



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 05:21 PM BST

PDB ID : 6JXD
Title : Human nucleosome core particle with cohesive end DNA termini
Authors : DeFalco, L.; Davey, C.A.
Deposited on : 2019-04-23
Resolution : 2.25 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 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	:	2.13
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)	:	2.13

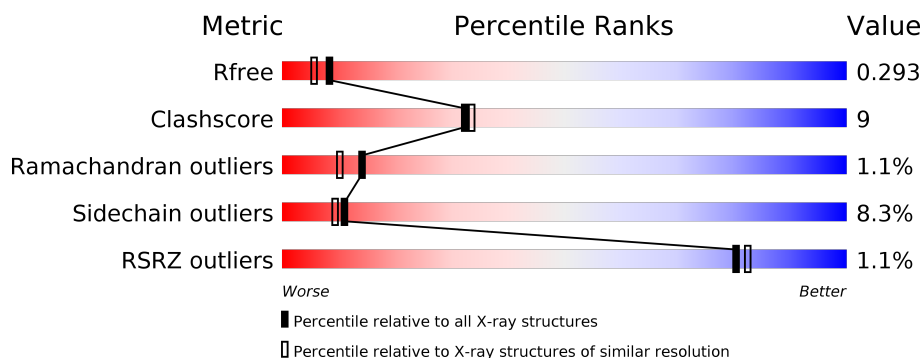
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 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 $\leq 5\%$. 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	A	98	<div> <div style="width: 95%;"></div> <div>95%</div> </div>
2	B	82	<div> <div style="width: 74%;"></div> <div>74%</div> <div style="width: 22%;"></div> <div>22%</div> </div>
3	C	107	<div> <div style="width: 78%;"></div> <div>78%</div> <div style="width: 19%;"></div> <div>19%</div> </div>
4	D	97	<div> <div style="width: 3%;"></div> <div>3%</div> <div style="width: 78%;"></div> <div>78%</div> <div style="width: 18%;"></div> <div>18%</div> </div>
4	H	97	<div> <div style="width: 4%;"></div> <div>4%</div> <div style="width: 73%;"></div> <div>73%</div> <div style="width: 19%;"></div> <div>19%</div> <div style="width: 8%;"></div> <div>8%</div> </div>
5	E	97	<div> <div style="width: 89%;"></div> <div>89%</div> <div style="width: 8%;"></div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	87	<div><div>%</div><div><div></div><div>90%</div><div>10%</div></div></div>
7	G	106	<div><div>%</div><div><div></div><div>75%</div><div>21%</div><div></div></div></div>
8	I	147	<div><div></div><div><div>54%</div><div>45%</div><div></div></div></div>
9	J	147	<div><div></div><div><div>61%</div><div>38%</div><div></div></div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12227 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 H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			

- 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
			830	523	164	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	12	ARG	-	expression tag	UNP P04908

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	97	Total	C	N	O	S	0	0	0
			765	480	142	141	2			
4	H	97	Total	C	N	O	S	0	0	0
			766	480	142	142	2			

- Molecule 5 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			

- Molecule 7 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	106	Total	C	N	O		0	0	0
			819	517	160	142				

- Molecule 8 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	147	Total	C	N	O	P	0	0	0
			3001	1425	546	883	147			

- Molecule 9 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	147	Total	C	N	O	P	0	0	0
			3028	1434	564	883	147			

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	I	6	Total	Mn	0	0
			6	6		
10	A	1	Total	Mn	0	0
			1	1		
10	J	9	Total	Mn	0	0
			9	9		
10	E	1	Total	Mn	0	0
			1	1		

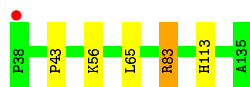
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	5	Total	O	0	0
			5	5		
11	B	6	Total	O	0	0
			6	6		
11	C	8	Total	O	0	0
			8	8		
11	D	3	Total	O	0	0
			3	3		
11	E	7	Total	O	0	0
			7	7		
11	F	4	Total	O	0	0
			4	4		
11	G	5	Total	O	0	0
			5	5		
11	H	4	Total	O	0	0
			4	4		
11	I	6	Total	O	0	0
			6	6		
11	J	4	Total	O	0	0
			4	4		

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.

