



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 06:51 pm GMT

PDB ID : 2F7M
Title : Crystal Structure of Unliganded Human FPPS
Authors : Rondeau, J.-M.; Bitsch, F.; Bourgier, E.; Geiser, M.; Hemmig, R.; Kroemer, M.; Lehmann, S.; Ramage, P.; Rieffel, S.; Strauss, A.; Green, J.R.; Jahnke, W.
Deposited on : 2005-12-01
Resolution : 2.30 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

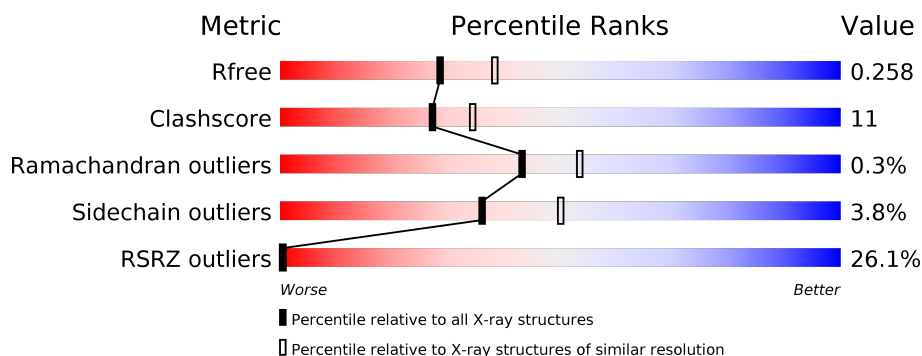
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	F	350	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2816 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	F	341	2757	1778	451	516	12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	4	GLY	-	CLONING ARTIFACT	UNP P14324
F	5	PRO	-	CLONING ARTIFACT	UNP P14324

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



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

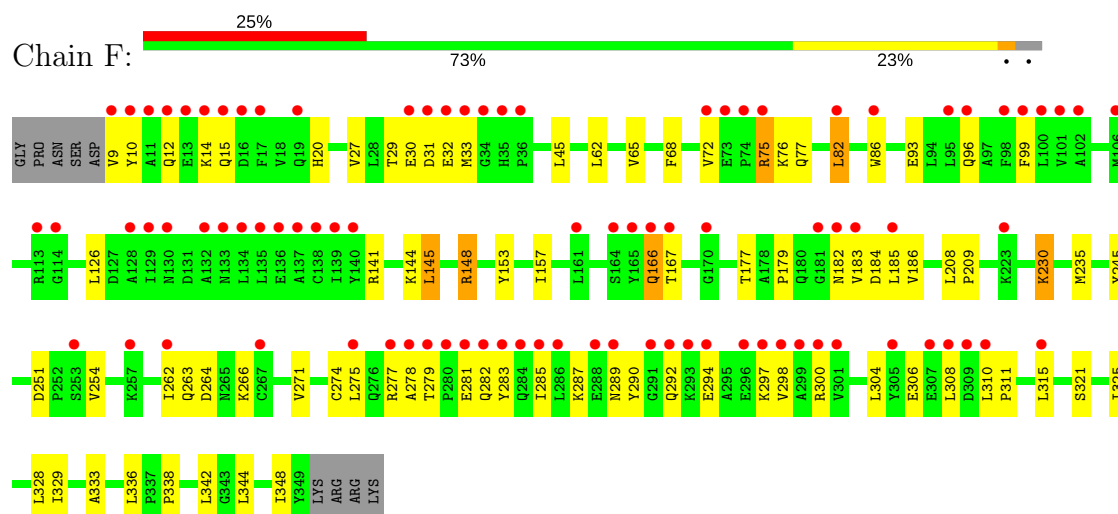
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	54	Total	O	0	0
			54	54		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.89Å 110.89Å 77.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.69 – 2.30 41.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.69-2.30) 99.5 (41.69-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.49 (at 2.29Å)	Xtriage
Refinement program	CNS, CNX 2005	Depositor
R, R_{free}	0.225 , 0.257 0.225 , 0.258	Depositor DCC
R_{free} test set	1955 reflections (8.97%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2816	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: 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	F	0.37	0/2816	0.50	0/3815

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	F	2757	0	2735	60	0
2	F	5	0	0	0	0
3	F	54	0	0	0	0
All	All	2816	0	2735	60	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 11.

