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

Feb 22, 2017 – 04:55 AM EST

| | | |
|---|---|---|
| PDB ID | : | 5MNI |
| Title | : | Escherichia coli AGPase mutant R130A apo form |
| Authors | : | Cifuente, J.O.; Comino, N.; Marina, A.; Orrantia, A.; Eguskiza, A.; Guerin, M.E. |
| Deposited on | : | 2016-12-13 |
| Resolution | : | 3.09 Å(reported) |

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

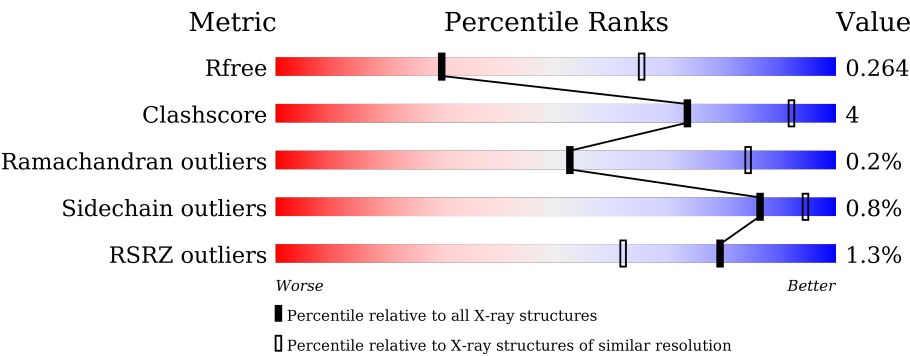| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | unknown |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20028442 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20028442 |

# 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 3.09 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 | Percentile Ranks | Value |
|--------|------------------|-------|
| Rfree | | 0.264 |
| Clashscore | | 4 |
| Ramachandran outliers | | 0.2% |
| Sidechain outliers | | 0.8% |
| RSRZ outliers | | 1.3% |

*Worse*             *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|--------|--------------------------|-----------------------------------------------------|
| $R_{free}$ | 91344 | 1114 (3.14-3.06) |
| Clashscore | 102246 | 1222 (3.14-3.06) |
| Ramachandran outliers | 100387 | 1174 (3.14-3.06) |
| Sidechain outliers | 100360 | 1174 (3.14-3.06) |
| RSRZ outliers | 91569 | 1119 (3.14-3.06) |

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 | 431 | %  83%  8% · 8% |
| 1 | B | 431 | 84%  9% · 6% |
| 1 | C | 431 | %  81%  10%  9% |
| 1 | D | 431 | 2%  86%  8%  5% |
| 1 | E | 431 | 87%  6%  7% |
| 1 | F | 431 | 2%  83%  7%  10% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | G | 431 | %<br>84% 7% 9% |
| 1 | H | 431 | 4%<br>80% 10% 9% |

# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 45964 atoms, of which 22263 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 Glucose-1-phosphate adenylyltransferase.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1 | E | 401 | Total | C | H | N | O | S | 0 | 3 | 0 |
| | | | 5912 | 1922 | 2886 | 521 | 562 | 21 | | | |
| 1 | G | 393 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 5661 | 1862 | 2738 | 499 | 543 | 19 | | | |
| 1 | H | 393 | Total | C | H | N | O | S | 0 | 2 | 0 |
| | | | 5304 | 1774 | 2512 | 485 | 516 | 17 | | | |
| 1 | F | 390 | Total | C | H | N | O | S | 0 | 2 | 0 |
| | | | 5786 | 1881 | 2825 | 505 | 555 | 20 | | | |
| 1 | A | 396 | Total | C | H | N | O | S | 0 | 2 | 0 |
| | | | 5737 | 1880 | 2778 | 510 | 551 | 18 | | | |
| 1 | B | 406 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 5945 | 1944 | 2887 | 518 | 576 | 20 | | | |
| 1 | D | 409 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 5795 | 1909 | 2788 | 521 | 557 | 20 | | | |
| 1 | C | 394 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 5824 | 1891 | 2849 | 514 | 550 | 20 | | | |

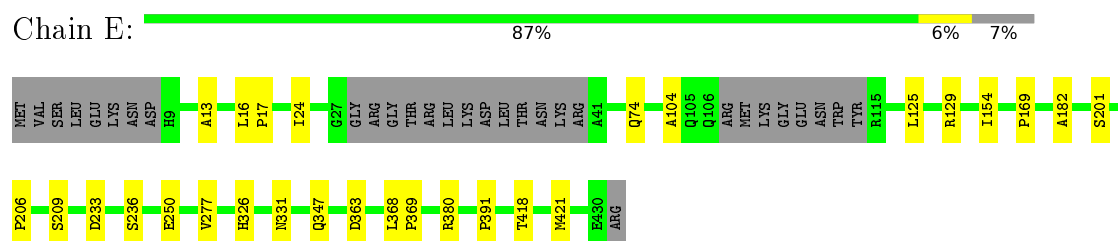There are 8 discrepancies between the modelled and reference sequences:

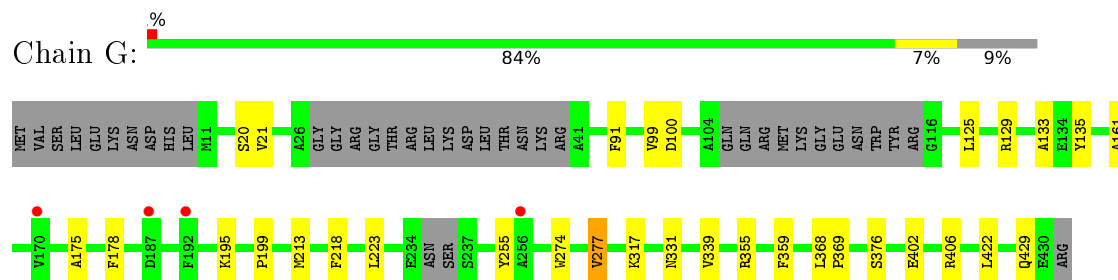| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| E | 130 | ALA | ARG | engineered mutation | UNP P0A6V1 |
| G | 130 | ALA | ARG | engineered mutation | UNP P0A6V1 |
| H | 130 | ALA | ARG | engineered mutation | UNP P0A6V1 |
| F | 130 | ALA | ARG | engineered mutation | UNP P0A6V1 |
| A | 130 | ALA | ARG | engineered mutation | UNP P0A6V1 |
| B | 130 | ALA | ARG | engineered mutation | UNP P0A6V1 |
| D | 130 | ALA | ARG | engineered mutation | UNP P0A6V1 |
| C | 130 | ALA | ARG | engineered mutation | UNP P0A6V1 |

# 3 Residue-property plots ⓘ

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

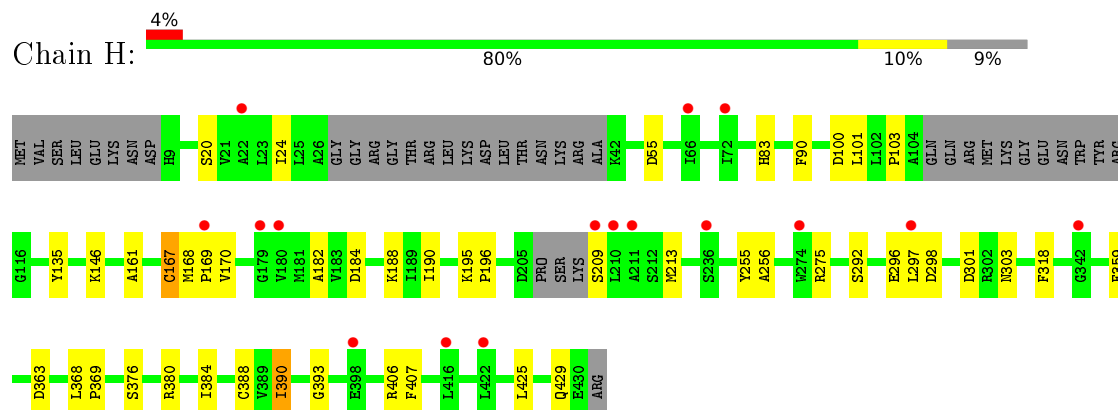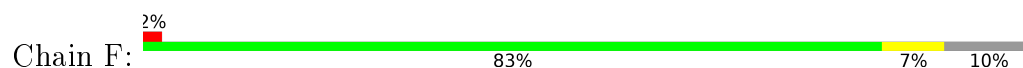- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain E:

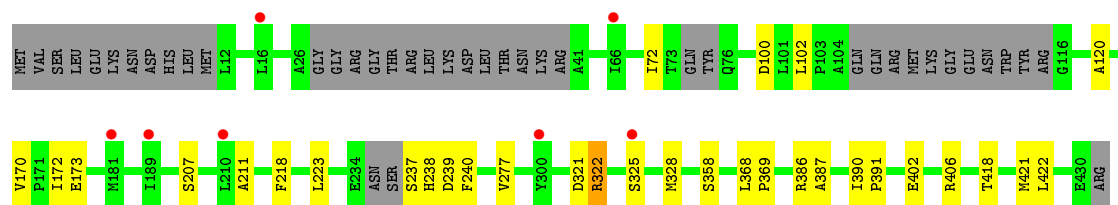- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain G:

- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain H:

- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain F:

MET VAL SER LEU GLU LYS ASN ASP HIS LEU MET L12 L16 A26 GLY ARG GLY THR ARG LEU LYS ASP LEU THR ASN LYS ARG A41 I66 I72 T73 GLN TYR Q76 D100 L101 L102 P103 A104 GLN GLN ARG MET LYS GLY GLU ASN TRP TYR ARG G116 A120

V170 P171 I172 E173 M181 I189 S207 L210 A211 F218 L223 E234 ASN SER S237 H238 D239 F240 V277 Y300 D321 R322 S325 M328 S358 L368 P369 R386 A387 I390 P391 E402 R406 T418 M421 L422 E430 ARG

- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain A: 83% 8% 8%

MET VAL SER LEU GLU LYS ASN ASP HIS L10 A13 R14 I24 L25 A26 GLY ARG GLY THR ARG LEU LYS ASP LEU THR ASN LYS ARG A41 H46 K50 I72 T73 Q74 TYR Q76 D100 L101 L102 P103 A104 GLN GLN ARG MET LYS GLY GLU ASN TRP TYR ARG G116

R129 A130 Y131 I138 L139 H143 I154 P169 S209 E228 R232 I245 P246 W274 R275 D276 V277 Y283 M328 N331 V344 Q347 F351 F359 S364 L368 P369 S376 V389 G397 D403 F407 M421 L422 R423

Q429 E430 R431

- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain B: 84% 9% 6%

MET VAL SER LEU GLU LYS ASN ASP HIS L10 L16 P17 G27 GLY ARG GLY THR ARG LEU LYS ASP LEU THR N38 K42 P43 Q74 Q85 E94 D100 A104 Q105 Q106 ARG MET LYS GLY GLU M112 W113 Y114 T117 L125 R129 Q147 M152

