



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:44 PM UTC

PDB ID : 3FP9 / pdb_00003fp9
Title : Crystal structure of Intern Domain of proteasome-associated ATPase, Mycobacterium tuberculosis
Authors : Li, H.; Wang, T.
Deposited on : 2009-01-04
Resolution : 2.00 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

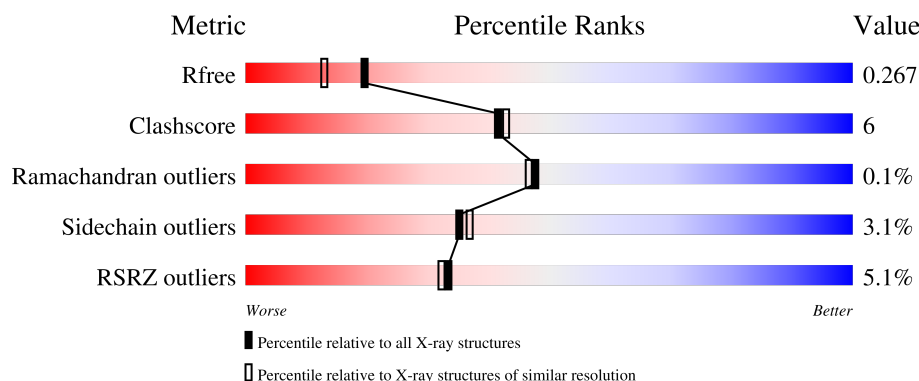
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	153	5% 83% 13% ..
1	B	153	3% 78% 14% 8%
1	C	153	5% 76% 15% 8%
1	D	153	2% 79% 12% 7%
1	E	153	0% 69% 14% 15%

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Mol	Chain	Length	Quality of chain
1	F	153	7%78%13%8%
1	G	153	7%77%15%7%
1	H	153	7%72%19%8%
1	I	153	5%76%15%8%
1	J	153	4%71%22%7%
1	K	153	5%80%10%8%
1	L	153	5%71%16%12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13735 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 Proteasome-associated ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1144	715	197	230	2			
1	B	141	Total	C	N	O	S	0	0	0
			1079	676	187	214	2			
1	C	141	Total	C	N	O	S	0	0	0
			1079	676	187	214	2			
1	D	142	Total	C	N	O	S	0	0	0
			1087	680	188	217	2			
1	E	130	Total	C	N	O	S	0	0	0
			989	622	169	196	2			
1	F	140	Total	C	N	O	S	0	0	0
			1071	672	186	211	2			
1	G	142	Total	C	N	O	S	0	0	0
			1083	678	188	215	2			
1	H	141	Total	C	N	O	S	0	0	0
			1079	676	187	214	2			
1	I	141	Total	C	N	O	S	0	0	0
			1079	676	187	214	2			
1	J	142	Total	C	N	O	S	0	0	0
			1087	680	188	217	2			
1	K	140	Total	C	N	O	S	0	0	0
			1071	672	186	211	2			
1	L	134	Total	C	N	O	S	0	0	0
			1021	642	177	200	2			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	MET	-	initiating methionine	UNP P63345
A	246	LEU	-	expression tag	UNP P63345
A	247	VAL	-	expression tag	UNP P63345
A	248	PRO	-	expression tag	UNP P63345
A	249	ARG	-	expression tag	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
B	97	MET	-	initiating methionine	UNP P63345
B	246	LEU	-	expression tag	UNP P63345
B	247	VAL	-	expression tag	UNP P63345
B	248	PRO	-	expression tag	UNP P63345
B	249	ARG	-	expression tag	UNP P63345
C	97	MET	-	initiating methionine	UNP P63345
C	246	LEU	-	expression tag	UNP P63345
C	247	VAL	-	expression tag	UNP P63345
C	248	PRO	-	expression tag	UNP P63345
C	249	ARG	-	expression tag	UNP P63345
D	97	MET	-	initiating methionine	UNP P63345
D	246	LEU	-	expression tag	UNP P63345
D	247	VAL	-	expression tag	UNP P63345
D	248	PRO	-	expression tag	UNP P63345
D	249	ARG	-	expression tag	UNP P63345
E	97	MET	-	initiating methionine	UNP P63345
E	246	LEU	-	expression tag	UNP P63345
E	247	VAL	-	expression tag	UNP P63345
E	248	PRO	-	expression tag	UNP P63345
E	249	ARG	-	expression tag	UNP P63345
F	97	MET	-	initiating methionine	UNP P63345
F	246	LEU	-	expression tag	UNP P63345
F	247	VAL	-	expression tag	UNP P63345
F	248	PRO	-	expression tag	UNP P63345
F	249	ARG	-	expression tag	UNP P63345
G	97	MET	-	initiating methionine	UNP P63345
G	246	LEU	-	expression tag	UNP P63345
G	247	VAL	-	expression tag	UNP P63345
G	248	PRO	-	expression tag	UNP P63345
G	249	ARG	-	expression tag	UNP P63345
H	97	MET	-	initiating methionine	UNP P63345
H	246	LEU	-	expression tag	UNP P63345
H	247	VAL	-	expression tag	UNP P63345
H	248	PRO	-	expression tag	UNP P63345
H	249	ARG	-	expression tag	UNP P63345
I	97	MET	-	initiating methionine	UNP P63345
I	246	LEU	-	expression tag	UNP P63345
I	247	VAL	-	expression tag	UNP P63345
I	248	PRO	-	expression tag	UNP P63345
I	249	ARG	-	expression tag	UNP P63345
J	97	MET	-	initiating methionine	UNP P63345
J	246	LEU	-	expression tag	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
J	247	VAL	-	expression tag	UNP P63345
J	248	PRO	-	expression tag	UNP P63345
J	249	ARG	-	expression tag	UNP P63345
K	97	MET	-	initiating methionine	UNP P63345
K	246	LEU	-	expression tag	UNP P63345
K	247	VAL	-	expression tag	UNP P63345
K	248	PRO	-	expression tag	UNP P63345
K	249	ARG	-	expression tag	UNP P63345
L	97	MET	-	initiating methionine	UNP P63345
L	246	LEU	-	expression tag	UNP P63345
L	247	VAL	-	expression tag	UNP P63345
L	248	PRO	-	expression tag	UNP P63345
L	249	ARG	-	expression tag	UNP P63345

