



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 18, 2023 – 04:07 PM EDT

PDB ID : 1UE6  
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 : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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 : 2.36  
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) : 2.36

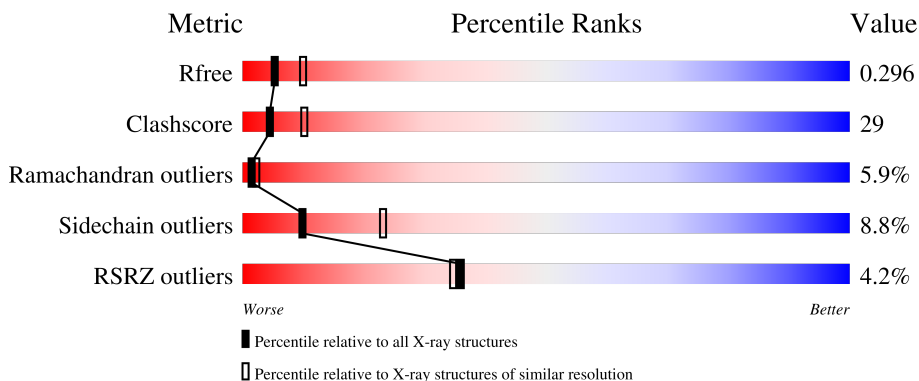
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	 3% 40% 21% 5% 33%
1	B	164	 3% 32% 30% 35%
1	C	164	 2% 34% 23% 8% 35%
1	D	164	 3% 34% 27% 37%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3289 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
			Total	C	N	O	S			
1	A	110	784	489	139	155	1	0	0	0
1	B	106	751	466	134	150	1	0	0	0
1	C	106	781	486	144	150	1	0	0	0
1	D	104	744	465	133	145	1	0	0	0

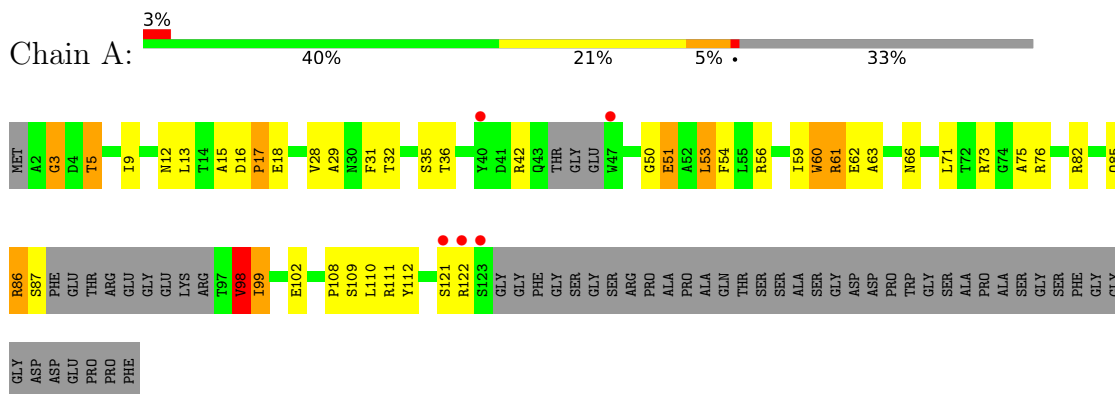
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		
2	B	66	Total	O	0	0
			66	66		
2	C	56	Total	O	0	0
			56	56		
2	D	43	Total	O	0	0
			43	43		

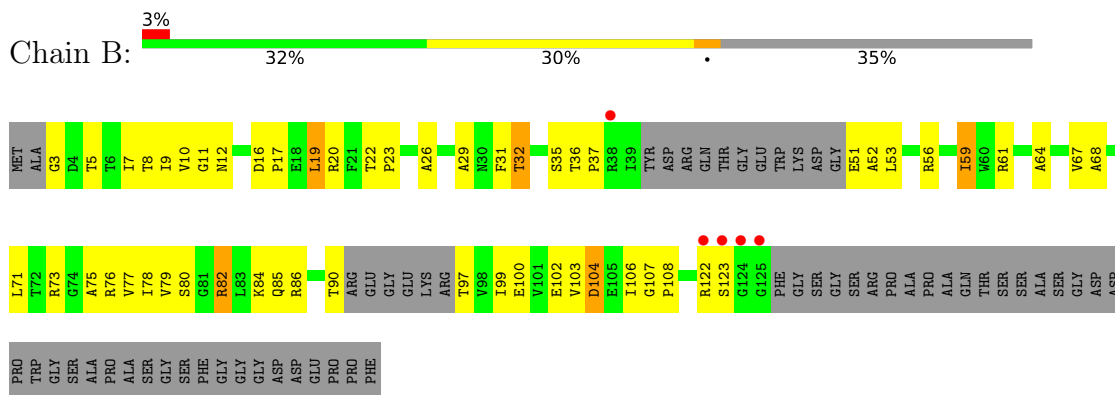
### 3 Residue-property plots [i](#)

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.

