



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:40 AM GMT

PDB ID : 3OR1
Title : Crystal structure of dissimilatory sulfite reductase I (DsrI)
Authors : Hsieh, Y.C.; Liu, M.Y.; Wang, V.C.C.; Chiang, Y.L.; Liu, E.H.; Wu, W.G.;
Chan, S.I.; Chen, C.J.
Deposited on : 2010-09-06
Resolution : 1.76 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

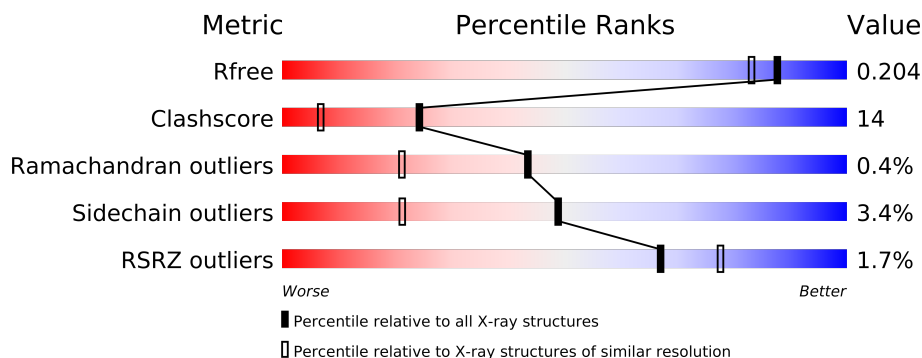
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.76 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 1134 (1.76-1.76) |
| Clashscore | 79885 | 1304 (1.76-1.76) |
| Ramachandran outliers | 78287 | 1288 (1.76-1.76) |
| Sidechain outliers | 78261 | 1288 (1.76-1.76) |
| RSRZ outliers | 66119 | 1135 (1.76-1.76) |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 437 | |
| 1 | D | 437 | |
| 2 | B | 386 | |
| 2 | E | 386 | |
| 3 | C | 105 | |
| 3 | F | 105 | |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 4 | SO3 | A | 6575 | - | X |
| 4 | SO3 | D | 6576 | - | X |

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15467 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Sulfite reductase alpha.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 435 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3422 | 2163 | 585 | 646 | 28 | | | |
| 1 | D | 435 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3422 | 2163 | 585 | 646 | 28 | | | |

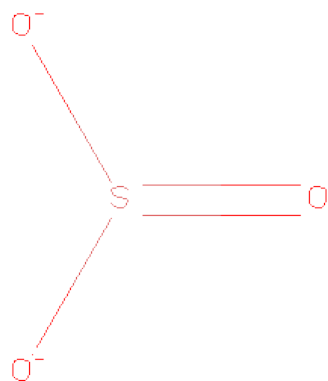
- Molecule 2 is a protein called Sulfite reductase beta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 385 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2999 | 1912 | 519 | 542 | 26 | | | |
| 2 | E | 385 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2999 | 1912 | 519 | 542 | 26 | | | |

- Molecule 3 is a protein called Sulfite reductase gama.

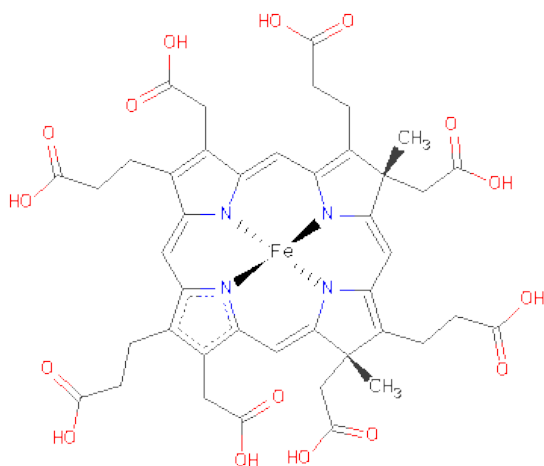
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | C | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 787 | 508 | 125 | 149 | 5 | | | |
| 3 | F | 104 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 787 | 508 | 125 | 149 | 5 | | | |

- Molecule 4 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | A | 1 | Total | O | S | 0 | 0 |
| | | | 4 | 3 | 1 | | |
| 4 | D | 1 | Total | O | S | 0 | 0 |
| | | | 4 | 3 | 1 | | |

- Molecule 5 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{42}FeN_4O_{16}$).



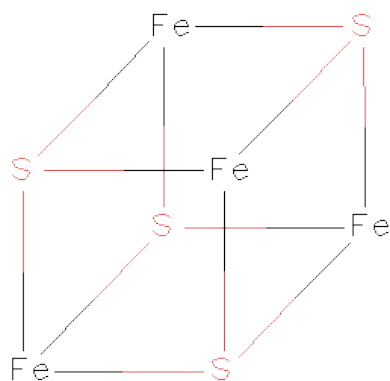
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 5 | A | 1 | Total | C | Fe | N | O | 0 |
| | | | 63 | 42 | 1 | 4 | 16 | |
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 62 | 42 | 4 | 16 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---------|---------|
| 5 | D | 1 | Total | C | Fe | N | O | |
| | | | 63 | 42 | 1 | 4 | 16 | |
| 5 | E | 1 | Total | C | N | O | | |
| | | | 62 | 42 | 4 | 16 | | |

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 6 | A | 1 | Total | Fe | S | | |
| | | | 8 | 4 | 4 | 0 | 0 |
| 6 | A | 1 | Total | Fe | S | | |
| | | | 8 | 4 | 4 | 0 | 0 |
| 6 | B | 1 | Total | Fe | S | | |
| | | | 8 | 4 | 4 | 0 | 0 |
| 6 | B | 1 | Total | Fe | S | | |
| | | | 8 | 4 | 4 | 0 | 0 |
| 6 | D | 1 | Total | Fe | S | | |
| | | | 8 | 4 | 4 | 0 | 0 |
| 6 | D | 1 | Total | Fe | S | | |
| | | | 8 | 4 | 4 | 0 | 0 |
| 6 | E | 1 | Total | Fe | S | | |
| | | | 8 | 4 | 4 | 0 | 0 |
| 6 | E | 1 | Total | Fe | S | | |
| | | | 8 | 4 | 4 | 0 | 0 |

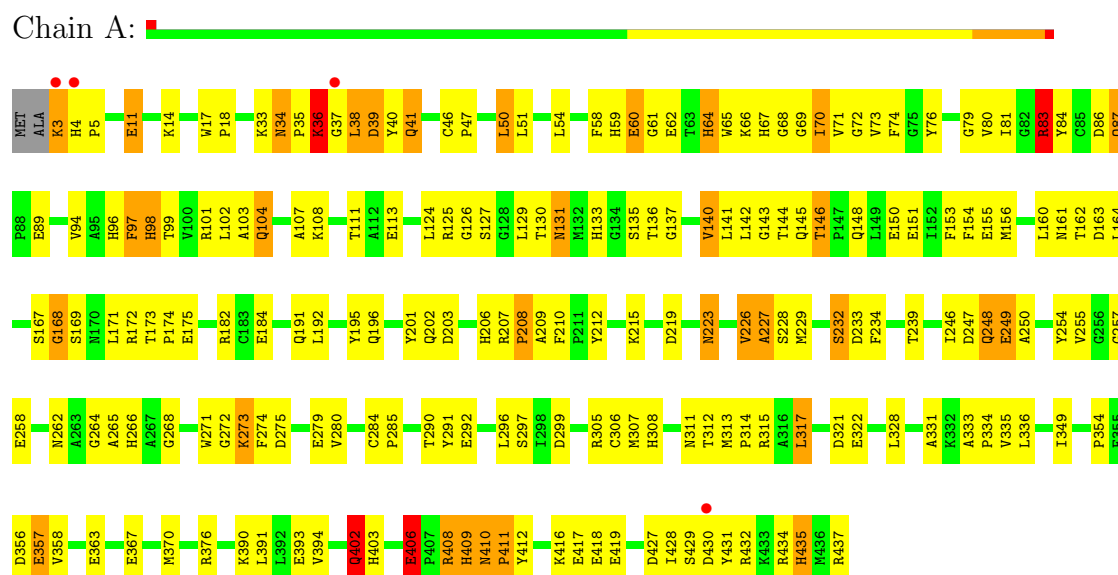
- Molecule 7 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 7 | A | 164 | Total 164 | O 164 | 0 | 0 |
| 7 | B | 160 | Total 160 | O 160 | 0 | 0 |
| 7 | C | 12 | Total 12 | O 12 | 0 | 0 |
| 7 | D | 220 | Total 220 | O 220 | 0 | 0 |
| 7 | E | 155 | Total 155 | O 155 | 0 | 0 |
| 7 | F | 18 | Total 18 | O 18 | 0 | 0 |

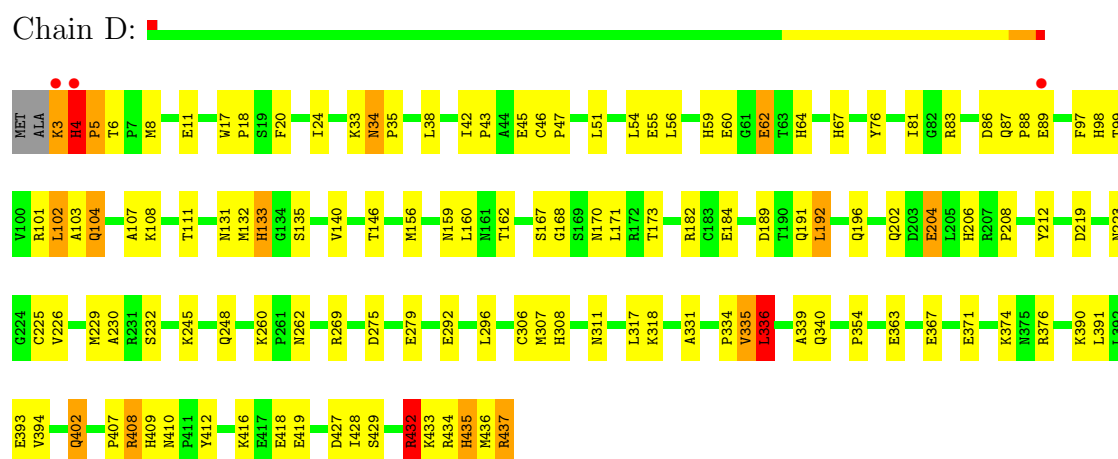
3 Residue-property plots

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.

• Molecule 1: Sulfite reductase alpha

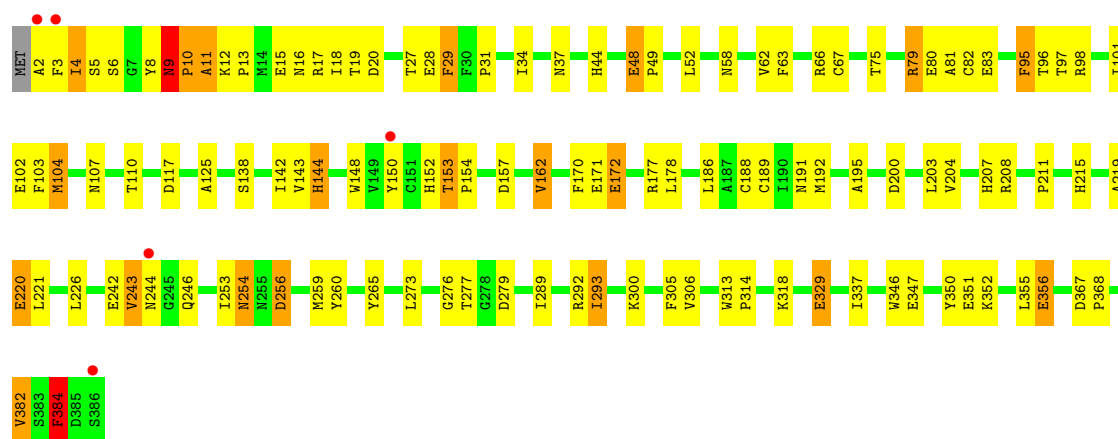


• Molecule 1: Sulfite reductase alpha



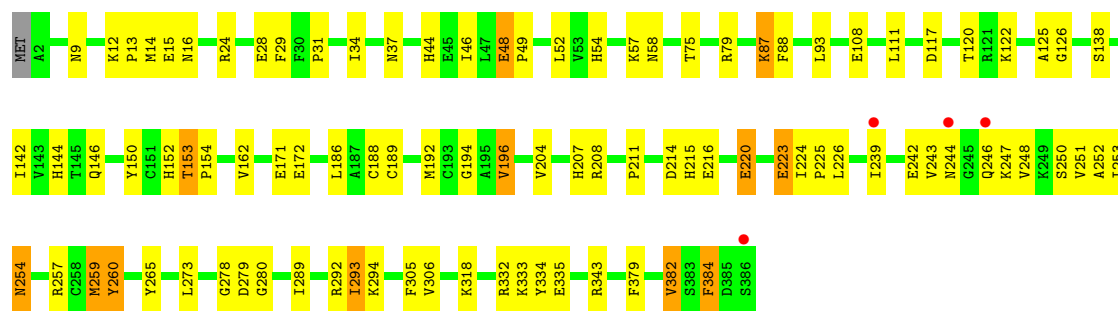
• Molecule 2: Sulfite reductase beta





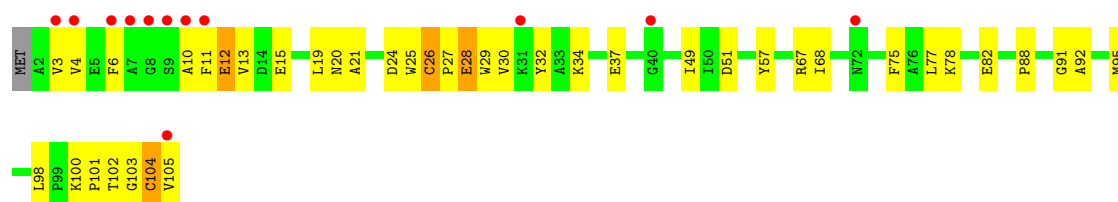
- Molecule 2: Sulfite reductase beta

Chain E:



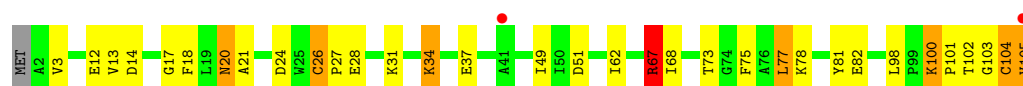
- Molecule 3: Sulfite reductase gama

Chain C:



- Molecule 3: Sulfite reductase gama

Chain F:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 114.72Å 60.48Å 132.91Å 90.00° 94.30° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 1.76 29.48 – 1.70 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (30.00-1.76) 99.1 (29.48-1.70) | Depositor EDS |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | 0.06 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.96 (at 1.70Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.193 , 0.212 0.201 , 0.204 | Depositor DCC |
| R_{free} test set | 10018 reflections (5.31%) | DCC |
| Wilson B-factor (Å ²) | 22.0 | Xtriage |
| Anisotropy | 0.292 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.39 , 35.8 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Outliers | 0 of 198600 reflections | Xtriage |
| F_o, F_c correlation | 0.96 | EDS |
| Total number of atoms | 15467 | wwPDB-VP |
| Average B, all atoms (Å ²) | 25.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, SO3, SRM

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 | 2.36 | 257/3512 (7.3%) | 1.23 | 27/4751 (0.6%) |
| 1 | D | 1.23 | 58/3512 (1.7%) | 1.08 | 21/4751 (0.4%) |
| 2 | B | 1.93 | 133/3076 (4.3%) | 0.99 | 12/4170 (0.3%) |
| 2 | E | 1.52 | 67/3076 (2.2%) | 0.84 | 11/4170 (0.3%) |
| 3 | C | 1.26 | 9/808 (1.1%) | 0.77 | 1/1090 (0.1%) |
| 3 | F | 1.60 | 17/808 (2.1%) | 1.27 | 4/1090 (0.4%) |
| All | All | 1.78 | 541/14792 (3.7%) | 1.05 | 76/20022 (0.4%) |

