Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:02 PM BST

PDB ID	:	6HKT
Title	:	Structure of an H1-bound 6-nucleosome array
Authors	:	Garcia-Saez, I.; Dimitrov, S.; Petosa, C.
Deposited on	:	2018-09-08
Resolution	:	9.70 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 ①) were used in the production of this report:

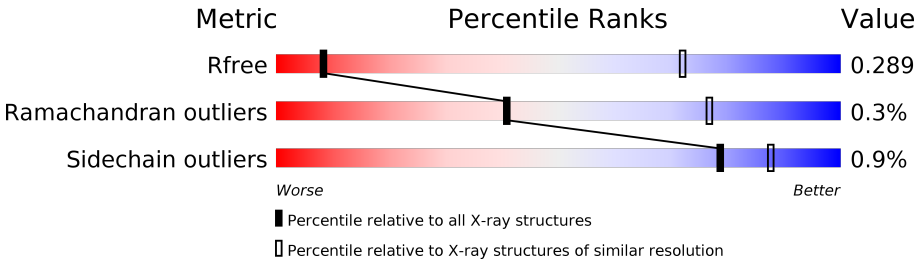
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 9.70 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	1005 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	139	70% 30%
1	E	139	70% 29%
1	K	139	70% 30%
1	O	139	71% 29%
1	U	139	70% 30%
1	Y	139	71% 29%
1	a	139	71% 29%
1	e	139	68% 30%
1	k	139	71% 29%

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Mol	Chain	Length	Quality of chain
1	o	139	70% 30%
1	u	139	71% 29%
1	y	139	70% 30%
2	B	106	76% 23%
2	F	106	77% 23%
2	L	106	77% 23%
2	P	106	77% 23%
2	V	106	77% 23%
2	Z	106	76% 23%
2	b	106	76% 23%
2	f	106	77% 23%
2	l	106	76% 23%
2	p	106	77% 23%
2	v	106	77% 23%
2	z	106	77% 23%
3	0	133	78% 21%
3	2	133	76% 23%
3	C	133	76% 23%
3	G	133	78% 21%
3	M	133	77% 23%
3	Q	133	78% 21%
3	W	133	76% 23%
3	c	133	78% 21%
3	g	133	76% 23%
3	m	133	78% 21%

