



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:52 PM UTC

PDB ID : 6RTH / pdb_00006rth
Title : Crystal structure of the ligand-free glycosyltransferase domain from the YGT toxin
Authors : Wirth, C.; Bogdanovic, X.; Kao, W.-C.; Hunte, C.
Deposited on : 2019-05-23
Resolution : 3.40 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

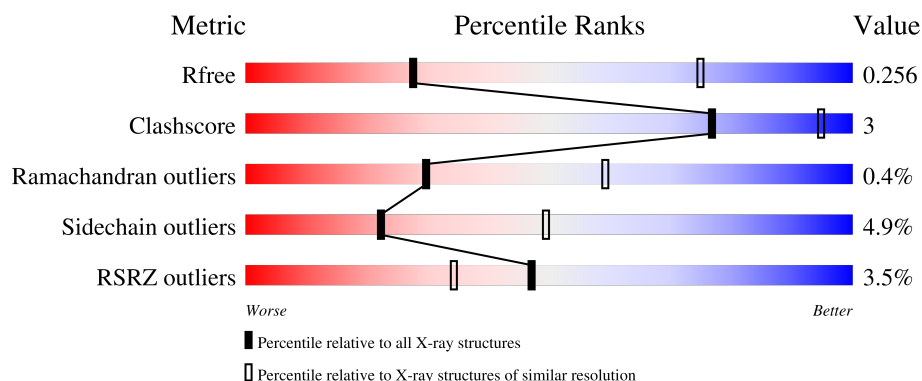
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

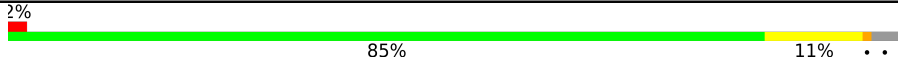
The reported resolution of this entry is 3.40 Å.

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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	521	
1	B	521	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8080 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 RTX toxin and Ca²⁺-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	43	0	0
			4073	2583	680	798	12			
1	B	496	Total	C	N	O	S	59	0	0
			4007	2545	667	783	12			

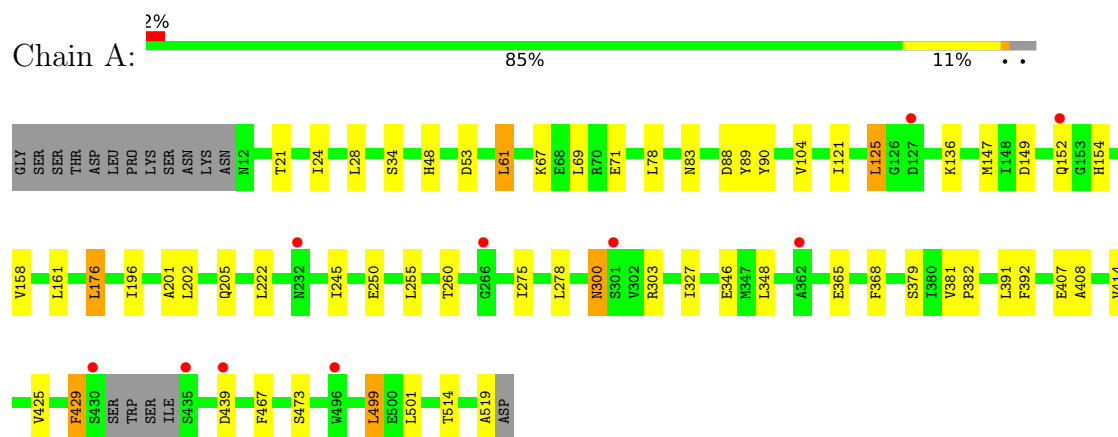
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP C4SH25
A	1	SER	-	expression tag	UNP C4SH25
B	0	GLY	-	expression tag	UNP C4SH25
B	1	SER	-	expression tag	UNP C4SH25

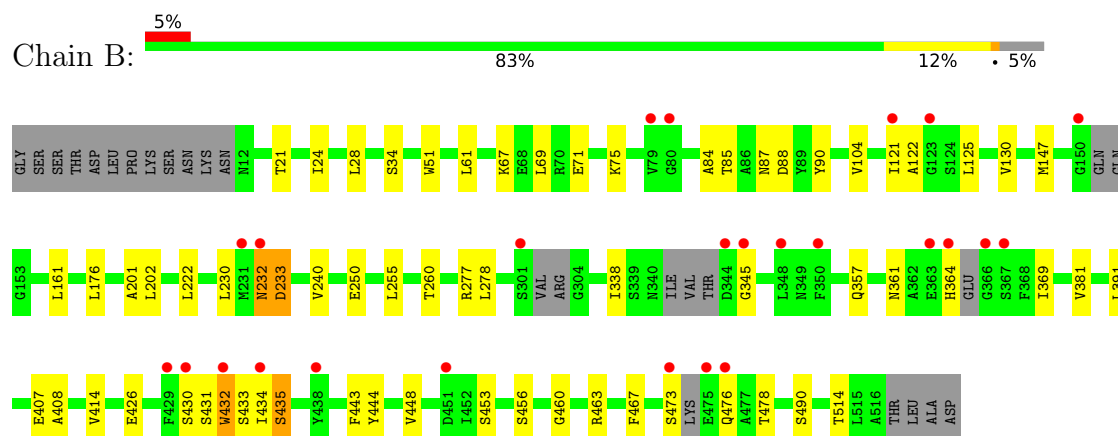
3 Residue-property plots [i](#)

