

wwPDB X-ray Structure Validation Summary Report (i)

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
$\operatorname{Resolution}$:	9.70 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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	Similar resolution $(\#Entries, resolution, range(Å))$
	(#Entries)	$(\#$ Entries, resolution range(\mathbf{A}))
R_{free}	130704	$1005\ (11.50\text{-}3.90)$
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	А	139	70%	30%
1	Е	139	70%	• 29%
1	K	139	70%	30%
1	0	139	71%	29%
1	U	139	70%	30%
1	Y	139	71%	29%
1	a	139	71%	29%
1	е	139	68% .	30%
1	k	139	71%	29%



Continued from previous page...

Mol	Chain	Length	Quality of chain				
1	0	139	70%	30%			
1	u	139	71%	29%	_		
1	У	139	70%	30%	_		
2	В	106	76%	• 23%	_		
2	F	106	77%	23%	_		
2	L	106	77%	23%	_		
2	Р	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	р	106	77%	23%	_		
2	v	106	77%	23%	_		
2	Z	106	77%	23%	_		
3	0	133	78%	• 21%	_		
3	2	133	76%	• 23%	_		
3	С	133	76%	• 23%			
3	G	133	78%	• 21%			
3	М	133	77%	• 23%			
3	Q	133	78%	• 21%			
3	W	133	76%	• 23%	_		
3	с	133	78%	• 21%	_		
3	g	133	76%	• 23%	_		
3	m	133	78%	• 21%	_		



Chain Length Quality of chain Mol 3 13376% q 23% • 3 133W • 78% 21% 4 1 12973% 26% • 3 1294 71% 26% • D 4 129• 73% 26% Η 1294 72% 26% • Ν 1294 73% • 26% R 4129• 72% 26% Х 1294 72% 26% • d 1294 71% • 26% 1294 \mathbf{h} • 72% 26% 129• 4n 71% 26% 4 129r 72% • 26% 129• 4 х 72% 26% Ι 1122599% • J . 11226 98%





2 Entry composition (i)

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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	07	Total	С	Ν	Ο	S	0	0	0
	A	91	801	505	155	137	4	0	0	0
1	F	0.8	Total	С	Ν	Ο	S	0	0	0
	Ľ	90	807	508	156	139	4	0	0	0
1	9	08	Total	С	Ν	Ο	\mathbf{S}	0	0	Ο
	a	90	807	508	156	139	4	0	0	0
1	0	07	Total	С	Ν	Ο	S	0	0	Ο
	е	91	801	505	155	137	4	0	0	0
1	K	07	Total	С	Ν	Ο	\mathbf{S}	0	0	Ο
L	17	31	801	505	155	137	4	0	0	0
1	0	08	Total	С	Ν	Ο	\mathbf{S}	0	0	Ο
L L	0	90	807	508	156	139	4	0	0	0
1	Ŀ	0.8	Total	С	Ν	Ο	\mathbf{S}	0	0	Ο
L L	K	90	807	508	156	139	4	0	0	0
1	0	07	Total	С	Ν	Ο	\mathbf{S}	0	0	Ο
L L	0	31	801	505	155	137	4	0	0	0
1	T	07	Total	С	Ν	Ο	\mathbf{S}	0	0	Ο
L	U	31	801	505	155	137	4	0	0	0
1	V	0.8	Total	С	Ν	Ο	\mathbf{S}	0	0	Ο
L	T	90	807	508	156	139	4	0	0	0
1	11	98	Total	С	Ν	Ο	S	0	0	0
	u	30	807	508	156	139	4		0	0
1	v	97	Total	С	Ν	Ο	S	0	0	0
	У	31	801	505	155	137	4		0	0

• Molecule 1 is a protein called Histone H3.1.

