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

Oct 17, 2021 – 03:51 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 1M3K |
| Title | : | biosynthetic thiolase, inactive C89A mutant |
| Authors | : | Kursula, P.; Ojala, J.; Lambeir, A.-M.; Wierenga, R.K. |
| Deposited on | : | 2002-06-28 |
| Resolution | : | 1.70 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 following versions of software and data (see references (1)) were used in the production of this report:

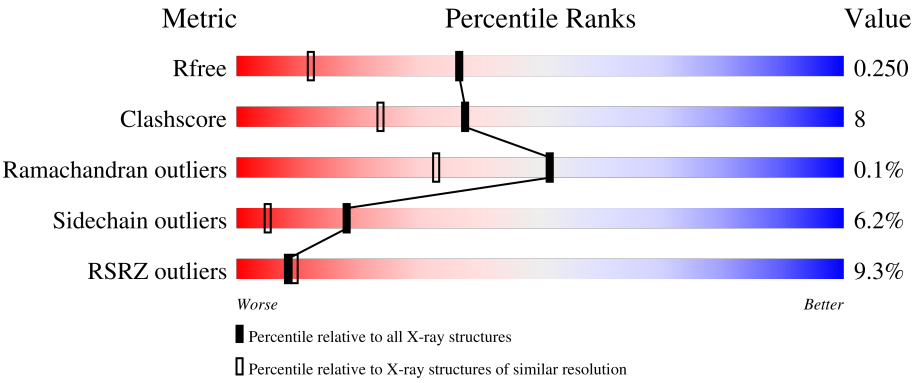
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.23.2 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.23.2 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 4298 (1.70-1.70) |
| Clashscore | 141614 | 4695 (1.70-1.70) |
| Ramachandran outliers | 138981 | 4610 (1.70-1.70) |
| Sidechain outliers | 138945 | 4610 (1.70-1.70) |
| RSRZ outliers | 127900 | 4222 (1.70-1.70) |

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 | A | 392 | 2% 85% 13% · |
| 1 | B | 392 | 2% 87% 12% · |
| 1 | C | 392 | 11% 84% 16% · |
| 1 | D | 392 | 23% 78% 21% · |

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12527 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

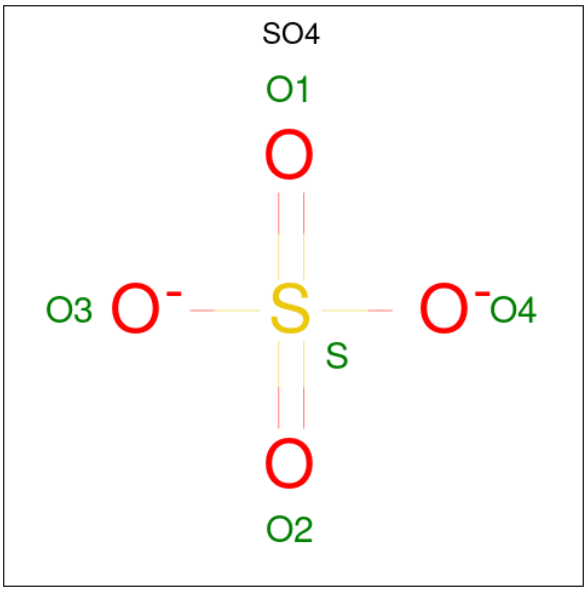
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 392 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 2834 | 1759 | 512 | 543 | 20 | | | |
| 1 | B | 392 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 2834 | 1759 | 512 | 543 | 20 | | | |
| 1 | C | 392 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 2834 | 1759 | 512 | 543 | 20 | | | |
| 1 | D | 392 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 2834 | 1759 | 512 | 543 | 20 | | | |

There are 12 discrepancies between the modelled and reference sequences:

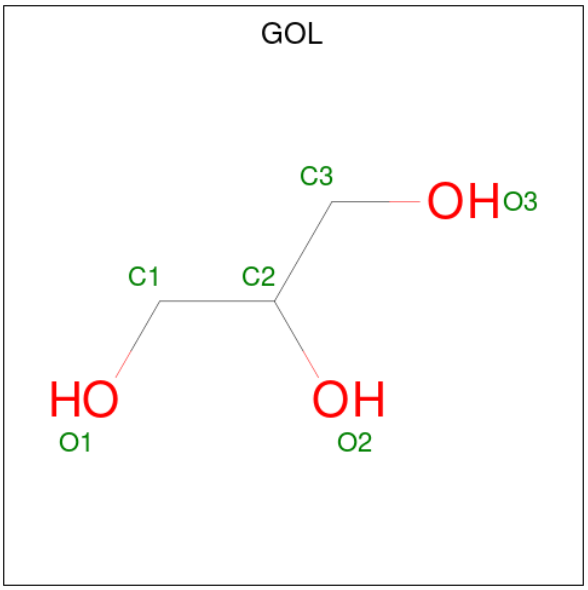
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 10 | ALA | - | insertion | UNP P07097 |
| A | 89 | ALA | CYS | engineered mutation | UNP P07097 |
| A | 129 | ARG | ALA | conflict | UNP P07097 |
| B | 10 | ALA | - | insertion | UNP P07097 |
| B | 89 | ALA | CYS | engineered mutation | UNP P07097 |
| B | 129 | ARG | ALA | conflict | UNP P07097 |
| C | 10 | ALA | - | insertion | UNP P07097 |
| C | 89 | ALA | CYS | engineered mutation | UNP P07097 |
| C | 129 | ARG | ALA | conflict | UNP P07097 |
| D | 10 | ALA | - | insertion | UNP P07097 |
| D | 89 | ALA | CYS | engineered mutation | UNP P07097 |
| D | 129 | ARG | ALA | conflict | UNP P07097 |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: $O_4S$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | A | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 2 | A | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 2 | B | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 2 | B | 1 | Total O S<br>5 4 1 | 0 | 0 |

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 1 | Total C O<br>6 3 3 | 0 | 0 |
| 3 | B | 1 | Total C O<br>6 3 3 | 0 | 0 |

- Molecule 4 is water.

