

Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 04:43 PM EDT

| PDB ID | : | 3RDE |
|--------------|---|--|
| Title | : | Crystal structure of the catalytic domain of porcine leukocyte 12-lipoxygenase |
| Authors | : | Funk, M.O.; Xu, S.; Marnett, L.J.; Mueser, T.C. |
| Deposited on | : | 2011-04-01 |
| Resolution | : | 1.89 Å(reported) |
| | | |

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

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

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

| MolProbity | : | 4.02b-467 |
|--------------------------------|---|--|
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| buster-report | : | 1.1.7(2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.89 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.



| Motria | Whole archive | Similar resolution |
|-----------------------|---------------------|---|
| Metric | $(\# { m Entries})$ | $(\# { m Entries}, { m resolution} { m range}({ m \AA}))$ |
| R _{free} | 130704 | 6207 (1.90-1.90) |
| Clashscore | 141614 | 6847 (1.90-1.90) |
| Ramachandran outliers | 138981 | 6760 (1.90-1.90) |
| Sidechain outliers | 138945 | 6760 (1.90-1.90) |
| RSRZ outliers | 127900 | 6082 (1.90-1.90) |

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

| Mol | Chain | Length | Quality of chain | | |
|-----|-------|--------|------------------|-----|-----|
| 1 | А | 573 | % 83% | 12% | ••• |
| 1 | В | 573 | % • 84% | 11% | ••• |
| 1 | С | 573 | <u>6%</u> 80% | 15% | ••• |
| 1 | D | 573 | 87% | 8% | ••• |



3RDE

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19031 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|-------|------|-----|-----|--------------|---------|-------|---|
| 1 | Λ | 559 | Total | С | Ν | 0 | \mathbf{S} | 12 | n | 0 |
| | A | 552 | 4412 | 2824 | 760 | 804 | 24 | 13 | 0 | |
| 1 | Р | 559 | Total | С | Ν | Ο | \mathbf{S} | 0 | 1 | 0 |
| | | 552 | 4421 | 2829 | 762 | 806 | 24 | 9 | 4 | U |
| 1 | 1 0 | 7 559 | Total | С | Ν | 0 | S | 43 | 1 | 0 |
| | 552 | 4398 | 2816 | 756 | 802 | 24 | 40 | 1 | 0 | |
| 1 D | 552 | Total | С | Ν | 0 | S | 35 | 1 | Ο | |
| | | 4416 | 2826 | 758 | 808 | 24 | | 4 | 0 | |

• Molecule 1 is a protein called Arachidonate 12-lipoxygenase, 12S-type.

There are 96 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Actual Comment | |
|-------|---------|----------|--------|-----------------------|------------|
| А | 91 | MET | - | initiating methionine | UNP P16469 |
| А | 92 | GLY | - | expression tag | UNP P16469 |
| А | 93 | SER | - | expression tag | UNP P16469 |
| А | 94 | SER | - | expression tag | UNP P16469 |
| А | 95 | HIS | - | expression tag | UNP P16469 |
| А | 96 | HIS | - | expression tag | UNP P16469 |
| А | 97 | HIS | - | expression tag | UNP P16469 |
| А | 98 | HIS | - | expression tag | UNP P16469 |
| А | 99 | HIS | - | expression tag | UNP P16469 |
| А | 100 | HIS | - | expression tag | UNP P16469 |
| А | 101 | SER | - | expression tag | UNP P16469 |
| А | 102 | SER | - | expression tag | UNP P16469 |
| А | 103 | GLY | - | expression tag | UNP P16469 |
| А | 104 | LEU | - | expression tag | UNP P16469 |
| А | 105 | VAL | - | expression tag | UNP P16469 |
| А | 106 | PRO | - | expression tag | UNP P16469 |
| А | 107 | ARG | - | expression tag | UNP P16469 |
| A | 108 | GLY | - | expression tag | UNP P16469 |
| A | 109 | SER | - | expression tag | UNP P16469 |
| А | 110 | HIS | - | expression tag | UNP P16469 |
| А | 111 | MET | - | expression tag | UNP P16469 |



| 3RDE |
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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| A | 210 | SER | CYS | engineered mutation | UNP P16469 |
| A | 218 | ARG | GLN | engineered mutation | UNP P16469 |
| A | 292 | SER | CYS | engineered mutation | UNP P16469 |
| В | 91 | MET | _ | initiating methionine | UNP P16469 |
| В | 92 | GLY | - | expression tag | UNP P16469 |
| В | 93 | SER | - | expression tag | UNP P16469 |
| В | 94 | SER | - | expression tag | UNP P16469 |
| В | 95 | HIS | - | expression tag | UNP P16469 |
| В | 96 | HIS | - | expression tag | UNP P16469 |
| В | 97 | HIS | - | expression tag | UNP P16469 |
| В | 98 | HIS | - | expression tag | UNP P16469 |
| В | 99 | HIS | - | expression tag | UNP P16469 |
| В | 100 | HIS | - | expression tag | UNP P16469 |
| В | 101 | SER | - | expression tag | UNP P16469 |
| В | 102 | SER | - | expression tag | UNP P16469 |
| В | 103 | GLY | - | expression tag | UNP P16469 |
| В | 104 | LEU | - | expression tag | UNP P16469 |
| В | 105 | VAL | - | expression tag | UNP P16469 |
| В | 106 | PRO | - | expression tag | UNP P16469 |
| В | 107 | ARG | - | expression tag | UNP P16469 |
| В | 108 | GLY | - | expression tag | UNP P16469 |
| В | 109 | SER | - | expression tag | UNP P16469 |
| В | 110 | HIS | - | expression tag | UNP P16469 |
| В | 111 | MET | - | expression tag | UNP P16469 |
| В | 210 | SER | CYS | engineered mutation | UNP P16469 |
| В | 218 | ARG | GLN | engineered mutation | UNP P16469 |
| В | 292 | SER | CYS | engineered mutation | UNP P16469 |
| С | 91 | MET | - | initiating methionine | UNP P16469 |
| С | 92 | GLY | - | expression tag | UNP P16469 |
| С | 93 | SER | - | expression tag | UNP P16469 |
| С | 94 | SER | - | expression tag | UNP P16469 |
| С | 95 | HIS | - | expression tag | UNP P16469 |
| С | 96 | HIS | - | expression tag | UNP P16469 |
| С | 97 | HIS | - | expression tag | UNP P16469 |
| С | 98 | HIS | - | expression tag | UNP P16469 |
| С | 99 | HIS | - | expression tag | UNP P16469 |
| С | 100 | HIS | - | expression tag | UNP P16469 |
| C | 101 | SER | - | expression tag | UNP P16469 |
| C | 102 | SER | - | expression tag | UNP P16469 |
| C | 103 | GLY | - | expression tag | UNP P16469 |
| C | 104 | LEU | - | expression tag | UNP P16469 |
| С | 105 | VAL | - | expression tag | UNP P16469 |



| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| С | 106 | PRO | - | expression tag | UNP P16469 |
| С | 107 | ARG | - | expression tag | UNP P16469 |
| С | 108 | GLY | - | expression tag | UNP P16469 |
| С | 109 | SER | - | expression tag | UNP P16469 |
| С | 110 | HIS | - | expression tag | UNP P16469 |
| С | 111 | MET | - | expression tag | UNP P16469 |
| С | 210 | SER | CYS | engineered mutation | UNP P16469 |
| С | 218 | ARG | GLN | engineered mutation | UNP P16469 |
| С | 292 | SER | CYS | engineered mutation | UNP P16469 |
| D | 91 | MET | - | initiating methionine | UNP P16469 |
| D | 92 | GLY | - | expression tag | UNP P16469 |
| D | 93 | SER | - | expression tag | UNP P16469 |
| D | 94 | SER | - | expression tag | UNP P16469 |
| D | 95 | HIS | - | expression tag | UNP P16469 |
| D | 96 | HIS | - | expression tag | UNP P16469 |
| D | 97 | HIS | - | expression tag | UNP P16469 |
| D | 98 | HIS | - | expression tag | UNP P16469 |
| D | 99 | HIS | - | expression tag | UNP P16469 |
| D | 100 | HIS | - | expression tag | UNP P16469 |
| D | 101 | SER | - | expression tag | UNP P16469 |
| D | 102 | SER | - | expression tag | UNP P16469 |
| D | 103 | GLY | - | expression tag | UNP P16469 |
| D | 104 | LEU | - | expression tag | UNP P16469 |
| D | 105 | VAL | - | expression tag | UNP P16469 |
| D | 106 | PRO | - | expression tag | UNP P16469 |
| D | 107 | ARG | - | expression tag | UNP P16469 |
| D | 108 | GLY | - | expression tag | UNP P16469 |
| D | 109 | SER | - | expression tag | UNP P16469 |
| D | 110 | HIS | - | expression tag | UNP P16469 |
| D | 111 | MET | - | expression tag | UNP P16469 |
| D | 210 | SER | CYS | engineered mutation | UNP P16469 |
| D | 218 | ARG | GLN | engineered mutation | UNP P16469 |
| D | 292 | SER | CYS | engineered mutation | UNP P16469 |

• Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 2 | А | 1 | Total K 1 1 | 0 | 0 |
| 2 | D | 1 | Total K 1 1 | 0 | 0 |



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | А | 1 | Total Fe 1 1 | 0 | 0 |
| 3 | В | 1 | Total Fe 1 1 | 0 | 0 |
| 3 | С | 1 | Total Fe 1 1 | 0 | 0 |
| 3 | D | 1 | Total Fe 1 1 | 0 | 0 |

• Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

• Molecule 4 is $3-\{4-[(tridec-2-yn-1-yloxy)methyl]phenyl\}$ propanoic acid (three-letter code: OYP) (formula: $C_{23}H_{34}O_3$).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 4 | А | 1 | Total C O | 0 | 0 |
| Т | 11 | I | 26 23 3 | 0 | 0 |
| 4 | В | 1 | Total C O | 0 | 0 |
| 4 | D | 1 | 26 23 3 | 0 | 0 |
| 4 | С | 1 | Total C O | 0 | 0 |
| 4 | U | 1 | 26 23 3 | 0 | 0 |
| 4 | Л | 1 | Total C O | 0 | 0 |
| 4 | D | | 26 23 3 | 0 | 0 |

• Molecule 5 is water.



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5 | А | 393 | Total O 393 393 | 0 | 0 |
| 5 | В | 386 | Total O 386 386 | 0 | 0 |
| 5 | С | 187 | Total O 187 187 | 0 | 0 |
| 5 | D | 308 | Total O 308 308 | 0 | 0 |



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Arachidonate 12-lipoxygenase, 12S-type

N54

H6: E6: E6: 163

F332 F332 565 9337 565 9336 568 9337 570 60 571 813 573 836 573 837 570 8336 571 813 573 837 570 837 571 814 600 7361 615 846 616 1412 616 1412 616 1412 616 1412 616 1412 616 1412 63 1463 657 1466 658 7463 650 846 651 1465 653 1466 654 146 653 1465 654 146 657 1466 658 1465 658 1466 658 1466 658 1466 659 6465 650 8406 650 8406 651 8466 650 850 650 860

• Molecule 1: Arachidonate 12-lipoxygenase, 12S-type

| Chain D: | 87% | 8% • • |
|--|---|---|
| MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLZ ARG CII2 GII2 MET MET | R115 116 116 1116 1116 1123 6123 6123 6123 6 | 1157 1157 1157 1170 1170 1173 1173 1173 1173 1173 117 |
| 8212 8213 8214 8214 8214 8214 8214 8256 66 8267 6267 6307 8307 8307 8307 8307 8307 | R323 E324 F327 H356 1389 L429 A449 A449 A449 | L466 E470 E475 E476 C500 C500 D513 P517 V530 |
| | | |



4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|-----------|
| Space group | P 1 21 1 | Depositor |
| Cell constants | 83.45Å 181.54Å 91.61Å | Deperitor |
| a, b, c, α , β , γ | 90.00° 92.86° 90.00° | Depositor |
| $\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$ | 48.97 - 1.89 | Depositor |
| Resolution (A) | 48.97 - 1.89 | EDS |
| % Data completeness | 99.4 (48.97-1.89) | Depositor |
| (in resolution range) | 99.4 (48.97-1.89) | EDS |
| R _{merge} | (Not available) | Depositor |
| R_{sym} | 0.10 | Depositor |
| $< I/\sigma(I) > 1$ | 2.87 (at 1.90Å) | Xtriage |
| Refinement program | REFMAC | Depositor |
| D D. | 0.172 , 0.214 | Depositor |
| Π, Π_{free} | 0.179 , 0.218 | DCC |
| R_{free} test set | 6468 reflections $(3.01%)$ | wwPDB-VP |
| Wilson B-factor $(Å^2)$ | 19.8 | Xtriage |
| Anisotropy | 0.042 | Xtriage |
| Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$ | 0.37, 47.0 | EDS |
| L-test for twinning ² | $< L >=0.49, < L^2>=0.32$ | Xtriage |
| Estimated twinning fraction | 0.029 for h,-k,-l | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 19031 | wwPDB-VP |
| Average B, all atoms $(Å^2)$ | 22.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, K, OYP

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).

| Mal | Chain | Bo | ond lengths | В | ond angles |
|-------|-------|------|-----------------|------|-----------------|
| INIOI | Chain | RMSZ | # Z > 5 | RMSZ | # Z > 5 |
| 1 | А | 1.27 | 9/4527~(0.2%) | 1.04 | 14/6144~(0.2%) |
| 1 | В | 1.24 | 10/4536~(0.2%) | 1.01 | 11/6156~(0.2%) |
| 1 | С | 1.17 | 6/4510~(0.1%) | 0.96 | 5/6122~(0.1%) |
| 1 | D | 1.17 | 5/4531~(0.1%) | 0.99 | 12/6150~(0.2%) |
| All | All | 1.22 | 30/18104~(0.2%) | 1.00 | 42/24572~(0.2%) |

