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

Feb 1, 2016 – 01:46 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 3UW6 |
| Title | : | Crystal Structure of Engineered Protein, Northeast Structural Genomics Consortium Target OR120 |
| Authors | : | Seetharaman, J.; Lew, S; Nivon, L; Baker, D; Bjelic, S; Ciccosanti, C; Sahdev, S; Xiao, R; Everett, J.K; Acton, T.B; Montelione, G.T; Tong, L; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG) |
| Deposited on | : | 2011-11-30 |
| Resolution | : | 2.30 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

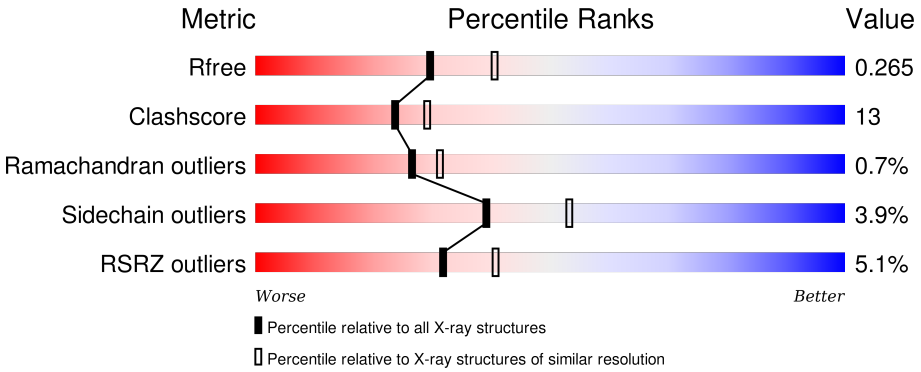
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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)) |
|---|---|---|
| $R_{free}$ | 91344 | 3852 (2.30-2.30) |
| Clashscore | 102246 | 4452 (2.30-2.30) |
| Ramachandran outliers | 100387 | 4410 (2.30-2.30) |
| Sidechain outliers | 100360 | 4409 (2.30-2.30) |
| RSRZ outliers | 91569 | 3857 (2.30-2.30) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | 390 | 3% 73% 20% • 5% |
| 1 | B | 390 | 4% 71% 22% •• 5% |
| 1 | C | 390 | 7% 71% 22% •• 5% |

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8977 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 Alanine racemase.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 372 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 2929 | 1876 | 520 | 519 | 4 | 10 | | | |
| 1 | B | 371 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 2914 | 1867 | 516 | 518 | 4 | 9 | | | |
| 1 | C | 370 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 2900 | 1858 | 515 | 514 | 4 | 9 | | | |

- Molecule 2 is water.

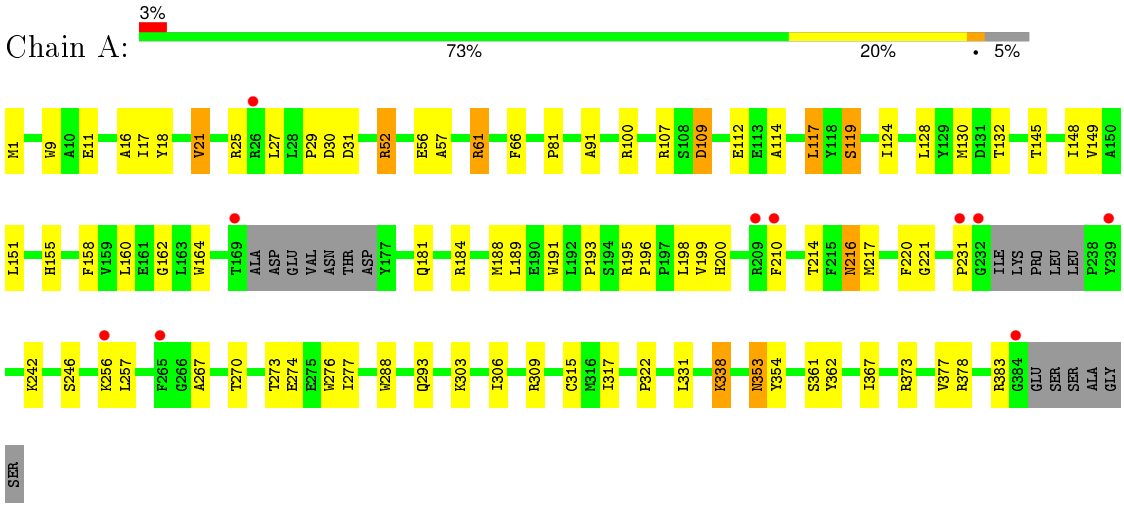
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | A | 80 | Total | O | 0 | 0 |
| | | | 80 | 80 | | |
| 2 | B | 80 | Total | O | 0 | 0 |
| | | | 80 | 80 | | |
| 2 | C | 74 | Total | O | 0 | 0 |
| | | | 74 | 74 | | |

# 3 Residue-property plots (i)

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

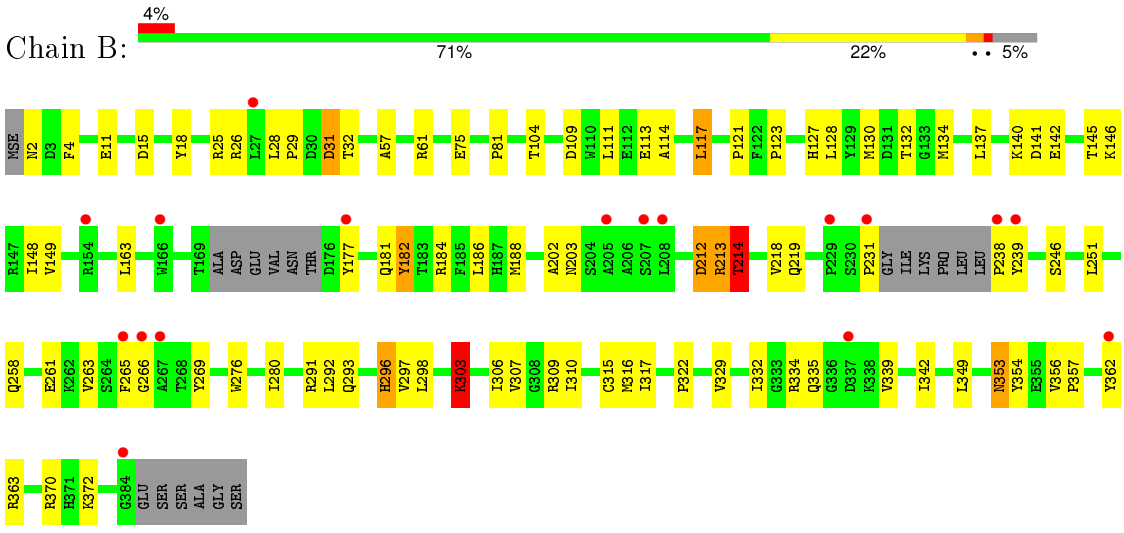
- Molecule 1: Alanine racemase

Chain A:



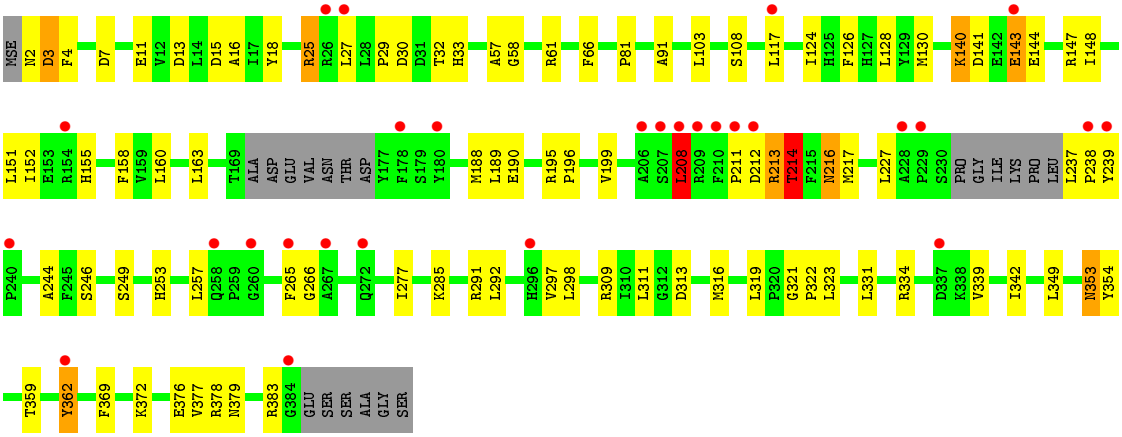

- Molecule 1: Alanine racemase

Chain B:




- Molecule 1: Alanine racemase

Chain C:


MSE N2 D3 F4 D7 E11 V12 D13 L14 D15 A16 I17 Y18 R25 R26 L27 L28 P29 D30 D31 T32 H33 A57 G58 R61 F66 P81 A91 L103 S108 L117 I124 H125 F126 H127 L128 Y129 M130 K140 D141 E142 E143 E144 R147 I148
L151 I152 E153 R154 H155 F158 V159 L160 L163 T169 ALA ASP GLU VAL ASN THR ASP Y177 F178 S179 Y180 M188 L189 E190 R195 P196 V199 A206 S207 L208 R209 F210 P211 D212 R213 T214 P215 N216 M217 L227 A228 P229 S230 PRO GLY ILE LYS PRO LEU L237 P238 Y239
P240 A244 F245 S246 S249 H253 L257 Q258 P259 G260 F265 G266 A267 Q272 I277 K285 R291 L292 H296 V297 L298 R309 I310 L311 G312 D313 M316 L319 P320 G321 P322 L323 L331 R334 D337 K338 V339 I342 L349 N353 Y354
T359 Y362 F369 K372 E376 V377 R378 N379 R383 G384 GLU SER SER ALA GLY SER

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 41 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 112.35Å 112.35Å 237.06Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.47 – 2.30<br>37.66 – 2.13 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 94.5 (30.47-2.30)<br>98.1 (37.66-2.13) | Depositor<br>EDS |
| $R_{merge}$ | 0.07 | Depositor |
| $R_{sym}$ | 0.06 | Depositor |
| $< I/\sigma(I) >$ [1] | 5.42 (at 2.14Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, $R_{free}$ | 0.215 , 0.259<br>0.227 , 0.265 | Depositor<br>DCC |
| $R_{free}$ test set | 6477 reflections (10.92%) | DCC |
| Wilson B-factor (Å$^2$) | 35.7 | Xtriage |
| Anisotropy | 0.415 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.36 , 41.7 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.31$ | Xtriage |
| Outliers | 0 of 160943 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 8977 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 42.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 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 | 0.53 | 3/2995 (0.1%) | 0.65 | 5/4051 (0.1%) |
| 1 | B | 0.80 | 14/2980 (0.5%) | 0.65 | 2/4035 (0.0%) |
| 1 | C | 1.15 | 37/2965 (1.2%) | 0.74 | 8/4014 (0.2%) |
| All | All | 0.86 | 54/8940 (0.6%) | 0.68 | 15/12100 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 1 | B | 0 | 1 |
| 1 | C | 0 | 2 |
| All | All | 0 | 4 |

