



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:22 PM UTC

PDB ID : 1IV3 / pdb_00001iv3
Title : Structure of 2C-Methyl-D-erythritol-2,4-cyclodiphosphate Synthase (bound form MG atoms)
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Deposited on : 2002-03-11
Resolution : 1.52 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

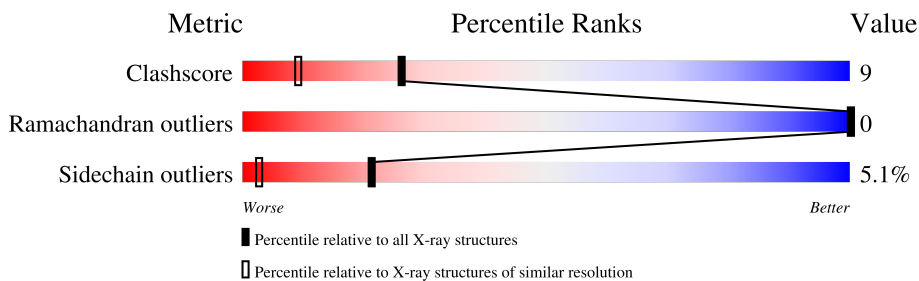
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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))
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	152	82% 16% ..
1	B	152	79% 17% ..
1	C	152	71% 23% . ..
1	D	152	76% 21% ..
1	E	152	72% 21% . ..
1	F	152	81% 15% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7475 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 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	B	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	C	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	D	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	E	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	F	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	LEU	engineered mutation	UNP Q8RQP5
A	81	MET	LEU	engineered mutation	UNP Q8RQP5
A	120	MET	LEU	engineered mutation	UNP Q8RQP5
B	241	MET	LEU	engineered mutation	UNP Q8RQP5
B	281	MET	LEU	engineered mutation	UNP Q8RQP5
B	320	MET	LEU	engineered mutation	UNP Q8RQP5
C	441	MET	LEU	engineered mutation	UNP Q8RQP5
C	481	MET	LEU	engineered mutation	UNP Q8RQP5
C	520	MET	LEU	engineered mutation	UNP Q8RQP5
D	1041	MET	LEU	engineered mutation	UNP Q8RQP5
D	1081	MET	LEU	engineered mutation	UNP Q8RQP5
D	1120	MET	LEU	engineered mutation	UNP Q8RQP5
E	1241	MET	LEU	engineered mutation	UNP Q8RQP5
E	1281	MET	LEU	engineered mutation	UNP Q8RQP5
E	1320	MET	LEU	engineered mutation	UNP Q8RQP5
F	1441	MET	LEU	engineered mutation	UNP Q8RQP5
F	1481	MET	LEU	engineered mutation	UNP Q8RQP5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1520	MET	LEU	engineered mutation	UNP Q8RQP5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total 112	O 112	0	0
3	B	94	Total 94	O 94	0	0
3	C	90	Total 90	O 90	0	0
3	D	87	Total 87	O 87	0	0
3	E	90	Total 90	O 90	0	0
3	F	84	Total 84	O 84	0	0

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.

Note EDS was not executed.

- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain A: 



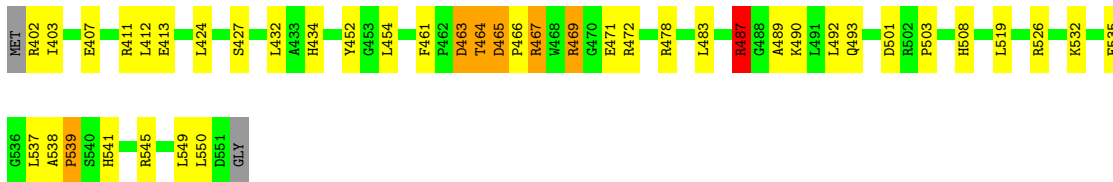
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain B: 



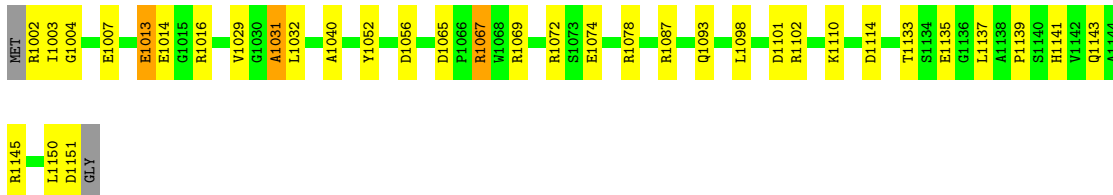
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain C: 



