wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 02:17 pm GMT

PDB ID	:	5OY7
Title	:	Structure of the 4_601_157 tetranucleosome (P1 form)
Authors	:	Ekundayo, B.; Richmond, T.J.; Schalch, T.
Deposited on	:	2017-09-07
Resolution	:	5.77 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

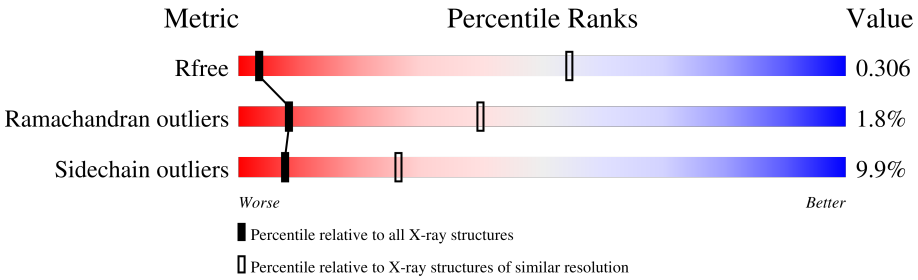
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 5.77 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	1008 (7.70-3.86)
Ramachandran outliers	138981	1003 (7.70-3.86)
Sidechain outliers	138945	1005 (7.70-3.82)

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 >=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	D	126	64% 10% • 25%
1	H	126	62% 12% 26%
1	L	126	65% 9% • 25%
1	P	126	63% 11% 26%
1	T	126	65% 9% • 25%
1	X	126	63% 11% 26%
1	b	126	65% 9% • 25%
1	f	126	63% 11% 26%

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Mol	Chain	Length	Quality of chain
2	A	135	64% 8% 28%
2	E	135	68% 28%
2	I	135	64% 8% 28%
2	M	135	68% 28%
2	Q	135	64% 8% 28%
2	U	135	68% 28%
2	Y	135	64% 8% 28%
2	c	135	68% 28%
3	B	102	73% 9% 19%
3	F	102	73% 24%
3	J	102	73% 9% 19%
3	N	102	73% 24%
3	R	102	73% 8% 20%
3	V	102	73% 24%
3	Z	102	74% 8% 19%
3	d	102	73% 24%
4	C	130	72% 7% 21%
4	G	130	74% 7% 19%
4	K	130	72% 7% 21%
4	O	130	74% 7% 19%
4	S	130	72% 7% 21%
4	W	130	74% 7% 19%
4	a	130	72% 7% 21%
4	e	130	74% 7% 19%
5	g	634	73% 25%

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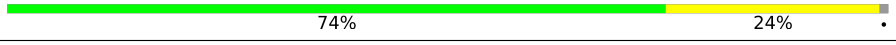
Mol	Chain	Length	Quality of chain
6	h	628	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 49215 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 H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
1	P	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			
1	D	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
1	H	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			
1	T	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
1	X	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			
1	b	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
1	f	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	29	THR	SER	conflict	UNP P02281
P	29	THR	SER	conflict	UNP P02281
D	29	THR	SER	conflict	UNP P02281
H	29	THR	SER	conflict	UNP P02281
T	29	THR	SER	conflict	UNP P02281
X	29	THR	SER	conflict	UNP P02281
b	29	THR	SER	conflict	UNP P02281
f	29	THR	SER	conflict	UNP P02281

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
2	Q	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			
2	I	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			
2	A	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			
2	E	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
2	U	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			
2	Y	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			
2	c	97	Total	C	N	O	S	0	0	0
			801	504	155	139	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	102	ALA	GLY	conflict	UNP Q92133
M	111	ALA	GLY	conflict	UNP Q92133
Q	102	ALA	GLY	conflict	UNP Q92133
Q	111	ALA	GLY	conflict	UNP Q92133
I	102	ALA	GLY	conflict	UNP Q92133
I	111	ALA	GLY	conflict	UNP Q92133
A	102	ALA	GLY	conflict	UNP Q92133
A	111	ALA	GLY	conflict	UNP Q92133
E	102	ALA	GLY	conflict	UNP Q92133
E	111	ALA	GLY	conflict	UNP Q92133
U	102	ALA	GLY	conflict	UNP Q92133
U	111	ALA	GLY	conflict	UNP Q92133
Y	102	ALA	GLY	conflict	UNP Q92133
Y	111	ALA	GLY	conflict	UNP Q92133
c	102	ALA	GLY	conflict	UNP Q92133
c	111	ALA	GLY	conflict	UNP Q92133

