



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 12:23 PM JST

PDB ID : 8HXX
EMDB ID : EMD-35081
Title : Cryo-EM structure of the histone deacetylase complex Rpd3S
Authors : Cui, H.; Wang, H.
Deposited on : 2023-01-05
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary 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**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

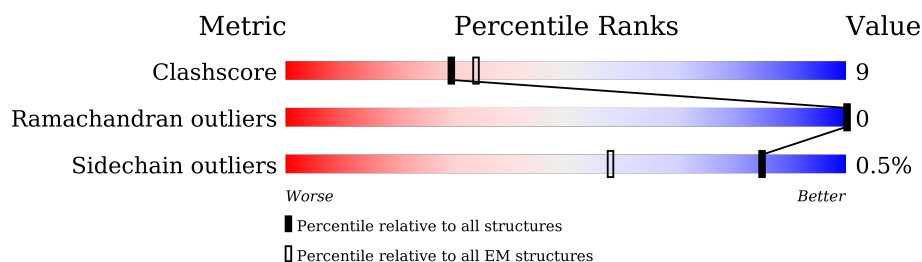
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	K	1536	
2	L	433	
3	M	401	
3	O	401	
4	N	684	
4	P	684	
5	E	135	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14873 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 Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	549	Total	C	N	O	S	0	0
			4597	2954	774	854	15		

- Molecule 2 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	384	Total	C	N	O	S	0	0
			3048	1941	512	569	26		

- Molecule 3 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	183	Total	C	N	O	S	0	0
			1483	950	239	285	9		
3	O	156	Total	C	N	O	S	0	0
			1275	823	204	240	8		

- Molecule 4 is a protein called RCO1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	375	Total	C	N	O	S	0	0
			3073	1953	529	573	18		
4	P	151	Total	C	N	O	S	0	0
			1249	802	206	231	10		

- Molecule 5 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	19	Total	C	N	O	0	0
			141	86	31	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	110	ALA	CYS	engineered mutation	UNP A0A310TTQ1

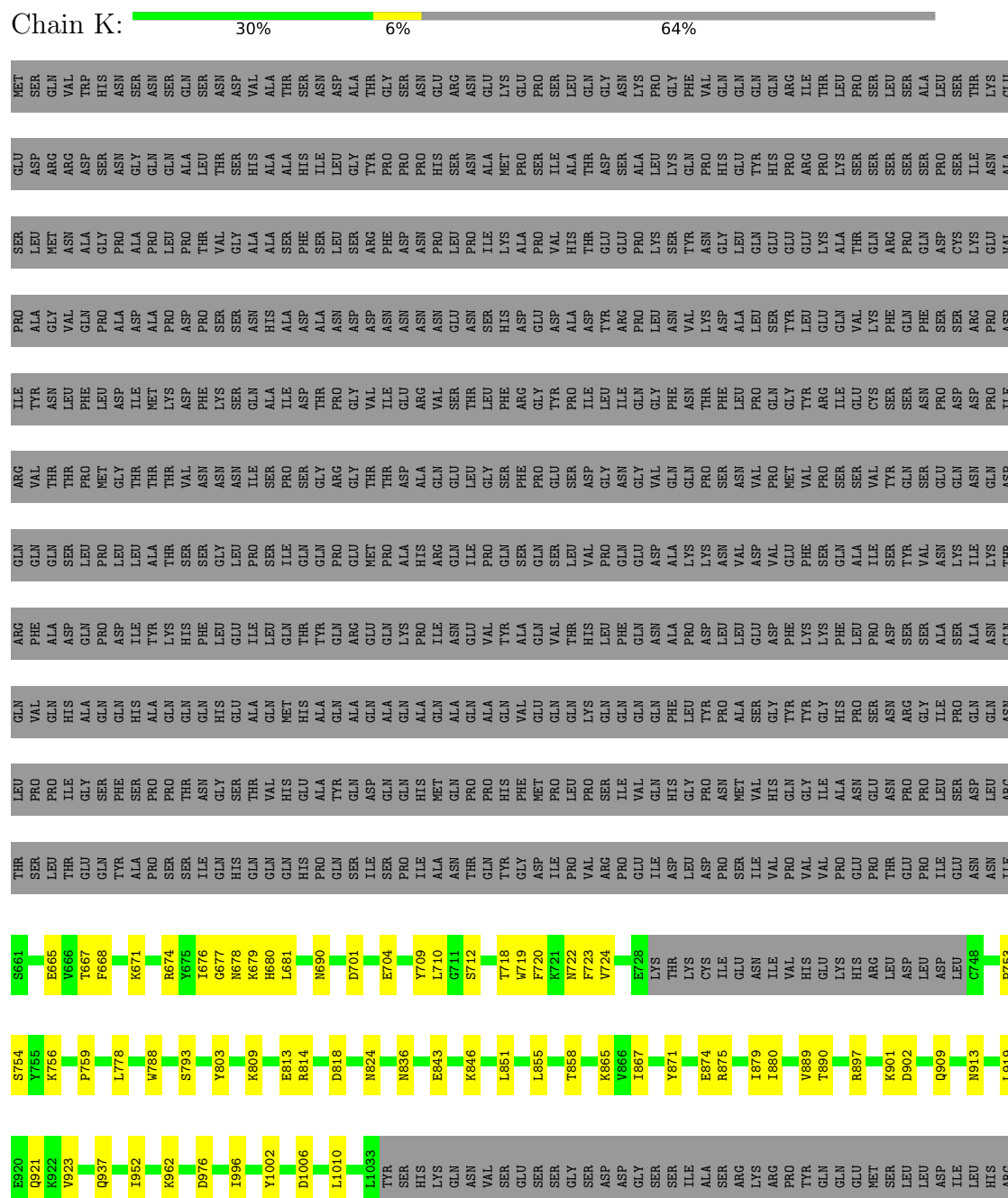
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	L	1	Total 1	Zn 1	0
6	N	4	Total 4	Zn 4	0
6	P	2	Total 2	Zn 2	0