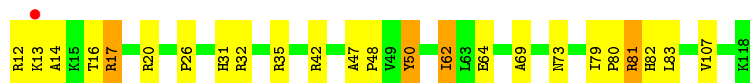
- Molecule 1: Histone H3.1



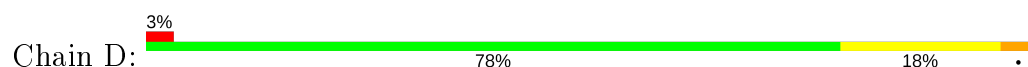
- Molecule 2: Histone H4



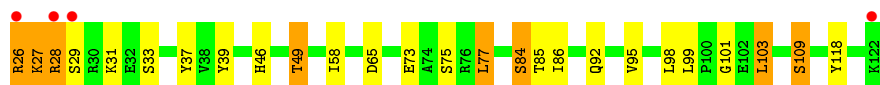
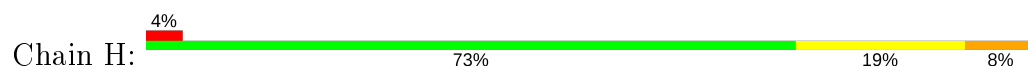
- Molecule 3: Histone H2A type 1-B/E




- Molecule 4: Histone H2B type 1-J

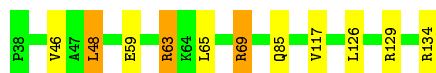


- Molecule 4: Histone H2B type 1-J




- Molecule 5: Histone H3.1

Chain E:  89% 8% .




- Molecule 6: Histone H4

Chain F:  90% 10% .



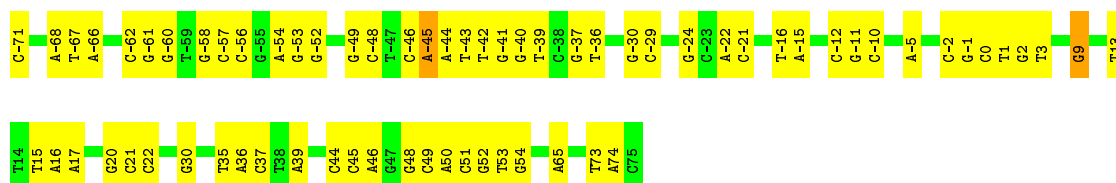
- Molecule 7: Histone H2A type 1-B/E

Chain G:  75% 21% .



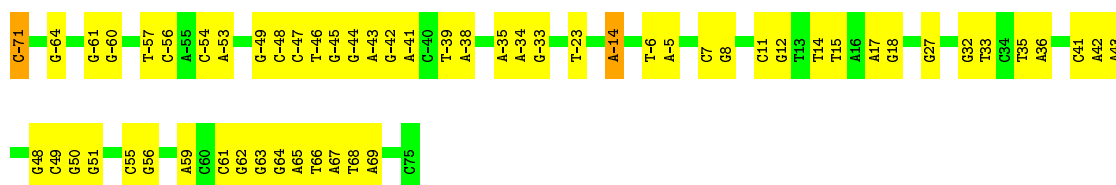
- Molecule 8: DNA (147-MER)

Chain I:  54% 45% .



- Molecule 9: DNA (147-MER)