All (541) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3 | F | 26 | CYS | CB-SG | -20.23 | 1.47 | 1.82 |
| 2 | B | 384 | PHE | CE1-CZ | -19.93 | 0.99 | 1.37 |
| 2 | E | 220 | GLU | CB-CG | -19.51 | 1.15 | 1.52 |
| 1 | A | 406 | GLU | CB-CG | -18.91 | 1.16 | 1.52 |
| 2 | B | 306 | VAL | CB-CG2 | -17.20 | 1.16 | 1.52 |
| 2 | B | 384 | PHE | CD1-CE1 | -16.73 | 1.05 | 1.39 |
| 1 | D | 335 | VAL | CB-CG1 | -16.48 | 1.18 | 1.52 |
| 2 | E | 28 | GLU | CD-OE1 | -16.30 | 1.07 | 1.25 |
| 2 | B | 243 | VAL | CB-CG2 | -16.23 | 1.18 | 1.52 |
| 2 | E | 220 | GLU | CD-OE2 | -15.94 | 1.08 | 1.25 |
| 2 | B | 28 | GLU | CD-OE2 | -15.56 | 1.08 | 1.25 |
| 2 | E | 48 | GLU | CB-CG | -15.35 | 1.23 | 1.52 |
| 2 | E | 306 | VAL | CB-CG2 | -15.27 | 1.20 | 1.52 |
| 2 | E | 196 | VAL | CB-CG2 | -13.45 | 1.24 | 1.52 |
| 2 | B | 102 | GLU | CD-OE1 | -13.26 | 1.11 | 1.25 |
| 2 | B | 220 | GLU | CB-CG | -12.96 | 1.27 | 1.52 |
| 2 | E | 243 | VAL | CB-CG2 | -12.88 | 1.25 | 1.52 |
| 1 | A | 58 | PHE | CE1-CZ | -12.33 | 1.14 | 1.37 |
| 2 | E | 220 | GLU | CG-CD | -11.70 | 1.34 | 1.51 |
| 2 | B | 80 | GLU | CD-OE1 | -11.67 | 1.12 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | E | 28 | GLU | CB-CG | -11.24 | 1.30 | 1.52 |
| 2 | E | 382 | VAL | CB-CG2 | -11.04 | 1.29 | 1.52 |
| 2 | B | 220 | GLU | CD-OE1 | -11.01 | 1.13 | 1.25 |
| 3 | F | 102 | THR | CB-OG1 | -10.98 | 1.21 | 1.43 |
| 2 | B | 220 | GLU | CG-CD | -10.89 | 1.35 | 1.51 |
| 2 | E | 384 | PHE | CE1-CZ | -10.82 | 1.16 | 1.37 |
| 3 | F | 103 | GLY | C-O | -10.80 | 1.06 | 1.23 |
| 3 | C | 103 | GLY | C-O | -10.75 | 1.06 | 1.23 |
| 1 | A | 209 | ALA | CA-CB | -10.70 | 1.29 | 1.52 |
| 1 | A | 98 | HIS | C-O | -10.65 | 1.03 | 1.23 |
| 2 | B | 329 | GLU | CD-OE1 | -10.54 | 1.14 | 1.25 |
| 1 | A | 58 | PHE | CD2-CE2 | -10.51 | 1.18 | 1.39 |
| 1 | A | 315 | ARG | CZ-NH2 | -10.45 | 1.19 | 1.33 |
| 1 | A | 68 | GLY | C-O | -10.43 | 1.06 | 1.23 |
| 3 | F | 102 | THR | C-O | -10.41 | 1.03 | 1.23 |
| 3 | F | 67 | ARG | CZ-NH2 | -10.38 | 1.19 | 1.33 |
| 1 | A | 83 | ARG | CD-NE | -10.36 | 1.28 | 1.46 |
| 3 | C | 26 | CYS | CB-SG | -10.25 | 1.64 | 1.82 |
| 2 | B | 384 | PHE | CE2-CZ | -10.22 | 1.18 | 1.37 |
| 2 | B | 52 | LEU | C-O | -10.14 | 1.04 | 1.23 |
| 1 | D | 11 | GLU | CD-OE1 | -10.14 | 1.14 | 1.25 |
| 1 | A | 229 | MET | CB-CG | -10.11 | 1.19 | 1.51 |
| 1 | D | 432 | ARG | CD-NE | -10.05 | 1.29 | 1.46 |
| 1 | A | 50 | LEU | CG-CD1 | -10.03 | 1.14 | 1.51 |
| 1 | A | 290 | THR | C-O | -9.90 | 1.04 | 1.23 |
| 2 | E | 48 | GLU | CD-OE1 | -9.89 | 1.14 | 1.25 |
| 1 | A | 232 | SER | CB-OG | -9.83 | 1.29 | 1.42 |
| 2 | B | 204 | VAL | CB-CG1 | -9.80 | 1.32 | 1.52 |
| 1 | D | 260 | LYS | CE-NZ | -9.74 | 1.24 | 1.49 |
| 1 | A | 418 | GLU | CB-CG | -9.71 | 1.33 | 1.52 |
| 1 | D | 42 | ILE | C-O | -9.70 | 1.04 | 1.23 |
| 2 | E | 384 | PHE | CG-CD2 | -9.67 | 1.24 | 1.38 |
| 2 | B | 102 | GLU | CD-OE2 | -9.66 | 1.15 | 1.25 |
| 1 | A | 393 | GLU | CD-OE1 | -9.65 | 1.15 | 1.25 |
| 1 | A | 74 | PHE | CE2-CZ | -9.64 | 1.19 | 1.37 |
| 1 | D | 269 | ARG | CZ-NH2 | -9.62 | 1.20 | 1.33 |
| 2 | E | 384 | PHE | CE2-CZ | -9.62 | 1.19 | 1.37 |
| 2 | B | 204 | VAL | CB-CG2 | -9.47 | 1.32 | 1.52 |
| 1 | A | 406 | GLU | CG-CD | -9.40 | 1.37 | 1.51 |
| 1 | A | 249 | GLU | CB-CG | -9.38 | 1.34 | 1.52 |
| 1 | A | 103 | ALA | C-O | -9.38 | 1.05 | 1.23 |
| 2 | B | 15 | GLU | CD-OE2 | -9.37 | 1.15 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 162 | THR | C-O | -9.34 | 1.05 | 1.23 |
| 1 | D | 171 | LEU | C-O | -9.32 | 1.05 | 1.23 |
| 1 | D | 374 | LYS | CD-CE | -9.31 | 1.27 | 1.51 |
| 1 | D | 269 | ARG | CZ-NH1 | -9.28 | 1.21 | 1.33 |
| 2 | B | 95 | PHE | CG-CD1 | -9.26 | 1.24 | 1.38 |
| 1 | A | 264 | GLY | C-O | -9.26 | 1.08 | 1.23 |
| 1 | A | 234 | PHE | CE1-CZ | -9.26 | 1.19 | 1.37 |
| 2 | B | 143 | VAL | CB-CG1 | -9.23 | 1.33 | 1.52 |
| 1 | A | 94 | VAL | C-O | -9.18 | 1.05 | 1.23 |
| 2 | B | 220 | GLU | CD-OE2 | -9.16 | 1.15 | 1.25 |
| 2 | E | 220 | GLU | CD-OE1 | -9.16 | 1.15 | 1.25 |
| 1 | A | 297 | SER | CB-OG | -9.13 | 1.30 | 1.42 |
| 3 | C | 37 | GLU | CD-OE1 | -9.11 | 1.15 | 1.25 |
| 1 | A | 155 | GLU | CD-OE2 | -9.10 | 1.15 | 1.25 |
| 1 | A | 254 | TYR | CD2-CE2 | -9.09 | 1.25 | 1.39 |
| 2 | E | 57 | LYS | CG-CD | -9.08 | 1.21 | 1.52 |
| 2 | B | 384 | PHE | CG-CD2 | -9.08 | 1.25 | 1.38 |
| 2 | B | 66 | ARG | CZ-NH1 | -9.03 | 1.21 | 1.33 |
| 1 | A | 154 | PHE | C-O | -8.98 | 1.06 | 1.23 |
| 2 | E | 384 | PHE | CB-CG | -8.98 | 1.36 | 1.51 |
| 1 | A | 60 | GLU | CD-OE2 | -8.97 | 1.15 | 1.25 |
| 2 | B | 350 | TYR | CG-CD2 | -8.94 | 1.27 | 1.39 |
| 1 | A | 150 | GLU | CD-OE1 | -8.89 | 1.15 | 1.25 |
| 1 | A | 130 | THR | C-O | -8.86 | 1.06 | 1.23 |
| 1 | D | 393 | GLU | CD-OE1 | -8.85 | 1.16 | 1.25 |
| 2 | E | 48 | GLU | CD-OE2 | -8.84 | 1.16 | 1.25 |
| 2 | B | 178 | LEU | C-O | -8.82 | 1.06 | 1.23 |
| 1 | A | 315 | ARG | CB-CG | -8.77 | 1.28 | 1.52 |
| 1 | A | 125 | ARG | C-O | -8.77 | 1.06 | 1.23 |
| 1 | A | 201 | TYR | CD1-CE1 | -8.77 | 1.26 | 1.39 |
| 2 | E | 125 | ALA | CA-CB | -8.75 | 1.34 | 1.52 |
| 2 | B | 27 | THR | C-O | -8.74 | 1.06 | 1.23 |
| 2 | B | 191 | ASN | CG-OD1 | -8.73 | 1.04 | 1.24 |
| 2 | E | 384 | PHE | CD1-CE1 | -8.73 | 1.21 | 1.39 |
| 1 | A | 249 | GLU | CD-OE1 | -8.72 | 1.16 | 1.25 |
| 1 | A | 124 | LEU | C-O | -8.69 | 1.06 | 1.23 |
| 2 | B | 66 | ARG | CZ-NH2 | -8.63 | 1.21 | 1.33 |
| 1 | A | 127 | SER | CB-OG | -8.62 | 1.31 | 1.42 |
| 2 | E | 16 | ASN | C-O | -8.61 | 1.06 | 1.23 |
| 3 | F | 104 | CYS | CB-SG | -8.61 | 1.67 | 1.82 |
| 2 | B | 95 | PHE | CE1-CZ | -8.58 | 1.21 | 1.37 |
| 1 | A | 58 | PHE | CG-CD2 | -8.58 | 1.25 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 417 | GLU | CD-OE2 | -8.57 | 1.16 | 1.25 |
| 1 | A | 437 | ARG | CB-CG | -8.56 | 1.29 | 1.52 |
| 1 | D | 335 | VAL | C-O | -8.53 | 1.07 | 1.23 |
| 2 | B | 162 | VAL | CB-CG1 | -8.51 | 1.34 | 1.52 |
| 2 | B | 351 | GLU | CD-OE1 | -8.51 | 1.16 | 1.25 |
| 1 | A | 210 | PHE | CG-CD1 | -8.50 | 1.26 | 1.38 |
| 1 | A | 65 | TRP | CG-CD1 | -8.49 | 1.24 | 1.36 |
| 1 | A | 431 | TYR | CD2-CE2 | -8.48 | 1.26 | 1.39 |
| 1 | A | 175 | GLU | CD-OE2 | -8.47 | 1.16 | 1.25 |
| 2 | B | 3 | PHE | C-O | -8.46 | 1.07 | 1.23 |
| 1 | D | 434 | ARG | C-O | -8.46 | 1.07 | 1.23 |
| 2 | B | 48 | GLU | CG-CD | -8.45 | 1.39 | 1.51 |
| 1 | A | 150 | GLU | CD-OE2 | -8.43 | 1.16 | 1.25 |
| 3 | F | 67 | ARG | CB-CG | -8.43 | 1.29 | 1.52 |
| 2 | E | 243 | VAL | CB-CG1 | -8.42 | 1.35 | 1.52 |
| 1 | A | 175 | GLU | CD-OE1 | -8.42 | 1.16 | 1.25 |
| 1 | A | 141 | LEU | C-O | -8.39 | 1.07 | 1.23 |
| 2 | B | 329 | GLU | CD-OE2 | -8.38 | 1.16 | 1.25 |
| 2 | B | 20 | ASP | CG-OD1 | -8.37 | 1.06 | 1.25 |
| 1 | A | 89 | GLU | CB-CG | -8.36 | 1.36 | 1.52 |
| 1 | A | 155 | GLU | CD-OE1 | -8.35 | 1.16 | 1.25 |
| 2 | E | 248 | VAL | CB-CG2 | -8.35 | 1.35 | 1.52 |
| 1 | A | 97 | PHE | CG-CD1 | -8.35 | 1.26 | 1.38 |
| 2 | B | 356 | GLU | C-O | -8.32 | 1.07 | 1.23 |
| 1 | A | 131 | ASN | C-O | -8.31 | 1.07 | 1.23 |
| 2 | E | 318 | LYS | C-O | -8.28 | 1.07 | 1.23 |
| 2 | B | 356 | GLU | CB-CG | -8.27 | 1.36 | 1.52 |
| 1 | A | 208 | PRO | C-O | -8.25 | 1.06 | 1.23 |
| 1 | D | 103 | ALA | CA-CB | -8.22 | 1.35 | 1.52 |
| 1 | A | 209 | ALA | C-O | -8.20 | 1.07 | 1.23 |
| 1 | D | 245 | LYS | C-O | -8.20 | 1.07 | 1.23 |
| 1 | A | 151 | GLU | CD-OE2 | -8.20 | 1.16 | 1.25 |
| 2 | B | 29 | PHE | CE1-CZ | -8.17 | 1.21 | 1.37 |
| 2 | B | 208 | ARG | CZ-NH1 | -8.16 | 1.22 | 1.33 |
| 1 | A | 171 | LEU | C-O | -8.15 | 1.07 | 1.23 |
| 1 | A | 322 | GLU | CD-OE1 | -8.09 | 1.16 | 1.25 |
| 2 | E | 194 | GLY | C-O | -8.09 | 1.10 | 1.23 |
| 1 | D | 62 | GLU | C-O | -8.06 | 1.08 | 1.23 |
| 1 | A | 182 | ARG | CZ-NH2 | -8.05 | 1.22 | 1.33 |
| 1 | A | 129 | LEU | C-O | -8.03 | 1.08 | 1.23 |
| 1 | A | 268 | GLY | C-O | -8.02 | 1.10 | 1.23 |
| 1 | A | 406 | GLU | CD-OE1 | -8.02 | 1.16 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 228 | SER | CB-OG | -7.99 | 1.31 | 1.42 |
| 2 | B | 243 | VAL | CB-CG1 | -7.98 | 1.36 | 1.52 |
| 1 | A | 431 | TYR | C-O | -7.95 | 1.08 | 1.23 |
| 1 | A | 146 | THR | C-O | -7.95 | 1.08 | 1.23 |
| 1 | D | 393 | GLU | CD-OE2 | -7.94 | 1.17 | 1.25 |
| 2 | B | 384 | PHE | CB-CG | -7.91 | 1.38 | 1.51 |
| 1 | A | 40 | TYR | C-O | -7.91 | 1.08 | 1.23 |
| 2 | B | 170 | PHE | CE2-CZ | -7.90 | 1.22 | 1.37 |
| 1 | A | 317 | LEU | C-O | -7.87 | 1.08 | 1.23 |
| 2 | B | 191 | ASN | CG-ND2 | -7.87 | 1.13 | 1.32 |
| 1 | A | 40 | TYR | CD1-CE1 | -7.86 | 1.27 | 1.39 |
| 2 | E | 28 | GLU | CD-OE2 | -7.86 | 1.17 | 1.25 |
| 1 | A | 87 | GLN | CG-CD | -7.85 | 1.32 | 1.51 |
| 2 | B | 226 | LEU | C-O | -7.84 | 1.08 | 1.23 |
| 1 | A | 274 | PHE | CD1-CE1 | -7.83 | 1.23 | 1.39 |
| 1 | A | 393 | GLU | C-O | -7.83 | 1.08 | 1.23 |
| 1 | A | 192 | LEU | C-O | -7.82 | 1.08 | 1.23 |
| 1 | A | 333 | ALA | C-O | -7.79 | 1.08 | 1.23 |
| 1 | A | 357 | GLU | C-O | -7.75 | 1.08 | 1.23 |
| 1 | A | 328 | LEU | C-O | -7.74 | 1.08 | 1.23 |
| 1 | D | 103 | ALA | C-O | -7.73 | 1.08 | 1.23 |
| 1 | A | 160 | LEU | CG-CD1 | -7.73 | 1.23 | 1.51 |
| 1 | A | 36 | LYS | CB-CG | -7.67 | 1.31 | 1.52 |
| 2 | E | 196 | VAL | C-O | -7.64 | 1.08 | 1.23 |
| 1 | D | 393 | GLU | CB-CG | -7.63 | 1.37 | 1.52 |
| 1 | A | 437 | ARG | C-O | -7.62 | 1.08 | 1.23 |
| 3 | C | 102 | THR | C-O | -7.60 | 1.08 | 1.23 |
| 1 | A | 168 | GLY | C-O | -7.59 | 1.11 | 1.23 |
| 1 | A | 144 | THR | C-O | -7.58 | 1.08 | 1.23 |
| 2 | B | 104 | MET | C-O | -7.57 | 1.08 | 1.23 |
| 1 | A | 257 | GLY | C-O | -7.56 | 1.11 | 1.23 |
| 1 | A | 135 | SER | CB-OG | -7.55 | 1.32 | 1.42 |
| 1 | D | 102 | LEU | C-O | -7.54 | 1.09 | 1.23 |
| 1 | A | 335 | VAL | CB-CG1 | -7.52 | 1.37 | 1.52 |
| 1 | D | 8 | MET | C-O | -7.52 | 1.09 | 1.23 |
| 1 | A | 232 | SER | C-O | -7.48 | 1.09 | 1.23 |
| 1 | A | 417 | GLU | CB-CG | -7.48 | 1.38 | 1.52 |
| 2 | B | 102 | GLU | CG-CD | -7.47 | 1.40 | 1.51 |
| 2 | B | 95 | PHE | CE2-CZ | -7.47 | 1.23 | 1.37 |
| 2 | B | 117 | ASP | C-O | -7.47 | 1.09 | 1.23 |
| 2 | E | 382 | VAL | CB-CG1 | -7.46 | 1.37 | 1.52 |
| 1 | A | 246 | ILE | C-O | -7.45 | 1.09 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3 | F | 98 | LEU | C-O | -7.45 | 1.09 | 1.23 |
| 2 | B | 350 | TYR | CG-CD1 | -7.44 | 1.29 | 1.39 |
| 1 | A | 83 | ARG | CZ-NH2 | -7.41 | 1.23 | 1.33 |
| 2 | E | 28 | GLU | C-O | -7.41 | 1.09 | 1.23 |
| 1 | A | 136 | THR | CB-CG2 | -7.41 | 1.27 | 1.52 |
| 2 | B | 27 | THR | CB-CG2 | -7.39 | 1.27 | 1.52 |
| 1 | A | 127 | SER | C-O | -7.38 | 1.09 | 1.23 |
| 1 | A | 315 | ARG | C-O | -7.37 | 1.09 | 1.23 |
| 1 | D | 245 | LYS | CD-CE | -7.34 | 1.32 | 1.51 |
| 2 | E | 24 | ARG | CG-CD | -7.33 | 1.33 | 1.51 |
| 1 | A | 431 | TYR | CE1-CZ | -7.31 | 1.29 | 1.38 |
| 1 | A | 125 | ARG | CZ-NH1 | -7.30 | 1.23 | 1.33 |
| 1 | D | 275 | ASP | C-O | -7.30 | 1.09 | 1.23 |
| 1 | A | 71 | VAL | CB-CG2 | -7.26 | 1.37 | 1.52 |
| 2 | B | 79 | ARG | CZ-NH1 | -7.25 | 1.23 | 1.33 |
| 2 | E | 306 | VAL | C-O | -7.25 | 1.09 | 1.23 |
| 2 | E | 9 | ASN | C-O | -7.25 | 1.09 | 1.23 |
| 2 | B | 215 | HIS | C-O | -7.23 | 1.09 | 1.23 |
| 1 | A | 356 | ASP | C-O | -7.20 | 1.09 | 1.23 |
| 2 | E | 382 | VAL | C-O | -7.20 | 1.09 | 1.23 |
| 2 | B | 6 | SER | C-O | -7.19 | 1.09 | 1.23 |
| 2 | B | 48 | GLU | CB-CG | -7.19 | 1.38 | 1.52 |
| 1 | A | 40 | TYR | CE1-CZ | -7.18 | 1.29 | 1.38 |
| 3 | F | 67 | ARG | CD-NE | -7.18 | 1.34 | 1.46 |
| 1 | A | 394 | VAL | CB-CG2 | -7.16 | 1.37 | 1.52 |
| 1 | A | 234 | PHE | C-O | -7.13 | 1.09 | 1.23 |
| 1 | A | 97 | PHE | C-O | -7.11 | 1.09 | 1.23 |
| 1 | D | 51 | LEU | C-O | -7.11 | 1.09 | 1.23 |
| 1 | D | 435 | HIS | C-O | -7.11 | 1.09 | 1.23 |
| 1 | A | 135 | SER | C-O | -7.10 | 1.09 | 1.23 |
| 1 | A | 145 | GLN | C-O | -7.07 | 1.09 | 1.23 |
| 1 | A | 210 | PHE | C-O | -7.06 | 1.09 | 1.23 |
| 1 | D | 391 | LEU | C-O | -7.04 | 1.09 | 1.23 |
| 1 | D | 437 | ARG | CD-NE | -7.04 | 1.34 | 1.46 |
| 2 | B | 80 | GLU | CD-OE2 | -7.04 | 1.18 | 1.25 |
| 1 | D | 432 | ARG | CZ-NH2 | -7.04 | 1.24 | 1.33 |
| 2 | B | 204 | VAL | C-O | -7.03 | 1.09 | 1.23 |
| 1 | D | 275 | ASP | CG-OD2 | -7.03 | 1.09 | 1.25 |
| 1 | A | 155 | GLU | C-O | -7.02 | 1.10 | 1.23 |
| 1 | A | 265 | ALA | C-O | -7.01 | 1.10 | 1.23 |
| 2 | B | 20 | ASP | CG-OD2 | -7.01 | 1.09 | 1.25 |
| 2 | B | 81 | ALA | C-O | -7.01 | 1.10 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 60 | GLU | CD-OE1 | -7.00 | 1.18 | 1.25 |
| 1 | D | 408 | ARG | CZ-NH2 | -6.99 | 1.24 | 1.33 |
| 2 | E | 343 | ARG | CZ-NH2 | -6.99 | 1.24 | 1.33 |
| 2 | E | 93 | LEU | C-O | -6.98 | 1.10 | 1.23 |
| 1 | A | 435 | HIS | C-O | -6.98 | 1.10 | 1.23 |
| 2 | B | 243 | VAL | C-O | -6.97 | 1.10 | 1.23 |
| 2 | B | 5 | SER | CB-OG | -6.97 | 1.33 | 1.42 |
| 1 | A | 96 | HIS | C-O | -6.95 | 1.10 | 1.23 |
| 1 | A | 74 | PHE | CG-CD2 | -6.93 | 1.28 | 1.38 |
| 1 | A | 249 | GLU | CD-OE2 | -6.93 | 1.18 | 1.25 |
| 1 | A | 192 | LEU | CG-CD1 | -6.89 | 1.26 | 1.51 |
| 1 | D | 374 | LYS | CG-CD | -6.88 | 1.29 | 1.52 |
| 1 | A | 137 | GLY | C-O | -6.88 | 1.12 | 1.23 |
| 2 | B | 305 | PHE | CE2-CZ | -6.88 | 1.24 | 1.37 |
| 1 | D | 11 | GLU | CB-CG | -6.88 | 1.39 | 1.52 |
| 2 | B | 350 | TYR | C-O | -6.88 | 1.10 | 1.23 |
| 2 | E | 223 | GLU | CD-OE1 | -6.87 | 1.18 | 1.25 |
| 2 | B | 305 | PHE | C-O | -6.85 | 1.10 | 1.23 |
| 1 | A | 356 | ASP | CG-OD2 | -6.84 | 1.09 | 1.25 |
| 1 | A | 254 | TYR | CD1-CE1 | -6.84 | 1.29 | 1.39 |
| 2 | B | 29 | PHE | CG-CD2 | -6.83 | 1.28 | 1.38 |
| 1 | A | 59 | HIS | C-O | -6.82 | 1.10 | 1.23 |
| 1 | D | 269 | ARG | C-O | -6.82 | 1.10 | 1.23 |
| 1 | A | 417 | GLU | C-O | -6.77 | 1.10 | 1.23 |
| 1 | A | 83 | ARG | NE-CZ | -6.76 | 1.24 | 1.33 |
| 1 | A | 70 | ILE | C-O | -6.75 | 1.10 | 1.23 |
| 2 | B | 203 | LEU | C-O | -6.74 | 1.10 | 1.23 |
| 2 | B | 11 | ALA | CA-CB | -6.73 | 1.38 | 1.52 |
| 1 | A | 36 | LYS | C-O | -6.73 | 1.10 | 1.23 |
| 2 | B | 384 | PHE | C-O | -6.73 | 1.10 | 1.23 |
| 2 | B | 384 | PHE | CG-CD1 | -6.72 | 1.28 | 1.38 |
| 1 | A | 195 | TYR | CG-CD2 | -6.71 | 1.30 | 1.39 |
| 1 | A | 299 | ASP | C-O | -6.71 | 1.10 | 1.23 |
| 1 | A | 148 | GLN | CD-OE1 | -6.71 | 1.09 | 1.24 |
| 1 | A | 266 | HIS | C-O | -6.70 | 1.10 | 1.23 |
| 2 | B | 103 | PHE | CE1-CZ | -6.70 | 1.24 | 1.37 |
| 1 | A | 41 | GLN | C-O | -6.69 | 1.10 | 1.23 |
| 1 | A | 4 | HIS | C-O | -6.69 | 1.10 | 1.23 |
| 1 | A | 411 | PRO | C-O | -6.67 | 1.09 | 1.23 |
| 2 | B | 178 | LEU | CG-CD2 | -6.67 | 1.27 | 1.51 |
| 2 | B | 171 | GLU | CB-CG | -6.66 | 1.39 | 1.52 |
| 2 | E | 117 | ASP | CG-OD1 | -6.66 | 1.10 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 210 | PHE | CE2-CZ | -6.66 | 1.24 | 1.37 |
| 2 | B | 306 | VAL | CB-CG1 | -6.64 | 1.39 | 1.52 |
| 1 | A | 140 | VAL | C-O | -6.63 | 1.10 | 1.23 |
| 3 | C | 67 | ARG | C-O | -6.63 | 1.10 | 1.23 |
| 1 | A | 408 | ARG | C-O | -6.63 | 1.10 | 1.23 |
| 2 | B | 79 | ARG | CZ-NH2 | -6.63 | 1.24 | 1.33 |
| 1 | A | 434 | ARG | CZ-NH1 | -6.62 | 1.24 | 1.33 |
| 1 | A | 173 | THR | C-O | -6.60 | 1.10 | 1.23 |
| 1 | A | 148 | GLN | C-O | -6.58 | 1.10 | 1.23 |
| 2 | E | 87 | LYS | C-O | -6.58 | 1.10 | 1.23 |
| 2 | E | 125 | ALA | C-O | -6.58 | 1.10 | 1.23 |
| 1 | A | 234 | PHE | CD2-CE2 | -6.58 | 1.26 | 1.39 |
| 1 | D | 428 | ILE | C-O | -6.57 | 1.10 | 1.23 |
| 1 | A | 432 | ARG | C-O | -6.56 | 1.10 | 1.23 |
| 1 | A | 210 | PHE | CD2-CE2 | -6.54 | 1.26 | 1.39 |
| 1 | A | 79 | GLY | C-O | -6.54 | 1.13 | 1.23 |
| 1 | A | 248 | GLN | CB-CG | -6.54 | 1.34 | 1.52 |
| 2 | B | 8 | TYR | C-O | -6.54 | 1.10 | 1.23 |
| 1 | A | 226 | VAL | CB-CG2 | -6.50 | 1.39 | 1.52 |
| 1 | A | 169 | SER | CB-OG | -6.48 | 1.33 | 1.42 |
| 1 | A | 223 | ASN | CG-OD1 | -6.48 | 1.09 | 1.24 |
| 1 | A | 35 | PRO | C-O | -6.47 | 1.10 | 1.23 |
| 1 | A | 201 | TYR | CE1-CZ | -6.46 | 1.30 | 1.38 |
| 1 | D | 340 | GLN | CD-OE1 | -6.46 | 1.09 | 1.24 |
| 2 | B | 143 | VAL | CB-CG2 | -6.45 | 1.39 | 1.52 |
| 1 | A | 182 | ARG | C-O | -6.44 | 1.11 | 1.23 |
| 2 | E | 24 | ARG | CZ-NH2 | -6.43 | 1.24 | 1.33 |
| 1 | A | 432 | ARG | CZ-NH2 | -6.42 | 1.24 | 1.33 |
| 2 | B | 6 | SER | CB-OG | -6.41 | 1.33 | 1.42 |
| 1 | A | 142 | LEU | C-O | -6.41 | 1.11 | 1.23 |
| 1 | A | 431 | TYR | CG-CD1 | -6.39 | 1.30 | 1.39 |
| 2 | B | 3 | PHE | CG-CD2 | -6.39 | 1.29 | 1.38 |
| 1 | A | 357 | GLU | CD-OE1 | -6.38 | 1.18 | 1.25 |
| 1 | D | 5 | PRO | CB-CG | -6.38 | 1.18 | 1.50 |
| 2 | E | 93 | LEU | CG-CD1 | -6.37 | 1.28 | 1.51 |
| 1 | A | 250 | ALA | C-O | -6.36 | 1.11 | 1.23 |
| 1 | A | 226 | VAL | C-O | -6.35 | 1.11 | 1.23 |
| 1 | A | 182 | ARG | CZ-NH1 | -6.34 | 1.24 | 1.33 |
| 1 | D | 408 | ARG | C-O | -6.34 | 1.11 | 1.23 |
| 1 | D | 101 | ARG | CZ-NH1 | -6.33 | 1.24 | 1.33 |
| 1 | A | 143 | GLY | C-O | -6.33 | 1.13 | 1.23 |
| 2 | E | 126 | GLY | C-O | -6.33 | 1.13 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | E | 223 | GLU | C-O | -6.32 | 1.11 | 1.23 |
| 1 | A | 101 | ARG | C-O | -6.32 | 1.11 | 1.23 |
| 1 | D | 62 | GLU | CD-OE1 | -6.31 | 1.18 | 1.25 |
| 2 | B | 208 | ARG | CZ-NH2 | -6.31 | 1.24 | 1.33 |
| 1 | D | 6 | THR | C-O | -6.30 | 1.11 | 1.23 |
| 1 | A | 431 | TYR | CE2-CZ | -6.30 | 1.30 | 1.38 |
| 1 | A | 202 | GLN | CG-CD | -6.30 | 1.36 | 1.51 |
| 1 | A | 321 | ASP | C-O | -6.29 | 1.11 | 1.23 |
| 1 | A | 291 | TYR | CD1-CE1 | -6.28 | 1.29 | 1.39 |
| 1 | A | 80 | VAL | C-O | -6.27 | 1.11 | 1.23 |
| 1 | A | 174 | PRO | C-O | -6.27 | 1.10 | 1.23 |
| 2 | B | 221 | LEU | C-O | -6.26 | 1.11 | 1.23 |
| 1 | A | 201 | TYR | C-O | -6.25 | 1.11 | 1.23 |
| 1 | A | 154 | PHE | CE2-CZ | -6.24 | 1.25 | 1.37 |
| 1 | A | 328 | LEU | CG-CD1 | -6.24 | 1.28 | 1.51 |
| 1 | A | 37 | GLY | C-O | -6.24 | 1.13 | 1.23 |
| 1 | A | 84 | TYR | C-O | -6.22 | 1.11 | 1.23 |
| 2 | B | 48 | GLU | CD-OE2 | -6.21 | 1.18 | 1.25 |
| 2 | B | 171 | GLU | C-O | -6.21 | 1.11 | 1.23 |
| 2 | B | 16 | ASN | C-O | -6.21 | 1.11 | 1.23 |
| 2 | E | 108 | GLU | CB-CG | -6.21 | 1.40 | 1.52 |
| 2 | E | 16 | ASN | CG-OD1 | -6.20 | 1.10 | 1.24 |
| 1 | A | 164 | LEU | CG-CD1 | -6.20 | 1.28 | 1.51 |
| 1 | A | 248 | GLN | CD-NE2 | -6.20 | 1.17 | 1.32 |
| 1 | A | 36 | LYS | CG-CD | -6.18 | 1.31 | 1.52 |
| 2 | B | 18 | ILE | C-O | -6.18 | 1.11 | 1.23 |
| 2 | B | 10 | PRO | C-O | -6.17 | 1.10 | 1.23 |
| 1 | A | 50 | LEU | C-O | -6.17 | 1.11 | 1.23 |
| 1 | A | 156 | MET | C-O | -6.16 | 1.11 | 1.23 |
| 1 | A | 394 | VAL | CB-CG1 | -6.16 | 1.40 | 1.52 |
| 2 | B | 177 | ARG | C-O | -6.16 | 1.11 | 1.23 |
| 2 | E | 57 | LYS | CB-CG | -6.15 | 1.35 | 1.52 |
| 1 | A | 273 | LYS | C-O | -6.15 | 1.11 | 1.23 |
| 2 | B | 277 | THR | C-O | -6.14 | 1.11 | 1.23 |
| 1 | D | 4 | HIS | C-O | -6.14 | 1.11 | 1.23 |
| 2 | E | 220 | GLU | C-O | -6.14 | 1.11 | 1.23 |
| 1 | A | 64 | HIS | C-O | -6.14 | 1.11 | 1.23 |
| 2 | B | 17 | ARG | CZ-NH1 | -6.14 | 1.25 | 1.33 |
| 2 | B | 17 | ARG | CZ-NH2 | -6.13 | 1.25 | 1.33 |
| 2 | B | 244 | ASN | C-O | -6.12 | 1.11 | 1.23 |
| 1 | A | 233 | ASP | C-O | -6.12 | 1.11 | 1.23 |
| 1 | A | 140 | VAL | CB-CG1 | -6.10 | 1.40 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 82 | CYS | C-O | -6.09 | 1.11 | 1.23 |
| 1 | A | 161 | ASN | CG-ND2 | -6.08 | 1.17 | 1.32 |
| 1 | A | 201 | TYR | CD2-CE2 | -6.07 | 1.30 | 1.39 |
| 3 | C | 15 | GLU | CD-OE2 | -6.07 | 1.19 | 1.25 |
| 1 | A | 437 | ARG | N-CA | -6.06 | 1.34 | 1.46 |
| 2 | B | 219 | ALA | C-O | -6.05 | 1.11 | 1.23 |
| 1 | A | 274 | PHE | CD2-CE2 | -6.05 | 1.27 | 1.39 |
| 1 | D | 336 | LEU | C-O | -6.04 | 1.11 | 1.23 |
| 3 | F | 37 | GLU | CD-OE1 | -6.02 | 1.19 | 1.25 |
| 1 | A | 250 | ALA | CA-CB | -6.02 | 1.39 | 1.52 |
| 1 | A | 229 | MET | C-O | -6.01 | 1.11 | 1.23 |
| 1 | D | 437 | ARG | CB-CG | -6.01 | 1.36 | 1.52 |
| 1 | A | 402 | GLN | C-O | -6.00 | 1.11 | 1.23 |
| 2 | B | 20 | ASP | C-O | -6.00 | 1.11 | 1.23 |
| 2 | E | 111 | LEU | C-O | -6.00 | 1.11 | 1.23 |
| 1 | A | 182 | ARG | CB-CG | -5.99 | 1.36 | 1.52 |
| 2 | B | 355 | LEU | C-O | -5.98 | 1.11 | 1.23 |
| 2 | E | 122 | LYS | CD-CE | -5.98 | 1.36 | 1.51 |
| 1 | A | 254 | TYR | CE2-CZ | -5.97 | 1.30 | 1.38 |
| 1 | A | 201 | TYR | CG-CD2 | -5.96 | 1.31 | 1.39 |
| 1 | D | 317 | LEU | C-O | -5.96 | 1.12 | 1.23 |
| 1 | A | 402 | GLN | CD-NE2 | -5.95 | 1.18 | 1.32 |
| 1 | A | 97 | PHE | CE2-CZ | -5.95 | 1.26 | 1.37 |
| 2 | E | 14 | MET | C-O | -5.95 | 1.12 | 1.23 |
| 1 | A | 336 | LEU | CG-CD2 | -5.94 | 1.29 | 1.51 |
| 1 | A | 210 | PHE | CE1-CZ | -5.93 | 1.26 | 1.37 |
| 2 | B | 79 | ARG | C-O | -5.93 | 1.12 | 1.23 |
| 2 | B | 103 | PHE | C-O | -5.91 | 1.12 | 1.23 |
| 1 | A | 201 | TYR | CG-CD1 | -5.91 | 1.31 | 1.39 |
| 2 | B | 144 | HIS | C-O | -5.91 | 1.12 | 1.23 |
| 2 | B | 8 | TYR | CG-CD2 | -5.90 | 1.31 | 1.39 |
| 1 | A | 97 | PHE | CD1-CE1 | -5.89 | 1.27 | 1.39 |
| 3 | F | 100 | LYS | C-O | -5.89 | 1.12 | 1.23 |
| 2 | B | 382 | VAL | CB-CG2 | -5.88 | 1.40 | 1.52 |
| 1 | A | 83 | ARG | C-O | -5.87 | 1.12 | 1.23 |
| 1 | A | 334 | PRO | CB-CG | -5.87 | 1.20 | 1.50 |
| 1 | A | 226 | VAL | CB-CG1 | -5.86 | 1.40 | 1.52 |
| 1 | A | 315 | ARG | CZ-NH1 | -5.84 | 1.25 | 1.33 |
| 1 | A | 406 | GLU | CA-CB | -5.84 | 1.41 | 1.53 |
| 1 | A | 234 | PHE | CG-CD2 | -5.83 | 1.29 | 1.38 |
| 1 | A | 153 | PHE | CE2-CZ | -5.83 | 1.26 | 1.37 |
| 1 | A | 271 | TRP | CG-CD1 | -5.82 | 1.28 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | D | 408 | ARG | CZ-NH1 | -5.82 | 1.25 | 1.33 |
| 3 | C | 13 | VAL | CB-CG2 | -5.80 | 1.40 | 1.52 |
| 1 | A | 150 | GLU | CG-CD | 5.80 | 1.60 | 1.51 |
| 2 | B | 352 | LYS | C-O | -5.80 | 1.12 | 1.23 |
| 1 | A | 66 | LYS | C-O | -5.79 | 1.12 | 1.23 |
| 2 | B | 98 | ARG | C-O | -5.77 | 1.12 | 1.23 |
| 1 | A | 248 | GLN | C-O | -5.77 | 1.12 | 1.23 |
| 1 | A | 434 | ARG | C-O | -5.77 | 1.12 | 1.23 |
| 1 | A | 393 | GLU | CB-CG | -5.76 | 1.41 | 1.52 |
| 1 | A | 210 | PHE | CD1-CE1 | -5.76 | 1.27 | 1.39 |
| 1 | A | 14 | LYS | CE-NZ | 5.75 | 1.63 | 1.49 |
| 3 | F | 100 | LYS | CD-CE | -5.75 | 1.36 | 1.51 |
| 1 | A | 94 | VAL | CB-CG1 | -5.75 | 1.40 | 1.52 |
| 1 | A | 409 | HIS | C-O | -5.74 | 1.12 | 1.23 |
| 1 | A | 61 | GLY | C-O | -5.74 | 1.14 | 1.23 |
| 1 | A | 228 | SER | C-O | -5.74 | 1.12 | 1.23 |
| 1 | A | 394 | VAL | C-O | -5.73 | 1.12 | 1.23 |
| 2 | B | 170 | PHE | C-O | -5.72 | 1.12 | 1.23 |
| 2 | E | 251 | VAL | CB-CG2 | -5.72 | 1.40 | 1.52 |
| 2 | B | 103 | PHE | CE2-CZ | -5.70 | 1.26 | 1.37 |
| 1 | A | 72 | GLY | C-O | -5.70 | 1.14 | 1.23 |
| 2 | B | 195 | ALA | CA-CB | -5.70 | 1.40 | 1.52 |
| 2 | B | 226 | LEU | CG-CD2 | -5.70 | 1.30 | 1.51 |
| 1 | A | 271 | TRP | CD1-NE1 | -5.69 | 1.28 | 1.38 |
| 2 | E | 15 | GLU | C-O | -5.68 | 1.12 | 1.23 |
| 1 | A | 5 | PRO | C-O | -5.68 | 1.11 | 1.23 |
| 2 | B | 162 | VAL | C-O | -5.67 | 1.12 | 1.23 |
| 1 | A | 150 | GLU | C-O | -5.66 | 1.12 | 1.23 |
| 2 | B | 97 | THR | C-O | -5.66 | 1.12 | 1.23 |
| 1 | A | 317 | LEU | CG-CD2 | -5.65 | 1.30 | 1.51 |
| 1 | D | 434 | ARG | CZ-NH2 | -5.65 | 1.25 | 1.33 |
| 1 | A | 65 | TRP | CD2-CE2 | -5.65 | 1.34 | 1.41 |
| 1 | A | 406 | GLU | C-O | -5.64 | 1.12 | 1.23 |
| 1 | D | 56 | LEU | CG-CD1 | -5.64 | 1.30 | 1.51 |
| 1 | A | 11 | GLU | C-O | -5.64 | 1.12 | 1.23 |
| 1 | A | 151 | GLU | CB-CG | -5.63 | 1.41 | 1.52 |
| 2 | B | 384 | PHE | CD2-CE2 | -5.63 | 1.27 | 1.39 |
| 1 | A | 255 | VAL | C-O | -5.63 | 1.12 | 1.23 |
| 3 | F | 98 | LEU | CG-CD1 | -5.62 | 1.31 | 1.51 |
| 1 | D | 43 | PRO | CB-CG | -5.62 | 1.21 | 1.50 |
| 2 | E | 117 | ASP | CG-OD2 | -5.61 | 1.12 | 1.25 |
| 2 | B | 8 | TYR | CG-CD1 | -5.60 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 40 | TYR | CZ-OH | -5.59 | 1.28 | 1.37 |
| 1 | D | 317 | LEU | CG-CD2 | -5.58 | 1.31 | 1.51 |
| 2 | B | 80 | GLU | C-O | -5.58 | 1.12 | 1.23 |
| 2 | B | 83 | GLU | C-O | -5.58 | 1.12 | 1.23 |
| 1 | A | 223 | ASN | C-O | -5.58 | 1.12 | 1.23 |
| 2 | E | 343 | ARG | CZ-NH1 | -5.58 | 1.25 | 1.33 |
| 1 | D | 318 | LYS | C-O | -5.57 | 1.12 | 1.23 |
| 2 | B | 276 | GLY | C-O | -5.55 | 1.14 | 1.23 |
| 1 | A | 73 | VAL | CB-CG2 | -5.55 | 1.41 | 1.52 |
| 1 | A | 403 | HIS | C-O | -5.54 | 1.12 | 1.23 |
| 3 | F | 100 | LYS | CB-CG | -5.52 | 1.37 | 1.52 |
| 2 | E | 318 | LYS | CE-NZ | -5.51 | 1.35 | 1.49 |
| 1 | A | 195 | TYR | CB-CG | -5.51 | 1.43 | 1.51 |
| 2 | B | 19 | THR | C-O | -5.50 | 1.12 | 1.23 |
| 2 | B | 350 | TYR | CD1-CE1 | -5.50 | 1.31 | 1.39 |
| 1 | D | 275 | ASP | CG-OD1 | -5.50 | 1.12 | 1.25 |
| 2 | B | 9 | ASN | C-O | -5.50 | 1.12 | 1.23 |
| 2 | E | 122 | LYS | C-O | -5.49 | 1.12 | 1.23 |
| 1 | D | 394 | VAL | CB-CG2 | -5.49 | 1.41 | 1.52 |
| 2 | B | 28 | GLU | CD-OE1 | -5.48 | 1.19 | 1.25 |
| 2 | B | 98 | ARG | CZ-NH1 | -5.48 | 1.25 | 1.33 |
| 1 | A | 38 | LEU | C-O | -5.47 | 1.12 | 1.23 |
| 2 | B | 103 | PHE | CD1-CE1 | -5.47 | 1.28 | 1.39 |
| 1 | D | 62 | GLU | CD-OE2 | -5.46 | 1.19 | 1.25 |
| 2 | B | 220 | GLU | N-CA | -5.46 | 1.35 | 1.46 |
| 2 | B | 170 | PHE | CD1-CE1 | -5.45 | 1.28 | 1.39 |
| 3 | C | 13 | VAL | CB-CG1 | -5.45 | 1.41 | 1.52 |
| 1 | A | 40 | TYR | CE2-CZ | -5.45 | 1.31 | 1.38 |
| 1 | A | 160 | LEU | CG-CD2 | -5.44 | 1.31 | 1.51 |
| 1 | A | 272 | GLY | C-O | -5.44 | 1.15 | 1.23 |
| 2 | B | 350 | TYR | CE1-CZ | -5.44 | 1.31 | 1.38 |
| 2 | E | 243 | VAL | C-O | -5.43 | 1.13 | 1.23 |
| 1 | A | 432 | ARG | C-N | -5.41 | 1.21 | 1.34 |
| 2 | E | 343 | ARG | C-O | -5.40 | 1.13 | 1.23 |
| 1 | A | 418 | GLU | C-O | -5.39 | 1.13 | 1.23 |
| 1 | A | 174 | PRO | CA-C | 5.37 | 1.63 | 1.52 |
| 2 | B | 103 | PHE | CD2-CE2 | -5.36 | 1.28 | 1.39 |
| 1 | A | 434 | ARG | CZ-NH2 | -5.35 | 1.26 | 1.33 |
| 1 | A | 74 | PHE | CG-CD1 | -5.35 | 1.30 | 1.38 |
| 1 | A | 80 | VAL | CB-CG2 | -5.33 | 1.41 | 1.52 |
| 2 | E | 384 | PHE | C-O | -5.33 | 1.13 | 1.23 |
| 2 | B | 350 | TYR | CD2-CE2 | -5.33 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | D | 292 | GLU | CD-OE1 | -5.31 | 1.19 | 1.25 |
| 1 | A | 40 | TYR | CD2-CE2 | -5.31 | 1.31 | 1.39 |
| 1 | D | 436 | MET | C-O | -5.30 | 1.13 | 1.23 |
| 1 | A | 51 | LEU | CG-CD2 | -5.30 | 1.32 | 1.51 |
| 1 | A | 370 | MET | CB-CG | -5.28 | 1.34 | 1.51 |
| 2 | B | 191 | ASN | C-O | -5.26 | 1.13 | 1.23 |
| 1 | A | 227 | ALA | CA-CB | -5.26 | 1.41 | 1.52 |
| 1 | A | 249 | GLU | C-O | -5.25 | 1.13 | 1.23 |
| 2 | E | 244 | ASN | C-O | -5.25 | 1.13 | 1.23 |
| 2 | E | 343 | ARG | NE-CZ | -5.25 | 1.26 | 1.33 |
| 1 | A | 71 | VAL | C-O | -5.24 | 1.13 | 1.23 |
| 2 | B | 67 | CYS | C-O | -5.24 | 1.13 | 1.23 |
| 1 | D | 204 | GLU | CD-OE2 | -5.23 | 1.19 | 1.25 |
| 1 | A | 203 | ASP | C-O | -5.23 | 1.13 | 1.23 |
| 2 | E | 120 | THR | C-O | -5.22 | 1.13 | 1.23 |
| 2 | E | 57 | LYS | CD-CE | -5.22 | 1.38 | 1.51 |
| 2 | B | 66 | ARG | NE-CZ | -5.21 | 1.26 | 1.33 |
| 1 | D | 318 | LYS | CE-NZ | -5.20 | 1.36 | 1.49 |
| 2 | E | 384 | PHE | CG-CD1 | -5.20 | 1.30 | 1.38 |
| 1 | D | 133 | HIS | C-O | -5.19 | 1.13 | 1.23 |
| 1 | A | 175 | GLU | CG-CD | 5.18 | 1.59 | 1.51 |
| 1 | A | 126 | GLY | C-O | -5.18 | 1.15 | 1.23 |
| 1 | A | 203 | ASP | CG-OD1 | -5.18 | 1.13 | 1.25 |
| 1 | A | 292 | GLU | CD-OE2 | -5.17 | 1.20 | 1.25 |
| 2 | B | 83 | GLU | C-N | -5.17 | 1.22 | 1.34 |
| 1 | A | 102 | LEU | C-O | -5.16 | 1.13 | 1.23 |
| 3 | C | 15 | GLU | CB-CG | -5.16 | 1.42 | 1.52 |
| 1 | A | 271 | TRP | C-O | -5.16 | 1.13 | 1.23 |
| 1 | A | 195 | TYR | C-O | -5.15 | 1.13 | 1.23 |
| 2 | B | 306 | VAL | C-O | -5.15 | 1.13 | 1.23 |
| 2 | B | 117 | ASP | CG-OD1 | -5.14 | 1.13 | 1.25 |
| 1 | A | 163 | ASP | C-O | -5.14 | 1.13 | 1.23 |
| 2 | B | 220 | GLU | CA-CB | -5.12 | 1.42 | 1.53 |
| 1 | A | 356 | ASP | CG-OD1 | -5.12 | 1.13 | 1.25 |
| 2 | E | 120 | THR | CA-CB | -5.11 | 1.40 | 1.53 |
| 1 | A | 358 | VAL | CB-CG2 | -5.11 | 1.42 | 1.52 |
| 1 | A | 275 | ASP | C-O | -5.11 | 1.13 | 1.23 |
| 1 | A | 154 | PHE | CD1-CE1 | -5.10 | 1.29 | 1.39 |
| 1 | A | 273 | LYS | CB-CG | -5.10 | 1.38 | 1.52 |
| 2 | E | 194 | GLY | N-CA | -5.10 | 1.38 | 1.46 |
| 1 | A | 101 | ARG | CZ-NH1 | -5.10 | 1.26 | 1.33 |
| 1 | A | 84 | TYR | CD2-CE2 | -5.09 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 246 | ILE | CB-CG2 | -5.08 | 1.37 | 1.52 |
| 2 | B | 329 | GLU | C-O | -5.07 | 1.13 | 1.23 |
| 3 | F | 104 | CYS | N-CA | -5.07 | 1.36 | 1.46 |
| 3 | F | 105 | VAL | C-O | -5.06 | 1.13 | 1.23 |
| 1 | A | 151 | GLU | CD-OE1 | -5.06 | 1.20 | 1.25 |
| 2 | B | 8 | TYR | CE2-CZ | -5.05 | 1.31 | 1.38 |
| 1 | A | 291 | TYR | CD2-CE2 | -5.04 | 1.31 | 1.39 |
| 2 | B | 102 | GLU | C-O | -5.04 | 1.13 | 1.23 |
| 1 | D | 336 | LEU | CG-CD1 | -5.04 | 1.33 | 1.51 |
| 2 | B | 351 | GLU | CB-CG | -5.04 | 1.42 | 1.52 |
| 3 | F | 37 | GLU | CD-OE2 | -5.04 | 1.20 | 1.25 |
| 1 | A | 299 | ASP | CG-OD1 | -5.03 | 1.13 | 1.25 |
| 1 | A | 65 | TRP | CB-CG | -5.03 | 1.41 | 1.50 |
| 1 | A | 153 | PHE | CD1-CE1 | -5.03 | 1.29 | 1.39 |
| 1 | A | 410 | ASN | C-O | -5.03 | 1.13 | 1.23 |
| 2 | B | 18 | ILE | CB-CG2 | -5.03 | 1.37 | 1.52 |
| 2 | E | 248 | VAL | C-O | -5.01 | 1.13 | 1.23 |

