



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:49 PM UTC

PDB ID : 4QRA / pdb_00004qra
Title : Structure and specificity of L-D-Transpeptidase from Mycobacterium tuberculosis and antibiotic resistance: Calcium binding promotes dimer formation
Authors : Gokulan, K.; Varughese, K.I.
Deposited on : 2014-06-30
Resolution : 2.29 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

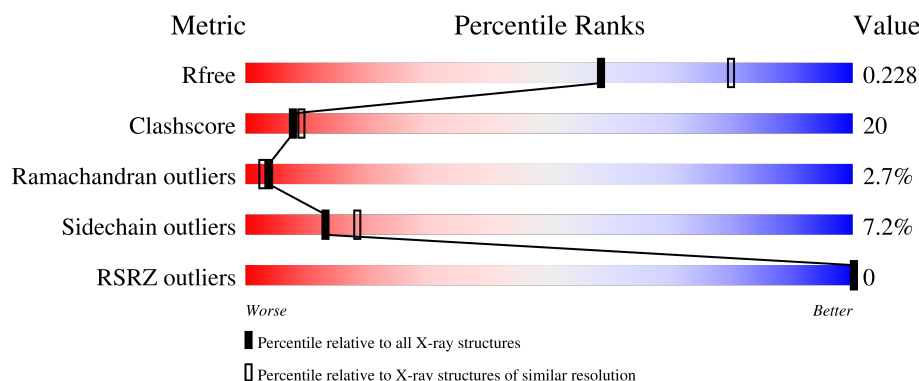
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	352	 73% 16% 5% • 5%
1	B	352	 76% 11% • • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5344 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 L,d-transpeptidase LdtB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2539	1590	445	496	8			
1	B	330	Total	C	N	O	S	0	0	0
			2507	1572	437	490	8			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

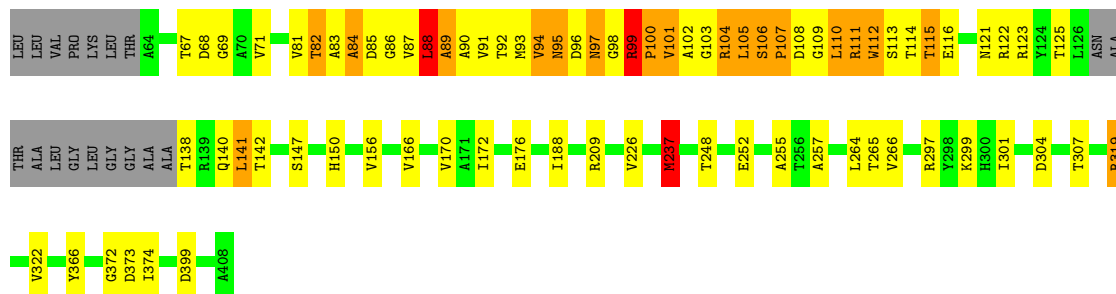
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	151	Total	O	0	0
			151	151		

3 Residue-property plots

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.

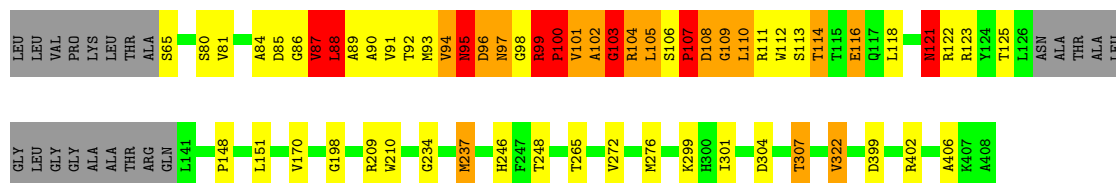
• Molecule 1: L,d-transpeptidase LdtB

Chain A: 



