



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2023 – 02:31 PM JST

PDB ID : 7COW  
Title : 353 bp di-nucleosome harboring cohesive DNA termini with linker histone H1.0  
Authors : Adhireksan, Z.; Sharma, D.; Lee, P.L.; Davey, C.A.  
Deposited on : 2020-08-05  
Resolution : 2.86 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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 : 2.36  
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) : 2.36

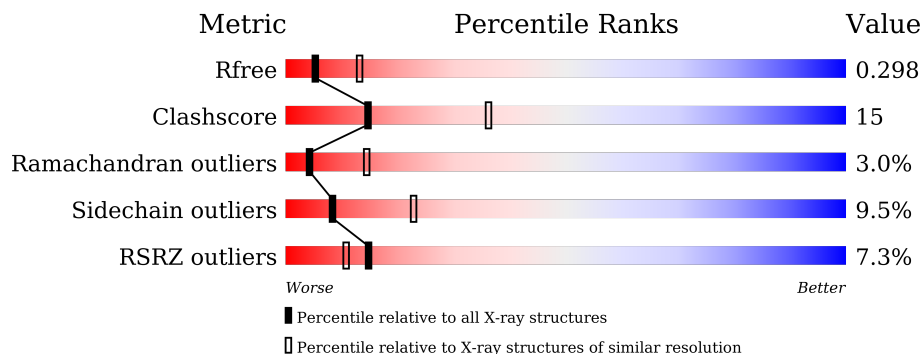
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.86 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 of 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	I	353	
2	J	353	
3	A	138	
3	E	138	
3	K	138	
3	O	138	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	B	105	
4	F	105	
4	L	105	
4	P	105	
5	C	132	
5	G	132	
5	M	132	
5	Q	132	
6	D	128	
6	H	128	
6	N	128	
6	R	128	
7	S	195	
7	T	195	

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
10	CL	C	201	-	-	X	-
10	CL	Q	201	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27785 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 (353-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	I	353	7230	3428	1369	2080	353	0	0	0

- Molecule 2 is a DNA chain called DNA (353-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	J	353	7245	3446	1288	2158	353	0	0	0

- Molecule 3 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	98	807	508	156	139	4	0	0	0
3	E	98	807	508	156	139	4	0	0	0
3	K	98	807	508	156	139	4	0	0	0
3	O	99	816	514	158	140	4	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431
K	-2	SER	-	expression tag	UNP P68431
K	-1	HIS	-	expression tag	UNP P68431
O	-2	SER	-	expression tag	UNP P68431
O	-1	HIS	-	expression tag	UNP P68431

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
4	F	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
4	L	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
4	P	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805
L	-2	SER	-	expression tag	UNP P62805
L	-1	HIS	-	expression tag	UNP P62805
P	-2	SER	-	expression tag	UNP P62805
P	-1	HIS	-	expression tag	UNP P62805

- Molecule 5 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	107	Total	C	N	O	0	0	0
			828	523	162	143			
5	G	106	Total	C	N	O	0	0	0
			819	517	160	142			
5	M	108	Total	C	N	O	0	0	0
			833	526	163	144			
5	Q	107	Total	C	N	O	0	0	0
			824	520	161	143			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908
M	-2	SER	-	expression tag	UNP P04908

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	HIS	-	expression tag	UNP P04908
Q	-2	SER	-	expression tag	UNP P04908
Q	-1	HIS	-	expression tag	UNP P04908

- Molecule 6 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	96	Total 755	C 474	N 138	O 141	S 2	0	0	0
6	H	97	Total 766	C 480	N 142	O 142	S 2	0	0	0
6	N	96	Total 755	C 474	N 138	O 141	S 2	0	0	0
6	R	96	Total 755	C 474	N 138	O 141	S 2	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP P06899
D	-1	HIS	-	expression tag	UNP P06899
H	-2	SER	-	expression tag	UNP P06899
H	-1	HIS	-	expression tag	UNP P06899
N	-2	SER	-	expression tag	UNP P06899
N	-1	HIS	-	expression tag	UNP P06899
R	-2	SER	-	expression tag	UNP P06899
R	-1	HIS	-	expression tag	UNP P06899

- Molecule 7 is a protein called Histone H1.0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	S	75	Total 575	C 358	N 108	O 108	S 1	0	0	0
7	T	75	Total 575	C 358	N 108	O 108	S 1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	0	GLY	-	expression tag	UNP P07305
S	1	PRO	-	expression tag	UNP P07305
T	0	GLY	-	expression tag	UNP P07305

