



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:09 PM UTC

PDB ID : 1UE6 / pdb_00001ue6
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 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

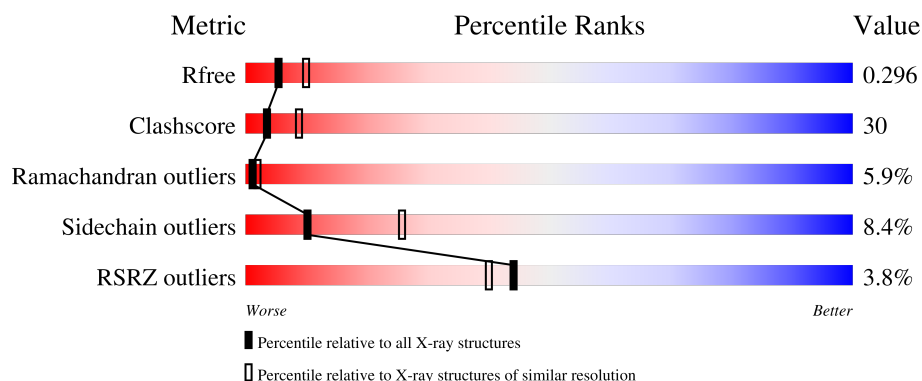
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	4% 36% 23% 7% 33%
1	B	164	2% 30% 31% • 35%
1	C	164	• 33% 23% 9% 35%
1	D	164	2% 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
1	A	110	Total	C	N	O	S	0	0	0
			784	489	139	155	1			
1	B	106	Total	C	N	O	S	0	0	0
			751	466	134	150	1			
1	C	106	Total	C	N	O	S	0	0	0
			781	486	144	150	1			
1	D	104	Total	C	N	O	S	0	0	0
			744	465	133	145	1			

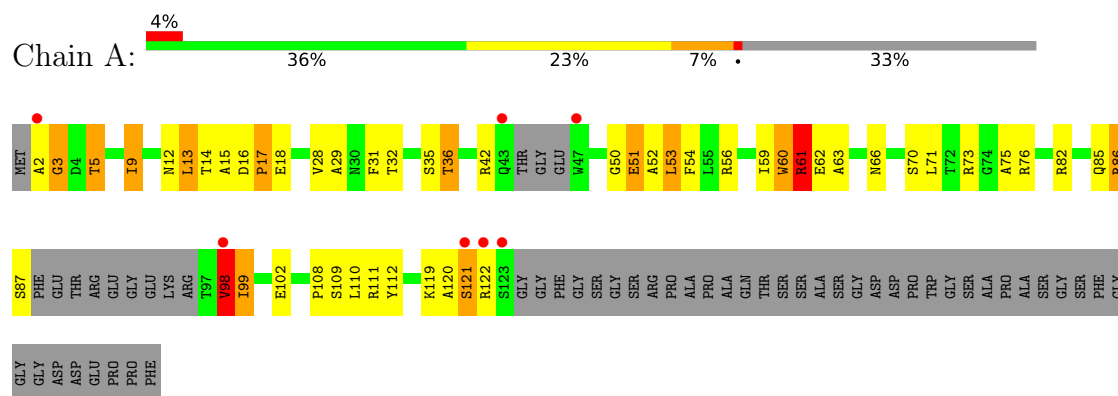
- Molecule 2 is water.

