



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:35 PM GMT

PDB ID : 1KX4  
Title : X-Ray Structure of the Nucleosome Core Particle, NCP146b, at 2.6 Å Resolution  
Authors : Davey, C.A.; Sargent, D.F.; Luger, K.; Maeder, A.W.; Richmond, T.J.  
Deposited on : 2002-01-31  
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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

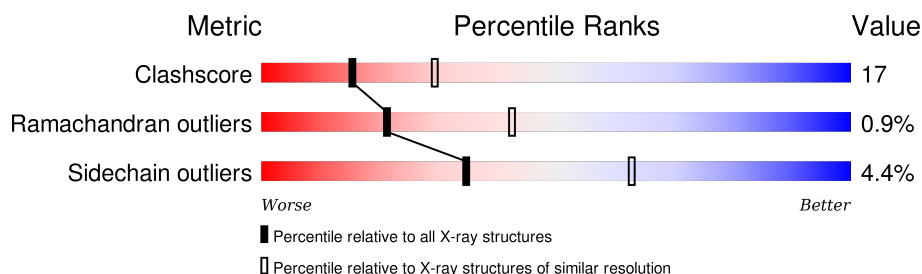
# 1 Overall quality at a glance

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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)


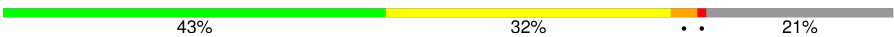

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	135	
2	E	135	
3	B	102	
3	F	102	
4	C	128	

*Continued on next page...*

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Mol	Chain	Length	Quality of chain
4	G	128	 53% 25% • 18%
5	D	125	 43% 32% • • 21%
5	H	125	 51% 22% • 25%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12438 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'(ATCTCCAAATATCCCTTGCGGATCGTAG AAAAAGTGTGTCAAACCTGCGCTATCAAAGGGAACTTCAACTGAATTCAGTTG AAGTTTCCCTTTGATAGCGCAGTTTGACACACTTTTTCTACGATCCGCAAGGGA TATTTGGAGAT)3').

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	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			
2	E	97	Total	C	N	O	S	0	0	0
			801	504	155	139	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 3 is a protein called histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

- Molecule 4 is a protein called histone H2A.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			

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 5 is a protein called histone H2B.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	99	Total	C	N	O	S	0	0	0
			785	493	146	144	2			
5	H	94	Total	C	N	O	S	0	0	0
			736	463	132	139	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 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mn	0	0
			1	1		
6	A	1	Total	Mn	0	0
			1	1		
6	I	4	Total	Mn	0	0
			4	4		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total Cl 1 1	0	0
7	A	1	Total Cl 1 1	0	0
7	C	1	Total Cl 1 1	0	0
7	E	1	Total Cl 1 1	0	0

- Molecule 8 is water.

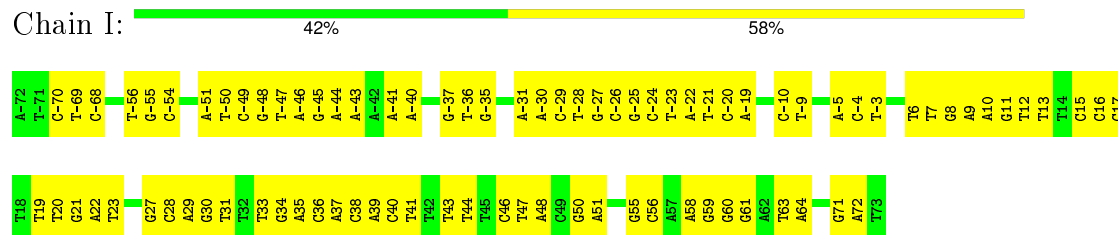
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	56	Total O 56 56	0	0
8	B	40	Total O 40 40	0	0
8	C	37	Total O 37 37	0	0
8	D	20	Total O 20 20	0	0
8	E	31	Total O 31 31	0	0
8	F	27	Total O 27 27	0	0
8	G	44	Total O 44 44	0	0
8	H	31	Total O 31 31	0	0
8	I	73	Total O 73 73	0	0
8	J	74	Total O 74 74	0	0