All (76) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 83 | ARG | NE-CZ-NH2 | -28.06 | 106.27 | 120.30 |
| 3 | F | 67 | ARG | NE-CZ-NH1 | 25.12 | 132.86 | 120.30 |
| 1 | D | 432 | ARG | NE-CZ-NH2 | -22.41 | 109.09 | 120.30 |
| 1 | D | 437 | ARG | NE-CZ-NH2 | -18.76 | 110.92 | 120.30 |
| 3 | F | 67 | ARG | NE-CZ-NH2 | -17.91 | 111.34 | 120.30 |
| 1 | D | 432 | ARG | NE-CZ-NH1 | 16.75 | 128.68 | 120.30 |
| 1 | A | 315 | ARG | NE-CZ-NH2 | 15.66 | 128.13 | 120.30 |
| 1 | D | 269 | ARG | NE-CZ-NH2 | 15.48 | 128.04 | 120.30 |
| 1 | A | 83 | ARG | NE-CZ-NH1 | 14.31 | 127.46 | 120.30 |
| 1 | D | 102 | LEU | CB-CG-CD1 | -14.18 | 86.89 | 111.00 |
| 2 | B | 20 | ASP | CB-CG-OD1 | 12.51 | 129.56 | 118.30 |
| 1 | A | 315 | ARG | NE-CZ-NH1 | -12.20 | 114.20 | 120.30 |
| 1 | D | 437 | ARG | NE-CZ-NH1 | 12.14 | 126.37 | 120.30 |
| 1 | D | 434 | ARG | NE-CZ-NH1 | 12.04 | 126.32 | 120.30 |
| 1 | D | 427 | ASP | CB-CG-OD1 | 11.17 | 128.35 | 118.30 |
| 2 | B | 329 | GLU | OE1-CD-OE2 | -11.08 | 110.01 | 123.30 |
| 1 | D | 269 | ARG | NE-CZ-NH1 | -10.77 | 114.91 | 120.30 |
| 1 | A | 356 | ASP | CB-CG-OD1 | 10.50 | 127.75 | 118.30 |
| 2 | B | 256 | ASP | CB-CG-OD2 | -10.21 | 109.11 | 118.30 |
| 2 | E | 24 | ARG | NE-CZ-NH1 | 10.18 | 125.39 | 120.30 |
| 3 | F | 67 | ARG | CD-NE-CZ | 9.70 | 137.19 | 123.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 39 | ASP | CB-CG-OD1 | 9.25 | 126.62 | 118.30 |
| 1 | D | 275 | ASP | CB-CG-OD1 | 9.01 | 126.41 | 118.30 |
| 1 | D | 434 | ARG | NE-CZ-NH2 | -8.24 | 116.18 | 120.30 |
| 2 | E | 117 | ASP | CB-CG-OD1 | 8.05 | 125.54 | 118.30 |
| 1 | D | 101 | ARG | NE-CZ-NH2 | 8.03 | 124.31 | 120.30 |
| 1 | A | 102 | LEU | CA-CB-CG | 7.89 | 133.45 | 115.30 |
| 2 | B | 256 | ASP | CB-CG-OD1 | 7.75 | 125.27 | 118.30 |
| 1 | D | 432 | ARG | CD-NE-CZ | 7.67 | 134.34 | 123.60 |
| 1 | D | 427 | ASP | CB-CG-OD2 | -7.63 | 111.43 | 118.30 |
| 2 | E | 257 | ARG | NE-CZ-NH1 | 7.61 | 124.11 | 120.30 |
| 1 | A | 408 | ARG | NE-CZ-NH1 | -7.33 | 116.63 | 120.30 |
| 1 | A | 182 | ARG | NE-CZ-NH2 | 7.32 | 123.96 | 120.30 |
| 1 | A | 356 | ASP | OD1-CG-OD2 | -7.23 | 109.57 | 123.30 |
| 2 | E | 220 | GLU | CG-CD-OE2 | -7.18 | 103.95 | 118.30 |
| 1 | A | 36 | LYS | CD-CE-NZ | 6.93 | 127.63 | 111.70 |
| 1 | A | 160 | LEU | CB-CG-CD2 | 6.90 | 122.73 | 111.00 |
| 2 | B | 192 | MET | CG-SD-CE | 6.90 | 111.24 | 100.20 |
| 2 | B | 117 | ASP | CB-CG-OD1 | 6.77 | 124.39 | 118.30 |
| 2 | B | 384 | PHE | CD1-CE1-CZ | 6.62 | 128.04 | 120.10 |
| 3 | C | 104 | CYS | O-C-N | 6.58 | 133.22 | 122.70 |
| 1 | D | 437 | ARG | CD-NE-CZ | 6.49 | 132.68 | 123.60 |
| 1 | A | 406 | GLU | CB-CA-C | -6.43 | 97.55 | 110.40 |
| 1 | A | 273 | LYS | CD-CE-NZ | 6.42 | 126.45 | 111.70 |
| 2 | E | 117 | ASP | OD1-CG-OD2 | -6.41 | 111.11 | 123.30 |
| 2 | E | 220 | GLU | CB-CA-C | -6.34 | 97.71 | 110.40 |
| 2 | E | 220 | GLU | CG-CD-OE1 | 6.27 | 130.85 | 118.30 |
| 1 | A | 321 | ASP | CB-CG-OD1 | 6.22 | 123.89 | 118.30 |
| 1 | A | 83 | ARG | CD-NE-CZ | 6.20 | 132.28 | 123.60 |
| 2 | E | 120 | THR | OG1-CB-CG2 | 6.08 | 123.99 | 110.00 |
| 2 | B | 384 | PHE | CG-CD2-CE2 | -5.97 | 114.23 | 120.80 |
| 1 | D | 101 | ARG | NE-CZ-NH1 | -5.89 | 117.35 | 120.30 |
| 1 | A | 299 | ASP | CB-CG-OD1 | 5.79 | 123.51 | 118.30 |
| 2 | B | 220 | GLU | OE1-CD-OE2 | 5.71 | 130.15 | 123.30 |
| 1 | D | 408 | ARG | NE-CZ-NH2 | 5.69 | 123.15 | 120.30 |
| 1 | A | 247 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 2 | E | 120 | THR | CA-CB-OG1 | 5.61 | 120.79 | 109.00 |
| 2 | E | 117 | ASP | CB-CG-OD2 | 5.59 | 123.33 | 118.30 |
| 1 | D | 4 | HIS | CB-CA-C | 5.58 | 121.55 | 110.40 |
| 3 | F | 104 | CYS | C-N-CA | 5.55 | 135.59 | 121.70 |
| 1 | D | 4 | HIS | N-CA-CB | 5.43 | 120.37 | 110.60 |
| 2 | B | 352 | LYS | CD-CE-NZ | 5.40 | 124.12 | 111.70 |
| 2 | E | 257 | ARG | NH1-CZ-NH2 | -5.37 | 113.49 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 163 | ASP | CB-CG-OD1 | 5.35 | 123.11 | 118.30 |
| 2 | B | 143 | VAL | CG1-CB-CG2 | -5.33 | 102.37 | 110.90 |
| 1 | A | 125 | ARG | NE-CZ-NH1 | 5.31 | 122.96 | 120.30 |
| 1 | A | 247 | ASP | CB-CG-OD2 | -5.30 | 113.53 | 118.30 |
| 1 | A | 83 | ARG | NH1-CZ-NH2 | 5.25 | 125.18 | 119.40 |
| 1 | A | 334 | PRO | CA-N-CD | -5.25 | 104.15 | 111.50 |
| 1 | D | 391 | LEU | CB-CG-CD2 | 5.22 | 119.87 | 111.00 |
| 1 | A | 317 | LEU | CB-CG-CD1 | 5.21 | 119.86 | 111.00 |
| 1 | A | 432 | ARG | NE-CZ-NH2 | 5.16 | 122.88 | 120.30 |
| 1 | D | 269 | ARG | CB-CG-CD | 5.10 | 124.87 | 111.60 |
| 1 | A | 207 | ARG | NE-CZ-NH2 | 5.09 | 122.85 | 120.30 |
| 1 | A | 275 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |
| 2 | B | 52 | LEU | CA-CB-CG | 5.04 | 126.88 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3422 | 0 | 3275 | 99 | 0 |
| 1 | D | 3422 | 0 | 3275 | 113 | 0 |
| 2 | B | 2999 | 0 | 2963 | 79 | 0 |
| 2 | E | 2999 | 0 | 2963 | 78 | 0 |
| 3 | C | 787 | 0 | 757 | 49 | 0 |
| 3 | F | 787 | 0 | 758 | 46 | 0 |
| 4 | A | 4 | 0 | 0 | 0 | 0 |
| 4 | D | 4 | 0 | 0 | 0 | 0 |
| 5 | A | 63 | 0 | 33 | 12 | 0 |
| 5 | B | 62 | 0 | 35 | 8 | 0 |
| 5 | D | 63 | 0 | 35 | 10 | 0 |
| 5 | E | 62 | 0 | 34 | 5 | 0 |
| 6 | A | 16 | 0 | 0 | 0 | 0 |
| 6 | B | 16 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6 | D | 16 | 0 | 0 | 0 | 0 |
| 6 | E | 16 | 0 | 0 | 0 | 0 |
| 7 | A | 164 | 0 | 0 | 10 | 0 |
| 7 | B | 160 | 0 | 0 | 4 | 0 |
| 7 | C | 12 | 0 | 0 | 1 | 0 |
| 7 | D | 220 | 0 | 0 | 8 | 0 |
| 7 | E | 155 | 0 | 0 | 3 | 0 |
| 7 | F | 18 | 0 | 0 | 0 | 0 |
| All | All | 15467 | 0 | 14128 | 408 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (408) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:A:580:SRM:HHA | 3:C:104:CYS:SG | 1.36 | 1.62 |
| 5:D:582:SRM:HHA | 3:F:104:CYS:SG | 1.47 | 1.51 |
| 5:A:580:SRM:CHA | 3:C:104:CYS:SG | 2.10 | 1.39 |
| 7:A:6631:HOH:O | 3:C:105:VAL:CG2 | 1.75 | 1.34 |
| 5:D:582:SRM:CHA | 3:F:104:CYS:SG | 2.20 | 1.29 |
| 1:A:427:ASP:OD2 | 1:A:429:SER:HB3 | 1.38 | 1.24 |
| 1:D:3:LYS:HA | 1:D:4:HIS:HB3 | 1.14 | 1.12 |
| 1:A:3:LYS:O | 1:A:3:LYS:HG3 | 1.41 | 1.07 |
| 1:D:167:SER:HB2 | 3:F:105:VAL:HG21 | 1.33 | 1.06 |
| 2:E:382:VAL:CG2 | 2:E:384:PHE:HD1 | 1.68 | 1.06 |
| 3:F:13:VAL:HG11 | 3:F:17:GLY:HA2 | 1.40 | 1.04 |
| 5:B:581:SRM:HBA1 | 5:B:581:SRM:HMA3 | 1.36 | 1.02 |
| 3:C:3:VAL:HG22 | 3:C:12:GLU:OE2 | 1.61 | 0.99 |
| 7:A:6631:HOH:O | 3:C:105:VAL:HG21 | 1.39 | 0.99 |
| 1:D:3:LYS:O | 1:D:3:LYS:HD3 | 1.63 | 0.98 |
| 7:D:6726:HOH:O | 3:F:105:VAL:HG23 | 1.63 | 0.97 |
| 2:E:196:VAL:HG11 | 2:E:204:VAL:HG22 | 1.47 | 0.97 |
| 1:A:39:ASP:OD1 | 2:B:2:ALA:HA | 1.65 | 0.96 |
| 5:B:581:SRM:CBA | 5:B:581:SRM:HMA3 | 1.92 | 0.94 |
| 1:D:3:LYS:CA | 1:D:4:HIS:HB3 | 1.97 | 0.94 |
| 2:B:382:VAL:CG2 | 2:B:384:PHE:HD1 | 1.80 | 0.94 |
| 1:A:70:ILE:HG12 | 3:C:100:LYS:HD2 | 1.49 | 0.94 |
| 5:E:583:SRM:HMA3 | 5:E:583:SRM:HBA1 | 1.48 | 0.93 |
| 3:C:26:CYS:SG | 3:C:28:GLU:HG2 | 2.10 | 0.91 |
| 2:B:382:VAL:HG23 | 2:B:384:PHE:HD1 | 1.34 | 0.91 |
| 2:E:196:VAL:HG11 | 2:E:204:VAL:CG2 | 2.01 | 0.90 |
| 2:E:382:VAL:HG23 | 2:E:384:PHE:HD1 | 1.36 | 0.90 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:104:GLN:HE21 | 1:D:104:GLN:H | 1.20 | 0.89 |
| 3:C:3:VAL:CG2 | 3:C:12:GLU:OE2 | 2.21 | 0.88 |
| 1:D:97:PHE:O | 2:E:150:TYR:HE1 | 1.59 | 0.86 |
| 1:A:69:GLY:O | 1:A:70:ILE:HD13 | 1.74 | 0.86 |
| 2:E:382:VAL:HG21 | 2:E:384:PHE:HD1 | 1.40 | 0.85 |
| 1:D:34:ASN:HD21 | 1:D:38:LEU:H | 1.23 | 0.85 |
| 1:A:97:PHE:O | 2:B:150:TYR:CE1 | 2.30 | 0.84 |
| 1:A:104:GLN:HE21 | 1:A:104:GLN:H | 1.25 | 0.83 |
| 1:A:97:PHE:O | 2:B:150:TYR:HE1 | 1.61 | 0.83 |
| 1:D:104:GLN:NE2 | 1:D:104:GLN:H | 1.77 | 0.82 |
| 5:B:581:SRM:HBA1 | 5:B:581:SRM:CMA | 2.10 | 0.81 |
| 7:D:6726:HOH:O | 3:F:105:VAL:CG2 | 2.21 | 0.80 |
| 7:A:6631:HOH:O | 3:C:105:VAL:HG23 | 1.52 | 0.80 |
| 1:D:3:LYS:HA | 1:D:4:HIS:CB | 2.02 | 0.80 |
| 1:D:402:GLN:H | 1:D:402:GLN:HE21 | 1.29 | 0.80 |
| 1:D:3:LYS:O | 1:D:3:LYS:CG | 2.30 | 0.80 |
| 3:F:26:CYS:SG | 3:F:28:GLU:OE2 | 2.41 | 0.79 |
| 1:D:3:LYS:O | 1:D:3:LYS:CD | 2.30 | 0.79 |
| 1:D:97:PHE:O | 2:E:150:TYR:CE1 | 2.36 | 0.79 |
| 2:B:382:VAL:CG2 | 2:B:384:PHE:CD1 | 2.65 | 0.79 |
| 3:C:105:VAL:OXT | 3:C:105:VAL:HG12 | 1.82 | 0.78 |
| 2:B:37:ASN:HD21 | 2:B:58:ASN:HD21 | 1.29 | 0.78 |
| 2:E:37:ASN:HD21 | 2:E:58:ASN:HD21 | 1.28 | 0.78 |
| 1:D:170:ASN:ND2 | 1:D:208:PRO:HG3 | 1.99 | 0.78 |
| 1:A:104:GLN:H | 1:A:104:GLN:NE2 | 1.82 | 0.77 |
| 1:D:131:ASN:HB2 | 1:D:140:VAL:HB | 1.66 | 0.77 |
| 1:D:416:LYS:HB2 | 1:D:419:GLU:HG3 | 1.66 | 0.77 |
| 2:E:382:VAL:CG2 | 2:E:384:PHE:CD1 | 2.61 | 0.77 |
| 1:A:34:ASN:HD21 | 1:A:38:LEU:H | 1.32 | 0.76 |
| 2:E:382:VAL:HG23 | 2:E:384:PHE:CD1 | 2.20 | 0.76 |
| 3:F:28:GLU:HA | 3:F:31:LYS:HE2 | 1.67 | 0.76 |
| 2:E:382:VAL:HG21 | 2:E:384:PHE:CD1 | 2.21 | 0.76 |
| 3:C:49:ILE:HD11 | 3:C:75:PHE:HD1 | 1.50 | 0.75 |
| 1:D:308:HIS:HD2 | 2:E:292:ARG:HE | 1.35 | 0.75 |
| 3:F:13:VAL:HG11 | 3:F:17:GLY:CA | 2.15 | 0.74 |
| 2:E:208:ARG:HD2 | 2:E:305:PHE:CE1 | 2.23 | 0.73 |
| 1:D:262:ASN:ND2 | 2:E:292:ARG:HH22 | 1.86 | 0.73 |
| 1:A:69:GLY:C | 1:A:70:ILE:HD13 | 2.09 | 0.73 |
| 3:F:13:VAL:HG12 | 3:F:14:ASP:N | 2.02 | 0.73 |
| 1:D:5:PRO:HG2 | 1:D:5:PRO:O | 1.88 | 0.72 |
| 1:A:83:ARG:CD | 2:B:150:TYR:O | 2.38 | 0.72 |
| 2:B:382:VAL:HG21 | 2:B:384:PHE:CD1 | 2.24 | 0.72 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:402:GLN:H | 1:D:402:GLN:NE2 | 1.88 | 0.72 |
| 1:D:408:ARG:HH11 | 1:D:410:ASN:HD21 | 1.38 | 0.71 |
| 1:A:402:GLN:HE21 | 1:A:402:GLN:H | 1.37 | 0.71 |
| 1:A:46:CYS:HB3 | 1:A:47:PRO:HD3 | 1.72 | 0.71 |
| 1:D:104:GLN:HE22 | 1:D:173:THR:HG21 | 1.54 | 0.71 |
| 1:A:83:ARG:HD3 | 2:B:150:TYR:O | 1.91 | 0.70 |
| 1:A:3:LYS:O | 1:A:3:LYS:CG | 2.30 | 0.70 |
| 3:C:49:ILE:HD11 | 3:C:75:PHE:CD1 | 2.26 | 0.70 |
| 1:A:167:SER:HB2 | 3:C:105:VAL:HG21 | 1.73 | 0.70 |
| 1:A:308:HIS:HD2 | 2:B:292:ARG:HE | 1.37 | 0.70 |
| 5:D:582:SRM:O1A | 2:E:150:TYR:HD2 | 1.74 | 0.69 |
| 1:D:184:GLU:OE1 | 2:E:44:HIS:HD2 | 1.75 | 0.69 |
| 1:D:81:ILE:CD1 | 3:F:105:VAL:HG22 | 2.22 | 0.69 |
| 2:B:9:ASN:C | 2:B:9:ASN:HD22 | 1.93 | 0.69 |
| 1:A:427:ASP:OD2 | 1:A:429:SER:CB | 2.29 | 0.69 |
| 1:A:70:ILE:HG12 | 3:C:100:LYS:CD | 2.23 | 0.69 |
| 3:F:105:VAL:HG12 | 3:F:105:VAL:OXT | 1.91 | 0.69 |
| 1:D:83:ARG:H | 1:D:98:HIS:HD2 | 1.40 | 0.69 |
| 1:D:104:GLN:N | 1:D:104:GLN:HE21 | 1.90 | 0.69 |
| 1:A:285:PRO:HG3 | 2:B:293:ILE:HA | 1.75 | 0.68 |
| 3:F:26:CYS:SG | 3:F:28:GLU:HG2 | 2.33 | 0.68 |
| 1:A:427:ASP:CG | 1:A:429:SER:HB3 | 2.12 | 0.68 |
| 1:A:427:ASP:OD2 | 1:A:430:ASP:OD1 | 2.12 | 0.67 |
| 1:A:83:ARG:H | 1:A:98:HIS:HD2 | 1.40 | 0.67 |
| 1:A:248:GLN:HE22 | 1:A:296:LEU:H | 1.42 | 0.67 |
| 1:D:3:LYS:HG3 | 1:D:3:LYS:O | 1.93 | 0.67 |
| 1:D:170:ASN:HD22 | 1:D:208:PRO:HG3 | 1.60 | 0.67 |
| 1:D:223:ASN:HD21 | 1:D:311:ASN:HD21 | 1.40 | 0.67 |
| 5:B:581:SRM:HBA1 | 5:B:581:SRM:C1A | 2.24 | 0.66 |
| 2:E:293:ILE:HG22 | 2:E:294:LYS:HD2 | 1.78 | 0.66 |
| 1:A:167:SER:OG | 3:C:105:VAL:HG11 | 1.95 | 0.66 |
| 3:F:13:VAL:CG1 | 3:F:17:GLY:HA2 | 2.23 | 0.66 |
| 2:E:208:ARG:HD3 | 2:E:278:GLY:O | 1.96 | 0.66 |
| 2:E:224:ILE:HB | 2:E:225:PRO:HD3 | 1.78 | 0.66 |
| 2:B:9:ASN:ND2 | 2:B:11:ALA:H | 1.94 | 0.65 |
| 1:A:408:ARG:HH11 | 1:A:410:ASN:HD21 | 1.44 | 0.65 |
| 2:B:4:ILE:HG13 | 2:B:4:ILE:O | 1.95 | 0.65 |
| 1:A:411:PRO:HG3 | 2:E:192:MET:CE | 2.26 | 0.64 |
| 5:D:582:SRM:HMA2 | 3:F:104:CYS:SG | 2.38 | 0.64 |
| 1:D:376:ARG:NH1 | 1:D:376:ARG:HB3 | 2.14 | 0.63 |
| 3:C:3:VAL:HG22 | 3:C:12:GLU:HG3 | 1.81 | 0.63 |
| 2:E:239:ILE:HG12 | 2:E:252:ALA:HB2 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:46:CYS:HB3 | 1:D:47:PRO:HD3 | 1.81 | 0.63 |
| 5:B:581:SRM:C1A | 5:B:581:SRM:CBA | 2.76 | 0.62 |
| 1:A:104:GLN:HE21 | 1:A:104:GLN:N | 1.97 | 0.62 |
| 1:D:3:LYS:HE2 | 1:D:4:HIS:ND1 | 2.14 | 0.62 |
| 1:A:402:GLN:NE2 | 1:A:402:GLN:H | 1.97 | 0.61 |
| 1:A:223:ASN:HD21 | 1:A:311:ASN:HD21 | 1.48 | 0.61 |
| 3:F:3:VAL:HG22 | 3:F:12:GLU:HG2 | 1.82 | 0.61 |
| 1:A:36:LYS:HB2 | 7:A:6638:HOH:O | 1.99 | 0.61 |
| 3:F:78:LYS:O | 3:F:82:GLU:HG3 | 2.00 | 0.61 |
| 2:B:142:ILE:O | 2:B:144:HIS:HD2 | 1.84 | 0.61 |
| 2:B:207:HIS:HD2 | 2:B:279:ASP:OD1 | 1.83 | 0.61 |
| 3:C:78:LYS:O | 3:C:82:GLU:HG3 | 2.01 | 0.61 |
| 5:A:580:SRM:C1A | 3:C:104:CYS:SG | 2.84 | 0.61 |
| 1:D:418:GLU:H | 1:D:418:GLU:CD | 2.03 | 0.61 |
| 3:C:11:PHE:HE2 | 3:C:26:CYS:HG | 1.48 | 0.60 |
| 2:B:107:ASN:ND2 | 2:B:110:THR:H | 1.99 | 0.60 |
| 5:D:582:SRM:C1A | 3:F:104:CYS:SG | 2.88 | 0.60 |
| 3:C:26:CYS:HB2 | 3:C:27:PRO:CD | 2.31 | 0.60 |
| 2:E:247:LYS:HZ3 | 2:E:247:LYS:HB3 | 1.65 | 0.60 |
| 1:A:410:ASN:HD22 | 1:A:412:TYR:H | 1.50 | 0.60 |
| 1:D:156:MET:HE3 | 1:D:162:THR:HB | 1.83 | 0.60 |
| 5:B:581:SRM:NA | 5:B:581:SRM:HBA2 | 2.17 | 0.59 |
| 1:A:435:HIS:HD2 | 1:D:86:ASP:OD2 | 1.85 | 0.59 |
| 2:B:11:ALA:C | 2:B:13:PRO:HD3 | 2.22 | 0.59 |
| 3:F:13:VAL:CG1 | 3:F:17:GLY:CA | 2.79 | 0.59 |
| 2:B:367:ASP:N | 2:B:368:PRO:HD2 | 2.18 | 0.59 |
| 1:D:230:ALA:HB2 | 2:E:289:ILE:HD13 | 1.84 | 0.59 |
| 1:D:167:SER:OG | 3:F:105:VAL:HG11 | 2.03 | 0.58 |
| 1:D:196:GLN:HE22 | 1:D:354:PRO:HA | 1.68 | 0.58 |
| 1:A:206:HIS:HD2 | 7:A:6580:HOH:O | 1.85 | 0.58 |
| 2:B:382:VAL:HG23 | 2:B:384:PHE:CD1 | 2.26 | 0.58 |
| 1:D:248:GLN:HE22 | 1:D:296:LEU:H | 1.50 | 0.58 |
| 1:A:313:MET:HE3 | 1:A:317:LEU:HD11 | 1.84 | 0.58 |
| 1:A:62:GLU:OE1 | 1:D:435:HIS:HE1 | 1.86 | 0.58 |
| 2:B:75:THR:O | 2:B:79:ARG:HG3 | 2.04 | 0.58 |
| 2:E:37:ASN:ND2 | 2:E:58:ASN:HD21 | 2.01 | 0.58 |
| 1:A:98:HIS:HA | 2:B:150:TYR:OH | 2.03 | 0.58 |
| 1:D:45:GLU:H | 1:D:45:GLU:CD | 2.08 | 0.58 |
| 1:D:34:ASN:ND2 | 1:D:38:LEU:H | 1.97 | 0.57 |
| 1:D:98:HIS:HE1 | 1:D:146:THR:OG1 | 1.86 | 0.57 |
| 3:F:67:ARG:HG3 | 3:F:68:ILE:N | 2.20 | 0.57 |
| 1:D:363:GLU:O | 1:D:367:GLU:HG3 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 7:B:949:HOH:O | 1:D:432:ARG:HD3 | 2.04 | 0.57 |
| 1:D:416:LYS:HB3 | 1:D:418:GLU:OE2 | 2.03 | 0.57 |
| 1:D:3:LYS:C | 1:D:3:LYS:HD3 | 2.24 | 0.57 |
| 3:F:49:ILE:HD11 | 3:F:75:PHE:HD1 | 1.69 | 0.57 |
| 1:A:108:LYS:HD3 | 1:A:133:HIS:CE1 | 2.40 | 0.57 |
| 2:B:300:LYS:HB3 | 1:D:407:PRO:HG2 | 1.87 | 0.57 |
| 3:F:13:VAL:HG12 | 3:F:14:ASP:H | 1.70 | 0.56 |
| 2:B:48:GLU:HB3 | 2:B:49:PRO:CD | 2.35 | 0.56 |
| 1:A:131:ASN:HB2 | 1:A:140:VAL:HB | 1.86 | 0.56 |
| 2:B:153:THR:N | 2:B:154:PRO:CD | 2.67 | 0.56 |
| 5:D:582:SRM:O1A | 2:E:150:TYR:CD2 | 2.57 | 0.56 |
| 3:C:3:VAL:HG21 | 3:C:12:GLU:OE2 | 2.05 | 0.56 |
| 2:B:9:ASN:ND2 | 2:B:9:ASN:C | 2.56 | 0.56 |
| 1:A:184:GLU:OE1 | 2:B:44:HIS:HD2 | 1.87 | 0.56 |
| 2:E:247:LYS:NZ | 2:E:247:LYS:HB3 | 2.22 | 0.55 |
| 2:B:200:ASP:HB3 | 2:B:337:ILE:HD12 | 1.87 | 0.55 |
| 3:C:4:VAL:O | 3:C:10:ALA:HA | 2.06 | 0.55 |
| 1:A:33:LYS:HG3 | 7:A:6734:HOH:O | 2.07 | 0.55 |
| 1:A:81:ILE:CD1 | 3:C:105:VAL:HG22 | 2.37 | 0.54 |
| 5:A:580:SRM:O1A | 2:B:150:TYR:HD2 | 1.91 | 0.54 |
| 1:A:305:ARG:NH2 | 2:E:379:PHE:O | 2.39 | 0.54 |
| 1:D:308:HIS:CD2 | 2:E:292:ARG:HE | 2.21 | 0.54 |
| 1:A:227:ALA:CB | 2:B:289:ILE:HD13 | 2.37 | 0.54 |
| 1:A:376:ARG:HB3 | 1:A:376:ARG:NH1 | 2.21 | 0.54 |
| 3:F:21:ALA:HB3 | 3:F:24:ASP:OD2 | 2.06 | 0.54 |
| 1:D:229:MET:HB3 | 2:E:289:ILE:HD11 | 1.90 | 0.54 |
| 1:D:206:HIS:HD2 | 7:D:6634:HOH:O | 1.90 | 0.54 |
| 1:A:83:ARG:HD2 | 2:B:150:TYR:O | 2.07 | 0.54 |
| 3:C:3:VAL:HG22 | 3:C:12:GLU:CD | 2.27 | 0.54 |
| 3:F:49:ILE:HD13 | 3:F:73:THR:HG21 | 1.90 | 0.54 |
| 3:C:91:GLY:O | 3:C:95:MET:HG3 | 2.07 | 0.54 |
| 1:A:411:PRO:HG3 | 2:E:192:MET:HE2 | 1.90 | 0.53 |
| 1:A:435:HIS:HE1 | 1:D:62:GLU:OE1 | 1.91 | 0.53 |
| 1:D:306:CYS:O | 1:D:307:MET:HB2 | 2.08 | 0.53 |
| 1:A:306:CYS:O | 1:A:307:MET:HB2 | 2.09 | 0.53 |
| 7:A:6604:HOH:O | 2:B:125:ALA:HB3 | 2.07 | 0.53 |
| 1:D:376:ARG:HB3 | 1:D:376:ARG:HH11 | 1.74 | 0.53 |
| 2:B:37:ASN:ND2 | 2:B:58:ASN:HD21 | 2.03 | 0.53 |
| 5:A:580:SRM:HMA2 | 3:C:104:CYS:SG | 2.49 | 0.53 |
| 3:F:13:VAL:HG13 | 3:F:18:PHE:O | 2.09 | 0.53 |
| 1:D:334:PRO:HD2 | 7:E:841:HOH:O | 2.09 | 0.53 |
| 1:A:227:ALA:HB1 | 2:B:289:ILE:HD13 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:390:LYS:HD3 | 1:D:390:LYS:O | 2.08 | 0.52 |
| 1:A:50:LEU:C | 1:A:50:LEU:HD13 | 2.29 | 0.52 |
| 3:F:13:VAL:CG1 | 3:F:14:ASP:N | 2.72 | 0.52 |
| 3:F:13:VAL:CG1 | 3:F:17:GLY:C | 2.77 | 0.52 |
| 2:B:186:LEU:C | 2:B:186:LEU:HD23 | 2.29 | 0.52 |
| 2:E:146:GLN:HE21 | 2:E:150:TYR:HB3 | 1.74 | 0.52 |
| 2:B:300:LYS:CB | 1:D:407:PRO:HG2 | 2.40 | 0.52 |
| 5:D:582:SRM:HBA1 | 5:D:582:SRM:HHB | 1.91 | 0.52 |
| 2:E:280:GLY:HA3 | 2:E:305:PHE:CE1 | 2.45 | 0.52 |
| 1:D:410:ASN:HD22 | 1:D:412:TYR:H | 1.57 | 0.52 |
| 2:E:48:GLU:HB2 | 2:E:49:PRO:CD | 2.40 | 0.52 |
| 1:A:349:ILE:HD11 | 1:A:357:GLU:HB3 | 1.92 | 0.52 |
| 1:A:70:ILE:HG13 | 3:C:101:PRO:HD2 | 1.92 | 0.52 |
| 2:E:153:THR:N | 2:E:154:PRO:CD | 2.72 | 0.52 |
| 3:C:3:VAL:HG22 | 3:C:12:GLU:CG | 2.40 | 0.52 |
| 2:E:220:GLU:HB3 | 3:F:20:ASN:O | 2.10 | 0.51 |
| 2:B:254:ASN:HD21 | 2:B:256:ASP:HB2 | 1.76 | 0.51 |
| 5:E:583:SRM:NA | 5:E:583:SRM:HBA2 | 2.25 | 0.51 |
| 1:D:334:PRO:HG2 | 2:E:192:MET:CE | 2.40 | 0.51 |
| 1:D:168:GLY:HA2 | 3:F:105:VAL:HB | 1.93 | 0.51 |
| 1:A:67:HIS:HE1 | 2:B:265:TYR:O | 1.93 | 0.51 |
| 3:C:21:ALA:HB3 | 3:C:24:ASP:OD2 | 2.11 | 0.51 |
| 1:A:280:VAL:HG11 | 1:A:313:MET:HE1 | 1.92 | 0.51 |
| 3:C:25:TRP:CE3 | 3:C:26:CYS:HA | 2.45 | 0.50 |
| 1:D:34:ASN:N | 1:D:35:PRO:HD3 | 2.26 | 0.50 |
| 1:A:67:HIS:CE1 | 2:B:265:TYR:O | 2.64 | 0.50 |
| 2:B:243:VAL:HG23 | 2:B:243:VAL:O | 2.11 | 0.50 |
| 1:D:429:SER:O | 1:D:433:LYS:HG3 | 2.12 | 0.50 |
| 1:D:55:GLU:OE2 | 1:D:59:HIS:HE1 | 1.94 | 0.50 |
| 2:B:12:LYS:N | 2:B:13:PRO:HD3 | 2.27 | 0.50 |
| 2:B:211:PRO:HB3 | 2:B:273:LEU:HB3 | 1.94 | 0.50 |
| 1:A:111:THR:HG23 | 2:B:29:PHE:HD2 | 1.75 | 0.50 |
| 1:A:262:ASN:ND2 | 2:B:292:ARG:HH22 | 2.09 | 0.50 |
| 1:D:170:ASN:HB3 | 1:D:208:PRO:HA | 1.93 | 0.50 |
| 2:E:211:PRO:HG2 | 2:E:253:ILE:CD1 | 2.42 | 0.50 |
| 1:A:390:LYS:O | 1:A:390:LYS:HD3 | 2.11 | 0.49 |
| 1:D:160:LEU:N | 1:D:160:LEU:HD12 | 2.26 | 0.49 |
| 2:B:9:ASN:HD22 | 2:B:10:PRO:N | 2.09 | 0.49 |
| 3:F:49:ILE:HD11 | 3:F:75:PHE:CD1 | 2.47 | 0.49 |
| 3:F:77:LEU:HD22 | 3:F:81:TYR:CD1 | 2.47 | 0.49 |
| 5:D:582:SRM:HMA2 | 3:F:104:CYS:CB | 2.43 | 0.49 |
| 1:D:279:GLU:O | 1:D:308:HIS:HE1 | 1.96 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:E:242:GLU:HA | 2:E:246:GLN:O | 2.12 | 0.49 |
| 2:E:239:ILE:C | 2:E:239:ILE:HD12 | 2.33 | 0.49 |
| 1:D:87:GLN:N | 1:D:88:PRO:HD3 | 2.27 | 0.49 |
| 5:A:580:SRM:HMA2 | 3:C:104:CYS:CB | 2.43 | 0.48 |
| 1:D:168:GLY:N | 3:F:105:VAL:HB | 2.28 | 0.48 |
| 2:E:293:ILE:HG22 | 2:E:294:LYS:CD | 2.42 | 0.48 |
| 1:A:67:HIS:HA | 2:B:152:HIS:CD2 | 2.48 | 0.48 |
| 1:D:170:ASN:HB2 | 1:D:204:GLU:O | 2.13 | 0.48 |
| 1:D:99:THR:HG23 | 1:D:140:VAL:HG13 | 1.96 | 0.48 |
| 5:B:581:SRM:NA | 5:B:581:SRM:CBA | 2.74 | 0.48 |
| 2:B:153:THR:N | 2:B:154:PRO:HD2 | 2.29 | 0.48 |
| 3:C:6:PHE:CD2 | 3:C:32:TYR:HB2 | 2.48 | 0.48 |
| 2:B:314:PRO:O | 2:B:318:LYS:HG2 | 2.13 | 0.48 |
| 3:C:12:GLU:HB3 | 3:C:20:ASN:HD22 | 1.78 | 0.48 |
| 1:A:60:GLU:OE1 | 1:A:64:HIS:HE1 | 1.96 | 0.48 |
| 1:D:67:HIS:HD2 | 7:D:6692:HOH:O | 1.94 | 0.48 |
| 2:B:138:SER:HB2 | 2:B:172:GLU:O | 2.14 | 0.48 |
| 1:A:196:GLN:HE22 | 1:A:354:PRO:HA | 1.78 | 0.48 |
| 1:A:285:PRO:CG | 2:B:293:ILE:HA | 2.44 | 0.48 |
| 1:D:159:ASN:C | 1:D:160:LEU:HD12 | 2.34 | 0.48 |
| 2:E:215:HIS:HD2 | 2:E:250:SER:OG | 1.97 | 0.48 |
| 2:E:207:HIS:HD2 | 2:E:279:ASP:OD1 | 1.97 | 0.47 |
| 1:D:3:LYS:HE2 | 1:D:3:LYS:HB2 | 1.78 | 0.47 |
| 2:B:31:PRO:HG2 | 2:B:34:ILE:CG1 | 2.44 | 0.47 |
| 1:D:81:ILE:HD12 | 3:F:105:VAL:HG22 | 1.96 | 0.47 |
| 1:A:168:GLY:HA2 | 3:C:105:VAL:HB | 1.96 | 0.47 |
| 1:D:107:ALA:HB3 | 1:D:191:GLN:HE21 | 1.78 | 0.47 |
| 5:A:580:SRM:C4D | 3:C:104:CYS:SG | 2.92 | 0.47 |
| 2:B:9:ASN:HD21 | 2:B:11:ALA:HB3 | 1.80 | 0.47 |
| 1:A:239:THR:OG1 | 1:A:305:ARG:HD2 | 2.14 | 0.47 |
| 1:A:17:TRP:CD2 | 1:A:18:PRO:HD2 | 2.49 | 0.47 |
| 5:A:580:SRM:O1A | 2:B:150:TYR:CD2 | 2.68 | 0.46 |
| 1:A:83:ARG:H | 1:A:98:HIS:CD2 | 2.28 | 0.46 |
| 2:B:254:ASN:HD22 | 2:B:254:ASN:C | 2.18 | 0.46 |
| 1:D:98:HIS:HA | 2:E:150:TYR:OH | 2.16 | 0.46 |
| 3:F:26:CYS:SG | 3:F:28:GLU:CG | 3.02 | 0.46 |
| 2:E:171:GLU:HG3 | 7:E:934:HOH:O | 2.15 | 0.46 |
| 1:A:167:SER:CB | 3:C:105:VAL:HG11 | 2.46 | 0.46 |
| 5:E:583:SRM:CBA | 5:E:583:SRM:C1A | 2.93 | 0.46 |
| 1:A:107:ALA:HB3 | 1:A:191:GLN:HE21 | 1.81 | 0.46 |
| 2:E:142:ILE:O | 2:E:144:HIS:HD2 | 1.98 | 0.46 |
| 2:B:242:GLU:HA | 2:B:246:GLN:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:104:GLN:N | 1:D:104:GLN:NE2 | 2.54 | 0.46 |
| 2:E:211:PRO:HB3 | 2:E:273:LEU:HB3 | 1.97 | 0.46 |
| 3:C:105:VAL:OXT | 3:C:105:VAL:CG1 | 2.55 | 0.46 |
| 1:A:363:GLU:O | 1:A:367:GLU:HG3 | 2.14 | 0.46 |
| 2:B:144:HIS:CG | 2:B:162:VAL:HG21 | 2.50 | 0.46 |
| 1:A:313:MET:N | 1:A:314:PRO:HD3 | 2.31 | 0.46 |
| 3:C:11:PHE:CE2 | 3:C:29:TRP:HB2 | 2.51 | 0.46 |
| 1:D:168:GLY:CA | 3:F:105:VAL:HB | 2.46 | 0.46 |
| 1:A:279:GLU:O | 1:A:308:HIS:HE1 | 1.99 | 0.46 |
| 1:D:76:TYR:CD1 | 1:D:206:HIS:HB3 | 2.51 | 0.46 |
| 2:B:382:VAL:HG22 | 1:D:402:GLN:OE1 | 2.16 | 0.45 |
| 1:A:411:PRO:HG3 | 2:E:192:MET:HE1 | 1.96 | 0.45 |
| 2:B:172:GLU:HA | 2:B:172:GLU:OE1 | 2.14 | 0.45 |
| 1:A:406:GLU:HG3 | 7:A:6681:HOH:O | 2.16 | 0.45 |
| 1:D:20:PHE:O | 1:D:24:ILE:HG13 | 2.16 | 0.45 |
| 7:D:6726:HOH:O | 3:F:105:VAL:HG21 | 2.03 | 0.45 |
| 2:E:186:LEU:C | 2:E:186:LEU:HD23 | 2.36 | 0.45 |
| 1:D:189:ASP:CG | 1:D:192:LEU:HB2 | 2.37 | 0.45 |
| 2:B:96:THR:HB | 5:B:581:SRM:HAB1 | 1.98 | 0.45 |
| 5:A:580:SRM:HDD1 | 3:C:104:CYS:SG | 2.57 | 0.45 |
| 1:A:113:GLU:HG3 | 7:A:6608:HOH:O | 2.16 | 0.45 |
| 1:D:371:GLU:HG2 | 7:D:6743:HOH:O | 2.15 | 0.45 |
| 1:A:97:PHE:O | 2:B:150:TYR:CZ | 2.68 | 0.45 |
| 1:D:34:ASN:HD21 | 1:D:38:LEU:N | 2.02 | 0.45 |
| 1:A:416:LYS:HB2 | 1:A:419:GLU:HG3 | 1.97 | 0.45 |
| 1:D:104:GLN:HE22 | 1:D:173:THR:CG2 | 2.25 | 0.45 |
| 2:B:62:VAL:O | 2:B:62:VAL:HG13 | 2.17 | 0.45 |
| 2:E:214:ASP:OD1 | 2:E:216:GLU:HG2 | 2.17 | 0.45 |
| 3:F:26:CYS:SG | 3:F:27:PRO:N | 2.89 | 0.45 |
| 1:A:232:SER:O | 1:A:331:ALA:HB3 | 2.15 | 0.45 |
| 2:B:48:GLU:HB3 | 2:B:49:PRO:HD2 | 1.99 | 0.45 |
| 1:D:3:LYS:CD | 1:D:3:LYS:C | 2.82 | 0.44 |
| 2:B:63:PHE:O | 2:B:104:MET:HA | 2.17 | 0.44 |
| 2:B:211:PRO:HG2 | 2:B:253:ILE:CD1 | 2.47 | 0.44 |
| 1:D:225:CYS:HA | 5:E:583:SRM:C1C | 2.48 | 0.44 |
| 1:A:98:HIS:HE1 | 1:A:146:THR:OG1 | 2.01 | 0.44 |
| 1:A:64:HIS:HD2 | 1:A:86:ASP:OD1 | 2.00 | 0.44 |
| 1:D:170:ASN:HD22 | 1:D:208:PRO:CG | 2.29 | 0.44 |
| 1:D:45:GLU:N | 1:D:45:GLU:CD | 2.71 | 0.44 |
| 1:A:60:GLU:OE1 | 1:A:64:HIS:CE1 | 2.70 | 0.44 |
| 2:E:223:GLU:HB3 | 3:F:62:ILE:HG22 | 1.99 | 0.44 |
| 2:E:333:LYS:O | 2:E:334:TYR:HB2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 7:D:6620:HOH:O | 2:E:44:HIS:HE1 | 2.00 | 0.43 |
| 3:C:57:TYR:CD1 | 3:C:98:LEU:HD22 | 2.53 | 0.43 |
| 3:F:100:LYS:HG3 | 3:F:101:PRO:HD2 | 1.99 | 0.43 |
| 2:E:138:SER:HB2 | 2:E:172:GLU:O | 2.18 | 0.43 |
| 1:D:219:ASP:OD1 | 1:D:226:VAL:HG12 | 2.18 | 0.43 |
| 3:F:13:VAL:HG13 | 3:F:18:PHE:N | 2.34 | 0.43 |
| 2:E:208:ARG:HD2 | 2:E:305:PHE:CD1 | 2.53 | 0.43 |
| 2:E:75:THR:O | 2:E:79:ARG:HG3 | 2.18 | 0.43 |
| 1:D:308:HIS:HD2 | 2:E:292:ARG:NE | 2.10 | 0.43 |
| 2:B:346:TRP:CE2 | 1:D:407:PRO:HD2 | 2.53 | 0.43 |
| 2:E:48:GLU:HB2 | 2:E:49:PRO:HD2 | 2.00 | 0.43 |
| 1:A:41:GLN:NE2 | 2:B:4:ILE:HG23 | 2.34 | 0.43 |
| 3:C:4:VAL:HG11 | 3:C:32:TYR:CE2 | 2.54 | 0.43 |
| 2:E:246:GLN:HA | 2:E:246:GLN:OE1 | 2.18 | 0.43 |
| 1:D:232:SER:O | 1:D:331:ALA:HB3 | 2.18 | 0.43 |
| 1:A:86:ASP:OD1 | 1:A:87:GLN:HG2 | 2.17 | 0.43 |
| 1:A:83:ARG:NH1 | 5:A:580:SRM:O1A | 2.52 | 0.43 |
| 1:A:308:HIS:CD2 | 2:B:292:ARG:HE | 2.25 | 0.43 |
| 1:D:334:PRO:HG3 | 1:D:339:ALA:HB2 | 2.00 | 0.43 |
| 1:D:67:HIS:CE1 | 2:E:265:TYR:O | 2.72 | 0.43 |
| 2:E:12:LYS:N | 2:E:13:PRO:HD3 | 2.34 | 0.43 |
| 2:B:148:TRP:CE3 | 2:B:157:ASP:HB2 | 2.53 | 0.43 |
| 2:B:347:GLU:HG2 | 7:B:814:HOH:O | 2.17 | 0.43 |
| 1:D:67:HIS:HE1 | 2:E:265:TYR:O | 2.01 | 0.43 |
| 2:B:152:HIS:C | 2:B:154:PRO:HD2 | 2.39 | 0.42 |
| 1:D:135:SER:HB2 | 5:D:582:SRM:HHC | 2.01 | 0.42 |
| 3:C:19:LEU:HD21 | 3:C:29:TRP:CE3 | 2.54 | 0.42 |
| 1:A:76:TYR:CD1 | 1:A:206:HIS:HB3 | 2.55 | 0.42 |
| 1:A:312:THR:C | 1:A:314:PRO:HD3 | 2.39 | 0.42 |
| 1:D:17:TRP:CD2 | 1:D:18:PRO:HD2 | 2.53 | 0.42 |
| 1:D:156:MET:SD | 1:D:160:LEU:HD22 | 2.60 | 0.42 |
| 2:B:44:HIS:HE1 | 7:B:837:HOH:O | 2.03 | 0.42 |
| 3:F:77:LEU:HD22 | 3:F:81:TYR:CE1 | 2.55 | 0.42 |
| 1:D:335:VAL:HA | 1:D:336:LEU:HA | 1.85 | 0.42 |
| 3:C:11:PHE:HB3 | 3:C:19:LEU:CD2 | 2.49 | 0.42 |
| 1:D:416:LYS:HB2 | 1:D:419:GLU:CG | 2.44 | 0.42 |
| 2:B:367:ASP:N | 2:B:368:PRO:CD | 2.82 | 0.42 |
| 5:E:583:SRM:C1A | 5:E:583:SRM:HBA2 | 2.50 | 0.42 |
| 2:E:254:ASN:HD22 | 2:E:254:ASN:C | 2.21 | 0.42 |
| 1:A:81:ILE:HD11 | 3:C:105:VAL:HG22 | 2.00 | 0.42 |
| 2:B:384:PHE:N | 2:B:384:PHE:CD1 | 2.84 | 0.42 |
| 3:F:13:VAL:HG13 | 3:F:17:GLY:C | 2.39 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:182:ARG:HD3 | 2:E:54:HIS:CE1 | 2.54 | 0.42 |
| 2:E:87:LYS:HD3 | 2:E:88:PHE:CE1 | 2.55 | 0.42 |
| 5:D:582:SRM:CCA | 2:E:150:TYR:HD2 | 2.32 | 0.41 |
| 2:E:211:PRO:HG2 | 2:E:253:ILE:HD13 | 2.01 | 0.41 |
| 1:A:428:ILE:HD13 | 2:E:214:ASP:HB2 | 2.02 | 0.41 |
| 2:E:332:ARG:O | 2:E:335:GLU:HB2 | 2.20 | 0.41 |
| 1:A:219:ASP:OD1 | 1:A:226:VAL:HG12 | 2.20 | 0.41 |
| 1:D:376:ARG:CB | 1:D:376:ARG:HH11 | 2.33 | 0.41 |
| 2:E:223:GLU:HB2 | 2:E:226:LEU:HD12 | 2.01 | 0.41 |
| 5:A:580:SRM:CCA | 2:B:150:TYR:HD2 | 2.34 | 0.41 |
| 1:D:202:GLN:OE1 | 1:D:206:HIS:HE1 | 2.04 | 0.41 |
| 3:C:30:VAL:HG13 | 3:C:95:MET:HE3 | 2.02 | 0.41 |
| 2:B:31:PRO:HG2 | 2:B:34:ILE:HG12 | 2.01 | 0.41 |
| 1:D:111:THR:HG23 | 2:E:29:PHE:HD2 | 1.84 | 0.41 |
| 1:A:284:CYS:HA | 1:A:285:PRO:HD3 | 1.92 | 0.41 |
| 1:D:83:ARG:H | 1:D:98:HIS:CD2 | 2.29 | 0.41 |
| 2:E:152:HIS:C | 2:E:154:PRO:HD2 | 2.40 | 0.41 |
| 1:A:428:ILE:CD1 | 2:E:214:ASP:HB2 | 2.50 | 0.41 |
| 2:B:95:PHE:CE2 | 2:B:101:ILE:HG12 | 2.56 | 0.41 |
| 1:A:11:GLU:O | 1:A:11:GLU:HG3 | 2.20 | 0.41 |
| 3:C:68:ILE:HD12 | 7:C:514:HOH:O | 2.19 | 0.41 |
| 1:D:132:MET:HA | 1:D:133:HIS:HA | 1.88 | 0.41 |
| 1:A:99:THR:N | 2:B:150:TYR:OH | 2.53 | 0.41 |
| 2:E:239:ILE:O | 2:E:239:ILE:HD12 | 2.20 | 0.41 |
| 7:B:949:HOH:O | 1:D:437:ARG:HD2 | 2.20 | 0.41 |
| 1:D:102:LEU:HA | 1:D:102:LEU:HD12 | 1.80 | 0.41 |
| 1:D:408:ARG:HH11 | 1:D:410:ASN:ND2 | 2.13 | 0.41 |
| 2:E:207:HIS:HE1 | 7:E:954:HOH:O | 2.03 | 0.41 |
| 1:D:108:LYS:HD3 | 1:D:133:HIS:CE1 | 2.56 | 0.41 |
| 1:D:409:HIS:HD2 | 7:D:6621:HOH:O | 2.03 | 0.41 |
| 1:A:409:HIS:HD2 | 7:A:6614:HOH:O | 2.04 | 0.41 |
| 2:E:46:ILE:HG12 | 2:E:52:LEU:HD22 | 2.03 | 0.41 |
| 1:D:60:GLU:OE1 | 1:D:64:HIS:CE1 | 2.74 | 0.41 |
| 1:A:172:ARG:HB2 | 1:A:215:LYS:HG2 | 2.03 | 0.41 |
| 1:A:427:ASP:CG | 1:A:429:SER:H | 2.25 | 0.41 |
| 2:B:313:TRP:N | 2:B:314:PRO:HD3 | 2.35 | 0.41 |
| 1:A:376:ARG:HB3 | 1:A:376:ARG:HH11 | 1.85 | 0.40 |
| 2:E:144:HIS:CG | 2:E:162:VAL:HG21 | 2.56 | 0.40 |
| 3:C:57:TYR:CG | 3:C:98:LEU:HD22 | 2.57 | 0.40 |
| 3:F:13:VAL:CG1 | 3:F:14:ASP:H | 2.34 | 0.40 |
| 3:F:26:CYS:SG | 3:F:28:GLU:CD | 2.99 | 0.40 |
| 2:E:259:MET:C | 2:E:260:TYR:CG | 2.93 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|----------------|-------------|----------|
| 2:E:31:PRO:HG2 | 2:E:34:ILE:CG1 | 2.51 | 0.40 |
| 5:A:580:SRM:CDD | 3:C:104:CYS:SG | 3.09 | 0.40 |
| 3:C:88:PRO:O | 3:C:92:ALA:HB3 | 2.22 | 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 | 433/437 (99%) | 418 (96%) | 15 (4%) | 0 | 100 | 100 |
| 1 | D | 433/437 (99%) | 422 (98%) | 10 (2%) | 1 (0%) | 56 | 34 |
| 2 | B | 383/386 (99%) | 365 (95%) | 16 (4%) | 2 (0%) | 38 | 15 |
| 2 | E | 383/386 (99%) | 369 (96%) | 12 (3%) | 2 (0%) | 38 | 15 |
| 3 | C | 102/105 (97%) | 98 (96%) | 3 (3%) | 1 (1%) | 22 | 6 |
| 3 | F | 102/105 (97%) | 99 (97%) | 2 (2%) | 1 (1%) | 22 | 6 |
| All | All | 1836/1856 (99%) | 1771 (96%) | 58 (3%) | 7 (0%) | 43 | 21 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 4 | HIS |
| 3 | C | 34 | LYS |
| 3 | F | 34 | LYS |
| 2 | E | 293 | ILE |
| 2 | E | 153 | THR |
| 2 | B | 153 | THR |
| 2 | B | 293 | ILE |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 364/365 (100%) | 350 (96%) | 14 (4%) | 44 | 17 |
| 1 | D | 364/365 (100%) | 352 (97%) | 12 (3%) | 50 | 22 |
| 2 | B | 324/325 (100%) | 312 (96%) | 12 (4%) | 45 | 18 |
| 2 | E | 324/325 (100%) | 319 (98%) | 5 (2%) | 76 | 59 |
| 3 | C | 79/80 (99%) | 75 (95%) | 4 (5%) | 33 | 9 |
| 3 | F | 79/80 (99%) | 74 (94%) | 5 (6%) | 25 | 6 |
| All | All | 1534/1540 (100%) | 1482 (97%) | 52 (3%) | 49 | 21 |