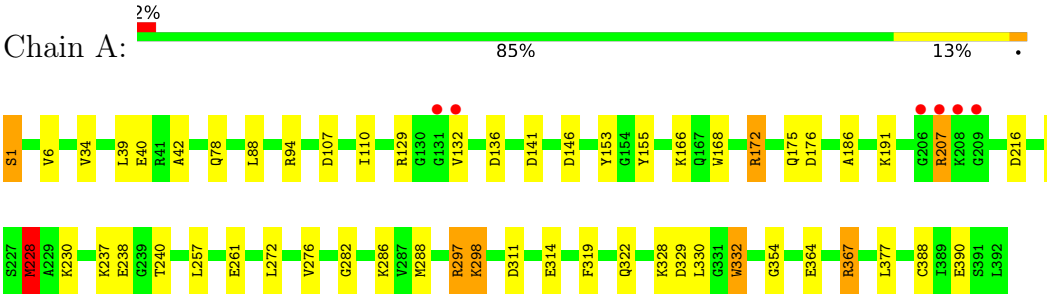
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | A | 416 | Total O<br>416 416 | 0 | 0 |
| 4 | B | 425 | Total O<br>425 425 | 0 | 0 |
| 4 | C | 152 | Total O<br>152 152 | 0 | 0 |
| 4 | D | 166 | Total O<br>166 166 | 0 | 0 |

# 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.

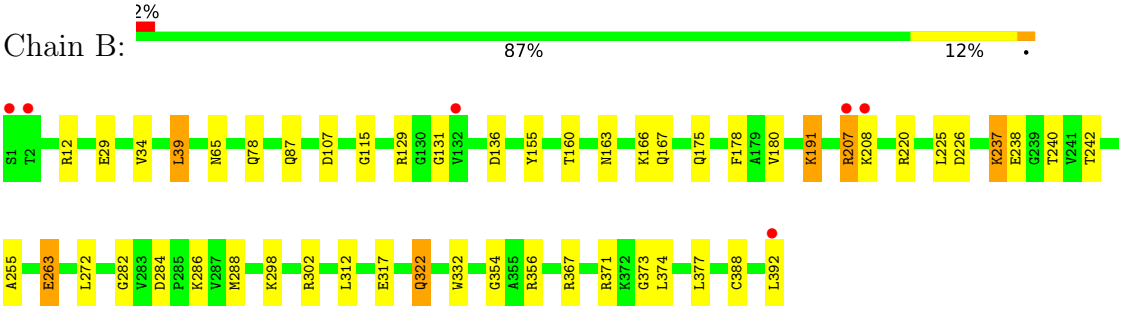
• Molecule 1: Acetyl-CoA acetyltransferase

Chain A:



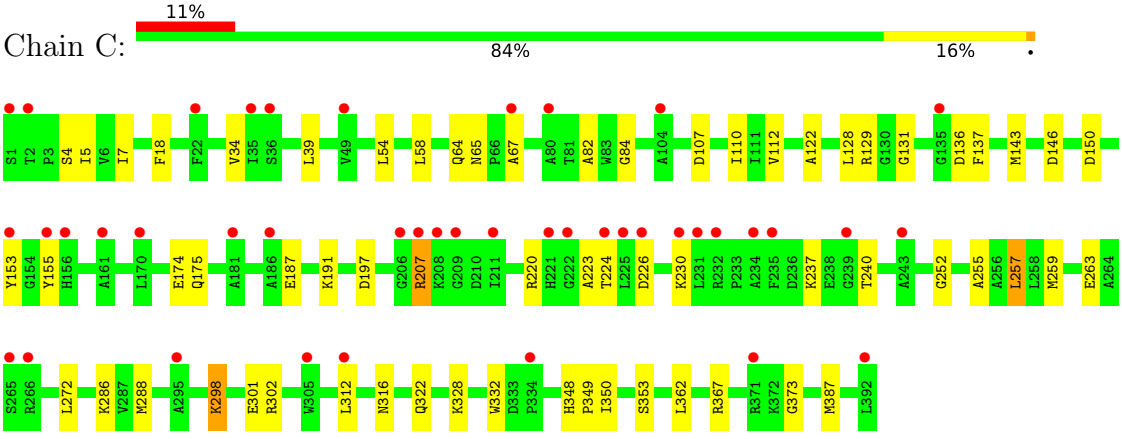

• Molecule 1: Acetyl-CoA acetyltransferase

Chain B:



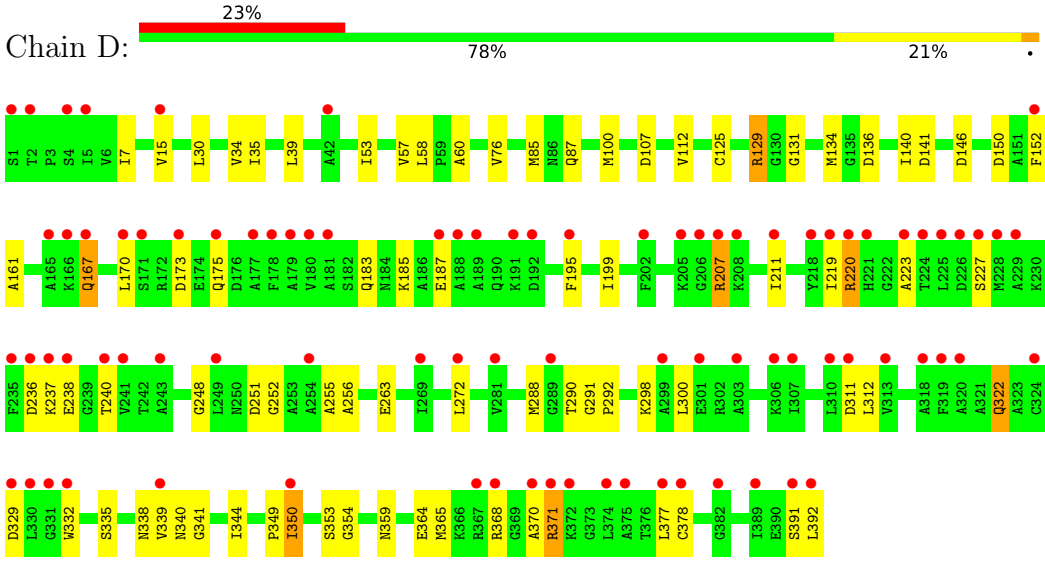

• Molecule 1: Acetyl-CoA acetyltransferase

Chain C:




• Molecule 1: Acetyl-CoA acetyltransferase

Chain D:


23%
78%
21%
S1 T2 P3 S4 I5 V6 I7 V15 L30 V34 I35 L39 A42 I53 V57 L58 P59 A60 V76 M85 N86 Q87 M100 D107 V112 C125 R129 G130 G131 M134 G135 D136 I140 D141 D146 D150 A151 F152 Y153 G154 Y155
A161 A165 K166 Q167 L170 S171 R172 D173 E174 Q175 D176 A177 F178 A179 V180 A181 S182 Q183 N184 K185 A186 E187 A188 A189 Q190 K191 D192 F195 I199 F202 K205 G206 R207 K208 I211 Y218 I219 R220 H221 G222 A223 T224 L225 D226 S227 M228 A229 K230 L231 R232 P233 A234
F235 D236 K237 E238 G239 T240 V241 T242 A243 G248 L249 N250 D251 G252 A253 A254 A255 A256 E263 I269 L272 V281 M288 G289 T290 G291 P292 K298 A299 L300 E301 R302 A303 K306 I307 L310 D311 L312 V313 A318 F319 A320 A321 Q322 A323 C324 A325 V326 N327 K328
D329 L330 G331 W332 S335 N338 V339 N340 G341 I344 P349 I350 S353 G354 N359 E364 M365 K366 R367 R368 G369 A370 R371 K372 G373 L374 A375 T376 L377 C378 G382 I389 E390 S391 L392

