



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 07:10 PM EST

PDB ID : 3LVS
Title : Crystal structure of farnesyl diphosphate synthase from rhodobacter capsulatus sb1003
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Deposited on : 2010-02-22
Resolution : 2.15 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 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)
Xtrriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

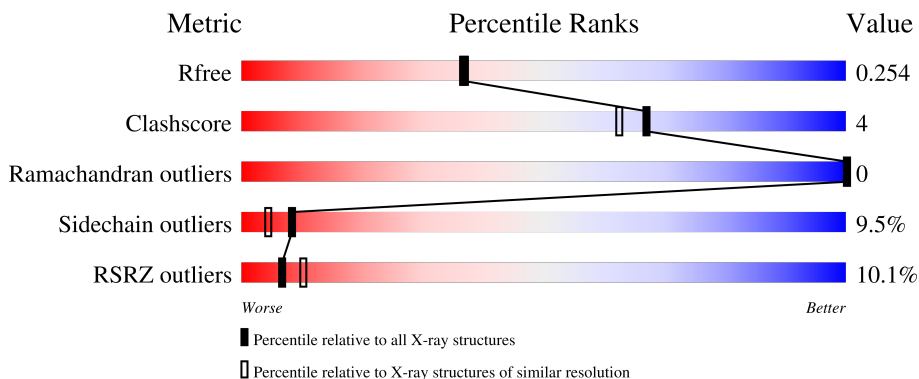
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	298	
1	B	298	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4105 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 FARNESYL DIPHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	Total 1961	C 1229	N 339	O 383	S 10	0	2	0
1	B	274	Total 1987	C 1245	N 345	O 387	S 10	0	2	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

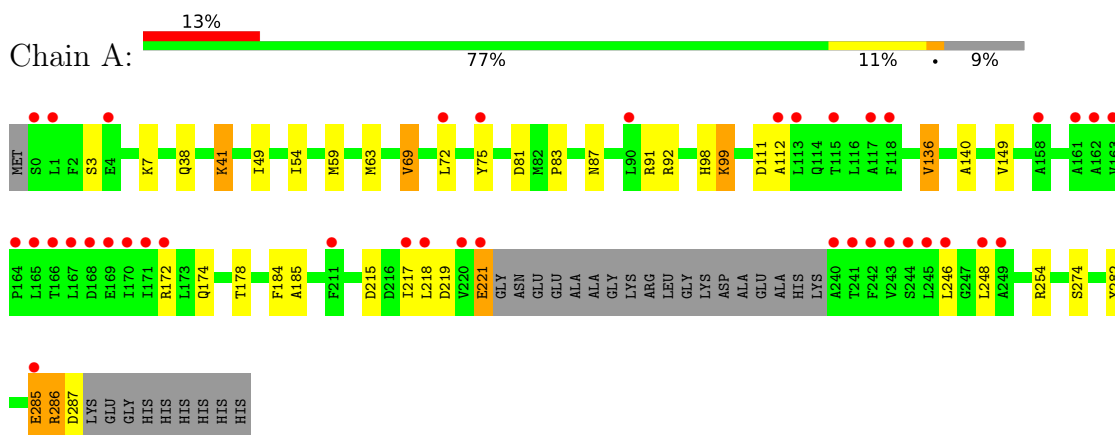
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	56	Total O 56 56	0	0
4	B	69	Total O 69 69	0	0

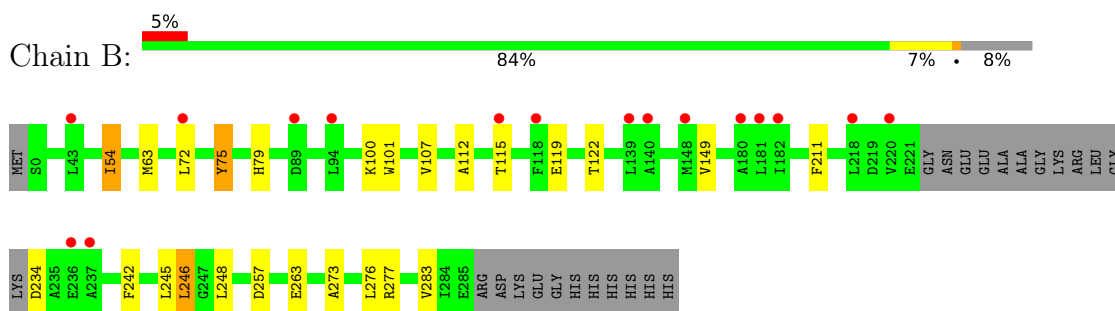
3 Residue-property plots [i](#)

