



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 9, 2023 – 09:15 pm GMT

PDB ID : 7QRH
Title : Crystal structure of the 5-(aminomethyl)furan-3-yl methyl phosphate kinase MfnE from *Methanococcus vannielii*.
Authors : Maddock, R.M.A.; Race, P.R.; Burton, N.M.
Deposited on : 2022-01-11
Resolution : 2.36 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

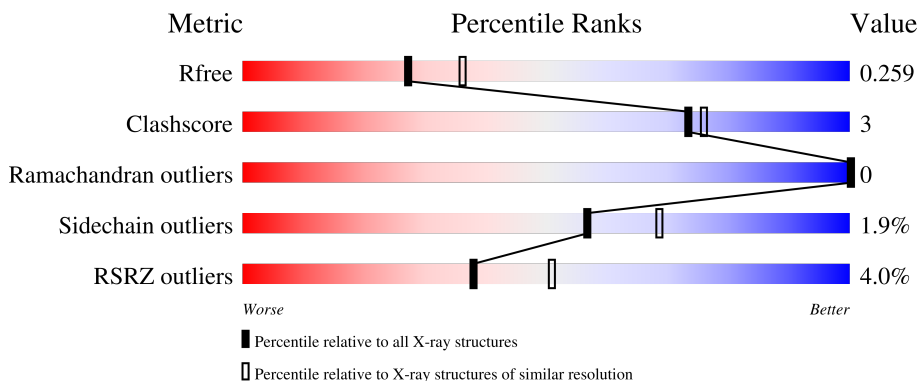
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	AAA	228	
1	BBB	228	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6643 atoms, of which 3371 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 Aspartate/glutamate/uridylylate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	209	3293	1040	1679	261	309	4	78	0	0
1	BBB	211	3322	1048	1692	263	315	4	78	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-18	MET	-	initiating methionine	UNP A6UQ44
AAA	-17	ALA	-	expression tag	UNP A6UQ44
AAA	-16	HIS	-	expression tag	UNP A6UQ44
AAA	-15	HIS	-	expression tag	UNP A6UQ44
AAA	-14	HIS	-	expression tag	UNP A6UQ44
AAA	-13	HIS	-	expression tag	UNP A6UQ44
AAA	-12	HIS	-	expression tag	UNP A6UQ44
AAA	-11	HIS	-	expression tag	UNP A6UQ44
AAA	-10	SER	-	expression tag	UNP A6UQ44
AAA	-9	SER	-	expression tag	UNP A6UQ44
AAA	-8	GLY	-	expression tag	UNP A6UQ44
AAA	-7	LEU	-	expression tag	UNP A6UQ44
AAA	-6	GLU	-	expression tag	UNP A6UQ44
AAA	-5	VAL	-	expression tag	UNP A6UQ44
AAA	-4	LEU	-	expression tag	UNP A6UQ44
AAA	-3	PHE	-	expression tag	UNP A6UQ44
AAA	-2	GLN	-	expression tag	UNP A6UQ44
AAA	-1	GLY	-	expression tag	UNP A6UQ44
AAA	0	PRO	-	expression tag	UNP A6UQ44
BBB	-18	MET	-	initiating methionine	UNP A6UQ44
BBB	-17	ALA	-	expression tag	UNP A6UQ44
BBB	-16	HIS	-	expression tag	UNP A6UQ44
BBB	-15	HIS	-	expression tag	UNP A6UQ44
BBB	-14	HIS	-	expression tag	UNP A6UQ44
BBB	-13	HIS	-	expression tag	UNP A6UQ44

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-12	HIS	-	expression tag	UNP A6UQ44
BBB	-11	HIS	-	expression tag	UNP A6UQ44
BBB	-10	SER	-	expression tag	UNP A6UQ44
BBB	-9	SER	-	expression tag	UNP A6UQ44
BBB	-8	GLY	-	expression tag	UNP A6UQ44
BBB	-7	LEU	-	expression tag	UNP A6UQ44
BBB	-6	GLU	-	expression tag	UNP A6UQ44
BBB	-5	VAL	-	expression tag	UNP A6UQ44
BBB	-4	LEU	-	expression tag	UNP A6UQ44
BBB	-3	PHE	-	expression tag	UNP A6UQ44
BBB	-2	GLN	-	expression tag	UNP A6UQ44
BBB	-1	GLY	-	expression tag	UNP A6UQ44
BBB	0	PRO	-	expression tag	UNP A6UQ44

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	8	Total	O	0	0
			8	8		

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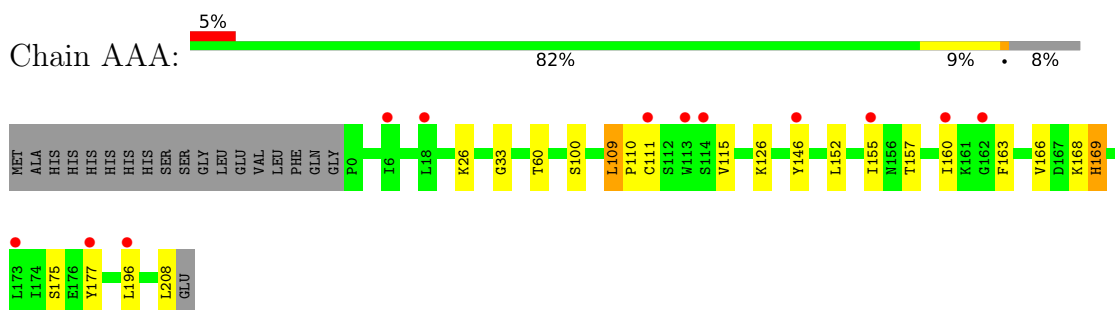
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	BBB	10	Total	O	0	0
			10	10		