All (54) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | B | 303 | LYS | CB-CG | -14.42 | 1.13 | 1.52 |
| 1 | B | 213 | ARG | CA-CB | -14.06 | 1.23 | 1.53 |
| 1 | C | 376 | GLU | CD-OE1 | -13.63 | 1.10 | 1.25 |
| 1 | C | 376 | GLU | CD-OE2 | -13.24 | 1.11 | 1.25 |
| 1 | C | 377 | VAL | CB-CG2 | -13.19 | 1.25 | 1.52 |
| 1 | C | 3 | ASP | CB-CG | -12.28 | 1.25 | 1.51 |
| 1 | B | 214 | THR | CB-CG2 | -11.77 | 1.13 | 1.52 |
| 1 | C | 4 | PHE | CD2-CE2 | -11.74 | 1.15 | 1.39 |
| 1 | C | 4 | PHE | CD1-CE1 | -11.27 | 1.16 | 1.39 |
| 1 | C | 379 | ASN | C-O | -10.99 | 1.02 | 1.23 |
| 1 | C | 377 | VAL | CB-CG1 | -10.77 | 1.30 | 1.52 |
| 1 | C | 4 | PHE | CE2-CZ | -10.21 | 1.18 | 1.37 |
| 1 | C | 376 | GLU | C-O | -9.28 | 1.05 | 1.23 |
| 1 | C | 2 | ASN | C-O | -9.27 | 1.05 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 4 | PHE | CG-CD2 | -9.15 | 1.25 | 1.38 |
| 1 | C | 4 | PHE | CE1-CZ | -9.10 | 1.20 | 1.37 |
| 1 | C | 378 | ARG | CZ-NH2 | -9.01 | 1.21 | 1.33 |
| 1 | B | 214 | THR | C-O | -9.01 | 1.06 | 1.23 |
| 1 | B | 213 | ARG | C-O | -8.81 | 1.06 | 1.23 |
| 1 | C | 3 | ASP | C-O | -8.79 | 1.06 | 1.23 |
| 1 | C | 379 | ASN | CG-ND2 | -8.71 | 1.11 | 1.32 |
| 1 | C | 3 | ASP | CG-OD2 | -8.53 | 1.05 | 1.25 |
| 1 | C | 378 | ARG | CZ-NH1 | -8.27 | 1.22 | 1.33 |
| 1 | A | 119 | SER | C-O | -8.09 | 1.07 | 1.23 |
| 1 | C | 379 | ASN | CG-OD1 | -8.08 | 1.06 | 1.24 |
| 1 | B | 296 | HIS | C-O | -7.94 | 1.08 | 1.23 |
| 1 | C | 378 | ARG | C-O | -7.75 | 1.08 | 1.23 |
| 1 | C | 3 | ASP | CG-OD1 | -7.74 | 1.07 | 1.25 |
| 1 | C | 4 | PHE | C-O | -7.64 | 1.08 | 1.23 |
| 1 | B | 303 | LYS | CA-CB | -7.57 | 1.37 | 1.53 |
| 1 | C | 377 | VAL | C-O | -7.57 | 1.08 | 1.23 |
| 1 | B | 212 | ASP | CG-OD2 | -7.41 | 1.08 | 1.25 |
| 1 | B | 212 | ASP | C-O | -7.37 | 1.09 | 1.23 |
| 1 | C | 214 | THR | CB-CG2 | -7.30 | 1.28 | 1.52 |
| 1 | B | 303 | LYS | CG-CD | -7.19 | 1.28 | 1.52 |
| 1 | A | 119 | SER | CA-CB | -7.15 | 1.42 | 1.52 |
| 1 | C | 4 | PHE | CG-CD1 | -7.08 | 1.28 | 1.38 |
| 1 | C | 211 | PRO | CA-C | -7.05 | 1.38 | 1.52 |
| 1 | C | 378 | ARG | CB-CG | -6.88 | 1.33 | 1.52 |
| 1 | A | 119 | SER | CB-OG | -6.66 | 1.33 | 1.42 |
| 1 | C | 208 | LEU | N-CA | -6.64 | 1.33 | 1.46 |
| 1 | B | 303 | LYS | C-O | -6.45 | 1.11 | 1.23 |
| 1 | C | 376 | GLU | CG-CD | -6.19 | 1.42 | 1.51 |
| 1 | C | 213 | ARG | C-O | -5.91 | 1.12 | 1.23 |
| 1 | B | 212 | ASP | CG-OD1 | -5.87 | 1.11 | 1.25 |
| 1 | C | 211 | PRO | N-CA | -5.87 | 1.37 | 1.47 |
| 1 | C | 377 | VAL | CA-CB | -5.78 | 1.42 | 1.54 |
| 1 | C | 211 | PRO | C-O | -5.74 | 1.11 | 1.23 |
| 1 | C | 2 | ASN | CG-OD1 | -5.74 | 1.11 | 1.24 |
| 1 | C | 214 | THR | CA-CB | -5.70 | 1.38 | 1.53 |
| 1 | B | 214 | THR | N-CA | -5.55 | 1.35 | 1.46 |
| 1 | C | 4 | PHE | CB-CG | -5.40 | 1.42 | 1.51 |
| 1 | B | 303 | LYS | N-CA | -5.08 | 1.36 | 1.46 |
| 1 | C | 214 | THR | C-O | -5.05 | 1.13 | 1.23 |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 378 | ARG | NE-CZ-NH1 | 12.08 | 126.34 | 120.30 |
| 1 | B | 212 | ASP | CB-CG-OD1 | 8.48 | 125.93 | 118.30 |
| 1 | A | 378 | ARG | N-CA-CB | -8.10 | 96.03 | 110.60 |
| 1 | C | 3 | ASP | CB-CG-OD1 | 7.63 | 125.17 | 118.30 |
| 1 | C | 378 | ARG | NE-CZ-NH2 | -7.61 | 116.49 | 120.30 |
| 1 | C | 2 | ASN | N-CA-C | 7.57 | 131.43 | 111.00 |
| 1 | C | 376 | GLU | OE1-CD-OE2 | -6.19 | 115.88 | 123.30 |
| 1 | C | 378 | ARG | CG-CD-NE | 6.04 | 124.48 | 111.80 |
| 1 | A | 377 | VAL | N-CA-C | -6.01 | 94.77 | 111.00 |
| 1 | A | 378 | ARG | N-CA-C | -5.80 | 95.34 | 111.00 |
| 1 | B | 231 | PRO | N-CA-CB | 5.62 | 110.04 | 103.30 |
| 1 | A | 231 | PRO | N-CA-CB | 5.49 | 109.89 | 103.30 |
| 1 | A | 377 | VAL | CB-CA-C | -5.38 | 101.17 | 111.40 |
| 1 | C | 214 | THR | CA-CB-CG2 | -5.18 | 105.14 | 112.40 |
| 1 | C | 208 | LEU | CA-CB-CG | -5.07 | 103.65 | 115.30 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 362 | TYR | Sidechain |
| 1 | B | 362 | TYR | Sidechain |
| 1 | C | 213 | ARG | Peptide |
| 1 | C | 362 | TYR | Sidechain |

## 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 | 2929 | 0 | 2900 | 66 | 0 |
| 1 | B | 2914 | 0 | 2865 | 72 | 0 |
| 1 | C | 2900 | 0 | 2861 | 97 | 1 |
| 2 | A | 80 | 0 | 0 | 4 | 1 |
| 2 | B | 80 | 0 | 0 | 1 | 0 |
| 2 | C | 74 | 0 | 0 | 2 | 0 |
| All | All | 8977 | 0 | 8626 | 229 | 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 13.

