



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:35 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)

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

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	:	4-5-2 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

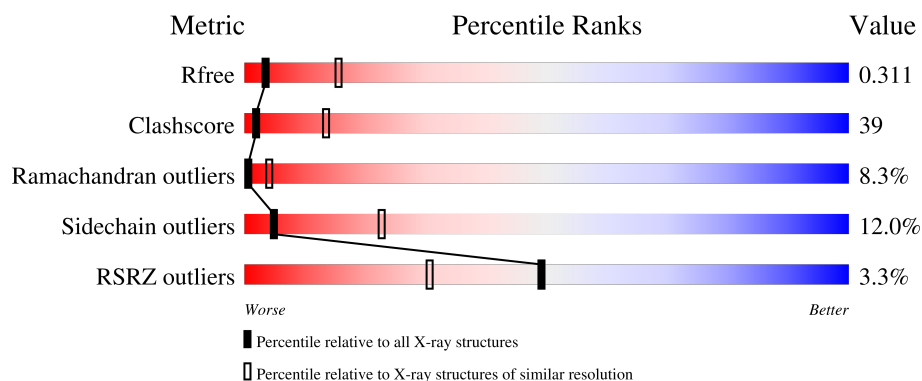
1 Overall quality at a glance

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 (#Entries)	Similar resolution (#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 ≥ 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.

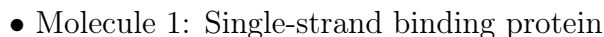
- Molecule 1 is a protein called Single-strand binding protein.

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.

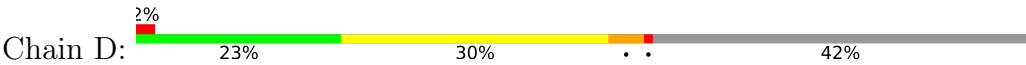
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	O	0	0
			51	51		
2	B	18	Total	O	0	0
			18	18		
2	C	46	Total	O	0	0
			46	46		
2	D	68	Total	O	0	0
			68	68		

- 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
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
V30
F31
T32
V33
A34
ARG
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
THR
SER
SER
ALA
SER
GLY
ASP
ASP
PRO
TRP
GLY
SER
ALA
PRO
ALA
SER
GLY
PHE
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, α , β , γ	60.22Å 116.72Å 177.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.3 (15.00-3.20) 93.2 (15.00-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 3.17Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.313 0.236 , 0.311	Depositor DCC
R_{free} test set	1042 reflections (10.31%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 99.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

All (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
1	C	25	GLY	N-CA-C	-7.29	104.54	115.32
1	D	115	ALA	CB-CA-C	-7.07	106.89	117.07
1	B	117	VAL	N-CA-C	6.94	123.77	109.34
1	C	84	LYS	N-CA-C	6.89	120.58	110.17
1	A	104	ASP	N-CA-C	-6.67	104.78	113.12
1	A	117	VAL	N-CA-C	6.66	123.18	109.34
1	A	63	ALA	N-CA-C	-6.65	104.65	112.89
1	C	22	THR	CA-C-N	6.53	128.00	119.84
1	C	22	THR	C-N-CA	6.53	128.00	119.84
1	A	22	THR	CA-C-N	6.34	127.76	119.84
1	A	22	THR	C-N-CA	6.34	127.76	119.84
1	C	94	GLU	N-CA-C	-6.16	97.68	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	LYS	N-CA-C	5.95	123.47	110.80
1	D	70	SER	N-CA-C	5.92	120.52	113.12
1	A	37	PRO	N-CA-CB	5.79	109.33	103.25
1	A	115	ALA	N-CA-C	5.53	116.82	108.46
1	D	37	PRO	N-CA-CB	5.51	109.04	103.25
1	A	60	TRP	N-CA-C	5.44	119.04	109.80
1	D	114	THR	N-CA-C	5.25	117.84	109.65
1	A	70	SER	N-CA-C	5.20	119.85	112.93
1	B	117	VAL	CA-C-N	5.20	131.48	121.54
1	B	117	VAL	C-N-CA	5.20	131.48	121.54
1	D	103	VAL	N-CA-C	5.18	115.07	108.12
1	A	55	LEU	N-CA-C	5.12	116.98	108.02
1	C	68	ALA	CA-C-N	5.11	131.30	121.54
1	C	68	ALA	C-N-CA	5.11	131.30	121.54
1	C	107	GLY	CA-C-N	5.08	125.32	119.83
1	C	107	GLY	C-N-CA	5.08	125.32	119.83
1	B	85	GLN	N-CA-C	5.03	114.88	108.24
1	B	25	GLY	N-CA-C	-5.01	108.40	115.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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.

