



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:07 AM GMT

PDB ID : 3O3W  
Title : Crystal Structure of BH2092 protein (residues 14-131) from *Bacillus halodurans*, Northeast Structural Genomics Consortium Target BhR228A  
Authors : Forouhar, F.; Neely, H.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Ciccocanti, C.; Lee, D.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2010-07-26  
Resolution : 2.91 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.

---

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

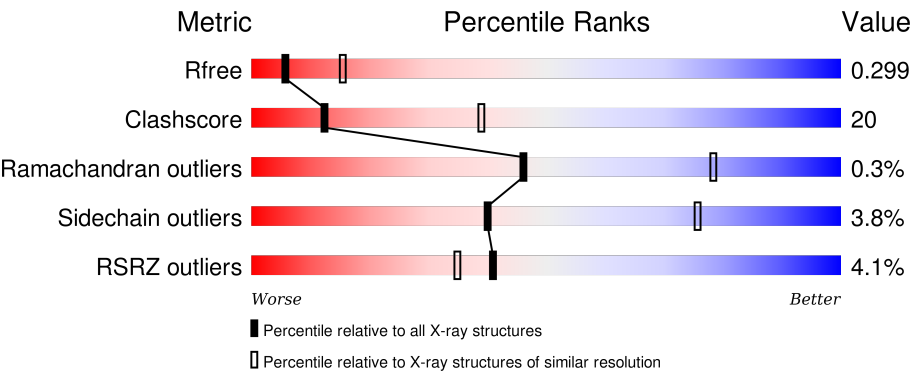
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.91 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.



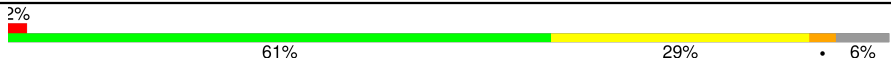

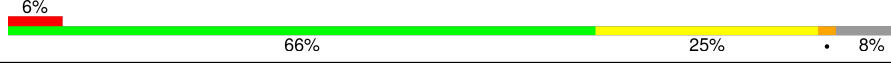
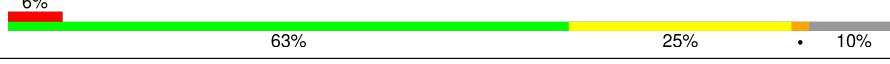
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1643 (2.94-2.90)                                      |
| Clashscore            | 102246                      | 1871 (2.94-2.90)                                      |
| Ramachandran outliers | 100387                      | 1824 (2.94-2.90)                                      |
| Sidechain outliers    | 100360                      | 1826 (2.94-2.90)                                      |
| RSRZ outliers         | 91569                       | 1650 (2.94-2.90)                                      |

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     | 126    | <div><div>2%</div><div>63%29%6%</div></div> |
| 1   | B     | 126    | <div><div>2%</div><div>60%31%7%</div></div> |
| 1   | C     | 126    | <div><div>2%</div><div>60%30%6%</div></div> |
| 1   | D     | 126    | <div><div>%</div><div>65%25%10%</div></div> |
| 1   | E     | 126    | <div><div>2%</div><div>55%36%6%</div></div> |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | F     | 126    |  |
| 1   | G     | 126    |  |
| 1   | H     | 126    |  |
| 1   | I     | 126    |  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8353 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 BH2092 protein.

| Mol | Chain | Residues | Atoms |     |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 118      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 928   | 591 | 159 | 174 | 3 | 1  |         |         |       |
| 1   | B     | 117      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 928   | 591 | 158 | 175 | 3 | 1  |         |         |       |
| 1   | C     | 118      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 933   | 594 | 159 | 176 | 3 | 1  |         |         |       |
| 1   | D     | 114      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 907   | 578 | 155 | 170 | 3 | 1  |         |         |       |
| 1   | E     | 118      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 933   | 594 | 159 | 176 | 3 | 1  |         |         |       |
| 1   | F     | 118      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 929   | 591 | 161 | 173 | 3 | 1  |         |         |       |
| 1   | G     | 114      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 907   | 578 | 155 | 170 | 3 | 1  |         |         |       |
| 1   | H     | 116      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 919   | 586 | 157 | 172 | 3 | 1  |         |         |       |
| 1   | I     | 113      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 890   | 567 | 153 | 166 | 3 | 1  |         |         |       |

There are 72 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 132     | LEU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| A     | 133     | GLU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| A     | 134     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| A     | 135     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| A     | 136     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| A     | 137     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| A     | 138     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| A     | 139     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| B     | 132     | LEU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| B     | 133     | GLU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| B     | 134     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 135     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| B     | 136     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| B     | 137     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| B     | 138     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| B     | 139     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| C     | 132     | LEU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| C     | 133     | GLU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| C     | 134     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| C     | 135     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| C     | 136     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| C     | 137     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| C     | 138     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| C     | 139     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| D     | 132     | LEU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| D     | 133     | GLU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| D     | 134     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| D     | 135     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| D     | 136     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| D     | 137     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| D     | 138     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| D     | 139     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| E     | 132     | LEU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| E     | 133     | GLU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| E     | 134     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| E     | 135     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| E     | 136     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| E     | 137     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| E     | 138     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| E     | 139     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| F     | 132     | LEU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| F     | 133     | GLU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| F     | 134     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| F     | 135     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| F     | 136     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| F     | 137     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| F     | 138     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| F     | 139     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| G     | 132     | LEU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| G     | 133     | GLU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| G     | 134     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| G     | 135     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| G     | 136     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| G     | 137     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| G     | 138     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| G     | 139     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| H     | 132     | LEU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| H     | 133     | GLU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| H     | 134     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| H     | 135     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| H     | 136     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| H     | 137     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| H     | 138     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| H     | 139     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| I     | 132     | LEU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| I     | 133     | GLU      | -      | EXPRESSION TAG | UNP Q9KB42 |
| I     | 134     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| I     | 135     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| I     | 136     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| I     | 137     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| I     | 138     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |
| I     | 139     | HIS      | -      | EXPRESSION TAG | UNP Q9KB42 |

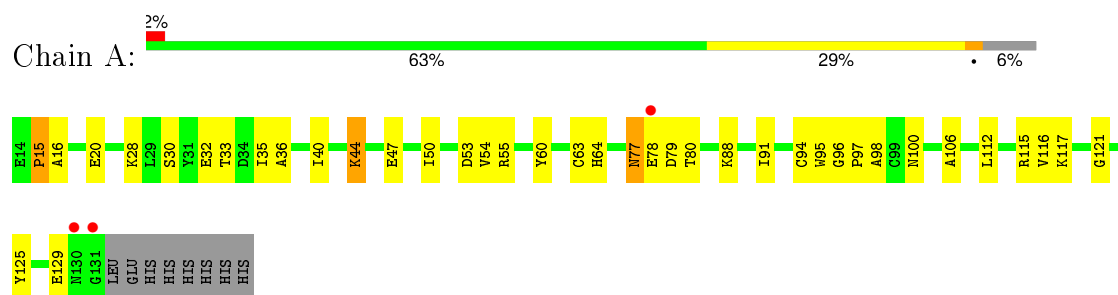
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 2   | A     | 14       | Total O<br>14 14 | 0       | 0       |
| 2   | B     | 9        | Total O<br>9 9   | 0       | 0       |
| 2   | C     | 6        | Total O<br>6 6   | 0       | 0       |
| 2   | D     | 10       | Total O<br>10 10 | 0       | 0       |
| 2   | E     | 11       | Total O<br>11 11 | 0       | 0       |
| 2   | F     | 7        | Total O<br>7 7   | 0       | 0       |
| 2   | G     | 10       | Total O<br>10 10 | 0       | 0       |
| 2   | H     | 2        | Total O<br>2 2   | 0       | 0       |
| 2   | I     | 10       | Total O<br>10 10 | 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: BH2092 protein



