



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:42 PM GMT

PDB ID : 4A8J  
Title : Crystal Structure of the Elongator subcomplex Elp456  
Authors : Glatt, S.; Mueller, C.W.  
Deposited on : 2011-11-21  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

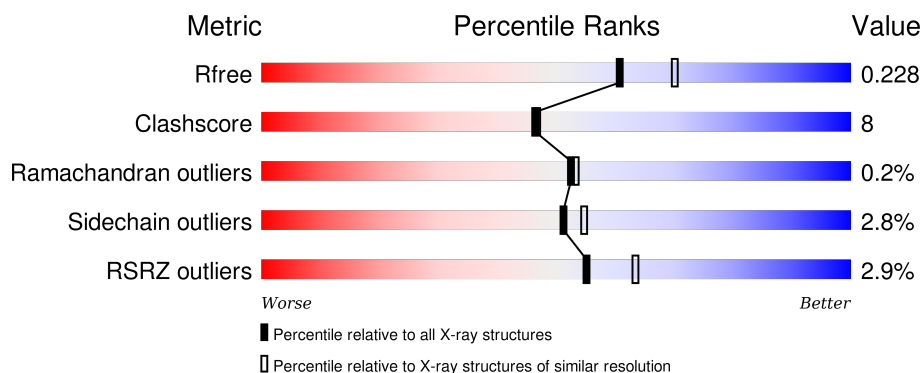
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 3939 (2.10-2.10)                                      |
| Clashscore            | 102246                      | 4460 (2.10-2.10)                                      |
| Ramachandran outliers | 100387                      | 4413 (2.10-2.10)                                      |
| Sidechain outliers    | 100360                      | 4414 (2.10-2.10)                                      |
| RSRZ outliers         | 91569                       | 3948 (2.10-2.10)                                      |

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  $\geq 3$ , 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  $\leq 5\%$ . 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   | A     | 361    | <div> <div>2%</div> <div>67% 9% 23%</div> </div>  |
| 1   | D     | 361    | <div> <div>2%</div> <div>69% 8% 22%</div> </div>  |
| 2   | B     | 270    | <div> <div>4%</div> <div>62% 18% 19%</div> </div> |
| 2   | E     | 270    | <div> <div>5%</div> <div>60% 20% 18%</div> </div> |
| 3   | C     | 280    | <div> <div>2%</div> <div>80% 14% 6%</div> </div>  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 3   | F     | 280    | <div><div><div>%</div><div><div></div></div><div>81%</div><div>12%</div><div>• 6%</div></div></div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13005 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 ELONGATOR COMPLEX PROTEIN 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 277      | Total | C    | N   | O   | Se | 26      | 0       | 0     |
|     |       |          | 2203  | 1419 | 376 | 399 | 9  |         |         |       |
| 1   | D     | 280      | Total | C    | N   | O   | Se | 34      | 0       | 0     |
|     |       |          | 2222  | 1432 | 379 | 402 | 9  |         |         |       |

- Molecule 2 is a protein called ELONGATOR COMPLEX PROTEIN 5.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 2   | B     | 220      | Total | C    | N   | O   | S | Se | 28      | 0       | 0     |
|     |       |          | 1781  | 1143 | 290 | 341 | 3 | 4  |         |         |       |
| 2   | E     | 221      | Total | C    | N   | O   | S | Se | 30      | 0       | 0     |
|     |       |          | 1787  | 1146 | 291 | 343 | 3 | 4  |         |         |       |

- Molecule 3 is a protein called ELONGATOR COMPLEX PROTEIN 6.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 3   | C     | 263      | Total | C    | N   | O   | S | Se | 25      | 0       | 0     |
|     |       |          | 2080  | 1324 | 352 | 397 | 4 | 3  |         |         |       |
| 3   | F     | 262      | Total | C    | N   | O   | S | Se | 14      | 0       | 0     |
|     |       |          | 2070  | 1319 | 350 | 394 | 4 | 3  |         |         |       |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -6      | MSE      | -      | EXPRESSION TAG | UNP Q04868 |
| C     | -5      | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| C     | -4      | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| C     | -3      | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| C     | -2      | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| C     | -1      | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| C     | 0       | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| F     | -6      | MSE      | -      | EXPRESSION TAG | UNP Q04868 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | -5      | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| F     | -4      | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| F     | -3      | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| F     | -2      | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| F     | -1      | HIS      | -      | EXPRESSION TAG | UNP Q04868 |
| F     | 0       | HIS      | -      | EXPRESSION TAG | UNP Q04868 |

