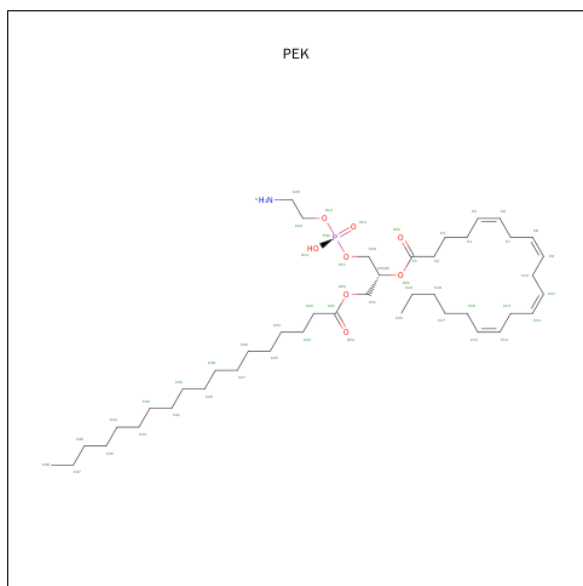
- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 22 | C | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 22 | G | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 22 | P | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |
| 22 | T | 1 | Total | C | O | P | 0 | 0 |
| | | | 100 | 81 | 17 | 2 | | |

- Molecule 23 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).

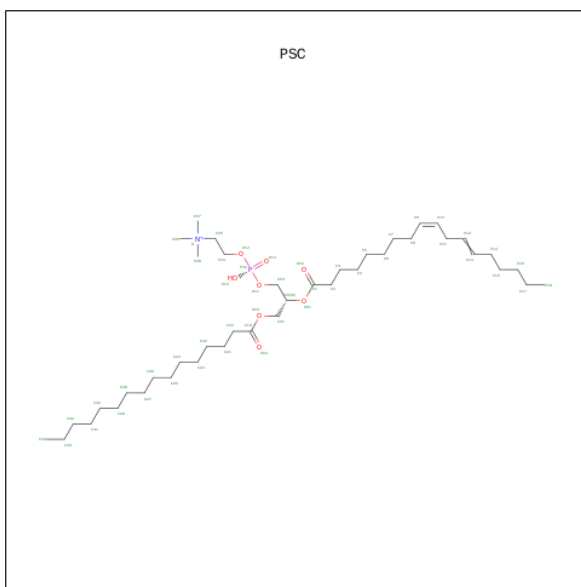


| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 23 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 23 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 23 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 23 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 23 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |
| 23 | T | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | | |

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

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

- Molecule 25 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: C₄₂H₈₁NO₈P).

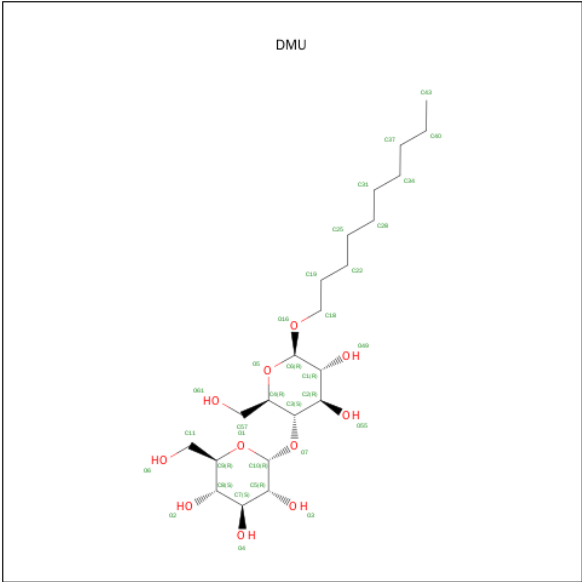


| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 25 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |
| 25 | O | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | | |

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 26 | S | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 26 | F | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 27 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 28 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 28 | A | 227 | Total | O | 0 | 0 |
| | | | 227 | 227 | | |
| 28 | B | 180 | Total | O | 0 | 0 |
| | | | 180 | 180 | | |
| 28 | C | 116 | Total | O | 0 | 0 |
| | | | 116 | 116 | | |
| 28 | D | 109 | Total | O | 0 | 0 |
| | | | 109 | 109 | | |
| 28 | E | 68 | Total | O | 0 | 0 |
| | | | 68 | 68 | | |
| 28 | F | 80 | Total | O | 0 | 0 |
| | | | 80 | 80 | | |
| 28 | G | 59 | Total | O | 0 | 0 |
| | | | 59 | 59 | | |
| 28 | H | 71 | Total | O | 0 | 0 |
| | | | 71 | 71 | | |
| 28 | I | 61 | Total | O | 0 | 0 |
| | | | 61 | 61 | | |
| 28 | J | 21 | Total | O | 0 | 0 |
| | | | 21 | 21 | | |

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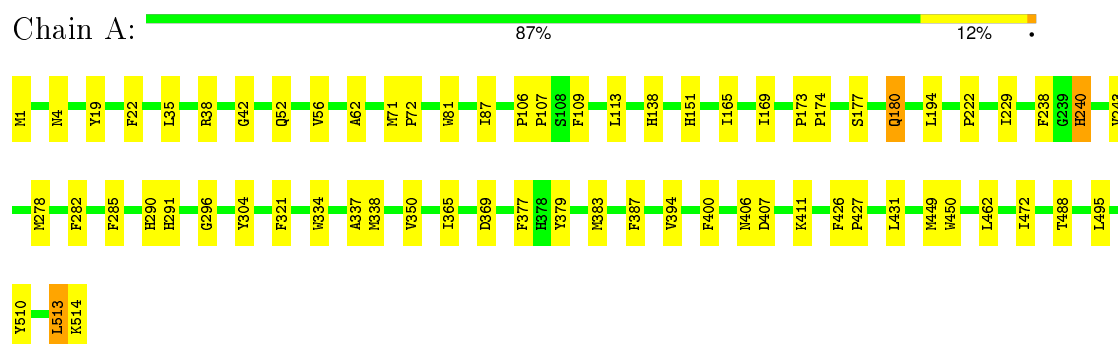
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 28 | K | 37 | Total 37 | O 37 | 0 | 0 |
| 28 | L | 23 | Total 23 | O 23 | 0 | 0 |
| 28 | M | 32 | Total 32 | O 32 | 0 | 0 |
| 28 | N | 217 | Total 217 | O 217 | 0 | 0 |
| 28 | O | 146 | Total 146 | O 146 | 0 | 0 |
| 28 | P | 120 | Total 120 | O 120 | 0 | 0 |
| 28 | Q | 73 | Total 73 | O 73 | 0 | 0 |
| 28 | R | 32 | Total 32 | O 32 | 0 | 0 |
| 28 | S | 54 | Total 54 | O 54 | 0 | 0 |
| 28 | T | 58 | Total 58 | O 58 | 0 | 0 |
| 28 | U | 65 | Total 65 | O 65 | 0 | 0 |
| 28 | V | 36 | Total 36 | O 36 | 0 | 0 |
| 28 | W | 13 | Total 13 | O 13 | 0 | 0 |
| 28 | X | 29 | Total 29 | O 29 | 0 | 0 |
| 28 | Y | 25 | Total 25 | O 25 | 0 | 0 |
| 28 | Z | 18 | Total 18 | O 18 | 0 | 0 |

3 Residue-property plots

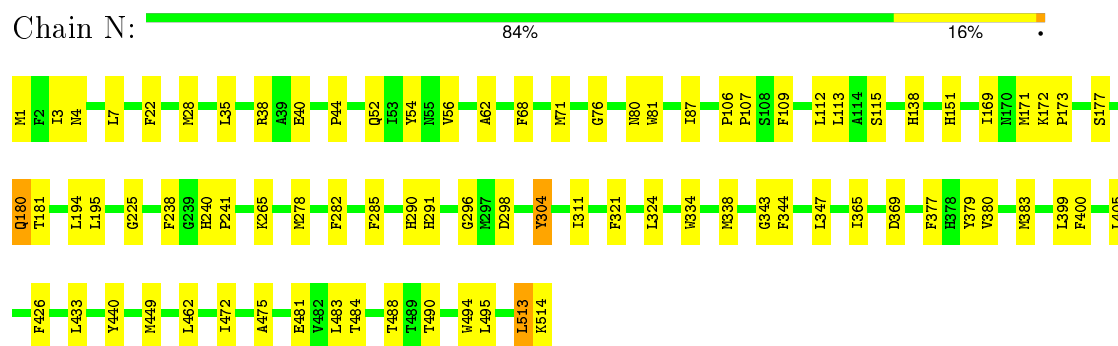
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

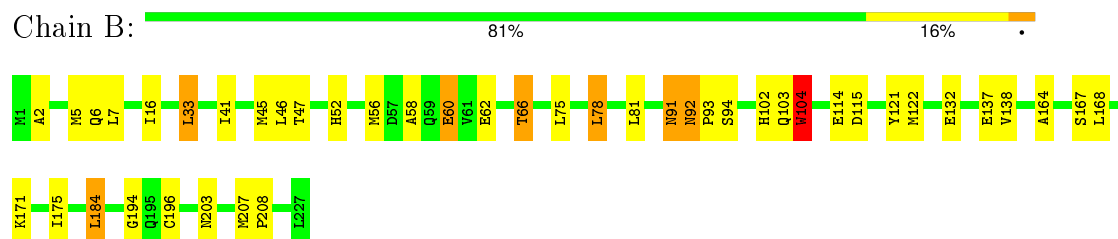
• Molecule 1: Cytochrome c oxidase polypeptide I



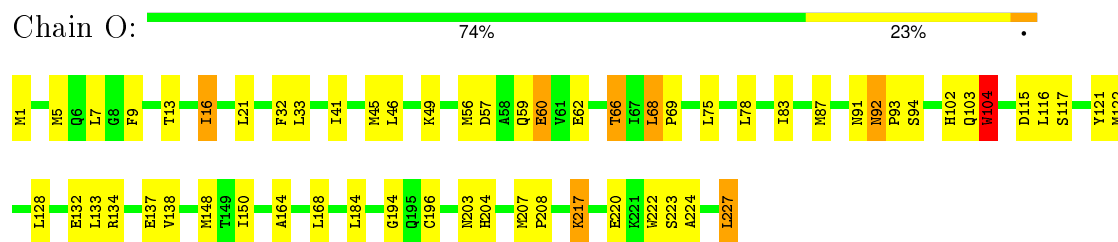
• Molecule 1: Cytochrome c oxidase polypeptide I



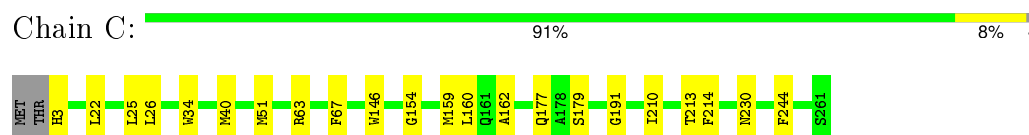
• Molecule 2: Cytochrome c oxidase polypeptide II



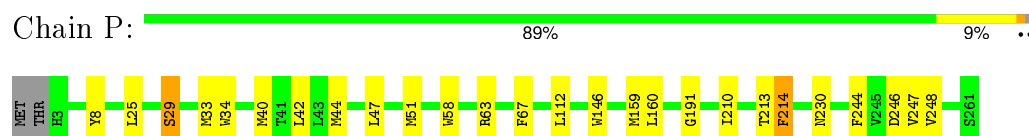
• Molecule 2: Cytochrome c oxidase polypeptide II



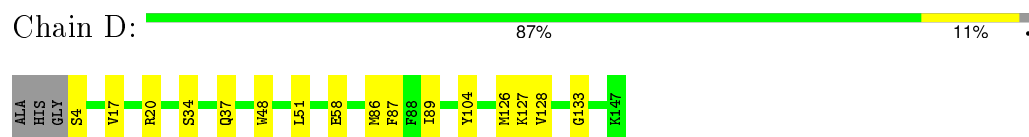
- Molecule 3: Cytochrome c oxidase polypeptide III



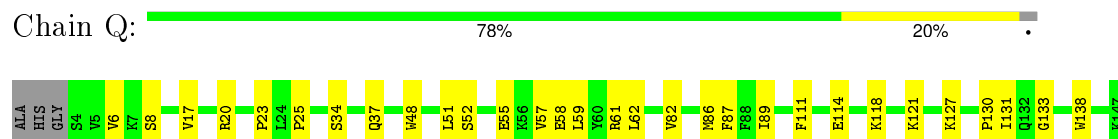
- Molecule 3: Cytochrome c oxidase polypeptide III



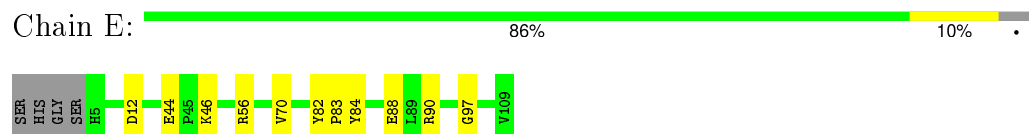
- Molecule 4: Cytochrome c oxidase subunit IV isoform 1



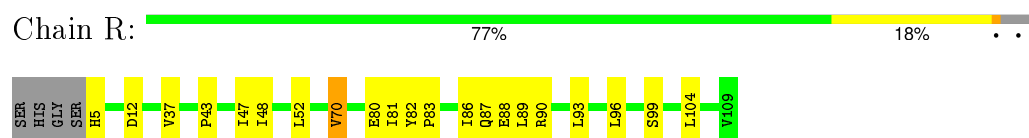
- Molecule 4: Cytochrome c oxidase subunit IV isoform 1




- Molecule 5: Cytochrome c oxidase polypeptide Va



- Molecule 5: Cytochrome c oxidase polypeptide Va




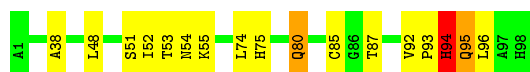
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  78% 19% ..



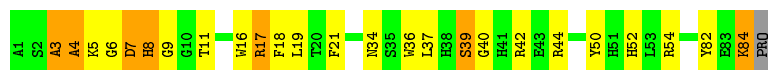
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  83% 14% ..



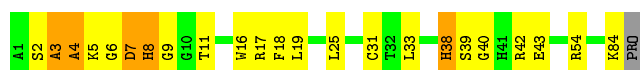
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  69% 21% 8% .



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  72% 21% 6% .



- Molecule 8: Cytochrome c oxidase polypeptide VIb

Chain H:  82% 9% 7% .




- Molecule 8: Cytochrome c oxidase polypeptide VIb

Chain U:  74% 16% 7% .




- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  85% 14% .



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  85% 15%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J: 86% 10% ..



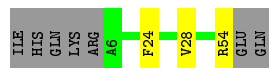
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W: 95% ...



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K: 82% 5% 13%



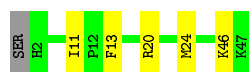
- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X: 77% 9% 13%



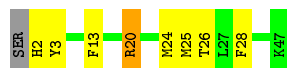
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L: 87% 11% .



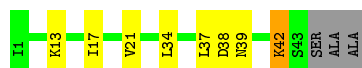
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y: 81% 15% ..

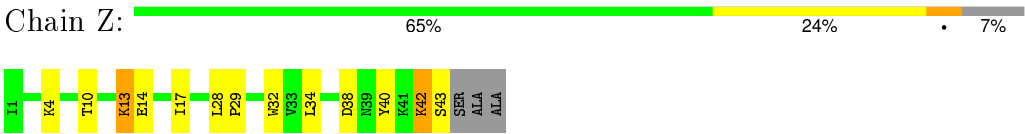


- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M: 76% 15% 7%



● Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 182.59Å 205.14Å 178.25Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 1.80 | Depositor |
| % Data completeness (in resolution range) | (Not available) (40.00-1.80) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | X-PLOR | Depositor |
| R, R_{free} | 0.202 , 0.227 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 32636 | wwPDB-VP |
| Average B, all atoms (Å ²) | 36.0 | wwPDB-VP |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CHD, HEA, SAC, CDL, PSC, PEK, 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 | 0.51 | 0/4156 | 0.68 | 0/5678 |
| 1 | N | 0.50 | 0/4156 | 0.67 | 0/5678 |
| 2 | B | 0.48 | 0/1860 | 0.79 | 3/2534 (0.1%) |
| 2 | O | 0.52 | 0/1860 | 0.82 | 3/2534 (0.1%) |
| 3 | C | 0.51 | 0/2197 | 0.59 | 0/3005 |
| 3 | P | 0.48 | 0/2197 | 0.61 | 0/3005 |
| 4 | D | 0.48 | 0/1229 | 0.66 | 1/1658 (0.1%) |
| 4 | Q | 0.51 | 0/1229 | 0.66 | 1/1658 (0.1%) |
| 5 | E | 0.49 | 0/871 | 0.66 | 0/1182 |
| 5 | R | 0.50 | 0/871 | 0.68 | 0/1182 |
| 6 | F | 0.48 | 0/765 | 0.81 | 2/1038 (0.2%) |
| 6 | S | 0.51 | 0/765 | 0.82 | 2/1038 (0.2%) |
| 7 | G | 0.52 | 0/690 | 0.69 | 0/937 |
| 7 | T | 0.55 | 0/690 | 0.73 | 1/937 (0.1%) |
| 8 | H | 0.47 | 0/682 | 0.68 | 0/921 |
| 8 | U | 0.49 | 0/682 | 0.67 | 0/921 |
| 9 | I | 0.53 | 0/605 | 0.60 | 0/802 |
| 9 | V | 0.53 | 0/605 | 0.62 | 0/802 |
| 10 | J | 0.47 | 0/471 | 0.60 | 0/636 |
| 10 | W | 0.48 | 0/471 | 0.64 | 0/636 |
| 11 | K | 0.50 | 0/398 | 0.67 | 0/546 |
| 11 | X | 0.49 | 0/398 | 0.66 | 0/546 |
| 12 | L | 0.50 | 0/393 | 0.56 | 0/526 |
| 12 | Y | 0.54 | 0/393 | 0.58 | 0/526 |
| 13 | M | 0.47 | 0/345 | 0.62 | 0/470 |
| 13 | Z | 0.43 | 0/345 | 0.61 | 0/470 |
| All | All | 0.50 | 0/29324 | 0.68 | 13/39866 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 1 | N | 0 | 2 |
| 8 | U | 0 | 1 |
| All | All | 0 | 5 |

There are no bond length outliers.