All (229) 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:B:296:HIS:ND1 | 1:B:303:LYS:HE2 | 1.20 | 1.46 |
| 1:B:296:HIS:CE1 | 1:B:303:LYS:HE2 | 1.72 | 1.23 |
| 1:C:91:ALA:HA | 1:C:117:LEU:CD2 | 1.71 | 1.19 |
| 1:C:208:LEU:CD2 | 1:C:239:TYR:OH | 1.94 | 1.15 |
| 1:B:296:HIS:ND1 | 1:B:303:LYS:CE | 2.13 | 1.11 |
| 1:B:296:HIS:CE1 | 1:B:303:LYS:CE | 2.39 | 1.06 |
| 1:C:91:ALA:HA | 1:C:117:LEU:HD21 | 1.38 | 1.04 |
| 1:B:296:HIS:CE1 | 1:B:303:LYS:NZ | 2.38 | 0.92 |
| 1:C:199:VAL:H | 1:C:216:ASN:HD21 | 1.15 | 0.90 |
| 1:C:208:LEU:HD21 | 1:C:239:TYR:OH | 1.70 | 0.90 |
| 1:C:91:ALA:HA | 1:C:117:LEU:HD23 | 1.52 | 0.89 |
| 1:A:25:ARG:HD3 | 1:A:25:ARG:O | 1.74 | 0.88 |
| 1:A:353:ASN:HD22 | 1:A:354:TYR:H | 1.16 | 0.88 |
| 1:C:128:LEU:HD21 | 1:C:148:ILE:HG21 | 1.54 | 0.87 |
| 1:A:216:ASN:H | 1:A:216:ASN:HD22 | 1.18 | 0.87 |
| 1:A:199:VAL:H | 1:A:216:ASN:HD21 | 1.20 | 0.86 |
| 1:A:132:THR:HG23 | 1:A:184:ARG:CG | 2.07 | 0.84 |
| 1:A:132:THR:O | 1:A:132:THR:HG22 | 1.76 | 0.83 |
| 1:A:17:ILE:O | 1:A:21:VAL:HG12 | 1.79 | 0.83 |
| 1:B:25:ARG:O | 1:B:25:ARG:HD3 | 1.78 | 0.82 |
| 1:A:130:MSE:HE3 | 1:A:188:MSE:HB3 | 1.64 | 0.80 |
| 1:A:353:ASN:HD22 | 1:A:354:TYR:N | 1.82 | 0.78 |
| 1:C:208:LEU:HD22 | 1:C:239:TYR:OH | 1.82 | 0.77 |
| 1:B:296:HIS:HE1 | 1:B:303:LYS:NZ | 1.82 | 0.75 |
| 1:C:322:PRO:O | 1:C:323:LEU:HD12 | 1.85 | 0.75 |
| 1:C:128:LEU:CD2 | 1:C:148:ILE:HG21 | 2.16 | 0.75 |
| 1:A:114:ALA:HA | 1:A:117:LEU:HD22 | 1.68 | 0.75 |
| 1:C:353:ASN:HD22 | 1:C:354:TYR:H | 1.35 | 0.74 |
| 1:C:91:ALA:CA | 1:C:117:LEU:CD2 | 2.61 | 0.74 |
| 1:C:163:LEU:HG | 1:C:196:PRO:HG3 | 1.70 | 0.73 |
| 1:B:212:ASP:OD1 | 1:B:214:THR:CG2 | 2.36 | 0.72 |
| 1:A:132:THR:HG21 | 1:A:181:GLN:HA | 1.72 | 0.72 |
| 1:C:216:ASN:H | 1:C:216:ASN:HD22 | 1.36 | 0.71 |
| 1:C:91:ALA:CA | 1:C:117:LEU:HD21 | 2.19 | 0.71 |
| 1:B:266:GLY:HA3 | 1:B:309:ARG:HB2 | 1.72 | 0.71 |
| 1:C:208:LEU:HD21 | 1:C:239:TYR:HH | 1.55 | 0.71 |
| 1:B:332:ILE:HD13 | 1:B:342:ILE:HD13 | 1.72 | 0.71 |
| 1:B:130:MSE:SE | 1:B:163:LEU:HD21 | 2.41 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:132:THR:O | 1:B:184:ARG:HG2 | 1.91 | 0.70 |
| 1:A:216:ASN:ND2 | 1:A:216:ASN:H | 1.88 | 0.70 |
| 1:B:334:ARG:HB2 | 1:B:339:VAL:HG12 | 1.75 | 0.68 |
| 1:A:132:THR:CG2 | 1:A:184:ARG:HB3 | 2.24 | 0.68 |
| 1:A:132:THR:HG23 | 1:A:184:ARG:HB3 | 1.75 | 0.68 |
| 1:A:52:ARG:HD2 | 2:A:400:HOH:O | 1.93 | 0.68 |
| 1:C:195:ARG:NH2 | 1:C:199:VAL:HG21 | 2.08 | 0.68 |
| 1:C:124:ILE:HD13 | 1:C:126:PHE:CZ | 2.29 | 0.68 |
| 1:B:353:ASN:HD22 | 1:B:354:TYR:H | 1.43 | 0.67 |
| 1:C:29:PRO:HG2 | 1:C:32:THR:HG23 | 1.77 | 0.67 |
| 1:A:91:ALA:HA | 1:A:117:LEU:HD11 | 1.76 | 0.67 |
| 1:A:61:ARG:HG3 | 1:A:81:PRO:HB2 | 1.76 | 0.67 |
| 1:C:321:GLY:O | 1:C:323:LEU:HD13 | 1.95 | 0.67 |
| 1:A:107:ARG:NH1 | 1:A:109:ASP:HB2 | 2.10 | 0.66 |
| 1:A:256:LYS:HD3 | 1:A:276:TRP:CZ2 | 2.31 | 0.66 |
| 1:B:296:HIS:HE1 | 1:B:303:LYS:HZ1 | 1.43 | 0.65 |
| 1:C:199:VAL:H | 1:C:216:ASN:ND2 | 1.90 | 0.65 |
| 1:B:297:VAL:HG11 | 1:B:329:VAL:CG1 | 2.27 | 0.65 |
| 1:B:212:ASP:O | 1:B:213:ARG:CB | 2.30 | 0.64 |
| 1:A:353:ASN:ND2 | 1:A:354:TYR:H | 1.94 | 0.64 |
| 1:A:132:THR:HG23 | 1:A:184:ARG:CB | 2.28 | 0.64 |
| 1:A:199:VAL:H | 1:A:216:ASN:ND2 | 1.96 | 0.62 |
| 1:C:147:ARG:O | 1:C:151:LEU:HD23 | 2.00 | 0.62 |
| 1:C:353:ASN:HD22 | 1:C:354:TYR:N | 1.98 | 0.61 |
| 1:C:216:ASN:HD22 | 1:C:216:ASN:N | 1.95 | 0.61 |
| 1:C:334:ARG:HB2 | 1:C:339:VAL:HG12 | 1.82 | 0.61 |
| 1:A:61:ARG:HD2 | 1:A:217:MSE:HE1 | 1.82 | 0.60 |
| 1:C:216:ASN:ND2 | 1:C:216:ASN:H | 2.00 | 0.60 |
| 1:B:353:ASN:HD22 | 1:B:354:TYR:N | 1.99 | 0.60 |
| 1:A:132:THR:O | 1:A:132:THR:CG2 | 2.48 | 0.60 |
| 1:A:257:LEU:HD11 | 1:A:277:ILE:HD12 | 1.84 | 0.59 |
| 1:C:27:LEU:HD21 | 1:C:238:PRO:HG2 | 1.83 | 0.59 |
| 1:B:145:THR:O | 1:B:149:VAL:HG23 | 2.02 | 0.59 |
| 1:B:114:ALA:HA | 1:B:117:LEU:CD2 | 2.33 | 0.58 |
| 1:B:291:ARG:HE | 1:C:291:ARG:NE | 2.01 | 0.58 |
| 1:A:100:ARG:HG3 | 1:A:100:ARG:HH11 | 1.68 | 0.58 |
| 1:B:363:ARG:HG2 | 1:C:66:PHE:HZ | 1.67 | 0.58 |
| 1:C:128:LEU:HD21 | 1:C:148:ILE:CG2 | 2.29 | 0.58 |
