



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 07:54 AM EDT

PDB ID : 5N7X  
Title : CRYSTAL STRUCTURE OF STREPTAVIDIN WITH PEPTIDE EWWH-PQFEQKAK  
Authors : Lyamichev, V.; Goodrich, L.; Sullivan, E.; Bannen, R.; Benz, J.; Albert, T.; Patel, J.  
Deposited on : 2017-02-21  
Resolution : 1.12 Å(reported)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

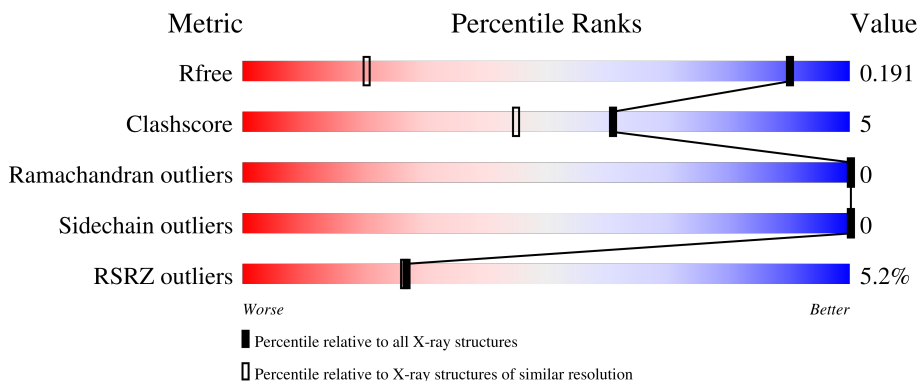
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.12 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1168 (1.14-1.10)                                      |
| Clashscore            | 141614                      | 1205 (1.14-1.10)                                      |
| Ramachandran outliers | 138981                      | 1168 (1.14-1.10)                                      |
| Sidechain outliers    | 138945                      | 1165 (1.14-1.10)                                      |
| RSRZ outliers         | 127900                      | 1146 (1.14-1.10)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 183    |                  |
| 1   | B     | 183    |                  |
| 1   | E     | 183    |                  |
| 1   | F     | 183    |                  |
| 1   | H     | 183    |                  |

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| Mol | Chain | Length | Quality of chain     |
|-----|-------|--------|----------------------|
| 1   | K     | 183    | <p>3% 63% 5% 33%</p> |
| 1   | M     | 183    | <p>3% 61% 5% 34%</p> |
| 1   | O     | 183    | <p>2% 64% 5% 33%</p> |
| 2   | C     | 12     | <p>17% 92% 8%</p>    |
| 2   | D     | 12     | <p>17% 92% 8%</p>    |
| 2   | G     | 12     | <p>8% 83% 8% 8%</p>  |
| 2   | I     | 12     | <p>8% 83% 8% 8%</p>  |
| 2   | J     | 12     | <p>8% 92% 8%</p>     |
| 2   | L     | 12     | <p>8% 92% 8%</p>     |
| 2   | N     | 12     | <p>8% 92% 8%</p>     |
| 2   | P     | 12     | <p>8% 92% 8%</p>     |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9634 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 Streptavidin.

| Mol | Chain | Residues | Atoms        |          |          |          | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|---------|-------|
|     |       |          | Total        | C        | N        | O        |         |         |       |
| 1   | A     | 122      | Total<br>957 | C<br>602 | N<br>162 | O<br>193 | 0       | 10      | 0     |
| 1   | B     | 121      | Total<br>945 | C<br>596 | N<br>160 | O<br>189 | 0       | 9       | 0     |
| 1   | E     | 122      | Total<br>945 | C<br>594 | N<br>159 | O<br>192 | 0       | 8       | 0     |
| 1   | F     | 122      | Total<br>939 | C<br>590 | N<br>158 | O<br>191 | 0       | 7       | 0     |
| 1   | H     | 122      | Total<br>952 | C<br>599 | N<br>162 | O<br>191 | 6       | 9       | 0     |
| 1   | K     | 122      | Total<br>951 | C<br>599 | N<br>158 | O<br>194 | 0       | 10      | 0     |
| 1   | M     | 121      | Total<br>944 | C<br>595 | N<br>161 | O<br>188 | 0       | 8       | 0     |
| 1   | O     | 122      | Total<br>939 | C<br>590 | N<br>158 | O<br>191 | 0       | 7       | 0     |