All (30) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | В | 488 | GLU | CD-OE1 | 5.95 | 1.32 | 1.25 |
| 1 | С | 498 | ALA | CA-CB | 5.94 | 1.65 | 1.52 |
| 1 | А | 600 | CYS | CB-SG | 5.91 | 1.92 | 1.82 |
| 1 | С | 461 | TYR | CE2-CZ | -5.86 | 1.30 | 1.38 |
| 1 | С | 155 | SER | C-N | -5.84 | 1.20 | 1.34 |
| 1 | D | 227 | ALA | CA-CB | 5.75 | 1.64 | 1.52 |
| 1 | В | 612 | GLU | CB-CG | 5.60 | 1.62 | 1.52 |
| 1 | В | 369 | ALA | CA-CB | 5.57 | 1.64 | 1.52 |
| 1 | В | 641 | ARG | CG-CD | -5.57 | 1.38 | 1.51 |
| 1 | А | 653 | ARG | CB-CG | -5.53 | 1.37 | 1.52 |
| 1 | А | 223 | TRP | NE1-CE2 | -5.53 | 1.30 | 1.37 |
| 1 | А | 431 | ARG | CG-CD | 5.50 | 1.65 | 1.51 |
| 1 | А | 575 | GLU | CG-CD | 5.50 | 1.60 | 1.51 |
| 1 | С | 480 | VAL | CB-CG1 | 5.45 | 1.64 | 1.52 |
| 1 | А | 275 | PHE | CE2-CZ | 5.43 | 1.47 | 1.37 |
| 1 | В | 470 | GLU | C-N | -5.40 | 1.21 | 1.34 |
| 1 | С | 148 | GLY | N-CA | 5.32 | 1.54 | 1.46 |
| 1 | А | 458 | SER | CB-OG | -5.28 | 1.35 | 1.42 |
| 1 | D | 475 | TYR | CD1-CE1 | 5.26 | 1.47 | 1.39 |
| 1 | А | 180 | ALA | CA-CB | 5.18 | 1.63 | 1.52 |
| 1 | С | 134 | ALA | CA-CB | 5.17 | 1.63 | 1.52 |
| 1 | В | 365 | GLY | C-O | 5.16 | 1.31 | 1.23 |



| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | В | 299 | VAL | CB-CG2 | 5.13 | 1.63 | 1.52 |
| 1 | D | 449 | ALA | CA-CB | 5.12 | 1.63 | 1.52 |
| 1 | В | 605 | VAL | CB-CG2 | 5.12 | 1.63 | 1.52 |
| 1 | D | 463 | GLN | CG-CD | 5.11 | 1.62 | 1.51 |
| 1 | D | 160 | ASP | CB-CG | -5.08 | 1.41 | 1.51 |
| 1 | В | 181 | LYS | CD-CE | 5.06 | 1.64 | 1.51 |
| 1 | В | 575 | GLU | CG-CD | 5.06 | 1.59 | 1.51 |
| 1 | А | 418 | VAL | CB-CG2 | 5.04 | 1.63 | 1.52 |

Continued from previous page...

All (42) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|--------|------|------------|--------|------------------|---------------|
| 1 | D | 129 | ARG | NE-CZ-NH2 | -10.74 | 114.93 | 120.30 |
| 1 | D | 129 | ARG | NE-CZ-NH1 | 9.22 | 124.91 | 120.30 |
| 1 | В | 129 | ARG | NE-CZ-NH2 | -8.85 | 115.88 | 120.30 |
| 1 | В | 129 | ARG | NE-CZ-NH1 | 6.32 | 123.46 | 120.30 |
| 1 | D | 170 | ASP | CB-CG-OD1 | 6.02 | 123.72 | 118.30 |
| 1 | В | 221 | ASP | CB-CG-OD1 | 5.97 | 123.67 | 118.30 |
| 1 | А | 202 | ASP | CB-CG-OD1 | 5.91 | 123.62 | 118.30 |
| 1 | D | 496 | LEU | CA-CB-CG | 5.91 | 128.88 | 115.30 |
| 1 | А | 312 | LEU | CB-CG-CD1 | 5.87 | 120.98 | 111.00 |
| 1 | А | 501 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 1 | А | 136 | ARG | NE-CZ-NH1 | 5.85 | 123.22 | 120.30 |
| 1 | А | 416 | ASP | CB-CG-OD2 | -5.81 | 113.07 | 118.30 |
| 1 | А | 170 | ASP | CB-CG-OD1 | 5.74 | 123.46 | 118.30 |
| 1 | А | 349 | ARG | NE-CZ-NH2 | -5.72 | 117.44 | 120.30 |
| 1 | D | 513 | ASP | CB-CG-OD1 | 5.70 | 123.43 | 118.30 |
| 1 | В | 431 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 1 | А | 395[A] | ARG | NE-CZ-NH2 | -5.65 | 117.48 | 120.30 |
| 1 | А | 395[B] | ARG | NE-CZ-NH2 | -5.65 | 117.48 | 120.30 |
| 1 | С | 349 | ARG | NE-CZ-NH2 | -5.58 | 117.51 | 120.30 |
| 1 | D | 246 | VAL | CG1-CB-CG2 | 5.51 | 119.71 | 110.90 |
| 1 | А | 604 | MET | CG-SD-CE | 5.47 | 108.96 | 100.20 |
| 1 | D | 513 | ASP | CB-CG-OD2 | -5.45 | 113.39 | 118.30 |
| 1 | D | 123 | GLY | N-CA-C | 5.43 | 126.69 | 113.10 |
| 1 | В | 172 | ARG | NE-CZ-NH2 | -5.40 | 117.60 | 120.30 |
| 1 | D | 170 | ASP | CB-CG-OD2 | -5.39 | 113.45 | 118.30 |
| 1 | D | 429 | LEU | CB-CG-CD2 | -5.38 | 101.85 | 111.00 |
| 1 | A | 496 | LEU | CA-CB-CG | 5.37 | 127.66 | 115.30 |
| 1 | В | 538 | THR | O-C-N | -5.36 | 114.10 | 123.20 |
| 1 | D | 349 | ARG | NE-CZ-NH2 | -5.33 | 117.63 | 120.30 |
| 1 | А | 487 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |



| Mol | Chain | Res | Type | Atoms | | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|-----------|-------|------------------|---------------|
| 1 | А | 431 | ARG | NE-CZ-NH2 | -5.28 | 117.66 | 120.30 |
| 1 | D | 115 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 1 | В | 431 | ARG | NE-CZ-NH2 | -5.21 | 117.70 | 120.30 |
| 1 | А | 403 | ARG | NE-CZ-NH1 | 5.19 | 122.89 | 120.30 |
| 1 | В | 141 | ARG | NE-CZ-NH2 | -5.13 | 117.73 | 120.30 |
| 1 | В | 597 | LEU | CB-CG-CD2 | 5.13 | 119.72 | 111.00 |
| 1 | В | 278 | ASP | CB-CG-OD1 | 5.11 | 122.90 | 118.30 |
| 1 | С | 326 | SER | C-N-CD | -5.09 | 109.39 | 120.60 |
| 1 | С | 254 | PHE | C-N-CD | -5.09 | 109.41 | 120.60 |
| 1 | С | 599 | ARG | CG-CD-NE | -5.07 | 101.15 | 111.80 |
| 1 | С | 243 | ARG | NE-CZ-NH1 | 5.05 | 122.82 | 120.30 |
| 1 | В | 349 | ARG | NE-CZ-NH2 | -5.00 | 117.80 | 120.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | А | 4412 | 0 | 4407 | 42 | 0 |
| 1 | В | 4421 | 0 | 4414 | 43 | 0 |
| 1 | С | 4398 | 0 | 4389 | 56 | 0 |
| 1 | D | 4416 | 0 | 4404 | 36 | 0 |
| 2 | А | 1 | 0 | 0 | 0 | 0 |
| 2 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | А | 1 | 0 | 0 | 0 | 0 |
| 3 | В | 1 | 0 | 0 | 0 | 0 |
| 3 | С | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | А | 26 | 0 | 33 | 0 | 0 |
| 4 | В | 26 | 0 | 33 | 0 | 0 |
| 4 | С | 26 | 0 | 33 | 1 | 0 |
| 4 | D | 26 | 0 | 33 | 0 | 0 |
| 5 | А | 393 | 0 | 0 | 1 | 0 |
| 5 | B | 386 | 0 | 0 | 2 | 0 |
| 5 | С | 187 | 0 | 0 | 0 | 0 |



