



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2017 – 08:00 AM EST

PDB ID : 5ONG
Title : X-Ray crystal structure of a nucleosome core particle with its DNA site-specifically crosslinked to the histone octamer
Authors : Frouws, T.D.; Barth, P.D.; Richmond, T.J.
Deposited on : 2017-08-03
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

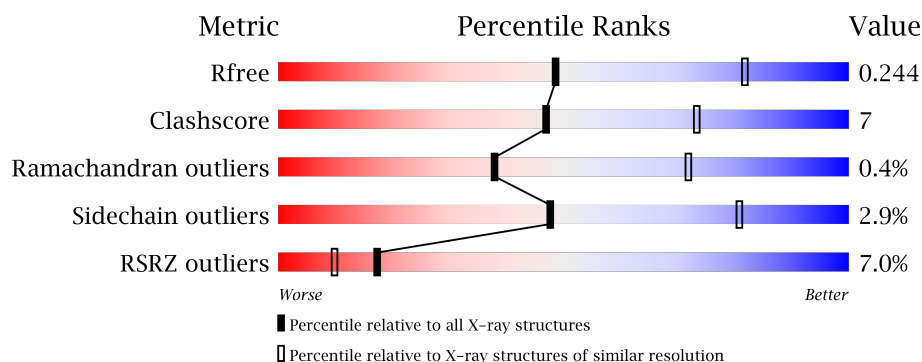
1 Overall quality at a glance

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 ≥ 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>21%</div> <div> <div></div> <div>57%</div> <div>43%</div> </div> </div>
2	J	147	<div> <div>21%</div> <div> <div></div> <div>60%</div> <div>40%</div> </div> </div>
3	A	135	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>11%</div> <div>•</div> <div>29%</div> </div> </div>
3	E	135	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>10%</div> <div>•</div> <div>28%</div> </div> </div>
4	B	103	<div> <div></div> <div> <div></div> <div>62%</div> <div>14%</div> <div>24%</div> </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	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12111 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	97	Total	C	N	O	S	0	0	0
			794	501	152	138	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
			618	391	120	106	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			

- Molecule 5 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	106	Total	C	N	O		0	0	0
			820	517	160	143				
5	G	106	Total	C	N	O		0	0	0
			818	516	160	142				

- Molecule 6 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	94	Total	C	N	O	S	0	0	0
			735	463	132	138	2			
6	H	93	Total	C	N	O	S	0	0	0
			726	457	130	137	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	10	Total	Mn	0	0
			10	10		
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	Cl	0	0
			1	1		
8	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total 1	Cl 1	0	0
8	E	1	Total 1	Cl 1	0	0

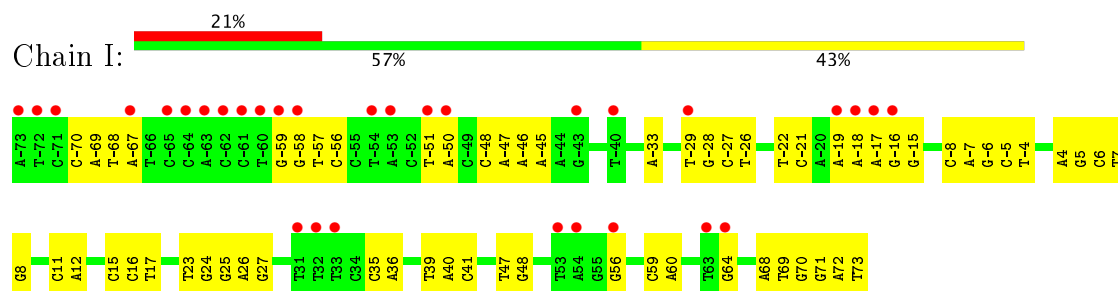
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	I	16	Total 16	O 16	0	0
9	J	17	Total 17	O 17	0	0
9	A	3	Total 3	O 3	0	0
9	B	4	Total 4	O 4	0	0
9	C	12	Total 12	O 12	0	0
9	D	5	Total 5	O 5	0	0
9	E	10	Total 10	O 10	0	0
9	F	11	Total 11	O 11	0	0
9	G	4	Total 4	O 4	0	0
9	H	5	Total 5	O 5	0	0