- Molecule 2 is a protein called GLU-TRP-VAL-HIS-PRO-GLN-PHE-GLU-GLN-LYS-ALA-LYS Peptide.

| Mol | Chain | Residues | Atoms       |         |         |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------------|---------|---------|---------|---------|---------|-------|
|     |       |          | Total       | C       | N       | O       |         |         |       |
| 2   | C     | 11       | Total<br>99 | C<br>65 | N<br>17 | O<br>17 | 0       | 0       | 0     |
| 2   | D     | 11       | Total<br>99 | C<br>65 | N<br>17 | O<br>17 | 0       | 0       | 0     |
| 2   | G     | 11       | Total<br>99 | C<br>65 | N<br>17 | O<br>17 | 0       | 0       | 0     |
| 2   | I     | 11       | Total<br>99 | C<br>65 | N<br>17 | O<br>17 | 0       | 0       | 0     |
| 2   | J     | 11       | Total<br>99 | C<br>65 | N<br>17 | O<br>17 | 0       | 0       | 0     |
| 2   | L     | 11       | Total<br>99 | C<br>65 | N<br>17 | O<br>17 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 2   | N     | 11       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 99    | 65 | 17 | 17 |         |         |       |
| 2   | P     | 11       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 99    | 65 | 17 | 17 |         |         |       |

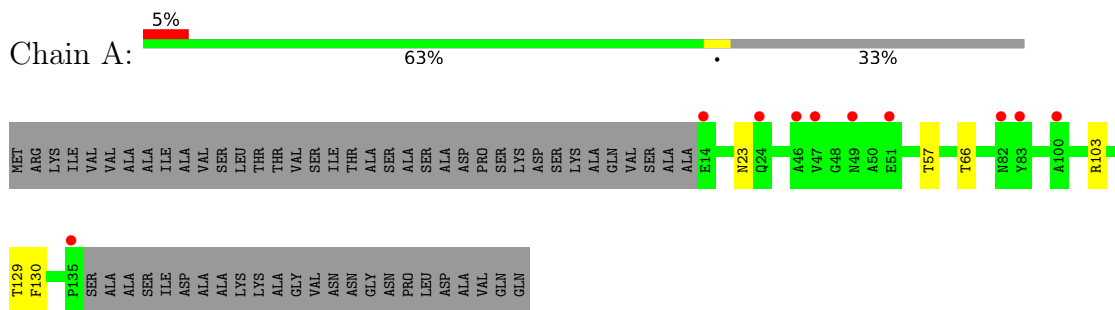
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 129      | Total | O   | 0       | 0       |
|     |       |          | 129   | 129 |         |         |
| 3   | B     | 153      | Total | O   | 0       | 0       |
|     |       |          | 153   | 153 |         |         |
| 3   | C     | 11       | Total | O   | 0       | 0       |
|     |       |          | 11    | 11  |         |         |
| 3   | D     | 9        | Total | O   | 0       | 0       |
|     |       |          | 9     | 9   |         |         |
| 3   | E     | 150      | Total | O   | 0       | 0       |
|     |       |          | 150   | 150 |         |         |
| 3   | F     | 140      | Total | O   | 0       | 0       |
|     |       |          | 140   | 140 |         |         |
| 3   | G     | 10       | Total | O   | 0       | 0       |
|     |       |          | 10    | 10  |         |         |
| 3   | H     | 148      | Total | O   | 0       | 0       |
|     |       |          | 148   | 148 |         |         |
| 3   | I     | 10       | Total | O   | 0       | 0       |
|     |       |          | 10    | 10  |         |         |
| 3   | J     | 24       | Total | O   | 0       | 0       |
|     |       |          | 24    | 24  |         |         |
| 3   | K     | 147      | Total | O   | 0       | 0       |
|     |       |          | 147   | 147 |         |         |
| 3   | L     | 14       | Total | O   | 0       | 0       |
|     |       |          | 14    | 14  |         |         |
| 3   | M     | 158      | Total | O   | 0       | 0       |
|     |       |          | 158   | 158 |         |         |
| 3   | N     | 11       | Total | O   | 0       | 0       |
|     |       |          | 11    | 11  |         |         |
| 3   | O     | 136      | Total | O   | 0       | 0       |
|     |       |          | 136   | 136 |         |         |
| 3   | P     | 20       | Total | O   | 0       | 0       |
|     |       |          | 20    | 20  |         |         |

