



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:32 PM UTC

PDB ID : 8Z9U / pdb_00008z9u
Title : Crystal structure of the Methermicoccus shengliensis ZC-1 2-methoxybenzoic acid methyltransferase (MtxA)
Authors : Yang, Q.; Wang, S.X.; Bai, L.P.
Deposited on : 2024-04-23
Resolution : 1.91 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

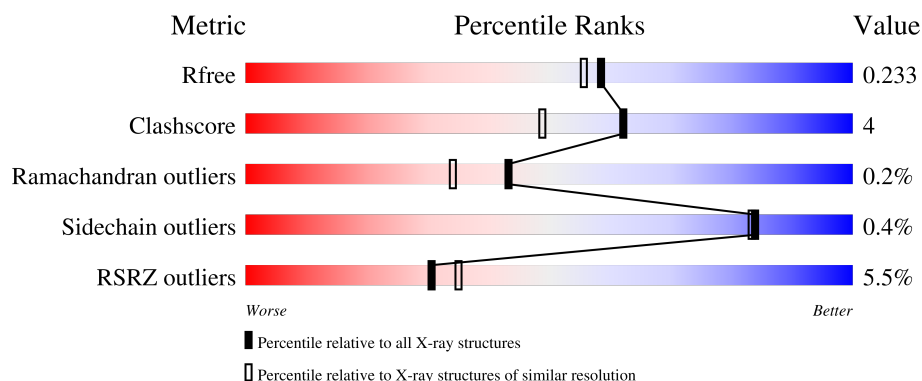
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	3% 74% 7% 19%
1	B	344	6% 76% 8% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4628 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 Tetrahydromethanopterin S-methyltransferase subunit H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	287	Total	C	N	O	S	0	0	0
			2196	1417	350	422	7			
1	A	279	Total	C	N	O	S	0	0	0
			2141	1381	341	411	8			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	290	MET	-	expression tag	UNP A0A832VZ83
B	291	GLY	-	expression tag	UNP A0A832VZ83
B	292	TRP	-	expression tag	UNP A0A832VZ83
B	293	SER	-	expression tag	UNP A0A832VZ83
B	294	HIS	-	expression tag	UNP A0A832VZ83
B	295	PRO	-	expression tag	UNP A0A832VZ83
B	296	GLN	-	expression tag	UNP A0A832VZ83
B	297	PHE	-	expression tag	UNP A0A832VZ83
B	298	GLU	-	expression tag	UNP A0A832VZ83
B	299	LYS	-	expression tag	UNP A0A832VZ83
B	300	GLY	-	expression tag	UNP A0A832VZ83
B	301	GLY	-	expression tag	UNP A0A832VZ83
B	302	GLY	-	expression tag	UNP A0A832VZ83
B	303	SER	-	expression tag	UNP A0A832VZ83
B	304	GLY	-	expression tag	UNP A0A832VZ83
B	305	GLY	-	expression tag	UNP A0A832VZ83
B	306	GLY	-	expression tag	UNP A0A832VZ83
B	307	SER	-	expression tag	UNP A0A832VZ83
B	308	GLY	-	expression tag	UNP A0A832VZ83
B	309	GLY	-	expression tag	UNP A0A832VZ83
B	310	SER	-	expression tag	UNP A0A832VZ83
B	311	SER	-	expression tag	UNP A0A832VZ83
B	312	ALA	-	expression tag	UNP A0A832VZ83
B	313	TRP	-	expression tag	UNP A0A832VZ83
B	314	SER	-	expression tag	UNP A0A832VZ83

