



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:44 pm BST

PDB ID : 5WA3
Title : Pyridine synthase, TbtD, from thiomuracin biosynthesis
Authors : Cogan, D.P.; Nair, S.K.
Deposited on : 2017-06-24
Resolution : 2.80 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	:	2.11
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

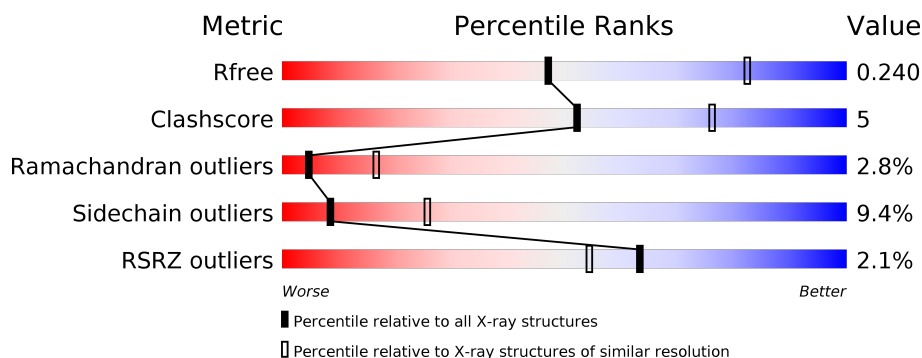
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 ≥ 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	361	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	361	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>16%</div> <div>•</div> <div>15%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4874 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 Pyridine synthase TbtD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2448	1549	462	431	6			
1	B	306	Total	C	N	O	S	0	0	0
			2426	1535	459	426	6			

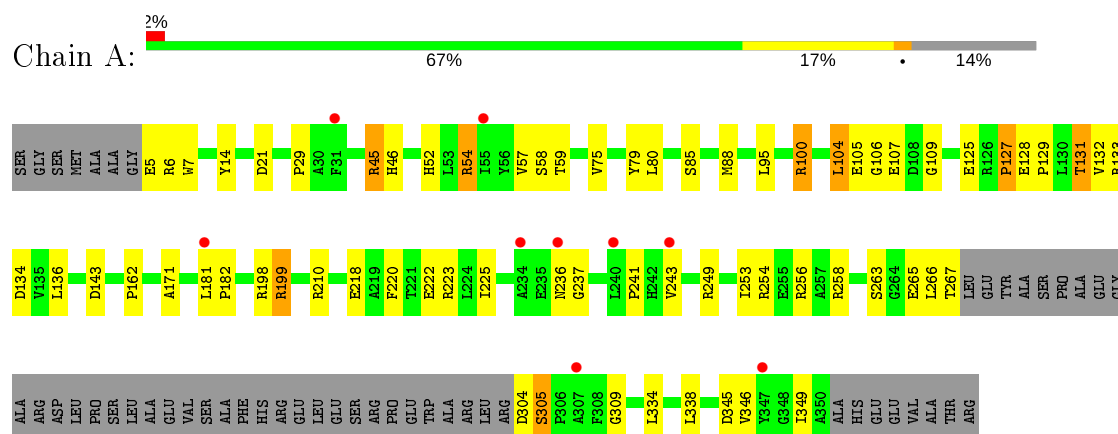
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP D6Y504
A	-1	GLY	-	expression tag	UNP D6Y504
A	0	SER	-	expression tag	UNP D6Y504
B	-2	SER	-	expression tag	UNP D6Y504
B	-1	GLY	-	expression tag	UNP D6Y504
B	0	SER	-	expression tag	UNP D6Y504

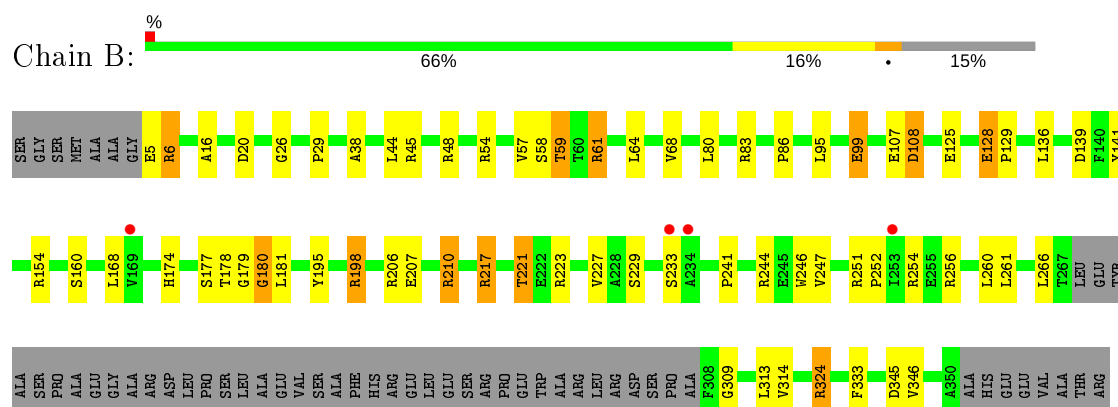
3 Residue-property plots [i](#)