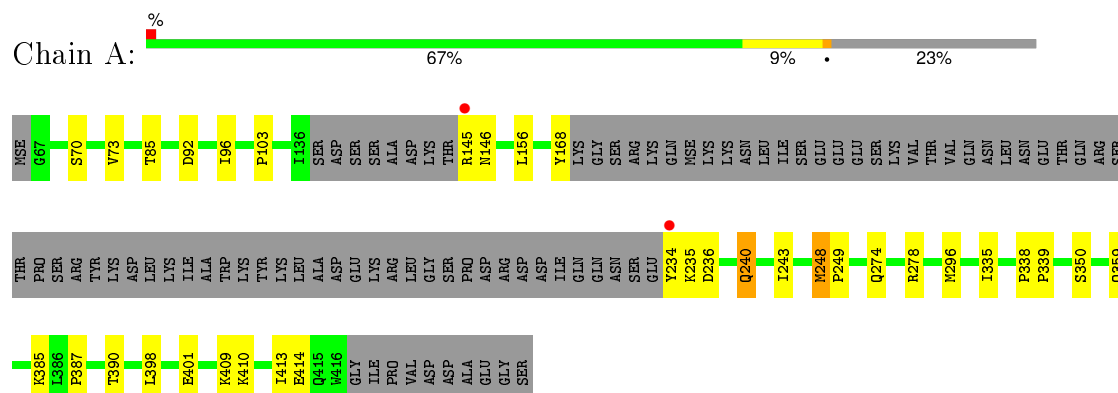
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | A     | 213      | Total O<br>213 213 | 0       | 0       |
| 4   | B     | 113      | Total O<br>113 113 | 0       | 0       |
| 4   | C     | 131      | Total O<br>131 131 | 0       | 0       |
| 4   | D     | 187      | Total O<br>187 187 | 0       | 0       |
| 4   | E     | 96       | Total O<br>96 96   | 0       | 0       |
| 4   | F     | 122      | Total O<br>122 122 | 0       | 0       |

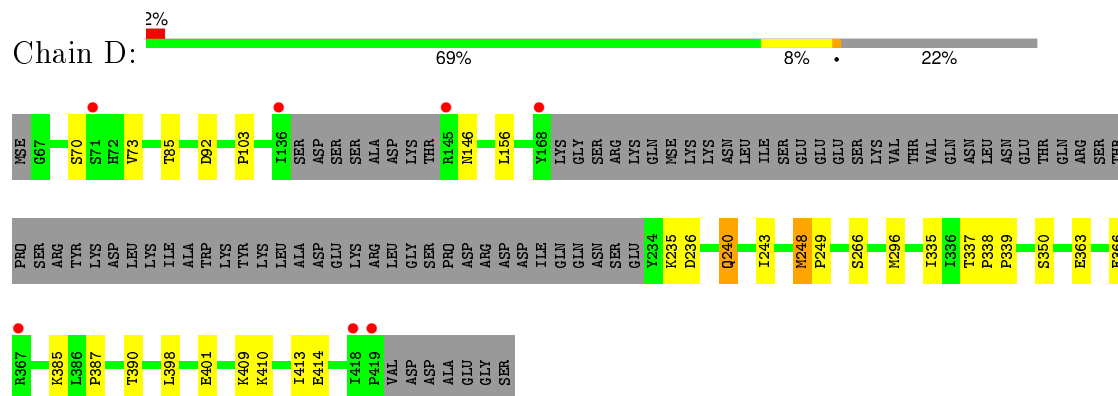
### 3 Residue-property plots [i](#)

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.

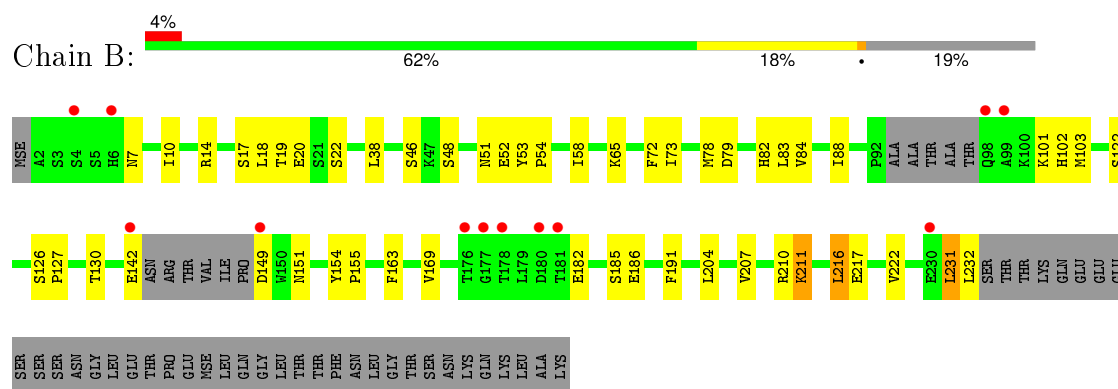
#### • Molecule 1: ELONGATOR COMPLEX PROTEIN 4



#### • Molecule 1: ELONGATOR COMPLEX PROTEIN 4



#### • Molecule 2: ELONGATOR COMPLEX PROTEIN 5



Chain E:

5% 60% 20% 18%

MSE A2 S3 S4 S5 S6 N7 T10 R14 S17 L18 T19 E20 S21 S22 L38 S46 K47 S48 K49 G50 N51 E52 Y53 P54 F58 I73 M78 D79 H82 L83 V84 I88 P92 A94 A95 T96 Q98 A99 K100 K101 M102 M103 I117 S126 P127 T130 E142 A143 T144 T145 I146 P147 M148 W149 L150 N151 Y154 P155 D156 L161 V169 V173 T176 E182 S185 E186 F191 D200 L204 V207 R210 K211 L216 E217 V222 N223 S224 N225 L231 L232 T233 T234 L235

Chain C:

2%

80%

14%

6%

MSE HIS HIS HIS HIS HIS MSE GLY SER VAL Q5 F12 P19 A20 H21 Q24 D25 S26 N27 F32 S38 Q41 T46 L49 E53 SER SER SER SER M68 R74 L79 K97 F112 M116 I117 K120 P121 A122 I125 M139

