



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 06:22 PM BST

PDB ID : 5OJ6  
Title : Crystal structure of the chicken MDGA1 ectodomain in complex with the human neuroligin 1 (NL1(-A-B)) cholinesterase domain.  
Authors : Elegheert, J.; Clayton, A.J.; Aricescu, A.R.  
Deposited on : 2017-07-20  
Resolution : 3.30 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

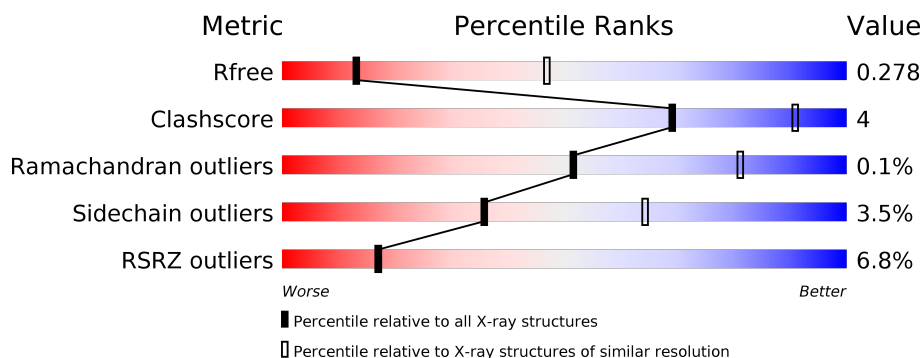
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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  $\geq 3$ , 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	575	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
2	B	910	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>8%</div> <div>24%</div> </div> </div>
3	C	3	<div> <div></div> <div>100%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9810 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 Neuroligin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4278	2748	709	804	17			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	THR	-	expression tag	UNP Q8N2Q7
A	45	GLY	-	expression tag	UNP Q8N2Q7
A	?	-	GLY	deletion	UNP Q8N2Q7
A	?	-	ASN	deletion	UNP Q8N2Q7
A	?	-	ARG	deletion	UNP Q8N2Q7
A	?	-	TRP	deletion	UNP Q8N2Q7
A	?	-	SER	deletion	UNP Q8N2Q7
A	?	-	ASN	deletion	UNP Q8N2Q7
A	?	-	SER	deletion	UNP Q8N2Q7
A	?	-	THR	deletion	UNP Q8N2Q7
A	?	-	LYS	deletion	UNP Q8N2Q7
A	636	ARG	-	expression tag	UNP Q8N2Q7
A	637	THR	-	expression tag	UNP Q8N2Q7
A	638	LYS	-	expression tag	UNP Q8N2Q7
A	639	HIS	-	expression tag	UNP Q8N2Q7
A	640	HIS	-	expression tag	UNP Q8N2Q7
A	641	HIS	-	expression tag	UNP Q8N2Q7
A	642	HIS	-	expression tag	UNP Q8N2Q7
A	643	HIS	-	expression tag	UNP Q8N2Q7
A	644	HIS	-	expression tag	UNP Q8N2Q7

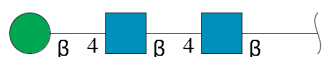
- Molecule 2 is a protein called MAM domain-containing glycosylphosphatidylinositol anchor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	689	Total	C	N	O	S	0	0	0
			5381	3396	930	1028	27			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	LYS	ARG	engineered mutation	UNP Q0WYX8
B	920	GLY	-	expression tag	UNP Q0WYX8
B	921	THR	-	expression tag	UNP Q0WYX8
B	922	LYS	-	expression tag	UNP Q0WYX8
B	923	HIS	-	expression tag	UNP Q0WYX8
B	924	HIS	-	expression tag	UNP Q0WYX8
B	925	HIS	-	expression tag	UNP Q0WYX8
B	926	HIS	-	expression tag	UNP Q0WYX8
B	927	HIS	-	expression tag	UNP Q0WYX8
B	928	HIS	-	expression tag	UNP Q0WYX8

