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

Feb 1, 2016 – 02:10 AM GMT

| | | |
|---|---|---|
| PDB ID | : | 2FZ2 |
| Title | : | Structure of Turnip Yellow Mosaic Virus at 100 K |
| Authors | : | Larson, S.B.; Lucas, R.W.; McPherson, A. |
| Deposited on | : | 2006-02-08 |
| Resolution | : | 2.90 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:

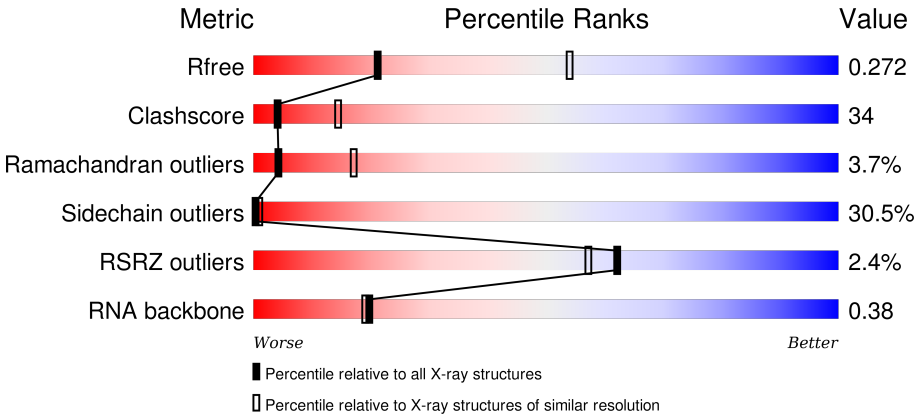
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| 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 2.90 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 | 1451 (2.90-2.90) |
| Clashscore | 102246 | 1668 (2.90-2.90) |
| Ramachandran outliers | 100387 | 1630 (2.90-2.90) |
| Sidechain outliers | 100360 | 1632 (2.90-2.90) |
| RSRZ outliers | 91569 | 1456 (2.90-2.90) |
| RNA backbone | 2183 | 1093 (3.30-2.50) |

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. 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 | D | 3 | 100%<br>33%<br>67% |
| 2 | A | 189 | 3%<br>40%<br>32%<br>14%<br>13% |
| 2 | B | 189 | 2%<br>39%<br>44%<br>15% |
| 2 | C | 189 | %<br>36%<br>48%<br>16% |

# 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4122 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 RNA chain called 5'-R(*CP*CP*C)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | D | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 57 | 27 | 9 | 19 | 2 | | | |

- Molecule 2 is a protein called Coat protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 164 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1231 | 792 | 195 | 237 | 7 | | | |
| 2 | B | 189 | Total | C | N | O | S | 6 | 0 | 0 |
| | | | 1417 | 909 | 225 | 275 | 8 | | | |
| 2 | C | 189 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1417 | 909 | 225 | 275 | 8 | | | |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 99 | GLN | ASN | VARIANT | UNP P20125 |
| A | 123 | GLN | ASN | VARIANT | UNP P20125 |
| A | 138 | GLN | ASN | VARIANT | UNP P20125 |
| B | 99 | GLN | ASN | VARIANT | UNP P20125 |
| B | 123 | GLN | ASN | VARIANT | UNP P20125 |
| B | 138 | GLN | ASN | VARIANT | UNP P20125 |
| C | 99 | GLN | ASN | VARIANT | UNP P20125 |
| C | 123 | GLN | ASN | VARIANT | UNP P20125 |
| C | 138 | GLN | ASN | VARIANT | UNP P20125 |

# 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.

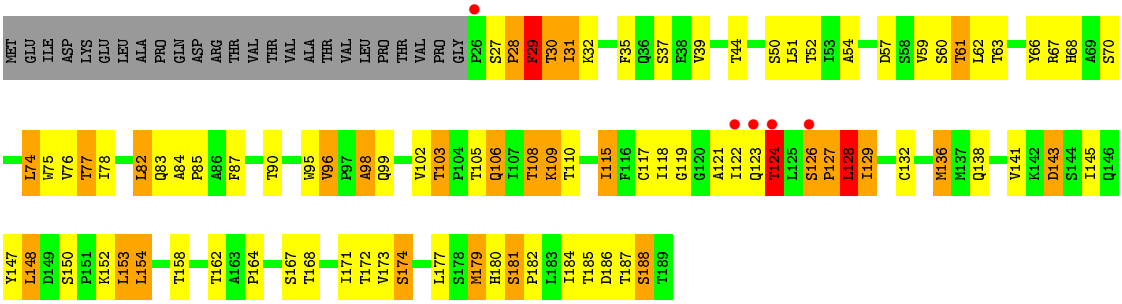
- Molecule 1: 5'-R(*CP*CP*C)-3'

Chain D:



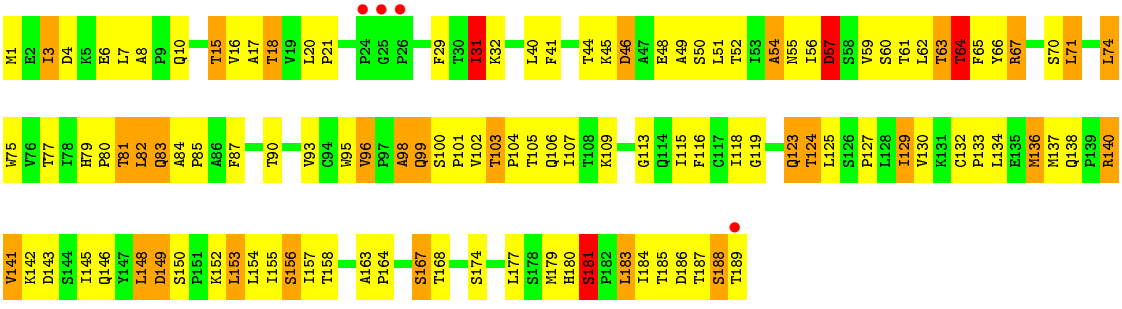
- Molecule 2: Coat protein

Chain A:

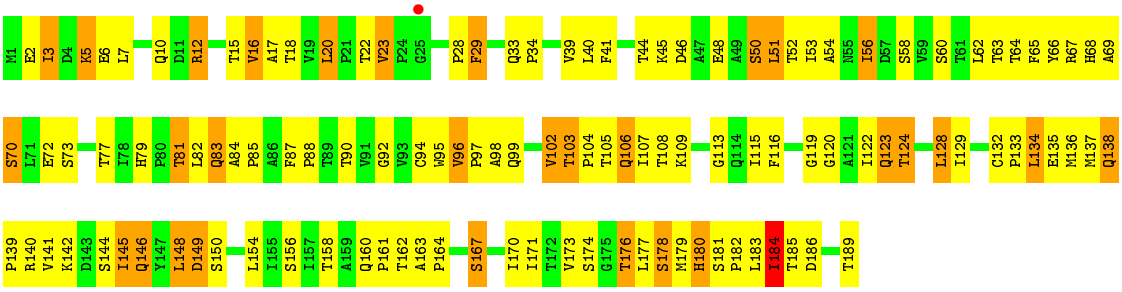

- Molecule 2: Coat protein

Chain B:


- Molecule 2: Coat protein

Chain C:


M1 E2 I3 D4 K5 E6 L7 Q10 D11 R12 T15 V16 A17 T18 V19 L20 P21 T22 V23 P24 G25 P28 F29 Q33 P34 V39 L40 F41 T44 K45 D46 A47 E48 A49 S50 L51 T52 I53 A54 N55 I56 D57 S58 V59 S60 T61 L62 T63 T64 F65 Y66 R67 H68 A69
S70 L71 E72 S73 T77 I78 H79 P80 T81 L82 Q83 A84 P85 A86 F87 P88 T89 T90 V91 G92 V93 C94 W95 V96 P97 A98 Q99 V102 T103 P104 T105 Q106 I107 T108 K109 G113 Q114 I115 F116 G119 G120 A121 I122 Q123 T124 L128 I129 G132 P133 L134 E135 M136 M137 Q138
P139 R140 V141 K142 D143 S144 I145 Q146 Y147 L148 D149 S150 L154 I155 S156 I157 T158 A159 Q160 P161 T162 A163 P164 S167 I170 I171 T172 V173 S174 G175 T176 L177 S178 M179 H180 S181 P182 L183 I184 T185 D186 T189

