



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:15 am BST

PDB ID : 3MGS  
Title : Binding of Cesium ions to the Nucleosome Core particle  
Authors : Mohideen, K.; Muhammad, R.; Davey, C.A.  
Deposited on : 2010-04-07  
Resolution : 3.15 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

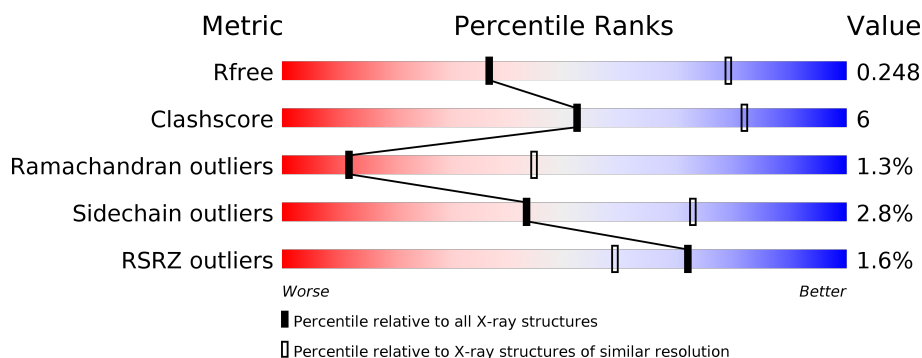
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 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	135	<div> <div>0.5%</div> <div> <div></div> <div>64%</div> <div>9%</div> <div>27%</div> </div> </div>
1	E	135	<div> <div>0.5%</div> <div> <div></div> <div>64%</div> <div>7%</div> <div>27%</div> </div> </div>
2	B	102	<div> <div>0.5%</div> <div> <div></div> <div>65%</div> <div>11%</div> <div>23%</div> </div> </div>
2	F	102	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>15%</div> </div> </div>
3	C	119	<div> <div></div> <div> <div></div> <div>77%</div> <div>9%</div> <div>13%</div> </div> </div>
3	G	119	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	125	
4	H	125	
5	I	147	
6	J	147	

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
8	CS	C	120	-	-	-	X
8	CS	H	123	-	-	-	X
8	CS	I	78	-	-	-	X
8	CS	I	79	-	-	-	X
8	CS	I	80	-	-	-	X
8	CS	J	74	-	-	-	X
8	CS	J	75	-	-	-	X
9	MN	I	3141	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12207 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 H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			817	515	158	141	3			
1	E	99	Total	C	N	O	S	0	0	0
			817	515	158	141	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	SEE REMARK 999	UNP P84233
E	102	ALA	GLY	SEE REMARK 999	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	79	Total	C	N	O	S	0	0	0
			627	395	121	110	1			
2	F	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	104	Total	C	N	O		0	0	0
			804	507	157	140				
3	G	106	Total	C	N	O		0	0	0
			818	516	160	142				

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	99	Total	C	N	O	S	0	0	0
			785	493	146	144	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	99	Total	C	N	O	S	0	0	0
			785	493	146	144	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	SEE REMARK 999	UNP P02281
H	29	THR	SER	SEE REMARK 999	UNP P02281

- Molecule 5 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	147	Total	C	N	O	P	0	0	0
			3011	1440	546	879	146			

- Molecule 6 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	147	Total	C	N	O	P	0	0	0
			3010	1440	543	881	146			

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total Cs 1 1	0	0
8	J	2	Total Cs 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	7	Total	Cs	0	0
			7	7		
8	D	1	Total	Cs	0	0
			1	1		
8	C	1	Total	Cs	0	0
			1	1		

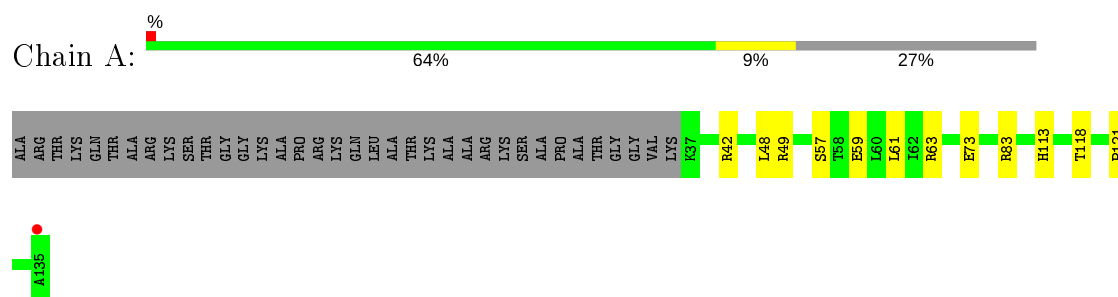
- Molecule 9 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	7	Total	Mn	0	0
			7	7		
9	I	6	Total	Mn	0	0
			6	6		
9	E	1	Total	Mn	0	0
			1	1		