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	PRO	-	expression tag	UNP P07305

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	I	2	Total Ca 2 2	0	0
8	J	1	Total Ca 1 1	0	0

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	I	2	Total K 2 2	0	0
9	J	3	Total K 3 3	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Cl 1 1	0	0
10	G	1	Total Cl 1 1	0	0
10	M	1	Total Cl 1 1	0	0
10	Q	1	Total Cl 1 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total O 1 1	0	0
11	E	1	Total O 1 1	0	0
11	F	1	Total O 1 1	0	0
11	K	1	Total O 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

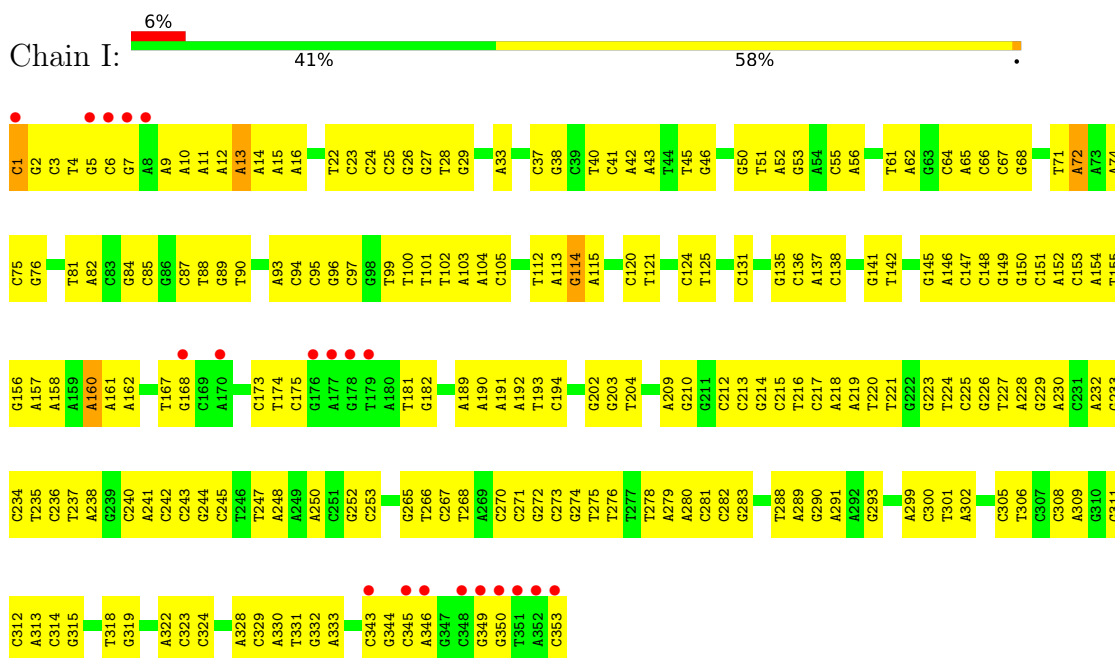
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	2	Total O 2 2	0	0
11	P	3	Total O 3 3	0	0



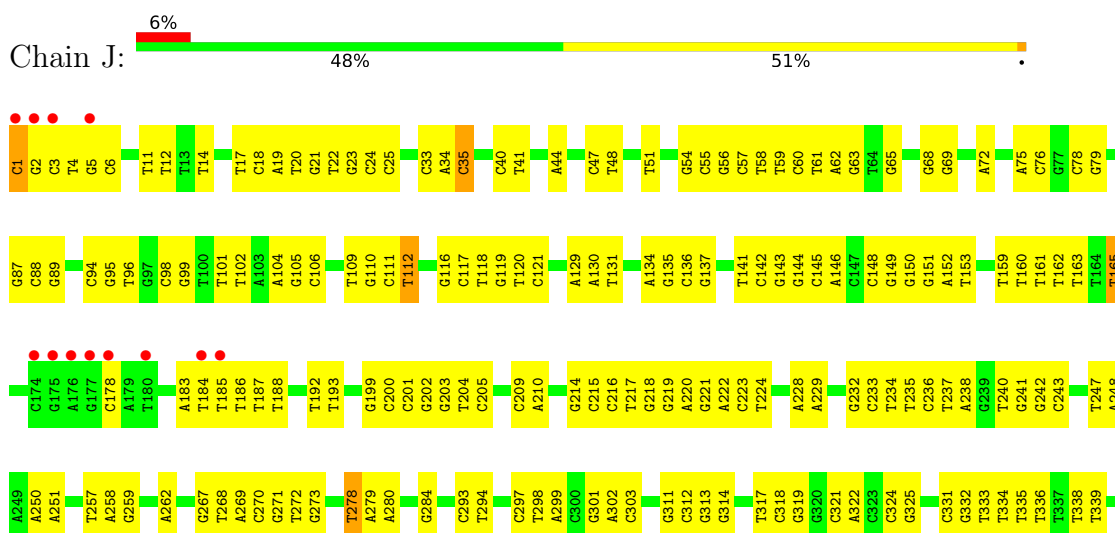
### 3 Residue-property plots [i](#)