There are 36 discrepancies between the modelled and reference sequences:

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



Chain	Residue	Modelled	Actual	Comment	Reference
Е	-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
е	-3	GLY	-	expression tag	UNP P68431
е	-2	SER	-	expression tag	UNP P68431
е	-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
0	-3	GLY	-	expression tag	UNP P68431
0	-2	SER	-	expression tag	UNP P68431
0	-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
0	-3	GLY	-	expression tag	UNP P68431
0	-2	SER	-	expression tag	UNP P68431
0	-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
у	-3	GLY	-	expression tag	UNP P68431
у	-2	SER	-	expression tag	UNP P68431
у	-1	HIS	-	expression tag	UNP P68431

• Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
	р	80	Total	С	Ν	0	S	0	0	0
	D	02	653	412	127	113	1	0	0	0
2	F	80	Total	С	Ν	0	S	0	0	0
	Ľ	02	653	412	127	113	1	0	0	0
0	h	o 82	Total	С	Ν	Ο	S	0	0	0
	U		653	412	127	113	1	0	0	0
<u></u>	0 f	80	Total	С	Ν	Ο	S	0	0	0
	1	02	653	412	127	113	1	0	0	0



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Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
	т	0.0	Total	С	Ν	Ο	\mathbf{S}	0	0	0
		02	653	412	127	113	1	0	0	0
2	р	80	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	L	02	653	412	127	113	1	0	0	0
2	1	80	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	1	02	653	412	127	113	1	0	0	0
2	n	80	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	p	02	653	412	127	113	1	0	0	0
2	V	0.0	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	v	02	653	412	127	113	1	0	0	0
2	7	80	Total	С	Ν	Ο	S	0	0	0
		02	653	412	127	113	1	0	0	0
2	17	80	Total	С	Ν	Ο	S	0	0	0
	v	02	653	412	127	113	1	0	0	0
2	7	80	Total	С	Ν	0	S	0	0	0
	L	82	653	412	127	113	1	0		0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	-3	GLY	-	expression tag	UNP P62805
В	-2	SER	-	expression tag	UNP P62805
В	-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
Р	-3	GLY	-	expression tag	UNP P62805
Р	-2	SER	-	expression tag	UNP P62805
Р	-1	HIS	-	expression tag	UNP P62805
1	-3	GLY	-	expression tag	UNP P62805
1	-2	SER	-	expression tag	UNP P62805
1	-1	HIS	-	expression tag	UNP P62805
р	-3	GLY	-	expression tag	UNP P62805
р	-2	SER	-	expression tag	UNP P62805



Chain	Residue	Modelled	Actual	Comment	Reference
р	-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		Ato	\mathbf{ms}		ZeroOcc	AltConf	Trace
3	С	103	Total 796	${ m C} 502$	$rac{N}{155}$	O 139	0	0	0
3	G	105	Total 810	C 511	N 158	O 141	0	0	0
3	с	105	Total 810	C 511	N 158	O 141	0	0	0
3	g	103	Total 796	${ m C} 502$	N 155	O 139	0	0	0
3	М	103	Total 796	${ m C} 502$	N 155	O 139	0	0	0
3	Q	105	Total 810	C 511	N 158	O 141	0	0	0
3	m	105	Total 810	C 511	N 158	O 141	0	0	0
3	q	103	Total 796	${ m C} 502$	N 155	O 139	0	0	0
3	W	103	Total 796	${ m C} 502$	N 155	O 139	0	0	0
3	0	105	Total 810	C 511	N 158	O 141	0	0	0
3	W	105	Total 810	C 511	N 158	O 141	0	0	0
3	2	103	Total 796	C 502	N 155	O 139	0	0	0

There are 36 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
С	-3	GLY	-	expression tag	UNP P04908
С	-2	SER	-	expression tag	UNP P04908
С	-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
с	-3	GLY	-	expression tag	UNP P04908
с	-2	SER	-	expression tag	UNP P04908
с	-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
М	-3	GLY	-	expression tag	UNP P04908
М	-2	SER	-	expression tag	UNP P04908
М	-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		At	oms			ZeroOcc	AltConf	Trace
4	4 D 96	Total	С	Ν	Ο	S	0	0	0	
4		90	755	474	138	141	2	0	0	0
4	п	05	Total	С	Ν	Ο	S	0	0	0
4	4 П	90	745	468	136	139	2	0	0	0



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4	d	05	Total	С	Ν	Ο	S	0	0	0
4	4 u	90	745	468	136	139	2	0	0	0
4	h	96	Total	С	Ν	Ο	S	0	0	0
	11	30	755	474	138	141	2	0	0	0
4	N	96	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	11	30	755	474	138	141	2	0	0	0
4	R	95	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	10	50	745	468	136	139	2	0		0
	n	95	Total	С	Ν	Ο	\mathbf{S}	0	0	Ο
	11		745	468	136	139	2			0
	r 06	96	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	1	50	755	474	138	141	2	0	0	0
4	X	96	Total	С	Ν	Ο	\mathbf{S}	0	0	0
-		50	755	474	138	141	2	0	0	0
4	1	95	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	1	50	745	468	136	139	2	0	0	0
4	v	95	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	л	50	745	468	136	139	2	0	0	0
4	3	96	Total	С	Ν	Ο	\mathbf{S}	0	0	0
T	0	30	755	474	138	141	2			U

