



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:15 AM UTC

PDB ID : 5NR9 / pdb_00005nr9
Title : A Native Ternary Complex of Alpha-1,3-Galactosyltransferase (alpha-3GalT)
Supports a Conserved Reaction Mechanism for Retaining Glycosyltransferases
- Unliganded alpha-3GalT
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Deposited on : 2017-04-22
Resolution : 1.70 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
Mogul : 2022.3.0, CSD as543be (2022)
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

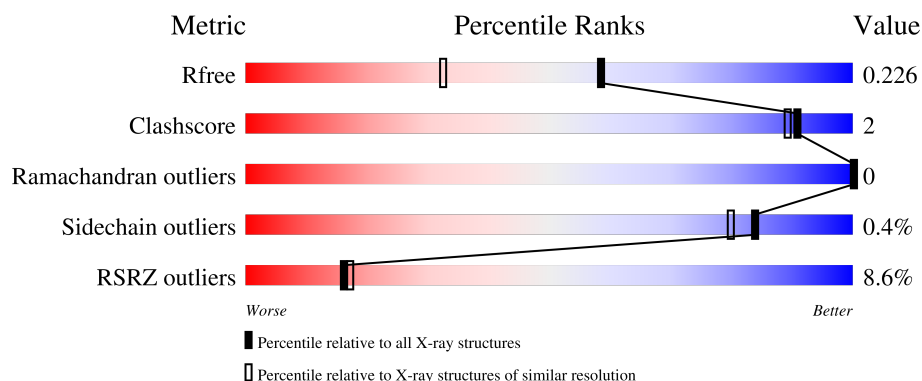
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	292	8% 90% 5%
1	B	292	8% 93% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9718 atoms, of which 4415 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.

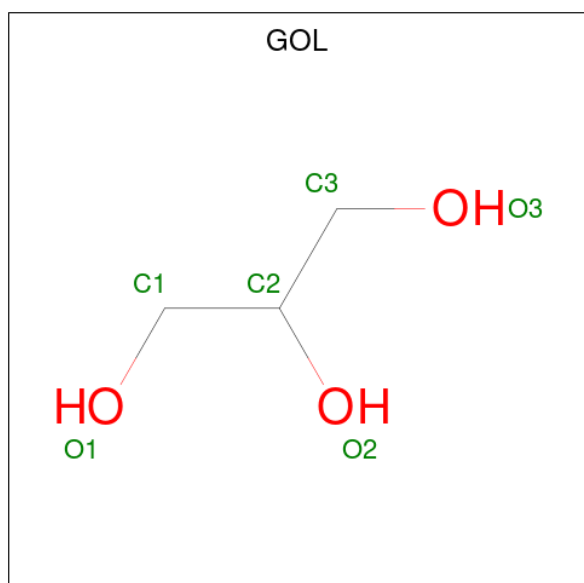
- Molecule 1 is a protein called N-acetylglucosaminide alpha-1,3-galactosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	278	Total	C	H	N	O	S	0	5	0
			4482	1498	2198	369	404	13			
1	B	280	Total	C	H	N	O	S	0	9	0
			4505	1508	2201	372	412	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	expression tag	UNP P14769
A	78	SER	-	expression tag	UNP P14769
A	79	MET	-	expression tag	UNP P14769
B	77	GLY	-	expression tag	UNP P14769
B	78	SER	-	expression tag	UNP P14769
B	79	MET	-	expression tag	UNP P14769

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C H O 14 3 8 3	0	0
2	B	1	Total C H O 14 3 8 3	0	0

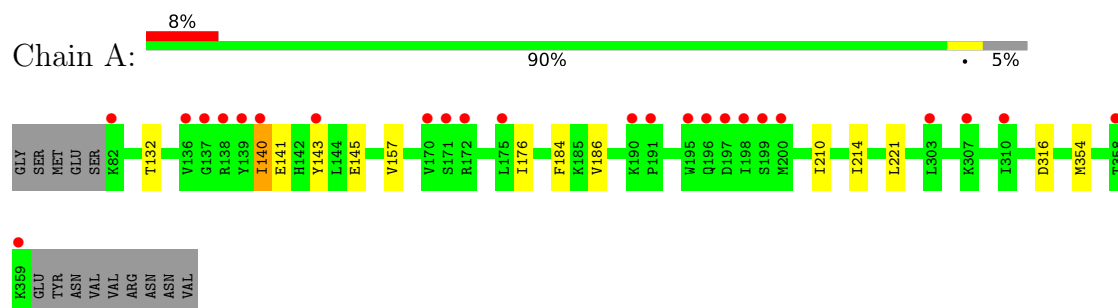
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	357	Total O 357 357	0	0
3	B	340	Total O 340 340	0	0

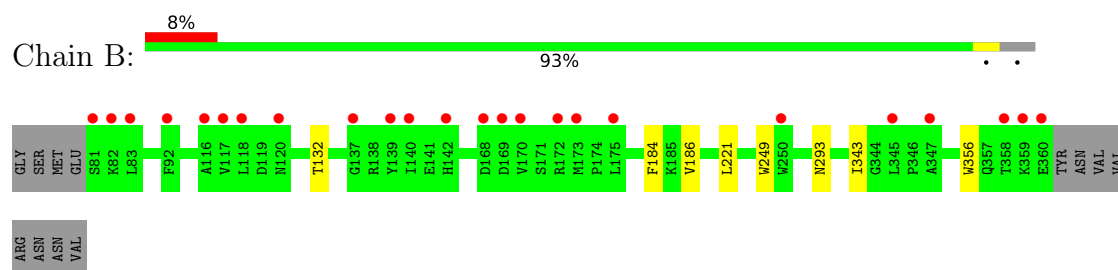
3 Residue-property plots [i](#)