V158 L161 E165 C178 K179 I182 N186 S187 D188 I192 Y195 S202 Q205 N206 K209 M216 T226 GLY PHE A229 V232 R273

Chain F:

| Residue | Count | Percentage |
|---------|-------|------------|
| MSE     | 1     | 1%         |
| HIS     | 1     | 1%         |
| HIS     | 1     | 1%         |
| HIS     | 1     | 1%         |
| HIS     | 1     | 1%         |
| HIS     | 1     | 1%         |
| MSE     | 1     | 1%         |
| GLY     | 1     | 1%         |
| SER     | 1     | 1%         |
| VAL     | 1     | 1%         |
| Q5      | 1     | 1%         |
| F12     | 1     | 1%         |
| P19     | 1     | 1%         |
| A20     | 1     | 1%         |
| H21     | 1     | 1%         |
| D25     | 1     | 1%         |
| S26     | 1     | 1%         |
| T35     | 1     | 1%         |
| S38     | 1     | 1%         |
| Q41     | 1     | 1%         |
| L49     | 1     | 1%         |
| H62     | 1     | 1%         |
| GLU     | 1     | 1%         |
| SER     | 1     | 1%         |
| SER     | 1     | 1%         |
| SER     | 1     | 1%         |
| SER     | 1     | 1%         |
| H68     | 1     | 1%         |
| R74     | 1     | 1%         |
| L79     | 1     | 1%         |
| H84     | 1     | 1%         |
| K97     | 1     | 1%         |
| I117    | 1     | 1%         |
| R122    | 1     | 1%         |
| Q138    | 1     | 1%         |
| V158    | 1     | 1%         |
| L161    | 1     | 1%         |
| R176    | 1     | 1%         |
| Q177    | 1     | 1%         |
| K178    | 1     | 1%         |
| K179    | 1     | 1%         |
| I182    | 1     | 1%         |
| M186    | 1     | 1%         |
| I192    | 1     | 1%         |
| Y195    | 1     | 1%         |
| S202    | 1     | 1%         |
| Q205    | 1     | 1%         |
| M206    | 1     | 1%         |
| K209    | 1     | 1%         |
| M216    | 1     | 1%         |
| I217    | 1     | 1%         |
| M218    | 1     | 1%         |
| L219    | 1     | 1%         |
| N220    | 1     | 1%         |
| T236    | 1     | 1%         |
| GLY     | 1     | 1%         |
| PHE     | 1     | 1%         |
| A229    | 1     | 1%         |
| V232    | 1     | 1%         |
| K273    | 1     | 1%         |

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 105.73Å 124.89Å 146.42Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 46.20 – 2.10<br>46.20 – 2.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.8 (46.20-2.10)<br>99.0 (46.20-2.10)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.13  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.27 (at 2.10Å)   | Xtriage          |
| Refinement program  | PHENIX (PHENIX.REFINE)                                      | Depositor        |
| R, $R_{free}$   | 0.201 , 0.231<br>0.196 , 0.228                              | Depositor<br>DCC |
| $R_{free}$ test set   | 5598 reflections (5.00%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 30.5  | Xtriage          |
| Anisotropy  | 0.754   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 61.1   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Outliers  | 5 of 112115 reflections (0.004%)                            | Xtriage          |
| $F_o, F_c$ correlation  | 0.96  | EDS              |
| Total number of atoms   | 13005   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 42.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.52 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.5003e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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     | 0.46         | 0/2243         | 0.58        | 0/3022         |
| 1   | D     | 0.46         | 0/2263         | 0.58        | 0/3050         |
| 2   | B     | 0.43         | 0/1812         | 0.56        | 1/2451 (0.0%)  |
| 2   | E     | 0.42         | 0/1818         | 0.55        | 0/2459         |
| 3   | C     | 0.48         | 1/2120 (0.0%)  | 0.59        | 0/2878         |
| 3   | F     | 0.50         | 1/2110 (0.0%)  | 0.60        | 0/2865         |
| All | All   | 0.46         | 2/12366 (0.0%) | 0.58        | 1/16725 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | C     | 178 | CYS  | CB-SG | -5.45 | 1.73        | 1.81     |
| 3   | F     | 178 | CYS  | CB-SG | -5.19 | 1.73        | 1.81     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | B     | 211 | LYS  | CD-CE-NZ | 5.70 | 124.80      | 111.70   |

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     | 2203  | 0        | 2255     | 27      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | D     | 2222  | 0        | 2276     | 22      | 0            |
| 2   | B     | 1781  | 0        | 1775     | 34      | 0            |
| 2   | E     | 1787  | 0        | 1780     | 45      | 0            |
| 3   | C     | 2080  | 0        | 2056     | 30      | 0            |
| 3   | F     | 2070  | 0        | 2051     | 28      | 0            |
| 4   | A     | 213   | 0        | 0        | 8       | 0            |
| 4   | B     | 113   | 0        | 0        | 3       | 0            |
| 4   | C     | 131   | 0        | 0        | 4       | 0            |
| 4   | D     | 187   | 0        | 0        | 4       | 0            |
| 4   | E     | 96    | 0        | 0        | 5       | 0            |
| 4   | F     | 122   | 0        | 0        | 5       | 0            |
| All | All   | 13005 | 0        | 12193    | 181     | 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.