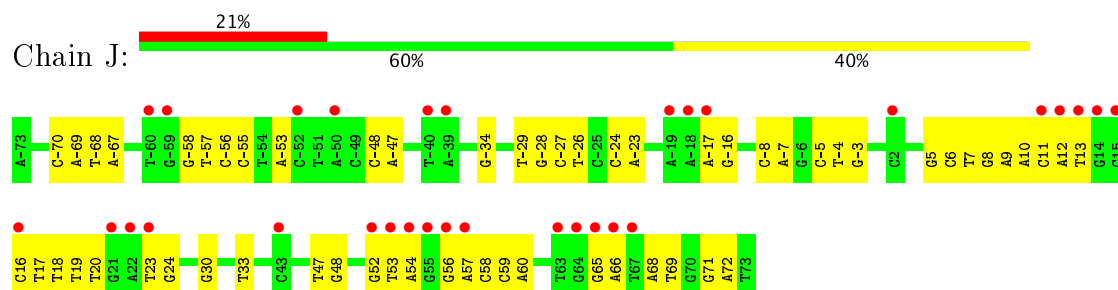
3 Residue-property plots [i](#)

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

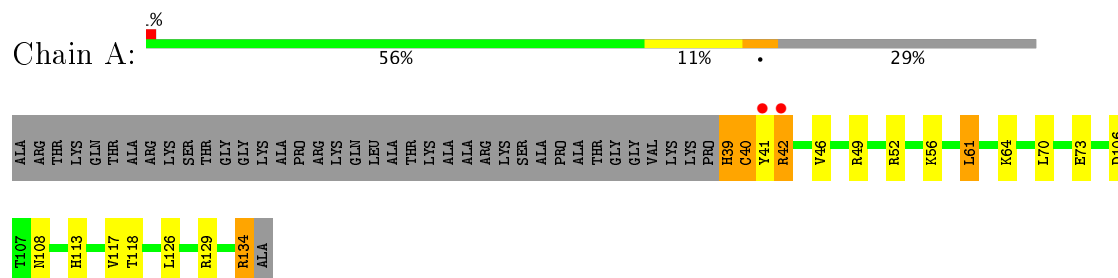
• Molecule 1: DNA (147-MER)



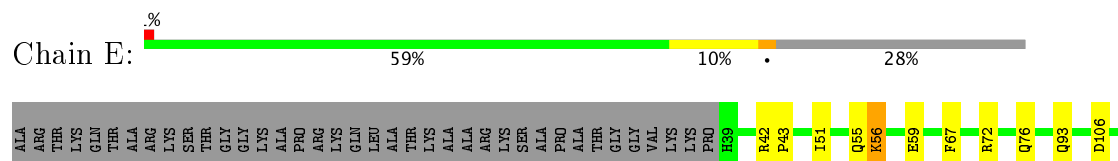
• Molecule 2: DNA (147-MER)