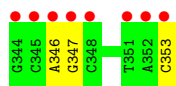
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA (353-MER)

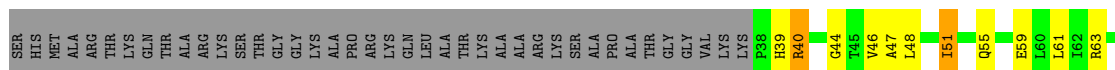


- Molecule 2: DNA (353-MER)

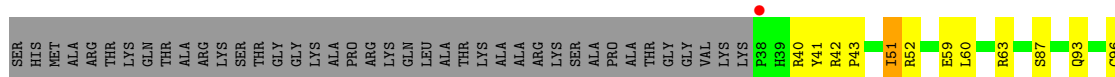




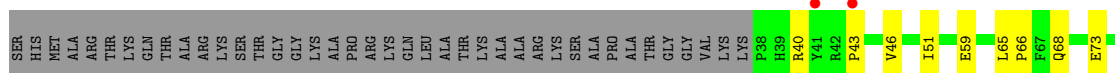
- Molecule 3: Histone H3.1



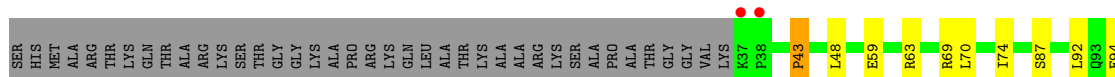
- Molecule 3: Histone H3.1



- Molecule 3: Histone H3.1

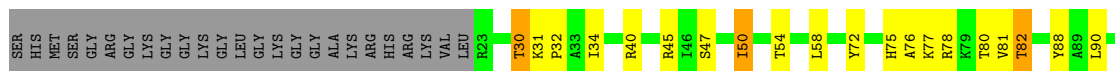


- Molecule 3: Histone H3.1

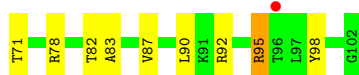
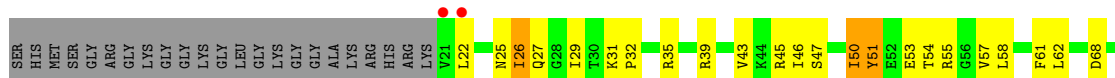


- Molecule 4: Histone H4

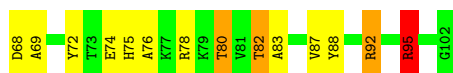
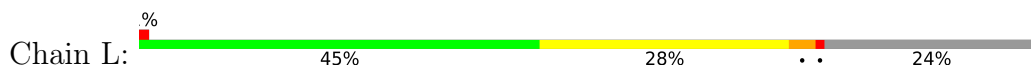