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6 | S | 94 | HIS | N-CA-C | 6.25 | 127.89 | 111.00 |
| 2 | B | 103 | GLN | CA-C-N | -6.20 | 103.55 | 117.20 |
| 6 | F | 94 | HIS | N-CA-C | 5.99 | 127.18 | 111.00 |
| 7 | T | 33 | LEU | CA-CB-CG | 5.91 | 128.88 | 115.30 |
| 2 | O | 103 | GLN | CA-C-N | -5.82 | 104.40 | 117.20 |
| 2 | B | 184 | LEU | CA-CB-CG | 5.72 | 128.46 | 115.30 |
| 6 | F | 93 | PRO | N-CA-C | 5.69 | 126.90 | 112.10 |
| 4 | D | 133 | GLY | N-CA-C | 5.63 | 127.17 | 113.10 |
| 2 | B | 104 | TRP | N-CA-C | 5.47 | 125.78 | 111.00 |
| 4 | Q | 133 | GLY | N-CA-C | 5.43 | 126.67 | 113.10 |
| 2 | O | 227 | LEU | CA-CB-CG | 5.40 | 127.72 | 115.30 |
| 6 | S | 93 | PRO | N-CA-C | 5.33 | 125.94 | 112.10 |
| 2 | O | 104 | TRP | N-CA-C | 5.27 | 125.23 | 111.00 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 19 | TYR | Sidechain |
| 1 | A | 240 | HIS | Sidechain |
| 1 | N | 240 | HIS | Sidechain |
| 1 | N | 304 | TYR | Sidechain |
| 8 | U | 11 | TYR | Sidechain |

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 | 4027 | 0 | 4001 | 62 | 0 |
| 1 | N | 4027 | 0 | 4001 | 72 | 0 |
| 2 | B | 1824 | 0 | 1833 | 33 | 0 |
| 2 | O | 1824 | 0 | 1833 | 49 | 0 |
| 3 | C | 2110 | 0 | 2027 | 17 | 0 |
| 3 | P | 2110 | 0 | 2027 | 24 | 0 |
| 4 | D | 1195 | 0 | 1183 | 15 | 0 |
| 4 | Q | 1195 | 0 | 1183 | 25 | 0 |
| 5 | E | 852 | 0 | 845 | 6 | 0 |
| 5 | R | 852 | 0 | 845 | 11 | 0 |
| 6 | F | 748 | 0 | 728 | 16 | 0 |
| 6 | S | 748 | 0 | 728 | 12 | 0 |
| 7 | G | 675 | 0 | 644 | 25 | 0 |
| 7 | T | 675 | 0 | 644 | 21 | 0 |
| 8 | H | 662 | 0 | 623 | 5 | 0 |
| 8 | U | 662 | 0 | 623 | 8 | 0 |
| 9 | I | 601 | 0 | 613 | 8 | 0 |
| 9 | V | 601 | 0 | 613 | 11 | 0 |
| 10 | J | 460 | 0 | 459 | 6 | 0 |
| 10 | W | 460 | 0 | 459 | 2 | 0 |
| 11 | K | 384 | 0 | 366 | 2 | 0 |
| 11 | X | 384 | 0 | 366 | 8 | 0 |
| 12 | L | 380 | 0 | 380 | 13 | 0 |
| 12 | Y | 380 | 0 | 380 | 10 | 0 |
| 13 | M | 335 | 0 | 352 | 5 | 0 |
| 13 | Z | 335 | 0 | 352 | 6 | 0 |
| 14 | A | 1 | 0 | 0 | 0 | 0 |
| 14 | N | 1 | 0 | 0 | 0 | 0 |
| 15 | A | 1 | 0 | 0 | 0 | 0 |
| 15 | N | 1 | 0 | 0 | 0 | 0 |
| 16 | A | 1 | 0 | 0 | 0 | 0 |
| 16 | N | 1 | 0 | 0 | 0 | 0 |
| 17 | A | 120 | 0 | 108 | 4 | 0 |
| 17 | N | 120 | 0 | 108 | 3 | 0 |
| 18 | A | 63 | 0 | 110 | 11 | 0 |
| 18 | D | 63 | 0 | 110 | 15 | 0 |
| 18 | L | 63 | 0 | 110 | 25 | 0 |
| 18 | N | 126 | 0 | 220 | 38 | 0 |
| 18 | Q | 63 | 0 | 110 | 15 | 0 |
| 19 | A | 102 | 0 | 152 | 7 | 0 |
| 19 | C | 102 | 0 | 152 | 7 | 0 |
| 19 | N | 102 | 0 | 152 | 5 | 0 |
| 19 | P | 102 | 0 | 152 | 8 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20 | B | 2 | 0 | 0 | 0 | 0 |
| 20 | O | 2 | 0 | 0 | 0 | 0 |
| 21 | B | 29 | 0 | 39 | 1 | 0 |
| 21 | C | 58 | 0 | 78 | 3 | 0 |
| 21 | J | 29 | 0 | 39 | 2 | 0 |
| 21 | O | 29 | 0 | 39 | 1 | 0 |
| 21 | P | 58 | 0 | 78 | 2 | 0 |
| 21 | W | 29 | 0 | 39 | 2 | 0 |
| 22 | C | 100 | 0 | 156 | 14 | 0 |
| 22 | G | 100 | 0 | 156 | 14 | 0 |
| 22 | P | 100 | 0 | 156 | 18 | 0 |
| 22 | T | 100 | 0 | 156 | 15 | 0 |
| 23 | C | 106 | 0 | 154 | 7 | 0 |
| 23 | G | 53 | 0 | 77 | 10 | 0 |
| 23 | P | 106 | 0 | 154 | 6 | 0 |
| 23 | T | 53 | 0 | 77 | 9 | 0 |
| 24 | C | 1 | 0 | 0 | 0 | 0 |
| 24 | P | 1 | 0 | 0 | 0 | 0 |
| 25 | E | 52 | 0 | 80 | 13 | 0 |
| 25 | O | 52 | 0 | 80 | 21 | 0 |
| 26 | F | 1 | 0 | 0 | 0 | 0 |
| 26 | S | 1 | 0 | 0 | 0 | 0 |
| 27 | M | 33 | 0 | 36 | 0 | 0 |
| 27 | Z | 33 | 0 | 36 | 0 | 0 |
| 28 | A | 227 | 0 | 0 | 2 | 0 |
| 28 | B | 180 | 0 | 0 | 8 | 0 |
| 28 | C | 116 | 0 | 0 | 1 | 0 |
| 28 | D | 109 | 0 | 0 | 3 | 0 |
| 28 | E | 68 | 0 | 0 | 2 | 0 |
| 28 | F | 80 | 0 | 0 | 2 | 0 |
| 28 | G | 59 | 0 | 0 | 3 | 0 |
| 28 | H | 71 | 0 | 0 | 1 | 0 |
| 28 | I | 61 | 0 | 0 | 2 | 0 |
| 28 | J | 21 | 0 | 0 | 0 | 0 |
| 28 | K | 37 | 0 | 0 | 0 | 0 |
| 28 | L | 23 | 0 | 0 | 1 | 0 |
| 28 | M | 32 | 0 | 0 | 0 | 0 |
| 28 | N | 217 | 0 | 0 | 5 | 0 |
| 28 | O | 146 | 0 | 0 | 1 | 0 |
| 28 | P | 120 | 0 | 0 | 1 | 0 |
| 28 | Q | 73 | 0 | 0 | 5 | 0 |
| 28 | R | 32 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28 | S | 54 | 0 | 0 | 3 | 0 |
| 28 | T | 58 | 0 | 0 | 2 | 0 |
| 28 | U | 65 | 0 | 0 | 1 | 0 |
| 28 | V | 36 | 0 | 0 | 2 | 0 |
| 28 | W | 13 | 0 | 0 | 0 | 0 |
| 28 | X | 29 | 0 | 0 | 1 | 0 |
| 28 | Y | 25 | 0 | 0 | 1 | 0 |
| 28 | Z | 18 | 0 | 0 | 0 | 0 |
| All | All | 32636 | 0 | 31222 | 551 | 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 9.

