



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:43 AM GMT

PDB ID : 3FP9
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

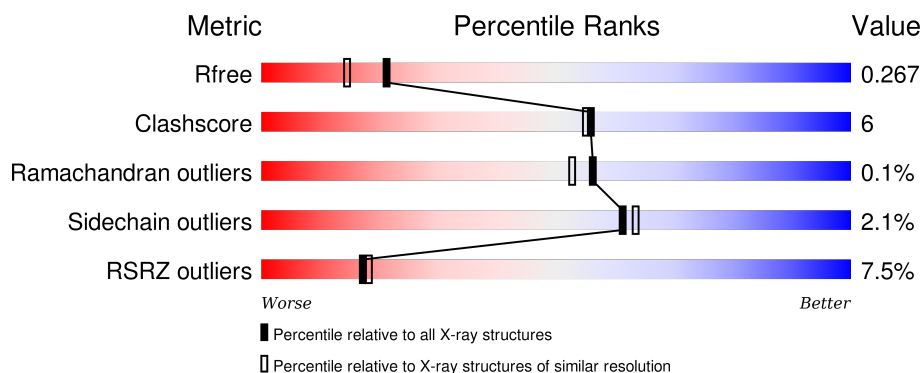
1 Overall quality at a glance

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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	<div> <div>7%</div> <div>86%10%..</div> </div>
1	B	153	<div> <div>6%</div> <div>80%12%8%</div> </div>
1	C	153	<div> <div>8%</div> <div>77%15%8%</div> </div>
1	D	153	<div> <div>4%</div> <div>80%13%7%</div> </div>
1	E	153	<div> <div>2%</div> <div>75%10%•15%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

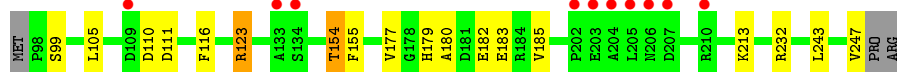
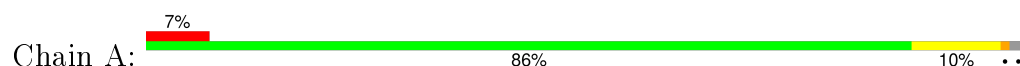
- Molecule 2 is water.

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

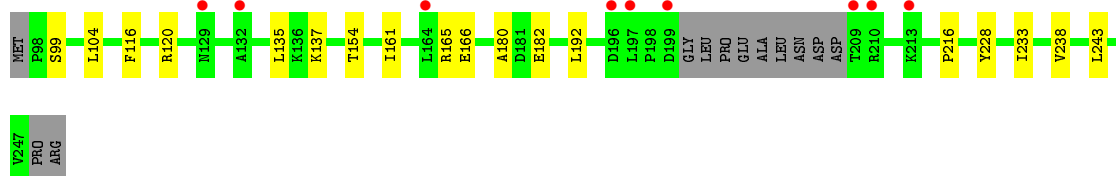
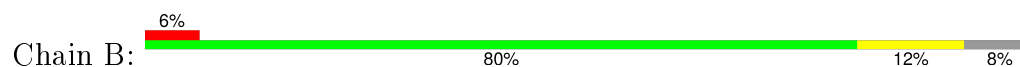
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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 ($\text{RSRZ} > 2$). 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.

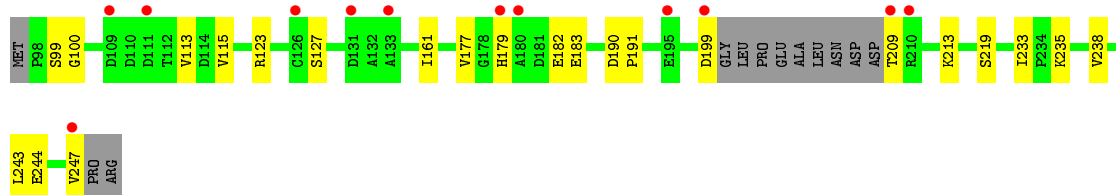
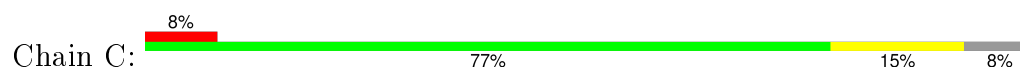
- Molecule 1: Proteasome-associated ATPase



