Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:19 PM GMT

PDB ID	:	3WTP
Title	:	Crystal Structure of the heterotypic nucleosome containing human CENP-A and H3.3
Authors	:	Arimura, Y.; Shirayama, K.; Horikoshi, N.; Fujita, R.; Kagawa, W.; Fukagawa, T.; Almouzni, G.; Kurumizaka, H.
Deposited on	:	2014-04-14
Resolution	:	2.67 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:

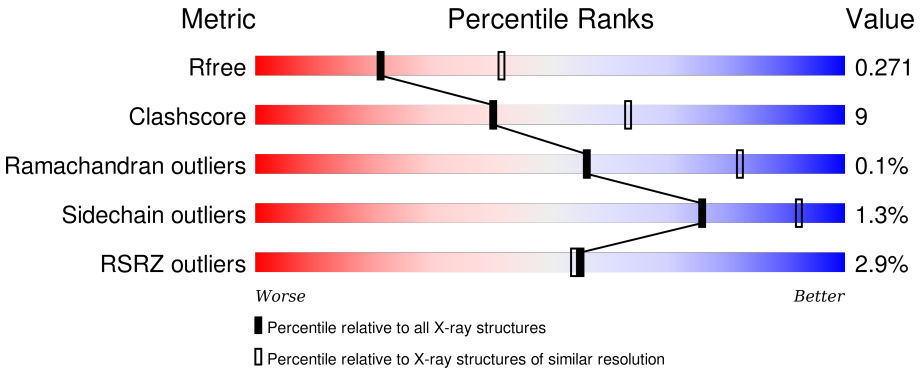
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.67 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	143	3% 43% 17% • 38%
2	B	106	61% 12% 26%
2	F	106	% 70% 10% 20%
3	C	133	2% 72% 8% • 20%
3	G	133	2% 65% 12% 23%

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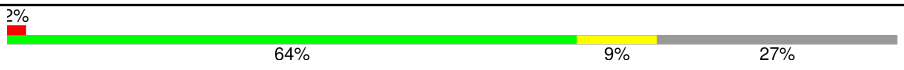
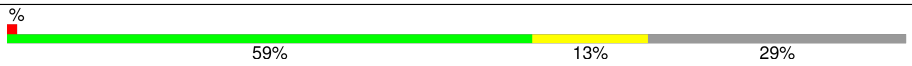
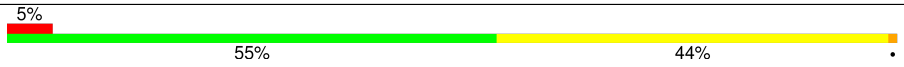
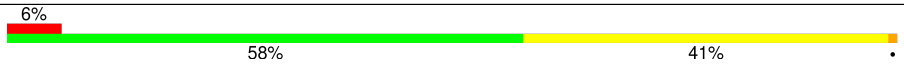
Mol	Chain	Length	Quality of chain
4	D	129	
4	H	129	
5	E	140	
6	I	146	
6	J	146	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11916 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-like centromeric protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	0	0
			732	477	136	118	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P49450
A	-1	SER	-	EXPRESSION TAG	UNP P49450
A	0	HIS	-	EXPRESSION TAG	UNP P49450

- 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	85	Total	C	N	O	S	0	0	0
			682	430	136	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 type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	107	Total	C	N	O	0	0	0
			824	520	161	143			
3	G	103	Total	C	N	O	0	0	0
			794	500	155	139			

There are 6 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
G	-3	GLY	-	EXPRESSION TAG	UNP P04908
G	-2	SER	-	EXPRESSION TAG	UNP P04908
G	-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	94	Total	C	N	O	S	0	0	0
			740	465	135	138	2			
4	H	93	Total	C	N	O	S	0	0	0
			725	456	130	137	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 H3.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	100	Total	C	N	O	S	0	0	0
			820	518	160	140	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	GLY	-	EXPRESSION TAG	UNP P84243
E	-3	PRO	-	EXPRESSION TAG	UNP P84243
E	-2	GLY	-	EXPRESSION TAG	UNP P84243
E	-1	HIS	-	EXPRESSION TAG	UNP P84243

