Full wwPDB X-ray Structure Validation Report ⓘ

Feb 7, 2017 – 11:59 AM EST

PDB ID	:	5B1M
Title	:	The mouse nucleosome structure containing H3.1
Authors	:	Urahama, T.; Machida, S.; Horikoshi, N.; Osakabe, A.; Tachiwana, H.; Taguchi, H.; Kurumizaka, H.
Deposited on	:	2015-12-08
Resolution	:	2.34 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:

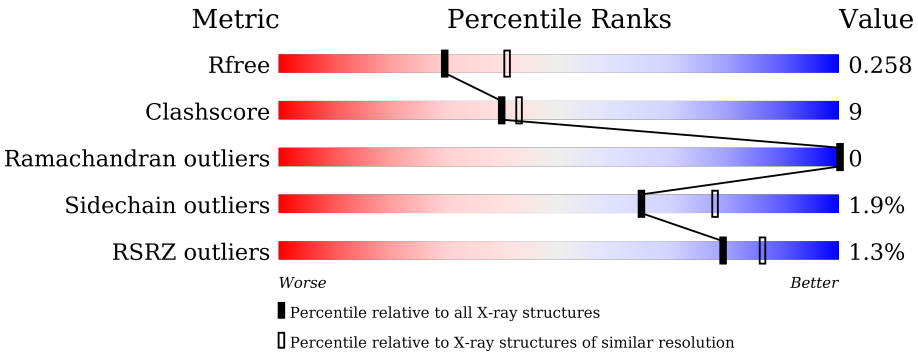
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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 <=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	139	58% 12% 30%
1	E	139	3% 58% 13% 29%
2	B	106	60% 13% 26%
2	F	106	2% 63% 15% 21%
3	C	133	71% 9% 19%
3	G	133	70% 8% 22%

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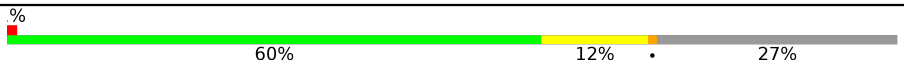
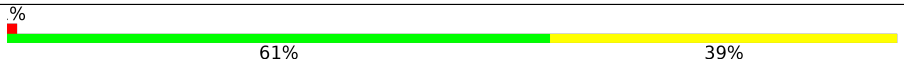
Mol	Chain	Length	Quality of chain
4	D	129	
4	H	129	
5	I	146	
5	J	146	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12071 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 Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	E	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68433
A	-2	SER	-	expression tag	UNP P68433
A	-1	HIS	-	expression tag	UNP P68433
E	-3	GLY	-	expression tag	UNP P68433
E	-2	SER	-	expression tag	UNP P68433
E	-1	HIS	-	expression tag	UNP P68433

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
2	F	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62806
B	-2	SER	-	expression tag	UNP P62806
B	-1	HIS	-	expression tag	UNP P62806
F	-3	GLY	-	expression tag	UNP P62806
F	-2	SER	-	expression tag	UNP P62806
F	-1	HIS	-	expression tag	UNP P62806

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	108	Total	C	N	O	0	0	0
			835	526	165	144			
3	G	104	Total	C	N	O	0	0	0
			805	508	157	140			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P22752
C	-2	SER	-	expression tag	UNP P22752
C	-1	HIS	-	expression tag	UNP P22752
G	-3	GLY	-	expression tag	UNP P22752
G	-2	SER	-	expression tag	UNP P22752
G	-1	HIS	-	expression tag	UNP P22752

- Molecule 4 is a protein called Histone H2B type 3-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	94	Total	C	N	O	S	0	0	0
			736	461	134	139	2			
4	H	92	Total	C	N	O	S	0	0	0
			721	453	129	137	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP Q9D2U9
D	-2	SER	-	expression tag	UNP Q9D2U9
D	-1	HIS	-	expression tag	UNP Q9D2U9
H	-3	GLY	-	expression tag	UNP Q9D2U9
H	-2	SER	-	expression tag	UNP Q9D2U9
H	-1	HIS	-	expression tag	UNP Q9D2U9

- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			
5	J	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			

- Molecule 6 is water.

