



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2017 – 07:44 AM EST

PDB ID : 5ONW  
Title : X-Ray crystal structure of a nucleosome core particle with its DNA site-specifically crosslinked to the histone octamer and the two H2A/H2B dimers crosslinked via H2A N38C  
Authors : Frouws, T.D.; Barth, P.D.; Richmond, T.J.  
Deposited on : 2017-08-04  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

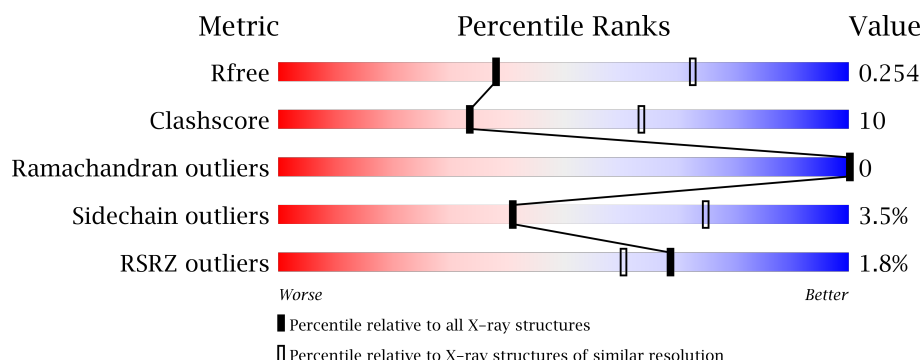
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	I	147	<div> <div>5%</div> <div>58%</div> <div>42%</div> </div>
2	J	147	<div> <div>%</div> <div>54%</div> <div>46%</div> </div>
3	A	135	<div> <div>%</div> <div>54%</div> <div>16%</div> <div>29%</div> </div>
3	E	135	<div> <div>%</div> <div>55%</div> <div>15%</div> <div>30%</div> </div>
4	B	103	<div> <div>%</div> <div>50%</div> <div>24%</div> <div>24%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	103	
5	C	129	
5	G	129	
6	D	122	
6	H	122	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MN	E	201	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12069 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 DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	I	147	Total	C	N	O	P	S	0	0	0
			3014	1440	548	879	146	1			

- Molecule 2 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	J	147	Total	C	N	O	P	S	0	0	0
			3013	1440	545	881	146	1			

- Molecule 3 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	96	Total	C	N	O	S	0	0	0
			789	498	151	137	3			
3	E	95	Total	C	N	O	S	0	0	0
			778	492	147	136	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	CYS	ARG	engineered mutation	UNP P84233
A	102	ALA	GLY	conflict	UNP P84233
A	110	ALA	CYS	engineered mutation	UNP P84233
E	40	CYS	ARG	engineered mutation	UNP P84233
E	102	ALA	GLY	conflict	UNP P84233
E	110	ALA	CYS	engineered mutation	UNP P84233

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	86	Total	C	N	O	S	0	0	0
			694	436	140	117	1			

- Molecule 5 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	103	Total	C	N	O	S	0	0	0
			793	500	154	138	1			
5	G	105	Total	C	N	O	S	0	0	0
			807	509	157	140	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	38	CYS	ASN	engineered mutation	UNP Q6AZJ8
G	38	CYS	ASN	engineered mutation	UNP Q6AZJ8

- Molecule 6 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	96	Total	C	N	O	S	0	0	0
			757	475	140	140	2			
6	H	92	Total	C	N	O	S	0	0	0
			719	453	129	135	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	9	Total	Mn	0	0
			9	9		
7	I	9	Total	Mn	0	0
			9	9		
7	D	1	Total	Mn	0	0
			1	1		
7	E	1	Total	Mn	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

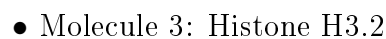
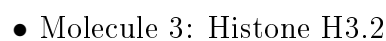
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total 1	Cl 1	0	0
8	A	1	Total 1	Cl 1	0	0
8	C	1	Total 1	Cl 1	0	0
8	E	1	Total 1	Cl 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	I	5	Total 5	O 5	0	0
9	J	5	Total 5	O 5	0	0
9	A	4	Total 4	O 4	0	0
9	B	6	Total 6	O 6	0	0
9	C	8	Total 8	O 8	0	0
9	D	4	Total 4	O 4	0	0
9	E	11	Total 11	O 11	0	0
9	F	10	Total 10	O 10	0	0
9	G	6	Total 6	O 6	0	0
9	H	3	Total 3	O 3	0	0



