



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:04 AM UTC

PDB ID : 2P5T / pdb\_00002p5t  
Title : Molecular and structural characterization of the PezAT chromosomal toxin-antitoxin system of the human pathogen *Streptococcus pneumoniae*  
Authors : Loll, B.; Meinhart, A.  
Deposited on : 2007-03-16  
Resolution : 3.20 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

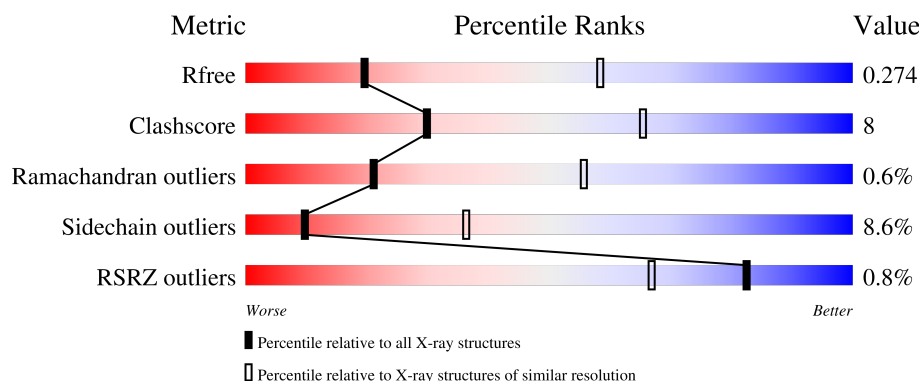
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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   | X     | 33     |                  |
| 2   | A     | 158    |                  |
| 2   | C     | 158    |                  |
| 2   | E     | 158    |                  |
| 2   | G     | 158    |                  |

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| Mol | Chain | Length | Quality of chain                                                                       |
|-----|-------|--------|----------------------------------------------------------------------------------------|
| 3   | B     | 253    | <div><div></div><div>73%</div><div>20%</div><div></div><div></div></div>               |
| 3   | D     | 253    | <div><div></div><div>72%</div><div>22%</div><div></div><div></div></div>               |
| 3   | F     | 253    | <div><div></div><div>%</div><div>77%</div><div>16%</div><div></div><div>5%</div></div> |
| 3   | H     | 253    | <div><div></div><div>2%</div><div>69%</div><div>24%</div><div></div><div></div></div>  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11093 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 fragment of PezA helix-turn-helix motif.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 1   | X     | 33       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 132   | 66 | 33 | 33 |         |         |       |

- Molecule 2 is a protein called Putative transcriptional regulator PezA.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | A     | 92       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 759   | 478 | 122 | 156 | 3 |         |         |       |
| 2   | C     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 767   | 483 | 123 | 157 | 4 |         |         |       |
| 2   | E     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 784   | 493 | 126 | 161 | 4 |         |         |       |
| 2   | G     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 767   | 483 | 123 | 157 | 4 |         |         |       |

- Molecule 3 is a protein called PezT.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | B     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1979  | 1253 | 342 | 381 | 3 |         |         |       |
| 3   | D     | 247      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2002  | 1268 | 345 | 385 | 4 |         |         |       |
| 3   | F     | 240      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1944  | 1232 | 332 | 377 | 3 |         |         |       |
| 3   | H     | 242      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1959  | 1242 | 334 | 379 | 4 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 109     | GLY      | ARG    | conflict | UNP Q97QZ1 |
| B     | 228     | PHE      | LEU    | conflict | UNP Q97QZ1 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 109     | GLY      | ARG    | conflict | UNP Q97QZ1 |
| D     | 228     | PHE      | LEU    | conflict | UNP Q97QZ1 |
| F     | 109     | GLY      | ARG    | conflict | UNP Q97QZ1 |
| F     | 228     | PHE      | LEU    | conflict | UNP Q97QZ1 |
| H     | 109     | GLY      | ARG    | conflict | UNP Q97QZ1 |
| H     | 228     | PHE      | LEU    | conflict | UNP Q97QZ1 |

### 3 Residue-property plots [i](#)

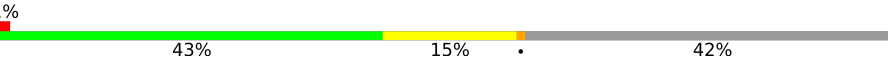
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