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
Н	-6	GLY	-	expression tag	UNP P06899
Н	-5	SER	-	expression tag	UNP P06899
Н	-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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Continu					
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
Х	-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
5	Ι	1122	Total 22861	m C 10850	N 4162	O 6727	Р 1122	0	0	0

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

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
6	J	1122	Total 23141	C 10945	N 4337	O 6737	Р 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.

Chain A:	70%	30%
GLY SER MET MET MET MET ALA ALA ALA ALA ALA ALA CLYS SER SER SER CLYS SER ALA ALA ALA ALA CLYS SER SER CLYS SER CLYS CLYS CLYS CLYS CLYS CLYS CLYS CLYS	LEU LEU LTRR LTRR LTRR LTRR ALA ALA ALA ALA CTR CTR CTR CTR CTR CTR CTR CTR CTR CTR	
• Molecule 1: Histone H3.1		
Chain E:	70% .	29%
GLY BER HIS NET NET NET ARG CLN ALA ALA ALA ALA CLYS SER SER CLY CLYS SER CLYS SER CLYS SER CLYS CLYS CLYS CLYS CLYS CLYS CLYS CLYS	LEUN LEUN LYS LYS LYS LYS ALA ALA ALA ALA ALA ALA CLY VAL LYS CLY VAL LYS CLY VAL LYS CLY VAL LYS CLY VAL ALA	
• Molecule 1: Histone H3.1		
Chain a:	71%	29%
CLAR CONTRACT CONTRAC	LEU LUN LUN LUN LUN ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
• Molecule 1: Histone H3.1		
Chain e:	68% ·	30%
GLY SER HIS NET ARG ALA ARG CLN CLNS SER SER SER CLNS SER CLNS SER CLNS SER CLNS SER CLNS SER CLNS SER CLNS CLNS CLNS CLNS CLNS CLNS CLNS CLNS	LEU LAN LAN LAN LAN LAN LAN ALA ALA ALA ALA	R134 ALA
• Molecule 1: Histone H3.1		
Chain K:	70%	30%
CLA CLARK CALLER CLARK ALLA ALLA ALLA ALLA ALLA ALLA ALLA ALL	LEU LUN LUN LUN LUN ALA ALA ALA ALA ALA ALA CUN CUN CUN CUN CUN CUN CUN CUN CUN CUN	
• Molecule 1: Histone H3.1		
Chain O:	71%	29%

• Molecule 1: Histone H3.1



GLY SER MET MET MET ALA ALA ALA ALA ALA ALA ALA CLYS SER CLYS SER CLYS SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	LEU LEU THR TTR TTR TTR ALA ALA ALA ALA ALA ALA ALA CLY CLY CLY CLY CLY CLY CLY CLY	A135
• Molecule 1: Histone H3.1		
Chain k:	71%	29%
017 8.58 8.88 MHLS MHLS ALA ALA ALA ALA ALA ALA ALA ALA ALA A	L LUI ALLA ALLA ALLA ALLA ALLA ALLA ALLA A	A135
• Molecule 1: Histone H3.1		-
Chain o:	70%	30%
GLY SER MALA ALA ALA ALA ALA CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	L LULAL ALLA ALLA ALLA ALLA ALLA ALLA AL	R134 ALA
• Molecule 1: Histone H3.1		
Chain U:	70%	30%
CLY SER MET ALLA ALLA ALLA ALCA CLY CLY SER CLY SER CLY SER CLY SER CLY SER CLY SER CLY SER CLY SER CLY SER CLY SER CLY CLY SER SER SER SER SER SER SER SER SER SER	L ULU L ULU ALLA ALLA ALLA ALLA ALLA ALL	R134 ALA
• Molecule 1: Histone H3.1		
Chain Y:	71%	29%
GLY SER NET ALA ALA ALA ALA CLY CLY SER ARG GLY CLY SER ARG CLY CLY SER ARG CLY CLY SER ARG CLY CLY SER ARG CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	L LULAN ALLA ALLA ALLA ALLA ALLA ALLA ALLA	A135
• Molecule 1: Histone H3.1	_	-
Chain u:	71%	29%
GLY SUBBA MALA A ALA A ALA A ALA C	L CUIT A ALA A ALA	A 135
• Molecule 1: Histone H3.1	_	-
Chain y:	70%	30%
GLY SER MET MET THR MET THR ALA ALA ARG GLY SER ALA ALA ALA ALA ALA ALA ALA	LEU LEU ALLA ALLA ALLA ALLA ALLA ALLA AL	R134 ALA
• Molecule 2: Histone H4		-