All (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
1:D:7:ILE:HG12	1:D:8:THR:H	1.33	0.91
1:D:76:ARG:HG2	1:D:109:SER:HB3	1.53	0.91
1:A:29:ALA:HB3	1:A:59:ILE:HG23	1.55	0.89
1:C:22:THR:HB	1:C:23:PRO:CD	1.99	0.89
1:A:9:ILE:HD12	1:A:55:LEU:HD12	1.54	0.88
1:A:56:ARG:H	1:A:56:ARG:HD3	1.39	0.87
1:A:59:ILE:HD13	1:A:67:VAL:HG21	1.55	0.86
1:D:36:THR:HG23	1:D:52:ALA:H	1.39	0.85
1:A:28:VAL:HG22	1:A:60:TRP:NE1	1.95	0.81
1:A:117:VAL:HG12	1:A:118:ASN:N	1.95	0.81
1:A:79:VAL:HG22	1:A:106:ILE:HD13	1.61	0.81
1:A:85:GLN:HE22	1:B:54:PHE:H	1.29	0.81
1:D:14:THR:OG1	1:D:32:THR:HG23	1.81	0.80
1:B:116:LYS:HE2	1:B:117:VAL:H	1.45	0.80
1:C:21:PHE:HA	1:C:26:ALA:O	1.83	0.78
1:D:7:ILE:HG12	1:D:8:THR:N	1.96	0.78
1:C:28:VAL:HG22	1:C:60:TRP:NE1	1.99	0.78
1:D:76:ARG:CG	1:D:109:SER:HB3	2.13	0.78
1:C:71:LEU:HD13	1:C:77:VAL:HG11	1.67	0.76
1:C:23:PRO:HD2	2:C:176:HOH:O	1.84	0.76
1:A:56:ARG:H	1:A:56:ARG:CD	1.96	0.76
1:A:84:LYS:HD2	1:A:102:GLU:OE2	1.85	0.76
1:C:79:VAL:HG22	1:C:106:ILE:CD1	2.16	0.76
1:B:82:ARG:HG3	1:B:82:ARG:HH11	1.51	0.75
1:A:19:LEU:HD23	1:A:20:ARG:N	2.01	0.75
1:B:85:GLN:O	1:B:86:ARG:HB2	1.85	0.74
1:C:22:THR:HB	2:C:176:HOH:O	1.88	0.74
1:B:67:VAL:HG13	1:B:71:LEU:HD12	1.69	0.73
1:B:14:THR:OG1	1:B:32:THR:HG23	1.88	0.73
1:A:42:ARG:NH1	1:A:42:ARG:HB3	2.03	0.73
1:A:117:VAL:CG1	1:A:118:ASN:H	1.95	0.73
1:A:79:VAL:HG22	1:A:106:ILE:CD1	2.20	0.71
1:A:20:ARG:O	1:A:27:ALA:HA	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:HD12	1:D:5:THR:HG21	1.70	0.71
1:D:53:LEU:CD1	1:D:55:LEU:HG	2.21	0.70
1:C:12:ASN:HA	1:C:75:ALA:O	1.93	0.69
1:B:87:SER:HB3	1:B:97:THR:HG22	1.74	0.68
1:A:53:LEU:HD11	1:A:55:LEU:HG	1.75	0.68
1:B:117:VAL:HG23	1:B:118:ASN:N	2.09	0.68
1:D:117:VAL:HG13	1:D:118:ASN:N	2.07	0.68
1:A:85:GLN:NE2	1:B:54:PHE:H	1.91	0.68
1:C:82:ARG:NH2	1:C:102:GLU:HG2	2.09	0.68
1:A:29:ALA:HB3	1:A:59:ILE:CG2	2.22	0.68
1:A:22:THR:HB	1:A:23:PRO:HD2	1.74	0.67
1:C:19:LEU:HD23	1:C:20:ARG:H	1.60	0.67
1:A:29:ALA:HB2	1:A:64:ALA:HB1	1.76	0.66
1:B:52:ALA:HB1	1:B:54:PHE:HE1	1.60	0.66
1:A:53:LEU:CD1	1:A:55:LEU:HG	2.25	0.66
1:B:59:ILE:HD12	1:B:106:ILE:HG21	1.78	0.66
1:B:6:THR:HG22	1:B:82:ARG:HG2	1.79	0.64
1:C:21:PHE:O	1:C:22:THR:OG1	2.13	0.64
1:A:63:ALA:O	1:A:67:VAL:HG23	1.98	0.64
1:B:14:THR:HG1	1:B:32:THR:HG23	1.61	0.64