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		

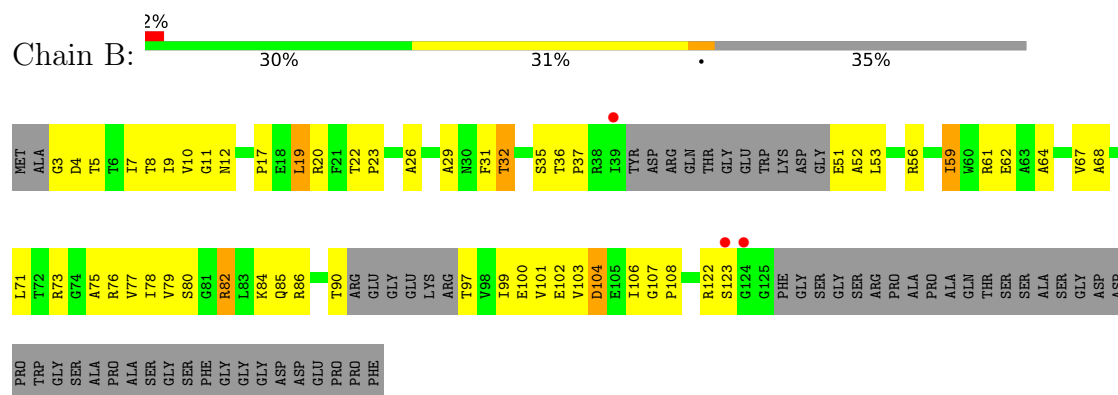
3 Residue-property plots [i](#)

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.

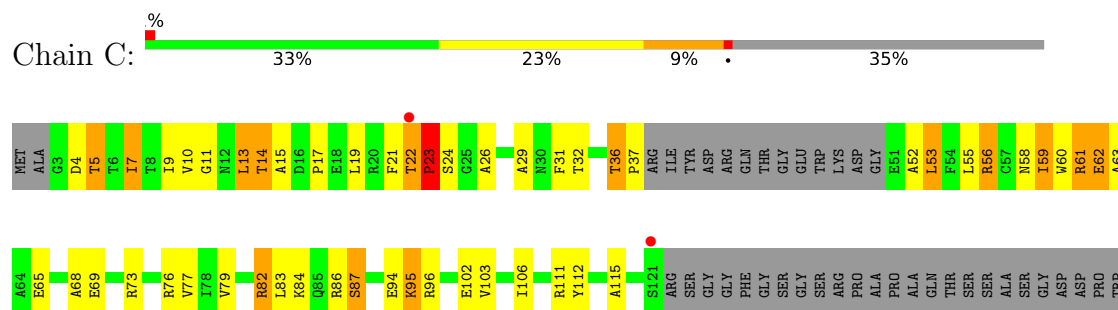
• Molecule 1: Single-strand binding protein



• Molecule 1: Single-strand binding protein

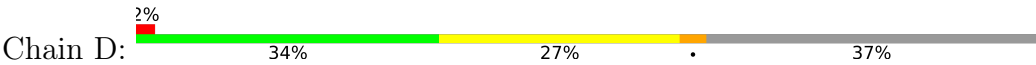


• Molecule 1: Single-strand binding protein



GLY
SER
ALA
PRO
ALA
SER
GLY
SER
PHE
GLY
GLY
GLY
GLY
ASP
ASP
GLU
PRO
PRO
PHE

● Molecule 1: Single-strand binding protein



MET
ALA
G3
D4
T5
T6
I7
I8
I9
L13
T14
A15
D16
P17
E18
L19
R20
F21
G25
A26
A27
V28
A29
T32
S35
T36
P37
R38
I39
Y40
ASP
ARG
GLN
THR
GLY
GLU
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
GLY
GLY
GLU
GLU
R95
R96
T97
V98
I99
E100
V101
E102
V103
I106
T114
K119
ALA
SER
ARG
SER
GLY
GLY
PHE
GLY
SER
GLY
SER
ARG
PRO
ALA
PRO
ALA
GLN
THR
SER
SER
ALA
SER
GLY
W60
ASP
R61
E62
TRP
GLY
SER
ALA
PRO

ALA
SER
GLY
SER
PHE
GLY
GLY
GLY
ASP
ASP
GLU
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	60.36Å 117.62Å 175.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (15.00-2.70) 92.4 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.71Å)	Xtriage
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 ²)	53.4	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.7	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	0.93	EDS
Total number of atoms	3289	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage'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.*

