# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:25 pm BST

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|---|---|---|
| PDB ID | : | 6FBM |
| Title | : | Crystal structure of GNIP1Aa from Chromobacterium piscinae |
| Authors | : | Freigang, J.; Zaitseva, J. |
| Deposited on | : | 2017-12-19 |
| Resolution | : | 2.50 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 ⓘ symbol.

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

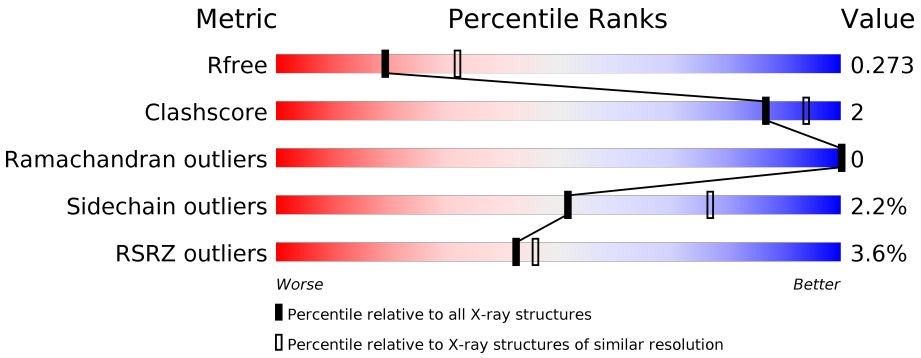
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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 | 4661 (2.50-2.50) |
| Clashscore | 141614 | 5346 (2.50-2.50) |
| Ramachandran outliers | 138981 | 5231 (2.50-2.50) |
| Sidechain outliers | 138945 | 5233 (2.50-2.50) |
| RSRZ outliers | 127900 | 4559 (2.50-2.50) |

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 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 | 536 | 2% 92% |
| 1 | B | 536 | 2% 91% 6% |
| 1 | C | 536 | 4% 92% 5% |
| 1 | D | 536 | 5% 90% 7% |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16588 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 Gram-negative insecticidal protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 521 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4034 | 2527 | 695 | 785 | 27 | | | |
| 1 | B | 521 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4034 | 2527 | 695 | 785 | 27 | | | |
| 1 | C | 521 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4034 | 2527 | 695 | 785 | 27 | | | |
| 1 | D | 521 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4034 | 2527 | 695 | 785 | 27 | | | |

- Molecule 2 is water.

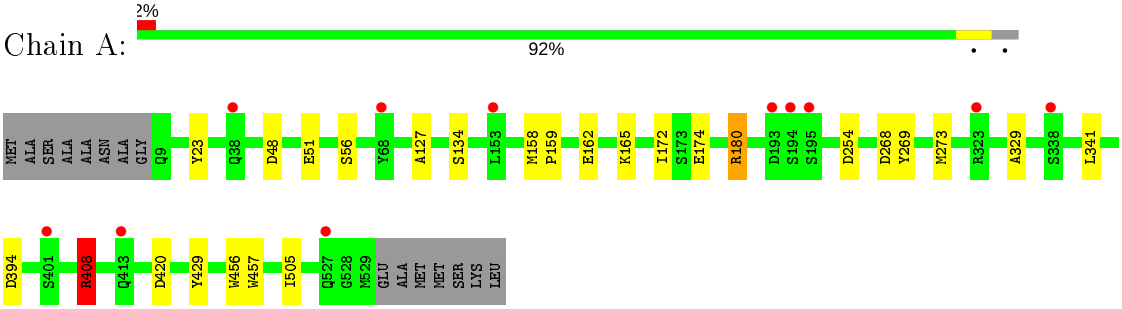
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | A | 120 | Total | O | 0 | 0 |
| | | | 120 | 120 | | |
| 2 | B | 116 | Total | O | 0 | 0 |
| | | | 116 | 116 | | |
| 2 | C | 105 | Total | O | 0 | 0 |
| | | | 105 | 105 | | |
| 2 | D | 111 | Total | O | 0 | 0 |
| | | | 111 | 111 | | |