1:C:79:VAL:HG13	1:C:103:VAL:HG13	1.81	0.62
1:C:57:CYS:HB3	1:C:103:VAL:CG2	2.29	0.62
1:D:22:THR:OG1	1:D:26:ALA:HB3	1.99	0.62
1:D:53:LEU:HD11	1:D:55:LEU:HG	1.81	0.62
1:D:77:VAL:HB	1:D:106:ILE:HD11	1.81	0.62
1:A:21:PHE:HA	1:A:26:ALA:O	2.00	0.62
1:C:67:VAL:HG22	1:C:106:ILE:HG21	1.82	0.61
1:A:61:ARG:HD2	1:A:61:ARG:N	2.16	0.61
1:C:30:ASN:O	1:C:31:PHE:HB3	2.00	0.61
1:C:59:ILE:HG21	1:C:67:VAL:HG21	1.83	0.60
1:B:59:ILE:CD1	1:B:106:ILE:HG21	2.32	0.59
1:B:87:SER:CB	1:B:97:THR:HG22	2.32	0.59
1:A:122:ARG:O	1:A:123:SER:CB	2.50	0.59
1:D:79:VAL:HG22	1:D:106:ILE:HD13	1.85	0.59
1:C:111:ARG:HG3	1:C:112:TYR:CD2	2.38	0.58
1:D:117:VAL:HG22	1:D:118:ASN:N	2.17	0.58
1:B:17:PRO:HG2	1:B:68:ALA:HA	1.83	0.58
1:D:13:LEU:HD22	1:D:31:PHE:HB2	1.85	0.58
1:B:4:ASP:HB2	2:B:169:HOH:O	2.04	0.58
1:A:20:ARG:HD3	1:A:22:THR:CG2	2.34	0.58
1:A:67:VAL:CG2	1:A:106:ILE:HG21	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:NH1	1:A:42:ARG:CB	2.68	0.57
1:A:80:SER:HB3	1:A:105:GLU:HB2	1.87	0.56
1:B:82:ARG:HG3	1:B:82:ARG:NH1	2.19	0.56
1:C:56:ARG:N	1:C:56:ARG:HD2	2.20	0.56
1:B:7:ILE:HG12	1:B:8:THR:N	2.19	0.56
1:D:59:ILE:HD11	1:D:63:ALA:HB1	1.87	0.56
1:A:60:TRP:HB3	1:A:61:ARG:HD2	1.87	0.56
1:A:19:LEU:HD21	1:A:27:ALA:CB	2.31	0.56
1:C:7:ILE:HG12	1:C:8:THR:N	2.21	0.56
1:B:82:ARG:NH2	1:B:102:GLU:CG	2.69	0.56
1:B:116:LYS:HE2	1:B:117:VAL:N	2.17	0.56
1:A:42:ARG:HB3	1:A:42:ARG:CZ	2.35	0.55
1:C:79:VAL:HG22	1:C:106:ILE:HD12	1.89	0.55
1:A:19:LEU:HD23	1:A:20:ARG:H	1.70	0.55
1:A:9:ILE:CG2	1:A:79:VAL:HB	2.37	0.55
1:B:22:THR:HG1	1:B:24:SER:HG	1.53	0.54
1:A:81:GLY:HA2	1:A:104:ASP:OD1	2.08	0.54
1:D:67:VAL:HG21	1:D:106:ILE:HG21	1.90	0.53
1:B:17:PRO:CG	1:B:68:ALA:HA	2.38	0.53
1:B:28:VAL:HG22	1:B:60:TRP:CD1	2.44	0.53
1:A:42:ARG:CB	1:A:42:ARG:HH11	2.22	0.53
1:B:13:LEU:O	1:B:74:GLY:N	2.41	0.53
1:A:41:ASP:O	1:A:42:ARG:HG2	2.09	0.52
1:D:56:ARG:HD3	1:D:56:ARG:N	2.24	0.52
1:B:79:VAL:HG22	1:B:106:ILE:HD13	1.91	0.52
1:B:82:ARG:NH2	1:B:102:GLU:HG3	2.25	0.52
1:D:76:ARG:HG2	1:D:109:SER:CB	2.33	0.52
1:C:19:LEU:HD23	1:C:20:ARG:N	2.24	0.52
1:D:71:LEU:HD13	1:D:77:VAL:HG11	1.92	0.52
1:C:9:ILE:N	1:C:9:ILE:HD12	2.26	0.51
1:C:4:ASP:O	1:C:5:THR:HG22	2.11	0.51
1:D:81:GLY:HA2	1:D:104:ASP:OD1	2.11	0.51
1:D:34:ALA:HA	1:D:53:LEU:O	2.11	0.51
1:B:19:LEU:HD23	1:B:20:ARG:H	1.76	0.50