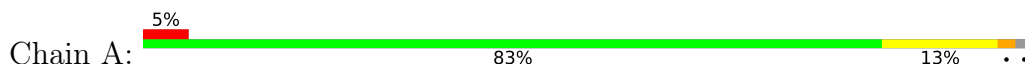
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	95	Total O 95 95	0	0
2	B	95	Total O 95 95	0	0
2	C	98	Total O 98 98	0	0
2	D	80	Total O 80 80	0	0
2	E	78	Total O 78 78	0	0
2	F	69	Total O 69 69	0	0
2	G	52	Total O 52 52	0	0
2	H	61	Total O 61 61	0	0
2	I	58	Total O 58 58	0	0
2	J	65	Total O 65 65	0	0
2	K	65	Total O 65 65	0	0
2	L	50	Total O 50 50	0	0

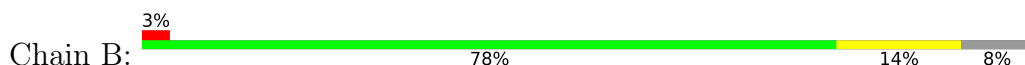
3 Residue-property plots [i](#)

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.

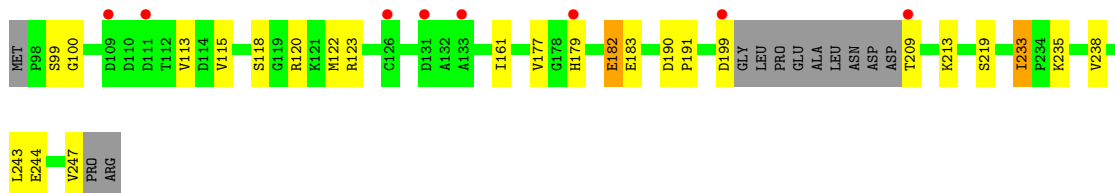
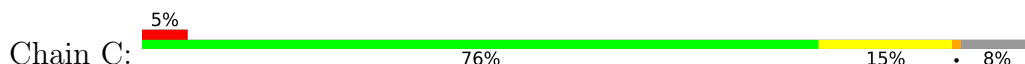
- Molecule 1: Proteasome-associated ATPase



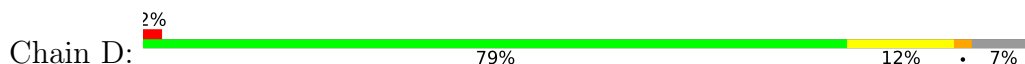
- Molecule 1: Proteasome-associated ATPase



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- Molecule 1: Proteasome-associated ATPase

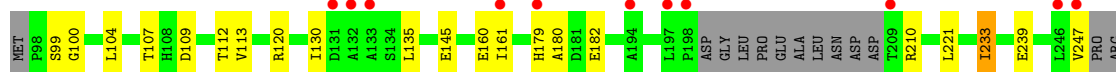
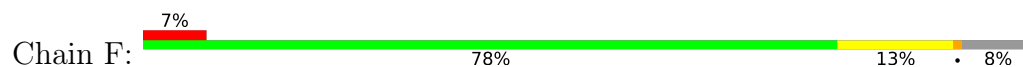