LEU  
GLU  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

• Molecule 1: BH2092 protein

Chain E:  2% 55% 36% 6%

GLU PRO A16 N17 P18 N19 R23 M26 K28 K29 S30 Y31 E32 T33 D34 I35 A36 K44 E47 I50 D53 V54 R55 Y60 A61 E62 C63 H64 I65 P66 S70 G73 N74 K75 I76 N77 E78 D79 T80 K82 K88 I91 C94 W95 G96 P97

A98 A106 L112 R115 V116 K117 I120 G121 Y125 E129 G131 G132 E133 HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: BH2092 protein

Chain F:  2% 61% 29% 6%

GLU P15 A16 N17 E20 D34 I35 K43 K44 G45 TTR G48 I49 I50 D53 V54 R55 Y60 C63 H64 I65 P66 G73 N74 K75 I76 N77 E78 D79 T80 R83 K88 V89 I90 I91 C94 W95 G96 A106 L112 R115 V116 K117 G121

Y125 E129 N130 G131 E133 HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: BH2092 protein

Chain G:  11% 57% 32% 10%

GLU PRO ALA N17 P18 N19 S30 T33 D34 I35 A36 D37 L38 S39 I40 D41 I42 K43 K44 G45 Y46 E47 G48 I49 I50 D53 V54 R55 D56 Y60 K61 E62 C63 H64 I65 P66 G73 N74 K75 I76 N77 E78 D79 T80 S85 K86 E87 K88 V89 I90 I91 C94

K95 G96 N100 A106 R115 V116 K117 I120 G121 W126 R127 K128 N130 GLU LEU HIS HIS HIS HIS HIS HIS

• Molecule 1: BH2092 protein

Chain H:  6% 66% 25% 8%

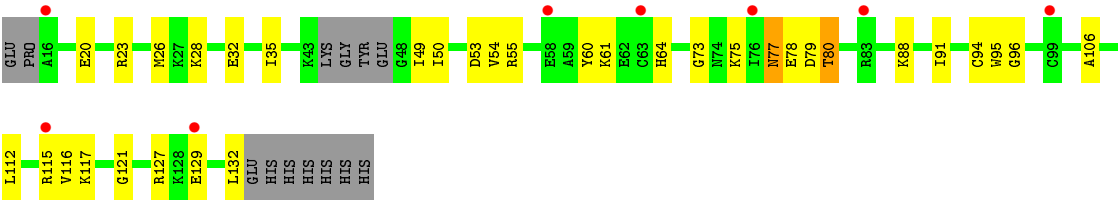
GLU PRO ALA N17 P18 Y31 T35 A36 D37 I40 K44 G45 Y46 E47 I50 D53 V54 R55 Y60 C63 H64 I67 N77 E78 D79 T80 K88 I91 C94 W95 G96 A106 L112 R115 V116 K117 G121 Y125 W126 R127 K128 E129

L132 GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: BH2092 protein

Chain I:  6% 63% 25% 10%





## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 31   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 114.24 Å   114.24 Å   85.45 Å<br>90.00°   90.00°   120.00°     | Depositor        |
| Resolution (Å)  | 19.79 – 2.91<br>28.56 – 2.91                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.9 (19.79-2.91)<br>99.5 (28.56-2.91)                         | Depositor<br>EDS |
| $R_{merge}$   | 0.17   | Depositor        |
| $R_{sym}$   | 0.17   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.74 (at 2.90 Å)   | Xtriage          |
| Refinement program  | CNS 1.2  | Depositor        |
| R, $R_{free}$   | 0.250   ,   0.292<br>0.261   ,   0.299                         | Depositor<br>DCC |
| $R_{free}$ test set   | 2694 reflections (9.91%)                                       | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 33.1   | Xtriage          |
| Anisotropy  | 0.009  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33   ,   2.1   | EDS              |
| Estimated twinning fraction   | 0.098 for -h,-k,l<br>0.099 for h,-h-k,-l<br>0.286 for -k,-h,-l | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$    | Xtriage          |
| Outliers  | 0 of 54750 reflections   | Xtriage          |
| $F_o, F_c$ correlation  | 0.87   | EDS              |
| Total number of atoms   | 8353   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 31.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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, 0.375 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     | 0.48         | 0/946   | 0.61        | 0/1275         |
| 1   | B     | 0.45         | 0/945   | 0.58        | 0/1272         |
| 1   | C     | 0.49         | 0/950   | 1.26        | 3/1279 (0.2%)  |
| 1   | D     | 0.45         | 0/924   | 0.57        | 0/1244         |
| 1   | E     | 0.47         | 0/950   | 0.60        | 0/1279         |
| 1   | F     | 0.45         | 0/946   | 0.59        | 0/1272         |
| 1   | G     | 0.46         | 0/924   | 0.55        | 0/1244         |
| 1   | H     | 0.42         | 0/936   | 0.55        | 0/1260         |
| 1   | I     | 0.46         | 0/905   | 0.56        | 0/1218         |
| All | All   | 0.46         | 0/8426  | 0.69        | 3/11343 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|-----------|--------|------------------------|---------------------|
| 1   | C     | 23  | ARG  | NE-CZ-NH1 | -27.41 | 106.60                 | 120.30              |
| 1   | C     | 23  | ARG  | NE-CZ-NH2 | 25.63  | 133.12                 | 120.30              |
| 1   | C     | 23  | ARG  | CD-NE-CZ  | 12.99  | 141.78                 | 123.60              |

