



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:05 pm GMT

PDB ID : 1F66  
Title : 2.6 Å CRYSTAL STRUCTURE OF A NUCLEOSOME CORE PARTICLE  
CONTAINING THE VARIANT HISTONE H2A.Z  
Authors : Suto, R.K.; Clarkson, M.J.; Tremethick, D.J.; Luger, K.  
Deposited on : 2000-06-20  
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

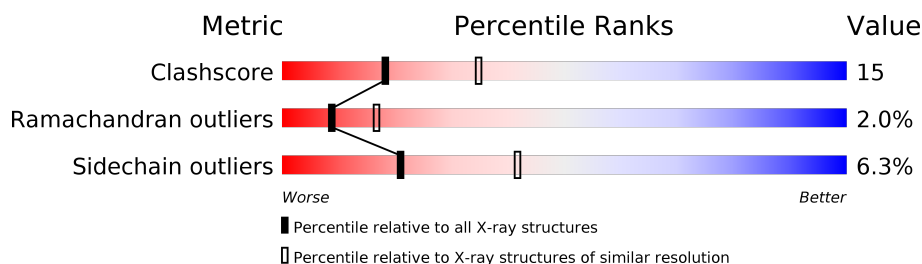
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	I	146	
1	J	146	
2	A	136	
2	E	136	
3	B	103	
3	F	103	
4	C	128	

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Mol	Chain	Length	Quality of chain
4	G	128	<div><div></div><div>59%18%6%•16%</div></div>
5	D	126	<div><div></div><div>56%17%••25%</div></div>
5	H	126	<div><div></div><div>59%14%•25%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12397 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 PALINDROMIC 146 BASE PAIR DNA FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			
1	J	146	Total	C	N	O	P	0	0	0
			2990	1430	541	874	145			

- Molecule 2 is a protein called HISTONE H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	100	Total	C	N	O	S	0	0	0
			826	521	160	142	3			
2	E	103	Total	C	N	O	S	0	0	0
			841	530	163	145	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	GLU	GLY	CONFLICT	UNP Q7ZT64
A	517	VAL	ILE	CONFLICT	UNP Q7ZT64
E	634	GLU	GLY	CONFLICT	UNP Q7ZT64
E	717	VAL	ILE	CONFLICT	UNP Q7ZT64

- Molecule 3 is a protein called HISTONE H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
3	F	86	Total	C	N	O	S	0	0	0
			694	436	140	117	1			

- Molecule 4 is a protein called HISTONE H2A.Z.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	103	Total	C	N	O	0	0	0
			781	490	152	139			
4	G	107	Total	C	N	O	0	0	0
			807	506	158	143			

- Molecule 5 is a protein called HISTONE H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			
5	H	95	Total	C	N	O	S	0	0	0
			745	469	134	140	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1229	THR	SER	CONFLICT	UNP P02281
H	1429	THR	SER	CONFLICT	UNP P02281

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mn	0	0
			1	1		
6	J	5	Total	Mn	0	0
			5	5		
6	I	7	Total	Mn	0	0
			7	7		
6	C	1	Total	Mn	0	0
			1	1		
6	E	1	Total	Mn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	27	Total	O	0	0
			27	27		
7	B	24	Total	O	0	0
			24	24		
7	C	31	Total	O	0	0
			31	31		

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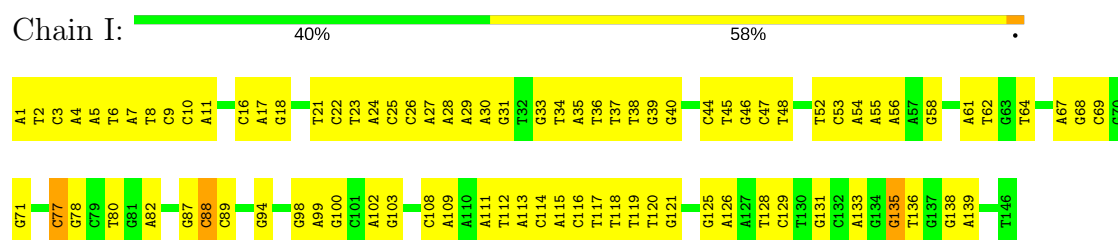
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	25	Total 25	O 25	0	0
7	E	43	Total 43	O 43	0	0
7	F	26	Total 26	O 26	0	0
7	G	16	Total 16	O 16	0	0
7	H	15	Total 15	O 15	0	0
7	I	62	Total 62	O 62	0	0
7	J	56	Total 56	O 56	0	0

