



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:34 AM UTC

PDB ID : 1UE7 / pdb\_00001ue7  
Title : Crystal structure of the single-stranded dna-binding protein from mycobacterium tuberculosis  
Authors : Saikrishnan, K.; Jeyakanthan, J.; Venkatesh, J.; Acharya, N.; Sekar, K.; Varshney, U.; Vijayan, M.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2003-05-09  
Resolution : 3.20 Å(reported)

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

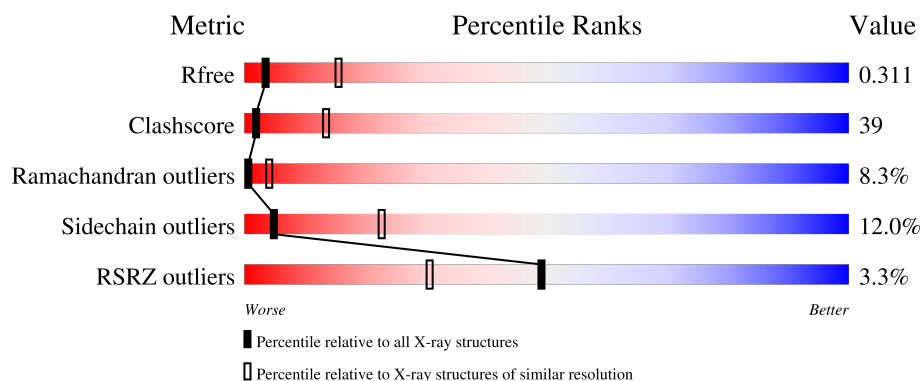
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 164    |                  |
| 1   | B     | 164    |                  |
| 1   | C     | 164    |                  |
| 1   | D     | 164    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3036 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 Single-strand binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 758   | 468 | 141 | 148 | 1 |         |         |       |
| 1   | B     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 440 | 125 | 139 | 1 |         |         |       |
| 1   | C     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 712   | 445 | 126 | 140 | 1 |         |         |       |
| 1   | D     | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 678   | 425 | 117 | 135 | 1 |         |         |       |

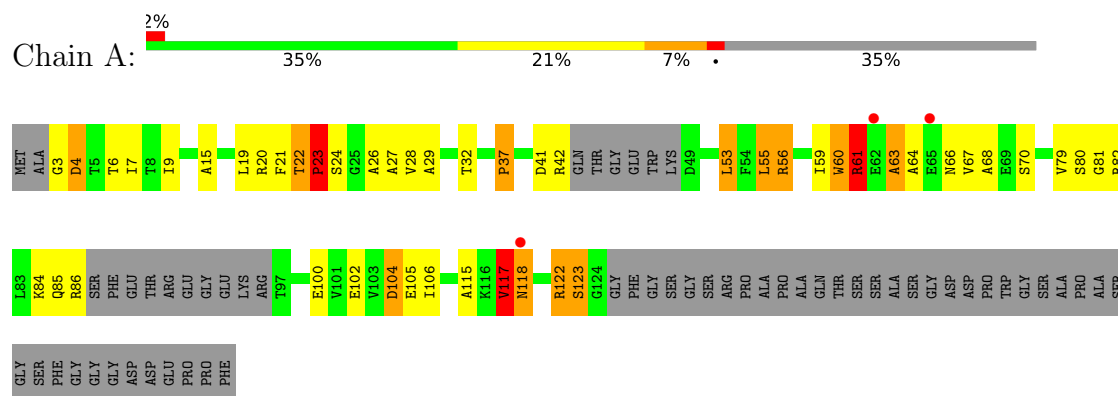
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 51       | Total | O  | 0       | 0       |
|     |       |          | 51    | 51 |         |         |
| 2   | B     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 2   | C     | 46       | Total | O  | 0       | 0       |
|     |       |          | 46    | 46 |         |         |
| 2   | D     | 68       | Total | O  | 0       | 0       |
|     |       |          | 68    | 68 |         |         |

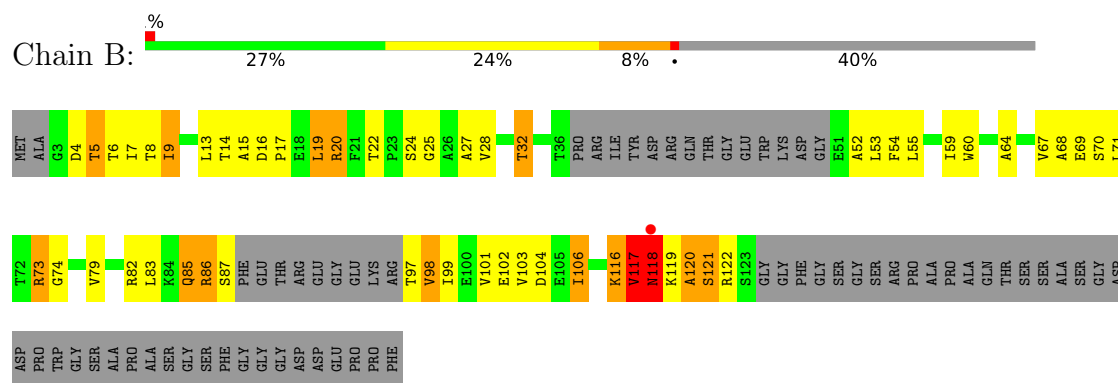
### 3 Residue-property plots [i](#)

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.