- Molecule 1: Proteasome-associated ATPase

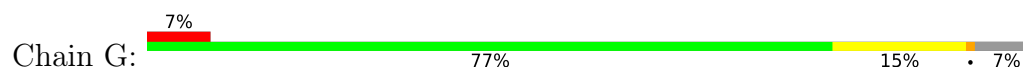




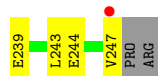
- Molecule 1: Proteasome-associated ATPase



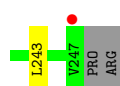
- Molecule 1: Proteasome-associated ATPase



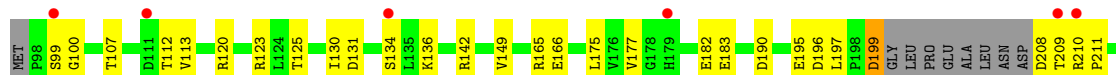
- Molecule 1: Proteasome-associated ATPase

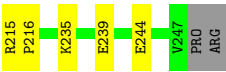


- Molecule 1: Proteasome-associated ATPase

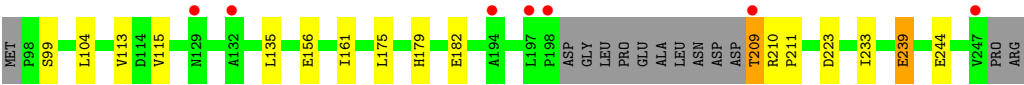
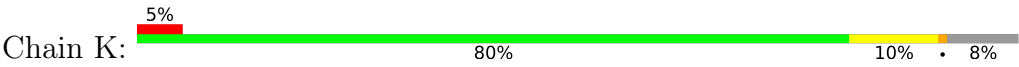


- Molecule 1: Proteasome-associated ATPase

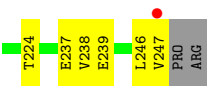




● Molecule 1: Proteasome-associated ATPase



● Molecule 1: Proteasome-associated ATPase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.86Å 74.99Å 200.85Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.00) 98.0 (20.00-2.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.266 0.214 , 0.267	Depositor DCC
R_{free} test set	7416 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l 0.009 for k,h,-l 0.019 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13735	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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	1.26	4/1161 (0.3%)	1.08	3/1579 (0.2%)
1	B	1.25	2/1094 (0.2%)	1.06	2/1485 (0.1%)
1	C	1.16	1/1094 (0.1%)	1.01	3/1485 (0.2%)
1	D	1.13	4/1102 (0.4%)	0.99	1/1496 (0.1%)
1	E	1.23	5/1002 (0.5%)	1.01	0/1360
1	F	1.09	2/1086 (0.2%)	1.03	2/1474 (0.1%)
1	G	0.94	0/1098	0.97	1/1490 (0.1%)
1	H	1.12	3/1094 (0.3%)	1.03	2/1485 (0.1%)
1	I	1.02	0/1094	1.03	4/1485 (0.3%)
1	J	1.02	2/1102 (0.2%)	1.03	0/1496
1	K	1.01	0/1086	1.03	0/1474
1	L	1.04	1/1035 (0.1%)	0.97	0/1403
All	All	1.11	24/13048 (0.2%)	1.02	18/17712 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	GLY	C-N	-11.27	1.23	1.33
1	E	190	ASP	C-O	-9.25	1.15	1.24
1	A	99	SER	C-N	-8.94	1.24	1.33
1	F	100	GLY	N-CA	6.66	1.49	1.44
1	A	103	VAL	CA-CB	6.62	1.62	1.54
1	D	233	ILE	CA-CB	6.43	1.60	1.53
1	J	190	ASP	C-O	-6.02	1.18	1.24
1	E	154	THR	C-O	-5.92	1.16	1.24
1	D	103	VAL	CA-CB	5.89	1.61	1.54
1	D	180	ALA	CA-CB	-5.71	1.45	1.53
1	E	103	VAL	CA-CB	5.56	1.60	1.54
1	F	233	ILE	CA-CB	5.46	1.59	1.53
1	H	152	ALA	CA-CB	-5.41	1.45	1.53
1	J	100	GLY	N-CA	5.26	1.48	1.44
1	C	233	ILE	CA-CB	5.26	1.59	1.53
1	D	120	ARG	C-O	-5.24	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	150	VAL	C-O	-5.20	1.18	1.24
1	E	155	PHE	C-O	-5.18	1.17	1.23
1	E	169	ALA	C-O	-5.15	1.18	1.24
1	H	126	CYS	C-O	-5.08	1.18	1.23
1	A	190	ASP	C-O	-5.07	1.19	1.24
1	B	152	ALA	CA-CB	-5.03	1.45	1.53
1	A	152	ALA	CA-CB	-5.02	1.42	1.53
1	L	224	THR	C-O	-5.01	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	SER	O-C-N	-6.78	114.37	123.19
1	H	210	ARG	CA-C-N	6.71	127.11	119.93
1	H	210	ARG	C-N-CA	6.71	127.11	119.93
1	A	179	HIS	N-CA-C	6.09	118.42	111.11
1	I	197	LEU	CA-C-N	6.04	126.35	119.83
1	I	197	LEU	C-N-CA	6.04	126.35	119.83
1	I	154	THR	CB-CA-C	-5.77	108.77	117.07
1	C	120	ARG	N-CA-C	5.76	117.83	109.07
1	D	120	ARG	N-CA-C	5.74	117.80	109.07
1	G	120	ARG	N-CA-C	5.52	117.19	108.96
1	C	118	SER	CB-CA-C	-5.36	103.97	111.80
1	F	179	HIS	N-CA-C	5.17	117.66	111.71
1	B	190	ASP	CA-C-N	-5.15	114.31	119.56
1	B	190	ASP	C-N-CA	-5.15	114.31	119.56
1	I	179	HIS	N-CA-C	5.08	117.48	111.33
1	A	199	ASP	N-CA-C	5.07	117.70	111.82
1	F	112	THR	N-CA-C	-5.05	103.26	110.59
1	C	233	ILE	N-CA-C	-5.04	102.21	107.60