• Molecule 1: L,d-transpeptidase LdtB

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.76Å 88.13Å 90.51Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	34.86 – 2.29 34.86 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.5 (34.86-2.29) 97.6 (34.86-2.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.49 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.182 , 0.226 0.190 , 0.228	Depositor DCC
R_{free} test set	1964 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.459 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5344	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.35	9/2603 (0.3%)	1.17	9/3561 (0.3%)
1	B	1.25	7/2571 (0.3%)	1.11	4/3518 (0.1%)
All	All	1.30	16/5174 (0.3%)	1.14	13/7079 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	TRP	C-N	-28.97	0.95	1.33
1	A	399	ASP	C-O	-6.00	1.17	1.24
1	A	99	ARG	C-N	5.67	1.41	1.33
1	B	399	ASP	C-O	-5.46	1.17	1.24
1	A	100	PRO	N-CD	5.39	1.55	1.47
1	B	406	ALA	C-O	-5.38	1.17	1.24
1	A	373	ASP	C-O	-5.28	1.16	1.23
1	B	107	PRO	N-CD	5.28	1.55	1.47
1	A	372	GLY	C-O	-5.27	1.16	1.24
1	B	402	ARG	C-O	-5.27	1.17	1.24
1	A	237	MET	C-O	-5.22	1.17	1.24
1	A	374	ILE	C-O	-5.21	1.18	1.24
1	B	322	VAL	C-O	-5.21	1.18	1.24
1	A	266	VAL	C-O	-5.18	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	VAL	C-O	-5.10	1.18	1.24
1	B	265	THR	C-O	-5.00	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	SER	N-CA-C	14.71	121.37	108.13
1	A	112	TRP	O-C-N	-12.98	107.43	123.27
1	B	95	ASN	N-CA-C	9.78	125.58	110.42
1	B	99	ARG	C-N-CD	-7.91	92.58	125.00
1	A	99	ARG	CA-C-N	-6.74	112.82	119.76
1	A	99	ARG	C-N-CA	-6.74	112.82	119.76
1	A	112	TRP	CA-C-N	5.71	131.47	122.21
1	A	112	TRP	C-N-CA	5.71	131.47	122.21
1	A	88	LEU	CA-C-N	5.50	132.06	121.54
1	A	88	LEU	C-N-CA	5.50	132.06	121.54
1	A	82	THR	N-CA-C	5.33	118.13	109.06
1	B	103	GLY	N-CA-C	-5.22	100.80	113.18
1	B	89	ALA	N-CA-C	5.02	118.44	111.71

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	VAL	Peptide
1	A	88	LEU	Peptide
1	A	94	VAL	Peptide
1	B	100	PRO	Peptide
1	B	121	ASN	Peptide

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	2539	0	2425	96	0
1	B	2507	0	2393	100	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	146	0	0	1	0
3	B	151	0	0	3	0
All	All	5344	0	4818	196	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 20.