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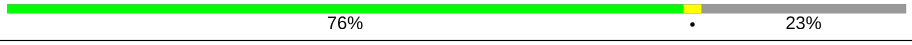
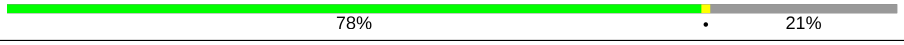
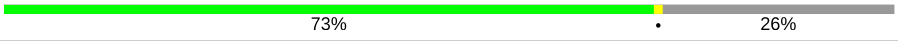
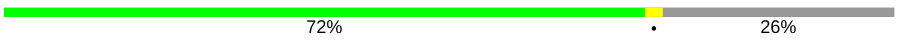
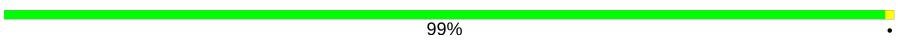
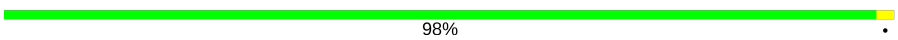
Mol	Chain	Length	Quality of chain
3	q	133	
3	w	133	
4	1	129	
4	3	129	
4	D	129	
4	H	129	
4	N	129	
4	R	129	
4	X	129	
4	d	129	
4	h	129	
4	n	129	
4	r	129	
4	x	129	
5	I	1122	
6	J	1122	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 82122 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	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	E	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	a	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	e	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	K	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	O	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	k	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	o	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	U	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			
1	Y	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	u	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			
1	y	97	Total	C	N	O	S	0	0	0
			801	505	155	137	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	HIS	-	expression tag	UNP P68431
a	-3	GLY	-	expression tag	UNP P68431
a	-2	SER	-	expression tag	UNP P68431
a	-1	HIS	-	expression tag	UNP P68431
e	-3	GLY	-	expression tag	UNP P68431
e	-2	SER	-	expression tag	UNP P68431
e	-1	HIS	-	expression tag	UNP P68431
K	-3	GLY	-	expression tag	UNP P68431
K	-2	SER	-	expression tag	UNP P68431
K	-1	HIS	-	expression tag	UNP P68431
O	-3	GLY	-	expression tag	UNP P68431
O	-2	SER	-	expression tag	UNP P68431
O	-1	HIS	-	expression tag	UNP P68431
k	-3	GLY	-	expression tag	UNP P68431
k	-2	SER	-	expression tag	UNP P68431
k	-1	HIS	-	expression tag	UNP P68431
o	-3	GLY	-	expression tag	UNP P68431
o	-2	SER	-	expression tag	UNP P68431
o	-1	HIS	-	expression tag	UNP P68431
U	-3	GLY	-	expression tag	UNP P68431
U	-2	SER	-	expression tag	UNP P68431
U	-1	HIS	-	expression tag	UNP P68431
Y	-3	GLY	-	expression tag	UNP P68431
Y	-2	SER	-	expression tag	UNP P68431
Y	-1	HIS	-	expression tag	UNP P68431
u	-3	GLY	-	expression tag	UNP P68431
u	-2	SER	-	expression tag	UNP P68431
u	-1	HIS	-	expression tag	UNP P68431
y	-3	GLY	-	expression tag	UNP P68431
y	-2	SER	-	expression tag	UNP P68431
y	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	F	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	b	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	f	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	P	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	l	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	p	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	V	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	Z	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	v	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	z	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805
L	-3	GLY	-	expression tag	UNP P62805
L	-2	SER	-	expression tag	UNP P62805
L	-1	HIS	-	expression tag	UNP P62805
P	-3	GLY	-	expression tag	UNP P62805
P	-2	SER	-	expression tag	UNP P62805
P	-1	HIS	-	expression tag	UNP P62805
l	-3	GLY	-	expression tag	UNP P62805
l	-2	SER	-	expression tag	UNP P62805
l	-1	HIS	-	expression tag	UNP P62805
p	-3	GLY	-	expression tag	UNP P62805
p	-2	SER	-	expression tag	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
p	-1	HIS	-	expression tag	UNP P62805
V	-3	GLY	-	expression tag	UNP P62805
V	-2	SER	-	expression tag	UNP P62805
V	-1	HIS	-	expression tag	UNP P62805
Z	-3	GLY	-	expression tag	UNP P62805
Z	-2	SER	-	expression tag	UNP P62805
Z	-1	HIS	-	expression tag	UNP P62805
v	-3	GLY	-	expression tag	UNP P62805
v	-2	SER	-	expression tag	UNP P62805
v	-1	HIS	-	expression tag	UNP P62805
z	-3	GLY	-	expression tag	UNP P62805
z	-2	SER	-	expression tag	UNP P62805
z	-1	HIS	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	G	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	c	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	g	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	M	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	Q	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	m	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	q	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	W	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	0	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	w	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	2	103	Total	C	N	O	0	0	0
			796	502	155	139			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908
M	-3	GLY	-	expression tag	UNP P04908
M	-2	SER	-	expression tag	UNP P04908
M	-1	HIS	-	expression tag	UNP P04908
Q	-3	GLY	-	expression tag	UNP P04908
Q	-2	SER	-	expression tag	UNP P04908
Q	-1	HIS	-	expression tag	UNP P04908
m	-3	GLY	-	expression tag	UNP P04908
m	-2	SER	-	expression tag	UNP P04908
m	-1	HIS	-	expression tag	UNP P04908
q	-3	GLY	-	expression tag	UNP P04908
q	-2	SER	-	expression tag	UNP P04908
q	-1	HIS	-	expression tag	UNP P04908
W	-3	GLY	-	expression tag	UNP P04908
W	-2	SER	-	expression tag	UNP P04908
W	-1	HIS	-	expression tag	UNP P04908
0	-3	GLY	-	expression tag	UNP P04908
0	-2	SER	-	expression tag	UNP P04908
0	-1	HIS	-	expression tag	UNP P04908
w	-3	GLY	-	expression tag	UNP P04908
w	-2	SER	-	expression tag	UNP P04908
w	-1	HIS	-	expression tag	UNP P04908
2	-3	GLY	-	expression tag	UNP P04908
2	-2	SER	-	expression tag	UNP P04908
2	-1	HIS	-	expression tag	UNP P04908