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: RTX toxin and Ca^{2+} -binding protein



- Molecule 1: RTX toxin and Ca^{2+} -binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.18Å 161.74Å 162.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 30.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.40) 98.9 (30.00-3.40)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.227 , 0.249 0.241 , 0.256	Depositor DCC
R_{free} test set	922 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.048 for -h,l,k	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8080	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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	0.76	0/4148	1.43	7/5616 (0.1%)
1	B	0.76	1/4080 (0.0%)	1.44	12/5519 (0.2%)
All	All	0.76	1/8228 (0.0%)	1.43	19/11135 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	ILE	CA-CB	5.67	1.57	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	431	SER	CA-C-N	7.76	131.01	120.38
1	B	431	SER	C-N-CA	7.76	131.01	120.38
1	B	75	LYS	CA-C-N	6.47	128.95	120.28
1	B	75	LYS	C-N-CA	6.47	128.95	120.28
1	B	407	GLU	CA-C-N	6.26	130.22	120.82
1	B	407	GLU	C-N-CA	6.26	130.22	120.82
1	A	407	GLU	CA-C-N	6.19	130.11	120.82
1	A	407	GLU	C-N-CA	6.19	130.11	120.82
1	A	88	ASP	CA-CB-CG	5.95	118.55	112.60
1	B	443	PHE	CA-CB-CG	5.79	119.59	113.80
1	B	433	SER	CA-C-N	5.78	129.13	120.69
1	B	433	SER	C-N-CA	5.78	129.13	120.69
1	A	149	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	346	GLU	CA-C-N	5.37	127.42	120.44
1	A	346	GLU	C-N-CA	5.37	127.42	120.44
1	A	379	SER	CA-CB-OG	5.19	121.48	111.10
1	B	345	GLY	CA-C-N	5.17	127.73	120.28
1	B	345	GLY	C-N-CA	5.17	127.73	120.28
1	B	233	ASP	CA-CB-CG	5.07	117.67	112.60

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	4073	0	3999	25	0
1	B	4007	0	3914	21	0
All	All	8080	0	7913	46	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 3.

All (46) 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:232:ASN:HB3	1:B:240:VAL:HG21	1.78	0.65
1:A:245:ILE:HG23	1:A:275:ILE:HD12	1.82	0.61
1:A:61:LEU:HD21	1:A:136:LYS:HD3	1.86	0.58
1:A:28:LEU:H	1:A:147:MET:HE1	1.69	0.58
1:B:90:TYR:HB3	1:B:381:VAL:HG22	1.87	0.57
1:B:28:LEU:H	1:B:147:MET:HE1	1.69	0.56
1:B:250:GLU:HG3	1:B:255:LEU:HD12	1.87	0.56
1:A:250:GLU:HG3	1:A:255:LEU:HD12	1.87	0.56
1:A:425:VAL:O	1:A:429:PHE:HB2	2.07	0.55
1:B:473:SER:HB3	1:B:476:GLN:HB3	1.89	0.54
1:A:176:LEU:HD12	1:A:196:ILE:HG23	1.89	0.54
1:B:361:ASN:HD22	1:B:364:HIS:H	1.56	0.53
1:A:300:ASN:HD22	1:A:300:ASN:N	2.10	0.50
1:B:69:LEU:HD13	1:B:121:ILE:HG23	1.94	0.49
1:B:430:SER:C	1:B:432:TRP:H	2.22	0.48
1:A:69:LEU:HD13	1:A:121:ILE:HG23	1.96	0.47
1:A:90:TYR:HB3	1:A:381:VAL:HG22	1.95	0.47
1:A:467:PHE:HD1	1:A:501:LEU:HD23	1.79	0.47
1:B:222:LEU:HD21	1:B:278:LEU:HD22	1.96	0.47
1:A:161:LEU:HD11	1:A:201:ALA:HA	1.97	0.46
1:A:303:ARG:NE	1:A:303:ARG:HA	2.31	0.46
1:A:90:TYR:CE1	1:A:382:PRO:HD3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:HD22	1:A:300:ASN:H	1.64	0.45
1:A:250:GLU:HB3	1:A:260:THR:HG21	1.98	0.45
1:B:250:GLU:HB3	1:B:260:THR:HG21	1.98	0.44
1:A:499:LEU:HD11	1:A:519:ALA:HB2	2.00	0.44
1:B:161:LEU:HD11	1:B:201:ALA:HA	1.99	0.44
1:B:67:LYS:O	1:B:71:GLU:HG3	2.18	0.43
1:A:176:LEU:HD22	1:A:327:ILE:HD11	2.01	0.43
1:A:408:ALA:HB1	1:A:414:VAL:HB	2.00	0.43
1:B:122:ALA:HB1	1:B:130:VAL:HA	1.99	0.43
1:A:67:LYS:O	1:A:71:GLU:HG3	2.19	0.43
1:B:408:ALA:HB1	1:B:414:VAL:HB	2.01	0.43
1:A:48:HIS:O	1:A:154:HIS:HB3	2.18	0.43
1:A:78:LEU:HD11	1:A:89:TYR:CE1	2.54	0.43
1:A:222:LEU:HD21	1:A:278:LEU:HD22	1.99	0.43
1:A:53:ASP:CG	1:A:158:VAL:HG21	2.44	0.42
1:B:432:TRP:HE3	1:B:432:TRP:HA	1.84	0.42
1:B:432:TRP:HA	1:B:432:TRP:CE3	2.55	0.41
1:B:34:SER:HB3	1:B:255:LEU:HD22	2.01	0.41
1:A:34:SER:HB3	1:A:255:LEU:HD22	2.03	0.41
1:B:444:TYR:O	1:B:448:VAL:HG23	2.20	0.41
1:B:463:ARG:O	1:B:467:PHE:HD2	2.04	0.41
1:A:368:PHE:HD1	1:A:392:PHE:HB3	1.86	0.41
1:B:51:TRP:CZ3	1:B:161:LEU:HB2	2.56	0.40
1:B:460:GLY:HA2	1:B:463:ARG:HG2	2.03	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	500/521 (96%)	479 (96%)	20 (4%)	1 (0%)	43 71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	484/521 (93%)	464 (96%)	17 (4%)	3 (1%)	21 50
All	All	984/1042 (94%)	943 (96%)	37 (4%)	4 (0%)	30 59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	ASP
1	B	435	SER
1	B	84	ALA
1	A	125	LEU