- Molecule 1: DNA (147-MER)





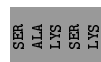
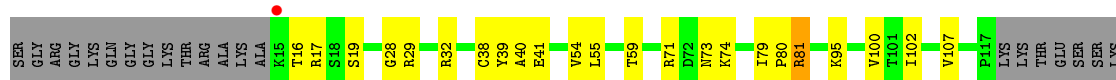
- Molecule 4: Histone H4



- Molecule 4: Histone H4



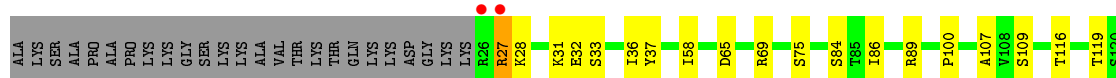
- Molecule 5: Histone H2A



- Molecule 5: Histone H2A



- Molecule 6: Histone H2B 1.1



- Molecule 6: Histone H2B 1.1



Chain H: 64%11%25%

ALA	LYS	SER	ALA	PRO	ALA	PRO	LYS	GLY	SER	LYS	LYS	ALA	VAL	THR	LYS	THR	GLN	LYS	ASP	GLY	LYS	LYS	ARG	ARG	LYS	THR	R30	Y37	K43	I58	E68	E73	A74	S75	R76	L77	N81	K82	R83	S84	T85	I86	K105	V108	T112	A121	LYS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.56Å 183.83Å 109.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.50 – 2.80 29.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.50-2.80) 98.4 (29.50-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.80Å)	Xtriage
Refinement program	PHENIX (dev_2447: ???)	Depositor
R, $R_{free}$	0.208 , 0.254 0.207 , 0.254	Depositor DCC
$R_{free}$ test set	2658 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.4	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 76.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: CL, MN, G47

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	I	0.56	0/3352	1.00	0/5169
2	J	0.56	0/3350	0.99	0/5166
3	A	0.27	0/800	0.43	0/1074
3	E	0.28	0/789	0.43	0/1060
4	B	0.30	0/626	0.47	0/837
4	F	0.28	0/702	0.47	0/937
5	C	0.27	0/803	0.47	0/1085
5	G	0.25	0/817	0.42	0/1103
6	D	0.27	0/768	0.41	0/1032
6	H	0.26	0/730	0.39	0/983
All	All	0.45	0/12737	0.80	0/18446

There are no bond length outliers.

There are no bond angle outliers.

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	I	3014	0	1663	54	0
2	J	3013	0	1664	58	0
3	A	789	0	824	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	778	0	811	19	0
4	B	619	0	659	26	0
4	F	694	0	742	15	0
5	C	793	0	844	15	0
5	G	807	0	862	16	0
6	D	757	0	786	14	0
6	H	719	0	740	14	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	I	9	0	0	0	0
7	J	9	0	0	1	0
8	A	1	0	0	1	0
8	C	1	0	0	1	0
8	E	1	0	0	0	0
8	G	1	0	0	0	0
9	A	4	0	0	1	0
9	B	6	0	0	1	0
9	C	8	0	0	0	0
9	D	4	0	0	1	0
9	E	11	0	0	0	0
9	F	10	0	0	1	0
9	G	6	0	0	0	0
9	H	3	0	0	1	0
9	I	5	0	0	0	0
9	J	5	0	0	1	0
All	All	12069	0	9595	206	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 10.