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 64 2 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 511.53Å 511.53Å 303.76Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 59.12 – 2.90<br>59.72 – 2.60 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 42.8 (59.12-2.90)<br>32.3 (59.72-2.60) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.11 | Depositor |
| $< I/\sigma(I) >$ [1] | 0.62 (at 2.61Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.276 , 0.289<br>0.261 , 0.272 | Depositor<br>DCC |
| $R_{free}$ test set | 10857 reflections (5.30%) | DCC |
| Wilson B-factor (Å$^2$) | 38.3 | Xtriage |
| Anisotropy | 0.263 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.33 , 40.5 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Outliers | 0 of 247626 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.80 | EDS |
| Total number of atoms | 4122 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 29.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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 | D | 0.91 | 0/62 | 1.44 | 3/94 (3.2%) |
| 2 | A | 0.58 | 0/1263 | 0.86 | 0/1735 |
| 2 | B | 0.57 | 0/1452 | 0.85 | 1/1997 (0.1%) |
| 2 | C | 0.59 | 0/1452 | 0.85 | 0/1997 |
| All | All | 0.59 | 0/4229 | 0.86 | 4/5823 (0.1%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 1 | C | O4'-C1'-N1 | 6.87 | 113.70 | 108.20 |
| 1 | D | 1 | C | O5'-C5'-C4' | 5.43 | 122.01 | 111.70 |
| 2 | B | 31 | ILE | CB-CA-C | -5.27 | 101.06 | 111.60 |
| 1 | D | 1 | C | O4'-C4'-C3' | -5.04 | 98.96 | 104.00 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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 | D | 57 | 0 | 35 | 1 | 0 |
| 2 | A | 1231 | 0 | 1258 | 80 | 0 |
| 2 | B | 1417 | 0 | 1454 | 102 | 0 |
| 2 | C | 1417 | 0 | 1454 | 110 | 0 |
| All | All | 4122 | 0 | 4201 | 281 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (281) 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) |
|---|---|---|---|
| 2:B:81:THR:HG23 | 2:B:83:GLN:H | 1.16 | 1.10 |
| 2:C:83:GLN:HA | 2:C:83:GLN:HE21 | 1.23 | 1.00 |
| 2:C:102:VAL:HG12 | 2:C:106:GLN:HG3 | 1.43 | 0.98 |
| 2:B:153:LEU:HD13 | 2:B:155:ILE:HD11 | 1.46 | 0.97 |
| 2:C:81:THR:HG23 | 2:C:83:GLN:H | 1.30 | 0.93 |
| 2:C:145:ILE:HD12 | 2:C:146:GLN:H | 1.34 | 0.92 |
| 2:B:103:THR:H | 2:B:106:GLN:HE21 | 1.14 | 0.91 |
| 2:C:160:GLN:HG3 | 2:C:161:PRO:HD2 | 1.52 | 0.90 |
| 2:B:103:THR:HG23 | 2:B:106:GLN:HG3 | 1.53 | 0.88 |
| 2:C:123:GLN:HE21 | 2:C:123:GLN:C | 1.79 | 0.86 |
| 2:B:59:VAL:O | 2:B:63:THR:HG23 | 1.76 | 0.85 |
| 2:A:129:ILE:HD13 | 2:A:129:ILE:H | 1.41 | 0.84 |
| 2:C:138:GLN:HE21 | 2:C:138:GLN:C | 1.80 | 0.84 |
| 2:A:30:THR:CG2 | 2:A:180:HIS:HB3 | 2.08 | 0.84 |
| 2:C:134:LEU:HD22 | 2:C:134:LEU:H | 1.43 | 0.84 |
| 2:C:138:GLN:HE21 | 2:C:138:GLN:CA | 1.92 | 0.83 |
| 2:A:102:VAL:HG13 | 2:A:106:GLN:HG3 | 1.61 | 0.82 |
| 2:B:81:THR:CG2 | 2:B:83:GLN:H | 1.92 | 0.81 |
| 2:A:30:THR:HG23 | 2:A:180:HIS:HB3 | 1.61 | 0.81 |
| 2:C:184:ILE:HD12 | 2:C:184:ILE:H | 1.47 | 0.80 |
| 2:B:18:THR:HB | 2:C:20:LEU:HB3 | 1.61 | 0.79 |
| 2:C:88:PRO:HG3 | 2:C:120:GLY:HA3 | 1.63 | 0.79 |
| 2:A:124:THR:O | 2:A:124:THR:HG23 | 1.83 | 0.79 |
| 2:C:15:THR:HG22 | 2:C:136:MET:HB2 | 1.64 | 0.78 |
| 2:A:98:ALA:HB3 | 2:A:148:LEU:O | 1.84 | 0.77 |
| 2:A:29:PHE:HE2 | 2:A:181:SER:H | 1.33 | 0.77 |
| 2:C:119:GLY:H | 2:C:124:THR:HB | 1.50 | 0.76 |
| 2:A:77:THR:HG23 | 2:A:129:ILE:HG22 | 1.66 | 0.76 |
| 2:A:78:ILE:HB | 2:A:128:LEU:HD23 | 1.68 | 0.76 |
| 2:C:83:GLN:HA | 2:C:83:GLN:NE2 | 2.01 | 0.74 |
| 2:B:153:LEU:CD1 | 2:B:155:ILE:HD11 | 2.16 | 0.74 |
| 2:A:84:ALA:HB3 | 2:A:85:PRO:HD3 | 1.69 | 0.74 |
| 2:B:16:VAL:HG22 | 2:B:17:ALA:N | 2.03 | 0.73 |
| 2:C:66:TYR:O | 2:C:142:LYS:HE2 | 1.89 | 0.73 |
| 2:C:81:THR:CG2 | 2:C:83:GLN:H | 2.01 | 0.73 |
| 2:C:68:HIS:HB2 | 2:C:180:HIS:CE1 | 2.25 | 0.72 |
| 2:B:153:LEU:HD13 | 2:B:155:ILE:CD1 | 2.20 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:128:LEU:HD22 | 2:A:128:LEU:N | 2.05 | 0.72 |
| 2:C:40:LEU:HD12 | 2:C:41:PHE:H | 1.55 | 0.72 |
| 2:A:30:THR:HG22 | 2:A:179:MET:O | 1.92 | 0.70 |
| 2:B:138:GLN:HB3 | 2:B:149:ASP:O | 1.92 | 0.70 |
| 2:A:127:PRO:C | 2:A:128:LEU:HD22 | 2.13 | 0.69 |
| 2:B:81:THR:HG23 | 2:B:82:LEU:N | 2.08 | 0.69 |
| 2:A:90:THR:HB | 2:A:158:THR:HB | 1.75 | 0.69 |
| 2:A:68:HIS:HD2 | 2:A:143:ASP:OD1 | 1.77 | 0.67 |
