Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 12:59 AM EDT

PDB ID	:	6VCZ
Title	:	Crystal structure of Arabidopsis thaliana S-adenosylmethionine Synthase 2 (AtMAT2)
Authors	:	Sekula, B.; Ruszkowski, M.; Dauter, Z.
Deposited on	:	2019-12-23
Resolution	:	1.52 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
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 1.52 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 8 unique types of molecules in this entry. The entry contains 7107 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.

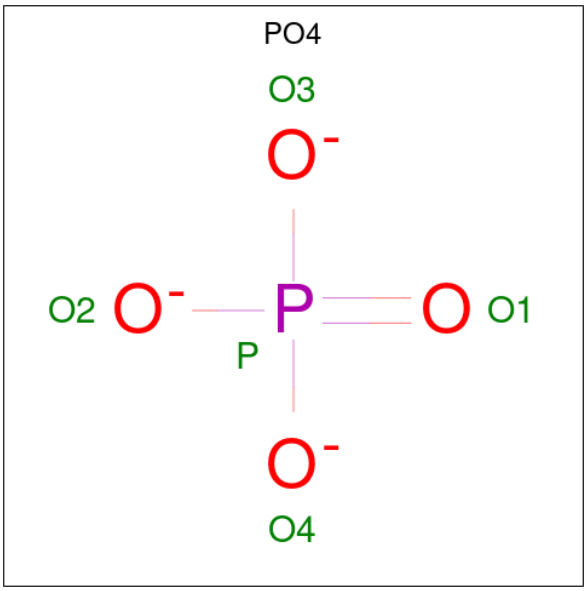
- Molecule 1 is a protein called S-adenosylmethionine synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	378	2976	1883	509	566	18	0	10	0
1	B	380	3012	1908	513	573	18	0	14	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P17562
A	-1	ASN	-	expression tag	UNP P17562
A	0	ALA	-	expression tag	UNP P17562
A	393	LEU	-	expression tag	UNP P17562
A	394	ASN	-	expression tag	UNP P17562
A	395	ASN	-	expression tag	UNP P17562
A	396	ILE	-	expression tag	UNP P17562
A	397	GLY	-	expression tag	UNP P17562
A	398	SER	-	expression tag	UNP P17562
A	399	GLY	-	expression tag	UNP P17562
B	-2	SER	-	expression tag	UNP P17562
B	-1	ASN	-	expression tag	UNP P17562
B	0	ALA	-	expression tag	UNP P17562
B	393	LEU	-	expression tag	UNP P17562
B	394	ASN	-	expression tag	UNP P17562
B	395	ASN	-	expression tag	UNP P17562
B	396	ILE	-	expression tag	UNP P17562
B	397	GLY	-	expression tag	UNP P17562
B	398	SER	-	expression tag	UNP P17562
B	399	GLY	-	expression tag	UNP P17562

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

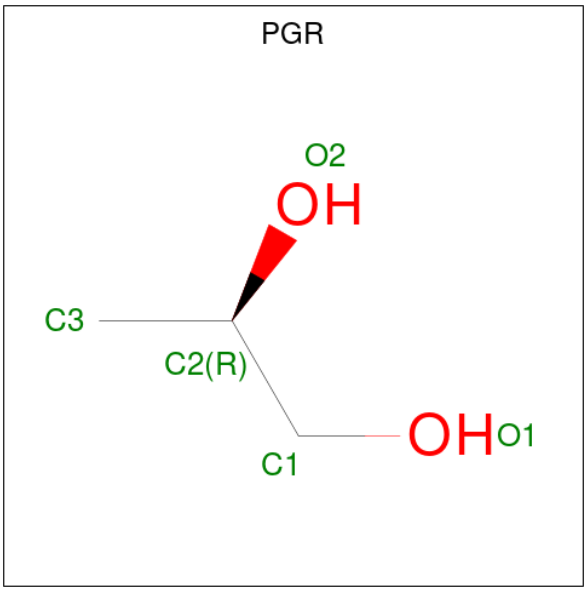


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

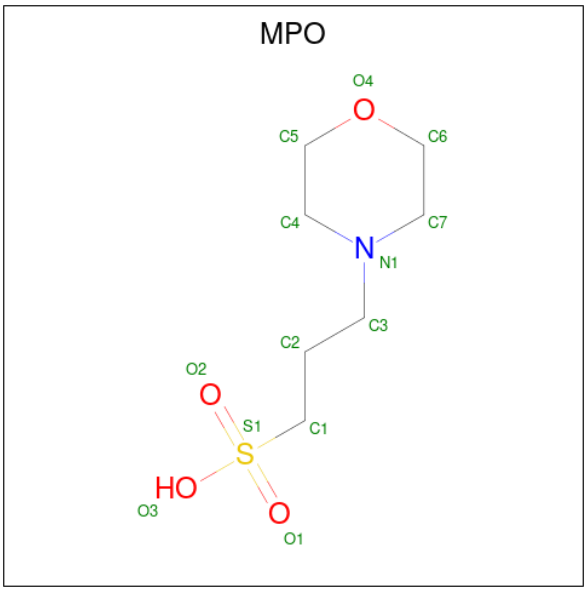
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0
3	B	4	Total Mg 4 4	0	0

- Molecule 4 is R-1,2-PROPANEDIOL (three-letter code: PGR) (formula: $C_3H_8O_2$).