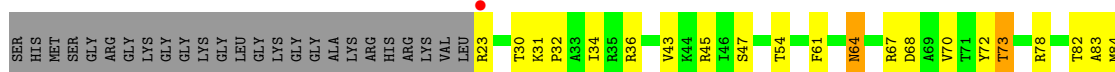
- Molecule 4: Histone H4



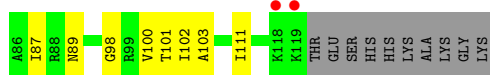
- Molecule 4: Histone H4



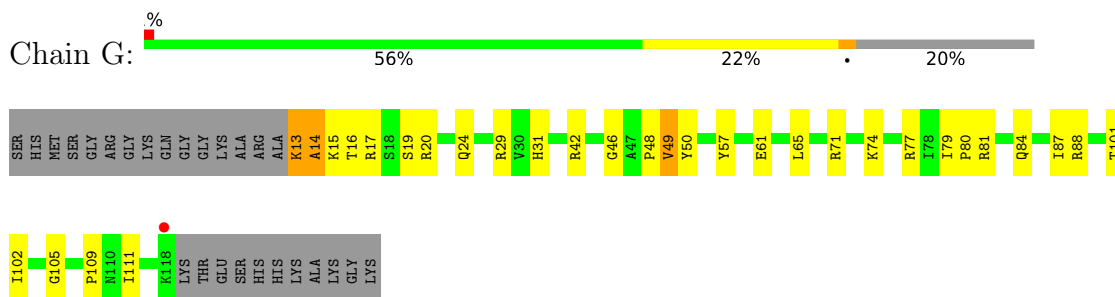
- Molecule 4: Histone H4



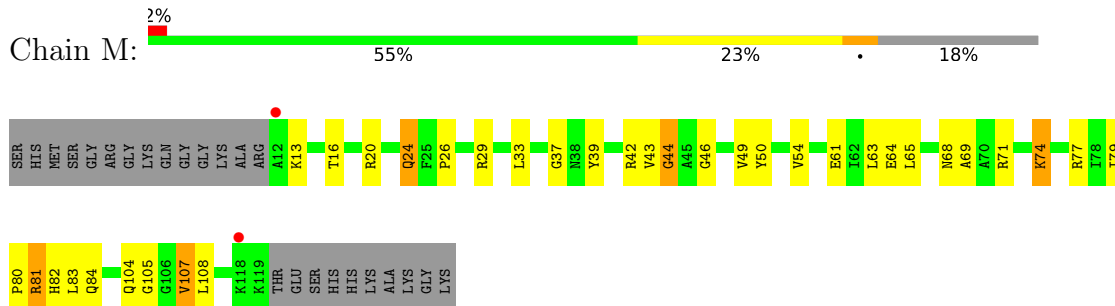
- Molecule 5: Histone H2A type 1-B/E



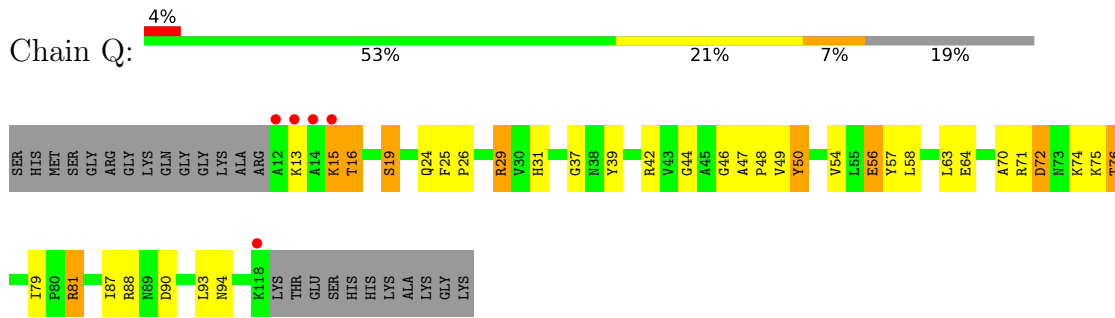
- Molecule 5: Histone H2A type 1-B/E



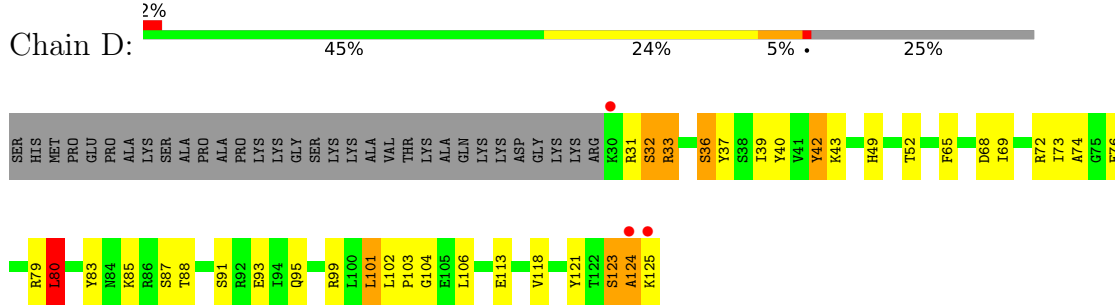
• Molecule 5: Histone H2A type 1-B/E



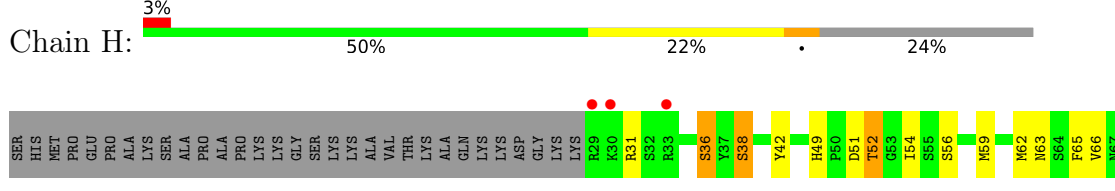
• Molecule 5: Histone H2A type 1-B/E



• Molecule 6: Histone H2B type 1-J



• Molecule 6: Histone H2B type 1-J





PRO  
LYS  
LYS  
ALA  
SER  
LYS  
PRO  
LYS  
LYS  
ALA  
ALA  
SER  
LYS  
ALA  
PRO  
THR  
LYS  
LYS  
PRO  
LYS  
LYS  
ALA  
THR  
PRO  
VAL  
VAL  
LYS  
LYS  
ALA  
LYS  
LYS  
LEU  
ALA  
ALA  
THR  
PRO  
LYS  
LYS  
LYS  
ALA  
LYS  
LYS  
PRO  
THR  
VAL  
VAL  
LYS  
LYS  
ALA  
LYS  
PRO  
VAL  
VAL  
LYS  
ALA  
SER  
SER  
PRO  
LYS  
LYS  
ALA  
PRO  
VAL

LYS  
PRO  
LYS  
ALA  
SER  
SER  
ALA  
LYS  
ARG  
ALA  
GLY  
LYS  
LYS

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.22Å 105.05Å 171.13Å 86.59° 88.95° 88.25°	Depositor
Resolution (Å)	49.35 – 2.86 49.30 – 2.86	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.35-2.86) 97.4 (49.30-2.86)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.225 , 0.297 0.230 , 0.298	Depositor DCC