| 1:B:184:ARG:O | 1:B:188:MSE:HG3 | 2.03 | 0.58 |
| 1:C:124:ILE:O | 1:C:124:ILE:HG23 | 2.04 | 0.57 |
| 1:C:311:LEU:HD21 | 1:C:316:MSE:HE1 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:296:HIS:CE1 | 1:B:303:LYS:HZ3 | 2.22 | 0.57 |
| 1:C:297:VAL:CG2 | 1:C:331:LEU:HD13 | 2.34 | 0.57 |
| 1:B:61:ARG:HG2 | 1:B:81:PRO:HB2 | 1.86 | 0.57 |
| 1:C:208:LEU:CD2 | 1:C:239:TYR:HH | 2.09 | 0.56 |
| 1:B:251:LEU:HD21 | 1:B:317:ILE:HD11 | 1.87 | 0.56 |
| 1:C:266:GLY:HA3 | 1:C:309:ARG:HB2 | 1.85 | 0.56 |
| 1:C:297:VAL:HG22 | 1:C:298:LEU:H | 1.71 | 0.56 |
| 1:B:291:ARG:NE | 1:C:291:ARG:NE | 2.54 | 0.56 |
| 1:C:227:LEU:HD21 | 1:C:342:ILE:HD12 | 1.88 | 0.56 |
| 1:C:322:PRO:C | 1:C:323:LEU:HD12 | 2.26 | 0.56 |
| 1:B:356:VAL:HB | 1:B:357:PRO:HD3 | 1.87 | 0.56 |
| 1:C:297:VAL:HG23 | 1:C:331:LEU:HD13 | 1.87 | 0.55 |
| 1:A:216:ASN:HD22 | 1:A:216:ASN:N | 1.83 | 0.55 |
| 1:A:130:MSE:CE | 1:A:188:MSE:HB3 | 2.36 | 0.55 |
| 1:C:163:LEU:O | 1:C:163:LEU:HD12 | 2.07 | 0.55 |
| 1:A:132:THR:HG23 | 1:A:184:ARG:HG3 | 1.87 | 0.55 |
| 1:C:128:LEU:HG | 1:C:160:LEU:HD11 | 1.90 | 0.54 |
| 1:A:353:ASN:ND2 | 1:A:354:TYR:N | 2.55 | 0.54 |
| 1:B:212:ASP:OD1 | 1:B:214:THR:HG23 | 2.07 | 0.54 |
| 1:A:52:ARG:O | 1:A:56:GLU:HG3 | 2.06 | 0.54 |
| 1:B:297:VAL:HG12 | 1:B:298:LEU:N | 2.22 | 0.54 |
| 1:C:3:ASP:N | 1:C:3:ASP:OD2 | 2.34 | 0.54 |
| 1:C:238:PRO:HG2 | 1:C:239:TYR:HD1 | 1.73 | 0.53 |
| 1:B:142:GLU:O | 1:B:146:LYS:HG2 | 2.08 | 0.53 |
| 1:A:267:ALA:HB2 | 1:A:309:ARG:HD2 | 1.91 | 0.53 |
| 1:C:141:ASP:OD2 | 1:C:143:GLU:HB2 | 2.09 | 0.53 |
| 1:B:114:ALA:HA | 1:B:117:LEU:HD22 | 1.90 | 0.53 |
| 1:C:292:LEU:HG | 1:C:349:LEU:HD21 | 1.90 | 0.52 |
| 1:A:293:GLN:O | 1:A:306:ILE:O | 2.27 | 0.52 |
| 1:A:184:ARG:O | 1:A:188:MSE:HG3 | 2.09 | 0.52 |
| 1:B:263:VAL:HG23 | 1:B:269:TYR:HB3 | 1.92 | 0.52 |
| 1:A:124:ILE:HD12 | 2:A:409:HOH:O | 2.09 | 0.52 |
| 1:A:315:CYS:HB2 | 2:A:401:HOH:O | 2.09 | 0.51 |
| 1:C:309:ARG:HG2 | 1:C:309:ARG:HH11 | 1.76 | 0.51 |
| 1:A:160:LEU:HD22 | 1:A:196:PRO:HB3 | 1.91 | 0.51 |
| 1:A:128:LEU:HD11 | 1:A:148:ILE:HG21 | 1.92 | 0.51 |
| 1:B:181:GLN:O | 1:B:182:TYR:HB2 | 2.10 | 0.51 |
| 1:C:316:MSE:SE | 1:C:316:MSE:N | 2.94 | 0.50 |
| 1:B:306:ILE:HG21 | 1:B:310:ILE:HD11 | 1.93 | 0.50 |
| 1:C:33:HIS:O | 1:C:217:MSE:HA | 2.12 | 0.50 |
| 1:C:195:ARG:HH22 | 1:C:199:VAL:HG21 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:75:GLU:OE1 | 1:C:383:ARG:HA | 2.11 | 0.50 |
| 1:C:297:VAL:HG22 | 1:C:298:LEU:N | 2.26 | 0.50 |
| 1:B:28:LEU:HD11 | 1:B:218:VAL:HG21 | 1.94 | 0.50 |
| 1:C:237:LEU:N | 1:C:238:PRO:HD2 | 2.27 | 0.49 |
| 1:A:29:PRO:HG2 | 1:A:31:ASP:OD1 | 2.13 | 0.49 |
| 1:B:32:THR:HG21 | 1:B:218:VAL:HG13 | 1.94 | 0.49 |
| 1:C:25:ARG:HG3 | 1:C:58:GLY:HA3 | 1.94 | 0.49 |
| 1:B:128:LEU:HB2 | 1:B:163:LEU:HD23 | 1.95 | 0.48 |
| 1:B:113:GLU:O | 1:B:117:LEU:HD22 | 2.13 | 0.48 |
| 1:A:27:LEU:C | 1:A:27:LEU:HD23 | 2.33 | 0.48 |
| 1:C:130:MSE:HE3 | 1:C:188:MSE:HE2 | 1.94 | 0.48 |
| 1:B:266:GLY:C | 1:B:309:ARG:HD2 | 2.34 | 0.48 |
| 1:C:103:LEU:HD12 | 1:C:124:ILE:HD11 | 1.94 | 0.48 |
| 1:B:18:TYR:CD1 | 1:B:57:ALA:HB2 | 2.49 | 0.48 |
| 1:B:238:PRO:HG2 | 1:B:239:TYR:CD1 | 2.49 | 0.47 |
| 1:C:199:VAL:HG23 | 1:C:199:VAL:O | 2.15 | 0.47 |
| 1:A:288:TRP:CE2 | 1:A:331:LEU:HD23 | 2.49 | 0.47 |
| 1:C:11:GLU:HB2 | 1:C:246:SER:OG | 2.15 | 0.47 |
| 1:C:334:ARG:CB | 1:C:339:VAL:HG12 | 2.45 | 0.47 |
| 1:C:128:LEU:O | 1:C:163:LEU:HA | 2.14 | 0.47 |
| 1:C:257:LEU:HD11 | 1:C:277:ILE:HD12 | 1.95 | 0.47 |
| 1:A:132:THR:HG23 | 1:A:184:ARG:HG2 | 1.94 | 0.47 |
| 1:B:128:LEU:HD21 | 1:B:148:ILE:HG21 | 1.98 | 0.46 |
| 1:A:155:HIS:HB3 | 1:A:158:PHE:HB2 | 1.96 | 0.46 |
| 1:B:297:VAL:CG1 | 1:B:329:VAL:CG1 | 2.94 | 0.46 |
| 1:C:334:ARG:HH11 | 1:C:334:ARG:HB2 | 1.80 | 0.46 |
| 1:B:316:MSE:N | 1:B:316:MSE:SE | 2.98 | 0.46 |
| 1:A:303:LYS:HE2 | 1:A:338:LYS:HG3 | 1.97 | 0.46 |
| 1:A:61:ARG:CD | 1:A:217:MSE:HE1 | 2.46 | 0.46 |
| 1:B:291:ARG:C | 1:B:293:GLN:H | 2.19 | 0.46 |
| 1:C:11:GLU:HG2 | 1:C:369:PHE:HE1 | 1.80 | 0.46 |
| 1:B:140:LYS:HG3 | 1:B:141:ASP:OD1 | 2.16 | 0.46 |
| 1:B:128:LEU:HB2 | 1:B:163:LEU:CD2 | 2.47 | 0.46 |
