



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 04:02 AM GMT

PDB ID : 4FP4  
Title : Crystal structure of isoprenoid synthase a3mx09 (target efi-501993) from pyrobaculum calidifontis  
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Deposited on : 2012-06-21  
Resolution : 2.00 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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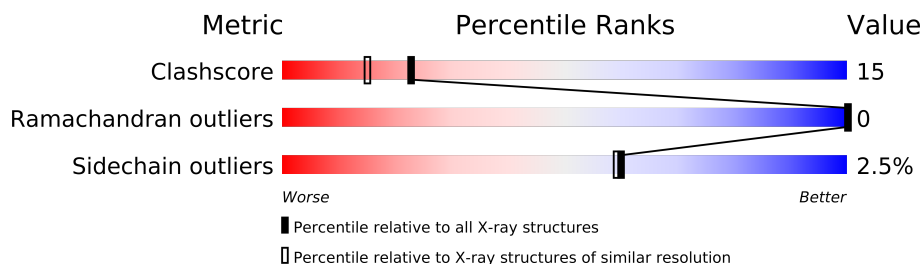
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	<b>FAILED</b>
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	285	
1	B	285	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3887 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Polyprenyl synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	1	0
			1913	1227	334	346	6			
1	B	234	Total	C	N	O	S	0	1	0
			1840	1181	322	332	5			

There are 48 discrepancies between the modelled and reference sequences:

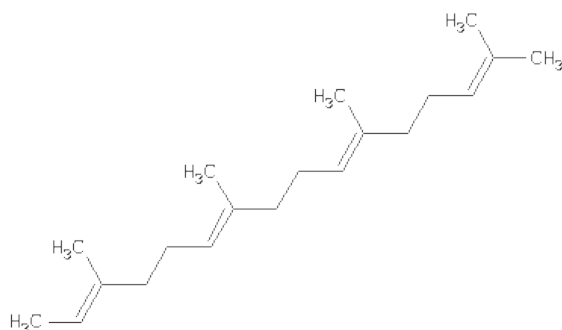
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP A3MX09
A	0	VAL	-	EXPRESSION TAG	UNP A3MX09
A	262	ALA	-	EXPRESSION TAG	UNP A3MX09
A	263	GLU	-	EXPRESSION TAG	UNP A3MX09
A	264	ASN	-	EXPRESSION TAG	UNP A3MX09
A	265	LEU	-	EXPRESSION TAG	UNP A3MX09
A	266	TYR	-	EXPRESSION TAG	UNP A3MX09
A	267	PHE	-	EXPRESSION TAG	UNP A3MX09
A	268	GLN	-	EXPRESSION TAG	UNP A3MX09
A	269	SER	-	EXPRESSION TAG	UNP A3MX09
A	270	HIS	-	EXPRESSION TAG	UNP A3MX09
A	271	HIS	-	EXPRESSION TAG	UNP A3MX09
A	272	HIS	-	EXPRESSION TAG	UNP A3MX09
A	273	HIS	-	EXPRESSION TAG	UNP A3MX09
A	274	HIS	-	EXPRESSION TAG	UNP A3MX09
A	275	HIS	-	EXPRESSION TAG	UNP A3MX09
A	276	TRP	-	EXPRESSION TAG	UNP A3MX09
A	277	SER	-	EXPRESSION TAG	UNP A3MX09
A	278	HIS	-	EXPRESSION TAG	UNP A3MX09
A	279	PRO	-	EXPRESSION TAG	UNP A3MX09
A	280	GLN	-	EXPRESSION TAG	UNP A3MX09
A	281	PHE	-	EXPRESSION TAG	UNP A3MX09
A	282	GLU	-	EXPRESSION TAG	UNP A3MX09
A	283	LYS	-	EXPRESSION TAG	UNP A3MX09
B	-1	MET	-	EXPRESSION TAG	UNP A3MX09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	VAL	-	EXPRESSION TAG	UNP A3MX09
B	262	ALA	-	EXPRESSION TAG	UNP A3MX09
B	263	GLU	-	EXPRESSION TAG	UNP A3MX09
B	264	ASN	-	EXPRESSION TAG	UNP A3MX09
B	265	LEU	-	EXPRESSION TAG	UNP A3MX09
B	266	TYR	-	EXPRESSION TAG	UNP A3MX09
B	267	PHE	-	EXPRESSION TAG	UNP A3MX09
B	268	GLN	-	EXPRESSION TAG	UNP A3MX09
B	269	SER	-	EXPRESSION TAG	UNP A3MX09
B	270	HIS	-	EXPRESSION TAG	UNP A3MX09
B	271	HIS	-	EXPRESSION TAG	UNP A3MX09
B	272	HIS	-	EXPRESSION TAG	UNP A3MX09
B	273	HIS	-	EXPRESSION TAG	UNP A3MX09
B	274	HIS	-	EXPRESSION TAG	UNP A3MX09
B	275	HIS	-	EXPRESSION TAG	UNP A3MX09
B	276	TRP	-	EXPRESSION TAG	UNP A3MX09
B	277	SER	-	EXPRESSION TAG	UNP A3MX09
B	278	HIS	-	EXPRESSION TAG	UNP A3MX09
B	279	PRO	-	EXPRESSION TAG	UNP A3MX09
B	280	GLN	-	EXPRESSION TAG	UNP A3MX09
B	281	PHE	-	EXPRESSION TAG	UNP A3MX09
B	282	GLU	-	EXPRESSION TAG	UNP A3MX09
B	283	LYS	-	EXPRESSION TAG	UNP A3MX09