1:B:119:LYS:O	1:B:120:ALA:HB3	2.12	0.50
1:C:7:ILE:HG23	1:C:9:ILE:HD11	1.93	0.50
1:C:73:ARG:O	1:C:73:ARG:HG3	2.10	0.50
1:B:59:ILE:HG23	1:B:64:ALA:HA	1.92	0.50
1:D:29:ALA:HB3	1:D:59:ILE:CG2	2.40	0.50
1:D:59:ILE:HG23	1:D:64:ALA:HA	1.94	0.50
1:C:35:SER:O	1:C:52:ALA:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LEU:HD21	1:B:27:ALA:HB1	1.94	0.50
1:C:15:ALA:HA	1:C:73:ARG:CB	2.42	0.50
1:A:20:ARG:HD3	1:A:22:THR:HG23	1.92	0.50
1:B:117:VAL:HG23	1:B:118:ASN:H	1.78	0.49
1:D:36:THR:HG23	1:D:52:ALA:N	2.18	0.49
1:D:111:ARG:HD3	1:D:112:TYR:CZ	2.48	0.49
1:B:53:LEU:HD11	1:B:55:LEU:HD12	1.94	0.49
1:C:95:LYS:HB2	2:C:204:HOH:O	2.13	0.49
1:C:57:CYS:HB3	1:C:103:VAL:HG23	1.94	0.49
1:C:109:SER:C	1:C:111:ARG:H	2.21	0.49
1:B:8:THR:HA	1:B:79:VAL:O	2.13	0.48
1:C:21:PHE:CA	1:C:26:ALA:O	2.57	0.48
1:B:82:ARG:NH2	1:B:102:GLU:HG2	2.28	0.48
1:D:12:ASN:HA	1:D:75:ALA:O	2.13	0.48
1:B:16:ASP:O	1:B:17:PRO:C	2.57	0.48
1:B:120:ALA:O	1:B:121:SER:CB	2.62	0.48
1:D:31:PHE:CE2	1:D:57:CYS:HB2	2.48	0.48
1:D:3:GLY:N	2:D:174:HOH:O	2.46	0.48
1:D:73:ARG:C	1:D:75:ALA:H	2.22	0.48
1:D:117:VAL:CG1	1:D:118:ASN:H	2.06	0.48
1:C:15:ALA:HA	1:C:73:ARG:HB2	1.95	0.47
1:C:83:LEU:HD11	1:D:7:ILE:HD12	1.94	0.47
1:D:33:VAL:HG21	1:D:79:VAL:HG21	1.97	0.47
1:B:98:VAL:HG12	1:B:99:ILE:H	1.78	0.47
1:D:60:TRP:HZ3	1:D:102:GLU:OE2	1.98	0.47
1:A:85:GLN:O	1:A:86:ARG:HB2	2.15	0.47
1:B:82:ARG:NH1	1:B:104:ASP:OD2	2.48	0.47
1:C:7:ILE:HG22	1:C:81:GLY:O	2.15	0.47
1:A:19:LEU:HD22	1:A:21:PHE:CE1	2.50	0.46
1:C:28:VAL:HG22	1:C:60:TRP:CE2	2.49	0.46
1:A:67:VAL:HG22	1:A:106:ILE:HG21	1.96	0.46
1:C:23:PRO:CD	2:C:176:HOH:O	2.54	0.46
1:B:79:VAL:CG1	1:B:103:VAL:HG22	2.45	0.46
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.81	0.46
1:C:5:THR:HG23	1:C:5:THR:O	2.14	0.46
1:C:76:ARG:HG2	1:C:109:SER:HB3	1.98	0.46
1:A:9:ILE:HD12	1:A:55:LEU:CD1	2.38	0.46
1:C:30:ASN:O	1:C:31:PHE:CB	2.65	0.45
1:C:62:GLU:O	1:C:65:GLU:N	2.50	0.45
1:D:60:TRP:CZ3	1:D:102:GLU:OE2	2.70	0.45
1:B:117:VAL:CG2	1:B:118:ASN:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:CG	1:A:100:GLU:HG2	2.46	0.45
1:C:23:PRO:O	1:C:24:SER:OG	2.29	0.45
1:D:4:ASP:OD1	1:D:5:THR:N	2.49	0.45
1:A:82:ARG:NH1	1:A:104:ASP:OD2	2.50	0.45
1:B:83:LEU:HD22	1:B:99:ILE:CG2	2.47	0.45
1:B:15:ALA:HA	1:B:73:ARG:HG2	1.99	0.45