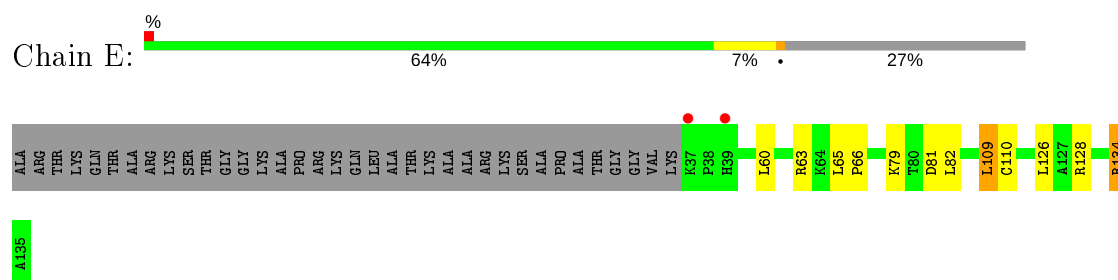
### 3 Residue-property plots [i](#)

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.

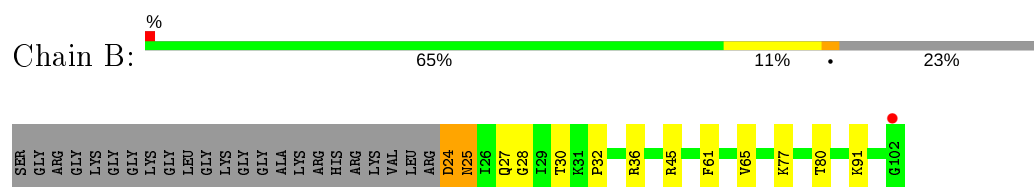
- Molecule 1: Histone H3.2



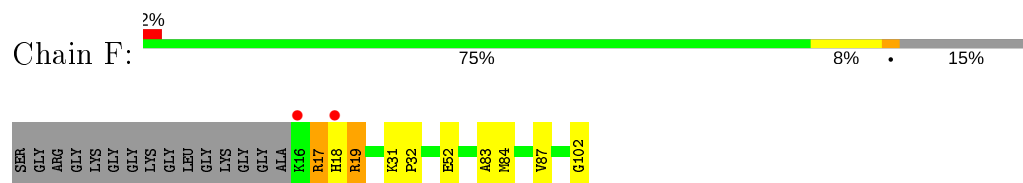
- Molecule 1: Histone H3.2



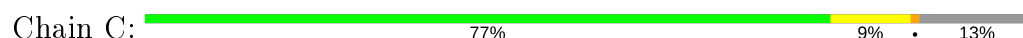
- Molecule 2: Histone H4



- Molecule 2: Histone H4

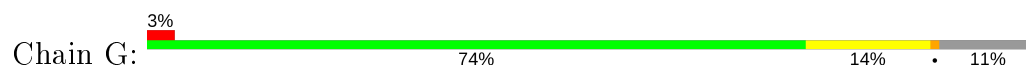


- Molecule 3: Histone H2A

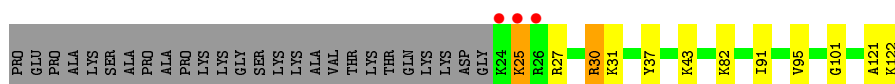




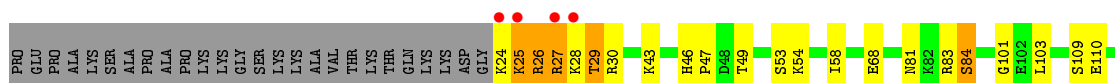
- Molecule 3: Histone H2A



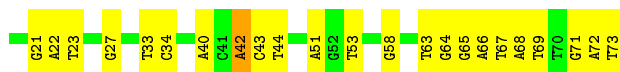
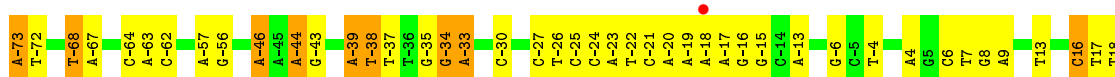
- Molecule 4: Histone H2B 1.1