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	1144	0	1142	11	0
1	B	1079	0	1084	17	0
1	C	1079	0	1084	16	0
1	D	1087	0	1088	13	0
1	E	989	0	994	14	0
1	F	1071	0	1080	11	0
1	G	1083	0	1087	18	0
1	H	1079	0	1084	25	0
1	I	1079	0	1084	17	0
1	J	1087	0	1088	20	0
1	K	1071	0	1080	15	0
1	L	1021	0	1033	22	0
2	A	95	0	0	0	0
2	B	95	0	0	1	0
2	C	98	0	0	2	0
2	D	80	0	0	0	0
2	E	78	0	0	3	0
2	F	69	0	0	1	0
2	G	52	0	0	1	0
2	H	61	0	0	0	0
2	I	58	0	0	1	0
2	J	65	0	0	1	0
2	K	65	0	0	0	0
2	L	50	0	0	1	0
All	All	13735	0	12928	166	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 6.

All (166) 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:LEU:CD2	1:B:135:LEU:HB3	1.97	0.93
1:L:237:GLU:HB3	1:L:239:GLU:OE1	1.71	0.91
1:L:247:VAL:HG12	1:L:247:VAL:O	1.74	0.86
1:L:110:ASP:O	1:L:111:ASP:HB2	1.75	0.83
1:L:104:LEU:HD21	1:L:135:LEU:HB3	1.61	0.80
1:K:210:ARG:HB2	1:K:211:PRO:CD	2.13	0.78
1:H:209:THR:HG23	1:H:210:ARG:H	1.49	0.76
1:C:219:SER:OG	1:C:235:LYS:HE3	1.86	0.74
1:G:199:ASP:HB3	1:G:213:LYS:HD3	1.68	0.73
1:J:199:ASP:N	1:J:199:ASP:OD1	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:107:THR:HG22	1:L:113:VAL:HG12	1.73	0.71
1:L:247:VAL:O	1:L:247:VAL:CG1	2.38	0.71
1:G:185:VAL:HG23	1:H:161:ILE:HD11	1.73	0.69
1:B:104:LEU:HD21	1:B:135:LEU:HB3	1.74	0.69
1:G:161:ILE:HD11	1:L:185:VAL:HG23	1.74	0.69
1:H:127:SER:OG	1:H:128:PRO:HD2	1.93	0.68
1:F:104:LEU:CD2	1:F:135:LEU:HB3	2.24	0.67
1:E:104:LEU:HD22	1:E:135:LEU:HB3	1.77	0.67
1:F:161:ILE:HD13	1:F:221:LEU:HA	1.75	0.67
1:H:120:ARG:NH1	1:I:118:SER:OG	2.28	0.66
1:K:182:GLU:HG2	1:K:182:GLU:O	1.96	0.64
1:H:180:ALA:N	1:H:182:GLU:OE2	2.30	0.64
1:K:210:ARG:HB2	1:K:211:PRO:HD3	1.79	0.63
1:L:104:LEU:CD2	1:L:135:LEU:HB3	2.30	0.62
1:C:123:ARG:HB3	1:D:99:SER:HB2	1.81	0.62
1:G:216:PRO:HD2	1:H:244:GLU:HG2	1.82	0.61
1:I:225:LYS:HD3	2:I:254:HOH:O	2.00	0.61
1:G:161:ILE:CD1	1:G:233:ILE:HG13	2.32	0.60
1:L:110:ASP:OD2	1:L:123:ARG:NH2	2.34	0.60
1:B:104:LEU:HD21	1:B:135:LEU:CB	2.32	0.60
1:G:209:THR:HG23	1:G:210:ARG:HG2	1.82	0.60
1:H:110:ASP:O	1:H:111:ASP:HB2	2.00	0.60
1:H:182:GLU:O	1:H:182:GLU:HG2	2.02	0.60
1:K:210:ARG:CB	1:K:211:PRO:CD	2.80	0.60
1:K:210:ARG:HB2	1:K:211:PRO:HD2	1.84	0.59
1:G:112:THR:HG22	1:G:125:THR:HG22	1.83	0.59
1:B:104:LEU:HD22	1:B:135:LEU:HB3	1.83	0.58
1:L:246:LEU:O	1:L:247:VAL:C	2.45	0.58
1:I:239:GLU:CD	1:I:239:GLU:H	2.09	0.58
1:A:123:ARG:HB3	1:B:99:SER:HB2	1.85	0.57
1:E:107:THR:HG22	1:E:113:VAL:HG12	1.86	0.57
1:H:185:VAL:HG23	1:I:161:ILE:HD11	1.84	0.57
1:I:123:ARG:HB3	1:J:99:SER:OG	2.05	0.57
1:L:239:GLU:H	1:L:239:GLU:CD	2.12	0.57
1:K:104:LEU:CD2	1:K:135:LEU:HB3	2.34	0.57
1:H:107:THR:HG22	1:H:113:VAL:HG12	1.86	0.57
1:A:213:LYS:O	1:A:213:LYS:HG3	2.04	0.56
1:C:190:ASP:N	1:C:191:PRO:HD2	2.20	0.56
1:G:99:SER:HB3	1:G:143:LEU:O	2.06	0.56
1:D:161:ILE:HD11	1:D:233:ILE:HG13	1.87	0.56