All (181) 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:240:GLN:OE1 | 1:D:410:LYS:HE3  | 1.56                     | 1.06              |
| 1:A:240:GLN:OE1 | 1:A:410:LYS:HE3  | 1.55                     | 1.04              |
| 2:E:54:PRO:HG2  | 2:E:102:HIS:ND1  | 1.74                     | 1.03              |
| 3:F:35:THR:OG1  | 3:F:220:ASN:ND2  | 1.99                     | 0.94              |
| 2:E:92:PRO:HD3  | 2:E:102:HIS:CD2  | 2.04                     | 0.92              |
| 1:A:168:TYR:O   | 4:A:2073:HOH:O   | 1.96                     | 0.82              |
| 2:E:156:ASP:OD2 | 4:E:2063:HOH:O   | 2.01                     | 0.78              |
| 2:E:46:SER:O    | 2:E:51:ASN:HB2   | 1.84                     | 0.76              |
| 2:E:18:LEU:HD21 | 2:E:103:MSE:CE   | 2.17                     | 0.74              |
| 3:C:26:SER:HA   | 3:C:179:LYS:NZ   | 2.03                     | 0.74              |
| 3:F:19:PRO:HB3  | 3:F:21:HIS:CE1   | 2.23                     | 0.74              |
| 2:E:54:PRO:HG2  | 2:E:102:HIS:CE1  | 2.23                     | 0.73              |
| 3:C:112:PHE:CE2 | 3:C:117:ILE:HD11 | 2.24                     | 0.73              |
| 3:F:26:SER:HA   | 3:F:179:LYS:NZ   | 2.04                     | 0.73              |
| 2:B:46:SER:O    | 2:B:51:ASN:HB2   | 1.88                     | 0.73              |
| 2:B:18:LEU:HD21 | 2:B:103:MSE:CE   | 2.19                     | 0.72              |
| 3:C:19:PRO:HB3  | 3:C:21:HIS:CE1   | 2.24                     | 0.71              |
| 2:E:149:ASP:N   | 4:E:2055:HOH:O   | 2.24                     | 0.70              |
| 3:C:112:PHE:HE2 | 3:C:117:ILE:HD11 | 1.57                     | 0.69              |
| 2:B:149:ASP:N   | 4:B:2066:HOH:O   | 2.24                     | 0.69              |
| 2:E:14:ARG:NH1  | 2:E:20:GLU:OE1   | 2.24                     | 0.69              |
| 2:E:92:PRO:CD   | 2:E:102:HIS:CD2  | 2.77                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:2134:HOH:O   | 2:B:151:ASN:ND2  | 2.27                     | 0.68              |
| 3:F:41:GLN:NE2   | 4:F:2018:HOH:O   | 2.27                     | 0.67              |
| 1:D:366:GLU:OE1  | 2:E:3:SER:HB3    | 1.94                     | 0.67              |
| 3:C:41:GLN:NE2   | 4:C:2022:HOH:O   | 2.28                     | 0.66              |
| 2:E:92:PRO:HD3   | 2:E:102:HIS:NE2  | 2.11                     | 0.65              |
| 2:B:54:PRO:HG2   | 2:B:102:HIS:CE1  | 2.31                     | 0.65              |
| 3:F:25:ASP:O     | 4:F:2011:HOH:O   | 2.14                     | 0.65              |
| 1:A:234:TYR:N    | 4:A:2076:HOH:O   | 2.30                     | 0.65              |
| 3:C:165:GLU:OE1  | 4:C:2076:HOH:O   | 2.15                     | 0.64              |
| 1:A:278:ARG:NH2  | 4:A:2121:HOH:O   | 2.17                     | 0.64              |
| 2:E:7:ASN:OD1    | 4:E:2002:HOH:O   | 2.15                     | 0.64              |
| 3:C:139:ASN:ND2  | 4:C:2068:HOH:O   | 2.31                     | 0.63              |
| 1:A:398:LEU:HG   | 1:A:401:GLU:HG3  | 1.80                     | 0.63              |
| 2:E:78:MSE:HE3   | 2:E:83:LEU:HD13  | 1.80                     | 0.62              |
| 2:B:78:MSE:HE3   | 2:B:83:LEU:HD13  | 1.81                     | 0.62              |
| 3:C:205:GLN:NE2  | 3:C:206:ASN:OD1  | 2.33                     | 0.61              |
| 3:C:205:GLN:OE1  | 3:C:209:LYS:NZ   | 2.28                     | 0.61              |
| 4:D:2112:HOH:O   | 2:E:151:ASN:ND2  | 2.33                     | 0.61              |
| 1:D:398:LEU:HG   | 1:D:401:GLU:HG3  | 1.82                     | 0.61              |
| 3:F:205:GLN:OE1  | 3:F:209:LYS:NZ   | 2.26                     | 0.60              |
| 2:B:163:PHE:O    | 4:B:2076:HOH:O   | 2.16                     | 0.60              |
| 3:F:205:GLN:NE2  | 3:F:206:ASN:OD1  | 2.34                     | 0.60              |
| 2:E:18:LEU:HD21  | 2:E:103:MSE:HE2  | 1.84                     | 0.59              |
| 2:B:54:PRO:HG2   | 2:B:102:HIS:ND1  | 2.17                     | 0.59              |
| 2:E:79:ASP:OD1   | 2:E:82:HIS:ND1   | 2.35                     | 0.59              |
| 2:B:18:LEU:HD21  | 2:B:103:MSE:HE2  | 1.84                     | 0.59              |
| 1:A:350:SER:HB3  | 1:A:387:PRO:HD3  | 1.85                     | 0.59              |
| 2:E:22:SER:O     | 2:E:130:THR:HG23 | 2.04                     | 0.58              |
| 3:C:12:PHE:CZ    | 3:C:216:MSE:HE1  | 2.39                     | 0.58              |
| 1:A:240:GLN:OE1  | 1:A:410:LYS:CE   | 2.43                     | 0.57              |
| 3:C:26:SER:HA    | 3:C:179:LYS:HZ3  | 1.69                     | 0.56              |
| 3:F:12:PHE:CZ    | 3:F:216:MSE:HE1  | 2.40                     | 0.56              |
| 2:E:18:LEU:HD21  | 2:E:103:MSE:HE3  | 1.86                     | 0.56              |
| 1:A:73:VAL:HG21  | 1:A:236:ASP:HB2  | 1.86                     | 0.56              |
| 3:F:26:SER:HA    | 3:F:179:LYS:HZ1  | 1.68                     | 0.56              |
| 2:E:49:LYS:O     | 4:E:2014:HOH:O   | 2.18                     | 0.55              |
| 2:E:231:LEU:HG   | 2:E:232:LEU:H    | 1.70                     | 0.55              |
| 1:D:73:VAL:HG21  | 1:D:236:ASP:HB2  | 1.88                     | 0.55              |
| 2:E:58:ILE:N     | 2:E:58:ILE:HD12  | 2.22                     | 0.55              |
| 1:A:243:ILE:HD12 | 1:A:409:LYS:O    | 2.07                     | 0.54              |