All (551) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G:84:LYS:HD2 | 7:G:84:LYS:H | 1.14 | 1.08 |
| 3:P:63:ARG:HE | 22:P:4270:CDL:HA22 | 1.24 | 1.03 |
| 22:C:3270:CDL:H662 | 19:C:3267:PGV:H182 | 1.41 | 1.03 |
| 7:T:84:LYS:H | 7:T:84:LYS:HD2 | 1.23 | 1.02 |
| 3:C:63:ARG:HE | 22:C:3270:CDL:HA22 | 1.23 | 1.01 |
| 10:W:33:ARG:HG2 | 21:W:4060:CHD:H152 | 1.46 | 0.94 |
| 18:N:4522:TGL:HC31 | 12:Y:13:PHE:HA | 1.51 | 0.93 |
| 4:D:34:SER:H | 4:D:37:GLN:HE21 | 1.16 | 0.89 |
| 23:C:3264:PEK:H161 | 23:C:3264:PEK:H102 | 1.55 | 0.89 |
| 4:Q:114:GLU:HB3 | 28:Q:2622:HOH:O | 1.73 | 0.89 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:H | 1.93 | 0.87 |
| 9:I:5:ALA:HB2 | 28:I:2536:HOH:O | 1.73 | 0.86 |
| 6:F:85:CYS:SG | 6:F:87:THR:HG23 | 2.15 | 0.86 |
| 22:P:4270:CDL:H242 | 22:P:4270:CDL:H661 | 1.59 | 0.84 |
| 18:N:4521:TGL:H101 | 18:N:4521:TGL:H271 | 1.58 | 0.84 |
| 18:A:3521:TGL:H241 | 18:A:3521:TGL:HA91 | 1.60 | 0.83 |
| 7:T:5:LYS:HD2 | 23:T:3263:PEK:H382 | 1.61 | 0.83 |
| 22:C:3270:CDL:H242 | 22:C:3270:CDL:H661 | 1.60 | 0.82 |
| 22:P:4270:CDL:H662 | 19:P:4267:PGV:H182 | 1.61 | 0.81 |
| 25:O:4230:PSC:H21 | 25:O:4230:PSC:H222 | 1.64 | 0.80 |
| 12:L:20:ARG:HH12 | 18:L:3522:TGL:HC61 | 1.45 | 0.80 |
| 3:P:67:PHE:HE1 | 22:P:4270:CDL:H1 | 1.45 | 0.80 |
| 4:Q:114:GLU:HG2 | 28:Q:1465:HOH:O | 1.81 | 0.79 |
| 25:E:3230:PSC:H21 | 25:E:3230:PSC:H222 | 1.65 | 0.79 |
| 2:O:224:ALA:O | 2:O:227:LEU:HG | 1.83 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:426:PHE:CE1 | 18:A:3521:TGL:H282 | 2.19 | 0.77 |
| 23:P:4264:PEK:H161 | 23:P:4264:PEK:H102 | 1.64 | 0.77 |
| 1:N:113:LEU:CD1 | 18:N:4522:TGL:H292 | 2.16 | 0.76 |
| 2:O:49:LYS:NZ | 18:Q:4523:TGL:HC71 | 2.00 | 0.76 |
| 19:N:4524:PGV:H321 | 19:N:4524:PGV:H162 | 1.68 | 0.76 |
| 5:E:82:TYR:HB3 | 5:E:83:PRO:HD3 | 1.69 | 0.75 |
| 18:N:4521:TGL:H241 | 18:N:4521:TGL:HA91 | 1.67 | 0.74 |
| 2:O:56:MET:HA | 25:O:4230:PSC:H202 | 1.70 | 0.74 |
| 1:N:433:LEU:HD11 | 18:N:4521:TGL:OB1 | 1.88 | 0.74 |
| 19:A:3524:PGV:H321 | 19:A:3524:PGV:H162 | 1.70 | 0.74 |
| 3:P:210:ILE:HG23 | 19:P:4267:PGV:H102 | 1.70 | 0.74 |
| 10:J:33:ARG:HG2 | 21:J:3060:CHD:H152 | 1.68 | 0.74 |
| 12:L:13:PHE:HA | 18:L:3522:TGL:HC31 | 1.68 | 0.74 |
| 13:M:42:LYS:HE3 | 13:M:42:LYS:HA | 1.68 | 0.74 |
| 2:O:217:LYS:HA | 2:O:217:LYS:HE2 | 1.69 | 0.73 |
| 9:V:63:MET:HB3 | 9:V:68:ILE:HD11 | 1.70 | 0.73 |
| 5:R:43:PRO:HB2 | 5:R:48:ILE:HD11 | 1.68 | 0.73 |
| 22:C:3270:CDL:C66 | 19:C:3267:PGV:H182 | 2.18 | 0.72 |
| 28:B:4263:HOH:O | 18:D:3523:TGL:HC52 | 1.89 | 0.72 |
| 1:N:1:FME:HCN | 1:N:4:ASN:H | 1.55 | 0.72 |
| 1:A:282:PHE:HA | 7:T:4:ALA:HB3 | 1.72 | 0.72 |
| 4:D:34:SER:H | 4:D:37:GLN:NE2 | 1.88 | 0.71 |
| 3:C:67:PHE:HE1 | 22:C:3270:CDL:H1 | 1.55 | 0.71 |
| 18:D:3523:TGL:H242 | 18:D:3523:TGL:HA81 | 1.73 | 0.71 |
| 6:S:85:CYS:SG | 6:S:87:THR:HG23 | 2.31 | 0.70 |
| 18:Q:4523:TGL:HG12 | 18:Q:4523:TGL:HC21 | 1.73 | 0.70 |
| 6:S:94:HIS:CG | 6:S:95:GLN:H | 2.09 | 0.70 |
| 18:N:4521:TGL:H101 | 18:N:4521:TGL:C27 | 2.20 | 0.70 |
| 1:N:334:TRP:CH2 | 2:O:46:LEU:HD13 | 2.27 | 0.69 |
| 22:P:4270:CDL:H662 | 19:P:4267:PGV:C18 | 2.21 | 0.69 |
| 3:C:210:ILE:HG23 | 19:C:3267:PGV:H102 | 1.75 | 0.69 |
| 1:A:334:TRP:HZ3 | 18:D:3523:TGL:HA62 | 1.57 | 0.68 |
| 7:T:38:HIS:NE2 | 22:T:4269:CDL:H111 | 2.09 | 0.68 |
| 3:P:246:ASP:HB2 | 28:P:1524:HOH:O | 1.91 | 0.68 |
| 7:G:5:LYS:HB3 | 1:N:278:MET:SD | 2.33 | 0.68 |
| 19:P:4267:PGV:H161 | 19:P:4267:PGV:H12 | 1.76 | 0.68 |
| 18:D:3523:TGL:HC31 | 28:D:3613:HOH:O | 1.93 | 0.67 |
| 1:N:334:TRP:CZ3 | 18:Q:4523:TGL:HA42 | 2.30 | 0.67 |
| 1:A:229:ILE:HD11 | 2:B:175:ILE:HD13 | 1.76 | 0.67 |
| 3:P:29:SER:HB3 | 3:P:42:LEU:HD13 | 1.77 | 0.67 |
| 1:N:472:ILE:HD13 | 18:N:4522:TGL:HA92 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:G:84:LYS:N | 7:G:84:LYS:HD2 | 1.99 | 0.67 |
| 7:T:84:LYS:H | 7:T:84:LYS:CD | 2.03 | 0.66 |
| 6:S:94:HIS:CD2 | 6:S:95:GLN:N | 2.63 | 0.66 |
| 9:V:10:ARG:HD2 | 28:V:2590:HOH:O | 1.94 | 0.66 |
| 12:L:20:ARG:NH2 | 18:L:3522:TGL:HC32 | 2.11 | 0.66 |
| 25:E:3230:PSC:C07 | 9:I:10:ARG:HH21 | 2.09 | 0.66 |
| 2:O:41:ILE:HD13 | 25:O:4230:PSC:H342 | 1.79 | 0.65 |
| 1:A:337:ALA:HB2 | 1:A:394:VAL:HG23 | 1.77 | 0.65 |
| 7:G:84:LYS:H | 7:G:84:LYS:CD | 1.97 | 0.65 |
| 22:C:3270:CDL:H812 | 19:C:3267:PGV:H181 | 1.79 | 0.65 |
| 2:B:92:ASN:HB3 | 28:B:4260:HOH:O | 1.97 | 0.64 |
| 18:A:3521:TGL:H283 | 18:A:3521:TGL:HB92 | 1.79 | 0.64 |
| 4:D:58:GLU:HG3 | 28:D:3555:HOH:O | 1.98 | 0.63 |
| 18:N:4521:TGL:HB91 | 2:O:32:PHE:CE2 | 2.33 | 0.63 |
| 1:N:483:LEU:HD13 | 4:Q:6:VAL:HB | 1.80 | 0.63 |
| 18:Q:4523:TGL:H122 | 18:Q:4523:TGL:HB82 | 1.79 | 0.63 |
| 5:R:89:LEU:O | 5:R:93:LEU:HG | 1.99 | 0.63 |
| 18:D:3523:TGL:H122 | 18:D:3523:TGL:HB82 | 1.80 | 0.63 |
| 18:Q:4523:TGL:HA81 | 18:Q:4523:TGL:H242 | 1.80 | 0.62 |
| 6:S:75:HIS:H | 6:S:80:GLN:HE22 | 1.46 | 0.62 |
| 1:A:194:LEU:HD22 | 1:A:285:PHE:HE2 | 1.64 | 0.62 |
| 2:O:68:LEU:HD22 | 25:O:4230:PSC:H171 | 1.82 | 0.62 |
| 6:F:92:VAL:O | 6:F:92:VAL:HG23 | 1.99 | 0.62 |
| 28:N:2197:HOH:O | 18:Q:4523:TGL:HG2 | 1.98 | 0.62 |
| 19:C:3267:PGV:H12 | 19:C:3267:PGV:H161 | 1.81 | 0.61 |
| 4:Q:58:GLU:O | 4:Q:62:LEU:HG | 2.00 | 0.61 |
| 1:N:449:MET:SD | 2:O:5:MET:HG2 | 2.40 | 0.61 |
| 28:B:4247:HOH:O | 18:D:3523:TGL:H352 | 2.00 | 0.61 |
| 1:N:472:ILE:HG21 | 18:N:4522:TGL:HA81 | 1.83 | 0.60 |
| 1:A:334:TRP:CZ3 | 18:D:3523:TGL:HA42 | 2.37 | 0.60 |
| 2:O:49:LYS:HZ2 | 18:Q:4523:TGL:HC71 | 1.65 | 0.60 |
| 1:N:68:PHE:HE2 | 1:N:112:LEU:HD13 | 1.66 | 0.59 |
| 1:N:472:ILE:HG21 | 18:N:4522:TGL:CA8 | 2.32 | 0.59 |
| 2:B:41:ILE:HD13 | 25:E:3230:PSC:H342 | 1.84 | 0.59 |
| 25:O:4230:PSC:C07 | 9:V:10:ARG:HE | 2.15 | 0.59 |
| 3:P:160:LEU:HD13 | 21:P:4271:CHD:H181 | 1.84 | 0.59 |
| 9:V:65:LYS:O | 11:X:54:ARG:NH1 | 2.35 | 0.59 |
| 1:N:194:LEU:HD22 | 1:N:285:PHE:HE2 | 1.67 | 0.59 |
| 4:Q:127:LYS:O | 4:Q:130:PRO:HD3 | 2.02 | 0.59 |
| 1:A:151:HIS:CD2 | 23:C:3264:PEK:H382 | 2.38 | 0.59 |
| 1:N:112:LEU:HG | 28:N:1389:HOH:O | 2.01 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:L:20:ARG:NH1 | 18:L:3522:TGL:HC61 | 2.17 | 0.58 |
| 7:G:8:HIS:HD2 | 23:G:4263:PEK:H252 | 1.66 | 0.58 |
| 1:A:407:ASP:O | 1:A:411:LYS:HG3 | 2.04 | 0.58 |
| 18:N:4521:TGL:H281 | 18:N:4521:TGL:HB81 | 1.83 | 0.58 |
| 8:U:50:VAL:HG21 | 28:U:2545:HOH:O | 2.02 | 0.58 |
| 1:A:1:FME:HCN | 1:A:4:ASN:H | 1.68 | 0.58 |
| 25:E:3230:PSC:H072 | 9:I:10:ARG:HH21 | 1.67 | 0.58 |
| 1:N:81:TRP:HZ2 | 18:N:4522:TGL:C28 | 2.17 | 0.58 |
| 12:L:24:MET:HG3 | 28:L:2411:HOH:O | 2.04 | 0.58 |
| 12:Y:20:ARG:NH1 | 28:Y:1514:HOH:O | 2.36 | 0.58 |
| 22:P:4270:CDL:H812 | 19:P:4267:PGV:H181 | 1.86 | 0.57 |
| 1:A:426:PHE:CD1 | 18:A:3521:TGL:H282 | 2.38 | 0.57 |
| 2:O:104:TRP:CG | 2:O:203:ASN:HB2 | 2.39 | 0.57 |
| 12:L:11:ILE:HG22 | 18:L:3522:TGL:H271 | 1.86 | 0.57 |
| 2:O:41:ILE:CD1 | 25:O:4230:PSC:H342 | 2.34 | 0.57 |
| 1:A:449:MET:SD | 2:B:5:MET:HG2 | 2.45 | 0.57 |
| 1:N:113:LEU:HD13 | 18:N:4522:TGL:H292 | 1.84 | 0.57 |
| 22:G:3269:CDL:HB32 | 1:N:304:TYR:HD1 | 1.69 | 0.57 |
| 1:A:282:PHE:HA | 7:T:4:ALA:CB | 2.35 | 0.57 |
| 1:A:321:PHE:CD2 | 25:E:3230:PSC:H341 | 2.40 | 0.57 |
| 7:G:8:HIS:CD2 | 23:G:4263:PEK:H252 | 2.39 | 0.57 |
| 7:G:5:LYS:HD2 | 23:G:4263:PEK:H382 | 1.87 | 0.56 |
| 9:I:5:ALA:O | 9:I:7:PRO:HD3 | 2.04 | 0.56 |
| 22:T:4269:CDL:HA62 | 22:T:4269:CDL:H322 | 1.87 | 0.56 |
| 5:R:12:ASP:HA | 5:R:47:ILE:HD11 | 1.87 | 0.56 |
| 19:A:3524:PGV:H141 | 4:D:87:PHE:CD2 | 2.41 | 0.56 |
| 1:A:296:GLY:HA2 | 8:H:23:GLN:OE1 | 2.05 | 0.56 |
| 2:O:59:GLN:HG3 | 2:O:59:GLN:O | 2.06 | 0.56 |
| 1:N:22:PHE:HA | 18:N:4522:TGL:HB72 | 1.88 | 0.56 |
| 22:G:3269:CDL:HA62 | 22:G:3269:CDL:H322 | 1.87 | 0.56 |
| 3:C:213:THR:HG23 | 22:C:3270:CDL:H762 | 1.88 | 0.55 |
| 1:N:514:LYS:HA | 6:S:38:ALA:HB3 | 1.88 | 0.55 |
| 23:C:3264:PEK:C16 | 23:C:3264:PEK:H102 | 2.34 | 0.55 |
| 7:T:5:LYS:CD | 23:T:3263:PEK:H382 | 2.35 | 0.55 |
| 5:E:84:TYR:O | 5:E:88:GLU:HG2 | 2.07 | 0.55 |
| 4:D:17:VAL:HG12 | 28:D:3556:HOH:O | 2.06 | 0.55 |
| 3:C:160:LEU:HD13 | 21:C:3271:CHD:H181 | 1.88 | 0.55 |
| 1:A:334:TRP:CZ3 | 18:D:3523:TGL:HA62 | 2.41 | 0.54 |
| 1:A:472:ILE:HG21 | 18:L:3522:TGL:HA81 | 1.90 | 0.54 |
| 1:N:151:HIS:CD2 | 23:P:4264:PEK:H382 | 2.42 | 0.54 |
| 13:M:17:ILE:O | 13:M:21:VAL:HG23 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:177:SER:H | 1:A:180:GLN:HE21 | 1.54 | 0.54 |
| 1:N:54:TYR:HB2 | 28:N:1075:HOH:O | 2.07 | 0.54 |
| 13:Z:10:THR:HA | 13:Z:14:GLU:OE2 | 2.07 | 0.54 |
| 4:D:127:LYS:HD2 | 28:I:371:HOH:O | 2.07 | 0.54 |
| 2:B:56:MET:HG2 | 25:E:3230:PSC:H211 | 1.89 | 0.54 |
| 19:N:4524:PGV:H41 | 19:N:4524:PGV:H232 | 1.90 | 0.54 |
| 17:N:515:HEA:HMC1 | 17:N:515:HEA:HBC1 | 1.90 | 0.54 |
| 2:B:102:HIS:O | 2:B:104:TRP:N | 2.41 | 0.53 |
| 18:A:3521:TGL:HC52 | 2:B:7:LEU:HD12 | 1.90 | 0.53 |
| 7:G:17:ARG:HD2 | 28:G:289:HOH:O | 2.06 | 0.53 |
| 1:A:222:PRO:HD2 | 28:B:4240:HOH:O | 2.07 | 0.53 |
| 10:J:40:LEU:HD12 | 21:J:3060:CHD:H183 | 1.89 | 0.53 |
| 28:B:4144:HOH:O | 18:D:3523:TGL:HC72 | 2.08 | 0.53 |
| 7:G:8:HIS:CE1 | 23:G:4263:PEK:H331 | 2.44 | 0.53 |
| 7:G:19:LEU:HD21 | 23:G:4263:PEK:H362 | 1.90 | 0.53 |
| 12:Y:20:ARG:NH2 | 12:Y:24:MET:HG3 | 2.22 | 0.53 |
| 7:G:4:ALA:HB3 | 1:N:282:PHE:HA | 1.90 | 0.53 |
| 3:C:3:HIS:HE1 | 6:F:31:TYR:OH | 1.90 | 0.53 |
| 4:Q:118:LYS:HG3 | 28:Q:1465:HOH:O | 2.08 | 0.53 |
| 18:A:3521:TGL:H283 | 18:A:3521:TGL:CB9 | 2.38 | 0.53 |
| 1:A:81:TRP:HZ2 | 18:L:3522:TGL:H282 | 1.74 | 0.53 |
| 22:T:4269:CDL:H392 | 22:T:4269:CDL:H161 | 1.90 | 0.53 |
| 2:O:150:ILE:HD12 | 2:O:184:LEU:HD22 | 1.91 | 0.53 |
| 1:N:107:PRO:HB3 | 3:P:25:LEU:HB2 | 1.91 | 0.53 |
| 22:P:4270:CDL:C66 | 19:P:4267:PGV:H182 | 2.36 | 0.52 |
| 11:X:24:PHE:O | 11:X:28:VAL:HG12 | 2.10 | 0.52 |
| 7:G:3:ALA:O | 7:G:4:ALA:HB2 | 2.09 | 0.52 |
| 2:O:128:LEU:HD11 | 2:O:134:ARG:HA | 1.92 | 0.52 |
| 8:H:49:ASP:O | 8:H:52:VAL:HG22 | 2.10 | 0.52 |
| 12:L:20:ARG:HH12 | 18:L:3522:TGL:CC6 | 2.16 | 0.52 |
| 22:G:3269:CDL:H392 | 22:G:3269:CDL:H161 | 1.92 | 0.52 |
| 1:N:265:LYS:HE3 | 28:S:2510:HOH:O | 2.08 | 0.52 |
| 1:N:296:GLY:HA2 | 8:U:23:GLN:OE1 | 2.09 | 0.52 |
| 1:A:1:FME:HE2 | 1:A:1:FME:HA | 1.90 | 0.52 |
| 1:N:52:GLN:O | 1:N:56:VAL:HG23 | 2.10 | 0.52 |
| 2:B:122:MET:HB2 | 2:B:208:PRO:HD2 | 1.91 | 0.52 |
| 28:B:4241:HOH:O | 23:P:4265:PEK:H031 | 2.09 | 0.52 |
| 18:Q:4523:TGL:CG1 | 18:Q:4523:TGL:HC21 | 2.39 | 0.52 |
| 18:N:4521:TGL:HB91 | 2:O:32:PHE:CD2 | 2.46 | 0.51 |
| 2:O:56:MET:HG2 | 25:O:4230:PSC:H211 | 1.92 | 0.51 |
| 23:G:4263:PEK:H132 | 3:P:247:VAL:HG11 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:F:95:GLN:OE1 | 6:F:95:GLN:HA | 2.09 | 0.51 |
| 7:T:11:TPO:HG22 | 7:T:16:TRP:HE1 | 1.75 | 0.51 |
| 1:A:334:TRP:CH2 | 2:B:46:LEU:HD13 | 2.45 | 0.51 |
| 3:C:146:TRP:CZ2 | 7:G:17:ARG:HG3 | 2.45 | 0.51 |
| 3:P:213:THR:HG23 | 22:P:4270:CDL:H762 | 1.92 | 0.51 |
| 19:A:3524:PGV:H41 | 19:A:3524:PGV:H232 | 1.90 | 0.51 |
| 1:A:194:LEU:HD22 | 1:A:285:PHE:CE2 | 2.45 | 0.51 |
| 1:N:113:LEU:HD12 | 18:N:4522:TGL:H292 | 1.93 | 0.51 |
| 1:N:324:LEU:HD13 | 2:O:41:ILE:CG2 | 2.39 | 0.51 |
| 12:L:20:ARG:HH22 | 18:L:3522:TGL:HC32 | 1.74 | 0.51 |
| 12:L:13:PHE:HB3 | 18:L:3522:TGL:HG12 | 1.93 | 0.51 |
| 6:F:64:GLU:O | 6:F:65:ASP:HB2 | 2.11 | 0.51 |
| 6:F:25:ARG:HD2 | 28:F:154:HOH:O | 2.10 | 0.51 |
| 3:C:191:GLY:HA3 | 28:G:143:HOH:O | 2.11 | 0.50 |
| 2:O:83:ILE:O | 2:O:87:MET:HG3 | 2.12 | 0.50 |
| 18:N:4522:TGL:CG1 | 12:Y:13:PHE:HB3 | 2.41 | 0.50 |
| 7:T:3:ALA:O | 7:T:4:ALA:HB2 | 2.11 | 0.50 |
| 7:G:37:LEU:HD21 | 22:G:3269:CDL:H361 | 1.93 | 0.50 |
| 1:N:87:ILE:O | 1:N:173:PRO:HD3 | 2.11 | 0.50 |
| 17:A:515:HEA:HMC1 | 17:A:515:HEA:HBC1 | 1.93 | 0.50 |
| 1:A:472:ILE:HG21 | 18:L:3522:TGL:CA8 | 2.41 | 0.50 |
| 1:A:229:ILE:HD11 | 2:B:175:ILE:CD1 | 2.41 | 0.50 |
| 1:N:488:THR:HB | 1:N:495:LEU:HD13 | 1.92 | 0.50 |
| 3:P:34:TRP:CD1 | 3:P:40:MET:HG2 | 2.47 | 0.50 |
| 6:S:51:SER:O | 6:S:94:HIS:N | 2.45 | 0.50 |
| 7:T:5:LYS:HB2 | 23:T:3263:PEK:H372 | 1.94 | 0.50 |
| 22:T:4269:CDL:H511 | 22:T:4269:CDL:H172 | 1.93 | 0.50 |
| 1:A:177:SER:H | 1:A:180:GLN:NE2 | 2.10 | 0.50 |
| 3:C:244:PHE:HA | 23:T:3263:PEK:H9 | 1.93 | 0.50 |
| 2:O:49:LYS:O | 4:Q:20:ARG:NH2 | 2.42 | 0.50 |
| 6:S:87:THR:HG21 | 28:S:1319:HOH:O | 2.12 | 0.50 |
| 23:G:4263:PEK:H9 | 3:P:244:PHE:HA | 1.94 | 0.50 |
| 11:X:54:ARG:HG3 | 11:X:54:ARG:NH2 | 2.25 | 0.50 |
| 18:L:3522:TGL:HC62 | 18:L:3522:TGL:HC22 | 1.93 | 0.50 |
| 22:G:3269:CDL:H511 | 22:G:3269:CDL:H172 | 1.92 | 0.50 |
| 5:R:81:ILE:HG12 | 9:V:7:PRO:HG2 | 1.93 | 0.50 |
| 23:C:3264:PEK:H32 | 23:C:3264:PEK:H71 | 1.93 | 0.50 |
| 8:U:7:LYS:O | 8:U:8:ILE:HG22 | 2.12 | 0.50 |
| 2:O:102:HIS:O | 2:O:104:TRP:N | 2.45 | 0.49 |
| 1:N:290:HIS:CD2 | 1:N:291:HIS:CD2 | 3.00 | 0.49 |
| 2:O:122:MET:HB2 | 2:O:208:PRO:HD2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:G:3269:CDL:H522 | 22:G:3269:CDL:H202 | 1.95 | 0.49 |
| 2:O:132:GLU:HB3 | 2:O:137:GLU:HG3 | 1.94 | 0.49 |
| 7:T:8:HIS:CD2 | 23:T:3263:PEK:H252 | 2.48 | 0.49 |
| 1:A:81:TRP:HZ2 | 18:L:3522:TGL:C28 | 2.26 | 0.49 |
| 1:N:379:TYR:O | 1:N:383:MET:HB2 | 2.12 | 0.49 |
| 4:Q:89:ILE:HD12 | 18:Q:4523:TGL:H311 | 1.95 | 0.49 |
| 1:N:514:LYS:HE2 | 28:S:1319:HOH:O | 2.12 | 0.49 |
| 7:G:34:ASN:HD22 | 22:G:3269:CDL:H151 | 1.78 | 0.49 |
| 6:F:8:THR:OG1 | 6:F:11:GLU:HG3 | 2.13 | 0.49 |
| 22:P:4270:CDL:H602 | 22:P:4270:CDL:H632 | 1.59 | 0.49 |
| 2:B:132:GLU:HB3 | 2:B:137:GLU:HG3 | 1.95 | 0.49 |
| 1:N:106:PRO:HB2 | 1:N:107:PRO:HD3 | 1.95 | 0.48 |
| 2:B:196:CYS:HB2 | 2:B:207:MET:HG3 | 1.95 | 0.48 |
| 22:C:3270:CDL:HA61 | 28:C:3618:HOH:O | 2.11 | 0.48 |
| 18:N:4521:TGL:OB1 | 18:N:4521:TGL:HB42 | 2.13 | 0.48 |
| 11:X:54:ARG:HH21 | 11:X:54:ARG:HG3 | 1.78 | 0.48 |
| 1:N:194:LEU:HD22 | 1:N:285:PHE:CE2 | 2.48 | 0.48 |
| 1:A:87:ILE:O | 1:A:173:PRO:HD3 | 2.13 | 0.48 |
| 6:S:92:VAL:HG23 | 6:S:92:VAL:O | 2.13 | 0.48 |
| 28:O:2266:HOH:O | 8:U:61:LYS:HD3 | 2.12 | 0.48 |
| 25:O:4230:PSC:H071 | 9:V:10:ARG:HE | 1.77 | 0.48 |
| 1:A:304:TYR:HD1 | 22:T:4269:CDL:HB32 | 1.79 | 0.48 |
| 2:B:78:LEU:HD12 | 22:T:4269:CDL:H351 | 1.94 | 0.48 |
| 1:A:472:ILE:HD13 | 18:L:3522:TGL:HA92 | 1.95 | 0.48 |
| 2:B:164:ALA:O | 2:B:194:GLY:HA3 | 2.13 | 0.48 |
| 25:O:4230:PSC:H212 | 25:O:4230:PSC:O01 | 2.14 | 0.48 |
| 2:O:49:LYS:HZ3 | 18:Q:4523:TGL:HC71 | 1.76 | 0.48 |
| 8:H:23:GLN:HG3 | 28:H:2167:HOH:O | 2.12 | 0.48 |
| 12:Y:2:HIS:ND1 | 12:Y:3:TYR:N | 2.62 | 0.48 |
| 10:W:50:LEU:HD22 | 10:W:50:LEU:O | 2.14 | 0.48 |
| 18:N:4521:TGL:HB91 | 2:O:32:PHE:HE2 | 1.75 | 0.48 |
| 1:A:427:PRO:HG3 | 18:A:3521:TGL:H351 | 1.95 | 0.48 |
| 2:B:41:ILE:O | 2:B:45:MET:HG2 | 2.14 | 0.48 |
| 19:N:4524:PGV:H141 | 4:Q:87:PHE:CD2 | 2.49 | 0.48 |
| 2:O:104:TRP:HA | 2:O:207:MET:SD | 2.54 | 0.48 |
| 1:A:81:TRP:CZ2 | 18:L:3522:TGL:H282 | 2.49 | 0.47 |
| 1:N:405:LEU:HD23 | 1:N:475:ALA:HB2 | 1.96 | 0.47 |
| 2:B:114:GLU:HB3 | 28:B:4162:HOH:O | 2.14 | 0.47 |
| 7:G:34:ASN:ND2 | 22:G:3269:CDL:H151 | 2.28 | 0.47 |
| 7:G:50:TYR:HB3 | 7:G:52:HIS:CE1 | 2.48 | 0.47 |
| 3:P:67:PHE:CE1 | 22:P:4270:CDL:H1 | 2.37 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:X:54:ARG:HH21 | 11:X:54:ARG:CG | 2.28 | 0.47 |
| 2:O:9:PHE:HB2 | 2:O:21:LEU:HD21 | 1.96 | 0.47 |
| 1:A:52:GLN:O | 1:A:56:VAL:HG23 | 2.15 | 0.47 |
| 2:B:81:LEU:HD13 | 22:T:4269:CDL:H122 | 1.96 | 0.47 |
| 7:G:4:ALA:CB | 1:N:282:PHE:HA | 2.44 | 0.47 |
| 2:B:33:LEU:HD13 | 9:I:31:PHE:CD1 | 2.50 | 0.47 |
| 18:N:4521:TGL:HC52 | 2:O:7:LEU:HD12 | 1.97 | 0.47 |
| 22:T:4269:CDL:H152 | 22:T:4269:CDL:H181 | 1.62 | 0.47 |
| 3:P:25:LEU:O | 3:P:29:SER:HB2 | 2.15 | 0.47 |
| 1:A:278:MET:SD | 7:T:5:LYS:HB3 | 2.54 | 0.47 |
| 25:E:3230:PSC:H62 | 25:E:3230:PSC:H241 | 1.97 | 0.47 |
| 18:D:3523:TGL:HC91 | 18:D:3523:TGL:HC62 | 1.75 | 0.47 |
| 1:A:365:ILE:HD11 | 28:A:3732:HOH:O | 2.14 | 0.47 |
| 5:R:37:VAL:HG11 | 5:R:70:VAL:HG21 | 1.95 | 0.47 |
| 21:W:4060:CHD:H161 | 21:W:4060:CHD:H212 | 1.74 | 0.47 |
| 2:B:58:ALA:O | 2:B:62:GLU:HG3 | 2.15 | 0.47 |
| 18:N:4521:TGL:H301 | 18:N:4521:TGL:HA92 | 1.96 | 0.46 |
| 1:A:379:TYR:O | 1:A:383:MET:HB2 | 2.14 | 0.46 |
| 1:A:290:HIS:CD2 | 1:A:291:HIS:CD2 | 3.02 | 0.46 |
| 18:N:4521:TGL:HB92 | 18:N:4521:TGL:H283 | 1.96 | 0.46 |
| 23:T:3263:PEK:H371 | 23:T:3263:PEK:H332 | 1.98 | 0.46 |
| 25:O:4230:PSC:H072 | 9:V:10:ARG:HE | 1.81 | 0.46 |
| 4:Q:131:ILE:HD12 | 4:Q:131:ILE:H | 1.81 | 0.46 |
| 7:G:39:SER:HB3 | 28:G:2466:HOH:O | 2.15 | 0.46 |
| 1:N:377:PHE:HA | 1:N:380:VAL:HG22 | 1.97 | 0.46 |
| 10:J:50:LEU:HD22 | 10:J:50:LEU:O | 2.15 | 0.46 |
| 22:C:3270:CDL:H632 | 22:C:3270:CDL:H602 | 1.55 | 0.46 |
| 22:C:3270:CDL:H652 | 22:C:3270:CDL:H621 | 1.56 | 0.46 |
| 18:A:3521:TGL:HG11 | 2:B:7:LEU:HB3 | 1.98 | 0.46 |
| 1:A:107:PRO:HB3 | 3:C:25:LEU:HB2 | 1.98 | 0.46 |
| 3:C:210:ILE:HD13 | 19:C:3267:PGV:H301 | 1.98 | 0.46 |
| 2:O:196:CYS:HB2 | 2:O:207:MET:HG3 | 1.98 | 0.46 |
| 1:N:347:LEU:HD13 | 1:N:383:MET:SD | 2.54 | 0.46 |
| 10:J:56:PRO:HD3 | 12:L:46:LYS:HE3 | 1.96 | 0.46 |
| 19:N:4524:PGV:H141 | 4:Q:87:PHE:CE2 | 2.51 | 0.46 |
| 4:Q:52:SER:OG | 4:Q:55:GLU:HG3 | 2.16 | 0.46 |
| 18:N:4522:TGL:H181 | 18:N:4522:TGL:OA1 | 2.15 | 0.46 |
| 28:Q:1465:HOH:O | 11:X:51:LYS:HD3 | 2.16 | 0.46 |
| 22:T:4269:CDL:H202 | 22:T:4269:CDL:H522 | 1.98 | 0.46 |
| 12:Y:20:ARG:HH21 | 12:Y:24:MET:CG | 2.29 | 0.46 |
| 19:A:3524:PGV:H141 | 4:D:87:PHE:CE2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:N:44:PRO:HG2 | 4:Q:111:PHE:CZ | 2.51 | 0.46 |
| 2:O:57:ASP:H | 25:O:4230:PSC:H201 | 1.80 | 0.46 |
| 1:A:22:PHE:HA | 18:L:3522:TGL:HB72 | 1.98 | 0.46 |
| 2:O:1:FME:SD | 2:O:133:LEU:CD1 | 3.04 | 0.46 |
| 1:N:426:PHE:CE1 | 18:N:4521:TGL:H282 | 2.50 | 0.45 |
| 22:P:4270:CDL:H642 | 22:P:4270:CDL:H191 | 1.98 | 0.45 |
| 1:N:343:GLY:HA2 | 18:Q:4523:TGL:H202 | 1.98 | 0.45 |
| 3:P:191:GLY:HA3 | 28:T:1143:HOH:O | 2.16 | 0.45 |
| 4:D:89:ILE:CD1 | 18:D:3523:TGL:H311 | 2.46 | 0.45 |
| 13:M:42:LYS:CE | 13:M:42:LYS:HA | 2.38 | 0.45 |
| 23:G:4263:PEK:H15 | 3:P:248:VAL:HG22 | 1.99 | 0.45 |
| 4:Q:130:PRO:HG2 | 4:Q:131:ILE:HD12 | 1.99 | 0.45 |
| 11:K:24:PHE:O | 11:K:28:VAL:HG12 | 2.17 | 0.45 |
| 22:P:4270:CDL:CB3 | 22:P:4270:CDL:HB21 | 2.46 | 0.45 |
| 2:O:57:ASP:H | 25:O:4230:PSC:C20 | 2.29 | 0.45 |
| 2:O:16:ILE:HD13 | 2:O:16:ILE:HA | 1.82 | 0.45 |
| 1:A:71:MET:HB2 | 1:A:72:PRO:HD3 | 1.99 | 0.45 |
| 1:N:62:ALA:HB2 | 17:N:515:HEA:HBD1 | 1.99 | 0.45 |
| 10:J:1:PHE:HD1 | 10:J:1:PHE:H1 | 1.64 | 0.45 |
| 1:A:1:FME:HA | 1:A:1:FME:CE | 2.47 | 0.45 |
| 22:G:3269:CDL:H551 | 22:G:3269:CDL:H582 | 1.69 | 0.45 |
| 4:Q:48:TRP:HB2 | 5:R:96:LEU:O | 2.16 | 0.45 |
| 22:C:3270:CDL:HB21 | 22:C:3270:CDL:CB3 | 2.47 | 0.45 |
| 22:C:3270:CDL:H642 | 22:C:3270:CDL:H191 | 1.99 | 0.45 |
| 1:N:28:MET:HE2 | 17:N:515:HEA:H271 | 1.97 | 0.45 |
| 1:N:171:MET:HG2 | 3:P:8:TYR:CE1 | 2.51 | 0.45 |
| 18:L:3522:TGL:H181 | 18:L:3522:TGL:OA1 | 2.17 | 0.45 |
| 6:S:55:LYS:HA | 6:S:74:LEU:O | 2.17 | 0.45 |
| 1:N:321:PHE:CD2 | 25:O:4230:PSC:H341 | 2.52 | 0.45 |
| 22:T:4269:CDL:H582 | 22:T:4269:CDL:H551 | 1.68 | 0.45 |
| 1:N:365:ILE:HD11 | 28:N:2145:HOH:O | 2.16 | 0.45 |
| 25:O:4230:PSC:H221 | 25:O:4230:PSC:H251 | 1.75 | 0.44 |
| 18:L:3522:TGL:H122 | 18:L:3522:TGL:H291 | 1.66 | 0.44 |
| 2:B:47:THR:HB | 18:D:3523:TGL:H332 | 1.99 | 0.44 |
| 6:F:92:VAL:O | 6:F:92:VAL:CG2 | 2.63 | 0.44 |
| 13:Z:32:TRP:CZ3 | 13:Z:40:TYR:OH | 2.70 | 0.44 |
| 3:C:22:LEU:O | 3:C:26:LEU:HG | 2.17 | 0.44 |
| 18:N:4521:TGL:H222 | 18:N:4521:TGL:HA91 | 1.57 | 0.44 |
| 2:B:91:ASN:HD22 | 2:B:92:ASN:N | 2.15 | 0.44 |
| 21:P:4271:CHD:H112 | 21:P:4271:CHD:H12A | 1.65 | 0.44 |
| 9:V:15:ARG:HD2 | 28:V:2350:HOH:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:Q:34:SER:H | 4:Q:37:GLN:HE21 | 1.65 | 0.44 |
| 4:Q:17:VAL:HG12 | 28:Q:2237:HOH:O | 2.17 | 0.44 |
| 3:P:146:TRP:CZ2 | 7:T:17:ARG:HG3 | 2.52 | 0.44 |
| 18:N:4522:TGL:HG12 | 12:Y:13:PHE:HB3 | 1.98 | 0.44 |
| 19:A:3524:PGV:H262 | 19:A:3524:PGV:H81 | 2.00 | 0.44 |
| 4:D:126:MET:HA | 9:I:68:ILE:HD13 | 2.00 | 0.44 |
| 2:B:94:SER:HB2 | 28:B:4194:HOH:O | 2.17 | 0.44 |
| 18:L:3522:TGL:HG12 | 18:L:3522:TGL:CC1 | 2.48 | 0.44 |
| 4:Q:86:MET:HG2 | 18:Q:4523:TGL:H312 | 1.98 | 0.44 |
| 23:G:4263:PEK:H332 | 23:G:4263:PEK:H371 | 2.00 | 0.44 |
| 1:A:106:PRO:HB2 | 1:A:107:PRO:HD3 | 1.99 | 0.44 |
| 1:N:344:PHE:CD1 | 1:N:344:PHE:C | 2.91 | 0.44 |
| 1:N:400:PHE:HB3 | 18:N:4522:TGL:H282 | 1.99 | 0.44 |
| 18:N:4522:TGL:HB52 | 18:N:4522:TGL:HB81 | 1.65 | 0.44 |
| 18:N:4521:TGL:C28 | 18:N:4521:TGL:HB81 | 2.48 | 0.44 |
| 4:Q:82:VAL:O | 4:Q:86:MET:HG3 | 2.17 | 0.44 |
| 23:C:3265:PEK:H131 | 23:C:3265:PEK:H102 | 1.79 | 0.44 |
| 7:G:11:TPO:HG22 | 7:G:16:TRP:HE1 | 1.83 | 0.44 |
| 2:O:68:LEU:CB | 2:O:69:PRO:HD3 | 2.48 | 0.44 |
| 2:B:104:TRP:CG | 2:B:203:ASN:HB2 | 2.53 | 0.44 |
| 5:R:87:GLN:HG2 | 5:R:88:GLU:N | 2.32 | 0.44 |
| 4:D:34:SER:N | 4:D:37:GLN:HE21 | 1.99 | 0.44 |
| 18:N:4521:TGL:CA9 | 18:N:4521:TGL:H241 | 2.41 | 0.44 |
| 1:A:350:VAL:HG21 | 18:A:3521:TGL:H271 | 2.00 | 0.44 |
| 2:O:56:MET:HA | 25:O:4230:PSC:C20 | 2.44 | 0.44 |
| 25:E:3230:PSC:H232 | 25:E:3230:PSC:H201 | 1.85 | 0.44 |
| 2:O:62:GLU:O | 2:O:66:THR:HB | 2.18 | 0.44 |
| 13:Z:13:LYS:O | 13:Z:17:ILE:HG13 | 2.17 | 0.44 |
| 3:P:47:LEU:O | 3:P:51:MET:HG2 | 2.18 | 0.44 |
| 25:O:4230:PSC:H241 | 25:O:4230:PSC:H62 | 1.98 | 0.44 |
| 9:V:63:MET:HB3 | 9:V:68:ILE:CD1 | 2.45 | 0.44 |
| 22:T:4269:CDL:H631 | 22:T:4269:CDL:H662 | 1.85 | 0.44 |
| 2:B:104:TRP:HA | 2:B:207:MET:SD | 2.58 | 0.44 |
| 1:A:35:LEU:HD11 | 1:A:462:LEU:HD13 | 1.99 | 0.44 |
| 7:T:19:LEU:HD21 | 23:T:3263:PEK:H362 | 2.00 | 0.43 |
| 12:L:11:ILE:CG2 | 18:L:3522:TGL:H271 | 2.48 | 0.43 |
| 19:N:4524:PGV:O05 | 19:N:4524:PGV:H032 | 2.18 | 0.43 |
| 22:G:3269:CDL:H212 | 1:N:311:ILE:HD12 | 2.00 | 0.43 |
| 1:A:383:MET:O | 1:A:387:PHE:HB2 | 2.18 | 0.43 |
| 6:F:52:ILE:HA | 6:F:94:HIS:HA | 1.99 | 0.43 |
| 1:A:488:THR:HB | 1:A:495:LEU:HD13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:N:4521:TGL:CB9 | 18:N:4521:TGL:H283 | 2.49 | 0.43 |
| 2:B:62:GLU:O | 2:B:66:THR:HB | 2.19 | 0.43 |
| 1:A:377:PHE:CD1 | 17:A:516:HEA:HAD1 | 2.53 | 0.43 |
| 25:E:3230:PSC:O01 | 25:E:3230:PSC:H212 | 2.17 | 0.43 |
| 7:G:7:ASP:O | 7:G:9:GLY:N | 2.51 | 0.43 |
| 1:N:35:LEU:HD11 | 1:N:462:LEU:HD13 | 2.00 | 0.43 |
| 4:D:86:MET:HG2 | 18:D:3523:TGL:H312 | 2.00 | 0.43 |
| 18:L:3522:TGL:HB81 | 18:L:3522:TGL:HB52 | 1.63 | 0.43 |
| 1:N:334:TRP:HH2 | 2:O:46:LEU:HD13 | 1.82 | 0.43 |
| 6:S:52:ILE:O | 6:S:94:HIS:ND1 | 2.52 | 0.43 |
| 5:R:82:TYR:N | 5:R:83:PRO:CD | 2.81 | 0.43 |
| 1:N:481:GLU:HB2 | 13:Z:4:LYS:HE2 | 1.99 | 0.43 |
| 5:R:99:SER:HB2 | 5:R:104:LEU:HD21 | 2.01 | 0.43 |
| 3:C:177:GLN:HA | 3:C:177:GLN:OE1 | 2.19 | 0.43 |
| 1:N:225:GLY:HA3 | 3:P:112:LEU:HD21 | 2.01 | 0.43 |
| 22:T:4269:CDL:H601 | 22:T:4269:CDL:H571 | 1.70 | 0.43 |
| 7:G:44:ARG:HD2 | 7:G:82:TYR:CE1 | 2.54 | 0.43 |
| 3:C:34:TRP:CD1 | 3:C:40:MET:HG2 | 2.53 | 0.43 |
| 1:A:431:LEU:HD21 | 1:A:450:TRP:HB2 | 2.01 | 0.43 |
| 4:Q:131:ILE:N | 4:Q:131:ILE:HD12 | 2.34 | 0.43 |
| 23:C:3265:PEK:H383 | 22:G:3269:CDL:H272 | 2.01 | 0.43 |
| 2:O:1:FME:SD | 2:O:133:LEU:HD13 | 2.58 | 0.43 |
| 1:N:81:TRP:CZ2 | 18:N:4522:TGL:C28 | 3.00 | 0.43 |
| 18:N:4522:TGL:HA41 | 12:Y:25:MET:HG2 | 1.99 | 0.43 |
| 2:O:41:ILE:O | 2:O:45:MET:HG2 | 2.18 | 0.43 |
| 22:T:4269:CDL:H732 | 22:T:4269:CDL:H762 | 1.94 | 0.43 |
| 2:O:164:ALA:O | 2:O:194:GLY:HA3 | 2.18 | 0.43 |
| 5:E:97:GLY:HA2 | 28:E:3252:HOH:O | 2.19 | 0.43 |
| 4:Q:23:PRO:O | 4:Q:25:PRO:HD3 | 2.18 | 0.43 |
| 1:A:400:PHE:HB2 | 18:L:3522:TGL:H252 | 2.00 | 0.43 |
| 2:B:56:MET:HA | 25:E:3230:PSC:H202 | 2.01 | 0.43 |
| 8:U:37:HIS:CD2 | 8:U:76:ARG:CZ | 3.02 | 0.43 |
| 4:Q:57:VAL:O | 4:Q:61:ARG:HG2 | 2.19 | 0.43 |
| 2:B:52:HIS:HE1 | 25:E:3230:PSC:H02 | 1.83 | 0.42 |
| 1:N:334:TRP:HZ3 | 18:Q:4523:TGL:HA62 | 1.83 | 0.42 |
| 13:M:42:LYS:HE3 | 13:M:42:LYS:CA | 2.46 | 0.42 |
| 6:F:55:LYS:HA | 6:F:74:LEU:O | 2.18 | 0.42 |
| 2:O:220:GLU:O | 2:O:223:SER:HB2 | 2.18 | 0.42 |
| 3:P:58:TRP:CZ3 | 19:P:4267:PGV:H81 | 2.54 | 0.42 |
| 1:N:324:LEU:HD13 | 2:O:41:ILE:HG22 | 2.01 | 0.42 |
| 1:N:513:LEU:HD22 | 1:N:513:LEU:HA | 1.89 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:P:63:ARG:HE | 22:P:4270:CDL:CA2 | 2.11 | 0.42 |
| 4:Q:89:ILE:CD1 | 18:Q:4523:TGL:H311 | 2.49 | 0.42 |
| 6:S:94:HIS:CG | 6:S:95:GLN:N | 2.84 | 0.42 |
| 1:N:399:LEU:HB2 | 1:N:494:TRP:CZ3 | 2.55 | 0.42 |
| 10:J:2:GLU:HB2 | 10:J:4:ARG:NH1 | 2.35 | 0.42 |
| 1:A:240:HIS:O | 1:A:243:VAL:HG22 | 2.19 | 0.42 |
| 18:A:3521:TGL:OB1 | 18:A:3521:TGL:HB42 | 2.18 | 0.42 |
| 18:D:3523:TGL:HB21 | 18:D:3523:TGL:OG1 | 2.19 | 0.42 |
| 1:N:112:LEU:HD23 | 1:N:112:LEU:C | 2.40 | 0.42 |
| 12:Y:20:ARG:HH21 | 12:Y:24:MET:HG3 | 1.85 | 0.42 |
| 2:O:121:TYR:O | 2:O:138:VAL:HA | 2.18 | 0.42 |
| 1:A:165:ILE:O | 1:A:169:ILE:HG12 | 2.18 | 0.42 |
| 25:E:3230:PSC:C14 | 25:E:3230:PSC:H343 | 2.49 | 0.42 |
| 3:C:146:TRP:CD2 | 3:C:162:ALA:HB2 | 2.55 | 0.42 |
| 7:G:7:ASP:O | 1:N:169:ILE:HD12 | 2.20 | 0.42 |
| 2:O:116:LEU:HD12 | 2:O:117:SER:N | 2.35 | 0.42 |
| 7:G:5:LYS:HB2 | 23:G:4263:PEK:H372 | 2.02 | 0.42 |
| 23:C:3265:PEK:H232 | 7:G:21:PHE:CD2 | 2.54 | 0.42 |
| 6:F:25:ARG:HB3 | 28:F:145:HOH:O | 2.19 | 0.42 |
| 13:Z:28:LEU:HB2 | 13:Z:29:PRO:HD3 | 2.01 | 0.42 |
| 1:A:426:PHE:HE1 | 18:A:3521:TGL:H282 | 1.74 | 0.42 |
| 12:L:13:PHE:HB3 | 18:L:3522:TGL:CG1 | 2.49 | 0.42 |
| 5:R:48:ILE:O | 5:R:52:LEU:HG | 2.20 | 0.42 |
| 25:O:4230:PSC:H201 | 25:O:4230:PSC:H232 | 1.84 | 0.42 |
| 4:Q:138:TRP:CH2 | 11:X:50:PRO:HG2 | 2.54 | 0.42 |
| 2:O:92:ASN:HA | 2:O:93:PRO:HD2 | 1.82 | 0.42 |
| 18:N:4522:TGL:H232 | 18:N:4522:TGL:H272 | 2.02 | 0.42 |
| 25:E:3230:PSC:H251 | 25:E:3230:PSC:H221 | 1.73 | 0.42 |
| 22:G:3269:CDL:H152 | 22:G:3269:CDL:H181 | 1.63 | 0.42 |
| 7:T:7:ASP:O | 7:T:9:GLY:N | 2.52 | 0.42 |
| 5:E:46:LYS:HG2 | 28:E:3281:HOH:O | 2.19 | 0.41 |
| 22:P:4270:CDL:H312 | 22:P:4270:CDL:H151 | 2.03 | 0.41 |
| 22:C:3270:CDL:H312 | 22:C:3270:CDL:H151 | 2.02 | 0.41 |
| 2:B:92:ASN:HA | 2:B:93:PRO:HD2 | 1.92 | 0.41 |
| 1:A:62:ALA:HB2 | 17:A:515:HEA:HBD1 | 2.01 | 0.41 |
| 1:N:3:ILE:HG23 | 1:N:7:LEU:HD22 | 2.02 | 0.41 |
| 8:H:60:TYR:C | 8:H:60:TYR:CD1 | 2.92 | 0.41 |
| 22:P:4270:CDL:H372 | 22:P:4270:CDL:H192 | 2.02 | 0.41 |
| 7:T:2:SER:O | 7:T:3:ALA:HB3 | 2.21 | 0.41 |
| 21:C:3271:CHD:H222 | 21:C:3271:CHD:H162 | 1.79 | 0.41 |
| 1:N:265:LYS:HB2 | 1:N:490:THR:HG21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:X:8:ASP:HB2 | 28:X:2472:HOH:O | 2.19 | 0.41 |
| 21:O:3085:CHD:H212 | 21:O:3085:CHD:H12 | 2.01 | 0.41 |
| 9:I:65:LYS:O | 11:K:54:ARG:NH1 | 2.51 | 0.41 |
| 28:A:3739:HOH:O | 4:D:20:ARG:HG3 | 2.21 | 0.41 |
| 1:A:174:PRO:HB2 | 6:F:35:ALA:HB2 | 2.02 | 0.41 |
| 1:N:426:PHE:CD1 | 18:N:4521:TGL:H282 | 2.56 | 0.41 |
| 18:D:3523:TGL:HA52 | 18:D:3523:TGL:HB71 | 2.03 | 0.41 |
| 21:C:3271:CHD:H112 | 21:C:3271:CHD:H12A | 1.63 | 0.41 |
| 1:N:440:TYR:HE2 | 2:O:204:HIS:CE1 | 2.37 | 0.41 |
| 9:V:35:TYR:C | 9:V:37:PHE:H | 2.24 | 0.41 |
| 12:L:20:ARG:HH22 | 18:L:3522:TGL:CC6 | 2.33 | 0.41 |
| 23:P:4264:PEK:H71 | 23:P:4264:PEK:H32 | 2.01 | 0.41 |
| 2:O:116:LEU:HD21 | 2:O:222:TRP:CH2 | 2.55 | 0.41 |
| 1:A:42:GLY:HA3 | 4:D:104:TYR:OH | 2.21 | 0.41 |
| 5:E:12:ASP:OD1 | 5:E:44:GLU:HG3 | 2.20 | 0.41 |
| 5:R:86:ILE:HA | 5:R:86:ILE:HD13 | 1.88 | 0.41 |
| 1:A:514:LYS:HA | 6:F:38:ALA:HB3 | 2.03 | 0.41 |
| 3:C:51:MET:SD | 22:C:3270:CDL:H622 | 2.61 | 0.41 |
| 18:N:4522:TGL:H342 | 12:Y:28:PHE:HA | 2.03 | 0.41 |
| 7:T:8:HIS:CE1 | 23:T:3263:PEK:H331 | 2.56 | 0.41 |
| 18:Q:4523:TGL:HB31 | 18:Q:4523:TGL:HA32 | 2.03 | 0.41 |
| 19:A:3524:PGV:H032 | 19:A:3524:PGV:O05 | 2.19 | 0.41 |
| 1:A:406:ASN:HD21 | 19:A:3524:PGV:C3 | 2.34 | 0.41 |
| 22:G:3269:CDL:HB32 | 1:N:304:TYR:CD1 | 2.51 | 0.41 |
| 4:D:126:MET:HG3 | 4:D:128:VAL:HG23 | 2.02 | 0.41 |
| 1:A:510:TYR:CD2 | 6:F:49:VAL:HG13 | 2.56 | 0.41 |
| 25:O:4230:PSC:C14 | 25:O:4230:PSC:H343 | 2.51 | 0.41 |
| 2:B:168:LEU:HD13 | 2:B:184:LEU:HG | 2.03 | 0.41 |
| 8:U:9:LYS:HB3 | 8:U:10:ASN:H | 1.57 | 0.41 |
| 19:C:3268:PGV:H202 | 19:C:3268:PGV:H231 | 1.83 | 0.41 |
| 22:P:4270:CDL:H561 | 22:P:4270:CDL:H532 | 1.83 | 0.41 |
| 18:N:4521:TGL:H101 | 18:N:4521:TGL:C28 | 2.50 | 0.41 |
| 2:O:13:THR:HB | 2:O:168:LEU:HD23 | 2.03 | 0.41 |
| 1:N:177:SER:H | 1:N:180:GLN:NE2 | 2.19 | 0.41 |
| 2:B:2:ALA:HA | 2:B:6:GLN:OE1 | 2.21 | 0.41 |
| 2:B:121:TYR:O | 2:B:138:VAL:HA | 2.21 | 0.41 |
| 3:P:214:PHE:CD1 | 19:P:4267:PGV:H71 | 2.55 | 0.41 |
| 3:P:51:MET:SD | 22:P:4270:CDL:H622 | 2.61 | 0.41 |
| 18:N:4522:TGL:CC6 | 18:N:4522:TGL:HC22 | 2.51 | 0.41 |
| 1:A:426:PHE:HB3 | 1:A:427:PRO:HD3 | 2.03 | 0.41 |
| 25:O:4230:PSC:H042 | 25:O:4230:PSC:H062 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:P:4265:PEK:H383 | 22:T:4269:CDL:H272 | 2.03 | 0.41 |
| 22:G:3269:CDL:H601 | 22:G:3269:CDL:H571 | 1.71 | 0.41 |
| 7:T:17:ARG:HD3 | 28:T:1289:HOH:O | 2.21 | 0.41 |
| 1:A:35:LEU:HA | 1:A:35:LEU:HD23 | 1.95 | 0.41 |
| 3:C:154:GLY:HA2 | 6:F:6:VAL:HB | 2.03 | 0.41 |
| 1:N:172:LYS:HD2 | 1:N:181:THR:CG2 | 2.50 | 0.41 |
| 9:V:73:LYS:HE3 | 9:V:73:LYS:HB3 | 1.86 | 0.41 |
| 1:N:76:GLY:O | 1:N:80:ASN:HB2 | 2.21 | 0.41 |
| 21:B:4085:CHD:H12 | 21:B:4085:CHD:H212 | 2.03 | 0.41 |
| 8:U:64:CYS:HA | 8:U:65:PRO:HD3 | 1.98 | 0.41 |
| 25:O:4230:PSC:C02 | 25:O:4230:PSC:H212 | 2.51 | 0.41 |
| 3:P:40:MET:O | 3:P:44:MET:HG2 | 2.21 | 0.41 |
| 13:Z:42:LYS:HE3 | 13:Z:43:SER:N | 2.36 | 0.41 |
| 9:I:35:TYR:C | 9:I:37:PHE:H | 2.25 | 0.41 |
| 4:Q:51:LEU:HD21 | 4:Q:59:LEU:CD1 | 2.51 | 0.41 |
| 23:P:4264:PEK:C16 | 23:P:4264:PEK:H102 | 2.43 | 0.40 |
| 6:F:51:SER:O | 6:F:94:HIS:N | 2.54 | 0.40 |
| 25:O:4230:PSC:H343 | 25:O:4230:PSC:C13 | 2.51 | 0.40 |
| 8:U:50:VAL:HG12 | 8:U:50:VAL:O | 2.21 | 0.40 |
| 4:D:48:TRP:CH2 | 5:E:56:ARG:HA | 2.56 | 0.40 |
| 22:P:4270:CDL:H641 | 22:P:4270:CDL:H231 | 2.02 | 0.40 |
| 7:T:8:HIS:CD2 | 23:T:3263:PEK:H231 | 2.55 | 0.40 |
| 1:A:113:LEU:CD1 | 18:L:3522:TGL:H292 | 2.51 | 0.40 |
| 7:T:31:CYS:SG | 22:T:4269:CDL:H532 | 2.61 | 0.40 |
| 8:H:36:PHE:CD1 | 8:H:57:ARG:HB2 | 2.56 | 0.40 |
| 13:M:37:LEU:HA | 13:M:37:LEU:HD23 | 1.85 | 0.40 |
| 7:T:25:LEU:HD23 | 7:T:25:LEU:HA | 1.89 | 0.40 |
| 2:O:68:LEU:HB3 | 2:O:69:PRO:HD3 | 2.04 | 0.40 |
| 1:N:40:GLU:HG2 | 1:N:54:TYR:CD2 | 2.57 | 0.40 |
| 17:A:515:HEA:HMB1 | 17:A:515:HEA:H11 | 1.98 | 0.40 |
| 1:A:513:LEU:HA | 1:A:513:LEU:HD22 | 1.81 | 0.40 |
| 1:N:71:MET:HE1 | 1:N:195:LEU:HD21 | 2.04 | 0.40 |
| 1:N:298:ASP:HB3 | 28:N:1369:HOH:O | 2.21 | 0.40 |
| 2:B:16:ILE:HA | 2:B:16:ILE:HD13 | 1.84 | 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 | 512/514 (100%) | 496 (97%) | 16 (3%) | 0 | 100 | 100 |
| 1 | N | 512/514 (100%) | 500 (98%) | 12 (2%) | 0 | 100 | 100 |
| 2 | B | 225/227 (99%) | 208 (92%) | 14 (6%) | 3 (1%) | 15 | 4 |
| 2 | O | 225/227 (99%) | 206 (92%) | 16 (7%) | 3 (1%) | 15 | 4 |
| 3 | C | 257/261 (98%) | 252 (98%) | 5 (2%) | 0 | 100 | 100 |
| 3 | P | 257/261 (98%) | 252 (98%) | 5 (2%) | 0 | 100 | 100 |
| 4 | D | 142/147 (97%) | 138 (97%) | 4 (3%) | 0 | 100 | 100 |
| 4 | Q | 142/147 (97%) | 138 (97%) | 4 (3%) | 0 | 100 | 100 |
| 5 | E | 103/109 (94%) | 103 (100%) | 0 | 0 | 100 | 100 |
| 5 | R | 103/109 (94%) | 102 (99%) | 1 (1%) | 0 | 100 | 100 |
| 6 | F | 96/98 (98%) | 89 (93%) | 4 (4%) | 3 (3%) | 5 | 0 |
| 6 | S | 96/98 (98%) | 89 (93%) | 4 (4%) | 3 (3%) | 5 | 0 |
| 7 | G | 81/85 (95%) | 68 (84%) | 6 (7%) | 7 (9%) | 1 | 0 |
| 7 | T | 81/85 (95%) | 65 (80%) | 9 (11%) | 7 (9%) | 1 | 0 |
| 8 | H | 77/85 (91%) | 70 (91%) | 5 (6%) | 2 (3%) | 7 | 1 |
| 8 | U | 77/85 (91%) | 70 (91%) | 5 (6%) | 2 (3%) | 7 | 1 |
| 9 | I | 71/73 (97%) | 67 (94%) | 4 (6%) | 0 | 100 | 100 |
| 9 | V | 71/73 (97%) | 67 (94%) | 4 (6%) | 0 | 100 | 100 |
| 10 | J | 56/59 (95%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 10 | W | 56/59 (95%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 11 | K | 47/56 (84%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 11 | X | 47/56 (84%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 12 | L | 44/47 (94%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 12 | Y | 44/47 (94%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 13 | M | 41/46 (89%) | 41 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 13 | Z | 41/46 (89%) | 41 (100%) | 0 | 0 | 100 | 100 |
| All | All | 3504/3614 (97%) | 3350 (96%) | 124 (4%) | 30 (1%) | 21 | 7 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 95 | GLN |
| 7 | G | 4 | ALA |
| 7 | G | 7 | ASP |
| 7 | G | 8 | HIS |
| 7 | G | 39 | SER |
| 6 | S | 94 | HIS |
| 6 | S | 95 | GLN |
| 7 | T | 4 | ALA |
| 7 | T | 7 | ASP |
| 7 | T | 8 | HIS |
| 7 | T | 39 | SER |
| 2 | B | 60 | GLU |
| 6 | F | 94 | HIS |
| 7 | G | 3 | ALA |
| 7 | G | 40 | GLY |
| 8 | H | 8 | ILE |
| 2 | O | 104 | TRP |
| 7 | T | 3 | ALA |
| 8 | U | 8 | ILE |
| 2 | B | 104 | TRP |
| 2 | O | 60 | GLU |
| 7 | T | 40 | GLY |
| 6 | F | 96 | LEU |
| 8 | H | 46 | LYS |
| 6 | S | 96 | LEU |
| 7 | G | 6 | GLY |
| 7 | T | 6 | GLY |
| 8 | U | 46 | LYS |
| 2 | O | 92 | ASN |
| 2 | B | 92 | ASN |