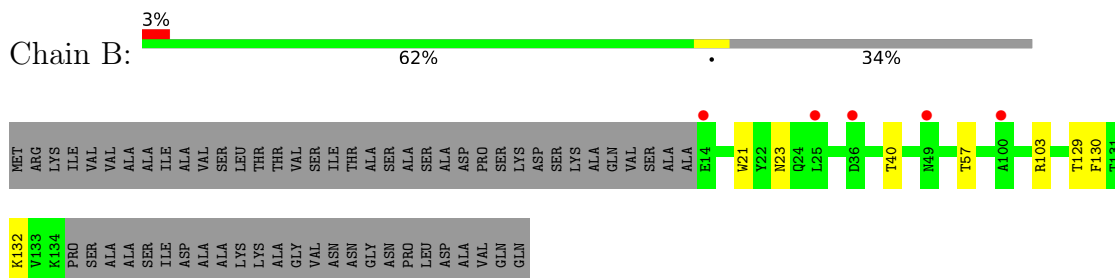
### 3 Residue-property plots [i](#)

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

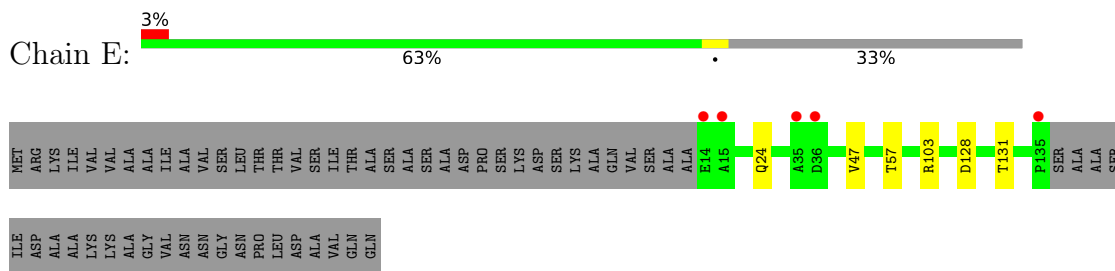
- Molecule 1: Streptavidin



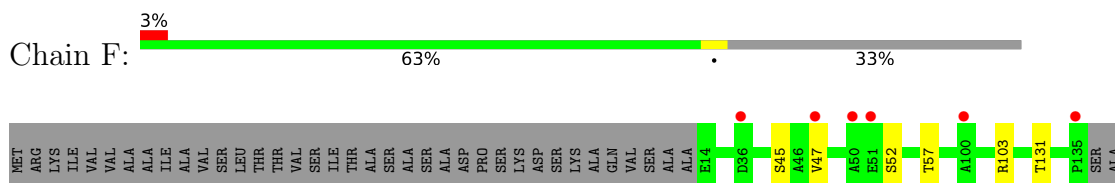
- Molecule 1: Streptavidin



- Molecule 1: Streptavidin



- Molecule 1: Streptavidin



ALA  
SER  
ILE  
ASP  
VAL  
VAL  
ALA  
LYS  
LYS  
LYS  
ALA  
GLY  
VAL  
VAL  
ASN  
ASN  
GLY  
PRO  
LEU  
ASP  
SER  
THR  
THR  
VAL  
SER  
ILE  
THR  
SER  
ALA  
SER  
SER  
ALA  
ALA  
ASP  
PRO  
SER  
SER  
SER  
LYS  
LYS  
ALA  
GLN  
VAL  
VAL  
GLN

● Molecule 1: Streptavidin



MET ARG LYS LYS ILE ASP VAL VAL ALA LYS LYS ILE ILE ASP VAL VAL ASN ASN GLY PRO LEU ASP SER LEU THR THR VAL SER ILE THR SER ALA SER SER ALA ALA ASP PRO SER SER ASP SER SER LYS LYS ALA GLN VAL VAL SER SER ALA ALA ALA E14 A16 A35 D36 M49 S52 R103 T131 P135 SER ALA ALA ALA SER ILE ASP SER ALA