| 2:A:126:SER:O | 2:A:128:LEU:N | 2.27 | 0.67 |
| 2:C:81:THR:HG23 | 2:C:82:LEU:N | 2.08 | 0.67 |
| 2:C:77:THR:HB | 2:C:79:HIS:CE1 | 2.30 | 0.67 |
| 2:B:102:VAL:HA | 2:B:106:GLN:NE2 | 2.10 | 0.66 |
| 2:B:81:THR:HG21 | 2:B:167:SER:O | 1.96 | 0.66 |
| 2:B:102:VAL:HG13 | 2:B:106:GLN:HB2 | 1.78 | 0.66 |
| 2:B:103:THR:H | 2:B:106:GLN:NE2 | 1.92 | 0.66 |
| 2:B:77:THR:HB | 2:B:79:HIS:CE1 | 2.30 | 0.66 |
| 2:C:145:ILE:HD12 | 2:C:146:GLN:N | 2.09 | 0.65 |
| 2:A:103:THR:O | 2:A:106:GLN:HG2 | 1.97 | 0.65 |
| 2:B:74:LEU:HD22 | 2:B:75:TRP:N | 2.10 | 0.65 |
| 2:A:186:ASP:OD1 | 2:A:188:SER:HB3 | 1.96 | 0.65 |
| 2:B:71:LEU:HD13 | 2:B:177:LEU:CD2 | 2.27 | 0.64 |
| 2:B:81:THR:HG23 | 2:B:83:GLN:N | 2.00 | 0.64 |
| 2:C:81:THR:HG21 | 2:C:167:SER:O | 1.97 | 0.64 |
| 2:B:83:GLN:HA | 2:B:83:GLN:HE21 | 1.62 | 0.64 |
| 2:A:99:GLN:O | 2:A:99:GLN:HG2 | 1.95 | 0.64 |
| 2:C:40:LEU:HD12 | 2:C:41:PHE:N | 2.12 | 0.64 |
| 2:B:15:THR:HB | 2:C:182:PRO:HD2 | 1.80 | 0.64 |
| 2:C:96:VAL:HG22 | 2:C:97:PRO:HD2 | 1.80 | 0.63 |
| 2:C:161:PRO:HG2 | 2:C:162:THR:H | 1.64 | 0.63 |
| 2:B:103:THR:N | 2:B:106:GLN:HE21 | 1.92 | 0.62 |
| 2:B:20:LEU:HD12 | 2:B:20:LEU:O | 1.98 | 0.62 |
| 2:B:74:LEU:HD22 | 2:B:75:TRP:H | 1.63 | 0.62 |
| 2:C:99:GLN:OE1 | 2:C:149:ASP:HB3 | 1.99 | 0.62 |
| 2:C:123:GLN:HE21 | 2:C:124:THR:N | 1.96 | 0.62 |
| 2:B:61:THR:O | 2:B:64:THR:HB | 1.98 | 0.62 |
| 2:C:64:THR:O | 2:C:65:PHE:HB2 | 1.98 | 0.62 |
| 2:A:184:ILE:HD12 | 2:A:184:ILE:H | 1.65 | 0.62 |
| 2:B:138:GLN:HB3 | 2:B:149:ASP:C | 2.21 | 0.61 |
| 2:B:66:TYR:O | 2:B:142:LYS:HE2 | 2.01 | 0.61 |
| 2:B:95:TRP:CE2 | 2:B:132:CYS:HB2 | 2.36 | 0.61 |
| 2:C:138:GLN:HG3 | 2:C:149:ASP:OD2 | 1.99 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:163:ALA:HB1 | 2:B:164:PRO:HD2 | 1.83 | 0.61 |
| 2:B:154:LEU:C | 2:B:155:ILE:HD12 | 2.20 | 0.61 |
| 2:C:92:GLY:HA2 | 2:C:115:ILE:HD13 | 1.83 | 0.60 |
| 2:B:103:THR:HG22 | 2:B:106:GLN:NE2 | 2.16 | 0.60 |
| 2:A:77:THR:CG2 | 2:A:129:ILE:HG22 | 2.31 | 0.60 |
| 2:A:30:THR:HG22 | 2:A:180:HIS:HB3 | 1.84 | 0.60 |
| 2:C:138:GLN:NE2 | 2:C:138:GLN:CA | 2.62 | 0.60 |
| 2:C:138:GLN:HB2 | 2:C:149:ASP:O | 2.00 | 0.60 |
| 2:B:32:LYS:HA | 2:B:177:LEU:O | 2.01 | 0.60 |
| 2:A:31:ILE:HD12 | 2:A:31:ILE:O | 2.02 | 0.60 |
| 2:C:123:GLN:NE2 | 2:C:123:GLN:C | 2.54 | 0.59 |
| 2:B:71:LEU:HD13 | 2:B:177:LEU:HD21 | 1.84 | 0.59 |
| 2:C:95:TRP:CE2 | 2:C:132:CYS:HB2 | 2.37 | 0.59 |
| 2:C:104:PRO:O | 2:C:107:ILE:HG13 | 2.02 | 0.59 |
| 2:B:17:ALA:O | 2:C:23:VAL:HG13 | 2.03 | 0.59 |
| 2:C:53:ILE:O | 2:C:56:ILE:HG13 | 2.02 | 0.59 |
| 2:A:39:VAL:HG22 | 2:A:171:ILE:O | 2.02 | 0.58 |
| 2:C:149:ASP:OD2 | 2:C:149:ASP:N | 2.36 | 0.58 |
| 2:C:50:SER:HB3 | 2:C:154:LEU:CD2 | 2.32 | 0.58 |
| 2:B:3:ILE:H | 2:B:3:ILE:HD12 | 1.68 | 0.58 |
| 2:B:90:THR:HB | 2:B:158:THR:HB | 1.85 | 0.58 |
| 2:A:67:ARG:HH12 | 2:C:17:ALA:HB2 | 1.68 | 0.58 |
| 2:B:16:VAL:CG2 | 2:B:17:ALA:N | 2.66 | 0.58 |
| 2:A:35:PHE:O | 2:A:174:SER:HB3 | 2.03 | 0.57 |
| 2:A:118:ILE:HD12 | 2:A:118:ILE:N | 2.19 | 0.57 |
| 2:B:18:THR:OG1 | 2:C:144:SER:HB2 | 2.04 | 0.57 |
| 2:B:87:PHE:CD1 | 2:B:164:PRO:HB3 | 2.40 | 0.57 |
| 2:A:124:THR:O | 2:A:124:THR:CG2 | 2.53 | 0.56 |
| 2:A:153:LEU:HD22 | 2:A:154:LEU:N | 2.19 | 0.56 |
| 2:B:8:ALA:O | 2:B:130:VAL:HG22 | 2.06 | 0.56 |
| 2:C:184:ILE:H | 2:C:184:ILE:CD1 | 2.09 | 0.55 |
| 2:C:119:GLY:N | 2:C:124:THR:HB | 2.20 | 0.55 |
| 2:B:84:ALA:N | 2:B:85:PRO:HD2 | 2.21 | 0.55 |
| 2:C:97:PRO:HD3 | 2:C:137:MET:HE1 | 1.89 | 0.55 |
| 2:C:83:GLN:HE21 | 2:C:83:GLN:CA | 2.04 | 0.55 |
| 2:B:149:ASP:OD2 | 2:B:149:ASP:N | 2.40 | 0.54 |
| 2:C:103:THR:O | 2:C:106:GLN:HG2 | 2.07 | 0.54 |
| 2:A:127:PRO:O | 2:A:128:LEU:O | 2.25 | 0.54 |
| 2:A:185:THR:HG23 | 2:A:186:ASP:N | 2.22 | 0.54 |
| 2:C:90:THR:HB | 2:C:158:THR:HB | 1.90 | 0.53 |
| 2:B:81:THR:CG2 | 2:B:168:THR:HA | 2.39 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:32:LYS:HA | 2:A:177:LEU:O | 2.07 | 0.53 |
| 2:A:129:ILE:H | 2:A:129:ILE:CD1 | 2.16 | 0.53 |
| 2:A:109:LYS:HB3 | 2:B:186:ASP:OD1 | 2.08 | 0.53 |
| 2:C:77:THR:HG23 | 2:C:129:ILE:CD1 | 2.39 | 0.53 |
| 2:C:33:GLN:HB3 | 2:C:62:LEU:HD13 | 1.91 | 0.52 |
| 2:B:20:LEU:HB3 | 2:C:20:LEU:HD11 | 1.90 | 0.52 |
| 2:C:50:SER:HB3 | 2:C:154:LEU:HD23 | 1.90 | 0.52 |
| 2:A:95:TRP:CE2 | 2:A:132:CYS:HB2 | 2.43 | 0.52 |
| 2:C:10:GLN:HE22 | 2:C:95:TRP:H | 1.58 | 0.52 |