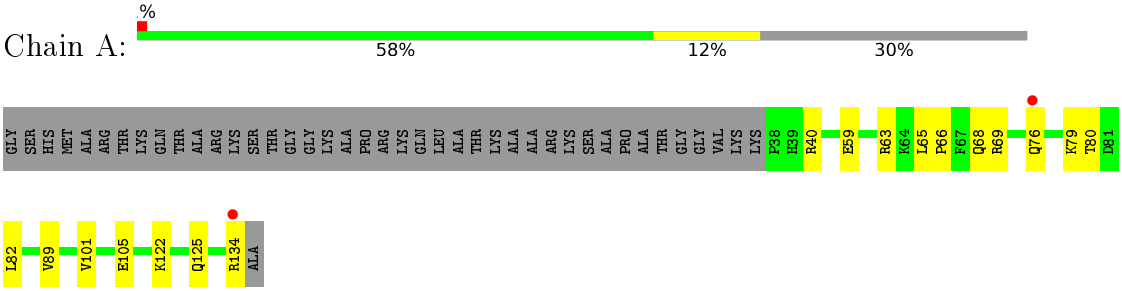
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	C	12	Total O 12 12	0	0
6	D	7	Total O 7 7	0	0
6	E	16	Total O 16 16	0	0
6	F	11	Total O 11 11	0	0
6	G	4	Total O 4 4	0	0
6	H	4	Total O 4 4	0	0
6	I	11	Total O 11 11	0	0
6	J	13	Total O 13 13	0	0

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 (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.

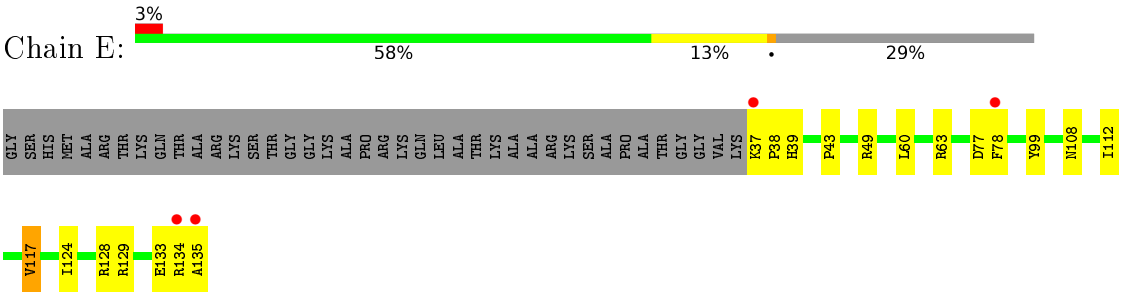
- Molecule 1: Histone H3.1

Chain A:



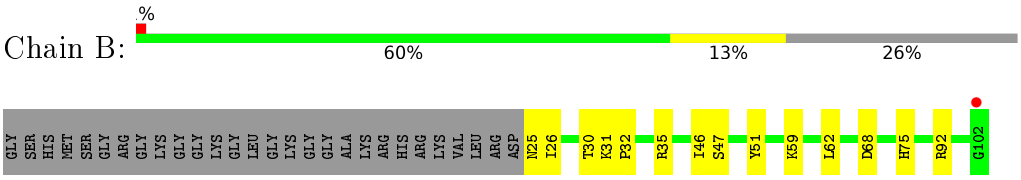
- Molecule 1: Histone H3.1

Chain E:



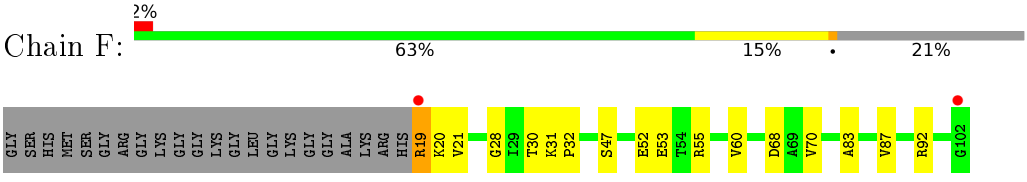
- Molecule 2: Histone H4

Chain B:



- Molecule 2: Histone H4

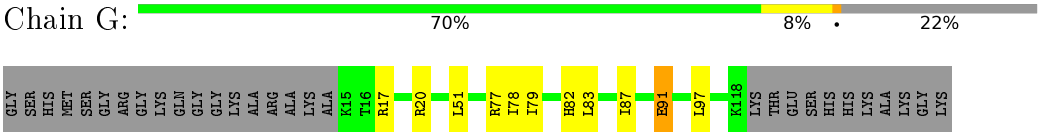
Chain F:



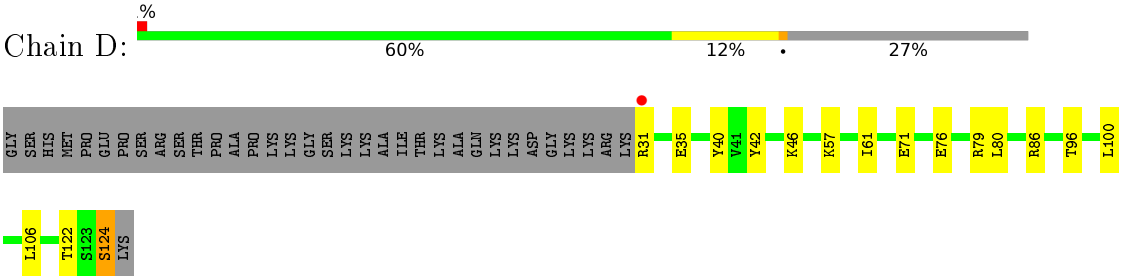
- Molecule 3: Histone H2A type 1

Chain C:

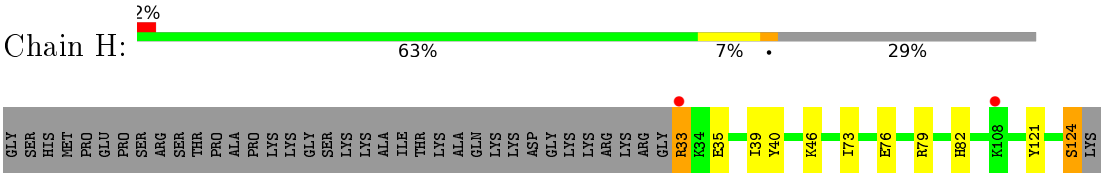
• Molecule 3: Histone H2A type 1



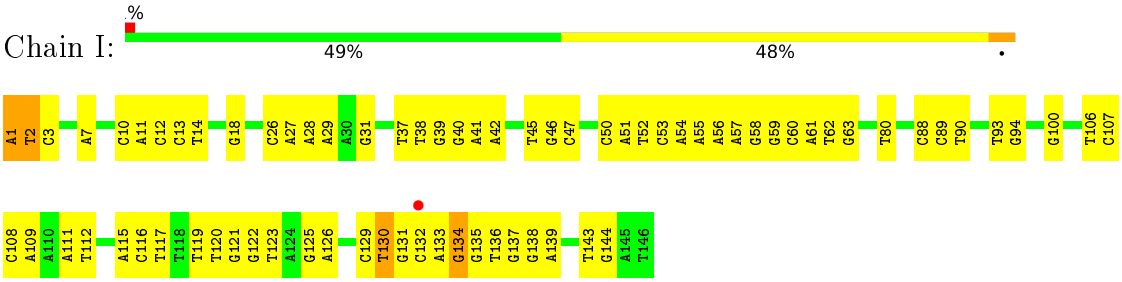
• Molecule 4: Histone H2B type 3-A



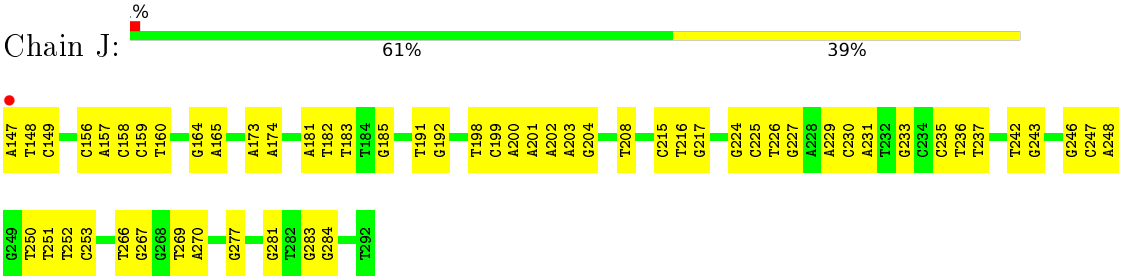
• Molecule 4: Histone H2B type 3-A



• Molecule 5: DNA (146-MER)