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

5.1 Standard geometry

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	0.59	1/792 (0.1%)	1.23	12/1078 (1.1%)
1	B	0.48	0/758	1.00	1/1032 (0.1%)
1	C	0.67	1/790 (0.1%)	1.12	3/1072 (0.3%)
1	D	0.49	0/750	1.05	3/1020 (0.3%)
All	All	0.56	2/3090 (0.1%)	1.11	19/4202 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	THR	CA-CB	8.48	1.67	1.53
1	A	98	VAL	CA-CB	5.38	1.61	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	LEU	N-CA-C	14.38	131.03	112.34
1	D	13	LEU	N-CA-C	9.02	123.92	113.19
1	A	13	LEU	N-CA-C	8.84	123.32	112.54
1	A	99	ILE	N-CA-C	-7.95	96.98	108.11
1	A	98	VAL	N-CA-C	7.53	125.00	109.34
1	A	120	ALA	N-CA-C	5.91	118.37	107.73
1	A	9	ILE	CB-CA-C	-5.73	102.08	110.62
1	C	14	THR	N-CA-CB	5.70	120.12	110.49
1	C	103	VAL	N-CA-C	5.68	116.34	108.84
1	B	101	VAL	N-CA-C	5.61	116.03	108.17
1	A	36	THR	CA-C-N	5.58	125.55	120.03
1	A	36	THR	C-N-CA	5.58	125.55	120.03
1	D	97	THR	N-CA-C	5.53	117.91	109.95
1	A	119	LYS	N-CA-C	5.51	115.12	107.73
1	A	70	SER	N-CA-C	5.39	117.97	111.40
1	A	52	ALA	N-CA-C	5.32	118.02	110.10
1	D	37	PRO	N-CA-CB	5.29	108.81	103.25
1	A	121	SER	N-CA-C	5.17	121.81	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ARG	CB-CA-C	-5.02	109.27	115.89

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	784	0	738	45	0
1	B	751	0	713	54	0
1	C	781	0	763	60	0
1	D	744	0	709	41	0
2	A	64	0	0	0	0
2	B	66	0	0	3	0
2	C	56	0	0	2	0
2	D	43	0	0	2	0
All	All	3289	0	2923	177	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 30.