| 2:A:123:GLN:CD | 2:A:123:GLN:O | 2.47 | 0.52 |
| 2:B:98:ALA:HA | 2:B:152:LYS:HB2 | 1.92 | 0.52 |
| 2:A:123:GLN:O | 2:A:124:THR:HG22 | 2.10 | 0.51 |
| 2:A:28:PRO:O | 2:A:29:PHE:HB3 | 2.11 | 0.51 |
| 2:A:29:PHE:C | 2:A:29:PHE:CD2 | 2.84 | 0.51 |
| 2:B:185:THR:OG1 | 2:B:186:ASP:N | 2.42 | 0.51 |
| 2:B:16:VAL:HG22 | 2:B:17:ALA:H | 1.73 | 0.51 |
| 2:B:99:GLN:O | 2:B:99:GLN:HG2 | 2.09 | 0.51 |
| 2:B:125:LEU:HD23 | 2:B:125:LEU:N | 2.25 | 0.51 |
| 2:A:50:SER:C | 2:A:51:LEU:HD23 | 2.31 | 0.51 |
| 2:C:77:THR:HG23 | 2:C:129:ILE:HD13 | 1.93 | 0.51 |
| 2:C:87:PHE:CD1 | 2:C:164:PRO:HB3 | 2.46 | 0.51 |
| 2:B:104:PRO:O | 2:B:107:ILE:HG13 | 2.11 | 0.50 |
| 2:C:69:ALA:O | 2:C:141:VAL:HG22 | 2.11 | 0.50 |
| 2:C:185:THR:OG1 | 2:C:186:ASP:N | 2.44 | 0.50 |
| 2:A:59:VAL:HG12 | 2:A:60:SER:N | 2.25 | 0.50 |
| 2:B:83:GLN:NE2 | 2:B:83:GLN:HA | 2.27 | 0.50 |
| 2:C:29:PHE:HD1 | 2:C:29:PHE:H | 1.56 | 0.50 |
| 2:B:31:ILE:O | 2:B:31:ILE:HD12 | 2.12 | 0.50 |
| 2:C:51:LEU:HD23 | 2:C:51:LEU:O | 2.12 | 0.50 |
| 2:B:66:TYR:N | 2:B:66:TYR:CD1 | 2.80 | 0.50 |
| 2:A:68:HIS:HE1 | 2:C:16:VAL:O | 1.95 | 0.50 |
| 2:C:15:THR:CG2 | 2:C:136:MET:HB2 | 2.37 | 0.49 |
| 2:A:76:VAL:O | 2:A:129:ILE:HA | 2.12 | 0.49 |
| 2:C:29:PHE:CD1 | 2:C:29:PHE:N | 2.77 | 0.49 |
| 2:B:16:VAL:CG2 | 2:B:17:ALA:H | 2.25 | 0.49 |
| 2:A:59:VAL:C | 2:A:61:THR:N | 2.65 | 0.49 |
| 2:C:163:ALA:HB1 | 2:C:164:PRO:HD2 | 1.94 | 0.49 |
| 2:C:81:THR:HG23 | 2:C:83:GLN:N | 2.13 | 0.49 |
| 2:C:103:THR:HG23 | 2:C:106:GLN:CD | 2.33 | 0.49 |
| 2:C:138:GLN:HB2 | 2:C:149:ASP:C | 2.33 | 0.49 |
| 2:B:15:THR:O | 2:B:15:THR:HG23 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:124:THR:C | 2:B:125:LEU:HD23 | 2.32 | 0.49 |
| 2:A:82:LEU:HD23 | 2:A:83:GLN:N | 2.27 | 0.49 |
| 2:A:117:CYS:C | 2:A:118:ILE:HD12 | 2.33 | 0.49 |
| 2:A:103:THR:OG1 | 2:A:105:THR:HG23 | 2.13 | 0.49 |
| 2:A:87:PHE:CG | 2:A:164:PRO:HB3 | 2.47 | 0.49 |
| 2:C:17:ALA:HB1 | 2:C:138:GLN:HG2 | 1.95 | 0.48 |
| 2:A:128:LEU:N | 2:A:128:LEU:CD2 | 2.76 | 0.48 |
| 2:A:129:ILE:HD13 | 2:A:129:ILE:N | 2.20 | 0.48 |
| 2:A:29:PHE:HZ | 2:A:182:PRO:HD3 | 1.76 | 0.48 |
| 2:B:15:THR:CG2 | 2:B:136:MET:HG3 | 2.42 | 0.48 |
| 2:C:63:THR:O | 2:C:64:THR:C | 2.51 | 0.48 |
| 2:C:95:TRP:CD1 | 2:C:132:CYS:HA | 2.48 | 0.48 |
| 2:A:108:THR:HG23 | 2:A:115:ILE:HD12 | 1.96 | 0.48 |
| 2:A:103:THR:HG23 | 2:A:106:GLN:CD | 2.34 | 0.48 |
| 2:A:59:VAL:C | 2:A:61:THR:H | 2.17 | 0.48 |
| 2:B:4:ASP:O | 2:B:127:PRO:HD2 | 2.14 | 0.48 |
| 2:C:12:ARG:HB3 | 2:C:136:MET:CE | 2.44 | 0.48 |
| 2:C:34:PRO:HA | 2:C:176:THR:HA | 1.95 | 0.48 |
| 2:B:155:ILE:N | 2:B:155:ILE:HD12 | 2.29 | 0.47 |
| 2:A:68:HIS:CD2 | 2:A:143:ASP:OD1 | 2.62 | 0.47 |
| 2:B:77:THR:HG23 | 2:B:129:ILE:HG22 | 1.95 | 0.47 |
| 2:B:80:PRO:HG2 | 2:B:125:LEU:O | 2.14 | 0.47 |
| 2:C:68:HIS:CG | 2:C:180:HIS:HE1 | 2.32 | 0.47 |
| 2:B:71:LEU:HD13 | 2:B:177:LEU:HD23 | 1.96 | 0.47 |
| 2:C:69:ALA:HA | 2:C:178:SER:O | 2.15 | 0.47 |
| 2:B:96:VAL:HG13 | 2:B:100:SER:HB3 | 1.94 | 0.47 |
| 2:B:81:THR:HG22 | 2:B:168:THR:HA | 1.95 | 0.47 |
| 2:A:143:ASP:HB2 | 2:A:147:TYR:HE1 | 1.79 | 0.47 |
| 2:C:84:ALA:N | 2:C:85:PRO:CD | 2.78 | 0.47 |
| 2:B:59:VAL:O | 2:B:60:SER:C | 2.51 | 0.47 |
| 2:B:54:ALA:HA | 2:B:141:VAL:HG12 | 1.96 | 0.47 |
| 2:B:6:GLU:C | 2:B:7:LEU:HD23 | 2.35 | 0.47 |
| 2:C:123:GLN:NE2 | 2:C:123:GLN:CA | 2.78 | 0.47 |
| 2:B:48:GLU:HB3 | 2:B:104:PRO:HG2 | 1.96 | 0.47 |
| 2:B:46:ASP:N | 2:B:46:ASP:OD2 | 2.48 | 0.47 |
| 2:B:186:ASP:OD1 | 2:B:188:SER:HB3 | 2.16 | 0.46 |
| 2:C:64:THR:O | 2:C:65:PHE:CB | 2.63 | 0.46 |
| 2:A:66:TYR:CD1 | 2:A:66:TYR:N | 2.84 | 0.46 |
| 2:A:87:PHE:CD1 | 2:A:164:PRO:HB3 | 2.50 | 0.46 |
| 2:A:29:PHE:CG | 2:A:29:PHE:O | 2.68 | 0.46 |
| 2:B:99:GLN:HB3 | 2:B:148:LEU:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:160:GLN:CG | 2:C:161:PRO:HD2 | 2.37 | 0.46 |
| 2:C:134:LEU:CD2 | 2:C:134:LEU:H | 2.20 | 0.45 |
| 2:B:153:LEU:HD22 | 2:B:155:ILE:CD1 | 2.46 | 0.45 |
| 2:A:82:LEU:O | 2:A:85:PRO:HD2 | 2.17 | 0.45 |
| 2:B:54:ALA:HA | 2:B:141:VAL:CG1 | 2.46 | 0.45 |
| 2:B:102:VAL:HA | 2:B:106:GLN:HE22 | 1.80 | 0.45 |
| 2:B:20:LEU:HD12 | 2:B:20:LEU:C | 2.35 | 0.45 |
| 2:A:28:PRO:O | 2:A:29:PHE:CB | 2.64 | 0.45 |
| 2:C:103:THR:HG23 | 2:C:106:GLN:NE2 | 2.31 | 0.45 |
| 2:C:128:LEU:C | 2:C:129:ILE:HG12 | 2.37 | 0.45 |
| 2:B:180:HIS:HD2 | 2:B:181:SER:HB2 | 1.82 | 0.45 |