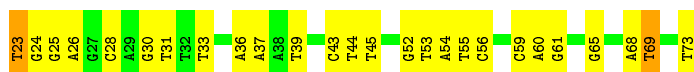
- Molecule 4: Histone H2B 1.1



- Molecule 5: DNA (147-MER)



- Molecule 6: DNA (147-MER)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.51Å 109.67Å 182.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.07 – 3.15 94.02 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (94.07-3.15) 99.7 (94.02-3.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 3.13Å)	Xtriage
Refinement program	REFMAC Rigid Body	Depositor
R, $R_{free}$	0.216 , 0.238 0.225 , 0.248	Depositor DCC
$R_{free}$ test set	774 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: CS, MN, CL

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	0.49	0/829	0.61	0/1111
1	E	0.60	0/829	0.65	0/1111
2	B	0.56	0/634	0.62	0/848
2	F	0.63	0/711	0.66	0/948
3	C	0.54	0/814	0.62	0/1099
3	G	0.48	0/828	0.63	0/1117
4	D	0.53	0/796	0.63	0/1065
4	H	0.52	0/796	0.61	0/1065
5	I	0.78	0/3378	1.48	45/5212 (0.9%)
6	J	0.78	0/3376	1.55	47/5209 (0.9%)
All	All	0.68	0/12991	1.20	92/18785 (0.5%)

There are no bond length outliers.