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Chain	Residue	Modelled	Actual	Comment	Reference
B	315	HIS	-	expression tag	UNP A0A832VZ83
B	316	PRO	-	expression tag	UNP A0A832VZ83
B	317	GLN	-	expression tag	UNP A0A832VZ83
B	318	PHE	-	expression tag	UNP A0A832VZ83
B	319	GLU	-	expression tag	UNP A0A832VZ83
B	320	LYS	-	expression tag	UNP A0A832VZ83
B	321	ASP	-	expression tag	UNP A0A832VZ83
B	322	TYR	-	expression tag	UNP A0A832VZ83
B	323	LYS	-	expression tag	UNP A0A832VZ83
B	324	ASP	-	expression tag	UNP A0A832VZ83
B	325	ASP	-	expression tag	UNP A0A832VZ83
B	326	ASP	-	expression tag	UNP A0A832VZ83
B	327	ASP	-	expression tag	UNP A0A832VZ83
B	328	LYS	-	expression tag	UNP A0A832VZ83
B	329	ASP	-	expression tag	UNP A0A832VZ83
B	330	TYR	-	expression tag	UNP A0A832VZ83
B	331	LYS	-	expression tag	UNP A0A832VZ83
B	332	ASP	-	expression tag	UNP A0A832VZ83
B	333	ASP	-	expression tag	UNP A0A832VZ83
B	334	ASP	-	expression tag	UNP A0A832VZ83
B	335	ASP	-	expression tag	UNP A0A832VZ83
B	336	LYS	-	expression tag	UNP A0A832VZ83
B	337	ASP	-	expression tag	UNP A0A832VZ83
B	338	TYR	-	expression tag	UNP A0A832VZ83
B	339	LYS	-	expression tag	UNP A0A832VZ83
B	340	ASP	-	expression tag	UNP A0A832VZ83
B	341	ASP	-	expression tag	UNP A0A832VZ83
B	342	ASP	-	expression tag	UNP A0A832VZ83
B	343	ASP	-	expression tag	UNP A0A832VZ83
B	344	LYS	-	expression tag	UNP A0A832VZ83
A	290	MET	-	expression tag	UNP A0A832VZ83
A	291	GLY	-	expression tag	UNP A0A832VZ83
A	292	TRP	-	expression tag	UNP A0A832VZ83
A	293	SER	-	expression tag	UNP A0A832VZ83
A	294	HIS	-	expression tag	UNP A0A832VZ83
A	295	PRO	-	expression tag	UNP A0A832VZ83
A	296	GLN	-	expression tag	UNP A0A832VZ83
A	297	PHE	-	expression tag	UNP A0A832VZ83
A	298	GLU	-	expression tag	UNP A0A832VZ83
A	299	LYS	-	expression tag	UNP A0A832VZ83
A	300	GLY	-	expression tag	UNP A0A832VZ83
A	301	GLY	-	expression tag	UNP A0A832VZ83