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 84.37Å 79.20Å 148.86Å<br>90.00° 92.32° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 1.70<br>19.84 – 1.70 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 90.1 (20.00-1.70)<br>81.4 (19.84-1.70) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.08 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.91 (at 1.70Å) | Xtriage |
| Refinement program | REFMAC | Depositor |
| R, $R_{free}$ | 0.199 , 0.243<br>0.211 , 0.250 | Depositor<br>DCC |
| $R_{free}$ test set | 8981 reflections (4.64%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 17.8 | Xtriage |
| Anisotropy | 0.440 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.37 , 50.1 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.37$, $< L^2 > = 0.19$ | Xtriage |
| Estimated twinning fraction | 0.155 for h,-k,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 12527 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 16.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 1.06 | 6/2880 (0.2%) | 1.05 | 11/3890 (0.3%) |
| 1 | B | 1.03 | 3/2880 (0.1%) | 1.06 | 9/3890 (0.2%) |
| 1 | C | 0.61 | 0/2880 | 0.83 | 7/3890 (0.2%) |
| 1 | D | 0.56 | 0/2880 | 0.79 | 5/3890 (0.1%) |
| All | All | 0.85 | 9/11520 (0.1%) | 0.94 | 32/15560 (0.2%) |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 317 | GLU | CD-OE1 | 6.37 | 1.32 | 1.25 |
| 1 | A | 314 | GLU | CD-OE1 | 6.01 | 1.32 | 1.25 |
| 1 | A | 94 | ARG | CZ-NH1 | -5.66 | 1.25 | 1.33 |
| 1 | B | 115 | GLY | CA-C | -5.52 | 1.43 | 1.51 |
| 1 | B | 178 | PHE | CE2-CZ | 5.45 | 1.47 | 1.37 |
| 1 | A | 34 | VAL | CB-CG1 | -5.40 | 1.41 | 1.52 |
| 1 | A | 319 | PHE | CE2-CZ | 5.36 | 1.47 | 1.37 |
| 1 | A | 186 | ALA | CA-CB | -5.13 | 1.41 | 1.52 |
| 1 | A | 42 | ALA | CA-CB | -5.04 | 1.41 | 1.52 |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 367 | ARG | NE-CZ-NH1 | 9.85 | 125.22 | 120.30 |
| 1 | B | 367 | ARG | NE-CZ-NH2 | -9.83 | 115.39 | 120.30 |
| 1 | A | 107 | ASP | CB-CG-OD2 | 8.45 | 125.90 | 118.30 |
| 1 | A | 141 | ASP | CB-CG-OD2 | 7.88 | 125.39 | 118.30 |
| 1 | B | 107 | ASP | CB-CG-OD2 | 7.82 | 125.34 | 118.30 |
| 1 | D | 146 | ASP | CB-CG-OD2 | 7.30 | 124.87 | 118.30 |
| 1 | D | 136 | ASP | CB-CG-OD2 | 7.01 | 124.61 | 118.30 |
| 1 | A | 311 | ASP | CB-CG-OD2 | 7.00 | 124.60 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 228 | MET | CG-SD-CE | 6.61 | 110.78 | 100.20 |
| 1 | B | 12 | ARG | NE-CZ-NH2 | -6.57 | 117.01 | 120.30 |
| 1 | C | 146 | ASP | CB-CG-OD2 | 6.38 | 124.04 | 118.30 |
| 1 | A | 146 | ASP | CB-CG-OD2 | 6.21 | 123.88 | 118.30 |
| 1 | D | 329 | ASP | CB-CG-OD2 | 5.98 | 123.69 | 118.30 |
| 1 | B | 284 | ASP | CB-CG-OD2 | 5.94 | 123.65 | 118.30 |
| 1 | C | 150 | ASP | CB-CG-OD2 | 5.92 | 123.62 | 118.30 |
| 1 | A | 226 | ASP | CB-CG-OD2 | 5.91 | 123.62 | 118.30 |
| 1 | A | 94 | ARG | NE-CZ-NH2 | 5.74 | 123.17 | 120.30 |
| 1 | A | 297 | ARG | NE-CZ-NH1 | 5.71 | 123.15 | 120.30 |
| 1 | B | 136 | ASP | CB-CG-OD2 | 5.66 | 123.39 | 118.30 |
| 1 | C | 302 | ARG | NE-CZ-NH1 | 5.52 | 123.06 | 120.30 |
| 1 | D | 173 | ASP | CB-CG-OD2 | 5.48 | 123.23 | 118.30 |
| 1 | C | 197 | ASP | CB-CG-OD2 | 5.33 | 123.10 | 118.30 |
| 1 | D | 107 | ASP | CB-CG-OD2 | 5.32 | 123.09 | 118.30 |
| 1 | C | 107 | ASP | CB-CG-OD2 | 5.29 | 123.07 | 118.30 |
| 1 | A | 176 | ASP | CB-CG-OD2 | 5.26 | 123.04 | 118.30 |
| 1 | B | 39 | LEU | CA-CB-CG | 5.23 | 127.34 | 115.30 |
| 1 | C | 367 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | A | 216 | ASP | CB-CG-OD2 | 5.11 | 122.89 | 118.30 |
| 1 | B | 302 | ARG | NE-CZ-NH1 | 5.11 | 122.85 | 120.30 |
| 1 | A | 172 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 1 | B | 129 | ARG | NE-CZ-NH2 | -5.05 | 117.78 | 120.30 |
| 1 | C | 136 | ASP | CB-CG-OD1 | 5.03 | 122.82 | 118.30 |

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 | A | 2834 | 0 | 2842 | 31 | 0 |
| 1 | B | 2834 | 0 | 2842 | 48 | 0 |
| 1 | C | 2834 | 0 | 2842 | 39 | 0 |
| 1 | D | 2834 | 0 | 2842 | 58 | 0 |
| 2 | A | 10 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | B | 10 | 0 | 0 | 0 | 0 |
| 3 | A | 6 | 0 | 7 | 2 | 0 |
| 3 | B | 6 | 0 | 8 | 0 | 0 |
| 4 | A | 416 | 0 | 0 | 17 | 0 |
| 4 | B | 425 | 0 | 0 | 29 | 1 |
| 4 | C | 152 | 0 | 0 | 18 | 0 |
| 4 | D | 166 | 0 | 0 | 36 | 0 |
| All | All | 12527 | 0 | 11383 | 174 | 1 |