Chain J:  61% 38% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.31Å 109.66Å 183.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.08 – 2.25 91.91 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (92.08-2.25) 99.6 (91.91-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.239 , 0.292 0.239 , 0.293	Depositor DCC
R_{free} test set	2022 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12227	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.66	0/819	0.90	0/1097
2	B	0.70	0/645	0.88	0/862
3	C	0.70	0/840	0.88	0/1132
4	D	0.77	0/776	0.88	0/1040
4	H	0.76	0/777	0.83	0/1040
5	E	0.75	0/813	0.94	1/1090 (0.1%)
6	F	0.73	0/711	0.97	1/948 (0.1%)
7	G	0.70	0/829	0.85	0/1118
8	I	0.51	1/3363 (0.0%)	0.89	4/5183 (0.1%)
9	J	0.51	2/3399 (0.1%)	0.89	2/5246 (0.0%)
All	All	0.62	3/12972 (0.0%)	0.89	8/18756 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	-71	DC	OP3-P	-10.18	1.49	1.61
9	J	-71	DC	OP3-P	-9.25	1.50	1.61
9	J	-14	DA	O3'-P	-5.21	1.54	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	39	DA	O5'-P-OP1	-8.73	97.85	105.70
9	J	-23	DT	O5'-P-OP2	-6.65	99.71	105.70
8	I	9	DG	O5'-P-OP2	-6.11	100.20	105.70
5	E	69	ARG	NE-CZ-NH2	-5.74	117.43	120.30
8	I	13	DT	O5'-P-OP1	-5.50	100.75	105.70
6	F	35	ARG	NE-CZ-NH1	5.45	123.03	120.30
8	I	-45	DA	C4'-C3'-O3'	5.37	123.12	109.70
9	J	48	DG	O5'-P-OP2	-5.33	100.90	105.70