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

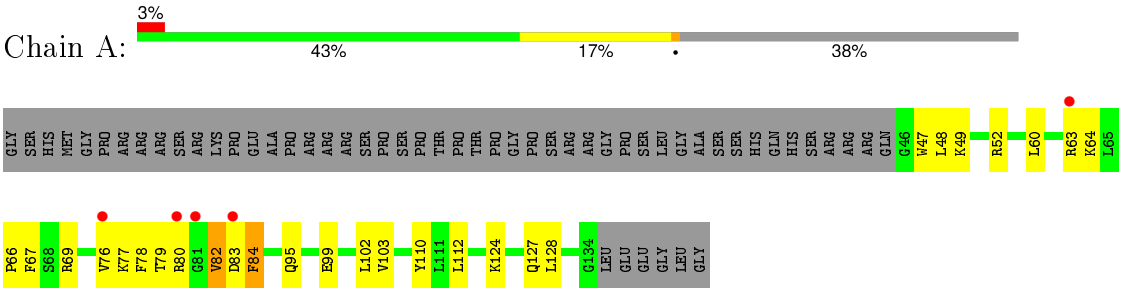
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			
6	J	146	Total	C	N	O	P	0	0	0
			2990	1431	540	874	145			

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.

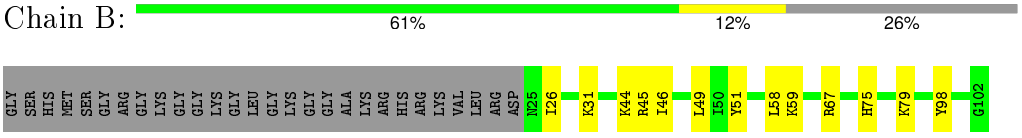
- Molecule 1: Histone H3-like centromeric protein A

Chain A:



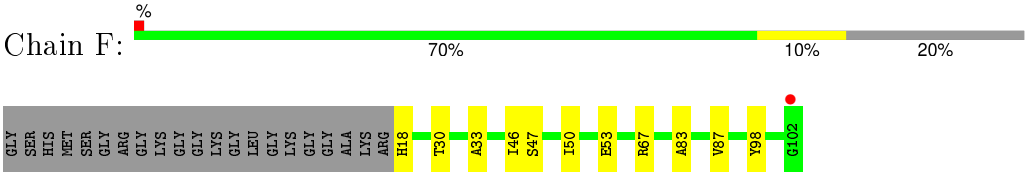
- Molecule 2: Histone H4

Chain B:



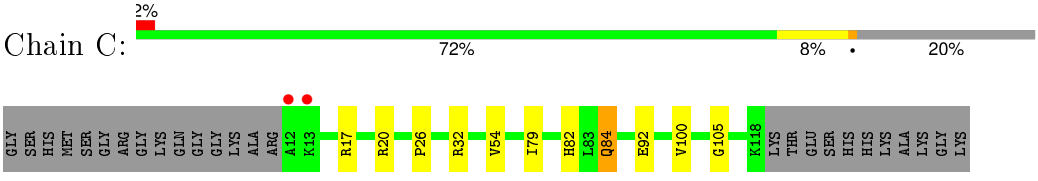
- Molecule 2: Histone H4

Chain F:



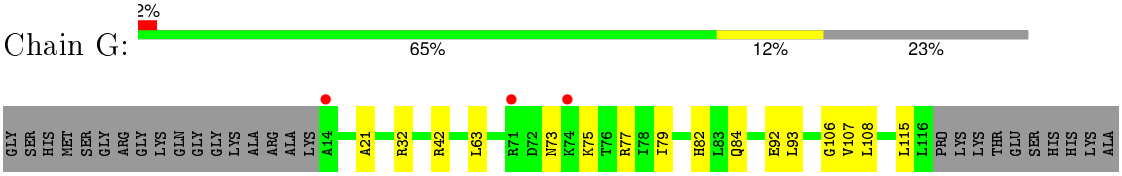
- Molecule 3: Histone H2A type 1-B/E

Chain C:



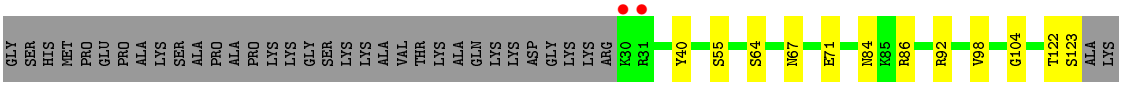
- Molecule 3: Histone H2A type 1-B/E

Chain G:



- Molecule 4: Histone H2B type 1-J

Chain D:

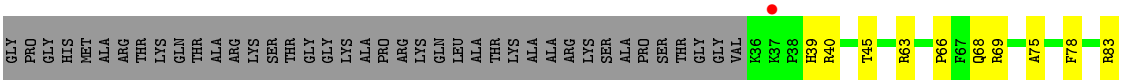


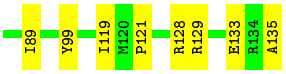
- Molecule 4: Histone H2B type 1-J

Chain H:

- Molecule 5: Histone H3.3

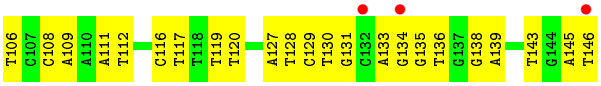
Chain E:





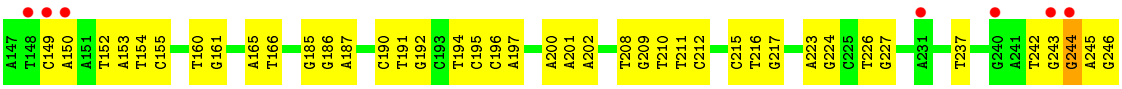
- Molecule 6: DNA (146-MER)

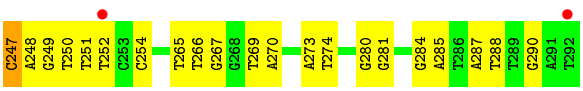
Chain I:



- 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	98.12Å 107.67Å 168.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.67 – 2.67 48.67 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.67-2.67) 97.1 (48.67-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.229 , 0.270 0.231 , 0.271	Depositor DCC
R_{free} test set	2553 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 50743 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11916	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.35	0/747	0.53	0/1006
2	B	0.33	0/626	0.55	0/837
2	F	0.43	0/690	0.60	0/923
3	C	0.38	0/834	0.55	0/1125
3	G	0.34	0/803	0.55	0/1084
4	D	0.41	0/751	0.59	0/1008
4	H	0.40	0/736	0.58	0/990
5	E	0.43	0/832	0.58	0/1115
6	I	0.79	0/3354	1.04	1/5175 (0.0%)
6	J	0.83	1/3354 (0.0%)	1.06	3/5175 (0.1%)
All	All	0.64	1/12727 (0.0%)	0.87	4/18438 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	244	DG	C3'-O3'	-5.74	1.36	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	247	DC	O4'-C1'-N1	7.55	113.29	108.00
6	J	212	DC	O4'-C1'-N1	5.31	111.72	108.00
6	J	191	DT	O4'-C1'-N1	5.30	111.71	108.00
6	I	39	DG	O4'-C1'-N9	5.29	111.70	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	732	0	770	26	0
2	B	619	0	659	12	0
2	F	682	0	729	12	0
3	C	824	0	884	8	0
3	G	794	0	846	19	0
4	D	740	0	766	10	0
4	H	725	0	745	11	0
5	E	820	0	865	19	0
6	I	2990	0	1652	72	0
6	J	2990	0	1652	54	0
All	All	11916	0	9568	186	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 (186) 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)
6:I:128:DT:H2"	6:I:129:DC:H5"	1.53	0.90
4:D:86:ARG:HH12	6:I:39:DG:H3'	1.36	0.89
5:E:69:ARG:NH2	6:I:90:DT:OP2	2.07	0.88
1:A:79:THR:HG21	1:A:82:VAL:HG22	1.59	0.84
6:J:194:DT:H2"	6:J:195:DC:H5"	1.60	0.83
1:A:48:LEU:HD11	1:A:52:ARG:NH1	1.99	0.77
6:J:249:DG:H2"	6:J:250:DT:H5"	1.69	0.75
6:J:242:DT:H2"	6:J:243:DG:H5"	1.70	0.73
6:J:245:DA:H2"	6:J:246:DG:C8	2.27	0.69
3:G:77:ARG:HH22	6:J:166:DT:H4'	1.58	0.68
6:J:243:DG:H2"	6:J:244:DG:C8	2.29	0.68
3:G:77:ARG:NH2	6:J:166:DT:H4'	2.09	0.67
1:A:79:THR:CG2	1:A:82:VAL:HG22	2.24	0.66
6:I:51:DA:H2"	6:I:52:DT:H5"	1.78	0.66
5:E:121:PRO:HB3	2:F:53:GLU:HG3	1.78	0.65
1:A:124:LYS:HA	1:A:127:GLN:HG2	1.79	0.65
6:I:40:DG:H2"	6:I:41:DA:C8	2.32	0.64
6:I:97:DG:H2"	6:I:98:DG:C8	2.32	0.64
6:I:119:DT:H1'	6:I:120:DT:H5'	1.79	0.64
6:I:99:DA:H2"	6:I:100:DG:C8	2.34	0.63
6:I:26:DC:H42	6:J:267:DG:H1	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:86:ARG:NH2	6:J:187:DA:OP2	2.33	0.62
6:I:143:DT:H3	6:J:150:DA:H61	1.48	0.61
6:I:47:DC:H2"	6:I:48:DT:C6	2.35	0.61
