

Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2023 – 04:07 PM EDT

PDB ID : 4RA7

Title : Structure of a putative peptidoglycan glycosyltransferase from Atopobium

parvulum in complex with nafcillin

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Deposited on : 2014-09-09

Resolution : 1.94 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 (i) 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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : FAILED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

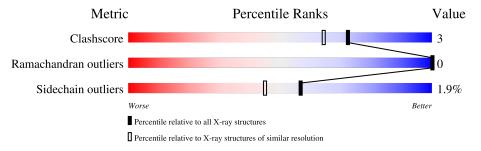
Validation Pipeline (wwPDB-VP) : 2.35.1

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 1.94 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain		
1	A	453	84%	7%	8%
1	В	453	85%	7%	8%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6414 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 Peptidoglycan glycosyltransferase.

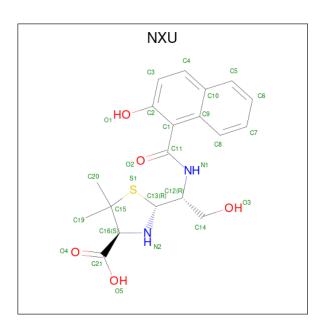
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	A	416	Total 2996	C 1863	N 508	_	S 2	Se 13	0	1	0
1	В	416	Total 2996	_	N 507	_	S 2	Se 13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	SER	-	expression tag	UNP C8W8H7
A	503	ASN	-	expression tag	UNP C8W8H7
A	504	ALA	-	expression tag	UNP C8W8H7
В	502	SER	-	expression tag	UNP C8W8H7
В	503	ASN	-	expression tag	UNP C8W8H7
В	504	ALA	-	expression tag	UNP C8W8H7

• Molecule 2 is (2R,4S)-2-[(1R)-2-hydroxy-1- $\{[(2-hydroxynaphthalen-1-yl)carbonyl]amino }ethyl]-5,5-dimethyl-1,3-thiazolidine-4-carboxylic acid (three-letter code: NXU) (formula: <math>C_{19}H_{22}N_2O_5S$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
9	Λ	1	Total	С	N	О	S	0	0	
2	A	1	27	19	2	5	1	0	ı	
9	D	1	Total	С	N	О	S	0	0	
2	Б	1	27	19	2	5	1	U	0	

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	195	Total O 195 195	0	0
3	В	172	Total O 173 173	0	1

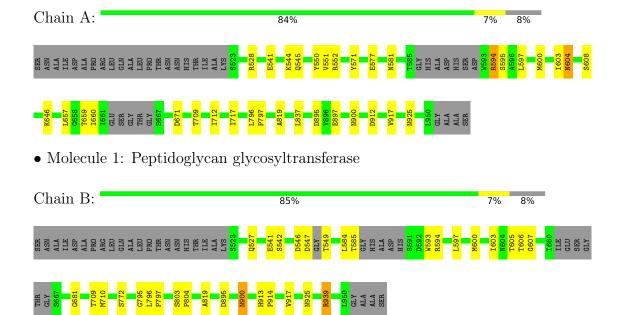


3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: Peptidoglycan glycosyltransferase





4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	68.40Å 70.06Å 114.57Å	Depositor
a, b, c, α , β , γ	90.00° 96.97° 90.00°	Depositor
Resolution (Å)	30.00 - 1.94	Depositor
% Data completeness	99.3 (30.00-1.94)	Depositor
(in resolution range)	, , ,	•
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.89 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.161 , 0.199	Depositor
Wilson B-factor (\mathring{A}^2)	38.0	Xtriage
Anisotropy	0.219	Xtriage
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6414	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.66	0/3034	0.77	1/4118 (0.0%)	
1	В	0.68	0/3034	0.79	0/4118	
All	All	0.67	0/6068	0.78	1/8236 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	604	ASN	N-CA-C	8.64	134.33	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	2996	0	2916	22	0
1	В	2996	0	2918	19	0
2	A	27	0	18	0	0
2	В	27	0	17	1	0
3	A	195	0	0	2	0
3	В	173	0	0	2	0
All	All	6414	0	5869	41	0