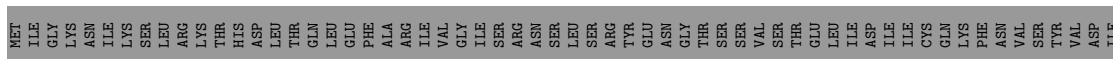
- Molecule 1: fragment of PezA helix-turn-helix motif

Chain X:  100%

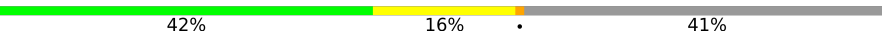
There are no outlier residues recorded for this chain.

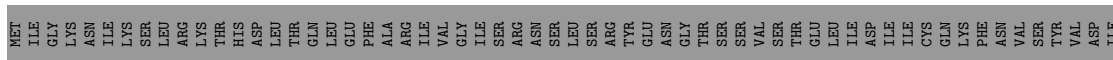
- Molecule 2: Putative transcriptional regulator PezA

Chain A:  %

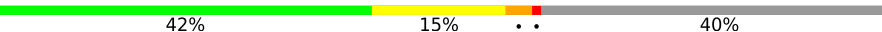


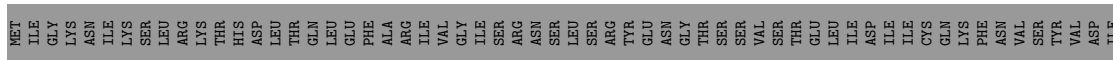
- Molecule 2: Putative transcriptional regulator PezA

Chain C:  %

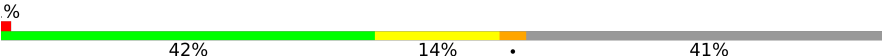


- Molecule 2: Putative transcriptional regulator PezA

Chain E:  %



- Molecule 2: Putative transcriptional regulator PezA

Chain G:  %

MET ILE GLY LYS ASP ASN ILE LYS SER LEU ARG LYS THR HIS ASP LEU THR GLN LEU GLU PHE ARG ILE VAL GLY ILE SER ARG ASN SER LEU SER ARG TYR TYR VAL ASP ILE

VAL GLY GLU ASP M66 M67 M68 M69 V70 Y73 K78 I79 K83 G86 D98 I104 P110 M114 S115 D116 L121 I122 N125 I126 Y127 L128 V129 D133 E134 I135 E136 R137 Y141 I145 L149 E150 I151 R155 M156 V157 A158

• Molecule 3: PezT

Chain B: 73% 20%

MET GLU I3 Q4 R20 S21 T22 T23 R24 P32 I33 Q40 K45 T46 Q53 Q58 I62 R69 S70 Q79 Q80 E81 Y82 G83 K84 V87 E88 Y89 M111 L112 L113 T117 L118 R119 T120 V121 D122 V123 L131 Y136 E137 V138 T143 A144 T145

S153 R157 E160 L161 T164 N165 Q168 A168 ARG ALA THR PRO LYS GLU H176 H177 D178 F179 I180 E198 R199 Q204 Q205 D206 Y207 S208 Y211 Q71 D212 S213 K214 E215 N216 V223 L227 E238 N248 E249 L250 L251 E252 K253

• Molecule 3: PezT

Chain D: 72% 22%

M1 E2 I3 T7 R17 R24 Q25 A141 K26 T35 L36 L37 T46 T51 G52 Q53 Q58 N59 I60 I61 I62 I63 D64 G65 D66 R69 S70 Q71 H72 H73 H74 H75 Q79 Q87 E88 T89 K91 G95 E99 S100 L108 L113 T114 E115 L118

R119 T120 V121 L131 Y136 L140 A141 L142 T145 K146 P147 Y151 R157 N165 P166 Q168 ALA ARG ALA THR P173 K174 E175 H176 H177 L200 Q201 L202 Y203 Q204 V210 Y211 T218 S219 D222 V223 F229 V235 E236 K237 E244 L251 GLU LYS

• Molecule 3: PezT

Chain F: 77% 16% 5%

MET E2 I3 T7 D8 K12 L19 L23 R24 T23 K27 S28 S41 T46 H49 N59 I60 S70 Q79 Y82 G83 M111 L112 L113 T117 L118 R119 T120 V121 D122 V123 P124 A144 T145 K146 S150 E160 I163 I164 H165 PRO ASN GLN