K159 G160 A161 R162 A197 Y222 L223 D230 H238 D239 F240 G241 K242 D243 L244 I245 P246 Y255 A256 V277 L313 D321 I340 S358 L368 P369 R378 V395 I396 G397 E398 R405 R406 E430 ARG

- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain D: 86% 8% 5%

MET VAL SER LEU GLU LYS ASN ASP HIS L10 I24 D35 H46 V99 A104 GLN ARG MET LYS GLY GLU ASN TRP TYR ARG GLY T117 A120 A211 I138 D148 A161 R162 V170 F178 K208 S209 L210 A211 S212 M213 Y216 D221 Y222 L226

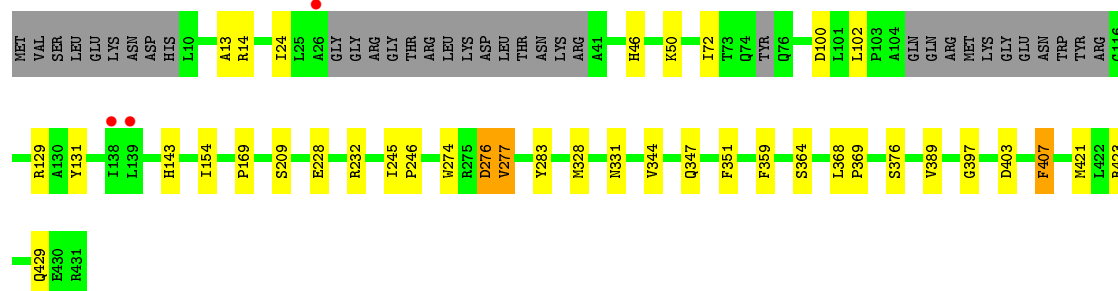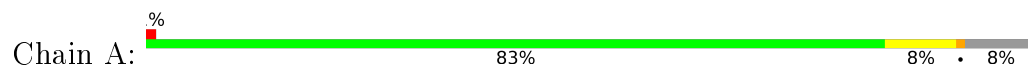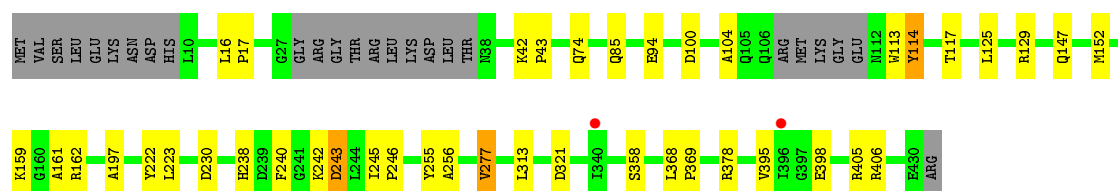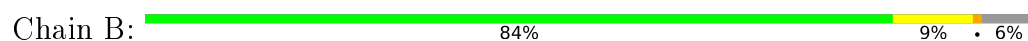D239 F240 L244 I245 I248 Y255 W274 R307 T308 F351 D363 L368 P369 L379 R380 V389 G397 D403 Y408 V417 L422 Q429 E430 ARG

- Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain C: 81% 10% 9%

MET VAL SER LEU GLU LYS ASN ASP HIS L10 M11 L12 Q15 G27 GLY ARG GLY THR ARG LEU LYS ASP LEU THR ASN LYS ARG A41 K42 P43 H46 F91 V99 D100 A104 GLN GLN ARG MET LYS GLY GLU ASN TRP TYR ARG G116 T117 L125 R129 K159

G160 A161 R162 C163 P169 V170 V180 M181 P200 K208 S209 E228 D233 GLU ASN SER S237 H238 D239 F240 G241 Y255 A256 V277 R307 T308 Y309 N310 E311 Q347 F351 N357 S358 F359 S364 L368 P369 R375 S376 P391 E402 D403

R406 T418 M421 E430 ARG

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 94.22Å   147.60Å   125.57Å<br>90.00°   91.52°    90.00° | Depositor |
| Resolution (Å) | 73.80   –   3.09<br>95.62   –   3.09 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.5 (73.80-3.09)<br>88.9 (95.62-3.09) | Depositor<br>EDS |
| $R_{merge}$ | 0.09 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $<I/\sigma(I)>$ [1] | 1.91 (at 3.07Å) | Xtriage |
| Refinement program | PHENIX (1.10.1_2155: ???) | Depositor |
| R, $R_{free}$ | 0.235   ,   0.273<br>0.227   ,   0.264 | Depositor<br>DCC |
| $R_{free}$ test set | 2828 reflections (5.06%) | DCC |
| Wilson B-factor (Å$^2$) | 75.4 | Xtriage |
| Anisotropy | 0.231 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.35 , 44.8 | EDS |
| L-test for twinning [2] | $<|L|> = 0.50$, $<L^2> = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.023 for h,-k,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.90 | EDS |
| Total number of atoms | 45964 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 92.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

## 5.1 Standard geometry (i)

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 | 0.33 | 0/3023 | 0.50 | 0/4120 |
| 1 | B | 0.34 | 0/3126 | 0.48 | 0/4261 |
| 1 | C | 0.32 | 0/3039 | 0.48 | 0/4136 |
| 1 | D | 0.36 | 0/3073 | 0.51 | 0/4197 |
| 1 | E | 0.33 | 0/3091 | 0.48 | 0/4209 |
| 1 | F | 0.32 | 0/3024 | 0.48 | 0/4117 |
| 1 | G | 0.31 | 0/2988 | 0.47 | 0/4080 |
| 1 | H | 0.32 | 0/2851 | 0.50 | 0/3908 |
| All | All | 0.33 | 0/24215 | 0.49 | 0/33028 |

There are no bond length outliers.