GLY SER MET SER MET SER ARG GLY GLY GLY GLY GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C	
• Molecule 2: Histone H4	
Chain F: 77%	23%
617 SER NET SER SER NET SER CUT CUT CUT CUT CUT CUT CUT CUT CUT CUT	
• Molecule 2: Histone H4	
Chain b: 76%	• 23%
01Y SER HET SER HET SER SER ARG 01Y CITY CITY CITY CITY CITY CITY CITY CIT	
• Molecule 2: Histone H4	
Chain f: 77%	23%
CLY SER HIS NET SER CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	
• Molecule 2: Histone H4	
Chain L: 77%	23%
CLY SER HIS NET SER SER CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	
• Molecule 2: Histone H4	
Chain P: 77%	23%
GLY SER HIS MET SER HIS GLY GLY GLY GLY GLY CLY GLY GLY CLY GLY GLY CLY GLY GLY CLY GLY GLY CLY GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C	
• Molecule 2: Histone H4	
Chain I: 76%	• 23%
CLY SER MET SER MET SER CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	
• Molecule 2: Histone H4	
Chain p: 77%	23%



GLY SER HIS NET SER SER SER ARG GLY CLY GLY GLY ARG GLY ARG CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	
• Molecule 2: Histone H4	
Chain V: 77%	23%
GLY BER BER BER BER BER BER BER BER GLY GLY GLY GLY GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C	
• Molecule 2: Histone H4	
Chain Z: 76%	• 23%
CLY SER MET SER SER SER SER SER CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	
• Molecule 2: Histone H4	
Chain v: 77%	23%
GLY BER BER BER BER BER BER BER BER GLY GLY GLY GLY GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C	
• Molecule 2: Histone H4	
Chain z: 77%	23%
GLY HIS MET MET MET SER SER SER SER GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY	
\bullet Molecule 3: Histone H2A type 1-B/E	
Chain C: 76%	• 23%
617 8187 MET 8187 8187 8187 8178 8178 817 1178 817 1178	SX11 RTID
\bullet Molecule 3: Histone H2A type 1-B/E	
Chain G: 78%	• 21%
GLY SER SER MET SER MET SER GLY GLY GLY GLY MIA MIA MIA MIA MIA MIA MIA MIA MIA MIA	
• Molecule 3: Histone H2A type 1-B/E	
• Molecule 5. Instelle HER type I D/H	



GLY SER MET MET MET SER GLY GLY GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA	KI18 THR SELU SELU SELU HIS ALA ALA CLY CLY CLY	
• Molecule 3: Histone H2A t	ype $1-B/E$	
Chain g:	76%	• 23%
6LY SER MET MET MET MET MET GLY GLY GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	162 162 163 164 174 174 174 174 175 1175 1175 1175 117	
• Molecule 3: Histone H2A t	ype $1-B/E$	
Chain M:	77%	• 23%
GLY SIER MET MET MET SIER SIER CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	R81 LYS THR CLU CLUS CLUS CLUS CLUS CLUS CLUS	
• Molecule 3: Histone H2A t	ype $1-B/E$	
Chain Q:	78%	• 21%
GLY SER MET MET MET SER GLY GLY GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	K118 THR THR SER HIS HIS HIS LVS LVS CLV CLV LVS	
• Molecule 3: Histone H2A t	ype $1-B/E$	
Chain m:	78%	• 21%
GLY MET MET MET MET MET GLY GLY GLY GLY GLY GLY A14 A14 A14 A14 A14 A14 A14 A14 A14 A14	KALB HIT SIRH ALKS LVS LVS LVS LVS LVS LVS LVS LVS LVS LV	
• Molecule 3: Histone H2A t	ype $1-B/E$	
Chain q:	76%	• 23%
CLY SER MET MET MET MET SER CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	162 181 191 191 191 192 192 192 192 192 192 19	
• Molecule 3: Histone H2A t	ype $1-B/E$	
Chain W:	76%	• 23%
GLY MET MET MET MET MET GLY GLY GLY GLY GLY GLY GLY GLY GLY GLY	162 162 181 178 178 178 178 178 178 178 178 178	
• Molecule 3: Histone H2A t	ype $1-B/E$	
Chain 0:	78%	• 21%