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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | D | 308 | 0 | 0 | 3 | 0 |
| All | All | 19031 | 0 | 17746 | 177 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom_1 | Atom_2 | Interatomic | Clash |
|---------------------|--------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:391:ILE:CG2 | 1:A:392:PRO:HD3 | 1.54 | 1.37 |
| 1:B:485:LYS:N | 1:B:485:LYS:HD3 | 1.47 | 1.14 |
| 1:B:485:LYS:H | 1:B:485:LYS:CD | 1.63 | 1.09 |
| 1:B:485:LYS:HD3 | 1:B:485:LYS:H | 0.91 | 1.07 |
| 1:A:391:ILE:CG2 | 1:A:392:PRO:CD | 2.31 | 1.07 |
| 1:A:500[B]:CYS:SG | 1:A:520:LEU:HG | 2.00 | 1.01 |
| 1:A:391:ILE:HG22 | 1:A:392:PRO:HD3 | 1.03 | 1.00 |
| 1:A:391:ILE:HG22 | 1:A:392:PRO:CD | 1.90 | 0.99 |
| 1:C:129:ARG:HD3 | 1:C:495:GLU:OE2 | 1.65 | 0.96 |
| 1:A:391:ILE:HG23 | 1:A:392:PRO:HD3 | 1.48 | 0.95 |
| 1:C:288:ASN:ND2 | 1:C:290:ILE:HD11 | 1.85 | 0.92 |
| 1:A:391:ILE:HG23 | 1:A:392:PRO:CD | 1.99 | 0.91 |
| 1:D:542:SER:HB3 | 5:D:764:HOH:O | 1.71 | 0.90 |
| 1:A:192:LEU:HG | 1:A:196:MET:HE1 | 1.55 | 0.88 |
| 1:B:656[B]:ARG:HH11 | 1:B:656[B]:ARG:HG3 | 1.39 | 0.87 |
| 1:C:157:GLY:O | 1:C:160:ASP:HB2 | 1.76 | 0.86 |
| 1:D:117:VAL:O | 1:D:120:ASP:HB2 | 1.77 | 0.85 |
| 1:C:204:PHE:O | 1:C:207:ILE:HD13 | 1.76 | 0.84 |
| 1:A:114:ALA:O | 1:A:115:ARG:HD2 | 1.79 | 0.83 |
| 1:C:255:PRO:HD3 | 1:C:328:LEU:HD13 | 1.60 | 0.82 |
| 1:A:391:ILE:HG23 | 1:A:392:PRO:N | 1.95 | 0.79 |
| 1:D:124:LEU:HD13 | 1:D:125:PHE:CE1 | 2.19 | 0.78 |
| 1:D:124:LEU:HD13 | 1:D:125:PHE:CD1 | 2.19 | 0.77 |
| 1:C:207:ILE:HD13 | 1:C:207:ILE:H | 1.47 | 0.77 |
| 1:D:145:TRP:H | 1:D:152:ASN:HD21 | 1.35 | 0.73 |
| 1:C:145:TRP:H | 1:C:152:ASN:HD21 | 1.36 | 0.72 |
| 1:A:220:ARG:HD3 | 5:A:758:HOH:O | 1.87 | 0.72 |
| 1:A:145:TRP:H | 1:A:152:ASN:HD21 | 1.36 | 0.71 |
| 1:A:192:LEU:CG | 1:A:196:MET:HE1 | 2.19 | 0.71 |
| 1:A:500[B]:CYS:HG | 1:A:520:LEU:HG | 1.55 | 0.69 |
| 1:B:307:GLN:NE2 | 1:B:313:LEU:HD12 | 2.08 | 0.68 |
| 1:A:391:ILE:HG21 | 1:A:614:TYR:CE1 | 2.29 | 0.67 |



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| Atom-1 | Atom-2 | Interatomic | Clash |
|--------------------|---------------------|--------------|-------------|
| | Atom-2 | distance (Å) | overlap (Å) |
| 1:C:179:LEU:HD22 | 4:C:664:OYP:O2 | 1.93 | 0.67 |
| 1:C:204:PHE:O | 1:C:207:ILE:CD1 | 2.43 | 0.67 |
| 1:A:192:LEU:CD1 | 1:A:196:MET:HE1 | 2.26 | 0.66 |
| 1:C:500[B]:CYS:SG | 1:C:517:PRO:HB2 | 2.36 | 0.66 |
| 1:C:356:HIS:HE1 | 1:C:544:ASN:O | 1.79 | 0.66 |
| 1:B:656[B]:ARG:HG3 | 1:B:656[B]:ARG:NH1 | 2.08 | 0.65 |
| 1:D:466:LEU:O | 1:D:470:GLU:HG3 | 1.98 | 0.63 |
| 1:D:542:SER:CB | 5:D:764:HOH:O | 2.39 | 0.63 |
| 1:A:172:ARG:O | 1:A:176:GLU:HG3 | 1.99 | 0.63 |
| 1:A:205:ASN:ND2 | 1:A:220:ARG:HH11 | 1.97 | 0.63 |
| 1:C:155:SER:OG | 1:C:160:ASP:HB3 | 1.99 | 0.62 |
| 1:B:178:SER:C | 1:B:596[B]:GLN:HE22 | 2.03 | 0.61 |
| 1:D:169:GLU:HG2 | 1:D:173:ILE:HD12 | 1.82 | 0.61 |
| 1:C:288:ASN:CG | 1:C:290:ILE:HD11 | 2.21 | 0.61 |
| 1:A:114:ALA:O | 1:A:115:ARG:CD | 2.50 | 0.60 |
| 1:A:205:ASN:HD22 | 1:A:220:ARG:HH11 | 1.50 | 0.59 |
| 1:B:145:TRP:H | 1:B:152:ASN:HD21 | 1.49 | 0.58 |
| 1:B:193:ASN:HD22 | 1:B:206:ARG:HH21 | 1.49 | 0.58 |
| 1:C:600:CYS:O | 1:C:602:PRO:HD3 | 2.02 | 0.58 |
| 1:A:642:ASN:HB3 | 1:A:648:PRO:HB3 | 1.85 | 0.58 |
| 1:D:169:GLU:CG | 1:D:173:ILE:HD12 | 2.34 | 0.58 |
| 1:D:117:VAL:O | 1:D:120:ASP:CB | 2.51 | 0.57 |
| 1:D:124:LEU:CD1 | 1:D:125:PHE:CD1 | 2.86 | 0.57 |
| 1:B:281:LEU:HG | 1:B:429:LEU:HD11 | 1.85 | 0.57 |
| 1:D:117:VAL:C | 1:D:120:ASP:HB2 | 2.25 | 0.57 |
| 1:C:545:HIS:CE1 | 1:C:663:ILE:HG23 | 2.41 | 0.56 |
| 1:C:454:LEU:CD2 | 1:C:466:LEU:HD11 | 2.35 | 0.55 |
| 1:C:444:PRO:HD2 | 1:C:469:TRP:CE3 | 2.42 | 0.54 |
| 1:B:281:LEU:HG | 1:B:429:LEU:CD1 | 2.37 | 0.54 |
| 1:D:124:LEU:CD1 | 1:D:125:PHE:HD1 | 2.20 | 0.54 |
| 1:C:429:LEU:HD12 | 1:C:429:LEU:O | 2.07 | 0.54 |
| 1:B:178:SER:OG | 1:B:596[B]:GLN:OE1 | 2.25 | 0.54 |
| 1:C:223:TRP:HA | 1:C:228:LEU:HD23 | 1.88 | 0.54 |
| 1:C:129:ARG:NH1 | 1:C:495:GLU:OE1 | 2.41 | 0.54 |
| 1:C:356:HIS:CE1 | 1:C:544:ASN:O | 2.60 | 0.54 |
| 1:A:194:VAL:HG12 | 1:A:584:PHE:HZ | 1.73 | 0.53 |
| 1:D:356:HIS:HE1 | 1:D:544:ASN:O | 1.91 | 0.53 |
| 1:C:650:GLU:OE1 | 1:C:653:ARG:HD3 | 2.10 | 0.52 |
| 1:A:391:ILE:HG21 | 1:A:614:TYR:CD1 | 2.45 | 0.52 |
| 1:D:129:ARG:CD | 1:D:495:GLU:OE2 | 2.58 | 0.52 |
| 1:C:205:ASN:HD21 | 1:C:220:ARG:HD2 | 1.73 | 0.52 |



