



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 10:20 AM EDT

PDB ID : 6N0X
Title : Crystal structure of Anaerolinea thermophila mevalonate 5-phosphate decarboxylase complexed with (R)-MVAP
Authors : Noel, J.P.; Thomas, S.T.; Louie, G.V.
Deposited on : 2018-11-07
Resolution : 1.44 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 : 1.8.5 (274361), 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) : 2.35.1

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 1.44 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 3 unique types of molecules in this entry. The entry contains 31274 atoms, of which 14514 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 Diphosphomevalonate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	321	4852	1544	2411	427	459	11	0	0	0
1	B	320	4839	1539	2405	426	458	11	0	0	0
1	C	324	4888	1558	2424	431	464	11	0	0	0
1	D	323	4880	1555	2419	431	464	11	0	0	0
1	E	320	4856	1542	2419	427	457	11	0	0	0
1	F	317	4786	1526	2376	419	454	11	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

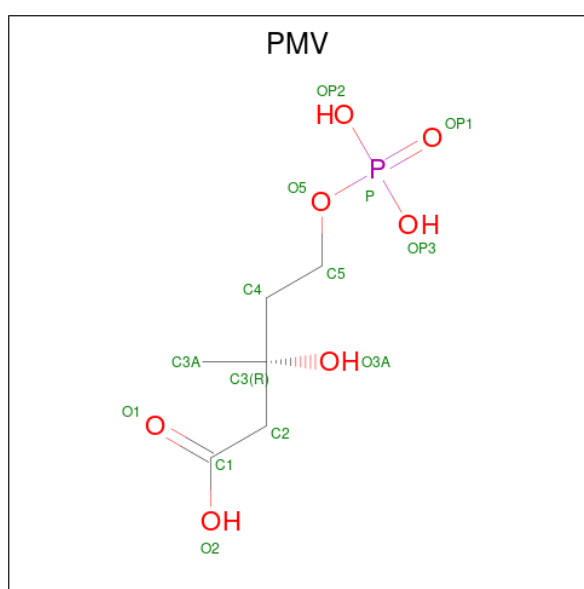
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP E8N6F3
A	-2	SER	-	expression tag	UNP E8N6F3
A	-1	HIS	-	expression tag	UNP E8N6F3
A	0	GLY	-	expression tag	UNP E8N6F3
B	-3	GLY	-	expression tag	UNP E8N6F3
B	-2	SER	-	expression tag	UNP E8N6F3
B	-1	HIS	-	expression tag	UNP E8N6F3
B	0	GLY	-	expression tag	UNP E8N6F3
C	-3	GLY	-	expression tag	UNP E8N6F3
C	-2	SER	-	expression tag	UNP E8N6F3
C	-1	HIS	-	expression tag	UNP E8N6F3
C	0	GLY	-	expression tag	UNP E8N6F3
D	-3	GLY	-	expression tag	UNP E8N6F3
D	-2	SER	-	expression tag	UNP E8N6F3
D	-1	HIS	-	expression tag	UNP E8N6F3
D	0	GLY	-	expression tag	UNP E8N6F3
E	-3	GLY	-	expression tag	UNP E8N6F3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	SER	-	expression tag	UNP E8N6F3
E	-1	HIS	-	expression tag	UNP E8N6F3
E	0	GLY	-	expression tag	UNP E8N6F3
F	-3	GLY	-	expression tag	UNP E8N6F3
F	-2	SER	-	expression tag	UNP E8N6F3
F	-1	HIS	-	expression tag	UNP E8N6F3
F	0	GLY	-	expression tag	UNP E8N6F3

- Molecule 2 is (3R)-3-HYDROXY-3-METHYL-5-(PHOSPHONOXY)PENTANOIC ACID (three-letter code: PMV) (formula: C₆H₁₃O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
2	A	1	Total	C	H	O	P	0	0
			24	6	10	7	1		
2	B	1	Total	C	H	O	P	0	0
			24	6	10	7	1		
2	C	1	Total	C	H	O	P	0	0
			24	6	10	7	1		
2	D	1	Total	C	H	O	P	0	0
			24	6	10	7	1		
2	E	1	Total	C	H	O	P	0	0
			24	6	10	7	1		
2	F	1	Total	C	H	O	P	0	0
			24	6	10	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	362	Total 362	O 362	0	0
3	B	357	Total 357	O 357	0	0
3	C	352	Total 352	O 352	0	0
3	D	371	Total 371	O 371	0	0
3	E	289	Total 289	O 289	0	0
3	F	298	Total 298	O 298	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 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.60Å 135.63Å 105.70Å 90.00° 97.72° 90.00°	Depositor
Resolution (Å)	37.57 – 1.44	Depositor
% Data completeness (in resolution range)	89.8 (37.57-1.44)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.44Å)	Xtrriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.172 , 0.196	Depositor
Wilson B-factor (Å ²)	18.3	Xtrriage
Anisotropy	0.133	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	31274	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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](#)

