Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2016 – 01:35 AM EDT

PDB ID	:	5B33
Title	:	The crystal structure of the H2AZ nucleosome with H3.3.
Authors	:	Horikoshi, N.; Taguchi, H.; Arimura, Y.; Kurumizaka, H.
Deposited on	:	2016-02-08
Resolution	:	2.92 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:

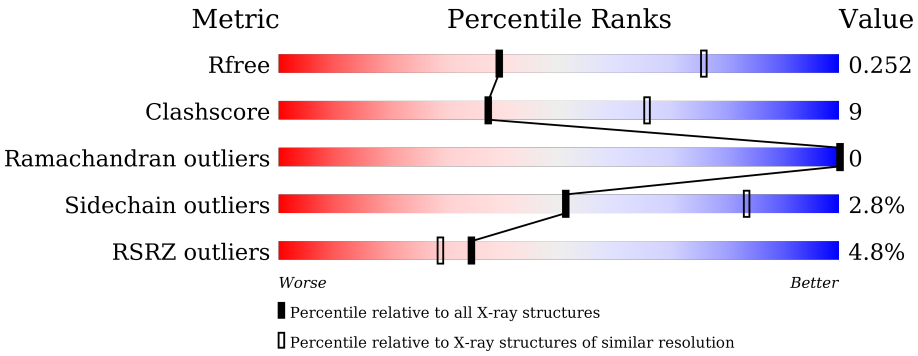
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.92 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	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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	63% 7% 30%
1	E	139	63% 8% 29%
2	B	106	64% 8% 26%
2	F	106	67% 11% 21%
3	C	131	68% 11% 20%
3	G	131	63% 13% 21%

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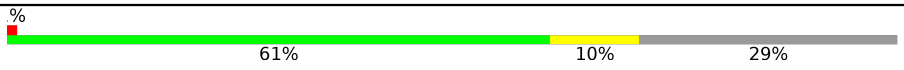
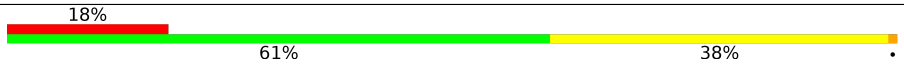
Mol	Chain	Length	Quality of chain
4	D	129	
4	H	129	
5	I	146	
5	J	146	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11893 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	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 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.Z.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	0	0	0
			794	498	155	141			
3	G	104	Total	C	N	O	0	0	0
			789	495	154	140			

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	92	Total	C	N	O	S	0	0	0
			719	453	129	135	2			
4	H	92	Total	C	N	O	S	0	0	0
			719	453	129	135	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

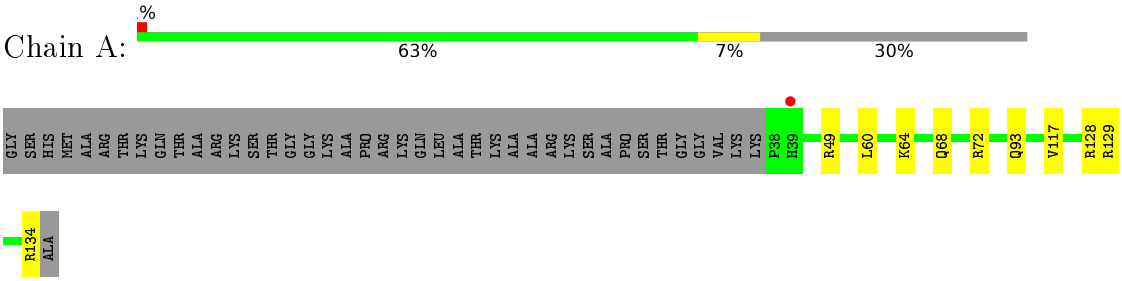
- Molecule 5 is a DNA chain called DNA (146-MER).