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	807	0	844	7	0
2	B	638	0	676	11	0
3	C	830	0	892	21	0
4	D	765	0	797	19	0
4	H	766	0	797	25	1
5	E	801	0	839	6	0
6	F	703	0	755	2	0
7	G	819	0	879	26	0
8	I	3001	0	1651	67	1
9	J	3028	0	1651	63	0
10	A	1	0	0	0	0
10	E	1	0	0	0	0
10	I	6	0	0	0	0
10	J	9	0	0	0	0
11	A	5	0	0	0	0
11	B	6	0	0	2	0
11	C	8	0	0	1	0
11	D	3	0	0	1	0
11	E	7	0	0	0	0
11	F	4	0	0	0	0
11	G	5	0	0	0	0
11	H	4	0	0	5	0
11	I	6	0	0	3	0
11	J	4	0	0	2	0
All	All	12227	0	9781	192	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:GLY:HA3	11:B:205:HOH:O	1.34	1.20
7:G:17:ARG:HH22	9:J:-43:DA:P	1.71	1.12
4:H:26:ARG:HH12	8:I:52:DG:P	1.85	0.99
3:C:73:ASN:HB3	11:C:204:HOH:O	1.64	0.96
7:G:17:ARG:NH1	9:J:-43:DA:OP2	2.00	0.94
7:G:17:ARG:NH2	9:J:-43:DA:OP2	2.04	0.91
9:J:65:DA:H2''	9:J:66:DT:H5''	1.58	0.84
4:H:46:HIS:HB3	4:H:49:THR:HG23	1.60	0.82
9:J:-71:DC:C6	9:J:-71:DC:H5'	2.16	0.80
8:I:-67:DT:H2''	8:I:-66:DA:OP2	1.82	0.79
4:H:39:TYR:OH	9:J:-53:DA:OP2	2.00	0.79
9:J:7:DC:H2'	9:J:8:DG:C8	2.18	0.79
7:G:17:ARG:CZ	9:J:-43:DA:OP2	2.31	0.77
9:J:-46:DT:H2''	9:J:-45:DG:C8	2.20	0.76
4:H:26:ARG:NH1	8:I:52:DG:P	2.59	0.74
8:I:-45:DA:H4'	8:I:-44:DA:OP1	1.88	0.72
8:I:-16:DT:H2''	8:I:-15:DA:C8	2.25	0.72
4:H:73:GLU:HG3	11:H:201:HOH:O	1.90	0.70
8:I:36:DA:H1'	8:I:37:DC:H5'	1.74	0.69
4:H:98:LEU:HB2	11:H:204:HOH:O	1.91	0.69
4:H:26:ARG:NH1	8:I:52:DG:OP1	2.26	0.69
4:H:95:VAL:HG13	4:H:99:LEU:HD12	1.75	0.69
4:D:73:GLU:OE1	11:D:201:HOH:O	2.10	0.68
1:A:43:PRO:HG2	8:I:-5:DA:H5'	1.75	0.68
2:B:95:ARG:NH1	11:B:201:HOH:O	2.27	0.67
8:I:-2:DC:H2''	8:I:-1:DG:C8	2.30	0.66
9:J:-71:DC:H6	9:J:-71:DC:H5'	1.59	0.66
2:B:35:ARG:NH1	2:B:51:TYR:OH	2.30	0.65
8:I:36:DA:H4'	8:I:37:DC:OP1	1.97	0.65
9:J:-45:DG:H2''	9:J:-44:DG:C8	2.32	0.65
4:H:46:HIS:HB3	4:H:49:THR:CG2	2.27	0.64
8:I:49:DC:H2'	8:I:50:DA:C8	2.33	0.63
7:G:17:ARG:HH21	7:G:17:ARG:HG2	1.63	0.62
3:C:26:PRO:HG3	4:D:37:TYR:CE2	2.34	0.62
5:E:63:ARG:CZ	9:J:-14:DA:H4'	2.29	0.61
8:I:15:DT:H2''	8:I:16:DA:C8	2.35	0.61
4:H:73:GLU:OE1	11:H:201:HOH:O	2.16	0.61
8:I:-46:DC:H2''	8:I:-45:DA:C8	2.36	0.61
9:J:-49:DG:H2'	9:J:-48:DC:C6	2.35	0.61
4:D:62:PHE:CE1	4:D:66:ILE:CD1	2.84	0.61
7:G:78:ILE:HA	7:G:82:HIS:HD1	1.64	0.61
3:C:81:ARG:NH2	3:C:107:VAL:O	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:53:DT:H2''	8:I:54:DG:C8	2.36	0.60
8:I:48:DG:H5''	11:I:203:HOH:O	2.01	0.60
7:G:17:ARG:NH2	7:G:17:ARG:HG2	2.15	0.60
7:G:17:ARG:NH2	9:J:-43:DA:P	2.57	0.60
9:J:55:DC:H2''	9:J:56:DG:C8	2.37	0.59
1:A:83:ARG:HG2	8:I:-24:DG:H4'	1.83	0.59
9:J:-54:DC:H2''	9:J:-53:DA:C8	2.38	0.59
4:H:28:ARG:HB3	8:I:50:DA:H4'	1.86	0.58
8:I:-57:DC:H2''	8:I:-56:DC:C6	2.39	0.58
9:J:-41:DA:OP1	9:J:-41:DA:H4'	2.05	0.57
9:J:62:DG:H2''	9:J:63:DG:OP2	2.04	0.57
3:C:32:ARG:HD3	8:I:-44:DA:OP2	2.04	0.57
9:J:35:DT:H2''	9:J:36:DA:C8	2.39	0.57
1:A:83:ARG:O	2:B:80:THR:HA	2.05	0.57