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	82	Total	C	N	O	S	0	0	0
			654	412	128	113	1			
3	J	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
3	B	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
3	F	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
3	V	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
3	Z	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
3	d	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	O	105	Total	C	N	O	0	0	0
			809	510	158	141			
4	C	103	Total	C	N	O	0	0	0
			795	501	155	139			
4	G	105	Total	C	N	O	0	0	0
			809	510	158	141			
4	K	103	Total	C	N	O	0	0	0
			795	501	155	139			
4	S	103	Total	C	N	O	0	0	0
			795	501	155	139			
4	W	105	Total	C	N	O	0	0	0
			809	510	158	141			
4	a	103	Total	C	N	O	0	0	0
			795	501	155	139			
4	e	105	Total	C	N	O	0	0	0
			809	510	158	141			

- Molecule 5 is a DNA chain called DNA (619-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	g	619	Total	C	N	O	P	0	0	0
			12605	5987	2278	3721	619			

- Molecule 6 is a DNA chain called DNA (619-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	h	619	Total 12774	C 6041	N 2407	O 3707	P 619	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	O	1	Total 1	Cl 1	1	0
7	C	1	Total 1	Cl 1	1	0
7	G	1	Total 1	Cl 1	1	0
7	K	1	Total 1	Cl 1	1	0
7	S	1	Total 1	Cl 1	1	0
7	W	1	Total 1	Cl 1	1	0
7	a	1	Total 1	Cl 1	1	0
7	e	1	Total 1	Cl 1	1	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 H2B 1.1

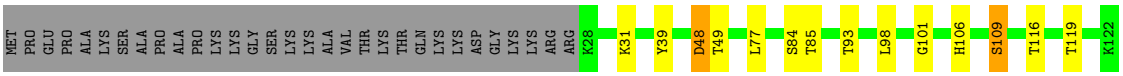
Chain L:

• Molecule 1: Histone H2B 1.1

Chain P:

• Molecule 1: Histone H2B 1.1

Chain D:



• Molecule 1: Histone H2B 1.1

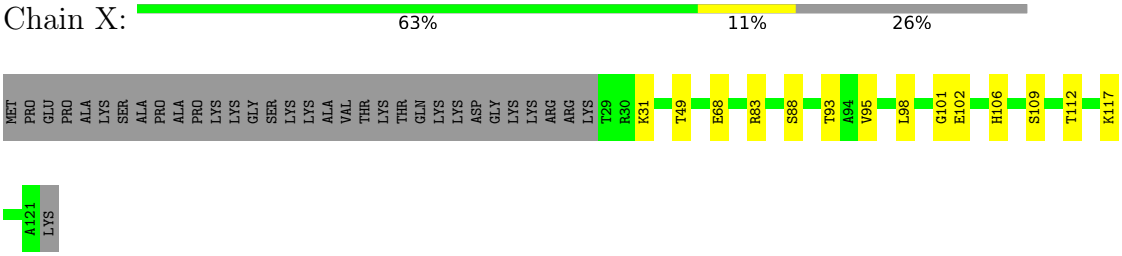
Chain H:

• Molecule 1: Histone H2B 1.1

Chain T:

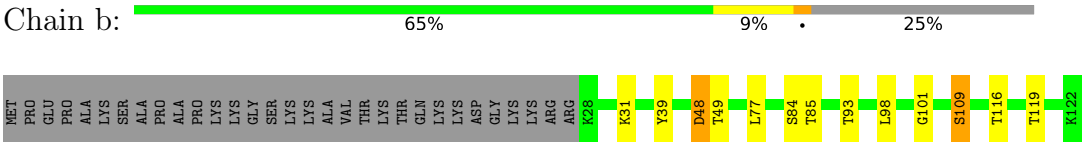
• Molecule 1: Histone H2B 1.1

Chain X:



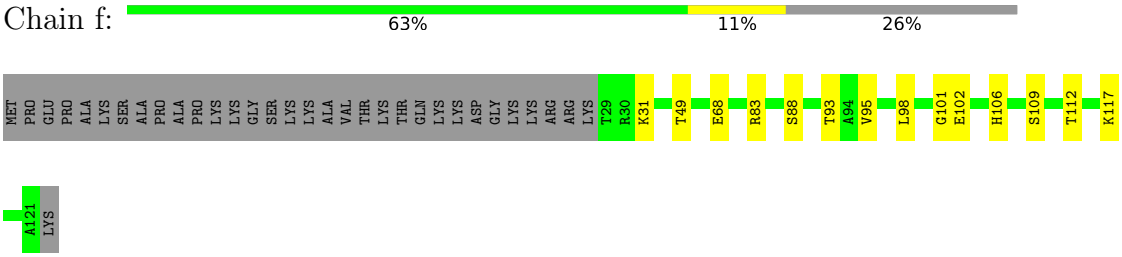
• Molecule 1: Histone H2B 1.1

Chain b:



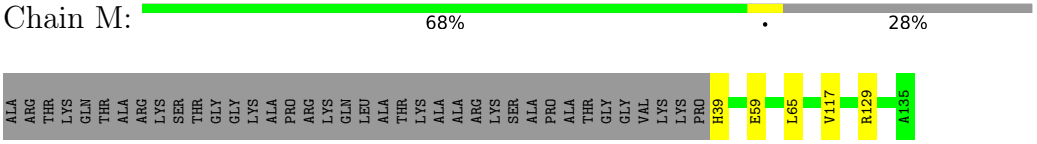
• Molecule 1: Histone H2B 1.1

Chain f:



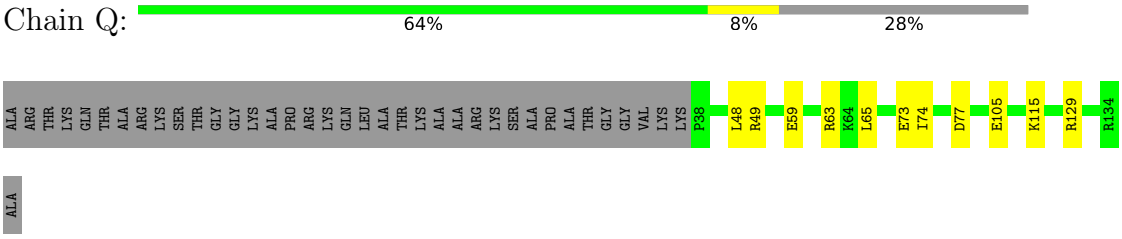
• Molecule 2: Histone H3

Chain M:



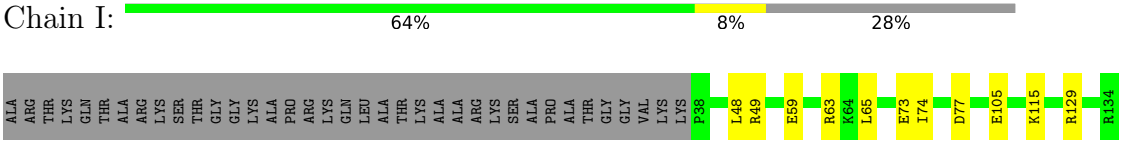
• Molecule 2: Histone H3

Chain Q:



• Molecule 2: Histone H3

Chain I:

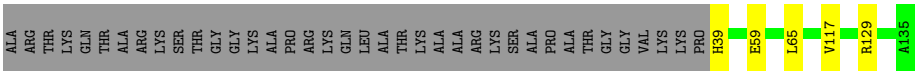


• Molecule 2: Histone H3

Chain A:

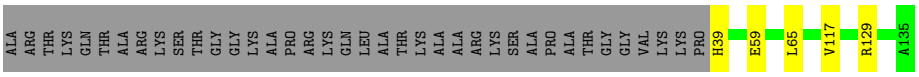
• Molecule 2: Histone H3

Chain E:



• Molecule 2: Histone H3

Chain U:

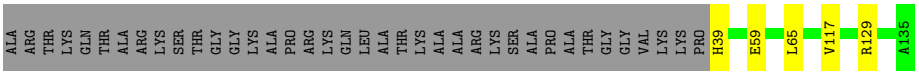


• Molecule 2: Histone H3

Chain Y:

• Molecule 2: Histone H3

Chain c:

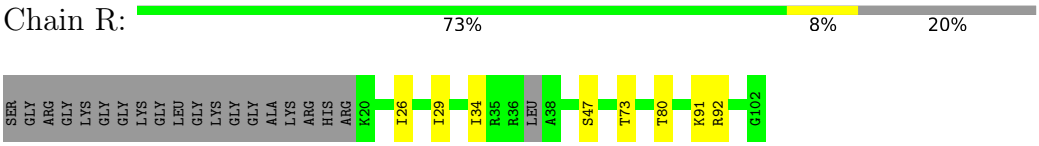


• Molecule 3: Histone H4

Chain N:

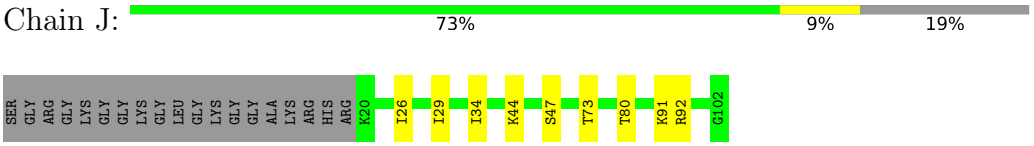
• Molecule 3: Histone H4

Chain R:



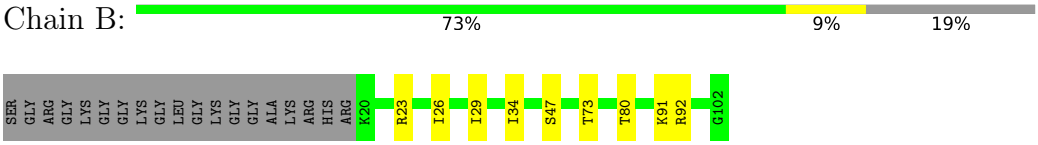
• Molecule 3: Histone H4

Chain J:



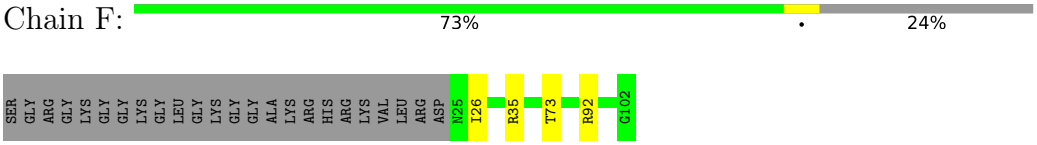
• Molecule 3: Histone H4

Chain B:



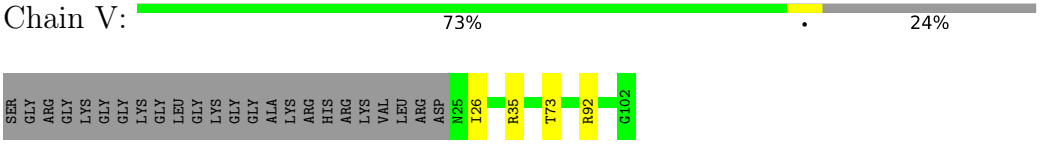
• Molecule 3: Histone H4

Chain F:



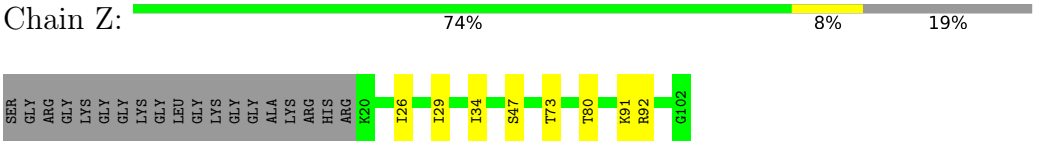
• Molecule 3: Histone H4

Chain V:



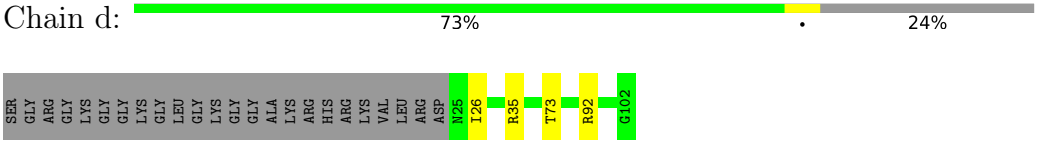
• Molecule 3: Histone H4

Chain Z:



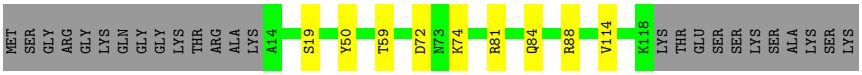
• Molecule 3: Histone H4

Chain d:



• Molecule 4: Histone H2A

Chain O:

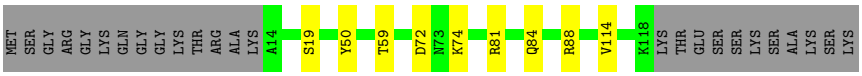


• Molecule 4: Histone H2A

Chain C:

• Molecule 4: Histone H2A

Chain G:



• Molecule 4: Histone H2A

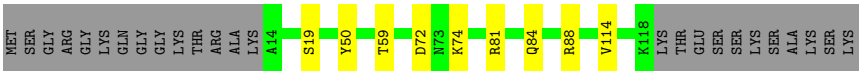
Chain K:

• Molecule 4: Histone H2A

Chain S:

• Molecule 4: Histone H2A

Chain W:

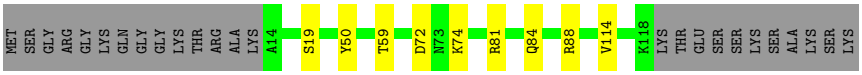


• Molecule 4: Histone H2A

Chain a:

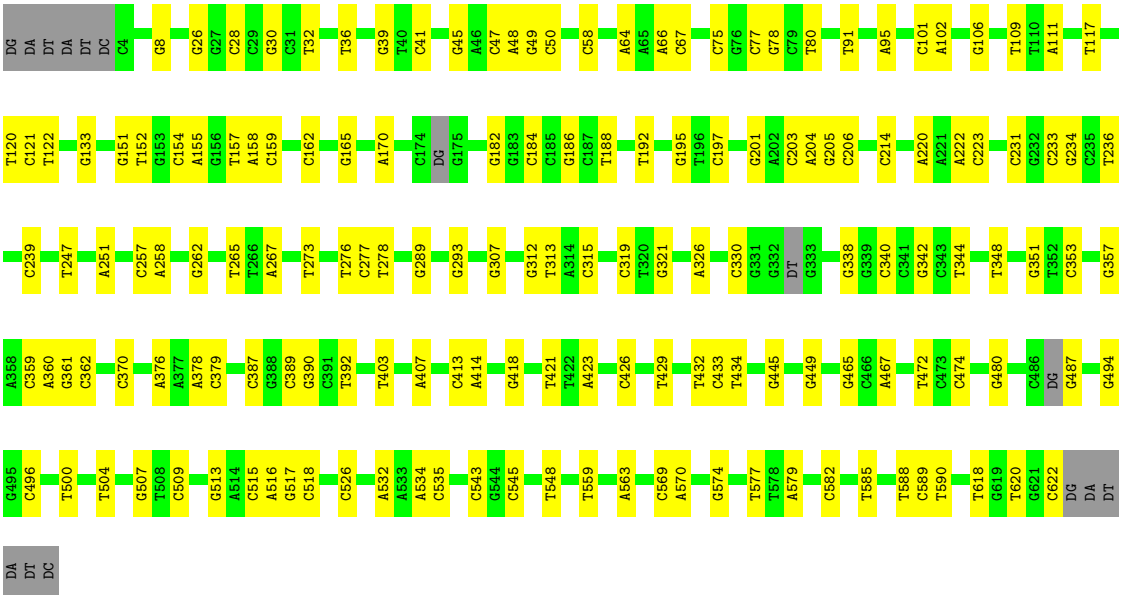
• Molecule 4: Histone H2A

Chain e:



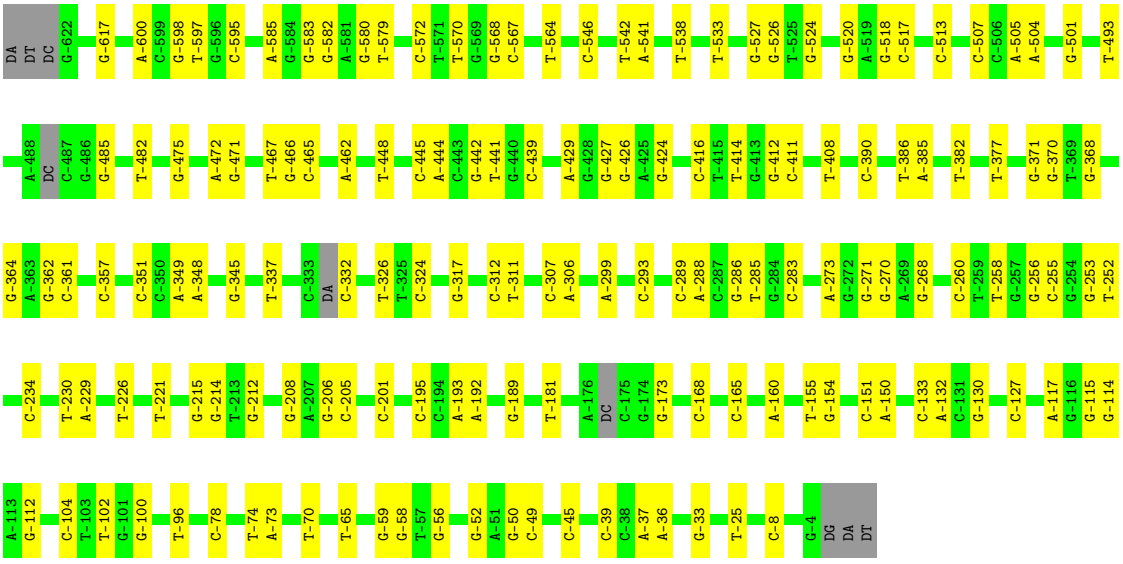
• Molecule 5: DNA (619-MER)

Chain g:



• Molecule 6: DNA (619-MER)

