



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:47 am BST

PDB ID : 6B02  
Title : Crystal structure of CfFPPS2 (apo form), a lepidopteran type-II farnesyl diphosphate synthase  
Authors : Picard, M.-E.; Cusson, M.; Shi, R.  
Deposited on : 2017-09-13  
Resolution : 2.82 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.

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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
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

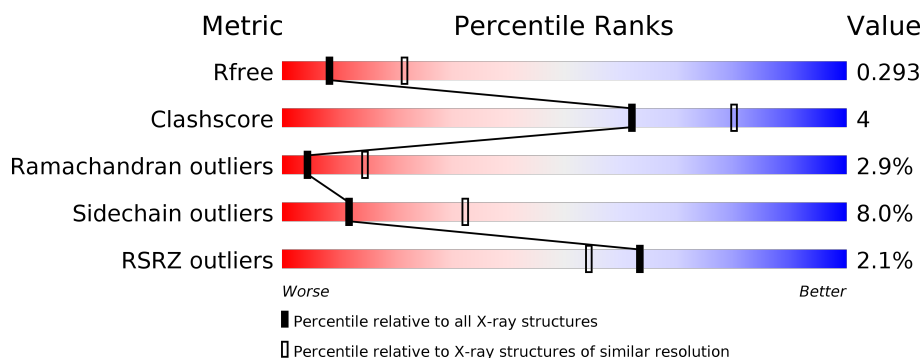
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	341	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	341	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5324 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.

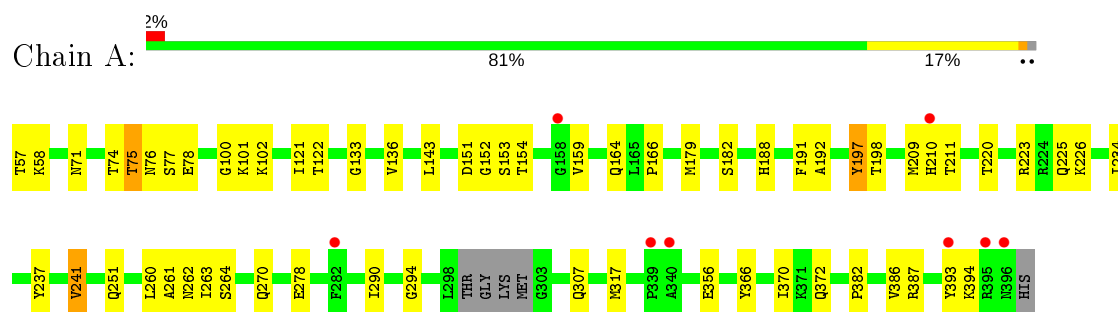
- Molecule 1 is a protein called Farnesyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2682	1724	429	510	19			
1	B	329	Total	C	N	O	S	0	0	0
			2642	1703	424	496	19			

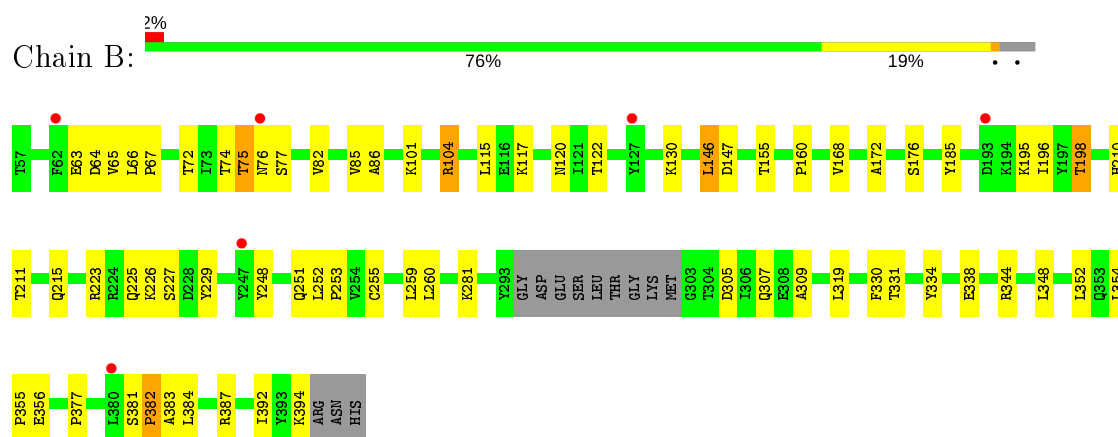
### 3 Residue-property plots [i](#)