All (196) 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:B:104:ARG:HB3	1:B:112:TRP:CZ2	1.32	1.62
1:B:104:ARG:CB	1:B:112:TRP:CZ2	1.86	1.55
1:B:101:VAL:CG2	1:B:116:GLU:OE2	1.64	1.45
1:B:98:GLY:O	1:B:100:PRO:HD3	1.13	1.28
1:B:86:GLY:CA	1:B:87:VAL:HG12	1.65	1.25
1:B:104:ARG:HB2	1:B:112:TRP:CE2	1.75	1.19
1:B:98:GLY:O	1:B:100:PRO:CD	1.91	1.17
1:B:104:ARG:HH11	1:B:105:LEU:CD1	1.62	1.11
1:B:101:VAL:HG21	1:B:116:GLU:CD	1.75	1.09
1:A:97:ASN:HB3	1:A:98:GLY:HA3	1.12	1.09
1:B:86:GLY:HA2	1:B:87:VAL:HG12	1.21	1.09
1:A:94:VAL:HB	1:A:95:ASN:HB3	1.34	1.06
1:A:95:ASN:HB2	1:A:99:ARG:HA	1.10	1.06
1:B:98:GLY:C	1:B:100:PRO:HD3	1.81	1.06
1:B:99:ARG:HH21	1:B:99:ARG:HG2	1.20	1.04
1:B:104:ARG:HB2	1:B:112:TRP:CZ2	1.80	1.04
1:B:104:ARG:HH11	1:B:105:LEU:HD12	1.16	1.04
1:B:121:ASN:HB2	1:B:122:ARG:HG2	1.36	1.04
1:B:107:PRO:HD3	1:B:111:ARG:O	1.59	1.03
1:A:101:VAL:HG22	1:A:102:ALA:H	1.18	1.03
1:B:104:ARG:CG	1:B:112:TRP:HZ2	1.71	1.03
1:A:95:ASN:HB2	1:A:99:ARG:CA	1.90	1.02
1:A:83:ALA:HB3	1:A:110:LEU:HD23	1.44	1.00
1:B:109:GLY:C	1:B:110:LEU:HD23	1.86	1.00
1:A:105:LEU:HD12	1:A:106:SER:HA	1.42	0.99
1:B:86:GLY:HA3	1:B:87:VAL:HG12	1.44	0.98
1:A:103:GLY:O	1:A:105:LEU:N	1.97	0.97
1:B:104:ARG:CB	1:B:112:TRP:HZ2	1.42	0.97
1:B:104:ARG:HB3	1:B:112:TRP:CH2	2.00	0.96
1:B:121:ASN:CB	1:B:122:ARG:HG2	1.97	0.95
1:B:101:VAL:HG23	1:B:102:ALA:H	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:VAL:HG21	1:B:116:GLU:OE2	0.77	0.94
1:A:104:ARG:O	1:A:105:LEU:HG	1.65	0.94
1:B:104:ARG:CB	1:B:112:TRP:CE2	2.42	0.93
1:B:96:ASP:H	1:B:100:PRO:HG2	1.28	0.93
1:B:104:ARG:NH1	1:B:105:LEU:CD1	2.32	0.93
1:A:89:ALA:HB1	1:A:90:ALA:C	1.96	0.90
1:A:97:ASN:CB	1:A:98:GLY:HA3	2.01	0.90
1:B:84:ALA:O	1:B:85:ASP:OD2	1.90	0.89
1:B:86:GLY:HA2	1:B:87:VAL:CG1	2.03	0.89
1:B:86:GLY:CA	1:B:87:VAL:CG1	2.49	0.88
1:A:89:ALA:HA	1:A:90:ALA:HB3	1.54	0.87
1:B:121:ASN:HB3	1:B:122:ARG:HA	1.56	0.87
1:B:104:ARG:HB2	1:B:112:TRP:NE1	1.90	0.86
1:A:95:ASN:CB	1:A:99:ARG:HA	2.01	0.85
1:A:96:ASP:OD1	1:A:97:ASN:N	2.09	0.84
1:A:105:LEU:O	1:A:106:SER:OG	1.95	0.83
1:B:86:GLY:HA3	1:B:87:VAL:O	1.78	0.83
1:A:97:ASN:HB3	1:A:98:GLY:CA	2.04	0.83
1:A:105:LEU:HD12	1:A:106:SER:CA	2.09	0.82
1:B:104:ARG:NE	1:B:104:ARG:O	2.13	0.82
1:B:101:VAL:CG2	1:B:116:GLU:CD	2.44	0.79
1:A:95:ASN:HA	1:A:100:PRO:O	1.82	0.78
1:A:98:GLY:C	1:A:100:PRO:HD3	2.07	0.78
1:A:88:LEU:HB3	1:A:89:ALA:HB3	1.65	0.78
1:B:99:ARG:HG2	1:B:99:ARG:NH2	1.95	0.77
1:A:105:LEU:HD12	1:A:106:SER:N	2.00	0.76
1:B:95:ASN:HB2	1:B:100:PRO:HG2	1.66	0.76
1:B:94:VAL:CG2	1:B:125:THR:HB	2.17	0.74
1:B:104:ARG:CG	1:B:112:TRP:CZ2	2.56	0.73
1:A:89:ALA:HB1	1:A:90:ALA:O	1.89	0.73
1:B:96:ASP:N	1:B:100:PRO:HG2	2.03	0.73
1:B:95:ASN:HA	1:B:100:PRO:HB2	1.71	0.72
1:A:88:LEU:HD22	1:A:88:LEU:N	2.04	0.72
1:A:88:LEU:HB3	1:A:89:ALA:CB	2.20	0.71
1:B:104:ARG:NH1	1:B:105:LEU:HD12	1.96	0.71