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			

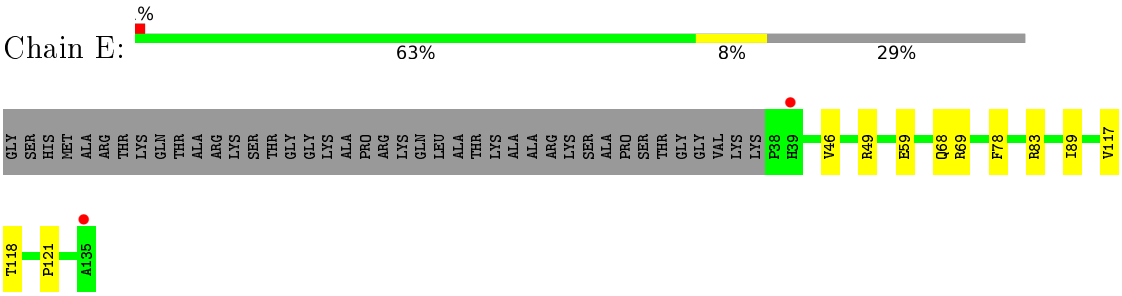
3 Residue-property plots (i)

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.

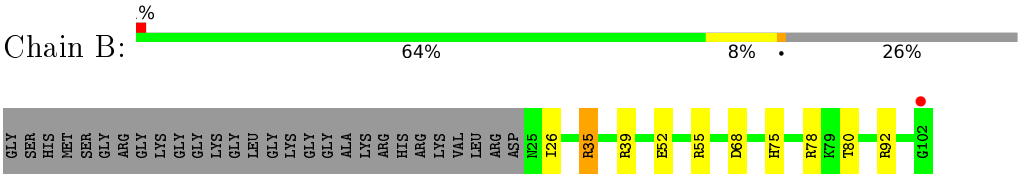
- Molecule 1: Histone H3.3



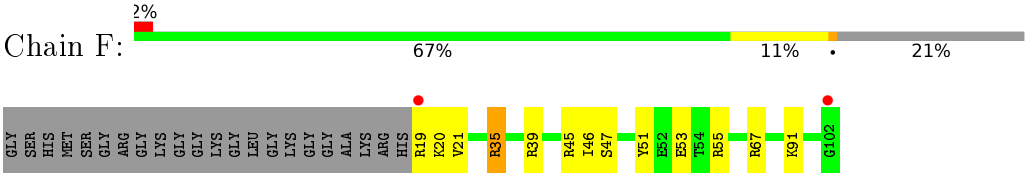
- Molecule 1: Histone H3.3



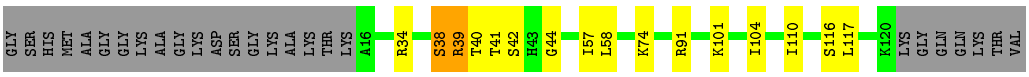
- Molecule 2: Histone H4



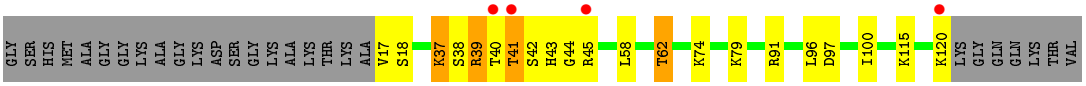
- Molecule 2: Histone H4



- Molecule 3: Histone H2A.Z

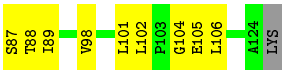


• Molecule 3: Histone H2A.Z

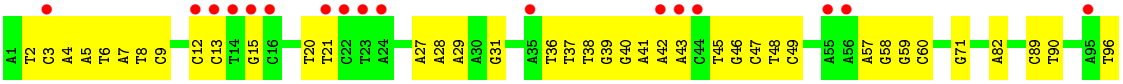


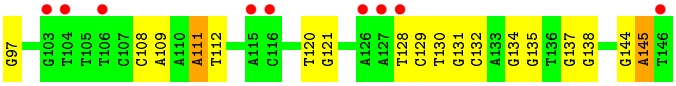
• Molecule 4: Histone H2B type 1-J

• Molecule 4: Histone H2B type 1-J

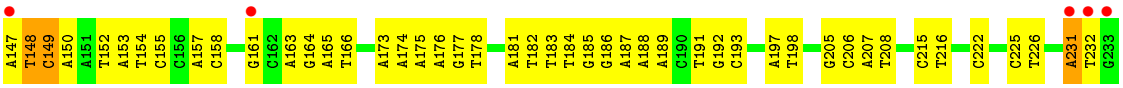


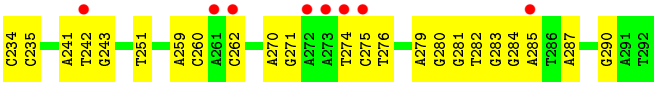
• Molecule 5: DNA (146-MER)