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

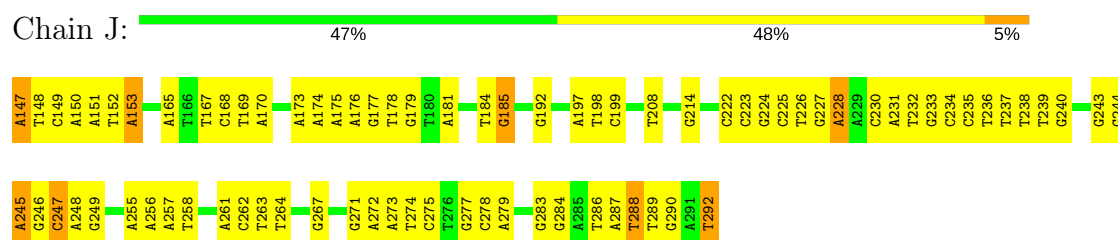
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

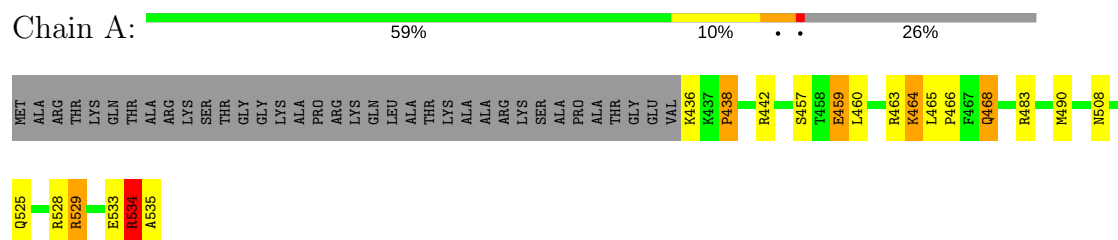
#### • Molecule 1: PALINDROMIC 146 BASE PAIR DNA FRAGMENT



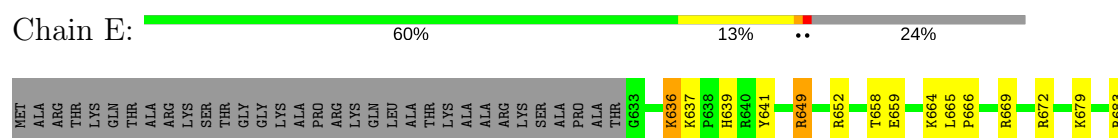
#### • Molecule 1: PALINDROMIC 146 BASE PAIR DNA FRAGMENT



#### • Molecule 2: HISTONE H3

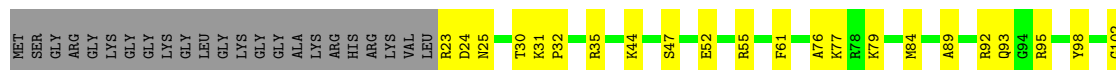


#### • Molecule 2: HISTONE H3

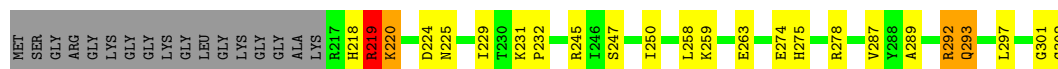




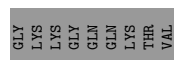
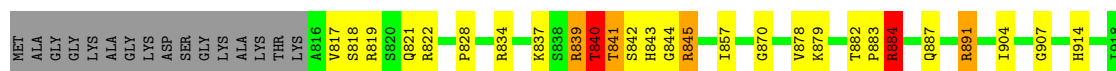
• Molecule 3: HISTONE H4



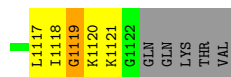
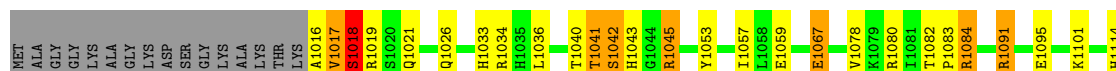
• Molecule 3: HISTONE H4