• Molecule 5: DNA (146-MER)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.72Å 107.66Å 168.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.59 – 2.34 49.76 – 2.33	Depositor EDS
% Data completeness (in resolution range)	96.2 (39.59-2.34) 94.0 (49.76-2.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.211 , 0.259 0.210 , 0.258	Depositor DCC
R_{free} test set	3640 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 27.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12071	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.41	0/813	0.60	0/1090
1	E	0.57	0/828	0.67	0/1109
2	B	0.45	0/626	0.65	0/837
2	F	0.57	1/680 (0.1%)	0.72	1/908 (0.1%)
3	C	0.45	0/845	0.62	0/1139
3	G	0.51	2/815 (0.2%)	0.59	0/1100
4	D	0.46	0/747	0.57	0/1004
4	H	0.47	0/732	0.55	0/985
5	I	0.92	1/3354 (0.0%)	1.07	8/5175 (0.2%)
5	J	0.87	0/3354	1.06	4/5175 (0.1%)
All	All	0.73	4/12794 (0.0%)	0.90	13/18522 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	19	ARG	NE-CZ	-5.86	1.25	1.33
3	G	91	GLU	CD-OE1	-5.65	1.19	1.25
3	G	91	GLU	CD-OE2	-5.39	1.19	1.25
5	I	130	DT	C1'-N1	5.11	1.55	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	19	ARG	NE-CZ-NH1	-6.79	116.91	120.30
5	J	233	DG	O4'-C1'-N9	6.38	112.47	108.00
5	I	139	DA	O4'-C4'-C3'	-6.25	102.00	104.50
5	I	119	DT	O4'-C1'-N1	-6.09	103.74	108.00
5	J	224	DG	O4'-C1'-N9	-5.98	103.81	108.00
5	I	134	DG	O4'-C1'-N9	5.75	112.03	108.00
5	J	208	DT	O5'-P-OP2	-5.58	100.68	105.70
5	I	130	DT	N3-C4-O4	5.44	123.16	119.90
5	J	281	DG	O4'-C4'-C3'	-5.29	102.38	104.50
5	I	2	DT	N3-C4-O4	5.11	122.97	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1	DA	C1'-O4'-C4'	-5.09	105.00	110.10
5	I	130	DT	C5-C4-O4	-5.04	121.37	124.90
5	I	1	DA	O4'-C1'-N9	5.02	111.51	108.00

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	801	0	839	10	0
1	E	816	0	856	24	0
2	B	619	0	659	11	0
2	F	673	0	722	12	0
3	C	835	0	897	15	0
3	G	805	0	861	10	0
4	D	736	0	756	15	0
4	H	721	0	740	8	0
5	I	2990	0	1652	73	0
5	J	2990	0	1652	46	0
6	A	7	0	0	0	0
6	C	12	0	0	0	0
6	D	7	0	0	1	0
6	E	16	0	0	1	0
6	F	11	0	0	0	0
6	G	4	0	0	0	0
6	H	4	0	0	0	0
6	I	11	0	0	3	0
6	J	13	0	0	2	0
All	All	12071	0	9634	190	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 9.

