Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 07:00 AM EDT

PDB ID	:	6V79
Title	:	Crystal structure of Danio rerio histone deacetylase 6 catalytic domain 2 (CD2) complexed with NF2376
Authors	:	Osko, J.D.; Christianson, D.W.
Deposited on	:	2019-12-08
Resolution	:	2.04 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-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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 6 unique types of molecules in this entry. The entry contains 5771 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 Hdac6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	357	2748	1734	487	509	18	2	1	0
1	B	357	2733	1724	484	507	18	2	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	SER	-	expression tag	UNP A7YT55
A	436	ASN	-	expression tag	UNP A7YT55
A	437	ALA	-	expression tag	UNP A7YT55
A	438	GLY	-	expression tag	UNP A7YT55
A	439	GLY	-	expression tag	UNP A7YT55
B	435	SER	-	expression tag	UNP A7YT55
B	436	ASN	-	expression tag	UNP A7YT55
B	437	ALA	-	expression tag	UNP A7YT55
B	438	GLY	-	expression tag	UNP A7YT55
B	439	GLY	-	expression tag	UNP A7YT55

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

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

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

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

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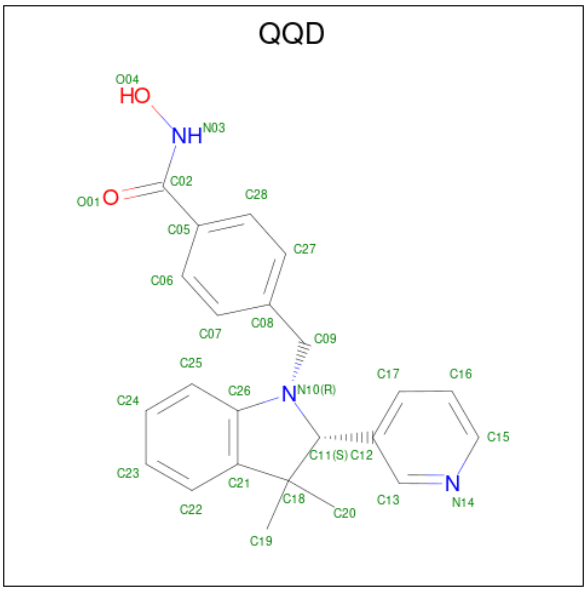
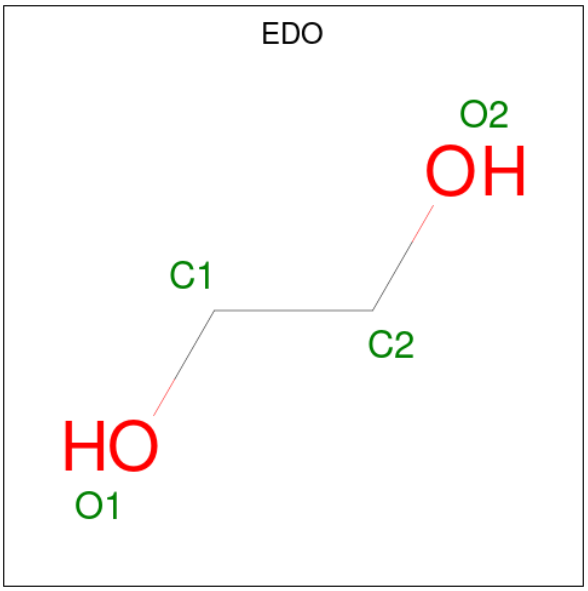
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	B	2	2	2	0	0

- Molecule 4 is 4-{[(2S)-3,3-dimethyl-2-(pyridin-3-yl)-2,3-dihydro-1H-indol-1-yl]methyl}-N-hydroxybenzamide (three-letter code: QQD) (formula: $C_{23}H_{23}N_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	28	23	3	2	0	0
			Total	C	N	O		
4	B	1	28	23	3	2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	116	116	116	0	0
			Total	O		
6	B	108	108	108	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 a, b, c, α, β, γ	48.25Å 108.14Å 74.34Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	74.34 – 2.04	Depositor
% Data completeness (in resolution range)	96.1 (74.34-2.04)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.195 , 0.234	Depositor
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.719	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.197 for h,-k,-l	Xtriage
Total number of atoms	5771	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

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 9 ligands modelled in this entry, 6 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	QQD	B	804	2	30,31,31	2.31	7 (23%)	42,45,45	1.31	6 (14%)
5	EDO	A	805	-	3,3,3	0.41	0	2,2,2	0.44	0
4	QQD	A	804	2	30,31,31	2.38	7 (23%)	42,45,45	1.21	6 (14%)