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	H	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	h	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	N	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	R	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	n	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	r	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	X	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	1	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	x	95	Total	C	N	O	S	0	0	0
			745	468	136	139	2			
4	3	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP P06899
D	-5	SER	-	expression tag	UNP P06899
D	-4	HIS	-	expression tag	UNP P06899
H	-6	GLY	-	expression tag	UNP P06899
H	-5	SER	-	expression tag	UNP P06899
H	-4	HIS	-	expression tag	UNP P06899
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899
N	-6	GLY	-	expression tag	UNP P06899
N	-5	SER	-	expression tag	UNP P06899
N	-4	HIS	-	expression tag	UNP P06899
R	-6	GLY	-	expression tag	UNP P06899
R	-5	SER	-	expression tag	UNP P06899
R	-4	HIS	-	expression tag	UNP P06899
n	-6	GLY	-	expression tag	UNP P06899

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Chain	Residue	Modelled	Actual	Comment	Reference
n	-5	SER	-	expression tag	UNP P06899
n	-4	HIS	-	expression tag	UNP P06899
r	-6	GLY	-	expression tag	UNP P06899
r	-5	SER	-	expression tag	UNP P06899
r	-4	HIS	-	expression tag	UNP P06899
X	-6	GLY	-	expression tag	UNP P06899
X	-5	SER	-	expression tag	UNP P06899
X	-4	HIS	-	expression tag	UNP P06899
1	-6	GLY	-	expression tag	UNP P06899
1	-5	SER	-	expression tag	UNP P06899
1	-4	HIS	-	expression tag	UNP P06899
x	-6	GLY	-	expression tag	UNP P06899
x	-5	SER	-	expression tag	UNP P06899
x	-4	HIS	-	expression tag	UNP P06899
3	-6	GLY	-	expression tag	UNP P06899
3	-5	SER	-	expression tag	UNP P06899
3	-4	HIS	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (1122-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	I	1122	22861	10850	4162	6727	1122	0	0	0

- Molecule 6 is a DNA chain called DNA (1122-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	J	1122	23141	10945	4337	6737	1122	0	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. 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. 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

Chain A:

- Molecule 1: Histone H3.1

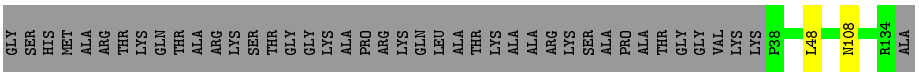
Chain E:

- Molecule 1: Histone H3.1

Chain a:

- Molecule 1: Histone H3.1

Chain e:



- Molecule 1: Histone H3.1

Chain K:

- Molecule 1: Histone H3.1

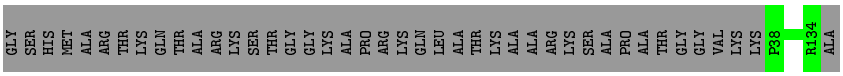
Chain O:

- Molecule 1: Histone H3.1

Chain k:

- Molecule 1: Histone H3.1

Chain o:



- Molecule 1: Histone H3.1

Chain U:

- Molecule 1: Histone H3.1

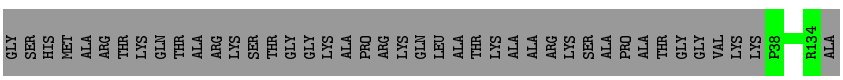
Chain Y:

- Molecule 1: Histone H3.1

Chain u:

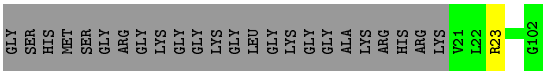
- Molecule 1: Histone H3.1

Chain y:



- Molecule 2: Histone H4

Chain B:

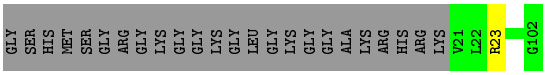


• Molecule 2: Histone H4

Chain F:

• Molecule 2: Histone H4

Chain b:



• Molecule 2: Histone H4

Chain f:

• Molecule 2: Histone H4

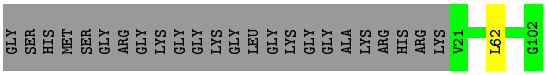
Chain L:

• Molecule 2: Histone H4

Chain P:

• Molecule 2: Histone H4

Chain l:



• Molecule 2: Histone H4

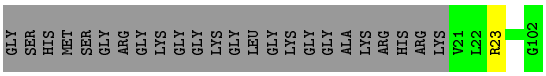
Chain p:

• Molecule 2: Histone H4

Chain V:

• Molecule 2: Histone H4

Chain Z:



• Molecule 2: Histone H4

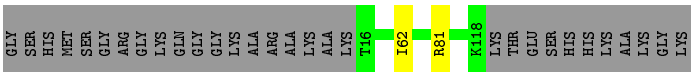
Chain v:

• Molecule 2: Histone H4

Chain z:

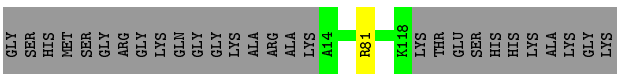
• Molecule 3: Histone H2A type 1-B/E

Chain C:



• Molecule 3: Histone H2A type 1-B/E

Chain G:



• Molecule 3: Histone H2A type 1-B/E

Chain c:

• Molecule 3: Histone H2A type 1-B/E

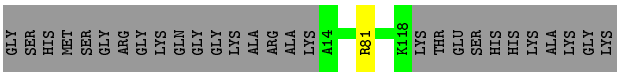
Chain g:

• Molecule 3: Histone H2A type 1-B/E

Chain M:

• Molecule 3: Histone H2A type 1-B/E

Chain Q:

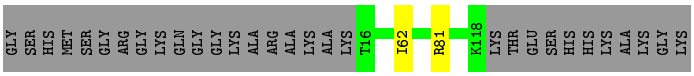


• Molecule 3: Histone H2A type 1-B/E

Chain m:

• Molecule 3: Histone H2A type 1-B/E

Chain q:



• Molecule 3: Histone H2A type 1-B/E

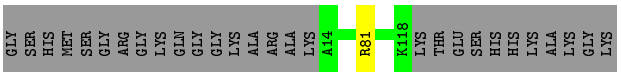
Chain W:

• Molecule 3: Histone H2A type 1-B/E

Chain 0:

• Molecule 3: Histone H2A type 1-B/E

Chain w:



• Molecule 3: Histone H2A type 1-B/E

Chain 2:

• Molecule 4: Histone H2B type 1-J

Chain D:

• Molecule 4: Histone H2B type 1-J

Chain H:

• Molecule 4: Histone H2B type 1-J

Chain d:

• Molecule 4: Histone H2B type 1-J

Chain h:

• Molecule 4: Histone H2B type 1-J

Chain N:

• Molecule 4: Histone H2B type 1-J

Chain R:

• Molecule 4: Histone H2B type 1-J

Chain n:

• Molecule 4: Histone H2B type 1-J

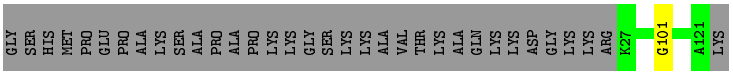
Chain r:

• Molecule 4: Histone H2B type 1-J

Chain X:

• Molecule 4: Histone H2B type 1-J

Chain 1:



• Molecule 4: Histone H2B type 1-J

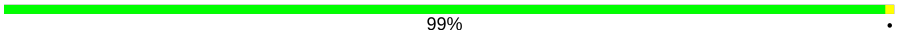
Chain x:

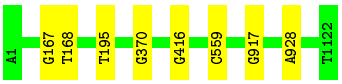
• Molecule 4: Histone H2B type 1-J

Chain 3:

- Molecule 5: DNA (1122-MER)

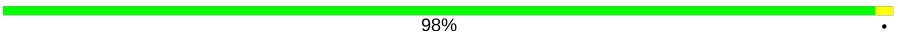
Chain I:

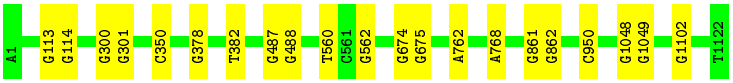




- Molecule 6: DNA (1122-MER)