The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 3.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1		$\operatorname{distance} \left(\operatorname{\AA} \right)$	overlap (Å)
1:A:545:GLN:HE22	1:A:551:VAL:HB	1.41	0.86
1:A:608:SER:HB2	1:A:837:LEU:O	1.97	0.64
1:A:571:TYR:HE2	1:A:657:LEU:O	1.81	0.62
1:A:796:LEU:HD12	1:A:797:PRO:HD2	1.83	0.61
1:B:527:GLN:HG2	1:B:606:THR:HG23	1.83	0.61
1:A:912:ASP:HB2	3:A:1112:HOH:O	2.03	0.58
1:B:939:ARG:HD2	3:B:1214:HOH:O	2.03	0.56
1:B:681:GLY:O	1:B:795:GLY:HA3	2.06	0.56
1:A:897:GLU:N	1:A:897:GLU:OE1	2.38	0.56
1:A:571:TYR:OH	1:A:660:ILE:O	2.20	0.55
1:B:594:ARG:HB2	1:B:600:MSE:HE3	1.90	0.54
1:B:597:LEU:HD22	1:B:600:MSE:HE2	1.90	0.54
1:A:604:ASN:OD1	1:A:604:ASN:C	2.48	0.51
1:A:594:ARG:HB2	1:A:600:MSE:HE3	1.91	0.51
1:A:541:GLU:O	1:A:552:ARG:HD2	2.12	0.50
1:B:803:SER:HB2	1:B:804:PRO:HD2	1.95	0.49
1:B:900:ASN:HB3	1:B:925:ASN:O	2.14	0.48
1:A:528:ARG:NH2	1:A:581:ASN:OD1	2.37	0.47
1:A:597:LEU:HB2	1:A:600:MSE:HE2	1.97	0.47
1:B:597:LEU:HD12	1:B:597:LEU:N	2.30	0.47
1:A:528:ARG:NH1	1:A:577:GLU:O	2.47	0.47
1:A:712:ILE:HD12	1:A:717:ILE:HG13	1.97	0.46
1:A:646:LYS:NZ	1:A:671:ASP:OD2	2.49	0.45
1:B:594:ARG:HB2	1:B:600:MSE:CE	2.46	0.45
1:B:772:SER:HB3	3:B:1142:HOH:O	2.16	0.44
1:B:913:HIS:N	1:B:914:PRO:HD3	2.33	0.44
1:A:597:LEU:HD12	1:A:597:LEU:N	2.32	0.43
1:B:796:LEU:HD12	1:B:797:PRO:HD2	2.01	0.43
1:A:608:SER:CB	1:A:837:LEU:O	2.65	0.43
1:B:547:ASP:O	1:B:549:THR:N	2.52	0.43
1:B:546:ASP:O	1:B:547:ASP:C	2.57	0.42
1:A:895:ASP:HB2	3:A:1232:HOH:O	2.19	0.42
1:A:544:LYS:HB2	1:A:550:TYR:CE1	2.53	0.42
1:B:527:GLN:HE21	1:B:542:SER:HB2	1.85	0.42
1:A:819:ALA:HA	1:A:917:VAL:HG21	2.01	0.42
1:B:593:TRP:CE2	1:B:594:ARG:HB3	2.54	0.42
1:A:900:ASN:CG	1:A:925:ASN:O	2.58	0.42

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Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:659:THR:OG1	1:A:660:ILE:N	2.50	0.41
1:B:584:LEU:O	1:B:607:GLY:HA3	2.21	0.41
1:B:895:ASP:CG	2:B:1001:NXU:H23	2.41	0.41
1:B:819:ALA:HA	1:B:917:VAL:HG21	2.04	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	Percenti	les
1	A	411/453 (91%)	399 (97%)	12 (3%)	0	100 10	00
1	В	408/453 (90%)	396 (97%)	12 (3%)	0	100 10	00
All	All	819/906 (90%)	795 (97%)	24 (3%)	0	100 10	00

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	Percer	ntiles
1	A	315/330 (96%)	311 (99%)	4 (1%)	69	62
1	В	316/330 (96%)	308 (98%)	8 (2%)	47	35
All	All	631/660 (96%)	619 (98%)	12 (2%)	57	45



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

Mol	Chain	Res	Type
1	A	594	ARG
1	A	595	SER
1	A	603	ILE
1	A	709	THR
1	В	541	GLU
1	В	585	THR
1	В	603	ILE
1	В	605	THR
1	В	709	THR
1	В	710	MSE
1	В	900	ASN
1	В	939	ARG

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

Mol	Chain	Res	Type
1	A	570	GLN
1	A	718	HIS
1	A	925	ASN
1	A	943	GLN
1	В	527	GLN
1	В	545	GLN
1	В	570	GLN
1	В	722	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 monosaccharides in this entry.



5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