4:D:86:ARG:NH1	6:I:39:DG:H3'	2.13	0.61
6:J:265:DT:H2"	6:J:266:DT:H5"	1.83	0.60
1:A:78:PHE:CE1	2:B:67:ARG:HG3	2.38	0.59
6:I:133:DA:H2"	6:I:134:DG:H5"	1.84	0.59
6:I:3:DC:H2"	6:I:4:DA:C8	2.38	0.59
5:E:39:HIS:HD2	6:I:6:DT:H5'	1.67	0.58
6:I:38:DT:H2"	6:I:39:DG:C8	2.38	0.58
6:J:266:DT:H2"	6:J:267:DG:C8	2.38	0.58
6:J:287:DA:H2'	6:J:288:DT:C6	2.39	0.58
4:H:76:GLU:OE1	4:H:79:ARG:NH1	2.37	0.58
1:A:110:TYR:HE2	3:G:115:LEU:HD11	1.67	0.57
2:F:46:ILE:HG23	2:F:50:ILE:HG12	1.86	0.57
3:G:75:LYS:HE2	6:I:131:DG:OP1	2.04	0.57
6:J:190:DC:H4'	6:J:190:DC:OP1	2.04	0.57
1:A:84:PHE:CE1	2:B:79:LYS:HA	2.39	0.57
1:A:48:LEU:HD13	1:A:52:ARG:HG3	1.87	0.57
6:I:96:DT:H2"	6:I:97:DG:H5"	1.86	0.56
3:C:84:GLN:HG3	3:C:105:GLY:HA3	1.86	0.56
1:A:49:LYS:NZ	6:J:155:DC:H5'	2.21	0.56
3:G:63:LEU:HD13	4:H:45:LEU:HB2	1.87	0.55
6:J:208:DT:H2"	6:J:209:DG:C8	2.41	0.55
3:C:17:ARG:HA	3:C:20:ARG:HD2	1.87	0.55
6:J:243:DG:H2"	6:J:244:DG:H8	1.70	0.54
6:I:103:DG:H2"	6:I:104:DT:H5"	1.89	0.54
6:J:248:DA:H2"	6:J:249:DG:H5"	1.90	0.53
6:J:215:DC:H2"	6:J:216:DT:H71	1.90	0.53
6:I:98:DG:H2"	6:I:99:DA:C8	2.43	0.53
6:I:135:DG:H2"	6:I:136:DT:O4'	2.08	0.53
5:E:68:GLN:HG2	5:E:89:ILE:HG21	1.90	0.53
2:F:18:HIS:O	2:F:18:HIS:ND1	2.41	0.53
6:I:130:DT:H2"	6:I:131:DG:OP2	2.08	0.53
6:I:134:DG:H2"	6:I:135:DG:H8	1.74	0.53
5:E:63:ARG:HE	5:E:66:PRO:HG2	1.73	0.53
5:E:69:ARG:HH22	6:I:90:DT:P	2.30	0.52
6:I:69:DC:H2"	6:I:70:DT:H71	1.90	0.52
6:I:12:DC:H42	6:J:281:DG:H1	1.56	0.52
3:G:92:GLU:OE2	4:H:104:GLY:O	2.28	0.52
4:D:64:SER:HB3	2:F:98:TYR:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:129:DC:H2"	6:I:130:DT:C7	2.38	0.52
1:A:84:PHE:HE1	2:B:79:LYS:HA	1.73	0.52
1:A:82:VAL:HG21	1:A:84:PHE:CD2	2.45	0.52
6:J:200:DA:H2"	6:J:201:DA:H5'	1.92	0.52
6:I:89:DC:H2"	6:I:90:DT:H71	1.92	0.52
1:A:124:LYS:HA	1:A:127:GLN:CG	2.40	0.51
4:H:99:ARG:NH2	4:H:108:LYS:NZ	2.59	0.51
6:I:64:DT:H5'	6:I:64:DT:H6	1.74	0.51
6:I:38:DT:H2"	6:I:39:DG:N7	2.26	0.51
3:G:42:ARG:CZ	6:I:111:DA:H4'	2.40	0.51
2:B:98:TYR:CD1	4:H:64:SER:HB3	2.46	0.51
6:I:105:DT:H2"	6:I:106:DT:OP2	2.11	0.51
6:J:273:DA:H2"	6:J:274:DT:H5"	1.94	0.50
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.47	0.50
1:A:95:GLN:O	1:A:99:GLU:HG3	2.12	0.49
6:I:88:DC:H2"	6:I:89:DC:C5	2.47	0.49
6:I:22:DC:H1'	6:I:23:DT:H5'	1.94	0.49
6:J:223:DA:H2"	6:J:224:DG:C8	2.47	0.49
6:I:129:DC:H2"	6:I:130:DT:H71	1.95	0.49
6:J:149:DC:H2"	6:J:150:DA:H8	1.78	0.48
3:G:84:GLN:NE2	3:G:106:GLY:O	2.46	0.48
6:I:38:DT:H2"	6:I:39:DG:C5	2.47	0.48
5:E:128:ARG:HD2	5:E:133:GLU:OE1	2.14	0.48