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Chain	Residue	Modelled	Actual	Comment	Reference
A	302	GLY	-	expression tag	UNP A0A832VZ83
A	303	SER	-	expression tag	UNP A0A832VZ83
A	304	GLY	-	expression tag	UNP A0A832VZ83
A	305	GLY	-	expression tag	UNP A0A832VZ83
A	306	GLY	-	expression tag	UNP A0A832VZ83
A	307	SER	-	expression tag	UNP A0A832VZ83
A	308	GLY	-	expression tag	UNP A0A832VZ83
A	309	GLY	-	expression tag	UNP A0A832VZ83
A	310	SER	-	expression tag	UNP A0A832VZ83
A	311	SER	-	expression tag	UNP A0A832VZ83
A	312	ALA	-	expression tag	UNP A0A832VZ83
A	313	TRP	-	expression tag	UNP A0A832VZ83
A	314	SER	-	expression tag	UNP A0A832VZ83
A	315	HIS	-	expression tag	UNP A0A832VZ83
A	316	PRO	-	expression tag	UNP A0A832VZ83
A	317	GLN	-	expression tag	UNP A0A832VZ83
A	318	PHE	-	expression tag	UNP A0A832VZ83
A	319	GLU	-	expression tag	UNP A0A832VZ83
A	320	LYS	-	expression tag	UNP A0A832VZ83
A	321	ASP	-	expression tag	UNP A0A832VZ83
A	322	TYR	-	expression tag	UNP A0A832VZ83
A	323	LYS	-	expression tag	UNP A0A832VZ83
A	324	ASP	-	expression tag	UNP A0A832VZ83
A	325	ASP	-	expression tag	UNP A0A832VZ83
A	326	ASP	-	expression tag	UNP A0A832VZ83
A	327	ASP	-	expression tag	UNP A0A832VZ83
A	328	LYS	-	expression tag	UNP A0A832VZ83
A	329	ASP	-	expression tag	UNP A0A832VZ83
A	330	TYR	-	expression tag	UNP A0A832VZ83
A	331	LYS	-	expression tag	UNP A0A832VZ83
A	332	ASP	-	expression tag	UNP A0A832VZ83
A	333	ASP	-	expression tag	UNP A0A832VZ83
A	334	ASP	-	expression tag	UNP A0A832VZ83
A	335	ASP	-	expression tag	UNP A0A832VZ83
A	336	LYS	-	expression tag	UNP A0A832VZ83
A	337	ASP	-	expression tag	UNP A0A832VZ83
A	338	TYR	-	expression tag	UNP A0A832VZ83
A	339	LYS	-	expression tag	UNP A0A832VZ83
A	340	ASP	-	expression tag	UNP A0A832VZ83
A	341	ASP	-	expression tag	UNP A0A832VZ83
A	342	ASP	-	expression tag	UNP A0A832VZ83
A	343	ASP	-	expression tag	UNP A0A832VZ83

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Chain	Residue	Modelled	Actual	Comment	Reference
A	344	LYS	-	expression tag	UNP A0A832VZ83

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	131	Total 131	O 131	0	0
2	A	160	Total 160	O 160	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.72Å 83.21Å 132.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.01 – 1.91 39.01 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.01-1.91) 100.0 (39.01-1.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.91Å)	Xtriage
Refinement program	PHENIX v1.20.1_4487	Depositor
R, R_{free}	0.212 , 0.233 0.212 , 0.233	Depositor DCC
R_{free} test set	3494 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4628	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 4.68% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	A	0.30	0/2180	0.54	0/2940
1	B	0.33	0/2235	0.61	4/3016 (0.1%)
All	All	0.32	0/4415	0.57	4/5956 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	TYR	CA-C-N	-5.90	105.34	122.46
1	B	209	TYR	C-N-CA	-5.90	105.34	122.46
1	B	216	GLY	CA-C-N	-5.64	113.69	122.37
1	B	216	GLY	C-N-CA	-5.64	113.69	122.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	A	2141	0	2183	19	0
1	B	2196	0	2237	18	0
2	A	160	0	0	5	0
2	B	131	0	0	6	0
All	All	4628	0	4420	36	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 4.