• 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	104.80Å 109.87Å 181.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.01 – 2.92 45.77 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.01-2.92) 97.6 (45.77-2.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.42 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.205 , 0.252 0.208 , 0.252	Depositor DCC
R_{free} test set	2316 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11893	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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	0.55	0/809	0.65	0/1085
1	E	0.66	0/815	0.71	0/1092
2	B	0.56	0/626	0.65	0/837
2	F	0.65	0/680	0.73	0/908
3	C	0.59	0/805	0.74	0/1084
3	G	0.52	0/800	0.71	0/1077
4	D	0.59	0/730	0.65	0/982
4	H	0.54	0/730	0.66	0/982
5	I	0.87	2/3354 (0.1%)	1.02	1/5175 (0.0%)
5	J	0.85	0/3354	1.05	4/5175 (0.1%)
All	All	0.74	2/12703 (0.0%)	0.90	5/18397 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	111	DA	C3'-O3'	-5.56	1.36	1.44
5	I	60	DC	C3'-O3'	-5.03	1.37	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	231	DA	O4'-C1'-N9	5.53	111.87	108.00
5	I	145	DA	O4'-C1'-N9	5.42	111.80	108.00
5	J	148	DT	C3'-C2'-C1'	-5.22	96.24	102.50
5	J	208	DT	OP2-P-O3'	5.21	116.67	105.20
5	J	149	DC	O4'-C4'-C3'	-5.01	102.50	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	7	0
1	E	803	0	840	10	0
2	B	619	0	659	11	0
2	F	673	0	722	10	0
3	C	794	0	840	19	0
3	G	789	0	835	27	0
4	D	719	0	740	15	0
4	H	719	0	740	20	0
5	I	2990	0	1652	59	0
5	J	2990	0	1652	65	0
All	All	11893	0	9515	192	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 (192) 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:J:182:DT:H2"	5:J:183:DT:H5"	1.56	0.88
3:G:41:THR:H	3:G:44:GLY:HA3	1.41	0.84
5:J:270:DA:H2"	5:J:271:DG:H5"	1.59	0.83
3:G:43:HIS:CE1	4:H:87:SER:HB3	2.13	0.82
5:J:259:DA:H2"	5:J:260:DC:H5"	1.62	0.81
5:J:197:DA:H2"	5:J:198:DT:H5"	1.67	0.76
5:J:173:DA:H2"	5:J:174:DA:C8	2.25	0.71
3:G:58:LEU:O	3:G:62:THR:HG23	1.90	0.71
5:I:37:DT:H2"	5:I:38:DT:C6	2.27	0.70
5:I:132:DC:H42	5:J:161:DG:H1	1.37	0.70
5:J:275:DC:H2"	5:J:276:DT:H5'	1.74	0.69
5:I:36:DT:H2"	5:I:37:DT:H5"	1.76	0.68
5:J:205:DG:H2"	5:J:206:DC:H5"	1.75	0.68
5:I:89:DC:H2"	5:I:90:DT:H71	1.74	0.66
5:I:5:DA:H2"	5:I:6:DT:H5"	1.77	0.66
5:J:175:DA:H2"	5:J:176:DA:C8	2.31	0.66
5:J:284:DG:H2"	5:J:285:DA:C8	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:ARG:HG2	2:F:46:ILE:HD12	1.77	0.65
5:J:152:DT:H2'	5:J:153:DA:C8	2.32	0.63
4:D:86:ARG:NH1	5:I:40:DG:OP1	2.32	0.63
4:D:73:ILE:HD13	4:D:101:LEU:HD12	1.82	0.62
5:J:274:DT:H2"	5:J:275:DC:C6	2.35	0.62
5:I:111:DA:H2'	5:I:112:DT:C6	2.35	0.61
4:H:104:GLY:O	4:H:105:GLU:HB2	1.99	0.61
