Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 03:52 PM JST

PDB ID	:	5XM0
Title	:	The mouse nucleosome structure containing H2A, H2B type3-A, H3.3, and H4
Authors	:	Taguchi, H.; Horikoshi, N.; Kurumizaka, H.
Deposited on	:	2017-05-12
Resolution	:	2.87 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

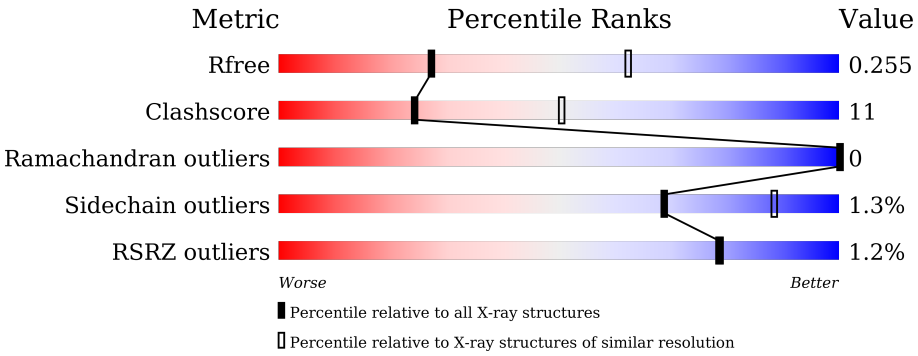
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.87 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}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	57% 12% • 30%
1	E	139	55% 13% • 30%
2	B	106	% 59% 13% • 26%
2	F	106	% 70% 8% • 21%
3	C	133	68% 11% 21%
3	G	133	% 71% 7% 22%

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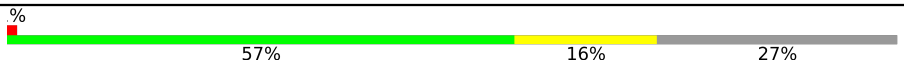
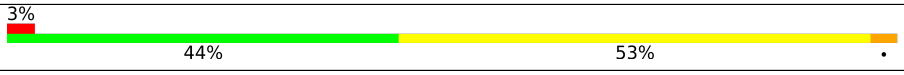
Mol	Chain	Length	Quality of chain
4	D	129	
4	H	129	
5	I	146	
5	J	146	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11950 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	97	Total	C	N	O	S	0	0	0
			797	503	155	137	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P84244
A	-2	SER	-	expression tag	UNP P84244
A	-1	HIS	-	expression tag	UNP P84244
E	-3	GLY	-	expression tag	UNP P84244
E	-2	SER	-	expression tag	UNP P84244
E	-1	HIS	-	expression tag	UNP P84244

- 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-B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	0	0	0
			810	511	158	141			
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 C0HKE1
C	-2	SER	-	expression tag	UNP C0HKE1
C	-1	HIS	-	expression tag	UNP C0HKE1
G	-3	GLY	-	expression tag	UNP C0HKE1
G	-2	SER	-	expression tag	UNP C0HKE1
G	-1	HIS	-	expression tag	UNP C0HKE1

- 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.

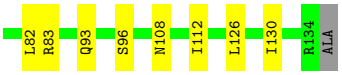
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	C	3	Total O 3 3	0	0
6	D	2	Total O 2 2	0	0
6	E	3	Total O 3 3	0	0
6	G	1	Total O 1 1	0	0
6	J	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

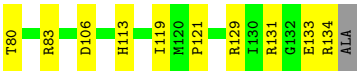
• Molecule 1: Histone H3.3

Chain A:



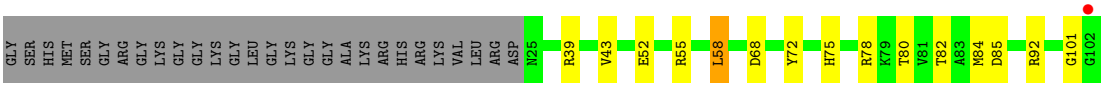
• Molecule 1: Histone H3.3

Chain E:



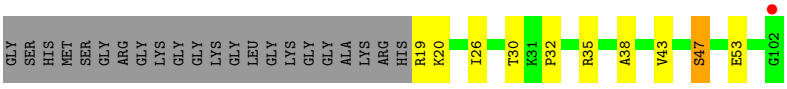
• Molecule 2: Histone H4

Chain B:



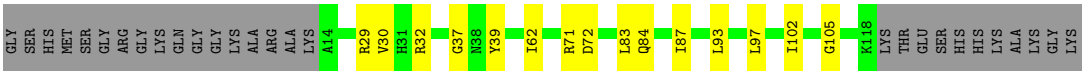
• Molecule 2: Histone H4

Chain F:



• Molecule 3: Histone H2A type 1-B

Chain C:

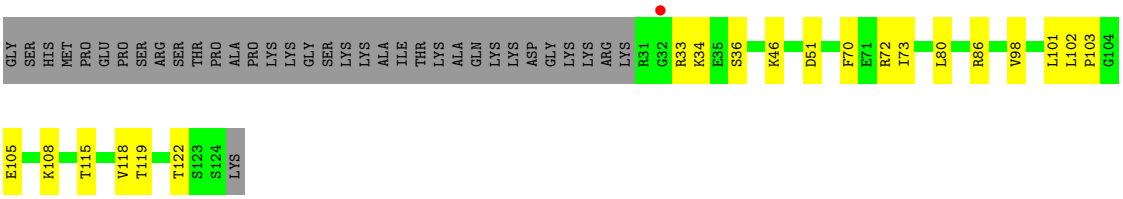


• Molecule 3: Histone H2A type 1-B

Chain G:

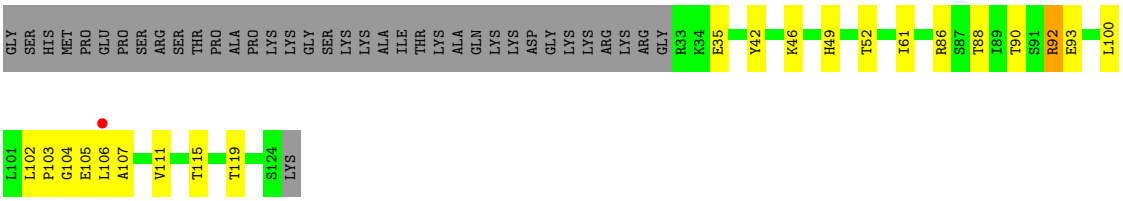
• Molecule 4: Histone H2B type 3-A

Chain D:



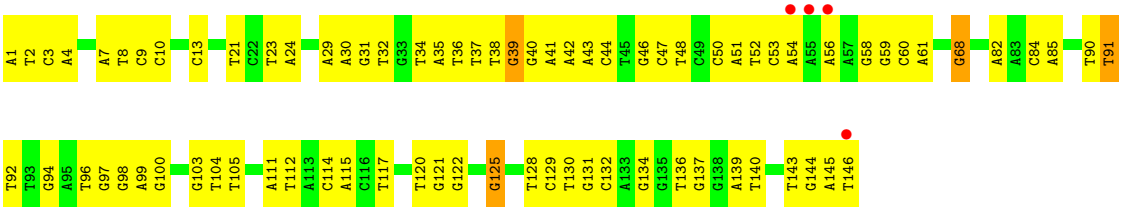
• Molecule 4: Histone H2B type 3-A

Chain H:



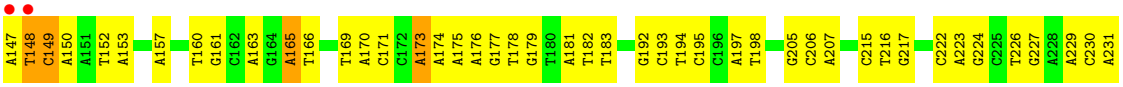
• Molecule 5: DNA (146-MER)

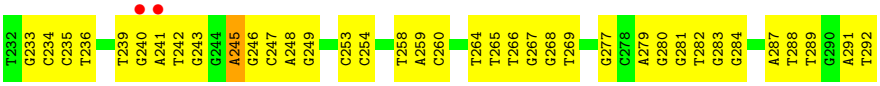
Chain I:



• Molecule 5: DNA (146-MER)

Chain J:




T232 G233 C234 C235 T236 T239 G240 A241 T242 G243 G244 A245 G246 C247 A248 G249 C253 C254 T258 A259 C260 T264 T265 T266 G267 G268 T269 G277 C278 A279 G280 G281 T282 G283 G284 A287 T288 T289 G290 A291 T292

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	106.52Å 110.09Å 182.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 2.87 48.90 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.90-2.87) 99.5 (48.90-2.87)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.48 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.219 , 0.255 0.219 , 0.255	Depositor DCC
R_{free} test set	2494 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	57.9	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11950	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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	0.53	1/809 (0.1%)	0.66	0/1085
1	E	0.66	1/809 (0.1%)	1.00	6/1085 (0.6%)
2	B	0.51	0/626	0.73	0/837
2	F	0.60	0/680	0.74	0/908
3	C	0.59	0/820	0.69	0/1107
3	G	0.45	0/815	0.62	0/1100
4	D	0.62	1/747 (0.1%)	0.82	2/1004 (0.2%)
4	H	0.58	0/732	0.72	0/985
5	I	0.86	2/3354 (0.1%)	1.09	8/5175 (0.2%)
5	J	0.84	3/3354 (0.1%)	1.11	8/5175 (0.2%)
All	All	0.73	8/12746 (0.1%)	0.96	24/18461 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	91	DT	C2'-C1'	7.80	1.60	1.52
5	J	277	DG	C3'-O3'	-6.90	1.34	1.44
1	E	77	ASP	CB-CG	6.50	1.65	1.51
1	A	59	GLU	CD-OE1	-5.78	1.19	1.25
4	D	105	GLU	CD-OE1	5.37	1.31	1.25
5	I	68	DG	C3'-O3'	-5.15	1.37	1.44
5	J	245	DA	C3'-O3'	-5.14	1.37	1.44
5	J	224	DG	C3'-O3'	-5.13	1.37	1.44

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	77	ASP	CB-CG-OD1	14.98	131.78	118.30
4	D	108	LYS	CD-CE-NZ	-9.81	89.13	111.70
1	E	77	ASP	CB-CG-OD2	-9.14	110.07	118.30
5	J	149	DC	O4'-C4'-C3'	-8.56	100.86	106.00
1	E	129	ARG	NE-CZ-NH1	-6.67	116.96	120.30
4	D	108	LYS	CA-CB-CG	-6.49	99.11	113.40
1	E	56	LYS	CA-CB-CG	6.29	127.23	113.40
5	J	148	DT	O4'-C1'-N1	6.21	112.34	108.00
1	E	56	LYS	CB-CA-C	-6.15	98.11	110.40
5	I	39	DG	O4'-C1'-N9	6.03	112.22	108.00
1	E	63	ARG	NE-CZ-NH1	5.78	123.19	120.30
5	J	165	DA	C1'-O4'-C4'	-5.67	104.43	110.10
5	I	125	DG	O4'-C1'-N9	5.61	111.92	108.00
5	I	56	DA	O4'-C1'-N9	5.57	111.90	108.00
5	I	94	DG	O4'-C1'-N9	5.57	111.90	108.00
5	J	165	DA	O4'-C1'-N9	5.55	111.88	108.00
5	I	143	DT	O4'-C1'-N1	5.45	111.81	108.00
5	J	163	DA	O4'-C1'-N9	5.32	111.72	108.00
5	J	173	DA	O4'-C4'-C3'	-5.29	102.38	104.50
5	J	243	DG	C3'-C2'-C1'	-5.21	96.24	102.50
5	J	149	DC	C4'-C3'-C2'	-5.20	98.42	103.10
5	I	68	DG	O4'-C1'-N9	5.15	111.60	108.00
5	I	21	DT	O4'-C1'-N1	5.09	111.56	108.00
5	I	91	DT	O5'-P-OP1	-5.08	101.13	105.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	103	PRO	Peptide

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	14	0
1	E	797	0	835	19	0
2	B	619	0	659	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	673	0	722	10	0
3	C	810	0	866	13	0
3	G	805	0	861	14	0
4	D	736	0	756	14	0
4	H	721	0	740	19	0
5	I	2990	0	1652	70	0
5	J	2990	0	1652	79	0
6	A	1	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
6	E	3	0	0	0	0
6	G	1	0	0	0	0
6	J	2	0	0	0	0
All	All	11950	0	9578	215	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 11.