1:B:107:PRO:HG2	1:B:109:GLY:H	1.56	0.71
1:B:101:VAL:CG2	1:B:102:ALA:H	2.01	0.71
1:B:101:VAL:HG23	1:B:102:ALA:N	2.04	0.70
1:B:95:ASN:HB2	1:B:100:PRO:CG	2.21	0.70
1:B:95:ASN:HB2	1:B:100:PRO:HD2	1.74	0.69
1:B:104:ARG:HE	1:B:104:ARG:C	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:CB	1:A:89:ALA:HB3	2.21	0.69
1:B:110:LEU:HD23	1:B:110:LEU:N	2.04	0.69
1:A:105:LEU:HA	1:A:112:TRP:NE1	2.07	0.69
1:B:88:LEU:HD23	1:B:88:LEU:C	2.18	0.69
1:B:93:MET:HA	1:B:125:THR:O	1.94	0.68
1:A:96:ASP:O	1:A:97:ASN:HB2	1.94	0.68
1:A:101:VAL:CG2	1:A:102:ALA:H	2.02	0.67
1:B:93:MET:HE1	1:B:114:THR:HG23	1.75	0.67
1:A:109:GLY:O	1:A:110:LEU:HB2	1.93	0.66
1:B:86:GLY:HA3	1:B:87:VAL:CG1	2.17	0.66
1:B:88:LEU:HD23	1:B:88:LEU:O	1.96	0.66
1:B:121:ASN:HB3	1:B:122:ARG:CA	2.26	0.66
1:A:91:VAL:O	1:A:92:THR:HG23	1.97	0.65
1:A:297:ARG:HG3	1:A:366:TYR:CE2	2.32	0.64
1:B:104:ARG:NH1	1:B:105:LEU:HD13	2.12	0.64
1:A:96:ASP:HB2	1:A:123:ARG:O	1.98	0.63
1:B:95:ASN:HB2	1:B:100:PRO:CD	2.28	0.63
1:A:116:GLU:HA	1:A:116:GLU:OE1	1.98	0.63
1:A:101:VAL:HG22	1:A:102:ALA:N	1.99	0.62
1:B:121:ASN:HB2	1:B:122:ARG:CG	2.22	0.62
1:A:87:VAL:HG12	1:A:88:LEU:N	2.15	0.61
1:B:104:ARG:HH11	1:B:105:LEU:HD13	1.59	0.61
1:A:297:ARG:HB3	1:A:297:ARG:CZ	2.30	0.61
1:A:98:GLY:CA	1:A:100:PRO:HD3	2.31	0.60
1:B:104:ARG:HD3	1:B:104:ARG:H	1.66	0.60
1:A:93:MET:HE1	1:A:114:THR:CG2	2.32	0.59
1:A:140:GLN:O	1:A:141:LEU:HD13	2.02	0.59
1:A:94:VAL:CB	1:A:95:ASN:HB3	2.24	0.58
1:A:94:VAL:HG11	1:A:99:ARG:NH2	2.17	0.58
1:B:102:ALA:O	1:B:103:GLY:O	2.20	0.58
1:B:109:GLY:CA	1:B:110:LEU:HD23	2.34	0.58
1:A:156:VAL:HG21	1:A:226:VAL:HG21	1.84	0.58
1:A:95:ASN:OD1	1:A:96:ASP:N	2.37	0.57
1:B:304:ASP:O	1:B:307:THR:HG23	2.05	0.56
1:A:110:LEU:C	1:A:111:ARG:HG3	2.31	0.56
1:A:105:LEU:CD1	1:A:106:SER:HA	2.28	0.56
1:B:93:MET:HE1	1:B:114:THR:CG2	2.36	0.55
1:A:172:ILE:HD13	1:A:188:ILE:HD13	1.89	0.55
1:B:86:GLY:CA	1:B:87:VAL:CB	2.85	0.54
1:A:107:PRO:HB3	1:A:108:ASP:HA	1.89	0.54
1:A:304:ASP:OD2	1:A:319:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD12	1:A:105:LEU:C	2.33	0.54
1:B:96:ASP:H	1:B:100:PRO:CG	2.10	0.53
1:B:107:PRO:O	1:B:108:ASP:HB2	2.08	0.53
1:A:94:VAL:HG11	1:A:99:ARG:HH21	1.72	0.53
1:A:104:ARG:O	1:A:105:LEU:CG	2.47	0.53
1:A:105:LEU:HA	1:A:112:TRP:CE2	2.43	0.52
1:A:88:LEU:N	1:A:88:LEU:CD2	2.73	0.52
1:A:83:ALA:HB3	1:A:110:LEU:CD2	2.28	0.52
1:A:156:VAL:CG2	1:A:226:VAL:HG21	2.40	0.52
1:A:95:ASN:O	1:A:99:ARG:N	2.42	0.52
1:A:105:LEU:CD1	1:A:106:SER:N	2.73	0.51
1:A:140:GLN:C	1:A:141:LEU:HD13	2.35	0.51
1:A:86:GLY:C	1:A:87:VAL:HG23	2.36	0.51
1:A:93:MET:HE1	1:A:114:THR:HG23	1.92	0.51
1:A:95:ASN:HB2	1:A:99:ARG:C	2.34	0.51
1:B:95:ASN:CB	1:B:100:PRO:HG2	2.40	0.51
1:B:234:GLY:O	1:B:237:MET:HB3	2.11	0.51
1:B:299:LYS:NZ	3:B:632:HOH:O	2.44	0.50
1:B:104:ARG:HB3	1:B:112:TRP:HZ2	1.07	0.50
1:A:93:MET:O	1:A:102:ALA:HB2	2.12	0.50
1:A:87:VAL:CG1	1:A:88:LEU:N	2.75	0.49
