



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:03 PM GMT

PDB ID : 3FP9
Title : Crystal structure of Intern Domain of proteasome-associatedATPase, Mycobacterium tuberculosis
Authors : Li, H.; Wang, T.
Deposited on : 2009-01-04
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

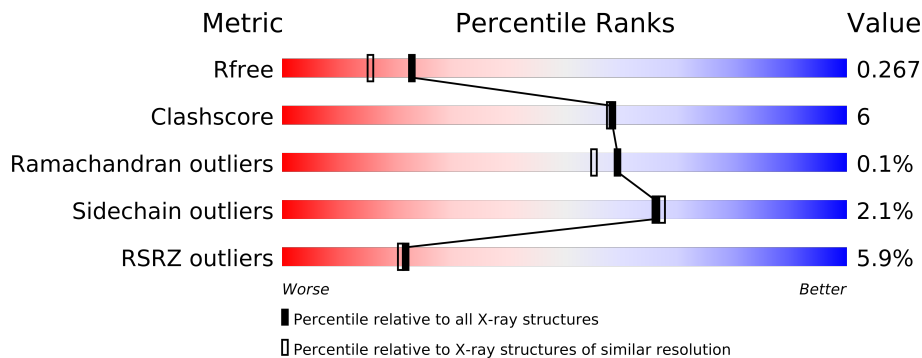
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	153	
1	B	153	
1	C	153	
1	D	153	
1	E	153	
1	F	153	
1	G	153	
1	H	153	
1	I	153	
1	J	153	
1	K	153	
1	L	153	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13735 atoms, of which 0 are hydrogen and 0 are deuterium.

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-associatedATPase.

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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-associatedATPase

Chain A: 



- Molecule 1: Proteasome-associatedATPase

Chain B: 



- Molecule 1: Proteasome-associatedATPase

Chain C: 



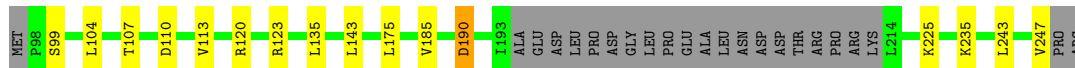
- Molecule 1: Proteasome-associatedATPase

Chain D: 



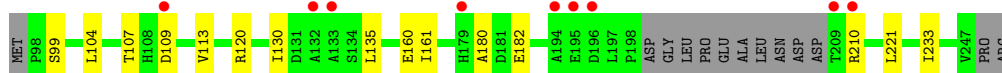
- Molecule 1: Proteasome-associatedATPase

Chain E: 

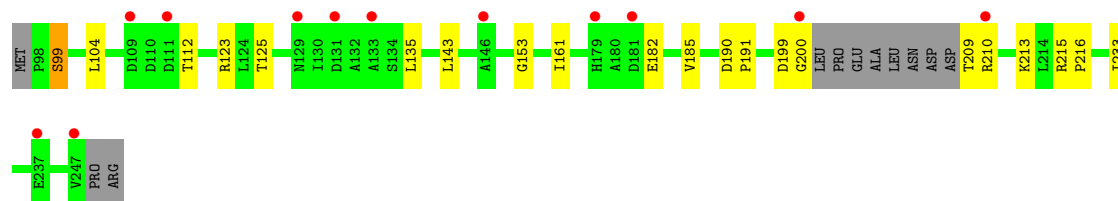


- Molecule 1: Proteasome-associatedATPase

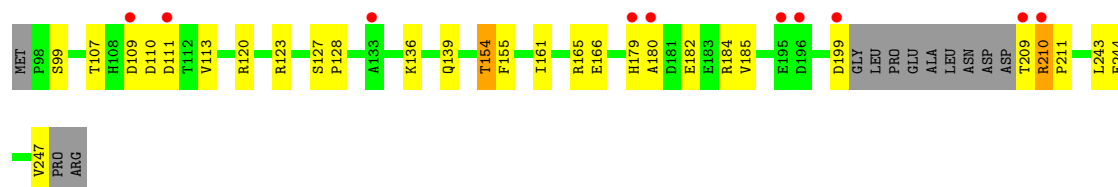
Chain F: 