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	-6	DG	O4'-C1'-N9	-12.20	99.46	108.00
6	J	22	DA	O4'-C1'-N9	9.94	114.96	108.00
6	J	-35	DG	O4'-C1'-N9	-8.37	102.14	108.00
5	I	-19	DA	O4'-C1'-N9	8.27	113.79	108.00
6	J	-62	DC	O4'-C1'-N1	8.27	113.79	108.00
5	I	9	DA	O4'-C1'-N9	-8.16	102.29	108.00
6	J	-40	DT	O4'-C1'-N1	7.79	113.45	108.00
6	J	-35	DG	O4'-C4'-C3'	-7.62	101.43	106.00
5	I	-39	DA	O4'-C1'-N9	7.44	113.21	108.00
6	J	60	DA	O4'-C1'-N9	-7.32	102.88	108.00
5	I	64	DG	O4'-C1'-N9	7.24	113.06	108.00
5	I	71	DG	O4'-C1'-N9	7.22	113.06	108.00
6	J	23	DT	O4'-C1'-N1	7.20	113.04	108.00
5	I	43	DC	O4'-C1'-N1	7.11	112.97	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	54	DA	O4'-C1'-N9	7.05	112.94	108.00
5	I	-63	DA	O4'-C1'-N9	6.97	112.88	108.00
5	I	8	DG	O4'-C1'-N9	-6.96	103.13	108.00
6	J	-19	DA	O4'-C1'-N9	6.94	112.86	108.00
6	J	-56	DG	O4'-C1'-N9	6.81	112.77	108.00
5	I	73	DT	O4'-C1'-N1	6.75	112.72	108.00
5	I	-38	DT	O4'-C1'-N1	6.68	112.68	108.00
6	J	-12	DT	N3-C2-O2	-6.57	118.36	122.30
5	I	22	DA	O4'-C1'-N9	6.57	112.60	108.00
5	I	-33	DA	O4'-C1'-N9	-6.52	103.44	108.00
5	I	-62	DC	O4'-C1'-N1	6.47	112.53	108.00
6	J	-4	DT	N3-C2-O2	-6.38	118.47	122.30
5	I	-64	DC	O4'-C1'-N1	6.38	112.47	108.00
6	J	56	DC	O4'-C1'-N1	6.35	112.45	108.00
5	I	-73	DA	O4'-C1'-N9	6.34	112.44	108.00
6	J	25	DG	O4'-C1'-N9	6.32	112.42	108.00
5	I	-4	DT	C4-C5-C7	6.27	122.76	119.00
5	I	44	DT	P-O3'-C3'	6.22	127.16	119.70
6	J	21	DG	C3'-C2'-C1'	-6.20	95.06	102.50
5	I	-17	DA	O4'-C1'-N9	6.14	112.30	108.00
5	I	21	DG	O4'-C1'-N9	6.13	112.29	108.00
6	J	53	DT	C1'-O4'-C4'	-6.13	103.97	110.10
5	I	68	DA	O4'-C1'-N9	-6.12	103.72	108.00
6	J	-4	DT	O4'-C1'-N1	-6.10	103.73	108.00
6	J	21	DG	P-O3'-C3'	6.07	126.99	119.70
5	I	53	DT	O4'-C1'-N1	6.07	112.25	108.00
6	J	69	DT	C4-C5-C7	6.05	122.63	119.00
5	I	-4	DT	C6-C5-C7	-6.00	119.30	122.90
5	I	58	DG	O4'-C1'-N9	-6.00	103.80	108.00
6	J	-44	DA	O4'-C1'-N9	6.00	112.20	108.00
6	J	52	DG	O4'-C1'-N9	5.91	112.14	108.00
5	I	16	DC	O4'-C1'-C2'	-5.89	101.19	105.90
5	I	42	DA	O4'-C1'-N9	5.85	112.10	108.00
5	I	-4	DT	O4'-C1'-N1	-5.85	103.90	108.00
6	J	55	DT	O4'-C1'-N1	5.79	112.05	108.00
6	J	-68	DT	O4'-C1'-N1	5.70	111.99	108.00
6	J	-31	DA	O4'-C1'-N9	5.68	111.98	108.00
5	I	-23	DA	O4'-C1'-N9	-5.64	104.05	108.00
5	I	-34	DG	O4'-C1'-N9	5.60	111.92	108.00
6	J	69	DT	C6-C5-C7	-5.58	119.55	122.90
6	J	4	DA	O4'-C1'-N9	-5.58	104.09	108.00
5	I	-20	DA	P-O3'-C3'	5.58	126.39	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	26	DA	O4'-C1'-N9	-5.56	104.11	108.00
5	I	58	DG	P-O3'-C3'	5.51	126.31	119.70
5	I	67	DT	C1'-O4'-C4'	-5.49	104.61	110.10
5	I	63	DT	C4-C5-C7	5.45	122.27	119.00
5	I	13	DT	N3-C2-O2	-5.41	119.05	122.30
6	J	-24	DC	O4'-C1'-N1	-5.40	104.22	108.00
6	J	65	DG	O4'-C1'-N9	5.39	111.77	108.00
5	I	40	DA	O4'-C1'-N9	5.38	111.77	108.00
5	I	23	DT	O4'-C1'-N1	5.38	111.77	108.00
5	I	7	DT	P-O3'-C3'	5.37	126.14	119.70
5	I	-46	DA	P-O3'-C3'	5.34	126.11	119.70
6	J	-23	DA	O4'-C1'-N9	-5.32	104.27	108.00
6	J	61	DG	O4'-C1'-N9	5.29	111.70	108.00
6	J	-33	DA	P-O3'-C3'	5.28	126.03	119.70
6	J	45	DT	O4'-C1'-N1	5.28	111.69	108.00
6	J	-3	DG	O4'-C1'-N9	-5.28	104.31	108.00
5	I	-73	DA	P-O3'-C3'	5.26	126.02	119.70
6	J	28	DC	O4'-C1'-N1	-5.23	104.34	108.00
6	J	-3	DG	P-O3'-C3'	5.18	125.92	119.70
6	J	-66	DT	C3'-C2'-C1'	-5.18	96.29	102.50
6	J	-30	DC	O4'-C1'-N1	5.18	111.62	108.00
5	I	-44	DA	C1'-O4'-C4'	-5.15	104.95	110.10
6	J	-45	DA	O4'-C1'-N9	5.15	111.61	108.00
6	J	21	DG	C1'-O4'-C4'	-5.15	104.95	110.10
6	J	59	DC	N1-C2-O2	5.15	121.99	118.90
5	I	67	DT	C3'-C2'-C1'	-5.13	96.34	102.50
6	J	-55	DA	C1'-O4'-C4'	-5.11	104.99	110.10
5	I	-30	DC	O4'-C1'-N1	5.11	111.58	108.00
6	J	0	DT	P-O3'-C3'	5.08	125.80	119.70
5	I	67	DT	O4'-C1'-N1	5.06	111.55	108.00
5	I	-68	DT	P-O3'-C3'	5.06	125.77	119.70
6	J	53	DT	O4'-C1'-C2'	-5.05	101.86	105.90
5	I	-4	DT	N3-C2-O2	-5.03	119.28	122.30
5	I	69	DT	O4'-C1'-N1	-5.03	104.48	108.00
6	J	-72	DT	O4'-C1'-N1	5.02	111.51	108.00
6	J	-58	DC	C1'-O4'-C4'	-5.00	105.09	110.10