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| Atom 1 | Atom 2 | Interatomic | Clash |
|-------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:B:573:THR:OG1 | 1:B:575:GLU:HG2 | 2.10 | 0.52 |
| 1:B:124:LEU:C | 1:B:124:LEU:CD1 | 2.78 | 0.51 |
| 1:B:129:ARG:CD | 1:B:495:GLU:OE2 | 2.57 | 0.51 |
| 1:B:356:HIS:HE1 | 1:B:544:ASN:O | 1.94 | 0.51 |
| 1:B:124:LEU:CD1 | 1:B:124:LEU:O | 2.59 | 0.51 |
| 1:B:124:LEU:O | 1:B:124:LEU:HD13 | 2.10 | 0.51 |
| 1:C:156:THR:OG1 | 1:C:160:ASP:OD2 | 2.28 | 0.51 |
| 1:D:129:ARG:HD3 | 1:D:495:GLU:OE2 | 2.11 | 0.50 |
| 1:C:204:PHE:HA | 1:C:207:ILE:CD1 | 2.41 | 0.50 |
| 1:D:307:GLN:NE2 | 1:D:313:LEU:HD12 | 2.27 | 0.50 |
| 1:B:485:LYS:H | 1:B:485:LYS:CE | 2.22 | 0.50 |
| 1:C:405:ARG:O | 1:C:410:SER:HB3 | 2.11 | 0.50 |
| 1:C:336:ASP:HB3 | 1:C:337:PRO:HD2 | 1.93 | 0.50 |
| 1:D:238:ASN:HB2 | 1:D:356:HIS:HB2 | 1.93 | 0.49 |
| 1:C:205:ASN:ND2 | 1:C:220:ARG:HD2 | 2.27 | 0.49 |
| 1:D:208:PHE:CZ | 1:D:212:GLN:HG3 | 2.47 | 0.49 |
| 1:B:258:MET:CE | 1:B:333:LEU:HD11 | 2.43 | 0.49 |
| 1:D:193:ASN:HD22 | 1:D:206:ARG:HH21 | 1.60 | 0.48 |
| 1:A:500[B]:CYS:SG | 1:A:520:LEU:CG | 2.89 | 0.48 |
| 1:B:466:LEU:O | 1:B:470:GLU:HG3 | 2.13 | 0.48 |
| 1:A:600:CYS:O | 1:A:602:PRO:HD3 | 2.12 | 0.48 |
| 1:B:160:ASP:OD1 | 1:B:160:ASP:C | 2.52 | 0.48 |
| 1:B:193:ASN:ND2 | 1:B:206:ARG:HH21 | 2.11 | 0.48 |
| 1:C:391:ILE:CG2 | 1:C:392:PRO:HD3 | 2.44 | 0.48 |
| 1:D:193:ASN:ND2 | 1:D:206:ARG:HH21 | 2.12 | 0.48 |
| 1:A:341:TRP:CD1 | 1:A:345:LYS:HE2 | 2.48 | 0.47 |
| 1:C:285:ILE:HG13 | 1:C:429:LEU:HD22 | 1.95 | 0.47 |
| 1:C:500[B]:CYS:SG | 1:C:520:LEU:HG | 2.54 | 0.47 |
| 1:A:358:LEU:HD12 | 1:A:429:LEU:HD23 | 1.95 | 0.47 |
| 1:C:356:HIS:CD2 | 1:C:552:TYR:OH | 2.67 | 0.47 |
| 1:C:153:ILE:HG22 | 1:C:370:GLU:OE2 | 2.14 | 0.47 |
| 1:C:307:GLN:HB3 | 1:C:308:PRO:HD2 | 1.96 | 0.47 |
| 1:B:170:ASP:OD1 | 1:B:171:LYS:N | 2.38 | 0.47 |
| 1:B:129:ARG:HD2 | 1:B:495:GLU:OE2 | 2.15 | 0.46 |
| 1:D:124:LEU:HD13 | 1:D:125:PHE:HE1 | 1.79 | 0.46 |
| 1:D:157:GLY:O | 1:D:160:ASP:HB2 | 2.15 | 0.46 |
| 1:B:129:ARG:HD3 | 1:B:495:GLU:OE2 | 2.14 | 0.46 |
| 1:C:117:VAL:HG13 | 1:C:129:ARG:NH1 | 2.31 | 0.46 |
| 1:C:155:SER:OG | 1:C:160:ASP:CB | 2.63 | 0.46 |
| 1:A:463:GLN:NE2 | 1:A:641:ARG:HH11 | 2.14 | 0.46 |
| 1:C:281:LEU:HG | 1:C:429:LEU:HD11 | 1.97 | 0.46 |