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 | 426/426 (100%) | 418 (98%) | 8 (2%) | 65 | 52 |
| 1 | N | 426/426 (100%) | 415 (97%) | 11 (3%) | 54 | 37 |
| 2 | B | 210/210 (100%) | 200 (95%) | 10 (5%) | 31 | 14 |
| 2 | O | 210/210 (100%) | 197 (94%) | 13 (6%) | 23 | 8 |
| 3 | C | 224/226 (99%) | 220 (98%) | 4 (2%) | 66 | 54 |
| 3 | P | 224/226 (99%) | 219 (98%) | 5 (2%) | 60 | 45 |
| 4 | D | 128/129 (99%) | 126 (98%) | 2 (2%) | 70 | 59 |
| 4 | Q | 128/129 (99%) | 126 (98%) | 2 (2%) | 70 | 59 |
| 5 | E | 92/95 (97%) | 90 (98%) | 2 (2%) | 60 | 45 |
| 5 | R | 92/95 (97%) | 88 (96%) | 4 (4%) | 35 | 17 |
| 6 | F | 81/81 (100%) | 79 (98%) | 2 (2%) | 55 | 39 |
| 6 | S | 81/81 (100%) | 77 (95%) | 4 (5%) | 31 | 13 |
| 7 | G | 67/68 (98%) | 61 (91%) | 6 (9%) | 12 | 3 |
| 7 | T | 67/68 (98%) | 62 (92%) | 5 (8%) | 17 | 5 |
| 8 | H | 71/75 (95%) | 69 (97%) | 2 (3%) | 51 | 35 |
| 8 | U | 71/75 (95%) | 67 (94%) | 4 (6%) | 26 | 10 |
| 9 | I | 57/57 (100%) | 53 (93%) | 4 (7%) | 19 | 6 |
| 9 | V | 57/57 (100%) | 55 (96%) | 2 (4%) | 43 | 25 |
| 10 | J | 49/50 (98%) | 48 (98%) | 1 (2%) | 63 | 49 |
| 10 | W | 49/50 (98%) | 48 (98%) | 1 (2%) | 63 | 49 |
| 11 | K | 39/46 (85%) | 39 (100%) | 0 | 100 | 100 |
| 11 | X | 39/46 (85%) | 38 (97%) | 1 (3%) | 54 | 37 |
| 12 | L | 39/40 (98%) | 39 (100%) | 0 | 100 | 100 |
| 12 | Y | 39/40 (98%) | 37 (95%) | 2 (5%) | 29 | 12 |
| 13 | M | 37/38 (97%) | 32 (86%) | 5 (14%) | 5 | 1 |
| 13 | Z | 37/38 (97%) | 33 (89%) | 4 (11%) | 8 | 2 |
| All | All | 3040/3082 (99%) | 2936 (97%) | 104 (3%) | 44 | 26 |