1:B:94:VAL:HG22	1:B:125:THR:HB	1.93	0.49
1:B:246:HIS:HB2	3:B:560:HOH:O	2.11	0.49
1:B:95:ASN:HA	1:B:100:PRO:CB	2.40	0.49
1:A:299:LYS:NZ	3:A:736:HOH:O	2.45	0.49
1:B:121:ASN:CA	1:B:122:ARG:HG2	2.43	0.49
1:A:93:MET:HA	1:A:125:THR:O	2.13	0.48
1:A:88:LEU:CB	1:A:89:ALA:CB	2.87	0.48
1:A:176:GLU:HG3	1:A:237:MET:HE1	1.95	0.48
1:B:81:VAL:HG22	1:B:112:TRP:HB3	1.95	0.47
1:A:103:GLY:HA3	1:A:115:THR:H	1.79	0.47
1:A:110:LEU:C	1:A:111:ARG:CG	2.86	0.47
1:B:90:ALA:C	1:B:91:VAL:HG23	2.40	0.47
1:A:98:GLY:HA3	1:A:100:PRO:HD3	1.96	0.46
1:A:121:ASN:OD1	1:A:147:SER:CB	2.62	0.46
1:B:90:ALA:C	1:B:91:VAL:CG2	2.89	0.46
1:A:255:ALA:HA	1:A:265:THR:O	2.15	0.46
1:A:88:LEU:HD22	1:A:88:LEU:H	1.77	0.46
1:B:101:VAL:O	1:B:102:ALA:CB	2.63	0.46
1:B:104:ARG:HG2	1:B:112:TRP:CZ2	2.48	0.46
1:B:110:LEU:N	1:B:110:LEU:CD2	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ASP:HA	1:B:97:ASN:HA	1.71	0.45
1:A:99:ARG:N	1:A:100:PRO:CD	2.79	0.45
1:B:104:ARG:HD3	1:B:104:ARG:N	2.31	0.45
1:B:148:PRO:HG2	1:B:151:LEU:HD21	1.99	0.45
1:B:90:ALA:O	1:B:91:VAL:HG22	2.17	0.44
1:B:90:ALA:O	1:B:91:VAL:CG2	2.65	0.44
1:B:65:SER:HB3	1:B:80:SER:O	2.18	0.44
1:A:98:GLY:C	1:A:100:PRO:CD	2.86	0.43
1:B:123:ARG:NH2	3:B:649:HOH:O	2.51	0.43
1:A:150:HIS:HB2	1:A:237:MET:HE3	1.99	0.43
1:B:121:ASN:CB	1:B:122:ARG:CA	2.96	0.43
1:A:95:ASN:HB2	1:A:99:ARG:HG2	2.00	0.43
1:A:85:ASP:OD1	1:A:85:ASP:N	2.34	0.43
1:A:101:VAL:CG2	1:A:102:ALA:N	2.70	0.43
1:A:103:GLY:C	1:A:105:LEU:N	2.74	0.43
1:A:107:PRO:CB	1:A:108:ASP:HA	2.48	0.42
1:A:257:ALA:HB2	1:A:264:LEU:HD13	2.00	0.42
1:B:88:LEU:C	1:B:88:LEU:CD2	2.89	0.42
1:A:123:ARG:HD2	1:A:142:THR:CG2	2.50	0.42
1:B:198:GLY:HA3	1:B:210:TRP:CZ2	2.53	0.42
1:A:106:SER:C	1:A:107:PRO:O	2.61	0.42
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.85	0.42
1:A:95:ASN:O	1:A:100:PRO:HD2	2.18	0.42
1:A:82:THR:HG22	1:A:83:ALA:O	2.19	0.42
1:A:88:LEU:HB3	1:A:89:ALA:HB2	2.01	0.42
1:B:109:GLY:HA3	1:B:110:LEU:HD23	2.00	0.42
1:A:68:ASP:OD1	1:A:69:GLY:N	2.53	0.42
1:A:103:GLY:C	1:A:105:LEU:H	2.13	0.42
1:B:101:VAL:CG2	1:B:102:ALA:N	2.71	0.41
1:A:96:ASP:HB3	1:A:122:ARG:HB3	2.02	0.41
1:A:106:SER:O	1:A:107:PRO:O	2.38	0.41
1:B:86:GLY:HA3	1:B:87:VAL:C	2.41	0.41
1:B:170:VAL:O	1:B:209:ARG:HA	2.19	0.41
1:B:198:GLY:HA3	1:B:210:TRP:CH2	2.56	0.41
1:A:170:VAL:O	1:A:209:ARG:HA	2.20	0.41
1:A:95:ASN:OD1	1:A:96:ASP:CA	2.69	0.41
1:A:83:ALA:O	1:A:84:ALA:CB	2.69	0.41
1:A:93:MET:CE	1:A:114:THR:CG2	2.99	0.41
1:A:166:VAL:HG21	1:A:252:GLU:HG3	2.03	0.41
1:B:101:VAL:HG23	1:B:116:GLU:CD	2.36	0.40
1:B:104:ARG:O	1:B:104:ARG:CD	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:PRO:O	1:B:108:ASP:CB	2.69	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	330/352 (94%)	308 (93%)	14 (4%)	8 (2%)	4	4
1	B	326/352 (93%)	305 (94%)	11 (3%)	10 (3%)	3	2
All	All	656/704 (93%)	613 (93%)	25 (4%)	18 (3%)	4	3