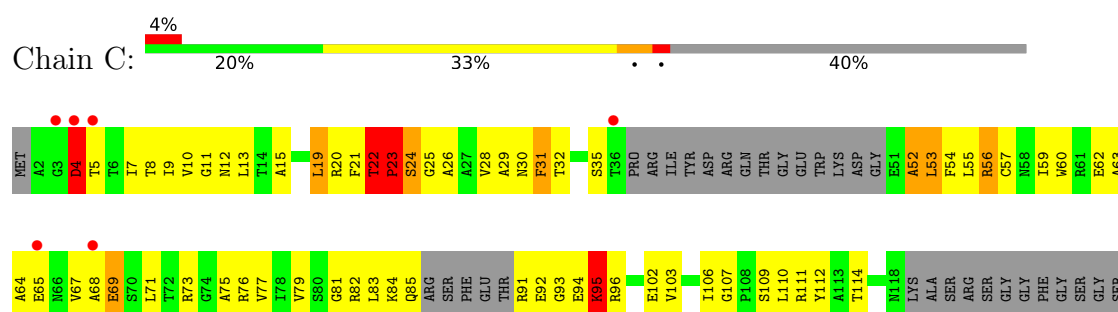
#### • Molecule 1: Single-strand binding protein



#### • Molecule 1: Single-strand binding protein

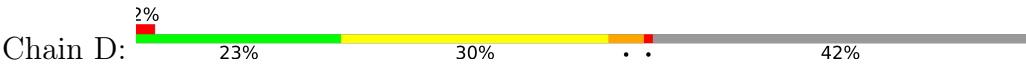


#### • Molecule 1: Single-strand binding protein



ARG  
PRO  
ALA  
PRO  
PRO  
ALA  
GLN  
THR  
SER  
SER  
ALA  
SER  
GLY  
ASP  
ASP  
PRO  
TRP  
GLY  
SER  
ALA  
ALA  
PRO  
ALA  
SER  
GLY  
GLY  
SER  
PHE  
GLY  
GLY  
GLY  
ASP  
ASP  
GLU  
PRO  
PRO  
PHE

● Molecule 1: Single-strand binding protein



MET  
ALA  
G3  
D4  
T5  
T6  
I7  
T8  
I9  
N12  
L13  
T14  
E18  
L19  
T22  
P23  
S24  
G25  
A26  
A27  
V28  
A29  
K30  
F31  
T32  
V33  
A34  
S35  
T36  
P37  
R38  
ILE  
TYR  
ASP  
ARG  
GLN  
THR  
GLY  
GLY  
TRP  
LYS  
ASP  
GLY  
E51  
A52  
L53  
F54  
L55  
R56  
C57  
N58  
I59  
W60  
R61  
E62  
A63  
A64

V67  
S70  
L71  
T72  
R73  
G74  
R76  
V77  
I78  
V79  
S80  
G81  
R82  
L83  
K84  
Q85  
R86  
S87  
PHE  
GLU  
THR  
ARG  
GLU  
GLY  
GLY  
LYS  
ARG  
T97  
V101  
E102  
V103  
D104  
F105  
I106  
S109  
L110  
R111  
Y112  
A113  
T114  
A115  
K116  
V117  
N118  
LYS  
ALA  
SER  
ARG  
SER  
GLY  
GLY  
PHE  
GLY  
SER  
GLY

SER  
ARG  
PRO  
ALA  
PRO  
ALA  
GLN  
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ASP  
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PRO  
ALA  
SER  
GLY  
PHE  
GLY  
GLY  
GLY  
ASP  
ASP  
GLU  
PRO  
PRO  
PHE

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | I 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 60.22Å 116.72Å 177.88Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 15.00 – 3.20<br>15.00 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.3 (15.00-3.20)<br>93.2 (15.00-3.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.62 (at 3.17Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.235 , 0.313<br>0.236 , 0.311                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1042 reflections (10.31%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 64.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.357                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 99.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                        | EDS              |
| Total number of atoms                                                   | 3036                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 59.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.67         | 2/764 (0.3%)  | 1.22        | 11/1037 (1.1%) |
| 1   | B     | 0.55         | 0/711         | 1.09        | 6/968 (0.6%)   |
| 1   | C     | 0.60         | 1/718 (0.1%)  | 1.24        | 11/976 (1.1%)  |
| 1   | D     | 0.55         | 0/684         | 1.35        | 7/934 (0.7%)   |
| All | All   | 0.59         | 3/2877 (0.1%) | 1.23        | 35/3915 (0.9%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 69  | GLU  | CA-C  | -6.39 | 1.44        | 1.52     |
| 1   | A     | 3   | GLY  | N-CA  | 5.91  | 1.55        | 1.45     |
| 1   | A     | 4   | ASP  | N-CA  | 5.37  | 1.53        | 1.46     |