All (52) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | LYS |
| 1 | A | 34 | ASN |
| 1 | A | 36 | LYS |
| 1 | A | 54 | LEU |
| 1 | A | 83 | ARG |
| 1 | A | 104 | GLN |
| 1 | A | 208 | PRO |
| 1 | A | 212 | TYR |
| 1 | A | 249 | GLU |
| 1 | A | 258 | GLU |
| 1 | A | 273 | LYS |
| 1 | A | 391 | LEU |
| 1 | A | 402 | GLN |
| 1 | A | 406 | GLU |
| 2 | B | 4 | ILE |
| 2 | B | 9 | ASN |
| 2 | B | 172 | GLU |
| 2 | B | 188 | CYS |
| 2 | B | 189 | CYS |
| 2 | B | 220 | GLU |
| 2 | B | 254 | ASN |
| 2 | B | 259 | MET |
| 2 | B | 260 | TYR |
| 2 | B | 329 | GLU |
| 2 | B | 356 | GLU |
| 2 | B | 384 | PHE |
| 3 | C | 12 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 28 | GLU |
| 3 | C | 51 | ASP |
| 3 | C | 77 | LEU |
| 1 | D | 3 | LYS |
| 1 | D | 4 | HIS |
| 1 | D | 33 | LYS |
| 1 | D | 34 | ASN |
| 1 | D | 54 | LEU |
| 1 | D | 89 | GLU |
| 1 | D | 104 | GLN |
| 1 | D | 192 | LEU |
| 1 | D | 212 | TYR |
| 1 | D | 336 | LEU |
| 1 | D | 402 | GLN |
| 1 | D | 432 | ARG |
| 2 | E | 188 | CYS |
| 2 | E | 189 | CYS |
| 2 | E | 254 | ASN |
| 2 | E | 259 | MET |
| 2 | E | 260 | TYR |
| 3 | F | 20 | ASN |
| 3 | F | 34 | LYS |
| 3 | F | 51 | ASP |
| 3 | F | 67 | ARG |
| 3 | F | 77 | LEU |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 34 | ASN |
| 1 | A | 64 | HIS |
| 1 | A | 67 | HIS |
| 1 | A | 98 | HIS |
| 1 | A | 104 | GLN |
| 1 | A | 161 | ASN |
| 1 | A | 196 | GLN |
| 1 | A | 206 | HIS |
| 1 | A | 248 | GLN |
| 1 | A | 262 | ASN |
| 1 | A | 308 | HIS |
| 1 | A | 311 | ASN |
| 1 | A | 402 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 409 | HIS |
| 1 | A | 410 | ASN |
| 1 | A | 435 | HIS |
| 2 | B | 9 | ASN |
| 2 | B | 37 | ASN |
| 2 | B | 44 | HIS |
| 2 | B | 107 | ASN |
| 2 | B | 144 | HIS |
| 2 | B | 191 | ASN |
| 2 | B | 207 | HIS |
| 2 | B | 215 | HIS |
| 2 | B | 254 | ASN |
| 2 | B | 263 | ASN |
| 1 | D | 34 | ASN |
| 1 | D | 64 | HIS |
| 1 | D | 67 | HIS |
| 1 | D | 98 | HIS |
| 1 | D | 104 | GLN |
| 1 | D | 161 | ASN |
| 1 | D | 170 | ASN |
| 1 | D | 196 | GLN |
| 1 | D | 206 | HIS |
| 1 | D | 248 | GLN |
| 1 | D | 262 | ASN |
| 1 | D | 308 | HIS |
| 1 | D | 311 | ASN |
| 1 | D | 375 | ASN |
| 1 | D | 402 | GLN |
| 1 | D | 409 | HIS |
| 1 | D | 410 | ASN |
| 1 | D | 435 | HIS |
| 2 | E | 37 | ASN |
| 2 | E | 44 | HIS |
| 2 | E | 144 | HIS |
| 2 | E | 146 | GLN |
| 2 | E | 191 | ASN |
| 2 | E | 207 | HIS |
| 2 | E | 215 | HIS |
| 2 | E | 254 | ASN |
| 2 | E | 263 | ASN |
| 3 | F | 47 | GLN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 ligands 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$ |
| 5 | SRM | A | 580 | 2,4 | 70,70,70 | 2.24 | 15 (21%) | 94,112,112 | 3.27 | 29 (30%) |
| 4 | SO3 | A | 6575 | 5 | 3,3,3 | 1.11 | 0 | 2,3,3 | 0.55 | 0 |
| 6 | SF4 | A | 803 | 1 | 12,12,12 | 24.18 | 11 (91%) | 0,24,24 | 0.00 | - |
| 6 | SF4 | A | 804 | 1 | 12,12,12 | 19.10 | 12 (100%) | 0,24,24 | 0.00 | - |
| 5 | SRM | B | 581 | - | 66,66,70 | 1.67 | 8 (12%) | 92,98,112 | 4.78 | 26 (28%) |
| 6 | SF4 | B | 801 | 2 | 12,12,12 | 15.68 | 9 (75%) | 0,24,24 | 0.00 | - |
| 6 | SF4 | B | 802 | 2 | 12,12,12 | 10.47 | 11 (91%) | 0,24,24 | 0.00 | - |
| 5 | SRM | D | 582 | 2,4 | 70,70,70 | 1.88 | 11 (15%) | 94,112,112 | 2.82 | 28 (29%) |
| 4 | SO3 | D | 6576 | 5 | 3,3,3 | 1.07 | 0 | 2,3,3 | 0.74 | 0 |
| 6 | SF4 | D | 807 | 1 | 12,12,12 | 20.72 | 11 (91%) | 0,24,24 | 0.00 | - |
| 6 | SF4 | D | 808 | 1 | 12,12,12 | 28.69 | 12 (100%) | 0,24,24 | 0.00 | - |
| 5 | SRM | E | 583 | - | 66,66,70 | 1.70 | 10 (15%) | 92,98,112 | 4.06 | 28 (30%) |
| 6 | SF4 | E | 805 | 2 | 12,12,12 | 17.65 | 10 (83%) | 0,24,24 | 0.00 | - |
| 6 | SF4 | E | 806 | 2 | 12,12,12 | 15.67 | 9 (75%) | 0,24,24 | 0.00 | - |