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: Farnesyl diphosphate synthase



#### • Molecule 1: Farnesyl diphosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.68Å 113.68Å 131.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	98.45 – 2.82 46.08 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.8 (98.45-2.82) 98.8 (46.08-2.82)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.216 , 0.296 0.218 , 0.293	Depositor DCC
$R_{free}$ test set	1214 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.4	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5324	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.57	0/2738	0.75	0/3711
1	B	0.59	0/2698	0.76	1/3654 (0.0%)
All	All	0.58	0/5436	0.76	1/7365 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ARG	NE-CZ-NH1	5.38	122.99	120.30

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	2682	0	2648	24	0
1	B	2642	0	2635	27	0
All	All	5324	0	5283	47	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 (47) 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:B:74:THR:HG23	1:B:86:ALA:HB1	1.58	0.86
1:A:198:THR:HG22	1:B:198:THR:CG2	2.17	0.73
1:B:225:GLN:O	1:B:227:SER:N	2.23	0.71
1:A:151:ASP:O	1:A:153:SER:N	2.29	0.65
1:B:229:TYR:CD2	1:B:331:THR:HG22	2.36	0.61
1:B:74:THR:CG2	1:B:86:ALA:HB1	2.29	0.60
1:B:319:LEU:HD21	1:B:330:PHE:CD1	2.37	0.59
1:A:143:LEU:CD2	1:A:211:THR:HG21	2.33	0.58
1:B:381:SER:O	1:B:384:LEU:N	2.40	0.55
1:A:198:THR:HG22	1:B:198:THR:HG21	1.89	0.54
1:A:143:LEU:HD22	1:A:211:THR:HG21	1.90	0.53
1:A:382:PRO:O	1:A:386:VAL:HG23	2.10	0.51
1:A:261:ALA:O	1:A:263:ILE:HG13	2.09	0.51
1:B:381:SER:O	1:B:382:PRO:C	2.49	0.51
1:A:154:THR:HA	1:A:164:GLN:HE21	1.76	0.50
1:B:381:SER:O	1:B:383:ALA:N	2.45	0.50
1:B:348:LEU:O	1:B:352:LEU:HG	2.14	0.48
1:A:75:THR:HG22	1:A:76:ASN:N	2.28	0.48
1:A:237:TYR:O	1:A:241:VAL:HG13	2.14	0.47
1:A:188:HIS:O	1:A:192:ALA:HB2	2.15	0.47
1:A:366:TYR:CE1	1:A:393:TYR:CD2	3.03	0.47
1:B:354:LEU:N	1:B:355:PRO:CD	2.78	0.47
1:A:290:ILE:O	1:A:294:GLY:N	2.48	0.46
1:A:209:MET:HG2	1:B:185:TYR:OH	2.16	0.46
1:B:147:ASP:OD1	1:B:215:GLN:NE2	2.49	0.46
1:B:75:THR:O	1:B:77:SER:OG	2.29	0.46
1:B:65:VAL:HG21	1:B:130:LYS:HB3	1.97	0.45
1:A:278:GLU:HG3	1:A:372:GLN:HE22	1.82	0.45
1:B:155:THR:HA	1:B:160:PRO:HA	1.98	0.45
1:A:261:ALA:O	1:A:263:ILE:N	2.50	0.45
1:A:234:ILE:HD13	1:A:317:MET:HE3	1.99	0.45
1:A:366:TYR:CE2	1:A:370:ILE:HG13	2.52	0.44
1:B:229:TYR:HD2	1:B:331:THR:HG22	1.79	0.43
1:B:309:ALA:HA	1:B:334:TYR:CE2	2.54	0.43
1:B:75:THR:O	1:B:77:SER:N	2.52	0.43
1:A:191:PHE:O	1:A:197:TYR:HB2	2.20	0.42
1:A:143:LEU:HD22	1:A:211:THR:CG2	2.49	0.42
1:B:146:LEU:HD23	1:B:146:LEU:N	2.35	0.42
1:B:146:LEU:HD21	1:B:176:SER:HB2	2.00	0.42
1:B:252:LEU:HB3	1:B:253:PRO:HD3	2.02	0.42
1:B:66:LEU:O	1:B:67:PRO:C	2.58	0.41
1:A:133:GLY:O	1:A:136:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:OE1	1:B:210:HIS:CE1	2.72	0.41
1:A:366:TYR:O	1:A:370:ILE:HG12	2.20	0.41
1:A:143:LEU:CD1	1:A:211:THR:HG21	2.51	0.41
1:B:82:VAL:HG12	1:B:85:VAL:HG23	2.03	0.40
1:B:196:ILE:HG21	1:B:259:LEU:O	2.21	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	332/341 (97%)	296 (89%)	26 (8%)	10 (3%)	4	14
1	B	325/341 (95%)	292 (90%)	24 (7%)	9 (3%)	5	15
All	All	657/682 (96%)	588 (90%)	50 (8%)	19 (3%)	4	15