All (60) 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:F:279:THR:OG1	1:F:282:GLN:HG2	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:LYS:HA	1:F:62:LEU:HD21	1.77	0.65
1:F:179:PRO:HB2	1:F:182:ASN:HB2	1.79	0.65
1:F:321:SER:O	1:F:325:ILE:HG12	1.99	0.63
1:F:9:VAL:HG23	1:F:10:TYR:HD1	1.63	0.63
1:F:12:GLN:O	1:F:15:GLN:HG2	2.00	0.61
1:F:144:LYS:O	1:F:148:ARG:HB2	2.01	0.61
1:F:68:PHE:CE1	1:F:72:VAL:HG21	2.35	0.60
1:F:77:GLN:HB3	1:F:82:LEU:HD11	1.84	0.60
1:F:277:ARG:HG3	1:F:277:ARG:HH11	1.67	0.60
1:F:68:PHE:HE2	1:F:82:LEU:HD12	1.68	0.59
1:F:75:ARG:HH21	1:F:76:LYS:HE3	1.68	0.57
1:F:185:LEU:HD12	1:F:283:TYR:HE1	1.71	0.56
1:F:9:VAL:HG23	1:F:10:TYR:CD1	2.39	0.56
1:F:30:GLU:HG3	1:F:31:ASP:N	2.20	0.56
1:F:304:LEU:O	1:F:308:LEU:HG	2.07	0.55
1:F:283:TYR:CZ	1:F:287:LYS:HD2	2.43	0.54
1:F:99:PHE:CE2	1:F:167:THR:HG21	2.43	0.54
1:F:93:GLU:O	1:F:96:GLN:HB3	2.07	0.53
1:F:251:ASP:OD2	1:F:254:VAL:HG23	2.09	0.52
1:F:292:GLN:HE21	1:F:297:LYS:NZ	2.08	0.51
1:F:245:TYR:HE1	1:F:311:PRO:HA	1.74	0.51
1:F:310:LEU:N	1:F:311:PRO:CD	2.74	0.50
1:F:27:VAL:HA	1:F:30:GLU:HG2	1.93	0.49
1:F:30:GLU:C	1:F:32:GLU:H	2.15	0.49
1:F:271:VAL:O	1:F:275:LEU:HG	2.13	0.49
1:F:263:GLN:HG3	1:F:298:VAL:HG21	1.94	0.49
1:F:65:VAL:HG21	1:F:86:TRP:CE3	2.48	0.48
1:F:14:LYS:HD3	1:F:14:LYS:O	2.13	0.47
1:F:20:HIS:CD2	1:F:86:TRP:HB3	2.49	0.47
1:F:289:ASN:HD22	1:F:297:LYS:HB3	1.78	0.47
1:F:333:ALA:O	1:F:336:LEU:HB2	2.14	0.47
1:F:264:ASP:HB3	1:F:266:LYS:HE3	1.97	0.47
1:F:279:THR:OG1	1:F:281:GLU:HG2	2.15	0.47
1:F:27:VAL:CG1	1:F:145:LEU:HD23	2.46	0.46
1:F:148:ARG:HG2	1:F:148:ARG:HH11	1.80	0.46
1:F:277:ARG:HG3	1:F:277:ARG:NH1	2.30	0.46
1:F:29:THR:O	1:F:33:MET:HG2	2.16	0.46
1:F:274:CYS:HB2	1:F:310:LEU:HD11	1.97	0.45
1:F:31:ASP:OD1	1:F:141:ARG:NH2	2.50	0.45
1:F:294:GLU:OE2	1:F:297:LYS:HD2	2.16	0.45
1:F:75:ARG:HE	1:F:76:LYS:HG3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:ASP:OD1	1:F:186:VAL:HB	2.18	0.44
1:F:297:LYS:O	1:F:300:ARG:HB3	2.18	0.44
1:F:235:MET:HE3	1:F:348:ILE:HD11	1.99	0.44
1:F:177:THR:C	1:F:179:PRO:HD3	2.38	0.44
1:F:281:GLU:O	1:F:285:ILE:HG13	2.18	0.44
1:F:278:ALA:HB1	1:F:282:GLN:HB2	1.99	0.43
1:F:235:MET:HE1	1:F:344:LEU:HB2	2.00	0.43
1:F:325:ILE:O	1:F:329:ILE:HG13	2.18	0.43
1:F:338:PRO:O	1:F:342:LEU:HG	2.18	0.43
1:F:336:LEU:HD12	1:F:336:LEU:N	2.34	0.43
1:F:166:GLN:HB2	1:F:166:GLN:HE21	1.54	0.42
1:F:208:LEU:HB3	1:F:209:PRO:HD3	2.00	0.42
1:F:153:TYR:CZ	1:F:157:ILE:HD11	2.54	0.42
1:F:262:ILE:HA	1:F:290:TYR:CE1	2.55	0.41
1:F:300:ARG:HA	1:F:300:ARG:HD2	1.77	0.41
1:F:279:THR:H	1:F:282:GLN:CG	2.33	0.41
1:F:235:MET:HE1	1:F:344:LEU:CB	2.51	0.41
1:F:230:LYS:HE2	1:F:230:LYS:HB2	1.64	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	F	339/350 (97%)	327 (96%)	11 (3%)	1 (0%)	43 53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	183	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	F	292/300 (97%)	281 (96%)	11 (4%)	36 50