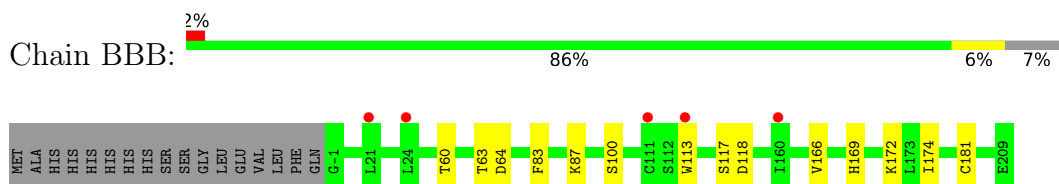
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Aspartate/glutamate/uridylylate kinase



- Molecule 1: Aspartate/glutamate/uridylylate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.15Å 86.15Å 234.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.72 – 2.36 74.61 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.5 (74.72-2.36) 99.6 (74.61-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.37Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.204 , 0.258 0.210 , 0.259	Depositor DCC
R_{free} test set	1097 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtrriage
Anisotropy	0.184	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6643	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.91% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	AAA	0.71	0/1640	0.85	0/2221
1	BBB	0.72	0/1656	0.83	0/2242
All	All	0.72	0/3296	0.84	0/4463

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	1614	1679	1674	15	0
1	BBB	1630	1692	1688	7	0
2	AAA	5	0	0	1	0
2	BBB	5	0	0	0	0
3	AAA	8	0	0	0	0
3	BBB	10	0	0	0	0
All	All	3272	3371	3362	22	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 3.

All (22) 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:AAA:110:PRO:HD2	1:AAA:169:HIS:NE2	1.95	0.80
1:AAA:110:PRO:HD2	1:AAA:169:HIS:HE2	1.45	0.79
1:BBB:64:ASP:OD2	1:BBB:100:SER:HB3	1.92	0.69
1:AAA:109:LEU:HD12	1:AAA:109:LEU:H	1.66	0.58
1:BBB:60:THR:CG2	1:BBB:100:SER:HA	2.36	0.56
1:AAA:60:THR:HG22	1:AAA:100:SER:HB2	1.88	0.54
1:AAA:126:LYS:HG3	1:AAA:177:TYR:CD2	2.45	0.51
1:AAA:110:PRO:O	1:AAA:115:VAL:HG21	2.12	0.50
1:BBB:118:ASP:OD2	1:BBB:166:VAL:HA	2.11	0.50
1:AAA:157:THR:O	1:AAA:160:ILE:HG22	2.12	0.49
1:AAA:26:LYS:HE2	1:AAA:196:LEU:O	2.14	0.47
1:AAA:110:PRO:HD2	1:AAA:169:HIS:CE1	2.50	0.46
1:BBB:174:ILE:HD12	1:BBB:181:CYS:HB2	1.99	0.45
1:AAA:33:GLY:HA3	2:AAA:301:SO4:O4	2.17	0.45
1:AAA:152:LEU:HD13	1:AAA:155:ILE:HD13	1.98	0.44
1:AAA:160:ILE:HD11	1:AAA:166:VAL:HG21	2.01	0.43
1:BBB:169:HIS:ND1	1:BBB:172:LYS:NZ	2.67	0.43
1:AAA:60:THR:HG22	1:AAA:100:SER:CB	2.49	0.43
1:BBB:63:THR:HG21	1:BBB:117:SER:OG	2.18	0.43
1:BBB:83:PHE:CE1	1:BBB:87:LYS:HE3	2.56	0.41
1:AAA:175:SER:HB2	1:AAA:208:LEU:HD13	2.02	0.40
1:AAA:175:SER:CB	1:AAA:208:LEU:HD13	2.52	0.40

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	AAA	207/228 (91%)	199 (96%)	8 (4%)	0	100	100
1	BBB	209/228 (92%)	202 (97%)	7 (3%)	0	100	100
All	All	416/456 (91%)	401 (96%)	15 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	184/202 (91%)	178 (97%)	6 (3%)	38	46
1	BBB	186/202 (92%)	185 (100%)	1 (0%)	88	94
All	All	370/404 (92%)	363 (98%)	7 (2%)	57	68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	109	LEU
1	AAA	111	CYS
1	AAA	146	TYR
1	AAA	163	PHE
1	AAA	168	LYS
1	AAA	169	HIS
1	BBB	113	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

2 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	SO4	BBB	301	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	AAA	301	-	4,4,4	0.33	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	301	SO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	209/228 (91%)	0.55	12 (5%) 23 34	63, 81, 145, 170	0
1	BBB	211/228 (92%)	0.51	5 (2%) 59 68	60, 75, 108, 138	0
All	All	420/456 (92%)	0.53	17 (4%) 38 51	60, 78, 135, 170	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	160	ILE	5.4
1	AAA	114	SER	5.3
1	AAA	113	TRP	5.1
1	BBB	113	TRP	4.4
1	AAA	146	TYR	4.1
1	AAA	18	LEU	3.1
1	BBB	111	CYS	2.9
1	AAA	155	ILE	2.6
1	AAA	162	GLY	2.5
1	BBB	160	ILE	2.4
1	AAA	173	LEU	2.3
1	AAA	111	CYS	2.3
1	BBB	24	LEU	2.2
1	BBB	21	LEU	2.1
1	AAA	6	ILE	2.1
1	AAA	177	TYR	2.1
1	AAA	196	LEU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	AAA	301	5/5	0.92	0.13	98,116,134,135	0
2	SO4	BBB	301	5/5	0.96	0.15	95,99,105,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.