The worst 5 of 35 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 115 | ALA  | N-CA-C | 23.22 | 127.82      | 108.78   |
| 1   | C     | 4   | ASP  | N-CA-C | 10.21 | 126.10      | 109.96   |
| 1   | B     | 118 | ASN  | N-CA-C | 8.49  | 128.88      | 110.80   |
| 1   | A     | 4   | ASP  | N-CA-C | 8.45  | 128.79      | 110.80   |
| 1   | D     | 115 | ALA  | CA-C-O | 7.85  | 122.49      | 117.94   |

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     | 758   | 0        | 725      | 61      | 0            |
| 1   | B     | 705   | 0        | 690      | 53      | 0            |
| 1   | C     | 712   | 0        | 704      | 60      | 0            |
| 1   | D     | 678   | 0        | 655      | 50      | 0            |
| 2   | A     | 51    | 0        | 0        | 1       | 0            |
| 2   | B     | 18    | 0        | 0        | 1       | 0            |
| 2   | C     | 46    | 0        | 0        | 4       | 0            |
| 2   | D     | 68    | 0        | 0        | 1       | 0            |
| All | All   | 3036  | 0        | 2774     | 219     | 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 39.

The worst 5 of 219 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:22:THR:HB    | 1:C:23:PRO:HD2 | 1.06                     | 1.02              |
| 1:A:117:VAL:HG12 | 1:A:118:ASN:H  | 1.27                     | 0.99              |
| 1:C:22:THR:CB    | 1:C:23:PRO:HD2 | 1.93                     | 0.97              |
| 1:D:117:VAL:HG13 | 1:D:118:ASN:H  | 1.29                     | 0.94              |
| 1:A:19:LEU:HD21  | 1:A:27:ALA:HB1 | 1.53                     | 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     | 100/164 (61%) | 75 (75%) | 16 (16%) | 9 (9%)   | 0           | 3 |
| 1   | B     | 92/164 (56%)  | 74 (80%) | 11 (12%) | 7 (8%)   | 1           | 5 |
| 1   | C     | 92/164 (56%)  | 72 (78%) | 11 (12%) | 9 (10%)  | 0           | 2 |
| 1   | D     | 89/164 (54%)  | 75 (84%) | 8 (9%)   | 6 (7%)   | 1           | 7 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|----------|-------------|
| All | All   | 373/656 (57%) | 296 (79%) | 46 (12%) | 31 (8%)  | 0 4         |

5 of 31 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ASP  |
| 1   | A     | 23  | PRO  |
| 1   | A     | 24  | SER  |
| 1   | A     | 118 | ASN  |
| 1   | A     | 122 | ARG  |

### 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     | 73/126 (58%)  | 65 (89%)  | 8 (11%)  | 6 26        |
| 1   | B     | 71/126 (56%)  | 60 (84%)  | 11 (16%) | 2 14        |
| 1   | C     | 72/126 (57%)  | 63 (88%)  | 9 (12%)  | 4 21        |
| 1   | D     | 68/126 (54%)  | 62 (91%)  | 6 (9%)   | 9 35        |
| All | All   | 284/504 (56%) | 250 (88%) | 34 (12%) | 5 23        |

5 of 34 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 7   | ILE  |
| 1   | D     | 19  | LEU  |
| 1   | D     | 36  | THR  |
| 1   | B     | 69  | GLU  |
| 1   | B     | 32  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 12  | ASN  |
| 1   | B     | 58  | ASN  |
| 1   | D     | 12  | ASN  |
| 1   | C     | 30  | ASN  |
| 1   | A     | 85  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 106/164 (64%) | -0.03  | 3 (2%) 55 35  | 17, 57, 102, 102      | 0     |
| 1   | B     | 98/164 (59%)  | -0.04  | 1 (1%) 79 63  | 14, 57, 97, 102       | 0     |
| 1   | C     | 98/164 (59%)  | 0.15   | 6 (6%) 27 17  | 17, 60, 102, 102      | 0     |
| 1   | D     | 95/164 (57%)  | -0.05  | 3 (3%) 50 31  | 22, 50, 97, 101       | 0     |
| All | All   | 397/656 (60%) | 0.01   | 13 (3%) 49 30 | 14, 57, 101, 102      | 0     |

The worst 5 of 13 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 4   | ASP  | 3.9  |
| 1   | B     | 118 | ASN  | 3.0  |
| 1   | C     | 65  | GLU  | 3.0  |
| 1   | C     | 68  | ALA  | 2.7  |
| 1   | C     | 36  | THR  | 2.7  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.