5:I:144:DG:H1	5:J:149:DC:H42	1.47	0.61
5:I:135:DG:H1	5:J:158:DC:H42	1.47	0.61
3:C:34:ARG:NH1	5:I:29:DA:OP1	2.32	0.61
1:A:129:ARG:HE	1:A:134:ARG:CZ	2.14	0.60
5:J:241:DA:H2"	5:J:242:DT:H5'	1.84	0.60
5:J:184:DT:H2"	5:J:185:DG:N7	2.17	0.60
5:I:120:DT:H2"	5:I:121:DG:C8	2.37	0.59
5:J:147:DA:C6	5:J:148:DT:C4	2.91	0.59
2:B:92:ARG:HH21	4:D:101:LEU:HD23	1.67	0.59
5:J:150:DA:H5"	5:J:150:DA:H8	1.68	0.59
3:G:45:ARG:HH11	5:J:185:DG:H5'	1.68	0.59
5:I:45:DT:H2'	5:I:46:DG:C8	2.39	0.58
3:C:104:ILE:HG23	4:D:61:ILE:HD12	1.85	0.58
3:G:39:ARG:HD3	4:H:74:ALA:HB1	1.85	0.58
4:H:33:ARG:HG3	4:H:34:LYS:HD2	1.85	0.58
5:I:57:DA:N6	5:J:235:DC:H42	2.03	0.57
5:I:108:DC:H2"	5:I:109:DA:C8	2.39	0.57
1:E:49:ARG:HD2	5:I:8:DT:OP1	2.05	0.57
5:J:234:DC:H2"	5:J:235:DC:C5	2.39	0.57
5:I:134:DG:H2'	5:I:135:DG:C8	2.39	0.57
5:I:20:DT:H2"	5:I:21:DT:H5"	1.86	0.57
5:J:150:DA:C8	5:J:150:DA:H5"	2.39	0.56
3:C:41:THR:H	3:C:44:GLY:HA3	1.68	0.56
5:J:181:DA:H2"	5:J:182:DT:H5"	1.86	0.56
1:A:60:LEU:HD22	1:A:93:GLN:HG2	1.87	0.56
5:I:42:DA:H2"	5:I:43:DA:H5'	1.86	0.55
5:I:40:DG:H5"	5:I:40:DG:H8	1.71	0.55
3:G:37:LYS:NZ	5:I:112:DT:OP1	2.32	0.55
5:J:148:DT:H72	5:J:149:DC:H41	1.70	0.55
5:J:197:DA:C2'	5:J:198:DT:H5"	2.37	0.55
2:F:35:ARG:NH1	2:F:35:ARG:HB3	2.22	0.54
1:A:49:ARG:HD2	5:J:155:DC:OP1	2.07	0.54
5:I:3:DC:H2"	5:I:4:DA:C8	2.42	0.54
5:I:128:DT:H2"	5:I:129:DC:H6	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:6:DT:H2"	5:I:7:DA:C8	2.43	0.54
5:I:128:DT:H2"	5:I:129:DC:C6	2.43	0.53
2:F:20:LYS:HD2	2:F:21:VAL:H	1.74	0.53
2:B:52:GLU:OE2	2:B:55:ARG:NH1	2.42	0.53
5:J:174:DA:H2"	5:J:175:DA:C8	2.44	0.53
5:I:46:DG:H2"	5:I:47:DC:H5"	1.90	0.53
3:C:39:ARG:NH2	4:D:75:GLY:HA2	2.24	0.53
4:H:40:TYR:O	4:H:44:VAL:HG23	2.10	0.53
2:F:35:ARG:HB3	2:F:35:ARG:CZ	2.39	0.52
5:J:215:DC:H2"	5:J:216:DT:H71	1.92	0.52
2:B:75:HIS:CD2	4:D:80:LEU:HD22	2.45	0.52
1:E:68:GLN:HG3	1:E:89:ILE:HD13	1.91	0.52
1:A:68:GLN:CD	1:A:72:ARG:HH21	2.13	0.51
4:D:88:THR:HG22	5:I:39:DG:OP1	2.10	0.51
3:C:57:ILE:HD13	4:D:98:VAL:HG22	1.93	0.51
4:D:98:VAL:HG13	4:D:102:LEU:HD22	1.92	0.51
5:I:137:DG:H1'	5:I:138:DG:C8	2.45	0.51
3:C:41:THR:O	3:G:42:SER:N	2.44	0.51
3:G:43:HIS:NE2	4:H:87:SER:HB3	2.25	0.51
4:D:115:THR:O	4:D:119:THR:HG23	2.11	0.50
2:B:92:ARG:HB3	2:B:92:ARG:CZ	2.41	0.50
5:I:8:DT:H2"	5:I:9:DC:H5"	1.93	0.50
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.93	0.50
1:A:60:LEU:HD12	1:A:64:LYS:HE2	1.92	0.50
5:I:135:DG:N2	5:J:158:DC:N3	2.48	0.50
3:G:18:SER:HA	5:J:177:DG:H5"	1.93	0.50
3:G:39:ARG:HD3	4:H:74:ALA:CB	2.42	0.49
3:G:17:VAL:HB	5:J:178:DT:OP1	2.12	0.49
1:E:78:PHE:CZ	2:F:67:ARG:HB2	2.47	0.49
5:I:128:DT:H2"	5:I:129:DC:H5'	1.95	0.49