8:I:-62:DC:H2'	8:I:-61:DG:C8	2.40	0.57
4:D:73:GLU:HG3	4:D:98:LEU:HD12	1.86	0.57
4:D:62:PHE:CE1	4:D:66:ILE:HD11	2.40	0.56
8:I:49:DC:H2''	8:I:50:DA:O5'	2.05	0.56
3:C:80:PRO:HB3	4:D:58:ILE:CD1	2.36	0.55
8:I:-22:DA:H2''	8:I:-21:DC:C5	2.42	0.55
8:I:-58:DG:N2	9:J:59:DA:C2	2.73	0.55
3:C:17:ARG:HD3	8:I:-43:DT:P	2.46	0.55
9:J:61:DC:H2'	11:J:203:HOH:O	2.06	0.54
7:G:21:ALA:HB2	4:H:118:TYR:HB2	1.88	0.54
3:C:42:ARG:NH1	4:D:85:THR:OG1	2.41	0.54
8:I:-40:DG:H2''	8:I:-39:DT:OP2	2.08	0.54
4:D:28:ARG:N	9:J:51:DG:OP1	2.35	0.54
9:J:-48:DC:H2''	9:J:-47:DC:C6	2.42	0.54
9:J:-49:DG:H2''	9:J:-48:DC:H5'	1.90	0.54
9:J:50:DG:H2''	9:J:51:DG:H5''	1.90	0.54
3:C:62:ILE:HD11	3:C:83:LEU:HD22	1.89	0.53
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.43	0.53
7:G:17:ARG:NH2	9:J:-43:DA:OP1	2.39	0.53
9:J:-71:DC:H6	9:J:-71:DC:C5'	2.22	0.53
3:C:17:ARG:HA	3:C:20:ARG:HD2	1.90	0.52
7:G:81:ARG:NH2	7:G:107:VAL:O	2.40	0.52
1:A:83:ARG:HG2	8:I:-24:DG:O3'	2.09	0.52
7:G:29:ARG:NH2	4:H:33:SER:O	2.43	0.52
8:I:-66:DA:C2	9:J:67:DA:C2	2.98	0.52
4:D:62:PHE:CE1	4:D:66:ILE:HD13	2.45	0.51
8:I:-16:DT:C2'	8:I:-15:DA:C8	2.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ARG:HD3	8:I:-43:DT:OP1	2.11	0.51
6:F:68:ASP:OD2	6:F:93:GLN:NE2	2.44	0.51
9:J:11:DC:H2"	9:J:12:DG:C8	2.46	0.51
8:I:73:DT:H2"	8:I:74:DA:N7	2.25	0.51
9:J:-61:DG:H2"	9:J:-60:DG:OP2	2.12	0.50
9:J:-42:DG:H2"	9:J:-41:DA:H5"	1.94	0.50
9:J:-47:DC:H2"	9:J:-46:DT:H72	1.91	0.50
7:G:32:ARG:NH1	9:J:-44:DG:OP2	2.41	0.50
4:H:95:VAL:HG13	4:H:99:LEU:CD1	2.42	0.50
9:J:-39:DT:H2"	9:J:-38:DA:C8	2.46	0.50
9:J:14:DT:H1'	9:J:15:DT:H5'	1.93	0.49
3:C:50:TYR:OH	4:D:92:GLN:NE2	2.41	0.49
9:J:7:DC:H4'	9:J:8:DG:OP1	2.13	0.49
8:I:20:DG:H2"	8:I:21:DC:O5'	2.13	0.49
9:J:65:DA:C2'	9:J:66:DT:H5"	2.35	0.49
4:H:84:SER:OG	9:J:-35:DA:H3'	2.13	0.49
8:I:44:DC:H4'	8:I:45:DC:OP1	2.12	0.49
8:I:-68:DA:C2	9:J:69:DA:C2	3.01	0.48
3:C:12:ARG:HH22	8:I:-41:DG:H5'	1.78	0.48
7:G:17:ARG:CG	7:G:17:ARG:HH21	2.26	0.48
8:I:65:DA:C2	9:J:-64:DG:C2	3.01	0.48
9:J:-71:DC:C6	9:J:-71:DC:C5'	2.92	0.48
3:C:64:GLU:OE2	4:D:45:VAL:CG1	2.62	0.48
9:J:17:DA:H1'	9:J:18:DG:H5'	1.97	0.47
2:B:94:GLY:C	2:B:95:ARG:HG2	2.35	0.47
2:B:101:GLY:O	2:B:102:GLY:C	2.52	0.47
8:I:-12:DC:H2"	8:I:-11:DG:C8	2.50	0.47
9:J:-6:DT:H2"	9:J:-5:DA:C8	2.50	0.47
7:G:50:TYR:OH	4:H:92:GLN:NE2	2.34	0.47
8:I:-66:DA:OP2	8:I:-66:DA:H8	1.97	0.47
3:C:26:PRO:HG3	4:D:37:TYR:CZ	2.50	0.47
4:D:30:ARG:HG3	9:J:49:DC:H4'	1.96	0.47
8:I:35:DT:H1'	8:I:36:DA:N7	2.30	0.47
9:J:17:DA:C6	9:J:18:DG:C6	3.03	0.46
9:J:-35:DA:C5	9:J:-34:DA:C6	3.04	0.46
9:J:50:DG:C2'	9:J:51:DG:H5"	2.45	0.46
8:I:21:DC:H2'	8:I:22:DC:C6	2.51	0.46
8:I:45:DC:H2"	8:I:46:DA:OP2	2.15	0.46
5:E:69:ARG:NH2	8:I:17:DA:P	2.88	0.46
9:J:-57:DT:H2"	9:J:-56:DC:C5	2.50	0.46
2:B:31:LYS:N	2:B:32:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:ALA:O	3:C:73:ASN:ND2	2.48	0.46
