wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 08:59 AM EDT

PDB ID	:	6VK5
Title	:	Crystal Structure of Methylosinus trichosporium OB3b Soluble Methane Monooxygenase Hydroxylase and Regulatory Component Complex
Authors	:	Jones, J.C.; Banerjee, R.; Shi, K.; Aihara, H.; Lipscomb, J.D.
Deposited on	:	2020-01-18
Resolution	:	1.86 Å(reported)

This is a wwPDB X-ray Structure 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/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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (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)	:	2.35.1

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 1.86 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 9 unique types of molecules in this entry. The entry contains 40070 atoms, of which 19003 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 Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	515	Total	C	H	N	O	S	0	0	0
			8145	2676	3970	723	764	12			
1	E	515	Total	C	H	N	O	S	0	2	0
			8164	2682	3981	724	765	12			

- Molecule 2 is a protein called Methane monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	392	Total	C	H	N	O	S	0	0	0
			6196	2033	3010	556	592	5			
2	F	392	Total	C	H	N	O	S	0	3	0
			6224	2040	3024	559	596	5			

- Molecule 3 is a protein called Methane monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	168	Total	C	H	N	O	S	0	0	0
			2762	874	1400	234	253	1			
3	G	168	Total	C	H	N	O	S	0	0	0
			2762	874	1400	234	253	1			

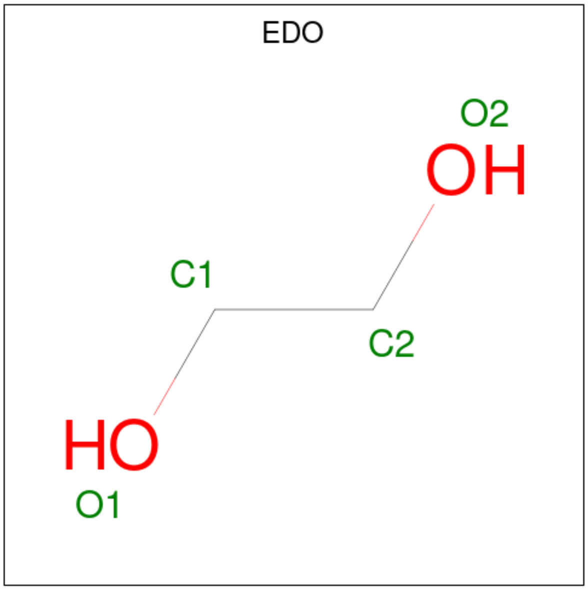
- Molecule 4 is a protein called Methane monooxygenase regulatory protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	132	Total	C	H	N	O	S	0	0	0
			1997	639	995	162	198	3			
4	H	137	Total	C	H	N	O	S	0	0	0
			2071	662	1033	167	206	3			

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Fe 2	0	0
5	E	2	Total 2	Fe 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 10	C 2	H 6	O 2	0	0
6	A	1	Total 10	C 2	H 6	O 2	0	0
6	A	1	Total 10	C 2	H 6	O 2	0	0
6	A	1	Total 10	C 2	H 6	O 2	0	0
6	A	1	Total 10	C 2	H 6	O 2	0	0
6	A	1	Total 10	C 2	H 6	O 2	0	0
6	A	1	Total 10	C 2	H 6	O 2	0	0
6	A	1	Total 10	C 2	H 6	O 2	0	0
6	A	1	Total 10	C 2	H 6	O 2	0	0
6	A	1	Total 10	C 2	H 6	O 2	0	0