| 2:B:58:ILE:N     | 2:B:58:ILE:HD12  | 2.24                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:17:SER:OG    | 2:B:19:THR:HG23  | 2.09                     | 0.53              |
| 1:D:243:ILE:HD12 | 1:D:409:LYS:O    | 2.07                     | 0.53              |
| 3:F:138:GLN:HG3  | 4:F:2077:HOH:O   | 2.09                     | 0.53              |
| 3:F:218:ASN:HD21 | 3:F:220:ASN:HD21 | 1.56                     | 0.53              |
| 2:E:19:THR:OG1   | 2:E:20:GLU:N     | 2.41                     | 0.52              |
| 2:B:22:SER:O     | 2:B:130:THR:HG23 | 2.09                     | 0.52              |
| 1:D:266:SER:HB3  | 3:F:117:ILE:HD12 | 1.91                     | 0.52              |
| 2:B:18:LEU:HD21  | 2:B:103:MSE:HE3  | 1.91                     | 0.52              |
| 3:C:116:ASN:O    | 3:C:125:ILE:HG12 | 2.10                     | 0.52              |
| 2:B:79:ASP:OD1   | 2:B:82:HIS:ND1   | 2.36                     | 0.52              |
| 3:F:26:SER:HA    | 3:F:179:LYS:HZ2  | 1.73                     | 0.52              |
| 1:A:338:PRO:HB3  | 3:C:192:ILE:HG21 | 1.92                     | 0.52              |
| 2:B:19:THR:OG1   | 2:B:20:GLU:N     | 2.43                     | 0.52              |
| 1:D:350:SER:HB3  | 1:D:387:PRO:HD3  | 1.92                     | 0.52              |
| 1:A:385:LYS:HG3  | 1:A:390:THR:HG21 | 1.91                     | 0.52              |
| 2:E:173:VAL:O    | 4:E:2072:HOH:O   | 2.19                     | 0.51              |
| 2:B:231:LEU:HG   | 2:B:232:LEU:H    | 1.75                     | 0.51              |
| 1:D:338:PRO:HB3  | 3:F:192:ILE:HG21 | 1.91                     | 0.51              |
| 2:E:17:SER:OG    | 2:E:19:THR:HG23  | 2.11                     | 0.51              |
| 3:C:26:SER:HA    | 3:C:179:LYS:HZ1  | 1.72                     | 0.50              |
| 1:A:335:ILE:HD12 | 4:A:2159:HOH:O   | 2.10                     | 0.50              |
| 3:F:84:HIS:HE1   | 4:F:2018:HOH:O   | 1.94                     | 0.50              |
| 2:B:73:ILE:CG2   | 2:B:78:MSE:HE1   | 2.41                     | 0.50              |
| 1:A:274:GLN:OE1  | 4:A:2119:HOH:O   | 2.19                     | 0.50              |
| 2:B:10:ILE:O     | 2:B:14:ARG:HG3   | 2.11                     | 0.50              |
| 2:B:84:VAL:O     | 2:B:88:ILE:HG13  | 2.12                     | 0.49              |
| 1:A:85:THR:HA    | 1:A:103:PRO:HA   | 1.94                     | 0.49              |
| 1:D:85:THR:HA    | 1:D:103:PRO:HA   | 1.95                     | 0.49              |
| 3:F:49:LEU:HD13  | 3:F:182:ILE:HD13 | 1.95                     | 0.49              |
| 1:D:73:VAL:HG21  | 1:D:236:ASP:CB   | 2.43                     | 0.48              |
| 2:E:126:SER:OG   | 2:E:127:PRO:HD2  | 2.14                     | 0.48              |
| 1:D:235:LYS:O    | 1:D:236:ASP:HB2  | 2.12                     | 0.48              |
| 2:E:231:LEU:HG   | 2:E:232:LEU:N    | 2.28                     | 0.48              |
| 2:E:18:LEU:CD2   | 2:E:103:MSE:HE3  | 2.44                     | 0.48              |
| 2:E:10:ILE:O     | 2:E:14:ARG:HG3   | 2.13                     | 0.48              |
| 3:C:38:SER:HB3   | 3:C:186:ASN:HD21 | 1.79                     | 0.48              |
| 2:B:182:GLU:O    | 2:B:186:GLU:HG2  | 2.14                     | 0.48              |
| 3:F:38:SER:HB3   | 3:F:186:ASN:HD21 | 1.79                     | 0.47              |
| 3:C:12:PHE:HZ    | 3:C:216:MSE:HE1  | 1.78                     | 0.47              |
| 2:E:92:PRO:HD3   | 2:E:102:HIS:HD2  | 1.69                     | 0.47              |
| 2:B:231:LEU:HG   | 2:B:232:LEU:N    | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:73:ILE:CG2   | 2:E:78:MSE:HE1   | 2.44                     | 0.47              |
| 3:F:202:SER:HA   | 3:F:205:GLN:HG3  | 1.97                     | 0.47              |
| 3:C:179:LYS:HD2  | 3:C:179:LYS:HA   | 1.65                     | 0.47              |
| 2:B:73:ILE:CG2   | 2:B:78:MSE:CE    | 2.93                     | 0.47              |
| 2:E:18:LEU:HD22  | 2:E:18:LEU:N     | 2.29                     | 0.46              |
| 1:A:73:VAL:CG2   | 1:A:236:ASP:HB2  | 2.44                     | 0.46              |
| 1:D:73:VAL:CG2   | 1:D:236:ASP:HB2  | 2.45                     | 0.46              |
| 1:D:338:PRO:HB2  | 1:D:339:PRO:HD3  | 1.97                     | 0.46              |
| 2:B:53:TYR:CD1   | 2:B:101:LYS:HB3  | 2.51                     | 0.46              |
| 2:B:126:SER:OG   | 2:B:127:PRO:HD2  | 2.16                     | 0.46              |
| 2:E:53:TYR:CD1   | 2:E:101:LYS:HB3  | 2.51                     | 0.46              |
| 1:A:235:LYS:O    | 1:A:236:ASP:HB2  | 2.15                     | 0.46              |
| 1:A:73:VAL:HG21  | 1:A:236:ASP:CB   | 2.46                     | 0.46              |
| 1:D:385:LYS:HG3  | 1:D:390:THR:HG21 | 1.96                     | 0.46              |
| 2:E:182:GLU:O    | 2:E:186:GLU:HG2  | 2.16                     | 0.45              |
| 2:B:18:LEU:HD22  | 2:B:18:LEU:N     | 2.31                     | 0.45              |
| 3:F:202:SER:HA   | 3:F:205:GLN:CG   | 2.47                     | 0.45              |
| 2:E:84:VAL:O     | 2:E:88:ILE:HG13  | 2.16                     | 0.45              |
| 3:F:12:PHE:HZ    | 3:F:216:MSE:HE1  | 1.80                     | 0.45              |
| 1:D:240:GLN:OE1  | 1:D:410:LYS:CE   | 2.45                     | 0.45              |
| 2:E:154:TYR:CD1  | 2:E:155:PRO:HD2  | 2.52                     | 0.44              |
| 1:A:338:PRO:HB2  | 1:A:339:PRO:HD3  | 1.98                     | 0.44              |
| 2:E:73:ILE:CG2   | 2:E:78:MSE:CE    | 2.95                     | 0.44              |