All (104) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 38 | ARG |
| 1 | A | 109 | PHE |
| 1 | A | 138 | HIS |
| 1 | A | 180 | GLN |
| 1 | A | 238 | PHE |
| 1 | A | 338 | MET |
| 1 | A | 369 | ASP |
| 1 | A | 513 | LEU |
| 2 | B | 33 | LEU |
| 2 | B | 60 | GLU |
| 2 | B | 66 | THR |
| 2 | B | 75 | LEU |
| 2 | B | 78 | LEU |
| 2 | B | 91 | ASN |
| 2 | B | 104 | TRP |
| 2 | B | 115 | ASP |
| 2 | B | 167 | SER |
| 2 | B | 171 | LYS |
| 3 | C | 159 | MET |
| 3 | C | 179 | SER |
| 3 | C | 214 | PHE |
| 3 | C | 230 | ASN |
| 4 | D | 4 | SER |
| 4 | D | 51 | LEU |
| 5 | E | 70 | VAL |
| 5 | E | 90 | ARG |
| 6 | F | 48 | LEU |
| 6 | F | 87 | THR |
| 7 | G | 17 | ARG |
| 7 | G | 18 | PHE |
| 7 | G | 36 | TRP |
| 7 | G | 42 | ARG |
| 7 | G | 54 | ARG |
| 7 | G | 84 | LYS |
| 8 | H | 29 | CYS |
| 8 | H | 60 | TYR |
| 9 | I | 8 | GLN |
| 9 | I | 15 | ARG |
| 9 | I | 37 | PHE |
| 9 | I | 61 | GLU |
| 10 | J | 50 | LEU |
| 13 | M | 13 | LYS |
| 13 | M | 34 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | M | 38 | ASP |
| 13 | M | 39 | ASN |
| 13 | M | 42 | LYS |
| 1 | N | 38 | ARG |
| 1 | N | 109 | PHE |
| 1 | N | 115 | SER |
| 1 | N | 138 | HIS |
| 1 | N | 180 | GLN |
| 1 | N | 238 | PHE |
| 1 | N | 241 | PRO |
| 1 | N | 338 | MET |
| 1 | N | 369 | ASP |
| 1 | N | 484 | THR |
| 1 | N | 513 | LEU |
| 2 | O | 16 | ILE |
| 2 | O | 33 | LEU |
| 2 | O | 60 | GLU |
| 2 | O | 66 | THR |
| 2 | O | 68 | LEU |
| 2 | O | 75 | LEU |
| 2 | O | 78 | LEU |
| 2 | O | 91 | ASN |
| 2 | O | 94 | SER |
| 2 | O | 104 | TRP |
| 2 | O | 115 | ASP |
| 2 | O | 148 | MET |
| 2 | O | 217 | LYS |
| 3 | P | 29 | SER |
| 3 | P | 33 | MET |
| 3 | P | 159 | MET |
| 3 | P | 214 | PHE |
| 3 | P | 230 | ASN |
| 4 | Q | 8 | SER |
| 4 | Q | 121 | LYS |
| 5 | R | 5 | HIS |
| 5 | R | 70 | VAL |
| 5 | R | 80 | GLU |
| 5 | R | 90 | ARG |
| 6 | S | 48 | LEU |
| 6 | S | 53 | THR |
| 6 | S | 54 | ASN |
| 6 | S | 80 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | T | 18 | PHE |
| 7 | T | 38 | HIS |
| 7 | T | 42 | ARG |
| 7 | T | 43 | GLU |
| 7 | T | 54 | ARG |
| 8 | U | 9 | LYS |
| 8 | U | 21 | PRO |
| 8 | U | 29 | CYS |
| 8 | U | 60 | TYR |
| 9 | V | 8 | GLN |
| 9 | V | 29 | LEU |
| 10 | W | 50 | LEU |
| 11 | X | 54 | ARG |
| 12 | Y | 20 | ARG |
| 12 | Y | 26 | THR |
| 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 (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 80 | ASN |
| 1 | A | 98 | ASN |
| 1 | A | 151 | HIS |
| 1 | A | 178 | GLN |
| 1 | A | 180 | GLN |
| 1 | A | 512 | ASN |
| 2 | B | 10 | GLN |
| 2 | B | 181 | GLN |
| 3 | C | 3 | HIS |
| 3 | C | 50 | ASN |
| 3 | C | 68 | GLN |
| 4 | D | 37 | GLN |
| 4 | D | 109 | HIS |
| 5 | E | 94 | ASN |
| 7 | G | 8 | HIS |
| 7 | G | 34 | ASN |
| 9 | I | 8 | GLN |
| 11 | K | 35 | GLN |
| 1 | N | 80 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 98 | ASN |
| 1 | N | 178 | GLN |
| 1 | N | 180 | GLN |
| 1 | N | 512 | ASN |
| 2 | O | 91 | ASN |
| 2 | O | 181 | GLN |
| 2 | O | 195 | GLN |
| 3 | P | 3 | HIS |
| 3 | P | 68 | GLN |
| 4 | Q | 37 | GLN |
| 4 | Q | 101 | HIS |
| 5 | R | 94 | ASN |
| 6 | S | 54 | ASN |
| 6 | S | 80 | GLN |
| 6 | S | 94 | HIS |
| 9 | V | 8 | GLN |
| 10 | W | 57 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 1 | FME | A | 1 | 1 | 8,9,10 | 0.58 | 0 | 6,9,11 | 1.31 | 2 (33%) |
| 2 | FME | B | 1 | 2 | 8,9,10 | 0.80 | 0 | 6,9,11 | 2.08 | 1 (16%) |
| 7 | TPO | G | 11 | 7 | 8,10,11 | 1.39 | 1 (12%) | 7,14,16 | 1.01 | 0 |
| 9 | SAC | I | 1 | 9 | 7,8,9 | 2.56 | 2 (28%) | 7,9,11 | 2.07 | 2 (28%) |
| 1 | FME | N | 1 | 1 | 8,9,10 | 0.72 | 0 | 6,9,11 | 2.01 | 2 (33%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FME | O | 1 | 2 | 8,9,10 | 0.59 | 0 | 6,9,11 | 1.41 | 1 (16%) |
| 7 | TPO | T | 11 | 7 | 8,10,11 | 1.37 | 1 (12%) | 7,14,16 | 1.03 | 1 (14%) |
| 9 | SAC | V | 1 | 9 | 7,8,9 | 2.65 | 2 (28%) | 7,9,11 | 2.18 | 4 (57%) |

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 | - | 0/6/8/10 | 0/0/0/0 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 7 | G | 11 | TPO | CB-CA | 2.80 | 1.59 | 1.54 |
| 7 | T | 11 | TPO | CB-CA | 3.15 | 1.59 | 1.54 |
| 9 | I | 1 | SAC | CA-N | 4.26 | 1.52 | 1.46 |
| 9 | V | 1 | SAC | CA-N | 4.36 | 1.52 | 1.46 |
| 9 | I | 1 | SAC | OAC-C1A | 5.02 | 1.34 | 1.23 |
| 9 | V | 1 | SAC | OAC-C1A | 5.10 | 1.35 | 1.23 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | B | 1 | FME | CA-N-CN | -4.79 | 115.46 | 122.82 |
| 1 | N | 1 | FME | CA-N-CN | -4.24 | 116.30 | 122.82 |
| 9 | V | 1 | SAC | CA-N-C1A | -3.28 | 110.25 | 121.37 |
| 2 | O | 1 | FME | CA-N-CN | -2.96 | 118.27 | 122.82 |
| 9 | I | 1 | SAC | CA-N-C1A | -2.58 | 112.62 | 121.37 |
| 1 | N | 1 | FME | O-C-CA | -2.31 | 119.35 | 125.44 |
| 9 | V | 1 | SAC | OAC-C1A-C2A | -2.21 | 118.00 | 122.06 |
| 1 | A | 1 | FME | CA-N-CN | -2.17 | 119.48 | 122.82 |
| 7 | T | 11 | TPO | O-C-CA | -2.07 | 119.98 | 125.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 1 | FME | O-C-CA | -2.04 | 120.05 | 125.44 |
| 9 | V | 1 | SAC | C2A-C1A-N | 2.54 | 120.97 | 116.11 |
| 9 | V | 1 | SAC | CB-CA-N | 2.63 | 116.36 | 110.60 |
| 9 | I | 1 | SAC | CB-CA-N | 3.79 | 118.90 | 110.60 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 1 | N | 1 | FME | O1-CN-N-CA |
| 1 | A | 1 | FME | O1-CN-N-CA |
| 2 | B | 1 | FME | O1-CN-N-CA |
| 2 | O | 1 | FME | O1-CN-N-CA |

There are no ring outliers.

5 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 1 | FME | 3 | 0 |
| 7 | G | 11 | TPO | 1 | 0 |
| 1 | N | 1 | FME | 1 | 0 |
| 2 | O | 1 | FME | 2 | 0 |
| 7 | T | 11 | TPO | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 42 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 |
| 19 | PGV | A | 3266 | - | 50,50,50 | 0.91 | 1 (2%) | 51,56,56 | 0.81 | 2 (3%) |
| 18 | TGL | A | 3521 | - | 62,62,62 | 0.96 | 4 (6%) | 65,65,65 | 1.13 | 7 (10%) |
| 19 | PGV | A | 3524 | - | 50,50,50 | 1.09 | 4 (8%) | 51,56,56 | 1.08 | 6 (11%) |
| 17 | HEA | A | 515 | 1 | 40,67,67 | 1.44 | 6 (15%) | 41,103,103 | 1.71 | 11 (26%) |
| 17 | HEA | A | 516 | 1 | 40,67,67 | 1.51 | 6 (15%) | 41,103,103 | 1.42 | 6 (14%) |
| 20 | CUA | B | 228 | 2 | 0,1,1 | 0.00 | - | 0,0,0 | 0.00 | - |
| 21 | CHD | B | 4085 | - | 29,32,32 | 0.70 | 0 | 48,51,51 | 1.85 | 14 (29%) |
| 23 | PEK | C | 3264 | - | 51,52,52 | 1.49 | 4 (7%) | 52,57,57 | 1.34 | 7 (13%) |
| 23 | PEK | C | 3265 | - | 51,52,52 | 1.67 | 10 (19%) | 52,57,57 | 1.05 | 4 (7%) |
| 19 | PGV | C | 3267 | - | 50,50,50 | 0.81 | 1 (2%) | 51,56,56 | 0.96 | 4 (7%) |
| 19 | PGV | C | 3268 | - | 50,50,50 | 1.11 | 4 (8%) | 51,56,56 | 0.60 | 0 |
| 22 | CDL | C | 3270 | - | 99,99,99 | 0.78 | 3 (3%) | 101,111,111 | 0.91 | 5 (4%) |
| 21 | CHD | C | 3271 | - | 29,32,32 | 0.76 | 1 (3%) | 48,51,51 | 3.62 | 21 (43%) |
| 21 | CHD | C | 3525 | - | 29,32,32 | 0.77 | 0 | 48,51,51 | 1.59 | 10 (20%) |
| 18 | TGL | D | 3523 | - | 62,62,62 | 1.13 | 3 (4%) | 65,65,65 | 1.12 | 7 (10%) |
| 25 | PSC | E | 3230 | - | 51,51,51 | 1.24 | 4 (7%) | 55,59,59 | 1.10 | 4 (7%) |
| 22 | CDL | G | 3269 | - | 99,99,99 | 0.96 | 5 (5%) | 101,111,111 | 0.92 | 8 (7%) |
| 23 | PEK | G | 4263 | - | 51,52,52 | 1.71 | 9 (17%) | 52,57,57 | 0.95 | 2 (3%) |
| 21 | CHD | J | 3060 | - | 29,32,32 | 0.83 | 1 (3%) | 48,51,51 | 3.27 | 24 (50%) |
| 18 | TGL | L | 3522 | - | 62,62,62 | 1.35 | 7 (11%) | 65,65,65 | 1.23 | 4 (6%) |
| 27 | DMU | M | 3526 | - | 34,34,34 | 3.21 | 8 (23%) | 45,45,45 | 4.41 | 20 (44%) |
| 19 | PGV | N | 4266 | - | 50,50,50 | 1.03 | 3 (6%) | 51,56,56 | 1.12 | 4 (7%) |
| 18 | TGL | N | 4521 | - | 62,62,62 | 0.97 | 4 (6%) | 65,65,65 | 1.10 | 4 (6%) |
| 18 | TGL | N | 4522 | - | 62,62,62 | 1.38 | 7 (11%) | 65,65,65 | 1.14 | 5 (7%) |
| 19 | PGV | N | 4524 | - | 50,50,50 | 1.09 | 4 (8%) | 51,56,56 | 1.02 | 6 (11%) |
| 17 | HEA | N | 515 | 1 | 40,67,67 | 1.38 | 6 (15%) | 41,103,103 | 1.71 | 12 (29%) |
| 17 | HEA | N | 516 | 1 | 40,67,67 | 1.44 | 5 (12%) | 41,103,103 | 1.40 | 7 (17%) |
| 20 | CUA | O | 228 | 2 | 0,1,1 | 0.00 | - | 0,0,0 | 0.00 | - |
| 21 | CHD | O | 3085 | - | 29,32,32 | 0.73 | 0 | 48,51,51 | 1.87 | 17 (35%) |
| 25 | PSC | O | 4230 | - | 51,51,51 | 1.20 | 3 (5%) | 55,59,59 | 1.11 | 3 (5%) |
| 23 | PEK | P | 4264 | - | 51,52,52 | 1.49 | 5 (9%) | 52,57,57 | 1.44 | 12 (23%) |
| 23 | PEK | P | 4265 | - | 51,52,52 | 1.71 | 12 (23%) | 52,57,57 | 1.03 | 4 (7%) |
| 19 | PGV | P | 4267 | - | 50,50,50 | 0.99 | 2 (4%) | 51,56,56 | 1.11 | 5 (9%) |
| 19 | PGV | P | 4268 | - | 50,50,50 | 1.11 | 4 (8%) | 51,56,56 | 0.63 | 0 |
| 22 | CDL | P | 4270 | - | 99,99,99 | 0.81 | 3 (3%) | 101,111,111 | 0.89 | 4 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 21 | CHD | P | 4271 | - | 29,32,32 | 0.73 | 0 | 48,51,51 | 3.56 | 22 (45%) |
| 21 | CHD | P | 4525 | - | 29,32,32 | 0.81 | 1 (3%) | 48,51,51 | 1.63 | 9 (18%) |
| 18 | TGL | Q | 4523 | - | 62,62,62 | 1.11 | 3 (4%) | 65,65,65 | 1.06 | 5 (7%) |
| 23 | PEK | T | 3263 | - | 51,52,52 | 1.71 | 10 (19%) | 52,57,57 | 0.92 | 2 (3%) |
| 22 | CDL | T | 4269 | - | 99,99,99 | 0.92 | 4 (4%) | 101,111,111 | 0.93 | 7 (6%) |
| 21 | CHD | W | 4060 | - | 29,32,32 | 0.92 | 1 (3%) | 48,51,51 | 3.23 | 25 (52%) |
| 27 | DMU | Z | 4526 | - | 34,34,34 | 3.18 | 8 (23%) | 45,45,45 | 4.36 | 20 (44%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 19 | PGV | A | 3266 | - | - | 0/55/55/55 | 0/0/0/0 |
| 18 | TGL | A | 3521 | - | - | 0/65/65/65 | 0/0/0/0 |
| 19 | PGV | A | 3524 | - | - | 0/55/55/55 | 0/0/0/0 |
| 17 | HEA | A | 515 | 1 | 3/3/7/16 | 0/24/76/76 | 0/0/8/8 |
| 17 | HEA | A | 516 | 1 | 3/3/7/16 | 0/24/76/76 | 0/0/8/8 |
| 20 | CUA | B | 228 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 21 | CHD | B | 4085 | - | - | 0/7/74/74 | 0/4/4/4 |
| 23 | PEK | C | 3264 | - | - | 0/56/56/56 | 0/0/0/0 |
| 23 | PEK | C | 3265 | - | - | 0/56/56/56 | 0/0/0/0 |
| 19 | PGV | C | 3267 | - | - | 0/55/55/55 | 0/0/0/0 |
| 19 | PGV | C | 3268 | - | - | 0/55/55/55 | 0/0/0/0 |
| 22 | CDL | C | 3270 | - | - | 0/110/110/110 | 0/0/0/0 |
| 21 | CHD | C | 3271 | - | 5/5/12/12 | 0/7/74/74 | 0/4/4/4 |
| 21 | CHD | C | 3525 | - | - | 0/7/74/74 | 0/4/4/4 |
| 18 | TGL | D | 3523 | - | - | 2/65/65/65 | 0/0/0/0 |
| 25 | PSC | E | 3230 | - | - | 0/55/55/55 | 0/0/0/0 |
| 22 | CDL | G | 3269 | - | - | 0/110/110/110 | 0/0/0/0 |
| 23 | PEK | G | 4263 | - | - | 0/56/56/56 | 0/0/0/0 |
| 21 | CHD | J | 3060 | - | 5/5/12/12 | 0/7/74/74 | 0/4/4/4 |
| 18 | TGL | L | 3522 | - | - | 0/65/65/65 | 0/0/0/0 |
| 27 | DMU | M | 3526 | - | 5/5/10/10 | 0/19/59/59 | 0/2/2/2 |
| 19 | PGV | N | 4266 | - | - | 0/55/55/55 | 0/0/0/0 |
| 18 | TGL | N | 4521 | - | - | 0/65/65/65 | 0/0/0/0 |
| 18 | TGL | N | 4522 | - | - | 0/65/65/65 | 0/0/0/0 |
| 19 | PGV | N | 4524 | - | - | 0/55/55/55 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 17 | HEA | N | 515 | 1 | 3/3/7/16 | 0/24/76/76 | 0/0/8/8 |
| 17 | HEA | N | 516 | 1 | 3/3/7/16 | 0/24/76/76 | 0/0/8/8 |
| 20 | CUA | O | 228 | 2 | - | 0/0/0/0 | 0/0/0/0 |
| 21 | CHD | O | 3085 | - | - | 0/7/74/74 | 0/4/4/4 |
| 25 | PSC | O | 4230 | - | - | 0/55/55/55 | 0/0/0/0 |
| 23 | PEK | P | 4264 | - | - | 0/56/56/56 | 0/0/0/0 |
| 23 | PEK | P | 4265 | - | - | 0/56/56/56 | 0/0/0/0 |
| 19 | PGV | P | 4267 | - | - | 0/55/55/55 | 0/0/0/0 |
| 19 | PGV | P | 4268 | - | - | 0/55/55/55 | 0/0/0/0 |
| 22 | CDL | P | 4270 | - | - | 0/110/110/110 | 0/0/0/0 |
| 21 | CHD | P | 4271 | - | 5/5/12/12 | 0/7/74/74 | 0/4/4/4 |
| 21 | CHD | P | 4525 | - | - | 0/7/74/74 | 0/4/4/4 |
| 18 | TGL | Q | 4523 | - | - | 1/65/65/65 | 0/0/0/0 |
| 23 | PEK | T | 3263 | - | - | 0/56/56/56 | 0/0/0/0 |
| 22 | CDL | T | 4269 | - | - | 0/110/110/110 | 0/0/0/0 |
| 21 | CHD | W | 4060 | - | 5/5/12/12 | 0/7/74/74 | 0/4/4/4 |
| 27 | DMU | Z | 4526 | - | 5/5/10/10 | 0/19/59/59 | 0/2/2/2 |

