Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2016 – 01:20 AM EDT

PDB ID	:	5B32
Title	:	The crystal structure of the heterotypic H2AZ/H2A nucleosome with H3.3.
Authors	:	Horikoshi, N.; Taguchi, H.; Arimura, Y.; Kurumizaka, H.
Deposited on	:	2016-02-08
Resolution	:	2.35 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

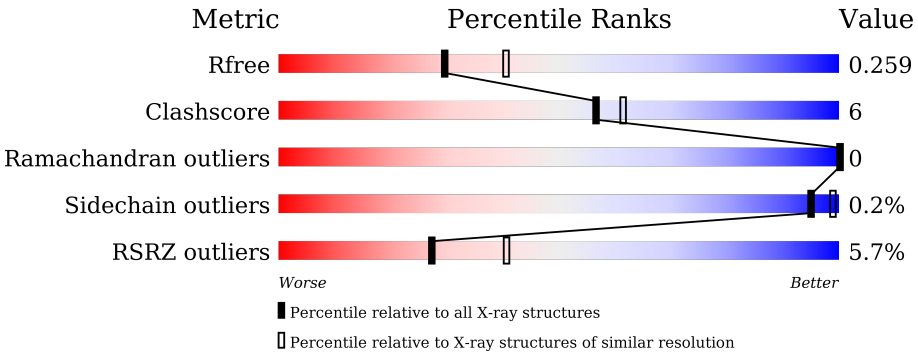
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	6% 60% 9% 30%
1	E	139	63% 8% 29%
2	B	106	65% 8% 26%
2	F	106	67% 11% 22%
3	C	133	3% 72% 9% 19%
4	D	129	68% 28%

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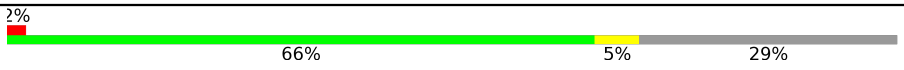
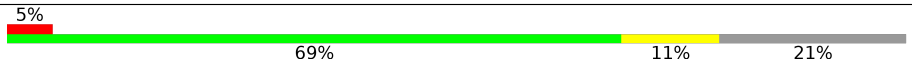
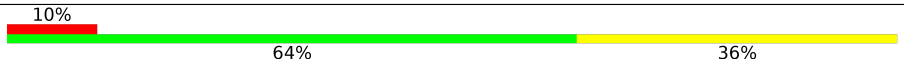
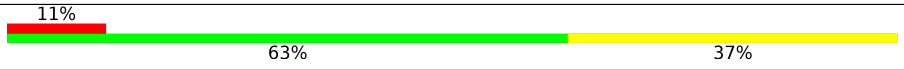
Mol	Chain	Length	Quality of chain
4	H	129	
5	G	131	
6	I	146	
6	J	146	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12022 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 H3.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			797	503	155	137	2			
1	E	98	Total	C	N	O	S	0	0	0
			803	506	156	139	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P84243
A	-2	SER	-	expression tag	UNP P84243
A	-1	HIS	-	expression tag	UNP P84243
E	-3	GLY	-	expression tag	UNP P84243
E	-2	SER	-	expression tag	UNP P84243
E	-1	HIS	-	expression tag	UNP P84243

- 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	83	Total	C	N	O	S	0	0	0
			668	422	132	113	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	108	Total	C	N	O	0	0	0
			835	526	165	144			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	93	Total	C	N	O	S	0	0	0
			725	456	130	137	2			
4	H	91	Total	C	N	O	S	0	0	0
			708	447	125	134	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P06899
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
H	-3	GLY	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899

- Molecule 5 is a protein called Histone H2A.Z.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	104	Total	C	N	O	0	0	0
			785	492	153	140			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP P0C0S5
G	-2	SER	-	expression tag	UNP P0C0S5
G	-1	HIS	-	expression tag	UNP P0C0S5

- Molecule 6 is a DNA chain called DNA (146-MER).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Cl	0	0
			1	1		
7	A	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	E	1	Total	Cl	0	0
			1	1		

