



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 10:04 pm GMT

PDB ID : 1KX5  
Title : X-Ray Structure of the Nucleosome Core Particle, NCP147, at 1.9 Å Resolution  
Authors : Davey, C.A.; Sargent, D.F.; Luger, K.; Maeder, A.W.; Richmond, T.J.  
Deposited on : 2002-01-31  
Resolution : 1.94 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

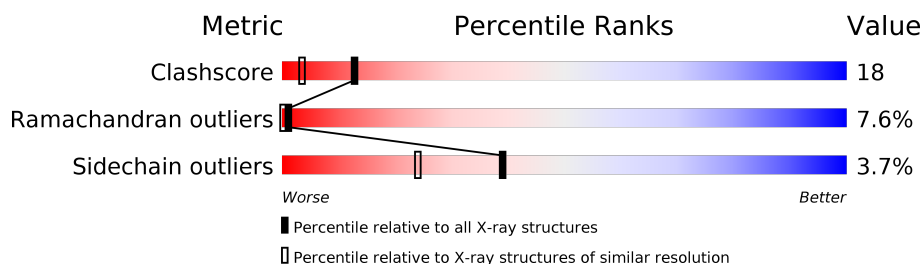
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	3430 (1.96-1.92)
Ramachandran outliers	110173	3395 (1.96-1.92)
Sidechain outliers	110143	3395 (1.96-1.92)

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	147	
2	J	147	
3	A	135	
3	E	135	
4	B	102	
4	F	102	
5	C	128	

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Mol	Chain	Length	Quality of chain
5	G	128	<div><div></div><div>74%</div><div>23%</div><div></div><div></div></div>
6	D	125	<div><div></div><div>66%</div><div>24%</div><div>6%</div><div></div><div></div></div>
6	H	125	<div><div></div><div>66%</div><div>26%</div><div>5%</div><div></div><div></div></div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 16755 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called DNA (5'(ATCAATATCCACCTGCAGATACTACCAA AAGTGTATTTGGAACTGCTCCATCAAAAGGCATGTTTCAGCTGGAATCCAGCT GAACATGCCTTTTGGATGGAGCAGTTTCCAAATACACTTTTGGTAGTATCTGCA GGTGGATATTGAT)3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	147	Total	C	N	O	P	0	0	0
			3011	1440	546	879	146			

- Molecule 2 is a DNA chain called DNA (5'(ATCAATATCCACCTGCAGATACTACCAA AAGTGTATTTGGAACTGCTCCATCAAAAGGCATGTTTCAGCTGGATTCCAGCT GAACATGCCTTTTGGATGGAGCAGTTTCCAAATACACTTTTGGTAGTATCTGCA GGTGGATATTGAT)3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	147	Total	C	N	O	P	0	0	0
			3010	1440	543	881	146			

- Molecule 3 is a protein called histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	135	Total	C	N	O	S	134	0	0
			1074	670	215	186	3			
3	E	135	Total	C	N	O	S	94	0	0
			1074	670	215	186	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	CONFLICT	UNP P16105
E	102	ALA	GLY	CONFLICT	UNP P16105

- Molecule 4 is a protein called histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	102	Total	C	N	O	S	74	0	0
			792	494	163	134	1			
4	F	102	Total	C	N	O	S	42	0	0
			792	494	163	134	1			

- Molecule 5 is a protein called histone H2A.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	128	Total	C	N	O	S	98	0	0
			978	608	195	175				
5	G	128	Total	C	N	O	S	105	0	0
			978	608	195	175				

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	VARIANT	UNP P06897
C	123	SER	ALA	CONFLICT	UNP P06897
C	?	-	ALA	DELETION	UNP P06897
G	99	ARG	GLY	VARIANT	UNP P06897
G	123	SER	ALA	CONFLICT	UNP P06897
G	?	-	ALA	DELETION	UNP P06897

- Molecule 6 is a protein called histone H2B.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	122	Total	C	N	O	S	106	0	0
			949	595	178	174	2			
6	H	122	Total	C	N	O	S	139	0	0
			949	595	178	174	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	VARIANT	UNP P02281
H	29	THR	SER	VARIANT	UNP P02281

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	6	Total	Mn	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	7	Total 7	Mn 7	0	0
7	E	1	Total 1	Mn 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total 1	Cl 1	0	0
8	A	1	Total 1	Cl 1	0	0
8	D	1	Total 1	Cl 1	0	0
8	E	1	Total 1	Cl 1	0	0

- Molecule 9 is water.

