wwPDB X-ray Structure Validation Summary Report (i)

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 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 1.44 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
1	A	321	Total	C	H	N	O	S	0	0	0
			4852	1544	2411	427	459	11			
1	B	320	Total	C	H	N	O	S	0	0	0
			4839	1539	2405	426	458	11			
1	C	324	Total	C	H	N	O	S	0	0	0
			4888	1558	2424	431	464	11			
1	D	323	Total	C	H	N	O	S	0	0	0
			4880	1555	2419	431	464	11			
1	E	320	Total	C	H	N	O	S	0	0	0
			4856	1542	2419	427	457	11			
1	F	317	Total	C	H	N	O	S	0	0	0
			4786	1526	2376	419	454	11			

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

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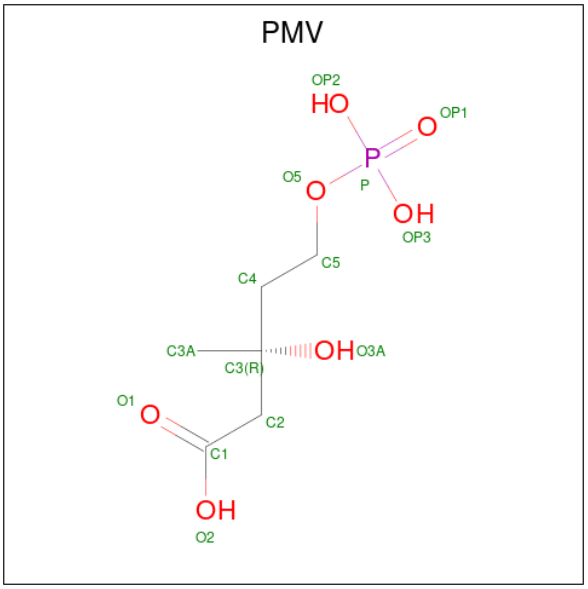
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	SER	-	expression tag	UNP E8N6F3
E	-1	HIS	-	expression tag	UNP E8N6F3
E	0	GLY	-	expression tag	UNP E8N6F3
F	-3	GLY	-	expression tag	UNP E8N6F3
F	-2	SER	-	expression tag	UNP E8N6F3
F	-1	HIS	-	expression tag	UNP E8N6F3
F	0	GLY	-	expression tag	UNP E8N6F3

- Molecule 2 is (3R)-3-HYDROXY-3-METHYL-5-(PHOSPHONOOXY)PENTANOIC ACID (three-letter code: PMV) (formula: $C_6H_{13}O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 O 362 362	0	0
3	B	357	Total O 357 357	0	0
3	C	352	Total O 352 352	0	0
3	D	371	Total O 371 371	0	0
3	E	289	Total O 289 289	0	0
3	F	298	Total O 298 298	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	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
$< I/\sigma(I) >$ [1]	1.94 (at 1.44Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.172 , 0.196	Depositor
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.133	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31274	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage'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.*

[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

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

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 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

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.