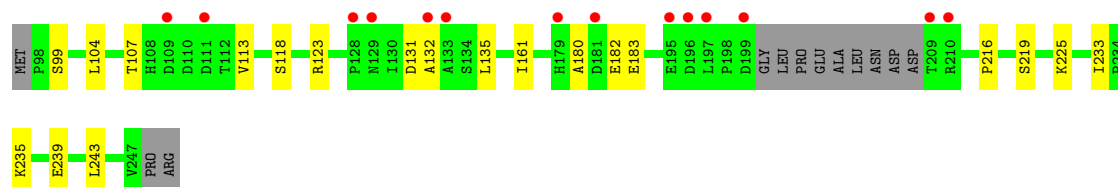
- Molecule 1: Proteasome-associatedATPase

Chain G: 

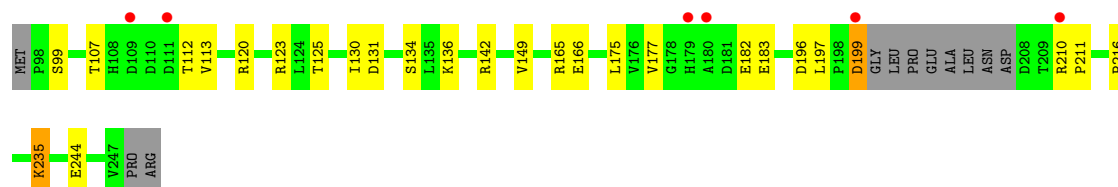
- Molecule 1: Proteasome-associatedATPase

Chain H: 

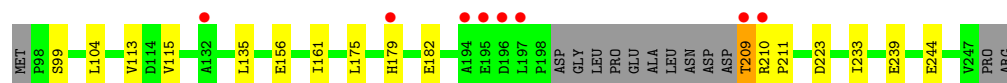
- Molecule 1: Proteasome-associatedATPase

Chain I: 

- Molecule 1: Proteasome-associatedATPase

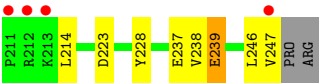
Chain J: 

- Molecule 1: Proteasome-associatedATPase

Chain K: 

- Molecule 1: Proteasome-associatedATPase

Chain L: 



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 19.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.00) 98.1 (19.87-2.00)	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 0.215 , 0.267	Depositor DCC
R_{free} test set	7416 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.8	EDS
Estimated twinning fraction	0.009 for -k,-h,-l 0.009 for k,h,-l 0.019 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 147570 reflections	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.