6 ligands are modelled in this entry.

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
2	PMV	A	1001	-	12,13,13	1.29	1 (8%)	13,19,19	1.35	3 (23%)
2	PMV	B	401	-	12,13,13	1.13	1 (8%)	13,19,19	1.09	1 (7%)
2	PMV	F	401	-	12,13,13	1.04	1 (8%)	13,19,19	1.38	2 (15%)
2	PMV	E	401	-	12,13,13	1.08	1 (8%)	13,19,19	0.99	0
2	PMV	D	401	-	12,13,13	1.05	0	13,19,19	1.06	1 (7%)
2	PMV	C	401	-	12,13,13	1.17	1 (8%)	13,19,19	1.55	3 (23%)

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	PMV	A	1001	-	-	4/13/13/13	-
2	PMV	B	401	-	-	3/13/13/13	-
2	PMV	F	401	-	-	5/13/13/13	-
2	PMV	E	401	-	-	4/13/13/13	-
2	PMV	D	401	-	-	4/13/13/13	-
2	PMV	C	401	-	-	7/13/13/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PMV	C2-C3	-2.83	1.51	1.54
2	F	401	PMV	C2-C3	-2.77	1.51	1.54
2	B	401	PMV	C2-C3	-2.48	1.52	1.54
2	A	1001	PMV	C2-C3	-2.47	1.52	1.54
2	E	401	PMV	P-OP3	-2.06	1.46	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	PMV	P-O5-C5	2.99	126.53	118.30
2	C	401	PMV	O2-C1-C2	2.78	123.29	114.35
2	A	1001	PMV	P-O5-C5	2.71	125.77	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	PMV	OP2-P-O5	2.36	113.02	106.73
2	F	401	PMV	OP3-P-OP2	2.33	116.52	107.64
2	C	401	PMV	O1-C1-C2	-2.32	116.16	122.94
2	B	401	PMV	P-O5-C5	2.30	124.63	118.30
2	F	401	PMV	OP2-P-O5	-2.21	100.86	106.73
2	A	1001	PMV	OP3-P-O5	-2.05	101.27	106.73
2	D	401	PMV	P-O5-C5	2.01	123.83	118.30

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	PMV	C5-O5-P-OP2
2	A	1001	PMV	C5-O5-P-OP3
2	A	1001	PMV	C5-O5-P-OP1
2	B	401	PMV	C5-O5-P-OP2
2	B	401	PMV	C5-O5-P-OP3
2	B	401	PMV	C5-O5-P-OP1
2	C	401	PMV	C5-O5-P-OP2
2	C	401	PMV	C5-O5-P-OP3
2	C	401	PMV	C5-O5-P-OP1
2	D	401	PMV	C5-O5-P-OP2
2	D	401	PMV	C5-O5-P-OP3
2	D	401	PMV	C5-O5-P-OP1
2	E	401	PMV	C5-O5-P-OP2
2	E	401	PMV	C5-O5-P-OP3
2	E	401	PMV	C5-O5-P-OP1
2	F	401	PMV	C5-O5-P-OP2
2	F	401	PMV	C5-O5-P-OP3
2	F	401	PMV	C5-O5-P-OP1
2	A	1001	PMV	C3A-C3-C4-C5
2	C	401	PMV	C3A-C3-C4-C5
2	D	401	PMV	C3A-C3-C4-C5
2	C	401	PMV	C2-C3-C4-C5
2	F	401	PMV	O2-C1-C2-C3
2	C	401	PMV	O1-C1-C2-C3
2	C	401	PMV	O2-C1-C2-C3
2	E	401	PMV	O2-C1-C2-C3
2	F	401	PMV	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 [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.