



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:09 am BST

PDB ID : 4MND  
Title : Crystal structure of Archaeoglobus fulgidus IPCT-DIPPS bifunctional membrane protein  
Authors : Nogly, P.; Gushchin, I.; Remeeva, A.; Esteves, A.M.; Ishchenko, A.; Ma, P.; Grudinin, S.; Borges, N.; Round, E.; Moraes, I.; Borshchevskiy, V.; Santos, H.; Gordeliy, V.; Archer, M.  
Deposited on : 2013-09-10  
Resolution : 2.66 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](mailto: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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

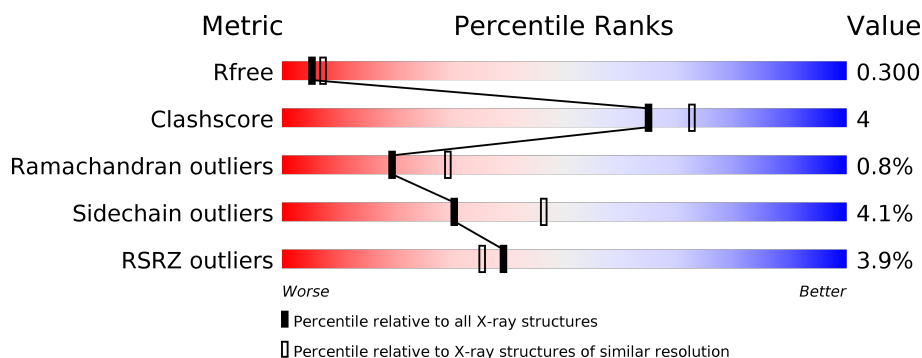
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	479	<div> <div>3%</div> <div>73%</div> <div>11%</div> <div>15%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3160 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 CTP L-myo-inositol-1-phosphate cytidylyltransferase/CDP-L-myo-inositol myo-inositolphosphotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	1	0
			3112	2030	510	559	13			

There are 43 discrepancies between the modelled and reference sequences:

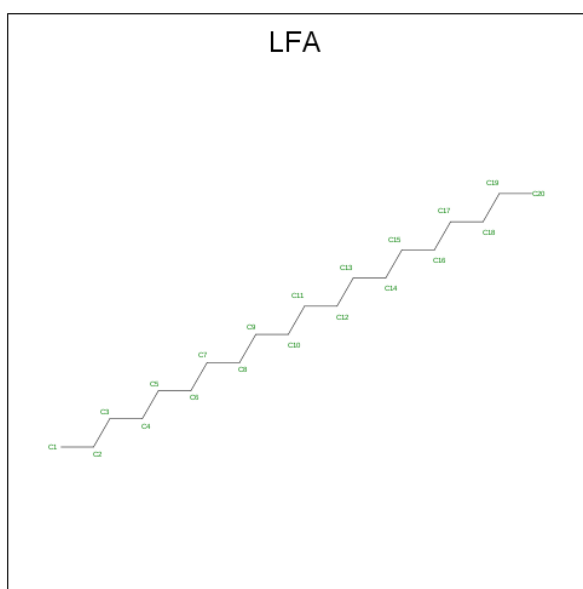
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	EXPRESSION TAG	UNP O29976
A	34	ALA	-	EXPRESSION TAG	UNP O29976
A	35	SER	-	EXPRESSION TAG	UNP O29976
A	36	TRP	-	EXPRESSION TAG	UNP O29976
A	37	SER	-	EXPRESSION TAG	UNP O29976
A	38	HIS	-	EXPRESSION TAG	UNP O29976
A	39	PRO	-	EXPRESSION TAG	UNP O29976
A	40	GLN	-	EXPRESSION TAG	UNP O29976
A	41	PHE	-	EXPRESSION TAG	UNP O29976
A	42	GLU	-	EXPRESSION TAG	UNP O29976
A	43	LYS	-	EXPRESSION TAG	UNP O29976
A	44	GLY	-	EXPRESSION TAG	UNP O29976
A	45	ALA	-	EXPRESSION TAG	UNP O29976
A	46	LEU	-	EXPRESSION TAG	UNP O29976
A	47	GLU	-	EXPRESSION TAG	UNP O29976
A	48	VAL	-	EXPRESSION TAG	UNP O29976
A	49	LEU	-	EXPRESSION TAG	UNP O29976
A	50	PHE	-	EXPRESSION TAG	UNP O29976
A	51	GLN	-	EXPRESSION TAG	UNP O29976
A	52	GLY	-	EXPRESSION TAG	UNP O29976
A	53	PRO	-	EXPRESSION TAG	UNP O29976
A	54	GLY	-	EXPRESSION TAG	UNP O29976
A	491	GLU	-	EXPRESSION TAG	UNP O29976
A	492	LEU	-	EXPRESSION TAG	UNP O29976
A	493	ALA	-	EXPRESSION TAG	UNP O29976
A	494	LEU	-	EXPRESSION TAG	UNP O29976

