



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 28, 2022 – 12:03 AM JST

PDB ID : 7VG4
Title : 10,5-methenyltetrahydrofolate cyclohydrolase from *Methylobacterium extorquens* AM1 strain
Authors : Kim, S.; Lee, S.; Kim, I.-K.; Seo, H.; Kim, K.-J.
Deposited on : 2021-09-14
Resolution : 2.77 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 ⓘ 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
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

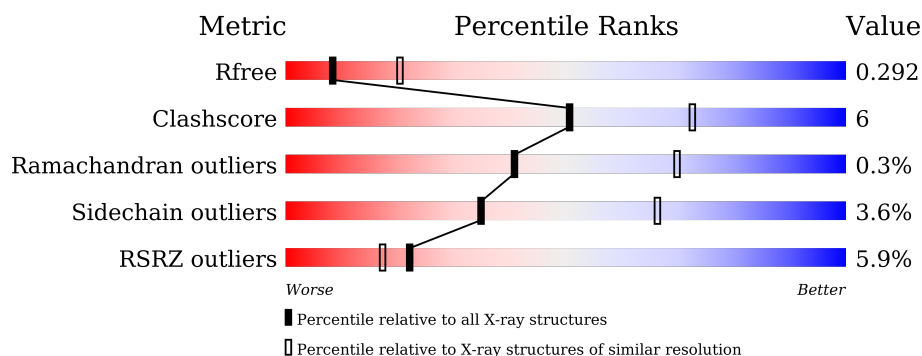
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	216	<div> <div>79%</div> <div>15%</div> <div>6%</div> </div>
1	B	216	<div> <div>4%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
1	C	216	<div> <div>6%</div> <div>81%</div> <div>13%</div> <div>5%</div> </div>
1	D	216	<div> <div>4%</div> <div>76%</div> <div>18%</div> <div>6%</div> </div>
1	E	216	<div> <div>4%</div> <div>75%</div> <div>16%</div> <div>9%</div> </div>
1	F	216	<div> <div>13%</div> <div>70%</div> <div>15%</div> <div>14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8805 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 Methenyltetrahydrofolate cyclohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1485	924	254	299	8			
1	B	206	Total	C	N	O	S	0	0	0
			1504	935	258	303	8			
1	C	205	Total	C	N	O	S	0	0	0
			1500	933	257	302	8			
1	D	204	Total	C	N	O	S	0	0	0
			1492	929	255	300	8			
1	E	196	Total	C	N	O	S	0	0	0
			1420	883	244	285	8			
1	F	186	Total	C	N	O	S	0	0	0
			1343	832	232	271	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	LEU	-	expression tag	UNP Q49135
A	210	GLU	-	expression tag	UNP Q49135
A	211	HIS	-	expression tag	UNP Q49135
A	212	HIS	-	expression tag	UNP Q49135
A	213	HIS	-	expression tag	UNP Q49135
A	214	HIS	-	expression tag	UNP Q49135
A	215	HIS	-	expression tag	UNP Q49135
A	216	HIS	-	expression tag	UNP Q49135
B	209	LEU	-	expression tag	UNP Q49135
B	210	GLU	-	expression tag	UNP Q49135
B	211	HIS	-	expression tag	UNP Q49135
B	212	HIS	-	expression tag	UNP Q49135
B	213	HIS	-	expression tag	UNP Q49135
B	214	HIS	-	expression tag	UNP Q49135
B	215	HIS	-	expression tag	UNP Q49135
B	216	HIS	-	expression tag	UNP Q49135
C	209	LEU	-	expression tag	UNP Q49135

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Chain	Residue	Modelled	Actual	Comment	Reference
C	210	GLU	-	expression tag	UNP Q49135
C	211	HIS	-	expression tag	UNP Q49135
C	212	HIS	-	expression tag	UNP Q49135
C	213	HIS	-	expression tag	UNP Q49135
C	214	HIS	-	expression tag	UNP Q49135
C	215	HIS	-	expression tag	UNP Q49135
C	216	HIS	-	expression tag	UNP Q49135
D	209	LEU	-	expression tag	UNP Q49135
D	210	GLU	-	expression tag	UNP Q49135
D	211	HIS	-	expression tag	UNP Q49135
D	212	HIS	-	expression tag	UNP Q49135
D	213	HIS	-	expression tag	UNP Q49135
D	214	HIS	-	expression tag	UNP Q49135
D	215	HIS	-	expression tag	UNP Q49135
D	216	HIS	-	expression tag	UNP Q49135
E	209	LEU	-	expression tag	UNP Q49135
E	210	GLU	-	expression tag	UNP Q49135
E	211	HIS	-	expression tag	UNP Q49135
E	212	HIS	-	expression tag	UNP Q49135
E	213	HIS	-	expression tag	UNP Q49135
E	214	HIS	-	expression tag	UNP Q49135
E	215	HIS	-	expression tag	UNP Q49135
E	216	HIS	-	expression tag	UNP Q49135
F	209	LEU	-	expression tag	UNP Q49135
F	210	GLU	-	expression tag	UNP Q49135
F	211	HIS	-	expression tag	UNP Q49135
F	212	HIS	-	expression tag	UNP Q49135
F	213	HIS	-	expression tag	UNP Q49135
F	214	HIS	-	expression tag	UNP Q49135
F	215	HIS	-	expression tag	UNP Q49135
F	216	HIS	-	expression tag	UNP Q49135

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	18	Total O 18 18	0	0
2	B	13	Total O 13 13	0	0
2	C	15	Total O 15 15	0	0
2	D	7	Total O 7 7	0	0