$R_{free}$ test set	2099 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.7	Xtrriage
Anisotropy	0.024	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 78.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	27785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, K, CA

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	0.47	3/8122 (0.0%)	0.91	5/12523 (0.0%)
2	J	0.46	5/8116 (0.1%)	0.91	6/12532 (0.0%)
3	A	0.66	0/819	0.85	0/1097
3	E	0.68	0/819	0.87	0/1097
3	K	0.67	0/819	0.86	0/1097
3	O	0.65	0/828	0.83	0/1109
4	B	0.67	0/645	0.87	0/862
4	F	0.70	0/660	0.90	0/883
4	L	0.72	0/645	0.96	1/862 (0.1%)
4	P	0.72	0/645	0.90	0/862
5	C	0.70	0/838	0.90	0/1129
5	G	0.68	0/829	0.85	0/1118
5	M	0.68	0/843	0.86	0/1136
5	Q	0.67	0/834	0.88	0/1125
6	D	0.71	0/766	0.92	0/1026
6	H	0.69	0/777	0.88	0/1040
6	N	0.72	0/766	0.85	0/1026
6	R	0.83	2/766 (0.3%)	0.93	1/1026 (0.1%)
7	S	0.74	0/581	0.89	0/775
7	T	0.72	0/581	0.84	0/775
All	All	0.58	10/29699 (0.0%)	0.90	13/43100 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1	DC	OP3-P	-10.15	1.49	1.61
1	I	1	DC	OP3-P	-10.07	1.49	1.61
6	R	71	GLU	CD-OE2	8.81	1.35	1.25
2	J	112	DT	O3'-P	-6.83	1.52	1.61
6	R	71	GLU	CD-OE1	6.83	1.33	1.25