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	VAL	-	EXPRESSION TAG	UNP O29976
A	496	PRO	-	EXPRESSION TAG	UNP O29976
A	497	ARG	-	EXPRESSION TAG	UNP O29976
A	498	GLY	-	EXPRESSION TAG	UNP O29976
A	499	SER	-	EXPRESSION TAG	UNP O29976
A	500	SER	-	EXPRESSION TAG	UNP O29976
A	501	ALA	-	EXPRESSION TAG	UNP O29976
A	502	HIS	-	EXPRESSION TAG	UNP O29976
A	503	HIS	-	EXPRESSION TAG	UNP O29976
A	504	HIS	-	EXPRESSION TAG	UNP O29976
A	505	HIS	-	EXPRESSION TAG	UNP O29976
A	506	HIS	-	EXPRESSION TAG	UNP O29976
A	507	HIS	-	EXPRESSION TAG	UNP O29976
A	508	HIS	-	EXPRESSION TAG	UNP O29976
A	509	HIS	-	EXPRESSION TAG	UNP O29976
A	510	HIS	-	EXPRESSION TAG	UNP O29976
A	511	HIS	-	EXPRESSION TAG	UNP O29976

- Molecule 2 is EICOSANE (three-letter code: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 10 10	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 8 8	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

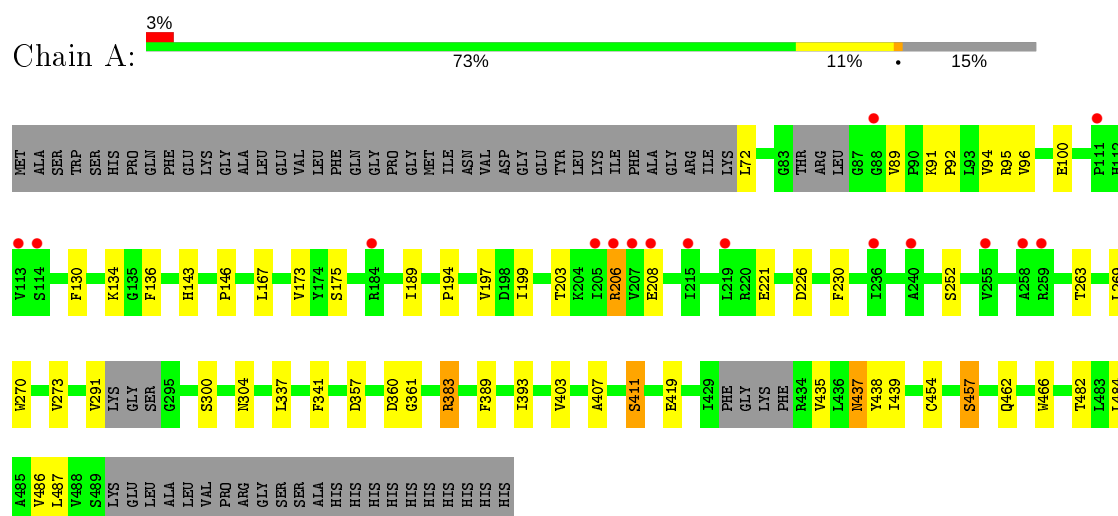
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: CTP L-myo-inositol-1-phosphate cytidylyltransferase/CDP-L-myo-inositol myo-inositolphosphotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.37Å 107.58Å 123.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.85 – 2.66 53.79 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.7 (53.85-2.66) 99.8 (53.79-2.66)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.243 , 0.300 0.253 , 0.300	Depositor DCC
$R_{free}$ test set	838 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.6	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 65.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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