1:H:136:LYS:O	1:H:139:GLN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:SER:HB3	1:E:143:LEU:O	2.06	0.56
1:G:123:ARG:HB3	1:H:99:SER:HB2	1.88	0.56
1:K:113:VAL:HG23	1:K:115:VAL:HG23	1.88	0.56
1:I:180:ALA:N	1:I:182:GLU:OE2	2.37	0.56
1:L:180:ALA:N	1:L:182:GLU:OE2	2.37	0.56
1:A:243:LEU:O	1:A:247:VAL:HG23	2.06	0.55
1:G:161:ILE:HD11	1:L:185:VAL:CG2	2.36	0.55
1:I:131:ASP:OD1	1:I:131:ASP:C	2.48	0.55
1:L:238:VAL:HG23	2:L:259:HOH:O	2.06	0.55
1:C:243:LEU:O	1:C:247:VAL:HG23	2.08	0.54
1:E:185:VAL:HG23	1:F:161:ILE:HD11	1.90	0.54
1:H:123:ARG:HB3	1:I:99:SER:HB2	1.90	0.54
1:A:180:ALA:N	1:A:182:GLU:OE2	2.39	0.53
1:J:216:PRO:HD2	1:K:244:GLU:HG2	1.90	0.53
1:C:161:ILE:HD11	1:C:233:ILE:HG13	1.91	0.53
1:D:239:GLU:H	1:D:239:GLU:CD	2.16	0.53
1:I:104:LEU:HD22	1:I:135:LEU:HB3	1.91	0.53
1:A:177:VAL:HG22	1:A:183:GLU:HG2	1.90	0.52
1:J:165:ARG:HD3	1:J:175:LEU:HD13	1.90	0.52
1:H:127:SER:OG	1:H:128:PRO:CD	2.58	0.52
1:H:243:LEU:O	1:H:247:VAL:HG23	2.09	0.52
1:I:107:THR:HG22	1:I:113:VAL:HG12	1.92	0.52
1:C:183:GLU:OE2	1:D:235:LYS:NZ	2.36	0.51
1:C:113:VAL:HG23	1:C:115:VAL:HG23	1.93	0.51
1:I:216:PRO:HD2	1:J:244:GLU:HG2	1.93	0.51
1:J:120:ARG:HD2	2:J:649:HOH:O	2.10	0.51
1:H:210:ARG:HB2	1:H:211:PRO:HD2	1.92	0.51
1:A:110:ASP:O	1:A:111:ASP:HB2	2.12	0.50
1:F:107:THR:HG22	1:F:113:VAL:HG12	1.93	0.50
1:E:225:LYS:HD2	2:E:37:HOH:O	2.11	0.49
1:J:131:ASP:O	1:J:134:SER:HB3	2.12	0.49
1:L:144:ASN:ND2	1:L:148:THR:HB	2.27	0.49
1:B:216:PRO:HD2	1:C:244:GLU:HG2	1.94	0.49
1:I:104:LEU:CD2	1:I:135:LEU:HB3	2.44	0.48
1:L:99:SER:HB2	1:L:143:LEU:O	2.13	0.48
1:E:243:LEU:O	1:E:247:VAL:HG23	2.13	0.48
1:B:165:ARG:NH1	1:B:166:GLU:OE1	2.47	0.48
1:L:130:ILE:HD11	1:L:151:GLU:HA	1.95	0.48
1:E:110:ASP:OD2	1:E:123:ARG:NH2	2.47	0.48
1:D:110:ASP:OD2	1:D:123:ARG:NH2	2.45	0.48
1:G:104:LEU:HD22	1:G:135:LEU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:239:GLU:H	1:K:239:GLU:CD	2.22	0.47
1:L:167:ILE:HD11	1:L:214:LEU:HB2	1.96	0.47
1:J:130:ILE:HD12	1:J:149:VAL:HG12	1.97	0.47
1:G:161:ILE:HD11	1:G:233:ILE:HG13	1.96	0.47
2:E:258:HOH:O	1:F:160:GLU:HG3	2.15	0.47
1:H:210:ARG:HB2	1:H:211:PRO:CD	2.45	0.47
1:A:154:THR:HB	1:A:155:PHE:H	1.41	0.46
1:F:161:ILE:HD12	1:F:233:ILE:HG13	1.98	0.46
1:D:137:LYS:HB3	1:D:228:TYR:OH	2.15	0.46
1:E:120:ARG:HD2	2:E:839:HOH:O	2.15	0.46
1:C:199:ASP:OD1	1:C:213:LYS:HE3	2.14	0.46
1:G:182:GLU:HA	1:H:179:HIS:HB2	1.96	0.46
1:I:219:SER:OG	1:I:235:LYS:HE3	2.15	0.46
1:L:110:ASP:O	1:L:111:ASP:CB	2.50	0.46
1:F:180:ALA:N	1:F:182:GLU:OE2	2.40	0.46
1:G:182:GLU:HA	1:H:179:HIS:CB	2.45	0.46
1:J:123:ARG:HB3	1:K:99:SER:HB2	1.98	0.46
1:C:238:VAL:HG12	2:C:566:HOH:O	2.16	0.45
1:G:216:PRO:CD	1:H:244:GLU:HG2	2.47	0.45
1:A:105:LEU:HD11	1:A:116:PHE:HB2	1.97	0.45
1:J:210:ARG:HB2	1:J:211:PRO:HD2	1.99	0.45
1:H:109:ASP:C	1:H:109:ASP:OD2	2.60	0.45
1:C:182:GLU:HA	1:D:179:HIS:HB3	1.99	0.45
1:H:210:ARG:CB	1:H:211:PRO:CD	2.95	0.45
