Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 07:29 PM EDT

PDB ID	:	3QAS
Title	:	Structure of Undecaprenyl Diphosphate synthase
Authors	:	Cao, R.; Oldfield, E.
Deposited on	:	2011-01-11
Resolution	:	1.70 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:

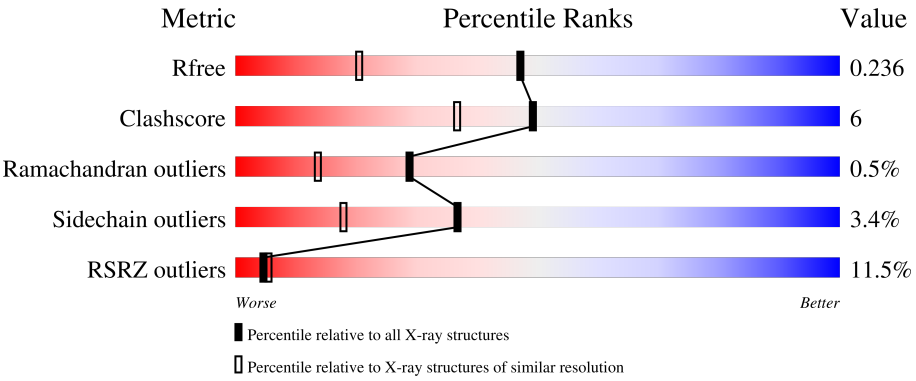
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	253	11% 77% 10% • 12%
1	B	253	9% 68% 13% • 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3795 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 Undecaprenyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	211	Total	C	N	O	S	0	0	0
			1673	1049	315	304	5			
1	A	223	Total	C	N	O	S	0	0	0
			1778	1116	332	324	6			

- Molecule 2 is water.

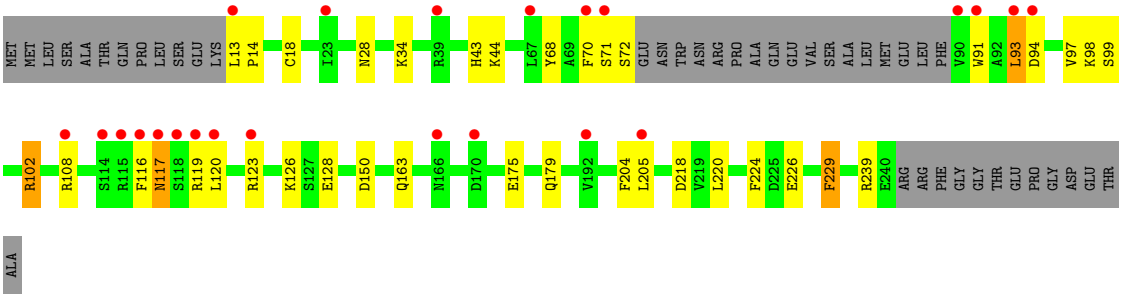
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	151	Total	O	0	0
			151	151		
2	A	193	Total	O	0	0
			193	193		

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.

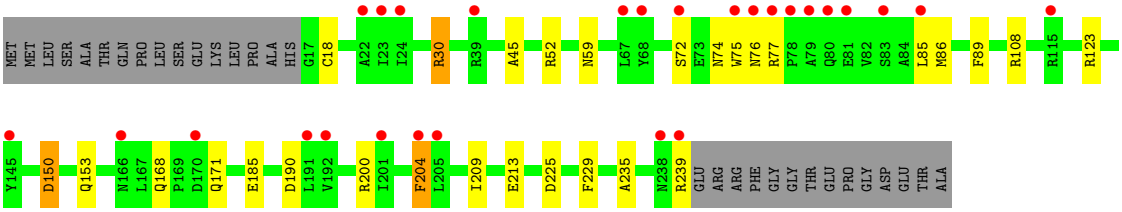
• Molecule 1: Undecaprenyl pyrophosphate synthase

Chain B:



• Molecule 1: Undecaprenyl pyrophosphate synthase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.63Å 68.76Å 111.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.95 – 1.70 27.95 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (27.95-1.70) 99.5 (27.95-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.72 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.184 , 0.224 0.202 , 0.236	Depositor DCC
R_{free} test set	2711 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3795	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.25	3/1814 (0.2%)	1.11	8/2451 (0.3%)
1	B	1.25	6/1706 (0.4%)	1.14	9/2303 (0.4%)
All	All	1.25	9/3520 (0.3%)	1.13	17/4754 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	18	CYS	CB-SG	-9.76	1.65	1.82
1	A	18	CYS	CB-SG	-7.97	1.68	1.82
1	B	224	PHE	CD2-CE2	6.50	1.52	1.39
1	A	89	PHE	CE1-CZ	5.51	1.47	1.37
1	A	45	ALA	CA-CB	5.41	1.63	1.52
1	B	224	PHE	CD1-CE1	5.27	1.49	1.39
1	B	226	GLU	CD-OE1	5.20	1.31	1.25
1	B	128	GLU	CB-CG	5.17	1.61	1.52
1	B	229	PHE	CD2-CE2	5.07	1.49	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	239	ARG	NE-CZ-NH1	-10.42	115.09	120.30
1	B	239	ARG	NE-CZ-NH2	7.81	124.20	120.30
1	A	123	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	204	PHE	CB-CG-CD2	-7.41	115.61	120.80
1	B	224	PHE	CB-CG-CD2	-6.11	116.53	120.80
1	B	218	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	52	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	B	150	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	150	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	225	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	68	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	B	218	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	190	ASP	CB-CG-OD2	-5.18	113.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	ILE	CG1-CB-CG2	5.13	122.68	111.40
1	A	150	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	200	ARG	CG-CD-NE	-5.05	101.19	111.80
1	B	205	LEU	CB-CG-CD1	-5.03	102.45	111.00

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	1778	0	1741	15	0
1	B	1673	0	1637	27	0
2	A	193	0	0	2	0
2	B	151	0	0	9	0
All	All	3795	0	3378	40	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 6.

All (40) 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:93:LEU:O	1:B:97:VAL:HG23	1.52	1.09
1:B:91:TRP:HA	2:B:267:HOH:O	1.61	1.00
1:B:98:LYS:O	1:B:102:ARG:HG2	1.65	0.96
1:A:108:ARG:NH1	1:A:185:GLU:OE2	2.05	0.90
1:A:213:GLU:OE2	1:A:239:ARG:HD3	1.90	0.72
1:B:28:ASN:HD22	1:B:43:HIS:HD2	1.37	0.71
1:A:168:GLN:HB2	1:A:171:GLN:HG3	1.76	0.67
1:B:13:LEU:HD12	1:B:14:PRO:HD2	1.75	0.66
1:A:150:ASP:O	1:A:153:GLN:HG3	2.00	0.62
1:B:119:ARG:HB3	2:B:352:HOH:O	2.03	0.58
1:A:235:ALA:O	1:A:239:ARG:HD2	2.06	0.56
1:B:108:ARG:HD2	2:B:318:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PHE:CE2	1:B:72:SER:HA	2.41	0.55
1:B:117:ASN:HB2	2:B:352:HOH:O	2.07	0.54
1:B:28:ASN:HD22	1:B:43:HIS:CD2	2.24	0.53
1:B:91:TRP:CZ2	1:B:120:LEU:HD22	2.45	0.52
1:B:175:GLU:O	1:B:179:GLN:HG2	2.09	0.51
1:B:163:GLN:HE22	1:A:168:GLN:NE2	2.08	0.50
1:B:119:ARG:CB	2:B:352:HOH:O	2.59	0.50
1:B:34:LYS:HE2	1:B:220:LEU:HD11	1.94	0.49
1:B:91:TRP:HZ2	1:B:120:LEU:HD22	1.76	0.49
1:B:98:LYS:O	1:B:102:ARG:CG	2.51	0.49
1:A:74:ASN:HA	1:A:77:ARG:HD3	1.95	0.48
1:B:117:ASN:ND2	2:B:352:HOH:O	2.47	0.47
1:B:163:GLN:HE22	1:A:168:GLN:HE22	1.62	0.47
1:B:179:GLN:NE2	2:B:308:HOH:O	2.34	0.47
1:A:108:ARG:HH12	1:A:185:GLU:CD	2.16	0.47
1:A:30:ARG:HE	1:A:30:ARG:HB2	1.51	0.46
1:A:86:MET:HE3	2:A:260:HOH:O	2.15	0.45
1:B:99:SER:HA	1:B:102:ARG:HG3	1.99	0.45
1:B:70:PHE:CD2	1:B:72:SER:HB3	2.52	0.45
1:B:94:ASP:OD2	1:B:123:ARG:HD3	2.18	0.43
1:A:239:ARG:HH21	1:A:239:ARG:HG2	1.83	0.43
1:A:59:ASN:ND2	2:A:257:HOH:O	2.50	0.43
1:A:76:ASN:O	1:A:76:ASN:CG	2.56	0.43
1:B:117:ASN:CB	2:B:352:HOH:O	2.64	0.43
1:B:179:GLN:HG3	2:B:338:HOH:O	2.19	0.42
1:A:76:ASN:O	1:A:77:ARG:HG3	2.19	0.42
1:B:70:PHE:CE2	1:B:72:SER:HB3	2.54	0.42
1:B:116:PHE:N	1:B:116:PHE:CD1	2.89	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	221/253 (87%)	216 (98%)	4 (2%)	1 (0%)	29	13
1	B	207/253 (82%)	203 (98%)	3 (1%)	1 (0%)	29	13
All	All	428/506 (85%)	419 (98%)	7 (2%)	2 (0%)	29	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	PHE
1	B	204	PHE