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	817	0	858	10	0
1	E	817	0	858	11	0
2	B	627	0	663	10	0
2	F	703	0	755	7	0
3	C	804	0	859	11	0
3	G	818	0	877	16	0
4	D	785	0	825	7	0
4	H	785	0	825	16	0
5	I	3011	0	1662	30	0
6	J	3010	0	1662	36	0
7	A	1	0	0	1	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	H	1	0	0	0	0
8	I	7	0	0	0	0
8	J	2	0	0	1	0
9	E	1	0	0	0	0
9	I	6	0	0	0	0
9	J	7	0	0	1	0
All	All	12207	0	9844	119	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 6.

All (119) 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)
8:J:74:CS:CS	9:J:3136:MN:MN	1.47	1.02
6:J:16:DC:H2"	6:J:17:DT:H71	1.58	0.84
5:I:-22:DT:H2"	5:I:-21:DC:H5"	1.61	0.82
6:J:-69:DA:H2"	6:J:-68:DT:H5"	1.71	0.73
6:J:16:DC:H2"	6:J:17:DT:C7	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-47:DA:H2''	6:J:-46:DA:C8	2.28	0.68
4:H:27:ARG:HA	6:J:30:DG:H5''	1.75	0.68
6:J:-5:DC:H2''	6:J:-4:DT:H71	1.77	0.67
4:D:43:LYS:HE2	4:D:43:LYS:HA	1.77	0.67
4:H:25:LYS:HE2	6:J:-47:DA:H5''	1.78	0.66
5:I:-18:DA:H61	6:J:18:DT:H3	1.43	0.65
5:I:-25:DC:H1'	5:I:-24:DC:C6	2.31	0.65
3:G:13:LYS:HE2	6:J:-44:DA:N3	2.11	0.65
5:I:42:DA:H61	6:J:-42:DT:H3	1.46	0.63
5:I:-44:DA:H2''	5:I:-43:DG:H8	1.65	0.62
6:J:-72:DT:H2''	6:J:-71:DC:H5'	1.82	0.61
5:I:65:DG:H2''	5:I:66:DA:OP2	2.00	0.61
6:J:-68:DT:H2''	6:J:-67:DA:C8	2.36	0.60
3:C:17:ARG:HH22	3:C:31:HIS:CD2	2.20	0.60
3:G:13:LYS:HB3	6:J:-43:DG:H4'	1.84	0.58
5:I:-16:DG:H4'	5:I:-15:DG:H5'	1.87	0.57
5:I:-73:DA:H2''	5:I:-72:DT:OP2	2.06	0.56
1:A:63:ARG:NE	5:I:-13:DA:H5''	2.21	0.56
5:I:-33:DA:H61	6:J:33:DT:H3	1.52	0.56
3:C:17:ARG:HH12	3:C:31:HIS:HD2	1.53	0.55
1:E:81:ASP:HA	2:F:19:ARG:HH12	1.72	0.55
2:B:61:PHE:O	2:B:65:VAL:HG23	2.07	0.55
1:A:83:ARG:O	2:B:80:THR:HA	2.06	0.54
5:I:-73:DA:H61	6:J:73:DT:H3	1.54	0.54
1:A:57:SER:HB2	1:A:59:GLU:OE2	2.08	0.54
4:H:24:LYS:HD3	5:I:51:DA:H4'	1.89	0.54
3:G:31:HIS:CD2	3:G:48:PRO:HG3	2.42	0.54
5:I:-39:DA:H61	6:J:39:DT:H3	1.56	0.53
6:J:3:DC:H2''	6:J:4:DA:N7	2.23	0.53
5:I:-67:DA:C2	6:J:68:DA:C2	2.97	0.53
3:G:73:ASN:N	3:G:73:ASN:HD22	2.08	0.52
2:F:84:MET:HE1	2:F:102:GLY:HA3	1.91	0.52
4:H:28:LYS:O	4:H:29:THR:C	2.48	0.51
2:F:84:MET:CE	2:F:102:GLY:HA3	2.40	0.51
5:I:-27:DC:H2''	5:I:-26:DT:H72	1.92	0.51
5:I:-25:DC:H1'	5:I:-24:DC:C5	2.46	0.50
6:J:-68:DT:H2''	6:J:-67:DA:H8	1.76	0.50
2:B:30:THR:HB	2:B:32:PRO:HD2	1.92	0.50
2:F:83:ALA:O	2:F:87:VAL:HG23	2.11	0.49
5:I:-38:DT:H2''	5:I:-37:DT:OP2	2.11	0.49
3:C:17:ARG:HH22	3:C:31:HIS:HD2	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:91:ILE:O	4:D:95:VAL:HG23	2.12	0.49
6:J:23:DT:H2"	6:J:24:DG:OP2	2.12	0.49
3:G:79:ILE:HB	3:G:80:PRO:CD	2.43	0.49
4:H:81:ASN:O	4:H:83:ARG:HG2	2.13	0.49
3:C:31:HIS:CG	3:C:48:PRO:HG3	2.48	0.48
5:I:-44:DA:H2"	5:I:-43:DG:C8	2.46	0.48
4:H:26:ARG:C	4:H:28:LYS:H	2.16	0.48
4:H:30:ARG:HD3	6:J:-46:DA:H4'	1.95	0.48
