

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 3, 2023 – 03:12 AM EDT

PDB ID : 6ODA

Title : Crystal structure of HDAC8 in complex with compound 2

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Deposited on : 2019-03-26

Resolution : 2.88 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 (i) 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 (1)) were used in the production of this report:

MolProbity : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : FAILED

buster-report : 1.1.7 (2018)

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) : 2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.88 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 5 unique types of molecules in this entry. The entry contains 8516 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					AltConf	Trace
1 Λ	2004	Total	С	N	О	S	9	4	0	
1	1 A	364	2839	1819	472	527	21	3	4	
1	В	363	Total	С	N	О	S	3	3	0
1	Б	303	2834	1814	470	530	20			
1	1 0	252	Total	С	N	О	S	2	2	0
	353	2756	1770	458	509	19	3			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q9BY41
A	-22	HIS	-	expression tag	UNP Q9BY41
A	-21	HIS	-	expression tag	UNP Q9BY41
A	-20	HIS	-	expression tag	UNP Q9BY41
A	-19	HIS	-	expression tag	UNP Q9BY41
A	-18	HIS	-	expression tag	UNP Q9BY41
A	-17	HIS	-	expression tag	UNP Q9BY41
A	-16	SER	-	expression tag	UNP Q9BY41
A	-15	SER	-	expression tag	UNP Q9BY41
A	-14	GLY	-	expression tag	UNP Q9BY41
A	-13	VAL	-	expression tag	UNP Q9BY41
A	-12	ASP	-	expression tag	UNP Q9BY41
A	-11	LEU	-	expression tag	UNP Q9BY41
A	-10	GLY	-	expression tag	UNP Q9BY41
A	-9	THR	-	expression tag	UNP Q9BY41
A	-8	GLU	-	expression tag	UNP Q9BY41
A	-7	ASN	-	expression tag	UNP Q9BY41
A	-6	LEU	-	expression tag	UNP Q9BY41
A	-5	TYR	-	expression tag	UNP Q9BY41
A	-4	PHE	-	expression tag	UNP Q9BY41
A	-3	GLN	-	expression tag	UNP Q9BY41
A	-2	SER	-	expression tag	UNP Q9BY41
A	-1	ASN	-	expression tag	UNP Q9BY41