All (177) 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
1:C:31:PHE:CE1	1:C:59:ILE:HD11	2.16	0.80
1:D:20:ARG:HD2	1:D:21:PHE:H	1.45	0.78
1:B:77:VAL:HB	1:B:106:ILE:HD11	1.66	0.76
1:A:87:SER:CB	1:A:98:VAL:HG11	2.16	0.75
1:A:63:ALA:HA	1:A:66:ASN:HD22	1.51	0.75
1:B:31:PHE:HE1	1:B:59:ILE:HD11	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:GLU:HA	1:D:95:LYS:CB	2.17	0.74
1:D:5:THR:CG2	1:D:83:LEU:H	2.00	0.74
1:A:82:ARG:HH22	1:B:37:PRO:HB3	1.54	0.73
1:C:79:VAL:HG22	1:C:106:ILE:CD1	2.18	0.70
1:A:32:THR:HG21	1:A:56:ARG:HH11	1.56	0.70
1:B:79:VAL:HG22	1:B:106:ILE:HD13	1.75	0.69
1:B:82:ARG:HH11	1:B:82:ARG:HB2	1.57	0.68
1:C:31:PHE:CZ	1:C:59:ILE:HD11	2.27	0.68
1:C:32:THR:HG22	1:C:56:ARG:HG2	1.74	0.68
1:D:26:ALA:HB2	2:D:165:HOH:O	1.94	0.67
1:C:32:THR:HG23	1:C:56:ARG:HH11	1.58	0.67
1:A:54:PHE:N	1:B:85:GLN:NE2	2.42	0.66
1:C:36:THR:H	1:C:37:PRO:HD2	1.59	0.66
1:D:5:THR:HG21	1:D:83:LEU:H	1.61	0.65
1:D:5:THR:HG21	1:D:83:LEU:HB2	1.78	0.65
1:C:32:THR:HG23	1:C:56:ARG:NH1	2.13	0.63
1:B:17:PRO:CG	1:B:68:ALA:HA	2.29	0.63
1:C:65:GLU:O	1:C:69:GLU:HG2	1.97	0.63
1:B:32:THR:HG22	1:B:56:ARG:HG3	1.82	0.62
1:A:98:VAL:HG12	1:A:98:VAL:O	1.98	0.62
1:B:106:ILE:HD12	1:B:107:GLY:H	1.64	0.61
1:A:71:LEU:CD2	1:A:108:PRO:HG3	2.28	0.61
1:C:15:ALA:HA	1:C:73:ARG:HB3	1.82	0.61
1:C:94:GLU:OE2	1:C:94:GLU:HA	2.00	0.61
1:D:53:LEU:HD22	1:D:55:LEU:HG	1.82	0.61
1:B:31:PHE:CE1	1:B:59:ILE:HD11	2.33	0.61
1:A:29:ALA:HB3	1:A:59:ILE:CG2	2.30	0.61
1:B:17:PRO:HG2	1:B:68:ALA:HA	1.83	0.61
1:D:3:GLY:C	1:D:5:THR:H	2.08	0.61
1:A:3:GLY:HA3	1:B:10:VAL:O	2.01	0.60
1:D:39:ILE:O	1:D:39:ILE:HG13	2.00	0.60
1:A:9:ILE:HG23	1:B:5:THR:HG22	1.84	0.60
1:A:18:GLU:O	1:A:29:ALA:HA	2.01	0.60
1:A:3:GLY:O	1:B:35:SER:HB2	2.00	0.59
1:D:5:THR:HG22	1:D:83:LEU:H	1.69	0.58
1:C:53:LEU:HD23	1:D:85:GLN:HG3	1.85	0.58
1:A:28:VAL:HG22	1:A:60:TRP:NE1	2.19	0.57
1:B:22:THR:HB	1:B:23:PRO:HD2	1.85	0.57
1:C:84:LYS:HZ1	1:D:51:GLU:HG2	1.68	0.57
1:C:84:LYS:NZ	1:D:51:GLU:HG2	2.20	0.57
1:A:53:LEU:O	1:A:53:LEU:HD23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:THR:CG2	1:C:56:ARG:HH11	2.17	0.56
1:D:28:VAL:HG22	1:D:60:TRP:CD1	2.39	0.56
1:A:54:PHE:N	1:B:85:GLN:HE22	1.96	0.56
1:C:9:ILE:HG22	1:C:10:VAL:N	2.21	0.56
1:D:9:ILE:HD11	1:D:101:VAL:HG21	1.87	0.56
1:C:5:THR:HG23	1:C:82:ARG:NH1	2.20	0.56
1:B:79:VAL:CG2	1:B:106:ILE:HD13	2.35	0.56
1:B:84:LYS:HD2	1:B:102:GLU:HG2	1.87	0.56