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| A + a 1 | | | Clash |
|--------------------|-------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:C:129:ARG:HH11 | 1:C:495:GLU:CD | 2.18 | 0.46 |
| 1:A:194:VAL:HG12 | 1:A:584:PHE:CZ | 2.51 | 0.45 |
| 1:A:638:ILE:HG21 | 1:A:653:ARG:HG2 | 1.98 | 0.45 |
| 1:B:173:ILE:HA | 1:B:173:ILE:HD12 | 1.67 | 0.45 |
| 1:C:207:ILE:H | 1:C:207:ILE:CD1 | 2.21 | 0.45 |
| 1:A:238:ASN:HB2 | 1:A:356:HIS:HB2 | 1.98 | 0.45 |
| 1:B:444:PRO:HD2 | 1:B:469:TRP:CE3 | 2.52 | 0.45 |
| 1:A:258:MET:HE1 | 1:A:333:LEU:HD11 | 1.97 | 0.45 |
| 1:C:337:PRO:HG2 | 1:C:340:VAL:CG2 | 2.47 | 0.45 |
| 1:A:444:PRO:HD2 | 1:A:469:TRP:CE3 | 2.52 | 0.44 |
| 1:B:610:HIS:HD2 | 1:B:659:ASN:HD21 | 1.65 | 0.44 |
| 1:C:204:PHE:HA | 1:C:207:ILE:HD11 | 1.98 | 0.44 |
| 1:C:237:THR:HG22 | 1:C:356:HIS:CE1 | 2.52 | 0.44 |
| 1:A:405:ARG:O | 1:A:410:SER:HB3 | 2.17 | 0.44 |
| 1:B:656[B]:ARG:NH1 | 1:B:656[B]:ARG:CG | 2.76 | 0.44 |
| 1:A:192:LEU:O | 1:A:196:MET:HE2 | 2.18 | 0.44 |
| 1:B:527:CYS:HB3 | 5:B:832:HOH:O | 2.18 | 0.44 |
| 1:C:279:PHE:HB2 | 1:C:300:PRO:HD2 | 2.00 | 0.44 |
| 1:C:198:TRP:HH2 | 1:C:207:ILE:HD12 | 1.82 | 0.44 |
| 1:D:638:ILE:HG21 | 1:D:653:ARG:HG2 | 1.99 | 0.44 |
| 1:C:255:PRO:CD | 1:C:328:LEU:HD13 | 2.42 | 0.43 |
| 1:A:244:HIS:HE1 | 1:A:272:GLY:O | 2.01 | 0.43 |
| 1:A:545:HIS:CE1 | 1:A:663:ILE:HG23 | 2.53 | 0.43 |
| 1:B:356:HIS:CE1 | 1:B:544:ASN:O | 2.71 | 0.43 |
| 1:D:323:ARG:HA | 1:D:323:ARG:HD3 | 1.75 | 0.43 |
| 1:B:496:LEU:HD21 | 1:B:526:LEU:HD13 | 1.99 | 0.43 |
| 1:B:500[B]:CYS:SG | 1:B:517:PRO:HB2 | 2.58 | 0.43 |
| 1:C:337:PRO:HG2 | 1:C:340:VAL:HG21 | 2.00 | 0.43 |
| 1:D:117:VAL:HA | 1:D:120:ASP:HB2 | 1.99 | 0.43 |
| 1:D:129:ARG:HD2 | 1:D:495:GLU:OE2 | 2.19 | 0.43 |
| 1:A:595:TRP:CZ2 | 1:A:599:ARG:HD2 | 2.54 | 0.43 |
| 1:D:389:LEU:HD23 | 1:D:530:VAL:HG11 | 2.01 | 0.43 |
| 1:D:610:HIS:CD2 | 1:D:610:HIS:H | 2.36 | 0.43 |
| 1:B:610:HIS:HE1 | 5:B:836:HOH:O | 2.02 | 0.42 |
| 1:C:205:ASN:ND2 | 1:C:220:ARG:HH11 | 2.17 | 0.42 |
| 1:C:246:VAL:C | 1:C:269:LEU:HD21 | 2.39 | 0.42 |
| 1:C:319:LEU:HD23 | 1:C:319:LEU:HA | 1.85 | 0.42 |
| 1:D:500[A]:CYS:SG | 1:D:517:PRO:HG2 | 2.59 | 0.42 |
| 1:A:215:LEU:HD23 | 1:A:550:ASP:HB3 | 2.00 | 0.42 |
| 1:C:238:ASN:HB2 | 1:C:356:HIS:HB2 | 2.01 | 0.42 |
| 1:C:463:GLN:O | 1:C:467:ARG:HD3 | 2.18 | 0.42 |



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| A 4 1 | A 4 D | Interatomic | Clash | |
|------------------|-------------------|-------------------------|-------------|--|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) | |
| 1:B:610:HIS:CD2 | 1:B:610:HIS:H | 2.36 | 0.42 | |
| 1:B:626:LYS:HE3 | 1:B:630:GLU:OE2 | 2.19 | 0.42 | |
| 1:B:261:LEU:HA | 1:B:264:GLN:HG2 | 2.01 | 0.42 | |
| 1:A:145:TRP:CG | 1:A:405:ARG:HD2 | 2.54 | 0.42 | |
| 1:C:653:ARG:O | 1:C:657:VAL:HG23 | 2.20 | 0.42 | |
| 1:B:307:GLN:NE2 | 1:B:313:LEU:CD1 | 2.82 | 0.41 | |
| 1:C:247:GLU:N | 1:C:269:LEU:HD21 | 2.35 | 0.41 | |
| 1:B:238:ASN:HB2 | 1:B:356:HIS:HB2 | 2.01 | 0.41 | |
| 1:D:206:ARG:HD3 | 5:D:757:HOH:O | 2.20 | 0.41 | |
| 1:B:124:LEU:C | 1:B:124:LEU:HD12 | 2.41 | 0.41 | |
| 1:D:356:HIS:CE1 | 1:D:544:ASN:O | 2.73 | 0.41 | |
| 1:C:296:TYR:CE2 | 1:C:565:PRO:HG3 | 2.56 | 0.41 | |
| 1:D:261:LEU:HA | 1:D:264:GLN:HG2 | 2.02 | 0.41 | |
| 1:C:488:GLU:HG3 | 1:C:492:GLU:OE2 | 2.20 | 0.41 | |
| 1:C:205:ASN:HD22 | 1:C:220:ARG:HH11 | 1.68 | 0.41 | |
| 1:A:590:GLN:O | 1:A:594:THR:HG23 | 2.21 | 0.41 | |
| 1:B:357:GLU:HA | 1:B:357:GLU:OE1 | 2.21 | 0.41 | |
| 1:D:124:LEU:H | 1:D:124:LEU:HG | 1.48 | 0.41 | |
| 1:D:129:ARG:HD3 | 1:D:381:PRO:HG3 | 2.02 | 0.41 | |
| 1:D:155[B]:SER:O | 1:D:155[B]:SER:OG | 2.24 | 0.41 | |
| 1:B:230:GLY:HA3 | 1:B:312:LEU:O | 2.21 | 0.40 | |
| 1:A:638:ILE:HG21 | 1:A:653:ARG:CG | 2.52 | 0.40 | |

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Perce | ntiles |
|-----|-------|---------------|-----------|---------|----------|-------|--------|
| 1 | А | 553/573~(96%) | 539~(98%) | 13 (2%) | 1 (0%) | 47 | 38 |
| 1 | В | 554/573~(97%) | 543~(98%) | 10 (2%) | 1 (0%) | 47 | 38 |
| 1 | С | 551/573~(96%) | 531 (96%) | 17 (3%) | 3~(0%) | 29 | 18 |



| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percer | ntiles | |
|-----|-------|-----------------|------------|---------|----------|--------|--------|--|
| 1 | D | 554/573~(97%) | 540 (98%) | 11 (2%) | 3~(0%) | 29 | 18 | |
| All | All | 2212/2292~(96%) | 2153 (97%) | 51 (2%) | 8 (0%) | 41 | 24 | |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | В | 121 | PRO |
| 1 | D | 155[A] | SER |
| 1 | D | 155[B] | SER |
| 1 | С | 256 | PRO |
| 1 | С | 326 | SER |
| 1 | А | 407 | GLY |
| 1 | D | 120 | ASP |
| 1 | С | 407 | GLY |

