W O R L D W I D E
wwPDB
P R O T E I N D A T A B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2023 – 01:36 AM EDT

PDB ID	:	6N44
Title	:	Sheep Galectin-11 (LGALS11) complex with glycerol
Authors	:	Beddoe, T.C.; Sakthivel, D.
Deposited on	:	2018-11-17
Resolution	:	2.00 Å(reported)

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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 2.00 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9987 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 Galectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1095	709	178	201	7			
1	B	135	Total	C	N	O	S	0	0	0
			1064	691	173	194	6			
1	C	133	Total	C	N	O	S	0	0	0
			1049	680	171	192	6			
1	D	135	Total	C	N	O	S	0	0	0
			1068	693	174	195	6			
1	E	135	Total	C	N	O	S	0	0	0
			1050	679	171	194	6			
1	F	133	Total	C	N	O	S	0	0	0
			1048	683	170	189	6			
1	G	131	Total	C	N	O	S	0	0	0
			1044	680	169	189	6			
1	H	135	Total	C	N	O	S	0	0	0
			1060	688	172	194	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PRO	-	expression tag	UNP A0A0A7EMW6
A	0	GLY	-	expression tag	UNP A0A0A7EMW6
B	-1	PRO	-	expression tag	UNP A0A0A7EMW6
B	0	GLY	-	expression tag	UNP A0A0A7EMW6
C	-1	PRO	-	expression tag	UNP A0A0A7EMW6
C	0	GLY	-	expression tag	UNP A0A0A7EMW6
D	-1	PRO	-	expression tag	UNP A0A0A7EMW6
D	0	GLY	-	expression tag	UNP A0A0A7EMW6
E	-1	PRO	-	expression tag	UNP A0A0A7EMW6
E	0	GLY	-	expression tag	UNP A0A0A7EMW6
F	-1	PRO	-	expression tag	UNP A0A0A7EMW6
F	0	GLY	-	expression tag	UNP A0A0A7EMW6
G	-1	PRO	-	expression tag	UNP A0A0A7EMW6

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W O R L D W I D E
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PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP A0A0A7EMW6
H	-1	PRO	-	expression tag	UNP A0A0A7EMW6
H	0	GLY	-	expression tag	UNP A0A0A7EMW6

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
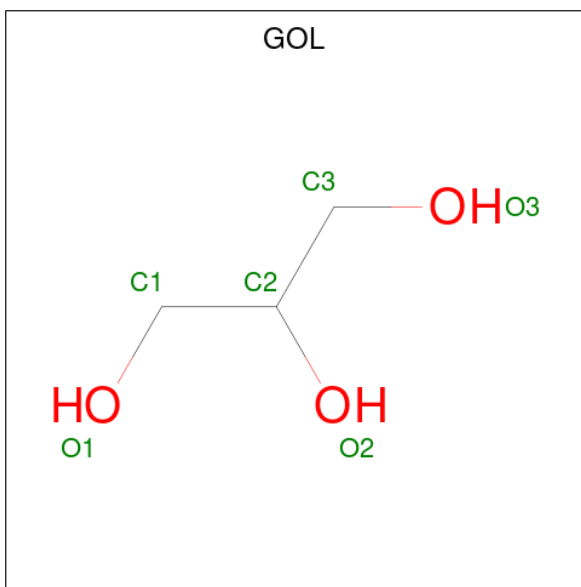
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total	O	0	0
			203	203		
3	B	183	Total	O	0	0
			183	183		
3	C	169	Total	O	0	0
			169	169		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	195	Total 195	O 195	0	0
3	E	199	Total 199	O 199	0	0
3	F	190	Total 190	O 190	0	0
3	G	159	Total 159	O 159	0	0
3	H	181	Total 181	O 181	0	0

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

3 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.17Å 127.45Å 141.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.38 – 2.00	Depositor
% Data completeness (in resolution range)	98.3 (38.38-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.93 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.10_2148	Depositor
R, R_{free}	0.192 , 0.238	Depositor
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.431	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9987	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

4.2 Too-close contacts ⓘ

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

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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

4.3.2 Protein sidechains ⓘ

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

4.3.3 RNA ⓘ

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

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

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

5 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	D	201	-	5,5,5	0.36	0	5,5,5	0.22	0
2	GOL	F	201	-	5,5,5	0.36	0	5,5,5	0.47	0
2	GOL	B	201	-	5,5,5	0.35	0	5,5,5	0.28	0
2	GOL	C	201	-	5,5,5	0.31	0	5,5,5	0.42	0
2	GOL	H	201	-	5,5,5	0.34	0	5,5,5	0.16	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	D	201	-	-	4/4/4/4	-
2	GOL	F	201	-	-	1/4/4/4	-
2	GOL	B	201	-	-	4/4/4/4	-
2	GOL	C	201	-	-	1/4/4/4	-
2	GOL	H	201	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	GOL	C1-C2-C3-O3
2	D	201	GOL	O1-C1-C2-C3
2	D	201	GOL	C1-C2-C3-O3
2	H	201	GOL	C1-C2-C3-O3
2	D	201	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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

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

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

5.3 Carbohydrates ⓘ

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

5.4 Ligands ⓘ

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

5.5 Other polymers ⓘ

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