1:E:128:ARG:HH12	1:E:134:ARG:HE	1.61	0.48
3:G:17:ARG:HH12	3:G:31:HIS:HD2	1.60	0.48
5:I:-57:DA:H2"	5:I:-56:DG:OP2	2.15	0.47
6:J:68:DA:H1'	6:J:69:DT:H5'	1.96	0.47
3:C:15:LYS:HG2	3:C:20:ARG:NH1	2.29	0.47
1:A:49:ARG:HD2	6:J:-66:DT:P	2.55	0.47
3:G:31:HIS:CE1	3:G:35:ARG:NH2	2.83	0.47
4:D:121:ALA:O	4:D:122:LYS:HB2	2.15	0.47
3:G:79:ILE:HB	3:G:80:PRO:HD2	1.97	0.47
2:F:17:ARG:HD2	2:F:17:ARG:HA	1.71	0.47
6:J:-5:DC:H2"	6:J:-4:DT:C7	2.45	0.47
1:A:121:PRO:HD2	7:A:3147:CL:CL	2.52	0.46
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.50	0.46
4:H:46:HIS:HB3	4:H:49:THR:OG1	2.15	0.46
6:J:43:DC:H2"	6:J:44:DT:O5'	2.15	0.46
3:C:17:ARG:HH12	3:C:31:HIS:CD2	2.34	0.46
1:A:42:ARG:NH1	5:I:72:DA:OP1	2.48	0.46
1:E:79:LYS:HB3	1:E:82:LEU:HD11	1.98	0.46
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.51	0.46
1:E:65:LEU:HB3	1:E:66:PRO:HD3	1.98	0.46
3:G:37:GLY:HA3	3:G:39:TYR:CE1	2.50	0.46
5:I:16:DC:H2"	5:I:17:DT:H71	1.98	0.46
2:F:31:LYS:N	2:F:32:PRO:HD2	2.32	0.45
4:H:43:LYS:O	4:H:47:PRO:HG3	2.16	0.45
4:H:26:ARG:HA	6:J:31:DT:OP1	2.16	0.45
3:C:26:PRO:HG3	4:D:37:TYR:CE1	2.52	0.45
1:A:118:THR:HA	2:B:45:ARG:O	2.17	0.44
3:G:102:ILE:HG23	4:H:58:ILE:HD12	1.98	0.44
6:J:-48:DC:H2"	6:J:-47:DA:N7	2.33	0.44
3:G:41:GLU:OE1	4:H:84:SER:HB2	2.18	0.44
2:B:91:LYS:NZ	4:H:68:GLU:OE1	2.51	0.44
5:I:-68:DT:H2"	5:I:-67:DA:C8	2.53	0.44
1:E:134:ARG:HA	1:E:134:ARG:HD3	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ASP:HB3	2:B:25:ASN:H	1.51	0.43
2:B:24:ASP:HA	2:B:27:GLN:HB2	1.99	0.43
1:E:65:LEU:O	1:E:66:PRO:C	2.56	0.43
5:I:4:DA:C2	6:J:-3:DG:N2	2.87	0.43
5:I:-6:DG:O6	6:J:5:DG:C6	2.71	0.43
1:E:110:CYS:SG	1:E:126:LEU:HD23	2.58	0.43
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.54	0.43
3:G:15:LYS:HD2	3:G:15:LYS:HA	1.80	0.42
6:J:-25:DC:H1'	6:J:-24:DC:C5	2.54	0.42
1:E:81:ASP:HA	2:F:19:ARG:NH1	2.35	0.42
4:D:31:LYS:HD3	4:D:31:LYS:HA	1.92	0.42
3:C:31:HIS:CE1	3:C:35:ARG:NH2	2.88	0.42
1:E:109:LEU:HA	1:E:109:LEU:HD12	1.75	0.42
1:A:61:LEU:HD13	2:B:36:ARG:HB3	2.01	0.42
1:A:73:GLU:OE1	2:B:25:ASN:ND2	2.52	0.42
3:G:57:TYR:HB2	4:H:110:GLU:HG3	2.02	0.42
5:I:6:DC:H42	6:J:-6:DG:H1	1.68	0.42
2:B:28:GLY:O	2:B:30:THR:HG23	2.20	0.41
3:C:118:LYS:NZ	3:C:118:LYS:HA	2.35	0.41
4:D:25:LYS:HE3	4:D:25:LYS:HB2	1.89	0.41
3:G:47:ALA:N	3:G:48:PRO:HD2	2.36	0.41
4:H:28:LYS:HE2	6:J:-47:DA:H4'	2.02	0.41
4:D:30:ARG:HD2	5:I:-46:DA:H4'	2.03	0.41
5:I:-35:DG:C6	5:I:-34:DG:C6	3.09	0.41
3:G:77:ARG:NH2	6:J:-55:DA:H4'	2.36	0.41
6:J:36:DA:H2''	6:J:37:DA:OP2	2.21	0.41
4:H:54:LYS:O	4:H:58:ILE:HG12	2.20	0.41
5:I:33:DT:H1'	5:I:34:DC:H5'	2.02	0.41
6:J:-25:DC:H1'	6:J:-24:DC:C6	2.56	0.41
5:I:27:DG:C6	6:J:-28:DG:O6	2.74	0.40
3:C:37:GLY:HA3	3:C:39:TYR:CE1	2.57	0.40
1:E:63:ARG:NH1	5:I:18:DT:OP1	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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