All (190) 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)
2:F:68:ASP:OD2	2:F:92:ARG:NH1	2.01	0.93
5:I:134:DG:H1	5:J:159:DC:H42	1.23	0.87
3:C:11:ARG:HH12	5:I:31:DG:H4'	1.42	0.85
5:I:45:DT:H2'	5:I:46:DG:C8	2.16	0.81
5:I:100:DG:N7	6:I:202:HOH:O	2.12	0.80
5:I:115:DA:H2"	5:I:116:DC:H5"	1.64	0.79
2:B:35:ARG:NH1	2:B:51:TYR:OH	2.16	0.78
4:H:76:GLU:OE1	4:H:79:ARG:NH1	2.17	0.77
1:E:77:ASP:OD2	6:E:201:HOH:O	2.01	0.76
4:D:76:GLU:OE2	4:D:79:ARG:NH1	2.19	0.75
5:J:266:DT:H2"	5:J:267:DG:C8	2.21	0.75
3:C:11:ARG:HH12	5:I:31:DG:C4'	1.99	0.75
5:I:130:DT:H2"	5:I:131:DG:C8	2.22	0.74
5:I:134:DG:N2	5:J:159:DC:N3	2.35	0.74
2:B:75:HIS:CD2	4:D:96:THR:HG21	2.23	0.73
5:J:191:DT:H2"	5:J:192:DG:C8	2.24	0.73
5:I:108:DC:H2"	5:I:109:DA:N7	2.03	0.72
5:J:266:DT:H2"	5:J:267:DG:N7	2.04	0.71
4:D:71:GLU:OE1	6:D:201:HOH:O	2.08	0.71
5:I:38:DT:H2"	5:I:39:DG:C8	2.26	0.70
5:J:173:DA:H2"	5:J:174:DA:C8	2.26	0.70
1:A:40:ARG:NH2	5:J:229:DA:N3	2.41	0.69
5:I:51:DA:H2"	5:I:52:DT:H5"	1.75	0.68
4:D:80:LEU:HD13	4:D:96:THR:HG23	1.77	0.67
5:J:156:DC:H2"	5:J:157:DA:N7	2.10	0.67
5:I:80:DT:OP2	6:I:201:HOH:O	2.11	0.67
1:E:43:PRO:HG2	5:J:215:DC:H5'	1.76	0.66
5:I:89:DC:H2"	5:I:90:DT:H71	1.77	0.65
5:J:158:DC:H2"	5:J:159:DC:H5"	1.79	0.64
5:I:143:DT:H2"	5:I:144:DG:C8	2.33	0.63
5:I:134:DG:H1'	5:I:135:DG:N7	2.12	0.63
5:J:181:DA:H2"	5:J:182:DT:H5"	1.81	0.63
5:J:147:DA:H8	5:J:148:DT:H72	1.63	0.62
5:I:1:DA:H4'	5:I:2:DT:C2	2.34	0.62
1:E:63:ARG:HH21	2:F:30:THR:HG23	1.66	0.61
3:C:84:GLN:HG3	3:C:105:GLY:HA3	1.83	0.60
3:C:11:ARG:HH11	3:C:11:ARG:HG3	1.67	0.60
1:E:128:ARG:HH22	1:E:134:ARG:CZ	2.15	0.60
5:I:136:DT:H2'	5:I:137:DG:C4	2.36	0.60
5:I:40:DG:H2"	5:I:41:DA:C8	2.36	0.59
5:I:111:DA:H2"	5:I:112:DT:H5'	1.83	0.59
5:I:18:DG:N7	6:I:204:HOH:O	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ARG:HH11	5:I:90:DT:H5"	1.67	0.59
5:J:185:DG:N7	6:J:302:HOH:O	2.31	0.59
5:J:164:DG:H2"	5:J:165:DA:H5"	1.85	0.58
3:G:87:ILE:HD12	3:G:97:LEU:HD12	1.84	0.58
5:J:147:DA:C8	5:J:148:DT:H72	2.39	0.58
1:A:76:GLN:HG3	1:A:80:THR:HA	1.84	0.58
5:I:47:DC:H42	5:J:246:DG:H1	1.51	0.57
3:C:11:ARG:NH1	5:I:31:DG:H4'	2.17	0.57
5:I:37:DT:H1'	5:I:38:DT:H5'	1.87	0.56
5:J:216:DT:H2"	5:J:217:DG:C8	2.40	0.56
5:I:108:DC:H2"	5:I:109:DA:C5	2.41	0.56
5:J:250:DT:H2'	5:J:251:DT:H71	1.86	0.56
5:I:60:DC:H2"	5:I:61:DA:C8	2.41	0.56
5:I:10:DC:H2"	5:I:11:DA:H8	1.71	0.55
5:J:283:DG:H1'	5:J:284:DG:C8	2.41	0.55
5:I:120:DT:H2"	5:I:121:DG:C8	2.42	0.55
5:I:1:DA:H4'	5:I:2:DT:N1	2.22	0.54
5:I:58:DG:H2"	5:I:59:DG:C8	2.42	0.54
5:I:131:DG:H2"	5:I:132:DC:C5	2.43	0.54
2:F:83:ALA:O	2:F:87:VAL:HG23	2.08	0.54
5:J:252:DT:H2"	5:J:253:DC:C6	2.43	0.53
5:J:277:DG:H5"	5:J:277:DG:H8	1.73	0.53
5:I:115:DA:C2'	5:I:116:DC:H5"	2.36	0.53
1:E:63:ARG:NH1	5:I:90:DT:H5"	2.24	0.53
5:I:12:DC:H2'	5:I:13:DC:C6	2.43	0.53
2:B:26:ILE:HD12	2:B:59:LYS:HD2	1.91	0.53
3:G:77:ARG:HH11	3:G:77:ARG:HB3	1.73	0.53
1:E:108:ASN:O	1:E:112:ILE:HG12	2.10	0.52
4:H:33:ARG:NH2	4:H:35:GLU:OE1	2.39	0.52