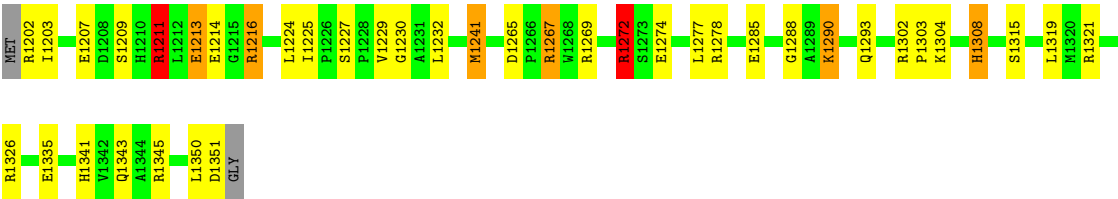
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain D: 

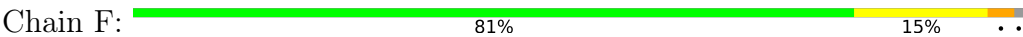


- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain E: 



● Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.18Å 106.18Å 148.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.52	Depositor
% Data completeness (in resolution range)	93.5 (20.00-1.52)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.202 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7475	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

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: MG

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	0.49	0/1173	1.30	5/1587 (0.3%)
1	B	0.50	0/1173	1.28	5/1587 (0.3%)
1	C	0.52	0/1173	1.48	14/1587 (0.9%)
1	D	0.49	0/1173	1.40	10/1587 (0.6%)
1	E	0.50	0/1173	1.47	10/1587 (0.6%)
1	F	0.48	0/1173	1.38	5/1587 (0.3%)
All	All	0.50	0/7038	1.39	49/9522 (0.5%)

There are no bond length outliers.

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	487	ARG	CD-NE-CZ	12.73	142.23	124.40
1	E	1350	LEU	CA-C-N	8.11	136.29	121.70
1	E	1350	LEU	C-N-CA	8.11	136.29	121.70
1	E	1351	ASP	CA-CB-CG	-7.44	105.16	112.60
1	C	550	LEU	CA-C-N	6.89	134.11	121.70

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	1152	0	1182	25	0
1	B	1152	0	1182	18	0
1	C	1152	0	1182	28	0
1	D	1152	0	1182	32	0
1	E	1152	0	1182	35	0
1	F	1152	0	1180	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	112	0	0	1	0
3	B	94	0	0	1	0
3	C	90	0	0	1	0
3	D	87	0	0	1	0
3	E	90	0	0	4	0
3	F	84	0	0	1	0
All	All	7475	0	7090	132	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 9.

The worst 5 of 132 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:E:1216:ARG:NH2	1:E:1232:LEU:HD12	1.63	1.13
1:E:1216:ARG:NH2	1:E:1232:LEU:CD1	2.28	0.97
1:E:1216:ARG:HH21	1:E:1232:LEU:HD12	1.28	0.90
1:C:483:LEU:HD22	1:C:487:ARG:HH22	1.39	0.86
1:D:1065:ASP:OD1	1:D:1067:ARG:HG3	1.84	0.78

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	148/152 (97%)	145 (98%)	3 (2%)	0	100	100
1	B	148/152 (97%)	147 (99%)	1 (1%)	0	100	100
1	C	148/152 (97%)	143 (97%)	5 (3%)	0	100	100
1	D	148/152 (97%)	145 (98%)	3 (2%)	0	100	100
1	E	148/152 (97%)	146 (99%)	2 (1%)	0	100	100
1	F	148/152 (97%)	146 (99%)	2 (1%)	0	100	100
All	All	888/912 (97%)	872 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	121/122 (99%)	116 (96%)	5 (4%)	27	4
1	B	121/122 (99%)	114 (94%)	7 (6%)	18	2
1	C	121/122 (99%)	112 (93%)	9 (7%)	13	1
1	D	121/122 (99%)	119 (98%)	2 (2%)	53	24
1	E	121/122 (99%)	113 (93%)	8 (7%)	15	1
1	F	121/122 (99%)	115 (95%)	6 (5%)	22	3
All	All	726/732 (99%)	689 (95%)	37 (5%)	21	3

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1267	ARG
1	F	1463	ASP
1	E	1272	ARG
1	F	1416	ARG
1	C	424	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1341	HIS
1	F	1508	HIS
1	F	1543	GLN
1	F	1541	HIS
1	C	508	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.