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 8.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:225:LEU:HG | 4:A:9889:HOH:O | 1.51 | 1.08 |
| 1:A:228:MET:SD | 4:A:488:HOH:O | 2.19 | 1.00 |
| 1:C:353:SER:HA | 4:C:505:HOH:O | 1.63 | 0.96 |
| 1:A:225:LEU:HD21 | 4:A:523:HOH:O | 1.67 | 0.95 |
| 1:B:371:ARG:HD3 | 4:B:476:HOH:O | 1.69 | 0.92 |
| 4:C:483:HOH:O | 1:D:87:GLN:HA | 1.70 | 0.89 |
| 1:C:65:ASN:ND2 | 4:C:483:HOH:O | 2.06 | 0.87 |
| 1:D:183:GLN:HG2 | 4:D:539:HOH:O | 1.75 | 0.85 |
| 1:D:252:GLY:HA3 | 4:D:515:HOH:O | 1.75 | 0.84 |
| 4:A:432:HOH:O | 1:B:65:ASN:HB2 | 1.77 | 0.84 |
| 1:B:163:ASN:ND2 | 4:B:416:HOH:O | 2.12 | 0.83 |
| 1:D:141:ASP:HA | 4:D:446:HOH:O | 1.79 | 0.82 |
| 1:D:125:CYS:SG | 4:D:431:HOH:O | 2.37 | 0.81 |
| 1:B:191:LYS:HB3 | 1:B:191:LYS:NZ | 1.97 | 0.80 |
| 1:D:185:LYS:O | 4:D:409:HOH:O | 2.01 | 0.79 |
| 4:A:9993:HOH:O | 1:C:131:GLY:HA3 | 1.82 | 0.78 |
| 1:D:152:PHE:CE2 | 4:D:503:HOH:O | 2.37 | 0.77 |
| 1:A:6:VAL:HG11 | 4:A:530:HOH:O | 1.84 | 0.76 |
| 1:C:110:ILE:HG22 | 4:C:528:HOH:O | 1.86 | 0.76 |
| 1:C:67:ALA:HB1 | 4:C:524:HOH:O | 1.86 | 0.75 |
| 1:D:150:ASP:HB2 | 4:D:494:HOH:O | 1.86 | 0.73 |
| 1:B:160:THR:HA | 4:B:416:HOH:O | 1.89 | 0.71 |
| 1:B:388:CYS:HA | 4:B:444:HOH:O | 1.90 | 0.71 |
| 1:D:251:ASP:O | 4:D:551:HOH:O | 2.07 | 0.71 |
| 1:B:322:GLN:HB3 | 4:B:524:HOH:O | 1.90 | 0.71 |
| 1:D:57:VAL:HG21 | 1:D:350:ILE:HG22 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:223:ALA:HB3 | 4:D:487:HOH:O | 1.91 | 0.70 |
| 1:C:143:MET:HB2 | 4:C:399:HOH:O | 1.91 | 0.69 |
| 1:A:207:ARG:H | 1:A:207:ARG:HD3 | 1.56 | 0.69 |
| 1:D:53:ILE:HG22 | 4:D:460:HOH:O | 1.93 | 0.68 |
| 1:D:370:ALA:HB1 | 4:D:538:HOH:O | 1.94 | 0.68 |
| 1:D:290:THR:HA | 4:D:502:HOH:O | 1.93 | 0.67 |
| 1:C:58:LEU:HD13 | 4:C:399:HOH:O | 1.93 | 0.67 |
| 1:D:344:ILE:HG22 | 4:D:539:HOH:O | 1.96 | 0.65 |
| 1:B:388:CYS:SG | 4:B:444:HOH:O | 2.55 | 0.65 |
| 1:D:340:ASN:ND2 | 1:D:364:GLU:OE1 | 2.23 | 0.64 |
| 1:B:191:LYS:HB3 | 1:B:191:LYS:HZ3 | 1.62 | 0.64 |
| 1:D:7:ILE:HG23 | 1:D:256:ALA:HB1 | 1.81 | 0.63 |
| 1:C:82:ALA:HB1 | 4:C:524:HOH:O | 1.97 | 0.63 |
| 1:C:252:GLY:HA2 | 4:C:459:HOH:O | 2.00 | 0.62 |
| 1:B:87:GLN:C | 4:B:9970:HOH:O | 2.38 | 0.61 |
| 1:B:191:LYS:NZ | 1:B:191:LYS:CB | 2.64 | 0.60 |
| 1:D:30:LEU:HD11 | 4:D:543:HOH:O | 2.00 | 0.60 |
| 1:D:15:VAL:HG13 | 4:D:551:HOH:O | 2.01 | 0.60 |
| 1:D:170:LEU:HB3 | 4:D:496:HOH:O | 2.02 | 0.60 |
| 1:B:191:LYS:HB3 | 4:B:475:HOH:O | 2.02 | 0.59 |
| 1:A:228:MET:HG3 | 4:A:9831:HOH:O | 2.02 | 0.59 |
| 1:A:129:ARG:O | 4:A:9993:HOH:O | 2.16 | 0.58 |
| 3:A:5393:GOL:C1 | 4:A:511:HOH:O | 2.25 | 0.58 |
| 1:B:374:LEU:HB2 | 4:B:444:HOH:O | 2.02 | 0.58 |
| 1:D:57:VAL:HG21 | 1:D:350:ILE:CG2 | 2.32 | 0.58 |
| 1:B:166:LYS:HG3 | 4:B:480:HOH:O | 2.03 | 0.58 |
| 1:D:233:PRO:HB2 | 1:D:236:ASP:O | 2.04 | 0.57 |
| 1:A:88:LEU:HG | 4:A:432:HOH:O | 2.04 | 0.57 |
| 1:A:298:LYS:HE3 | 2:A:9722:SO4:O3 | 2.05 | 0.57 |
| 1:D:220:ARG:NH1 | 4:D:479:HOH:O | 2.37 | 0.57 |
| 1:B:175:GLN:HE22 | 1:B:240:THR:CG2 | 2.18 | 0.57 |
| 1:B:29:GLU:HG2 | 4:B:497:HOH:O | 2.05 | 0.57 |
| 1:D:85:MET:HG3 | 4:D:460:HOH:O | 2.04 | 0.56 |
| 1:A:172:ARG:NH1 | 4:A:501:HOH:O | 2.38 | 0.56 |
| 1:B:34:VAL:HG12 | 1:B:255:ALA:HB3 | 1.87 | 0.56 |
| 1:D:338:ASN:HB3 | 1:D:341:GLY:O | 2.05 | 0.55 |
| 1:A:168:TRP:CH2 | 1:A:329:ASP:HB2 | 2.41 | 0.55 |
| 1:D:392:LEU:HG | 4:D:500:HOH:O | 2.06 | 0.55 |
| 1:D:251:ASP:C | 4:D:551:HOH:O | 2.46 | 0.54 |
| 1:B:29:GLU:CG | 4:B:497:HOH:O | 2.54 | 0.54 |
| 1:A:207:ARG:H | 1:A:207:ARG:CD | 2.20 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:191:LYS:HD2 | 4:B:475:HOH:O | 2.08 | 0.53 |
| 1:C:349:PRO:HG2 | 4:C:505:HOH:O | 2.09 | 0.53 |
| 1:B:191:LYS:HB3 | 1:B:191:LYS:HZ2 | 1.73 | 0.53 |
| 1:C:129:ARG:CG | 4:C:509:HOH:O | 2.57 | 0.53 |
| 1:A:168:TRP:HH2 | 1:A:329:ASP:HB2 | 1.75 | 0.52 |
| 1:B:374:LEU:CB | 4:B:444:HOH:O | 2.58 | 0.52 |
| 1:D:140:ILE:HG22 | 4:D:431:HOH:O | 2.10 | 0.52 |
| 1:C:257:LEU:CD1 | 1:C:259:MET:CE | 2.87 | 0.52 |
| 1:B:87:GLN:HA | 4:B:9970:HOH:O | 2.09 | 0.52 |
| 1:C:175:GLN:HE22 | 1:C:240:THR:HG21 | 1.74 | 0.52 |
| 1:B:240:THR:C | 4:B:510:HOH:O | 2.47 | 0.52 |
| 1:C:257:LEU:CD1 | 1:C:259:MET:HE2 | 2.39 | 0.52 |
| 1:D:349:PRO:HB3 | 4:D:551:HOH:O | 2.09 | 0.51 |
| 1:C:122:ALA:HA | 4:C:514:HOH:O | 2.11 | 0.51 |
| 1:B:87:GLN:CA | 4:B:9970:HOH:O | 2.59 | 0.50 |
| 1:B:242:THR:CG2 | 4:B:510:HOH:O | 2.59 | 0.50 |
| 1:B:242:THR:HG23 | 4:B:510:HOH:O | 2.12 | 0.50 |
| 1:B:312:LEU:HB3 | 4:B:479:HOH:O | 2.11 | 0.50 |
| 1:B:225:LEU:HB2 | 4:B:515:HOH:O | 2.11 | 0.50 |
| 1:D:15:VAL:HG22 | 4:D:515:HOH:O | 2.11 | 0.50 |
| 1:D:60:ALA:O | 4:D:519:HOH:O | 2.20 | 0.50 |
| 1:A:40:GLU:HG3 | 4:A:9951:HOH:O | 2.12 | 0.49 |
| 1:A:228:MET:CE | 4:A:488:HOH:O | 2.54 | 0.49 |
| 1:B:175:GLN:HE22 | 1:B:240:THR:HG23 | 1.76 | 0.49 |
| 1:A:276:VAL:CG2 | 1:A:388:CYS:HB2 | 2.42 | 0.49 |
| 1:B:226:ASP:HB3 | 4:B:509:HOH:O | 2.12 | 0.49 |
| 1:B:180:VAL:HG11 | 4:B:515:HOH:O | 2.12 | 0.49 |
| 1:C:7:ILE:HD13 | 1:C:362:LEU:HD11 | 1.94 | 0.48 |