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     | 928   | 0        | 927      | 43      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 928   | 0        | 930      | 35      | 0            |
| 1   | C     | 933   | 0        | 935      | 56      | 1            |
| 1   | D     | 907   | 0        | 910      | 41      | 0            |
| 1   | E     | 933   | 0        | 935      | 59      | 0            |
| 1   | F     | 929   | 0        | 934      | 47      | 1            |
| 1   | G     | 907   | 0        | 910      | 35      | 0            |
| 1   | H     | 919   | 0        | 924      | 28      | 0            |
| 1   | I     | 890   | 0        | 897      | 41      | 0            |
| 2   | A     | 14    | 0        | 0        | 1       | 0            |
| 2   | B     | 9     | 0        | 0        | 2       | 0            |
| 2   | C     | 6     | 0        | 0        | 1       | 0            |
| 2   | D     | 10    | 0        | 0        | 1       | 0            |
| 2   | E     | 11    | 0        | 0        | 4       | 0            |
| 2   | F     | 7     | 0        | 0        | 2       | 0            |
| 2   | G     | 10    | 0        | 0        | 4       | 0            |
| 2   | H     | 2     | 0        | 0        | 0       | 0            |
| 2   | I     | 10    | 0        | 0        | 6       | 0            |
| All | All   | 8353  | 0        | 8302     | 324     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (324) 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:C:78:GLU:OE1   | 1:E:26:MSE:HE2   | 1.37                     | 1.24              |
| 1:I:49:ILE:HD12  | 1:I:91:ILE:HD12  | 1.37                     | 1.07              |
| 1:E:115:ARG:HH12 | 1:F:15:PRO:HB2   | 1.17                     | 1.05              |
| 1:D:23:ARG:NH2   | 1:I:20:GLU:HB2   | 1.73                     | 1.03              |
| 1:G:35:ILE:HG21  | 1:G:129:GLU:HG3  | 1.42                     | 0.98              |
| 1:B:28:LYS:HD2   | 2:B:144:HOH:O    | 1.66                     | 0.96              |
| 1:A:16:ALA:N     | 1:C:115:ARG:HH12 | 1.65                     | 0.95              |
| 1:D:23:ARG:NH2   | 1:I:20:GLU:CB    | 2.31                     | 0.92              |
| 1:D:23:ARG:HH21  | 1:I:20:GLU:CB    | 1.87                     | 0.86              |
| 1:A:15:PRO:C     | 1:C:115:ARG:HH12 | 1.79                     | 0.86              |
| 1:G:100:ASN:HB2  | 2:G:143:HOH:O    | 1.75                     | 0.86              |
| 1:E:115:ARG:HH22 | 1:F:15:PRO:C     | 1.81                     | 0.84              |
| 1:E:115:ARG:HH12 | 1:F:15:PRO:CB    | 1.91                     | 0.84              |
| 1:F:43:LYS:HD3   | 1:F:44:LYS:N     | 1.91                     | 0.83              |
| 1:B:77:ASN:HD22  | 1:B:79:ASP:H     | 1.26                     | 0.83              |
| 1:E:94:CYS:HB3   | 2:E:9:HOH:O      | 1.79                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:77:ASN:HD22 | 1:D:79:ASP:H     | 1.26                     | 0.83              |
| 1:C:77:ASN:HD22 | 1:C:79:ASP:H     | 1.28                     | 0.82              |
| 1:C:35:ILE:HG21 | 1:C:129:GLU:HG3  | 1.59                     | 0.82              |
| 1:I:77:ASN:HD22 | 1:I:79:ASP:H     | 1.28                     | 0.82              |
| 1:F:77:ASN:HD22 | 1:F:79:ASP:H     | 1.30                     | 0.80              |
| 1:B:35:ILE:HG21 | 1:B:129:GLU:HG3  | 1.64                     | 0.80              |
| 1:I:35:ILE:HG21 | 1:I:129:GLU:HG3  | 1.64                     | 0.79              |
| 1:E:77:ASN:HD22 | 1:E:79:ASP:H     | 1.29                     | 0.79              |
| 1:B:129:GLU:HB2 | 1:B:130:ASN:HD22 | 1.47                     | 0.78              |
| 1:E:35:ILE:HG21 | 1:E:129:GLU:HG3  | 1.63                     | 0.78              |
| 1:G:77:ASN:HD22 | 1:G:79:ASP:H     | 1.30                     | 0.78              |
| 1:H:77:ASN:HD22 | 1:H:79:ASP:H     | 1.30                     | 0.77              |
| 1:A:16:ALA:N    | 1:C:115:ARG:NH1  | 2.32                     | 0.77              |
| 1:A:77:ASN:HD22 | 1:A:79:ASP:H     | 1.31                     | 0.77              |
| 1:E:115:ARG:NH1 | 1:F:15:PRO:HB2   | 1.98                     | 0.77              |
| 1:D:23:ARG:NH2  | 1:I:20:GLU:CG    | 2.47                     | 0.76              |
| 1:I:26:MSE:HE3  | 2:I:148:HOH:O    | 1.84                     | 0.76              |
| 1:C:78:GLU:CD   | 1:E:26:MSE:HE2   | 2.05                     | 0.76              |
| 1:H:35:ILE:HG21 | 1:H:129:GLU:HG3  | 1.68                     | 0.74              |
| 1:C:82:LYS:NZ   | 1:E:19:ASN:HD22  | 1.85                     | 0.73              |
| 1:F:129:GLU:HA  | 2:F:140:HOH:O    | 1.89                     | 0.73              |
| 1:C:78:GLU:OE1  | 1:E:26:MSE:CE    | 2.29                     | 0.72              |
| 1:D:35:ILE:HG21 | 1:D:129:GLU:HG3  | 1.71                     | 0.72              |
| 1:E:63:CYS:SG   | 1:E:132:LEU:HD13 | 2.29                     | 0.71              |
| 1:F:35:ILE:HG21 | 1:F:129:GLU:HG3  | 1.72                     | 0.71              |
| 1:B:63:CYS:SG   | 1:B:132:LEU:HD13 | 2.31                     | 0.71              |
| 1:C:82:LYS:HZ1  | 1:E:19:ASN:HD22  | 1.37                     | 0.70              |
| 1:A:35:ILE:HG21 | 1:A:129:GLU:HG3  | 1.72                     | 0.70              |
| 1:H:17:ASN:HD22 | 1:H:18:PRO:HD2   | 1.55                     | 0.70              |
| 1:A:15:PRO:C    | 1:C:115:ARG:HH22 | 1.94                     | 0.69              |
| 1:I:127:ARG:HG2 | 1:I:132:LEU:HD21 | 1.74                     | 0.68              |
| 1:H:17:ASN:HD22 | 1:H:18:PRO:CD    | 2.07                     | 0.68              |
| 1:E:30:SER:O    | 1:F:15:PRO:HB3   | 1.92                     | 0.68              |
| 1:A:106:ALA:HA  | 1:A:116:VAL:HG21 | 1.76                     | 0.68              |
| 1:E:44:LYS:HA   | 1:E:44:LYS:HE3   | 1.75                     | 0.68              |
| 1:C:79:ASP:OD2  | 1:E:23:ARG:HG2   | 1.94                     | 0.68              |
| 1:I:106:ALA:HA  | 1:I:116:VAL:HG21 | 1.76                     | 0.67              |
| 1:D:23:ARG:HH21 | 1:I:20:GLU:HB2   | 1.51                     | 0.67              |
| 1:G:106:ALA:HA  | 1:G:116:VAL:HG21 | 1.77                     | 0.67              |
| 1:H:47:GLU:O    | 1:H:88:LYS:HE3   | 1.95                     | 0.67              |
| 1:A:15:PRO:CB   | 1:C:115:ARG:HH12 | 2.09                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:106:ALA:HA  | 1:D:116:VAL:HG21 | 1.76                     | 0.66              |
| 1:E:47:GLU:O    | 1:E:88:LYS:HE3   | 1.95                     | 0.66              |
| 1:B:106:ALA:HA  | 1:B:116:VAL:HG21 | 1.77                     | 0.66              |
| 1:H:106:ALA:HA  | 1:H:116:VAL:HG21 | 1.77                     | 0.66              |
| 1:E:106:ALA:HA  | 1:E:116:VAL:HG21 | 1.78                     | 0.66              |
| 1:G:47:GLU:O    | 1:G:88:LYS:HE3   | 1.95                     | 0.65              |
| 1:D:23:ARG:NH2  | 1:I:20:GLU:HG3   | 2.12                     | 0.65              |
| 1:A:15:PRO:HB2  | 1:C:115:ARG:HH12 | 1.61                     | 0.65              |
| 1:F:106:ALA:HA  | 1:F:116:VAL:HG21 | 1.78                     | 0.65              |
| 1:B:77:ASN:HD22 | 1:B:79:ASP:N     | 1.95                     | 0.64              |
| 1:G:18:PRO:HB2  | 2:G:147:HOH:O    | 1.97                     | 0.64              |
| 1:A:15:PRO:HB2  | 1:C:115:ARG:NH1  | 2.13                     | 0.64              |
| 1:A:15:PRO:HG2  | 1:C:115:ARG:NH1  | 2.13                     | 0.64              |
| 1:A:47:GLU:O    | 1:A:88:LYS:HE3   | 1.97                     | 0.64              |
| 1:D:77:ASN:HD22 | 1:D:79:ASP:N     | 1.95                     | 0.64              |