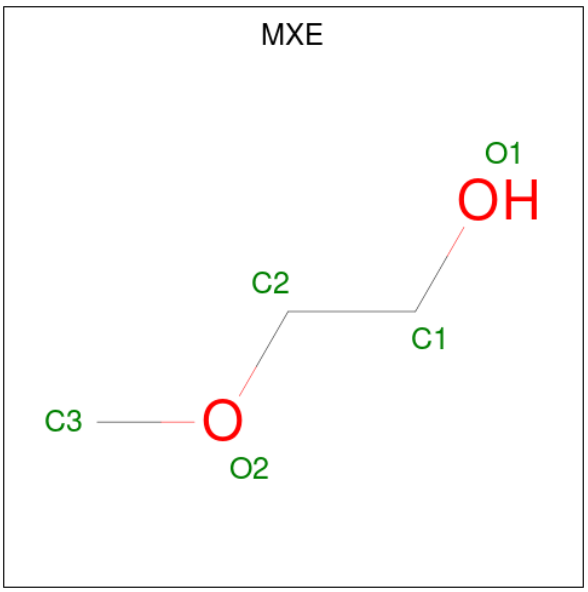
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	5	3	2	0	0
			Total	C	O		
4	B	1	5	3	2	0	0

- Molecule 5 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



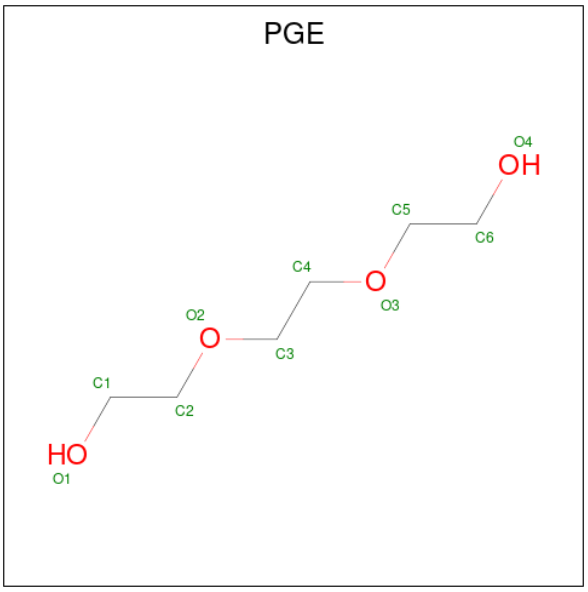
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	13	7	1	4	1	0	0

- Molecule 6 is 2-METHOXYETHANOL (three-letter code: MXE) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 5 3 2	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 10 6 4	0	0
7	B	1	Total C O 10 6 4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	498	501	501	0	3
			Total	O		
8	B	516	523	523	0	7

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	62.80Å 99.28Å 86.93Å 90.00° 109.74° 90.00°	Depositor
Resolution (Å)	42.44 – 1.52	Depositor
% Data completeness (in resolution range)	99.8 (42.44-1.52)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.160 , 0.180	Depositor
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.099	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
Total number of atoms	7107	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.26% 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 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
2	PO4	B	404	3	4,4,4	0.56	0	6,6,6	0.37	0
4	PGR	A	408	-	3,4,4	0.23	0	1,4,4	0.08	0
6	MXE	B	410	-	4,4,4	0.06	0	3,3,3	0.27	0
2	PO4	A	404	-	4,4,4	1.02	0	6,6,6	0.51	0
4	PGR	B	411	-	3,4,4	0.27	0	1,4,4	0.33	0
2	PO4	A	403	-	4,4,4	0.69	0	6,6,6	0.46	0
2	PO4	B	402	3	4,4,4	0.70	0	6,6,6	0.92	0
5	MPO	B	409	-	13,13,13	0.82	1 (7%)	17,17,17	1.10	2 (11%)
7	PGE	B	412	-	9,9,9	0.23	0	8,8,8	0.26	0
2	PO4	A	401	3	4,4,4	1.16	0	6,6,6	0.47	0
2	PO4	B	403	-	4,4,4	0.91	0	6,6,6	0.70	0
2	PO4	A	402	3	4,4,4	1.03	0	6,6,6	0.73	0
2	PO4	B	401	3	4,4,4	1.19	0	6,6,6	0.53	0
7	PGE	B	413	-	9,9,9	0.25	0	8,8,8	0.23	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
4	PGR	A	408	-	-	0/2/2/2	-
7	PGE	B	412	-	-	4/7/7/7	-
4	PGR	B	411	-	-	1/2/2/2	-
5	MPO	B	409	-	-	4/7/15/15	0/1/1/1
6	MXE	B	410	-	-	1/2/2/2	-
7	PGE	B	413	-	-	4/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	409	MPO	O2-S1	2.51	1.52	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	409	MPO	O3-S1-O1	2.85	118.24	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	409	MPO	C2-C1-S1	-2.15	109.96	113.25

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	411	PGR	O1-C1-C2-O2
5	B	409	MPO	C2-C3-N1-C7
7	B	412	PGE	O1-C1-C2-O2
7	B	412	PGE	O3-C5-C6-O4
7	B	413	PGE	O2-C3-C4-O3
5	B	409	MPO	C2-C3-N1-C4
7	B	412	PGE	O2-C3-C4-O3
7	B	413	PGE	O1-C1-C2-O2
7	B	413	PGE	O3-C5-C6-O4
5	B	409	MPO	C1-C2-C3-N1
7	B	412	PGE	C3-C4-O3-C5
7	B	413	PGE	C3-C4-O3-C5
5	B	409	MPO	S1-C1-C2-C3
6	B	410	MXE	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 (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.