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	152	GLY
1	A	197	TYR
1	A	262	ASN
1	B	172	ALA
1	B	223	ARG
1	B	226	LYS
1	B	76	ASN
1	B	305	ASP
1	A	74	THR
1	A	225	GLN
1	B	75	THR
1	A	394	LYS

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Mol	Chain	Res	Type
1	A	100	GLY
1	B	377	PRO
1	B	382	PRO
1	A	166	PRO
1	A	121	ILE
1	B	168	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	294/304 (97%)	272 (92%)	22 (8%)	13	35
1	B	291/304 (96%)	266 (91%)	25 (9%)	10	29
All	All	585/608 (96%)	538 (92%)	47 (8%)	12	32

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	THR
1	A	58	LYS
1	A	71	ASN
1	A	77	SER
1	A	101	LYS
1	A	102	LYS
1	A	122	THR
1	A	159	VAL
1	A	179	MET
1	A	182	SER
1	A	210	HIS
1	A	220	THR
1	A	223	ARG
1	A	226	LYS
1	A	241	VAL
1	A	251	GLN
1	A	260	LEU

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Mol	Chain	Res	Type
1	A	264	SER
1	A	270	GLN
1	A	307	GLN
1	A	356	GLU
1	A	387	ARG
1	B	63	GLU
1	B	64	ASP
1	B	72	THR
1	B	101	LYS
1	B	104	ARG
1	B	115	LEU
1	B	117	LYS
1	B	120	ASN
1	B	122	THR
1	B	146	LEU
1	B	195	LYS
1	B	198	THR
1	B	211	THR
1	B	248	TYR
1	B	251	GLN
1	B	255	CYS
1	B	260	LEU
1	B	281	LYS
1	B	307	GLN
1	B	338	GLU
1	B	344	ARG
1	B	356	GLU
1	B	387	ARG
1	B	392	ILE
1	B	394	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	216	HIS
1	A	372	GLN
1	A	390	HIS
1	B	174	ASN
1	B	205	ASN
1	B	262	ASN
1	B	270	GLN

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Mol	Chain	Res	Type
1	B	320	GLN
1	B	390	HIS

### 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](#)

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, 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	336/341 (98%)	0.07	8 (2%) 59 49	76, 107, 143, 177	0
1	B	329/341 (96%)	-0.01	6 (1%) 68 61	69, 101, 135, 183	0
All	All	665/682 (97%)	0.03	14 (2%) 63 54	69, 105, 142, 183	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	ASN	8.8
1	B	76	ASN	4.1
1	A	339	PRO	3.4
1	A	395	ARG	3.2
1	A	282	PHE	3.1
1	B	193	ASP	2.9
1	B	62	PHE	2.9
1	A	158	GLY	2.6
1	B	380	LEU	2.4
1	B	127	TYR	2.4
1	A	393	TYR	2.3
1	A	340	ALA	2.2
1	A	210	HIS	2.1
1	B	247	TYR	2.1

### 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 carbohydrates 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.