| 1:A:107:ARG:HH12 | 1:A:109:ASP:HB2 | 1.80 | 0.46 |
| 1:C:152:ILE:HG23 | 1:C:158:PHE:HB3 | 1.98 | 0.45 |
| 1:A:195:ARG:NH2 | 1:A:214:THR:O | 2.49 | 0.45 |
| 1:C:124:ILE:HG23 | 1:C:126:PHE:CE2 | 2.52 | 0.45 |
| 1:A:1:MSE:HG2 | 1:A:383:ARG:HB2 | 1.98 | 0.45 |
| 1:A:91:ALA:CA | 1:A:117:LEU:HD11 | 2.45 | 0.45 |
| 1:A:117:LEU:C | 1:A:117:LEU:HD23 | 2.37 | 0.45 |
| 1:B:15:ASP:OD2 | 1:B:370:ARG:HD2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:202:ALA:HB2 | 1:B:219:GLN:OE1 | 2.17 | 0.45 |
| 1:C:353:ASN:HD22 | 1:C:353:ASN:N | 2.15 | 0.45 |
| 1:B:266:GLY:CA | 1:B:309:ARG:HB2 | 2.44 | 0.45 |
| 1:A:164:TRP:HA | 1:A:200:HIS:O | 2.17 | 0.44 |
| 1:B:269:TYR:CE2 | 1:B:307:VAL:HB | 2.52 | 0.44 |
| 1:B:182:TYR:O | 1:B:186:LEU:HG | 2.17 | 0.44 |
| 1:B:137:LEU:HB2 | 1:C:253:HIS:CD2 | 2.52 | 0.44 |
| 1:A:9:TRP:CD1 | 1:A:367:ILE:HD12 | 2.52 | 0.44 |
| 1:C:7:ASP:O | 1:C:249:SER:HA | 2.17 | 0.44 |
| 1:B:26:ARG:HH11 | 1:B:26:ARG:HB3 | 1.83 | 0.44 |
| 1:A:162:GLY:HA2 | 1:A:198:LEU:O | 2.18 | 0.44 |
| 1:C:16:ALA:HB3 | 1:C:244:ALA:HB2 | 2.00 | 0.44 |
| 1:C:362:TYR:CD1 | 1:C:362:TYR:N | 2.84 | 0.44 |
| 1:C:140:LYS:H | 1:C:140:LYS:HD3 | 1.82 | 0.44 |
| 1:C:238:PRO:HG2 | 1:C:239:TYR:CD1 | 2.53 | 0.44 |
| 1:B:276:TRP:CE3 | 1:B:322:PRO:HB3 | 2.53 | 0.44 |
| 1:A:188:MSE:HA | 1:A:191:TRP:CD2 | 2.53 | 0.44 |
| 1:C:155:HIS:HB3 | 1:C:158:PHE:HB2 | 2.00 | 0.44 |
| 1:B:296:HIS:H | 1:B:296:HIS:CD2 | 2.34 | 0.43 |
| 1:C:32:THR:HA | 1:C:216:ASN:O | 2.18 | 0.43 |
| 1:C:124:ILE:CG2 | 1:C:126:PHE:CE2 | 3.02 | 0.43 |
| 1:C:61:ARG:HH11 | 1:C:61:ARG:HG2 | 1.83 | 0.43 |
| 1:B:104:THR:HA | 1:B:127:HIS:O | 2.18 | 0.43 |
| 1:B:263:VAL:HG23 | 1:B:263:VAL:O | 2.19 | 0.43 |
| 1:C:13:ASP:OD1 | 1:C:15:ASP:HB2 | 2.18 | 0.43 |
| 1:C:334:ARG:NH1 | 1:C:334:ARG:HB2 | 2.33 | 0.43 |
| 1:A:306:ILE:HA | 1:A:317:ILE:HG22 | 2.00 | 0.43 |
| 1:B:276:TRP:CZ3 | 1:B:322:PRO:HB3 | 2.53 | 0.43 |
| 1:B:26:ARG:HB3 | 1:B:26:ARG:NH1 | 2.33 | 0.43 |
| 1:C:61:ARG:HD3 | 1:C:81:PRO:HB2 | 2.00 | 0.43 |
| 1:C:195:ARG:NH2 | 1:C:214:THR:O | 2.51 | 0.43 |
| 1:A:276:TRP:CZ2 | 1:A:322:PRO:HB3 | 2.54 | 0.43 |
| 1:C:29:PRO:HG2 | 1:C:32:THR:CG2 | 2.47 | 0.43 |
| 1:C:353:ASN:N | 1:C:353:ASN:ND2 | 2.65 | 0.43 |
| 1:C:237:LEU:N | 1:C:238:PRO:CD | 2.82 | 0.43 |
| 1:B:280:ILE:HD11 | 1:B:315:CYS:SG | 2.59 | 0.42 |
| 1:B:292:LEU:HG | 1:B:349:LEU:HD21 | 1.99 | 0.42 |
| 1:C:27:LEU:HD12 | 1:C:27:LEU:N | 2.34 | 0.42 |
| 1:A:257:LEU:CD1 | 1:A:277:ILE:HD12 | 2.50 | 0.42 |
| 1:C:25:ARG:O | 1:C:25:ARG:HD3 | 2.19 | 0.42 |
| 1:C:108:SER:HB3 | 1:C:144:GLU:HG3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:18:TYR:CD1 | 1:C:57:ALA:HB2 | 2.55 | 0.42 |
| 1:B:134:MSE:HE1 | 1:B:177:TYR:CZ | 2.55 | 0.42 |
| 1:B:4:PHE:HB2 | 2:C:399:HOH:O | 2.19 | 0.42 |
| 1:C:353:ASN:ND2 | 1:C:354:TYR:H | 2.11 | 0.42 |
| 1:A:273:THR:OG1 | 1:A:274:GLU:N | 2.52 | 0.42 |
| 1:A:18:TYR:CD1 | 1:A:57:ALA:HB2 | 2.55 | 0.42 |
| 1:C:359:THR:HB | 2:C:413:HOH:O | 2.20 | 0.42 |
| 1:A:25:ARG:HD3 | 1:A:25:ARG:C | 2.34 | 0.42 |
| 1:C:311:LEU:CD2 | 1:C:316:MSE:HE1 | 2.50 | 0.41 |
| 1:A:11:GLU:HB2 | 1:A:246:SER:OG | 2.20 | 0.41 |
| 1:C:124:ILE:CG2 | 1:C:124:ILE:O | 2.67 | 0.41 |
| 1:B:11:GLU:HB2 | 1:B:246:SER:OG | 2.20 | 0.41 |
| 1:B:29:PRO:C | 1:B:31:ASP:H | 2.24 | 0.41 |
| 1:C:319:LEU:HD13 | 1:C:323:LEU:HB2 | 2.02 | 0.41 |
| 1:A:16:ALA:HB1 | 1:A:242:LYS:HG3 | 2.02 | 0.41 |
| 1:C:285:LYS:HE2 | 1:C:313:ASP:OD1 | 2.20 | 0.41 |
| 1:A:145:THR:O | 1:A:149:VAL:HG23 | 2.20 | 0.41 |
| 1:B:363:ARG:HG2 | 1:C:66:PHE:CZ | 2.52 | 0.41 |
| 1:C:189:LEU:HD23 | 1:C:189:LEU:O | 2.21 | 0.41 |
| 1:B:258:GLN:O | 1:B:261:GLU:HB2 | 2.21 | 0.41 |
| 1:B:332:ILE:HD13 | 1:B:342:ILE:CD1 | 2.46 | 0.40 |
| 1:C:297:VAL:HG21 | 1:C:331:LEU:HD13 | 2.03 | 0.40 |
| 1:A:373:ARG:HB2 | 1:A:373:ARG:NH1 | 2.35 | 0.40 |
| 1:A:66:PHE:HB2 | 2:A:398:HOH:O | 2.20 | 0.40 |
| 1:B:123:PRO:HB3 | 2:B:469:HOH:O | 2.20 | 0.40 |
| 1:A:112:GLU:HG2 | 1:A:151:LEU:HD11 | 2.03 | 0.40 |
| 1:C:353:ASN:ND2 | 1:C:354:TYR:N | 2.68 | 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:117:LEU:CD1 | 2:A:443:HOH:O[8_654] | 2.18 | 0.02 |

