



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 05:15 am GMT

PDB ID : 4BZ9
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with J1075
Authors : Marek, M.; Romier, C.
Deposited on : 2013-07-24
Resolution : 2.00 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**
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.00 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 13756 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 protein called HISTONE DEACETYLASE 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	Total 3174	C 2047	N 528	O 584	S 15	0	2	0
1	B	414	Total 3301	C 2123	N 553	O 609	S 16	0	0	0
1	C	413	Total 3299	C 2128	N 552	O 603	S 16	0	1	0
1	D	398	Total 3184	C 2054	N 530	O 586	S 14	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	GLY	-	expression tag	UNP A5H660
A	442	SER	-	expression tag	UNP A5H660
A	443	LEU	-	expression tag	UNP A5H660
A	444	VAL	-	expression tag	UNP A5H660
A	445	PRO	-	expression tag	UNP A5H660
A	446	ARG	-	expression tag	UNP A5H660
B	441	GLY	-	expression tag	UNP A5H660
B	442	SER	-	expression tag	UNP A5H660
B	443	LEU	-	expression tag	UNP A5H660
B	444	VAL	-	expression tag	UNP A5H660
B	445	PRO	-	expression tag	UNP A5H660
B	446	ARG	-	expression tag	UNP A5H660
C	441	GLY	-	expression tag	UNP A5H660
C	442	SER	-	expression tag	UNP A5H660
C	443	LEU	-	expression tag	UNP A5H660
C	444	VAL	-	expression tag	UNP A5H660
C	445	PRO	-	expression tag	UNP A5H660
C	446	ARG	-	expression tag	UNP A5H660
D	441	GLY	-	expression tag	UNP A5H660
D	442	SER	-	expression tag	UNP A5H660
D	443	LEU	-	expression tag	UNP A5H660

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Chain	Residue	Modelled	Actual	Comment	Reference
D	444	VAL	-	expression tag	UNP A5H660
D	445	PRO	-	expression tag	UNP A5H660
D	446	ARG	-	expression tag	UNP A5H660

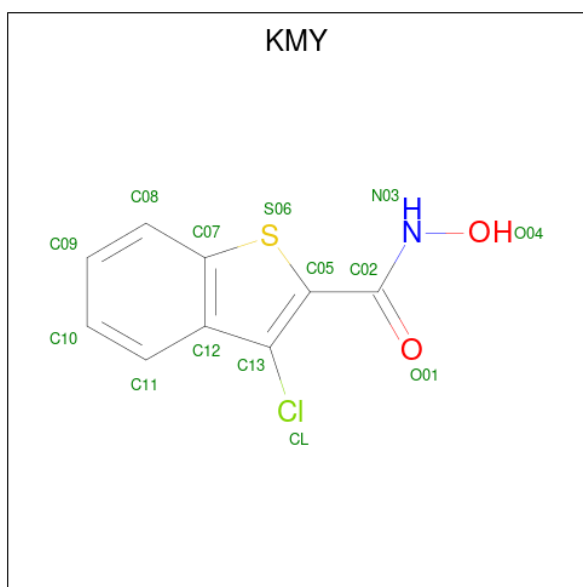
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

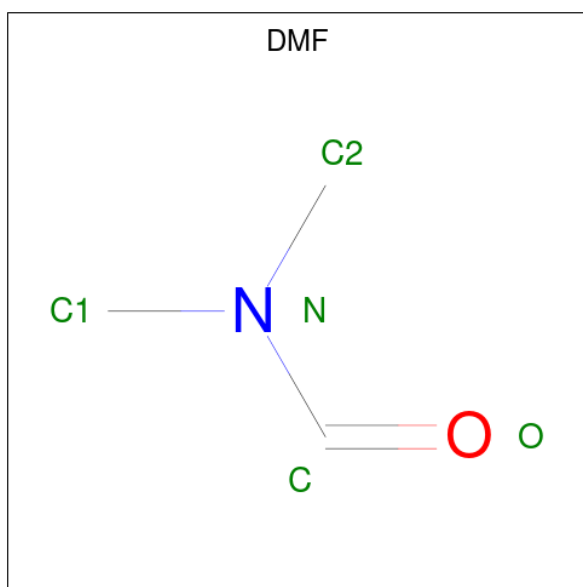
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is 3-chlorobenzothiophene-2-carbohydroxamic acid (three-letter code: KMY) (formula: C₉H₆ClNO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
4	A	1	Total	C	Cl	N	O	S	0	0
			14	9	1	1	2	1		
4	A	1	Total	C	Cl	N	O	S	0	0
			14	9	1	1	2	1		
4	B	1	Total	C	Cl	N	O	S	0	0
			14	9	1	1	2	1		
4	B	1	Total	C	Cl	N	O	S	0	0
			14	9	1	1	2	1		
4	C	1	Total	C	Cl	N	O	S	0	0
			14	9	1	1	2	1		
4	C	1	Total	C	Cl	N	O	S	0	0
			14	9	1	1	2	1		
4	D	1	Total	C	Cl	N	O	S	0	0
			14	9	1	1	2	1		
4	D	1	Total	C	Cl	N	O	S	0	0
			14	9	1	1	2	1		

- Molecule 5 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C₃H₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	138	Total O 138 138	0	0
7	B	178	Total O 178 178	0	0
7	C	186	Total O 186 186	0	0
7	D	130	Total O 130 130	0	0

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

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.28Å 70.32Å 98.13Å 77.93° 75.59° 85.54°	Depositor
Resolution (Å)	20.16 – 2.00	Depositor
% Data completeness (in resolution range)	97.1 (20.16-2.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.00Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.191 , 0.221	Depositor
Wilson B-factor (Å ²)	19.3	Xtrriage
Anisotropy	0.272	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.074 for -k,-h,-l	Xtrriage
Total number of atoms	13756	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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 monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 12 are monoatomic - leaving 16 for Mogul analysis.