# 3 Residue-property plots

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

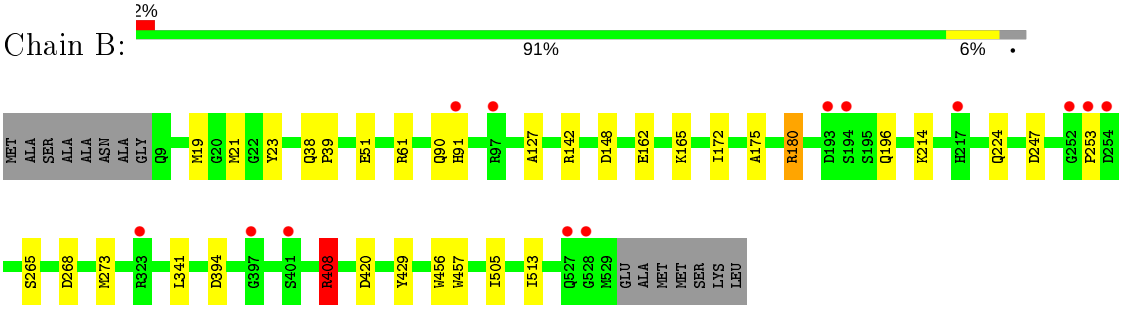
- Molecule 1: Gram-negative insecticidal protein

Chain A:



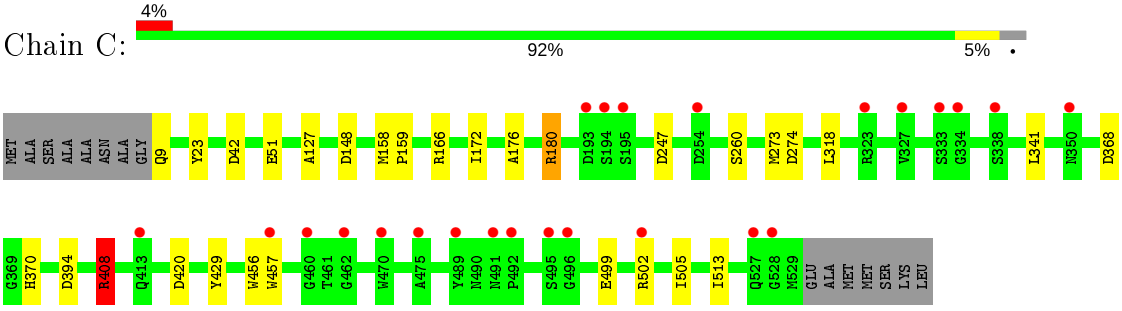

- Molecule 1: Gram-negative insecticidal protein

Chain B:



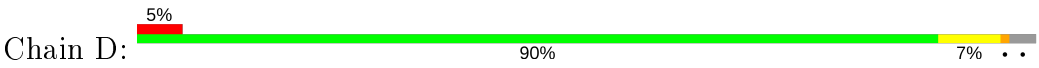

- Molecule 1: Gram-negative insecticidal protein

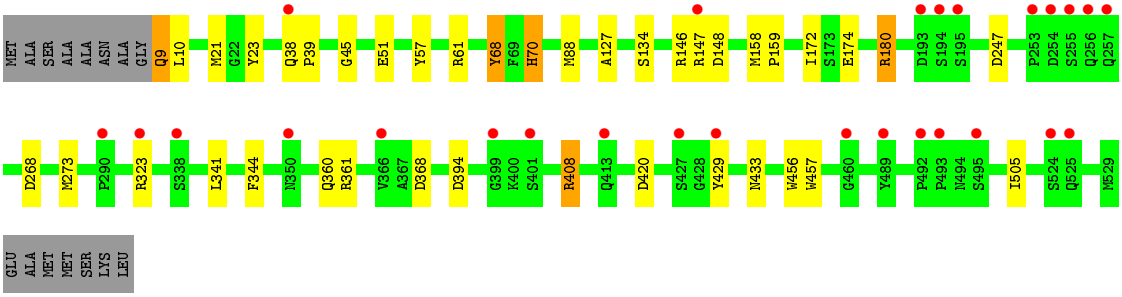
Chain C:




- Molecule 1: Gram-negative insecticidal protein

Chain D:




MET ALA SER ALA ALA ASN ALA GLY Q9 L10 M21 G22 Y23 Q38 P39 G45 E51 Y57 R61 Y68 F69 H70 M88 A127 S134 R146 R147 D148 M158 P159 I172 S173 E174 R180 D193 S194 S195 D247 P253 D254 S255 Q256 Q257
D268 M273 P290 R323 S338 L341 F344 N350 Q360 R361 V366 A367 D368 D394 G399 K400 S401 R408 Q413 D420 S427 G428 Y429 N433 W456 W457 G460 Y489 P492 P493 N494 S495 I505 S524 Q525 M529
GLU ALA MET MET SER LYS LEU

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 78.68Å 143.19Å 209.62Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 14.99 – 2.50<br>14.99 – 2.50 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 96.7 (14.99-2.50)<br>97.2 (14.99-2.50) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.11 | Depositor |
| $< I/\sigma(I) >$ [1] | 3.31 (at 2.51Å) | Xtriage |
| Refinement program | REFMAC 5.8.0158 2016/10/03 | Depositor |
| R, $R_{free}$ | 0.230 , 0.271<br>0.233 , 0.273 | Depositor<br>DCC |
| $R_{free}$ test set | 4016 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 21.5 | Xtriage |
| Anisotropy | 0.032 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.36 , 29.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.46$, $< L^2 > = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.89 | EDS |
| Total number of atoms | 16588 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 27.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1995e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.59 | 0/4129 | 0.78 | 4/5589 (0.1%) |
| 1 | B | 0.61 | 1/4129 (0.0%) | 0.79 | 5/5589 (0.1%) |
| 1 | C | 0.63 | 0/4129 | 0.80 | 5/5589 (0.1%) |
| 1 | D | 0.62 | 0/4129 | 0.81 | 5/5589 (0.1%) |
| All | All | 0.61 | 1/16516 (0.0%) | 0.80 | 19/22356 (0.1%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 265 | SER | CB-OG | 6.08 | 1.50 | 1.42 |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 142 | ARG | NE-CZ-NH2 | -7.57 | 116.52 | 120.30 |
| 1 | D | 57 | TYR | CB-CG-CD1 | -7.25 | 116.65 | 121.00 |
| 1 | D | 57 | TYR | CB-CG-CD2 | 6.77 | 125.06 | 121.00 |
| 1 | A | 408 | ARG | NE-CZ-NH2 | 6.46 | 123.53 | 120.30 |
| 1 | B | 408 | ARG | NE-CZ-NH2 | 6.33 | 123.47 | 120.30 |
| 1 | A | 180 | ARG | NE-CZ-NH1 | 6.33 | 123.46 | 120.30 |
| 1 | C | 408 | ARG | NE-CZ-NH1 | -6.30 | 117.15 | 120.30 |
| 1 | C | 408 | ARG | NE-CZ-NH2 | 6.22 | 123.41 | 120.30 |
| 1 | D | 268 | ASP | CB-CG-OD1 | 6.21 | 123.89 | 118.30 |
| 1 | A | 408 | ARG | NE-CZ-NH1 | -5.97 | 117.31 | 120.30 |
| 1 | C | 180 | ARG | NE-CZ-NH1 | 5.95 | 123.28 | 120.30 |
| 1 | B | 408 | ARG | NE-CZ-NH1 | -5.70 | 117.45 | 120.30 |
| 1 | C | 42 | ASP | CB-CG-OD2 | -5.61 | 113.25 | 118.30 |
| 1 | B | 180 | ARG | NE-CZ-NH1 | 5.59 | 123.09 | 120.30 |
| 1 | B | 268 | ASP | CB-CG-OD2 | 5.38 | 123.14 | 118.30 |
| 1 | D | 68 | TYR | CA-CB-CG | 5.37 | 123.61 | 113.40 |
| 1 | D | 180 | ARG | NE-CZ-NH1 | 5.29 | 122.94 | 120.30 |
| 1 | C | 166 | ARG | NE-CZ-NH1 | 5.09 | 122.85 | 120.30 |
| 1 | A | 268 | ASP | CB-CG-OD2 | 5.08 | 122.88 | 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 | 4034 | 0 | 3895 | 15 | 0 |
| 1 | B | 4034 | 0 | 3895 | 15 | 0 |
| 1 | C | 4034 | 0 | 3895 | 18 | 1 |
| 1 | D | 4034 | 0 | 3895 | 19 | 1 |
| 2 | A | 120 | 0 | 0 | 2 | 0 |
| 2 | B | 116 | 0 | 0 | 0 | 0 |
| 2 | C | 105 | 0 | 0 | 2 | 0 |
| 2 | D | 111 | 0 | 0 | 0 | 0 |
| All | All | 16588 | 0 | 15580 | 65 | 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 2.