## 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 | 366/390 (94%) | 355 (97%) | 9 (2%) | 2 (0%) | 34 | 41 |
| 1 | B | 365/390 (94%) | 347 (95%) | 16 (4%) | 2 (0%) | 34 | 41 |
| 1 | C | 364/390 (93%) | 351 (96%) | 9 (2%) | 4 (1%) | 17 | 18 |
| All | All | 1095/1170 (94%) | 1053 (96%) | 34 (3%) | 8 (1%) | 26 | 31 |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 265 | PHE |
| 1 | C | 212 | ASP |
| 1 | C | 214 | THR |
| 1 | B | 182 | TYR |
| 1 | C | 265 | PHE |
| 1 | C | 30 | ASP |
| 1 | A | 221 | GLY |
| 1 | A | 193 | PRO |

### 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 | 304/314 (97%) | 289 (95%) | 15 (5%) | 31 | 41 |
| 1 | B | 300/314 (96%) | 288 (96%) | 12 (4%) | 38 | 52 |
| 1 | C | 299/314 (95%) | 291 (97%) | 8 (3%) | 52 | 70 |
| All | All | 903/942 (96%) | 868 (96%) | 35 (4%) | 39 | 53 |

All (35) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 21 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 30 | ASP |
| 1 | A | 52 | ARG |
| 1 | A | 61 | ARG |
| 1 | A | 109 | ASP |
| 1 | A | 117 | LEU |
| 1 | A | 119 | SER |
| 1 | A | 189 | LEU |
| 1 | A | 210 | PHE |
| 1 | A | 216 | ASN |
| 1 | A | 220 | PHE |
| 1 | A | 270 | THR |
| 1 | A | 338 | LYS |
| 1 | A | 353 | ASN |
| 1 | A | 361 | SER |
| 1 | B | 2 | ASN |
| 1 | B | 31 | ASP |
| 1 | B | 109 | ASP |
| 1 | B | 111 | LEU |
| 1 | B | 117 | LEU |
| 1 | B | 121 | PRO |
| 1 | B | 203 | ASN |
| 1 | B | 214 | THR |
| 1 | B | 303 | LYS |
| 1 | B | 335 | GLN |
| 1 | B | 353 | ASN |
| 1 | B | 372 | LYS |
| 1 | C | 25 | ARG |
| 1 | C | 140 | LYS |
| 1 | C | 143 | GLU |
| 1 | C | 190 | GLU |
| 1 | C | 208 | LEU |
| 1 | C | 216 | ASN |
| 1 | C | 353 | ASN |
| 1 | C | 372 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 5 | HIS |
| 1 | A | 99 | GLN |
| 1 | A | 181 | GLN |
| 1 | A | 203 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 216 | ASN |
| 1 | A | 258 | GLN |
| 1 | A | 293 | GLN |
| 1 | A | 348 | HIS |
| 1 | A | 353 | ASN |
| 1 | B | 5 | HIS |
| 1 | B | 157 | HIS |
| 1 | B | 203 | ASN |
| 1 | B | 293 | GLN |
| 1 | B | 296 | HIS |
| 1 | B | 348 | HIS |
| 1 | B | 353 | ASN |
| 1 | C | 23 | ASN |
| 1 | C | 33 | HIS |
| 1 | C | 125 | HIS |
| 1 | C | 216 | ASN |
| 1 | C | 272 | GLN |
| 1 | C | 353 | ASN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no carbohydrates in this entry.