• Molecule 3: Histone H3.2



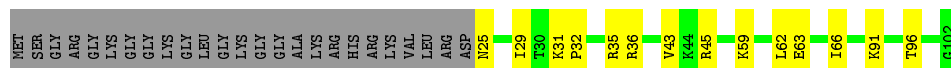
• Molecule 3: Histone H3.2





• Molecule 4: Histone H4

Chain B: 62% 14% 24%



• Molecule 4: Histone H4

Chain F: 69% 13% 18%



• Molecule 5: Histone H2A

Chain C: 2% 73% 9% 18%



• Molecule 5: Histone H2A

Chain G: 2% 71% 11% 18%



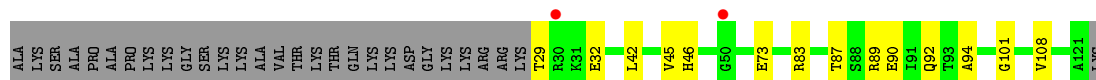
• Molecule 6: Histone H2B 1.1

Chain D: 69% 7% 23%



• Molecule 6: Histone H2B 1.1

Chain H: 2% 65% 11% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.24Å 183.13Å 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)	89.4 (29.50-2.80) 89.5 (29.50-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.80Å)	Xtriage
Refinement program	PHENIX (dev_2447: ???)	Depositor
R, R_{free}	0.206 , 0.247 0.202 , 0.244	Depositor DCC
R_{free} test set	4810 reflections (10.07%)	DCC
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.042 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12111	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.51	0/3352	0.95	0/5169
2	J	0.50	0/3350	0.97	0/5166
3	A	0.26	0/800	0.40	0/1074
3	E	0.25	0/805	0.38	0/1081
4	B	0.24	0/625	0.42	0/837
4	F	0.24	0/680	0.43	0/908
5	C	0.23	0/830	0.41	0/1120
5	G	0.25	0/828	0.41	0/1117
6	D	0.24	0/746	0.40	0/1004
6	H	0.24	0/737	0.39	0/993
All	All	0.40	0/12753	0.77	0/18469

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	47	0
2	J	3013	0	1664	47	0
3	A	789	0	824	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	794	0	829	12	0
4	B	618	0	659	12	0
4	F	673	0	722	6	0
5	C	820	0	879	10	0
5	G	818	0	877	12	0
6	D	735	0	760	9	0
6	H	726	0	747	10	0
7	E	1	0	0	0	0
7	I	10	0	0	0	0
7	J	9	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	G	1	0	0	0	0
9	A	3	0	0	0	0
9	B	4	0	0	0	0
9	C	12	0	0	0	0
9	D	5	0	0	0	0
9	E	10	0	0	1	0
9	F	11	0	0	1	0
9	G	4	0	0	1	0
9	H	5	0	0	0	0
9	I	16	0	0	0	0
9	J	17	0	0	1	0
All	All	12111	0	9624	152	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 7.