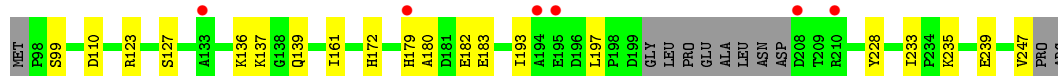
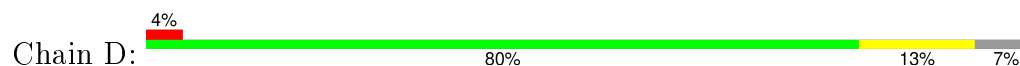
- Molecule 1: Proteasome-associated ATPase



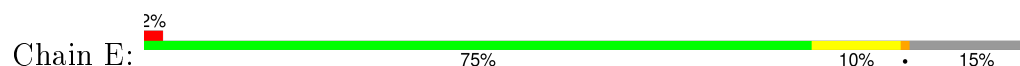
- Molecule 1: Proteasome-associated ATPase

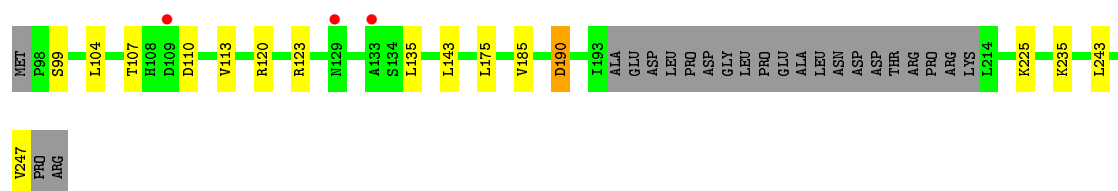


- Molecule 1: Proteasome-associated ATPase

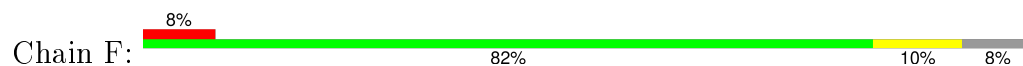


- Molecule 1: Proteasome-associated ATPase

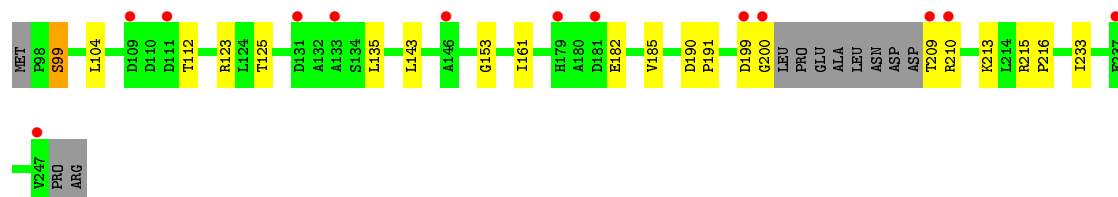
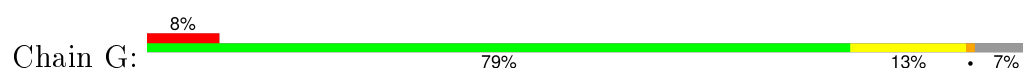




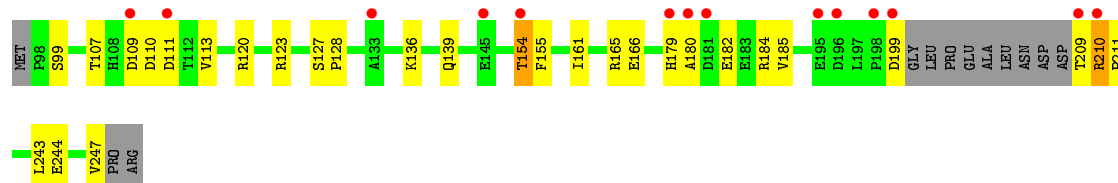
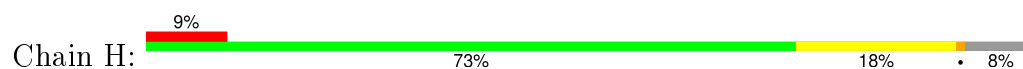
- Molecule 1: Proteasome-associated ATPase