6:I:116:DC:H2'	6:I:117:DT:H72	1.94	0.48
1:A:79:THR:HG23	1:A:82:VAL:H	1.79	0.48
6:I:56:DA:H2"	6:I:57:DA:C8	2.49	0.48
5:E:40:ARG:NH2	6:I:82:DA:N3	2.62	0.48
6:I:6:DT:H2"	6:I:7:DA:H5'	1.96	0.47
6:I:108:DC:H2"	6:I:109:DA:N7	2.29	0.47
6:J:210:DT:H2'	6:J:211:DT:H71	1.95	0.47
6:I:145:DA:H2"	6:I:146:DT:H5"	1.95	0.47
1:A:63:ARG:O	1:A:66:PRO:HD2	2.15	0.47
6:I:39:DG:H1	6:J:254:DC:H42	1.62	0.47
6:I:138:DG:H2"	6:I:139:DA:OP2	2.14	0.47
6:I:119:DT:H5'	6:I:119:DT:H6	1.80	0.47
6:I:101:DC:H42	6:J:192:DG:H1	1.61	0.47
6:J:251:DT:H2"	6:J:252:DT:OP2	2.15	0.47
6:J:216:DT:H2"	6:J:217:DG:C8	2.50	0.47
1:A:60:LEU:HD13	1:A:95:GLN:OE1	2.15	0.47
2:F:83:ALA:O	2:F:87:VAL:HG23	2.15	0.47
5:E:83:ARG:HD2	6:I:100:DG:H5"	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ILE:O	6:J:227:DG:H3'	2.15	0.47
6:J:154:DT:H2"	6:J:155:DC:C6	2.50	0.46
3:C:54:VAL:HG21	4:D:98:VAL:HG21	1.98	0.46
5:E:75:ALA:O	5:E:78:PHE:N	2.49	0.46
6:J:152:DT:H2"	6:J:153:DA:H5'	1.97	0.46
5:E:63:ARG:HH12	2:F:33:ALA:HB2	1.80	0.46
2:B:75:HIS:O	4:D:92:ARG:NH1	2.29	0.46
1:A:67:PHE:CG	1:A:95:GLN:HG3	2.51	0.46
3:C:92:GLU:OE2	4:D:104:GLY:O	2.34	0.46
1:A:47:TRP:CE2	2:B:44:LYS:HE3	2.51	0.46
6:J:284:DG:H2"	6:J:285:DA:OP2	2.16	0.45
6:I:127:DA:H2"	6:I:128:DT:H5"	1.97	0.45
6:J:194:DT:C2'	6:J:195:DC:H5"	2.39	0.45
6:I:94:DG:H2"	6:I:95:DA:OP2	2.16	0.45
2:B:31:LYS:HG3	2:B:51:TYR:CE1	2.51	0.45
6:I:55:DA:H2"	6:I:56:DA:H5"	1.99	0.45
2:B:31:LYS:HG3	2:B:51:TYR:CZ	2.52	0.45
3:G:108:LEU:HA	3:G:108:LEU:HD12	1.79	0.45
1:A:48:LEU:HD11	1:A:52:ARG:HH11	1.80	0.45
6:I:111:DA:H2'	6:I:112:DT:C7	2.46	0.45
6:J:250:DT:H2'	6:J:251:DT:H71	1.98	0.45
6:I:50:DC:H2"	6:I:51:DA:H8	1.82	0.45
6:I:47:DC:H42	6:J:246:DG:H1	1.64	0.44
6:I:111:DA:H2"	6:I:112:DT:H5'	1.99	0.44
6:J:196:DC:H2"	6:J:197:DA:C8	2.52	0.44
1:A:64:LYS:HE2	1:A:64:LYS:HB3	1.50	0.44
6:I:26:DC:N4	6:J:267:DG:H1	2.12	0.44
6:I:51:DA:C5	6:I:52:DT:C4	3.06	0.44
6:I:143:DT:H3	6:J:150:DA:N6	2.14	0.44
1:A:76:VAL:HA	1:A:79:THR:HG22	1.98	0.44
5:E:45:THR:OG1	6:J:290:DG:OP1	2.29	0.44
4:D:67:ASN:O	4:D:71:GLU:HG3	2.18	0.44
3:G:73:ASN:O	3:G:73:ASN:OD1	2.35	0.44
6:I:50:DC:H2"	6:I:51:DA:C8	2.53	0.44
6:I:52:DT:H2"	6:I:53:DC:O4'	2.18	0.44
6:J:244:DG:C6	6:J:245:DA:C6	3.06	0.44
6:J:269:DT:H2"	6:J:270:DA:C8	2.53	0.44
6:J:185:DG:C5	6:J:186:DG:C6	3.06	0.43
1:A:69:ARG:NH2	6:J:237:DT:OP2	2.52	0.43
6:J:165:DA:H2"	6:J:166:DT:H5'	2.01	0.43
6:I:111:DA:H2'	6:I:112:DT:H72	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:ARG:HG3	5:E:135:ALA:HB3	2.01	0.43
1:A:77:LYS:HD2	1:A:77:LYS:HA	1.76	0.43
3:G:75:LYS:HE2	6:I:131:DG:P	2.59	0.43