of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/135 (72%)	97 (100%)	0	0	100	100
1	E	97/135 (72%)	95 (98%)	2 (2%)	0	100	100
2	B	77/102 (76%)	75 (97%)	1 (1%)	1 (1%)	12	44
2	F	85/102 (83%)	82 (96%)	1 (1%)	2 (2%)	6	30
3	C	102/119 (86%)	99 (97%)	3 (3%)	0	100	100
3	G	104/119 (87%)	95 (91%)	8 (8%)	1 (1%)	15	51
4	D	97/125 (78%)	93 (96%)	2 (2%)	2 (2%)	7	33
4	H	97/125 (78%)	90 (93%)	3 (3%)	4 (4%)	3	18
All	All	756/962 (79%)	726 (96%)	20 (3%)	10 (1%)	12	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	27	ARG
4	D	101	GLY
4	H	26	ARG
4	H	29	THR
4	H	101	GLY
2	B	25	ASN
2	F	19	ARG
3	G	14	ALA
4	H	27	ARG
2	F	18	HIS

### 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	86/110 (78%)	85 (99%)	1 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	86/110 (78%)	83 (96%)	3 (4%)	36	67
2	B	64/78 (82%)	62 (97%)	2 (3%)	40	70
2	F	72/78 (92%)	70 (97%)	2 (3%)	43	73
3	C	83/92 (90%)	82 (99%)	1 (1%)	71	87
3	G	84/92 (91%)	83 (99%)	1 (1%)	71	87
4	D	85/105 (81%)	82 (96%)	3 (4%)	36	67
4	H	85/105 (81%)	80 (94%)	5 (6%)	19	51
All	All	645/770 (84%)	627 (97%)	18 (3%)	43	73

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

Mol	Chain	Res	Type
1	A	48	LEU
2	B	24	ASP
2	B	77	LYS
3	C	118	LYS
4	D	25	LYS
4	D	30	ARG
4	D	82	LYS
1	E	60	LEU
1	E	109	LEU
1	E	134	ARG
2	F	17	ARG
2	F	52	GLU
3	G	73	ASN
4	H	25	LYS
4	H	53	SER
4	H	84	SER
4	H	103	LEU
4	H	109	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
3	C	31	HIS
3	C	38	ASN
4	D	92	GLN