| 1:I:94:CYS:SG   | 1:I:95:TRP:N     | 2.70                     | 0.64              |
| 1:B:47:GLU:O    | 1:B:88:LYS:HE3   | 1.97                     | 0.64              |
| 1:C:106:ALA:HA  | 1:C:116:VAL:HG21 | 1.80                     | 0.64              |
| 1:G:87:GLU:HB2  | 2:G:142:HOH:O    | 1.98                     | 0.63              |
| 1:C:82:LYS:NZ   | 1:E:19:ASN:ND2   | 2.47                     | 0.63              |
| 1:C:77:ASN:HD22 | 1:C:79:ASP:N     | 1.97                     | 0.62              |
| 1:H:77:ASN:HD22 | 1:H:79:ASP:N     | 1.98                     | 0.62              |
| 1:G:44:LYS:NZ   | 1:G:44:LYS:HB2   | 2.15                     | 0.62              |
| 1:E:77:ASN:HD22 | 1:E:79:ASP:N     | 1.98                     | 0.62              |
| 1:E:70:SER:HB3  | 2:E:141:HOH:O    | 1.99                     | 0.61              |
| 1:B:66:PRO:HA   | 1:B:133:GLU:OE1  | 2.01                     | 0.61              |
| 1:C:82:LYS:NZ   | 1:E:23:ARG:NH2   | 2.49                     | 0.60              |
| 1:G:35:ILE:HG21 | 1:G:129:GLU:CG   | 2.27                     | 0.60              |
| 1:E:66:PRO:HG3  | 1:E:133:GLU:HB2  | 1.82                     | 0.60              |
| 1:D:77:ASN:ND2  | 1:D:79:ASP:HB2   | 2.17                     | 0.60              |
| 1:I:77:ASN:HD22 | 1:I:79:ASP:N     | 1.98                     | 0.60              |
| 1:G:77:ASN:HD22 | 1:G:79:ASP:N     | 1.98                     | 0.60              |
| 1:E:33:THR:O    | 1:E:120:ILE:HG12 | 2.01                     | 0.60              |
| 1:A:15:PRO:CB   | 1:C:115:ARG:NH1  | 2.65                     | 0.60              |
| 1:D:30:SER:O    | 1:D:117:LYS:HE3  | 2.02                     | 0.59              |
| 1:G:94:CYS:SG   | 1:G:95:TRP:N     | 2.74                     | 0.59              |
| 1:D:23:ARG:HH21 | 1:I:20:GLU:CA    | 2.15                     | 0.59              |
| 1:F:77:ASN:HD22 | 1:F:79:ASP:N     | 1.99                     | 0.59              |
| 1:A:15:PRO:C    | 1:C:115:ARG:NH1  | 2.53                     | 0.59              |
| 1:C:130:ASN:OD1 | 2:C:140:HOH:O    | 2.16                     | 0.59              |
| 1:A:77:ASN:HD22 | 1:A:79:ASP:N     | 1.99                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:23:ARG:NH1   | 2:I:146:HOH:O    | 2.37                     | 0.58              |
| 1:A:15:PRO:O     | 1:C:115:ARG:NH2  | 2.22                     | 0.57              |
| 1:G:77:ASN:ND2   | 1:G:79:ASP:HB2   | 2.19                     | 0.57              |
| 1:H:77:ASN:ND2   | 1:H:79:ASP:HB2   | 2.18                     | 0.57              |
| 1:A:77:ASN:ND2   | 1:A:79:ASP:HB2   | 2.20                     | 0.57              |
| 1:A:30:SER:O     | 1:A:117:LYS:HE3  | 2.03                     | 0.57              |
| 1:G:44:LYS:HB2   | 1:G:44:LYS:HZ2   | 1.70                     | 0.56              |
| 1:C:132:LEU:C    | 1:C:132:LEU:HD12 | 2.26                     | 0.56              |
| 1:C:33:THR:O     | 1:C:120:ILE:HG12 | 2.05                     | 0.56              |
| 1:F:17:ASN:ND2   | 1:F:20:GLU:HB2   | 2.20                     | 0.56              |
| 1:I:77:ASN:ND2   | 1:I:79:ASP:HB2   | 2.21                     | 0.56              |
| 1:F:66:PRO:HA    | 1:F:133:GLU:OE2  | 2.06                     | 0.56              |
| 1:H:31:TYR:OH    | 1:I:20:GLU:HG2   | 2.05                     | 0.56              |
| 1:H:17:ASN:HD22  | 1:H:18:PRO:N     | 2.04                     | 0.56              |
| 1:C:47:GLU:O     | 1:C:88:LYS:HE3   | 2.06                     | 0.56              |
| 1:D:23:ARG:HH22  | 1:I:20:GLU:CG    | 2.17                     | 0.55              |
| 1:B:77:ASN:ND2   | 1:B:79:ASP:HB2   | 2.20                     | 0.55              |
| 1:H:40:ILE:HG22  | 1:H:44:LYS:HD2   | 1.89                     | 0.55              |
| 1:H:63:CYS:SG    | 1:H:132:LEU:HD13 | 2.46                     | 0.55              |
| 1:F:77:ASN:ND2   | 1:F:79:ASP:HB2   | 2.21                     | 0.55              |
| 1:F:49:ILE:HG22  | 1:F:89:VAL:HB    | 1.89                     | 0.55              |
| 1:G:35:ILE:CG2   | 1:G:129:GLU:HG3  | 2.27                     | 0.54              |
| 1:E:77:ASN:ND2   | 1:E:79:ASP:HB2   | 2.22                     | 0.54              |
| 1:H:40:ILE:O     | 1:H:44:LYS:HG3   | 2.07                     | 0.54              |
| 1:D:23:ARG:CZ    | 1:I:20:GLU:HB2   | 2.36                     | 0.54              |
| 1:A:54:VAL:HG12  | 1:A:54:VAL:O     | 2.08                     | 0.54              |
| 1:C:77:ASN:ND2   | 1:C:79:ASP:HB2   | 2.23                     | 0.53              |
| 1:E:115:ARG:HH22 | 1:F:15:PRO:N     | 2.07                     | 0.53              |
| 1:D:77:ASN:HD21  | 1:D:79:ASP:HB2   | 1.72                     | 0.52              |
| 1:H:96:GLY:HA2   | 1:H:121:GLY:O    | 2.09                     | 0.52              |
| 1:E:82:LYS:HB2   | 2:E:146:HOH:O    | 2.09                     | 0.52              |
| 1:B:128:LYS:HA   | 2:B:143:HOH:O    | 2.10                     | 0.52              |
| 1:B:77:ASN:HD21  | 1:B:79:ASP:HB2   | 1.74                     | 0.52              |
| 1:G:30:SER:O     | 1:G:117:LYS:HE3  | 2.10                     | 0.52              |
| 1:F:116:VAL:HG22 | 1:F:117:LYS:N    | 2.24                     | 0.52              |
| 1:I:80:THR:CG2   | 2:I:142:HOH:O    | 2.57                     | 0.52              |
| 1:C:94:CYS:SG    | 1:C:95:TRP:N     | 2.81                     | 0.52              |
| 1:A:116:VAL:HG22 | 1:A:117:LYS:N    | 2.25                     | 0.52              |
| 1:D:23:ARG:HH22  | 1:I:20:GLU:HG3   | 1.73                     | 0.52              |
| 1:I:77:ASN:HD21  | 1:I:79:ASP:HB2   | 1.75                     | 0.51              |
| 1:F:17:ASN:HD21  | 1:F:20:GLU:HB2   | 1.75                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:17:ASN:ND2   | 1:H:18:PRO:HD2   | 2.24                     | 0.51              |
| 1:C:54:VAL:HG12  | 1:C:54:VAL:O     | 2.09                     | 0.51              |
| 1:B:33:THR:O     | 1:B:120:ILE:HG12 | 2.10                     | 0.51              |
| 1:H:116:VAL:HG22 | 1:H:117:LYS:N    | 2.25                     | 0.51              |
| 1:A:98:ALA:O     | 1:B:34:ASP:HB2   | 2.10                     | 0.51              |
| 1:A:77:ASN:HD21  | 1:A:79:ASP:HB2   | 1.75                     | 0.51              |
| 1:H:77:ASN:HD21  | 1:H:79:ASP:HB2   | 1.74                     | 0.51              |
| 1:H:94:CYS:SG    | 1:H:95:TRP:N     | 2.76                     | 0.51              |
| 1:G:96:GLY:HA2   | 1:G:121:GLY:O    | 2.10                     | 0.51              |
| 1:E:117:LYS:NZ   | 1:F:15:PRO:HG3   | 2.26                     | 0.51              |
| 1:F:77:ASN:HD21  | 1:F:79:ASP:HB2   | 1.75                     | 0.51              |
| 1:C:60:TYR:O     | 1:C:64:HIS:HD2   | 1.94                     | 0.51              |
| 1:G:53:ASP:OD1   | 1:G:55:ARG:HD3   | 2.11                     | 0.51              |
| 1:D:47:GLU:O     | 1:D:88:LYS:HE3   | 2.10                     | 0.51              |
| 1:E:53:ASP:OD1   | 1:E:55:ARG:HD3   | 2.11                     | 0.50              |
| 1:E:115:ARG:HH12 | 1:F:16:ALA:H     | 1.58                     | 0.50              |
| 1:B:116:VAL:HG22 | 1:B:117:LYS:N    | 2.27                     | 0.50              |
| 1:I:116:VAL:HG22 | 1:I:117:LYS:N    | 2.26                     | 0.50              |
| 1:E:94:CYS:SG    | 1:E:95:TRP:N     | 2.78                     | 0.50              |
| 1:I:53:ASP:OD1   | 1:I:55:ARG:HD3   | 2.12                     | 0.50              |
| 1:F:53:ASP:OD1   | 1:F:55:ARG:HD3   | 2.12                     | 0.50              |
| 1:F:94:CYS:SG    | 1:F:95:TRP:N     | 2.75                     | 0.49              |