All (206) 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)
1:I:48:DC:N3	2:J:48:DG:N2	2.06	1.04
4:B:29:ILE:HD11	4:B:55:ARG:HG3	1.47	0.96
1:I:48:DG:N2	2:J:-47:DA:C2	2.36	0.94
3:A:39:HIS:CG	3:A:40:CYS:H	1.87	0.92
3:A:39:HIS:O	3:A:40:CYS:HB2	1.72	0.86
8:C:201:CL:CL	9:D:302:HOH:O	2.32	0.84
2:J:-14:DC:OP2	9:J:201:HOH:O	1.98	0.82
4:F:95:ARG:NH2	9:F:201:HOH:O	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:DC:H42	2:J:48:DG:H1	1.27	0.81
1:I:72:DA:H5''	3:A:39:HIS:NE2	1.96	0.81
1:I:48:DG:N2	2:J:-47:DA:H2	1.79	0.79
1:I:10:DA:H5''	3:E:39:HIS:N	1.98	0.77
2:J:48:DG:H2''	2:J:49:DG:H5''	1.68	0.75
4:B:42:GLY:O	9:B:201:HOH:O	2.05	0.74
3:A:39:HIS:CD2	3:A:40:CYS:H	2.04	0.74
3:A:39:HIS:CG	3:A:40:CYS:N	2.57	0.73
3:E:50:GLU:OE2	4:F:35:ARG:NH1	2.24	0.70
2:J:56:DG:H2''	2:J:57:DA:C8	2.27	0.69
3:E:61:LEU:O	4:F:36:ARG:NH1	2.25	0.69
3:A:73:GLU:OE1	9:A:301:HOH:O	2.10	0.68
4:B:44:LYS:HD3	5:G:115:LEU:HB2	1.75	0.68
4:B:75:HIS:O	6:D:89:ARG:NH2	2.27	0.68
4:B:29:ILE:HD12	4:B:34:ILE:HD11	1.76	0.68
5:G:102:ILE:HG23	6:H:58:ILE:HD13	1.75	0.67
1:I:-13:DA:H3'	4:B:30:THR:HB	1.77	0.67
1:I:48:DG:H2''	1:I:49:DG:C8	2.31	0.66
2:J:-51:DT:H2'	2:J:-50:DA:C8	2.31	0.65
5:G:37:GLY:HA3	5:G:39:TYR:CE2	2.31	0.65
2:J:-69:DA:H2''	2:J:-68:DT:H5''	1.79	0.65
1:I:72:DA:H2''	1:I:73:DT:H5''	1.79	0.65
3:A:79:LYS:NZ	3:A:80:THR:O	2.30	0.64
3:E:61:LEU:HD13	4:F:36:ARG:HB3	1.80	0.64
1:I:48:DG:H2''	1:I:49:DG:H8	1.62	0.64
2:J:-51:DT:H2'	2:J:-50:DA:H8	1.63	0.63
5:C:55:LEU:O	5:C:59:THR:HG23	1.99	0.63
4:F:30:THR:HB	4:F:32:PRO:HD2	1.82	0.62
2:J:72:DA:H2''	2:J:73:DT:H5''	1.81	0.62
5:G:42:ARG:HB2	6:H:85:THR:HG22	1.81	0.61
5:C:81:ARG:NH2	5:C:107:VAL:O	2.33	0.61
5:C:29:ARG:NH1	6:D:33:SER:O	2.34	0.61
4:B:78:ARG:NH2	4:B:85:ASP:OD2	2.33	0.60
3:E:59:GLU:N	3:E:59:GLU:OE1	2.34	0.60
2:J:-4:DT:H2''	2:J:-3:DG:C8	2.36	0.60
2:J:44:DT:H2''	2:J:45:DT:H5''	1.84	0.60
2:J:71:DG:O6	7:J:101:MN:MN	1.60	0.59
1:I:51:DA:H2''	1:I:52:DG:H5''	1.84	0.59
5:C:102:ILE:HG23	6:D:58:ILE:HD13	1.84	0.59
2:J:-28:DG:H1'	2:J:-27:DC:H5'	1.85	0.59
2:J:16:DC:H2'	2:J:17:DT:C6	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:-5:DC:H2"	2:J:-4:DT:H71	1.85	0.58
3:E:116:ARG:NH2	3:E:123:ASP:OD2	2.38	0.57
4:B:29:ILE:CD1	4:B:34:ILE:HD11	2.34	0.57
6:H:77:LEU:O	6:H:81:ASN:ND2	2.36	0.56
5:G:79:ILE:HG12	5:G:82:HIS:CE1	2.41	0.56
3:A:63:ARG:HE	3:A:66:PRO:HG2	1.71	0.56