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
4	KMY	B	700	2	9,15,15	3.35	2 (22%)	9,21,21	1.60	1 (11%)
4	KMY	A	700	2	9,15,15	3.22	2 (22%)	9,21,21	1.54	1 (11%)
5	DMF	A	901	-	4,4,4	0.78	0	4,4,4	0.24	0
4	KMY	D	700	2	9,15,15	3.21	2 (22%)	9,21,21	1.65	1 (11%)
5	DMF	C	900	-	4,4,4	0.77	0	4,4,4	0.76	0
5	DMF	C	901	-	4,4,4	0.65	0	4,4,4	0.45	0
4	KMY	D	701	-	9,15,15	3.25	2 (22%)	9,21,21	1.76	1 (11%)
4	KMY	C	700	2	9,15,15	3.41	2 (22%)	9,21,21	1.61	1 (11%)
5	DMF	D	900	-	4,4,4	0.66	0	4,4,4	0.33	0
4	KMY	A	701	-	9,15,15	3.24	3 (33%)	9,21,21	1.74	1 (11%)
4	KMY	B	701	-	9,15,15	3.27	2 (22%)	9,21,21	1.78	2 (22%)
5	DMF	D	901	-	4,4,4	0.75	0	4,4,4	0.38	0
4	KMY	C	701	-	9,15,15	3.06	2 (22%)	9,21,21	2.06	3 (33%)
6	GOL	D	800	-	5,5,5	0.71	0	5,5,5	1.05	0
6	GOL	B	800	-	5,5,5	0.75	0	5,5,5	1.01	0
5	DMF	C	902	-	4,4,4	0.76	0	4,4,4	0.26	0

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
4	KMY	B	700	2	-	0/2/6/6	0/2/2/2
4	KMY	A	700	2	-	0/2/6/6	0/2/2/2
5	DMF	A	901	-	-	0/2/2/2	-
4	KMY	D	700	2	-	0/2/6/6	0/2/2/2
5	DMF	C	900	-	-	0/2/2/2	-
5	DMF	C	901	-	-	0/2/2/2	-
4	KMY	D	701	-	-	0/2/6/6	0/2/2/2
4	KMY	C	700	2	-	0/2/6/6	0/2/2/2
5	DMF	D	900	-	-	0/2/2/2	-
4	KMY	A	701	-	-	0/2/6/6	0/2/2/2
4	KMY	B	701	-	-	0/2/6/6	0/2/2/2
5	DMF	D	901	-	-	0/2/2/2	-
4	KMY	C	701	-	-	0/2/6/6	0/2/2/2
6	GOL	D	800	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	800	-	-	1/4/4/4	-
5	DMF	C	902	-	-	0/2/2/2	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	700	KMY	C02-N03	9.00	1.44	1.32
4	B	701	KMY	C02-N03	8.80	1.44	1.32
4	B	700	KMY	C02-N03	8.75	1.44	1.32
4	D	701	KMY	C02-N03	8.67	1.44	1.32
4	A	701	KMY	C02-N03	8.56	1.43	1.32
4	A	700	KMY	C02-N03	8.37	1.43	1.32
4	D	700	KMY	C02-N03	8.13	1.43	1.32
4	C	701	KMY	C02-N03	8.07	1.43	1.32
4	D	700	KMY	O04-N03	-4.31	1.29	1.40
4	B	700	KMY	O04-N03	-4.24	1.29	1.40
4	C	700	KMY	O04-N03	-4.23	1.29	1.40
4	A	700	KMY	O04-N03	-4.21	1.29	1.40
4	A	701	KMY	O04-N03	-3.75	1.30	1.40
4	D	701	KMY	O04-N03	-3.68	1.30	1.40
4	B	701	KMY	O04-N03	-3.52	1.31	1.40
4	C	701	KMY	O04-N03	-3.51	1.31	1.40
4	A	701	KMY	C09-C08	2.06	1.41	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	KMY	C11-C12-C13	-4.36	125.35	134.33
4	A	701	KMY	C11-C12-C13	-4.35	125.36	134.33
4	B	701	KMY	C11-C12-C13	-4.33	125.40	134.33
4	C	701	KMY	C11-C12-C13	-4.21	125.66	134.33
4	D	700	KMY	C11-C12-C13	-4.08	125.91	134.33
4	C	700	KMY	C11-C12-C13	-4.03	126.03	134.33
4	B	700	KMY	C11-C12-C13	-4.00	126.09	134.33
4	A	700	KMY	C11-C12-C13	-3.88	126.32	134.33
4	C	701	KMY	C05-C02-N03	3.32	120.55	115.18
4	C	701	KMY	O01-C02-N03	-2.40	118.47	122.94
4	B	701	KMY	C05-C02-N03	2.14	118.64	115.18

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	800	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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