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	450/466 (97%)	431 (96%)	19 (4%)	26 52
1	B	441/466 (95%)	416 (94%)	25 (6%)	18 45
All	All	891/932 (96%)	847 (95%)	44 (5%)	22 49

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	24	ILE
1	A	61	LEU
1	A	83	ASN
1	A	104	VAL
1	A	125	LEU
1	A	152	GLN
1	A	176	LEU
1	A	202	LEU
1	A	205	GLN
1	A	300	ASN
1	A	348	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	365	GLU
1	A	391	LEU
1	A	429	PHE
1	A	439	ASP
1	A	473	SER
1	A	499	LEU
1	A	514	THR
1	B	21	THR
1	B	24	ILE
1	B	61	LEU
1	B	85	THR
1	B	87	ASN
1	B	88	ASP
1	B	104	VAL
1	B	125	LEU
1	B	176	LEU
1	B	202	LEU
1	B	230	LEU
1	B	232	ASN
1	B	277	ARG
1	B	338	ILE
1	B	357	GLN
1	B	391	LEU
1	B	426	GLU
1	B	432	TRP
1	B	434	ILE
1	B	435	SER
1	B	453	SER
1	B	456	SER
1	B	478	THR
1	B	490	SER
1	B	514	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	156	GLN
1	A	170	ASN
1	A	205	GLN
1	A	300	ASN
1	A	386	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	476	GLN
1	A	498	GLN
1	B	92	GLN
1	B	103	ASN
1	B	156	GLN
1	B	164	GLN
1	B	170	ASN
1	B	205	GLN
1	B	300	ASN
1	B	349	ASN
1	B	361	ASN
1	B	374	ASN
1	B	493	ASN

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 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	504/521 (96%)	0.47	10 (1%)	65 49	14, 40, 66, 88	11 (2%)
1	B	496/521 (95%)	0.61	25 (5%)	34 25	13, 43, 84, 105	14 (2%)
All	All	1000/1042 (95%)	0.54	35 (3%)	47 34	13, 42, 77, 105	25 (2%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	344	ASP	4.3
1	B	430	SER	3.8
1	B	367	SER	3.6
1	B	475	GLU	3.4
1	B	348	LEU	3.4
1	B	150	GLY	3.0
1	B	79	VAL	2.8
1	A	430	SER	2.8
1	A	439	ASP	2.7
1	A	152	GLN	2.6
1	B	80	GLY	2.6
1	B	434	ILE	2.6
1	B	366	GLY	2.6
1	B	363	GLU	2.6
1	B	301	SER	2.5
1	B	432	TRP	2.5
1	A	362	ALA	2.4
1	B	438	TYR	2.4
1	A	301	SER	2.4
1	A	266	GLY	2.3
1	B	364	HIS	2.3
1	B	231	MET	2.3
1	B	232	ASN	2.3
1	B	350	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	496	TRP	2.3
1	A	127	ASP	2.3
1	B	123	GLY	2.2
1	A	232	ASN	2.2
1	B	429	PHE	2.2
1	B	476	GLN	2.1
1	A	435	SER	2.1
1	B	473	SER	2.1
1	B	451	ASP	2.1
1	B	345	GLY	2.1
1	B	121	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 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.