The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	71	GLU	OE1-CD-OE2	7.10	131.82	123.30
4	L	95	ARG	NE-CZ-NH1	7.08	123.84	120.30
2	J	284	DG	C1'-O4'-C4'	-6.04	104.06	110.10
2	J	165	DT	C1'-O4'-C4'	-5.95	104.15	110.10
1	I	114	DG	C1'-O4'-C4'	-5.91	104.19	110.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	7230	0	3948	232	0
2	J	7245	0	3987	173	0
3	A	807	0	844	18	0
3	E	807	0	844	17	0
3	K	807	0	844	19	0
3	O	816	0	856	10	0
4	B	638	0	676	19	0
4	F	653	0	696	27	0
4	L	638	0	676	29	0
4	P	638	0	676	25	0
5	C	828	0	892	37	1
5	G	819	0	879	20	0
5	M	833	0	897	30	0
5	Q	824	0	884	35	1
6	D	755	0	784	38	0
6	H	766	0	797	19	1
6	N	755	0	784	29	1
6	R	755	0	784	49	0
7	S	575	0	604	33	0
7	T	575	0	604	29	0
8	I	2	0	0	0	0
8	J	1	0	0	0	0
9	I	2	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	3	0	0	0	0
10	C	1	0	0	2	0
10	G	1	0	0	0	0
10	M	1	0	0	1	0
10	Q	1	0	0	2	0
11	B	1	0	0	0	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
11	K	1	0	0	0	0
11	L	2	0	0	0	0
11	P	3	0	0	0	0
All	All	27785	0	21956	754	2

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 15.

The worst 5 of 754 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:J:210:DA:OP2	6:R:42:TYR:OH	1.76	1.02
7:S:62:GLU:O	7:S:64:ALA:N	1.98	0.96
2:J:318:DC:H4'	2:J:319:DG:OP1	1.65	0.96
1:I:167:DT:H5''	7:T:42:ARG:HD2	1.46	0.95
2:J:203:DG:H2''	2:J:204:DT:H5'	1.50	0.93

All (2) 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)
6:N:51:ASP:OD2	5:Q:57:TYR:OH[1_455]	2.10	0.10
5:C:61:GLU:OE1	6:H:51:ASP:OD2[1_455]	2.17	0.03

## 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	
3	A	96/138 (70%)	79 (82%)	16 (17%)	1 (1%)	15	40
3	E	96/138 (70%)	78 (81%)	16 (17%)	2 (2%)	7	22
3	K	96/138 (70%)	81 (84%)	14 (15%)	1 (1%)	15	40
3	O	97/138 (70%)	86 (89%)	10 (10%)	1 (1%)	15	40
4	B	78/105 (74%)	64 (82%)	12 (15%)	2 (3%)	5	17
4	F	80/105 (76%)	68 (85%)	9 (11%)	3 (4%)	3	10
4	L	78/105 (74%)	61 (78%)	16 (20%)	1 (1%)	12	33
4	P	78/105 (74%)	70 (90%)	7 (9%)	1 (1%)	12	33
5	C	105/132 (80%)	85 (81%)	14 (13%)	6 (6%)	1	4
5	G	104/132 (79%)	86 (83%)	15 (14%)	3 (3%)	4	15
5	M	106/132 (80%)	88 (83%)	14 (13%)	4 (4%)	3	10
5	Q	105/132 (80%)	89 (85%)	15 (14%)	1 (1%)	15	40
6	D	94/128 (73%)	77 (82%)	11 (12%)	6 (6%)	1	3
6	H	95/128 (74%)	76 (80%)	15 (16%)	4 (4%)	3	8
6	N	94/128 (73%)	80 (85%)	14 (15%)	0	100	100
6	R	94/128 (73%)	74 (79%)	16 (17%)	4 (4%)	2	8
7	S	73/195 (37%)	58 (80%)	8 (11%)	7 (10%)	0	1
7	T	73/195 (37%)	60 (82%)	10 (14%)	3 (4%)	3	9
All	All	1642/2402 (68%)	1360 (83%)	232 (14%)	50 (3%)	4	14

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	50	ILE
5	C	14	ALA
6	D	32	SER
6	D	33	ARG
5	G	17	ARG