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	4	Total	Mn	0	0
			4	4		
8	I	4	Total	Mn	0	0
			4	4		
8	D	1	Total	Mn	0	0
			1	1		
8	E	1	Total	Mn	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	6	Total	O	0	0
			6	6		
9	B	4	Total	O	0	0
			4	4		
9	C	7	Total	O	0	0
			7	7		
9	D	6	Total	O	0	0
			6	6		
9	E	17	Total	O	0	0
			17	17		

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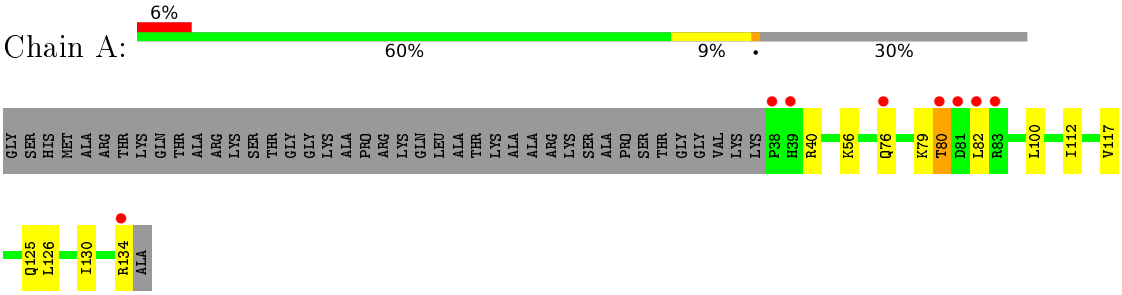
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	19	Total O 19 19	0	0
9	G	3	Total O 3 3	0	0
9	H	3	Total O 3 3	0	0
9	I	11	Total O 11 11	0	0
9	J	12	Total O 12 12	0	0

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.

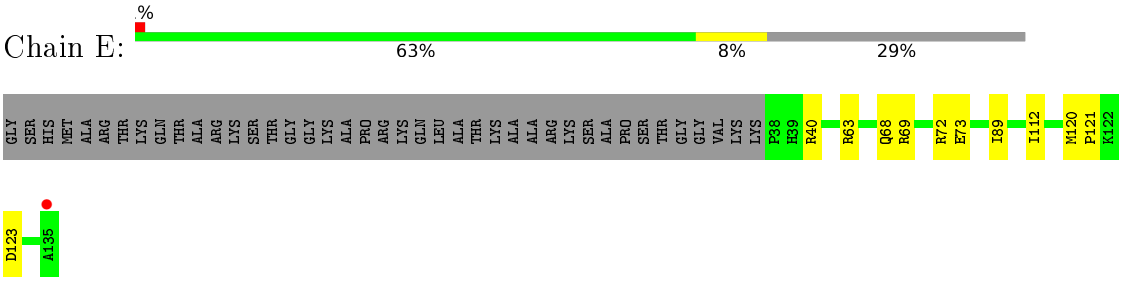
- Molecule 1: Histone H3.3

Chain A:



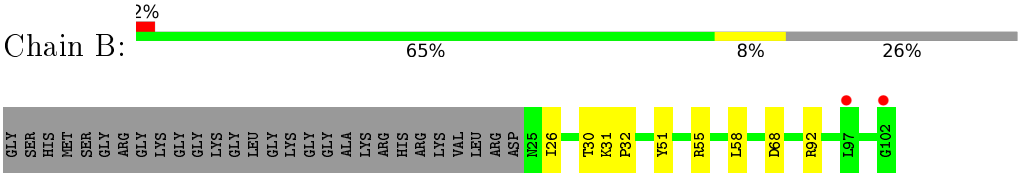
- Molecule 1: Histone H3.3

Chain E:



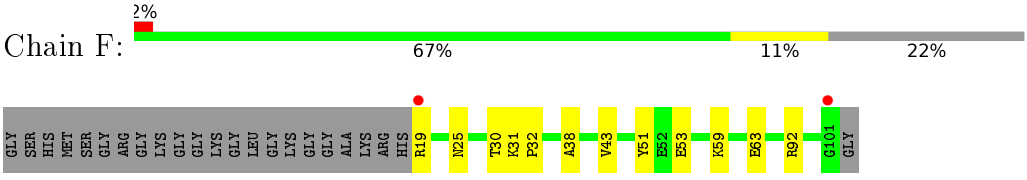
- Molecule 2: Histone H4

Chain B:



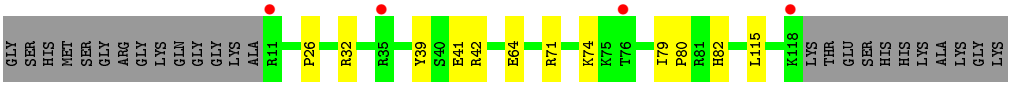
- Molecule 2: Histone H4

Chain F:



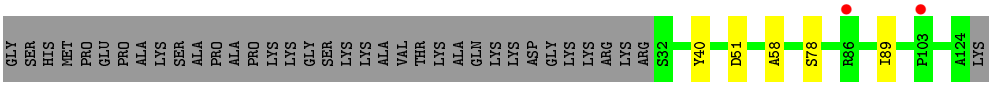
- Molecule 3: Histone H2A type 1-B/E

Chain C:



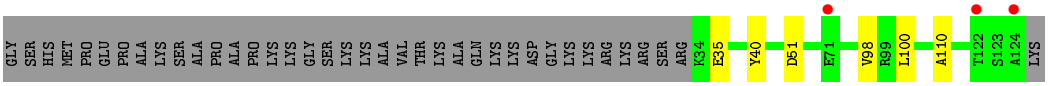
• Molecule 4: Histone H2B type 1-J

Chain D:



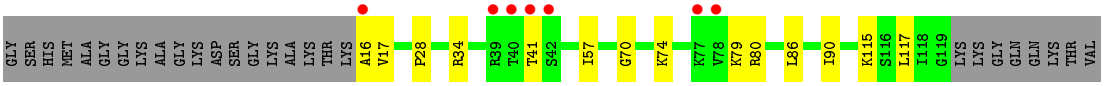
• Molecule 4: Histone H2B type 1-J

Chain H:



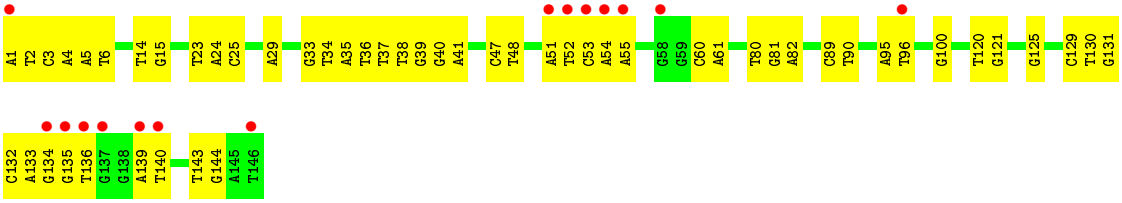
• Molecule 5: Histone H2A.Z

Chain G:



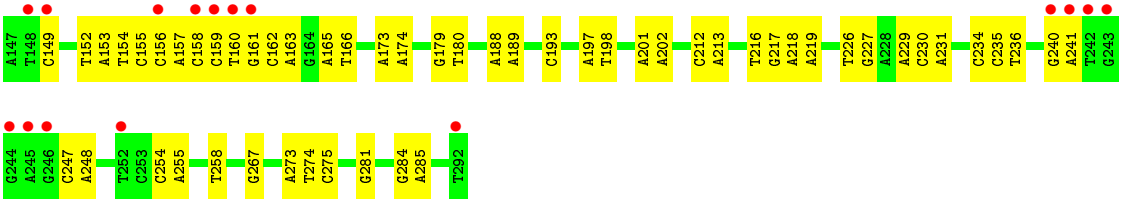
• Molecule 6: DNA (146-MER)

Chain I:



• Molecule 6: DNA (146-MER)

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.18Å 105.82Å 166.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.35 49.09 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.09-2.35) 99.0 (49.09-2.34)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.259 0.227 , 0.259	Depositor DCC
R_{free} test set	3646 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12022	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

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

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	0.21	0/809	0.36	0/1085
1	E	0.21	0/815	0.37	0/1092
2	B	0.20	0/626	0.39	0/837
2	F	0.20	0/675	0.39	0/903
3	C	0.20	0/845	0.37	0/1139
4	D	0.20	0/736	0.36	0/990
4	H	0.20	0/719	0.35	0/968
5	G	0.20	0/796	0.38	0/1073
6	I	0.48	0/3354	0.93	0/5175
6	J	0.49	0/3354	0.94	1/5175 (0.0%)
All	All	0.38	0/12729	0.74	1/18437 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	281	DG	O4'-C4'-C3'	-5.03	102.49	104.50

