

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	5NFA
Title	:	Structure of Galectin-3 CRD in complex with compound 3
Authors	:	Ronin, C.; Atmanene, C.; Gautier, F.M.; Djedaini Pilard, F.; Teletchea, S.;
		Ciesielski, F.; Vivat Hannah, V.; Grandjean, C.
Deposited on	:	2017-03-13
Resolution	:	1.59 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 following versions of software and data (see references (1)) were used in the production of this report:

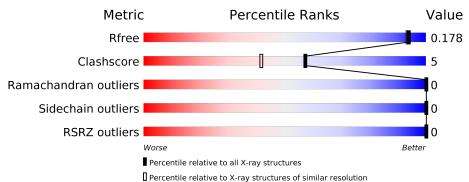
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.59 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R _{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665(1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563(1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 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% 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	А	147	82%	11%	• 6%
2	В	2	100%		



5NFA

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1374 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-3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	138	Total 1190	C 766	N 212	O 207	${ m S}{ m 5}$	0	16	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	GLY	-	expression tag	UNP P17931
А	105	SER	-	expression tag	UNP P17931

• Molecule 2 is an oligosaccharide called 3-O-[(3-methoxyphenyl)methyl]-beta-D-galactopyra nose-(1-4)-N-acetyl-2-(acetylamino)-2-deoxy-beta-D-glucopyranosylamine.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	В	2	Total C N 38 24 2	O 12	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	146	Total O 146 146	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: Galectin-3

Chain A:	in A: 82%					
GLY SER PRO TYR GLY GLY ALA ALA GLY GLY GLY	11 19 11 19					

 $\bullet \ {\rm Molecule \ 2: \ 3-O-[(3-methoxyphenyl)methyl]-beta-D-galactopyranose-(1-4)-N-acetyl-2-(acetylamino)-2-deoxy-beta-D-glucopyranosylamine}$

Chain B:

100%

TVD1 TVD2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	36.80Å 58.15 Å 63.07 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.75 - 1.59	Depositor
Resolution (A)	42.75 - 1.59	EDS
% Data completeness	99.2(42.75-1.59)	Depositor
(in resolution range)	99.2(42.75 - 1.59)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	$3.24 (at 1.58 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.8.0073$	Depositor
R, R_{free}	0.143 , 0.169	Depositor
Π, Π_{free}	0.156 , 0.178	DCC
R_{free} test set	941 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , 48.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1374	wwPDB-VP
Average B, all atoms $(Å^2)$	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.97% of the height of the origin peak. No significant pseudotranslation is detected.

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.



 $^{^1 {\}rm Intensities}$ 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: $\mathrm{TVM},\,\mathrm{TVD}$

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	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.13	1/1261~(0.1%)	1.15	6/1706~(0.4%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	193	GLU	CD-OE2	5.75	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	151	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	А	233	LYS	CA-CB-CG	7.18	129.20	113.40
1	А	207	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	А	207	ASP	CB-CG-OD1	6.30	123.97	118.30
1	А	144	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	А	154	ASP	CB-CG-OD2	-5.13	113.68	118.30

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	А	1190	0	1239	12	0

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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 5.

All (12) 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:205:GLU:OE1	1:A:208[A]:HIS:HE1	1.66	0.78
1:A:119:ASN:OD1	1:A:233:LYS:HG2	1.88	0.73
1:A:205:GLU:OE1	1:A:208[A]:HIS:CE1	2.45	0.68
1:A:140[B]:PRO:O	1:A:194[B]:SER:OG	2.09	0.68
1:A:140[A]:PRO:O	3:A:401:HOH:O	2.10	0.68
1:A:160:ASN:ND2	1:A:162:ARG:HE	1.96	0.64
1:A:119:ASN:OD1	1:A:233:LYS:CG	2.45	0.64
1:A:140[A]:PRO:HD3	3:A:481:HOH:O	2.03	0.56
1:A:203:LEU:HD23	1:A:210[A]:LYS:HE2	1.96	0.47
1:A:210[B]:LYS:HE3	1:A:210[B]:LYS:HB3	1.82	0.42
1:A:160:ASN:HD21	1:A:162:ARG:HE	1.65	0.41
1:A:158:HIS:O	1:A:173:CYS:HA	2.20	0.41

All (1) 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)
3:A:448:HOH:O	3:A:485:HOH:O[4_545]	2.16	0.04

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.