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 |
|-----|------|-------|------|------|---------|--------------|---------|
| 5 | SRM | A | 580 | 2,4 | - | 0/38/126/126 | 0/0/8/8 |
| 4 | SO3 | A | 6575 | 5 | - | 0/0/0/0 | 0/0/0/0 |
| 6 | SF4 | A | 803 | 1 | - | 0/0/48/48 | 0/0/5/5 |
| 6 | SF4 | A | 804 | 1 | - | 0/0/48/48 | 0/0/5/5 |
| 5 | SRM | B | 581 | - | - | 0/49/94/126 | 0/0/4/8 |
| 6 | SF4 | B | 801 | 2 | - | 0/0/48/48 | 0/0/5/5 |
| 6 | SF4 | B | 802 | 2 | - | 0/0/48/48 | 0/0/5/5 |
| 5 | SRM | D | 582 | 2,4 | - | 0/38/126/126 | 0/0/8/8 |
| 4 | SO3 | D | 6576 | 5 | - | 0/0/0/0 | 0/0/0/0 |
| 6 | SF4 | D | 807 | 1 | - | 0/0/48/48 | 0/0/5/5 |
| 6 | SF4 | D | 808 | 1 | - | 0/0/48/48 | 0/0/5/5 |
| 5 | SRM | E | 583 | - | - | 0/49/94/126 | 0/0/4/8 |
| 6 | SF4 | E | 805 | 2 | - | 0/0/48/48 | 0/0/5/5 |
| 6 | SF4 | E | 806 | 2 | - | 0/0/48/48 | 0/0/5/5 |