GLY RET RET RET RET RET RET RET RET RET RET	
\bullet Molecule 3: Histone H2A type 1-B/E	
Chain w: 78%	• 21%
GLY MET SER ARC ARC ARC CLY CLYS CLYS CLYS CLYS CLYS CLYS CLYS	
\bullet Molecule 3: Histone H2A type 1-B/E	
Chain 2: 76% .	23%
GLY SER MET SER MET SER ALX ALX ALA CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	
• Molecule 4: Histone H2B type 1-J	
Chain D: 73% ·	26%
GLY RER MET MET PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	
• Molecule 4: Histone H2B type 1-J	
Chain H: 72% ·	26%
GLY REF MET MET MET MET MET MET MET MET MET MET	
• Molecule 4: Histone H2B type 1-J	
Chain d: 71% ·	26%
GLY SER MET MET MET MET MET MET MET PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	
• Molecule 4: Histone H2B type 1-J	
Chain h: 72% ·	26%
GLY SER HETS HETS HETS HETS FRO GLU GLU GLU FRO FRO FRO FRO FRO FRO GLU CVS GLV CVS GLV CVS GLV CVS GLU CVS GLO CVS CVS GLO CVS CVS CVS CVS CVS CVS CVS CVS CVS CVS	
• Molecule 4: Histone H2B type 1-J	
Chain N: 73% .	26%



• Molecule 4: Histone H2B type 1-J

Chain R:	72% •	26%
GLY SER HIS MET PRO GLU PRO	LALA ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	
• Molecul	e 4: Histone H2B type 1-J	
Chain n:	71%	26%
GLY SER HIS MET PRO GLU	L ALA ALA PRIA PRIA PRIA PRIA PRIA PRIA PRIA PRI	2
• Molecul	e 4: Histone H2B type 1-J	
Chain r:	72%	26%
GLY SER HIS MET PRO GLU FRO	ALA ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	
• Molecul	e 4: Histone H2B type 1-J	
Chain X:	72% •	26%
GLY SER HIS MET PRO GLU PRO	LATA ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	
• Molecul	e 4: Histone H2B type 1-J	
Chain 1:	73% •	26%
GLY SER HIS MET PRO GLU GLU	LALA ALA SER PALA ALA ALA ALA LAS CLAS ALA ALA LAS ALA ALA CLAS ALA ALA LAS ALA CLAS ALA CLAS ALA CLAS ALA CLAS ALA CLAS ALA CLAS ALA CLAS ALA CLAS ALA CLAS ALA CLAS ALA CLAS ALA CLAS ALA CLAS CLAS	
• Molecul	e 4: Histone H2B type 1-J	
Chain x: '	72% •	26%
GLY SER HIS NET PRO GLU PRO	ATA ATA ATA ATA ATA ATA ATA ATA ATA ATA	
• Molecul	e 4: Histone H2B type 1-J	
Chain 3:	71% •	26%



• Molecule 5: DNA (1122-MER)

Chain I:



• Molecule 6: DNA (1122-MER)

99%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	111.08Å 238.76Å 674.37Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{B}_{\mathrm{ascolution}}(\mathbf{\hat{A}})$	49.07 - 9.70	Depositor
Resolution (A)	49.07 - 9.70	EDS
% Data completeness	99.8 (49.07-9.70)	Depositor
(in resolution range)	$99.8 \ (49.07 - 9.70)$	EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.23 (at 9.80 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
D D.	0.254 , 0.286	Depositor
Π, Π_{free}	0.255 , 0.289	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.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/813	0.37	0/1090
1	Е	0.24	0/819	0.37	0/1097
1	K	0.26	0/813	0.40	0/1090
1	0	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	е	0.26	0/813	0.43	1/1090~(0.1%)
1	k	0.25	0/819	0.41	0/1097
1	0	0.25	0/813	0.41	0/1090
1	u	0.27	0/819	0.39	0/1097
1	у	0.26	0/813	0.37	0/1090
2	В	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	Р	0.25	0/660	0.45	0/883
2	V	0.27	0/660	0.48	0/883
2	Ζ	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	р	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	С	0.24	0/806	0.41	0/1089
3	G	0.27	0/820	0.40	0/1107
3	М	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	с	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