There are no bond angle outliers.

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 | 2959 | 2778 | 2774 | 25 | 0 |
| 1 | B | 3058 | 2887 | 2886 | 30 | 0 |
| 1 | C | 2975 | 2849 | 2849 | 24 | 0 |
| 1 | D | 3007 | 2788 | 2788 | 33 | 2 |
| 1 | E | 3026 | 2886 | 2877 | 17 | 0 |
| 1 | F | 2961 | 2825 | 2821 | 19 | 2 |
| 1 | G | 2923 | 2738 | 2738 | 20 | 0 |
| 1 | H | 2792 | 2512 | 2510 | 32 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All | 23701 | 22263 | 22243 | 190 | 2 |

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 4.

All (190) 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:D:226:LEU:HG | 1:D:244:LEU:HD11 | 1.72 | 0.71 |
| 1:A:397:GLY:N | 1:A:403:ASP:OD2 | 2.28 | 0.67 |
| 1:H:146:LYS:NZ | 1:H:298:ASP:O | 2.28 | 0.67 |
| 1:B:243:ASP:N | 1:B:243:ASP:OD1 | 2.28 | 0.66 |
| 1:C:200:PRO:O | 1:C:209:SER:HB3 | 1.95 | 0.65 |
| 1:A:277:VAL:HG12 | 1:A:277:VAL:O | 1.97 | 0.64 |
| 1:G:277:VAL:HG12 | 1:G:277:VAL:O | 1.96 | 0.64 |
| 1:E:13:ALA:HA | 1:E:154:ILE:HD11 | 1.79 | 0.64 |
| 1:F:172:ILE:N | 1:F:207:SER:O | 2.29 | 0.63 |
| 1:B:114:TYR:CE1 | 1:B:242:LYS:HE2 | 2.35 | 0.62 |
| 1:D:240:PHE:HA | 1:D:244:LEU:HB3 | 1.81 | 0.62 |
| 1:E:182:ALA:HB2 | 1:B:113:TRP:CZ2 | 2.36 | 0.60 |
| 1:D:226:LEU:CG | 1:D:244:LEU:HD11 | 2.30 | 0.60 |
| 1:B:277:VAL:O | 1:B:277:VAL:HG12 | 2.01 | 0.60 |
| 1:A:14:ARG:NH2 | 1:D:148:ASP:OD2 | 2.36 | 0.59 |
| 1:C:159:LYS:NZ | 1:C:256:ALA:O | 2.36 | 0.58 |
| 1:D:161:ALA:HB2 | 1:D:255:TYR:CD1 | 2.38 | 0.58 |
| 1:D:417:VAL:CG1 | 1:D:422:LEU:HD21 | 2.32 | 0.58 |
| 1:H:301:ASP:OD1 | 1:H:303:ASN:N | 2.28 | 0.58 |
| 1:A:228:GLU:O | 1:A:232:ARG:CB | 2.51 | 0.58 |
| 1:A:50:LYS:HE3 | 1:B:313:LEU:O | 2.05 | 0.57 |
| 1:B:378:ARG:NH2 | 1:B:398:GLU:OE1 | 2.37 | 0.56 |
| 1:D:417:VAL:HG12 | 1:D:422:LEU:HD21 | 1.87 | 0.56 |
| 1:H:161:ALA:HB2 | 1:H:255:TYR:HD2 | 1.70 | 0.56 |
| 1:E:201:SER:HB2 | 1:E:206:PRO:HA | 1.88 | 0.55 |
| 1:B:117:THR:HG1 | 1:B:240:PHE:HD2 | 1.55 | 0.55 |
| 1:B:242:LYS:O | 1:B:246:PRO:HG2 | 2.06 | 0.55 |
| 1:D:221:ASP:OD1 | 1:D:221:ASP:N | 2.39 | 0.54 |
| 1:H:390:ILE:CD1 | 1:H:390:ILE:N | 2.70 | 0.54 |
| 1:D:216:TYR:CE1 | 1:D:245:ILE:HD11 | 2.43 | 0.54 |
| 1:D:216:TYR:CZ | 1:D:245:ILE:HD11 | 2.43 | 0.54 |
| 1:B:114:TYR:CZ | 1:B:242:LYS:HE3 | 2.42 | 0.54 |
| 1:A:407:PHE:HB3 | 1:A:421:MET:SD | 2.49 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:125:LEU:O | 1:B:129:ARG:HG3 | 2.08 | 0.53 |
| 1:E:125:LEU:O | 1:E:129:ARG:HG3 | 2.09 | 0.53 |
| 1:H:182:ALA:O | 1:H:190:ILE:N | 2.38 | 0.53 |
| 1:H:275:ARG:NH2 | 1:H:296:GLU:OE1 | 2.41 | 0.53 |
| 1:B:162:ARG:HB3 | 1:B:222:TYR:CD2 | 2.43 | 0.53 |
| 1:C:125:LEU:O | 1:C:129:ARG:HG3 | 2.09 | 0.53 |
| 1:D:170:VAL:O | 1:D:208:LYS:CB | 2.57 | 0.52 |
| 1:B:74:GLN:HA | 1:B:104:ALA:HB3 | 1.92 | 0.52 |
| 1:H:168:MET:HB2 | 1:H:213:MET:SD | 2.50 | 0.52 |
| 1:A:276:ASP:OD1 | 1:A:276:ASP:N | 2.39 | 0.52 |
| 1:G:422:LEU:HB2 | 1:G:429:GLN:NE2 | 2.26 | 0.51 |
| 1:H:390:ILE:HD12 | 1:H:390:ILE:N | 2.25 | 0.51 |
| 1:D:422:LEU:CB | 1:D:429:GLN:HE21 | 2.23 | 0.51 |
| 1:C:129:ARG:NH2 | 1:C:228:GLU:OE2 | 2.43 | 0.51 |
| 1:F:172:ILE:HG22 | 1:F:207:SER:O | 2.10 | 0.51 |
| 1:C:277:VAL:HG12 | 1:C:277:VAL:O | 2.10 | 0.51 |
| 1:E:182:ALA:HB2 | 1:B:113:TRP:HZ2 | 1.75 | 0.50 |
| 1:F:72:ILE:HG21 | 1:F:120:ALA:HB1 | 1.94 | 0.50 |
| 1:B:85:GLN:NE2 | 1:D:99:VAL:O | 2.39 | 0.50 |
| 1:A:46:HIS:HB3 | 1:A:351:PHE:CE2 | 2.46 | 0.50 |
| 1:B:395:VAL:O | 1:B:406:ARG:NH1 | 2.39 | 0.50 |
| 1:D:213:MET:CE | 1:D:274:TRP:CD1 | 2.95 | 0.49 |