### 5.3.2 Protein sidechains [i](#)

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	85/113 (75%)	80 (94%)	5 (6%)	19	45
3	E	85/113 (75%)	81 (95%)	4 (5%)	26	56
3	K	85/113 (75%)	82 (96%)	3 (4%)	36	67
3	O	86/113 (76%)	80 (93%)	6 (7%)	15	37
4	B	65/81 (80%)	62 (95%)	3 (5%)	27	56
4	F	67/81 (83%)	65 (97%)	2 (3%)	41	72
4	L	65/81 (80%)	60 (92%)	5 (8%)	13	32
4	P	65/81 (80%)	61 (94%)	4 (6%)	18	43
5	C	85/102 (83%)	73 (86%)	12 (14%)	3	9
5	G	84/102 (82%)	76 (90%)	8 (10%)	8	23
5	M	85/102 (83%)	81 (95%)	4 (5%)	26	56
5	Q	84/102 (82%)	73 (87%)	11 (13%)	4	10
6	D	82/107 (77%)	70 (85%)	12 (15%)	3	8
6	H	83/107 (78%)	71 (86%)	12 (14%)	3	8
6	N	82/107 (77%)	73 (89%)	9 (11%)	6	17
6	R	82/107 (77%)	73 (89%)	9 (11%)	6	17
7	S	62/158 (39%)	48 (77%)	14 (23%)	1	2
7	T	62/158 (39%)	52 (84%)	10 (16%)	2	6
All	All	1394/1928 (72%)	1261 (90%)	133 (10%)	8	23

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	S	53	TYR
7	S	84	THR
7	T	67	GLN
6	H	38	SER
6	H	36	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
7	S	67	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	S	83	GLN
6	H	95	GLN
6	H	49	HIS
7	T	67	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	353/353 (100%)	-0.18	20 (5%) 23 19	69, 146, 265, 317	0
2	J	353/353 (100%)	-0.18	20 (5%) 23 19	83, 145, 263, 358	0
3	A	98/138 (71%)	0.06	0 100 100	58, 85, 134, 163	0
3	E	98/138 (71%)	0.20	1 (1%) 82 81	39, 72, 117, 171	0
3	K	98/138 (71%)	0.11	3 (3%) 49 44	59, 85, 137, 167	0
3	O	99/138 (71%)	0.12	3 (3%) 50 45	53, 81, 134, 184	0
4	B	80/105 (76%)	0.09	0 100 100	51, 79, 117, 169	0
4	F	82/105 (78%)	0.50	3 (3%) 41 36	42, 65, 107, 242	0
4	L	80/105 (76%)	0.14	1 (1%) 77 76	55, 83, 123, 169	0
4	P	80/105 (76%)	0.18	3 (3%) 40 35	46, 75, 113, 172	0
5	C	107/132 (81%)	0.25	2 (1%) 66 64	41, 70, 117, 202	0
5	G	106/132 (80%)	0.01	1 (0%) 84 84	40, 78, 120, 152	0
5	M	108/132 (81%)	0.13	2 (1%) 66 64	50, 77, 123, 176	0
5	Q	107/132 (81%)	0.27	5 (4%) 31 27	42, 78, 148, 208	0
6	D	96/128 (75%)	0.21	3 (3%) 49 44	45, 71, 140, 167	0
6	H	97/128 (75%)	0.20	4 (4%) 37 31	50, 76, 169, 219	0
6	N	96/128 (75%)	0.22	2 (2%) 63 60	56, 81, 143, 196	0
6	R	96/128 (75%)	0.23	3 (3%) 49 44	54, 76, 148, 170	0
7	S	75/195 (38%)	2.39	34 (45%) 0 0	104, 167, 213, 284	1 (1%)
7	T	75/195 (38%)	5.93	63 (84%) 0 0	181, 241, 294, 319	1 (1%)
All	All	2384/3108 (76%)	0.32	173 (7%) 15 11	39, 93, 235, 358	2 (0%)

The worst 5 of 173 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	21	VAL	28.9
7	T	83	GLN	19.3
7	S	42	ARG	17.1
7	T	42	ARG	16.5
7	T	43	ALA	14.7

## 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, 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
8	CA	J	401	1/1	0.55	0.17	125,125,125,125	0
8	CA	I	401	1/1	0.86	0.05	119,119,119,119	0
9	K	I	404	1/1	0.86	0.08	110,110,110,110	0
9	K	I	403	1/1	0.89	0.19	116,116,116,116	0
9	K	J	404	1/1	0.89	0.07	134,134,134,134	0
10	CL	C	201	1/1	0.91	0.09	72,72,72,72	0
8	CA	I	402	1/1	0.92	0.05	116,116,116,116	0
9	K	J	403	1/1	0.92	0.07	97,97,97,97	0
10	CL	M	201	1/1	0.92	0.08	83,83,83,83	0
10	CL	Q	201	1/1	0.93	0.08	69,69,69,69	0
9	K	J	402	1/1	0.94	0.20	101,101,101,101	0
10	CL	G	201	1/1	0.94	0.08	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.