All (129) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 6 | D | 808 | SF4 | S1-FE4 | 51.49 | 2.67 | 2.33 |
| 6 | D | 807 | SF4 | S1-FE3 | 49.38 | 2.66 | 2.33 |
| 6 | D | 808 | SF4 | S3-FE1 | 46.17 | 2.64 | 2.33 |
| 6 | D | 808 | SF4 | S2-FE4 | 38.52 | 2.59 | 2.33 |
| 6 | A | 803 | SF4 | S4-FE2 | 37.04 | 2.58 | 2.33 |
| 6 | A | 804 | SF4 | S4-FE3 | 36.30 | 2.57 | 2.33 |
| 6 | A | 803 | SF4 | S2-FE4 | 35.27 | 2.57 | 2.33 |
| 6 | E | 805 | SF4 | S1-FE3 | 33.69 | 2.55 | 2.33 |
| 6 | A | 803 | SF4 | S1-FE3 | 32.92 | 2.55 | 2.33 |
| 6 | D | 808 | SF4 | S2-FE3 | 31.71 | 2.54 | 2.33 |
| 6 | D | 807 | SF4 | S1-FE2 | 31.65 | 2.54 | 2.33 |
| 6 | A | 803 | SF4 | S1-FE4 | 31.54 | 2.54 | 2.33 |
| 6 | B | 801 | SF4 | S1-FE2 | 30.97 | 2.54 | 2.33 |
| 6 | A | 803 | SF4 | S3-FE4 | -29.42 | 2.13 | 2.33 |
| 6 | E | 806 | SF4 | S1-FE3 | 29.42 | 2.53 | 2.33 |
| 6 | E | 806 | SF4 | S2-FE1 | 29.19 | 2.52 | 2.33 |
| 6 | A | 804 | SF4 | S3-FE4 | 29.03 | 2.52 | 2.33 |
| 6 | D | 808 | SF4 | S4-FE2 | 28.20 | 2.52 | 2.33 |
| 6 | E | 805 | SF4 | S3-FE2 | 28.12 | 2.52 | 2.33 |
| 6 | A | 803 | SF4 | S2-FE1 | 28.02 | 2.52 | 2.33 |
| 6 | D | 807 | SF4 | S3-FE4 | 26.84 | 2.51 | 2.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 6 | B | 801 | SF4 | S4-FE1 | -25.94 | 2.15 | 2.33 |
| 6 | D | 808 | SF4 | S3-FE2 | 23.46 | 2.49 | 2.33 |
| 6 | E | 805 | SF4 | S3-FE1 | 22.38 | 2.48 | 2.33 |
| 6 | A | 804 | SF4 | S3-FE1 | 21.98 | 2.48 | 2.33 |
| 6 | A | 804 | SF4 | S1-FE4 | 20.83 | 2.47 | 2.33 |
| 6 | B | 801 | SF4 | S2-FE1 | 20.44 | 2.47 | 2.33 |
| 6 | D | 808 | SF4 | S1-FE2 | 20.24 | 2.46 | 2.33 |
| 6 | E | 805 | SF4 | S2-FE3 | 19.20 | 2.46 | 2.33 |
| 6 | A | 804 | SF4 | S4-FE1 | 18.07 | 2.45 | 2.33 |
| 6 | E | 805 | SF4 | S4-FE2 | -17.84 | 2.21 | 2.33 |
| 6 | B | 802 | SF4 | S4-FE3 | 17.81 | 2.45 | 2.33 |
| 6 | B | 802 | SF4 | S4-FE1 | 17.28 | 2.44 | 2.33 |
| 6 | A | 803 | SF4 | S3-FE1 | 17.15 | 2.44 | 2.33 |
| 6 | D | 808 | SF4 | S3-FE4 | 17.10 | 2.44 | 2.33 |
| 6 | E | 806 | SF4 | S1-FE2 | 16.94 | 2.44 | 2.33 |
| 6 | A | 804 | SF4 | S4-FE2 | 16.65 | 2.44 | 2.33 |
| 6 | A | 804 | SF4 | S3-FE2 | -16.63 | 2.22 | 2.33 |
| 6 | E | 806 | SF4 | S4-FE1 | -16.58 | 2.22 | 2.33 |
| 6 | E | 805 | SF4 | S3-FE4 | 16.18 | 2.44 | 2.33 |
| 6 | D | 807 | SF4 | S3-FE1 | 16.01 | 2.44 | 2.33 |
| 6 | E | 806 | SF4 | S4-FE3 | 15.18 | 2.43 | 2.33 |
| 6 | D | 807 | SF4 | S3-FE2 | 14.80 | 2.43 | 2.33 |
| 6 | B | 801 | SF4 | S2-FE4 | 14.62 | 2.43 | 2.33 |
| 6 | D | 808 | SF4 | S4-FE1 | 14.56 | 2.43 | 2.33 |
| 6 | D | 808 | SF4 | S2-FE1 | 14.40 | 2.42 | 2.33 |
| 6 | B | 802 | SF4 | S3-FE2 | 14.22 | 2.42 | 2.33 |
| 6 | B | 802 | SF4 | S3-FE4 | -14.07 | 2.23 | 2.33 |
| 6 | A | 803 | SF4 | S3-FE2 | 13.74 | 2.42 | 2.33 |
| 6 | B | 801 | SF4 | S2-FE3 | 13.29 | 2.42 | 2.33 |
| 6 | E | 805 | SF4 | S4-FE3 | -13.03 | 2.24 | 2.33 |
| 6 | E | 806 | SF4 | S2-FE3 | 12.83 | 2.41 | 2.33 |
| 6 | B | 801 | SF4 | S1-FE3 | -12.79 | 2.24 | 2.33 |
| 6 | B | 801 | SF4 | S4-FE3 | -12.65 | 2.24 | 2.33 |
| 6 | E | 806 | SF4 | S3-FE1 | 12.63 | 2.41 | 2.33 |
| 6 | D | 807 | SF4 | S4-FE1 | -12.00 | 2.25 | 2.33 |
| 6 | D | 807 | SF4 | S2-FE1 | 11.96 | 2.41 | 2.33 |
| 6 | D | 807 | SF4 | S2-FE3 | 11.60 | 2.41 | 2.33 |
| 6 | B | 801 | SF4 | S3-FE2 | -11.37 | 2.25 | 2.33 |
| 6 | A | 804 | SF4 | S2-FE3 | 11.05 | 2.40 | 2.33 |
| 6 | A | 803 | SF4 | S4-FE3 | 11.02 | 2.40 | 2.33 |
| 6 | A | 804 | SF4 | S1-FE2 | 11.00 | 2.40 | 2.33 |
| 6 | B | 802 | SF4 | S2-FE3 | 10.61 | 2.40 | 2.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6 | D | 808 | SF4 | S1-FE3 | 10.59 | 2.40 | 2.33 |
| 5 | A | 580 | SRM | O1B-CCB | 9.34 | 1.55 | 1.22 |
| 6 | A | 804 | SF4 | S1-FE3 | 9.31 | 2.39 | 2.33 |
| 6 | E | 805 | SF4 | S1-FE4 | 9.16 | 2.39 | 2.33 |
| 6 | D | 807 | SF4 | S2-FE4 | 8.89 | 2.39 | 2.33 |
| 6 | E | 806 | SF4 | S3-FE2 | -8.01 | 2.27 | 2.33 |
| 6 | E | 805 | SF4 | S2-FE4 | 8.00 | 2.38 | 2.33 |
| 6 | B | 802 | SF4 | S2-FE1 | 7.87 | 2.38 | 2.33 |
| 6 | A | 804 | SF4 | S2-FE4 | 7.83 | 2.38 | 2.33 |
| 6 | A | 803 | SF4 | S2-FE3 | -7.44 | 2.28 | 2.33 |
| 6 | B | 801 | SF4 | S4-FE2 | -7.30 | 2.28 | 2.33 |
| 6 | B | 802 | SF4 | S1-FE2 | 7.22 | 2.38 | 2.33 |
| 5 | A | 580 | SRM | CBB-CCB | -6.90 | 1.32 | 1.50 |
| 5 | D | 582 | SRM | O1B-CCB | 6.88 | 1.46 | 1.22 |
| 6 | E | 806 | SF4 | S2-FE4 | 6.81 | 2.37 | 2.33 |
| 6 | E | 805 | SF4 | S4-FE1 | 6.70 | 2.37 | 2.33 |
| 5 | A | 580 | SRM | O2B-CCB | 6.36 | 1.53 | 1.30 |
| 5 | B | 581 | SRM | O1A-CCA | 6.28 | 1.44 | 1.22 |
| 6 | B | 802 | SF4 | S1-FE3 | 5.94 | 2.37 | 2.33 |
| 5 | E | 583 | SRM | O2A-CCA | -5.93 | 1.09 | 1.30 |
| 5 | D | 582 | SRM | O2B-CCB | 5.92 | 1.52 | 1.30 |
| 5 | B | 581 | SRM | O2A-CCA | 5.90 | 1.52 | 1.30 |
| 6 | A | 804 | SF4 | S2-FE1 | 5.57 | 2.37 | 2.33 |
| 5 | E | 583 | SRM | CBA-CAA | -5.35 | 1.36 | 1.52 |
| 5 | A | 580 | SRM | C3B-C4B | 4.83 | 1.59 | 1.35 |
| 6 | D | 808 | SF4 | S4-FE3 | -4.83 | 2.30 | 2.33 |
| 5 | D | 582 | SRM | C3B-C4B | 4.61 | 1.58 | 1.35 |
| 5 | A | 580 | SRM | FE-NC | 4.53 | 2.11 | 1.92 |
| 5 | D | 582 | SRM | FE-NC | 4.50 | 2.11 | 1.92 |
| 5 | E | 583 | SRM | CAB-C3B | 4.50 | 1.57 | 1.51 |
| 5 | B | 581 | SRM | CAB-C3B | 4.29 | 1.57 | 1.51 |
| 6 | B | 802 | SF4 | S4-FE2 | 3.93 | 2.35 | 2.33 |
| 5 | D | 582 | SRM | FE-ND | 3.80 | 2.08 | 1.92 |
| 5 | A | 580 | SRM | FE-ND | 3.77 | 2.08 | 1.92 |
| 6 | B | 802 | SF4 | S2-FE4 | 3.76 | 2.35 | 2.33 |
| 5 | D | 582 | SRM | C3A-C4A | 3.69 | 1.53 | 1.35 |
| 5 | A | 580 | SRM | C3A-C4A | 3.65 | 1.53 | 1.35 |
| 5 | A | 580 | SRM | FE-NA | 3.41 | 2.10 | 1.97 |
| 5 | A | 580 | SRM | FE-NB | 3.29 | 2.10 | 1.97 |
| 5 | E | 583 | SRM | C3B-C4B | 3.25 | 1.56 | 1.43 |
| 5 | D | 582 | SRM | FE-NA | 3.22 | 2.09 | 1.97 |
| 5 | B | 581 | SRM | CMB-C2B | 3.21 | 1.61 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | A | 580 | SRM | CMB-C2B | 3.17 | 1.61 | 1.54 |
| 6 | A | 803 | SF4 | S1-FE2 | -3.07 | 2.31 | 2.33 |
| 5 | E | 583 | SRM | C4C-CHD | 3.03 | 1.41 | 1.35 |
| 5 | B | 581 | SRM | C3B-C4B | 3.00 | 1.55 | 1.43 |
| 5 | D | 582 | SRM | CMB-C2B | 2.98 | 1.61 | 1.54 |
| 5 | D | 582 | SRM | FE-NB | 2.97 | 2.09 | 1.97 |
| 5 | E | 583 | SRM | CMB-C2B | 2.94 | 1.61 | 1.54 |
| 6 | B | 802 | SF4 | S1-FE4 | 2.90 | 2.35 | 2.33 |
| 5 | E | 583 | SRM | C1C-CHC | 2.69 | 1.40 | 1.35 |
| 6 | D | 807 | SF4 | S1-FE4 | 2.66 | 2.35 | 2.33 |
| 5 | D | 582 | SRM | CHC-C4B | -2.53 | 1.37 | 1.44 |
| 5 | A | 580 | SRM | CAA-C3A | -2.51 | 1.48 | 1.51 |
| 5 | E | 583 | SRM | CAA-C3A | -2.43 | 1.48 | 1.51 |
| 5 | B | 581 | SRM | C4C-CHD | 2.42 | 1.40 | 1.35 |
| 6 | D | 807 | SF4 | S4-FE2 | -2.38 | 2.31 | 2.33 |
| 5 | D | 582 | SRM | CAA-C3A | -2.36 | 1.48 | 1.51 |
| 5 | A | 580 | SRM | CAB-C3B | -2.29 | 1.49 | 1.51 |
| 5 | E | 583 | SRM | C3A-C4A | 2.28 | 1.52 | 1.43 |
| 5 | B | 581 | SRM | C1C-CHC | 2.25 | 1.39 | 1.35 |
| 5 | A | 580 | SRM | CHC-C4B | -2.17 | 1.38 | 1.44 |
| 5 | B | 581 | SRM | C3A-C4A | 2.15 | 1.52 | 1.43 |
| 5 | A | 580 | SRM | CDA-C2A | 2.10 | 1.61 | 1.53 |
| 5 | A | 580 | SRM | C2A-C1A | 2.09 | 1.56 | 1.51 |
| 5 | E | 583 | SRM | C4D-C3D | -2.07 | 1.42 | 1.45 |