Chain J:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.08Å 238.76Å 674.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 9.70 49.07 – 9.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.07-9.70) 99.8 (49.07-9.70)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 9.80Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.254 , 0.286 0.255 , 0.289	Depositor DCC
R_{free} test set	573 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	339.6	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.26 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.21$, $< L^2 > = 0.07$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	82122	wwPDB-VP
Average B, all atoms (Å^2)	544.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.25	0/813	0.37	0/1090
1	E	0.24	0/819	0.37	0/1097
1	K	0.26	0/813	0.40	0/1090
1	O	0.26	0/819	0.39	0/1097
1	U	0.25	0/813	0.38	0/1090
1	Y	0.24	0/819	0.39	0/1097
1	a	0.25	0/819	0.37	0/1097
1	e	0.26	0/813	0.43	1/1090 (0.1%)
1	k	0.25	0/819	0.41	0/1097
1	o	0.25	0/813	0.41	0/1090
1	u	0.27	0/819	0.39	0/1097
1	y	0.26	0/813	0.37	0/1090
2	B	0.26	0/660	0.45	0/883
2	F	0.25	0/660	0.46	0/883
2	L	0.25	0/660	0.46	0/883
2	P	0.25	0/660	0.45	0/883
2	V	0.27	0/660	0.48	0/883
2	Z	0.26	0/660	0.46	0/883
2	b	0.26	0/660	0.46	0/883
2	f	0.26	0/660	0.46	0/883
2	l	0.33	0/660	0.67	2/883 (0.2%)
2	p	0.28	0/660	0.49	0/883
2	v	0.26	0/660	0.48	0/883
2	z	0.26	0/660	0.46	0/883
3	0	0.26	0/820	0.40	0/1107
3	2	0.24	0/806	0.41	0/1089
3	C	0.24	0/806	0.41	0/1089
3	G	0.27	0/820	0.40	0/1107
3	M	0.24	0/806	0.39	0/1089
3	Q	0.24	0/820	0.41	0/1107
3	W	0.23	0/806	0.40	0/1089
3	c	0.29	0/820	0.43	0/1107
3	g	0.23	0/806	0.39	0/1089
3	m	0.24	0/820	0.40	0/1107

