



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 01:29 PM UTC

PDB ID : 1J8F / pdb_00001j8f
Title : HUMAN SIRT2 HISTONE DEACETYLASE
Authors : Pavletich, N.P.; Finnin, M.S.; Donigian, J.R.
Deposited on : 2001-05-21
Resolution : 1.70 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

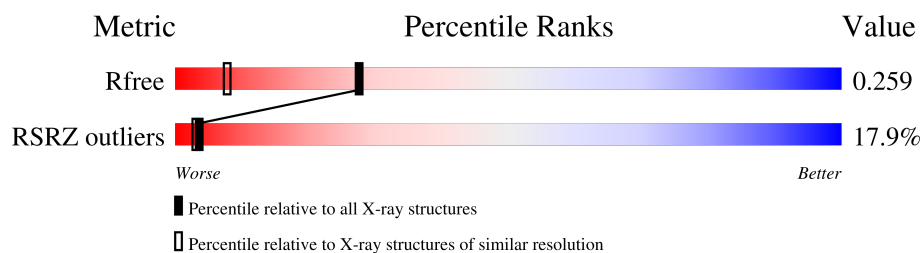
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11519 atoms, of which 3295 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 protein called SIRTUIN 2, ISOFORM 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	H	N	O	S	0	0	0
			3006	1590	527	411	458	20			
1	B	312	Total	C	H	N	O	S	0	0	0
			3007	1590	527	411	459	20			
1	C	303	Total	C	H	N	O	S	0	0	0
			2905	1536	509	398	443	19			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	275	Total	H	O	0	0
			825	550	275		
3	B	276	Total	H	O	0	0
			828	552	276		
3	C	315	Total	H	O	0	0
			945	630	315		