All (65) 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:C:499:GLU:OE2 | 1:C:502:ARG:NH2 | 2.19 | 0.76 |
| 1:B:196:GLN:HB3 | 1:B:224:GLN:HE21 | 1.59 | 0.68 |
| 1:C:499:GLU:CD | 1:C:502:ARG:NH2 | 2.52 | 0.63 |
| 1:C:370:HIS:CE1 | 2:C:698:HOH:O | 2.52 | 0.63 |
| 1:C:370:HIS:HE1 | 2:C:698:HOH:O | 1.83 | 0.59 |
| 1:B:408:ARG:HD3 | 1:B:505:ILE:HD11 | 1.85 | 0.57 |
| 1:C:408:ARG:HD3 | 1:C:505:ILE:HD11 | 1.84 | 0.57 |
| 1:D:408:ARG:HD3 | 1:D:505:ILE:HD11 | 1.85 | 0.56 |
| 1:A:408:ARG:HD3 | 1:A:505:ILE:HD11 | 1.85 | 0.56 |
| 1:A:269:TYR:OH | 1:D:45:GLY:HA3 | 2.06 | 0.55 |
| 1:C:158:MET:HE2 | 1:C:159:PRO:HD2 | 1.89 | 0.55 |
| 1:C:499:GLU:OE1 | 1:C:502:ARG:NH2 | 2.40 | 0.55 |
| 1:B:90:GLN:HB3 | 1:B:91:HIS:ND1 | 2.23 | 0.54 |
| 1:D:9:GLN:HE21 | 1:D:9:GLN:N | 2.06 | 0.54 |
| 1:D:180:ARG:HD3 | 1:D:273:MET:O | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:180:ARG:HD3 | 1:C:273:MET:O | 2.11 | 0.51 |
| 1:C:127:ALA:HB1 | 1:C:273:MET:HE3 | 1.92 | 0.51 |
| 1:D:127:ALA:HB1 | 1:D:273:MET:CE | 2.40 | 0.51 |
| 1:C:127:ALA:HB1 | 1:C:273:MET:CE | 2.41 | 0.51 |
| 1:B:127:ALA:HB1 | 1:B:273:MET:CE | 2.41 | 0.50 |
| 1:B:180:ARG:HD3 | 1:B:273:MET:O | 2.12 | 0.50 |
| 1:D:127:ALA:HB1 | 1:D:273:MET:HE3 | 1.92 | 0.50 |
| 1:A:127:ALA:HB1 | 1:A:273:MET:CE | 2.42 | 0.50 |
| 1:A:134:SER:HB3 | 1:A:174:GLU:HG3 | 1.94 | 0.49 |
| 1:A:180:ARG:HD3 | 1:A:273:MET:O | 2.11 | 0.49 |
| 1:A:254:ASP:OD2 | 1:B:253:PRO:O | 2.30 | 0.49 |
| 1:B:180:ARG:HB2 | 1:B:273:MET:HE2 | 1.94 | 0.49 |
| 1:A:180:ARG:HB2 | 1:A:273:MET:HE2 | 1.95 | 0.49 |
| 1:B:196:GLN:HB3 | 1:B:224:GLN:NE2 | 2.27 | 0.49 |
| 1:D:394:ASP:HB2 | 1:D:429:TYR:CE1 | 2.49 | 0.48 |
| 1:A:165:LYS:HE3 | 2:A:718:HOH:O | 2.13 | 0.48 |
| 1:B:394:ASP:HB2 | 1:B:429:TYR:CE1 | 2.49 | 0.47 |
| 1:D:344:PHE:CE1 | 1:D:360:GLN:NE2 | 2.83 | 0.47 |