ALA ARG THR PRO LYS HIS D178 F179 I180 V185 E198 D212 E215 Q225 F228 W232 S233 E236 K245 E249 K253

• Molecule 3: PezT

Chain H: 69% 24%

M1 T7 D8 S9 H13 A14 R17 R18 S21 R24 G25 K26 P32 I35 L36 L37 Q40 S41 G42 A43 R50 I51 K54 G58 I62 S70 H74 Q79 G83 K84 E88 A94 V98 S106 L113 L118 R119 T120

V121 D122 P124 K125 Q129 Y136 Q139 T145 E148 L152 G153 S153 T154 L155 E159 I163 T164 N165 P166 ASN GLN ALA ALA ALA THR PRO LYS GLU HIS D178 F179 M182 H183 I196 R199 Q204 R205 D206 R207 V210 T217 A221

L224 W232 L240 Q241 E244 K245 R246 L250 L251 E252 K253

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 80.52Å 102.86Å 254.44Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 47.67 – 3.20<br>47.67 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (47.67-3.20)<br>98.4 (47.67-3.20)                     | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.00 (at 3.19Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0005                                             | Depositor        |
| R, $R_{free}$                                                           | 0.214 , 0.277<br>0.211 , 0.274                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1726 reflections (4.91%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 90.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.014                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 79.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 11093                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 91.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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        |
| 2   | A     | 0.47         | 0/770   | 0.91        | 0/1039         |
| 2   | C     | 0.48         | 0/778   | 0.86        | 0/1049         |
| 2   | E     | 0.52         | 0/795   | 0.93        | 2/1071 (0.2%)  |
| 2   | G     | 0.53         | 0/778   | 0.92        | 1/1049 (0.1%)  |
| 3   | B     | 0.49         | 0/2010  | 0.85        | 0/2703         |
| 3   | D     | 0.49         | 0/2034  | 0.84        | 0/2736         |
| 3   | F     | 0.49         | 0/1972  | 0.86        | 0/2650         |
| 3   | H     | 0.54         | 0/1988  | 0.89        | 0/2672         |
| All | All   | 0.50         | 0/11125 | 0.87        | 3/14969 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | G     | 125 | ASN  | N-CA-C  | 6.54  | 119.40      | 111.82   |
| 2   | E     | 125 | ASN  | N-CA-C  | 6.23  | 118.07      | 111.28   |
| 2   | E     | 126 | ILE  | CB-CA-C | -5.61 | 104.70      | 112.04   |

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   | X     | 132   | 0        | 2        | 0       | 0            |
| 2   | A     | 759   | 0        | 740      | 22      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | C     | 767   | 0        | 749      | 22      | 0            |
| 2   | E     | 784   | 0        | 766      | 19      | 0            |
| 2   | G     | 767   | 0        | 749      | 23      | 0            |
| 3   | B     | 1979  | 0        | 1997     | 33      | 0            |
| 3   | D     | 2002  | 0        | 2023     | 38      | 0            |
| 3   | F     | 1944  | 0        | 1968     | 20      | 0            |
| 3   | H     | 1959  | 0        | 1987     | 43      | 0            |
| All | All   | 11093 | 0        | 10981    | 187     | 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 8.

The worst 5 of 187 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:G:104:ILE:HD11 | 3:H:17:ARG:HB2  | 1.51                     | 0.89              |
| 3:D:147:PRO:HB2  | 3:H:148:GLU:HG2 | 1.58                     | 0.85              |
| 2:G:79:ILE:HD13  | 3:H:50:ARG:HD2  | 1.61                     | 0.80              |
| 3:H:40:GLN:HB2   | 3:H:43:ALA:HB2  | 1.65                     | 0.79              |
| 2:C:131:THR:HG23 | 2:C:134:GLU:HB2 | 1.66                     | 0.77              |