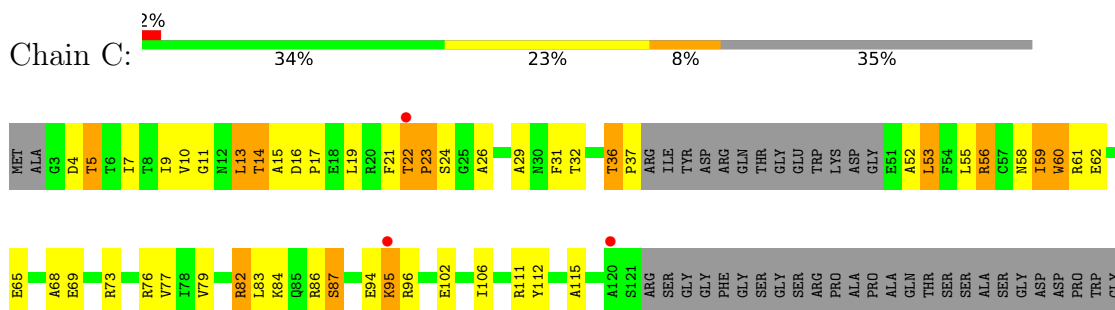
- Molecule 1: Single-strand binding protein



- Molecule 1: Single-strand binding protein



- Molecule 1: Single-strand binding protein



SER  
ALA  
PRO  
ALA  
SER  
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  
L13  
T14  
A15  
D16  
P17  
E18  
L19  
R20  
F21  
G25  
A26  
A27  
V28  
A29  
T32  
S35  
T36  
P37  
R38  
L39  
Y40  
ASP  
ARG  
GLN  
GLN  
THR  
GLY  
GLU  
TRP  
TRP  
LYS  
ASP  
GLY  
E51  
A52  
L53  
F54  
L55  
R56  
I59  
W60  
R61  
E62  
V67  
L71  
T72

R73  
V79  
L83  
K84  
Q85  
E89  
T90  
R91  
GLU  
GLY  
GLU  
K95  
V98  
I99  
F100  
V101  
E102  
V103  
I106  
T114  
K119  
ALA  
SER  
ARG  
SER  
GLY  
GLY  
PHE  
GLY  
SER  
SER  
GLY  
SER  
ARG  
PRO  
ALA  
PRO  
ALA  
GLN  
THR  
SER  
SER  
SER  
ALA  
SER  
GLY  
ASP  
ASP  
PRO  
PRO  
TRP  
GLY  
SER  
ALA  
ALA

SER  
GLY  
SER  
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 a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.36Å 117.62Å 175.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 19.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (15.00-2.70) 93.1 (19.77-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 2.71Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.231 , 0.295 0.231 , 0.296	Depositor DCC
$R_{free}$ test set	954 reflections (5.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtrriage
Anisotropy	0.434	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 82.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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	0.45	0/792	0.79	2/1078 (0.2%)
1	B	0.40	0/758	0.71	0/1032
1	C	0.51	1/790 (0.1%)	0.82	2/1072 (0.2%)
1	D	0.40	0/750	0.73	0/1020
All	All	0.44	1/3090 (0.0%)	0.76	4/4202 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	THR	CA-CB	5.56	1.67	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	LEU	N-CA-C	7.42	131.03	111.00
1	A	99	ILE	N-CA-C	-5.19	96.98	111.00
1	A	98	VAL	N-CA-C	5.19	125.00	111.00
1	C	14	THR	N-CA-CB	5.17	120.12	110.30

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	784	0	738	42	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	751	0	713	52	0
1	C	781	0	763	58	0
1	D	744	0	709	41	0
2	A	64	0	0	0	0
2	B	66	0	0	2	0
2	C	56	0	0	2	0
2	D	43	0	0	2	0
All	All	3289	0	2923	171	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 29.

The worst 5 of 171 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:79:VAL:HG22	1:C:106:ILE:HD13	1.41	1.01
1:A:54:PHE:H	1:B:85:GLN:HE22	1.20	0.87
1:A:76:ARG:HG2	1:A:109:SER:HB3	1.56	0.87
1:A:54:PHE:H	1:B:85:GLN:NE2	1.72	0.86
1:A:71:LEU:HD21	1:A:108:PRO:HG3	1.61	0.83

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	104/164 (63%)	85 (82%)	11 (11%)	8 (8%)	<a href="#">1</a> <a href="#">1</a>
1	B	100/164 (61%)	93 (93%)	4 (4%)	3 (3%)	<a href="#">4</a> <a href="#">10</a>
1	C	102/164 (62%)	82 (80%)	11 (11%)	9 (9%)	<a href="#">1</a> <a href="#">1</a>
1	D	98/164 (60%)	87 (89%)	7 (7%)	4 (4%)	<a href="#">3</a> <a href="#">6</a>

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	404/656 (62%)	347 (86%)	33 (8%)	24 (6%)	<b>1</b> <b>2</b>

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	86	ARG
1	A	121	SER
1	B	122	ARG
1	C	26	ALA

### 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	75/126 (60%)	70 (93%)	5 (7%)	<b>16</b> <b>37</b>
1	B	73/126 (58%)	65 (89%)	8 (11%)	<b>6</b> <b>14</b>
1	C	78/126 (62%)	68 (87%)	10 (13%)	<b>4</b> <b>10</b>
1	D	71/126 (56%)	68 (96%)	3 (4%)	<b>30</b> <b>58</b>
All	All	297/504 (59%)	271 (91%)	26 (9%)	<b>10</b> <b>23</b>

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	16	ASP
1	C	56	ARG
1	D	73	ARG
1	C	53	LEU
1	C	59	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	66	ASN
1	B	85	GLN
1	C	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 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	110/164 (67%)	-0.07	5 (4%) 33 31	23, 49, 115, 143	0
1	B	106/164 (64%)	-0.13	5 (4%) 31 30	26, 51, 106, 127	0
1	C	106/164 (64%)	-0.13	3 (2%) 53 54	25, 52, 105, 121	0
1	D	104/164 (63%)	-0.23	5 (4%) 30 28	18, 48, 103, 132	0
All	All	426/656 (64%)	-0.14	18 (4%) 36 35	18, 51, 110, 143	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	GLY	6.2
1	B	123	SER	6.1
1	A	122	ARG	6.1
1	A	47	TRP	5.3
1	A	123	SER	4.8

### 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.