### 3 Residue-property plots

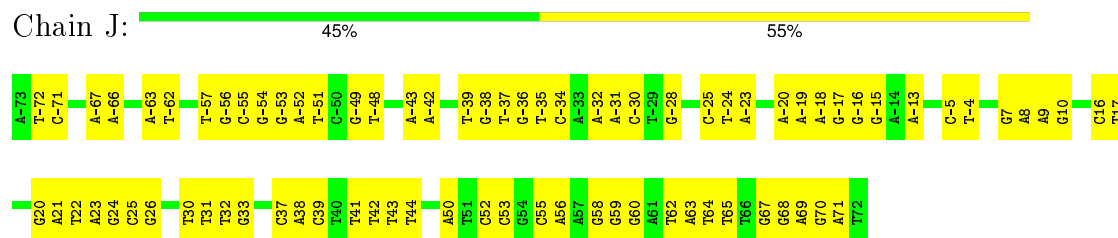
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

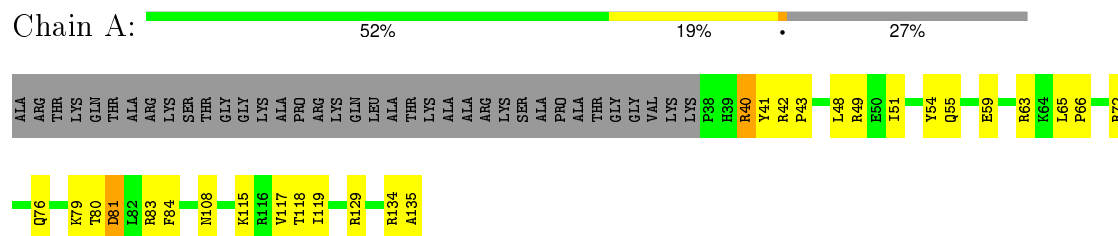
- Molecule 1: DNA (5'(ATCTCCAAATATCCCTTGCGGATCGTAGAAAAAGTGTGTCAAACTGCGCTATCAAAGGGAACTTCAACTGAATTCAGTTGAAAGTTTCCCTTTGATAGCGCAGTTTGACACACTTTTTCTACGATCCGCAAGGGATATTTGGAGAT)3')



- Molecule 1: DNA (5'(ATCTCCAAATATCCCTTGCGGATCGTAGAAAAAGTGTGTCAAACTGCGCTATCAAAGGGAACTTCAACTGAATTCAGTTGAAAGTTTCCCTTTGATAGCGCAGTTTGACACACTTTTTCTACGATCCGCAAGGGATATTTGGAGAT)3')