5:J:206:DC:H2"	5:J:207:DA:C8	2.47	0.49
5:I:7:DA:C2	5:J:287:DA:C2	3.01	0.48
5:J:187:DA:H2"	5:J:188:DA:C8	2.48	0.48
5:J:242:DT:H1'	5:J:243:DG:H5'	1.95	0.48
5:J:192:DG:H1'	5:J:193:DC:H5'	1.94	0.48
4:D:88:THR:HG23	4:D:90:THR:HG23	1.94	0.48
1:E:69:ARG:NH2	5:I:90:DT:OP2	2.46	0.48
5:I:71:DG:N2	5:J:222:DC:O2	2.37	0.48
1:E:59:GLU:OE2	1:E:59:GLU:N	2.46	0.48
3:G:91:ARG:HA	3:G:91:ARG:HD3	1.68	0.48
5:J:231:DA:H2"	5:J:232:DT:OP2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ARG:HH12	2:B:39:ARG:HH21	1.60	0.48
3:C:38:SER:O	3:G:41:THR:HG21	2.13	0.48
5:I:15:DG:H22	5:J:279:DA:H2	1.61	0.47
5:I:41:DA:N6	5:J:251:DT:O4	2.48	0.47
5:J:283:DG:H2"	5:J:284:DG:C8	2.50	0.47
5:I:144:DG:H1	5:J:149:DC:N4	2.10	0.47
5:I:15:DG:N2	5:J:279:DA:H2	2.13	0.47
5:J:173:DA:H2"	5:J:174:DA:N7	2.29	0.47
2:B:35:ARG:NH1	2:B:39:ARG:HH21	2.13	0.47
3:C:57:ILE:HD13	4:D:98:VAL:CG2	2.45	0.47
4:H:46:LYS:NZ	4:H:52:THR:O	2.40	0.47
2:B:92:ARG:HB3	2:B:92:ARG:NH1	2.30	0.46
3:G:79:LYS:HD3	5:I:130:DT:H5"	1.95	0.46
3:C:91:ARG:HA	3:C:91:ARG:HD3	1.69	0.46
3:G:91:ARG:NH1	3:G:97:ASP:OD1	2.43	0.46
5:I:130:DT:C4	5:I:131:DG:C6	3.03	0.46
5:J:205:DG:C2'	5:J:206:DC:H5"	2.43	0.46
3:C:42:SER:OG	3:G:37:LYS:O	2.26	0.46
1:E:46:VAL:HG21	5:I:82:DA:H3'	1.96	0.46
5:J:225:DC:H2"	5:J:226:DT:C7	2.46	0.46
5:I:27:DA:C6	5:I:28:DA:C6	3.04	0.46
2:F:51:TYR:O	2:F:55:ARG:HG3	2.17	0.45
3:G:42:SER:OG	3:G:43:HIS:N	2.48	0.45
5:I:6:DT:H2"	5:I:7:DA:H8	1.80	0.45
2:B:92:ARG:NH2	4:D:101:LEU:HD23	2.31	0.45
3:G:79:LYS:O	4:H:52:THR:HG23	2.17	0.45
5:I:129:DC:H2"	5:I:130:DT:C7	2.46	0.45
3:C:57:ILE:HG13	3:C:58:LEU:N	2.30	0.45
2:B:26:ILE:HG13	2:B:55:ARG:HB3	1.99	0.45
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.50	0.45
3:C:101:LYS:HA	3:C:101:LYS:HD3	1.47	0.45
5:I:12:DC:H2"	5:I:13:DC:H5'	1.98	0.45
5:J:275:DC:H2'	5:J:276:DT:H71	1.98	0.45
5:J:281:DG:H2"	5:J:282:DT:H5'	1.97	0.45
5:I:40:DG:H5"	5:I:40:DG:C8	2.51	0.44
4:D:46:LYS:HA	4:D:46:LYS:HD3	1.59	0.44
2:F:35:ARG:O	2:F:39:ARG:HG2	2.18	0.44
3:G:41:THR:C	3:G:44:GLY:H	2.21	0.44
4:H:42:TYR:CE2	4:H:46:LYS:HE2	2.52	0.44
5:I:13:DC:H42	5:J:280:DG:H1	1.65	0.44
5:J:284:DG:H2"	5:J:285:DA:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:191:DT:H2"	5:J:192:DG:C8	2.52	0.44
3:G:41:THR:O	3:G:44:GLY:N	2.45	0.44
4:H:98:VAL:HG13	4:H:102:LEU:HD22	1.99	0.44
3:G:38:SER:OG	3:G:38:SER:O	2.31	0.44
3:G:96:LEU:HD23	4:H:106:LEU:HD11	1.99	0.44
4:H:33:ARG:HB2	4:H:34:LYS:NZ	2.33	0.44
4:H:87:SER:OG	5:J:186:DG:OP1	2.34	0.44
3:G:40:THR:HG21	4:H:89:ILE:HD11	1.99	0.43
5:I:38:DT:C4	5:I:39:DG:N1	2.86	0.43
5:I:96:DT:H2"	5:I:97:DG:C5'	2.48	0.43
5:J:147:DA:C6	5:J:148:DT:C5	3.06	0.43
3:C:41:THR:HG22	3:C:42:SER:H	1.84	0.43
5:I:46:DG:H5"	5:I:46:DG:C8	2.54	0.43
