



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:15 AM GMT

PDB ID : 2GAM
Title : X-ray crystal structure of murine leukocyte-type Core 2 b1,6-N-acetylglucosaminyltransferase (C2GnT-L) in complex with Galb1,3GalNAc
Authors : Pak, J.E.; Rini, J.M.
Deposited on : 2006-03-09
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

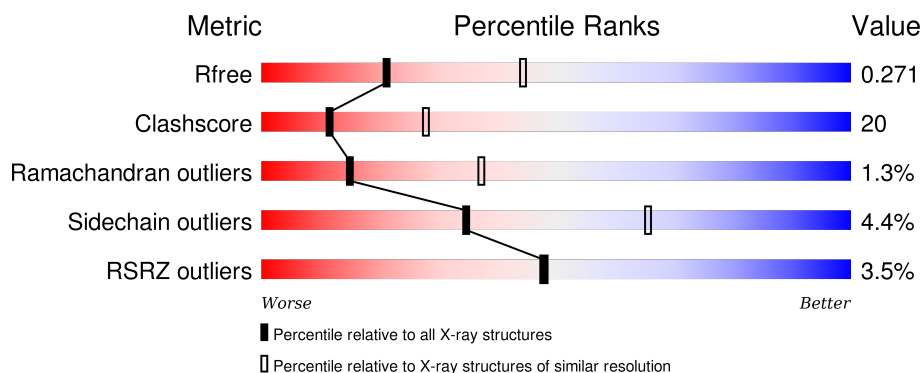
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	391	<div> <div>2%</div> <div>58% 32% 7%</div> </div>
1	B	391	<div> <div>%</div> <div>56% 32% 8%</div> </div>
1	C	391	<div> <div>5%</div> <div>54% 40% . .</div> </div>
1	D	391	<div> <div>5%</div> <div>59% 33% . 6%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12285 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 beta-1,6-N-acetylglucosaminyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2966	1903	505	537	21			
1	B	359	Total	C	N	O	S	0	0	0
			2919	1871	499	528	21			
1	C	374	Total	C	N	O	S	0	0	0
			3050	1958	522	549	21			
1	D	368	Total	C	N	O	S	0	0	0
			2994	1921	510	542	21			

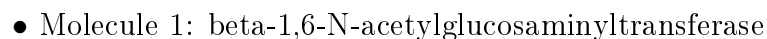
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			26	14	1	11		
2	B	2	Total	C	N	O	0	0
			26	14	1	11		
2	C	2	Total	C	N	O	0	0
			26	14	1	11		
2	D	2	Total	C	N	O	0	0
			26	14	1	11		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		
3	B	85	Total	O	0	0
			85	85		
3	C	58	Total	O	0	0
			58	58		
3	D	44	Total	O	0	0
			44	44		

- Chain C:  5% 54% 40% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.50 Å 80.58 Å 102.33 Å 73.61° 76.26° 64.56°	Depositor
Resolution (Å)	20.00 – 2.70 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.70) 90.9 (19.98-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.50 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.274 0.218 , 0.271	Depositor DCC
R_{free} test set	5592 reflections (10.17%)	DCC
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67650 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12285	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: GAL, NGA

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	0.39	0/3042	0.61	0/4125
1	B	0.41	0/2995	0.63	0/4060
1	C	0.39	0/3128	0.61	0/4238
1	D	0.37	0/3070	0.57	0/4161
All	All	0.39	0/12235	0.61	0/16584

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	TYR	Sidechain

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	2966	0	2937	103	0
1	B	2919	0	2882	115	0
1	C	3050	0	3028	149	0
1	D	2994	0	2962	117	0
2	A	26	0	24	0	0
2	B	26	0	24	1	0
2	C	26	0	24	0	0
2	D	26	0	24	1	0
3	A	65	0	0	4	0
3	B	85	0	0	3	0
3	C	58	0	0	2	0
3	D	44	0	0	3	0
All	All	12285	0	11905	476	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 20.