LYS  
LYS  
ALA  
VAL  
ASN  
ASN  
GLY  
ASN  
PRO  
LEU  
ASP  
SER  
VAL  
GLN

● Molecule 1: Streptavidin



MET ARG LYS LYS ILE ASP VAL VAL ALA LYS LYS ILE ILE ASP VAL VAL ASN ASN GLY THR THR VAL SER ILE THR SER ALA SER SER ALA ALA ASP PRO SER SER ASP SER SER LYS LYS ALA GLN VAL VAL SER SER ALA ALA ALA E14 N23 Q24 L25 D36 M49 T57 R103 T129 F130 T131 K132 V133 K134 P135 SER ALA

ALA  
SER  
ILE  
ASP  
VAL  
VAL  
ALA  
LYS  
LYS  
LYS  
ALA  
GLY  
VAL  
VAL  
ASN  
ASN  
GLY  
ASN  
PRO  
LEU  
ASP  
SER  
THR  
THR  
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ALA  
ALA  
ASP  
PRO  
SER  
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SER  
LYS  
LYS  
ALA  
GLN  
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VAL  
GLN

● Molecule 1: Streptavidin



MET ARG LYS LYS ILE ASP VAL VAL ALA LYS LYS ILE ILE ASP VAL VAL ASN ASN GLY THR THR VAL SER ILE THR SER ALA SER SER ALA ALA ASP PRO SER SER ASP SER SER LYS LYS ALA GLN VAL VAL SER SER ALA ALA ALA E14 N23 T42 S45 A46 W47 G48 M49 S52 R53 T57 R84 A100 M105

T129 F130 K134 PRO SER ALA ALA ALA ALA ILE ILE ASP VAL VAL ASN ASN GLY LYS LYS ALA VAL VAL ILE VAL ILE ASN ASN GLY PRO PRO SER ASP ASP ALA VAL VAL GLN

● Molecule 1: Streptavidin



MET ARG LYS LYS ILE ASP VAL VAL ALA LYS LYS ILE ILE ASP VAL VAL ASN ASN GLY THR THR VAL SER ILE THR SER ALA SER SER ALA ALA ASP PRO SER SER ASP SER SER LYS LYS ALA GLN VAL VAL SER SER ALA ALA ALA E14 D36 M49 Y54 R103 L110 T131 P135 SER ALA ALA ALA SER ILE ASP SER ALA

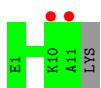
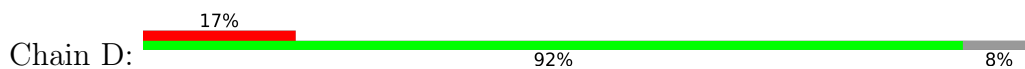
LYS  
LYS  
ALA  
GLY  
VAL  
ASN  
ASN  
GLY  
ASN  
PRO  
LEU  
ASP  
SER  
VAL  
GLN

● Molecule 2: GLU-TRP-VAL-HIS-PRO-GLN-PHE-GLU-GLN-LYS-ALA-LYS Peptide

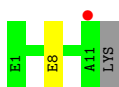
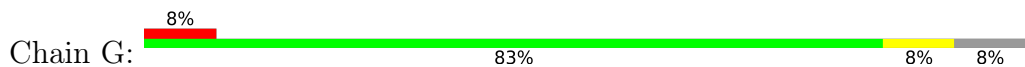


E1 K10 A11 LYS

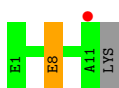
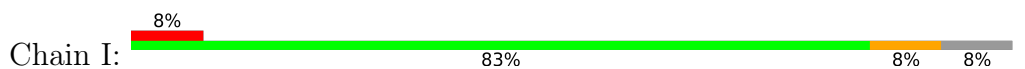
- Molecule 2: GLU-TRP-VAL-HIS-PRO-GLN-PHE-GLU-GLN-LYS-ALA-LYS Peptide



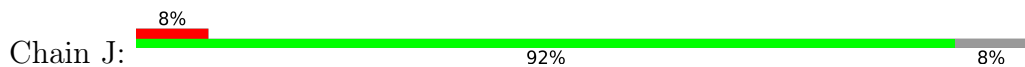
- Molecule 2: GLU-TRP-VAL-HIS-PRO-GLN-PHE-GLU-GLN-LYS-ALA-LYS Peptide



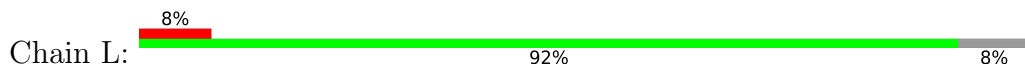
- Molecule 2: GLU-TRP-VAL-HIS-PRO-GLN-PHE-GLU-GLN-LYS-ALA-LYS Peptide