1:B:154:THR:HG21	2:B:481:HOH:O	2.17	0.45
1:E:104:LEU:CD2	1:E:135:LEU:HB3	2.45	0.45
1:K:161:ILE:HD11	1:K:233:ILE:HG13	1.99	0.45
1:L:144:ASN:HD21	1:L:148:THR:HB	1.82	0.44
1:E:247:VAL:HG22	1:I:243:LEU:HD11	1.99	0.44
1:C:122:MET:HE1	2:C:263:HOH:O	2.17	0.44
1:G:190:ASP:N	1:G:191:PRO:HD2	2.33	0.44
1:K:156:GLU:OE1	1:K:223:ASP:OD2	2.35	0.44
1:G:200:GLY:HA2	1:G:215:ARG:HH12	1.82	0.44
1:I:161:ILE:CD1	1:I:233:ILE:HG13	2.48	0.44
1:J:165:ARG:NH1	1:J:166:GLU:OE1	2.50	0.44
1:B:161:ILE:HD11	1:B:233:ILE:HG13	2.00	0.44
1:A:185:VAL:HG23	1:B:161:ILE:HD11	1.99	0.44
1:E:215:ARG:NH1	1:F:247:VAL:C	2.76	0.44
1:L:130:ILE:HD13	1:L:130:ILE:HA	1.79	0.43
1:B:120:ARG:HH21	1:C:100:GLY:HA3	1.82	0.43
1:H:165:ARG:NH1	1:H:166:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:GLU:OE1	1:E:235:LYS:NZ	2.42	0.43
1:F:120:ARG:NH2	2:F:665:HOH:O	2.52	0.43
1:L:99:SER:CB	1:L:143:LEU:O	2.67	0.43
1:A:239:GLU:H	1:A:239:GLU:CD	2.26	0.43
1:D:180:ALA:N	1:D:182:GLU:OE2	2.49	0.43
1:G:153:GLY:HA3	2:G:862:HOH:O	2.19	0.43
1:B:180:ALA:N	1:B:182:GLU:OE2	2.49	0.43
1:J:99:SER:OG	1:J:142:ARG:HD2	2.19	0.43
1:J:177:VAL:HG22	1:J:183:GLU:HG2	2.00	0.42
1:K:104:LEU:HD22	1:K:135:LEU:HB3	2.01	0.42
1:J:112:THR:HG22	1:J:125:THR:HG22	2.00	0.42
1:H:154:THR:HB	1:H:155:PHE:H	1.51	0.42
1:J:208:ASP:CG	1:J:209:THR:H	2.27	0.42
1:B:192:LEU:HD23	1:B:192:LEU:HA	1.88	0.42
1:E:108:HIS:HE1	1:E:114:ASP:CG	2.28	0.42
1:C:182:GLU:HA	1:D:179:HIS:CB	2.50	0.42
1:I:182:GLU:O	1:I:182:GLU:HG2	2.19	0.42
1:J:182:GLU:HA	1:K:179:HIS:HB3	2.01	0.42
1:D:136:LYS:O	1:D:139:GLN:HB2	2.20	0.42
1:B:243:LEU:HD23	1:B:243:LEU:HA	1.79	0.41
1:D:172:HIS:CD2	1:D:193:ILE:CD1	3.03	0.41
1:I:183:GLU:OE2	1:J:235:LYS:NZ	2.48	0.41
1:B:182:GLU:HA	1:C:179:HIS:HB2	2.03	0.41
1:J:215:ARG:O	1:J:216:PRO:C	2.65	0.40
1:K:209:THR:HB	1:K:210:ARG:H	1.58	0.40
1:H:209:THR:HG23	1:H:210:ARG:N	2.27	0.40
1:E:185:VAL:CG2	1:F:161:ILE:HD11	2.51	0.40
1:B:137:LYS:HB3	1:B:228:TYR:OH	2.22	0.40
1:J:107:THR:HG22	1:J:113:VAL:HG12	2.03	0.40
1:J:196:ASP:OD1	1:J:196:ASP:N	2.50	0.40
1:A:179:HIS:HB3	1:F:182:GLU:HA	2.03	0.40
1:B:182:GLU:HA	1:C:179:HIS:CB	2.52	0.40
1:D:161:ILE:CD1	1:D:233:ILE:HG13	2.51	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	148/153 (97%)	145 (98%)	3 (2%)	0	100	100
1	B	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	C	137/153 (90%)	135 (98%)	2 (2%)	0	100	100
1	D	138/153 (90%)	137 (99%)	1 (1%)	0	100	100
1	E	126/153 (82%)	125 (99%)	1 (1%)	0	100	100
1	F	136/153 (89%)	134 (98%)	2 (2%)	0	100	100
1	G	138/153 (90%)	135 (98%)	3 (2%)	0	100	100
1	H	137/153 (90%)	133 (97%)	4 (3%)	0	100	100
1	I	137/153 (90%)	134 (98%)	2 (2%)	1 (1%)	18	14
1	J	138/153 (90%)	134 (97%)	4 (3%)	0	100	100
1	K	136/153 (89%)	130 (96%)	6 (4%)	0	100	100
1	L	130/153 (85%)	123 (95%)	7 (5%)	0	100	100
All	All	1638/1836 (89%)	1600 (98%)	37 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	132	ALA