All (215) 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:I:145:DA:N1	5:J:147:DA:N6	2.01	1.07
5:I:104:DT:H2”	5:I:105:DT:H5”	1.50	0.94
5:I:51:DA:H2”	5:I:52:DT:H5”	1.50	0.93
5:J:229:DA:H2”	5:J:230:DC:H5”	1.56	0.88
5:J:165:DA:H2”	5:J:166:DT:H5”	1.57	0.86
5:I:47:DC:H2”	5:I:48:DT:H5”	1.61	0.83
3:C:84:GLN:HG3	3:C:105:GLY:HA3	1.60	0.82
1:A:50:GLU:HB2	2:B:39:ARG:HD2	1.62	0.81
5:I:128:DT:H2”	5:I:129:DC:H5”	1.63	0.81
2:B:82:THR:HG22	2:B:84:MET:H	1.47	0.80
4:H:104:GLY:N	4:H:105:GLU:O	2.15	0.79
4:H:104:GLY:H	4:H:105:GLU:C	1.86	0.79
5:I:43:DA:H1’	5:I:44:DC:H5”	1.67	0.75
5:J:149:DC:H1’	5:J:150:DA:H5”	1.70	0.74
5:I:40:DG:N2	5:J:253:DC:O2	2.21	0.74
2:B:78:ARG:NH2	2:B:85:ASP:OD2	2.21	0.73
5:I:36:DT:H2”	5:I:37:DT:H5”	1.71	0.73
5:I:42:DA:H2”	5:I:43:DA:H5’	1.71	0.73
2:F:19:ARG:HG2	2:F:20:LYS:N	2.04	0.72
5:I:132:DC:H42	5:J:161:DG:H1	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:8:DT:H2"	5:I:9:DC:H5"	1.73	0.71
5:J:259:DA:H2"	5:J:260:DC:H5"	1.72	0.71
3:G:15:LYS:CD	5:J:178:DT:OP1	2.38	0.71
3:G:102:ILE:HG23	4:H:61:ILE:HD13	1.73	0.69
5:J:247:DC:H2"	5:J:248:DA:N7	2.07	0.69
5:J:283:DG:H5'	5:J:283:DG:H8	1.58	0.69
5:J:279:DA:H2"	5:J:280:DG:H5"	1.74	0.69
5:J:291:DA:H2"	5:J:292:DT:H5"	1.75	0.68
2:F:19:ARG:HG2	2:F:20:LYS:H	1.55	0.68
4:H:103:PRO:HB2	4:H:105:GLU:O	1.96	0.66
5:J:205:DG:H2"	5:J:206:DC:H5"	1.79	0.65
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.79	0.65
5:J:152:DT:H2"	5:J:153:DA:H5"	1.79	0.64
4:D:86:ARG:HG3	4:D:86:ARG:HH11	1.62	0.64
5:I:40:DG:H2'	5:I:41:DA:C8	2.34	0.63
4:H:104:GLY:N	4:H:105:GLU:C	2.51	0.63
5:I:29:DA:H2"	5:I:30:DA:H5'	1.79	0.63
5:I:136:DT:H2'	5:I:137:DG:C8	2.34	0.63
5:J:197:DA:H1'	5:J:198:DT:H5"	1.81	0.63
2:B:52:GLU:OE2	2:B:55:ARG:NH1	2.32	0.62
5:J:175:DA:H2"	5:J:176:DA:C8	2.35	0.61
1:E:134:ARG:HB3	1:E:134:ARG:NH1	2.15	0.61
5:I:10:DC:H42	5:J:283:DG:H1	1.46	0.61
1:A:43:PRO:HG2	5:I:68:DG:H5'	1.82	0.61
1:E:42:ARG:NH1	5:J:215:DC:OP1	2.34	0.60
5:J:283:DG:H5'	5:J:283:DG:C8	2.36	0.60
1:E:63:ARG:NH2	5:I:91:DT:OP1	2.34	0.60
3:G:61:GLU:HG2	4:H:106:LEU:HD21	1.82	0.60
1:A:79:LYS:HB3	1:A:82:LEU:HD11	1.81	0.60
5:J:148:DT:H3	5:J:149:DC:N4	1.99	0.60
3:C:84:GLN:HG3	3:C:105:GLY:CA	2.30	0.59
5:I:38:DT:H2"	5:I:39:DG:O4'	2.03	0.59