| 1:D:422:LEU:HB3 | 1:D:429:GLN:HE21 | 1.77 | 0.49 |
| 1:D:389:VAL:N | 1:D:429:GLN:OE1 | 2.42 | 0.49 |
| 1:H:146:LYS:HE3 | 1:H:297:LEU:HD11 | 1.95 | 0.49 |
| 1:F:239:ASP:OD2 | 1:F:240:PHE:N | 2.45 | 0.49 |
| 1:H:169:PRO:HA | 1:H:209:SER:O | 2.13 | 0.49 |
| 1:C:161:ALA:HB2 | 1:C:255:TYR:CD1 | 2.48 | 0.49 |
| 1:C:402:GLU:HG3 | 1:C:406:ARG:HD2 | 1.95 | 0.49 |
| 1:H:170:VAL:N | 1:H:209:SER:O | 2.38 | 0.48 |
| 1:B:114:TYR:CD2 | 1:B:114:TYR:N | 2.81 | 0.48 |
| 1:D:222:TYR:OH | 1:D:248:ILE:HG23 | 2.14 | 0.48 |
| 1:E:368:LEU:HB3 | 1:E:369:PRO:CD | 2.43 | 0.48 |
| 1:C:403:ASP:OD1 | 1:C:406:ARG:NH1 | 2.47 | 0.47 |
| 1:D:170:VAL:HG21 | 1:D:211:ALA:HB2 | 1.95 | 0.47 |
| 1:A:368:LEU:HB3 | 1:A:369:PRO:CD | 2.44 | 0.47 |
| 1:H:101:LEU:O | 1:H:103:PRO:HD3 | 2.14 | 0.47 |
| 1:B:94:GLU:OE2 | 1:C:307:ARG:NH1 | 2.46 | 0.47 |
| 1:H:167:CYS:SG | 1:H:256:ALA:HB1 | 2.55 | 0.47 |
| 1:G:422:LEU:CB | 1:G:429:GLN:NE2 | 2.78 | 0.47 |
| 1:C:359:PHE:O | 1:C:376:SER:HA | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:429:GLN:HE21 | 1:H:429:GLN:N | 2.12 | 0.47 |
| 1:C:169:PRO:HA | 1:C:209:SER:O | 2.15 | 0.47 |
| 1:D:307:ARG:NH1 | 1:D:308:THR:O | 2.48 | 0.47 |
| 1:A:368:LEU:HB3 | 1:A:369:PRO:HD2 | 1.97 | 0.46 |
| 1:B:230:ASP:OD1 | 1:B:238:HIS:ND1 | 2.34 | 0.46 |
| 1:F:170:VAL:HG11 | 1:F:211:ALA:HB2 | 1.96 | 0.46 |
| 1:A:407:PHE:CB | 1:A:421:MET:SD | 3.03 | 0.46 |
| 1:C:239:ASP:OD1 | 1:C:241:GLY:N | 2.47 | 0.46 |
| 1:F:402:GLU:HG3 | 1:F:406:ARG:HD2 | 1.98 | 0.46 |
| 1:H:376:SER:O | 1:H:393:GLY:HA2 | 2.16 | 0.46 |
| 1:C:347:GLN:O | 1:C:364:SER:HA | 2.16 | 0.46 |
| 1:E:169:PRO:HA | 1:E:209:SER:O | 2.16 | 0.46 |
| 1:H:368:LEU:HB3 | 1:H:369:PRO:CD | 2.46 | 0.46 |
| 1:F:277:VAL:O | 1:F:277:VAL:HG12 | 2.15 | 0.46 |
| 1:G:368:LEU:HB3 | 1:G:369:PRO:CD | 2.46 | 0.46 |
| 1:H:55:ASP:OD1 | 1:H:83:HIS:NE2 | 2.37 | 0.46 |
| 1:D:363:ASP:O | 1:D:380:ARG:HA | 2.16 | 0.46 |
| 1:D:46:HIS:HB3 | 1:D:351:PHE:CE2 | 2.51 | 0.46 |
| 1:C:12:LEU:HA | 1:C:15:GLN:HG2 | 1.98 | 0.46 |
| 1:H:363:ASP:O | 1:H:380:ARG:HA | 2.15 | 0.46 |
| 1:B:368:LEU:HB3 | 1:B:369:PRO:CD | 2.45 | 0.45 |
| 1:E:363:ASP:O | 1:E:380:ARG:HA | 2.17 | 0.45 |
| 1:B:42:LYS:HB3 | 1:B:43:PRO:HD3 | 1.99 | 0.45 |
| 1:D:368:LEU:HB3 | 1:D:369:PRO:CD | 2.46 | 0.45 |
| 1:F:321:ASP:HB2 | 1:F:358:SER:HB3 | 1.97 | 0.45 |
| 1:H:359:PHE:O | 1:H:376:SER:HA | 2.16 | 0.45 |
| 1:A:129:ARG:NH1 | 1:A:228:GLU:OE2 | 2.50 | 0.45 |
| 1:H:195:LYS:N | 1:H:196:PRO:HD3 | 2.32 | 0.44 |
| 1:E:368:LEU:HB3 | 1:E:369:PRO:HD2 | 1.98 | 0.44 |
| 1:G:339:VAL:HB | 1:G:355:ARG:HD2 | 2.00 | 0.44 |
| 1:D:368:LEU:HB3 | 1:D:369:PRO:HD2 | 1.99 | 0.44 |
| 1:F:72:ILE:HD13 | 1:F:102:LEU:HB2 | 1.99 | 0.44 |
| 1:G:91:PHE:CE2 | 1:G:99:VAL:HG23 | 2.53 | 0.44 |
| 1:H:406:ARG:HB3 | 1:H:425:LEU:HD11 | 1.98 | 0.44 |
| 1:E:74:GLN:HA | 1:E:104:ALA:HB3 | 1.99 | 0.44 |
| 1:G:277:VAL:CG1 | 1:G:277:VAL:O | 2.65 | 0.44 |
| 1:A:13:ALA:HB1 | 1:A:154:ILE:HD11 | 1.99 | 0.44 |
| 1:C:181:MET:HE2 | 1:C:256:ALA:HB2 | 1.99 | 0.44 |
| 1:F:386:ARG:HG3 | 1:F:387:ALA:N | 2.32 | 0.44 |
| 1:B:147:GLN:OE1 | 1:B:152:MET:CE | 2.66 | 0.43 |
| 1:C:91:PHE:CE2 | 1:C:99:VAL:HG23 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:277:VAL:HG13 | 1:A:283:TYR:HA | 2.00 | 0.43 |
| 1:E:16:LEU:HB2 | 1:E:17:PRO:HD3 | 1.99 | 0.43 |
| 1:G:161:ALA:HB2 | 1:G:255:TYR:CD1 | 2.53 | 0.43 |
| 1:D:363:ASP:HB3 | 1:D:379:LEU:O | 2.18 | 0.43 |
| 1:H:384:ILE:HG22 | 1:H:388:CYS:HB2 | 2.00 | 0.43 |
| 1:B:159:LYS:NZ | 1:B:256:ALA:O | 2.43 | 0.43 |
| 1:D:117:THR:OG1 | 1:D:239:ASP:OD1 | 2.22 | 0.43 |