| 2:B:38:LEU:HD21  | 2:B:169:VAL:HG11 | 2.00                     | 0.44              |
| 3:C:122:ARG:HG3  | 3:C:158:VAL:HG11 | 2.00                     | 0.43              |
| 1:D:335:ILE:HD12 | 4:D:2131:HOH:O   | 2.16                     | 0.43              |
| 3:C:202:SER:HA   | 3:C:205:GLN:HG3  | 2.00                     | 0.43              |
| 3:F:122:ARG:HG3  | 3:F:158:VAL:HG11 | 2.00                     | 0.43              |
| 4:B:2016:HOH:O   | 3:F:176:ARG:NH2  | 2.17                     | 0.43              |
| 3:C:229:ALA:HB3  | 3:C:232:VAL:HG12 | 2.01                     | 0.43              |
| 2:B:154:TYR:CD1  | 2:B:155:PRO:HD2  | 2.54                     | 0.43              |
| 1:D:248:MSE:HA   | 1:D:249:PRO:HA   | 1.87                     | 0.43              |
| 3:C:38:SER:OG    | 3:C:188:ASP:OD2  | 2.31                     | 0.43              |
| 1:A:359:GLN:HG3  | 2:B:216:LEU:HD23 | 2.01                     | 0.43              |
| 1:A:92:ASP:HB3   | 1:A:413:ILE:HB   | 2.00                     | 0.43              |
| 2:E:200:ASP:O    | 2:E:224:SER:OG   | 2.36                     | 0.43              |
| 2:E:38:LEU:HD21  | 2:E:169:VAL:HG11 | 2.01                     | 0.43              |
| 3:C:49:LEU:HD13  | 3:C:182:ILE:HD13 | 2.01                     | 0.43              |
| 2:B:7:ASN:HB3    | 2:B:10:ILE:HD12  | 2.01                     | 0.43              |
| 2:E:54:PRO:CG    | 2:E:102:HIS:CE1  | 2.99                     | 0.42              |
| 2:B:18:LEU:CD2   | 2:B:103:MSE:HE3  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:120:LYS:HA   | 3:C:121:PRO:HD3  | 1.85                     | 0.42              |
| 1:D:156:LEU:HD12 | 1:D:296:MSE:HG3  | 2.00                     | 0.42              |
| 1:A:274:GLN:NE2  | 4:A:2120:HOH:O   | 2.25                     | 0.42              |
| 3:F:179:LYS:HD2  | 3:F:179:LYS:HA   | 1.72                     | 0.42              |
| 1:A:248:MSE:HA   | 1:A:249:PRO:HA   | 1.88                     | 0.42              |
| 2:B:207:VAL:HG22 | 2:B:217:GLU:HG3  | 2.01                     | 0.42              |
| 3:F:12:PHE:CE1   | 3:F:216:MSE:HE1  | 2.55                     | 0.42              |
| 3:C:122:ARG:HD2  | 3:C:161:LEU:HA   | 2.02                     | 0.42              |
| 2:B:204:LEU:HD22 | 2:B:222:VAL:HG21 | 2.02                     | 0.42              |
| 3:C:202:SER:HA   | 3:C:205:GLN:CG   | 2.50                     | 0.42              |
| 1:A:235:LYS:HA   | 4:A:2081:HOH:O   | 2.19                     | 0.42              |
| 3:F:122:ARG:HD2  | 3:F:161:LEU:HA   | 2.02                     | 0.42              |
| 1:A:156:LEU:HD12 | 1:A:296:MSE:HG3  | 2.02                     | 0.42              |
| 1:D:92:ASP:HB3   | 1:D:413:ILE:HB   | 2.02                     | 0.41              |
| 2:E:92:PRO:HD3   | 2:E:102:HIS:HE2  | 1.83                     | 0.41              |
| 2:E:78:MSE:HE3   | 2:E:83:LEU:CD1   | 2.46                     | 0.41              |
| 2:B:210:ARG:NE   | 2:B:216:LEU:HD13 | 2.35                     | 0.41              |
| 2:E:204:LEU:HD22 | 2:E:222:VAL:HG21 | 2.02                     | 0.41              |
| 1:D:337:THR:HG23 | 4:D:2132:HOH:O   | 2.20                     | 0.41              |
| 1:A:235:LYS:HG2  | 1:A:236:ASP:OD2  | 2.21                     | 0.41              |
| 2:E:210:ARG:NE   | 2:E:216:LEU:HD13 | 2.35                     | 0.41              |
| 3:C:26:SER:O     | 3:C:27:ASN:HB2   | 2.20                     | 0.41              |
| 1:A:350:SER:HB3  | 1:A:387:PRO:CD   | 2.48                     | 0.41              |
| 2:B:65:LYS:HG3   | 2:B:72:PHE:CD1   | 2.56                     | 0.41              |
| 3:C:12:PHE:CE1   | 3:C:216:MSE:HE1  | 2.56                     | 0.41              |
| 3:C:32:PHE:HB2   | 3:C:182:ILE:HG12 | 2.02                     | 0.41              |
| 3:F:229:ALA:HB3  | 3:F:232:VAL:HG12 | 2.03                     | 0.41              |
| 2:E:117:ILE:HD12 | 2:E:161:LEU:HD21 | 2.03                     | 0.41              |
| 3:C:122:ARG:HG3  | 3:C:158:VAL:CG1  | 2.51                     | 0.40              |
| 1:D:156:LEU:H    | 1:D:296:MSE:SE   | 2.54                     | 0.40              |
| 1:D:363:GLU:HB3  | 4:D:2151:HOH:O   | 2.21                     | 0.40              |
| 3:F:122:ARG:HG3  | 3:F:158:VAL:CG1  | 2.52                     | 0.40              |
| 1:A:96:ILE:HD13  | 1:A:96:ILE:HA    | 1.89                     | 0.40              |
| 3:F:5:GLN:O      | 4:F:2001:HOH:O   | 2.22                     | 0.40              |
| 3:C:5:GLN:O      | 4:C:2001:HOH:O   | 2.22                     | 0.40              |
| 2:E:207:VAL:HG22 | 2:E:217:GLU:HG3  | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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     | 271/361 (75%)   | 260 (96%)  | 11 (4%) | 0        | 100         | 100 |
| 1   | D     | 274/361 (76%)   | 263 (96%)  | 11 (4%) | 0        | 100         | 100 |
| 2   | B     | 214/270 (79%)   | 207 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 2   | E     | 215/270 (80%)   | 208 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 3   | C     | 257/280 (92%)   | 245 (95%)  | 11 (4%) | 1 (0%)   | 39          | 37  |
| 3   | F     | 256/280 (91%)   | 246 (96%)  | 8 (3%)  | 2 (1%)   | 24          | 17  |
| All | All   | 1487/1822 (82%) | 1429 (96%) | 55 (4%) | 3 (0%)   | 52          | 53  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | F     | 195 | TYR  |
| 3   | C     | 195 | TYR  |
| 3   | F     | 117 | ILE  |