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	QQD	B	804	2	-	0/14/34/34	0/4/4/4
5	EDO	A	805	-	-	0/1/1/1	-
4	QQD	A	804	2	-	0/14/34/34	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	804	QQD	C02-N03	8.79	1.44	1.32
4	B	804	QQD	C02-N03	8.19	1.43	1.32
4	B	804	QQD	C11-N10	5.00	1.52	1.47
4	A	804	QQD	C12-C11	4.68	1.58	1.51
4	A	804	QQD	C11-N10	4.59	1.52	1.47
4	B	804	QQD	C12-C11	4.33	1.57	1.51
4	A	804	QQD	C26-C21	2.61	1.42	1.39
4	A	804	QQD	O01-C02	-2.61	1.18	1.23
4	B	804	QQD	O01-C02	-2.49	1.18	1.23
4	B	804	QQD	C05-C02	2.37	1.55	1.50
4	A	804	QQD	C05-C02	2.30	1.55	1.50
4	B	804	QQD	C17-C12	2.29	1.42	1.39
4	B	804	QQD	C26-C21	2.27	1.42	1.39
4	A	804	QQD	C17-C12	2.16	1.42	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	804	QQD	C25-C26-C21	-3.41	118.36	121.76
4	A	804	QQD	C25-C26-C21	-3.19	118.58	121.76
4	B	804	QQD	C05-C02-N03	2.98	120.94	116.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	804	QQD	C26-N10-C11	2.62	111.14	108.87
4	B	804	QQD	C26-N10-C11	2.49	111.03	108.87
4	B	804	QQD	O01-C02-N03	-2.48	118.31	122.94
4	A	804	QQD	C12-C11-N10	2.45	116.64	112.35
4	A	804	QQD	C17-C12-C13	-2.36	114.38	116.88
4	A	804	QQD	C05-C02-N03	2.34	119.91	116.16
4	B	804	QQD	C17-C12-C13	-2.29	114.46	116.88
4	B	804	QQD	C17-C12-C11	2.20	125.34	120.70
4	A	804	QQD	C17-C12-C11	2.19	125.31	120.70

There are no chirality outliers.

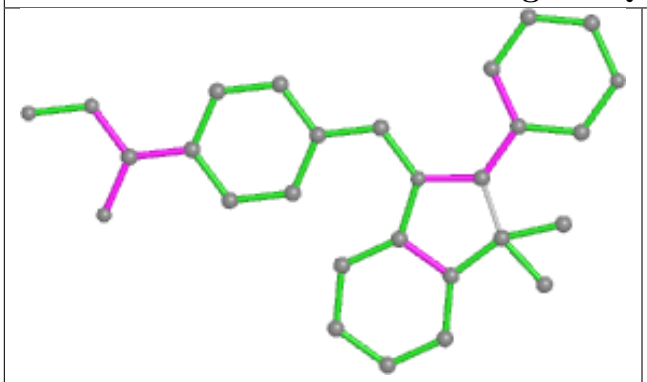
There are no torsion outliers.

There are no ring outliers.

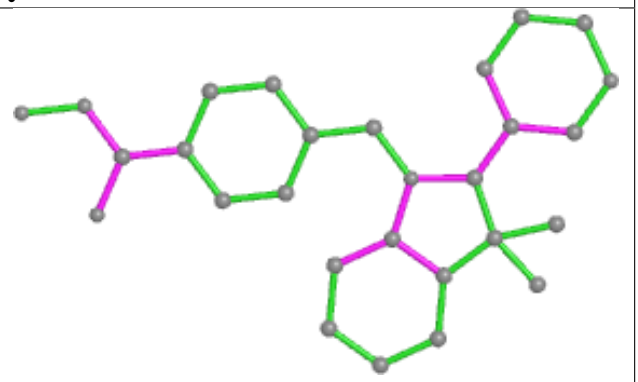
No monomer is involved in short contacts.

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.