- Molecule 2: GLU-TRP-VAL-HIS-PRO-GLN-PHE-GLU-GLN-LYS-ALA-LYS Peptide



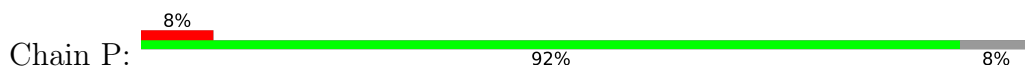
- Molecule 2: GLU-TRP-VAL-HIS-PRO-GLN-PHE-GLU-GLN-LYS-ALA-LYS Peptide



- Molecule 2: GLU-TRP-VAL-HIS-PRO-GLN-PHE-GLU-GLN-LYS-ALA-LYS Peptide



- Molecule 2: GLU-TRP-VAL-HIS-PRO-GLN-PHE-GLU-GLN-LYS-ALA-LYS Peptide







## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 57.91Å 64.81Å 81.16Å<br>96.31° 97.15° 84.09°                | Depositor        |
| Resolution (Å)  | 80.13 – 1.12<br>47.84 – 1.12                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.4 (80.13-1.12)<br>90.4 (47.84-1.12)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.03  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.59 (at 1.12Å)   | Xtrriage         |
| Refinement program  | REFMAC 5.8.0158   | Depositor        |
| R, $R_{free}$   | 0.160 , 0.186<br>0.169 , 0.191                              | Depositor<br>DCC |
| $R_{free}$ test set   | 20178 reflections (5.01%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 12.5  | Xtrriage         |
| Anisotropy  | 0.134   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 47.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.97  | EDS              |
| Total number of atoms   | 9634  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 20.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.27 % 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 1.0159e-04.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5        |
| 1   | A     | 0.70         | 0/1008        | 0.88        | 0/1379         |
| 1   | B     | 0.67         | 0/992         | 0.82        | 0/1357         |
| 1   | E     | 0.71         | 0/990         | 0.81        | 0/1355         |
| 1   | F     | 0.72         | 0/981         | 0.84        | 0/1343         |
| 1   | H     | 0.76         | 1/1000 (0.1%) | 0.84        | 0/1368         |
| 1   | K     | 0.75         | 0/1002        | 0.86        | 0/1373         |
| 1   | M     | 0.69         | 0/988         | 0.82        | 1/1351 (0.1%)  |
| 1   | O     | 0.72         | 0/981         | 0.83        | 2/1343 (0.1%)  |
| 2   | C     | 0.62         | 0/103         | 0.60        | 0/139          |
| 2   | D     | 0.59         | 0/103         | 0.61        | 0/139          |
| 2   | G     | 0.59         | 0/103         | 0.67        | 0/139          |
| 2   | I     | 0.85         | 1/103 (1.0%)  | 0.80        | 0/139          |
| 2   | J     | 0.62         | 0/103         | 0.61        | 0/139          |
| 2   | L     | 0.64         | 0/103         | 0.63        | 0/139          |
| 2   | N     | 0.57         | 0/103         | 0.59        | 0/139          |
| 2   | P     | 0.66         | 0/103         | 0.64        | 0/139          |
| All | All   | 0.71         | 2/8766 (0.0%) | 0.82        | 3/11981 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | I     | 8   | GLU  | CD-OE1 | 5.40  | 1.31        | 1.25     |
| 1   | H     | 135 | PRO  | C-O    | -5.34 | 1.12        | 1.23     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 110 | LEU  | CB-CG-CD1 | 6.00  | 121.20      | 111.00   |
| 1   | M     | 84  | ARG  | NE-CZ-NH1 | -5.78 | 117.41      | 120.30   |
| 1   | O     | 54  | TYR  | CB-CG-CD1 | 5.26  | 124.15      | 121.00   |