### 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 |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 250/315 (79%) | 244 (98%) | 6 (2%)   | 57          | 61 |
| 1   | D     | 252/315 (80%) | 247 (98%) | 5 (2%)   | 63          | 68 |
| 2   | B     | 207/246 (84%) | 198 (96%) | 9 (4%)   | 35          | 34 |
| 2   | E     | 208/246 (85%) | 198 (95%) | 10 (5%)  | 31          | 29 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 3   | C     | 244/257 (95%)   | 239 (98%)  | 5 (2%)   | 63          | 68 |
| 3   | F     | 243/257 (95%)   | 238 (98%)  | 5 (2%)   | 61          | 66 |
| All | All   | 1404/1636 (86%) | 1364 (97%) | 40 (3%)  | 51          | 55 |

All (40) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 70  | SER  |
| 1   | A     | 145 | ARG  |
| 1   | A     | 146 | ASN  |
| 1   | A     | 240 | GLN  |
| 1   | A     | 248 | MSE  |
| 1   | A     | 414 | GLU  |
| 2   | B     | 48  | SER  |
| 2   | B     | 52  | GLU  |
| 2   | B     | 122 | SER  |
| 2   | B     | 142 | GLU  |
| 2   | B     | 185 | SER  |
| 2   | B     | 191 | PHE  |
| 2   | B     | 211 | LYS  |
| 2   | B     | 216 | LEU  |
| 2   | B     | 231 | LEU  |
| 3   | C     | 68  | MSE  |
| 3   | C     | 74  | ARG  |
| 3   | C     | 79  | LEU  |
| 3   | C     | 97  | LYS  |
| 3   | C     | 216 | MSE  |
| 1   | D     | 70  | SER  |
| 1   | D     | 146 | ASN  |
| 1   | D     | 240 | GLN  |
| 1   | D     | 248 | MSE  |
| 1   | D     | 414 | GLU  |
| 2   | E     | 48  | SER  |
| 2   | E     | 52  | GLU  |
| 2   | E     | 101 | LYS  |
| 2   | E     | 122 | SER  |
| 2   | E     | 142 | GLU  |
| 2   | E     | 185 | SER  |
| 2   | E     | 191 | PHE  |
| 2   | E     | 211 | LYS  |
| 2   | E     | 216 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 231 | LEU  |
| 3   | F     | 68  | MSE  |
| 3   | F     | 74  | ARG  |
| 3   | F     | 79  | LEU  |
| 3   | F     | 97  | LYS  |
| 3   | F     | 216 | MSE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | F     | 220 | ASN  |