All (166) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 27 | M | 3526 | DMU | O7-C3 | -8.59 | 1.22 | 1.43 |
| 27 | Z | 4526 | DMU | O7-C3 | -8.39 | 1.22 | 1.43 |
| 27 | Z | 4526 | DMU | O16-C6 | -7.14 | 1.27 | 1.40 |
| 27 | M | 3526 | DMU | O1-C9 | -6.86 | 1.27 | 1.44 |
| 27 | Z | 4526 | DMU | O1-C9 | -6.79 | 1.27 | 1.44 |
| 27 | M | 3526 | DMU | O16-C6 | -6.73 | 1.28 | 1.40 |
| 27 | M | 3526 | DMU | O5-C4 | -6.56 | 1.27 | 1.44 |
| 27 | Z | 4526 | DMU | O7-C10 | -6.36 | 1.24 | 1.41 |
| 27 | M | 3526 | DMU | O7-C10 | -6.31 | 1.24 | 1.41 |
| 27 | M | 3526 | DMU | O16-C18 | -6.23 | 1.25 | 1.42 |
| 27 | Z | 4526 | DMU | O5-C4 | -6.19 | 1.28 | 1.44 |
| 27 | Z | 4526 | DMU | O1-C10 | -5.84 | 1.26 | 1.41 |
| 27 | Z | 4526 | DMU | O16-C18 | -5.82 | 1.26 | 1.42 |
| 27 | M | 3526 | DMU | O1-C10 | -5.60 | 1.27 | 1.41 |
| 27 | M | 3526 | DMU | O5-C6 | -4.55 | 1.30 | 1.41 |
| 27 | Z | 4526 | DMU | O5-C6 | -4.39 | 1.30 | 1.41 |
| 17 | A | 516 | HEA | C3C-C2C | -3.52 | 1.35 | 1.40 |
| 17 | A | 516 | HEA | C3A-C2A | -3.51 | 1.35 | 1.40 |
| 17 | N | 516 | HEA | C3A-CMA | -3.49 | 1.38 | 1.46 |
| 17 | N | 515 | HEA | C3A-C2A | -3.33 | 1.35 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 17 | N | 515 | HEA | C3A-CMA | -3.24 | 1.39 | 1.46 |
| 17 | A | 516 | HEA | C3A-CMA | -3.09 | 1.39 | 1.46 |
| 17 | A | 515 | HEA | C3A-CMA | -2.97 | 1.39 | 1.46 |
| 17 | N | 516 | HEA | C3A-C2A | -2.94 | 1.36 | 1.40 |
| 18 | N | 4521 | TGL | OG1-CG1 | -2.62 | 1.39 | 1.45 |
| 18 | A | 3521 | TGL | OG1-CG1 | -2.46 | 1.39 | 1.45 |
| 23 | P | 4264 | PEK | O03-C01 | -2.23 | 1.40 | 1.45 |
| 21 | C | 3271 | CHD | C10-C9 | -2.05 | 1.52 | 1.56 |
| 23 | G | 4263 | PEK | P-O11 | 2.04 | 1.68 | 1.59 |
| 22 | P | 4270 | CDL | OA8-CA7 | 2.07 | 1.39 | 1.33 |
| 22 | C | 3270 | CDL | OA8-CA7 | 2.08 | 1.39 | 1.33 |
| 23 | C | 3265 | PEK | O01-C1 | 2.09 | 1.40 | 1.34 |
| 25 | E | 3230 | PSC | C01-C02 | 2.10 | 1.56 | 1.50 |
| 18 | N | 4522 | TGL | CG3-CG2 | 2.10 | 1.56 | 1.50 |
| 19 | P | 4267 | PGV | O03-C19 | 2.10 | 1.39 | 1.33 |
| 21 | P | 4525 | CHD | C8-C9 | 2.10 | 1.58 | 1.53 |
| 23 | P | 4265 | PEK | C22-C21 | 2.14 | 1.57 | 1.50 |
| 19 | N | 4266 | PGV | O03-C19 | 2.16 | 1.39 | 1.33 |
| 18 | L | 3522 | TGL | CC2-CC1 | 2.16 | 1.57 | 1.50 |
| 23 | T | 3263 | PEK | C2-C1 | 2.17 | 1.57 | 1.50 |
| 19 | C | 3268 | PGV | C03-C02 | 2.18 | 1.56 | 1.50 |
| 19 | N | 4524 | PGV | C01-C02 | 2.18 | 1.56 | 1.50 |
| 25 | O | 4230 | PSC | C2-C1 | 2.20 | 1.57 | 1.50 |
| 19 | A | 3524 | PGV | C20-C19 | 2.21 | 1.57 | 1.50 |
| 23 | C | 3265 | PEK | P-O11 | 2.21 | 1.69 | 1.59 |
| 17 | A | 516 | HEA | C1A-NA | 2.22 | 1.39 | 1.36 |
| 23 | P | 4265 | PEK | P-O12 | 2.23 | 1.69 | 1.59 |
| 19 | P | 4268 | PGV | C03-C02 | 2.24 | 1.57 | 1.50 |
| 18 | L | 3522 | TGL | CG3-CG2 | 2.24 | 1.57 | 1.50 |
| 19 | A | 3524 | PGV | C01-C02 | 2.25 | 1.57 | 1.50 |
| 23 | T | 3263 | PEK | P-O11 | 2.27 | 1.69 | 1.59 |
| 23 | C | 3265 | PEK | C2-C1 | 2.28 | 1.57 | 1.50 |
| 17 | A | 515 | HEA | C3C-CAC | 2.29 | 1.52 | 1.47 |
| 19 | N | 4524 | PGV | C20-C19 | 2.30 | 1.57 | 1.50 |
| 22 | C | 3270 | CDL | CA3-CA4 | 2.31 | 1.57 | 1.50 |
| 22 | G | 3269 | CDL | CA6-CA4 | 2.31 | 1.57 | 1.50 |
| 23 | P | 4265 | PEK | O01-C1 | 2.32 | 1.41 | 1.34 |
| 22 | T | 4269 | CDL | C11-CA5 | 2.32 | 1.57 | 1.50 |
| 22 | T | 4269 | CDL | OA6-CA5 | 2.33 | 1.41 | 1.34 |
| 18 | N | 4522 | TGL | CC2-CC1 | 2.34 | 1.57 | 1.50 |
| 22 | P | 4270 | CDL | CA3-CA4 | 2.35 | 1.57 | 1.50 |
| 22 | G | 3269 | CDL | C11-CA5 | 2.36 | 1.57 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 19 | N | 4266 | PGV | C01-C02 | 2.36 | 1.57 | 1.50 |
| 18 | N | 4522 | TGL | CB2-CB1 | 2.36 | 1.57 | 1.50 |
| 18 | L | 3522 | TGL | OG3-CG3 | 2.37 | 1.50 | 1.45 |
| 23 | P | 4265 | PEK | P-O11 | 2.37 | 1.69 | 1.59 |
| 25 | E | 3230 | PSC | C2-C1 | 2.38 | 1.57 | 1.50 |
| 17 | A | 515 | HEA | C4A-NA | 2.43 | 1.40 | 1.36 |
| 18 | L | 3522 | TGL | OG2-CG2 | 2.45 | 1.52 | 1.46 |
| 19 | N | 4524 | PGV | P-O11 | 2.46 | 1.70 | 1.59 |
| 19 | A | 3524 | PGV | P-O11 | 2.46 | 1.70 | 1.59 |
| 23 | P | 4265 | PEK | C2-C1 | 2.46 | 1.58 | 1.50 |
| 17 | N | 515 | HEA | C1A-NA | 2.48 | 1.40 | 1.36 |
| 19 | C | 3268 | PGV | O01-C1 | 2.48 | 1.41 | 1.34 |
| 22 | C | 3270 | CDL | CA6-CA4 | 2.52 | 1.57 | 1.50 |
| 22 | T | 4269 | CDL | CB3-CB4 | 2.54 | 1.57 | 1.50 |
| 19 | P | 4268 | PGV | O01-C1 | 2.55 | 1.41 | 1.34 |
| 17 | A | 515 | HEA | C4B-NB | 2.56 | 1.40 | 1.36 |
| 18 | N | 4522 | TGL | OG3-CG3 | 2.57 | 1.50 | 1.45 |
| 23 | T | 3263 | PEK | C22-C21 | 2.60 | 1.58 | 1.50 |
| 22 | G | 3269 | CDL | CB3-CB4 | 2.63 | 1.58 | 1.50 |
| 23 | C | 3265 | PEK | C01-C02 | 2.65 | 1.58 | 1.50 |
| 23 | P | 4265 | PEK | C01-C02 | 2.69 | 1.58 | 1.50 |
| 17 | N | 515 | HEA | C4B-NB | 2.71 | 1.40 | 1.36 |
| 17 | N | 515 | HEA | C4A-NA | 2.71 | 1.40 | 1.36 |
| 21 | J | 3060 | CHD | C13-C17 | 2.72 | 1.60 | 1.55 |
| 19 | C | 3268 | PGV | C2-C1 | 2.75 | 1.58 | 1.50 |
| 23 | G | 4263 | PEK | C22-C21 | 2.75 | 1.58 | 1.50 |
| 18 | N | 4521 | TGL | OG3-CC1 | 2.80 | 1.41 | 1.33 |
| 22 | P | 4270 | CDL | CA6-CA4 | 2.81 | 1.58 | 1.50 |
| 23 | C | 3265 | PEK | O03-C21 | 2.82 | 1.41 | 1.33 |
| 19 | P | 4268 | PGV | C2-C1 | 2.85 | 1.59 | 1.50 |
| 18 | A | 3521 | TGL | OG3-CC1 | 2.85 | 1.41 | 1.33 |
| 17 | N | 516 | HEA | C4B-NB | 2.86 | 1.40 | 1.36 |
| 22 | G | 3269 | CDL | OA6-CA5 | 2.89 | 1.42 | 1.34 |
| 19 | C | 3267 | PGV | C12-C11 | 2.91 | 1.48 | 1.31 |
| 17 | A | 516 | HEA | C4B-NB | 2.96 | 1.40 | 1.36 |
| 17 | A | 515 | HEA | C1A-NA | 2.98 | 1.40 | 1.36 |
| 18 | N | 4521 | TGL | OG1-CA1 | 3.06 | 1.42 | 1.33 |
| 23 | P | 4265 | PEK | C03-C02 | 3.06 | 1.59 | 1.50 |
| 21 | W | 4060 | CHD | C13-C17 | 3.07 | 1.61 | 1.55 |
| 23 | T | 3263 | PEK | C01-C02 | 3.11 | 1.59 | 1.50 |
| 23 | G | 4263 | PEK | O03-C21 | 3.12 | 1.42 | 1.33 |
| 23 | C | 3265 | PEK | C03-C02 | 3.19 | 1.59 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 23 | P | 4265 | PEK | O03-C21 | 3.26 | 1.43 | 1.33 |
| 18 | A | 3521 | TGL | OG1-CA1 | 3.30 | 1.43 | 1.33 |
| 22 | G | 3269 | CDL | CB6-CB4 | 3.38 | 1.60 | 1.50 |
| 18 | D | 3523 | TGL | OG2-CB1 | 3.41 | 1.44 | 1.34 |
| 23 | G | 4263 | PEK | C01-C02 | 3.46 | 1.60 | 1.50 |
| 18 | A | 3521 | TGL | OG2-CB1 | 3.48 | 1.44 | 1.34 |
| 23 | T | 3263 | PEK | O03-C21 | 3.48 | 1.43 | 1.33 |
| 23 | T | 3263 | PEK | C03-C02 | 3.55 | 1.60 | 1.50 |
| 17 | N | 516 | HEA | C1D-ND | 3.59 | 1.41 | 1.36 |
| 22 | T | 4269 | CDL | CB6-CB4 | 3.60 | 1.60 | 1.50 |
| 19 | P | 4267 | PGV | C12-C11 | 3.66 | 1.52 | 1.31 |
| 17 | N | 515 | HEA | C1D-ND | 3.68 | 1.41 | 1.36 |
| 23 | G | 4263 | PEK | C03-C02 | 3.69 | 1.61 | 1.50 |
| 18 | Q | 4523 | TGL | OG3-CC1 | 3.75 | 1.44 | 1.33 |
| 17 | N | 516 | HEA | C4A-NA | 3.82 | 1.41 | 1.36 |
| 18 | N | 4521 | TGL | OG2-CB1 | 3.87 | 1.45 | 1.34 |
| 19 | N | 4266 | PGV | C12-C11 | 3.94 | 1.54 | 1.31 |
| 18 | L | 3522 | TGL | OG3-CC1 | 3.97 | 1.45 | 1.33 |
| 23 | P | 4265 | PEK | C15-C14 | 3.98 | 1.54 | 1.31 |
| 23 | P | 4264 | PEK | C6-C5 | 4.02 | 1.54 | 1.31 |
| 23 | C | 3265 | PEK | C15-C14 | 4.05 | 1.55 | 1.31 |
| 18 | Q | 4523 | TGL | OG2-CB1 | 4.06 | 1.46 | 1.34 |
| 19 | A | 3524 | PGV | C12-C11 | 4.07 | 1.55 | 1.31 |
| 23 | G | 4263 | PEK | C9-C8 | 4.07 | 1.55 | 1.31 |
| 23 | P | 4264 | PEK | C9-C8 | 4.09 | 1.55 | 1.31 |
| 19 | A | 3266 | PGV | C12-C11 | 4.09 | 1.55 | 1.31 |
| 23 | C | 3264 | PEK | C9-C8 | 4.11 | 1.55 | 1.31 |
| 19 | N | 4524 | PGV | C12-C11 | 4.11 | 1.55 | 1.31 |
| 25 | E | 3230 | PSC | C13-C12 | 4.13 | 1.55 | 1.31 |
| 23 | C | 3264 | PEK | C6-C5 | 4.13 | 1.55 | 1.31 |
| 23 | T | 3263 | PEK | C15-C14 | 4.17 | 1.55 | 1.31 |
| 23 | T | 3263 | PEK | C9-C8 | 4.18 | 1.55 | 1.31 |
| 23 | C | 3265 | PEK | C9-C8 | 4.19 | 1.55 | 1.31 |
| 17 | A | 516 | HEA | C1D-ND | 4.20 | 1.42 | 1.36 |
| 23 | P | 4265 | PEK | C9-C8 | 4.22 | 1.56 | 1.31 |
| 23 | G | 4263 | PEK | C15-C14 | 4.23 | 1.56 | 1.31 |
| 18 | D | 3523 | TGL | OG3-CC1 | 4.24 | 1.46 | 1.33 |
| 19 | C | 3268 | PGV | C12-C11 | 4.24 | 1.56 | 1.31 |
| 23 | P | 4265 | PEK | C6-C5 | 4.27 | 1.56 | 1.31 |
| 25 | E | 3230 | PSC | C10-C9 | 4.28 | 1.56 | 1.31 |
| 23 | C | 3265 | PEK | C12-C11 | 4.28 | 1.56 | 1.31 |
| 23 | G | 4263 | PEK | C6-C5 | 4.30 | 1.56 | 1.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 25 | O | 4230 | PSC | C13-C12 | 4.31 | 1.56 | 1.31 |
| 18 | N | 4522 | TGL | OG3-CC1 | 4.32 | 1.46 | 1.33 |
| 23 | P | 4265 | PEK | C12-C11 | 4.33 | 1.56 | 1.31 |
| 23 | C | 3265 | PEK | C6-C5 | 4.34 | 1.56 | 1.31 |
| 19 | P | 4268 | PGV | C12-C11 | 4.35 | 1.56 | 1.31 |
| 23 | T | 3263 | PEK | C6-C5 | 4.36 | 1.56 | 1.31 |
| 25 | O | 4230 | PSC | C10-C9 | 4.39 | 1.57 | 1.31 |
| 18 | Q | 4523 | TGL | OG1-CA1 | 4.39 | 1.46 | 1.33 |
| 23 | T | 3263 | PEK | C12-C11 | 4.47 | 1.57 | 1.31 |
| 18 | L | 3522 | TGL | OG1-CA1 | 4.53 | 1.47 | 1.33 |
| 23 | C | 3264 | PEK | C12-C11 | 4.55 | 1.58 | 1.31 |
| 23 | P | 4264 | PEK | C15-C14 | 4.59 | 1.58 | 1.31 |
| 23 | G | 4263 | PEK | C12-C11 | 4.67 | 1.58 | 1.31 |
| 23 | C | 3264 | PEK | C15-C14 | 4.68 | 1.58 | 1.31 |
| 17 | A | 515 | HEA | C1D-ND | 4.76 | 1.43 | 1.36 |
| 23 | P | 4264 | PEK | C12-C11 | 4.79 | 1.59 | 1.31 |
| 18 | D | 3523 | TGL | OG1-CA1 | 4.88 | 1.48 | 1.33 |
| 18 | N | 4522 | TGL | OG1-CA1 | 4.95 | 1.48 | 1.33 |
| 18 | N | 4522 | TGL | OG2-CB1 | 5.12 | 1.49 | 1.34 |
| 18 | L | 3522 | TGL | OG2-CB1 | 5.47 | 1.50 | 1.34 |