| 1:I:26:MSE:CE    | 2:I:148:HOH:O    | 2.51                     | 0.49              |
| 1:G:33:THR:O     | 1:G:120:ILE:HG12 | 2.12                     | 0.49              |
| 1:C:77:ASN:HD21  | 1:C:79:ASP:HB2   | 1.77                     | 0.49              |
| 1:C:116:VAL:HG22 | 1:C:117:LYS:N    | 2.28                     | 0.49              |
| 1:D:94:CYS:SG    | 1:D:95:TRP:N     | 2.80                     | 0.49              |
| 1:G:77:ASN:HD21  | 1:G:79:ASP:HB2   | 1.77                     | 0.49              |
| 1:D:96:GLY:HA2   | 1:D:121:GLY:O    | 2.13                     | 0.49              |
| 1:E:115:ARG:NH1  | 1:F:16:ALA:H     | 2.11                     | 0.49              |
| 1:A:15:PRO:CG    | 1:C:115:ARG:NH1  | 2.75                     | 0.49              |
| 1:G:116:VAL:HG22 | 1:G:117:LYS:N    | 2.28                     | 0.48              |
| 1:G:50:ILE:HD11  | 1:G:88:LYS:HD2   | 1.95                     | 0.48              |
| 1:E:115:ARG:NH1  | 1:F:16:ALA:N     | 2.61                     | 0.48              |
| 1:E:60:TYR:O     | 1:E:64:HIS:HD2   | 1.96                     | 0.48              |
| 1:D:43:LYS:NZ    | 1:D:43:LYS:HB3   | 2.28                     | 0.48              |
| 1:C:78:GLU:HG2   | 1:C:112:LEU:HD22 | 1.96                     | 0.48              |
| 1:C:64:HIS:O     | 1:C:132:LEU:HB2  | 2.13                     | 0.48              |
| 1:D:60:TYR:O     | 1:D:64:HIS:HD2   | 1.95                     | 0.48              |
| 1:E:115:ARG:HH22 | 1:F:15:PRO:CA    | 2.26                     | 0.48              |
| 1:H:17:ASN:HD22  | 1:H:17:ASN:C     | 2.17                     | 0.48              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:60:TYR:O     | 1:B:64:HIS:HD2   | 1.96                     | 0.48              |
| 1:H:53:ASP:OD1   | 1:H:55:ARG:HD3   | 2.13                     | 0.48              |
| 1:E:54:VAL:O     | 1:E:54:VAL:HG12  | 2.13                     | 0.48              |
| 1:H:60:TYR:O     | 1:H:64:HIS:HD2   | 1.96                     | 0.48              |
| 1:I:96:GLY:HA2   | 1:I:121:GLY:O    | 2.14                     | 0.48              |
| 1:E:116:VAL:HG22 | 1:E:117:LYS:N    | 2.29                     | 0.47              |
| 1:F:60:TYR:O     | 1:F:64:HIS:HD2   | 1.97                     | 0.47              |
| 1:A:15:PRO:CA    | 1:C:115:ARG:HH12 | 2.27                     | 0.47              |
| 1:I:54:VAL:HG12  | 1:I:54:VAL:O     | 2.13                     | 0.47              |
| 1:A:40:ILE:O     | 1:A:44:LYS:HG3   | 2.14                     | 0.47              |
| 1:E:77:ASN:HD21  | 1:E:79:ASP:HB2   | 1.78                     | 0.47              |
| 1:F:43:LYS:HD3   | 1:F:44:LYS:H     | 1.76                     | 0.47              |
| 1:F:50:ILE:HD11  | 1:F:88:LYS:HD2   | 1.95                     | 0.47              |
| 1:A:15:PRO:C     | 1:C:115:ARG:NH2  | 2.65                     | 0.47              |
| 1:D:116:VAL:HG22 | 1:D:117:LYS:N    | 2.30                     | 0.47              |
| 1:E:115:ARG:HH12 | 1:F:16:ALA:N     | 2.12                     | 0.47              |
| 1:E:30:SER:HB2   | 1:F:15:PRO:HA    | 1.96                     | 0.47              |
| 1:E:115:ARG:NH2  | 1:F:15:PRO:C     | 2.59                     | 0.47              |
| 1:E:98:ALA:O     | 1:F:34:ASP:HB2   | 2.15                     | 0.47              |
| 1:B:30:SER:O     | 1:B:117:LYS:HE3  | 2.14                     | 0.47              |
| 1:G:54:VAL:O     | 1:G:54:VAL:HG12  | 2.15                     | 0.47              |
| 1:B:54:VAL:O     | 1:B:54:VAL:HG12  | 2.14                     | 0.47              |
| 1:E:50:ILE:HD11  | 1:E:88:LYS:HD2   | 1.97                     | 0.47              |
| 1:A:60:TYR:O     | 1:A:64:HIS:HD2   | 1.97                     | 0.47              |
| 1:B:115:ARG:HG3  | 1:B:115:ARG:HH11 | 1.80                     | 0.47              |
| 1:G:91:ILE:HA    | 1:G:117:LYS:O    | 2.16                     | 0.46              |
| 1:F:94:CYS:HB3   | 2:F:142:HOH:O    | 2.15                     | 0.46              |
| 1:I:60:TYR:O     | 1:I:64:HIS:HD2   | 1.98                     | 0.46              |
| 1:D:19:ASN:HB2   | 2:D:6:HOH:O      | 2.15                     | 0.46              |
| 1:B:66:PRO:HG3   | 1:B:133:GLU:HB2  | 1.98                     | 0.46              |
| 1:I:115:ARG:HH11 | 1:I:115:ARG:HG3  | 1.80                     | 0.46              |
| 1:A:53:ASP:OD1   | 1:A:55:ARG:HD3   | 2.16                     | 0.46              |
| 1:A:16:ALA:O     | 1:C:115:ARG:NH1  | 2.49                     | 0.46              |
| 1:C:46:TYR:CZ    | 1:C:48:GLY:HA3   | 2.51                     | 0.46              |
| 1:F:54:VAL:O     | 1:F:54:VAL:HG12  | 2.15                     | 0.46              |
| 1:E:115:ARG:NH2  | 1:F:15:PRO:N     | 2.64                     | 0.45              |
| 1:G:60:TYR:O     | 1:G:64:HIS:HD2   | 1.98                     | 0.45              |
| 1:D:49:ILE:HD12  | 1:D:49:ILE:O     | 2.16                     | 0.45              |
| 1:B:129:GLU:CB   | 1:B:130:ASN:HD22 | 2.24                     | 0.45              |
| 1:A:94:CYS:SG    | 1:A:95:TRP:N     | 2.81                     | 0.45              |
| 1:C:115:ARG:HG3  | 1:C:115:ARG:HH11 | 1.80                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:121:GLY:HA3  | 1:C:125:TYR:CD2  | 2.52                     | 0.45              |
| 1:C:91:ILE:HA    | 1:C:117:LYS:O    | 2.16                     | 0.45              |
| 1:D:115:ARG:HG3  | 1:D:115:ARG:HH11 | 1.81                     | 0.45              |
| 1:E:17:ASN:H     | 1:E:18:PRO:CD    | 2.29                     | 0.45              |
| 1:I:78:GLU:HG2   | 1:I:112:LEU:HD22 | 1.99                     | 0.45              |
| 1:D:53:ASP:OD1   | 1:D:55:ARG:HD3   | 2.17                     | 0.45              |
| 1:E:36:ALA:N     | 2:E:143:HOH:O    | 2.45                     | 0.45              |
| 1:F:115:ARG:HH11 | 1:F:115:ARG:HG3  | 1.82                     | 0.44              |
| 1:C:63:CYS:HB2   | 1:C:132:LEU:CD1  | 2.47                     | 0.44              |
| 1:A:115:ARG:HH11 | 1:A:115:ARG:HG3  | 1.81                     | 0.44              |
| 1:C:96:GLY:HA2   | 1:C:121:GLY:O    | 2.16                     | 0.44              |
| 1:A:91:ILE:HA    | 1:A:117:LYS:O    | 2.18                     | 0.44              |
| 1:D:50:ILE:HD11  | 1:D:88:LYS:HD2   | 1.99                     | 0.44              |
| 1:F:78:GLU:HG2   | 1:F:112:LEU:HD22 | 2.00                     | 0.44              |
| 1:D:121:GLY:HA3  | 1:D:125:TYR:CD2  | 2.53                     | 0.44              |
| 1:G:48:GLY:HA2   | 1:G:88:LYS:HG2   | 2.00                     | 0.44              |
| 1:H:54:VAL:O     | 1:H:54:VAL:HG12  | 2.17                     | 0.44              |
| 1:G:115:ARG:HH11 | 1:G:115:ARG:HG3  | 1.82                     | 0.44              |
| 1:B:96:GLY:HA2   | 1:B:121:GLY:O    | 2.18                     | 0.44              |
| 1:A:50:ILE:HD11  | 1:A:88:LYS:HD2   | 1.98                     | 0.44              |
| 1:H:91:ILE:HA    | 1:H:117:LYS:O    | 2.17                     | 0.44              |
| 1:H:115:ARG:HG3  | 1:H:115:ARG:HH11 | 1.83                     | 0.44              |
| 1:A:96:GLY:HA2   | 1:A:121:GLY:O    | 2.17                     | 0.44              |
| 1:B:77:ASN:ND2   | 1:B:79:ASP:H     | 2.05                     | 0.44              |
| 1:D:91:ILE:HA    | 1:D:117:LYS:O    | 2.18                     | 0.44              |
| 1:B:115:ARG:NH1  | 1:C:16:ALA:N     | 2.66                     | 0.44              |
| 1:E:28:LYS:O     | 1:E:32:GLU:HG2   | 2.17                     | 0.44              |
| 1:F:96:GLY:HA2   | 1:F:121:GLY:O    | 2.18                     | 0.43              |
| 1:E:78:GLU:HG2   | 1:E:112:LEU:HD22 | 1.99                     | 0.43              |