8:I:-54:DA:P	11:I:201:HOH:O	2.74	0.46
9:J:-45:DG:H2''	9:J:-44:DG:H8	1.79	0.46
8:I:-11:DG:C4	8:I:-10:DC:C5	3.03	0.45
8:I:2:DG:C8	8:I:3:DT:H72	2.51	0.45
9:J:65:DA:C2	9:J:66:DT:C2	3.05	0.45
7:G:50:TYR:O	7:G:54:VAL:HG23	2.17	0.45
9:J:64:DG:H2''	9:J:65:DA:OP2	2.16	0.45
2:B:88:TYR:CE1	4:D:80:TYR:CE1	3.05	0.45
1:A:83:ARG:CG	8:I:-24:DG:O3'	2.64	0.45
8:I:44:DC:H2''	8:I:45:DC:O5'	2.17	0.45
8:I:50:DA:H2''	8:I:51:DC:OP2	2.16	0.45
9:J:-34:DA:H1'	9:J:-33:DG:C8	2.51	0.45
1:A:43:PRO:HG2	8:I:-5:DA:C5'	2.45	0.44
2:B:98:TYR:OH	4:H:65:ASP:OD2	2.19	0.44
8:I:-67:DT:C2'	8:I:-66:DA:OP2	2.61	0.44
4:H:98:LEU:HD13	11:H:204:HOH:O	2.17	0.44
8:I:-54:DA:C5	8:I:-53:DG:C6	3.05	0.44
3:C:12:ARG:HH12	8:I:-41:DG:H5''	1.81	0.44
8:I:50:DA:H2''	8:I:51:DC:H5'	2.00	0.44
7:G:32:ARG:CD	9:J:-44:DG:OP2	2.65	0.44
8:I:-54:DA:C6	8:I:-53:DG:C6	3.04	0.44
3:C:80:PRO:HG3	4:D:58:ILE:HD12	2.00	0.43
8:I:0:DC:H2''	8:I:1:DT:OP2	2.18	0.43
9:J:49:DC:H2''	9:J:50:DG:C8	2.53	0.43
4:D:79:HIS:NE2	7:G:38:ASN:OD1	2.45	0.43
7:G:27:VAL:HG11	7:G:49:VAL:HG22	2.01	0.43
7:G:26:PRO:HG3	4:H:37:TYR:CE2	2.53	0.43
8:I:-61:DG:H2''	8:I:-60:DG:C8	2.54	0.43
9:J:42:DA:H1'	9:J:43:DA:C8	2.54	0.42
9:J:-45:DG:C2	9:J:-44:DG:C2	3.07	0.42
9:J:-47:DC:H2''	9:J:-46:DT:C7	2.49	0.42
5:E:46:VAL:HG21	8:I:9:DG:H3'	2.00	0.42
7:G:81:ARG:HG3	7:G:81:ARG:O	2.19	0.42
8:I:35:DT:H1'	8:I:36:DA:C5	2.55	0.42
8:I:-37:DG:H2''	8:I:-36:DT:OP2	2.19	0.42
3:C:31:HIS:CE1	3:C:35:ARG:HE	2.37	0.42
7:G:87:ILE:HD13	7:G:102:ILE:HD11	2.01	0.42
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.51	0.42
8:I:-53:DG:H1'	8:I:-52:DG:C8	2.54	0.42
8:I:-49:DG:H1'	8:I:-48:DC:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:36:LYS:O	7:G:36:LYS:HG2	2.19	0.41
7:G:93:LEU:HD23	4:H:103:LEU:HD21	2.02	0.41
9:J:41:DC:H2''	9:J:42:DA:C8	2.55	0.41
4:D:62:PHE:CD1	4:D:66:ILE:HD13	2.55	0.41
8:I:-49:DG:H1'	8:I:-48:DC:C6	2.54	0.41
9:J:50:DG:H1'	9:J:51:DG:H5''	2.02	0.41
4:H:75:SER:HA	4:H:86:ILE:HD11	2.02	0.41
1:A:113:HIS:CG	5:E:126:LEU:HD22	2.54	0.41
4:H:49:THR:HG22	11:H:203:HOH:O	2.21	0.41
8:I:48:DG:C5'	11:I:203:HOH:O	2.64	0.41
9:J:67:DA:H2''	9:J:68:DT:H5'	2.03	0.41
7:G:14:ALA:HA	9:J:-42:DG:O5'	2.21	0.41
5:E:85:GLN:NE2	6:F:82:THR:HG22	2.36	0.41
3:C:64:GLU:OE2	4:D:45:VAL:HG13	2.20	0.41
7:G:80:PRO:HG3	4:H:58:ILE:HD12	2.03	0.41
8:I:73:DT:H2''	8:I:74:DA:C8	2.56	0.41
8:I:-30:DG:H2''	8:I:-29:DC:O5'	2.21	0.41
9:J:32:DG:H2''	9:J:33:DT:H71	2.02	0.41
4:D:29:SER:HB3	8:I:30:DG:OP1	2.21	0.40
5:E:48:LEU:HA	5:E:48:LEU:HD12	1.89	0.40
4:H:26:ARG:C	4:H:27:LYS:HD3	2.42	0.40
4:H:77:LEU:HA	4:H:77:LEU:HD13	1.94	0.40
3:C:47:ALA:HB3	3:C:48:PRO:HD3	2.02	0.40
8:I:-43:DT:H2''	8:I:-42:DT:H5'	2.03	0.40
8:I:54:DG:H2'	8:I:54:DG:OP2	2.22	0.40
2:B:30:THR:OG1	2:B:32:PRO:HG2	2.21	0.40
9:J:27:DG:OP2	11:J:201:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:109:SER:OG	8:I:-61:DG:OP1[3_755]	2.08	0.12