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3 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	78.94Å 119.07Å 218.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.70 15.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.70) 99.2 (15.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.63Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.260 0.227 , 0.259	Depositor DCC
R_{free} test set	2441 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11519	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	A	312/323 (96%)	1.04	57 (18%) 3 3	7, 18, 32, 44	0
1	B	312/323 (96%)	1.12	66 (21%) 2 2	6, 17, 33, 46	0
1	C	303/323 (93%)	0.79	43 (14%) 6 5	6, 13, 32, 43	0
All	All	927/969 (95%)	0.99	166 (17%) 3 3	6, 16, 33, 46	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	PHE	9.5
1	C	224	CYS	8.6
1	C	243	PHE	7.6
1	C	356	SER	7.1
1	B	99	PRO	7.1
1	C	266	VAL	6.7
1	C	310	ASP	6.6
1	B	100	SER	6.5
1	B	266	VAL	6.3
1	C	272	LEU	6.2
1	A	356	SER	6.0
1	C	273	ILE	5.9
1	A	101	THR	5.9
1	B	102	GLY	5.7
1	C	311	SER	5.6
1	B	311	SER	5.4
1	A	57	ARG	5.4
1	A	293	SER	5.3
1	A	266	VAL	5.3
1	A	102	GLY	5.3
1	B	58	LEU	5.2
1	B	101	THR	5.1
1	B	267	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	356	SER	5.1
1	A	268	PRO	5.1
1	A	100	SER	4.8
1	C	291	GLY	4.8
1	B	201	ARG	4.6
1	B	57	ARG	4.6
1	C	271	SER	4.6
1	B	214	PHE	4.6
1	A	58	LEU	4.6
1	C	99	PRO	4.5
1	C	241	ALA	4.5
1	B	217	VAL	4.5
1	A	60	ASP	4.4
1	C	100	SER	4.3
1	A	108	GLU	4.3
1	B	269	PHE	4.3
1	A	267	GLN	4.3
1	B	103	LEU	4.2
1	B	34	GLY	4.2
1	B	270	ALA	4.1
1	C	270	ALA	4.1
1	B	202	HIS	4.1
1	C	269	PHE	4.0
1	B	74	GLU	3.9
1	B	210	LYS	3.9
1	B	239	LEU	3.9
1	B	290	ALA	3.9
1	A	75	ARG	3.9
1	C	245	SER	3.8
1	C	240	PRO	3.8
1	B	215	SER	3.8
1	B	264	LEU	3.8
1	B	312	LYS	3.7
1	A	109	LYS	3.7
1	C	268	PRO	3.5
1	B	98	SER	3.5
1	C	313	LYS	3.5
1	A	105	ASP	3.5
1	C	265	GLN	3.5
1	A	223	ASP	3.5
1	C	312	LYS	3.5
1	B	265	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	248	GLN	3.4
1	B	108	GLU	3.4
1	B	111	HIS	3.4
1	B	243	PHE	3.4
1	B	291	GLY	3.3
1	C	239	LEU	3.2
1	B	206	LEU	3.1
1	A	310	ASP	3.1
1	C	355	GLN	3.1
1	B	204	TYR	3.1
1	B	278	LEU	3.1
1	C	292	GLN	3.1
1	A	106	ASN	3.1
1	A	269	PHE	3.1
1	A	103	LEU	3.0
1	A	224	CYS	3.0
1	B	292	GLN	3.0
1	B	213	ILE	3.0
1	B	106	ASN	3.0
1	B	240	PRO	3.0
1	A	355	GLN	2.9
1	A	265	GLN	2.9
1	A	312	LYS	2.9
1	B	207	SER	2.9
1	B	216	GLU	2.9
1	A	239	LEU	2.8
1	B	208	TRP	2.8
1	C	267	GLN	2.8
1	A	111	HIS	2.8
1	B	127	HIS	2.8
1	C	290	ALA	2.8
1	A	342	GLU	2.8
1	B	200	CYS	2.8
1	B	211	GLU	2.7
1	C	54	GLN	2.7
1	B	242	ARG	2.7
1	A	334	LEU	2.7
1	A	214	PHE	2.7
1	B	116	GLU	2.7
1	A	74	GLU	2.6
1	A	202	HIS	2.6
1	B	110	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	301	MET	2.6
1	A	221	CYS	2.6
1	A	39	ASP	2.6
1	A	297	LEU	2.6
1	C	211	GLU	2.6
1	C	288	GLU	2.6
1	B	114	TYR	2.6
1	B	198	ALA	2.6
1	B	212	LYS	2.6
1	A	201	ARG	2.6
1	B	220	LYS	2.5
1	C	223	ASP	2.5
1	C	98	SER	2.5
1	A	291	GLY	2.5
1	B	136	LYS	2.5
1	B	262	THR	2.5
1	B	313	LYS	2.4
1	C	242	ARG	2.4
1	B	268	PRO	2.4
1	A	180	GLN	2.4
1	C	247	MET	2.4
1	A	99	PRO	2.4
1	B	197	SER	2.4
1	B	225	GLN	2.4
1	B	226	SER	2.4
1	C	101	THR	2.4
1	C	252	LEU	2.3
1	C	274	SER	2.3
1	B	222	GLU	2.3
1	A	274	SER	2.3
1	A	288	GLU	2.3
1	A	311	SER	2.3
1	B	275	LYS	2.3
1	A	160	LEU	2.3
1	A	110	TYR	2.3
1	C	74	GLU	2.2
1	C	55	LYS	2.2
1	C	264	LEU	2.2
1	B	310	ASP	2.2
1	A	204	TYR	2.2
1	A	271	SER	2.2
1	C	307	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	217	VAL	2.1
1	B	221	CYS	2.1
1	A	112	LEU	2.1
1	A	98	SER	2.1
1	A	277	PRO	2.1
1	B	126	LYS	2.1
1	A	343	ASP	2.1
1	B	293	SER	2.1
1	A	77	ARG	2.1
1	A	295	PRO	2.1
1	B	115	PRO	2.1
1	A	142	GLN	2.0
1	A	294	ASP	2.0
1	B	73	SER	2.0
1	A	208	TRP	2.0
1	A	290	ALA	2.0
1	A	314	ALA	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	2001	1/1	0.94	0.07	33,33,33,33	0
2	ZN	C	3001	1/1	0.96	0.06	14,14,14,14	0
2	ZN	A	1001	1/1	0.98	0.07	27,27,27,27	0

5.5 Other polymers [i](#)

There are no such residues in this entry.