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: Pyridine synthase TbtD



• Molecule 1: Pyridine synthase TbtD



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	155.83Å 155.83Å 165.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	104.52 – 2.80 77.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (104.52-2.80) 93.9 (77.92-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.197 , 0.242 0.200 , 0.240	Depositor DCC
R_{free} test set	1729 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.087 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4874	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

5.1 Standard geometry

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	0.78	1/2515 (0.0%)	1.00	4/3428 (0.1%)
1	B	0.78	0/2492	1.01	9/3394 (0.3%)
All	All	0.78	1/5007 (0.0%)	1.01	13/6822 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLU	CD-OE1	5.66	1.31	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	54	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	20	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	45	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	20	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	256	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	217	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	61	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	256	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	21	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	198	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	154	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	198	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	SER	Peptide

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	A	2448	0	2402	25	0
1	B	2426	0	2383	32	0
All	All	4874	0	4785	53	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 5.

All (53) 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:6:ARG:HG2	1:B:125:GLU:OE2	1.86	0.76
1:B:64:LEU:HD12	1:B:68:VAL:CG2	2.24	0.68
1:A:334:LEU:O	1:A:334:LEU:HD23	1.98	0.62
1:A:220:PHE:CZ	1:A:338:LEU:HD13	2.34	0.62
1:B:64:LEU:HA	1:B:68:VAL:HG22	1.84	0.60
1:B:221:THR:HG22	1:B:346:VAL:CG1	2.34	0.57
1:B:217:ARG:NH1	1:B:345:ASP:OD2	2.38	0.56
1:B:217:ARG:O	1:B:221:THR:OG1	2.24	0.55
1:B:45:ARG:HD2	1:B:324:ARG:O	2.07	0.55
1:B:44:LEU:HD21	1:B:141:TYR:CE2	2.43	0.54
1:B:16:ALA:HB3	1:B:86:PRO:HD2	1.91	0.51
1:B:48:ARG:HD2	1:B:107:GLU:HG2	1.93	0.51
1:A:131:THR:OG1	1:A:132:VAL:N	2.44	0.51
1:A:6:ARG:O	1:A:58:SER:HA	2.11	0.50
1:A:334:LEU:HD23	1:A:334:LEU:C	2.32	0.50
1:A:100:ARG:HD3	1:A:104:LEU:HD22	1.93	0.49
1:A:29:PRO:HB2	1:A:75:VAL:HG11	1.94	0.49
1:A:52:HIS:NE2	1:A:54:ARG:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASP:OD2	1:B:217:ARG:NH2	2.49	0.45
1:B:26:GLY:C	1:B:29:PRO:HD2	2.36	0.45
1:A:7:TRP:O	1:A:125:GLU:HA	2.16	0.45
1:B:244:ARG:HA	1:B:247:VAL:HG12	1.98	0.45
1:B:38:ALA:HB2	1:B:59:THR:CG2	2.47	0.45
1:A:107:GLU:O	1:A:109:GLY:N	2.45	0.44
1:B:136:LEU:CD1	1:B:313:LEU:HD21	2.47	0.44
1:A:218:GLU:O	1:A:222:GLU:HG2	2.16	0.44
1:B:48:ARG:CD	1:B:107:GLU:HG2	2.48	0.44
1:A:181:LEU:N	1:A:182:PRO:HD2	2.32	0.44
1:B:223:ARG:O	1:B:227:VAL:HG23	2.18	0.44
1:B:168:LEU:HD22	1:B:246:TRP:CG	2.52	0.43
1:B:174:HIS:ND1	1:B:180:GLY:O	2.48	0.43
1:B:6:ARG:O	1:B:58:SER:HA	2.18	0.43
1:B:195:TYR:CG	1:B:333:PHE:CD2	3.07	0.43
1:A:210:ARG:CZ	1:B:210:ARG:HD2	2.49	0.43
1:A:46:HIS:HB3	1:A:52:HIS:NE2	2.34	0.43
1:A:136:LEU:HD21	1:A:253:ILE:HG23	2.00	0.43
1:B:38:ALA:HB2	1:B:59:THR:HG23	2.01	0.42
1:A:304:ASP:O	1:A:305:SER:C	2.58	0.42
1:B:5:GLU:O	1:B:6:ARG:HD2	2.20	0.42
1:A:199:ARG:N	1:A:199:ARG:HD3	2.35	0.42
1:A:198:ARG:C	1:A:199:ARG:HD3	2.40	0.42
1:B:95:LEU:O	1:B:99:GLU:HB2	2.20	0.41
1:A:171:ALA:HB2	1:A:243:VAL:HG23	2.02	0.41
1:A:210:ARG:CZ	1:B:210:ARG:CD	2.98	0.41
1:A:79:TYR:C	1:A:79:TYR:CD1	2.94	0.41
1:A:131:THR:HG23	1:A:134:ASP:OD2	2.20	0.41
1:B:107:GLU:O	1:B:108:ASP:HB2	2.21	0.41
1:B:128:GLU:CB	1:B:129:PRO:CD	2.99	0.41
1:B:261:LEU:HG	1:B:266:LEU:HD21	2.02	0.41
1:A:265:GLU:HB2	1:A:266:LEU:HD23	2.02	0.41
1:B:128:GLU:HB2	1:B:129:PRO:CD	2.51	0.40
1:A:210:ARG:CZ	1:B:210:ARG:NE	2.84	0.40
1:B:251:ARG:HB3	1:B:252:PRO:HD3	2.03	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	A	306/361 (85%)	272 (89%)	25 (8%)	9 (3%)	4	15
1	B	302/361 (84%)	269 (89%)	25 (8%)	8 (3%)	5	18
All	All	608/722 (84%)	541 (89%)	50 (8%)	17 (3%)	5	17