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	797	0	835	9	0
1	E	803	0	840	9	0
2	B	619	0	659	5	0
2	F	668	0	719	8	0
3	C	835	0	897	12	0
4	D	725	0	745	5	0
4	H	708	0	727	7	0
5	G	785	0	827	16	0
6	I	2990	0	1652	45	0
6	J	2990	0	1652	38	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
8	D	1	0	0	0	1
8	E	1	0	0	0	1
8	I	4	0	0	0	0
8	J	4	0	0	0	0
9	A	6	0	0	0	0
9	B	4	0	0	0	0
9	C	7	0	0	1	0
9	D	6	0	0	0	0
9	E	17	0	0	0	0
9	F	19	0	0	0	0
9	G	3	0	0	0	0
9	H	3	0	0	0	0
9	I	11	0	0	0	0
9	J	12	0	0	0	0
All	All	12022	0	9553	121	1

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 (121) 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)
5:G:74:LYS:NZ	4:H:51:ASP:OD2	1.85	1.08
5:G:115:LYS:HD2	5:G:115:LYS:H	1.28	0.98
6:I:144:DG:H1	6:J:149:DC:H42	1.22	0.86
3:C:64:GLU:OE2	9:C:301:HOH:O	2.03	0.76
3:C:32:ARG:NH1	6:I:29:DA:OP1	2.19	0.75
5:G:79:LYS:NZ	4:H:51:ASP:O	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:179:DG:H2"	6:J:180:DT:H5"	1.69	0.73
6:I:2:DT:H2"	6:I:3:DC:H5"	1.71	0.72
5:G:34:ARG:NH2	4:H:35:GLU:OE2	2.17	0.72
6:I:139:DA:H2"	6:I:140:DT:H5"	1.71	0.71
1:E:68:GLN:HG2	1:E:89:ILE:HG21	1.74	0.70
6:I:95:DA:H2"	6:I:96:DT:H5"	1.75	0.69
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.26	0.69
2:F:19:ARG:HD2	6:J:198:DT:H5"	1.76	0.68
1:A:79:LYS:HE3	1:A:82:LEU:HD21	1.76	0.67
1:E:69:ARG:NH2	6:I:90:DT:OP2	2.26	0.67
5:G:115:LYS:N	5:G:115:LYS:HD2	2.06	0.66
5:G:115:LYS:H	5:G:115:LYS:CD	2.07	0.65
2:F:92:ARG:NH2	4:H:100:LEU:O	2.27	0.65
6:I:51:DA:H2"	6:I:52:DT:H5"	1.79	0.64
6:J:153:DA:H2"	6:J:154:DT:H5"	1.78	0.64
6:I:25:DC:N4	6:J:267:DG:O6	2.31	0.63
6:I:131:DG:H1	6:J:162:DC:H42	1.46	0.63
6:I:134:DG:H2"	6:I:135:DG:H5'	1.80	0.63
6:J:226:DT:H2"	6:J:227:DG:C8	2.34	0.62
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.83	0.60
6:J:201:DA:H2"	6:J:202:DA:C8	2.39	0.57
6:J:274:DT:H1'	6:J:275:DC:H5'	1.86	0.57
1:E:40:ARG:NH2	6:I:82:DA:N3	2.54	0.56
1:A:117:VAL:HG13	5:G:117:LEU:HD22	1.87	0.56