| 1:F:322:ARG:HH11 | 1:F:322:ARG:HB3 | 1.82 | 0.43 |
| 1:E:326:HIS:CD2 | 1:F:328:MET:HB3 | 2.53 | 0.43 |
| 1:F:368:LEU:HB3 | 1:F:369:PRO:CD | 2.48 | 0.43 |
| 1:G:175:ALA:HB3 | 1:G:199:PRO:HG3 | 2.01 | 0.43 |
| 1:G:178:PHE:O | 1:G:195:LYS:HA | 2.18 | 0.43 |
| 1:D:24:ILE:N | 1:D:24:ILE:HD12 | 2.34 | 0.43 |
| 1:E:24:ILE:HD12 | 1:E:24:ILE:N | 2.34 | 0.43 |
| 1:E:233:ASP:OD1 | 1:E:236:SER:N | 2.51 | 0.43 |
| 1:F:390:ILE:HD13 | 1:F:422:LEU:HD11 | 2.01 | 0.43 |
| 1:G:125:LEU:O | 1:G:129:ARG:HG3 | 2.19 | 0.43 |
| 1:G:331:ASN:HA | 1:H:318:PHE:O | 2.19 | 0.43 |
| 1:A:100:ASP:OD2 | 1:A:131:TYR:OH | 2.31 | 0.42 |
| 1:A:347:GLN:O | 1:A:364:SER:HA | 2.18 | 0.42 |
| 1:B:368:LEU:HB3 | 1:B:369:PRO:HD2 | 2.00 | 0.42 |
| 1:C:170:VAL:O | 1:C:208:LYS:CB | 2.67 | 0.42 |
| 1:D:178:PHE:N | 1:D:178:PHE:CD2 | 2.86 | 0.42 |
| 1:G:368:LEU:HB3 | 1:G:369:PRO:HD2 | 2.00 | 0.42 |
| 1:H:168:MET:HB3 | 1:H:213:MET:HG2 | 2.00 | 0.42 |
| 1:B:321:ASP:HB2 | 1:B:358:SER:HB3 | 2.01 | 0.42 |
| 1:F:218:PHE:HB3 | 1:F:223:LEU:HB2 | 2.02 | 0.42 |
| 1:A:24:ILE:HD12 | 1:A:24:ILE:N | 2.34 | 0.42 |
| 1:A:389:VAL:H | 1:A:429:GLN:HE22 | 1.67 | 0.42 |
| 1:E:331:ASN:O | 1:E:347:GLN:HA | 2.19 | 0.42 |
| 1:G:359:PHE:O | 1:G:376:SER:HA | 2.20 | 0.42 |
| 1:A:169:PRO:HA | 1:A:209:SER:O | 2.19 | 0.42 |
| 1:B:223:LEU:HD23 | 1:B:223:LEU:C | 2.40 | 0.42 |
| 1:B:114:TYR:CZ | 1:B:242:LYS:CE | 3.02 | 0.42 |
| 1:D:162:ARG:HD2 | 1:D:222:TYR:HB2 | 2.01 | 0.42 |
| 1:E:418:THR:OG1 | 1:E:421:MET:HG3 | 2.19 | 0.42 |
| 1:G:213:MET:HE2 | 1:G:274:TRP:CD1 | 2.54 | 0.42 |
| 1:G:402:GLU:HG3 | 1:G:406:ARG:HD2 | 2.01 | 0.42 |
| 1:H:363:ASP:CG | 1:H:380:ARG:NH2 | 2.72 | 0.42 |
| 1:F:321:ASP:OD1 | 1:F:325:SER:N | 2.50 | 0.42 |
| 1:H:20:SER:HA | 1:H:135:TYR:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:161:ALA:HB2 | 1:B:255:TYR:CD1 | 2.55 | 0.42 |
| 1:C:42:LYS:HB3 | 1:C:43:PRO:HD3 | 2.01 | 0.42 |
| 1:E:250:GLU:OE1 | 1:B:197:ALA:N | 2.48 | 0.42 |
| 1:A:72:ILE:HA | 1:A:102:LEU:O | 2.20 | 0.42 |
| 1:C:357:ASN:HB3 | 1:C:375:ARG:HG2 | 2.01 | 0.42 |
| 1:H:368:LEU:HB3 | 1:H:369:PRO:HD2 | 2.02 | 0.42 |
| 1:D:222:TYR:CD1 | 1:D:222:TYR:C | 2.93 | 0.42 |
| 1:A:359:PHE:O | 1:A:376:SER:HA | 2.20 | 0.41 |
| 1:F:237:SER:O | 1:F:238:HIS:HB2 | 2.19 | 0.41 |
| 1:A:143:HIS:CD2 | 1:A:274:TRP:HZ2 | 2.39 | 0.41 |
| 1:C:117:THR:OG1 | 1:C:240:PHE:HD2 | 2.03 | 0.41 |
| 1:D:226:LEU:HD12 | 1:D:226:LEU:O | 2.20 | 0.41 |
| 1:F:418:THR:OG1 | 1:F:421:MET:HG3 | 2.20 | 0.41 |
| 1:H:161:ALA:HB2 | 1:H:255:TYR:CD2 | 2.53 | 0.41 |
| 1:D:397:GLY:N | 1:D:403:ASP:OD2 | 2.47 | 0.41 |
| 1:F:368:LEU:HB3 | 1:F:369:PRO:HD2 | 2.02 | 0.41 |
| 1:G:20:SER:HA | 1:G:135:TYR:O | 2.20 | 0.41 |
| 1:G:21:VAL:HG23 | 1:G:133:ALA:HB2 | 2.02 | 0.41 |
| 1:A:245:ILE:HB | 1:A:246:PRO:HD3 | 2.03 | 0.41 |
| 1:B:16:LEU:HB2 | 1:B:17:PRO:HD3 | 2.03 | 0.41 |
| 1:G:218:PHE:HB3 | 1:G:223:LEU:HB2 | 2.03 | 0.41 |
| 1:D:178:PHE:HE1 | 1:D:274:TRP:CZ3 | 2.38 | 0.41 |
| 1:H:24:ILE:HD12 | 1:H:24:ILE:N | 2.34 | 0.41 |
| 1:A:331:ASN:O | 1:A:347:GLN:HA | 2.21 | 0.41 |
| 1:C:418:THR:OG1 | 1:C:421:MET:HG3 | 2.20 | 0.41 |
| 1:H:184:ASP:N | 1:H:188:LYS:O | 2.54 | 0.41 |
| 1:C:368:LEU:HB3 | 1:C:369:PRO:HD2 | 2.03 | 0.41 |
| 1:C:309:TYR:CE2 | 1:C:311:GLU:HG2 | 2.56 | 0.40 |
| 1:G:317:LYS:NZ | 1:H:292:SER:O | 2.50 | 0.40 |
| 1:B:245:ILE:HB | 1:B:246:PRO:HD3 | 2.04 | 0.40 |
| 1:A:328:MET:HB2 | 1:A:344:VAL:HG22 | 2.04 | 0.40 |
| 1:C:46:HIS:HB3 | 1:C:351:PHE:CE2 | 2.57 | 0.40 |
| 1:H:90:PHE:C | 1:H:90:PHE:CD1 | 2.94 | 0.40 |
| 1:D:216:TYR:CE1 | 1:D:245:ILE:CD1 | 3.04 | 0.40 |