1:E:124:ILE:O	1:E:128:ARG:HG3	2.10	0.52
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.45	0.51
3:C:11:ARG:HG3	3:C:11:ARG:NH1	2.25	0.51
2:B:68:ASP:OD2	2:B:92:ARG:NH2	2.44	0.51
5:J:242:DT:H2"	5:J:243:DG:H5"	1.92	0.51
5:I:62:DT:H2"	5:I:63:DG:C8	2.46	0.50
5:J:230:DC:H2"	5:J:231:DA:C8	2.46	0.50
5:I:125:DG:H2'	5:I:126:DA:C8	2.46	0.50
5:J:201:DA:H2"	5:J:202:DA:C8	2.46	0.50
1:A:69:ARG:HD2	2:B:25:ASN:OD1	2.11	0.50
1:E:37:LYS:HB2	1:E:38:PRO:C	2.32	0.50
5:I:122:DG:H1'	5:I:123:DT:H5'	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LYS:HD3	1:A:82:LEU:HG	1.94	0.49
5:I:134:DG:H1'	5:I:135:DG:C8	2.47	0.49
1:A:125:GLN:CA	1:A:134:ARG:HH22	2.26	0.49
2:B:31:LYS:O	2:B:35:ARG:HG3	2.13	0.49
4:D:57:LYS:O	4:D:61:ILE:HG12	2.13	0.49
1:E:124:ILE:HD12	2:F:53:GLU:HG2	1.94	0.49
5:J:277:DG:C8	5:J:277:DG:H5"	2.46	0.49
1:A:65:LEU:HD12	1:A:69:ARG:HH21	1.77	0.49
3:C:115:LEU:HD23	1:E:117:VAL:HG22	1.95	0.49
1:E:129:ARG:HG3	1:E:135:ALA:HA	1.92	0.49
4:D:122:THR:C	4:D:124:SER:H	2.16	0.49
1:E:99:TYR:OH	1:E:133:GLU:OE1	2.27	0.49
3:C:84:GLN:HG3	3:C:105:GLY:CA	2.42	0.48
5:J:191:DT:H2"	5:J:192:DG:N7	2.27	0.48
2:B:92:ARG:HH21	4:D:100:LEU:HD22	1.78	0.48
5:I:111:DA:H2'	5:I:112:DT:C6	2.48	0.48
5:I:136:DT:H2'	5:I:137:DG:N9	2.28	0.48
2:B:46:ILE:O	5:J:227:DG:H3'	2.14	0.48
5:I:56:DA:H2"	5:I:57:DA:C8	2.48	0.48
5:I:38:DT:H2"	5:I:39:DG:N7	2.29	0.48
5:J:235:DC:H2"	5:J:236:DT:H71	1.95	0.48
5:I:10:DC:H2"	5:I:11:DA:C8	2.49	0.47
1:E:63:ARG:NH2	2:F:28:GLY:O	2.47	0.47
2:F:31:LYS:HB3	2:F:32:PRO:HD3	1.96	0.47
5:J:217:DG:N7	6:J:304:HOH:O	2.35	0.47
1:A:68:GLN:HG3	1:A:89:VAL:HG11	1.97	0.47
5:J:269:DT:H2"	5:J:270:DA:C8	2.50	0.47
5:J:225:DC:H2"	5:J:226:DT:H71	1.96	0.47
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.50	0.47
4:D:31:ARG:HA	4:D:31:ARG:HD3	1.73	0.46
5:J:147:DA:H2"	5:J:148:DT:H72	1.98	0.46
3:C:38:ASN:ND2	4:H:82:HIS:NE2	2.62	0.46
1:A:101:VAL:O	1:A:105:GLU:HG3	2.15	0.46
2:B:62:LEU:HD23	2:B:62:LEU:HA	1.77	0.46
1:E:78:PHE:HD2	2:F:70:VAL:HG11	1.80	0.46
5:I:10:DC:H42	5:J:283:DG:H1	1.64	0.46
5:I:137:DG:H2"	5:I:138:DG:C8	2.51	0.46
5:I:11:DA:H2"	5:I:12:DC:H6	1.80	0.46
5:I:132:DC:H2"	5:I:133:DA:C8	2.51	0.46
5:J:247:DC:H2"	5:J:248:DA:C8	2.50	0.46
4:D:31:ARG:HD2	5:J:270:DA:H4'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ARG:NH2	2:F:30:THR:HG23	2.30	0.46
5:I:1:DA:H1'	5:I:2:DT:C4	2.51	0.46
3:C:83:LEU:O	3:C:87:ILE:HG12	2.16	0.45
3:G:78:ILE:HA	3:G:82:HIS:HD1	1.81	0.45
2:F:30:THR:HB	2:F:32:PRO:HD2	1.99	0.45
5:I:28:DA:H1'	5:I:29:DA:C8	2.51	0.45
1:E:37:LYS:HD3	1:E:39:HIS:HB2	1.99	0.45
2:F:20:LYS:HE2	2:F:21:VAL:H	1.82	0.45
4:D:42:TYR:CE1	4:D:46:LYS:HE3	2.51	0.44
3:G:51:LEU:HD13	4:H:73:ILE:HG21	1.99	0.44
5:I:52:DT:H2"	5:I:53:DC:H5'	1.99	0.44
5:I:93:DT:H1'	5:I:94:DG:H5'	1.99	0.44
2:F:52:GLU:OE2	2:F:55:ARG:NH1	2.51	0.44
5:I:52:DT:C2'	5:I:53:DC:H5'	2.47	0.44
2:B:30:THR:HB	2:B:32:PRO:HD2	2.00	0.44
5:I:40:DG:H2"	5:I:41:DA:N7	2.32	0.44
3:C:32:ARG:NH2	4:D:35:GLU:OE2	2.44	0.44