3:C:39:ARG:CG	3:C:40:THR:HG22	2.49	0.43
5:I:58:DG:H2'	5:I:59:DG:C8	2.53	0.43
3:C:74:LYS:HE3	3:C:74:LYS:HB2	1.84	0.43
3:C:110:ILE:HD13	3:C:110:ILE:HA	1.84	0.43
5:J:157:DA:H8	5:J:157:DA:H5"	1.83	0.43
5:J:164:DG:H2"	5:J:165:DA:H5"	2.01	0.43
3:C:117:LEU:CD2	1:E:117:VAL:HG22	2.49	0.42
1:A:128:ARG:HD3	1:A:128:ARG:HH11	1.71	0.42
5:J:148:DT:H72	5:J:149:DC:N4	2.33	0.42
4:H:39:ILE:HD13	4:H:39:ILE:HA	1.90	0.42
5:I:89:DC:H2"	5:I:90:DT:C7	2.45	0.42
1:A:68:GLN:HG2	1:A:72:ARG:HE	1.85	0.42
4:H:62:MET:O	4:H:66:VAL:HG23	2.20	0.42
5:J:148:DT:C5	5:J:149:DC:C5	3.07	0.42
4:H:42:TYR:CZ	4:H:46:LYS:HE2	2.54	0.42
4:H:73:ILE:HD13	4:H:101:LEU:HD12	2.02	0.42
5:J:148:DT:H2"	5:J:149:DC:C5'	2.50	0.42
3:G:41:THR:CG2	3:G:42:SER:N	2.83	0.42
3:G:100:ILE:HD13	3:G:100:ILE:HG21	1.82	0.41
3:G:41:THR:N	3:G:44:GLY:HA3	2.22	0.41
5:J:165:DA:C8	5:J:166:DT:H72	2.55	0.41
4:H:78:SER:HA	4:H:89:ILE:HD11	2.00	0.41
5:I:2:DT:H2"	5:I:3:DC:C6	2.54	0.41
5:J:188:DA:H2'	5:J:189:DA:C8	2.55	0.41
5:I:145:DA:C2	5:J:148:DT:O4	2.73	0.41
5:I:46:DG:H2"	5:I:47:DC:C6	2.56	0.41
5:I:48:DT:H1'	5:I:49:DC:C6	2.55	0.41
5:J:163:DA:H2"	5:J:164:DG:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:ARG:HB3	2:F:20:LYS:H	1.35	0.41
3:G:74:LYS:HE3	3:G:74:LYS:HB2	1.81	0.41
3:C:117:LEU:HD23	1:E:117:VAL:HG22	2.03	0.41
3:C:39:ARG:HH21	4:D:75:GLY:HA2	1.86	0.40
5:I:37:DT:H2"	5:I:38:DT:C5	2.55	0.40
5:I:3:DC:H42	5:J:290:DG:H1	1.69	0.40
5:I:31:DG:H1	5:J:262:DC:H42	1.69	0.40
2:B:78:ARG:NH1	2:B:80:THR:O	2.55	0.40
5:I:46:DG:H5"	5:I:46:DG:H8	1.86	0.40
5:J:153:DA:H2"	5:J:154:DT:H5'	2.03	0.40
1:E:118:THR:HA	2:F:45:ARG:HB3	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%)	93 (98%)	2 (2%)	0	100	100
1	E	96/139 (69%)	94 (98%)	2 (2%)	0	100	100
2	B	76/106 (72%)	75 (99%)	1 (1%)	0	100	100
2	F	82/106 (77%)	81 (99%)	1 (1%)	0	100	100
3	C	103/131 (79%)	96 (93%)	7 (7%)	0	100	100
3	G	102/131 (78%)	93 (91%)	9 (9%)	0	100	100
4	D	90/129 (70%)	86 (96%)	4 (4%)	0	100	100
4	H	90/129 (70%)	85 (94%)	5 (6%)	0	100	100
All	All	734/1010 (73%)	703 (96%)	31 (4%)	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 94
1	E	83/112 (74%)	82 (99%)	1 (1%)	78 94
2	B	63/81 (78%)	62 (98%)	1 (2%)	70 91
2	F	69/81 (85%)	66 (96%)	3 (4%)	35 71
3	C	82/99 (83%)	79 (96%)	3 (4%)	41 76
3	G	82/99 (83%)	76 (93%)	6 (7%)	17 45
4	D	78/107 (73%)	78 (100%)	0	100 100
4	H	78/107 (73%)	76 (97%)	2 (3%)	54 84
All	All	618/798 (77%)	601 (97%)	17 (3%)	51 83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	VAL
2	B	35	ARG
3	C	38	SER
3	C	39	ARG
3	C	116	SER
1	E	83	ARG
2	F	35	ARG
2	F	47	SER
2	F	91	LYS
3	G	37	LYS
3	G	39	ARG
3	G	41	THR
3	G	62	THR
3	G	115	LYS
3	G	120	LYS
4	H	51	ASP
4	H	88	THR

