



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:06 AM UTC

PDB ID : 6EC7 / pdb_00006ec7
Title : Glutamylation domain, TbtB, from thiomuracin biosynthesis
Authors : Cogan, D.P.; Nair, S.K.
Deposited on : 2018-08-07
Resolution : 2.15 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

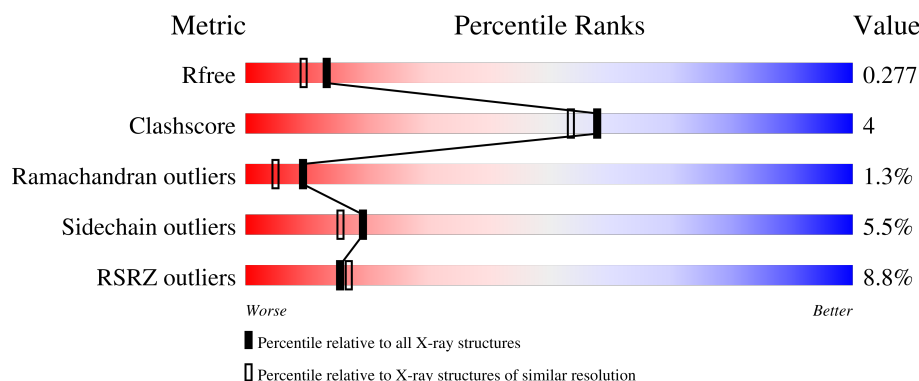
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	A	861	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6480 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 Lantibiotic dehydratase domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	796	6250	3966	1176	1092	16	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP D6Y502
A	-1	GLY	-	expression tag	UNP D6Y502
A	0	SER	-	expression tag	UNP D6Y502

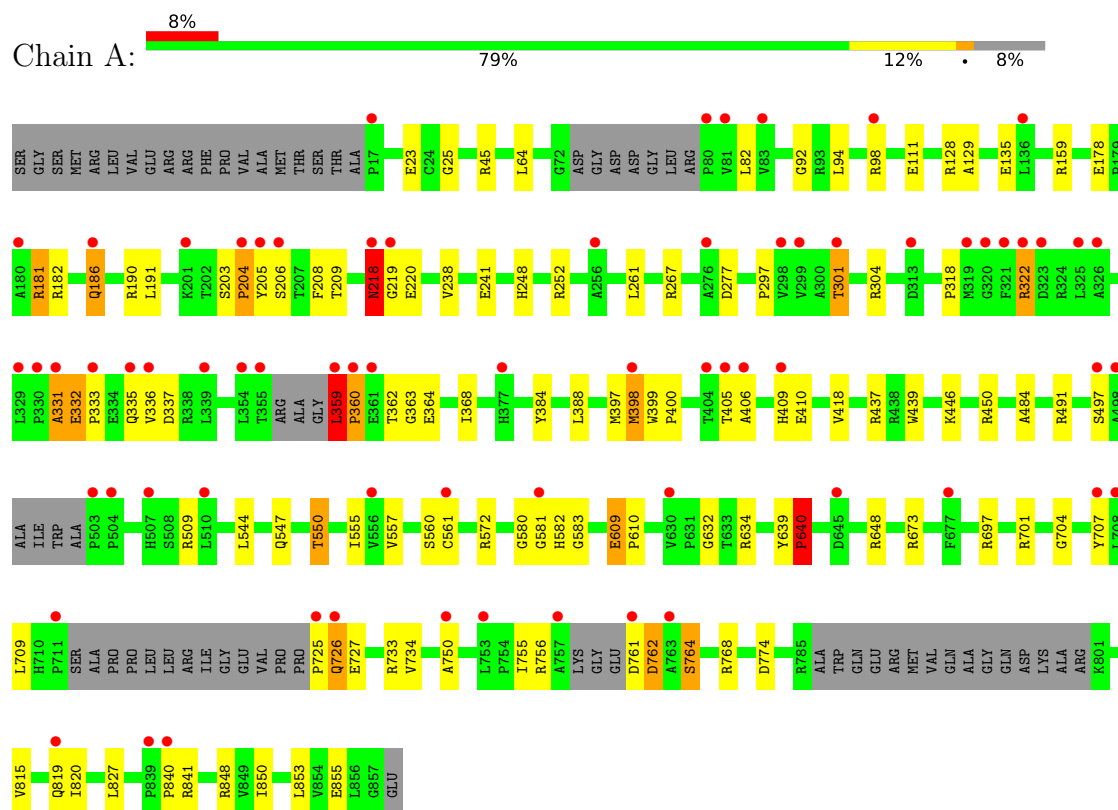
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	230	Total	O	0	0
			230	230		

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: Lantibiotic dehydratase domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.82Å 96.41Å 107.01Å 90.00° 98.76° 90.00°	Depositor
Resolution (Å)	105.76 – 2.15 105.76 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (105.76-2.15) 100.0 (105.76-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.214 , 0.277 0.221 , 0.277	Depositor DCC
R_{free} test set	2496 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.3	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	0.95	EDS
Total number of atoms	6480	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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](#)