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Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP Q9BY41
A	378	ILE	-	expression tag	UNP Q9BY41
A	379	GLU	-	expression tag	UNP Q9BY41
A	380	GLY	-	expression tag	UNP Q9BY41
A	381	ARG	-	expression tag	UNP Q9BY41
A	382	GLY	-	expression tag	UNP Q9BY41
A	383	SER	-	expression tag	UNP Q9BY41
A	384	HIS	-	expression tag	UNP Q9BY41
A	385	HIS	-	expression tag	UNP Q9BY41
A	386	HIS	-	expression tag	UNP Q9BY41
A	387	HIS	-	expression tag	UNP Q9BY41
A	388	HIS	-	expression tag	UNP Q9BY41
A	389	HIS	-	expression tag	UNP Q9BY41
В	-23	MET	-	expression tag	UNP Q9BY41
В	-22	HIS	-	expression tag	UNP Q9BY41
В	-21	HIS	-	expression tag	UNP Q9BY41
В	-20	HIS	-	expression tag	UNP Q9BY41
В	-19	HIS	-	expression tag	UNP Q9BY41
В	-18	HIS	-	expression tag	UNP Q9BY41
В	-17	HIS	-	expression tag	UNP Q9BY41
В	-16	SER	-	expression tag	UNP Q9BY41
В	-15	SER	-	expression tag	UNP Q9BY41
В	-14	GLY	-	expression tag	UNP Q9BY41
В	-13	VAL	-	expression tag	UNP Q9BY41
В	-12	ASP	-	expression tag	UNP Q9BY41
В	-11	LEU	-	expression tag	UNP Q9BY41
В	-10	GLY	-	expression tag	UNP Q9BY41
В	-9	THR	-	expression tag	UNP Q9BY41
В	-8	GLU	-	expression tag	UNP Q9BY41
В	-7	ASN	-	expression tag	UNP Q9BY41
В	-6	LEU	-	expression tag	UNP Q9BY41
В	-5	TYR	-	expression tag	UNP Q9BY41
В	-4	PHE	-	expression tag	UNP Q9BY41
В	-3	GLN	-	expression tag	UNP Q9BY41
В	-2	SER	-	expression tag	UNP Q9BY41
В	-1	ASN	-	expression tag	UNP Q9BY41
В	0	ALA	-	expression tag	UNP Q9BY41
В	378	ILE	-	expression tag	UNP Q9BY41
В	379	GLU	-	expression tag	UNP Q9BY41
В	380	GLY	-	expression tag	UNP Q9BY41
В	381	ARG	-	expression tag	UNP Q9BY41
В	382	GLY	-	expression tag	UNP Q9BY41
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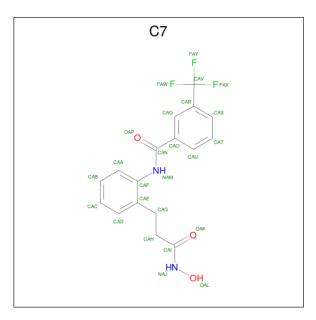
Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
В	383	SER	-	expression tag	UNP Q9BY41
В	384	HIS	-	expression tag	UNP Q9BY41
В	385	HIS	-	expression tag	UNP Q9BY41
В	386	HIS	-	expression tag	UNP Q9BY41
В	387	HIS	-	expression tag	UNP Q9BY41
В	388	HIS	-	expression tag	UNP Q9BY41
В	389	HIS	-	expression tag	UNP Q9BY41
С	-23	MET	-	expression tag	UNP Q9BY41
С	-22	HIS	-	expression tag	UNP Q9BY41
С	-21	HIS	-	expression tag	UNP Q9BY41
С	-20	HIS	-	expression tag	UNP Q9BY41
С	-19	HIS	-	expression tag	UNP Q9BY41
С	-18	HIS	-	expression tag	UNP Q9BY41
С	-17	HIS	-	expression tag	UNP Q9BY41
С	-16	SER	-	expression tag	UNP Q9BY41
С	-15	SER	-	expression tag	UNP Q9BY41
С	-14	GLY	-	expression tag	UNP Q9BY41
С	-13	VAL	-	expression tag	UNP Q9BY41
С	-12	ASP	-	expression tag	UNP Q9BY41
С	-11	LEU	-	expression tag	UNP Q9BY41
С	-10	GLY	-	expression tag	UNP Q9BY41
С	-9	THR	-	expression tag	UNP Q9BY41
С	-8	GLU	-	expression tag	UNP Q9BY41
С	-7	ASN	-	expression tag	UNP Q9BY41
С	-6	LEU	-	expression tag	UNP Q9BY41
С	-5	TYR	-	expression tag	UNP Q9BY41
С	-4	PHE	-	expression tag	UNP Q9BY41
С	-3	GLN	-	expression tag	UNP Q9BY41
С	-2	SER	-	expression tag	UNP Q9BY41
С	-1	ASN	-	expression tag	UNP Q9BY41
С	0	ALA	-	expression tag	UNP Q9BY41
С	378	ILE	-	expression tag	UNP Q9BY41
С	379	GLU	-	expression tag	UNP Q9BY41
С	380	GLY	-	expression tag	UNP Q9BY41
С	381	ARG		expression tag	UNP Q9BY41
С	382	GLY	-	expression tag	UNP Q9BY41
С	383	SER		expression tag	UNP Q9BY41
С	384	HIS		expression tag	UNP Q9BY41
С	385	HIS		expression tag	UNP Q9BY41
С	386	HIS		expression tag	UNP Q9BY41
С	387	HIS	-	expression tag	UNP Q9BY41
С	388	HIS	-	expression tag	UNP Q9BY41