4:F:68:ASP:OD2	4:F:93:GLN:NE2	2.39	0.55
5:G:55:LEU:O	5:G:59:THR:HG23	2.06	0.55
1:I:-61:DC:H2"	1:I:-60:DT:C6	2.42	0.55
5:G:116:LEU:HB3	5:G:117:PRO:HD2	1.89	0.54
1:I:48:DG:H21	2:J:-47:DA:H2	1.55	0.54
1:I:-5:DC:H2"	1:I:-4:DT:H71	1.90	0.54
3:A:116:ARG:NH2	3:A:123:ASP:OD2	2.41	0.54
4:B:89:ALA:O	4:B:93:GLN:HG2	2.08	0.53
1:I:39:DT:H2"	1:I:40:DA:H8	1.72	0.53
2:J:15:DC:H2"	2:J:16:DC:C6	2.43	0.53
2:J:64:DG:H2"	2:J:65:DG:C8	2.43	0.53
1:I:-47:DA:H2"	1:I:-46:DA:C8	2.44	0.53
2:J:-68:DT:H2"	2:J:-67:DA:C8	2.44	0.53
1:I:-26:DT:C6	1:I:-26:DT:H5'	2.43	0.53
5:C:95:LYS:HE3	6:D:100:PRO:HB3	1.89	0.53
3:E:51:ILE:O	3:E:55:GLN:HB2	2.08	0.52
2:J:-5:DC:H5'	3:E:43:PRO:HG2	1.91	0.52
5:G:43:VAL:HG12	6:H:86:ILE:HB	1.92	0.52
6:D:31:LYS:HD3	6:D:32:GLU:N	2.24	0.52
2:J:-21:DC:H2"	2:J:-20:DA:H5'	1.92	0.52
2:J:-55:DC:H2'	2:J:-54:DT:C6	2.45	0.52
5:G:39:TYR:OH	6:H:68:GLU:OE1	2.22	0.52
1:I:-48:DC:H2"	1:I:-47:DA:N7	2.25	0.52
1:I:-52:DC:H2'	1:I:-51:DT:C6	2.45	0.51
4:F:89:ALA:O	4:F:93:GLN:HG2	2.10	0.51
2:J:7:DT:H2"	2:J:8:DG:C8	2.46	0.51
2:J:54:DA:H1'	2:J:55:DG:H5'	1.92	0.51
2:J:-52:DC:H2"	2:J:-51:DT:H71	1.92	0.51
1:I:-6:DG:H2"	1:I:-5:DC:C6	2.46	0.51
2:J:-33:DA:P	6:H:83:ARG:HH21	2.33	0.51
3:A:108:ASN:ND2	4:B:42:GLY:O	2.44	0.50
4:F:57:VAL:O	4:F:60:VAL:HG13	2.11	0.50
1:I:28:DC:H2"	1:I:29:DA:C8	2.46	0.50
5:C:79:ILE:HB	5:C:80:PRO:HD2	1.91	0.50
3:E:62:ILE:HD11	4:F:37:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:-24:DC:H2"	1:I:-23:DA:C8	2.45	0.50
4:F:31:LYS:HG3	4:F:51:TYR:CE1	2.47	0.50
1:I:-44:DA:P	5:C:32:ARG:HH21	2.34	0.50
1:I:48:DG:H5"	6:H:37:TYR:OH	2.12	0.50
2:J:-33:DA:OP2	6:H:83:ARG:NH2	2.43	0.50
1:I:62:DG:C8	1:I:63:DT:H72	2.46	0.49
3:A:121:PRO:HG2	8:A:201:CL:CL	2.49	0.49
1:I:23:DT:H2"	1:I:24:DG:C8	2.47	0.49
2:J:-66:DT:OP1	3:A:49:ARG:HD3	2.12	0.49
3:A:113:HIS:CG	3:E:126:LEU:HD22	2.48	0.49
3:E:78:PHE:CZ	4:F:67:ARG:HG2	2.48	0.49
1:I:4:DA:H1'	1:I:5:DG:H5'	1.95	0.48
1:I:45:DT:H1'	1:I:46:DT:H5'	1.94	0.48
5:C:40:ALA:HB3	6:D:86:ILE:HG12	1.96	0.48
1:I:47:DT:H2"	1:I:48:DG:C8	2.48	0.48
1:I:-68:DT:H2"	1:I:-67:DA:C8	2.49	0.48
2:J:8:DG:H2"	2:J:9:DA:H8	1.80	0.47
3:E:54:TYR:CZ	4:F:36:ARG:HG2	2.50	0.47
1:I:7:DT:H2"	1:I:8:DG:C8	2.49	0.47
5:C:41:GLU:HB3	6:D:84:SER:HB2	1.96	0.47
3:A:118:THR:CG2	4:B:45:ARG:HE	2.28	0.47
2:J:59:DC:H2"	2:J:60:DA:C8	2.50	0.47
4:B:31:LYS:HG3	4:B:51:TYR:CE1	2.50	0.47