4:H:102:LEU:HB2	4:H:107:ALA:HB2	1.85	0.59
5:I:120:DT:H2"	5:I:121:DG:C8	2.38	0.58
5:J:264:DT:H1'	5:J:265:DT:H5"	1.84	0.58
3:C:29:ARG:NH1	4:D:36:SER:O	2.37	0.58
5:J:281:DG:H2"	5:J:282:DT:H5'	1.84	0.58
5:J:215:DC:H2"	5:J:216:DT:H71	1.86	0.57
1:A:42:ARG:HH21	5:I:68:DG:P	2.27	0.57
4:H:104:GLY:HA2	4:H:107:ALA:H	1.70	0.57
5:J:258:DT:H2"	5:J:259:DA:C8	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:ILE:HD12	4:D:98:VAL:HG22	1.86	0.56
5:I:125:DG:H22	5:J:169:DT:H3	1.53	0.56
5:J:148:DT:O2	5:J:149:DC:C5	2.58	0.56
4:D:98:VAL:HG13	4:D:102:LEU:HD22	1.87	0.56
3:G:15:LYS:HD3	5:J:178:DT:OP1	2.06	0.55
2:B:92:ARG:HB3	2:B:92:ARG:CZ	2.36	0.55
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.40	0.55
5:J:266:DT:H2"	5:J:267:DG:N7	2.22	0.55
3:G:83:LEU:O	3:G:87:ILE:HG12	2.07	0.54
5:I:130:DT:H2"	5:I:131:DG:H5"	1.88	0.54
5:I:144:DG:H1	5:J:149:DC:H42	1.55	0.54
4:D:118:VAL:O	4:D:122:THR:HG23	2.07	0.54
5:J:182:DT:H1'	5:J:183:DT:H5"	1.89	0.54
1:E:83:ARG:HD2	5:I:100:DG:H5"	1.89	0.54
3:C:32:ARG:NH1	5:I:29:DA:OP1	2.32	0.54
3:G:16:THR:HA	5:J:177:DG:H5"	1.90	0.54
1:E:69:ARG:NH2	5:I:90:DT:OP2	2.36	0.54
3:G:15:LYS:HG2	5:J:178:DT:OP1	2.08	0.54
5:J:241:DA:H2"	5:J:242:DT:H5'	1.89	0.54
1:A:60:LEU:HD22	1:A:93:GLN:HG2	1.90	0.53
1:A:108:ASN:O	1:A:112:ILE:HG12	2.08	0.53
5:I:9:DC:H2'	5:I:10:DC:C6	2.43	0.53
5:J:148:DT:H3	5:J:149:DC:H41	1.56	0.53
4:D:46:LYS:HA	4:D:46:LYS:HE2	1.90	0.53
3:G:79:ILE:H	3:G:82:HIS:CD2	2.25	0.53
2:B:82:THR:HG22	2:B:84:MET:N	2.21	0.53
5:I:84:DC:H2"	5:I:85:DA:C8	2.44	0.52
3:G:79:ILE:H	3:G:82:HIS:HD2	1.57	0.52
5:J:287:DA:H2"	5:J:288:DT:H5'	1.92	0.52
5:J:240:DG:H2"	5:J:241:DA:H5"	1.92	0.51
4:H:42:TYR:CZ	4:H:46:LYS:HE3	2.45	0.51
5:I:3:DC:H2"	5:I:4:DA:C8	2.45	0.51
5:J:170:DA:H2"	5:J:171:DC:H5"	1.92	0.51
1:E:49:ARG:HD2	5:I:8:DT:OP1	2.10	0.51
5:I:114:DC:H2'	5:I:115:DA:C8	2.45	0.51
5:J:148:DT:C2	5:J:149:DC:C5	2.98	0.51
4:H:49:HIS:HB3	4:H:52:THR:OG1	2.11	0.51
5:I:34:DT:H2'	5:I:35:DA:C8	2.45	0.51
5:J:157:DA:C8	5:J:157:DA:H5'	2.46	0.51
5:I:37:DT:H2"	5:I:38:DT:C6	2.46	0.50
5:J:222:DC:H2"	5:J:223:DA:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:129:DC:H2"	5:I:130:DT:H71	1.93	0.50
5:I:52:DT:H3	5:J:241:DA:H61	1.58	0.50
5:J:173:DA:H2"	5:J:174:DA:C8	2.47	0.50