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	q	0.25	0/806	0.42	0/1089
3	w	0.28	0/820	0.42	0/1107
4	1	0.26	0/756	0.39	0/1015
4	3	0.34	0/766	0.45	0/1026
4	D	0.24	0/766	0.39	0/1026
4	H	0.25	0/756	0.40	0/1015
4	N	0.24	0/766	0.39	0/1026
4	R	0.25	0/756	0.39	0/1015
4	X	0.24	0/766	0.39	0/1026
4	d	0.26	0/756	0.42	0/1015
4	h	0.24	0/766	0.40	0/1026
4	n	0.29	0/756	0.41	0/1015
4	r	0.27	0/766	0.44	0/1026
4	x	0.24	0/756	0.40	0/1015
5	I	0.56	0/25620	0.99	8/39502 (0.0%)
6	J	0.56	0/25990	1.00	33/40152 (0.1%)
All	All	0.46	0/88210	0.83	44/128794 (0.0%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	1048	DG	OP2-P-O3'	-11.49	79.92	105.20
6	J	300	DG	OP2-P-O3'	-11.41	80.10	105.20
6	J	861	DG	OP2-P-O3'	-11.41	80.10	105.20
6	J	487	DG	OP2-P-O3'	-11.39	80.14	105.20
6	J	674	DG	OP2-P-O3'	-11.34	80.25	105.20
6	J	113	DG	OP2-P-O3'	-11.28	80.39	105.20
2	l	62	LEU	CB-CG-CD2	-9.79	94.36	111.00
6	J	378	DG	O4'-C1'-N9	7.09	112.97	108.00
6	J	382	DT	O4'-C1'-N1	7.08	112.96	108.00
6	J	1102	DG	O4'-C1'-N9	6.29	112.40	108.00
6	J	300	DG	OP1-P-O3'	-6.27	91.41	105.20
6	J	861	DG	OP1-P-O3'	-6.25	91.45	105.20
6	J	113	DG	OP1-P-O3'	-6.25	91.45	105.20
6	J	674	DG	OP1-P-O3'	-6.22	91.51	105.20
6	J	487	DG	OP1-P-O3'	-6.21	91.54	105.20
6	J	1048	DG	OP1-P-O3'	-6.20	91.55	105.20
6	J	950	DC	O4'-C1'-N1	6.13	112.29	108.00
5	I	559	DC	O4'-C1'-N1	6.08	112.25	108.00
6	J	488	DG	OP1-P-OP2	5.95	128.52	119.60
6	J	862	DG	O5'-P-OP1	5.86	117.73	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	350	DC	O4'-C1'-N1	5.85	112.09	108.00
6	J	1049	DG	O5'-P-OP1	5.71	117.55	110.70
5	I	416	DG	OP2-P-O3'	5.70	117.74	105.20
5	I	168	DT	O4'-C1'-N1	5.69	111.98	108.00
6	J	768	DA	O4'-C1'-N9	5.69	111.98	108.00
6	J	114	DG	OP1-P-OP2	5.62	128.04	119.60
2	l	62	LEU	CA-CB-CG	5.62	128.22	115.30
6	J	301	DG	OP1-P-OP2	5.57	127.96	119.60
6	J	114	DG	O5'-P-OP1	5.56	117.38	110.70
6	J	675	DG	O5'-P-OP1	5.54	117.35	110.70
5	I	928	DA	O4'-C1'-N9	5.53	111.87	108.00
6	J	1049	DG	OP1-P-OP2	5.52	127.88	119.60
6	J	301	DG	O5'-P-OP1	5.50	117.30	110.70
6	J	862	DG	OP1-P-OP2	5.50	127.85	119.60
1	e	48	LEU	CB-CG-CD1	-5.46	101.73	111.00
6	J	560	DT	O4'-C1'-N1	5.37	111.76	108.00
5	I	195	DT	O4'-C1'-N1	5.34	111.74	108.00
6	J	762	DA	O4'-C1'-N9	5.26	111.68	108.00
6	J	562	DG	O4'-C1'-N9	5.21	111.64	108.00
5	I	917	DG	O4'-C1'-N9	5.14	111.60	108.00
6	J	488	DG	O5'-P-OP1	5.12	116.84	110.70
6	J	675	DG	OP1-P-OP2	5.04	127.16	119.60
5	I	167	DG	O4'-C1'-N9	5.01	111.51	108.00
5	I	370	DG	O4'-C1'-N9	5.01	111.51	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
1	A	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	E	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	K	95/139 (68%)	91 (96%)	4 (4%)	0	100	100
1	O	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	U	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	Y	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	a	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	e	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
1	k	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	o	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
1	u	96/139 (69%)	93 (97%)	3 (3%)	0	100	100
1	y	95/139 (68%)	93 (98%)	2 (2%)	0	100	100
2	B	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	F	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	L	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	P	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	V	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	Z	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	b	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	f	80/106 (76%)	79 (99%)	1 (1%)	0	100	100
2	l	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	p	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	v	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
2	z	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
3	0	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
3	2	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	C	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	G	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
3	M	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	Q	103/133 (77%)	102 (99%)	1 (1%)	0	100	100
3	W	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
3	c	103/133 (77%)	102 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	101/133 (76%)	99 (98%)	2 (2%)	0	100	100
3	m	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
3	q	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
3	w	103/133 (77%)	101 (98%)	2 (2%)	0	100	100
4	1	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	14	52
4	3	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	14	52
4	D	94/129 (73%)	89 (95%)	4 (4%)	1 (1%)	14	52
4	H	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	14	52
4	N	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	14	52
4	R	93/129 (72%)	92 (99%)	0	1 (1%)	14	52
4	X	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	14	52
4	d	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	14	52
4	h	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	14	52
4	n	93/129 (72%)	91 (98%)	1 (1%)	1 (1%)	14	52
4	r	94/129 (73%)	91 (97%)	2 (2%)	1 (1%)	14	52
4	x	93/129 (72%)	92 (99%)	0	1 (1%)	14	52
All	All	4452/6084 (73%)	4350 (98%)	90 (2%)	12 (0%)	41	77

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	GLY
4	H	101	GLY
4	d	101	GLY
4	h	101	GLY
4	N	101	GLY
4	R	101	GLY
4	n	101	GLY
4	r	101	GLY
4	X	101	GLY
4	1	101	GLY
4	x	101	GLY
4	3	101	GLY