6:I:51:DA:H61	6:J:242:DT:H3	1.66	0.43
5:E:39:HIS:CD2	6:I:6:DT:H5'	2.51	0.43
6:J:160:DT:H2"	6:J:161:DG:C8	2.54	0.43
6:I:90:DT:O4	6:J:202:DA:N6	2.52	0.43
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.54	0.43
2:F:46:ILE:HG23	2:F:50:ILE:CG1	2.49	0.43
6:J:280:DG:H2"	6:J:281:DG:H8	1.84	0.43
5:E:119:ILE:O	2:F:47:SER:HB3	2.19	0.43
2:B:45:ARG:HE	2:B:45:ARG:HB3	1.48	0.42
6:J:266:DT:H2"	6:J:267:DG:N7	2.33	0.42
3:C:32:ARG:NH1	6:I:29:DA:OP1	2.45	0.42
6:I:56:DA:H2"	6:I:57:DA:N7	2.35	0.42
5:E:63:ARG:NH1	2:F:30:THR:OG1	2.53	0.42
6:J:226:DT:H2"	6:J:227:DG:C8	2.55	0.42
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.54	0.42
5:E:99:TYR:OH	5:E:133:GLU:OE1	2.37	0.42
6:I:52:DT:C4	6:I:53:DC:C4	3.07	0.42
6:J:243:DG:C6	6:J:244:DG:C6	3.08	0.42
5:E:63:ARG:NH2	2:F:30:THR:H	2.18	0.41
4:H:76:GLU:HA	4:H:79:ARG:NH1	2.35	0.41
6:J:246:DG:C5	6:J:247:DC:C4	3.09	0.41
6:I:119:DT:C1'	6:I:120:DT:H5'	2.48	0.41
4:D:84:ASN:O	4:D:86:ARG:HG3	2.20	0.41
2:B:26:ILE:HD12	2:B:59:LYS:HD2	2.02	0.41
1:A:102:LEU:HD11	2:B:58:LEU:HD13	2.03	0.41
1:A:103:VAL:HG11	3:G:107:VAL:HG11	2.02	0.41
3:G:93:LEU:HA	3:G:93:LEU:HD23	1.94	0.41
3:G:42:ARG:NH1	6:I:111:DA:H4'	2.36	0.41
3:G:32:ARG:NH1	4:H:35:GLU:OE2	2.45	0.41
3:C:26:PRO:HG3	4:D:40:TYR:CZ	2.55	0.41
3:G:79:ILE:HG22	4:H:55:SER:HB2	2.02	0.41
6:I:51:DA:H2"	6:I:52:DT:O4'	2.20	0.40
6:I:7:DA:H2"	6:I:8:DT:OP2	2.21	0.40
3:G:21:ALA:HB2	4:H:121:TYR:HB2	2.04	0.40
1:A:112:LEU:HD22	1:A:128:LEU:HD23	2.02	0.40
4:H:46:LYS:HA	4:H:46:LYS:HD3	1.83	0.40
5:E:78:PHE:CZ	2:F:67:ARG:HB2	2.56	0.40
4:D:55:SER:HA	6:I:19:DA:H5"	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:77:ARG:CZ	6:J:166:DT:H4'	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	87/143 (61%)	84 (97%)	2 (2%)	1 (1%)	17 40
2	B	76/106 (72%)	75 (99%)	1 (1%)	0	100 100
2	F	83/106 (78%)	80 (96%)	3 (4%)	0	100 100
3	C	105/133 (79%)	102 (97%)	3 (3%)	0	100 100
3	G	101/133 (76%)	98 (97%)	3 (3%)	0	100 100
4	D	92/129 (71%)	89 (97%)	3 (3%)	0	100 100
4	H	91/129 (70%)	90 (99%)	1 (1%)	0	100 100
5	E	98/140 (70%)	97 (99%)	1 (1%)	0	100 100
All	All	733/1019 (72%)	715 (98%)	17 (2%)	1 (0%)	56 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	75/120 (62%)	72 (96%)	3 (4%)	38 67
2	B	63/81 (78%)	62 (98%)	1 (2%)	70 90
2	F	70/81 (86%)	70 (100%)	0	100 100
3	C	84/102 (82%)	83 (99%)	1 (1%)	78 93
3	G	81/102 (79%)	81 (100%)	0	100 100
4	D	81/107 (76%)	79 (98%)	2 (2%)	55 83
4	H	79/107 (74%)	78 (99%)	1 (1%)	76 92
5	E	85/112 (76%)	85 (100%)	0	100 100
All	All	618/812 (76%)	610 (99%)	8 (1%)	76 92