3:A:50:GLU:HB2	4:B:39:ARG:HD2	1.97	0.46
3:A:126:LEU:HD22	3:E:113:HIS:CG	2.50	0.46
3:E:42:ARG:HB3	3:E:43:PRO:HD2	1.96	0.46
4:B:26:ILE:HG23	4:B:27:GLN:NE2	2.30	0.46
1:I:15:DC:H2"	1:I:16:DC:C6	2.50	0.46
3:A:63:ARG:NE	3:A:66:PRO:HG2	2.31	0.46
4:B:30:THR:O	4:B:33:ALA:N	2.34	0.46
1:I:-54:DT:C2	1:I:-53:DA:C8	3.04	0.46
6:H:73:GLU:OE2	9:H:201:HOH:O	2.20	0.46
4:F:63:GLU:O	4:F:67:ARG:HG3	2.16	0.45
1:I:15:DC:H2"	1:I:16:DC:C5	2.50	0.45
3:A:46:VAL:O	3:A:50:GLU:HG3	2.16	0.45
2:J:45:DT:H1'	2:J:46:DT:H5'	1.98	0.45
2:J:-58:DG:H2"	2:J:-57:DT:C7	2.45	0.45
3:E:72:ARG:O	3:E:76:GLN:HB2	2.16	0.45
1:I:52:DG:C8	1:I:53:DT:H72	2.51	0.45
3:A:118:THR:HG22	4:B:45:ARG:HB3	1.99	0.45
6:D:65:ASP:OD1	6:D:69:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:-33:DA:H2''	1:I:-32:DA:H8	1.82	0.45
6:H:43:LYS:HD3	6:H:43:LYS:HA	1.59	0.45
2:J:-52:DC:C2'	2:J:-51:DT:H71	2.47	0.45
2:J:10:DA:H5''	3:A:39:HIS:N	2.32	0.45
3:A:118:THR:HG21	4:B:45:ARG:HE	1.81	0.44
1:I:-12:DT:H2''	1:I:-11:DG:C8	2.52	0.44
6:H:108:VAL:O	6:H:112:THR:HG22	2.18	0.44
1:I:-3:DG:H2''	1:I:-2:DG:C8	2.53	0.44
4:B:79:LYS:HE2	4:B:79:LYS:HB3	1.87	0.44
2:J:-12:DT:H2''	2:J:-11:DG:C8	2.53	0.44
2:J:16:DC:H4'	2:J:17:DT:OP1	2.18	0.44
2:J:39:DT:H2''	2:J:40:DA:H8	1.83	0.44
1:I:-45:DA:H5''	1:I:-45:DA:H8	1.83	0.44
1:I:-32:DA:H2''	1:I:-31:DA:H8	1.83	0.44
3:A:73:GLU:OE2	4:B:25:ASN:N	2.50	0.44
6:H:105:LYS:HD2	6:H:105:LYS:HA	1.81	0.44
2:J:-32:DA:C8	2:J:-32:DA:H5'	2.53	0.44
1:I:16:DC:H2''	1:I:17:DT:H71	2.00	0.43
1:I:48:DG:C8	1:I:49:DG:N7	2.86	0.43
2:J:-21:DC:H2'	2:J:-20:DA:H8	1.82	0.43
4:B:56:GLY:O	4:B:60:VAL:HG12	2.18	0.43
1:I:18:DT:OP1	3:E:63:ARG:NH1	2.43	0.43
3:A:61:LEU:HD13	4:B:36:ARG:HB3	2.01	0.43
1:I:18:DT:H1'	1:I:19:DT:H5'	2.00	0.43
2:J:8:DG:H2''	2:J:9:DA:C8	2.54	0.43
1:I:-53:DA:C4	1:I:-52:DC:C5	3.06	0.43
3:A:69:ARG:HB3	4:B:25:ASN:ND2	2.33	0.43
2:J:-21:DC:H2'	2:J:-20:DA:C8	2.53	0.43
5:C:17:ARG:NH2	5:C:28:GLY:HA2	2.33	0.42
1:I:59:DC:H2''	1:I:60:DA:N7	2.34	0.42
2:J:-22:DT:C2	2:J:-21:DC:C5	3.07	0.42
2:J:68:DA:H2''	2:J:69:DT:C6	2.54	0.42
6:D:36:ILE:HD11	6:D:37:TYR:CZ	2.54	0.42
1:I:72:DA:P	3:A:42:ARG:HE	2.42	0.42
6:D:27:ARG:HA	6:D:27:ARG:HD2	1.71	0.42
3:E:46:VAL:O	3:E:50:GLU:HG3	2.19	0.42
1:I:-4:DT:H2''	1:I:-3:DG:C8	2.54	0.42
1:I:-56:DC:H4'	1:I:-55:DC:OP1	2.19	0.42
4:B:98:TYR:CE2	5:G:100:VAL:HG11	2.53	0.42
3:E:62:ILE:HD12	3:E:97:GLU:HG2	2.00	0.42