4:H:35:GLU:HA	5:I:122:DG:H5"	1.92	0.50
4:D:51:ASP:OD1	4:D:51:ASP:N	2.39	0.49
5:I:117:DT:O2	5:J:177:DG:N2	2.45	0.49
5:J:206:DC:H2"	5:J:207:DA:C8	2.46	0.49
3:C:83:LEU:O	3:C:87:ILE:HG13	2.11	0.49
5:I:96:DT:H2"	5:I:97:DG:C8	2.47	0.49
5:I:46:DG:H2"	5:I:47:DC:H5"	1.93	0.49
2:F:19:ARG:CG	2:F:20:LYS:H	2.21	0.49
1:A:126:LEU:HD22	1:E:113:HIS:CG	2.48	0.48
1:E:43:PRO:HG2	5:J:215:DC:H5'	1.94	0.48
5:I:36:DT:C2'	5:I:37:DT:H5"	2.41	0.48
3:G:15:LYS:HD2	5:J:178:DT:P	2.53	0.48
5:I:9:DC:H2"	5:I:10:DC:H5'	1.96	0.48
5:J:181:DA:H2"	5:J:182:DT:H5"	1.95	0.48
5:J:234:DC:H2"	5:J:235:DC:C5	2.48	0.48
1:E:50:GLU:OE1	2:F:35:ARG:NH1	2.46	0.48
5:I:129:DC:H2"	5:I:130:DT:C7	2.43	0.48
5:J:165:DA:C2'	5:J:166:DT:H5"	2.36	0.48
5:I:91:DT:H1'	5:I:92:DT:H5'	1.95	0.48
5:J:245:DA:H2"	5:J:246:DG:N7	2.30	0.47
3:C:71:ARG:NH2	3:C:72:ASP:OD1	2.47	0.47
5:J:248:DA:H2"	5:J:249:DG:H5'	1.96	0.47
3:C:87:ILE:HD12	3:C:102:ILE:HD11	1.97	0.47
5:I:7:DA:C2	5:J:287:DA:C2	3.02	0.47
5:I:146:DT:H6	5:I:146:DT:H5'	1.80	0.47
2:B:84:MET:SD	2:B:101:GLY:HA3	2.54	0.47
1:E:63:ARG:CZ	5:I:91:DT:OP1	2.62	0.47
5:I:98:DG:H1	5:J:195:DC:H42	1.62	0.47
5:J:230:DC:H2'	5:J:231:DA:C8	2.50	0.47
3:G:15:LYS:CD	5:J:178:DT:P	3.03	0.47
4:D:115:THR:O	4:D:119:THR:HG23	2.15	0.47
4:D:86:ARG:HH21	5:I:40:DG:P	2.37	0.46
3:C:87:ILE:HD13	3:C:97:LEU:CD1	2.45	0.46
3:G:79:ILE:HG12	3:G:82:HIS:CD2	2.50	0.46
1:A:46:VAL:O	1:A:50:GLU:HG3	2.15	0.46
5:J:157:DA:H5'	5:J:157:DA:H8	1.80	0.46
5:J:216:DT:H2"	5:J:217:DG:C8	2.51	0.46
5:I:111:DA:H2'	5:I:112:DT:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LEU:O	2:B:58:LEU:HD22	2.15	0.46
2:F:30:THR:HB	2:F:32:PRO:HD2	1.98	0.46
5:J:205:DG:C2'	5:J:206:DC:H5"	2.46	0.46
3:G:15:LYS:HD2	5:J:177:DG:O3'	2.16	0.45
5:J:253:DC:H2'	5:J:254:DC:C5	2.51	0.45
1:A:50:GLU:CB	2:B:39:ARG:HD2	2.42	0.45
4:D:86:ARG:HH11	4:D:86:ARG:CG	2.28	0.45
3:G:15:LYS:CG	5:J:178:DT:OP1	2.63	0.45
1:A:68:GLN:HG2	1:A:72:ARG:HE	1.81	0.45
3:C:84:GLN:CG	3:C:105:GLY:HA3	2.39	0.45
2:F:38:ALA:HB1	2:F:43:VAL:HB	1.98	0.45
5:I:103:DG:H2"	5:I:104:DT:H5"	1.98	0.45
5:J:259:DA:C2'	5:J:260:DC:H5"	2.43	0.45
5:I:13:DC:H42	5:J:280:DG:H1	1.64	0.44
5:I:60:DC:H2"	5:I:61:DA:C8	2.52	0.44
4:D:33:ARG:HG3	5:J:269:DT:H4'	1.99	0.44