• Molecule 4: HISTONE H2A.Z



• Molecule 4: HISTONE H2A.Z



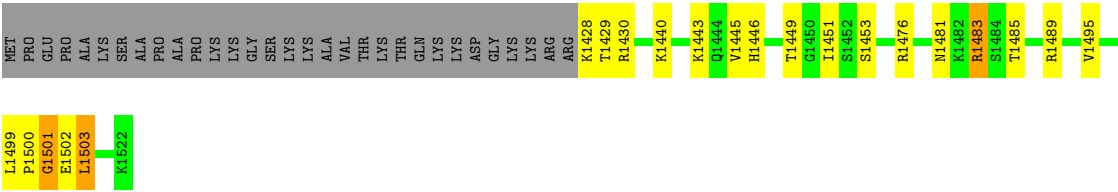
• Molecule 5: HISTONE H2B



• Molecule 5: HISTONE H2B







## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.66Å 183.21Å 109.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.6 (25.00-2.60)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.193 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12397	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.62	0/3354	0.82	1/5175 (0.0%)
1	J	0.62	0/3354	0.83	2/5175 (0.0%)
2	A	0.82	0/838	0.87	1/1122 (0.1%)
2	E	0.94	0/853	0.97	1/1142 (0.1%)
3	B	0.86	0/645	0.88	0/862
3	F	1.03	0/702	1.03	3/937 (0.3%)
4	C	0.84	0/792	0.92	2/1068 (0.2%)
4	G	0.72	0/818	0.93	3/1100 (0.3%)
5	D	0.84	0/756	0.84	0/1015
5	H	0.78	0/756	0.86	0/1015
All	All	0.74	0/12868	0.87	13/18611 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	8
1	J	0	10
3	B	0	1
5	D	0	1
All	All	0	20

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	728	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	J	227	DG	C5'-C4'-C3'	-6.47	102.45	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	884	ARG	NE-CZ-NH1	6.43	123.52	120.30
4	C	884	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	J	208	DT	OP2-P-O3'	6.26	118.98	105.20

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	121	DG	Sidechain
1	I	64	DT	Sidechain
1	I	67	DA	Sidechain
1	I	77	DC	Sidechain
1	I	88	DC	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2990	0	1651	83	0
1	J	2990	0	1651	96	0
2	A	826	0	871	22	0
2	E	841	0	884	27	0
3	B	638	0	676	18	0
3	F	694	0	742	18	0
4	C	781	0	824	41	0
4	G	807	0	856	39	0
5	D	745	0	773	30	0
5	H	745	0	773	22	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	7	0	0	0	0
6	J	5	0	0	0	0
7	A	27	0	0	0	0
7	B	24	0	0	2	0
7	C	31	0	0	0	0
7	D	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	43	0	0	1	0
7	F	26	0	0	1	0
7	G	16	0	0	1	0
7	H	15	0	0	2	0
7	I	62	0	0	5	0
7	J	56	0	0	3	0
All	All	12397	0	9701	325	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 325 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)
7:J:1048:HOH:O	4:G:1034:ARG:HD2	1.49	1.08
5:D:1243:LYS:HE2	5:D:1243:LYS:HA	1.40	1.03
4:C:839:ARG:HH11	4:C:839:ARG:HB2	1.26	0.98
2:E:636:LYS:HG2	2:E:637:LYS:H	1.26	0.97
4:C:822:ARG:NH2	5:D:1322:LYS:HB2	1.80	0.95

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	98/136 (72%)	94 (96%)	2 (2%)	2 (2%)	9	17
2	E	101/136 (74%)	96 (95%)	3 (3%)	2 (2%)	9	17
3	B	78/103 (76%)	78 (100%)	0	0	100	100
3	F	84/103 (82%)	77 (92%)	4 (5%)	3 (4%)	4	5
4	C	101/128 (79%)	93 (92%)	5 (5%)	3 (3%)	5	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	105/128 (82%)	94 (90%)	8 (8%)	3 (3%)	5	8
5	D	93/126 (74%)	91 (98%)	1 (1%)	1 (1%)	17	35
5	H	93/126 (74%)	89 (96%)	3 (3%)	1 (1%)	17	35
All	All	753/986 (76%)	712 (95%)	26 (4%)	15 (2%)	9	17

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	534	ARG
4	C	841	THR
5	D	1301	GLY
2	E	636	LYS
4	G	1017	VAL

### 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	
2	A	87/112 (78%)	82 (94%)	5 (6%)	24	47
2	E	88/112 (79%)	85 (97%)	3 (3%)	42	69
3	B	65/79 (82%)	62 (95%)	3 (5%)	31	58
3	F	71/79 (90%)	66 (93%)	5 (7%)	18	35
4	C	81/97 (84%)	74 (91%)	7 (9%)	12	23
4	G	83/97 (86%)	75 (90%)	8 (10%)	10	18
5	D	81/106 (76%)	76 (94%)	5 (6%)	21	42
5	H	81/106 (76%)	77 (95%)	4 (5%)	29	54
All	All	637/788 (81%)	597 (94%)	40 (6%)	21	42

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	1309	SER

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Mol	Chain	Res	Type
2	E	734	ARG
5	H	1453	SER
2	E	649	ARG
3	F	219	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	1292	GLN
4	G	1114	HIS
4	G	1033	HIS
3	B	75	HIS
2	E	639	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.