6:I:52:DT:H1'	6:I:53:DC:H5'	1.88	0.56
6:I:14:DT:H2"	6:I:15:DG:C8	2.42	0.55
6:I:38:DT:H2"	6:I:39:DG:C8	2.41	0.55
1:E:73:GLU:OE1	2:F:25:ASN:ND2	2.36	0.55
6:J:165:DA:H2"	6:J:166:DT:H5"	1.89	0.55
6:I:3:DC:H2"	6:I:4:DA:C8	2.41	0.55
6:I:36:DT:H2"	6:I:37:DT:H5"	1.88	0.54
6:I:40:DG:H2"	6:I:41:DA:H5'	1.90	0.54
6:J:152:DT:H2"	6:J:153:DA:C8	2.43	0.54
6:J:155:DC:H2"	6:J:156:DC:H5'	1.88	0.54
6:J:152:DT:H2"	6:J:153:DA:H5'	1.90	0.53
5:G:57:ILE:HG13	4:H:110:ALA:HB1	1.92	0.52
6:J:218:DA:H2"	6:J:219:DA:H5"	1.91	0.52
6:J:160:DT:H2"	6:J:161:DG:C8	2.46	0.51
6:I:23:DT:H2"	6:I:24:DA:H5"	1.91	0.51
6:I:131:DG:H2"	6:I:132:DC:C6	2.46	0.51
1:A:112:ILE:HD11	5:G:117:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:GLU:OE2	5:G:41:THR:HB	2.11	0.49
6:I:130:DT:H2"	6:I:131:DG:C8	2.46	0.49
6:J:273:DA:H2"	6:J:274:DT:H5"	1.94	0.49
1:A:126:LEU:O	1:A:130:ILE:HG12	2.13	0.49
6:J:254:DC:H2"	6:J:255:DA:N7	2.28	0.49
6:I:80:DT:H2"	6:I:81:DG:C8	2.48	0.48
3:C:80:PRO:HD3	4:D:58:ALA:HB2	1.94	0.48
2:F:31:LYS:HG3	2:F:51:TYR:CE1	2.48	0.48
6:I:60:DC:H2"	6:I:61:DA:C8	2.48	0.48
5:G:80:ARG:N	6:I:131:DG:OP1	2.44	0.48
6:I:54:DA:H2"	6:I:55:DA:C8	2.49	0.48
6:I:129:DC:H2"	6:I:130:DT:C5	2.49	0.48
6:J:216:DT:H2"	6:J:217:DG:C8	2.50	0.47
3:C:42:ARG:NH1	6:J:258:DT:H4'	2.29	0.47
6:I:14:DT:H2"	6:I:15:DG:N7	2.30	0.47
3:C:115:LEU:HD21	1:E:112:ILE:HD11	1.97	0.47
5:G:16:ALA:HB1	5:G:17:VAL:HG22	1.97	0.47
1:A:76:GLN:HG2	1:A:80:THR:HA	1.97	0.47
2:B:30:THR:HB	2:B:32:PRO:HD2	1.97	0.47
3:C:71:ARG:NH2	4:D:51:ASP:OD2	2.48	0.47
6:J:157:DA:H2"	6:J:158:DC:C5	2.50	0.47
6:J:248:DA:H5"	6:J:248:DA:H8	1.80	0.46
6:I:90:DT:O4	6:J:202:DA:N6	2.49	0.46
6:I:33:DG:H2'	6:I:34:DT:C6	2.51	0.46
6:I:89:DC:H2"	6:I:90:DT:H71	1.97	0.45
2:B:26:ILE:HG13	2:B:55:ARG:HB3	1.99	0.45
6:J:157:DA:H2"	6:J:158:DC:H5	1.82	0.45
6:I:100:DG:N2	6:J:193:DC:O2	2.49	0.45
2:F:59:LYS:HD3	2:F:63:GLU:OE2	2.16	0.45
6:I:135:DG:H2"	6:I:136:DT:C6	2.51	0.45