| 1:D:408:ARG:HG2 | 1:D:420:ASP:OD1 | 2.14 | 0.47 |
| 1:A:394:ASP:HB2 | 1:A:429:TYR:CE1 | 2.49 | 0.47 |
| 1:D:68:TYR:HB3 | 1:D:70:HIS:CE1 | 2.50 | 0.46 |
| 1:B:408:ARG:HG2 | 1:B:420:ASP:OD1 | 2.15 | 0.46 |
| 1:C:408:ARG:HG2 | 1:C:420:ASP:OD1 | 2.15 | 0.46 |
| 1:A:408:ARG:HG2 | 1:A:420:ASP:OD1 | 2.15 | 0.46 |
| 1:C:394:ASP:HB2 | 1:C:429:TYR:CE1 | 2.49 | 0.46 |
| 1:D:21:MET:HE2 | 1:D:39:PRO:HA | 1.98 | 0.45 |
| 1:D:341:LEU:HB2 | 1:D:456:TRP:CD1 | 2.51 | 0.45 |
| 1:C:23:TYR:CD1 | 1:C:172:ILE:HD11 | 2.52 | 0.45 |
| 1:D:134:SER:HB3 | 1:D:174:GLU:HG3 | 1.97 | 0.45 |
| 1:B:127:ALA:HB1 | 1:B:273:MET:HE3 | 1.99 | 0.45 |
| 1:C:341:LEU:HB2 | 1:C:456:TRP:CD1 | 2.52 | 0.45 |
| 1:B:341:LEU:HB2 | 1:B:456:TRP:CD1 | 2.52 | 0.44 |
| 1:A:341:LEU:HB2 | 1:A:456:TRP:CD1 | 2.52 | 0.44 |
| 1:D:23:TYR:CD1 | 1:D:172:ILE:HD11 | 2.52 | 0.44 |
| 1:D:158:MET:HE2 | 1:D:159:PRO:HD2 | 1.99 | 0.44 |
| 1:A:23:TYR:CD1 | 1:A:172:ILE:HD11 | 2.53 | 0.44 |
| 1:C:180:ARG:HB2 | 1:C:273:MET:HE2 | 2.00 | 0.44 |
| 1:D:180:ARG:HB2 | 1:D:273:MET:HE2 | 2.00 | 0.43 |
| 1:B:23:TYR:CD1 | 1:B:172:ILE:HD11 | 2.53 | 0.43 |
| 1:A:329:ALA:HB1 | 2:A:611:HOH:O | 2.18 | 0.43 |
| 1:A:158:MET:HE2 | 1:A:159:PRO:HD2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:19:MET:CE | 1:B:175:ALA:HB3 | 2.48 | 0.43 |
| 1:C:499:GLU:OE2 | 1:C:502:ARG:CZ | 2.67 | 0.42 |
| 1:C:318:LEU:HD12 | 1:C:513:ILE:HD11 | 2.02 | 0.42 |
| 1:A:127:ALA:HB1 | 1:A:273:MET:HE3 | 2.01 | 0.41 |
| 1:C:176:ALA:HB3 | 1:C:274:ASP:HB3 | 2.01 | 0.41 |
| 1:B:21:MET:HE2 | 1:B:39:PRO:HA | 2.02 | 0.41 |
| 1:D:360:GLN:HG2 | 1:D:368:ASP:OD2 | 2.21 | 0.41 |
| 1:D:344:PHE:CD1 | 1:D:360:GLN:NE2 | 2.88 | 0.40 |
| 1:D:10:LEU:HD12 | 1:D:45:GLY:HA2 | 2.04 | 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) |
|---|---|---|---|
| 1:C:368:ASP:O | 1:D:361:ARG:O[3_646] | 2.17 | 0.03 |