| 1:C:129:ARG:HG2 | 4:C:509:HOH:O | 2.13 | 0.48 |
| 1:A:282:GLY:HA3 | 1:B:78:GLN:O | 2.13 | 0.48 |
| 1:B:263:GLU:OE1 | 4:B:9846:HOH:O | 2.20 | 0.48 |
| 1:A:166:LYS:HB3 | 4:A:489:HOH:O | 2.13 | 0.48 |
| 1:D:291:GLY:N | 1:D:292:PRO:CD | 2.76 | 0.48 |
| 1:B:286:LYS:NZ | 4:B:9815:HOH:O | 2.28 | 0.47 |
| 1:B:34:VAL:CG1 | 1:B:255:ALA:HB3 | 2.43 | 0.47 |
| 1:B:374:LEU:C | 1:B:374:LEU:HD23 | 2.35 | 0.47 |
| 1:B:207:ARG:N | 1:B:207:ARG:HD3 | 2.29 | 0.47 |
| 1:C:112:VAL:HG22 | 1:C:257:LEU:HD23 | 1.96 | 0.47 |
| 1:C:54:LEU:O | 1:C:84:GLY:HA2 | 2.14 | 0.47 |
| 1:D:140:ILE:HB | 4:D:431:HOH:O | 2.15 | 0.47 |
| 1:A:237:LYS:N | 1:A:237:LYS:HD3 | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:131:GLY:HA2 | 1:D:131:GLY:HA2 | 1.97 | 0.47 |
| 1:B:208:LYS:NZ | 4:B:468:HOH:O | 2.48 | 0.47 |
| 1:C:64:GLN:O | 1:C:65:ASN:C | 2.54 | 0.47 |
| 1:D:34:VAL:CG1 | 1:D:255:ALA:HB3 | 2.45 | 0.47 |
| 1:C:223:ALA:HB1 | 4:C:523:HOH:O | 2.16 | 0.46 |
| 1:D:219:ILE:HD11 | 4:D:510:HOH:O | 2.15 | 0.46 |
| 4:A:9993:HOH:O | 1:C:131:GLY:CA | 2.52 | 0.46 |
| 1:A:110:ILE:HG23 | 1:A:257:LEU:HD21 | 1.98 | 0.46 |
| 1:B:191:LYS:CB | 1:B:191:LYS:HZ2 | 2.27 | 0.46 |
| 1:D:248:GLY:HA2 | 4:D:474:HOH:O | 2.16 | 0.46 |
| 1:B:356:ARG:HD2 | 1:B:356:ARG:C | 2.37 | 0.46 |
| 1:C:129:ARG:HG3 | 4:C:509:HOH:O | 2.16 | 0.45 |
| 1:C:174:GLU:OE2 | 1:C:328:LYS:NZ | 2.39 | 0.45 |
| 1:A:330:LEU:HD12 | 1:A:332:TRP:CZ2 | 2.51 | 0.45 |
| 1:A:261:GLU:HG3 | 4:A:530:HOH:O | 2.17 | 0.45 |
| 1:B:237:LYS:HD2 | 1:B:237:LYS:N | 2.31 | 0.45 |
| 1:A:225:LEU:C | 1:A:225:LEU:HD23 | 2.37 | 0.45 |
| 1:D:58:LEU:HB3 | 4:D:441:HOH:O | 2.16 | 0.45 |
| 1:D:322:GLN:O | 1:D:326:VAL:HG23 | 2.16 | 0.45 |
| 1:D:167:GLN:HB3 | 4:D:397:HOH:O | 2.17 | 0.45 |
| 1:B:373:GLY:CA | 4:B:479:HOH:O | 2.65 | 0.44 |
| 1:C:34:VAL:HG12 | 1:C:255:ALA:HB3 | 1.99 | 0.44 |
| 1:C:4:SER:C | 1:C:5:ILE:HD13 | 2.37 | 0.44 |
| 1:C:128:LEU:HD21 | 1:C:137:PHE:CZ | 2.52 | 0.44 |
| 1:D:211:ILE:HB | 4:D:554:HOH:O | 2.17 | 0.44 |
| 1:A:354:GLY:HA2 | 1:A:377:LEU:HD11 | 2.00 | 0.44 |
| 1:C:175:GLN:HE22 | 1:C:240:THR:CG2 | 2.30 | 0.44 |
| 1:D:76:VAL:HG23 | 4:D:540:HOH:O | 2.16 | 0.44 |
| 1:A:364:GLU:OE1 | 1:A:367:ARG:HD2 | 2.18 | 0.44 |
| 1:A:1:SER:O | 1:A:1:SER:OG | 2.29 | 0.43 |
| 1:D:207:ARG:N | 1:D:207:ARG:HD3 | 2.33 | 0.43 |
| 1:D:175:GLN:NE2 | 1:D:240:THR:OG1 | 2.51 | 0.43 |
| 1:D:335:SER:HA | 4:D:526:HOH:O | 2.18 | 0.43 |
| 1:D:335:SER:O | 1:D:339:VAL:HG12 | 2.19 | 0.43 |
| 1:C:153:TYR:CE2 | 1:C:286:LYS:HD3 | 2.53 | 0.43 |
| 1:D:312:LEU:HD13 | 1:D:368:ARG:HD2 | 2.00 | 0.43 |
| 1:B:392:LEU:HD23 | 4:B:471:HOH:O | 2.18 | 0.43 |
| 1:D:292:PRO:HD3 | 1:D:378:CYS:HB3 | 2.01 | 0.43 |
| 1:D:326:VAL:HG22 | 4:D:502:HOH:O | 2.18 | 0.43 |
| 1:D:300:LEU:HD22 | 4:D:427:HOH:O | 2.19 | 0.42 |
| 1:C:257:LEU:HD13 | 1:C:259:MET:HE2 | 1.99 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:365:MET:CE | 1:D:371:ARG:O | 2.67 | 0.42 |
| 1:A:276:VAL:HG11 | 1:A:390:GLU:HB2 | 2.01 | 0.42 |
| 1:C:316:ASN:HD21 | 1:C:348:HIS:CE1 | 2.37 | 0.42 |
| 1:D:195:PHE:HB3 | 1:D:199:ILE:HD12 | 2.02 | 0.42 |
| 1:A:175:GLN:HE22 | 1:A:240:THR:CG2 | 2.33 | 0.42 |
| 1:C:226:ASP:O | 1:C:230:LYS:HG3 | 2.19 | 0.42 |
| 1:C:312:LEU:O | 1:C:373:GLY:HA2 | 2.20 | 0.42 |
| 1:A:297:ARG:NE | 4:A:9987:HOH:O | 2.53 | 0.41 |
| 1:D:354:GLY:HA2 | 1:D:377:LEU:HD21 | 2.02 | 0.41 |
| 1:A:78:GLN:O | 1:B:282:GLY:HA3 | 2.20 | 0.41 |
| 1:D:35:ILE:HG12 | 1:D:112:VAL:HG11 | 2.02 | 0.41 |
| 1:C:18:PHE:CZ | 1:D:129:ARG:HD3 | 2.56 | 0.41 |
| 1:D:328:LYS:HA | 4:D:520:HOH:O | 2.20 | 0.41 |
| 1:D:100:MET:C | 1:D:100:MET:SD | 2.98 | 0.41 |
| 1:C:387:MET:HB2 | 4:C:497:HOH:O | 2.21 | 0.41 |
| 1:B:312:LEU:CB | 4:B:479:HOH:O | 2.68 | 0.41 |
| 1:B:354:GLY:HA2 | 1:B:377:LEU:HD11 | 2.03 | 0.41 |
| 1:C:298:LYS:HD3 | 1:C:301:GLU:OE1 | 2.21 | 0.40 |
| 1:C:65:ASN:CG | 4:C:483:HOH:O | 2.52 | 0.40 |
| 1:C:207:ARG:HG2 | 4:C:517:HOH:O | 2.20 | 0.40 |
| 1:A:153:TYR:CE2 | 1:A:286:LYS:HG3 | 2.56 | 0.40 |
| 1:C:257:LEU:HD11 | 1:C:259:MET:CE | 2.51 | 0.40 |
| 1:B:175:GLN:HE22 | 1:B:240:THR:HG21 | 1.86 | 0.40 |
| 1:D:161:ALA:HB2 | 4:D:415:HOH:O | 2.21 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:437:HOH:O | 4:B:9890:HOH:O[2_555] | 2.19 | 0.01 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 391/392 (100%) | 378 (97%) | 13 (3%) | 0 | 100 | 100 |
| 1 | B | 391/392 (100%) | 380 (97%) | 11 (3%) | 0 | 100 | 100 |
| 1 | C | 391/392 (100%) | 374 (96%) | 16 (4%) | 1 (0%) | 41 | 24 |
| 1 | D | 391/392 (100%) | 371 (95%) | 19 (5%) | 1 (0%) | 41 | 24 |
| All | All | 1564/1568 (100%) | 1503 (96%) | 59 (4%) | 2 (0%) | 51 | 33 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 350 | ILE |
| 1 | C | 350 | ILE |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 279/278 (100%) | 261 (94%) | 18 (6%) | 17 | 4 |
| 1 | B | 279/278 (100%) | 265 (95%) | 14 (5%) | 24 | 8 |
| 1 | C | 279/278 (100%) | 264 (95%) | 15 (5%) | 22 | 7 |
| 1 | D | 279/278 (100%) | 257 (92%) | 22 (8%) | 12 | 2 |
| All | All | 1116/1112 (100%) | 1047 (94%) | 69 (6%) | 18 | 5 |