1:A:63:ARG:O	1:A:66:PRO:HD2	2.18	0.44
5:I:2:DT:C2	5:I:3:DC:C5	3.06	0.44
5:J:215:DC:H2"	5:J:216:DT:H71	2.00	0.44
3:G:91:GLU:H	3:G:91:GLU:HG3	1.51	0.43
5:I:116:DC:H2'	5:I:117:DT:H72	2.00	0.43
5:I:88:DC:H2"	5:I:89:DC:C6	2.53	0.43
5:J:158:DC:C2'	5:J:159:DC:H5"	2.48	0.43
5:I:131:DG:OP2	5:I:131:DG:H2'	2.19	0.43
5:I:13:DC:H2'	5:I:14:DT:H71	2.00	0.43
5:I:89:DC:H2"	5:I:90:DT:C7	2.44	0.43
5:J:203:DA:H2"	5:J:204:DG:C8	2.54	0.43
5:J:159:DC:H2"	5:J:160:DT:O5'	2.19	0.43
1:A:66:PRO:HG3	5:J:237:DT:OP1	2.19	0.43
3:G:83:LEU:O	3:G:87:ILE:HG12	2.19	0.43
5:I:136:DT:H2'	5:I:137:DG:C8	2.54	0.43
5:I:47:DC:H5"	5:I:47:DC:H6	1.82	0.43
5:I:54:DA:H2"	5:I:55:DA:C8	2.54	0.43
5:I:106:DT:H1'	5:I:107:DC:H5'	1.99	0.42
4:D:42:TYR:HE1	4:D:46:LYS:HE3	1.84	0.42
5:J:200:DA:H2"	5:J:201:DA:C8	2.55	0.42
1:E:134:ARG:HH21	2:F:60:VAL:HG11	1.83	0.42
5:J:182:DT:H2'	5:J:183:DT:C6	2.54	0.42
3:G:17:ARG:HG2	4:H:121:TYR:HE1	1.84	0.42
4:D:46:LYS:HA	4:D:46:LYS:HD3	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:GLU:O	1:E:134:ARG:HG2	2.20	0.42
4:H:46:LYS:HA	4:H:46:LYS:HD3	1.81	0.42
4:H:39:ILE:HG13	4:H:40:TYR:N	2.35	0.42
5:I:130:DT:H2"	5:I:131:DG:H8	1.78	0.41
5:I:50:DC:H2"	5:I:51:DA:H8	1.84	0.41
5:J:198:DT:H2"	5:J:199:DC:C6	2.55	0.41
5:I:26:DC:H2"	5:I:27:DA:N7	2.35	0.41
3:C:35:ARG:NH1	3:C:36:LYS:HE3	2.36	0.41
1:E:43:PRO:HG2	5:J:215:DC:C5'	2.47	0.41
5:I:132:DC:H2"	5:I:133:DA:H8	1.85	0.41
5:J:226:DT:H2"	5:J:227:DG:C8	2.56	0.41
5:I:133:DA:H2"	5:I:134:DG:O4'	2.20	0.41
3:G:20:ARG:HH11	4:H:124:SER:HB2	1.85	0.41
5:I:50:DC:H2"	5:I:51:DA:C8	2.55	0.41
5:I:41:DA:H2"	5:I:42:DA:H8	1.85	0.41
1:E:60:LEU:HD23	1:E:60:LEU:HA	1.88	0.41
5:I:129:DC:C2'	5:I:130:DT:H72	2.51	0.41
1:E:49:ARG:HD3	5:I:7:DA:O3'	2.21	0.41
3:C:26:PRO:HG3	4:D:40:TYR:CE2	2.56	0.40
2:B:92:ARG:HD3	4:D:76:GLU:OE2	2.20	0.40
5:I:134:DG:O3'	5:I:135:DG:H8	2.04	0.40
3:G:77:ARG:HB3	3:G:77:ARG:NH1	2.36	0.40
1:E:37:LYS:HE2	1:E:37:LYS:HB3	1.76	0.40
3:C:115:LEU:CD2	1:E:117:VAL:HG22	2.51	0.40
5:J:148:DT:H2"	5:J:149:DC:H5'	2.04	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	95/139 (68%)	92 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	97/139 (70%)	94 (97%)	3 (3%)	0	100	100
2	B	76/106 (72%)	72 (95%)	4 (5%)	0	100	100
2	F	82/106 (77%)	81 (99%)	1 (1%)	0	100	100
3	C	106/133 (80%)	104 (98%)	2 (2%)	0	100	100
3	G	102/133 (77%)	100 (98%)	2 (2%)	0	100	100
4	D	92/129 (71%)	88 (96%)	4 (4%)	0	100	100
4	H	90/129 (70%)	87 (97%)	3 (3%)	0	100	100
All	All	740/1014 (73%)	718 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	85/113 (75%)	83 (98%)	2 (2%)	57	69
1	E	86/113 (76%)	85 (99%)	1 (1%)	78	88
2	B	63/81 (78%)	62 (98%)	1 (2%)	70	82
2	F	69/81 (85%)	67 (97%)	2 (3%)	50	62
3	C	85/102 (83%)	84 (99%)	1 (1%)	78	88
3	G	83/102 (81%)	83 (100%)	0	100	100
4	D	81/110 (74%)	78 (96%)	3 (4%)	41	53
4	H	80/110 (73%)	78 (98%)	2 (2%)	55	68
All	All	632/812 (78%)	620 (98%)	12 (2%)	65	78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	122	LYS