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     | 957   | 0        | 916      | 19      | 0            |
| 1   | B     | 945   | 0        | 910      | 17      | 0            |
| 1   | E     | 945   | 0        | 896      | 13      | 0            |
| 1   | F     | 939   | 0        | 888      | 12      | 0            |
| 1   | H     | 952   | 0        | 912      | 2       | 0            |
| 1   | K     | 951   | 0        | 909      | 13      | 0            |
| 1   | M     | 944   | 0        | 906      | 14      | 0            |
| 1   | O     | 939   | 0        | 888      | 1       | 0            |
| 2   | C     | 99    | 0        | 90       | 0       | 0            |
| 2   | D     | 99    | 0        | 90       | 0       | 0            |
| 2   | G     | 99    | 0        | 90       | 1       | 0            |
| 2   | I     | 99    | 0        | 90       | 1       | 0            |
| 2   | J     | 99    | 0        | 90       | 0       | 0            |
| 2   | L     | 99    | 0        | 90       | 0       | 0            |
| 2   | N     | 99    | 0        | 90       | 0       | 0            |
| 2   | P     | 99    | 0        | 90       | 0       | 0            |
| 3   | A     | 129   | 0        | 0        | 3       | 0            |
| 3   | B     | 153   | 0        | 0        | 3       | 0            |
| 3   | C     | 11    | 0        | 0        | 0       | 0            |
| 3   | D     | 9     | 0        | 0        | 0       | 0            |
| 3   | E     | 150   | 0        | 0        | 1       | 0            |
| 3   | F     | 140   | 0        | 0        | 1       | 0            |
| 3   | G     | 10    | 0        | 0        | 0       | 0            |
| 3   | H     | 148   | 0        | 0        | 0       | 0            |
| 3   | I     | 10    | 0        | 0        | 0       | 0            |
| 3   | J     | 24    | 0        | 0        | 0       | 0            |
| 3   | K     | 147   | 0        | 0        | 5       | 0            |
| 3   | L     | 14    | 0        | 0        | 0       | 0            |
| 3   | M     | 158   | 0        | 0        | 3       | 0            |
| 3   | N     | 11    | 0        | 0        | 0       | 0            |
| 3   | O     | 136   | 0        | 0        | 0       | 0            |
| 3   | P     | 20    | 0        | 0        | 0       | 0            |
| All | All   | 9634  | 0        | 7945     | 74      | 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 5.