- Molecule 2: histone H3



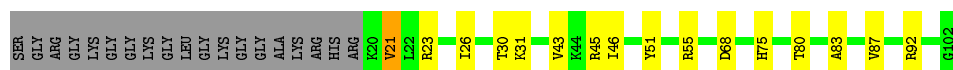
- Molecule 2: histone H3





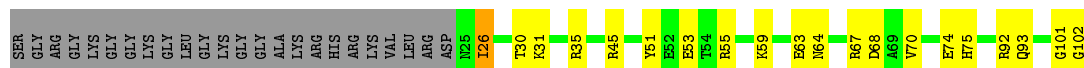
- Molecule 3: histone H4

Chain B: 66% 15% 19%



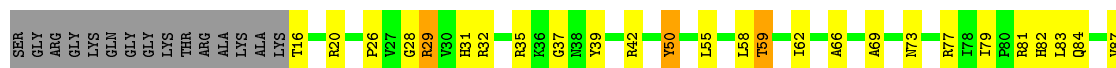
- Molecule 3: histone H4

Chain F: 57% 19% 24%



- Molecule 4: histone H2A.1

Chain C: 55% 22% 20%



- Molecule 4: histone H2A.1

Chain G: 53% 25% 18%



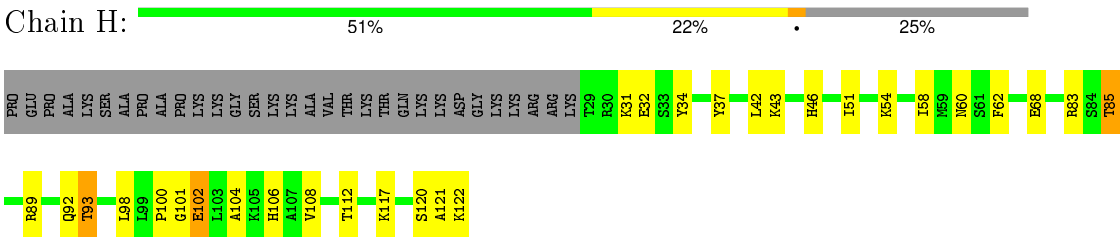
- Molecule 5: histone H2B.2

Chain D: 43% 32% 21%



- Molecule 5: histone H2B.2





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.30Å 175.69Å 109.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60	Depositor
% Data completeness (in resolution range)	91.6 (6.00-2.60)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.246 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	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	0.27	0/3354	0.66	0/5175
1	J	0.27	0/3354	0.66	0/5175
2	A	0.43	0/820	0.63	0/1099
2	E	0.37	0/812	0.55	0/1088
3	B	0.43	0/669	0.64	0/894
3	F	0.36	0/626	0.61	0/837
4	C	0.35	0/805	0.60	0/1088
4	G	0.40	0/819	0.62	0/1106
5	D	0.36	0/796	0.58	0/1065
5	H	0.38	0/747	0.60	0/1004
All	All	0.33	0/12802	0.64	0/18531

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
2	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	54	TYR	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	93	0
1	J	2990	0	1651	79	0
2	A	808	0	846	36	0
2	E	801	0	838	43	0
3	B	662	0	709	20	0
3	F	619	0	659	22	0
4	C	795	0	846	40	0
4	G	809	0	864	48	0
5	D	785	0	825	58	0
5	H	736	0	760	35	0
6	A	1	0	0	0	0
6	I	4	0	0	0	0
6	J	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
8	A	56	0	0	2	0
8	B	40	0	0	2	0
8	C	37	0	0	3	0
8	D	20	0	0	2	0
8	E	31	0	0	4	0
8	F	27	0	0	1	0
8	G	44	0	0	3	0
8	H	31	0	0	2	0
8	I	73	0	0	1	0
8	J	74	0	0	0	0
All	All	12438	0	9649	371	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 17.

The worst 5 of 371 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)
4:C:118:LYS:HE3	4:C:118:LYS:HA	1.34	1.06
4:C:42:ARG:HB2	5:D:85:THR:HG22	1.44	0.99
3:F:75:HIS:HD2	5:H:93:THR:HG21	1.25	0.97
1:I:-54:DC:H4'	4:C:77:ARG:HD2	1.47	0.96
2:A:129:ARG:HB2	2:A:129:ARG:HH11	1.33	0.92

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	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
2	E	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
3	B	81/102 (79%)	79 (98%)	2 (2%)	0	100	100
3	F	76/102 (74%)	75 (99%)	1 (1%)	0	100	100
4	C	101/128 (79%)	96 (95%)	5 (5%)	0	100	100
4	G	103/128 (80%)	100 (97%)	3 (3%)	0	100	100
5	D	97/125 (78%)	88 (91%)	3 (3%)	6 (6%)	2	2
5	H	92/125 (74%)	87 (95%)	4 (4%)	1 (1%)	17	36
All	All	741/980 (76%)	714 (96%)	20 (3%)	7 (1%)	21	42

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	102	GLU
5	D	29	THR
5	D	30	ARG
5	D	101	GLY
5	D	28	LYS

### 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	85/110 (77%)	80 (94%)	5 (6%)	24	47
2	E	84/110 (76%)	80 (95%)	4 (5%)	31	58
3	B	68/78 (87%)	67 (98%)	1 (2%)	72	90
3	F	63/78 (81%)	62 (98%)	1 (2%)	70	89
4	C	82/101 (81%)	77 (94%)	5 (6%)	23	46
4	G	83/101 (82%)	78 (94%)	5 (6%)	24	47
5	D	85/105 (81%)	82 (96%)	3 (4%)	43	71
5	H	80/105 (76%)	76 (95%)	4 (5%)	30	56
All	All	630/788 (80%)	602 (96%)	28 (4%)	35	63

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	93	THR
2	E	42	ARG
5	H	83	ARG
5	D	103	LEU
2	E	40	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	92	GLN
2	E	76	GLN
4	G	84	GLN
5	D	79	HIS
4	G	31	HIS

### 5.3.3 RNA ⓘ

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 10 ligands modelled in this entry, 10 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.