| 2:A:54:ALA:HB2 | 2:A:141:VAL:HB | 1.98 | 0.45 |
| 2:C:12:ARG:HB3 | 2:C:136:MET:HE3 | 1.98 | 0.45 |
| 2:C:82:LEU:HD23 | 2:C:82:LEU:H | 1.82 | 0.45 |
| 2:A:61:THR:HG22 | 2:A:62:LEU:N | 2.32 | 0.44 |
| 2:B:67:ARG:HG2 | 2:B:183:LEU:HB2 | 1.99 | 0.44 |
| 2:C:3:ILE:O | 2:C:5:LYS:N | 2.50 | 0.44 |
| 2:B:31:ILE:H | 2:B:31:ILE:HD12 | 1.82 | 0.44 |
| 2:A:37:SER:O | 2:A:172:THR:HA | 2.17 | 0.44 |
| 2:B:20:LEU:HA | 2:B:21:PRO:HD3 | 1.71 | 0.44 |
| 2:C:136:MET:HE2 | 2:C:136:MET:HB3 | 1.71 | 0.44 |
| 2:C:58:SER:O | 2:C:62:LEU:HG | 2.17 | 0.44 |
| 2:C:2:GLU:C | 2:C:3:ILE:HG13 | 2.37 | 0.44 |
| 2:B:56:ILE:O | 2:B:57:ASP:C | 2.55 | 0.44 |
| 2:C:39:VAL:HB | 2:C:171:ILE:HG22 | 2.00 | 0.43 |
| 2:B:95:TRP:CZ3 | 2:B:153:LEU:HG | 2.53 | 0.43 |
| 2:A:31:ILE:CD1 | 2:A:179:MET:HG3 | 2.48 | 0.43 |
| 2:B:20:LEU:O | 2:B:140:ARG:NH2 | 2.52 | 0.43 |
| 2:A:59:VAL:O | 2:A:63:THR:HG23 | 2.18 | 0.43 |
| 2:B:102:VAL:HG12 | 2:B:103:THR:N | 2.34 | 0.43 |
| 2:C:123:GLN:HG3 | 2:C:123:GLN:O | 2.19 | 0.43 |
| 2:B:18:THR:HG22 | 2:C:22:THR:HA | 2.01 | 0.43 |
| 2:B:133:PRO:HB2 | 2:B:136:MET:HE3 | 2.00 | 0.43 |
| 2:B:95:TRP:CH2 | 2:B:153:LEU:HG | 2.53 | 0.43 |
| 2:B:115:ILE:HD12 | 2:B:115:ILE:C | 2.39 | 0.42 |
| 2:B:82:LEU:HD23 | 2:B:82:LEU:H | 1.84 | 0.42 |
| 2:B:83:GLN:CA | 2:B:83:GLN:HE21 | 2.27 | 0.42 |
| 2:A:59:VAL:HG22 | 2:A:177:LEU:HD11 | 2.02 | 0.42 |
| 2:B:87:PHE:CG | 2:B:164:PRO:HB3 | 2.55 | 0.42 |
| 2:A:129:ILE:N | 2:A:129:ILE:CD1 | 2.80 | 0.42 |
| 2:C:73:SER:OG | 2:C:176:THR:HG23 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:145:ILE:CD1 | 2:C:146:GLN:H | 2.18 | 0.42 |
| 2:B:63:THR:O | 2:B:65:PHE:N | 2.53 | 0.42 |
| 2:C:56:ILE:H | 2:C:56:ILE:HG13 | 1.44 | 0.42 |
| 2:B:156:SER:O | 2:B:157:ILE:HD13 | 2.19 | 0.42 |
| 2:A:124:THR:OG1 | 2:A:127:PRO:HD3 | 2.19 | 0.42 |
| 2:C:10:GLN:HE22 | 2:C:94:CYS:HA | 1.84 | 0.42 |
| 2:C:87:PHE:CG | 2:C:164:PRO:HB3 | 2.54 | 0.42 |
| 2:B:119:GLY:O | 2:B:123:GLN:HG2 | 2.20 | 0.42 |
| 2:A:188:SER:HB2 | 2:C:109:LYS:HD2 | 2.02 | 0.42 |
| 2:C:133:PRO:HA | 2:C:135:GLU:OE1 | 2.20 | 0.42 |
| 2:A:119:GLY:C | 2:A:121:ALA:H | 2.23 | 0.42 |
| 2:B:40:LEU:HD12 | 2:B:41:PHE:H | 1.84 | 0.42 |
| 2:B:51:LEU:CD1 | 2:B:51:LEU:N | 2.82 | 0.42 |
| 2:C:138:GLN:HE21 | 2:C:138:GLN:HA | 1.78 | 0.41 |
| 2:C:33:GLN:HA | 2:C:34:PRO:HD3 | 1.94 | 0.41 |
| 2:C:92:GLY:CA | 2:C:115:ILE:HD13 | 2.49 | 0.41 |
| 2:A:118:ILE:O | 2:A:118:ILE:HG22 | 2.20 | 0.41 |
| 2:A:138:GLN:NE2 | 2:A:138:GLN:HA | 2.35 | 0.41 |
| 2:A:154:LEU:HA | 2:A:154:LEU:HD12 | 1.79 | 0.41 |
| 2:C:138:GLN:HE21 | 2:C:139:PRO:N | 2.18 | 0.41 |
| 2:C:138:GLN:NE2 | 2:C:138:GLN:HA | 2.33 | 0.41 |
| 2:A:27:SER:OG | 2:A:28:PRO:HD2 | 2.20 | 0.41 |
| 2:A:59:VAL:O | 2:A:61:THR:N | 2.53 | 0.41 |
| 2:A:136:MET:HE3 | 2:A:136:MET:HB2 | 2.00 | 0.41 |
| 2:C:122:ILE:HG13 | 2:C:122:ILE:O | 2.21 | 0.41 |
| 2:A:68:HIS:ND1 | 2:A:180:HIS:CE1 | 2.89 | 0.41 |
| 1:D:2:C:H1' | 2:C:12:ARG:HD3 | 2.02 | 0.41 |
| 2:C:28:PRO:HG2 | 2:C:180:HIS:CD2 | 2.55 | 0.41 |
| 2:A:96:VAL:HG12 | 2:A:152:LYS:HB3 | 2.02 | 0.41 |
| 2:C:98:ALA:HB3 | 2:C:148:LEU:O | 2.21 | 0.41 |
| 2:C:70:SER:OG | 2:C:140:ARG:HG2 | 2.20 | 0.41 |
| 2:C:17:ALA:CB | 2:C:138:GLN:HG2 | 2.51 | 0.40 |
| 2:A:74:LEU:HG | 2:A:75:TRP:N | 2.36 | 0.40 |
| 2:B:81:THR:HG21 | 2:B:168:THR:HA | 2.03 | 0.40 |
| 2:B:49:ALA:HB3 | 2:B:155:ILE:HB | 2.04 | 0.40 |
| 2:B:153:LEU:HD22 | 2:B:155:ILE:HD12 | 2.02 | 0.40 |
| 2:B:67:ARG:HG3 | 2:B:181:SER:O | 2.21 | 0.40 |
| 2:B:146:GLN:O | 2:C:145:ILE:HD13 | 2.21 | 0.40 |
| 2:C:115:ILE:HD13 | 2:C:115:ILE:HA | 1.85 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | A | 162/189 (86%) | 136 (84%) | 18 (11%) | 8 (5%) | 3 | 10 |
| 2 | B | 187/189 (99%) | 160 (86%) | 19 (10%) | 8 (4%) | 3 | 13 |
| 2 | C | 187/189 (99%) | 163 (87%) | 20 (11%) | 4 (2%) | 9 | 32 |
| All | All | 536/567 (94%) | 459 (86%) | 57 (11%) | 20 (4%) | 4 | 17 |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 28 | PRO |
| 2 | A | 29 | PHE |
| 2 | A | 98 | ALA |
| 2 | A | 124 | THR |
| 2 | A | 126 | SER |
| 2 | A | 127 | PRO |
| 2 | A | 128 | LEU |
| 2 | B | 64 | THR |
| 2 | B | 113 | GLY |
| 2 | B | 15 | THR |
| 2 | B | 57 | ASP |
| 2 | B | 98 | ALA |
| 2 | C | 113 | GLY |
| 2 | A | 181 | SER |
| 2 | B | 54 | ALA |
| 2 | C | 54 | ALA |
| 2 | C | 181 | SER |
| 2 | B | 101 | PRO |
| 2 | C | 184 | ILE |
| 2 | B | 181 | SER |