1:C:10:VAL:HB	1:D:4:ASP:HB3	1.88	0.56
1:A:76:ARG:HG2	1:A:109:SER:CB	2.33	0.55
1:C:111:ARG:HG2	1:C:112:TYR:CE2	2.41	0.55
1:A:32:THR:CG2	1:A:56:ARG:HD3	2.36	0.55
1:C:17:PRO:HG2	1:C:68:ALA:HA	1.87	0.55
1:B:19:LEU:HD23	1:B:20:ARG:H	1.71	0.55
1:A:99:ILE:HB	1:B:99:ILE:HD12	1.88	0.55
1:B:8:THR:HA	1:B:79:VAL:O	2.06	0.55
1:D:36:THR:HG22	1:D:52:ALA:HA	1.89	0.55
1:C:5:THR:CG2	1:C:82:ARG:HH12	2.19	0.54
1:C:7:ILE:HD12	1:C:7:ILE:O	2.07	0.54
1:C:22:THR:O	1:C:24:SER:N	2.41	0.54
1:C:87:SER:HA	1:C:96:ARG:O	2.07	0.54
1:B:29:ALA:H	1:B:64:ALA:HB1	1.72	0.54
1:C:22:THR:C	1:C:24:SER:N	2.65	0.54
1:A:82:ARG:NH2	1:B:37:PRO:HB3	2.23	0.53
1:C:76:ARG:HD2	2:C:180:HOH:O	2.09	0.53
1:B:84:LYS:HE3	1:B:102:GLU:HG3	1.90	0.53
1:B:71:LEU:HD21	1:B:108:PRO:HG3	1.89	0.53
1:C:77:VAL:HB	1:C:106:ILE:HD11	1.91	0.53
1:B:37:PRO:HG2	1:B:51:GLU:HG3	1.91	0.53
1:A:35:SER:HB3	1:A:53:LEU:CD2	2.39	0.53
1:D:67:VAL:HG21	1:D:106:ILE:HG21	1.90	0.53
1:C:10:VAL:O	1:D:4:ASP:HB3	2.09	0.52
1:B:77:VAL:HB	1:B:106:ILE:CD1	2.38	0.52
1:C:7:ILE:HG22	1:D:7:ILE:HB	1.91	0.52
1:D:19:LEU:C	1:D:19:LEU:HD13	2.34	0.52
1:C:15:ALA:HA	1:C:73:ARG:CB	2.40	0.51
1:C:5:THR:HG23	1:C:82:ARG:HH12	1.75	0.51
1:A:12:ASN:HA	1:A:75:ALA:O	2.10	0.51
1:B:106:ILE:HD12	1:B:107:GLY:N	2.25	0.50
1:C:82:ARG:NH1	1:C:82:ARG:HB2	2.26	0.50
1:A:82:ARG:HG2	1:A:102:GLU:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLY:O	1:C:76:ARG:HA	2.11	0.50
1:B:84:LYS:O	1:B:100:GLU:N	2.42	0.50
1:C:58:ASN:C	1:C:59:ILE:HD13	2.36	0.50
1:B:82:ARG:HH11	1:B:82:ARG:CB	2.22	0.50
1:B:12:ASN:HA	1:B:75:ALA:O	2.12	0.50
1:C:31:PHE:HE1	1:C:59:ILE:HD11	1.72	0.50
1:C:83:LEU:HD11	1:D:7:ILE:HD12	1.94	0.49
1:A:50:GLY:O	1:A:51:GLU:CB	2.59	0.49
1:B:11:GLY:O	1:B:76:ARG:HA	2.12	0.49
1:D:67:VAL:CG2	1:D:106:ILE:HG21	2.43	0.49
1:D:84:LYS:HD2	1:D:102:GLU:CG	2.43	0.49
1:A:82:ARG:HG3	1:A:82:ARG:HH11	1.78	0.48
1:B:3:GLY:N	2:B:175:HOH:O	2.46	0.48
1:C:7:ILE:CG2	1:D:7:ILE:HB	2.44	0.48
1:C:22:THR:O	1:C:23:PRO:C	2.56	0.48
1:C:95:LYS:HD3	1:C:95:LYS:H	1.78	0.48
1:B:29:ALA:N	1:B:64:ALA:HB1	2.28	0.48
1:D:17:PRO:HD2	1:D:71:LEU:O	2.14	0.48
1:A:13:LEU:HD22	1:A:31:PHE:HB2	1.96	0.48
1:D:53:LEU:HD23	1:D:54:PHE:N	2.29	0.48
1:C:13:LEU:C	1:C:15:ALA:H	2.22	0.48
1:A:111:ARG:HD3	1:A:112:TYR:CZ	2.49	0.48
1:D:13:LEU:O	1:D:14:THR:OG1	2.31	0.48
1:D:84:LYS:HD2	1:D:102:GLU:HG2	1.96	0.48
1:B:59:ILE:CD1	1:B:67:VAL:HG21	2.44	0.47
1:B:36:THR:HG22	1:B:52:ALA:HA	1.96	0.47