1:C:82:ARG:NH2	1:C:102:GLU:CG	2.78	0.45
1:B:22:THR:C	1:B:24:SER:N	2.74	0.44
1:D:56:ARG:CD	1:D:56:ARG:H	2.30	0.44
1:B:4:ASP:O	1:B:5:THR:C	2.60	0.44
1:C:29:ALA:HB2	1:C:64:ALA:HB1	1.99	0.44
1:C:76:ARG:HG2	1:C:109:SER:CB	2.48	0.44
1:D:56:ARG:N	1:D:56:ARG:CD	2.81	0.44
1:D:61:ARG:O	1:D:64:ALA:HB3	2.18	0.44
1:C:19:LEU:CD2	1:C:20:ARG:N	2.81	0.44
1:C:91:ARG:C	1:C:93:GLY:H	2.26	0.44
1:A:9:ILE:HG23	1:A:79:VAL:HB	2.00	0.43
1:B:82:ARG:NH1	1:B:104:ASP:CG	2.76	0.43
1:D:79:VAL:CG1	1:D:103:VAL:HG22	2.48	0.43
1:C:59:ILE:HG23	1:C:59:ILE:O	2.18	0.43
1:B:54:PHE:CD1	1:B:54:PHE:N	2.87	0.43
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.83	0.43
1:B:19:LEU:CD2	1:B:20:ARG:H	2.32	0.43
1:A:9:ILE:HG22	1:A:79:VAL:HB	2.00	0.43
1:B:82:ARG:NH1	1:B:82:ARG:CG	2.82	0.43
1:D:59:ILE:HD11	1:D:63:ALA:CB	2.49	0.42
1:B:79:VAL:HG22	1:B:106:ILE:CD1	2.48	0.42
1:D:83:LEU:HD23	1:D:101:VAL:HG22	2.01	0.42
1:A:60:TRP:HB3	1:A:61:ARG:H	1.61	0.42
1:B:83:LEU:HD22	1:B:99:ILE:HG21	2.02	0.42
1:A:56:ARG:HG3	1:A:100:GLU:HG2	2.00	0.42
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.84	0.42
1:A:67:VAL:O	1:A:67:VAL:HG12	2.19	0.42
1:D:24:SER:C	1:D:26:ALA:H	2.27	0.42
1:C:13:LEU:HD22	1:C:31:PHE:HD2	1.84	0.42
1:A:61:ARG:HD2	1:A:61:ARG:H	1.82	0.42
1:C:63:ALA:O	1:C:67:VAL:HG23	2.19	0.42
1:D:8:THR:HA	1:D:79:VAL:O	2.19	0.42
1:C:54:PHE:HD1	1:D:85:GLN:OE1	2.03	0.41
1:D:18:GLU:O	1:D:29:ALA:HA	2.19	0.41
1:A:20:ARG:HD3	1:A:22:THR:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NH2	1:A:102:GLU:OE2	2.53	0.41
1:B:9:ILE:HD11	1:B:101:VAL:HG21	2.03	0.41
1:A:22:THR:CB	1:A:23:PRO:HD2	2.45	0.41
1:C:12:ASN:OD1	1:C:76:ARG:HB2	2.21	0.41
1:C:67:VAL:CG2	1:C:106:ILE:HG21	2.50	0.41
1:C:9:ILE:HG12	1:C:55:LEU:HD12	2.03	0.41
1:D:29:ALA:HB3	1:D:59:ILE:HG22	2.01	0.41
1:B:116:LYS:HE2	1:B:116:LYS:CA	2.51	0.41
1:C:11:GLY:O	1:C:76:ARG:HA	2.21	0.41
1:C:28:VAL:HG22	1:C:60:TRP:CD1	2.55	0.41
1:C:30:ASN:C	1:C:31:PHE:CD1	2.99	0.41
1:A:15:ALA:HB1	2:A:189:HOH:O	2.21	0.40
1:D:9:ILE:CD1	1:D:55:LEU:HD12	2.52	0.40
1:A:28:VAL:HG22	1:A:60:TRP:HE1	1.78	0.40
1:A:66:ASN:C	1:A:68:ALA:N	2.77	0.40
1:C:9:ILE:HG22	1:C:10:VAL:N	2.36	0.40
1:D:79:VAL:HG12	1:D:80:SER:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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