All (69) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1 | SER |
| 1 | A | 39 | LEU |
| 1 | A | 132 | VAL |
| 1 | A | 136 | ASP |
| 1 | A | 155 | TYR |
| 1 | A | 191 | LYS |
| 1 | A | 207 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 220 | ARG |
| 1 | A | 228 | MET |
| 1 | A | 230 | LYS |
| 1 | A | 238 | GLU |
| 1 | A | 272 | LEU |
| 1 | A | 288 | MET |
| 1 | A | 298 | LYS |
| 1 | A | 322 | GLN |
| 1 | A | 328 | LYS |
| 1 | A | 332 | TRP |
| 1 | A | 367 | ARG |
| 1 | B | 39 | LEU |
| 1 | B | 155 | TYR |
| 1 | B | 167 | GLN |
| 1 | B | 191 | LYS |
| 1 | B | 207 | ARG |
| 1 | B | 220 | ARG |
| 1 | B | 237 | LYS |
| 1 | B | 238 | GLU |
| 1 | B | 263 | GLU |
| 1 | B | 272 | LEU |
| 1 | B | 288 | MET |
| 1 | B | 298 | LYS |
| 1 | B | 322 | GLN |
| 1 | B | 332 | TRP |
| 1 | C | 39 | LEU |
| 1 | C | 155 | TYR |
| 1 | C | 187 | GLU |
| 1 | C | 191 | LYS |
| 1 | C | 207 | ARG |
| 1 | C | 220 | ARG |
| 1 | C | 224 | THR |
| 1 | C | 237 | LYS |
| 1 | C | 257 | LEU |
| 1 | C | 263 | GLU |
| 1 | C | 272 | LEU |
| 1 | C | 288 | MET |
| 1 | C | 298 | LYS |
| 1 | C | 322 | GLN |
| 1 | C | 332 | TRP |
| 1 | D | 39 | LEU |
| 1 | D | 129 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 134 | MET |
| 1 | D | 155 | TYR |
| 1 | D | 167 | GLN |
| 1 | D | 187 | GLU |
| 1 | D | 207 | ARG |
| 1 | D | 220 | ARG |
| 1 | D | 227 | SER |
| 1 | D | 237 | LYS |
| 1 | D | 238 | GLU |
| 1 | D | 263 | GLU |
| 1 | D | 272 | LEU |
| 1 | D | 288 | MET |
| 1 | D | 298 | LYS |
| 1 | D | 311 | ASP |
| 1 | D | 322 | GLN |
| 1 | D | 332 | TRP |
| 1 | D | 353 | SER |
| 1 | D | 359 | ASN |
| 1 | D | 371 | ARG |
| 1 | D | 391 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 78 | GLN |
| 1 | A | 175 | GLN |
| 1 | A | 184 | ASN |
| 1 | B | 175 | GLN |
| 1 | B | 184 | ASN |
| 1 | C | 175 | GLN |
| 1 | C | 184 | ASN |
| 1 | C | 316 | ASN |
| 1 | D | 78 | GLN |
| 1 | D | 175 | GLN |
| 1 | D | 184 | ASN |
| 1 | D | 316 | ASN |