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	182/206 (88%)	177 (97%)	5 (3%)	44	26
1	B	170/206 (82%)	163 (96%)	7 (4%)	30	12
All	All	352/412 (85%)	340 (97%)	12 (3%)	37	18

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	44	LYS
1	B	71	SER
1	B	93	LEU
1	B	102	ARG
1	B	117	ASN
1	B	126	LYS
1	B	229	PHE
1	A	30	ARG
1	A	72	SER
1	A	75	TRP
1	A	85	LEU
1	A	229	PHE

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

sidechains are listed below:

Mol	Chain	Res	Type
1	B	43	HIS
1	B	59	ASN
1	B	166	ASN
1	A	43	HIS
1	A	59	ASN
1	A	163	GLN
1	A	168	GLN
1	A	179	GLN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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^{th} 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	223/253 (88%)	0.71	27 (12%)	4	5	14, 25, 54, 74	0
1	B	211/253 (83%)	0.60	23 (10%)	5	6	14, 25, 57, 75	0
All	All	434/506 (85%)	0.66	50 (11%)	4	5	14, 25, 54, 75	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	TRP	10.3
1	B	71	SER	8.3
1	B	91	TRP	7.6
1	A	79	ALA	7.4
1	A	76	ASN	6.4
1	A	80	GLN	5.6
1	B	119	ARG	4.9
1	B	115	ARG	4.9
1	B	70	PHE	4.8
1	A	23	ILE	4.6
1	B	116	PHE	4.4
1	A	115	ARG	4.1
1	B	118	SER	4.1
1	B	13	LEU	3.7
1	A	78	PRO	3.6
1	B	117	ASN	3.3
1	B	108	ARG	3.3
1	B	39	ARG	3.2
1	B	94	ASP	3.2
1	A	67	LEU	3.1
1	B	120	LEU	3.1
1	B	90	VAL	3.0
1	A	239	ARG	2.9
1	A	39	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	166	ASN	2.8
1	A	77	ARG	2.7
1	A	238	ASN	2.6
1	A	83	SER	2.6
1	A	204	PHE	2.6
1	B	23	ILE	2.5
1	B	93	LEU	2.5
1	A	22	ALA	2.5
1	A	166	ASN	2.5
1	A	24	ILE	2.4
1	A	192	VAL	2.4
1	A	191	LEU	2.4
1	B	123	ARG	2.3
1	A	68	TYR	2.3
1	B	114	SER	2.3
1	B	67	LEU	2.3
1	A	72	SER	2.3
1	A	201	ILE	2.3
1	A	81	GLU	2.2
1	B	205	LEU	2.2
1	A	205	LEU	2.2
1	A	170	ASP	2.2
1	A	145	TYR	2.1
1	B	192	VAL	2.1
1	A	85	LEU	2.0
1	B	170	ASP	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.