All (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
1	A	123	SER
1	B	121	SER
1	C	23	PRO
1	C	24	SER
1	C	69	GLU
1	C	95	LYS
1	C	96	ARG
1	D	36	THR
1	D	37	PRO
1	D	117	VAL
1	A	61	ARG
1	B	5	THR
1	B	73	ARG
1	C	31	PHE
1	B	86	ARG
1	B	122	ARG
1	D	52	ALA
1	D	116	LYS
1	C	52	ALA
1	B	117	VAL
1	B	120	ALA
1	C	110	LEU
1	D	4	ASP
1	A	37	PRO
1	A	117	VAL
1	C	22	THR

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	7	ILE
1	A	23	PRO
1	A	32	THR
1	A	53	LEU
1	A	56	ARG
1	A	61	ARG
1	A	117	VAL
1	B	9	ILE
1	B	19	LEU
1	B	20	ARG
1	B	32	THR
1	B	69	GLU
1	B	70	SER
1	B	98	VAL
1	B	106	ILE
1	B	116	LYS
1	B	117	VAL
1	B	118	ASN
1	C	4	ASP
1	C	19	LEU
1	C	23	PRO
1	C	32	THR
1	C	53	LEU
1	C	56	ARG
1	C	85	GLN
1	C	92	GLU
1	C	114	THR
1	D	7	ILE
1	D	19	LEU
1	D	28	VAL
1	D	32	THR
1	D	36	THR

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Mol	Chain	Res	Type
1	D	58	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

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

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, 95th 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 ²)	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

All (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
1	D	118	ASN	2.4
1	C	3	GLY	2.3
1	D	74	GLY	2.3
1	D	38	ARG	2.3
1	A	118	ASN	2.2
1	C	5	THR	2.1
1	A	65	GLU	2.1
1	A	62	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.