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	96/98 (98%)	96 (100%)	0	0	100	100
2	B	78/82 (95%)	77 (99%)	1 (1%)	0	100	100
3	C	105/107 (98%)	96 (91%)	7 (7%)	2 (2%)	8	4
4	D	95/97 (98%)	89 (94%)	4 (4%)	2 (2%)	7	3
4	H	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	4	1
5	E	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
6	F	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
7	G	104/106 (98%)	98 (94%)	5 (5%)	1 (1%)	15	13
All	All	753/771 (98%)	720 (96%)	25 (3%)	8 (1%)	14	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	28	ARG
4	D	101	GLY
4	H	101	GLY
3	C	14	ALA
7	G	14	ALA
4	H	28	ARG
4	H	29	SER
3	C	16	THR

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	85/85 (100%)	82 (96%)	3 (4%)	36	43
2	B	65/67 (97%)	59 (91%)	6 (9%)	9	7
3	C	85/85 (100%)	80 (94%)	5 (6%)	19	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	83/83 (100%)	74 (89%)	9 (11%)	6	4
4	H	83/83 (100%)	74 (89%)	9 (11%)	6	4
5	E	85/85 (100%)	78 (92%)	7 (8%)	11	10
6	F	72/72 (100%)	67 (93%)	5 (7%)	15	14
7	G	84/84 (100%)	75 (89%)	9 (11%)	6	4
All	All	642/644 (100%)	589 (92%)	53 (8%)	11	9