Chain h:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.62Å 161.47Å 227.91Å 78.94° 83.86° 83.74°	Depositor
Resolution (Å)	111.41 – 5.77 141.52 – 5.77	Depositor EDS
% Data completeness (in resolution range)	93.8 (111.41-5.77) 93.8 (141.52-5.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 5.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.219 , 0.238 0.289 , 0.306	Depositor DCC
R_{free} test set	1226 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	222.9	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 230.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	49215	wwPDB-VP
Average B, all atoms (Å^2)	246.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	D	0.49	0/756	0.64	0/1015
1	H	0.62	0/737	0.70	0/993
1	L	0.49	0/756	0.64	0/1015
1	P	0.62	0/737	0.70	0/993
1	T	0.49	0/756	0.64	0/1015
1	X	0.62	0/737	0.70	0/993
1	b	0.49	0/756	0.64	0/1015
1	f	0.62	0/737	0.70	0/993
2	A	0.66	0/814	0.73	0/1092
2	E	0.41	0/812	0.57	0/1088
2	I	0.66	0/814	0.73	0/1092
2	M	0.41	0/812	0.58	0/1088
2	Q	0.66	0/814	0.73	0/1092
2	U	0.41	0/812	0.57	0/1088
2	Y	0.66	0/814	0.73	0/1092
2	c	0.41	0/812	0.58	0/1088
3	B	0.67	0/669	0.84	0/894
3	F	0.45	0/626	0.61	0/837
3	J	0.67	0/669	0.89	1/894 (0.1%)
3	N	0.46	0/626	0.62	0/837
3	R	0.67	0/660	0.83	0/880
3	V	0.45	0/626	0.61	0/837
3	Z	0.67	0/669	0.83	0/894
3	d	0.46	0/626	0.61	0/837
4	C	0.42	0/805	0.61	0/1088
4	G	0.63	0/819	0.75	0/1106
4	K	0.43	0/805	0.61	0/1088
4	O	0.63	0/819	0.76	0/1106
4	S	0.42	0/805	0.61	0/1088
4	W	0.63	0/819	0.76	0/1106
4	a	0.43	0/805	0.61	0/1088
4	e	0.63	0/819	0.76	0/1106

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
5	g	0.80	28/14121 (0.2%)	1.34	144/21771 (0.7%)
6	h	0.82	29/14351 (0.2%)	1.36	165/22170 (0.7%)
All	All	0.70	57/52615 (0.1%)	1.12	310/76379 (0.4%)

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	h	-448	DT	O3'-P	26.30	1.92	1.61
6	h	-475	DG	C1'-N9	-8.79	1.34	1.47
5	g	622	DC	C1'-N1	7.52	1.59	1.49
5	g	151	DG	C1'-N9	-7.18	1.37	1.47
5	g	157	DT	C3'-O3'	7.08	1.53	1.44

The worst 5 of 310 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	h	-448	DT	P-O3'-C3'	29.45	155.04	119.70
5	g	158	DA	OP1-P-OP2	17.27	145.50	119.60
5	g	157	DT	OP1-P-O3'	-14.16	74.04	105.20
5	g	157	DT	OP2-P-O3'	-13.26	76.02	105.20
6	h	-448	DT	O3'-P-O5'	12.06	126.92	104.00

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	D	93/126 (74%)	82 (88%)	9 (10%)	2 (2%)	6 35
1	H	91/126 (72%)	80 (88%)	10 (11%)	1 (1%)	14 51
1	L	93/126 (74%)	82 (88%)	9 (10%)	2 (2%)	6 35
1	P	91/126 (72%)	80 (88%)	10 (11%)	1 (1%)	14 51
1	T	93/126 (74%)	81 (87%)	10 (11%)	2 (2%)	6 35
1	X	91/126 (72%)	80 (88%)	10 (11%)	1 (1%)	14 51
1	b	93/126 (74%)	82 (88%)	9 (10%)	2 (2%)	6 35
1	f	91/126 (72%)	80 (88%)	10 (11%)	1 (1%)	14 51
2	A	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4 26
2	E	95/135 (70%)	86 (90%)	9 (10%)	0	100 100
2	I	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4 26
2	M	95/135 (70%)	86 (90%)	9 (10%)	0	100 100
2	Q	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4 26
2	U	95/135 (70%)	86 (90%)	9 (10%)	0	100 100
2	Y	95/135 (70%)	83 (87%)	9 (10%)	3 (3%)	4 26
2	c	95/135 (70%)	86 (90%)	9 (10%)	0	100 100
3	B	81/102 (79%)	70 (86%)	8 (10%)	3 (4%)	3 24
3	F	76/102 (74%)	67 (88%)	9 (12%)	0	100 100
3	J	81/102 (79%)	70 (86%)	8 (10%)	3 (4%)	3 24
3	N	76/102 (74%)	67 (88%)	9 (12%)	0	100 100
3	R	78/102 (76%)	68 (87%)	7 (9%)	3 (4%)	3 24
3	V	76/102 (74%)	67 (88%)	9 (12%)	0	100 100
3	Z	81/102 (79%)	70 (86%)	8 (10%)	3 (4%)	3 24
3	d	76/102 (74%)	67 (88%)	9 (12%)	0	100 100
4	C	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3 23
4	G	103/130 (79%)	88 (85%)	15 (15%)	0	100 100
4	K	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3 23
4	O	103/130 (79%)	87 (84%)	16 (16%)	0	100 100
4	S	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3 23
4	W	103/130 (79%)	88 (85%)	15 (15%)	0	100 100
4	a	101/130 (78%)	88 (87%)	9 (9%)	4 (4%)	3 23
4	e	103/130 (79%)	88 (85%)	15 (15%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2937/3944 (74%)	2572 (88%)	313 (11%)	52 (2%)	8 40