5:C:16:THR:HG23	5:C:19:SER:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:39:TYR:HB3	6:H:75:SER:HB2	2.02	0.42
2:J:-24:DC:H2"	2:J:-23:DA:C8	2.54	0.42
4:B:29:ILE:HD12	4:B:34:ILE:CD1	2.49	0.42
2:J:13:DT:C4	2:J:14:DG:C6	3.08	0.42
2:J:15:DC:H2"	2:J:16:DC:C5	2.54	0.42
5:C:39:TYR:HB3	6:D:75:SER:HB2	2.01	0.42
1:I:-5:DC:H2"	1:I:-4:DT:C7	2.50	0.42
5:G:116:LEU:HA	5:G:116:LEU:HD23	1.85	0.41
4:B:62:LEU:O	4:B:66:ILE:HB	2.20	0.41
2:J:38:DA:C8	2:J:39:DT:H72	2.55	0.41
3:A:82:LEU:HA	3:A:82:LEU:HD23	1.94	0.41
4:B:26:ILE:HG23	4:B:27:GLN:HE21	1.85	0.41
3:A:122:LYS:HD3	3:E:113:HIS:CE1	2.56	0.41
5:G:62:ILE:HD13	5:G:93:LEU:HD13	2.02	0.41
2:J:-13:DA:H2'	2:J:-12:DT:H71	2.01	0.41
2:J:47:DT:H2"	2:J:48:DG:C5	2.55	0.41
2:J:16:DC:H2'	2:J:17:DT:C5	2.56	0.41
1:I:-34:DG:H1'	1:I:-33:DA:N7	2.36	0.41
2:J:-13:DA:OP1	4:F:36:ARG:NH2	2.54	0.41
2:J:4:DA:H2"	2:J:5:DG:OP2	2.20	0.41
2:J:20:DT:H1'	2:J:21:DG:H5'	2.03	0.41
6:D:116:THR:HA	6:D:119:THR:HG22	2.02	0.41
1:I:39:DT:H2"	1:I:40:DA:C8	2.55	0.41
5:C:100:VAL:HG11	4:F:98:TYR:CE2	2.56	0.41
1:I:61:DG:H2"	1:I:62:DG:H5"	2.03	0.41
2:J:-43:DG:C8	2:J:-42:DT:H72	2.56	0.41
5:G:88:ARG:HD3	5:G:88:ARG:HA	1.81	0.40
3:A:51:ILE:HG21	5:G:111:ILE:HG12	2.03	0.40
5:G:42:ARG:HE	6:H:85:THR:HG22	1.85	0.40
2:J:-65:DC:H2"	2:J:-64:DC:C6	2.56	0.40
5:C:54:VAL:HG13	6:D:107:ALA:HB1	2.03	0.40
1:I:-57:DT:H2"	1:I:-56:DC:C6	2.57	0.40
5:C:80:PRO:HB3	6:D:58:ILE:HD12	2.04	0.40
2:J:20:DT:C2	2:J:21:DG:C8	3.08	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	
3	A	94/135 (70%)	92 (98%)	2 (2%)	0	100	100
3	E	93/135 (69%)	89 (96%)	4 (4%)	0	100	100
4	B	76/103 (74%)	72 (95%)	4 (5%)	0	100	100
4	F	84/103 (82%)	77 (92%)	7 (8%)	0	100	100
5	C	101/129 (78%)	98 (97%)	3 (3%)	0	100	100
5	G	103/129 (80%)	97 (94%)	6 (6%)	0	100	100
6	D	94/122 (77%)	91 (97%)	3 (3%)	0	100	100
6	H	90/122 (74%)	90 (100%)	0	0	100	100
All	All	735/978 (75%)	706 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
3	A	83/109 (76%)	82 (99%)	1 (1%)	75	94
3	E	82/109 (75%)	80 (98%)	2 (2%)	54	85
4	B	63/79 (80%)	60 (95%)	3 (5%)	30	63
4	F	71/79 (90%)	67 (94%)	4 (6%)	25	57
5	C	82/101 (81%)	77 (94%)	5 (6%)	22	53
5	G	83/101 (82%)	79 (95%)	4 (5%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	D	82/102 (80%)	79 (96%)	3 (4%)	39	73
6	H	78/102 (76%)	78 (100%)	0	100	100
All	All	624/782 (80%)	602 (96%)	22 (4%)	41	75