All (111) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 5 | B | 581 | SRM | CAA-C3A-C2A | -34.48 | 88.33 | 123.49 |
| 5 | E | 583 | SRM | CAA-C3A-C2A | -22.56 | 100.49 | 123.49 |
| 5 | E | 583 | SRM | CAB-C3B-C2B | -16.85 | 106.31 | 123.49 |
| 5 | A | 580 | SRM | CAB-C3B-C4B | -16.62 | 101.29 | 126.43 |
| 5 | B | 581 | SRM | CAB-C3B-C2B | -16.05 | 107.13 | 123.49 |
| 5 | D | 582 | SRM | CAB-C3B-C4B | -15.31 | 103.26 | 126.43 |
| 5 | E | 583 | SRM | CAA-CBA-CCA | 13.00 | 137.67 | 113.53 |
| 5 | E | 583 | SRM | CAA-C3A-C4A | -12.36 | 97.48 | 126.39 |
| 5 | B | 581 | SRM | CAA-C3A-C4A | -11.32 | 99.92 | 126.39 |
| 5 | A | 580 | SRM | CAB-CBB-CCB | 11.24 | 134.41 | 113.53 |
| 5 | B | 581 | SRM | CAA-CBA-CCA | 10.15 | 132.38 | 113.53 |
| 5 | B | 581 | SRM | O2A-CCA-O1A | -8.98 | 100.45 | 123.30 |
| 5 | A | 580 | SRM | O2B-CCB-O1B | -8.70 | 101.16 | 123.30 |
| 5 | E | 583 | SRM | CBA-CAA-C3A | 8.59 | 132.22 | 113.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5 | A | 580 | SRM | CAB-C3B-C2B | -7.67 | 115.67 | 123.49 |
| 5 | A | 580 | SRM | CAA-C3A-C4A | -7.47 | 115.13 | 126.43 |
| 5 | D | 582 | SRM | CAA-C3A-C4A | -7.41 | 115.22 | 126.43 |
| 5 | D | 582 | SRM | C4A-NA-C1A | 6.94 | 109.93 | 106.86 |
| 5 | D | 582 | SRM | CAB-C3B-C2B | -6.66 | 116.70 | 123.49 |
| 5 | A | 580 | SRM | C4A-NA-C1A | 6.41 | 109.69 | 106.86 |
| 5 | A | 580 | SRM | CAA-C3A-C2A | -6.35 | 117.01 | 123.49 |
| 5 | B | 581 | SRM | CAB-C3B-C4B | -6.12 | 112.07 | 126.39 |
| 5 | D | 582 | SRM | CAA-C3A-C2A | -5.90 | 117.48 | 123.49 |
| 5 | E | 583 | SRM | CAB-C3B-C4B | -5.75 | 112.94 | 126.39 |
| 5 | D | 582 | SRM | CAB-CBB-CCB | 5.63 | 123.99 | 113.53 |
| 5 | A | 580 | SRM | CBB-CAB-C3B | 5.36 | 125.29 | 113.77 |
| 5 | A | 580 | SRM | CMA-C2A-CDA | 5.29 | 114.53 | 109.44 |
| 5 | D | 582 | SRM | CMA-C2A-CDA | 5.22 | 114.47 | 109.44 |
| 5 | E | 583 | SRM | CBD-CAD-C2D | -5.12 | 103.66 | 112.69 |
| 5 | D | 582 | SRM | C2B-C3B-C4B | -5.08 | 101.71 | 111.51 |
| 5 | A | 580 | SRM | C2B-C3B-C4B | -5.05 | 101.77 | 111.51 |
| 5 | B | 581 | SRM | CBD-CAD-C2D | -4.94 | 103.98 | 112.69 |
| 5 | E | 583 | SRM | C2B-C3B-C4B | -4.92 | 103.38 | 111.77 |
| 5 | A | 580 | SRM | C2A-C3A-C4A | -4.89 | 102.06 | 111.51 |
| 5 | D | 582 | SRM | C2A-C3A-C4A | -4.89 | 102.08 | 111.51 |
| 5 | A | 580 | SRM | C4B-NB-C1B | 4.89 | 109.02 | 106.86 |
| 5 | B | 581 | SRM | C2B-C3B-C4B | -4.76 | 103.67 | 111.77 |
| 5 | D | 582 | SRM | C4B-NB-C1B | 4.69 | 108.93 | 106.86 |
| 5 | E | 583 | SRM | C2B-CDB-CEB | 4.54 | 121.71 | 114.50 |
| 5 | E | 583 | SRM | C4D-C3D-C2D | 4.29 | 109.41 | 106.67 |
| 5 | B | 581 | SRM | O2A-CCA-CBA | 4.29 | 129.38 | 114.22 |
| 5 | B | 581 | SRM | C2A-C3A-C4A | -4.25 | 104.54 | 111.77 |
| 5 | B | 581 | SRM | C4D-C3D-C2D | 4.14 | 109.32 | 106.67 |
| 5 | E | 583 | SRM | C2A-C3A-C4A | -4.10 | 104.79 | 111.77 |
| 5 | A | 580 | SRM | C2C-C1C-NC | -4.06 | 106.59 | 109.64 |
| 5 | B | 581 | SRM | C2B-CDB-CEB | 3.92 | 120.74 | 114.50 |
| 5 | D | 582 | SRM | C2C-C1C-NC | -3.88 | 106.73 | 109.64 |
| 5 | B | 581 | SRM | C1D-C2D-C3D | -3.71 | 104.30 | 106.67 |
| 5 | E | 583 | SRM | C1C-C2C-C3C | 3.41 | 109.27 | 106.70 |
| 5 | A | 580 | SRM | C1C-C2C-C3C | 3.38 | 109.24 | 106.70 |
| 5 | A | 580 | SRM | C2A-CDA-CEA | 3.37 | 119.86 | 114.50 |
| 5 | B | 581 | SRM | CBA-CAA-C3A | 3.33 | 120.93 | 113.77 |
| 5 | E | 583 | SRM | C1D-C2D-C3D | -3.26 | 104.59 | 106.67 |
| 5 | B | 581 | SRM | C1C-C2C-C3C | 3.19 | 109.11 | 106.70 |
| 5 | B | 581 | SRM | CMA-C2A-CDA | 3.17 | 112.49 | 109.44 |
| 5 | D | 582 | SRM | O2B-CCB-O1B | -3.16 | 115.26 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5 | D | 582 | SRM | C1C-C2C-C3C | 3.16 | 109.08 | 106.70 |
| 5 | A | 580 | SRM | O1B-CCB-CBB | 3.15 | 133.85 | 123.03 |
| 5 | E | 583 | SRM | CMB-C2B-CDB | 3.09 | 112.42 | 109.44 |
| 5 | E | 583 | SRM | C4C-NC-C1C | 3.09 | 110.05 | 106.07 |
| 5 | B | 581 | SRM | CMB-C2B-CDB | 3.00 | 112.33 | 109.44 |
| 5 | E | 583 | SRM | O2A-CCA-O1A | -2.98 | 115.70 | 123.30 |
| 5 | D | 582 | SRM | C2A-CDA-CEA | 2.98 | 119.24 | 114.50 |
| 5 | D | 582 | SRM | O2B-CCB-CBB | 2.98 | 124.75 | 114.22 |
| 5 | B | 581 | SRM | C4D-CHA-C1A | 2.85 | 132.45 | 128.74 |
| 5 | A | 580 | SRM | C2A-C1A-NA | -2.83 | 108.56 | 112.11 |
| 5 | D | 582 | SRM | C2A-C1A-NA | -2.82 | 108.57 | 112.11 |
| 5 | A | 580 | SRM | C4C-C3C-C2C | -2.75 | 104.63 | 106.70 |
| 5 | E | 583 | SRM | C2C-CDC-CEC | 2.74 | 118.88 | 113.95 |
| 5 | E | 583 | SRM | CDB-C2B-C1B | -2.74 | 104.19 | 112.08 |
| 5 | B | 581 | SRM | C2C-CDC-CEC | 2.73 | 118.86 | 113.95 |
| 5 | A | 580 | SRM | CMB-C2B-CDB | 2.69 | 112.02 | 109.44 |
| 5 | B | 581 | SRM | C4C-NC-C1C | 2.64 | 109.47 | 106.07 |
| 5 | D | 582 | SRM | C3B-C4B-NB | -2.63 | 107.15 | 110.16 |
| 5 | D | 582 | SRM | C2C-CDC-CEC | 2.59 | 118.61 | 113.95 |
| 5 | A | 580 | SRM | C2C-CDC-CEC | 2.59 | 118.60 | 113.95 |
| 5 | A | 580 | SRM | CBC-CAC-C3C | 2.56 | 117.14 | 112.35 |
| 5 | E | 583 | SRM | C4D-CHA-C1A | 2.51 | 132.01 | 128.74 |
| 5 | D | 582 | SRM | C4C-C3C-C2C | -2.51 | 104.81 | 106.70 |
| 5 | E | 583 | SRM | C4C-C3C-C2C | -2.46 | 104.85 | 106.70 |
| 5 | B | 581 | SRM | C4D-ND-C1D | 2.46 | 109.02 | 105.95 |
| 5 | D | 582 | SRM | CMB-C2B-CDB | 2.44 | 111.78 | 109.44 |
| 5 | E | 583 | SRM | C2C-C1C-NC | -2.44 | 106.45 | 110.51 |
| 5 | D | 582 | SRM | C1D-C2D-C3D | -2.43 | 104.40 | 106.92 |
| 5 | B | 581 | SRM | CDB-C2B-C1B | -2.35 | 105.30 | 112.08 |
| 5 | B | 581 | SRM | C4C-C3C-C2C | -2.35 | 104.94 | 106.70 |
| 5 | E | 583 | SRM | C4D-ND-C1D | 2.33 | 108.86 | 105.95 |
| 5 | D | 582 | SRM | CBC-CAC-C3C | 2.33 | 116.70 | 112.35 |
| 5 | B | 581 | SRM | C2C-C1C-NC | -2.32 | 106.64 | 110.51 |
| 5 | A | 580 | SRM | C2A-C1A-CHA | 2.31 | 129.41 | 122.95 |
| 5 | D | 582 | SRM | C2A-C1A-CHA | 2.27 | 129.30 | 122.95 |
| 5 | E | 583 | SRM | CDA-C2A-C3A | -2.27 | 105.20 | 112.10 |
| 5 | D | 582 | SRM | C4C-NC-C1C | 2.26 | 108.97 | 105.58 |
| 5 | E | 583 | SRM | CAC-C3C-C4C | 2.22 | 128.67 | 124.67 |
| 5 | A | 580 | SRM | C1D-C2D-C3D | -2.22 | 104.62 | 106.92 |
| 5 | A | 580 | SRM | C4C-NC-C1C | 2.19 | 108.87 | 105.58 |
| 5 | D | 582 | SRM | O4D-CED-CDD | 2.17 | 119.25 | 113.80 |
| 5 | A | 580 | SRM | C2B-CDB-CEB | 2.16 | 117.94 | 114.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5 | A | 580 | SRM | CDB-C2B-C3B | -2.15 | 105.55 | 112.10 |
| 5 | A | 580 | SRM | C4A-CHB-C1B | 2.14 | 129.59 | 124.45 |
| 5 | B | 581 | SRM | CDA-C2A-C3A | -2.14 | 105.59 | 112.10 |
| 5 | E | 583 | SRM | CDC-C2C-C1C | -2.12 | 122.94 | 127.75 |
| 5 | A | 580 | SRM | CAC-C3C-C4C | 2.10 | 128.46 | 124.67 |
| 5 | B | 581 | SRM | O1A-CCA-CBA | 2.06 | 130.13 | 123.03 |
| 5 | D | 582 | SRM | C4D-ND-C1D | 2.05 | 109.47 | 106.76 |
| 5 | D | 582 | SRM | C4A-CHB-C1B | 2.04 | 129.34 | 124.45 |
| 5 | D | 582 | SRM | CAC-C3C-C4C | 2.04 | 128.34 | 124.67 |
| 5 | E | 583 | SRM | O2A-CCA-CBA | 2.03 | 121.41 | 114.22 |
| 5 | A | 580 | SRM | C4D-ND-C1D | 2.03 | 109.43 | 106.76 |
| 5 | E | 583 | SRM | O4D-CED-CDD | 2.02 | 118.88 | 113.80 |
| 5 | E | 583 | SRM | CMA-C2A-C3A | 2.00 | 119.91 | 112.50 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 435/437 (99%) | 0.10 | 4 (0%) 81 89 | 14, 23, 44, 74 | 0 |
| 1 | D | 435/437 (99%) | -0.15 | 3 (0%) 84 91 | 13, 19, 38, 73 | 0 |
| 2 | B | 385/386 (99%) | 0.06 | 5 (1%) 74 84 | 15, 23, 40, 59 | 0 |
| 2 | E | 385/386 (99%) | -0.07 | 4 (1%) 79 88 | 13, 21, 36, 78 | 0 |
| 3 | C | 104/105 (99%) | 0.67 | 12 (11%) 5 8 | 22, 33, 64, 79 | 0 |
| 3 | F | 104/105 (99%) | 0.25 | 2 (1%) 64 74 | 22, 29, 47, 66 | 0 |
| All | All | 1848/1856 (99%) | 0.04 | 30 (1%) 67 79 | 13, 23, 44, 79 | 0 |