## 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 | 519/536 (97%) | 504 (97%) | 15 (3%) | 0 | 100 | 100 |
| 1 | B | 519/536 (97%) | 504 (97%) | 15 (3%) | 0 | 100 | 100 |
| 1 | C | 519/536 (97%) | 505 (97%) | 14 (3%) | 0 | 100 | 100 |
| 1 | D | 519/536 (97%) | 503 (97%) | 16 (3%) | 0 | 100 | 100 |
| All | All | 2076/2144 (97%) | 2016 (97%) | 60 (3%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | 436/445 (98%) | 430 (99%) | 6 (1%) | 67 86 |
| 1 | B | 436/445 (98%) | 425 (98%) | 11 (2%) | 47 73 |
| 1 | C | 436/445 (98%) | 429 (98%) | 7 (2%) | 62 84 |
| 1 | D | 436/445 (98%) | 422 (97%) | 14 (3%) | 39 65 |
| All | All | 1744/1780 (98%) | 1706 (98%) | 38 (2%) | 52 77 |

All (38) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 48 | ASP |
| 1 | A | 51 | GLU |
| 1 | A | 56 | SER |
| 1 | A | 162 | GLU |
| 1 | A | 408 | ARG |
| 1 | A | 457 | TRP |
| 1 | B | 38 | GLN |
| 1 | B | 51 | GLU |
| 1 | B | 61 | ARG |
| 1 | B | 148 | ASP |
| 1 | B | 162 | GLU |
| 1 | B | 165 | LYS |
| 1 | B | 214 | LYS |
| 1 | B | 247 | ASP |
| 1 | B | 408 | ARG |
| 1 | B | 457 | TRP |
| 1 | B | 513 | ILE |
| 1 | C | 9 | GLN |
| 1 | C | 51 | GLU |
| 1 | C | 148 | ASP |
| 1 | C | 247 | ASP |
| 1 | C | 260 | SER |
| 1 | C | 408 | ARG |
| 1 | C | 457 | TRP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 9 | GLN |
| 1 | D | 38 | GLN |
| 1 | D | 51 | GLU |
| 1 | D | 61 | ARG |
| 1 | D | 70 | HIS |
| 1 | D | 88 | MET |
| 1 | D | 146 | ARG |
| 1 | D | 147 | ARG |
| 1 | D | 148 | ASP |
| 1 | D | 247 | ASP |
| 1 | D | 323 | ARG |
| 1 | D | 408 | ARG |
| 1 | D | 433 | ASN |
| 1 | D | 457 | TRP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 224 | GLN |
| 1 | C | 9 | GLN |
| 1 | C | 370 | HIS |
| 1 | D | 70 | HIS |

#### 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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 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, $95^{th}$ 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 | 521/536 (97%) | -0.08 | 11 (2%) | 63 | 66 | 9, 21, 46, 72 | 0 |
| 1 | B | 521/536 (97%) | 0.02 | 13 (2%) | 57 | 61 | 8, 25, 49, 78 | 0 |
| 1 | C | 521/536 (97%) | 0.14 | 24 (4%) | 32 | 34 | 6, 24, 58, 85 | 0 |
| 1 | D | 521/536 (97%) | 0.17 | 27 (5%) | 27 | 29 | 7, 29, 60, 95 | 0 |
| All | All | 2084/2144 (97%) | 0.06 | 75 (3%) | 42 | 46 | 6, 25, 55, 95 | 0 |