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	118	THR
4	B	45	ARG
4	B	60	VAL
4	B	95	ARG
5	C	38	CYS
5	C	71	ARG
5	C	73	ASN
5	C	74	LYS
5	C	81	ARG
6	D	27	ARG
6	D	28	LYS
6	D	109	SER
3	E	40	CYS
3	E	63	ARG
4	F	18	HIS
4	F	35	ARG
4	F	47	SER
4	F	60	VAL
5	G	38	CYS
5	G	50	TYR
5	G	81	ARG
5	G	115	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	25	ASN
4	B	27	GLN
6	D	64	ASN
5	G	104	GLN
5	G	112	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	G47	I	70	1,3,2,7	20,27,28	1.83	4 (20%)	22,38,41	2.40	4 (18%)
2	G47	J	70	1,3,2	20,27,28	1.82	4 (20%)	22,38,41	2.28	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G47	I	70	1,3,2,7	-	0/7/25/26	0/3/3/3
2	G47	J	70	1,3,2	-	0/7/25/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	70	G47	C7A-SG	-5.47	1.63	1.80
1	I	70	G47	C7A-SG	-5.29	1.63	1.80
2	J	70	G47	C6A-N2	-3.36	1.38	1.46
1	I	70	G47	C6A-N2	-3.36	1.38	1.46
2	J	70	G47	C8-N7	-2.04	1.30	1.34
1	I	70	G47	C6-C5	2.70	1.46	1.41
1	I	70	G47	C6-N1	3.50	1.39	1.33
2	J	70	G47	C6-N1	3.67	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	I	70	G47	C5-C6-N1	-8.37	111.56	123.48
2	J	70	G47	C5-C6-N1	-8.06	112.01	123.48
1	I	70	G47	C6-C5-C4	-3.08	117.78	120.84
2	J	70	G47	C6-C5-C4	-2.72	118.14	120.84
2	J	70	G47	C2-N3-C4	-2.69	112.05	115.11
1	I	70	G47	C2-N3-C4	-2.66	112.08	115.11
2	J	70	G47	C6-N1-C2	5.20	124.49	115.18
1	I	70	G47	C6-N1-C2	5.46	124.96	115.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	I	146/147 (99%)	0.33	8 (5%) 26 17	70, 140, 203, 235	0
2	J	146/147 (99%)	0.26	1 (0%) 87 83	73, 140, 194, 222	0
3	A	96/135 (71%)	0.16	2 (2%) 64 54	40, 71, 115, 178	0
3	E	95/135 (70%)	-0.03	1 (1%) 80 74	29, 52, 89, 148	0
4	B	78/103 (75%)	-0.04	1 (1%) 77 71	45, 66, 96, 118	0
4	F	86/103 (83%)	-0.20	1 (1%) 79 72	30, 51, 80, 153	0
5	C	103/129 (79%)	-0.20	1 (0%) 82 77	33, 55, 90, 114	0
5	G	105/129 (81%)	0.00	2 (1%) 67 58	45, 76, 117, 146	0
6	D	96/122 (78%)	-0.08	2 (2%) 64 54	38, 61, 111, 157	0
6	H	92/122 (75%)	-0.13	0 100 100	43, 74, 114, 135	0
All	All	1043/1272 (81%)	0.04	19 (1%) 69 60	29, 74, 173, 235	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	39	HIS	5.3
6	D	26	ARG	5.2
6	D	27	ARG	3.9
1	I	-61	DC	3.9
1	I	-64	DC	3.1
1	I	-62	DC	3.1
1	I	-60	DT	3.0
4	F	17	ARG	3.0
5	G	117	PRO	2.9
3	E	39	HIS	2.6
5	G	15	LYS	2.4
1	I	-18	DA	2.4
2	J	21	DG	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	32	DT	2.3
1	I	33	DT	2.3
3	A	76	GLN	2.2
4	B	30	THR	2.2
1	I	-16	DG	2.1
5	C	15	LYS	2.0