| 1:G:129:GLU:O    | 1:G:130:ASN:C    | 2.55                     | 0.43              |
| 1:G:38:LEU:HD12  | 1:G:126:TRP:CZ3  | 2.53                     | 0.43              |
| 1:B:94:CYS:SG    | 1:B:95:TRP:N     | 2.81                     | 0.43              |
| 1:F:43:LYS:HE2   | 1:F:43:LYS:HB2   | 1.69                     | 0.43              |
| 1:B:46:TYR:CE2   | 1:B:48:GLY:HA3   | 2.54                     | 0.43              |
| 1:A:28:LYS:O     | 1:A:32:GLU:HG2   | 2.17                     | 0.43              |
| 1:D:43:LYS:NZ    | 1:D:43:LYS:CB    | 2.81                     | 0.43              |
| 1:B:28:LYS:O     | 1:B:32:GLU:HG2   | 2.18                     | 0.43              |
| 1:C:89:VAL:HG13  | 1:C:115:ARG:O    | 2.18                     | 0.43              |
| 1:C:125:TYR:O    | 1:C:129:GLU:HG2  | 2.19                     | 0.43              |
| 1:B:91:ILE:HA    | 1:B:117:LYS:O    | 2.18                     | 0.43              |
| 1:C:53:ASP:OD1   | 1:C:55:ARG:HD3   | 2.19                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:115:ARG:NH1  | 1:E:17:ASN:OD1   | 2.52                     | 0.43              |
| 1:G:89:VAL:HG13  | 1:G:115:ARG:O    | 2.19                     | 0.43              |
| 1:I:77:ASN:ND2   | 1:I:79:ASP:H     | 2.07                     | 0.43              |
| 1:C:50:ILE:HD11  | 1:C:88:LYS:HD2   | 2.00                     | 0.43              |
| 1:D:98:ALA:O     | 1:E:34:ASP:HB2   | 2.19                     | 0.42              |
| 1:E:62:GLU:O     | 1:E:63:CYS:HB3   | 2.19                     | 0.42              |
| 1:F:91:ILE:HA    | 1:F:117:LYS:O    | 2.19                     | 0.42              |
| 1:B:50:ILE:HD11  | 1:B:88:LYS:HD2   | 2.01                     | 0.42              |
| 1:D:23:ARG:HH21  | 1:I:20:GLU:HA    | 1.84                     | 0.42              |
| 1:A:97:PRO:HB2   | 1:B:125:TYR:CE2  | 2.55                     | 0.42              |
| 1:E:73:GLY:C     | 1:E:75:LYS:H     | 2.23                     | 0.42              |
| 1:E:115:ARG:HH11 | 1:E:115:ARG:HG3  | 1.85                     | 0.42              |
| 1:E:30:SER:HB2   | 1:F:15:PRO:CA    | 2.49                     | 0.42              |
| 1:D:54:VAL:HG12  | 1:D:54:VAL:O     | 2.19                     | 0.42              |
| 1:A:125:TYR:O    | 1:A:129:GLU:HG2  | 2.18                     | 0.42              |
| 1:B:115:ARG:HH12 | 1:C:16:ALA:N     | 2.17                     | 0.42              |
| 1:F:63:CYS:SG    | 1:F:132:LEU:HD22 | 2.59                     | 0.42              |
| 1:G:73:GLY:C     | 1:G:75:LYS:H     | 2.23                     | 0.42              |
| 1:E:91:ILE:HA    | 1:E:117:LYS:O    | 2.19                     | 0.42              |
| 1:D:77:ASN:ND2   | 1:D:79:ASP:H     | 2.05                     | 0.42              |
| 1:H:50:ILE:HD11  | 1:H:88:LYS:HD2   | 2.01                     | 0.42              |
| 1:D:115:ARG:CZ   | 1:E:17:ASN:OD1   | 2.68                     | 0.42              |
| 1:I:50:ILE:HD11  | 1:I:88:LYS:HD2   | 2.01                     | 0.42              |
| 1:I:91:ILE:HA    | 1:I:117:LYS:O    | 2.20                     | 0.42              |
| 1:A:54:VAL:O     | 1:A:54:VAL:CG1   | 2.68                     | 0.42              |
| 1:B:121:GLY:HA3  | 1:B:125:TYR:CD2  | 2.55                     | 0.42              |
| 1:C:19:ASN:HB3   | 1:C:23:ARG:NH1   | 2.35                     | 0.42              |
| 1:A:100:ASN:HA   | 1:A:100:ASN:HD22 | 1.62                     | 0.42              |
| 1:G:127:ARG:O    | 1:G:130:ASN:HB2  | 2.20                     | 0.41              |
| 1:G:44:LYS:CB    | 1:G:44:LYS:NZ    | 2.82                     | 0.41              |
| 1:D:125:TYR:O    | 1:D:129:GLU:HG2  | 2.20                     | 0.41              |
| 1:D:46:TYR:HD2   | 1:D:49:ILE:HG13  | 1.85                     | 0.41              |
| 1:I:61:LYS:HB2   | 1:I:61:LYS:HE3   | 1.87                     | 0.41              |
| 1:B:78:GLU:HG2   | 1:B:112:LEU:HD22 | 2.02                     | 0.41              |
| 1:G:36:ALA:O     | 1:G:40:ILE:HG12  | 2.20                     | 0.41              |
| 1:F:73:GLY:C     | 1:F:75:LYS:H     | 2.23                     | 0.41              |
| 1:H:127:ARG:HG2  | 1:H:132:LEU:HD11 | 2.02                     | 0.41              |
| 1:I:75:LYS:HE3   | 2:I:142:HOH:O    | 2.21                     | 0.41              |
| 1:G:19:ASN:OD1   | 2:G:147:HOH:O    | 2.21                     | 0.41              |
| 1:F:121:GLY:HA3  | 1:F:125:TYR:CD2  | 2.56                     | 0.41              |
| 1:I:28:LYS:O     | 1:I:32:GLU:HG2   | 2.21                     | 0.41              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:77:ASN:ND2   | 1:C:79:ASP:H     | 2.06                     | 0.41              |
| 1:A:36:ALA:O     | 1:A:40:ILE:HG12  | 2.21                     | 0.41              |
| 1:E:121:GLY:HA3  | 1:E:125:TYR:CD2  | 2.56                     | 0.41              |
| 1:D:61:LYS:HB2   | 1:D:61:LYS:HE3   | 1.90                     | 0.41              |
| 1:I:54:VAL:HG13  | 1:I:73:GLY:CA    | 2.51                     | 0.41              |
| 1:E:96:GLY:HA2   | 1:E:121:GLY:O    | 2.21                     | 0.41              |
| 1:A:20:GLU:HG2   | 1:C:31:TYR:OH    | 2.21                     | 0.41              |
| 1:C:28:LYS:O     | 1:C:32:GLU:HG2   | 2.21                     | 0.41              |
| 1:H:121:GLY:HA3  | 1:H:125:TYR:CD2  | 2.56                     | 0.41              |
| 1:I:80:THR:HG23  | 2:I:142:HOH:O    | 2.20                     | 0.41              |
| 1:C:19:ASN:HB3   | 1:C:23:ARG:HH12  | 1.86                     | 0.40              |
| 1:A:78:GLU:HG2   | 1:A:112:LEU:HD22 | 2.02                     | 0.40              |
| 1:H:78:GLU:HG2   | 1:H:112:LEU:HD22 | 2.03                     | 0.40              |
| 1:I:53:ASP:OD2   | 1:I:55:ARG:NH1   | 2.53                     | 0.40              |
| 1:G:65:ILE:HA    | 1:G:66:PRO:HD3   | 1.99                     | 0.40              |
| 1:F:77:ASN:ND2   | 1:F:79:ASP:H     | 2.09                     | 0.40              |
| 1:A:33:THR:HA    | 2:A:11:HOH:O     | 2.20                     | 0.40              |
| 1:E:115:ARG:NH2  | 1:F:16:ALA:N     | 2.70                     | 0.40              |
| 1:B:73:GLY:C     | 1:B:75:LYS:H     | 2.25                     | 0.40              |
| 1:B:53:ASP:OD1   | 1:B:55:ARG:HD3   | 2.21                     | 0.40              |
| 1:D:100:ASN:HD22 | 1:D:100:ASN:HA   | 1.64                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------------|--------------------------|-------------------|
| 1:C:22:TYR:OH | 1:F:83:ARG:NH1[2_455] | 2.11                     | 0.09              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed        | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 116/126 (92%)   | 108 (93%) | 7 (6%)  | 1 (1%)   | 21          | 56  |
| 1   | B     | 115/126 (91%)   | 109 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 1   | C     | 116/126 (92%)   | 108 (93%) | 7 (6%)  | 1 (1%)   | 21          | 56  |
| 1   | D     | 112/126 (89%)   | 108 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 1   | E     | 116/126 (92%)   | 109 (94%) | 6 (5%)  | 1 (1%)   | 21          | 56  |
| 1   | F     | 114/126 (90%)   | 106 (93%) | 8 (7%)  | 0        | 100         | 100 |
| 1   | G     | 112/126 (89%)   | 103 (92%) | 9 (8%)  | 0        | 100         | 100 |
| 1   | H     | 114/126 (90%)   | 105 (92%) | 9 (8%)  | 0        | 100         | 100 |
| 1   | I     | 109/126 (86%)   | 102 (94%) | 7 (6%)  | 0        | 100         | 100 |
| All | All   | 1024/1134 (90%) | 958 (94%) | 63 (6%) | 3 (0%)   | 46          | 78  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 17  | ASN  |
| 1   | A     | 15  | PRO  |
| 1   | C     | 132 | LEU  |