All (152) 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:56:DG:N2	2:J:-56:DC:O2	2.06	0.88
4:F:40:ARG:O	9:F:201:HOH:O	1.95	0.84
1:I:-27:DC:H2''	1:I:-26:DT:H71	1.66	0.77
1:I:39:DT:OP2	5:G:35:ARG:NH2	2.20	0.74
3:E:51:ILE:O	3:E:55:GLN:HB2	1.91	0.71
3:A:61:LEU:O	4:B:36:ARG:NH2	2.24	0.69
1:I:-57:DT:H2'	1:I:-56:DC:C6	2.28	0.69
3:A:134:ARG:HD2	3:A:134:ARG:C	2.12	0.68
2:J:53:DT:H1'	2:J:54:DA:H5'	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:118:THR:OG1	4:B:45:ARG:NH1	2.26	0.67
2:J:10:DA:H2"	2:J:11:DC:H5"	1.78	0.66
1:I:-5:DC:H2"	1:I:-4:DT:H72	1.77	0.65
1:I:-19:DA:H1'	1:I:-18:DA:C8	2.32	0.65
1:I:72:DA:H2"	1:I:73:DT:H5"	1.78	0.64
2:J:10:DA:H5'	3:A:39:HIS:HD2	1.62	0.64
5:C:29:ARG:NH1	6:D:33:SER:O	2.32	0.63
2:J:11:DC:H2"	2:J:12:DA:C8	2.34	0.63
2:J:-27:DC:OP2	9:J:201:HOH:O	2.15	0.63
1:I:-69:DA:H1'	1:I:-68:DT:H5"	1.81	0.62
1:I:15:DC:H2"	1:I:16:DC:C5	2.34	0.62
3:E:56:LYS:NZ	9:E:302:HOH:O	2.33	0.61
6:H:92:GLN:HE21	6:H:108:VAL:HG13	1.66	0.60
2:J:10:DA:H5'	3:A:39:HIS:CD2	2.36	0.60
1:I:-48:DC:H2"	1:I:-47:DA:N7	2.17	0.60
3:A:117:VAL:HG13	5:G:115:LEU:HD22	1.85	0.59
5:G:63:LEU:HD13	6:H:42:LEU:HB2	1.84	0.58
1:I:-18:DA:H2"	1:I:-17:DA:C8	2.38	0.58
2:J:12:DA:H2"	2:J:13:DT:H5"	1.85	0.58
1:I:56:DG:N1	2:J:-56:DC:N3	2.34	0.58
1:I:35:DC:H2"	1:I:36:DA:N7	2.18	0.58
2:J:56:DG:H2"	2:J:57:DA:C8	2.38	0.58
2:J:16:DC:H2"	2:J:17:DT:H71	1.86	0.57
6:D:33:SER:HB2	6:D:60:ASN:OD1	2.05	0.57
5:C:39:TYR:HB3	6:D:75:SER:HB2	1.88	0.56
1:I:7:DT:H2"	1:I:8:DG:C8	2.41	0.56
2:J:-53:DA:H8	2:J:-53:DA:H5'	1.71	0.56
1:I:68:DA:H1'	1:I:69:DT:H5'	1.87	0.56
2:J:-34:DG:OP1	6:H:83:ARG:NH1	2.40	0.55
1:I:4:DA:H2"	1:I:5:DG:C8	2.42	0.55
2:J:-5:DC:H2"	2:J:-4:DT:H71	1.88	0.55
1:I:11:DC:H2"	1:I:12:DA:C8	2.41	0.55
2:J:52:DG:H2"	2:J:53:DT:H5'	1.88	0.55
3:E:42:ARG:HG2	3:E:43:PRO:HD2	1.87	0.55
1:I:-18:DA:H2"	1:I:-17:DA:H8	1.71	0.55
2:J:-58:DG:H2"	2:J:-57:DT:C5	2.42	0.55
4:F:31:LYS:HE2	4:F:35:ARG:HH12	1.73	0.53
1:I:-70:DC:H2"	1:I:-69:DA:C8	2.44	0.52
2:J:-27:DC:H2"	2:J:-26:DT:H72	1.92	0.52
2:J:30:DG:OP1	6:H:29:THR:OG1	2.25	0.52
3:A:106:ASP:OD1	3:E:129:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:32:ARG:NH2	6:H:32:GLU:OE2	2.42	0.52
3:E:67:PHE:CD1	3:E:93:GLN:HG2	2.45	0.52
2:J:-68:DT:H2"	2:J:-67:DA:C8	2.45	0.52
1:I:-59:DG:H2"	1:I:-58:DG:C8	2.45	0.52