### 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 |
|---|---|---|---|---|---|
| 2 | A | 145/167 (87%) | 108 (74%) | 37 (26%) | 1 2 |
| 2 | B | 167/167 (100%) | 112 (67%) | 55 (33%) | 0 1 |
| 2 | C | 167/167 (100%) | 113 (68%) | 54 (32%) | 0 1 |
| All | All | 479/501 (96%) | 333 (70%) | 146 (30%) | 0 1 |

All (146) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 29 | PHE |
| 2 | A | 30 | THR |
| 2 | A | 31 | ILE |
| 2 | A | 44 | THR |
| 2 | A | 52 | THR |
| 2 | A | 57 | ASP |
| 2 | A | 61 | THR |
| 2 | A | 70 | SER |
| 2 | A | 74 | LEU |
| 2 | A | 77 | THR |
| 2 | A | 82 | LEU |
| 2 | A | 96 | VAL |
| 2 | A | 103 | THR |
| 2 | A | 106 | GLN |
| 2 | A | 108 | THR |
| 2 | A | 109 | LYS |
| 2 | A | 110 | THR |
| 2 | A | 115 | ILE |
| 2 | A | 122 | ILE |
| 2 | A | 124 | THR |
| 2 | A | 128 | LEU |
| 2 | A | 129 | ILE |
| 2 | A | 136 | MET |
| 2 | A | 143 | ASP |
| 2 | A | 145 | ILE |
| 2 | A | 148 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 150 | SER |
| 2 | A | 153 | LEU |
| 2 | A | 154 | LEU |
| 2 | A | 162 | THR |
| 2 | A | 167 | SER |
| 2 | A | 168 | THR |
| 2 | A | 173 | VAL |
| 2 | A | 174 | SER |
| 2 | A | 179 | MET |
| 2 | A | 187 | THR |
| 2 | A | 188 | SER |
| 2 | B | 1 | MET |
| 2 | B | 3 | ILE |
| 2 | B | 10 | GLN |
| 2 | B | 18 | THR |
| 2 | B | 29 | PHE |
| 2 | B | 31 | ILE |
| 2 | B | 44 | THR |
| 2 | B | 45 | LYS |
| 2 | B | 46 | ASP |
| 2 | B | 50 | SER |
| 2 | B | 52 | THR |
| 2 | B | 55 | ASN |
| 2 | B | 57 | ASP |
| 2 | B | 62 | LEU |
| 2 | B | 63 | THR |
| 2 | B | 64 | THR |
| 2 | B | 67 | ARG |
| 2 | B | 70 | SER |
| 2 | B | 71 | LEU |
| 2 | B | 74 | LEU |
| 2 | B | 81 | THR |
| 2 | B | 82 | LEU |
| 2 | B | 83 | GLN |
| 2 | B | 93 | VAL |
| 2 | B | 96 | VAL |
| 2 | B | 99 | GLN |
| 2 | B | 103 | THR |
| 2 | B | 105 | THR |
| 2 | B | 109 | LYS |
| 2 | B | 116 | PHE |
| 2 | B | 118 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 123 | GLN |
| 2 | B | 124 | THR |
| 2 | B | 129 | ILE |
| 2 | B | 134 | LEU |
| 2 | B | 136 | MET |
| 2 | B | 137 | MET |
| 2 | B | 140 | ARG |
| 2 | B | 141 | VAL |
| 2 | B | 143 | ASP |
| 2 | B | 145 | ILE |
| 2 | B | 148 | LEU |
| 2 | B | 149 | ASP |
| 2 | B | 150 | SER |
| 2 | B | 153 | LEU |
| 2 | B | 156 | SER |
| 2 | B | 167 | SER |
| 2 | B | 174 | SER |
| 2 | B | 179 | MET |
| 2 | B | 181 | SER |
| 2 | B | 183 | LEU |
| 2 | B | 184 | ILE |
| 2 | B | 187 | THR |
| 2 | B | 188 | SER |
| 2 | B | 189 | THR |
| 2 | C | 3 | ILE |
| 2 | C | 5 | LYS |
| 2 | C | 6 | GLU |
| 2 | C | 7 | LEU |
| 2 | C | 12 | ARG |
| 2 | C | 16 | VAL |
| 2 | C | 18 | THR |
| 2 | C | 20 | LEU |
| 2 | C | 23 | VAL |
| 2 | C | 29 | PHE |
| 2 | C | 44 | THR |
| 2 | C | 45 | LYS |
| 2 | C | 46 | ASP |
| 2 | C | 48 | GLU |
| 2 | C | 50 | SER |
| 2 | C | 51 | LEU |
| 2 | C | 52 | THR |
| 2 | C | 56 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | C | 60 | SER |
| 2 | C | 67 | ARG |
| 2 | C | 70 | SER |
| 2 | C | 72 | GLU |
| 2 | C | 81 | THR |
| 2 | C | 83 | GLN |
| 2 | C | 96 | VAL |
| 2 | C | 102 | VAL |
| 2 | C | 103 | THR |
| 2 | C | 105 | THR |
| 2 | C | 106 | GLN |
| 2 | C | 108 | THR |
| 2 | C | 116 | PHE |
| 2 | C | 123 | GLN |
| 2 | C | 124 | THR |
| 2 | C | 128 | LEU |
| 2 | C | 134 | LEU |
| 2 | C | 138 | GLN |
| 2 | C | 145 | ILE |
| 2 | C | 146 | GLN |
| 2 | C | 148 | LEU |
| 2 | C | 149 | ASP |
| 2 | C | 150 | SER |
| 2 | C | 156 | SER |
| 2 | C | 167 | SER |
| 2 | C | 170 | ILE |
| 2 | C | 173 | VAL |
| 2 | C | 174 | SER |
| 2 | C | 176 | THR |
| 2 | C | 177 | LEU |
| 2 | C | 178 | SER |
| 2 | C | 179 | MET |
| 2 | C | 180 | HIS |
| 2 | C | 183 | LEU |
| 2 | C | 184 | ILE |
| 2 | C | 189 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 33 | GLN |
| 2 | A | 55 | ASN |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 68 | HIS |
| 2 | A | 180 | HIS |
| 2 | B | 33 | GLN |
| 2 | B | 79 | HIS |
| 2 | B | 83 | GLN |
| 2 | B | 106 | GLN |
| 2 | B | 114 | GLN |
| 2 | B | 180 | HIS |
| 2 | C | 10 | GLN |
| 2 | C | 55 | ASN |
| 2 | C | 79 | HIS |
| 2 | C | 83 | GLN |
| 2 | C | 106 | GLN |
| 2 | C | 123 | GLN |
| 2 | C | 138 | GLN |
| 2 | C | 180 | HIS |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | D | 2/3 (66%) | 0 | 0 |