### 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     | 96/104 (92%) | 92 (96%)  | 4 (4%)   | 36          | 72 |
| 1   | B     | 97/104 (93%) | 94 (97%)  | 3 (3%)   | 47          | 81 |
| 1   | C     | 97/104 (93%) | 93 (96%)  | 4 (4%)   | 37          | 73 |
| 1   | D     | 95/104 (91%) | 93 (98%)  | 2 (2%)   | 61          | 87 |
| 1   | E     | 97/104 (93%) | 91 (94%)  | 6 (6%)   | 23          | 54 |
| 1   | F     | 97/104 (93%) | 91 (94%)  | 6 (6%)   | 23          | 54 |
| 1   | G     | 95/104 (91%) | 92 (97%)  | 3 (3%)   | 46          | 81 |
| 1   | H     | 96/104 (92%) | 93 (97%)  | 3 (3%)   | 47          | 81 |
| 1   | I     | 93/104 (89%) | 91 (98%)  | 2 (2%)   | 60          | 87 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| All | All   | 863/936 (92%) | 830 (96%) | 33 (4%)  | 40          | 76 |

All (33) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | LYS  |
| 1   | A     | 63  | CYS  |
| 1   | A     | 77  | ASN  |
| 1   | A     | 80  | THR  |
| 1   | B     | 47  | GLU  |
| 1   | B     | 77  | ASN  |
| 1   | B     | 80  | THR  |
| 1   | C     | 44  | LYS  |
| 1   | C     | 47  | GLU  |
| 1   | C     | 77  | ASN  |
| 1   | C     | 80  | THR  |
| 1   | D     | 77  | ASN  |
| 1   | D     | 80  | THR  |
| 1   | E     | 17  | ASN  |
| 1   | E     | 44  | LYS  |
| 1   | E     | 77  | ASN  |
| 1   | E     | 80  | THR  |
| 1   | E     | 130 | ASN  |
| 1   | E     | 133 | GLU  |
| 1   | F     | 43  | LYS  |
| 1   | F     | 77  | ASN  |
| 1   | F     | 80  | THR  |
| 1   | F     | 130 | ASN  |
| 1   | F     | 132 | LEU  |
| 1   | F     | 133 | GLU  |
| 1   | G     | 77  | ASN  |
| 1   | G     | 80  | THR  |
| 1   | G     | 130 | ASN  |
| 1   | H     | 17  | ASN  |
| 1   | H     | 77  | ASN  |
| 1   | H     | 80  | THR  |
| 1   | I     | 77  | ASN  |
| 1   | I     | 80  | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 77  | ASN  |
| 1   | A     | 100 | ASN  |
| 1   | A     | 111 | GLN  |
| 1   | B     | 17  | ASN  |
| 1   | B     | 77  | ASN  |
| 1   | B     | 100 | ASN  |
| 1   | B     | 111 | GLN  |
| 1   | B     | 130 | ASN  |
| 1   | C     | 17  | ASN  |
| 1   | C     | 77  | ASN  |
| 1   | C     | 100 | ASN  |
| 1   | C     | 111 | GLN  |
| 1   | D     | 19  | ASN  |
| 1   | D     | 77  | ASN  |
| 1   | D     | 100 | ASN  |
| 1   | D     | 111 | GLN  |
| 1   | D     | 130 | ASN  |
| 1   | E     | 19  | ASN  |
| 1   | E     | 77  | ASN  |
| 1   | E     | 100 | ASN  |
| 1   | E     | 111 | GLN  |
| 1   | F     | 77  | ASN  |
| 1   | F     | 100 | ASN  |
| 1   | F     | 111 | GLN  |
| 1   | F     | 134 | HIS  |
| 1   | G     | 77  | ASN  |
| 1   | G     | 100 | ASN  |
| 1   | G     | 111 | GLN  |
| 1   | G     | 130 | ASN  |
| 1   | H     | 17  | ASN  |
| 1   | H     | 77  | ASN  |
| 1   | H     | 100 | ASN  |
| 1   | H     | 111 | GLN  |
| 1   | I     | 77  | ASN  |
| 1   | I     | 100 | ASN  |
| 1   | I     | 111 | GLN  |