### 5.3.3 RNA

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)

6 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 | $\#\|Z\| > 2$ |
| 2 | SO4 | B | 9719 | - | 4,4,4 | 0.18 | 0 | 6,6,6 | 0.24 | 0 |
| 2 | SO4 | A | 9720 | - | 4,4,4 | 0.06 | 0 | 6,6,6 | 0.41 | 0 |
| 2 | SO4 | A | 9722 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.59 | 0 |
| 3 | GOL | B | 6393 | - | 5,5,5 | 0.25 | 0 | 5,5,5 | 0.96 | 0 |
| 3 | GOL | A | 5393 | - | 5,5,5 | 1.07 | 1 (20%) | 5,5,5 | 1.19 | 1 (20%) |
| 2 | SO4 | B | 9721 | - | 4,4,4 | 0.23 | 0 | 6,6,6 | 0.21 | 0 |

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 |
|---|---|---|---|---|---|---|---|
| 3 | GOL | A | 5393 | - | - | 3/4/4/4 | - |
| 3 | GOL | B | 6393 | - | - | 3/4/4/4 | - |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | A | 5393 | GOL | O3-C3 | -2.25 | 1.32 | 1.42 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | A | 5393 | GOL | C3-C2-C1 | -2.05 | 103.75 | 111.70 |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | A | 5393 | GOL | O1-C1-C2-C3 |
| 3 | A | 5393 | GOL | C1-C2-C3-O3 |
| 3 | B | 6393 | GOL | C1-C2-C3-O3 |
| 3 | A | 5393 | GOL | O2-C2-C3-O3 |
| 3 | B | 6393 | GOL | O2-C2-C3-O3 |
| 3 | B | 6393 | GOL | O1-C1-C2-O2 |

There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | A | 9722 | SO4 | 1 | 0 |
| 3 | A | 5393 | GOL | 2 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 392/392 (100%) | -0.10 | 6 (1%) 73 77 | 5, 10, 25, 48 | 0 |
| 1 | B | 392/392 (100%) | -0.09 | 6 (1%) 73 77 | 5, 10, 25, 51 | 0 |
| 1 | C | 392/392 (100%) | 0.83 | 42 (10%) 6 7 | 3, 13, 26, 40 | 0 |
| 1 | D | 392/392 (100%) | 1.42 | 92 (23%) 0 0 | 2, 15, 27, 39 | 0 |
| All | All | 1568/1568 (100%) | 0.52 | 146 (9%) 8 9 | 2, 12, 26, 51 | 0 |