- Molecule 2 is GERAN-8-YL GERAN (three-letter code: GER) (formula:  $C_{20}H_{34}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 20 20	0	0

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total X 1 1	0	0
3	A	1	Total X 1 1	0	0

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 13 4 7 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	62	Total O 62 62	0	0
5	B	37	Total O 37 37	0	0



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.96Å 115.42Å 53.14Å 90.00° 110.84° 90.00°	Depositor
Resolution (Å)	38.57 – 2.00	Depositor
% Data completeness (in resolution range)	99.2 (38.57-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, $R_{free}$	0.185 , 0.228	Depositor
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.630	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 35416 reflections	Xtriage
Total number of atoms	3887	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 7.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, GER, UNL

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	0/1943	0.66	0/2624
1	B	0.47	0/1868	0.63	0/2523
All	All	0.48	0/3811	0.65	0/5147

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1913	0	2027	57	0
1	B	1840	0	1955	66	0
2	A	20	0	34	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	0	0	0
5	A	62	0	0	4	0
5	B	37	0	0	1	0
All	All	3887	0	4016	115	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 115 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:155:ARG:HD2	1:B:155:ARG:H	1.05	1.08
1:A:4:LEU:CD1	1:A:9:LEU:HD21	1.96	0.96
1:B:155:ARG:N	1:B:155:ARG:HD2	1.81	0.95
1:A:197:LEU:HD21	1:A:250:ALA:CB	1.96	0.94
1:A:211:ARG:N	1:A:212:PRO:CD	2.33	0.91

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	240/285 (84%)	230 (96%)	10 (4%)	0	100	100
1	B	231/285 (81%)	228 (99%)	3 (1%)	0	100	100
All	All	471/570 (83%)	458 (97%)	13 (3%)	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	203/243 (84%)	198 (98%)	5 (2%)	60	59
1	B	195/243 (80%)	189 (97%)	6 (3%)	52	49
All	All	398/486 (82%)	387 (97%)	11 (3%)	60	54

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	PRO
1	B	61	ARG
1	B	163	THR
1	A	200	TYR
1	B	155	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	91	GLN
1	A	94	GLN
1	A	231	HIS
1	B	85	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 3 are unknown - leaving 1 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	GER	A	301	-	19,19,19	0.52	0	22,22,22	1.92	6 (27%)

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	GER	A	301	-	-	0/20/20/20	0/0/0/0

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	GER	C14-C13-C15	4.31	121.94	115.39
2	A	301	GER	C9-C8-C10	3.80	121.16	115.39
2	A	301	GER	C6-C7-C8	-3.44	120.38	127.80
2	A	301	GER	C11-C12-C13	-3.12	121.07	127.80
2	A	301	GER	C4-C3-C5	2.20	118.74	115.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.