All (30) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | C | 105 | VAL | 6.2 |
| 3 | F | 105 | VAL | 5.3 |
| 1 | D | 3 | LYS | 4.7 |
| 2 | E | 386 | SER | 4.5 |
| 1 | D | 4 | HIS | 4.3 |
| 3 | C | 3 | VAL | 4.2 |
| 3 | C | 4 | VAL | 4.0 |
| 1 | A | 4 | HIS | 3.4 |
| 3 | C | 8 | GLY | 3.4 |
| 2 | B | 2 | ALA | 3.3 |
| 3 | C | 6 | PHE | 3.0 |
| 1 | A | 3 | LYS | 2.9 |
| 3 | F | 41 | ALA | 2.9 |
| 3 | C | 11 | PHE | 2.7 |
| 1 | D | 89 | GLU | 2.6 |
| 3 | C | 40 | GLY | 2.5 |
| 3 | C | 9 | SER | 2.5 |
| 3 | C | 7 | ALA | 2.5 |
| 1 | A | 430 | ASP | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 37 | GLY | 2.4 |
| 2 | B | 244 | ASN | 2.4 |
| 2 | B | 150 | TYR | 2.4 |
| 2 | E | 239 | ILE | 2.4 |
| 3 | C | 72 | ASN | 2.4 |
| 2 | B | 386 | SER | 2.3 |
| 2 | B | 3 | PHE | 2.2 |
| 3 | C | 10 | ALA | 2.2 |
| 3 | C | 31 | LYS | 2.1 |
| 2 | E | 244 | ASN | 2.1 |
| 2 | E | 246 | GLN | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 4 | SO3 | D | 6576 | 4/4 | 0.13 | 4.16 | 34,35,36,36 | 0 |
| 4 | SO3 | A | 6575 | 4/4 | 0.14 | 2.97 | 39,40,40,40 | 0 |
| 5 | SRM | B | 581 | 62/63 | 0.16 | 1.79 | 19,21,24,25 | 0 |
| 5 | SRM | E | 583 | 62/63 | 0.13 | 1.36 | 14,17,20,23 | 0 |
| 5 | SRM | D | 582 | 63/63 | 0.12 | 0.56 | 18,21,28,31 | 0 |
| 5 | SRM | A | 580 | 63/63 | 0.13 | 0.39 | 20,24,31,33 | 0 |
| 6 | SF4 | D | 808 | 8/8 | 0.10 | 0.26 | 13,18,21,22 | 0 |
| 6 | SF4 | A | 804 | 8/8 | 0.10 | -0.44 | 17,20,23,23 | 0 |
| 6 | SF4 | D | 807 | 8/8 | 0.06 | -0.47 | 17,21,22,22 | 0 |
| 6 | SF4 | A | 803 | 8/8 | 0.08 | -0.49 | 22,23,25,26 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|-----------------------------|-------|
| 6 | SF4 | E | 806 | 8/8 | 0.08 | -0.59 | 22,23,25,25 | 0 |
| 6 | SF4 | B | 802 | 8/8 | 0.07 | -0.78 | 21,22,22,24 | 0 |
| 6 | SF4 | E | 805 | 8/8 | 0.08 | -0.96 | 18,21,24,24 | 0 |
| 6 | SF4 | B | 801 | 8/8 | 0.07 | -1.06 | 17,23,24,24 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.