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 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: FARNESYL DIPHOSPHATE SYNTHASE



• Molecule 1: FARNESYL DIPHOSPHATE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.46Å 89.46Å 132.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 37.10 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.15) 99.4 (37.10-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.217 , 0.250 0.215 , 0.254	Depositor DCC
R_{free} test set	1116 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtrriage
Anisotropy	0.682	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4105	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: GOL, PO4

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	0.47	0/1991	0.63	0/2704
1	B	0.52	0/2018	0.61	0/2740
All	All	0.50	0/4009	0.62	0/5444

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	A	1961	0	1969	23	0
1	B	1987	0	1996	13	0
2	A	5	0	0	0	0
2	B	15	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	56	0	0	0	0
4	B	69	0	0	0	0
All	All	4105	0	3981	31	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 (31) 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:217:ILE:HD13	1:A:287:ASP:OD1	1.91	0.71
1:B:54:ILE:HD11	1:B:273:ALA:HA	1.79	0.65
1:B:75:TYR:CD1	1:B:75:TYR:C	2.69	0.65
1:A:217:ILE:O	1:A:221:GLU:HB2	2.03	0.58
1:A:83:PRO:HD3	1:A:98:HIS:CE1	2.40	0.57
1:B:54:ILE:HD12	1:B:276:LEU:HD12	1.87	0.56
1:A:41:LYS:HD3	1:A:286:ARG:HH12	1.70	0.56
1:B:75:TYR:CD1	1:B:75:TYR:O	2.60	0.55
1:A:149:VAL:HG11	1:B:112:ALA:HB2	1.90	0.53
1:A:217:ILE:HG21	1:A:287:ASP:CG	2.30	0.52
1:A:217:ILE:HG21	1:A:287:ASP:OD1	2.10	0.51
1:A:69:VAL:HG11	1:A:185:ALA:HB2	1.93	0.51
1:A:83:PRO:HD3	1:A:98:HIS:ND1	2.26	0.51
1:A:282:TYR:HA	1:A:285:GLU:HB2	1.94	0.48
1:A:219:ASP:OD1	1:A:219:ASP:N	2.47	0.48
1:A:91:ARG:HG2	1:A:92:ARG:HG3	1.96	0.46
1:B:75:TYR:HD1	1:B:75:TYR:O	1.97	0.46
1:A:111:ASP:OD1	1:B:79:HIS:CE1	2.69	0.45
1:A:286:ARG:HG2	1:A:286:ARG:H	1.54	0.45
1:B:100:LYS:HB3	1:B:101:TRP:CE3	2.51	0.45
1:B:263:GLU:HG2	1:B:277[A]:ARG:HB2	2.00	0.44
1:A:99:LYS:HA	1:A:99:LYS:HD2	1.44	0.44
1:A:69:VAL:HG13	1:A:184:PHE:CD2	2.54	0.42
1:A:49:ILE:HD13	1:A:59:MET:HE3	2.00	0.42
1:A:69:VAL:HG13	1:A:184:PHE:HD2	1.85	0.42
1:A:112:ALA:HB2	1:B:149:VAL:HG11	2.02	0.41
1:A:140:ALA:HB1	1:B:119:GLU:HB2	2.01	0.41
1:B:242:PHE:O	1:B:246:LEU:HB2	2.20	0.41
1:A:81:ASP:OD2	1:A:91:ARG:NH1	2.51	0.41
1:A:215:ASP:O	1:A:218:LEU:HB2	2.21	0.40
1:A:136:VAL:HG22	1:B:122:THR:CG2	2.51	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	A	268/298 (90%)	263 (98%)	5 (2%)	0	100	100
1	B	272/298 (91%)	266 (98%)	6 (2%)	0	100	100
All	All	540/596 (91%)	529 (98%)	11 (2%)	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	A	186/205 (91%)	164 (88%)	22 (12%)	5	2
1	B	188/205 (92%)	175 (93%)	13 (7%)	15	10
All	All	374/410 (91%)	339 (91%)	35 (9%)	8	4