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	1.03	0/1161	0.91	2/1579 (0.1%)
1	B	0.99	1/1094 (0.1%)	0.85	0/1485
1	C	0.95	0/1094	0.83	0/1485
1	D	0.90	0/1102	0.83	0/1496
1	E	0.96	0/1002	0.86	1/1360 (0.1%)
1	F	0.89	0/1086	0.83	0/1474
1	G	0.72	0/1098	0.78	0/1490
1	H	0.90	0/1094	0.84	1/1485 (0.1%)
1	I	0.81	0/1094	0.78	0/1485
1	J	0.82	0/1102	0.81	2/1496 (0.1%)
1	K	0.82	0/1086	0.83	0/1474
1	L	0.81	0/1035	0.78	2/1403 (0.1%)
All	All	0.89	1/13048 (0.0%)	0.83	8/17712 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	PHE	CD2-CE2	5.15	1.49	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	L	223	ASP	CB-CG-OD1	5.52	123.27	118.30
1	J	235	LYS	CD-CE-NZ	-5.33	99.44	111.70
1	H	184	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	99	SER	O-C-N	-5.19	114.37	123.20
1	L	122	MET	CG-SD-CE	5.09	108.35	100.20
1	J	197	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	232	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1144	0	1142	10	0
1	B	1079	0	1084	17	0
1	C	1079	0	1084	15	0
1	D	1087	0	1088	13	0
1	E	989	0	994	12	0
1	F	1071	0	1080	10	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	18	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	1	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	160	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (160) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:104:LEU:CD2	1:B:135:LEU:HB3	1.97	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:237:GLU:HB3	1:L:239:GLU:OE1	1.71	0.91
1:L:247:VAL:O	1:L:247:VAL:HG12	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
1:L:107:THR:HG22	1:L:113:VAL:HG12	1.73	0.71
1:L:247:VAL:CG1	1:L:247:VAL:O	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:L:110:ASP:OD2	1:L:123:ARG:NH2	2.34	0.60
1:G:161:ILE:CD1	1:G:233:ILE:HG13	2.32	0.60
1:B:104:LEU:HD21	1:B:135:LEU:CB	2.32	0.60
1:H:110:ASP:O	1:H:111:ASP:HB2	2.00	0.60
1:G:209:THR:HG23	1:G:210:ARG:HG2	1.82	0.60
1:K:210:ARG:CB	1:K:211:PRO:CD	2.80	0.60
1:H:182:GLU:O	1:H:182:GLU:HG2	2.02	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: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:I:123:ARG:HB3	1:J:99:SER:OG	2.05	0.57
1:H:185:VAL:HG23	1:I:161:ILE:HD11	1.84	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:213:LYS:HG3	1:A:213:LYS:O	2.04	0.56
1:G:99:SER:HB3	1:G:143:LEU:O	2.06	0.56
1:C:190:ASP:N	1:C:191:PRO:HD2	2.20	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
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:E:99:SER:HB3	1:E:143:LEU:O	2.06	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:G:161:ILE:HD11	1:L:185:VAL:CG2	2.36	0.55
1:A:243:LEU:O	1:A:247:VAL:HG23	2.06	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:L:246:LEU:O	1:L:247:VAL:C	2.45	0.54
1:I:239:GLU:H	1:I:239:GLU:CD	2.09	0.54
1:H:123:ARG:HB3	1:I:99:SER:HB2	1.90	0.54
1:D:183:GLU:OE1	1:E:235:LYS:NZ	2.42	0.53
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:L:239:GLU:H	1:L:239:GLU:CD	2.12	0.53
1:C:161:ILE:HD11	1:C:233:ILE:HG13	1.91	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:I:107:THR:HG22	1:I:113:VAL:HG12	1.92	0.52
1:H:243:LEU:O	1:H:247:VAL:HG23	2.09	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:I:131:ASP:OD1	1:I:131:ASP:C	2.48	0.50
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:J:131:ASP:O	1:J:134:SER:HB3	2.12	0.49
1:E:225:LYS:HD2	2:E:37:HOH:O	2.11	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:D:239:GLU:H	1:D:239:GLU:CD	2.16	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:G:104:LEU:HD22	1:G:135:LEU:HB3	1.94	0.48
1:D:110:ASP:OD2	1:D:123:ARG:NH2	2.45	0.48
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
1:H:210:ARG:HB2	1:H:211:PRO:CD	2.45	0.47
2:E:258:HOH:O	1:F:160:GLU:HG3	2.15	0.47
1:F:161:ILE:HD12	1:F:233:ILE:HG13	1.98	0.46
1:A:154:THR:HB	1:A:155:PHE:H	1.41	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:L:110:ASP:O	1:L:111:ASP:CB	2.50	0.46
1:I:219:SER:OG	1:I:235:LYS:HE3	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: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:F:180:ALA:N	1:F:182:GLU:OE2	2.40	0.46
1:G:216:PRO:CD	1:H:244:GLU:HG2	2.47	0.45
1:C:238:VAL:HG12	2:C:566:HOH:O	2.16	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:210:ARG:CB	1:H:211:PRO:CD	2.95	0.45
1:C:182:GLU:HA	1:D:179:HIS:HB3	1.99	0.45
1:E:104:LEU:CD2	1:E:135:LEU:HB3	2.45	0.45
1:B:154:THR:HG21	2:B:481:HOH:O	2.17	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: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: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:G:200:GLY:HA2	1:G:215:ARG:HH12	1.82	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:130:ILE:HA	1:L:130:ILE:HD13	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
1:L:99:SER:CB	1:L:143:LEU:O	2.67	0.43
1:F:120:ARG:NH2	2:F:665:HOH:O	2.52	0.43
1:D:180:ALA:N	1:D:182:GLU:OE2	2.49	0.43
1:I:182:GLU:HG2	1:I:182:GLU:O	2.19	0.43
1:G:153:GLY:HA3	2:G:862:HOH:O	2.19	0.43
1:J:99:SER:OG	1:J:142:ARG:HD2	2.19	0.43
1:K:239:GLU:CD	1:K:239:GLU:H	2.22	0.43
1:B:180:ALA:N	1:B:182:GLU:OE2	2.49	0.43
1:K:104:LEU:HD22	1:K:135:LEU:HB3	2.01	0.42
1:J:177:VAL:HG22	1:J:183:GLU:HG2	2.00	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:B:192:LEU:HA	1:B:192:LEU:HD23	1.88	0.42
1:C:182:GLU:HA	1:D:179:HIS:CB	2.50	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:HA	1:B:243:LEU:HD23	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: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:H:109:ASP:OD2	1:H:109:ASP:C	2.60	0.40
1:E:185:VAL:CG2	1:F:161:ILE:HD11	2.51	0.40
1:J:196:ASP:OD1	1:J:196:ASP:N	2.50	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:D:161:ILE:CD1	1:D:233:ILE:HG13	2.51	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