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 | D | 3/3 (100%) | 3.90 | 3 (100%) 0 0 | 183, 183, 183, 190 | 0 |
| 2 | A | 164/189 (86%) | -0.07 | 5 (3%) 54 47 | 7, 21, 100, 162 | 0 |
| 2 | B | 189/189 (100%) | -0.10 | 4 (2%) 67 62 | 9, 21, 61, 99 | 1 (0%) |
| 2 | C | 189/189 (100%) | -0.29 | 1 (0%) 91 90 | 9, 22, 51, 75 | 0 |
| All | All | 545/570 (95%) | -0.13 | 13 (2%) 62 57 | 7, 22, 69, 190 | 1 (0%) |

All (13) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | A | 26 | PRO | 13.2 |
| 2 | A | 123 | GLN | 8.6 |
| 2 | B | 24 | PRO | 5.4 |
| 2 | B | 25 | GLY | 5.2 |
| 1 | D | 1 | C | 4.8 |
| 2 | A | 124 | THR | 4.6 |
| 1 | D | 2 | C | 4.3 |
| 2 | A | 122 | ILE | 3.5 |
| 2 | A | 126 | SER | 3.3 |
| 1 | D | 3 | C | 2.7 |
| 2 | C | 25 | GLY | 2.3 |
| 2 | B | 26 | PRO | 2.3 |
| 2 | B | 189 | THR | 2.0 |

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

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

## 6.3 Carbohydrates

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.