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	124/127 (98%)	121 (98%)	3 (2%)	43	47
1	B	117/127 (92%)	114 (97%)	3 (3%)	40	44
1	C	117/127 (92%)	113 (97%)	4 (3%)	32	33
1	D	118/127 (93%)	115 (98%)	3 (2%)	42	45
1	E	107/127 (84%)	103 (96%)	4 (4%)	30	30
1	F	116/127 (91%)	110 (95%)	6 (5%)	21	18
1	G	117/127 (92%)	114 (97%)	3 (3%)	40	44
1	H	117/127 (92%)	114 (97%)	3 (3%)	40	44
1	I	117/127 (92%)	115 (98%)	2 (2%)	53	60
1	J	118/127 (93%)	113 (96%)	5 (4%)	26	25
1	K	116/127 (91%)	113 (97%)	3 (3%)	40	44
1	L	110/127 (87%)	106 (96%)	4 (4%)	31	31
All	All	1394/1524 (92%)	1351 (97%)	43 (3%)	35	37

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	THR
1	A	205	LEU
1	A	239	GLU
1	B	238	VAL
1	B	239	GLU
1	B	247	VAL
1	C	99	SER
1	C	177	VAL
1	C	182	GLU
1	C	209	THR
1	D	197	LEU
1	D	239	GLU
1	D	247	VAL
1	E	175	LEU
1	E	190	ASP
1	E	225	LYS
1	E	239	GLU
1	F	99	SER
1	F	109	ASP
1	F	130	ILE
1	F	145	GLU
1	F	210	ARG

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Mol	Chain	Res	Type
1	F	239	GLU
1	G	99	SER
1	G	239	GLU
1	G	247	VAL
1	H	154	THR
1	H	210	ARG
1	H	239	GLU
1	I	238	VAL
1	I	239	GLU
1	J	136	LYS
1	J	195	GLU
1	J	197	LEU
1	J	199	ASP
1	J	239	GLU
1	K	175	LEU
1	K	209	THR
1	K	239	GLU
1	L	99	SER
1	L	107	THR
1	L	145	GLU
1	L	193	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	179	HIS
1	B	108	HIS
1	C	108	HIS
1	D	108	HIS
1	D	172	HIS
1	E	108	HIS
1	F	108	HIS
1	F	172	HIS
1	F	179	HIS
1	G	108	HIS
1	G	172	HIS
1	H	172	HIS
1	I	108	HIS
1	I	179	HIS
1	J	108	HIS
1	K	108	HIS

