Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 02:54 AM EDT

PDB ID	:	6UUG
Title	:	Structure of methanesulfinate monooxygenase MsuC from Pseudomonas fluorescens at 1.69 angstrom resolution
Authors	:	Soule, J.; Gnann, A.D.; Gonzalez, R.; Parker, M.J.; McKenna, K.C.; Nguyen, S.V.; Phan, N.T.; Wicht, D.K.; Dowling, D.P.
Deposited on	:	2019-10-30
Resolution	:	1.69 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 (i)) were used in the production of this report:

MolProbity	:	FAILED
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 1.69 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 2 unique types of molecules in this entry. The entry contains 6483 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 Putative dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	3063	1936	557	563	7	0	6	0
1	B	387	3049	1931	548	563	7	0	5	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q3K9A0
A	-18	GLY	-	expression tag	UNP Q3K9A0
A	-17	SER	-	expression tag	UNP Q3K9A0
A	-16	SER	-	expression tag	UNP Q3K9A0
A	-15	HIS	-	expression tag	UNP Q3K9A0
A	-14	HIS	-	expression tag	UNP Q3K9A0
A	-13	HIS	-	expression tag	UNP Q3K9A0
A	-12	HIS	-	expression tag	UNP Q3K9A0
A	-11	HIS	-	expression tag	UNP Q3K9A0
A	-10	HIS	-	expression tag	UNP Q3K9A0
A	-9	SER	-	expression tag	UNP Q3K9A0
A	-8	SER	-	expression tag	UNP Q3K9A0
A	-7	GLY	-	expression tag	UNP Q3K9A0
A	-6	LEU	-	expression tag	UNP Q3K9A0
A	-5	VAL	-	expression tag	UNP Q3K9A0
A	-4	PRO	-	expression tag	UNP Q3K9A0
A	-3	ARG	-	expression tag	UNP Q3K9A0
A	-2	GLY	-	expression tag	UNP Q3K9A0
A	-1	SER	-	expression tag	UNP Q3K9A0
A	0	HIS	-	expression tag	UNP Q3K9A0
B	-19	MET	-	initiating methionine	UNP Q3K9A0
B	-18	GLY	-	expression tag	UNP Q3K9A0
B	-17	SER	-	expression tag	UNP Q3K9A0
B	-16	SER	-	expression tag	UNP Q3K9A0
B	-15	HIS	-	expression tag	UNP Q3K9A0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q3K9A0
B	-13	HIS	-	expression tag	UNP Q3K9A0
B	-12	HIS	-	expression tag	UNP Q3K9A0
B	-11	HIS	-	expression tag	UNP Q3K9A0
B	-10	HIS	-	expression tag	UNP Q3K9A0
B	-9	SER	-	expression tag	UNP Q3K9A0
B	-8	SER	-	expression tag	UNP Q3K9A0
B	-7	GLY	-	expression tag	UNP Q3K9A0
B	-6	LEU	-	expression tag	UNP Q3K9A0
B	-5	VAL	-	expression tag	UNP Q3K9A0
B	-4	PRO	-	expression tag	UNP Q3K9A0
B	-3	ARG	-	expression tag	UNP Q3K9A0
B	-2	GLY	-	expression tag	UNP Q3K9A0
B	-1	SER	-	expression tag	UNP Q3K9A0
B	0	HIS	-	expression tag	UNP Q3K9A0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	195	195	195	0	3
			Total	O		
2	B	176	176	176	0	1

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 2	Depositor
Cell constants a, b, c, α, β, γ	81.19Å 161.58Å 62.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.05 – 1.69	Depositor
% Data completeness (in resolution range)	99.7 (62.05-1.69)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.185 , 0.208	Depositor
Wilson B-factor (Å^2)	34.9	Xtriage
Anisotropy	0.174	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6483	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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)

There are no ligands in this entry.

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.