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	1.04	5/6398 (0.1%)	1.14	13/8702 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	557	VAL	N-CA	-7.04	1.39	1.46
1	A	734	VAL	C-O	-5.31	1.18	1.24
1	A	697	ARG	C-O	-5.16	1.18	1.24
1	A	241	GLU	CA-C	5.08	1.57	1.52
1	A	45	ARG	C-O	-5.04	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	LEU	CA-C-N	21.70	142.13	119.78
1	A	359	LEU	C-N-CA	21.70	142.13	119.78
1	A	764	SER	N-CA-C	-12.55	97.33	112.89
1	A	218	ASN	N-CA-C	8.81	129.57	110.80
1	A	707	TYR	N-CA-C	8.36	124.30	113.18
1	A	360	PRO	CA-C-O	-7.60	112.75	121.56
1	A	582	HIS	N-CA-C	-6.34	102.68	110.61
1	A	204	PRO	N-CA-C	6.05	123.59	113.78
1	A	762	ASP	N-CA-C	5.73	123.01	110.80
1	A	557	VAL	N-CA-C	-5.50	101.90	107.89
1	A	92	GLY	N-CA-C	5.40	122.26	114.10
1	A	580	GLY	N-CA-C	-5.27	105.87	111.93
1	A	632	GLY	N-CA-C	5.20	125.51	113.18

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	A	6250	0	6339	56	0
2	A	230	0	0	2	0
All	All	6480	0	6339	56	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 4.

All (56) 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:318:PRO:O	1:A:322:ARG:HG3	1.70	0.91
1:A:727:GLU:HA	2:A:901:HOH:O	1.76	0.85
1:A:318:PRO:O	1:A:322:ARG:CG	2.32	0.78
1:A:252:ARG:HD2	2:A:1107:HOH:O	1.92	0.70
1:A:547:GLN:O	1:A:550:THR:HG22	1.97	0.65
1:A:761:ASP:OD1	1:A:764:SER:OG	2.16	0.63
1:A:322:ARG:HD2	1:A:337:ASP:OD1	1.99	0.62
1:A:331:ALA:O	1:A:332:GLU:HB2	2.00	0.62
1:A:297:PRO:O	1:A:301:THR:HG23	2.01	0.60
1:A:128:ARG:HD2	1:A:129:ALA:N	2.17	0.59
1:A:301:THR:HG22	1:A:304:ARG:NH2	2.17	0.59
1:A:23:GLU:HB3	1:A:850:ILE:HG22	1.84	0.57
1:A:362:THR:HG22	1:A:363:GLY:N	2.19	0.56
1:A:384:TYR:CZ	1:A:388:LEU:HD11	2.41	0.56
1:A:267:ARG:NH2	1:A:640:PRO:O	2.39	0.55
1:A:450:ARG:NH1	1:A:704:GLY:O	2.40	0.54
1:A:405:THR:HG23	1:A:405:THR:O	2.08	0.54
1:A:853:LEU:C	1:A:853:LEU:HD23	2.34	0.53
1:A:384:TYR:CE2	1:A:388:LEU:HD11	2.47	0.49
1:A:399:TRP:CD2	1:A:400:PRO:HD2	2.48	0.49
1:A:484:ALA:O	1:A:491:ARG:NH2	2.46	0.49
1:A:186:GLN:NE2	1:A:190:ARG:HH11	2.12	0.48
1:A:439:TRP:CE2	1:A:544:LEU:HD22	2.49	0.48
1:A:159:ARG:NH2	1:A:410:GLU:OE1	2.46	0.48
1:A:609:GLU:HA	1:A:610:PRO:C	2.37	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASN:C	1:A:218:ASN:HD22	2.22	0.47
1:A:25:GLY:N	1:A:208:PHE:O	2.44	0.47
1:A:368:ILE:HG12	1:A:398:MET:HE1	1.97	0.47
1:A:218:ASN:C	1:A:218:ASN:ND2	2.73	0.46
1:A:764:SER:O	1:A:768:ARG:HG3	2.15	0.46
1:A:446:LYS:HD3	1:A:701:ARG:HA	1.96	0.46
1:A:248:HIS:O	1:A:252:ARG:HG3	2.16	0.46
1:A:332:GLU:HG3	1:A:335:GLN:HE21	1.80	0.46
1:A:23:GLU:CB	1:A:850:ILE:HG22	2.46	0.45
1:A:318:PRO:O	1:A:322:ARG:HG2	2.12	0.45
1:A:362:THR:CG2	1:A:363:GLY:N	2.81	0.44
1:A:815:VAL:O	1:A:819:GLN:HG2	2.17	0.44
1:A:405:THR:O	1:A:406:ALA:HB3	2.18	0.43
1:A:64:LEU:HD11	1:A:82:LEU:HD22	1.99	0.43
1:A:128:ARG:CD	1:A:129:ALA:N	2.80	0.43
1:A:359:LEU:HA	1:A:360:PRO:HD3	1.31	0.43
1:A:364:GLU:HB2	1:A:398:MET:HE2	2.00	0.43
1:A:639:TYR:O	1:A:640:PRO:C	2.62	0.43
1:A:437:ARG:HD2	1:A:561:CYS:HB2	2.00	0.43
1:A:725:PRO:O	1:A:726:GLN:CB	2.66	0.42
1:A:178:GLU:O	1:A:181:ARG:CB	2.68	0.41
1:A:331:ALA:O	1:A:332:GLU:CB	2.68	0.41
1:A:583:GLY:N	1:A:855:GLU:OE1	2.53	0.41
1:A:159:ARG:NH2	1:A:238:VAL:HG21	2.35	0.41
1:A:560:SER:HB3	1:A:581:GLY:O	2.21	0.41
1:A:218:ASN:ND2	1:A:219:GLY:O	2.53	0.41
1:A:841[B]:ARG:NH1	1:A:848:ARG:O	2.54	0.41
1:A:756:ARG:NH2	1:A:762:ASP:O	2.54	0.41
1:A:333:PRO:O	1:A:336:VAL:HG12	2.21	0.41
1:A:204:PRO:HA	1:A:209:THR:OG1	2.21	0.40
1:A:178:GLU:O	1:A:181:ARG:HB3	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	A	783/861 (91%)	747 (95%)	26 (3%)	10 (1%)	9	5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	331	ALA
1	A	640	PRO
1	A	750	ALA
1	A	205	TYR
1	A	277	ASP
1	A	398	MET
1	A	726	GLN
1	A	497	SER
1	A	182	ARG