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%)	30	20
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%)	59	55

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%)	122 (98%)	2 (2%)	75	77
1	B	117/127 (92%)	116 (99%)	1 (1%)	87	90
1	C	117/127 (92%)	113 (97%)	4 (3%)	49	45
1	D	118/127 (93%)	115 (98%)	3 (2%)	60	59
1	E	107/127 (84%)	105 (98%)	2 (2%)	69	71
1	F	116/127 (91%)	112 (97%)	4 (3%)	49	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	117/127 (92%)	116 (99%)	1 (1%)	87	90
1	H	117/127 (92%)	114 (97%)	3 (3%)	59	58
1	I	117/127 (92%)	117 (100%)	0	100	100
1	J	118/127 (93%)	116 (98%)	2 (2%)	73	75
1	K	116/127 (91%)	114 (98%)	2 (2%)	73	75
1	L	110/127 (87%)	105 (96%)	5 (4%)	38	31
All	All	1394/1524 (92%)	1365 (98%)	29 (2%)	66	67

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	154	THR
1	B	238	VAL
1	C	99	SER
1	C	127	SER
1	C	177	VAL
1	C	209	THR
1	D	127	SER
1	D	197	LEU
1	D	247	VAL
1	E	175	LEU
1	E	190	ASP
1	F	99	SER
1	F	109	ASP
1	F	130	ILE
1	F	210	ARG
1	G	99	SER
1	H	154	THR
1	H	199	ASP
1	H	210	ARG
1	J	136	LYS
1	J	199	ASP
1	K	175	LEU
1	K	209	THR
1	L	107	THR
1	L	145	GLU
1	L	193	ILE
1	L	228	TYR
1	L	239	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
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	G	108	HIS
1	G	172	HIS
1	H	172	HIS
1	I	108	HIS
1	J	108	HIS
1	K	108	HIS
1	L	108	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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 ⓘ