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	G47	I	70	25/26	0.91	0.19	-	108,130,149,180	0
2	G47	J	70	25/26	0.86	0.19	-	92,129,159,162	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	MN	E	201	1/1	0.97	0.25	2.30	51,51,51,51	0
8	CL	G	201	1/1	0.88	0.17	-0.38	70,70,70,70	0
8	CL	C	201	1/1	0.98	0.14	-1.36	72,72,72,72	0
7	MN	I	107	1/1	0.81	0.08	-	165,165,165,165	0
7	MN	I	101	1/1	0.75	0.10	-	165,165,165,165	0
7	MN	J	102	1/1	0.01	0.15	-	168,168,168,168	0
7	MN	I	108	1/1	0.89	0.20	-	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MN	J	108	1/1	0.22	0.24	-	175,175,175,175	0
7	MN	J	101	1/1	0.83	0.08	-	150,150,150,150	0
7	MN	I	104	1/1	0.90	0.22	-	136,136,136,136	0
7	MN	J	106	1/1	0.95	0.08	-	120,120,120,120	0
7	MN	J	105	1/1	0.96	0.24	-	120,120,120,120	0
7	MN	I	102	1/1	0.23	0.24	-	171,171,171,171	0
7	MN	I	106	1/1	0.52	0.17	-	143,143,143,143	0
7	MN	I	103	1/1	0.96	0.14	-	107,107,107,107	0
7	MN	J	107	1/1	0.82	0.11	-	153,153,153,153	0
7	MN	I	105	1/1	0.72	0.14	-	122,122,122,122	0
7	MN	I	109	1/1	0.32	0.29	-	151,151,151,151	0
8	CL	A	201	1/1	0.96	0.40	-	82,82,82,82	0
7	MN	J	109	1/1	0.85	0.10	-	121,121,121,121	0
8	CL	E	202	1/1	0.94	0.14	-	85,85,85,85	0
7	MN	J	104	1/1	0.92	0.26	-	103,103,103,103	0
7	MN	J	103	1/1	0.91	0.18	-	100,100,100,100	0
7	MN	D	201	1/1	0.88	0.10	-	128,128,128,128	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.