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     | 90/158 (57%) | 84 (93%) | 5 (6%)  | 1 (1%)   | 11 43       |
| 2   | C     | 91/158 (58%) | 87 (96%) | 3 (3%)  | 1 (1%)   | 11 43       |
| 2   | E     | 93/158 (59%) | 88 (95%) | 5 (5%)  | 0        | 100 100     |
| 2   | G     | 91/158 (58%) | 87 (96%) | 4 (4%)  | 0        | 100 100     |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 3   | B     | 240/253 (95%)   | 218 (91%)  | 21 (9%) | 1 (0%)   | 30          | 62 |
| 3   | D     | 243/253 (96%)   | 226 (93%)  | 15 (6%) | 2 (1%)   | 16          | 50 |
| 3   | F     | 236/253 (93%)   | 221 (94%)  | 13 (6%) | 2 (1%)   | 16          | 50 |
| 3   | H     | 238/253 (94%)   | 224 (94%)  | 13 (6%) | 1 (0%)   | 30          | 62 |
| All | All   | 1322/1644 (80%) | 1235 (93%) | 79 (6%) | 8 (1%)   | 21          | 56 |

5 of 8 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 164 | ILE  |
| 3   | F     | 24  | ARG  |
| 2   | A     | 106 | ASP  |
| 2   | C     | 104 | ILE  |
| 3   | D     | 177 | HIS  |

### 5.3.2 Protein sidechains ⓘ

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     | 86/147 (58%)    | 83 (96%)   | 3 (4%)   | 32          | 64 |
| 2   | C     | 87/147 (59%)    | 84 (97%)   | 3 (3%)   | 32          | 64 |
| 2   | E     | 89/147 (60%)    | 81 (91%)   | 8 (9%)   | 9           | 34 |
| 2   | G     | 87/147 (59%)    | 78 (90%)   | 9 (10%)  | 7           | 28 |
| 3   | B     | 219/226 (97%)   | 198 (90%)  | 21 (10%) | 8           | 32 |
| 3   | D     | 222/226 (98%)   | 200 (90%)  | 22 (10%) | 7           | 31 |
| 3   | F     | 215/226 (95%)   | 199 (93%)  | 16 (7%)  | 13          | 43 |
| 3   | H     | 217/226 (96%)   | 194 (89%)  | 23 (11%) | 6           | 27 |
| All | All   | 1222/1492 (82%) | 1117 (91%) | 105 (9%) | 10          | 36 |

5 of 105 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | F     | 3   | ILE  |
| 3   | F     | 198 | GLU  |
| 3   | H     | 196 | ILE  |
| 3   | F     | 23  | THR  |
| 3   | F     | 118 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 100 | GLN  |
| 3   | H     | 129 | GLN  |
| 3   | H     | 49  | HIS  |
| 3   | H     | 133 | ASN  |
| 3   | D     | 72  | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | X     | 0/33            | -      | -             | -                     | -     |
| 2   | A     | 92/158 (58%)    | -0.14  | 2 (2%) 62 42  | 78, 88, 97, 104       | 0     |
| 2   | C     | 93/158 (58%)    | -0.18  | 0 100 100     | 79, 90, 105, 112      | 0     |
| 2   | E     | 95/158 (60%)    | -0.24  | 0 100 100     | 79, 89, 107, 114      | 0     |
| 2   | G     | 93/158 (58%)    | -0.17  | 1 (1%) 78 61  | 79, 89, 108, 111      | 0     |
| 3   | B     | 244/253 (96%)   | -0.03  | 1 (0%) 88 79  | 78, 91, 106, 115      | 0     |
| 3   | D     | 247/253 (97%)   | -0.24  | 1 (0%) 88 79  | 79, 89, 105, 114      | 0     |
| 3   | F     | 240/253 (94%)   | -0.23  | 2 (0%) 82 67  | 74, 89, 114, 123      | 0     |
| 3   | H     | 242/253 (95%)   | -0.19  | 4 (1%) 69 49  | 75, 90, 112, 130      | 0     |
| All | All   | 1346/1677 (80%) | -0.17  | 11 (0%) 82 67 | 74, 90, 107, 130      | 0     |

The worst 5 of 11 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | H     | 178 | ASP  | 6.6  |
| 3   | F     | 178 | ASP  | 4.0  |
| 3   | B     | 3   | ILE  | 3.6  |
| 3   | H     | 179 | PHE  | 3.5  |
| 3   | H     | 164 | ILE  | 2.8  |

### 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 oligosaccharides 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.