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Chain	Residue	Modelled	Actual	Comment	Reference
С	389	HIS	-	expression tag	UNP Q9BY41

• Molecule 2 is N-{2-[3-(hydroxyamino)-3-oxopropyl]phenyl}-3-(trifluoromethyl)benza mide (three-letter code: C7) (formula:  $C_{17}H_{15}F_3N_2O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	
2	A	1	Total 25					0	0
2	В	1	Total 25	_			_	0	0
2	С	1	Total 25	C 17				0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0

• Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total K 2 2	0	0
4	В	2	Total K 2 2	0	0
4	С	2	Total K 2 2	0	0

#### • Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	В	1	Total O 1 1	0	0
5	С	1	Total O 1 1	0	0

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



# 3 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	87.75Å 91.29Å 92.70Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $94.09^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	50.00 - 2.88	Depositor	
% Data completeness	93.7 (50.00-2.88)	Depositor	
(in resolution range)	, , ,	•	
$R_{merge}$	0.11	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.25 (at 2.86Å)	Xtriage	
Refinement program	REFMAC 5.8.0158	Depositor	
$R, R_{free}$	0.199 , 0.249	Depositor	
Wilson B-factor $(\mathring{A}^2)$	52.7	Xtriage	
Anisotropy	0.120	Xtriage	
L-test for twinning <sup>2</sup>	$ < L > = 0.48, < L^2> = 0.30$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	8516	wwPDB-VP	
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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 Ty	Tuno	Chain	Res	Link	Bo	ond leng	$ ag{ths}$	Bond angles		
	туре				Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	C7	С	401	3	26,26,26	0.76	0	35,36,36	1.62	7 (20%)
2	C7	A	401	3	26,26,26	0.69	0	35,36,36	1.64	8 (22%)
2	C7	В	401	3	26,26,26	0.69	0	35,36,36	1.60	6 (17%)

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	C7	С	401	3	-	1/21/21/21	0/2/2/2
2	C7	A	401	3	-	1/21/21/21	0/2/2/2
2	C7	В	401	3	-	1/21/21/21	0/2/2/2

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	С	401	C7	CAH-CAG-CAE	4.98	125.46	112.57
2	В	401	C7	CAH-CAG-CAE	4.97	125.43	112.57
2	A	401	C7	CAH-CAG-CAE	4.92	125.29	112.57
2	С	401	C7	OAK-CAI-NAJ	-3.81	118.59	123.27
2	В	401	C7	OAP-CAN-CAO	-3.35	114.97	120.94
2	A	401	C7	OAP-CAN-CAO	-3.26	115.13	120.94
2	С	401	C7	OAP-CAN-CAO	-3.25	115.14	120.94
2	В	401	C7	CAO-CAN-NAM	2.99	122.50	115.92
2	A	401	C7	OAK-CAI-NAJ	-2.91	119.70	123.27
2	A	401	C7	CAO-CAN-NAM	2.88	122.27	115.92
2	A	401	C7	CAG-CAH-CAI	2.79	119.13	112.72
2	В	401	C7	OAK-CAI-NAJ	-2.73	119.92	123.27
2	С	401	C7	CAO-CAN-NAM	2.69	121.84	115.92
2	A	401	C7	OAK-CAI-CAH	2.61	126.79	122.02
2	С	401	C7	FAY-CAV-CAR	-2.59	107.25	112.93
2	С	401	C7	OAK-CAI-CAH	2.45	126.50	122.02
2	В	401	C7	OAK-CAI-CAH	2.42	126.45	122.02
2	В	401	C7	CAG-CAH-CAI	2.33	118.08	112.72
2	A	401	C7	FAX-CAV-CAR	-2.31	107.86	112.93



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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	С	401	C7	CAG-CAH-CAI	2.23	117.84	112.72
2	A	401	C7	CAQ-CAR-CAV	2.07	122.37	119.58

There are no chirality outliers.