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%)	0.33	1 (1%) 84 82	39, 51, 77, 100	0
1	E	98/139 (70%)	0.22	2 (2%) 68 64	31, 43, 71, 95	0
2	B	78/106 (73%)	0.26	1 (1%) 79 78	36, 49, 64, 70	0
2	F	84/106 (79%)	0.19	2 (2%) 62 57	31, 42, 64, 93	0
3	C	105/131 (80%)	0.24	0 100 100	34, 51, 97, 121	0
3	G	104/131 (79%)	0.32	4 (3%) 44 38	42, 63, 100, 116	0
4	D	92/129 (71%)	0.49	1 (1%) 82 80	38, 52, 74, 101	0
4	H	92/129 (71%)	0.31	0 100 100	42, 61, 87, 105	0
5	I	146/146 (100%)	0.83	26 (17%) 2 1	52, 113, 147, 160	0
5	J	146/146 (100%)	0.69	13 (8%) 12 8	60, 115, 147, 153	0
All	All	1042/1302 (80%)	0.42	50 (4%) 34 29	31, 59, 136, 160	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	146	DT	7.8
5	I	42	DA	4.8
5	J	273	DA	4.8
1	E	135	ALA	4.5
5	I	128	DT	3.9
5	I	55	DA	3.8
5	J	147	DA	3.7
5	I	43	DA	3.6
5	J	233	DG	3.5
1	A	39	HIS	3.4
5	I	15	DG	3.4
5	J	242	DT	3.4
5	I	14	DT	3.3