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 1 | А | 483/498~(97%) | 470 (97%) | 13 (3%) | 44 38 |
| 1 | В | 484/498~(97%) | 474 (98%) | 10 (2%) | 53 48 |
| 1 | С | 481/498~(97%) | 459 (95%) | 22~(5%) | 27 17 |
| 1 | D | 484/498~(97%) | 468 (97%) | 16 (3%) | 38 29 |
| All | All | 1932/1992~(97%) | 1871 (97%) | 61 (3%) | 40 30 |

All (61) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 168 | LEU |
| 1 | А | 218 | ARG |
| 1 | А | 258 | MET |
| 1 | А | 267 | LYS |
| 1 | А | 323 | ARG |
| 1 | А | 391 | ILE |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 458 | SER |
| 1 | А | 466 | LEU |
| 1 | А | 501 | ARG |
| 1 | А | 599 | ARG |
| 1 | А | 611 | GLU |
| 1 | А | 636 | LYS |
| 1 | А | 647 | LEU |
| 1 | В | 120 | ASP |
| 1 | В | 122 | GLN |
| 1 | В | 124 | LEU |
| 1 | В | 127 | LYS |
| 1 | В | 155 | SER |
| 1 | В | 173 | ILE |
| 1 | В | 286 | LYS |
| 1 | В | 485 | LYS |
| 1 | В | 604 | MET |
| 1 | В | 644 | LYS |
| 1 | С | 113 | THR |
| 1 | С | 129 | ARG |
| 1 | С | 139 | LEU |
| 1 | С | 147 | ASP |
| 1 | С | 160 | ASP |
| 1 | С | 207 | ILE |
| 1 | С | 258 | MET |
| 1 | С | 259 | GLU |
| 1 | С | 261 | LEU |
| 1 | С | 268 | GLU |
| 1 | С | 269 | LEU |
| 1 | С | 320 | GLN |
| 1 | С | 323 | ARG |
| 1 | C | 324 | GLU |
| 1 | C | 326 | SER |
| 1 | C | 429 | LEU |
| 1 | C | 477 | GLU |
| 1 | С | 501 | ARG |
| 1 | С | 612 | GLU |
| 1 | C | 616 | SER |
| 1 | С | 636 | LYS |
| 1 | C | 639 | GLU |
| 1 | D | 120 | ASP |
| 1 | D | 122 | GLN |
| 1 | D | 124 | LEU |



| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | D | 155[A] | SER |
| 1 | D | 155[B] | SER |
| 1 | D | 179 | LEU |
| 1 | D | 214 | LYS |
| 1 | D | 218 | ARG |
| 1 | D | 246 | VAL |
| 1 | D | 324 | GLU |
| 1 | D | 485 | LYS |
| 1 | D | 496 | LEU |
| 1 | D | 500[A] | CYS |
| 1 | D | 500[B] | CYS |
| 1 | D | 612 | GLU |
| 1 | D | 647 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | \mathbf{Res} | Type |
|-----|-------|----------------|------|
| 1 | А | 152 | ASN |
| 1 | А | 159 | HIS |
| 1 | А | 205 | ASN |
| 1 | А | 244 | HIS |
| 1 | А | 463 | GLN |
| 1 | А | 548 | GLN |
| 1 | В | 152 | ASN |
| 1 | В | 193 | ASN |
| 1 | В | 205 | ASN |
| 1 | В | 244 | HIS |
| 1 | В | 270 | GLN |
| 1 | В | 307 | GLN |
| 1 | В | 356 | HIS |
| 1 | В | 463 | GLN |
| 1 | В | 610 | HIS |
| 1 | С | 152 | ASN |
| 1 | С | 205 | ASN |
| 1 | С | 244 | HIS |
| 1 | С | 307 | GLN |
| 1 | С | 356 | HIS |
| 1 | С | 540 | GLN |
| 1 | С | 548 | GLN |
| 1 | С | 610 | HIS |
| 1 | D | 128 | HIS |
| 1 | D | 152 | ASN |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 193 | ASN |
| 1 | D | 205 | ASN |
| 1 | D | 244 | HIS |
| 1 | D | 270 | GLN |
| 1 | D | 295 | GLN |
| 1 | D | 307 | GLN |
| 1 | D | 356 | HIS |
| 1 | D | 540 | GLN |
| 1 | D | 610 | HIS |

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5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

| Mal | Turne | who Chain Bog | | Tiple | Bo | ond leng | $_{\rm sths}$ | Bond angles | | |
|------|-------|---------------|-----|-------|----------|----------|---------------|-------------|------|----------|
| WIOI | туре | Unain | nes | LIIIK | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | OYP | С | 664 | - | 26,26,26 | 0.72 | 0 | 29,29,29 | 1.27 | 3 (10%) |
| 4 | OYP | В | 664 | - | 26,26,26 | 0.65 | 0 | 29,29,29 | 1.25 | 3 (10%) |
| 4 | OYP | А | 664 | - | 26,26,26 | 0.72 | 1 (3%) | 29,29,29 | 1.23 | 5 (17%) |
| 4 | OYP | D | 664 | - | 26,26,26 | 0.66 | 0 | 29,29,29 | 1.73 | 6 (20%) |



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 |
|-----|------|-------|-----|------|------------------|------------|---------|
| 4 | OYP | С | 664 | - | - | 4/20/20/20 | 0/1/1/1 |
| 4 | OYP | В | 664 | - | - | 5/20/20/20 | 0/1/1/1 |
| 4 | OYP | А | 664 | - | - | 7/20/20/20 | 0/1/1/1 |
| 4 | OYP | D | 664 | - | - | 8/20/20/20 | 0/1/1/1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Ζ | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | А | 664 | OYP | O3-C10 | -2.48 | 1.33 | 1.42 |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|------------|-------|------------------|---------------|
| 4 | D | 664 | OYP | C7-C8-C9 | -6.00 | 96.95 | 113.76 |
| 4 | С | 664 | OYP | C10-O3-C11 | 3.52 | 119.53 | 113.34 |
| 4 | D | 664 | OYP | C7-C5-C4 | -3.36 | 112.73 | 121.23 |
| 4 | С | 664 | OYP | O3-C11-C12 | -3.34 | 100.63 | 112.06 |
| 4 | D | 664 | OYP | C1-C6-C5 | -2.94 | 116.99 | 121.03 |
| 4 | D | 664 | OYP | C3-C2-C1 | 2.93 | 122.78 | 118.17 |
| 4 | А | 664 | OYP | C10-O3-C11 | 2.83 | 118.32 | 113.34 |
| 4 | D | 664 | OYP | C4-C3-C2 | -2.66 | 117.37 | 121.03 |
| 4 | А | 664 | OYP | C10-C2-C1 | -2.60 | 114.55 | 120.66 |
| 4 | В | 664 | OYP | C3-C2-C1 | 2.57 | 122.20 | 118.17 |
| 4 | В | 664 | OYP | C10-C2-C3 | -2.50 | 114.80 | 120.66 |
| 4 | А | 664 | OYP | C4-C3-C2 | -2.32 | 117.83 | 121.03 |
| 4 | В | 664 | OYP | C6-C1-C2 | -2.31 | 117.85 | 121.03 |
| 4 | С | 664 | OYP | C7-C8-C9 | -2.22 | 107.53 | 113.76 |
| 4 | А | 664 | OYP | O1-C9-C8 | 2.21 | 121.14 | 114.03 |
| 4 | А | 664 | OYP | C10-C2-C3 | 2.08 | 125.53 | 120.66 |
| 4 | D | 664 | OYP | C6-C5-C4 | 2.01 | 121.33 | 118.17 |

