wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 06:10 PM EST

PDB ID	:	3IWB
Title	:	T. maritima AdoMetDC in processed form
Authors	:	Bale, S.; Kavita, B.; Ealick, S.E.
Deposited on	:	2009-09-02
Resolution	:	2.06 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 (1)) were used in the production of this report:

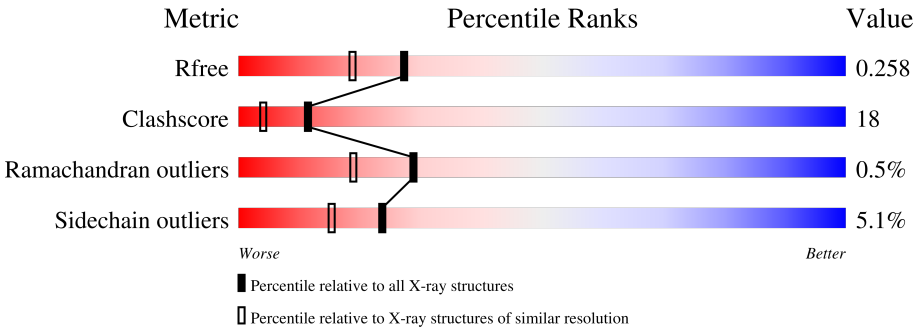
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.06 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	B	62	63% 32% 5%
1	D	62	61% 29% 5% 5%
2	A	68	54% 25% • 18%
2	C	68	51% 28% •• 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1983 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 decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	59	Total	C	N	O	S	0	0	0
			467	298	78	89	2			
1	D	59	Total	C	N	O	S	0	0	0
			467	298	78	89	2			

- Molecule 2 is a protein called S-adenosylmethionine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	56	Total	C	N	O	S	0	0	0
			467	302	81	83	1			
2	C	56	Total	C	N	O	S	0	0	0
			467	302	81	83	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	PYR	-	insertion	UNP Q9WZC3
C	63	PYR	-	insertion	UNP Q9WZC3

- Molecule 3 is water.

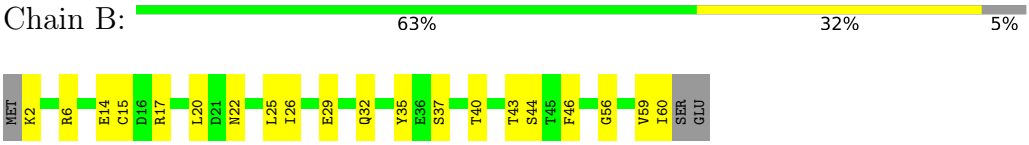
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	40	Total	O	0	0
			40	40		
3	A	21	Total	O	0	0
			21	21		
3	D	32	Total	O	0	0
			32	32		
3	C	22	Total	O	0	0
			22	22		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

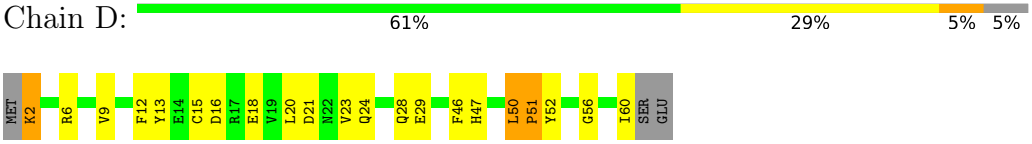
• Molecule 1: S-adenosylmethionine decarboxylase

Chain B:



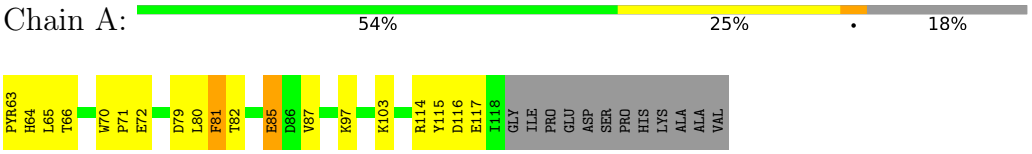
• Molecule 1: S-adenosylmethionine decarboxylase

Chain D:



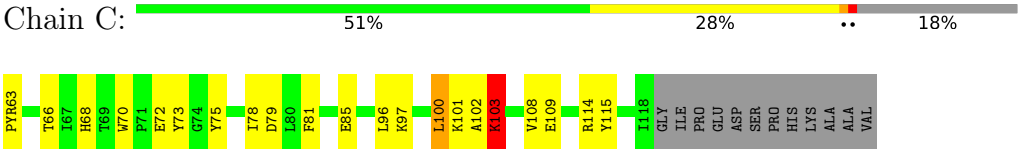
• Molecule 2: S-adenosylmethionine decarboxylase

Chain A:



• Molecule 2: S-adenosylmethionine decarboxylase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	104.71Å 104.71Å 69.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.03 – 2.06 38.03 – 2.06	Depositor EDS
% Data completeness (in resolution range)	94.5 (38.03-2.06) 94.6 (38.03-2.06)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.06Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.233 , 0.262 0.228 , 0.258	Depositor DCC
R_{free} test set	823 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 31.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.314 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1983	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYR

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.65	2/475 (0.4%)	0.66	0/642
1	D	0.55	1/475 (0.2%)	0.61	0/642
2	A	0.35	0/477	0.60	0/646
2	C	0.64	2/477 (0.4%)	0.75	0/646
All	All	0.56	5/1904 (0.3%)	0.66	0/2576

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	100	LEU	C-O	-6.00	1.11	1.23
2	C	103	LYS	C-O	-5.59	1.12	1.23
1	D	28	GLN	CD-OE1	-5.33	1.12	1.24
1	B	37	SER	CB-OG	-5.13	1.35	1.42
1	B	37	SER	C-O	-5.10	1.13	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	467	0	460	19	0
1	D	467	0	460	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	467	0	443	24	0
2	C	467	0	443	21	0
3	A	21	0	0	0	0
3	B	40	0	0	0	0
3	C	22	0	0	1	0
3	D	32	0	0	1	0
All	All	1983	0	1806	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 65 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:114:ARG:HD3	3:C:26:HOH:O	1.58	1.01
2:A:65:LEU:HD23	2:A:80:LEU:HA	1.45	0.99
2:A:65:LEU:HD22	2:A:80:LEU:CD2	1.93	0.97
2:A:65:LEU:HD22	2:A:80:LEU:HD22	1.49	0.91
2:A:65:LEU:CD2	2:A:80:LEU:HA	2.12	0.79

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	57/62 (92%)	57 (100%)	0	0	100 100
1	D	57/62 (92%)	55 (96%)	1 (2%)	1 (2%)	8 2
2	A	54/68 (79%)	54 (100%)	0	0	100 100
2	C	54/68 (79%)	53 (98%)	1 (2%)	0	100 100
All	All	222/260 (85%)	219 (99%)	2 (1%)	1 (0%)	29 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	51	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	51/54 (94%)	50 (98%)	1 (2%)	55 51
1	D	51/54 (94%)	48 (94%)	3 (6%)	19 11
2	A	47/56 (84%)	44 (94%)	3 (6%)	17 9
2	C	47/56 (84%)	44 (94%)	3 (6%)	17 9
All	All	196/220 (89%)	186 (95%)	10 (5%)	24 15

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	81	PHE
2	C	85	GLU
2	C	103	LYS
2	A	97	LYS
1	D	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	GLN
1	B	32	GLN
1	D	32	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.