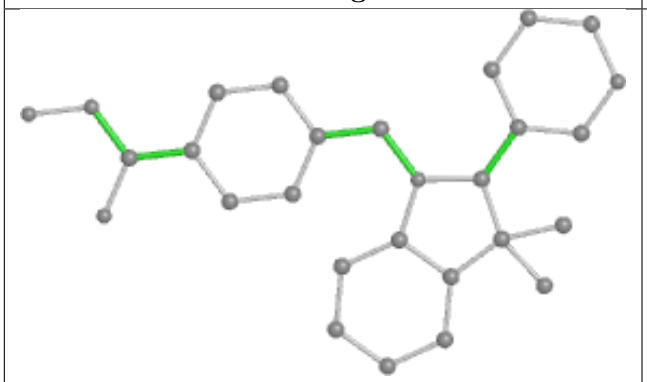
Ligand QQD B 804



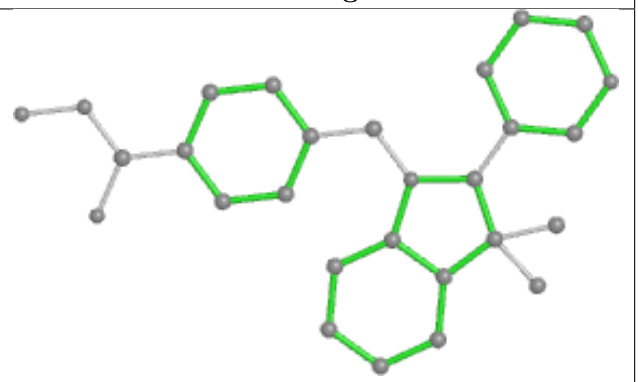
Bond lengths



Bond angles

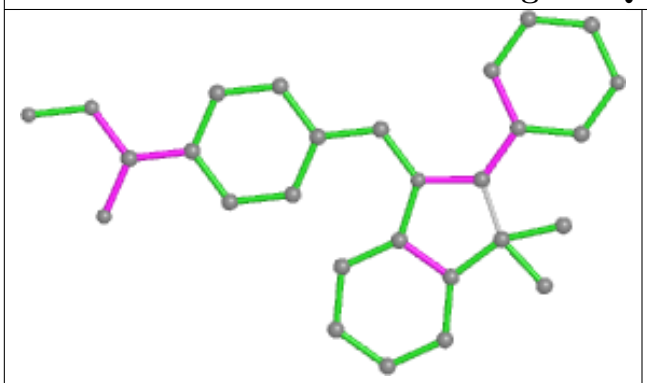


Torsions

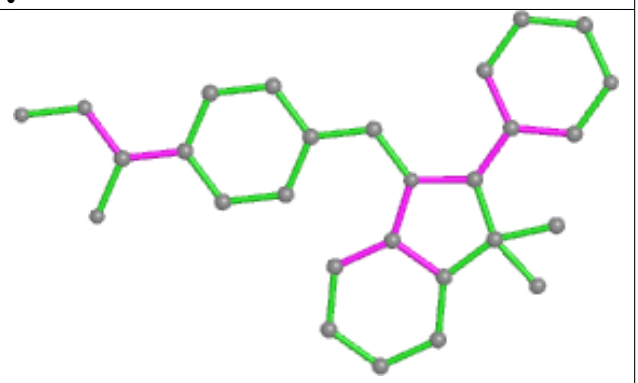


Rings

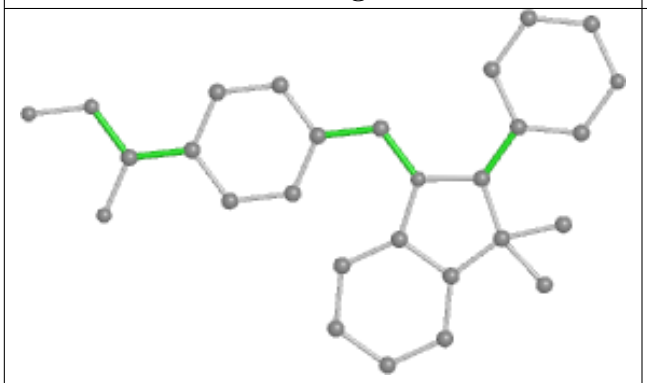
Ligand QQD A 804



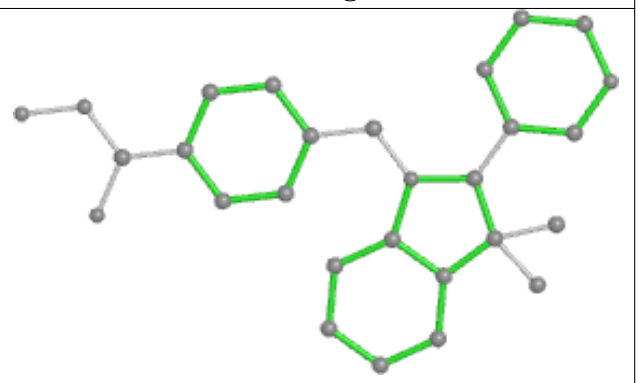
Bond lengths



Bond angles



Torsions



Rings

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.