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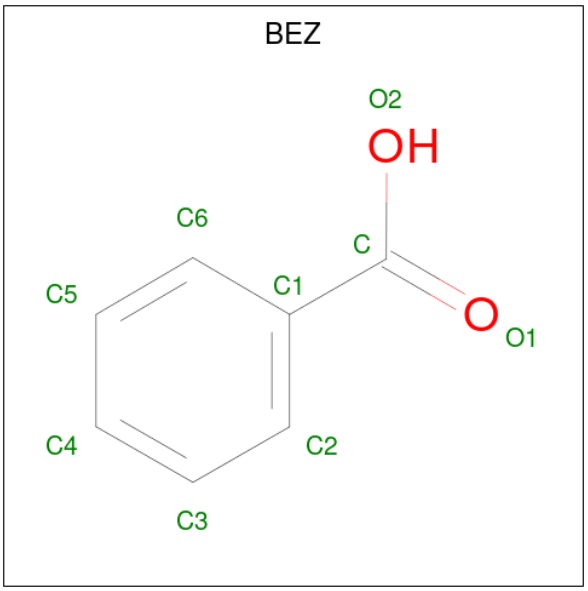
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total 10	C 2	H 6	O 2	0	0
6	B	1	Total 10	C 2	H 6	O 2	0	0
6	B	1	Total 10	C 2	H 6	O 2	0	0
6	C	1	Total 10	C 2	H 6	O 2	0	0
6	D	1	Total 10	C 2	H 6	O 2	0	0
6	D	1	Total 10	C 2	H 6	O 2	0	0
6	E	1	Total 10	C 2	H 6	O 2	0	0
6	E	1	Total 10	C 2	H 6	O 2	0	0
6	E	1	Total 10	C 2	H 6	O 2	0	0
6	E	1	Total 10	C 2	H 6	O 2	0	0
6	E	1	Total 10	C 2	H 6	O 2	0	0
6	E	1	Total 10	C 2	H 6	O 2	0	0
6	E	1	Total 10	C 2	H 6	O 2	0	0
6	F	1	Total 10	C 2	H 6	O 2	0	0
6	F	1	Total 10	C 2	H 6	O 2	0	0
6	F	1	Total 10	C 2	H 6	O 2	0	0
6	F	1	Total 10	C 2	H 6	O 2	0	0
6	G	1	Total 10	C 2	H 6	O 2	0	0
6	G	1	Total 10	C 2	H 6	O 2	0	0
6	H	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 7 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 14 7 5 2	0	0
7	E	1	Total C H O 14 7 5 2	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total Cl 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	293	Total O 293 293	0	0
9	B	257	Total O 258 258	0	1
9	C	105	Total O 105 105	0	0
9	D	40	Total O 40 40	0	0
9	E	296	Total O 296 296	0	0
9	F	257	Total O 258 258	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	111	Total O 111 111	0	0
9	H	55	Total O 55 55	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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.61Å 105.46Å 299.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.54 – 1.86	Depositor
% Data completeness (in resolution range)	99.7 (73.54-1.86)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.170 , 0.193	Depositor
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.229	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.030 for k,h,-l	Xtriage
Total number of atoms	40070	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 37 ligands modelled in this entry, 5 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
6	EDO	F	402	-	3,3,3	0.49	0	2,2,2	0.32	0
6	EDO	A	811	-	3,3,3	0.51	0	2,2,2	0.41	0
6	EDO	E	809	-	3,3,3	0.68	0	2,2,2	0.16	0
7	BEZ	E	810	5	9,9,9	1.59	1 (11%)	11,11,11	0.83	0
6	EDO	E	803	-	3,3,3	0.56	0	2,2,2	0.44	0
6	EDO	A	810	-	3,3,3	0.51	0	2,2,2	0.18	0
6	EDO	E	807	-	3,3,3	0.48	0	2,2,2	0.61	0
6	EDO	G	202	-	3,3,3	0.39	0	2,2,2	0.49	0