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: N-acetylactosaminide alpha-1,3-galactosyltransferase



- Molecule 1: N-acetylactosaminide alpha-1,3-galactosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.95Å 66.29Å 83.93Å 90.00° 102.59° 90.00°	Depositor
Resolution (Å)	81.91 – 1.70 81.91 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.8 (81.91-1.70) 99.6 (81.91-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.60Å)	Xtriage
Refinement program	PHENIX (dev_2219: ???)	Depositor
R, R_{free}	0.187 , 0.223 0.189 , 0.226	Depositor DCC
R_{free} test set	4769 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.1	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	0.96	EDS
Total number of atoms	9718	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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

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

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	0.55	0/2383	0.62	0/3233
1	B	0.52	0/2427	0.60	0/3294
All	All	0.54	0/4810	0.61	0/6527

There are no bond length outliers.

There are no bond angle outliers.

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	2284	2198	2175	9	0
1	B	2304	2201	2138	4	1
2	A	6	0	8	0	0
2	B	12	16	16	0	0
3	A	357	0	0	1	0
3	B	340	0	0	2	1
All	All	5303	4415	4337	15	2

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:A:140:ILE:O	1:A:143:TYR:N	2.46	0.49
1:B:249:TRP:CD1	1:B:343:ILE:HD11	2.51	0.46
1:A:157:VAL:HG13	3:A:754:HOH:O	2.17	0.45
1:A:184[A]:PHE:CD1	1:A:186:VAL:HG23	2.52	0.45
1:A:210:ILE:HA	1:A:214:ILE:HB	1.99	0.44
1:B:184[B]:PHE:CD1	1:B:186:VAL:HG23	2.53	0.43
1:A:140:ILE:O	1:A:141:GLU:C	2.63	0.41
1:A:132:THR:HG23	1:A:221:LEU:HD11	2.03	0.41
1:B:132:THR:HG23	1:B:221:LEU:HD11	2.03	0.41
1:B:356:TRP:CD1	1:B:356:TRP:N	2.88	0.41
1:A:145:GLU:HG3	1:A:176:ILE:HD11	2.03	0.40
1:A:184[A]:PHE:CE1	1:A:186:VAL:HG23	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:HD21	1:B:293:ASN:HD21[2_456]	1.32	0.28
3:B:523:HOH:O	3:B:751:HOH:O[2_456]	2.17	0.03

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	281/292 (96%)	275 (98%)	6 (2%)	0	100	100
1	B	287/292 (98%)	281 (98%)	6 (2%)	0	100	100
All	All	568/584 (97%)	556 (98%)	12 (2%)	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	A	243/262 (93%)	241 (99%)	2 (1%)	73	65
1	B	246/262 (94%)	246 (100%)	0	100	100
All	All	489/524 (93%)	487 (100%)	2 (0%)	84	80

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ILE
1	A	316	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	293	ASN
1	B	315	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 oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	401	-	5,5,5	0.27	0	5,5,5	0.17	0
2	GOL	A	401	-	5,5,5	0.49	0	5,5,5	0.40	0
2	GOL	B	402	-	5,5,5	0.47	0	5,5,5	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	4/4/4/4	-
2	GOL	B	402	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	A	401	GOL	O2-C2-C3-O3
2	A	401	GOL	O1-C1-C2-C3
2	B	401	GOL	O1-C1-C2-C3
2	B	401	GOL	O1-C1-C2-O2
2	B	402	GOL	O2-C2-C3-O3

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

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	278/292 (95%)	-0.01	24 (8%) 16 17	8, 21, 58, 70	2 (0%)
1	B	280/292 (95%)	0.24	24 (8%) 16 17	9, 27, 55, 78	4 (1%)
All	All	558/584 (95%)	0.11	48 (8%) 16 17	8, 24, 56, 78	6 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	TRP	6.3
1	A	140	ILE	4.1
1	B	360	GLU	4.0
1	B	139	TYR	3.8
1	A	170	VAL	3.7
1	B	170	VAL	3.7
1	A	175	LEU	3.5
1	A	303	LEU	3.4
1	B	358	THR	3.4
1	A	172	ARG	3.3
1	A	138	ARG	3.2
1	B	175	LEU	3.1
1	B	142	HIS	3.1
1	A	200	MET	3.1
1	A	82	LYS	3.0
1	B	250	TRP	2.9
1	A	199	SER	2.8
1	A	310	ILE	2.8
1	B	81	SER	2.8
1	A	139	TYR	2.7
1	B	345	LEU	2.7
1	A	359	LYS	2.7
1	A	198	ILE	2.7
1	A	358	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	83	LEU	2.6
1	B	92	PHE	2.6
1	A	196	GLN	2.5
1	B	359	LYS	2.5
1	B	168	ASP	2.4
1	B	173	MET	2.4
1	B	118	LEU	2.3
1	B	172	ARG	2.3
1	B	82	LYS	2.3
1	B	347	ALA	2.3
1	A	143	TYR	2.3
1	A	307	LYS	2.2
1	B	116	ALA	2.2
1	B	140	ILE	2.2
1	A	171	SER	2.2
1	A	136	VAL	2.1
1	B	117	VAL	2.1
1	A	137	GLY	2.1
1	B	137	GLY	2.1
1	A	197	ASP	2.1
1	A	190	LYS	2.1
1	B	169	ASP	2.1
1	A	191	PRO	2.1
1	B	120	ASN	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](#)

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($\text{\AA}^2$)	Q<0.9
2	GOL	A	401	6/6	0.87	0.14	23,45,51,55	0
2	GOL	B	402	6/6	0.90	0.10	27,33,39,43	0
2	GOL	B	401	6/6	0.92	0.10	27,37,54,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.