6:I:34:DT:H2'	6:I:35:DA:C8	2.53	0.44
6:J:234:DC:H1'	6:J:235:DC:H5'	1.98	0.44
5:G:86:LEU:O	5:G:90:ILE:HG12	2.17	0.44
6:I:39:DG:H1	6:J:254:DC:H42	1.63	0.44
6:I:143:DT:H2"	6:I:144:DG:C8	2.52	0.44
6:I:133:DA:H2'	6:I:134:DG:O4'	2.17	0.44
3:C:71:ARG:HE	3:C:71:ARG:HB2	1.63	0.44
6:I:131:DG:H2"	6:I:132:DC:C5	2.53	0.44
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.53	0.44
6:I:39:DG:H2"	6:I:40:DG:C8	2.53	0.44
6:J:162:DC:H2"	6:J:163:DA:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:235:DC:H2"	6:J:236:DT:C5	2.52	0.43
1:E:72:ARG:HH22	6:J:197:DA:P	2.41	0.43
3:C:26:PRO:HD3	4:D:40:TYR:CD1	2.54	0.43
1:E:63:ARG:HD2	6:I:90:DT:H4'	1.99	0.43
2:B:31:LYS:HG3	2:B:51:TYR:CE1	2.53	0.43
6:I:120:DT:H2"	6:I:121:DG:C8	2.53	0.43
6:I:125:DG:H5'	6:I:125:DG:C8	2.53	0.43
6:I:125:DG:H5'	6:I:125:DG:H8	1.84	0.43
6:I:47:DC:H2"	6:I:48:DT:C6	2.54	0.43
1:A:40:ARG:NH2	6:J:229:DA:N3	2.66	0.43
6:I:1:DA:H2"	6:I:2:DT:H5"	2.00	0.42
6:J:188:DA:H2"	6:J:189:DA:C8	2.54	0.42
3:C:74:LYS:N	3:C:74:LYS:HD2	2.35	0.42
6:J:240:DG:H2"	6:J:241:DA:O5'	2.19	0.42
5:G:70:GLY:O	5:G:74:LYS:HG3	2.20	0.42
5:G:57:ILE:HG12	4:H:98:VAL:HG21	2.01	0.42
6:J:212:DC:H2"	6:J:213:DA:C8	2.55	0.42
3:C:39:TYR:HB3	4:D:78:SER:HB2	2.02	0.42
1:E:120:MET:N	1:E:123:ASP:OD2	2.51	0.42
2:F:30:THR:HB	2:F:32:PRO:HD2	2.02	0.41
6:I:47:DC:H2"	6:I:48:DT:C5	2.55	0.41
1:A:125:GLN:HG2	1:A:134:ARG:HH22	1.85	0.41
2:F:38:ALA:HB1	2:F:43:VAL:HB	2.03	0.41
6:J:247:DC:H2"	6:J:248:DA:C8	2.56	0.41
1:A:100:LEU:HD11	2:B:58:LEU:HD13	2.03	0.41
5:G:28:PRO:HD3	4:H:40:TYR:CG	2.56	0.41
6:J:158:DC:H2'	6:J:159:DC:O4'	2.21	0.41
6:J:230:DC:H2"	6:J:231:DA:C8	2.55	0.41
1:A:56:LYS:HE3	1:A:56:LYS:HB2	1.91	0.41
4:D:78:SER:HA	4:D:89:ILE:HD11	2.02	0.41
6:I:5:DA:H2"	6:I:6:DT:H5'	2.03	0.40
6:J:173:DA:H2"	6:J:174:DA:C8	2.56	0.40
6:J:284:DG:H2"	6:J:285:DA:C8	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:301:MN:MN	8:E:301:MN:MN[3_544]	0.87	1.33