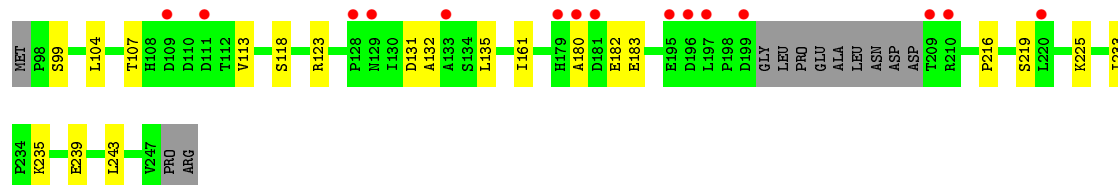
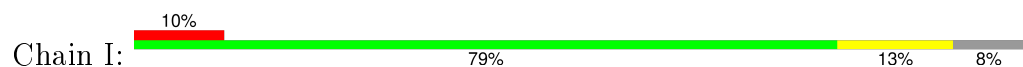
- Molecule 1: Proteasome-associated ATPase



- Molecule 1: Proteasome-associated ATPase

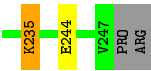


- Molecule 1: Proteasome-associated ATPase

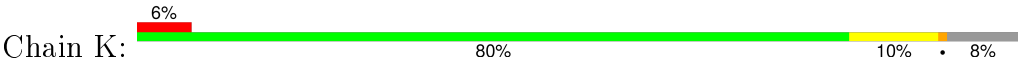


- Molecule 1: Proteasome-associated ATPase

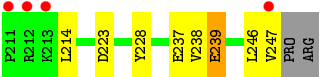




• Molecule 1: Proteasome-associated ATPase



• 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 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 0.214 , 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)	0.39 , 57.2	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 ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.03	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 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	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

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 (160) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:THR:HG22	1:H:113:VAL:HG12	1.86	0.57
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	26	19
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%)	56	53

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%)	70	73
1	B	117/127 (92%)	116 (99%)	1 (1%)	84	88
1	C	117/127 (92%)	113 (97%)	4 (3%)	44	41
1	D	118/127 (93%)	115 (98%)	3 (2%)	55	55
1	E	107/127 (84%)	105 (98%)	2 (2%)	65	67
1	F	116/127 (91%)	112 (97%)	4 (3%)	44	41
1	G	117/127 (92%)	116 (99%)	1 (1%)	84	88
1	H	117/127 (92%)	114 (97%)	3 (3%)	54	54
1	I	117/127 (92%)	117 (100%)	0	100	100
1	J	118/127 (93%)	116 (98%)	2 (2%)	68	71
1	K	116/127 (91%)	114 (98%)	2 (2%)	68	71
1	L	110/127 (87%)	105 (96%)	5 (4%)	34	29
All	All	1394/1524 (92%)	1365 (98%)	29 (2%)	61	63