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

Mol	Chain	Res	Type
1	A	80	ARG
1	A	83	ASP
1	A	84	PHE
2	B	49	LEU
3	C	84	GLN
4	D	122	THR
4	D	123	SER
4	H	39	ILE

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

Mol	Chain	Res	Type
3	C	73	ASN

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

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	89/143 (62%)	0.21	5 (5%) 28 25	27, 40, 70, 89	0
2	B	78/106 (73%)	0.11	0 100 100	29, 38, 52, 68	0
2	F	85/106 (80%)	0.07	1 (1%) 81 81	18, 24, 36, 68	0
3	C	107/133 (80%)	0.11	2 (1%) 70 69	19, 29, 45, 66	0
3	G	103/133 (77%)	0.16	3 (2%) 55 54	24, 36, 67, 79	0
4	D	94/129 (72%)	0.18	2 (2%) 67 66	20, 29, 49, 80	0
4	H	93/129 (72%)	0.16	0 100 100	20, 33, 58, 71	0
5	E	100/140 (71%)	0.05	1 (1%) 84 84	17, 26, 51, 80	0
6	I	146/146 (100%)	0.32	7 (4%) 34 32	38, 68, 121, 137	0
6	J	146/146 (100%)	0.38	9 (6%) 24 22	41, 72, 126, 132	0
All	All	1041/1311 (79%)	0.19	30 (2%) 55 54	17, 37, 102, 137	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	14	ALA	5.9
4	D	31	ARG	3.9
1	A	80	ARG	3.8
2	F	102	GLY	3.7
4	D	30	LYS	3.6
3	G	71	ARG	3.3
6	J	244	DG	3.2
6	J	148	DT	3.1
6	I	146	DT	3.1
6	J	149	DC	3.0
3	C	12	ALA	2.9
3	G	74	LYS	2.9
1	A	83	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	2.8
3	C	13	LYS	2.7
6	J	243	DG	2.7
6	J	231	DA	2.6
5	E	37	LYS	2.6
6	I	95	DA	2.5
1	A	76	VAL	2.5
6	J	292	DT	2.4
6	I	52	DT	2.4
6	I	132	DC	2.3
6	I	1	DA	2.3
6	J	240	DG	2.3
6	J	252	DT	2.2
6	J	150	DA	2.2
1	A	63	ARG	2.1
6	I	134	DG	2.0
6	I	53	DC	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.