All (2) 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:F:322:ARG:HH22 | 1:D:363:ASP:OD1[2_657] | 1.35 | 0.25 |
| 1:F:322:ARG:NH2 | 1:D:363:ASP:OD1[2_657] | 2.10 | 0.10 |

## 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 | 388/431 (90%) | 369 (95%) | 18 (5%) | 1 (0%) | 46 | 80 |
| 1 | B | 400/431 (93%) | 385 (96%) | 14 (4%) | 1 (0%) | 46 | 80 |
| 1 | C | 386/431 (90%) | 373 (97%) | 12 (3%) | 1 (0%) | 46 | 80 |
| 1 | D | 405/431 (94%) | 380 (94%) | 25 (6%) | 0 | 100 | 100 |
| 1 | E | 395/431 (92%) | 379 (96%) | 14 (4%) | 2 (0%) | 34 | 72 |
| 1 | F | 380/431 (88%) | 365 (96%) | 14 (4%) | 1 (0%) | 46 | 80 |
| 1 | G | 385/431 (89%) | 364 (94%) | 20 (5%) | 1 (0%) | 46 | 80 |
| 1 | H | 385/431 (89%) | 366 (95%) | 19 (5%) | 0 | 100 | 100 |
| All | All | 3124/3448 (91%) | 2981 (95%) | 136 (4%) | 7 (0%) | 52 | 84 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 391 | PRO |
| 1 | A | 277 | VAL |
| 1 | B | 277 | VAL |
| 1 | G | 277 | VAL |
| 1 | E | 277 | VAL |
| 1 | E | 391 | PRO |
| 1 | C | 391 | 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 | 297/372 (80%) | 294 (99%) | 3 (1%) | 82 | 93 |
| 1 | B | 314/372 (84%) | 310 (99%) | 4 (1%) | 76 | 91 |
| 1 | C | 307/372 (82%) | 305 (99%) | 2 (1%) | 88 | 95 |
| 1 | D | 294/372 (79%) | 292 (99%) | 2 (1%) | 88 | 95 |
| 1 | E | 311/372 (84%) | 311 (100%) | 0 | 100 | 100 |
| 1 | F | 309/372 (83%) | 306 (99%) | 3 (1%) | 82 | 93 |
| 1 | G | 294/372 (79%) | 293 (100%) | 1 (0%) | 94 | 97 |
| 1 | H | 258/372 (69%) | 254 (98%) | 4 (2%) | 70 | 89 |
| All | All | 2384/2976 (80%) | 2365 (99%) | 19 (1%) | 86 | 94 |