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	7	LYS
1	A	38	GLN
1	A	41	LYS
1	A	54	ILE
1	A	63	MET
1	A	69	VAL
1	A	72	LEU

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Mol	Chain	Res	Type
1	A	75	TYR
1	A	87	ASN
1	A	99	LYS
1	A	136	VAL
1	A	172	ARG
1	A	174	GLN
1	A	178	THR
1	A	221	GLU
1	A	246	LEU
1	A	248	LEU
1	A	254	ARG
1	A	274	SER
1	A	285	GLU
1	A	286	ARG
1	B	54	ILE
1	B	63	MET
1	B	72	LEU
1	B	75	TYR
1	B	107	VAL
1	B	115	THR
1	B	211	PHE
1	B	234	ASP
1	B	245	LEU
1	B	246	LEU
1	B	248	LEU
1	B	257	ASP
1	B	283	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	174	GLN
1	B	38	GLN
1	B	87	ASN

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](#)

6 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	PO4	B	297	-	4,4,4	0.87	0	6,6,6	0.46	0
3	GOL	B	300	-	5,5,5	0.42	0	5,5,5	0.14	0
3	GOL	A	298	-	5,5,5	0.38	0	5,5,5	0.22	0
2	PO4	A	297	-	4,4,4	0.96	0	6,6,6	0.58	0
2	PO4	B	299	-	4,4,4	0.89	0	6,6,6	0.35	0
2	PO4	B	298	-	4,4,4	0.88	0	6,6,6	0.47	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
3	GOL	A	298	-	-	2/4/4/4	-
3	GOL	B	300	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	298	GOL	C1-C2-C3-O3
3	A	298	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 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	270/298 (90%)	0.80	39 (14%) 2 3	35, 60, 111, 131	0
1	B	274/298 (91%)	0.31	16 (5%) 23 31	30, 53, 76, 107	0
All	All	544/596 (91%)	0.56	55 (10%) 7 10	30, 56, 102, 131	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	LEU	8.2
1	A	165	LEU	8.2
1	A	163	VAL	7.3
1	A	220	VAL	7.1
1	A	240	ALA	7.1
1	A	167	LEU	6.4
1	A	161	ALA	6.4
1	A	218	LEU	6.0
1	A	243	VAL	5.0
1	A	1	LEU	4.9
1	A	241	THR	4.9
1	A	244	SER	4.8
1	B	236	GLU	4.7
1	A	246	LEU	4.6
1	A	221	GLU	4.5
1	A	162	ALA	4.5
1	A	171	ILE	4.5
1	A	164	PRO	4.4
1	A	217	ILE	4.3
1	A	166	THR	4.1
1	B	237	ALA	4.1
1	A	249	ALA	3.9
1	A	245	LEU	3.8
1	B	218	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	181	LEU	3.3
1	A	169	GLU	3.3
1	A	242	PHE	3.3
1	A	158	ALA	3.2
1	A	0	SER	3.2
1	A	170	ILE	3.1
1	B	72	LEU	3.1
1	A	112	ALA	3.0
1	A	168	ASP	3.0
1	B	140	ALA	2.8
1	A	113	LEU	2.8
1	A	90	LEU	2.8
1	A	172	ARG	2.6
1	A	72	LEU	2.6
1	B	139	LEU	2.6
1	B	115	THR	2.5
1	B	182	ILE	2.5
1	A	211	PHE	2.4
1	A	115	THR	2.4
1	B	118	PHE	2.4
1	A	285	GLU	2.4
1	B	148	MET	2.3
1	B	89	ASP	2.3
1	B	180	ALA	2.3
1	B	220	VAL	2.3
1	B	43	LEU	2.2
1	A	75	TYR	2.2
1	A	118	PHE	2.2
1	B	94	LEU	2.1
1	A	117	ALA	2.1
1	A	4	GLU	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	PO4	A	297	5/5	0.90	0.38	48,50,56,58	5
3	GOL	B	300	6/6	0.91	0.13	60,70,72,74	0
2	PO4	B	298	5/5	0.91	0.24	57,62,63,64	5
3	GOL	A	298	6/6	0.92	0.13	66,74,75,78	0
2	PO4	B	297	5/5	0.93	0.30	45,49,58,59	5
2	PO4	B	299	5/5	0.96	0.09	85,88,94,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.