Chain Non-H H(model) H(added) Clashes Symm-Clashes Mol В $\mathbf{2}$ 380 0 0 0 3 2 А 0 0 1 146All All 1239121 13740

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Mol	Chain	Analysed	Favoured Allowed		Outliers	Percentiles	
1	А	152/147~(103%)	148 (97%)	4 (3%)	0	100 10	0

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	А	140/128~(109%)	140~(100%)	0	100 100	

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	160	ASN
1	А	222	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)

2 monosaccharides 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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles			
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
	2	TVD	В	1	2	18,18,18	1.83	3 (16%)	23,25,25	2.66	8 (34%)
	2	TVM	В	2	2	21,21,22	1.45	5 (23%)	28,28,30	1.49	6 (21%)

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).

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	\mathbf{Link}	Chirals	Torsions	Rings
2	TVD	В	1	2	-	0/10/30/30	0/1/1/1
2	TVM	В	2	2	-	0/9/26/29	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	В	1	TVD	C1-N1	5.07	1.49	1.43
2	В	2	TVM	O4-C4	3.24	1.50	1.43
2	В	1	TVD	C1-C2	3.22	1.56	1.53
2	В	1	TVD	O5-C1	-2.23	1.40	1.43
2	В	2	TVM	O2-C2	2.20	1.48	1.43
2	В	2	TVM	C30-C29	2.16	1.42	1.38
2	В	2	TVM	O3-C3	-2.07	1.39	1.43
2	В	2	TVM	C2-C3	-2.06	1.47	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	1	TVD	O5-C1-C2	-7.74	103.68	108.97
2	В	1	TVD	C1-N1-C9	-4.69	116.88	122.57
2	В	1	TVD	C3-C2-N2	-4.12	102.83	110.62
2	В	1	TVD	C5-O5-C1	3.86	117.76	112.52
2	В	2	TVM	C1-C2-C3	3.59	113.52	109.17
2	В	1	TVD	C8-C7-N2	-3.08	110.89	116.10
2	В	1	TVD	C2-N2-C7	-2.79	116.39	123.18
2	В	2	TVM	C29-C30-C25	2.73	122.73	119.73
2	В	1	TVD	O4-C4-C3	-2.67	104.17	110.35
2	В	2	TVM	C2-C3-C4	-2.52	108.47	110.66
2	В	2	TVM	C32-O31-C29	2.29	122.48	117.51
2	В	2	TVM	C28-C27-C26	2.22	123.39	120.25

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Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	2	TVM	C28-C29-C30	-2.15	117.58	120.53
2	В	1	TVD	O3-C3-C2	-2.09	105.44	109.66

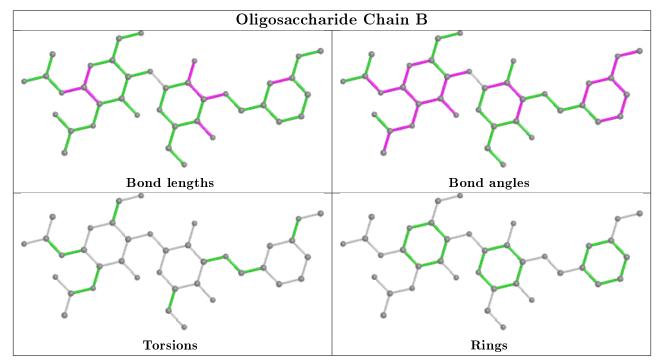
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



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	А	138/147~(93%)	-0.36	0 100 100	9, 13, 22, 39	0

There are no RSRZ outliers to report.

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

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

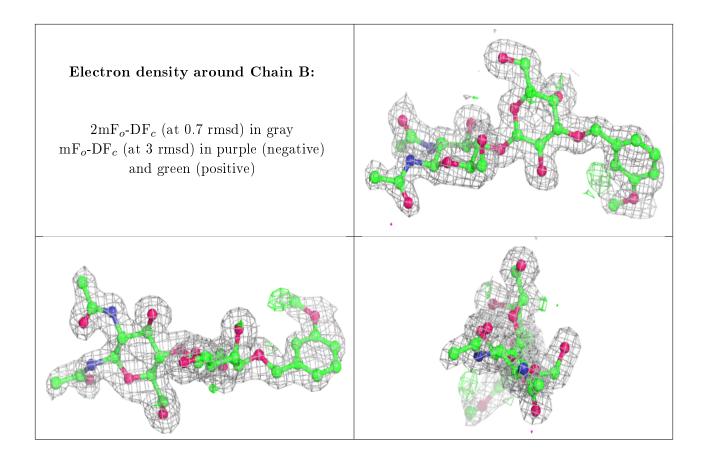
6.3 Carbohydrates (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
2	TVM	В	2	20/21	0.94	0.10	$12,\!18,\!38,\!40$	0
2	TVD	В	1	18/18	0.94	0.10	$14,\!22,\!37,\!39$	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