All (36) 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)
1:B:16:ASN:OD1	2:B:401:HOH:O	1.80	0.98
1:B:11:GLU:OE2	2:B:402:HOH:O	1.95	0.83
1:B:8:LYS:HG3	1:B:210:GLY:HA3	1.71	0.72
1:A:84:ARG:NH1	2:A:401:HOH:O	1.96	0.69
1:B:234:GLU:OE1	2:B:403:HOH:O	2.09	0.69
1:A:279:TYR:O	2:A:402:HOH:O	2.15	0.64
1:B:135:ASP:O	1:B:139:GLU:HG3	2.02	0.60
1:B:217:ALA:CB	1:B:243:ALA:HB1	2.32	0.59
1:B:9:ALA:HB1	1:B:16:ASN:HD21	1.68	0.56
1:A:43:GLU:HG3	2:A:486:HOH:O	2.07	0.54
1:A:200:LYS:O	1:A:204:GLU:HG3	2.08	0.54
2:B:500:HOH:O	1:A:192:VAL:HG11	2.08	0.52
1:A:84:ARG:NH2	2:A:403:HOH:O	2.26	0.50
1:A:42:ASP:OD2	1:A:45:LYS:HD2	2.13	0.48
1:A:218:HIS:HE1	1:A:256:LEU:O	1.96	0.48
1:A:113:GLU:HB2	2:A:401:HOH:O	2.15	0.47
1:A:88:GLU:HB2	1:A:114:TYR:OH	2.15	0.47
1:A:237:LYS:HE3	1:A:262:ASP:OD1	2.16	0.46
1:B:217:ALA:HB1	1:B:243:ALA:HB1	1.97	0.46
1:B:191:ASP:CG	1:B:193:PRO:HD2	2.39	0.46
1:A:78:MET:HE3	1:A:78:MET:HB3	1.69	0.45
1:B:161:SER:OG	1:B:200:LYS:HD3	2.15	0.45
1:B:83:ILE:O	1:B:87:MET:HG3	2.17	0.45
1:B:120:LEU:O	1:B:124:ILE:HG12	2.17	0.45
1:A:165:ILE:HD11	1:A:204:GLU:HB2	2.00	0.44
1:B:58:LYS:O	1:B:62:GLU:HG3	2.17	0.43
1:A:217:ALA:O	1:A:218:HIS:C	2.61	0.43
1:B:96:LYS:NZ	2:B:408:HOH:O	2.44	0.43
1:B:275:THR:HB	2:B:500:HOH:O	2.18	0.43
1:B:289:ILE:HG23	1:A:250:LEU:HD13	1.99	0.43
1:A:218:HIS:CE1	1:A:256:LEU:O	2.72	0.42
1:B:8:LYS:HG3	1:B:210:GLY:CA	2.45	0.42
1:A:242:MET:HE3	1:A:242:MET:HA	2.02	0.42
1:B:217:ALA:O	1:B:220:ALA:N	2.49	0.42
1:A:61:GLU:OE2	1:A:94:THR:OG1	2.36	0.41
1:A:216:GLY:HA3	1:A:256:LEU:O	2.21	0.41

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	A	277/344 (80%)	270 (98%)	6 (2%)	1 (0%)	30	19
1	B	285/344 (83%)	281 (99%)	4 (1%)	0	100	100
All	All	562/688 (82%)	551 (98%)	10 (2%)	1 (0%)	43	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	ASN

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	A	228/283 (81%)	227 (100%)	1 (0%)	84	83
1	B	233/283 (82%)	232 (100%)	1 (0%)	84	83
All	All	461/566 (81%)	459 (100%)	2 (0%)	84	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	PHE
1	A	124	ILE

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	16	ASN
1	A	69	ASN
1	A	145	ASN

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 oligosaccharides 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	279/344 (81%)	0.21	12 (4%) 40 44	18, 25, 36, 62	0
1	B	287/344 (83%)	0.35	19 (6%) 24 29	18, 26, 40, 54	0
All	All	566/688 (82%)	0.28	31 (5%) 30 35	18, 26, 39, 62	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	8.1
1	B	4	PHE	7.3
1	B	232	GLY	6.2
1	B	218	HIS	5.5
1	B	224	TRP	5.2
1	B	156	PHE	5.1
1	A	218	HIS	4.3
1	B	3	ARG	4.1
1	B	217	ALA	4.0
1	B	210	GLY	3.6
1	A	2	PHE	3.5
1	B	219	ASN	3.4
1	A	156	PHE	3.0
1	A	222	ALA	3.0
1	B	225	LYS	2.9
1	A	279	TYR	2.7
1	A	95	ASP	2.6
1	A	217	ALA	2.6
1	A	154	TYR	2.5
1	B	289	ILE	2.5
1	A	219	ASN	2.4
1	B	223	SER	2.4
1	B	234	GLU	2.2
1	A	113	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	5	GLY	2.2
1	B	279	TYR	2.1
1	A	65	ASP	2.1
1	B	190	MET	2.1
1	B	222	ALA	2.1
1	B	157	ASN	2.0
1	B	159	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.