### 5.6 Ligand geometry

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 | 362/390 (92%) | 0.12 | 10 (2%) | 56 | 66 | 20, 37, 64, 78 | 0 |
| 1 | B | 362/390 (92%) | 0.28 | 17 (4%) | 35 | 44 | 23, 39, 66, 82 | 0 |
| 1 | C | 361/390 (92%) | 0.33 | 28 (7%) | 16 | 22 | 25, 44, 74, 82 | 0 |
| All | All | 1085/1170 (92%) | 0.24 | 55 (5%) | 32 | 41 | 20, 40, 69, 82 | 0 |

All (55) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 207 | SER | 9.4 |
| 1 | B | 266 | GLY | 7.7 |
| 1 | C | 210 | PHE | 6.1 |
| 1 | B | 239 | TYR | 5.8 |
| 1 | B | 238 | PRO | 5.0 |
| 1 | C | 260 | GLY | 4.8 |
| 1 | A | 209 | ARG | 4.8 |
| 1 | C | 209 | ARG | 4.6 |
| 1 | C | 272 | GLN | 4.5 |
| 1 | B | 267 | ALA | 4.5 |
| 1 | B | 208 | LEU | 4.3 |
| 1 | C | 208 | LEU | 4.2 |
| 1 | A | 210 | PHE | 4.0 |
| 1 | C | 117 | LEU | 3.9 |
| 1 | A | 169 | THR | 3.9 |
| 1 | B | 205 | ALA | 3.9 |
| 1 | C | 27 | LEU | 3.8 |
| 1 | B | 265 | PHE | 3.4 |
| 1 | C | 207 | SER | 3.3 |
| 1 | A | 265 | PHE | 3.2 |
| 1 | C | 238 | PRO | 3.2 |
| 1 | B | 384 | GLY | 3.2 |
| 1 | B | 229 | PRO | 3.2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 26 | ARG | 3.2 |
| 1 | B | 337 | ASP | 3.1 |
| 1 | B | 177 | TYR | 3.0 |
| 1 | A | 384 | GLY | 2.9 |
| 1 | C | 384 | GLY | 2.9 |
| 1 | C | 154 | ARG | 2.9 |
| 1 | C | 178 | PHE | 2.9 |
| 1 | A | 239 | TYR | 2.8 |
| 1 | B | 27 | LEU | 2.8 |
| 1 | A | 232 | GLY | 2.8 |
| 1 | C | 206 | ALA | 2.8 |
| 1 | C | 240 | PRO | 2.7 |
| 1 | A | 231 | PRO | 2.6 |
| 1 | C | 212 | ASP | 2.6 |
| 1 | C | 229 | PRO | 2.5 |
| 1 | C | 267 | ALA | 2.5 |
| 1 | B | 231 | PRO | 2.4 |
| 1 | C | 228 | ALA | 2.4 |
| 1 | C | 239 | TYR | 2.4 |
| 1 | C | 180 | TYR | 2.3 |
| 1 | C | 26 | ARG | 2.3 |
| 1 | B | 166 | TRP | 2.3 |
| 1 | C | 362 | TYR | 2.2 |
| 1 | C | 211 | PRO | 2.2 |
| 1 | C | 258 | GLN | 2.2 |
| 1 | C | 265 | PHE | 2.2 |
| 1 | C | 337 | ASP | 2.1 |
| 1 | B | 154 | ARG | 2.1 |
| 1 | A | 256 | LYS | 2.1 |
| 1 | C | 143 | GLU | 2.1 |
| 1 | C | 296 | HIS | 2.1 |
| 1 | B | 362 | TYR | 2.1 |

## 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.