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 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 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%)	0.35	10 (6%) 21 22	17, 25, 56, 73	0
1	B	141/153 (92%)	0.33	9 (6%) 23 24	16, 24, 43, 56	0
1	C	141/153 (92%)	0.32	12 (8%) 13 14	15, 26, 49, 60	0
1	D	142/153 (92%)	0.18	6 (4%) 40 41	16, 27, 56, 73	0
1	E	130/153 (84%)	0.17	3 (2%) 64 64	18, 27, 45, 52	0
1	F	140/153 (91%)	0.52	13 (9%) 11 11	17, 28, 63, 71	0
1	G	142/153 (92%)	0.65	13 (9%) 11 12	22, 37, 64, 70	0
1	H	141/153 (92%)	0.51	14 (9%) 9 10	21, 34, 60, 71	0
1	I	141/153 (92%)	0.52	15 (10%) 8 9	20, 32, 58, 66	0
1	J	142/153 (92%)	0.38	7 (4%) 33 35	20, 31, 52, 70	0
1	K	140/153 (91%)	0.34	9 (6%) 23 24	21, 31, 55, 69	0
1	L	134/153 (87%)	0.55	15 (11%) 7 7	22, 34, 59, 67	0
All	All	1684/1836 (91%)	0.40	126 (7%) 17 18	15, 30, 58, 73	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	7.1
1	L	194	ALA	6.4
1	B	210	ARG	6.0
1	L	211	PRO	6.0
1	F	179	HIS	5.4
1	G	133	ALA	5.2
1	A	202	PRO	5.2
1	A	133	ALA	5.0
1	C	109	ASP	4.8
1	D	208	ASP	4.7
1	J	179	HIS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	206	ASN	4.4
1	H	209	THR	4.2
1	C	133	ALA	4.1
1	F	132	ALA	4.0
1	H	109	ASP	4.0
1	J	109	ASP	4.0
1	K	195	GLU	4.0
1	K	210	ARG	3.9
1	L	109	ASP	3.9
1	H	179	HIS	3.9
1	G	109	ASP	3.8
1	H	199	ASP	3.8
1	J	210	ARG	3.7
1	F	109	ASP	3.7
1	K	196	ASP	3.7
1	F	210	ARG	3.7
1	G	210	ARG	3.7
1	I	128	PRO	3.6
1	C	247	VAL	3.6
1	L	128	PRO	3.5
1	D	210	ARG	3.5
1	G	131	ASP	3.5
1	L	111	ASP	3.5
1	I	179	HIS	3.5
1	F	194	ALA	3.4
1	D	133	ALA	3.4
1	K	194	ALA	3.4
1	I	197	LEU	3.4
1	L	180	ALA	3.4
1	G	179	HIS	3.4
1	K	197	LEU	3.3
1	G	111	ASP	3.3
1	F	196	ASP	3.3
1	G	200	GLY	3.2
1	H	198	PRO	3.2
1	L	193	ILE	3.2
1	B	209	THR	3.2
1	H	210	ARG	3.2
1	B	199	ASP	3.2
1	F	133	ALA	3.2
1	D	179	HIS	3.1
1	I	210	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	180	ALA	3.1
1	A	203	GLU	3.1
1	C	210	ARG	3.1
1	C	179	HIS	3.0
1	L	179	HIS	3.0
1	H	195	GLU	3.0
1	G	199	ASP	3.0
1	I	109	ASP	3.0
1	L	212	ARG	3.0
1	H	133	ALA	2.9
1	C	199	ASP	2.9
1	L	133	ALA	2.9
1	J	111	ASP	2.8
1	A	134	SER	2.8
1	C	209	THR	2.8
1	I	181	ASP	2.7
1	I	196	ASP	2.7
1	J	199	ASP	2.7
1	L	181	ASP	2.7
1	I	129	ASN	2.7
1	L	213	LYS	2.7
1	F	195	GLU	2.6
1	J	180	ALA	2.6
1	F	197	LEU	2.6
1	K	132	ALA	2.6
1	J	208	ASP	2.6
1	C	195	GLU	2.6
1	G	237	GLU	2.6
1	G	181	ASP	2.6
1	E	109	ASP	2.5
1	I	209	THR	2.5
1	B	129	ASN	2.5
1	B	213	LYS	2.5
1	I	111	ASP	2.5
1	C	180	ALA	2.5
1	K	179	HIS	2.4
1	L	247	VAL	2.4
1	A	205	LEU	2.4
1	H	196	ASP	2.4
1	I	220	LEU	2.4
1	H	145	GLU	2.4
1	B	132	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	181	ASP	2.4
1	H	154	THR	2.4
1	I	195	GLU	2.4
1	E	129	ASN	2.4
1	F	111	ASP	2.3
1	I	199	ASP	2.3
1	H	181	ASP	2.3
1	I	180	ALA	2.3
1	L	134	SER	2.3
1	C	131	ASP	2.3
1	A	109	ASP	2.3
1	G	247	VAL	2.2
1	G	209	THR	2.2
1	K	209	THR	2.2
1	D	194	ALA	2.2
1	F	237	GLU	2.2
1	H	111	ASP	2.2
1	F	209	THR	2.2
1	G	146	ALA	2.2
1	C	126	CYS	2.2
1	A	210	ARG	2.2
1	B	196	ASP	2.2
1	I	133	ALA	2.2
1	C	111	ASP	2.1
1	L	129	ASN	2.1
1	E	133	ALA	2.1
1	B	197	LEU	2.1
1	K	220	LEU	2.1
1	A	207	ASP	2.1
1	B	164	LEU	2.1
1	D	195	GLU	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 carbohydrates 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.