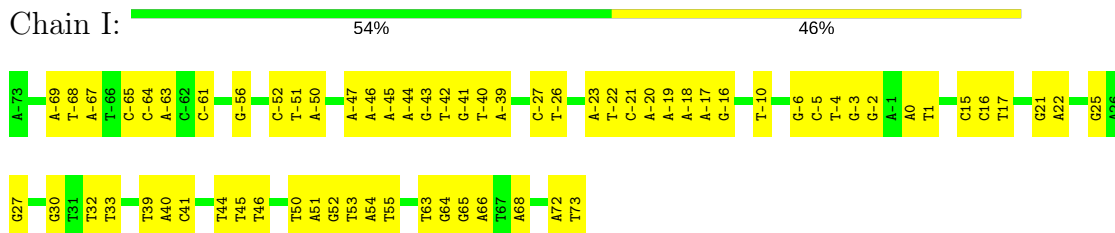
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	219	Total 219	O 219	0	0
9	B	129	Total 129	O 129	0	0
9	C	214	Total 214	O 214	0	0
9	D	196	Total 196	O 196	0	0
9	E	221	Total 221	O 221	0	0
9	F	202	Total 202	O 202	0	0
9	G	188	Total 188	O 188	0	0
9	H	179	Total 179	O 179	0	0
9	I	780	Total 780	O 780	0	0
9	J	802	Total 802	O 802	0	0

### 3 Residue-property plots

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.

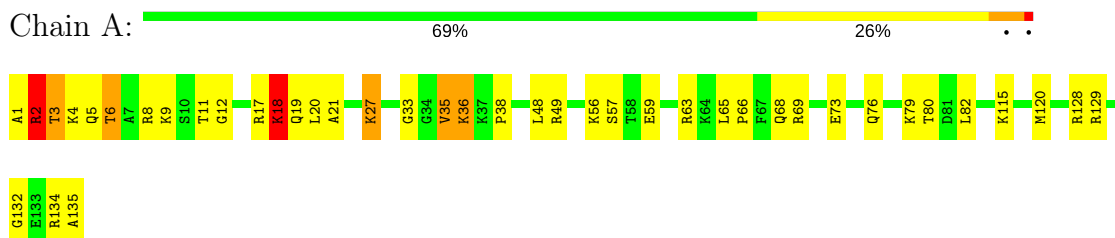
- Molecule 1: DNA (5'(ATCAATATCCACCTGCAGATACTACCAAAAGTGTATTTGGAAA CTGCTCCATCAAAAGGCATGTTTCAGCTGGAATCCAGCTGAACATGCCTTTTGGATGGA GCAGTTTCCAAATACACTTTTGGTAGTATCTGCAGGTGGATATTGAT)3')



- Molecule 2: DNA (5'(ATCAATATCCACCTGCAGATACTACCAAAAGTGTATTTGGAAA CTGCTCCATCAAAAGGCATGTTTCAGCTGGATTCCAGCTGAACATGCCTTTTGGATGGA GCAGTTTCCAAATACACTTTTGGTAGTATCTGCAGGTGGATATTGAT)3')



- Molecule 3: histone H3

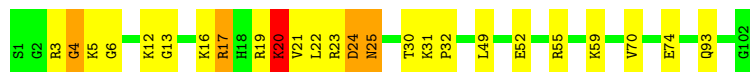


- Molecule 3: histone H3

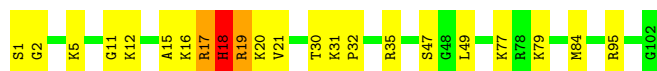
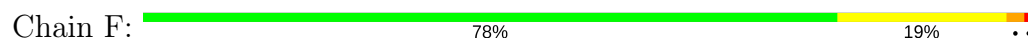