2:J:-53:DA:C8	2:J:-53:DA:H5'	2.44	0.51
1:I:-8:DC:H2"	1:I:-7:DA:C8	2.45	0.51
2:J:-55:DC:H4'	5:G:77:ARG:CZ	2.40	0.51
1:I:47:DT:H2"	1:I:48:DG:N7	2.25	0.51
2:J:23:DT:H2"	2:J:24:DG:C8	2.46	0.51
3:A:52:ARG:O	3:A:56:LYS:HG2	2.11	0.50
3:A:106:ASP:HB3	3:E:130:ILE:HD12	1.94	0.50
3:A:70:LEU:HD22	4:B:29:ILE:HD11	1.93	0.50
5:C:63:LEU:HD12	6:D:41:VAL:HG23	1.95	0.49
1:I:-58:DG:H2"	1:I:-57:DT:H71	1.94	0.49
1:I:-22:DT:H2"	1:I:-21:DC:H5"	1.94	0.49
5:G:67:GLY:HA3	6:H:46:HIS:CD2	2.47	0.49
2:J:-5:DC:H2"	2:J:-4:DT:C7	2.43	0.49
3:A:113:HIS:CG	3:E:126:LEU:HD22	2.48	0.49
3:E:72:ARG:O	3:E:76:GLN:HB2	2.12	0.49
1:I:47:DT:H2"	1:I:48:DG:C8	2.47	0.49
3:A:126:LEU:HD22	3:E:113:HIS:CG	2.47	0.49
3:E:126:LEU:O	3:E:130:ILE:HG12	2.13	0.49
3:A:56:LYS:NZ	5:G:109:PRO:HB3	2.28	0.48
2:J:-17:DA:H2"	2:J:-16:DG:C8	2.48	0.48
1:I:23:DT:H2"	1:I:24:DG:C8	2.49	0.48
3:A:73:GLU:OE1	4:B:25:ASN:ND2	2.25	0.48
2:J:68:DA:H1'	2:J:69:DT:H5'	1.94	0.48
2:J:71:DG:H1'	2:J:72:DA:C8	2.49	0.48
2:J:19:DT:H2"	2:J:20:DT:C6	2.48	0.48
6:H:87:THR:OG1	6:H:90:GLU:OE2	2.30	0.47
2:J:-48:DC:H2"	2:J:-47:DA:N7	2.30	0.47
2:J:-24:DC:H2"	2:J:-23:DA:C8	2.50	0.47
1:I:-5:DC:OP1	3:A:42:ARG:HD2	2.14	0.47
1:I:40:DA:H2"	1:I:41:DC:H5'	1.96	0.47
1:I:-68:DT:H2"	1:I:-67:DA:H8	1.79	0.47
2:J:59:DC:H2"	2:J:60:DA:N7	2.30	0.47
4:B:31:LYS:HE3	4:B:35:ARG:HH12	1.79	0.46
1:I:64:DG:C8	1:I:64:DG:H5'	2.50	0.46
2:J:-69:DA:H2"	2:J:-68:DT:H5"	1.97	0.46
3:A:108:ASN:HD21	5:G:115:LEU:HD11	1.81	0.46
4:B:96:THR:HG23	9:G:301:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:-70:DC:H2''	2:J:-69:DA:C8	2.50	0.46
1:I:-6:DG:H2''	1:I:-5:DC:C6	2.51	0.46
3:A:46:VAL:HA	3:A:49:ARG:HB2	1.98	0.46
4:B:59:LYS:NZ	4:B:63:GLU:OE2	2.43	0.46
2:J:57:DA:H2''	2:J:58:DC:C5	2.51	0.45
3:A:108:ASN:HB2	4:B:43:VAL:HG22	1.98	0.45
5:C:58:LEU:HD12	6:D:66:VAL:HG11	1.99	0.45
3:E:129:ARG:HG3	3:E:134:ARG:NH1	2.32	0.45
2:J:33:DT:H5'	2:J:33:DT:H6	1.82	0.45
5:C:102:ILE:HG23	6:D:58:ILE:HG12	1.98	0.45
1:I:-33:DA:OP2	6:D:83:ARG:NH1	2.49	0.45
1:I:6:DC:H2''	1:I:7:DT:C6	2.51	0.45
2:J:17:DT:H2'	2:J:18:DT:H71	1.98	0.45
5:C:64:GLU:HA	6:D:46:HIS:HE1	1.81	0.44
3:E:106:ASP:OD2	3:E:131:ARG:NH1	2.50	0.44
2:J:-8:DC:H2''	2:J:-7:DA:C8	2.52	0.44
1:I:25:DG:H1'	1:I:26:DA:C8	2.52	0.44
1:I:59:DC:H2''	1:I:60:DA:N7	2.32	0.44
1:I:-57:DT:H2''	1:I:-56:DC:C5'	2.48	0.43