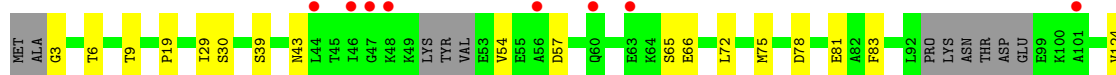
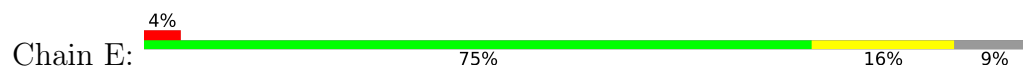
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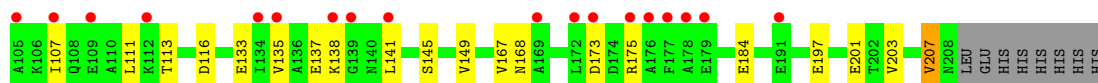
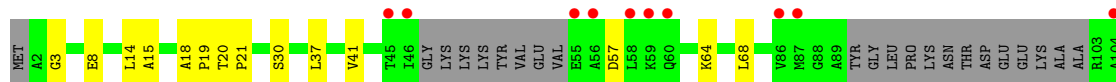
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	7	Total	O	0	0
			7	7		
2	F	1	Total	O	0	0
			1	1		



- Molecule 1: Methenyltetrahydrofolate cyclohydrolase



- Molecule 1: Methenyltetrahydrofolate cyclohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.74Å 67.73Å 88.59Å 80.14° 79.31° 79.42°	Depositor
Resolution (Å)	30.59 – 2.77 36.22 – 2.77	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.59-2.77) 94.6 (36.22-2.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.196 , 0.286 0.206 , 0.292	Depositor DCC
R_{free} test set	1405 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8805	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.75% 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

5.1 Standard geometry

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	0.72	0/1495	0.82	0/2017
1	B	0.74	0/1515	0.81	0/2045
1	C	0.73	0/1511	0.83	0/2040
1	D	0.74	0/1503	0.87	0/2029
1	E	0.73	0/1427	0.82	0/1922
1	F	0.73	0/1349	0.83	0/1820
All	All	0.73	0/8800	0.83	0/11873

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

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	1485	0	1511	23	0
1	B	1504	0	1533	13	0
1	C	1500	0	1530	16	0
1	D	1492	0	1524	23	0
1	E	1420	0	1451	20	0
1	F	1343	0	1366	17	0
2	A	18	0	0	0	0
2	B	13	0	0	0	0
2	C	15	0	0	0	0
2	D	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	7	0	0	0	0
2	F	1	0	0	0	0
All	All	8805	0	8915	100	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 6.

The worst 5 of 100 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:D:41:VAL:HG11	1:D:135:VAL:HG13	1.54	0.90
1:F:64:LYS:O	1:F:68:LEU:HG	1.77	0.85
1:A:41:VAL:HG11	1:A:135:VAL:HG13	1.73	0.70
1:D:155:TYR:CZ	1:D:159:ARG:HD2	2.28	0.68
1:E:6:THR:HG22	1:E:9:THR:H	1.62	0.64

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	200/216 (93%)	191 (96%)	9 (4%)	0	100	100
1	B	204/216 (94%)	191 (94%)	13 (6%)	0	100	100
1	C	203/216 (94%)	195 (96%)	7 (3%)	1 (0%)	29	58
1	D	202/216 (94%)	193 (96%)	9 (4%)	0	100	100
1	E	190/216 (88%)	176 (93%)	14 (7%)	0	100	100
1	F	180/216 (83%)	163 (91%)	15 (8%)	2 (1%)	14	38
All	All	1179/1296 (91%)	1109 (94%)	67 (6%)	3 (0%)	41	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	138	LYS
1	C	190	ALA
1	F	207	VAL

5.3.2 Protein sidechains ⓘ

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	150/162 (93%)	145 (97%)	5 (3%)	38	69
1	B	153/162 (94%)	150 (98%)	3 (2%)	55	82
1	C	153/162 (94%)	148 (97%)	5 (3%)	38	69
1	D	152/162 (94%)	143 (94%)	9 (6%)	19	46
1	E	143/162 (88%)	141 (99%)	2 (1%)	67	87
1	F	136/162 (84%)	128 (94%)	8 (6%)	19	46
All	All	887/972 (91%)	855 (96%)	32 (4%)	35	66

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	116	ASP
1	F	141	LEU
1	C	195	LEU
1	C	158	LEU
1	F	145	SER

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

5.3.3 RNA ⓘ

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 [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	A	204/216 (94%)	-0.18	3 (1%) 73 71	24, 45, 68, 103	0
1	B	206/216 (95%)	-0.03	9 (4%) 34 28	31, 49, 73, 106	0
1	C	205/216 (94%)	0.05	14 (6%) 17 12	30, 48, 72, 106	0
1	D	204/216 (94%)	0.03	8 (3%) 39 34	33, 48, 77, 89	0
1	E	196/216 (90%)	0.28	9 (4%) 32 26	39, 66, 95, 107	0
1	F	186/216 (86%)	0.74	28 (15%) 2 1	42, 70, 98, 108	0
All	All	1201/1296 (92%)	0.14	71 (5%) 22 17	24, 52, 90, 108	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	177	PHE	4.8
1	F	56	ALA	4.6
1	F	169	ALA	4.2
1	F	176	ALA	4.2
1	F	60	GLN	4.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.