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	65	LEU
1	A	83	ARG
2	B	23	ARG
2	B	24	ASP
2	B	26	ILE
2	B	47	SER
2	B	74	GLU
2	B	95	ARG
3	C	13	LYS
3	C	17	ARG
3	C	50	TYR
3	C	62	ILE
3	C	81	ARG
4	D	26	ARG
4	D	30	ARG
4	D	39	TYR
4	D	83	ARG
4	D	84	SER
4	D	85	THR
4	D	98	LEU
4	D	102	GLU
4	D	109	SER
5	E	48	LEU
5	E	59	GLU
5	E	63	ARG
5	E	65	LEU
5	E	117	VAL
5	E	129	ARG
5	E	134	ARG

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Mol	Chain	Res	Type
6	F	16	LYS
6	F	17	ARG
6	F	19	ARG
6	F	21	VAL
6	F	91	LYS
7	G	13	LYS
7	G	15	LYS
7	G	17	ARG
7	G	29	ARG
7	G	42	ARG
7	G	74	LYS
7	G	81	ARG
7	G	99	ARG
7	G	118	LYS
4	H	26	ARG
4	H	27	LYS
4	H	31	LYS
4	H	49	THR
4	H	77	LEU
4	H	84	SER
4	H	85	THR
4	H	103	LEU
4	H	109	SER

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

Mol	Chain	Res	Type
3	C	31	HIS
3	C	38	ASN
4	D	92	GLN
7	G	31	HIS
4	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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 17 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	A	98/98 (100%)	0.12	1 (1%) 82 84	40, 61, 97, 138	0
2	B	80/82 (97%)	0.06	1 (1%) 77 79	46, 57, 79, 125	0
3	C	107/107 (100%)	-0.02	1 (0%) 84 85	37, 53, 94, 156	0
4	D	97/97 (100%)	0.15	3 (3%) 49 52	41, 55, 107, 179	0
4	H	97/97 (100%)	0.42	4 (4%) 37 40	43, 62, 131, 184	0
5	E	97/97 (100%)	0.03	0 100 100	36, 48, 79, 145	0
6	F	87/87 (100%)	0.01	1 (1%) 80 82	37, 48, 78, 156	0
7	G	106/106 (100%)	0.04	1 (0%) 84 85	48, 63, 100, 127	0
8	I	147/147 (100%)	-0.60	0 100 100	61, 105, 141, 148	0
9	J	147/147 (100%)	-0.52	0 100 100	60, 108, 146, 159	0
All	All	1063/1065 (99%)	-0.08	12 (1%) 80 82	36, 64, 132, 184	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	28	ARG	8.5
4	H	26	ARG	8.0
4	H	122	LYS	7.1
4	H	29	SER	4.8
4	D	28	ARG	4.4
3	C	13	LYS	4.1
4	D	27	LYS	3.1
6	F	18	HIS	2.5
1	A	38	PRO	2.4
4	D	29	SER	2.3
7	G	118	LYS	2.3
2	B	102	GLY	2.0

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](#)

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. 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	B-factors(\AA^2)	Q<0.9
10	MN	J	102	1/1	0.74	0.12	119,119,119,119	0
10	MN	A	201	1/1	0.76	0.08	138,138,138,138	0
10	MN	J	107	1/1	0.77	0.07	122,122,122,122	0
10	MN	J	108	1/1	0.79	0.05	124,124,124,124	0
10	MN	J	106	1/1	0.89	0.10	107,107,107,107	0
10	MN	J	105	1/1	0.91	0.18	85,85,85,85	0
10	MN	I	104	1/1	0.92	0.21	127,127,127,127	0
10	MN	I	106	1/1	0.93	0.14	129,129,129,129	0
10	MN	I	102	1/1	0.94	0.10	113,113,113,113	0
10	MN	I	101	1/1	0.95	0.20	110,110,110,110	0
10	MN	J	109	1/1	0.96	0.05	106,106,106,106	0
10	MN	J	103	1/1	0.97	0.20	115,115,115,115	0
10	MN	I	105	1/1	0.97	0.19	99,99,99,99	0
10	MN	J	104	1/1	0.97	0.18	106,106,106,106	0
10	MN	J	101	1/1	0.97	0.15	86,86,86,86	0
10	MN	I	103	1/1	0.98	0.16	100,100,100,100	0
10	MN	E	201	1/1	1.00	0.17	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.