All (339) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 21 | C | 3271 | CHD | C17-C13-C12 | -10.29 | 108.56 | 117.68 |
| 21 | P | 4271 | CHD | C17-C13-C12 | -10.17 | 108.66 | 117.68 |
| 21 | C | 3271 | CHD | C19-C10-C9 | -7.79 | 99.50 | 111.18 |
| 27 | M | 3526 | DMU | C8-C7-C5 | -7.40 | 96.98 | 110.79 |
| 27 | Z | 4526 | DMU | C8-C7-C5 | -7.38 | 97.03 | 110.79 |
| 21 | P | 4271 | CHD | C19-C10-C9 | -7.10 | 100.53 | 111.18 |
| 19 | N | 4266 | PGV | C01-O03-C19 | -5.47 | 101.55 | 116.85 |
| 21 | W | 4060 | CHD | C15-C14-C8 | -5.36 | 110.54 | 118.32 |
| 21 | J | 3060 | CHD | C15-C14-C8 | -5.35 | 110.54 | 118.32 |
| 17 | A | 515 | HEA | CAD-C3D-C4D | -5.07 | 121.51 | 127.01 |
| 21 | J | 3060 | CHD | C18-C13-C14 | -4.97 | 103.38 | 111.22 |
| 21 | P | 4271 | CHD | C15-C14-C8 | -4.96 | 111.11 | 118.32 |
| 21 | C | 3271 | CHD | C15-C14-C8 | -4.96 | 111.12 | 118.32 |
| 21 | W | 4060 | CHD | C18-C13-C14 | -4.71 | 103.79 | 111.22 |
| 21 | C | 3271 | CHD | C19-C10-C1 | -4.63 | 100.41 | 108.20 |
| 21 | P | 4271 | CHD | C19-C10-C1 | -4.62 | 100.44 | 108.20 |
| 17 | N | 515 | HEA | CAD-C3D-C4D | -4.13 | 122.53 | 127.01 |
| 21 | J | 3060 | CHD | C17-C13-C12 | -4.07 | 114.07 | 117.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | B | 4085 | CHD | C16-C17-C13 | -3.94 | 99.68 | 103.60 |
| 17 | A | 516 | HEA | CAD-C3D-C4D | -3.82 | 122.86 | 127.01 |
| 17 | N | 515 | HEA | C27-C19-C18 | -3.81 | 116.02 | 123.50 |
| 21 | W | 4060 | CHD | C17-C13-C12 | -3.77 | 114.34 | 117.68 |
| 17 | A | 515 | HEA | C27-C19-C18 | -3.69 | 116.25 | 123.50 |
| 21 | B | 4085 | CHD | C15-C14-C13 | -3.68 | 99.93 | 103.60 |
| 21 | O | 3085 | CHD | C16-C17-C13 | -3.65 | 99.97 | 103.60 |
| 23 | C | 3264 | PEK | O03-C21-C22 | -3.65 | 100.78 | 111.90 |
| 21 | B | 4085 | CHD | O3-C3-C4 | -3.58 | 102.74 | 109.86 |
| 23 | C | 3264 | PEK | C30-C29-C28 | -3.58 | 96.05 | 114.53 |
| 19 | P | 4267 | PGV | C9-C10-C11 | -3.57 | 93.69 | 112.45 |
| 21 | B | 4085 | CHD | C15-C14-C8 | -3.57 | 113.14 | 118.32 |
| 21 | P | 4525 | CHD | C15-C14-C8 | -3.50 | 113.24 | 118.32 |
| 21 | O | 3085 | CHD | C15-C14-C8 | -3.49 | 113.26 | 118.32 |
| 25 | O | 4230 | PSC | C01-O03-C19 | -3.48 | 107.11 | 116.85 |
| 22 | P | 4270 | CDL | CB6-OB8-CB7 | -3.46 | 107.18 | 116.85 |
| 17 | N | 516 | HEA | CAD-C3D-C4D | -3.42 | 123.29 | 127.01 |
| 25 | E | 3230 | PSC | C01-O03-C19 | -3.42 | 107.30 | 116.85 |
| 21 | C | 3525 | CHD | C14-C13-C12 | -3.40 | 104.34 | 107.39 |
| 21 | B | 4085 | CHD | C14-C13-C12 | -3.35 | 104.39 | 107.39 |
| 23 | P | 4264 | PEK | C30-C29-C28 | -3.32 | 97.41 | 114.53 |
| 22 | C | 3270 | CDL | CB6-OB8-CB7 | -3.26 | 107.74 | 116.85 |
| 21 | J | 3060 | CHD | C19-C10-C9 | -3.26 | 106.29 | 111.18 |
| 23 | P | 4264 | PEK | O03-C21-C22 | -3.24 | 102.03 | 111.90 |
| 19 | A | 3266 | PGV | C01-O03-C19 | -3.17 | 107.98 | 116.85 |
| 21 | O | 3085 | CHD | C14-C13-C12 | -3.16 | 104.56 | 107.39 |
| 21 | C | 3525 | CHD | C15-C14-C8 | -3.11 | 113.80 | 118.32 |
| 17 | N | 515 | HEA | C17-C18-C19 | -3.05 | 121.14 | 127.76 |
| 21 | P | 4525 | CHD | C14-C8-C9 | -3.01 | 105.48 | 109.62 |
| 21 | O | 3085 | CHD | C15-C14-C13 | -2.98 | 100.63 | 103.60 |
| 27 | Z | 4526 | DMU | C2-C3-C4 | -2.95 | 104.18 | 110.84 |
| 19 | C | 3267 | PGV | C9-C10-C11 | -2.93 | 97.05 | 112.45 |
| 17 | A | 515 | HEA | C17-C18-C19 | -2.89 | 121.49 | 127.76 |
| 21 | W | 4060 | CHD | C19-C10-C9 | -2.88 | 106.86 | 111.18 |
| 22 | C | 3270 | CDL | OB6-CB5-C51 | -2.84 | 105.36 | 111.53 |
| 27 | M | 3526 | DMU | C2-C3-C4 | -2.83 | 104.45 | 110.84 |
| 17 | N | 515 | HEA | C26-C15-C14 | -2.82 | 117.96 | 123.50 |
| 23 | C | 3264 | PEK | C27-C26-C25 | -2.79 | 100.11 | 114.53 |
| 21 | O | 3085 | CHD | O3-C3-C4 | -2.77 | 104.35 | 109.86 |
| 21 | C | 3525 | CHD | C14-C8-C9 | -2.77 | 105.81 | 109.62 |
| 21 | C | 3271 | CHD | C18-C13-C14 | -2.70 | 106.95 | 111.22 |
| 19 | P | 4267 | PGV | C14-C13-C12 | -2.70 | 98.30 | 112.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | P | 4264 | PEK | C3-C2-C1 | -2.70 | 103.00 | 113.59 |
| 21 | B | 4085 | CHD | C19-C10-C1 | -2.65 | 103.74 | 108.20 |
| 19 | P | 4267 | PGV | O01-C1-C2 | -2.65 | 105.76 | 111.53 |
| 21 | B | 4085 | CHD | C14-C8-C9 | -2.65 | 105.98 | 109.62 |
| 23 | P | 4264 | PEK | C32-C31-C30 | -2.64 | 100.89 | 114.53 |
| 21 | O | 3085 | CHD | C14-C8-C9 | -2.64 | 105.99 | 109.62 |
| 23 | C | 3264 | PEK | C32-C31-C30 | -2.61 | 101.05 | 114.53 |
| 23 | P | 4264 | PEK | C34-C33-C32 | -2.55 | 101.36 | 114.53 |
| 19 | A | 3524 | PGV | C3-C2-C1 | -2.51 | 103.74 | 113.59 |
| 21 | O | 3085 | CHD | C19-C10-C1 | -2.47 | 104.05 | 108.20 |
| 17 | N | 515 | HEA | C13-C14-C15 | -2.45 | 122.44 | 127.76 |
| 17 | N | 515 | HEA | CMB-C2B-C1B | -2.43 | 124.35 | 128.36 |
| 17 | A | 515 | HEA | C13-C14-C15 | -2.42 | 122.49 | 127.76 |
| 18 | L | 3522 | TGL | OG3-CC1-OC1 | -2.42 | 117.25 | 123.49 |
| 23 | P | 4264 | PEK | C25-C24-C23 | -2.42 | 102.04 | 114.53 |
| 21 | W | 4060 | CHD | C19-C10-C5 | -2.41 | 106.00 | 110.25 |
| 21 | P | 4271 | CHD | C18-C13-C14 | -2.40 | 107.42 | 111.22 |
| 23 | C | 3264 | PEK | C25-C24-C23 | -2.38 | 102.25 | 114.53 |
| 17 | N | 516 | HEA | CMB-C2B-C1B | -2.38 | 124.43 | 128.36 |
| 23 | P | 4264 | PEK | C27-C26-C25 | -2.37 | 102.28 | 114.53 |
| 17 | A | 515 | HEA | C26-C15-C14 | -2.37 | 118.86 | 123.50 |
| 18 | N | 4521 | TGL | CG3-OG3-CC1 | -2.35 | 110.29 | 116.85 |
| 18 | N | 4522 | TGL | OG3-CC1-OC1 | -2.31 | 117.53 | 123.49 |
| 23 | C | 3264 | PEK | C3-C2-C1 | -2.30 | 104.54 | 113.59 |
| 19 | N | 4524 | PGV | C3-C2-C1 | -2.30 | 104.54 | 113.59 |
| 23 | P | 4264 | PEK | O03-C01-C02 | -2.28 | 102.56 | 108.69 |
| 23 | P | 4264 | PEK | C28-C27-C26 | -2.27 | 102.81 | 114.53 |
| 18 | N | 4521 | TGL | OG3-CC1-OC1 | -2.26 | 117.65 | 123.49 |
| 21 | C | 3525 | CHD | C19-C10-C9 | -2.25 | 107.80 | 111.18 |
| 18 | A | 3521 | TGL | OG3-CC1-OC1 | -2.25 | 117.69 | 123.49 |
| 18 | A | 3521 | TGL | CG3-OG3-CC1 | -2.25 | 110.56 | 116.85 |
| 17 | A | 515 | HEA | CMB-C2B-C1B | -2.23 | 124.67 | 128.36 |
| 22 | P | 4270 | CDL | OB6-CB5-C51 | -2.23 | 106.68 | 111.53 |
| 19 | A | 3524 | PGV | O01-C1-C2 | -2.23 | 106.69 | 111.53 |
| 19 | A | 3266 | PGV | O01-C1-C2 | -2.23 | 106.69 | 111.53 |
| 22 | C | 3270 | CDL | C52-C51-CB5 | -2.21 | 104.91 | 113.59 |
| 19 | N | 4524 | PGV | O01-C1-C2 | -2.20 | 106.74 | 111.53 |
| 17 | N | 516 | HEA | C20-C19-C18 | -2.19 | 116.89 | 121.05 |
| 21 | C | 3525 | CHD | O12-C12-C13 | -2.19 | 107.56 | 111.11 |
| 19 | C | 3267 | PGV | O01-C1-C2 | -2.19 | 106.76 | 111.53 |
| 21 | J | 3060 | CHD | C19-C10-C5 | -2.19 | 106.39 | 110.25 |
| 18 | D | 3523 | TGL | CG3-OG3-CC1 | -2.17 | 110.77 | 116.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17 | A | 515 | HEA | C21-C20-C19 | -2.15 | 105.70 | 112.71 |
| 21 | O | 3085 | CHD | C18-C13-C12 | -2.15 | 106.99 | 109.09 |
| 21 | C | 3525 | CHD | C16-C17-C13 | -2.14 | 101.47 | 103.60 |
| 22 | T | 4269 | CDL | OB8-CB7-C71 | -2.14 | 105.39 | 111.90 |
| 19 | N | 4266 | PGV | C3-C2-C1 | -2.13 | 105.22 | 113.59 |
| 19 | P | 4267 | PGV | C8-C9-C10 | -2.12 | 105.60 | 113.86 |
| 22 | P | 4270 | CDL | C52-C51-CB5 | -2.11 | 105.31 | 113.59 |
| 25 | E | 3230 | PSC | C14-C13-C12 | -2.10 | 110.71 | 125.34 |
| 19 | C | 3267 | PGV | C3-C2-C1 | -2.10 | 105.34 | 113.59 |
| 27 | Z | 4526 | DMU | C6-C1-C2 | -2.08 | 105.87 | 109.97 |
| 27 | M | 3526 | DMU | C6-C1-C2 | -2.08 | 105.87 | 109.97 |
| 19 | P | 4267 | PGV | C01-O03-C19 | -2.08 | 111.03 | 116.85 |
| 18 | Q | 4523 | TGL | CG3-OG3-CC1 | -2.08 | 111.04 | 116.85 |
| 17 | A | 516 | HEA | CMC-C2C-C1C | -2.08 | 124.93 | 128.36 |
| 18 | Q | 4523 | TGL | OG3-CC1-OC1 | -2.07 | 118.14 | 123.49 |
| 17 | N | 515 | HEA | C21-C20-C19 | -2.04 | 106.05 | 112.71 |
| 19 | C | 3267 | PGV | C8-C7-C6 | -2.04 | 104.00 | 114.53 |
| 22 | G | 3269 | CDL | OB8-CB7-C71 | -2.02 | 105.75 | 111.90 |
| 21 | O | 3085 | CHD | C13-C17-C20 | -2.01 | 117.06 | 119.50 |
| 18 | D | 3523 | TGL | OG1-CG1-CG2 | 2.00 | 114.08 | 108.69 |
| 19 | N | 4266 | PGV | O03-C01-C02 | 2.02 | 114.12 | 108.69 |
| 17 | A | 516 | HEA | C26-C15-C16 | 2.02 | 118.49 | 115.41 |
| 22 | G | 3269 | CDL | C79-C78-C77 | 2.02 | 124.98 | 114.53 |
| 19 | N | 4266 | PGV | C22-C21-C20 | 2.04 | 120.76 | 113.29 |
| 18 | N | 4521 | TGL | CB5-CB4-CB3 | 2.04 | 125.05 | 114.53 |
| 21 | P | 4271 | CHD | C11-C12-C13 | 2.04 | 113.28 | 111.20 |
| 21 | W | 4060 | CHD | C13-C14-C8 | 2.05 | 117.39 | 114.75 |
| 19 | N | 4524 | PGV | O01-C02-C01 | 2.05 | 115.58 | 108.36 |
| 19 | A | 3524 | PGV | O01-C02-C01 | 2.05 | 115.58 | 108.36 |
| 17 | N | 516 | HEA | C21-C20-C19 | 2.06 | 119.41 | 112.71 |
| 17 | N | 515 | HEA | CMD-C2D-C3D | 2.06 | 129.54 | 125.24 |
| 21 | O | 3085 | CHD | C18-C13-C14 | 2.06 | 114.47 | 111.22 |
| 21 | B | 4085 | CHD | C5-C6-C7 | 2.07 | 116.75 | 114.44 |
| 21 | P | 4271 | CHD | C1-C2-C3 | 2.07 | 113.79 | 110.43 |
| 21 | O | 3085 | CHD | C1-C10-C9 | 2.08 | 114.81 | 111.45 |
| 18 | A | 3521 | TGL | CB5-CB4-CB3 | 2.09 | 125.34 | 114.53 |
| 22 | P | 4270 | CDL | OA8-CA6-CA4 | 2.09 | 114.33 | 108.69 |
| 23 | P | 4264 | PEK | C8-C7-C6 | 2.10 | 118.98 | 112.00 |
| 18 | Q | 4523 | TGL | CB6-CB5-CB4 | 2.11 | 125.40 | 114.53 |
| 18 | D | 3523 | TGL | OG3-CC1-CC2 | 2.11 | 118.32 | 111.90 |
| 17 | A | 515 | HEA | CMC-C2C-C3C | 2.11 | 129.21 | 125.09 |
| 22 | T | 4269 | CDL | C80-C79-C78 | 2.12 | 125.45 | 114.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 22 | G | 3269 | CDL | C80-C79-C78 | 2.12 | 125.47 | 114.53 |
| 18 | D | 3523 | TGL | OG1-CA1-CA2 | 2.12 | 118.36 | 111.90 |
| 17 | A | 515 | HEA | CMD-C2D-C3D | 2.13 | 129.69 | 125.24 |
| 18 | A | 3521 | TGL | CC6-CC5-CC4 | 2.13 | 125.54 | 114.53 |
| 22 | C | 3270 | CDL | OB6-CB5-OB7 | 2.13 | 129.40 | 123.67 |
| 23 | P | 4265 | PEK | C14-C13-C12 | 2.15 | 119.14 | 112.00 |
| 18 | N | 4522 | TGL | OG1-CG1-CG2 | 2.15 | 114.48 | 108.69 |
| 21 | C | 3271 | CHD | C1-C2-C3 | 2.16 | 113.94 | 110.43 |
| 21 | P | 4525 | CHD | C1-C2-C3 | 2.16 | 113.94 | 110.43 |
| 22 | G | 3269 | CDL | C23-C22-C21 | 2.17 | 125.75 | 114.53 |
| 18 | D | 3523 | TGL | CB5-CB4-CB3 | 2.18 | 125.77 | 114.53 |
| 21 | J | 3060 | CHD | C4-C5-C10 | 2.18 | 115.06 | 112.66 |
| 21 | O | 3085 | CHD | C9-C11-C12 | 2.19 | 117.12 | 114.36 |
| 21 | B | 4085 | CHD | C17-C13-C14 | 2.19 | 102.27 | 100.05 |
| 18 | Q | 4523 | TGL | OG1-CA1-CA2 | 2.19 | 118.57 | 111.90 |
| 17 | A | 516 | HEA | C4B-C3B-C11 | 2.19 | 129.39 | 127.01 |
| 22 | G | 3269 | CDL | OB8-CB6-CB4 | 2.19 | 114.59 | 108.69 |
| 22 | T | 4269 | CDL | C20-C19-C18 | 2.19 | 125.86 | 114.53 |
| 17 | N | 516 | HEA | C4B-C3B-C11 | 2.20 | 129.39 | 127.01 |
| 21 | O | 3085 | CHD | C1-C2-C3 | 2.20 | 114.01 | 110.43 |
| 21 | P | 4525 | CHD | C17-C13-C12 | 2.21 | 119.64 | 117.68 |
| 21 | W | 4060 | CHD | C4-C5-C10 | 2.21 | 115.09 | 112.66 |
| 17 | N | 515 | HEA | C16-C15-C14 | 2.24 | 125.29 | 121.05 |
| 23 | P | 4264 | PEK | O03-C21-O04 | 2.24 | 129.27 | 123.49 |
| 23 | C | 3265 | PEK | C14-C13-C12 | 2.25 | 119.49 | 112.00 |
| 18 | A | 3521 | TGL | CB6-CB5-CB4 | 2.25 | 126.15 | 114.53 |
| 21 | B | 4085 | CHD | C9-C11-C12 | 2.26 | 117.22 | 114.36 |
| 21 | C | 3525 | CHD | C10-C9-C8 | 2.27 | 114.37 | 111.88 |
| 22 | T | 4269 | CDL | C23-C22-C21 | 2.28 | 126.30 | 114.53 |
| 22 | G | 3269 | CDL | C20-C19-C18 | 2.29 | 126.35 | 114.53 |
| 22 | C | 3270 | CDL | OA8-CA6-CA4 | 2.29 | 114.85 | 108.69 |
| 22 | T | 4269 | CDL | OB8-CB6-CB4 | 2.29 | 114.85 | 108.69 |
| 21 | J | 3060 | CHD | C14-C8-C7 | 2.29 | 114.92 | 111.74 |
| 17 | N | 515 | HEA | CMC-C2C-C3C | 2.32 | 129.62 | 125.09 |
| 27 | Z | 4526 | DMU | C10-O7-C3 | 2.32 | 124.06 | 118.01 |
| 21 | W | 4060 | CHD | C14-C8-C7 | 2.35 | 115.00 | 111.74 |
| 18 | D | 3523 | TGL | CB6-CB5-CB4 | 2.36 | 126.73 | 114.53 |
| 22 | T | 4269 | CDL | C22-C21-C20 | 2.38 | 126.82 | 114.53 |
| 23 | C | 3264 | PEK | O03-C21-O04 | 2.39 | 129.66 | 123.49 |
| 23 | G | 4263 | PEK | C03-C02-C01 | 2.39 | 117.67 | 112.07 |
| 21 | P | 4271 | CHD | C14-C8-C7 | 2.40 | 115.07 | 111.74 |
| 22 | G | 3269 | CDL | C22-C21-C20 | 2.41 | 126.99 | 114.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 18 | L | 3522 | TGL | OG1-CA1-CA2 | 2.42 | 119.27 | 111.90 |
| 21 | O | 3085 | CHD | C1-C10-C5 | 2.46 | 111.85 | 107.81 |
| 18 | A | 3521 | TGL | OG3-CC1-CC2 | 2.47 | 119.43 | 111.90 |
| 17 | A | 515 | HEA | C20-C19-C18 | 2.48 | 125.76 | 121.05 |
| 21 | C | 3525 | CHD | C1-C10-C5 | 2.49 | 111.89 | 107.81 |
| 18 | N | 4522 | TGL | OG1-CA1-CA2 | 2.49 | 119.48 | 111.90 |
| 19 | A | 3524 | PGV | O01-C02-C03 | 2.50 | 117.18 | 108.36 |
| 21 | W | 4060 | CHD | C1-C2-C3 | 2.52 | 114.52 | 110.43 |
| 21 | C | 3271 | CHD | C14-C8-C7 | 2.53 | 115.25 | 111.74 |
| 23 | P | 4264 | PEK | C11-C10-C9 | 2.53 | 120.43 | 112.00 |
| 21 | J | 3060 | CHD | C1-C2-C3 | 2.53 | 114.55 | 110.43 |
| 23 | P | 4265 | PEK | O03-C01-C02 | 2.54 | 115.51 | 108.69 |
| 21 | P | 4271 | CHD | C16-C15-C14 | 2.54 | 110.24 | 105.12 |
| 23 | T | 3263 | PEK | C03-C02-C01 | 2.54 | 118.02 | 112.07 |
| 19 | N | 4524 | PGV | O01-C02-C03 | 2.54 | 117.33 | 108.36 |
| 21 | C | 3525 | CHD | C5-C6-C7 | 2.55 | 117.28 | 114.44 |
| 21 | W | 4060 | CHD | C6-C5-C4 | 2.55 | 113.90 | 111.05 |
| 17 | A | 516 | HEA | CMC-C2C-C3C | 2.58 | 130.13 | 125.09 |
| 21 | P | 4271 | CHD | O12-C12-C13 | 2.58 | 115.30 | 111.11 |
| 21 | B | 4085 | CHD | C1-C10-C5 | 2.60 | 112.08 | 107.81 |
| 21 | P | 4525 | CHD | C6-C5-C10 | 2.61 | 115.54 | 112.66 |
| 17 | N | 516 | HEA | C3C-C4C-NC | 2.62 | 112.59 | 109.21 |
| 22 | G | 3269 | CDL | C19-C18-C17 | 2.63 | 128.12 | 114.53 |
| 21 | C | 3271 | CHD | C5-C6-C7 | 2.64 | 117.38 | 114.44 |
| 25 | E | 3230 | PSC | C15-C14-C13 | 2.64 | 126.31 | 112.45 |
| 23 | C | 3265 | PEK | O03-C01-C02 | 2.64 | 115.80 | 108.69 |
| 21 | B | 4085 | CHD | C5-C4-C3 | 2.65 | 116.85 | 112.91 |
| 22 | T | 4269 | CDL | C19-C18-C17 | 2.65 | 128.21 | 114.53 |
| 21 | C | 3271 | CHD | C15-C16-C17 | 2.66 | 110.47 | 105.12 |
| 21 | W | 4060 | CHD | C15-C16-C17 | 2.66 | 110.48 | 105.12 |
| 21 | C | 3271 | CHD | C16-C15-C14 | 2.67 | 110.50 | 105.12 |
| 21 | P | 4271 | CHD | C6-C5-C10 | 2.69 | 115.62 | 112.66 |
| 21 | C | 3271 | CHD | C6-C5-C10 | 2.71 | 115.64 | 112.66 |
| 21 | W | 4060 | CHD | C14-C13-C12 | 2.71 | 109.82 | 107.39 |
| 17 | N | 515 | HEA | C20-C19-C18 | 2.72 | 126.21 | 121.05 |
| 21 | P | 4525 | CHD | C9-C11-C12 | 2.72 | 117.80 | 114.36 |
| 21 | C | 3271 | CHD | O12-C12-C13 | 2.72 | 115.53 | 111.11 |
| 21 | B | 4085 | CHD | C1-C2-C3 | 2.73 | 114.86 | 110.43 |
| 23 | T | 3263 | PEK | O03-C01-C02 | 2.75 | 116.09 | 108.69 |
| 21 | C | 3271 | CHD | C5-C4-C3 | 2.75 | 117.01 | 112.91 |
| 21 | P | 4271 | CHD | C15-C16-C17 | 2.76 | 110.68 | 105.12 |
| 17 | A | 515 | HEA | C4B-C3B-C11 | 2.76 | 130.01 | 127.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 19 | N | 4524 | PGV | C03-C02-C01 | 2.77 | 118.54 | 112.07 |
| 21 | J | 3060 | CHD | C15-C16-C17 | 2.77 | 110.70 | 105.12 |
| 19 | A | 3524 | PGV | C03-C02-C01 | 2.77 | 118.55 | 112.07 |
| 25 | O | 4230 | PSC | C15-C14-C13 | 2.79 | 127.10 | 112.45 |
| 21 | P | 4525 | CHD | C1-C10-C5 | 2.81 | 112.42 | 107.81 |
| 21 | J | 3060 | CHD | C14-C13-C12 | 2.83 | 109.92 | 107.39 |
| 21 | P | 4271 | CHD | C1-C10-C9 | 2.83 | 116.01 | 111.45 |
| 21 | J | 3060 | CHD | C6-C5-C4 | 2.83 | 114.21 | 111.05 |
| 21 | B | 4085 | CHD | C10-C9-C8 | 2.88 | 115.05 | 111.88 |
| 21 | J | 3060 | CHD | C16-C15-C14 | 2.89 | 110.94 | 105.12 |
| 19 | N | 4524 | PGV | C02-O01-C1 | 2.92 | 124.89 | 117.89 |
| 21 | P | 4271 | CHD | C5-C4-C3 | 2.93 | 117.28 | 112.91 |
| 23 | G | 4263 | PEK | O03-C01-C02 | 2.94 | 116.61 | 108.69 |
| 23 | C | 3265 | PEK | C8-C7-C6 | 2.94 | 121.80 | 112.00 |
| 27 | M | 3526 | DMU | O7-C10-O1 | 2.98 | 118.22 | 110.68 |
| 21 | C | 3271 | CHD | C1-C10-C9 | 3.00 | 116.29 | 111.45 |
| 17 | N | 515 | HEA | C4B-C3B-C11 | 3.02 | 130.28 | 127.01 |
| 21 | W | 4060 | CHD | C16-C15-C14 | 3.02 | 111.20 | 105.12 |
| 27 | M | 3526 | DMU | C10-O7-C3 | 3.04 | 125.95 | 118.01 |
| 21 | P | 4525 | CHD | C5-C6-C7 | 3.05 | 117.84 | 114.44 |
| 23 | P | 4265 | PEK | C8-C7-C6 | 3.06 | 122.19 | 112.00 |
| 25 | O | 4230 | PSC | C16-C15-C14 | 3.09 | 125.93 | 113.86 |
| 21 | P | 4271 | CHD | C5-C6-C7 | 3.12 | 117.92 | 114.44 |
| 21 | J | 3060 | CHD | C5-C4-C3 | 3.18 | 117.64 | 112.91 |
| 23 | P | 4265 | PEK | C11-C10-C9 | 3.21 | 122.68 | 112.00 |
| 23 | C | 3265 | PEK | C11-C10-C9 | 3.26 | 122.86 | 112.00 |
| 21 | W | 4060 | CHD | C11-C9-C10 | 3.27 | 117.19 | 113.79 |
| 25 | E | 3230 | PSC | C16-C15-C14 | 3.28 | 126.67 | 113.86 |
| 27 | Z | 4526 | DMU | O7-C10-O1 | 3.33 | 119.11 | 110.68 |
| 21 | J | 3060 | CHD | C11-C9-C10 | 3.36 | 117.28 | 113.79 |
| 21 | W | 4060 | CHD | C5-C4-C3 | 3.37 | 117.93 | 112.91 |
| 17 | A | 516 | HEA | C27-C19-C20 | 3.38 | 120.57 | 115.41 |
| 21 | O | 3085 | CHD | C5-C4-C3 | 3.40 | 117.97 | 112.91 |
| 21 | J | 3060 | CHD | C2-C1-C10 | 3.49 | 119.06 | 112.84 |
| 18 | N | 4522 | TGL | OG2-CB1-CB2 | 3.51 | 119.16 | 111.53 |
| 21 | O | 3085 | CHD | C5-C6-C7 | 3.52 | 118.37 | 114.44 |
| 19 | A | 3524 | PGV | C02-O01-C1 | 3.54 | 126.38 | 117.89 |
| 21 | O | 3085 | CHD | C10-C9-C8 | 3.61 | 115.85 | 111.88 |
| 21 | W | 4060 | CHD | C2-C1-C10 | 3.66 | 119.37 | 112.84 |
| 17 | N | 516 | HEA | C27-C19-C20 | 3.66 | 121.00 | 115.41 |
| 21 | P | 4271 | CHD | C14-C13-C12 | 3.77 | 110.77 | 107.39 |
| 21 | P | 4271 | CHD | C4-C3-C2 | 3.84 | 115.42 | 110.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 21 | C | 3525 | CHD | C13-C17-C20 | 3.92 | 124.28 | 119.50 |
| 21 | C | 3271 | CHD | C14-C13-C12 | 4.01 | 110.98 | 107.39 |
| 18 | L | 3522 | TGL | OG2-CB1-CB2 | 4.03 | 120.28 | 111.53 |
| 18 | Q | 4523 | TGL | OG2-CB1-CB2 | 4.06 | 120.35 | 111.53 |
| 21 | W | 4060 | CHD | C1-C10-C5 | 4.08 | 114.52 | 107.81 |
| 21 | C | 3271 | CHD | C4-C3-C2 | 4.14 | 115.80 | 110.52 |
| 18 | N | 4522 | TGL | OG3-CG3-CG2 | 4.15 | 119.85 | 108.69 |
| 21 | P | 4525 | CHD | C13-C17-C20 | 4.20 | 124.61 | 119.50 |
| 27 | Z | 4526 | DMU | O7-C10-C5 | 4.22 | 118.37 | 108.10 |
| 21 | J | 3060 | CHD | C5-C6-C7 | 4.23 | 119.16 | 114.44 |
| 27 | M | 3526 | DMU | O7-C10-C5 | 4.28 | 118.52 | 108.10 |
| 21 | J | 3060 | CHD | C1-C10-C5 | 4.33 | 114.93 | 107.81 |
| 18 | A | 3521 | TGL | OG2-CB1-CB2 | 4.44 | 121.19 | 111.53 |
| 27 | M | 3526 | DMU | O7-C3-C4 | 4.46 | 121.05 | 109.32 |
| 21 | W | 4060 | CHD | C5-C6-C7 | 4.51 | 119.47 | 114.44 |
| 21 | W | 4060 | CHD | C4-C3-C2 | 4.57 | 116.34 | 110.52 |
| 18 | L | 3522 | TGL | OG3-CG3-CG2 | 4.58 | 121.02 | 108.69 |
| 18 | N | 4521 | TGL | OG2-CB1-CB2 | 4.61 | 121.55 | 111.53 |
| 18 | D | 3523 | TGL | OG2-CB1-CB2 | 4.62 | 121.57 | 111.53 |
| 21 | P | 4271 | CHD | C4-C5-C10 | 4.70 | 117.83 | 112.66 |
| 27 | Z | 4526 | DMU | O7-C3-C4 | 4.82 | 121.99 | 109.32 |
| 21 | J | 3060 | CHD | C11-C12-C13 | 4.99 | 116.27 | 111.20 |
| 27 | M | 3526 | DMU | O5-C6-O16 | 5.04 | 122.18 | 110.05 |
| 21 | W | 4060 | CHD | C9-C8-C7 | 5.05 | 117.89 | 111.92 |
| 21 | C | 3271 | CHD | C4-C5-C10 | 5.10 | 118.28 | 112.66 |
| 21 | J | 3060 | CHD | C4-C3-C2 | 5.10 | 117.03 | 110.52 |
| 21 | J | 3060 | CHD | C9-C8-C7 | 5.15 | 118.01 | 111.92 |
| 21 | J | 3060 | CHD | C6-C5-C10 | 5.17 | 118.35 | 112.66 |
| 21 | W | 4060 | CHD | C6-C5-C10 | 5.25 | 118.44 | 112.66 |
| 27 | Z | 4526 | DMU | O16-C6-C1 | 5.26 | 114.68 | 108.04 |
| 27 | M | 3526 | DMU | O5-C6-C1 | 5.40 | 121.35 | 110.28 |
| 21 | W | 4060 | CHD | C11-C12-C13 | 5.40 | 116.69 | 111.20 |
| 27 | Z | 4526 | DMU | C18-O16-C6 | 5.45 | 123.46 | 113.94 |
| 27 | Z | 4526 | DMU | O5-C6-O16 | 5.47 | 123.21 | 110.05 |
| 27 | Z | 4526 | DMU | O5-C6-C1 | 5.60 | 121.77 | 110.28 |
| 21 | P | 4271 | CHD | C9-C8-C7 | 5.70 | 118.65 | 111.92 |
| 21 | C | 3271 | CHD | C1-C10-C5 | 5.74 | 117.25 | 107.81 |
| 21 | C | 3271 | CHD | C9-C8-C7 | 5.77 | 118.73 | 111.92 |
| 21 | P | 4271 | CHD | C1-C10-C5 | 5.89 | 117.48 | 107.81 |
| 27 | M | 3526 | DMU | C18-O16-C6 | 6.07 | 124.56 | 113.94 |
| 27 | Z | 4526 | DMU | O7-C3-C2 | 6.24 | 123.27 | 107.17 |
| 27 | M | 3526 | DMU | O7-C3-C2 | 6.32 | 123.47 | 107.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | J | 3060 | CHD | C10-C9-C8 | 6.32 | 118.82 | 111.88 |
| 27 | M | 3526 | DMU | O16-C6-C1 | 6.34 | 116.04 | 108.04 |
| 21 | W | 4060 | CHD | C10-C9-C8 | 6.41 | 118.91 | 111.88 |
| 27 | Z | 4526 | DMU | O5-C4-C57 | 6.76 | 123.45 | 106.36 |
| 21 | J | 3060 | CHD | C13-C17-C20 | 6.83 | 127.82 | 119.50 |
| 21 | W | 4060 | CHD | C13-C17-C20 | 6.85 | 127.84 | 119.50 |
| 27 | M | 3526 | DMU | O5-C4-C57 | 6.88 | 123.75 | 106.36 |
| 27 | M | 3526 | DMU | O1-C9-C11 | 6.98 | 124.00 | 106.36 |
| 27 | Z | 4526 | DMU | O1-C9-C8 | 7.04 | 122.90 | 109.68 |
| 27 | M | 3526 | DMU | O5-C4-C3 | 7.13 | 124.81 | 109.75 |
| 27 | Z | 4526 | DMU | C7-C8-C9 | 7.22 | 122.79 | 110.20 |
| 27 | Z | 4526 | DMU | O1-C9-C11 | 7.25 | 124.68 | 106.36 |
| 27 | M | 3526 | DMU | O1-C9-C8 | 7.33 | 123.43 | 109.68 |
| 27 | M | 3526 | DMU | C7-C8-C9 | 7.38 | 123.06 | 110.20 |
| 27 | Z | 4526 | DMU | O5-C4-C3 | 7.38 | 125.34 | 109.75 |
| 27 | Z | 4526 | DMU | C6-O5-C4 | 8.15 | 129.56 | 113.75 |
| 27 | M | 3526 | DMU | C6-O5-C4 | 8.48 | 130.20 | 113.75 |
| 21 | W | 4060 | CHD | C17-C13-C14 | 9.31 | 109.46 | 100.05 |
| 21 | C | 3271 | CHD | C10-C9-C8 | 9.56 | 122.37 | 111.88 |
| 21 | J | 3060 | CHD | C17-C13-C14 | 9.65 | 109.81 | 100.05 |
| 21 | P | 4271 | CHD | C10-C9-C8 | 9.94 | 122.78 | 111.88 |
| 21 | P | 4271 | CHD | C17-C13-C14 | 10.07 | 110.22 | 100.05 |
| 27 | M | 3526 | DMU | C1-C2-C3 | 10.40 | 132.43 | 109.60 |
| 27 | Z | 4526 | DMU | C1-C2-C3 | 10.43 | 132.50 | 109.60 |
| 21 | C | 3271 | CHD | C17-C13-C14 | 10.48 | 110.64 | 100.05 |
| 27 | Z | 4526 | DMU | C10-C5-C7 | 11.04 | 131.73 | 109.97 |
| 27 | M | 3526 | DMU | C10-C5-C7 | 11.15 | 131.95 | 109.97 |