1:C:7:ILE:HD13	1:C:9:ILE:CD1	2.44	0.47
1:C:111:ARG:HG2	1:C:112:TYR:CD2	2.50	0.47
1:D:13:LEU:O	1:D:15:ALA:N	2.48	0.47
1:C:58:ASN:HB2	1:C:102:GLU:OE1	2.14	0.47
1:C:29:ALA:HB3	1:C:59:ILE:HG12	1.97	0.47
1:A:28:VAL:HG22	1:A:60:TRP:CD1	2.50	0.46
1:A:86:ARG:O	1:A:87:SER:CB	2.63	0.46
1:C:32:THR:CG2	1:C:56:ARG:HG2	2.44	0.46
1:B:22:THR:HG23	1:B:26:ALA:O	2.15	0.46
1:B:59:ILE:HG23	1:B:103:VAL:HB	1.98	0.46
1:C:53:LEU:HD11	1:C:55:LEU:HD11	1.97	0.46
1:C:60:TRP:HZ3	1:C:102:GLU:OE1	1.99	0.46
1:B:59:ILE:HD13	1:B:67:VAL:HG21	1.98	0.46
1:C:83:LEU:HB2	1:D:53:LEU:HD11	1.98	0.46
1:C:4:ASP:HB3	1:D:35:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:VAL:HG12	1:D:99:ILE:N	2.32	0.45
1:C:36:THR:N	1:C:37:PRO:HD2	2.29	0.45
1:C:37:PRO:HD2	2:D:167:HOH:O	2.17	0.45
1:A:9:ILE:HG23	1:B:5:THR:CG2	2.47	0.45
1:A:13:LEU:O	1:A:14:THR:OG1	2.34	0.45
1:C:59:ILE:HD13	1:C:59:ILE:N	2.32	0.45
1:D:25:GLY:O	1:D:26:ALA:C	2.58	0.45
1:C:21:PHE:O	1:C:22:THR:CB	2.65	0.45
1:B:4:ASP:CG	2:B:172:HOH:O	2.60	0.44
1:A:111:ARG:HG2	1:A:112:TYR:CD2	2.53	0.44
1:B:73:ARG:HH11	1:B:73:ARG:HG3	1.81	0.44
1:B:86:ARG:HA	1:B:86:ARG:HD2	1.62	0.44
1:C:32:THR:HG22	1:C:56:ARG:HA	2.00	0.44
1:A:61:ARG:HB3	1:A:62:GLU:H	1.60	0.44
1:C:62:GLU:O	1:C:63:ALA:C	2.60	0.44
1:B:37:PRO:HD3	2:B:174:HOH:O	2.17	0.44
1:C:9:ILE:CG2	1:C:10:VAL:N	2.81	0.43
1:D:32:THR:HG22	1:D:56:ARG:HA	2.01	0.43
1:A:29:ALA:HB3	1:A:59:ILE:HG22	2.00	0.43
1:D:20:ARG:CD	1:D:21:PHE:H	2.24	0.43
1:A:85:GLN:O	1:A:86:ARG:O	2.37	0.43
1:B:51:GLU:O	1:B:52:ALA:HB3	2.18	0.43
1:C:94:GLU:CG	2:C:176:HOH:O	2.67	0.43
1:A:2:ALA:O	1:A:3:GLY:C	2.62	0.42
1:D:28:VAL:HG22	1:D:60:TRP:NE1	2.34	0.42
1:D:29:ALA:HB3	1:D:59:ILE:CG2	2.50	0.42
1:A:16:ASP:O	1:A:17:PRO:O	2.38	0.42
1:B:19:LEU:CD2	1:B:20:ARG:N	2.83	0.42
1:D:15:ALA:HA	1:D:73:ARG:HB3	2.01	0.42
1:A:15:ALA:HA	1:A:73:ARG:HB2	2.02	0.42
1:A:110:LEU:HD23	1:A:110:LEU:HA	1.74	0.42
1:B:78:ILE:O	1:B:106:ILE:HD12	2.19	0.42
1:D:61:ARG:HB3	1:D:62:GLU:H	1.59	0.42
1:B:80:SER:O	1:B:104:ASP:HB2	2.21	0.41
1:C:111:ARG:O	1:C:112:TYR:HD2	2.03	0.41
1:C:61:ARG:O	1:C:62:GLU:C	2.64	0.41
1:C:86:ARG:O	1:C:87:SER:CB	2.69	0.41
1:A:2:ALA:N	1:B:36:THR:HG1	2.19	0.41
1:A:5:THR:HB	1:B:9:ILE:HG23	2.03	0.41
1:D:79:VAL:HG13	1:D:103:VAL:HG13	2.03	0.40
1:B:7:ILE:HG12	1:B:8:THR:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ARG:O	1:B:97:THR:HA	2.22	0.40
1:A:32:THR:HG21	1:A:56:ARG:HD3	2.03	0.40

