



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7MXZ
Title : Sy-CrtE apo structure
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Deposited on : 2021-05-19
Resolution : 1.47 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
Xtriage (Phenix) : 1.13
EDS : 2.28.1
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) : 2.28.1

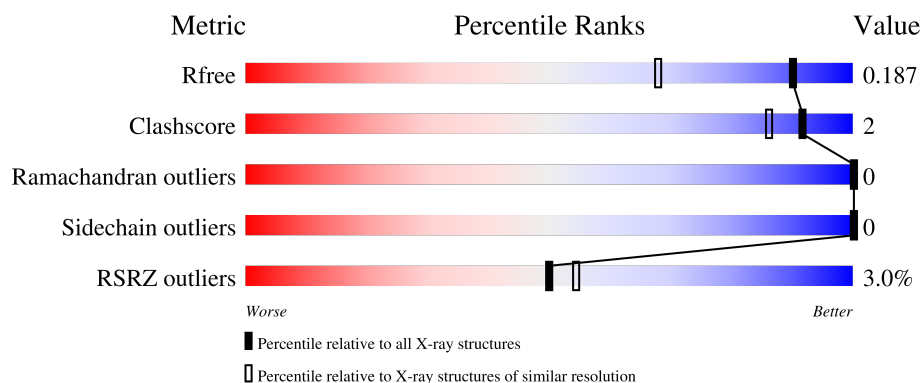
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

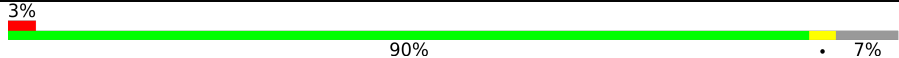

The reported resolution of this entry is 1.47 Å.

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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	AAA	310	
1	BBB	310	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5096 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 Geranylgeranyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	289	Total	C	N	O	S	0	9	0
			2249	1418	383	439	9			
1	BBB	284	Total	C	N	O	S	0	18	0
			2284	1439	394	441	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	303	LEU	-	expression tag	UNP P72683
AAA	304	GLU	-	expression tag	UNP P72683
AAA	305	HIS	-	expression tag	UNP P72683
AAA	306	HIS	-	expression tag	UNP P72683
AAA	307	HIS	-	expression tag	UNP P72683
AAA	308	HIS	-	expression tag	UNP P72683
AAA	309	HIS	-	expression tag	UNP P72683
AAA	310	HIS	-	expression tag	UNP P72683
BBB	303	LEU	-	expression tag	UNP P72683
BBB	304	GLU	-	expression tag	UNP P72683
BBB	305	HIS	-	expression tag	UNP P72683
BBB	306	HIS	-	expression tag	UNP P72683
BBB	307	HIS	-	expression tag	UNP P72683
BBB	308	HIS	-	expression tag	UNP P72683
BBB	309	HIS	-	expression tag	UNP P72683
BBB	310	HIS	-	expression tag	UNP P72683

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Mg	0	0
			1	1		
2	BBB	2	Total	Mg	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total 1	Cl 1	0	0
3	BBB	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

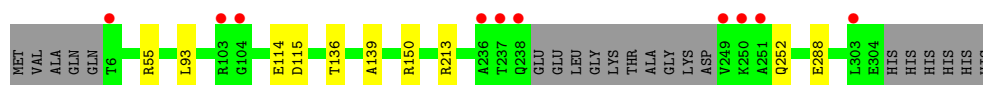
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	281	Total 281	O 281	0	0
4	BBB	277	Total 277	O 277	0	0

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: Geranylgeranyl pyrophosphate synthase

Chain AAA: 



- Molecule 1: Geranylgeranyl pyrophosphate synthase

Chain BBB: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	61.50Å 73.65Å 132.17Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	39.76 – 1.47 39.73 – 1.47	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.76-1.47) 98.2 (39.73-1.47)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.160 , 0.185 0.163 , 0.187	Depositor DCC
R_{free} test set	4987 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5096	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6136e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL

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	AAA	0.79	0/2281	0.89	4/3098 (0.1%)
1	BBB	0.78	1/2316 (0.0%)	0.91	3/3142 (0.1%)
All	All	0.79	1/4597 (0.0%)	0.90	7/6240 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	37	GLU	CD-OE1	6.20	1.32	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	150	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	AAA	213	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	BBB	213	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	AAA	150	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	BBB	96	MET	CA-CB-CG	-5.60	103.78	113.30
1	AAA	115	ASP	CB-CG-OD1	5.30	123.07	118.30
1	AAA	55	ARG	NE-CZ-NH2	-5.24	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	AAA	2249	0	2258	4	0
1	BBB	2284	0	2297	11	0
2	AAA	1	0	0	0	0
2	BBB	2	0	0	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
4	AAA	281	0	0	2	0
4	BBB	277	0	0	7	0
All	All	5096	0	4555	15	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 2.

All (15) 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:BBB:216[B]:ARG:HD2	4:BBB:553:HOH:O	1.65	0.94
1:BBB:216[B]:ARG:CD	4:BBB:553:HOH:O	2.22	0.86
1:BBB:216[B]:ARG:CG	4:BBB:553:HOH:O	2.24	0.84
1:BBB:216[B]:ARG:HG2	4:BBB:553:HOH:O	1.90	0.68
1:BBB:185:HIS:CE1	1:BBB:226[B]:GLN:HG2	2.31	0.65
1:AAA:288:GLU:OE1	4:AAA:501:HOH:O	2.15	0.62
1:BBB:185:HIS:NE2	1:BBB:226[B]:GLN:HG2	2.14	0.62
1:BBB:52:LYS:HE2	4:BBB:633:HOH:O	2.01	0.60
1:BBB:185:HIS:CD2	1:BBB:226[B]:GLN:HG2	2.45	0.50
1:AAA:252:GLN:CD	4:AAA:508:HOH:O	2.50	0.50
1:BBB:268[B]:GLN:HG3	4:BBB:628:HOH:O	2.15	0.47
1:AAA:136:THR:HG22	1:AAA:139:ALA:HB2	1.97	0.45
1:AAA:93:LEU:HD22	1:AAA:114[B]:GLU:HG3	1.99	0.44
1:BBB:39:ILE:HD12	1:BBB:39:ILE:HA	1.83	0.41
1:BBB:146[B]:GLN:HG2	4:BBB:544:HOH:O	2.21	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	AAA	294/310 (95%)	293 (100%)	1 (0%)	0	100	100
1	BBB	298/310 (96%)	297 (100%)	1 (0%)	0	100	100
All	All	592/620 (96%)	590 (100%)	2 (0%)	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	AAA	234/243 (96%)	234 (100%)	0	100	100
1	BBB	238/243 (98%)	238 (100%)	0	100	100
All	All	472/486 (97%)	472 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

Of 5 ligands modelled in this entry, 5 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

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 [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, 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	AAA	289/310 (93%)	-0.01	10 (3%) 44 48	10, 16, 32, 60	0
1	BBB	284/310 (91%)	-0.09	7 (2%) 57 61	10, 16, 32, 53	0
All	All	573/620 (92%)	-0.05	17 (2%) 50 54	10, 16, 32, 60	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	249	VAL	10.1
1	AAA	237	THR	9.3
1	AAA	238	GLN	5.5
1	BBB	235	THR	4.9
1	AAA	250	LYS	4.6
1	AAA	6	THR	4.2
1	BBB	251	ALA	3.7
1	BBB	104	GLY	3.6
1	AAA	236	ALA	3.5
1	BBB	236	ALA	3.4
1	AAA	303	LEU	3.4
1	AAA	251	ALA	3.0
1	AAA	103	ARG	2.6
1	AAA	104	GLY	2.4
1	BBB	303	LEU	2.4
1	BBB	103	ARG	2.2
1	BBB	101	PHE	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 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(\AA^2)	Q<0.9
2	MG	BBB	402	1/1	0.91	0.23	37,37,37,37	0
3	CL	AAA	402	1/1	0.96	0.05	23,23,23,23	0
3	CL	BBB	403	1/1	0.98	0.03	22,22,22,22	0
2	MG	BBB	401	1/1	1.00	0.04	11,11,11,11	0
2	MG	AAA	401	1/1	1.00	0.04	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.