All (42) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 27 | Z | 4526 | DMU | C4 |
| 27 | Z | 4526 | DMU | C6 |
| 27 | Z | 4526 | DMU | C5 |
| 27 | Z | 4526 | DMU | C2 |
| 27 | Z | 4526 | DMU | C9 |
| 21 | C | 3271 | CHD | C12 |
| 21 | C | 3271 | CHD | C8 |
| 21 | C | 3271 | CHD | C3 |
| 21 | C | 3271 | CHD | C9 |
| 21 | C | 3271 | CHD | C14 |
| 17 | A | 515 | HEA | ND |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 17 | A | 515 | HEA | NA |
| 17 | A | 515 | HEA | NB |
| 27 | M | 3526 | DMU | C4 |
| 27 | M | 3526 | DMU | C6 |
| 27 | M | 3526 | DMU | C5 |
| 27 | M | 3526 | DMU | C2 |
| 27 | M | 3526 | DMU | C9 |
| 17 | N | 516 | HEA | ND |
| 17 | N | 516 | HEA | NA |
| 17 | N | 516 | HEA | NB |
| 17 | A | 516 | HEA | ND |
| 17 | A | 516 | HEA | NA |
| 17 | A | 516 | HEA | NB |
| 21 | W | 4060 | CHD | C12 |
| 21 | W | 4060 | CHD | C8 |
| 21 | W | 4060 | CHD | C9 |
| 21 | W | 4060 | CHD | C14 |
| 21 | W | 4060 | CHD | C17 |
| 21 | P | 4271 | CHD | C12 |
| 21 | P | 4271 | CHD | C8 |
| 21 | P | 4271 | CHD | C3 |
| 21 | P | 4271 | CHD | C9 |
| 21 | P | 4271 | CHD | C14 |
| 17 | N | 515 | HEA | ND |
| 17 | N | 515 | HEA | NA |
| 17 | N | 515 | HEA | NB |
| 21 | J | 3060 | CHD | C12 |
| 21 | J | 3060 | CHD | C8 |
| 21 | J | 3060 | CHD | C9 |
| 21 | J | 3060 | CHD | C14 |
| 21 | J | 3060 | CHD | C17 |

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 18 | Q | 4523 | TGL | CG2-OG2-CB1-CB2 |
| 18 | D | 3523 | TGL | CG2-OG2-CB1-OB1 |
| 18 | D | 3523 | TGL | CG2-OG2-CB1-CB2 |

There are no ring outliers.

32 monomers are involved in 267 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 18 | A | 3521 | TGL | 11 | 0 |
| 19 | A | 3524 | PGV | 7 | 0 |
| 17 | A | 515 | HEA | 3 | 0 |
| 17 | A | 516 | HEA | 1 | 0 |
| 21 | B | 4085 | CHD | 1 | 0 |
| 23 | C | 3264 | PEK | 4 | 0 |
| 23 | C | 3265 | PEK | 3 | 0 |
| 19 | C | 3267 | PGV | 6 | 0 |
| 19 | C | 3268 | PGV | 1 | 0 |
| 22 | C | 3270 | CDL | 14 | 0 |
| 21 | C | 3271 | CHD | 3 | 0 |
| 18 | D | 3523 | TGL | 15 | 0 |
| 25 | E | 3230 | PSC | 13 | 0 |
| 22 | G | 3269 | CDL | 14 | 0 |
| 23 | G | 4263 | PEK | 10 | 0 |
| 21 | J | 3060 | CHD | 2 | 0 |
| 18 | L | 3522 | TGL | 25 | 0 |
| 18 | N | 4521 | TGL | 19 | 0 |
| 18 | N | 4522 | TGL | 19 | 0 |
| 19 | N | 4524 | PGV | 5 | 0 |
| 17 | N | 515 | HEA | 3 | 0 |
| 21 | O | 3085 | CHD | 1 | 0 |
| 25 | O | 4230 | PSC | 21 | 0 |
| 23 | P | 4264 | PEK | 4 | 0 |
| 23 | P | 4265 | PEK | 2 | 0 |
| 19 | P | 4267 | PGV | 8 | 0 |
| 22 | P | 4270 | CDL | 18 | 0 |
| 21 | P | 4271 | CHD | 2 | 0 |
| 18 | Q | 4523 | TGL | 15 | 0 |
| 23 | T | 3263 | PEK | 9 | 0 |
| 22 | T | 4269 | CDL | 15 | 0 |
| 21 | W | 4060 | CHD | 2 | 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.