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%)	1	1
1	B	100/164 (61%)	93 (93%)	4 (4%)	3 (3%)	3	8
1	C	102/164 (62%)	82 (80%)	11 (11%)	9 (9%)	0	0
1	D	98/164 (60%)	87 (89%)	7 (7%)	4 (4%)	2	5
All	All	404/656 (62%)	347 (86%)	33 (8%)	24 (6%)	1	2

All (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
1	C	52	ALA
1	D	37	PRO
1	D	52	ALA
1	A	3	GLY
1	A	17	PRO
1	A	122	ARG
1	C	62	GLU
1	A	42	ARG

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Mol	Chain	Res	Type
1	C	115	ALA
1	A	98	VAL
1	B	123	SER
1	C	14	THR
1	C	22	THR
1	D	14	THR
1	D	27	ALA
1	B	61	ARG
1	C	36	THR
1	C	87	SER
1	C	23	PRO

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	75/126 (60%)	70 (93%)	5 (7%)	15	36
1	B	73/126 (58%)	65 (89%)	8 (11%)	6	15
1	C	78/126 (62%)	68 (87%)	10 (13%)	4	11
1	D	71/126 (56%)	69 (97%)	2 (3%)	38	68
All	All	297/504 (59%)	272 (92%)	25 (8%)	10	26

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	36	THR
1	A	53	LEU
1	A	60	TRP
1	A	61	ARG
1	B	19	LEU
1	B	32	THR
1	B	53	LEU
1	B	59	ILE
1	B	62	GLU

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Mol	Chain	Res	Type
1	B	82	ARG
1	B	90	THR
1	B	104	ASP
1	C	5	THR
1	C	7	ILE
1	C	19	LEU
1	C	23	PRO
1	C	53	LEU
1	C	56	ARG
1	C	59	ILE
1	C	61	ARG
1	C	82	ARG
1	C	95	LYS
1	D	73	ARG
1	D	114	THR

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	66	ASN
1	B	30	ASN
1	B	58	ASN
1	B	85	GLN
1	C	85	GLN
1	D	12	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	110/164 (67%)	-0.01	7 (6%)	25 22	23, 49, 115, 143	0
1	B	106/164 (64%)	-0.16	3 (2%)	55 51	26, 51, 106, 127	0
1	C	106/164 (64%)	-0.12	2 (1%)	66 63	25, 52, 105, 121	0
1	D	104/164 (63%)	-0.13	4 (3%)	44 40	18, 48, 103, 132	0
All	All	426/656 (64%)	-0.10	16 (3%)	44 40	18, 51, 110, 143	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	TRP	3.3
1	A	43	GLN	3.2
1	B	123	SER	3.1
1	A	2	ALA	3.0
1	A	121	SER	3.0
1	C	121	SER	2.9
1	D	91	ARG	2.8
1	B	39	ILE	2.8
1	B	124	GLY	2.6
1	A	123	SER	2.5
1	A	98	VAL	2.4
1	C	22	THR	2.4
1	D	38	ARG	2.2
1	A	122	ARG	2.1
1	D	40	TYR	2.0
1	D	20	ARG	2.0

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.