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	101	GLY
2	Q	73	GLU
3	R	29	ILE
2	I	73	GLU
3	J	29	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	81/106 (76%)	69 (85%)	12 (15%)	3 15
1	H	79/106 (74%)	67 (85%)	12 (15%)	3 14
1	L	81/106 (76%)	69 (85%)	12 (15%)	3 15
1	P	79/106 (74%)	67 (85%)	12 (15%)	3 14
1	T	81/106 (76%)	69 (85%)	12 (15%)	3 15
1	X	79/106 (74%)	67 (85%)	12 (15%)	3 14
1	b	81/106 (76%)	69 (85%)	12 (15%)	3 15
1	f	79/106 (74%)	67 (85%)	12 (15%)	3 14
2	A	85/110 (77%)	77 (91%)	8 (9%)	8 28
2	E	84/110 (76%)	79 (94%)	5 (6%)	19 44
2	I	85/110 (77%)	77 (91%)	8 (9%)	8 28
2	M	84/110 (76%)	79 (94%)	5 (6%)	19 44
2	Q	85/110 (77%)	77 (91%)	8 (9%)	8 28
2	U	84/110 (76%)	79 (94%)	5 (6%)	19 44
2	Y	85/110 (77%)	77 (91%)	8 (9%)	8 28
2	c	84/110 (76%)	79 (94%)	5 (6%)	19 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	B	68/78 (87%)	63 (93%)	5 (7%)	13 38
3	F	63/78 (81%)	59 (94%)	4 (6%)	18 42
3	J	68/78 (87%)	63 (93%)	5 (7%)	13 38
3	N	63/78 (81%)	59 (94%)	4 (6%)	18 42
3	R	67/78 (86%)	62 (92%)	5 (8%)	13 37
3	V	63/78 (81%)	59 (94%)	4 (6%)	18 42
3	Z	68/78 (87%)	63 (93%)	5 (7%)	13 38
3	d	63/78 (81%)	59 (94%)	4 (6%)	18 42
4	C	82/102 (80%)	75 (92%)	7 (8%)	10 33
4	G	83/102 (81%)	74 (89%)	9 (11%)	6 23
4	K	82/102 (80%)	75 (92%)	7 (8%)	10 33
4	O	83/102 (81%)	74 (89%)	9 (11%)	6 23
4	S	82/102 (80%)	75 (92%)	7 (8%)	10 33
4	W	83/102 (81%)	74 (89%)	9 (11%)	6 23
4	a	82/102 (80%)	75 (92%)	7 (8%)	10 33
4	e	83/102 (81%)	74 (89%)	9 (11%)	6 23
All	All	2499/3168 (79%)	2251 (90%)	248 (10%)	8 26

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	84	GLN
2	c	117	VAL
4	S	118	LYS
2	c	59	GLU
1	f	31	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
4	S	112	GLN
4	W	84	GLN
4	W	31	HIS
3	Z	75	HIS
4	C	38	ASN

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

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	h	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	h	-448:DT	O3'	-447:DG	P	1.92

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.