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	0.67	0/3171	0.38	0/4290

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	3112	0	3105	26	0
2	A	38	0	72	0	0
3	A	1	0	0	0	0
4	A	9	0	0	0	0
All	All	3160	0	3177	26	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 (26) 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:A:437:ASN:O	1:A:439:ILE:N	2.24	0.68
1:A:300:SER:HA	1:A:304:ASN:HB2	1.79	0.64
1:A:484:LEU:HA	1:A:487:LEU:HD12	1.81	0.61
1:A:203:THR:HB	1:A:226:ASP:HB3	1.82	0.61
1:A:175:SER:HB3	1:A:269:LEU:HB3	1.86	0.56
1:A:89:VAL:HG13	1:A:94:VAL:HG22	1.91	0.52
1:A:143:HIS:HE1	1:A:146:PRO:HA	1.75	0.51
1:A:100:GLU:HG3	1:A:130:PHE:CZ	2.45	0.50
1:A:462:GLN:O	1:A:466:TRP:HD1	1.98	0.47
1:A:95:ARG:HA	1:A:100:GLU:HA	1.97	0.46
1:A:96:VAL:HG21	1:A:273:VAL:HG21	1.97	0.46
1:A:189:ILE:HD13	1:A:263:THR:HB	1.98	0.46
1:A:167:LEU:HB3	1:A:230:PHE:HB2	1.98	0.45
1:A:134:LYS:HB3	1:A:136:PHE:HD2	1.83	0.44
1:A:482:THR:O	1:A:486:VAL:HG23	2.17	0.44
1:A:360:ASP:OD2	1:A:361:GLY:N	2.52	0.43
1:A:194:PRO:HB2	1:A:197:VAL:HG22	2.00	0.43
1:A:389:PHE:O	1:A:393:ILE:HG12	2.19	0.42
1:A:437:ASN:O	1:A:439:ILE:HG22	2.19	0.42
1:A:206:ARG:HG3	1:A:221:GLU:O	2.20	0.41
1:A:407:ALA:O	1:A:411:SER:HB2	2.20	0.41
1:A:383:ARG:HD3	1:A:383:ARG:HA	1.72	0.41
1:A:91:LYS:HB2	1:A:92:PRO:HD3	2.03	0.40
1:A:206:ARG:NH2	1:A:208:GLU:HB2	2.36	0.40
1:A:173:VAL:O	1:A:270:TRP:HA	2.21	0.40
1:A:454:CYS:O	1:A:457:SER:HB3	2.21	0.40

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	401/479 (84%)	386 (96%)	12 (3%)	3 (1%)	22	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	TYR
1	A	435	VAL
1	A	437	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	315/403 (78%)	302 (96%)	13 (4%)	30	46

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	199	ILE
1	A	206	ARG
1	A	252	SER
1	A	291	VAL
1	A	337	LEU
1	A	341	PHE
1	A	357	ASP
1	A	383	ARG
1	A	403	VAL
1	A	411	SER
1	A	419	GLU
1	A	457	SER

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	LFA	A	602	-	11,11,19	0.44	0	10,10,18	0.62	0
2	LFA	A	601	-	9,9,19	0.35	0	8,8,18	0.52	0
2	LFA	A	604	-	7,7,19	0.44	0	6,6,18	0.48	0
2	LFA	A	603	-	7,7,19	0.43	0	6,6,18	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	602	-	-	0/9/9/17	-
2	LFA	A	601	-	-	0/7/7/17	-
2	LFA	A	604	-	-	0/5/5/17	-
2	LFA	A	603	-	-	0/5/5/17	-

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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	408/479 (85%)	0.40	16 (3%) 39 35	32, 60, 93, 125	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	ILE	5.7
1	A	259	ARG	4.7
1	A	240	ALA	4.2
1	A	255	VAL	3.5
1	A	207	VAL	3.4
1	A	258	ALA	3.0
1	A	111	PRO	2.7
1	A	215	ILE	2.6
1	A	88	GLY	2.4
1	A	219	LEU	2.4
1	A	208	GLU	2.3
1	A	114	SER	2.3
1	A	184	ARG	2.3
1	A	206	ARG	2.1
1	A	113	VAL	2.1
1	A	236	ILE	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	LFA	A	603	8/20	0.78	0.23	56,63,64,64	0
3	MG	A	605	1/1	0.81	0.10	58,58,58,58	0
2	LFA	A	602	12/20	0.88	0.20	49,57,64,69	0
2	LFA	A	604	8/20	0.91	0.16	60,68,71,71	0
2	LFA	A	601	10/20	0.92	0.15	44,46,50,50	0

## 6.5 Other polymers

There are no such residues in this entry.