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Mol	Chain	Res	Type
2	B	47	SER
3	C	11	ARG
4	D	86	ARG
4	D	106	LEU
4	D	124	SER
1	E	117	VAL
2	F	19	ARG
2	F	47	SER
4	H	33	ARG
4	H	124	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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, 95^{th} 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	97/139 (69%)	-0.06	2 (2%) 67 78	25, 37, 64, 76	0
1	E	99/139 (71%)	-0.15	4 (4%) 42 54	19, 28, 47, 65	0
2	B	78/106 (73%)	-0.05	1 (1%) 79 86	28, 38, 53, 63	0
2	F	84/106 (79%)	-0.21	2 (2%) 62 73	20, 27, 42, 70	0
3	C	108/133 (81%)	-0.24	0 100 100	21, 31, 50, 64	0
3	G	104/133 (78%)	-0.22	0 100 100	26, 36, 62, 73	0
4	D	94/129 (72%)	-0.25	1 (1%) 82 89	21, 32, 52, 70	0
4	H	92/129 (71%)	-0.04	2 (2%) 65 76	25, 36, 56, 73	0
5	I	146/146 (100%)	-0.37	1 (0%) 89 93	30, 58, 102, 106	0
5	J	146/146 (100%)	-0.33	1 (0%) 89 93	38, 60, 96, 109	0
All	All	1048/1306 (80%)	-0.21	14 (1%) 79 86	19, 38, 84, 109	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	147	DA	4.8
1	E	135	ALA	4.6
2	F	102	GLY	4.6
1	E	78	PHE	4.1
1	A	134	ARG	3.6
4	H	33	ARG	3.5
2	B	102	GLY	3.1
2	F	19	ARG	2.7
4	D	31	ARG	2.5
1	A	76	GLN	2.5
1	E	134	ARG	2.5
5	I	132	DC	2.2
1	E	37	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	H	108	LYS	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.