



Full wwPDB EM Validation Report ⓘ

May 17, 2026 – 12:14 AM JST

PDB ID : 9UZ7 / pdb_00009uz7
EMDB ID : EMD-64640
Title : Cryo-EM structure of the nucleosome core particle with site-specific DNA-histone crosslinking
Authors : Zhou, C.Z.; Li, H.T.; Shan, X.J.; Ji, G.Y.
Deposited on : 2025-05-16
Resolution : 3.24 Å(reported)
Based on initial model : 8JBX

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

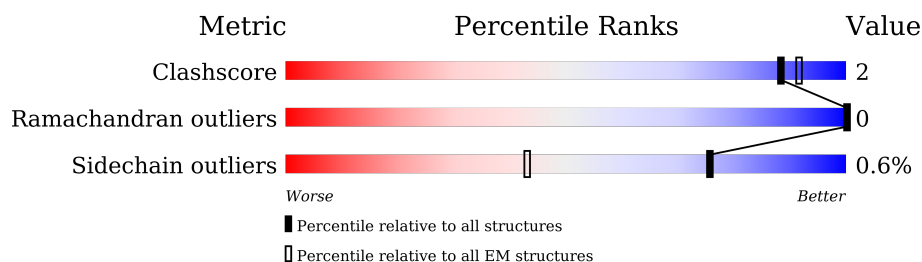
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.24 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.



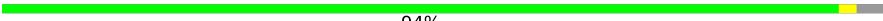
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	135	66% 31%
2	B	135	64% 7% 28%
3	C	102	77% 20%
3	D	102	77% 19%
4	E	129	78% 6% 16%
4	F	129	74% 8% 18%
5	G	125	73% 6% 22%
5	H	125	68% 11% 21%
6	I	145	91% 6%

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Mol	Chain	Length	Quality of chain
7	J	145	 94% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11818 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	93	Total	C	N	O	S	0	0
			753	473	142	135	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	SER	CYS	engineered mutation	UNP P68431
A	110	SER	CYS	engineered mutation	UNP P68431
A	115	CYS	LYS	engineered mutation	UNP P68431

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	97	Total	C	N	O	S	0	0
			801	502	155	141	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	96	SER	CYS	engineered mutation	UNP P68431
B	110	SER	CYS	engineered mutation	UNP P68431
B	115	YCM	LYS	engineered mutation	UNP P68431

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
3	D	83	Total	C	N	O	S	0	0
			662	418	129	114	1		

- Molecule 4 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	108	Total	C	N	O	0	0
			831	523	164	144		
4	F	106	Total	C	N	O	0	0
			819	515	162	142		

- Molecule 5 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	98	Total	C	N	O	S	0	0
			775	486	144	143	2		
5	H	99	Total	C	N	O	S	0	0
			784	492	146	144	2		

- Molecule 6 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	140	Total	C	N	O	P	0	0
			2889	1367	541	841	140		

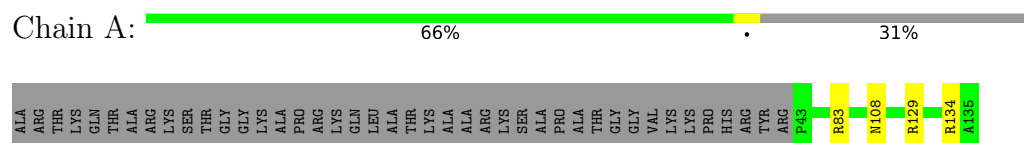
- Molecule 7 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	140	Total	C	N	O	P	0	0
			2851	1354	518	839	140		

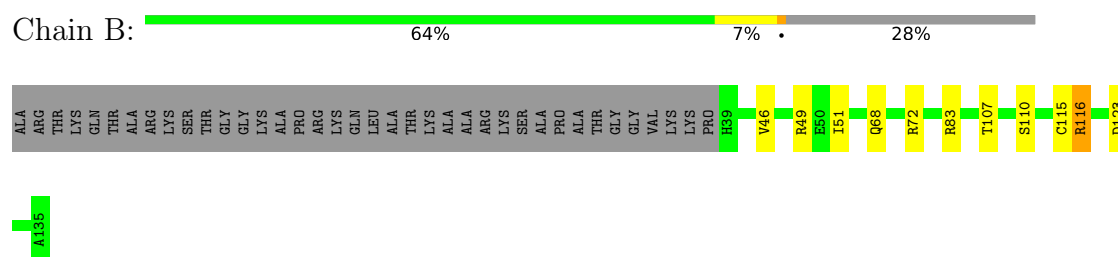
3 Residue-property plots [i](#)

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.