2:J:-4:DT:H2''	2:J:-3:DG:C8	2.54	0.43
2:J:6:DC:H2''	2:J:7:DT:C6	2.53	0.43
2:J:9:DA:H3'	3:A:46:VAL:HG11	2.01	0.43
2:J:47:DT:H2''	2:J:48:DG:N7	2.34	0.43
1:I:70:G47:H1'	1:I:71:DG:H5'	2.01	0.43
2:J:47:DT:H2''	2:J:48:DG:C8	2.54	0.43
4:B:91:LYS:HG3	4:B:96:THR:HG22	2.00	0.43
3:A:129:ARG:NH1	3:A:129:ARG:O	2.39	0.42
4:F:35:ARG:HG2	4:F:46:ILE:HD12	2.00	0.42
1:I:70:G47:H4'	3:A:41:TYR:HE1	1.83	0.42
2:J:56:DG:H2''	2:J:57:DA:H8	1.82	0.42
5:G:37:GLY:HA3	5:G:39:TYR:CE2	2.54	0.42
5:C:31:HIS:CG	5:C:48:PRO:HG3	2.54	0.42
1:I:26:DA:H2''	1:I:27:DG:C8	2.55	0.42
2:J:16:DC:H2''	2:J:17:DT:C7	2.49	0.42
4:B:91:LYS:HA	4:B:96:THR:HG22	2.02	0.42
3:A:64:LYS:HB3	3:A:64:LYS:HE3	1.94	0.42
1:I:16:DC:H2''	1:I:17:DT:C7	2.50	0.42
5:C:93:LEU:HD23	5:C:93:LEU:HA	1.93	0.42
4:F:77:LYS:HE3	6:H:89:ARG:NH2	2.34	0.42
5:G:79:ILE:HG12	5:G:82:HIS:CE1	2.55	0.42
5:G:31:HIS:O	5:G:35:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:55:LEU:O	5:C:59:THR:HG23	2.20	0.42
4:B:32:PRO:O	4:B:36:ARG:HG3	2.20	0.41
4:F:30:THR:HB	4:F:32:PRO:HD2	2.02	0.41
1:I:-16:DG:H1'	1:I:-15:DG:C8	2.54	0.41
2:J:-29:DT:H1'	2:J:-28:DG:C8	2.55	0.41
5:C:64:GLU:HA	6:D:46:HIS:CE1	2.56	0.41
1:I:-70:DC:H6	1:I:-70:DC:H5'	1.85	0.41
4:F:62:LEU:HA	4:F:65:VAL:HG22	2.03	0.41
1:I:-46:DA:C2	1:I:-45:DA:C4	3.08	0.41
1:I:-58:DG:H2''	1:I:-57:DT:C7	2.50	0.41
5:G:97:LEU:HB3	5:G:100:VAL:HG22	2.01	0.41
6:H:45:VAL:HG12	6:H:46:HIS:CD2	2.56	0.41
1:I:16:DC:H2''	1:I:17:DT:H71	2.03	0.41
2:J:65:DG:H2''	2:J:66:DA:C8	2.55	0.41
4:B:62:LEU:O	4:B:66:ILE:HB	2.21	0.41
6:H:73:GLU:HB3	6:H:94:ALA:HB1	2.02	0.41
1:I:-29:DT:H1'	1:I:-28:DG:N7	2.36	0.41
1:I:-51:DT:H2''	1:I:-50:DA:H5'	2.03	0.41
2:J:5:DG:H2''	2:J:6:DC:C5	2.56	0.40
2:J:7:DT:H2''	2:J:8:DG:C8	2.56	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%)	1 (1%)	1 (1%)	17	47
3	E	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
4	B	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
4	F	82/103 (80%)	77 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	104/129 (81%)	102 (98%)	2 (2%)	0	100	100
5	G	104/129 (81%)	102 (98%)	2 (2%)	0	100	100
6	D	92/122 (75%)	91 (99%)	0	1 (1%)	17	47
6	H	91/122 (75%)	89 (98%)	1 (1%)	1 (1%)	17	47
All	All	738/978 (76%)	722 (98%)	13 (2%)	3 (0%)	38	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	101	GLY
3	A	40	CYS
6	H	101	GLY