All (146) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 170 | LEU | 9.2 |
| 1 | C | 1 | SER | 9.1 |
| 1 | D | 1 | SER | 8.2 |
| 1 | D | 229 | ALA | 8.0 |
| 1 | D | 2 | THR | 7.3 |
| 1 | D | 232 | ARG | 6.6 |
| 1 | D | 392 | LEU | 6.6 |
| 1 | D | 228 | MET | 6.3 |
| 1 | B | 207 | ARG | 6.0 |
| 1 | D | 231 | LEU | 5.6 |
| 1 | D | 237 | LYS | 5.6 |
| 1 | C | 104 | ALA | 5.5 |
| 1 | D | 188 | ALA | 5.5 |
| 1 | D | 235 | PHE | 5.4 |
| 1 | C | 225 | LEU | 5.3 |
| 1 | C | 208 | LYS | 5.2 |
| 1 | A | 208 | LYS | 5.2 |
| 1 | D | 226 | ASP | 5.1 |
| 1 | D | 328 | LYS | 5.0 |
| 1 | D | 208 | LYS | 4.8 |
| 1 | C | 2 | THR | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 207 | ARG | 4.6 |
| 1 | C | 232 | ARG | 4.5 |
| 1 | D | 240 | THR | 4.5 |
| 1 | C | 211 | ILE | 4.4 |
| 1 | D | 224 | THR | 4.3 |
| 1 | C | 186 | ALA | 4.2 |
| 1 | C | 243 | ALA | 4.2 |
| 1 | D | 332 | TRP | 4.2 |
| 1 | D | 225 | LEU | 4.2 |
| 1 | D | 221 | HIS | 4.1 |
| 1 | C | 206 | GLY | 4.1 |
| 1 | D | 227 | SER | 4.0 |
| 1 | D | 219 | ILE | 4.0 |
| 1 | D | 325 | ALA | 4.0 |
| 1 | D | 167 | GLN | 3.9 |
| 1 | C | 231 | LEU | 3.9 |
| 1 | D | 371 | ARG | 3.9 |
| 1 | D | 152 | PHE | 3.9 |
| 1 | D | 238 | GLU | 3.8 |
| 1 | B | 1 | SER | 3.8 |
| 1 | A | 132 | VAL | 3.7 |
| 1 | C | 36 | SER | 3.6 |
| 1 | A | 209 | GLY | 3.6 |
| 1 | D | 206 | GLY | 3.6 |
| 1 | C | 221 | HIS | 3.6 |
| 1 | D | 377 | LEU | 3.6 |
| 1 | D | 223 | ALA | 3.6 |
| 1 | D | 382 | GLY | 3.6 |
| 1 | B | 392 | LEU | 3.5 |
| 1 | D | 236 | ASP | 3.4 |
| 1 | D | 330 | LEU | 3.4 |
| 1 | D | 339 | VAL | 3.3 |
| 1 | D | 269 | ILE | 3.3 |
| 1 | D | 220 | ARG | 3.2 |
| 1 | D | 306 | LYS | 3.2 |
| 1 | D | 173 | ASP | 3.2 |
| 1 | C | 67 | ALA | 3.2 |
| 1 | C | 234 | ALA | 3.2 |
| 1 | C | 80 | ALA | 3.2 |
| 1 | D | 324 | CYS | 3.2 |
| 1 | D | 378 | CYS | 3.2 |
| 1 | C | 153 | TYR | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 310 | LEU | 3.1 |
| 1 | D | 180 | VAL | 3.1 |
| 1 | D | 281 | VAL | 3.1 |
| 1 | D | 375 | ALA | 3.1 |
| 1 | D | 153 | TYR | 3.0 |
| 1 | A | 206 | GLY | 2.9 |
| 1 | D | 331 | GLY | 2.9 |
| 1 | D | 195 | PHE | 2.9 |
| 1 | D | 313 | VAL | 2.9 |
| 1 | B | 208 | LYS | 2.9 |
| 1 | D | 5 | ILE | 2.9 |
| 1 | D | 181 | ALA | 2.9 |
| 1 | D | 189 | ALA | 2.8 |
| 1 | D | 350 | ILE | 2.8 |
| 1 | B | 132 | VAL | 2.8 |
| 1 | C | 392 | LEU | 2.8 |
| 1 | D | 391 | SER | 2.8 |
| 1 | A | 131 | GLY | 2.7 |
| 1 | D | 155 | TYR | 2.7 |
| 1 | D | 178 | PHE | 2.7 |
| 1 | C | 226 | ASP | 2.7 |
| 1 | C | 209 | GLY | 2.7 |
| 1 | C | 334 | PRO | 2.7 |
| 1 | D | 307 | ILE | 2.7 |
| 1 | C | 235 | PHE | 2.7 |
| 1 | D | 303 | ALA | 2.6 |
| 1 | C | 135 | GLY | 2.6 |
| 1 | D | 289 | GLY | 2.6 |
| 1 | D | 15 | VAL | 2.6 |
| 1 | C | 224 | THR | 2.6 |
| 1 | C | 207 | ARG | 2.6 |
| 1 | C | 371 | ARG | 2.6 |
| 1 | C | 239 | GLY | 2.6 |
| 1 | A | 207 | ARG | 2.6 |
| 1 | D | 191 | LYS | 2.6 |
| 1 | D | 301 | GLU | 2.6 |
| 1 | D | 311 | ASP | 2.6 |
| 1 | D | 367 | ARG | 2.5 |
| 1 | D | 254 | ALA | 2.5 |
| 1 | D | 192 | ASP | 2.5 |
| 1 | C | 230 | LYS | 2.5 |
| 1 | D | 241 | VAL | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 299 | ALA | 2.4 |
| 1 | C | 312 | LEU | 2.4 |
| 1 | D | 165 | ALA | 2.4 |
| 1 | D | 389 | ILE | 2.4 |
| 1 | D | 175 | GLN | 2.4 |
| 1 | D | 368 | ARG | 2.4 |
| 1 | C | 49 | VAL | 2.4 |
| 1 | D | 329 | ASP | 2.3 |
| 1 | D | 166 | LYS | 2.3 |
| 1 | D | 374 | LEU | 2.3 |
| 1 | D | 370 | ALA | 2.3 |
| 1 | C | 222 | GLY | 2.3 |
| 1 | D | 171 | SER | 2.3 |
| 1 | D | 319 | PHE | 2.3 |
| 1 | D | 42 | ALA | 2.2 |
| 1 | D | 177 | ALA | 2.2 |
| 1 | D | 211 | ILE | 2.2 |
| 1 | D | 4 | SER | 2.2 |
| 1 | C | 35 | ILE | 2.2 |
| 1 | C | 22 | PHE | 2.2 |
| 1 | C | 156 | HIS | 2.2 |
| 1 | C | 295 | ALA | 2.2 |
| 1 | C | 266 | ARG | 2.2 |
| 1 | D | 249 | LEU | 2.2 |
| 1 | D | 318 | ALA | 2.2 |
| 1 | C | 265 | SER | 2.1 |
| 1 | D | 202 | PHE | 2.1 |
| 1 | C | 170 | LEU | 2.1 |
| 1 | C | 181 | ALA | 2.1 |
| 1 | D | 272 | LEU | 2.1 |
| 1 | C | 161 | ALA | 2.1 |
| 1 | D | 372 | LYS | 2.1 |
| 1 | B | 2 | THR | 2.1 |
| 1 | C | 155 | TYR | 2.1 |
| 1 | C | 305 | TRP | 2.1 |
| 1 | D | 179 | ALA | 2.1 |
| 1 | D | 243 | ALA | 2.1 |
| 1 | D | 187 | GLU | 2.1 |
| 1 | D | 320 | ALA | 2.0 |
| 1 | D | 205 | LYS | 2.0 |
| 1 | D | 218 | TYR | 2.0 |

## 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 | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | GOL | A | 5393 | 6/6 | 0.91 | 0.10 | 17,23,28,28 | 0 |
| 3 | GOL | B | 6393 | 6/6 | 0.93 | 0.11 | 9,24,30,31 | 0 |
| 2 | SO4 | A | 9722 | 5/5 | 0.94 | 0.15 | 65,65,68,69 | 0 |
| 2 | SO4 | B | 9721 | 5/5 | 0.97 | 0.08 | 42,45,51,54 | 0 |
| 2 | SO4 | B | 9719 | 5/5 | 0.98 | 0.07 | 67,67,68,69 | 0 |
| 2 | SO4 | A | 9720 | 5/5 | 0.98 | 0.10 | 44,49,52,55 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.