### 5.3.3 RNA ⓘ

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     | 117/126 (92%)   | 0.20   | 3 (2%) 59 54  | 12, 25, 46, 55        | 0     |
| 1   | B     | 116/126 (92%)   | 0.18   | 2 (1%) 73 70  | 6, 25, 47, 52         | 0     |
| 1   | C     | 117/126 (92%)   | 0.29   | 2 (1%) 73 70  | 11, 24, 44, 52        | 0     |
| 1   | D     | 113/126 (89%)   | 0.19   | 1 (0%) 85 84  | 10, 27, 47, 54        | 0     |
| 1   | E     | 117/126 (92%)   | 0.23   | 3 (2%) 59 54  | 5, 23, 46, 55         | 0     |
| 1   | F     | 117/126 (92%)   | 0.31   | 2 (1%) 73 70  | 9, 26, 46, 52         | 0     |
| 1   | G     | 113/126 (89%)   | 0.73   | 14 (12%) 5 3  | 22, 38, 57, 66        | 0     |
| 1   | H     | 115/126 (91%)   | 0.48   | 7 (6%) 25 18  | 24, 37, 55, 69        | 0     |
| 1   | I     | 112/126 (88%)   | 0.66   | 8 (7%) 19 13  | 25, 38, 55, 62        | 0     |
| All | All   | 1037/1134 (91%) | 0.36   | 42 (4%) 41 35 | 5, 31, 51, 69         | 0     |

All (42) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 83  | ARG  | 4.3  |
| 1   | G     | 115 | ARG  | 4.1  |
| 1   | G     | 130 | ASN  | 4.0  |
| 1   | H     | 47  | GLU  | 3.5  |
| 1   | A     | 131 | GLY  | 3.4  |
| 1   | I     | 16  | ALA  | 3.3  |
| 1   | A     | 130 | ASN  | 3.1  |
| 1   | G     | 43  | LYS  | 3.0  |
| 1   | G     | 78  | GLU  | 3.0  |
| 1   | I     | 58  | GLU  | 2.9  |
| 1   | I     | 76  | ILE  | 2.8  |
| 1   | C     | 129 | GLU  | 2.8  |
| 1   | H     | 17  | ASN  | 2.8  |
| 1   | D     | 130 | ASN  | 2.8  |
| 1   | I     | 99  | CYS  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 42  | ILE  | 2.7  |
| 1   | I     | 115 | ARG  | 2.7  |
| 1   | E     | 129 | GLU  | 2.7  |
| 1   | G     | 85  | SER  | 2.6  |
| 1   | I     | 129 | GLU  | 2.6  |
| 1   | E     | 16  | ALA  | 2.6  |
| 1   | H     | 67  | THR  | 2.5  |
| 1   | G     | 81  | THR  | 2.5  |
| 1   | G     | 44  | LYS  | 2.5  |
| 1   | H     | 129 | GLU  | 2.4  |
| 1   | G     | 34  | ASP  | 2.4  |
| 1   | F     | 15  | PRO  | 2.4  |
| 1   | I     | 63  | CYS  | 2.3  |
| 1   | B     | 78  | GLU  | 2.3  |
| 1   | H     | 121 | GLY  | 2.3  |
| 1   | G     | 62  | GLU  | 2.2  |
| 1   | B     | 87  | GLU  | 2.2  |
| 1   | A     | 78  | GLU  | 2.2  |
| 1   | F     | 129 | GLU  | 2.2  |
| 1   | H     | 46  | TYR  | 2.2  |
| 1   | G     | 79  | ASP  | 2.2  |
| 1   | C     | 78  | GLU  | 2.2  |
| 1   | H     | 37  | ASP  | 2.1  |
| 1   | G     | 60  | TYR  | 2.1  |
| 1   | G     | 45  | GLY  | 2.1  |
| 1   | G     | 56  | ASP  | 2.1  |
| 1   | E     | 78  | GLU  | 2.1  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.