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%)	78 (94%)	5 (6%)	22	54
3	E	83/109 (76%)	79 (95%)	4 (5%)	30	63
4	B	63/79 (80%)	63 (100%)	0	100	100
4	F	69/79 (87%)	65 (94%)	4 (6%)	23	55
5	C	85/101 (84%)	84 (99%)	1 (1%)	75	94
5	G	84/101 (83%)	82 (98%)	2 (2%)	54	85
6	D	80/102 (78%)	78 (98%)	2 (2%)	53	84
6	H	79/102 (78%)	79 (100%)	0	100	100
All	All	626/782 (80%)	608 (97%)	18 (3%)	48	81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	39	HIS

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Mol	Chain	Res	Type
3	A	40	CYS
3	A	42	ARG
3	A	61	LEU
3	A	134	ARG
5	C	101	THR
6	D	28	LYS
6	D	60	ASN
3	E	56	LYS
3	E	59	GLU
3	E	129	ARG
3	E	134	ARG
4	F	19	ARG
4	F	23	ARG
4	F	93	GLN
4	F	96	THR
5	G	51	LEU
5	G	77	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	108	ASN
6	D	44	GLN
6	D	46	HIS
6	H	92	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	20,27,28	1.37	2 (10%)	22,38,41	2.38	4 (18%)
2	G47	J	70	1,3,2,7	20,27,28	1.46	3 (15%)	22,38,41	2.38	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	-	2/7/25/26	0/3/3/3
2	G47	J	70	1,3,2,7	-	0/7/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	70	G47	C6A-N2	-3.42	1.38	1.46
1	I	70	G47	C6A-N2	-3.37	1.38	1.46
2	J	70	G47	C7A-SG	2.53	1.89	1.80
1	I	70	G47	C6-N1	3.46	1.39	1.33
2	J	70	G47	C6-N1	3.60	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	70	G47	C5-C6-N1	-8.34	111.61	123.48
1	I	70	G47	C5-C6-N1	-8.28	111.70	123.48
1	I	70	G47	C6-C5-C4	-3.03	117.83	120.84
2	J	70	G47	C6-C5-C4	-2.91	117.95	120.84
1	I	70	G47	C2-N3-C4	-2.65	112.08	115.11
2	J	70	G47	C2-N3-C4	-2.58	112.16	115.11
2	J	70	G47	C6-N1-C2	5.57	125.16	115.18
1	I	70	G47	C6-N1-C2	5.59	125.18	115.18