All (19) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 100 | ASP |
| 1 | H | 100 | ASP |
| 1 | H | 167 | CYS |
| 1 | H | 390 | ILE |
| 1 | H | 407 | PHE |
| 1 | F | 100 | ASP |
| 1 | F | 173 | GLU |
| 1 | F | 322 | ARG |
| 1 | A | 276 | ASP |
| 1 | A | 407 | PHE |
| 1 | A | 423 | ARG |
| 1 | B | 100 | ASP |
| 1 | B | 114 | TYR |
| 1 | B | 243 | ASP |
| 1 | B | 405 | ARG |
| 1 | D | 221 | ASP |
| 1 | D | 380 | ARG |
| 1 | C | 100 | ASP |
| 1 | C | 209 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 (i)

There are no such residues in this entry.

## 5.8   Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å²) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 396/431 (91%) | 0.11 | 3 (0%) | 87 | 75 | 49, 84, 128, 166 | 0 |
| 1 | B | 406/431 (94%) | 0.08 | 2 (0%) | 91 | 83 | 48, 77, 113, 164 | 0 |
| 1 | C | 394/431 (91%) | 0.16 | 3 (0%) | 87 | 75 | 47, 76, 114, 139 | 0 |
| 1 | D | 409/431 (94%) | 0.15 | 7 (1%) | 73 | 52 | 47, 84, 120, 161 | 0 |
| 1 | E | 401/431 (93%) | 0.05 | 0 | 100 | 100 | 50, 76, 113, 149 | 0 |
| 1 | F | 390/431 (90%) | 0.14 | 7 (1%) | 71 | 50 | 53, 83, 119, 162 | 0 |
| 1 | G | 393/431 (91%) | 0.18 | 4 (1%) | 84 | 69 | 55, 89, 139, 157 | 0 |
| 1 | H | 393/431 (91%) | 0.35 | 16 (4%) | 41 | 19 | 56, 105, 148, 172 | 0 |
| All | All | 3182/3448 (92%) | 0.15 | 42 (1%) | 79 | 62 | 47, 84, 130, 172 | 0 |

All (42) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 211 | ALA | 8.1 |
| 1 | H | 180 | VAL | 4.1 |
| 1 | H | 210 | LEU | 4.1 |
| 1 | H | 209 | SER | 3.3 |
| 1 | G | 256 | ALA | 3.3 |
| 1 | H | 416 | LEU | 3.2 |
| 1 | F | 300 | TYR | 3.1 |
| 1 | C | 180 | VAL | 3.0 |
| 1 | F | 325 | SER | 2.9 |
| 1 | A | 138 | ILE | 2.9 |
| 1 | H | 169 | PRO | 2.9 |
| 1 | F | 181 | MET | 2.9 |
| 1 | C | 200 | PRO | 2.7 |
| 1 | B | 340 | ILE | 2.7 |
| 1 | B | 396 | ILE | 2.6 |
| 1 | D | 35 | ASP | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 210 | LEU | 2.6 |
| 1 | H | 342 | GLY | 2.5 |
| 1 | H | 72 | ILE | 2.5 |
| 1 | F | 66 | ILE | 2.4 |
| 1 | H | 236 | SER | 2.4 |
| 1 | H | 422 | LEU | 2.3 |
| 1 | G | 187 | ASP | 2.3 |
| 1 | G | 170 | VAL | 2.3 |
| 1 | H | 398 | GLU | 2.2 |
| 1 | H | 297 | LEU | 2.2 |
| 1 | F | 210 | LEU | 2.2 |
| 1 | A | 139 | LEU | 2.2 |
| 1 | C | 163 | CYS | 2.2 |
| 1 | D | 117 | THR | 2.2 |
| 1 | D | 120 | ALA | 2.1 |
| 1 | H | 274 | TRP | 2.1 |
| 1 | D | 138 | ILE | 2.1 |
| 1 | D | 417 | VAL | 2.1 |
| 1 | F | 16 | LEU | 2.1 |
| 1 | H | 179 | GLY | 2.1 |
| 1 | A | 26 | ALA | 2.1 |
| 1 | F | 189 | ILE | 2.1 |
| 1 | G | 192 | PHE | 2.0 |
| 1 | D | 408 | TYR | 2.0 |
| 1 | H | 66 | ILE | 2.0 |
| 1 | H | 22 | ALA | 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.