The worst 5 of 476 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:D:151:CYS:HG	1:D:199:CYS:HG	1.10	0.96
1:D:372:CYS:HG	1:D:381:CYS:HG	0.98	0.95
1:A:372:CYS:HG	1:A:381:CYS:HG	1.10	0.95
1:C:79:THR:HG22	1:C:81:GLN:H	1.33	0.93
1:D:123:ILE:HD11	1:D:230:VAL:HG22	1.51	0.92

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	361/391 (92%)	341 (94%)	20 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	355/391 (91%)	321 (90%)	27 (8%)	7 (2%)	9	24
1	C	370/391 (95%)	339 (92%)	27 (7%)	4 (1%)	17	42
1	D	362/391 (93%)	322 (89%)	32 (9%)	8 (2%)	8	22
All	All	1448/1564 (93%)	1323 (91%)	106 (7%)	19 (1%)	15	37

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	383	PHE
1	D	87	ARG
1	D	114	LEU
1	C	365	ASN
1	D	86	PRO

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	327/351 (93%)	308 (94%)	19 (6%)	25	52
1	B	321/351 (92%)	305 (95%)	16 (5%)	30	60
1	C	336/351 (96%)	323 (96%)	13 (4%)	39	70
1	D	330/351 (94%)	320 (97%)	10 (3%)	48	79
All	All	1314/1404 (94%)	1256 (96%)	58 (4%)	35	65

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	242	LEU
1	B	369	TYR
1	D	309	MET
1	B	307	LYS
1	B	321	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	395	HIS
1	C	71	GLN
1	D	365	ASN
1	B	396	HIS
1	B	412	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

8 carbohydrates 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	GAL	A	501	2	11,11,12	0.51	0	14,15,17	0.34	0
2	NGA	A	502	2	15,15,15	0.51	0	17,21,21	0.65	0
2	GAL	B	503	2	11,11,12	0.38	0	14,15,17	0.35	0
2	NGA	B	504	2	15,15,15	0.48	0	17,21,21	0.60	0
2	GAL	C	505	2	11,11,12	0.44	0	14,15,17	0.49	0
2	NGA	C	506	2	15,15,15	0.40	0	17,21,21	0.75	0
2	GAL	D	507	2	11,11,12	0.39	0	14,15,17	0.46	0
2	NGA	D	508	2	15,15,15	0.42	0	17,21,21	0.79	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	GAL	A	501	2	-	0/2/19/22	0/1/1/1
2	NGA	A	502	2	-	0/6/26/26	0/1/1/1
2	GAL	B	503	2	-	0/2/19/22	0/1/1/1
2	NGA	B	504	2	-	0/6/26/26	0/1/1/1
2	GAL	C	505	2	-	0/2/19/22	0/1/1/1
2	NGA	C	506	2	-	0/6/26/26	0/1/1/1
2	GAL	D	507	2	-	0/2/19/22	0/1/1/1
2	NGA	D	508	2	-	0/6/26/26	0/1/1/1

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	GAL	1	0
2	D	508	NGA	1	0

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 [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	365/391 (93%)	-0.09	9 (2%) 61 61	19, 41, 72, 107	0
1	B	359/391 (91%)	-0.20	4 (1%) 82 83	18, 36, 70, 87	0
1	C	374/391 (95%)	-0.00	19 (5%) 32 30	21, 41, 90, 114	0
1	D	368/391 (94%)	0.09	19 (5%) 31 30	15, 46, 93, 113	0
All	All	1466/1564 (93%)	-0.05	51 (3%) 48 48	15, 41, 84, 114	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	80	VAL	5.4
1	D	86	PRO	4.7
1	A	86	PRO	4.7
1	C	81	GLN	4.4
1	C	45	HIS	4.4

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NGA	A	502	15/15	0.95	0.14	-0.09	25,31,35,38	0
2	GAL	C	505	11/12	0.96	0.13	-0.28	41,43,44,45	0
2	NGA	D	508	15/15	0.95	0.14	-1.01	29,32,33,37	0
2	NGA	C	506	15/15	0.92	0.13	-1.11	39,41,43,44	0
2	GAL	B	503	11/12	0.97	0.13	-1.12	27,30,31,32	0
2	GAL	D	507	11/12	0.98	0.08	-1.78	21,25,27,28	0
2	GAL	A	501	11/12	0.97	0.09	-2.62	19,23,24,24	0
2	NGA	B	504	15/15	0.97	0.09	-2.63	24,29,32,33	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.