



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 04:32 PM EDT

PDB ID : 3WYI
Title : Structure of S. aureus undecaprenyl diphosphate synthase
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Deposited on : 2014-08-29
Resolution : 2.00 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 types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

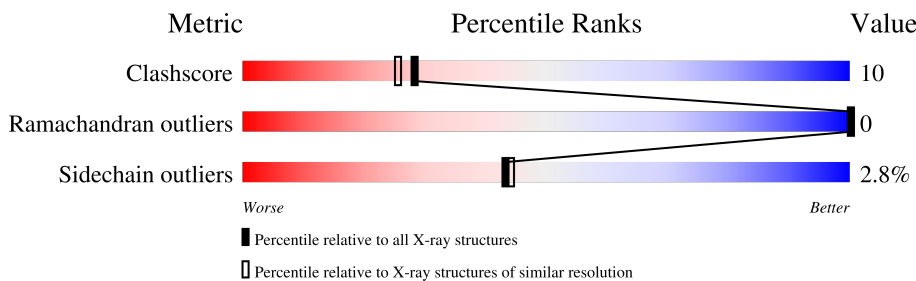
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	256	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2270 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 Isoprenyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1893	1211	318	357	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

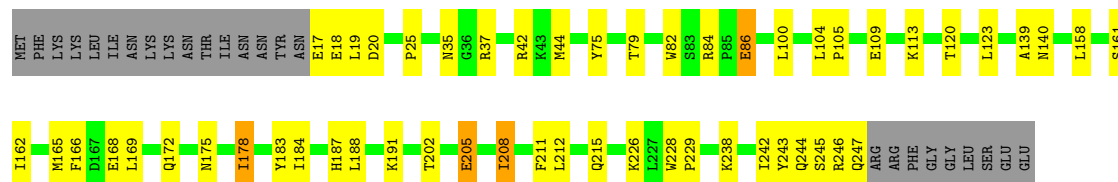
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	375	Total	O	0	0
			375	375		

Note EDS failed to run properly.

- Molecule 1: Isoprenyl transferase



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	62.08Å 62.08Å 133.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.227	Depositor
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.626	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
Total number of atoms	2270	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: MG

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	0.37	1/1933 (0.1%)	0.56	0/2610

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	PHE	C-O	-5.03	1.13	1.23

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	1893	0	1892	37	0
2	A	2	0	0	0	0
3	A	375	0	0	4	1
All	All	2270	0	1892	37	1

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 10.

All (37) 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:20:ASP:H	1:A:244:GLN:HE22	1.35	0.74
1:A:37:ARG:NH2	1:A:79:THR:HB	2.03	0.74
1:A:208:ILE:HD13	3:A:611:HOH:O	1.90	0.72
1:A:17:GLU:HG2	1:A:18:GLU:H	1.54	0.71
1:A:120:THR:HA	1:A:123:LEU:HD13	1.76	0.67
1:A:17:GLU:HG2	1:A:18:GLU:N	2.14	0.63
1:A:84:ARG:HA	1:A:86:GLU:OE2	2.04	0.58
1:A:246:ARG:O	1:A:247:GLN:HB2	2.05	0.57
1:A:105:PRO:O	1:A:109:GLU:HG3	2.04	0.57
1:A:183:TYR:O	1:A:187:HIS:HD2	1.86	0.57
1:A:165:MET:O	1:A:169:LEU:HG	2.06	0.55
1:A:17:GLU:CG	1:A:18:GLU:H	2.18	0.53
1:A:208:ILE:HD13	1:A:208:ILE:H	1.73	0.53
1:A:175:ASN:O	1:A:178:ILE:HD12	2.09	0.52
1:A:161:SER:O	1:A:165:MET:HG3	2.12	0.50
1:A:113:LYS:HE2	1:A:139:ALA:O	2.12	0.50
1:A:178:ILE:HD13	1:A:178:ILE:H	1.77	0.49
1:A:25:PRO:HG3	1:A:243:TYR:CE2	2.47	0.48
1:A:42:ARG:HH11	1:A:42:ARG:HG3	1.79	0.47
1:A:104:LEU:HB3	1:A:105:PRO:HD3	1.96	0.47
1:A:75:TYR:HB2	1:A:211:PHE:CE1	2.50	0.46
1:A:238:LYS:O	1:A:242:ILE:HG12	2.16	0.46
1:A:202:THR:HB	1:A:226:LYS:O	2.14	0.46
1:A:100:LEU:O	1:A:104:LEU:HB2	2.17	0.45
1:A:44:MET:HE2	3:A:714:HOH:O	2.15	0.45
1:A:82:TRP:HD1	1:A:205:GLU:OE2	1.99	0.45
1:A:158:LEU:O	1:A:162:ILE:HG13	2.17	0.45
1:A:178:ILE:H	1:A:178:ILE:CD1	2.29	0.44
1:A:184:ILE:O	1:A:188:LEU:HG	2.18	0.44
1:A:140:ASN:HB2	3:A:647:HOH:O	2.17	0.43
1:A:228:TRP:HB3	1:A:229:PRO:HD3	2.00	0.43
1:A:245:SER:C	1:A:247:GLN:H	2.21	0.42
1:A:123:LEU:HD12	3:A:636:HOH:O	2.18	0.42
1:A:35:ASN:HD21	1:A:228:TRP:HD1	1.68	0.42
1:A:178:ILE:HD13	1:A:178:ILE:N	2.34	0.41
1:A:168:GLU:O	1:A:172:GLN:HG3	2.20	0.41
1:A:212:LEU:HB3	1:A:215:GLN:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:759:HOH:O	3:A:759:HOH:O[5_674]	2.18	0.02

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	229/256 (90%)	221 (96%)	8 (4%)	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	211/234 (90%)	205 (97%)	6 (3%)	43	44

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	86	GLU
1	A	178	ILE
1	A	191	LYS
1	A	205	GLU
1	A	208	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	55	GLN
1	A	140	ASN
1	A	160	HIS
1	A	170	HIS
1	A	172	GLN
1	A	187	HIS
1	A	244	GLN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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 is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.