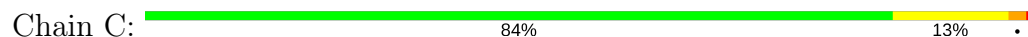
- Molecule 4: histone H4



- Molecule 4: histone H4



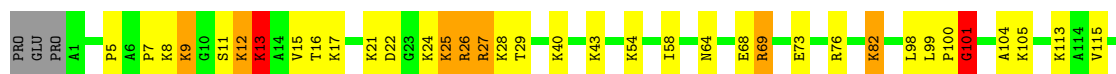
- Molecule 5: histone H2A.1



- Molecule 5: histone H2A.1



- Molecule 6: histone H2B.2



- Molecule 6: histone H2B.2





## 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, $\alpha$ , $\beta$ , $\gamma$	105.95Å 181.17Å 109.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.94	Depositor
% Data completeness (in resolution range)	95.6 (6.00-1.94)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.208 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	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, 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	I	0.41	0/3378	0.76	0/5212
2	J	0.42	0/3376	0.76	1/5209 (0.0%)
3	A	0.52	0/1088	0.68	0/1455
3	E	0.59	0/1088	0.79	2/1455 (0.1%)
4	B	0.53	0/800	0.75	0/1061
4	F	0.63	0/800	0.78	0/1061
5	C	0.57	0/988	0.68	0/1322
5	G	0.44	0/988	0.63	0/1322
6	D	0.56	0/962	0.71	3/1284 (0.2%)
6	H	0.44	0/962	0.62	0/1284
All	All	0.48	0/14430	0.73	6/20665 (0.0%)

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	1
2	J	0	7
All	All	0	8

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	37	LYS	N-CA-C	5.62	126.16	111.00
3	E	20	LEU	N-CA-C	5.39	125.55	111.00
6	D	69	ARG	NE-CZ-NH2	-5.36	117.62	120.30
6	D	101	GLY	N-CA-C	5.13	125.94	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	76	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	-6	DG	Sidechain
2	J	-12	DT	Sidechain
2	J	-3	DG	Sidechain
2	J	-6	DG	Sidechain
2	J	-73	DA	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	3011	0	1662	84	0
2	J	3010	0	1663	81	0
3	A	1074	0	1151	55	0
3	E	1074	0	1151	34	0
4	B	792	0	855	38	0
4	F	792	0	855	30	0
5	C	978	0	1054	33	0
5	G	978	0	1054	28	0
6	D	949	0	1017	49	0
6	H	949	0	1017	52	0
7	E	1	0	0	0	0
7	I	7	0	0	0	0
7	J	6	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	H	1	0	0	0	0
9	A	219	0	0	8	0
9	B	129	0	0	6	0
9	C	214	0	0	4	0
9	D	196	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	221	0	0	11	0
9	F	202	0	0	8	0
9	G	188	0	0	7	0
9	H	179	0	0	8	0
9	I	780	0	0	15	0
9	J	802	0	0	23	0
All	All	16755	0	11479	431	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 18.

The worst 5 of 431 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)
1:I:72:DA:H2''	1:I:73:DT:H5''	1.25	1.14
6:D:13:LYS:HG3	6:D:25:LYS:HA	1.25	1.12
5:C:12:ALA:HB1	5:C:15:LYS:HB3	1.29	1.07
1:I:42:DT:OP1	5:C:12:ALA:HB3	1.60	1.00
5:C:12:ALA:CB	5:C:15:LYS:HB3	1.92	0.99

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	
3	A	133/135 (98%)	106 (80%)	14 (10%)	13 (10%)	1	0
3	E	133/135 (98%)	105 (79%)	12 (9%)	16 (12%)	0	0
4	B	100/102 (98%)	83 (83%)	8 (8%)	9 (9%)	1	0
4	F	100/102 (98%)	88 (88%)	8 (8%)	4 (4%)	3	0
5	C	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	5	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	G	126/128 (98%)	106 (84%)	15 (12%)	5 (4%)	3	0
6	D	120/125 (96%)	101 (84%)	7 (6%)	12 (10%)	1	0
6	H	120/125 (96%)	104 (87%)	6 (5%)	10 (8%)	1	0
All	All	958/980 (98%)	806 (84%)	79 (8%)	73 (8%)	1	0

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	2	ARG
3	A	3	THR
3	A	4	LYS
4	B	24	ASP
6	D	5	PRO

### 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	
3	A	110/110 (100%)	105 (96%)	5 (4%)	32	16
3	E	110/110 (100%)	106 (96%)	4 (4%)	40	25
4	B	78/78 (100%)	76 (97%)	2 (3%)	51	39
4	F	78/78 (100%)	75 (96%)	3 (4%)	38	23
5	C	101/101 (100%)	96 (95%)	5 (5%)	28	13
5	G	101/101 (100%)	96 (95%)	5 (5%)	28	13
6	D	102/105 (97%)	99 (97%)	3 (3%)	48	34
6	H	102/105 (97%)	100 (98%)	2 (2%)	60	51
All	All	782/788 (99%)	753 (96%)	29 (4%)	39	24

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	25	LYS

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Mol	Chain	Res	Type
3	E	36	LYS
5	G	121	GLU
6	D	82	LYS
3	E	60	LEU

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

Mol	Chain	Res	Type
3	E	125	GLN
6	H	92	GLN
5	G	31	HIS
5	C	31	HIS
5	G	6	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.