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%)	0.24	8 (5%) 25 25	17, 25, 56, 73	0
1	B	141/153 (92%)	0.20	6 (4%) 34 32	16, 24, 43, 56	0
1	C	141/153 (92%)	0.18	8 (5%) 23 22	15, 26, 49, 60	0
1	D	142/153 (92%)	0.09	4 (2%) 50 50	16, 27, 56, 73	0
1	E	130/153 (84%)	0.05	0 100 100	18, 27, 45, 52	0
1	F	140/153 (91%)	0.36	9 (6%) 19 18	17, 28, 63, 71	0
1	G	142/153 (92%)	0.54	12 (8%) 11 10	22, 37, 64, 70	0
1	H	141/153 (92%)	0.38	10 (7%) 16 15	21, 34, 60, 71	0
1	I	141/153 (92%)	0.37	14 (9%) 8 7	20, 32, 58, 66	0
1	J	142/153 (92%)	0.29	6 (4%) 35 34	20, 31, 52, 70	0
1	K	140/153 (91%)	0.22	8 (5%) 23 22	21, 31, 55, 69	0
1	L	134/153 (87%)	0.41	14 (10%) 7 6	22, 34, 59, 67	0
All	All	1684/1836 (91%)	0.28	99 (5%) 22 21	15, 30, 58, 73	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	194	ALA	6.5
1	L	211	PRO	5.6
1	A	204	ALA	5.4
1	B	210	ARG	5.2
1	A	133	ALA	4.7
1	D	208	ASP	4.5
1	G	133	ALA	4.4
1	F	179	HIS	4.3
1	J	179	HIS	4.2
1	C	109	ASP	4.0
1	H	209	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	202	PRO	3.7
1	K	196	ASP	3.7
1	F	132	ALA	3.6
1	A	206	ASN	3.6
1	F	210	ARG	3.6
1	F	109	ASP	3.6
1	K	210	ARG	3.5
1	H	109	ASP	3.5
1	K	195	GLU	3.5
1	L	109	ASP	3.5
1	J	109	ASP	3.5
1	C	133	ALA	3.5
1	H	199	ASP	3.5
1	H	179	HIS	3.4
1	G	210	ARG	3.4
1	D	133	ALA	3.4
1	G	111	ASP	3.3
1	G	179	HIS	3.3
1	C	247	VAL	3.2
1	L	179	HIS	3.2
1	D	210	ARG	3.1
1	H	210	ARG	3.0
1	F	196	ASP	3.0
1	L	111	ASP	3.0
1	G	109	ASP	3.0
1	B	199	ASP	3.0
1	J	210	ARG	3.0
1	A	203	GLU	2.9
1	B	209	THR	2.9
1	L	193	ILE	2.9
1	I	179	HIS	2.9
1	G	237	GLU	2.9
1	I	128	PRO	2.9
1	I	210	ARG	2.8
1	A	134	SER	2.8
1	F	195	GLU	2.8
1	K	197	LEU	2.7
1	H	195	GLU	2.7
1	I	197	LEU	2.7
1	H	180	ALA	2.7
1	I	195	GLU	2.7
1	F	133	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	181	ASP	2.6
1	C	179	HIS	2.6
1	K	194	ALA	2.6
1	L	212	ARG	2.6
1	G	200	GLY	2.6
1	L	133	ALA	2.5
1	K	179	HIS	2.5
1	L	213	LYS	2.5
1	B	129	ASN	2.5
1	G	131	ASP	2.5
1	J	111	ASP	2.5
1	F	194	ALA	2.5
1	L	180	ALA	2.5
1	G	247	VAL	2.5
1	K	209	THR	2.4
1	G	129	ASN	2.4
1	I	129	ASN	2.4
1	I	109	ASP	2.3
1	C	210	ARG	2.3
1	B	132	ALA	2.3
1	J	199	ASP	2.3
1	I	209	THR	2.3
1	J	180	ALA	2.3
1	F	209	THR	2.3
1	L	181	ASP	2.3
1	B	213	LYS	2.2
1	I	133	ALA	2.2
1	H	196	ASP	2.2
1	L	247	VAL	2.2
1	H	133	ALA	2.2
1	L	134	SER	2.2
1	A	109	ASP	2.2
1	L	128	PRO	2.2
1	G	181	ASP	2.1
1	I	111	ASP	2.1
1	C	195	GLU	2.1
1	D	179	HIS	2.1
1	C	199	ASP	2.1
1	G	146	ALA	2.0
1	K	132	ALA	2.0
1	I	196	ASP	2.0
1	A	205	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	209	THR	2.0
1	I	199	ASP	2.0
1	I	132	ALA	2.0
1	H	111	ASP	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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.