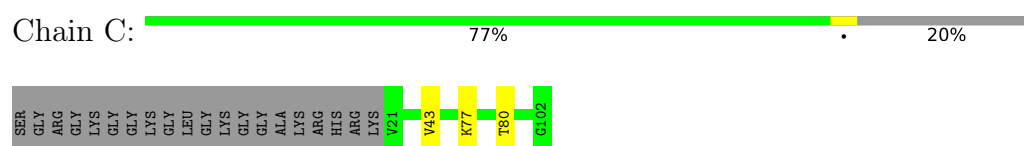
- Molecule 1: Histone H3.1



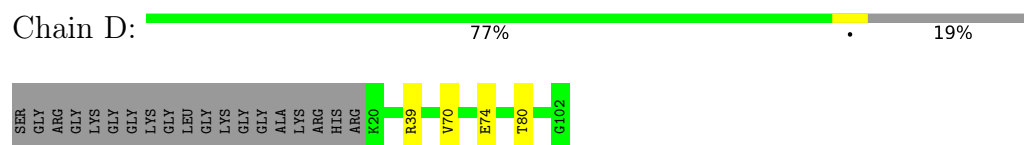
- Molecule 2: Histone H3.1



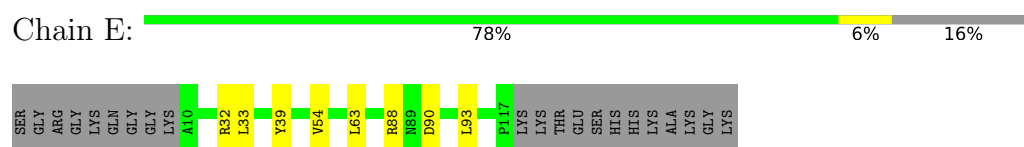
- Molecule 3: Histone H4



- Molecule 3: Histone H4

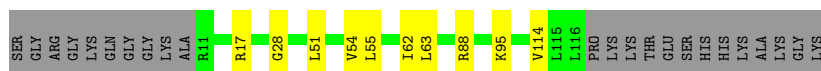


- Molecule 4: Histone H2A type 1-B/E



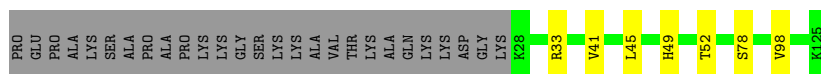
- Molecule 4: Histone H2A type 1-B/E

Chain F:  74% 8% 18%



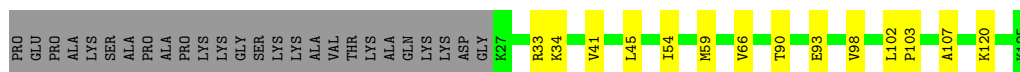
- Molecule 5: Histone H2B type 1-J

Chain G:  73% 6% 22%



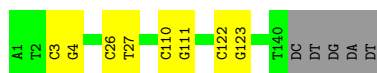
- Molecule 5: Histone H2B type 1-J

Chain H:  68% 11% 21%



- Molecule 6: DNA (145-MER)

Chain I:  91% 6% •



- Molecule 7: DNA (145-MER)

Chain J:  94% • •



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT	Depositor
Number of particles used	199160, 199160, 199160, 199160, 199160, 199160, 199160, 199160, 199160, 199160, 199160, 199160, 199160	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE, NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50, 50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor

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: YCM

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	A	0.19	0/762	0.38	0/1021
2	B	0.32	0/801	0.52	0/1072
3	C	0.23	0/660	0.49	0/883
3	D	0.26	0/669	0.52	0/894
4	E	0.17	0/841	0.39	0/1135
4	F	0.21	0/828	0.43	0/1116
5	G	0.17	0/786	0.44	0/1051
5	H	0.19	0/795	0.42	0/1062
6	I	0.27	0/3244	0.48	0/5010
7	J	0.22	0/3194	0.45	0/4922
All	All	0.23	0/12580	0.46	0/18166

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	A	753	0	787	3	0
2	B	801	0	830	7	0
3	C	653	0	696	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	662	0	709	3	0
4	E	831	0	889	7	0
4	F	819	0	877	8	0
5	G	775	0	810	6	0
5	H	784	0	823	12	0
6	I	2889	0	1572	5	0
7	J	2851	0	1571	2	0
All	All	11818	0	9564	40	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 2.