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	643/698 (92%)	608 (95%)	35 (5%)	20	16

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	98	ARG
1	A	111	GLU
1	A	135	GLU
1	A	181	ARG
1	A	186	GLN
1	A	191	LEU
1	A	203	SER
1	A	206	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	218	ASN
1	A	220	GLU
1	A	261	LEU
1	A	301	THR
1	A	322	ARG
1	A	332	GLU
1	A	359	LEU
1	A	397	MET
1	A	409	HIS
1	A	418	VAL
1	A	509	ARG
1	A	550	THR
1	A	555	ILE
1	A	572	ARG
1	A	609	GLU
1	A	634	ARG
1	A	640	PRO
1	A	648	ARG
1	A	673	ARG
1	A	709	LEU
1	A	733	ARG
1	A	755	ILE
1	A	774	ASP
1	A	820	ILE
1	A	827	LEU
1	A	840	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	218	ASN
1	A	335	GLN
1	A	409	HIS

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 oligosaccharides 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 [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	A	796/861 (92%)	0.60	70 (8%) 15 17	25, 45, 80, 128	1 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	ALA	6.1
1	A	503	PRO	6.0
1	A	205	TYR	5.8
1	A	498	ALA	5.6
1	A	206	SER	5.6
1	A	757	ALA	5.6
1	A	319	MET	4.9
1	A	725	PRO	4.9
1	A	80	PRO	4.8
1	A	360	PRO	4.6
1	A	711	PRO	4.3
1	A	355	THR	4.1
1	A	630	VAL	4.0
1	A	405	THR	3.9
1	A	359	LEU	3.6
1	A	323	ASP	3.6
1	A	330	PRO	3.6
1	A	504	PRO	3.3
1	A	763	ALA	3.3
1	A	840	PRO	3.3
1	A	219	GLY	3.2
1	A	329	LEU	3.2
1	A	839	PRO	3.1
1	A	81	VAL	3.1
1	A	276	ALA	3.1
1	A	510	LEU	3.1
1	A	180	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	186	GLN	3.0
1	A	404	THR	2.9
1	A	313	ASP	2.8
1	A	409	HIS	2.9
1	A	335	GLN	2.8
1	A	336	VAL	2.8
1	A	561	CYS	2.8
1	A	218	ASN	2.8
1	A	361	GLU	2.8
1	A	507	HIS	2.7
1	A	339	LEU	2.7
1	A	761	ASP	2.7
1	A	320	GLY	2.7
1	A	581	GLY	2.6
1	A	406	ALA	2.6
1	A	377	HIS	2.5
1	A	333	PRO	2.4
1	A	750	ALA	2.4
1	A	136	LEU	2.4
1	A	556	VAL	2.4
1	A	819	GLN	2.3
1	A	708	LEU	2.3
1	A	322	ARG	2.3
1	A	325	LEU	2.3
1	A	201	LYS	2.3
1	A	298	VAL	2.3
1	A	354	LEU	2.3
1	A	98	ARG	2.2
1	A	326	ALA	2.2
1	A	753	LEU	2.2
1	A	83	VAL	2.2
1	A	299	VAL	2.2
1	A	645	ASP	2.2
1	A	301	THR	2.2
1	A	321	PHE	2.1
1	A	256	ALA	2.1
1	A	204	PRO	2.1
1	A	677	PHE	2.1
1	A	497	SER	2.1
1	A	726	GLN	2.0
1	A	17	PRO	2.0
1	A	707	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	398	MET	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 oligosaccharides 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.