6	EDO	E	808	-	3,3,3	0.55	0	2,2,2	0.31	0
6	EDO	A	805	-	3,3,3	0.47	0	2,2,2	0.39	0
6	EDO	A	808	-	3,3,3	0.38	0	2,2,2	0.50	0
6	EDO	F	404	-	3,3,3	0.40	0	2,2,2	0.53	0
6	EDO	A	804	-	3,3,3	0.54	0	2,2,2	0.39	0
6	EDO	A	812	-	3,3,3	0.52	0	2,2,2	0.37	0
6	EDO	F	403	-	3,3,3	0.48	0	2,2,2	0.21	0
6	EDO	C	201	-	3,3,3	0.37	0	2,2,2	0.47	0
6	EDO	D	202	-	3,3,3	0.51	0	2,2,2	0.10	0
6	EDO	F	401	-	3,3,3	0.55	0	2,2,2	0.24	0
7	BEZ	A	813	5	9,9,9	1.62	1 (11%)	11,11,11	0.90	0
6	EDO	B	401	-	3,3,3	0.57	0	2,2,2	0.31	0
6	EDO	E	805	-	3,3,3	0.51	0	2,2,2	0.24	0
6	EDO	A	806	-	3,3,3	0.65	0	2,2,2	0.15	0
6	EDO	E	804	-	3,3,3	0.51	0	2,2,2	0.30	0
6	EDO	A	803	-	3,3,3	0.39	0	2,2,2	0.37	0
6	EDO	B	403	-	3,3,3	0.67	0	2,2,2	0.35	0
6	EDO	G	201	-	3,3,3	0.55	0	2,2,2	0.25	0
6	EDO	A	807	-	3,3,3	0.41	0	2,2,2	0.40	0
6	EDO	D	201	-	3,3,3	0.61	0	2,2,2	0.33	0
6	EDO	H	201	-	3,3,3	0.55	0	2,2,2	0.11	0
6	EDO	B	402	-	3,3,3	0.41	0	2,2,2	0.38	0
6	EDO	E	806	-	3,3,3	0.46	0	2,2,2	0.42	0
6	EDO	A	809	-	3,3,3	0.47	0	2,2,2	0.24	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
6	EDO	F	402	-	-	0/1/1/1	-
6	EDO	A	811	-	-	1/1/1/1	-
6	EDO	E	809	-	-	1/1/1/1	-
7	BEZ	E	810	5	-	0/4/4/4	0/1/1/1
6	EDO	E	803	-	-	1/1/1/1	-
6	EDO	A	810	-	-	0/1/1/1	-
6	EDO	E	807	-	-	0/1/1/1	-
6	EDO	G	202	-	-	0/1/1/1	-
6	EDO	E	808	-	-	0/1/1/1	-
6	EDO	A	805	-	-	0/1/1/1	-
6	EDO	A	808	-	-	1/1/1/1	-
6	EDO	F	404	-	-	1/1/1/1	-
6	EDO	A	804	-	-	0/1/1/1	-
6	EDO	A	812	-	-	0/1/1/1	-
6	EDO	F	403	-	-	1/1/1/1	-
6	EDO	C	201	-	-	0/1/1/1	-
6	EDO	D	202	-	-	0/1/1/1	-
6	EDO	F	401	-	-	1/1/1/1	-
7	BEZ	A	813	5	-	0/4/4/4	0/1/1/1
6	EDO	B	401	-	-	0/1/1/1	-
6	EDO	E	805	-	-	1/1/1/1	-
6	EDO	A	806	-	-	0/1/1/1	-
6	EDO	E	804	-	-	1/1/1/1	-
6	EDO	A	803	-	-	0/1/1/1	-
6	EDO	B	403	-	-	0/1/1/1	-
6	EDO	G	201	-	-	0/1/1/1	-
6	EDO	A	807	-	-	0/1/1/1	-
6	EDO	D	201	-	-	1/1/1/1	-
6	EDO	H	201	-	-	1/1/1/1	-
6	EDO	B	402	-	-	1/1/1/1	-
6	EDO	E	806	-	-	0/1/1/1	-
6	EDO	A	809	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	813	BEZ	C1-C	-4.39	1.40	1.49
7	E	810	BEZ	C1-C	-4.22	1.40	1.49

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	403	EDO	O1-C1-C2-O2
6	D	201	EDO	O1-C1-C2-O2
6	E	805	EDO	O1-C1-C2-O2
6	F	401	EDO	O1-C1-C2-O2
6	A	809	EDO	O1-C1-C2-O2

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.