All (40) 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)
6:I:3:DC:H2''	6:I:4:DG:C8	2.34	0.63
2:B:68:GLN:HG2	2:B:72:ARG:HE	1.63	0.62
5:G:33:ARG:HG3	6:I:122:DC:H4'	1.85	0.58
4:F:54:VAL:HG21	5:H:98:VAL:HG21	1.88	0.55
5:H:33:ARG:HG3	7:J:122:DC:H4'	1.89	0.54
4:E:54:VAL:HG21	5:G:98:VAL:HG21	1.90	0.52
2:B:107:THR:HG23	2:B:123:ASP:HB2	1.91	0.52
4:E:63:LEU:HD13	5:G:45:LEU:HB2	1.92	0.52
4:F:63:LEU:HD13	5:H:45:LEU:HB2	1.91	0.52
2:B:46:VAL:HG22	2:B:49:ARG:HH21	1.75	0.52
5:H:102:LEU:HB2	5:H:107:ALA:HB2	1.92	0.50
4:F:63:LEU:HD11	5:H:41:VAL:HG13	1.94	0.49
4:E:63:LEU:HD11	5:G:41:VAL:HG13	1.95	0.48
2:B:51:ILE:HG13	3:D:39:ARG:HD2	1.96	0.47
4:F:55:LEU:HD22	5:H:66:VAL:HG13	1.96	0.47
7:J:57:DC:H2''	7:J:58:DA:C8	2.49	0.47
4:F:95:LYS:HE3	5:H:103:PRO:HB3	1.97	0.46
1:A:83:ARG:HB2	3:C:80:THR:HG22	1.98	0.46
1:A:108:ASN:HB2	3:C:43:VAL:HG22	1.97	0.45
2:B:116:ARG:HH12	2:B:123:ASP:CG	2.24	0.45
5:H:90:THR:H	5:H:93:GLU:HG3	1.81	0.45
5:H:34:LYS:HE3	5:H:34:LYS:HB2	1.82	0.44
5:G:49:HIS:HB3	5:G:52:THR:HB	1.99	0.44
4:E:39:TYR:HB3	5:G:78:SER:HB2	1.99	0.43
2:B:110:SER:HB2	2:B:123:ASP:HB3	2.00	0.43
4:F:63:LEU:HD22	5:H:45:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:HH21	1:A:134:ARG:HE	1.67	0.42
5:H:54:ILE:HG21	5:H:59:MET:HE2	2.00	0.42
5:H:120:LYS:HE3	5:H:120:LYS:HB3	1.91	0.42
6:I:122:DC:H2"	6:I:123:DG:C8	2.55	0.42
2:B:83:ARG:HB2	3:D:80:THR:HG22	2.01	0.41
4:E:88:ARG:HA	4:E:88:ARG:HD3	1.87	0.41
3:C:77:LYS:HZ2	3:C:77:LYS:HG3	1.53	0.41
6:I:26:DC:H2"	6:I:27:DT:C5	2.56	0.41
6:I:110:DC:H2"	6:I:111:DG:C8	2.56	0.40
3:D:70:VAL:O	3:D:74:GLU:HG3	2.22	0.40
4:F:17:ARG:HH21	4:F:28:GLY:HA2	1.86	0.40
4:F:88:ARG:HA	4:F:88:ARG:HD3	1.88	0.40
4:E:32:ARG:HH21	4:E:33:LEU:HD21	1.85	0.40
4:E:90:ASP:HB3	4:E:93:LEU:HB2	2.04	0.40

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 PDB entries followed by that with respect to all EM entries.

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	A	91/135 (67%)	91 (100%)	0	0	100	100
2	B	94/135 (70%)	93 (99%)	1 (1%)	0	100	100
3	C	80/102 (78%)	78 (98%)	2 (2%)	0	100	100
3	D	81/102 (79%)	77 (95%)	4 (5%)	0	100	100
4	E	106/129 (82%)	102 (96%)	4 (4%)	0	100	100
4	F	104/129 (81%)	101 (97%)	3 (3%)	0	100	100
5	G	96/125 (77%)	94 (98%)	2 (2%)	0	100	100
5	H	97/125 (78%)	94 (97%)	3 (3%)	0	100	100
All	All	749/982 (76%)	730 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	A	80/110 (73%)	80 (100%)	0	100	100
2	B	83/109 (76%)	82 (99%)	1 (1%)	63	76
3	C	67/78 (86%)	67 (100%)	0	100	100
3	D	68/78 (87%)	68 (100%)	0	100	100
4	E	84/99 (85%)	84 (100%)	0	100	100
4	F	83/99 (84%)	80 (96%)	3 (4%)	31	60
5	G	84/104 (81%)	84 (100%)	0	100	100
5	H	85/104 (82%)	85 (100%)	0	100	100
All	All	634/781 (81%)	630 (99%)	4 (1%)	76	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	116	ARG
4	F	51	LEU
4	F	62	ILE
4	F	114	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
2	B	55	GLN
2	B	108	ASN
5	H	82	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	YCM	B	115	2	7,9,10	1.86	2 (28%)	4,10,12	1.84	2 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YCM	B	115	2	-	2/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	115	YCM	CE-NZ2	3.83	1.45	1.32
2	B	115	YCM	CB-CA	-2.13	1.48	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	115	YCM	CE-CD-SG	-2.64	105.81	113.59
2	B	115	YCM	CA-CB-SG	-2.37	105.05	113.74

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	115	YCM	CA-CB-SG-CD
2	B	115	YCM	SG-CD-CE-NZ2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.