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Mol	Chain	Res	Type	RSRZ
3	G	120	LYS	3.1
5	I	44	DC	3.1
5	I	24	DA	3.0
2	F	102	GLY	2.9
5	I	95	DA	2.9
2	F	19	ARG	2.9
5	I	116	DC	2.8
3	G	40	THR	2.8
5	I	21	DT	2.7
5	I	127	DA	2.7
2	B	102	GLY	2.7
5	I	106	DT	2.6
5	I	13	DC	2.6
5	J	262	DC	2.5
5	J	275	DC	2.5
5	J	285	DA	2.5
3	G	45	ARG	2.5
5	J	274	DT	2.5
5	J	272	DA	2.4
5	J	161	DG	2.4
5	I	22	DC	2.3
5	I	126	DA	2.3
5	J	261	DA	2.3
5	I	23	DT	2.2
5	I	35	DA	2.2
5	J	231	DA	2.2
4	D	124	ALA	2.2
5	I	56	DA	2.2
5	J	232	DT	2.1
5	I	3	DC	2.1
5	I	103	DG	2.1
5	I	16	DC	2.1
3	G	41	THR	2.1
5	I	104	DT	2.1
1	E	39	HIS	2.1
5	I	115	DA	2.1
5	I	12	DC	2.1

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

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.