All (3) torsion outliers are listed below:

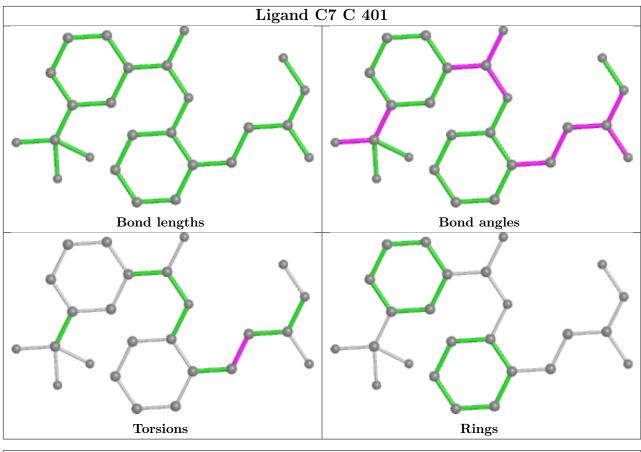
Mol	Chain	Res	Type	Atoms
2	A	401	C7	CAE-CAG-CAH-CAI
2	В	401	C7	CAE-CAG-CAH-CAI
2	С	401	C7	CAE-CAG-CAH-CAI

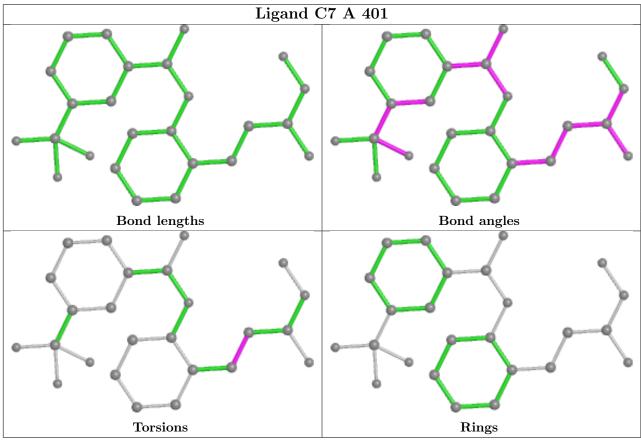
There are no ring outliers.

No monomer is involved in short contacts.

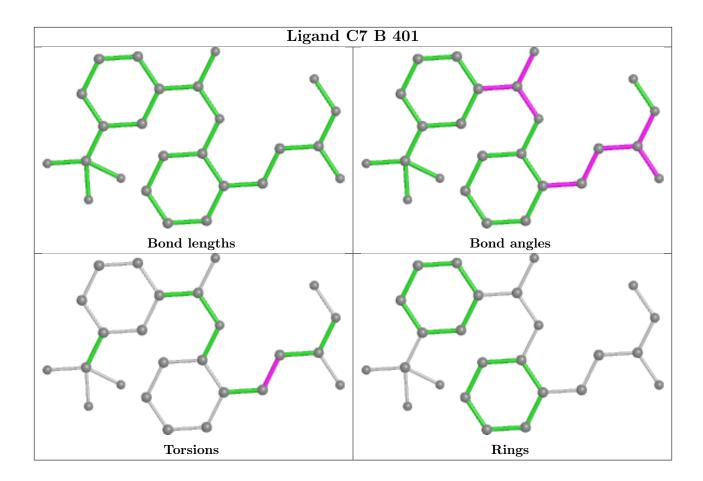
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











# 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 (i)

### 5.1 Protein, DNA and RNA chains (i)

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

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

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

### 5.3 Carbohydrates (i)

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

### 5.4 Ligands (i)

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

## 5.5 Other polymers (i)

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