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%)	94 (99%)	1 (1%)	0	100	100
1	E	96/139 (69%)	96 (100%)	0	0	100	100
2	B	76/106 (72%)	73 (96%)	3 (4%)	0	100	100
2	F	81/106 (76%)	79 (98%)	2 (2%)	0	100	100
3	C	106/133 (80%)	105 (99%)	1 (1%)	0	100	100
4	D	91/129 (70%)	89 (98%)	2 (2%)	0	100	100
4	H	89/129 (69%)	88 (99%)	1 (1%)	0	100	100
5	G	102/131 (78%)	98 (96%)	4 (4%)	0	100	100
All	All	736/1012 (73%)	722 (98%)	14 (2%)	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	83/112 (74%)	82 (99%)	1 (1%)	78	89
1	E	83/112 (74%)	83 (100%)	0	100	100
2	B	63/81 (78%)	63 (100%)	0	100	100
2	F	69/81 (85%)	69 (100%)	0	100	100
3	C	85/102 (83%)	85 (100%)	0	100	100
4	D	79/107 (74%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	H	77/107 (72%)	77 (100%)	0	100 100
5	G	81/99 (82%)	81 (100%)	0	100 100
All	All	620/801 (77%)	619 (100%)	1 (0%)	95 99

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	THR

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

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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%)	0.61	8 (8%) 14 23	26, 40, 74, 88	0
1	E	98/139 (70%)	0.31	1 (1%) 84 92	20, 30, 47, 72	0
2	B	78/106 (73%)	0.42	2 (2%) 59 71	27, 37, 53, 67	0
2	F	83/106 (78%)	0.46	2 (2%) 62 74	18, 29, 43, 64	0
3	C	108/133 (81%)	0.40	4 (3%) 45 59	25, 36, 57, 78	0
4	D	93/129 (72%)	0.48	2 (2%) 65 77	25, 36, 54, 63	0
4	H	91/129 (70%)	0.64	3 (3%) 50 63	25, 36, 56, 68	0
5	G	104/131 (79%)	0.69	7 (6%) 21 31	26, 40, 65, 74	0
6	I	146/146 (100%)	0.44	15 (10%) 9 15	30, 62, 109, 121	0
6	J	146/146 (100%)	0.46	16 (10%) 7 12	37, 64, 113, 122	0
All	All	1044/1304 (80%)	0.49	60 (5%) 27 41	18, 41, 91, 122	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	G	16	ALA	11.9
6	I	54	DA	6.4
6	I	139	DA	5.1
1	A	81	ASP	4.7
1	A	38	PRO	4.5
3	C	11	ARG	4.4
6	J	149	DC	4.3
6	J	292	DT	4.2
6	I	135	DG	4.2
6	J	241	DA	4.2
6	I	53	DC	4.1
5	G	42	SER	4.1
6	I	146	DT	4.0

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Mol	Chain	Res	Type	RSRZ
6	J	158	DC	3.9
6	J	243	DG	3.8
2	F	19	ARG	3.7
6	I	134	DG	3.5
5	G	77	LYS	3.5
6	J	159	DC	3.5
6	I	137	DG	3.4
5	G	40	THR	3.4
6	J	148	DT	3.3
1	A	82	LEU	3.3
1	A	83	ARG	3.2
3	C	118	LYS	3.2
6	I	52	DT	3.2
6	I	96	DT	3.2
1	A	80	THR	3.1
5	G	78	VAL	3.0
6	J	156	DC	2.9
6	I	58	DG	2.8
6	J	240	DG	2.7
6	J	246	DG	2.7
6	J	244	DG	2.7
2	F	101	GLY	2.7
3	C	35	ARG	2.6
1	A	76	GLN	2.6
1	E	135	ALA	2.6
6	I	1	DA	2.6
6	I	140	DT	2.6
4	H	71	GLU	2.6
1	A	39	HIS	2.5
4	H	124	ALA	2.5
4	D	103	PRO	2.5
5	G	41	THR	2.4
4	H	122	THR	2.3
6	J	161	DG	2.3
6	I	55	DA	2.3
5	G	39	ARG	2.3
2	B	102	GLY	2.2
6	J	245	DA	2.2
1	A	134	ARG	2.2
6	J	252	DT	2.2
4	D	86	ARG	2.1
6	J	160	DT	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	97	LEU	2.1
6	I	51	DA	2.0
6	I	136	DT	2.0
6	J	242	DT	2.0
3	C	76	THR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	CL	G	301	1/1	0.97	0.08	-1.78	40,40,40,40	0
7	CL	C	201	1/1	0.98	0.10	-2.15	42,42,42,42	0
8	MN	I	302	1/1	0.53	0.10	-2.86	80,80,80,80	0
8	MN	E	301	1/1	0.98	0.03	-5.24	59,59,59,59	0
8	MN	D	301	1/1	0.98	0.03	-5.60	55,55,55,55	0
8	MN	I	303	1/1	0.96	0.18	-	69,69,69,69	0
8	MN	J	401	1/1	0.90	0.15	-	67,67,67,67	0
8	MN	I	301	1/1	0.97	0.09	-	48,48,48,48	0
8	MN	J	403	1/1	0.79	0.15	-	63,63,63,63	0
8	MN	I	304	1/1	0.94	0.18	-	57,57,57,57	0
7	CL	A	301	1/1	0.99	0.16	-	54,54,54,54	0
7	CL	E	302	1/1	0.98	0.04	-	43,43,43,43	0
8	MN	J	404	1/1	0.98	0.06	-	92,92,92,92	0
8	MN	J	402	1/1	0.95	0.17	-	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.