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	45	LEU
1	F	75	ARG
1	F	82	LEU
1	F	126	LEU
1	F	145	LEU
1	F	148	ARG
1	F	166	GLN
1	F	230	LYS
1	F	306	GLU
1	F	315	LEU
1	F	328	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	12	GLN
1	F	23	GLN
1	F	83	GLN
1	F	162	GLN
1	F	166	GLN
1	F	182	ASN
1	F	282	GLN
1	F	289	ASN
1	F	292	GLN

5.3.3 RNA

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](#)

1 ligand is 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	F	1001	-	4,4,4	1.32	0	6,6,6	0.38	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	PO4	F	1001	-	-	0/0/0/0	0/0/0/0

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 [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	F	341/350 (97%)	1.22	89 (26%) 0 0	30, 59, 103, 109	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	10	TYR	7.1
1	F	33	MET	6.8
1	F	12	GLN	6.7
1	F	278	ALA	6.2
1	F	292	GLN	6.0
1	F	281	GLU	5.8
1	F	279	THR	5.3
1	F	15	GLN	5.0
1	F	32	GLU	4.9
1	F	284	GLN	4.9
1	F	11	ALA	4.7
1	F	294	GLU	4.6
1	F	183	VAL	4.6
1	F	286	LEU	4.5
1	F	31	ASP	4.4
1	F	9	VAL	4.4
1	F	296	GLU	4.4
1	F	293	LYS	4.3
1	F	285	ILE	4.2
1	F	288	GLU	4.2
1	F	30	GLU	4.0
1	F	282	GLN	3.9
1	F	300	ARG	3.9
1	F	82	LEU	3.9
1	F	99	PHE	3.8
1	F	135	LEU	3.6
1	F	86	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	95	LEU	3.5
1	F	13	GLU	3.4
1	F	35	HIS	3.3
1	F	140	TYR	3.3
1	F	289	ASN	3.3
1	F	275	LEU	3.3
1	F	299	ALA	3.2
1	F	305	TYR	3.2
1	F	98	PHE	3.2
1	F	291	GLY	3.2
1	F	102	ALA	3.2
1	F	182	ASN	3.1
1	F	34	GLY	3.1
1	F	139	ILE	3.1
1	F	298	VAL	3.1
1	F	164	SER	3.0
1	F	75	ARG	3.0
1	F	133	ASN	2.9
1	F	132	ALA	2.9
1	F	129	ILE	2.8
1	F	134	LEU	2.8
1	F	309	ASP	2.8
1	F	137	ALA	2.7
1	F	72	VAL	2.7
1	F	161	LEU	2.7
1	F	185	LEU	2.7
1	F	167	THR	2.7
1	F	114	GLY	2.7
1	F	106	MET	2.6
1	F	181	GLY	2.6
1	F	308	LEU	2.6
1	F	166	GLN	2.5
1	F	310	LEU	2.5
1	F	101	VAL	2.5
1	F	113	ARG	2.5
1	F	100	LEU	2.5
1	F	283	TYR	2.4
1	F	16	ASP	2.4
1	F	297	LYS	2.4
1	F	138	CYS	2.4
1	F	96	GLN	2.4
1	F	253	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	315	LEU	2.3
1	F	14	LYS	2.3
1	F	36	PRO	2.3
1	F	74	PRO	2.3
1	F	73	GLU	2.2
1	F	277	ARG	2.2
1	F	257	LYS	2.2
1	F	130	ASN	2.2
1	F	128	ALA	2.2
1	F	165	TYR	2.2
1	F	17	PHE	2.2
1	F	170	GLY	2.2
1	F	301	VAL	2.2
1	F	223	LYS	2.1
1	F	280	PRO	2.1
1	F	267	CYS	2.1
1	F	307	GLU	2.1
1	F	19	GLN	2.1
1	F	136	GLU	2.1
1	F	262	ILE	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 carbohydrates 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(\AA^2)	Q<0.9
2	PO4	F	1001	5/5	0.96	0.13	80,80,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.