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	A	97	ASN
1	A	99	ARG
1	A	104	ARG
1	B	96	ASP
1	B	102	ALA
1	A	95	ASN
1	A	110	LEU
1	B	87	VAL
1	B	88	LEU
1	B	100	PRO
1	B	103	GLY
1	B	108	ASP
1	B	121	ASN
1	A	89	ALA
1	A	107	PRO
1	B	94	VAL

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Mol	Chain	Res	Type
1	B	109	GLY

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	271/282 (96%)	254 (94%)	17 (6%)	16	23
1	B	268/282 (95%)	246 (92%)	22 (8%)	10	14
All	All	539/564 (96%)	500 (93%)	39 (7%)	13	18

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	71	VAL
1	A	81	VAL
1	A	88	LEU
1	A	99	ARG
1	A	105	LEU
1	A	111	ARG
1	A	113	SER
1	A	115	THR
1	A	138	THR
1	A	141	LEU
1	A	237	MET
1	A	248	THR
1	A	301	ILE
1	A	307	THR
1	A	319	ARG
1	A	322	VAL
1	B	87	VAL
1	B	88	LEU
1	B	92	THR
1	B	95	ASN
1	B	97	ASN

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Mol	Chain	Res	Type
1	B	99	ARG
1	B	101	VAL
1	B	104	ARG
1	B	105	LEU
1	B	106	SER
1	B	107	PRO
1	B	110	LEU
1	B	113	SER
1	B	114	THR
1	B	116	GLU
1	B	118	LEU
1	B	237	MET
1	B	248	THR
1	B	276	MET
1	B	301	ILE
1	B	307	THR
1	B	322	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	352	HIS

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	112:TRP	C	113:SER	N	0.95

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	334/352 (94%)	-1.24	0 100 100	19, 31, 105, 116	0
1	B	330/352 (93%)	-1.22	0 100 100	19, 31, 103, 114	0
All	All	664/704 (94%)	-1.23	0 100 100	19, 31, 104, 116	0

There are no RSRZ outliers to report.

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	501	1/1	1.00	0.02	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.