6HKT	
OTTLY T	

Mal	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	Н	0.25	0/756	0.40	0/1015
4	Ν	0.24	0/766	0.39	0/1026
4	R	0.25	0/756	0.39	0/1015
4	Х	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	Х	0.24	0/756	0.40	0/1015
5	Ι	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.

The worst 5 of 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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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



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	Perce	ntiles
1	А	95/139~(68%)	93~(98%)	2(2%)	0	100	100
1	Ε	96/139~(69%)	93~(97%)	3~(3%)	0	100	100
1	K	95/139~(68%)	91~(96%)	4 (4%)	0	100	100
1	Ο	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	е	95/139~(68%)	93~(98%)	2(2%)	0	100	100
1	k	96/139~(69%)	93~(97%)	3(3%)	0	100	100
1	О	95/139~(68%)	94 (99%)	1 (1%)	0	100	100
1	u	96/139~(69%)	93~(97%)	3 (3%)	0	100	100
1	у	95/139~(68%)	93~(98%)	2(2%)	0	100	100
2	В	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	Р	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	1	80/106 (76%)	78 (98%)	2(2%)	0	100	100
2	р	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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
3	2	101/133~(76%)	99~(98%)	2(2%)	0	100	100
3	С	101/133~(76%)	99~(98%)	2(2%)	0	100	100
3	G	103/133~(77%)	101~(98%)	2(2%)	0	100	100
3	М	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	с	103/133~(77%)	102~(99%)	1 (1%)	0	100	100
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	Н	93/129~(72%)	91~(98%)	1 (1%)	1 (1%)	14	52
4	Ν	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	$\overline{93/129}~(72\%)$	91 (98%)	1 (1%)	1 (1%)	14	52
4	r	94/129~(73%)	91 (97%)	2 (2%)	1 (1%)	14	52
4	X	$\overline{93/129}~(72\%)$	92 (99%)	0	1 (1%)	14	52
All	All	4452/6084~(73%)	4350 (98%)	90 (2%)	12 (0%)	41	77

Continued from previous page...

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	GLY
4	Н	101	GLY
4	d	101	GLY
4	h	101	GLY
4	N	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	Perce	ntiles
1	А	85/113~(75%)	85~(100%)	0	100	100
1	Ε	85/113~(75%)	84 (99%)	1 (1%)	71	83
1	K	85/113~(75%)	85 (100%)	0	100	100
1	О	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	е	85/113~(75%)	84 (99%)	1 (1%)	71	83
1	k	85/113~(75%)	85 (100%)	0	100	100
1	0	85/113~(75%)	85 (100%)	0	100	100
1	u	85/113~(75%)	85 (100%)	0	100	100
1	у	85/113~(75%)	85 (100%)	0	100	100
2	В	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	Р	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	1	67/81~(83%)	67 (100%)	0	100	100
2	р	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



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
3	С	82/102~(80%)	80~(98%)	2(2%)	49	69
3	G	83/102 (81%)	82~(99%)	1 (1%)	71	83
3	М	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	с	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	Η	81/107~(76%)	80~(99%)	1 (1%)	71	83
4	Ν	82/107~(77%)	81~(99%)	1 (1%)	71	83
4	R	81/107~(76%)	80~(99%)	1 (1%)	71	83
4	Х	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	Х	81/107 (76%)	80 (99%)	1 (1%)	71	83
All	All	3792/4836~(78%)	3757~(99%)	35 (1%)	78	87

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
4	Ν	31	LYS
4	n	53	SER
3	2	81	ARG
3	Q	81	ARG
4	R	85	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:



Mol	Chain	Res	Type
2	р	25	ASN
2	р	75	HIS
3	0	38	ASN
1	0	108	ASN
4	r	81	ASN

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)

There are no ligands in this entry.

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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

