



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:01 AM UTC

PDB ID : 3AV1 / pdb_00003av1
Title : The human nucleosome structure containing the histone variant H3.2
Authors : Tachiwana, H.; Osakabe, A.; Shiga, T.; Miya, Y.; Kimura, H.; Kagawa, W.; Kurumizaka, H.
Deposited on : 2011-02-18
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

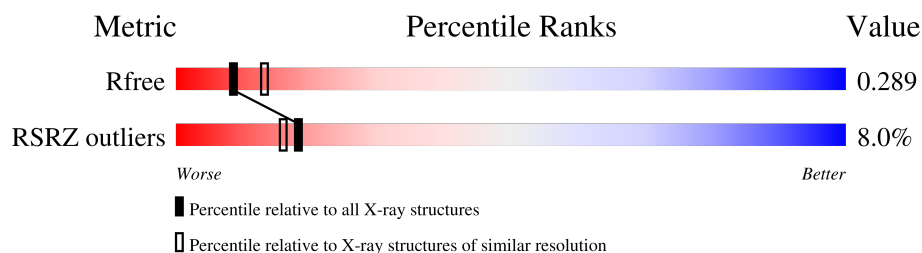
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

GLOBAL-STATISTICS INFOmissingINFO

2 Model quality [i](#)

2.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

2.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

2.3 Torsion angles [i](#)

2.3.1 Protein backbone [i](#)

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2.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

2.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

There are no non-standard protein/DNA/RNA residues in this entry.

2.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

2.6 Ligand geometry [i](#)

There are no ligands in this entry.

2.7 Other polymers [i](#)

There are no such residues in this entry.

2.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

3 Fit of model and data ⓘ

3.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	1-A	96/139 (69%)	0.07	4 (4%)	40	36	31, 42, 58, 79	0
1	1-E	99/139 (71%)	-0.04	4 (4%)	42	38	24, 34, 56, 84	0
2	1-B	78/106 (73%)	-0.04	1 (1%)	75	71	31, 40, 56, 64	0
2	1-F	84/106 (79%)	-0.20	2 (2%)	59	55	24, 34, 51, 79	0
3	1-C	105/133 (78%)	-0.03	2 (1%)	66	62	25, 39, 62, 76	0
3	1-G	104/133 (78%)	0.08	1 (0%)	79	76	32, 45, 68, 81	0
4	1-D	93/129 (72%)	0.27	5 (5%)	31	27	29, 42, 64, 84	0
4	1-H	92/129 (71%)	0.24	3 (3%)	49	45	32, 45, 71, 91	0
5	1-I	146/146 (100%)	1.43	33 (22%)	2	2	46, 99, 137, 155	0
5	1-J	49/146 (33%)	1.86	21 (42%)	0	0	67, 115, 146, 166	0
All	All	946/1306 (72%)	0.35	76 (8%)	18	16	24, 44, 123, 166	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	1-F	102	GLY	5.9
2	1-B	102	GLY	5.5
4	1-D	124	ALA	5.0
1	1-E	135	ALA	4.5
1	1-E	78	PHE	4.4
1	1-E	77	ASP	4.2
5	1-J	147	DA	4.1
2	1-F	101	GLY	3.9
5	1-I	146	DT	3.9
3	1-C	14	ALA	3.4
5	1-I	55	DA	3.4
5	1-J	148	DT	3.3
5	1-J	275	DC	3.2

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Mol	Chain	Res	Type	RSRZ
5	1-I	56	DA	3.1
5	1-I	39	DG	3.1
5	1-I	96	DT	3.0
1	1-A	39	HIS	3.0
1	1-E	37	LYS	3.0
5	1-I	136	DT	3.0
5	1-J	274	DT	3.0
5	1-I	58	DG	2.9
5	1-I	57	DA	2.9
5	1-I	127	DA	2.9
4	1-D	32	SER	2.9
4	1-H	124	ALA	2.9
5	1-J	284	DG	2.9
3	1-G	15	LYS	2.8
5	1-I	122	DG	2.8
5	1-J	241	DA	2.7
5	1-I	2	DT	2.7
5	1-I	128	DT	2.7
5	1-I	1	DA	2.7
5	1-J	244	DG	2.6
5	1-J	273	DA	2.6
5	1-I	53	DC	2.6
5	1-I	34	DT	2.6
5	1-I	31	DG	2.6
5	1-J	280	DG	2.6
4	1-D	123	SER	2.5
5	1-I	3	DC	2.5
5	1-J	283	DG	2.5
5	1-J	243	DG	2.4
4	1-H	121	TYR	2.4
1	1-A	134	ARG	2.4
5	1-I	145	DA	2.4
5	1-I	30	DA	2.4
5	1-I	40	DG	2.4
5	1-J	249	DG	2.4
5	1-J	272	DA	2.4
5	1-I	16	DC	2.4
5	1-I	8	DT	2.3
5	1-I	95	DA	2.3
5	1-I	114	DC	2.3
5	1-I	135	DG	2.3
5	1-J	245	DA	2.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	42	ARG	2.2
5	1-J	242	DT	2.2
5	1-J	267	DG	2.2
4	1-D	51	ASP	2.2
4	1-D	33	ARG	2.2
5	1-I	139	DA	2.2
4	1-H	39	ILE	2.2
5	1-I	97	DG	2.2
5	1-I	9	DC	2.1
5	1-J	240	DG	2.1
5	1-I	125	DG	2.1
5	1-J	271	DG	2.1
5	1-I	38	DT	2.1
5	1-J	263	DT	2.1
5	1-I	48	DT	2.1
1	1-A	63	ARG	2.0
3	1-C	118	LYS	2.0
5	1-I	12	DC	2.0
5	1-I	129	DC	2.0
5	1-J	252	DT	2.0
5	1-J	266	DT	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

3.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.4 Ligands [i](#)

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3.5 Other polymers [i](#)

There are no such residues in this entry.