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	70	G47	N3-C2-N2-C6A
1	I	70	G47	N1-C2-N2-C6A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	70	G47	2	0

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, 95th 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	I	146/147 (99%)	1.27	31 (21%) 1 1	70, 129, 180, 193	0
2	J	146/147 (99%)	1.31	31 (21%) 1 1	70, 126, 173, 218	0
3	A	96/135 (71%)	0.60	2 (2%) 64 54	39, 61, 98, 132	0
3	E	97/135 (71%)	0.51	1 (1%) 82 77	27, 45, 93, 138	0
4	B	78/103 (75%)	0.39	0 100 100	38, 57, 80, 86	0
4	F	84/103 (81%)	0.33	0 100 100	28, 45, 65, 106	0
5	C	106/129 (82%)	0.35	3 (2%) 53 43	26, 47, 79, 162	0
5	G	106/129 (82%)	0.49	3 (2%) 53 43	39, 67, 102, 144	0
6	D	94/122 (77%)	0.22	0 100 100	31, 51, 85, 115	0
6	H	93/122 (76%)	0.29	2 (2%) 62 52	35, 64, 97, 126	0
All	All	1046/1272 (82%)	0.65	73 (6%) 17 10	26, 64, 157, 218	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	G	119	LYS	8.5
5	C	120	THR	7.5
5	G	14	ALA	5.9
2	J	55	DG	5.8
2	J	54	DA	5.1
2	J	13	DT	4.9
1	I	-18	DA	4.8
1	I	-19	DA	4.3
1	I	-62	DC	4.3
1	I	56	DG	4.1
2	J	22	DA	4.1
1	I	-50	DA	4.0
2	J	21	DG	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	-60	DT	3.9
2	J	12	DA	3.9
2	J	56	DG	3.9
1	I	-73	DA	3.8
2	J	64	DG	3.7
1	I	-16	DG	3.7
2	J	14	DG	3.6
2	J	23	DT	3.6
2	J	53	DT	3.6
2	J	-39	DA	3.5
1	I	-51	DT	3.5
5	C	119	LYS	3.5
1	I	33	DT	3.3
1	I	-59	DG	3.2
2	J	57	DA	3.2
1	I	-64	DC	3.2
2	J	66	DA	3.2
1	I	-63	DA	3.2
1	I	54	DA	3.1
2	J	-40	DT	3.1
1	I	53	DT	3.0
2	J	2	DC	3.0
1	I	32	DT	3.0
1	I	64	DG	3.0
2	J	-50	DA	2.9
2	J	63	DT	2.9
1	I	-61	DC	2.9
1	I	-72	DT	2.8
2	J	65	DG	2.8
2	J	-60	DT	2.7
3	A	41	TYR	2.7
1	I	-71	DC	2.6
2	J	16	DC	2.6
1	I	-53	DA	2.6
2	J	43	DC	2.5
1	I	-58	DG	2.5
1	I	-54	DT	2.5
6	H	30	ARG	2.5
2	J	-17	DA	2.4
1	I	31	DT	2.4
1	I	-65	DC	2.4
2	J	11	DC	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	63	DT	2.4
2	J	67	DT	2.4
2	J	-19	DA	2.3
2	J	-18	DA	2.3
1	I	-29	DT	2.3
1	I	-40	DT	2.3
1	I	-67	DA	2.2
1	I	-17	DA	2.2
3	A	42	ARG	2.2
5	C	118	LYS	2.2
1	I	-43	DG	2.2
2	J	-59	DG	2.2
2	J	15	DC	2.1
5	G	15	LYS	2.1
3	E	135	ALA	2.1
2	J	-52	DC	2.1
2	J	52	DG	2.1
6	H	50	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	G47	I	70	25/26	0.89	0.21	-	101,118,149,165	0
2	G47	J	70	25/26	0.88	0.21	-	104,115,131,150	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	MN	E	201	1/1	0.99	0.26	1.39	42,42,42,42	0
8	CL	G	201	1/1	0.92	0.27	1.39	63,63,63,63	0
8	CL	D	201	1/1	0.91	0.20	0.38	68,68,68,68	0
7	MN	J	105	1/1	0.98	0.17	-1.72	93,93,93,93	0
7	MN	I	107	1/1	0.83	0.09	-	125,125,125,125	0
7	MN	I	101	1/1	0.62	0.07	-	148,148,148,148	0
7	MN	J	107	1/1	0.87	0.29	-	100,100,100,100	0
7	MN	J	102	1/1	0.77	0.53	-	128,128,128,128	0
7	MN	I	108	1/1	0.57	0.15	-	133,133,133,133	1
7	MN	I	105	1/1	0.86	0.22	-	103,103,103,103	0
8	CL	E	202	1/1	0.96	0.10	-	53,53,53,53	1
7	MN	I	103	1/1	0.69	0.29	-	174,174,174,174	0
7	MN	I	110	1/1	0.95	0.11	-	110,110,110,110	0
7	MN	J	108	1/1	0.92	0.23	-	101,101,101,101	0
7	MN	J	101	1/1	0.79	0.20	-	131,131,131,131	0
7	MN	I	104	1/1	0.81	0.11	-	154,154,154,154	0
7	MN	J	104	1/1	0.79	0.10	-	148,148,148,148	0
7	MN	I	109	1/1	0.83	0.19	-	103,103,103,103	1
7	MN	J	109	1/1	0.96	0.24	-	93,93,93,93	0
7	MN	J	103	1/1	0.76	0.08	-	133,133,133,133	0
7	MN	I	106	1/1	0.84	0.17	-	117,117,117,117	0
8	CL	A	201	1/1	0.82	0.21	-	50,50,50,50	1
7	MN	I	102	1/1	0.81	0.18	-	136,136,136,136	0
7	MN	J	106	1/1	0.89	0.09	-	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.