The worst 5 of 74 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:M:42[B]:THR:HG21 | 1:M:53[B]:ARG:HD2  | 1.42                     | 1.01              |
| 1:M:42[B]:THR:CG2  | 1:M:53[B]:ARG:CG   | 2.39                     | 1.00              |
| 1:M:42[B]:THR:HG21 | 1:M:53[B]:ARG:CD   | 1.93                     | 0.96              |
| 1:A:103:ARG:HH21   | 1:A:129[A]:THR:CG2 | 1.82                     | 0.91              |
| 1:K:103:ARG:HH21   | 1:K:129[A]:THR:CG2 | 1.82                     | 0.91              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 129/183 (70%) | 128 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | B     | 127/183 (69%) | 125 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | E     | 127/183 (69%) | 125 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | F     | 126/183 (69%) | 124 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | H     | 128/183 (70%) | 125 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | K     | 129/183 (70%) | 126 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | M     | 126/183 (69%) | 125 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | O     | 126/183 (69%) | 123 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 2   | C     | 9/12 (75%)    | 9 (100%)  | 0       | 0        | 100         | 100 |
| 2   | D     | 9/12 (75%)    | 9 (100%)  | 0       | 0        | 100         | 100 |
| 2   | G     | 9/12 (75%)    | 9 (100%)  | 0       | 0        | 100         | 100 |
| 2   | I     | 9/12 (75%)    | 9 (100%)  | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 2   | J     | 9/12 (75%)      | 9 (100%)   | 0       | 0        | 100         | 100 |
| 2   | L     | 9/12 (75%)      | 9 (100%)   | 0       | 0        | 100         | 100 |
| 2   | N     | 9/12 (75%)      | 9 (100%)   | 0       | 0        | 100         | 100 |
| 2   | P     | 9/12 (75%)      | 9 (100%)   | 0       | 0        | 100         | 100 |
| All | All   | 1090/1560 (70%) | 1073 (98%) | 17 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 99/134 (74%)   | 99 (100%)  | 0        | 100         | 100 |
| 1   | B     | 97/134 (72%)   | 97 (100%)  | 0        | 100         | 100 |
| 1   | E     | 97/134 (72%)   | 97 (100%)  | 0        | 100         | 100 |
| 1   | F     | 96/134 (72%)   | 96 (100%)  | 0        | 100         | 100 |
| 1   | H     | 98/134 (73%)   | 98 (100%)  | 0        | 100         | 100 |
| 1   | K     | 99/134 (74%)   | 99 (100%)  | 0        | 100         | 100 |
| 1   | M     | 96/134 (72%)   | 96 (100%)  | 0        | 100         | 100 |
| 1   | O     | 96/134 (72%)   | 96 (100%)  | 0        | 100         | 100 |
| 2   | C     | 10/11 (91%)    | 10 (100%)  | 0        | 100         | 100 |
| 2   | D     | 10/11 (91%)    | 10 (100%)  | 0        | 100         | 100 |
| 2   | G     | 10/11 (91%)    | 10 (100%)  | 0        | 100         | 100 |
| 2   | I     | 10/11 (91%)    | 10 (100%)  | 0        | 100         | 100 |
| 2   | J     | 10/11 (91%)    | 10 (100%)  | 0        | 100         | 100 |
| 2   | L     | 10/11 (91%)    | 10 (100%)  | 0        | 100         | 100 |
| 2   | N     | 10/11 (91%)    | 10 (100%)  | 0        | 100         | 100 |
| 2   | P     | 10/11 (91%)    | 10 (100%)  | 0        | 100         | 100 |
| All | All   | 858/1160 (74%) | 858 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 82  | ASN  |
| 1   | M     | 82  | ASN  |
| 1   | H     | 82  | ASN  |
| 1   | F     | 82  | ASN  |
| 1   | K     | 82  | 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 1   | A     | 122/183 (66%)   | 0.46   | 10 (8%) 11 12 | 11, 16, 35, 50        | 2 (1%)  |
| 1   | B     | 121/183 (66%)   | 0.33   | 5 (4%) 37 35  | 10, 16, 33, 56        | 2 (1%)  |
| 1   | E     | 122/183 (66%)   | 0.29   | 5 (4%) 37 35  | 10, 16, 30, 52        | 2 (1%)  |
| 1   | F     | 122/183 (66%)   | 0.31   | 6 (4%) 29 28  | 9, 15, 29, 49         | 2 (1%)  |
| 1   | H     | 122/183 (66%)   | 0.37   | 4 (3%) 46 45  | 9, 16, 30, 49         | 2 (1%)  |
| 1   | K     | 122/183 (66%)   | 0.43   | 6 (4%) 29 28  | 10, 15, 33, 48        | 2 (1%)  |
| 1   | M     | 121/183 (66%)   | 0.30   | 6 (4%) 28 28  | 9, 15, 31, 51         | 2 (1%)  |
| 1   | O     | 122/183 (66%)   | 0.24   | 3 (2%) 57 55  | 9, 16, 29, 50         | 2 (1%)  |
| 2   | C     | 11/12 (91%)     | 0.52   | 2 (18%) 1 2   | 13, 18, 50, 59        | 0       |
| 2   | D     | 11/12 (91%)     | 1.23   | 2 (18%) 1 2   | 15, 26, 53, 58        | 0       |
| 2   | G     | 11/12 (91%)     | 1.13   | 1 (9%) 9 10   | 12, 19, 39, 64        | 0       |
| 2   | I     | 11/12 (91%)     | 1.29   | 1 (9%) 9 10   | 12, 18, 44, 65        | 0       |
| 2   | J     | 11/12 (91%)     | 0.24   | 1 (9%) 9 10   | 12, 17, 35, 46        | 0       |
| 2   | L     | 11/12 (91%)     | 0.48   | 1 (9%) 9 10   | 16, 23, 45, 50        | 0       |
| 2   | N     | 11/12 (91%)     | 0.75   | 1 (9%) 9 10   | 15, 22, 49, 63        | 0       |
| 2   | P     | 11/12 (91%)     | 0.39   | 1 (9%) 9 10   | 12, 17, 36, 49        | 0       |
| All | All   | 1062/1560 (68%) | 0.38   | 55 (5%) 27 26 | 9, 16, 34, 65         | 16 (1%) |

The worst 5 of 55 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | I     | 11  | ALA  | 12.4 |
| 2   | G     | 11  | ALA  | 10.7 |
| 1   | K     | 135 | PRO  | 7.7  |
| 2   | D     | 11  | ALA  | 6.1  |
| 1   | A     | 49  | ASN  | 5.8  |



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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.