4:H:104:GLY:CA	4:H:107:ALA:HB3	2.47	0.44
5:I:1:DA:H2"	5:I:2:DT:H72	1.99	0.44
5:I:23:DT:H2"	5:I:24:DA:H5"	2.00	0.44
5:I:130:DT:C2'	5:I:131:DG:H5"	2.47	0.44
5:J:178:DT:H2"	5:J:179:DG:C8	2.52	0.44
1:E:79:LYS:HD3	1:E:80:THR:O	2.17	0.44
5:I:52:DT:H2"	5:I:53:DC:H5"	1.98	0.44
4:H:86:ARG:HH21	4:H:93:GLU:CD	2.21	0.44
4:D:72:ARG:HB3	4:D:101:LEU:CD1	2.48	0.44
1:E:46:VAL:HG21	5:I:82:DA:H3'	1.99	0.44
5:J:194:DT:H1'	5:J:195:DC:H5'	2.00	0.44
5:J:233:DG:H2"	5:J:234:DC:O4'	2.18	0.43
2:B:39:ARG:NH1	2:B:43:VAL:O	2.51	0.43
4:H:105:GLU:HB3	4:H:106:LEU:HA	2.01	0.43
5:I:2:DT:H2"	5:I:3:DC:C6	2.54	0.43
5:I:54:DA:H61	5:J:239:DT:H3	1.66	0.43
5:I:58:DG:H2'	5:I:59:DG:C8	2.54	0.43
5:I:114:DC:H2"	5:I:115:DA:H5'	2.01	0.43
3:C:87:ILE:HD13	3:C:97:LEU:HD12	2.00	0.43
5:J:226:DT:H2"	5:J:227:DG:C8	2.54	0.43
4:H:86:ARG:NH2	4:H:88:THR:O	2.52	0.43
5:J:288:DT:H1'	5:J:289:DT:H5"	2.00	0.43
4:H:107:ALA:O	4:H:111:VAL:HG23	2.19	0.43
4:H:115:THR:O	4:H:119:THR:HG23	2.19	0.43
2:B:72:TYR:OH	2:B:92:ARG:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:HD12	1:E:106:ASP:HB3	2.00	0.42
3:C:37:GLY:HA3	3:C:39:TYR:CE2	2.54	0.42
5:I:144:DG:H1	5:J:149:DC:N4	2.15	0.42
2:B:78:ARG:HD2	5:J:248:DA:H5'	2.02	0.42
5:I:139:DA:H2"	5:I:140:DT:H5'	2.02	0.42
1:A:42:ARG:NH2	5:I:68:DG:OP2	2.40	0.42
2:B:75:HIS:CD2	4:D:80:LEU:HD22	2.55	0.42
1:E:131:ARG:HD3	1:E:133:GLU:OE2	2.20	0.42
5:J:235:DC:O2	5:J:236:DT:N3	2.52	0.42
5:J:280:DG:H2"	5:J:281:DG:H8	1.85	0.41
1:E:134:ARG:HB3	1:E:134:ARG:CZ	2.49	0.41
5:I:31:DG:H1'	5:I:32:DT:H5'	2.01	0.41
4:H:86:ARG:HH22	4:H:90:THR:HG23	1.85	0.41
5:I:131:DG:H2"	5:I:132:DC:C6	2.55	0.41
1:E:46:VAL:O	1:E:50:GLU:HG3	2.21	0.41
4:H:92:ARG:HG2	4:H:92:ARG:HH11	1.85	0.41
5:I:99:DA:H1'	5:I:100:DG:H5'	2.01	0.41
1:A:57:SER:HB2	1:A:59:GLU:OE1	2.19	0.41
1:A:83:ARG:O	2:B:80:THR:HA	2.21	0.41
3:C:30:VAL:HG13	4:D:70:PHE:HE1	1.86	0.41
1:E:121:PRO:CB	2:F:53:GLU:HG3	2.48	0.41
5:J:192:DG:H1'	5:J:193:DC:H5'	2.02	0.41
5:J:235:DC:H2"	5:J:236:DT:C5	2.56	0.41
5:J:268:DG:H2"	5:J:269:DT:H71	2.02	0.41
5:J:283:DG:H2'	5:J:284:DG:C8	2.56	0.41
1:E:119:ILE:O	2:F:47:SER:HB3	2.21	0.40
5:I:50:DC:H2"	5:I:51:DA:C8	2.56	0.40
2:F:26:ILE:HD12	2:F:26:ILE:HA	1.96	0.40
5:I:145:DA:C2	5:I:146:DT:H73	2.57	0.40