All (75) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 254 | ASP | 6.3 |
| 1 | C | 492 | PRO | 5.1 |
| 1 | B | 194 | SER | 4.1 |
| 1 | D | 350 | ASN | 4.0 |
| 1 | C | 495 | SER | 3.6 |
| 1 | D | 255 | SER | 3.6 |
| 1 | A | 194 | SER | 3.5 |
| 1 | D | 253 | PRO | 3.4 |
| 1 | D | 195 | SER | 3.3 |
| 1 | C | 528 | GLY | 3.3 |
| 1 | C | 338 | SER | 3.3 |
| 1 | C | 475 | ALA | 3.1 |
| 1 | B | 91 | HIS | 3.1 |
| 1 | C | 489 | TYR | 3.1 |
| 1 | A | 195 | SER | 3.1 |
| 1 | B | 323 | ARG | 3.0 |
| 1 | B | 252 | GLY | 2.9 |
| 1 | B | 528 | GLY | 2.8 |
| 1 | C | 333 | SER | 2.8 |
| 1 | D | 401 | SER | 2.8 |
| 1 | C | 193 | ASP | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 217 | HIS | 2.7 |
| 1 | B | 397 | GLY | 2.7 |
| 1 | C | 334 | GLY | 2.7 |
| 1 | C | 527 | GLN | 2.7 |
| 1 | B | 527 | GLN | 2.7 |
| 1 | D | 429 | TYR | 2.7 |
| 1 | C | 413 | GLN | 2.7 |
| 1 | C | 194 | SER | 2.6 |
| 1 | C | 350 | ASN | 2.6 |
| 1 | C | 460 | GLY | 2.6 |
| 1 | B | 193 | ASP | 2.6 |
| 1 | D | 366 | VAL | 2.6 |
| 1 | C | 254 | ASP | 2.6 |
| 1 | B | 253 | PRO | 2.6 |
| 1 | D | 427 | SER | 2.6 |
| 1 | D | 492 | PRO | 2.6 |
| 1 | C | 502 | ARG | 2.6 |
| 1 | D | 193 | ASP | 2.6 |
| 1 | D | 194 | SER | 2.5 |
| 1 | A | 413 | GLN | 2.5 |
| 1 | B | 97 | ARG | 2.5 |
| 1 | A | 153 | LEU | 2.4 |
| 1 | D | 524 | SER | 2.4 |
| 1 | C | 457 | TRP | 2.4 |
| 1 | A | 527 | GLN | 2.4 |
| 1 | D | 493 | PRO | 2.4 |
| 1 | A | 401 | SER | 2.4 |
| 1 | C | 462 | GLY | 2.4 |
| 1 | B | 254 | ASP | 2.4 |
| 1 | C | 323 | ARG | 2.3 |
| 1 | D | 257 | GLN | 2.3 |
| 1 | D | 38 | GLN | 2.3 |
| 1 | D | 413 | GLN | 2.2 |
| 1 | A | 338 | SER | 2.2 |
| 1 | D | 338 | SER | 2.2 |
| 1 | A | 38 | GLN | 2.2 |
| 1 | C | 195 | SER | 2.2 |
| 1 | D | 399 | GLY | 2.1 |
| 1 | A | 68 | TYR | 2.1 |
| 1 | A | 193 | ASP | 2.1 |
| 1 | C | 491 | ASN | 2.1 |
| 1 | D | 256 | GLN | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 147 | ARG | 2.1 |
| 1 | D | 323 | ARG | 2.1 |
| 1 | D | 495 | SER | 2.1 |
| 1 | D | 489 | TYR | 2.1 |
| 1 | D | 525 | GLN | 2.1 |
| 1 | B | 401 | SER | 2.1 |
| 1 | C | 496 | GLY | 2.1 |
| 1 | C | 470 | TRP | 2.1 |
| 1 | D | 290 | PRO | 2.0 |
| 1 | C | 327 | VAL | 2.0 |
| 1 | D | 460 | GLY | 2.0 |
| 1 | A | 323 | ARG | 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 carbohydrates in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.