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 4 | А | 664 | OYP | O3-C11-C12-C13 |
| 4 | С | 664 | OYP | O3-C11-C12-C13 |



| Mol | Chain | \mathbf{Res} | Type | Atoms |
|-----|-------|----------------|------|-----------------|
| 4 | С | 664 | OYP | C12-C13-C14-C15 |
| 4 | D | 664 | OYP | C12-C13-C14-C15 |
| 4 | D | 664 | OYP | C5-C7-C8-C9 |
| 4 | А | 664 | OYP | C12-C11-O3-C10 |
| 4 | D | 664 | OYP | C12-C11-O3-C10 |
| 4 | В | 664 | OYP | C19-C20-C21-C22 |
| 4 | С | 664 | OYP | C12-C11-O3-C10 |
| 4 | В | 664 | OYP | C5-C7-C8-C9 |
| 4 | В | 664 | OYP | O3-C11-C12-C13 |
| 4 | А | 664 | OYP | C11-C12-C13-C14 |
| 4 | В | 664 | OYP | C7-C8-C9-O2 |
| 4 | В | 664 | OYP | C7-C8-C9-O1 |
| 4 | А | 664 | OYP | C5-C7-C8-C9 |
| 4 | D | 664 | OYP | C7-C8-C9-O2 |
| 4 | D | 664 | OYP | O3-C11-C12-C13 |
| 4 | D | 664 | OYP | C4-C5-C7-C8 |
| 4 | D | 664 | OYP | C6-C5-C7-C8 |
| 4 | А | 664 | OYP | C19-C20-C21-C22 |
| 4 | А | 664 | OYP | C7-C8-C9-O2 |
| 4 | А | 664 | OYP | C7-C8-C9-O1 |
| 4 | D | 664 | OYP | C7-C8-C9-O1 |
| 4 | С | 664 | OYP | C5-C7-C8-C9 |

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There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | С | 664 | OYP | 1 | 0 |

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









5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

| Mol | Chain | Analysed | < RSRZ > | #RSRZ>2 | | $OWAB(Å^2)$ | Q<0.9 |
|-----|-------|-----------------|-----------------|------------|----|----------------|-------|
| 1 | А | 550/573~(95%) | -0.24 | 5 (0%) 84 | 85 | 8, 16, 31, 47 | 0 |
| 1 | В | 551/573~(96%) | -0.24 | 5 (0%) 84 | 85 | 7, 17, 32, 53 | 0 |
| 1 | С | 546/573~(95%) | 0.31 | 32 (5%) 22 | 25 | 16, 28, 46, 63 | 0 |
| 1 | D | 547/573~(95%) | -0.19 | 11 (2%) 65 | 68 | 11, 20, 36, 56 | 0 |
| All | All | 2194/2292~(95%) | -0.09 | 53 (2%) 59 | 62 | 7, 20, 39, 63 | 0 |

All (53) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|----------------------|------|------|
| 1 | D | 123 | GLY | 7.4 |
| 1 | D | 120 | ASP | 6.8 |
| 1 | В | 121 | PRO | 6.0 |
| 1 | D | 124 | LEU | 5.7 |
| 1 | С | 614 | TYR | 5.0 |
| 1 | С | 328 | LEU | 4.3 |
| 1 | С | 327 | PRO | 4.2 |
| 1 | С | 163 | VAL | 4.2 |
| 1 | С | 255 | PRO | 3.9 |
| 1 | С | 254 | PHE | 3.8 |
| 1 | С | 571 | ASP | 3.6 |
| 1 | В | 124 | LEU | 3.6 |
| 1 | В | 256 | PRO | 3.6 |
| 1 | С | 128 | HIS | 3.4 |
| 1 | С | 569 | THR | 3.4 |
| 1 | С | 326 | SER | 3.2 |
| 1 | С | 616 | SER | 3.1 |
| 1 | С | 259 | GLU | 3.1 |
| 1 | D | 112 | GLY | 3.0 |
| 1 | D | 327 | PRO | 3.0 |
| 1 | С | 329 | PRO | 3.0 |



| Mol | Chain | Res | Type | RSRZ | |
|-----|-------|---------|---------|------|--|
| 1 | С | 139 LEU | | 2.9 | |
| 1 | В | 123 GLY | | 2.8 | |
| 1 | D | 256 PRO | | 2.8 | |
| 1 | С | 568 | THR | 2.8 | |
| 1 | А | 256 | PRO | 2.8 | |
| 1 | С | 336 | ASP | 2.7 | |
| 1 | С | 407 | GLY | 2.7 | |
| 1 | С | 572 ALA | | 2.7 | |
| 1 | С | 291 | 291 LEU | | |
| 1 | D | 125 | PHE | 2.7 | |
| 1 | С | 611 | GLU | 2.7 | |
| 1 | D | 257 | GLY | 2.6 | |
| 1 | А | 611 | GLU | 2.5 | |
| 1 | С | 253 | LYS | 2.5 | |
| 1 | А | 614 | TYR | 2.5 | |
| 1 | С | 575 | GLU | 2.4 | |
| 1 | В | 125 | PHE | 2.4 | |
| 1 | С | 613 | GLU | 2.4 | |
| 1 | А | 500[A] | CYS | 2.3 | |
| 1 | С | 332 | PHE | 2.3 | |
| 1 | С | 250 | ALA | 2.2 | |
| 1 | А | 391 | ILE | 2.2 | |
| 1 | С | 135 | GLU | 2.2 | |
| 1 | D | 128 | HIS | 2.2 | |
| 1 | D | 616 | SER | 2.2 | |
| 1 | С | 321 | LEU | 2.1 | |
| 1 | С | 612 | GLU | 2.1 | |
| 1 | D | 612 | GLU | 2.1 | |
| 1 | С | 164 | ASP | 2.1 | |
| 1 | С | 320 | GLN | 2.0 | |
| 1 | С | 412 | LEU | 2.0 | |
| 1 | С | 159 | HIS | 2.0 | |

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | ${f B}	ext{-factors}({ m \AA}^2)$ | Q < 0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------------|---------|
| 4 | OYP | С | 664 | 26/26 | 0.94 | 0.13 | 15,27,30,30 | 4 |
| 4 | OYP | D | 664 | 26/26 | 0.95 | 0.12 | 12,19,29,30 | 3 |
| 2 | K | D | 1 | 1/1 | 0.96 | 0.17 | $53,\!53,\!53,\!53$ | 0 |
| 4 | OYP | В | 664 | 26/26 | 0.96 | 0.14 | 9,19,26,30 | 3 |
| 4 | OYP | А | 664 | 26/26 | 0.97 | 0.12 | 8,16,21,24 | 3 |
| 2 | K | А | 2 | 1/1 | 0.98 | 0.29 | $57,\!57,\!57,\!57$ | 0 |
| 3 | FE2 | А | 1 | 1/1 | 1.00 | 0.10 | 8,8,8,8 | 0 |
| 3 | FE2 | В | 2 | 1/1 | 1.00 | 0.11 | 9,9,9,9 | 0 |
| 3 | FE2 | С | 3 | 1/1 | 1.00 | 0.08 | $17,\!17,\!17,\!17$ | 0 |
| 3 | FE2 | D | 4 | 1/1 | 1.00 | 0.10 | 12,12,12,12 | 0 |

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

















6.5 Other polymers (i)

There are no such residues in this entry.