3:C:62:ILE:HG12	3:C:93:LEU:HD13	2.03	0.40
5:I:134:DG:N2	5:J:160:DT:O2	2.54	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%)	94 (99%)	1 (1%)	0	100	100
1	E	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
2	B	76/106 (72%)	76 (100%)	0	0	100	100
2	F	82/106 (77%)	81 (99%)	1 (1%)	0	100	100
3	C	103/133 (77%)	100 (97%)	3 (3%)	0	100	100
3	G	102/133 (77%)	98 (96%)	4 (4%)	0	100	100
4	D	92/129 (71%)	87 (95%)	5 (5%)	0	100	100
4	H	90/129 (70%)	86 (96%)	4 (4%)	0	100	100
All	All	735/1014 (72%)	716 (97%)	19 (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	83/112 (74%)	82 (99%)	1 (1%)	71	89
1	E	83/112 (74%)	82 (99%)	1 (1%)	71	89
2	B	63/81 (78%)	62 (98%)	1 (2%)	62	85
2	F	69/81 (85%)	68 (99%)	1 (1%)	67	87
3	C	83/102 (81%)	83 (100%)	0	100	100
3	G	83/102 (81%)	82 (99%)	1 (1%)	71	89
4	D	81/110 (74%)	80 (99%)	1 (1%)	71	89
4	H	80/110 (73%)	78 (98%)	2 (2%)	47	77
All	All	625/810 (77%)	617 (99%)	8 (1%)	69	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	SER
2	B	58	LEU
4	D	34	LYS
1	E	79	LYS
2	F	47	SER
3	G	114	VAL
4	H	92	ARG
4	H	100	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	82	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 monosaccharides 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%)	-0.10	0 100 100	31, 43, 69, 96	0
1	E	97/139 (69%)	-0.18	0 100 100	24, 35, 60, 75	0
2	B	78/106 (73%)	-0.12	1 (1%) 77 77	30, 43, 55, 63	0
2	F	84/106 (79%)	-0.08	1 (1%) 79 78	24, 35, 53, 76	0
3	C	105/133 (78%)	-0.13	0 100 100	28, 40, 62, 81	0
3	G	104/133 (78%)	-0.14	1 (0%) 82 82	32, 47, 68, 91	0
4	D	94/129 (72%)	-0.06	1 (1%) 80 80	29, 43, 64, 116	0
4	H	92/129 (71%)	0.04	1 (1%) 80 80	31, 48, 68, 87	0
5	I	146/146 (100%)	0.24	4 (2%) 54 51	47, 97, 132, 149	0
5	J	146/146 (100%)	0.10	4 (2%) 54 51	53, 99, 130, 140	0
All	All	1043/1306 (79%)	-0.02	13 (1%) 79 78	24, 47, 118, 149	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	146	DT	7.4
5	J	148	DT	5.0
2	F	102	GLY	4.6
5	I	55	DA	3.8
5	I	54	DA	3.3
5	J	241	DA	3.0
5	J	147	DA	2.9
2	B	102	GLY	2.7
4	H	106	LEU	2.6
4	D	32	GLY	2.4
5	I	56	DA	2.1
5	J	240	DG	2.1
3	G	118	LYS	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 (i)

There are no monosaccharides 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.