### 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 ⓘ

### 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<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   | A     | 268/361 (74%)   | -0.35  | 2 (0%) 89 91  | 20, 33, 56, 88        | 8 (2%)  |
| 1   | D     | 271/361 (75%)   | -0.26  | 7 (2%) 59 66  | 21, 35, 61, 106       | 12 (4%) |
| 2   | B     | 216/270 (80%)   | 0.02   | 12 (5%) 28 36 | 27, 43, 75, 124       | 9 (4%)  |
| 2   | E     | 217/270 (80%)   | 0.09   | 14 (6%) 22 29 | 27, 44, 80, 144       | 9 (4%)  |
| 3   | C     | 260/280 (92%)   | -0.05  | 5 (1%) 70 75  | 22, 35, 75, 190       | 7 (2%)  |
| 3   | F     | 259/280 (92%)   | -0.03  | 3 (1%) 81 85  | 22, 34, 76, 208       | 7 (2%)  |
| All | All   | 1491/1822 (81%) | -0.11  | 43 (2%) 55 63 | 20, 36, 73, 208       | 52 (3%) |

All (43) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 142 | GLU  | 7.8  |
| 1   | D     | 419 | PRO  | 5.3  |
| 2   | B     | 6   | HIS  | 5.2  |
| 2   | B     | 142 | GLU  | 5.2  |
| 1   | D     | 418 | ILE  | 4.2  |
| 2   | B     | 99  | ALA  | 3.9  |
| 2   | E     | 52  | GLU  | 3.8  |
| 2   | B     | 176 | THR  | 3.6  |
| 2   | E     | 2   | ALA  | 3.3  |
| 3   | F     | 220 | ASN  | 3.3  |
| 2   | B     | 4   | SER  | 3.2  |
| 2   | B     | 180 | ASP  | 3.1  |
| 2   | E     | 99  | ALA  | 3.1  |
| 2   | E     | 150 | TRP  | 2.9  |
| 1   | D     | 145 | ARG  | 2.9  |
| 3   | C     | 229 | ALA  | 2.9  |
| 3   | C     | 117 | ILE  | 2.8  |
| 3   | F     | 226 | THR  | 2.7  |
| 1   | D     | 71  | SER  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 24  | GLN  | 2.7  |
| 2   | E     | 6   | HIS  | 2.6  |
| 2   | B     | 230 | GLU  | 2.6  |
| 2   | E     | 176 | THR  | 2.6  |
| 1   | A     | 145 | ARG  | 2.5  |
| 2   | B     | 178 | THR  | 2.5  |
| 2   | E     | 88  | ILE  | 2.5  |
| 2   | E     | 53  | TYR  | 2.5  |
| 2   | B     | 149 | ASP  | 2.4  |
| 2   | B     | 177 | GLY  | 2.4  |
| 1   | D     | 136 | ILE  | 2.4  |
| 1   | A     | 234 | TYR  | 2.3  |
| 3   | F     | 20  | ALA  | 2.3  |
| 2   | E     | 233 | SER  | 2.3  |
| 3   | C     | 46  | ILE  | 2.2  |
| 1   | D     | 367 | ARG  | 2.1  |
| 2   | E     | 3   | SER  | 2.1  |
| 1   | D     | 168 | TYR  | 2.1  |
| 2   | E     | 4   | SER  | 2.1  |
| 2   | B     | 181 | THR  | 2.1  |
| 3   | C     | 116 | ASN  | 2.1  |
| 2   | E     | 225 | ASN  | 2.0  |
| 2   | E     | 231 | LEU  | 2.0  |
| 2   | B     | 98  | GLN  | 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.