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	PRO
1	B	178	THR
1	B	181	LEU
1	A	106	GLY
1	B	108	ASP
1	B	128	GLU
1	B	309	GLY
1	A	128	GLU
1	A	237	GLY
1	A	309	GLY
1	A	236	ASN
1	A	241	PRO
1	A	129	PRO
1	B	179	GLY
1	B	180	GLY
1	B	241	PRO
1	A	349	ILE

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	245/285 (86%)	220 (90%)	25 (10%)	7	22
1	B	243/285 (85%)	222 (91%)	21 (9%)	10	30
All	All	488/570 (86%)	442 (91%)	46 (9%)	8	26

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	14	TYR
1	A	45	ARG
1	A	57	VAL
1	A	59	THR
1	A	80	LEU
1	A	85	SER
1	A	88	MET
1	A	95	LEU
1	A	100	ARG
1	A	104	LEU
1	A	127	PRO
1	A	131	THR
1	A	133	ARG
1	A	143	ASP
1	A	162	PRO
1	A	199	ARG
1	A	223	ARG
1	A	225	ILE
1	A	249	ARG
1	A	254	ARG
1	A	258	ARG
1	A	267	THR
1	A	305	SER
1	A	346	VAL
1	B	6	ARG
1	B	57	VAL
1	B	59	THR
1	B	61	ARG
1	B	80	LEU
1	B	83	ARG
1	B	99	GLU
1	B	139	ASP
1	B	160	SER

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Mol	Chain	Res	Type
1	B	177	SER
1	B	198	ARG
1	B	206	ARG
1	B	207	GLU
1	B	210	ARG
1	B	221	THR
1	B	229	SER
1	B	233	SER
1	B	254	ARG
1	B	260	LEU
1	B	314	VAL
1	B	324	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	98	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

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	A	310/361 (85%)	0.37	9 (2%) 51 41	50, 83, 147, 202	0
1	B	306/361 (84%)	0.35	4 (1%) 77 72	53, 85, 137, 195	0
All	All	616/722 (85%)	0.36	13 (2%) 63 54	50, 84, 141, 202	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	ALA	3.7
1	B	233	SER	3.4
1	B	169	VAL	2.9
1	A	236	ASN	2.7
1	A	240	LEU	2.5
1	A	307	ALA	2.3
1	B	253	ILE	2.3
1	A	347	TYR	2.2
1	A	181	LEU	2.2
1	A	31	PHE	2.2
1	A	243	VAL	2.1
1	A	234	ALA	2.1
1	A	55	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.