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Mol	Chain	Res	Type
1	E	39	HIS
1	E	125	GLN
3	G	31	HIS
3	G	73	ASN
3	G	110	ASN
4	H	44	GLN
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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 30 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 ⓘ

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<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	A	99/135 (73%)	0.22	1 (1%) 82 73	37, 53, 76, 90	0
1	E	99/135 (73%)	0.05	2 (2%) 65 50	30, 42, 69, 84	0
2	B	79/102 (77%)	0.01	1 (1%) 77 66	37, 48, 66, 76	0
2	F	87/102 (85%)	-0.00	2 (2%) 60 46	31, 40, 64, 98	0
3	C	104/119 (87%)	-0.13	0 100 100	32, 44, 61, 71	0
3	G	106/119 (89%)	-0.07	3 (2%) 53 36	37, 55, 78, 97	0
4	D	99/125 (79%)	0.13	3 (3%) 50 33	37, 51, 96, 118	0
4	H	99/125 (79%)	0.11	4 (4%) 38 23	42, 58, 96, 114	0
5	I	147/147 (100%)	-0.26	1 (0%) 87 81	58, 99, 130, 153	0
6	J	147/147 (100%)	-0.34	0 100 100	58, 102, 134, 146	0
All	All	1066/1256 (84%)	-0.06	17 (1%) 72 59	30, 56, 119, 153	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	24	LYS	8.6
4	D	24	LYS	6.3
4	H	25	LYS	5.2
2	F	18	HIS	4.7
2	B	102	GLY	4.5
4	D	25	LYS	4.3
3	G	13	LYS	4.1
4	H	27	ARG	4.0
1	A	135	ALA	4.0
3	G	118	LYS	3.6
4	H	28	LYS	2.8
1	E	37	LYS	2.6
4	D	26	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	39	HIS	2.2
2	F	16	LYS	2.1
3	G	114	VAL	2.0
5	I	-18	DA	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 ⓘ

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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
9	MN	J	3144	1/1	0.21	0.35	143,143,143,143	1
9	MN	I	3140	1/1	0.23	0.26	116,116,116,116	1
8	CS	C	120	1/1	0.32	1.08	100,100,100,100	0
9	MN	I	3141	1/1	0.34	0.40	125,125,125,125	1
8	CS	I	78	1/1	0.50	0.63	100,100,100,100	0
9	MN	I	3143	1/1	0.53	0.20	130,130,130,130	0
8	CS	I	79	1/1	0.61	0.68	100,100,100,100	0
8	CS	J	74	1/1	0.64	0.63	100,100,100,100	0
9	MN	J	3133	1/1	0.66	0.19	104,104,104,104	0
9	MN	I	3138	1/1	0.73	0.26	96,96,96,96	0
9	MN	I	3142	1/1	0.75	0.20	115,115,115,115	1
8	CS	I	80	1/1	0.75	0.55	100,100,100,100	0
8	CS	J	75	1/1	0.76	0.68	100,100,100,100	0
9	MN	J	3139	1/1	0.78	0.17	142,142,142,142	0
8	CS	H	123	1/1	0.79	0.59	100,100,100,100	0
9	MN	J	3134	1/1	0.80	0.14	108,108,108,108	0
8	CS	I	75	1/1	0.82	0.40	100,100,100,100	0
9	MN	I	3137	1/1	0.83	0.15	110,110,110,110	0
8	CS	I	76	1/1	0.83	0.52	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CL	C	3146	1/1	0.85	0.17	54,54,54,54	0
8	CS	I	74	1/1	0.85	0.42	100,100,100,100	0
8	CS	D	123	1/1	0.86	0.55	100,100,100,100	0
9	MN	J	3135	1/1	0.86	0.37	113,113,113,113	0
9	MN	J	3136	1/1	0.91	0.29	87,87,87,87	1
7	CL	G	3145	1/1	0.92	0.12	62,62,62,62	0
7	CL	A	3147	1/1	0.93	0.21	54,54,54,54	1
8	CS	I	77	1/1	0.94	0.55	100,100,100,100	0
7	CL	E	3148	1/1	0.97	0.24	47,47,47,47	1
9	MN	J	3131	1/1	0.98	0.30	94,94,94,94	0
9	MN	E	3132	1/1	0.98	0.33	52,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.