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Mol	Chain	Res	Type
1	K	179	HIS
1	L	108	HIS
1	L	179	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](#)

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	150/153 (98%)	-0.00	8 (5%) 32 31	17, 25, 56, 73	0
1	B	141/153 (92%)	-0.07	5 (3%) 47 46	16, 24, 43, 56	0
1	C	141/153 (92%)	-0.02	8 (5%) 29 28	15, 26, 49, 60	0
1	D	142/153 (92%)	-0.08	3 (2%) 63 63	16, 27, 56, 73	0
1	E	130/153 (84%)	-0.13	1 (0%) 82 82	18, 27, 45, 52	0
1	F	140/153 (91%)	0.21	11 (7%) 18 17	17, 28, 63, 71	0
1	G	142/153 (92%)	0.43	11 (7%) 19 18	22, 37, 64, 70	0
1	H	141/153 (92%)	0.38	11 (7%) 19 18	21, 34, 60, 71	0
1	I	141/153 (92%)	0.23	7 (4%) 34 33	20, 32, 58, 66	0
1	J	142/153 (92%)	0.20	6 (4%) 40 39	20, 31, 52, 70	0
1	K	140/153 (91%)	0.10	7 (5%) 34 33	21, 31, 55, 69	0
1	L	134/153 (87%)	0.33	8 (5%) 27 26	22, 34, 59, 67	0
All	All	1684/1836 (91%)	0.13	86 (5%) 33 32	15, 30, 58, 73	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	5.9
1	F	132	ALA	5.6
1	H	209	THR	4.6
1	F	209	THR	4.1
1	K	209	THR	4.1
1	A	133	ALA	4.1
1	G	209	THR	4.1
1	L	193	ILE	3.9
1	G	130	ILE	3.9
1	L	194	ALA	3.9
1	D	208	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	132	ALA	3.7
1	F	179	HIS	3.5
1	G	133	ALA	3.4
1	B	209	THR	3.4
1	F	247	VAL	3.3
1	C	199	ASP	3.3
1	C	133	ALA	3.2
1	F	133	ALA	3.2
1	L	111	ASP	3.2
1	H	247	VAL	3.1
1	J	179	HIS	3.0
1	F	198	PRO	3.0
1	F	194	ALA	3.0
1	H	132	ALA	3.0
1	H	179	HIS	3.0
1	I	209	THR	2.8
1	C	126	CYS	2.8
1	I	128	PRO	2.8
1	F	246	LEU	2.7
1	G	111	ASP	2.7
1	C	209	THR	2.7
1	I	247	VAL	2.7
1	L	179	HIS	2.7
1	C	131	ASP	2.7
1	A	132	ALA	2.6
1	C	111	ASP	2.6
1	A	247	VAL	2.6
1	B	247	VAL	2.6
1	G	129	ASN	2.5
1	B	132	ALA	2.5
1	H	180	ALA	2.5
1	A	202	PRO	2.5
1	L	211	PRO	2.5
1	B	210	ARG	2.5
1	L	247	VAL	2.5
1	H	127	SER	2.5
1	K	194	ALA	2.5
1	G	109	ASP	2.4
1	J	99	SER	2.4
1	H	199	ASP	2.4
1	K	247	VAL	2.4
1	J	134	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	209	THR	2.4
1	A	201	LEU	2.4
1	H	129	ASN	2.4
1	I	111	ASP	2.4
1	G	132	ALA	2.3
1	K	129	ASN	2.3
1	K	197	LEU	2.3
1	G	200	GLY	2.3
1	H	109	ASP	2.3
1	G	107	THR	2.3
1	J	209	THR	2.3
1	A	205	LEU	2.3
1	C	179	HIS	2.2
1	F	131	ASP	2.2
1	J	210	ARG	2.2
1	E	98	PRO	2.2
1	C	109	ASP	2.2
1	H	111	ASP	2.2
1	J	111	ASP	2.2
1	D	247	VAL	2.2
1	L	132	ALA	2.2
1	I	179	HIS	2.2
1	G	198	PRO	2.1
1	K	198	PRO	2.1
1	A	134	SER	2.1
1	B	129	ASN	2.1
1	H	128	PRO	2.1
1	F	197	LEU	2.1
1	F	161	ILE	2.1
1	I	133	ALA	2.1
1	L	109	ASP	2.0
1	G	179	HIS	2.0
1	I	180	ALA	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 ⓘ

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.