3 Residue-property plots

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: Transcriptional regulatory protein SIN3



Chain O: 26% 12% 61%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39789	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	K	0.29	0/4699	0.52	2/6334 (0.0%)
2	L	0.30	0/3127	0.54	0/4231
3	M	0.35	0/1509	0.58	2/2039 (0.1%)
3	O	0.36	0/1298	0.84	7/1755 (0.4%)
4	N	0.30	0/3144	0.58	3/4234 (0.1%)
4	P	0.34	0/1278	0.71	4/1716 (0.2%)
5	E	0.24	0/140	0.43	0/183
All	All	0.31	0/15195	0.59	18/20492 (0.1%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	N	383	ASP	CB-CG-OD1	9.85	127.16	118.30
1	K	1288	LEU	CA-CB-CG	7.89	133.45	115.30
3	O	319	PRO	CA-N-CD	-7.70	100.72	111.50
4	P	543	ASP	CB-CG-OD1	7.54	125.08	118.30
3	O	290	ASP	CB-CG-OD1	7.52	125.07	118.30

There are no chirality outliers.

There are no planarity outliers.

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	K	4597	0	4560	67	0
2	L	3048	0	2932	54	0
3	M	1483	0	1510	50	0
3	O	1275	0	1310	38	0
4	N	3073	0	3034	68	0
4	P	1249	0	1215	22	0
5	E	141	0	162	10	0
6	L	1	0	0	0	0
6	N	4	0	0	0	0
6	P	2	0	0	0	0
All	All	14873	0	14723	266	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 9.

The worst 5 of 266 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)
3:M:321:VAL:CG2	3:M:323:ILE:HG22	1.48	1.41
4:N:308:PHE:CE2	4:N:312:ILE:HD11	1.77	1.18
3:M:321:VAL:HG22	3:M:323:ILE:HG22	1.13	1.08
3:M:321:VAL:CG2	3:M:323:ILE:CG2	2.32	1.07
3:M:321:VAL:HG22	3:M:323:ILE:CG2	1.96	0.94

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	K	543/1536 (35%)	528 (97%)	15 (3%)	0	100	100
2	L	382/433 (88%)	370 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	181/401 (45%)	179 (99%)	2 (1%)	0	100	100
3	O	154/401 (38%)	147 (96%)	7 (4%)	0	100	100
4	N	365/684 (53%)	351 (96%)	14 (4%)	0	100	100
4	P	147/684 (22%)	142 (97%)	5 (3%)	0	100	100
5	E	15/135 (11%)	14 (93%)	1 (7%)	0	100	100
All	All	1787/4274 (42%)	1731 (97%)	56 (3%)	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	K	510/1391 (37%)	509 (100%)	1 (0%)	92	97
2	L	326/367 (89%)	325 (100%)	1 (0%)	91	96
3	M	172/359 (48%)	171 (99%)	1 (1%)	84	93
3	O	149/359 (42%)	148 (99%)	1 (1%)	81	91
4	N	356/653 (54%)	353 (99%)	3 (1%)	79	90
4	P	146/653 (22%)	145 (99%)	1 (1%)	81	91
5	E	13/108 (12%)	13 (100%)	0	100	100
All	All	1672/3890 (43%)	1664 (100%)	8 (0%)	85	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	P	268	GLN
3	O	288	TYR
4	N	551	PHE
4	N	85	LEU
4	N	569	PHE

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

Mol	Chain	Res	Type
3	M	358	GLN
3	M	389	ASN
4	N	519	ASN
3	O	295	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.