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	
1	A	85/113 (75%)	85 (100%)	0	100	100
1	E	85/113 (75%)	84 (99%)	1 (1%)	71	83
1	K	85/113 (75%)	85 (100%)	0	100	100
1	O	85/113 (75%)	85 (100%)	0	100	100
1	U	85/113 (75%)	85 (100%)	0	100	100
1	Y	85/113 (75%)	85 (100%)	0	100	100
1	a	85/113 (75%)	85 (100%)	0	100	100
1	e	85/113 (75%)	84 (99%)	1 (1%)	71	83
1	k	85/113 (75%)	85 (100%)	0	100	100
1	o	85/113 (75%)	85 (100%)	0	100	100
1	u	85/113 (75%)	85 (100%)	0	100	100
1	y	85/113 (75%)	85 (100%)	0	100	100
2	B	67/81 (83%)	67 (100%)	0	100	100
2	F	67/81 (83%)	67 (100%)	0	100	100
2	L	67/81 (83%)	67 (100%)	0	100	100
2	P	67/81 (83%)	67 (100%)	0	100	100
2	V	67/81 (83%)	67 (100%)	0	100	100
2	Z	67/81 (83%)	67 (100%)	0	100	100
2	b	67/81 (83%)	67 (100%)	0	100	100
2	f	67/81 (83%)	67 (100%)	0	100	100
2	l	67/81 (83%)	67 (100%)	0	100	100
2	p	67/81 (83%)	67 (100%)	0	100	100
2	v	67/81 (83%)	67 (100%)	0	100	100
2	z	67/81 (83%)	67 (100%)	0	100	100
3	0	83/102 (81%)	82 (99%)	1 (1%)	71	83
3	2	82/102 (80%)	81 (99%)	1 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	82/102 (80%)	80 (98%)	2 (2%)	49	69
3	G	83/102 (81%)	82 (99%)	1 (1%)	71	83
3	M	82/102 (80%)	81 (99%)	1 (1%)	71	83
3	Q	83/102 (81%)	82 (99%)	1 (1%)	71	83
3	W	82/102 (80%)	80 (98%)	2 (2%)	49	69
3	c	83/102 (81%)	82 (99%)	1 (1%)	71	83
3	g	82/102 (80%)	80 (98%)	2 (2%)	49	69
3	m	83/102 (81%)	82 (99%)	1 (1%)	71	83
3	q	82/102 (80%)	80 (98%)	2 (2%)	49	69
3	w	83/102 (81%)	82 (99%)	1 (1%)	71	83
4	1	81/107 (76%)	81 (100%)	0	100	100
4	3	82/107 (77%)	80 (98%)	2 (2%)	49	69
4	D	82/107 (77%)	81 (99%)	1 (1%)	71	83
4	H	81/107 (76%)	80 (99%)	1 (1%)	71	83
4	N	82/107 (77%)	81 (99%)	1 (1%)	71	83
4	R	81/107 (76%)	80 (99%)	1 (1%)	71	83
4	X	82/107 (77%)	80 (98%)	2 (2%)	49	69
4	d	81/107 (76%)	79 (98%)	2 (2%)	47	68
4	h	82/107 (77%)	80 (98%)	2 (2%)	49	69
4	n	81/107 (76%)	79 (98%)	2 (2%)	47	68
4	r	82/107 (77%)	80 (98%)	2 (2%)	49	69
4	x	81/107 (76%)	80 (99%)	1 (1%)	71	83
All	All	3792/4836 (78%)	3757 (99%)	35 (1%)	78	87

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	62	ILE
3	C	81	ARG
4	D	31	LYS
1	E	108	ASN
3	G	81	ARG
4	H	85	THR
3	c	81	ARG

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Mol	Chain	Res	Type
4	d	53	SER
4	d	85	THR
1	e	108	ASN
3	g	62	ILE
3	g	81	ARG
4	h	31	LYS
4	h	85	THR
3	M	81	ARG
4	N	31	LYS
3	Q	81	ARG
4	R	85	THR
3	m	81	ARG
4	n	53	SER
4	n	85	THR
3	q	62	ILE
3	q	81	ARG
4	r	31	LYS
4	r	85	THR
3	W	62	ILE
3	W	81	ARG
4	X	31	LYS
4	X	85	THR
3	0	81	ARG
3	w	81	ARG
4	x	85	THR
3	2	81	ARG
4	3	31	LYS
4	3	85	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	25	ASN
3	Q	38	ASN
4	R	64	ASN
2	l	25	ASN
1	o	108	ASN
2	p	25	ASN
2	p	75	HIS
3	q	31	HIS
4	r	81	ASN
3	0	38	ASN

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Mol	Chain	Res	Type
1	u	108	ASN
3	2	31	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.