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

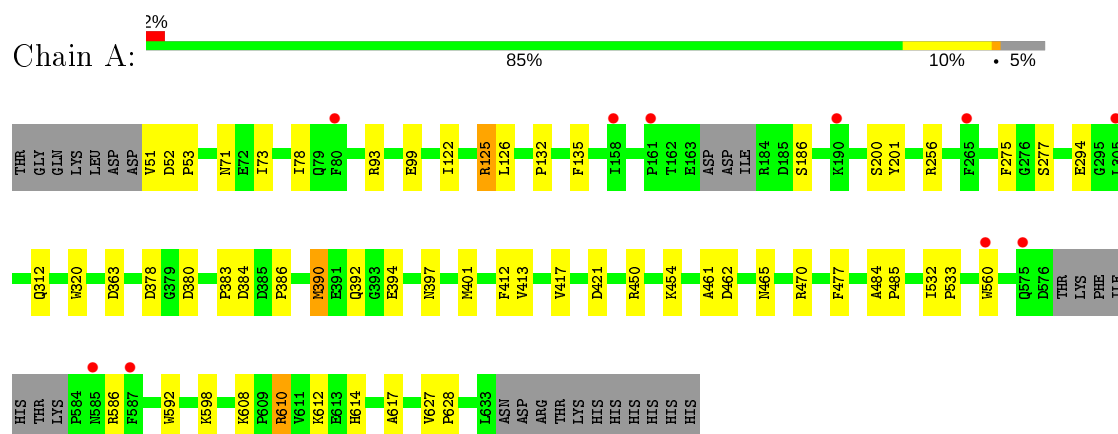


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

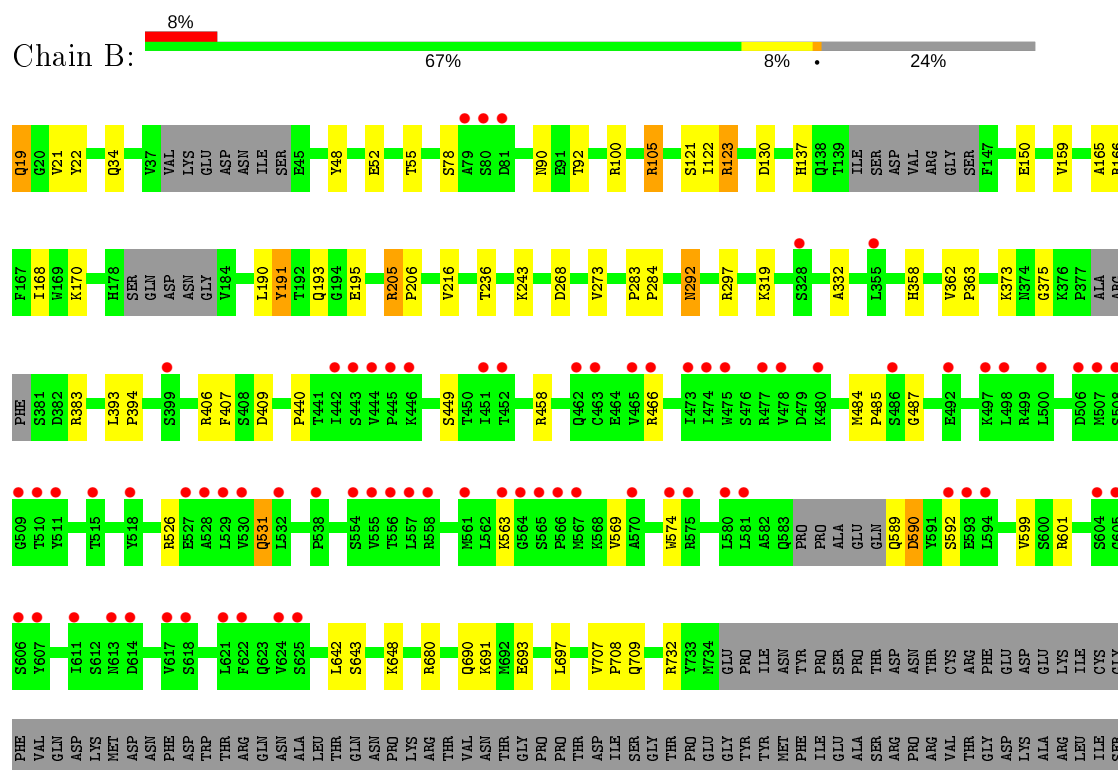
### 3 Residue-property plots

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: Neuroligin-1



#### • Molecule 2: MAM domain-containing glycosylphosphatidylinositol anchor protein 1



PRO  
LEU  
TYR  
ASN  
GLY  
ILE  
THR  
ALA  
LYS  
TYR  
CYS  
VAL  
SER  
PHE  
TYR  
HIS  
MET  
TYR  
GLY  
LYS  
HIS  
ILE  
GLY  
SER  
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ASN  
LEU  
LEU  
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ILE

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%

NA01  
NA02  
EM03

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.42Å 184.14Å 96.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.36 – 3.30 92.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (72.36-3.30) 98.4 (92.07-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.33Å)	Xtriage
Refinement program	PHENIX (dev_2044:)	Depositor
R, $R_{free}$	0.227 , 0.277 0.232 , 0.278	Depositor DCC
$R_{free}$ test set	1474 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.4	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 71.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BMA, NAG

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	0.24	0/4397	0.45	0/6003
2	B	0.23	0/5492	0.44	0/7476
All	All	0.23	0/9889	0.44	0/13479

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	4278	0	4117	31	0
2	B	5381	0	5360	41	2
3	C	39	0	34	0	0
4	B	112	0	104	4	1
All	All	9810	0	9615	71	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 4.

The worst 5 of 71 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)
2:B:100:ARG:NH2	2:B:130:ASP:OD1	2.20	0.74
1:A:51:VAL:HG13	1:A:52:ASP:H	1.59	0.68
1:A:93:ARG:NH1	1:A:99:GLU:OE2	2.27	0.67
2:B:574:TRP:NE1	2:B:592:SER:OG	2.31	0.64
1:A:397:ASN:OD1	2:B:78:SER:N	2.32	0.63

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)
2:B:643:SER:OG	4:B:1001:NAG:O4[4_477]	2.07	0.13
2:B:273:VAL:O	2:B:690:GLN:NE2[4_577]	2.09	0.11

## 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	541/575 (94%)	509 (94%)	32 (6%)	0	100	100
2	B	677/910 (74%)	621 (92%)	55 (8%)	1 (0%)	51	81
All	All	1218/1485 (82%)	1130 (93%)	87 (7%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	599	VAL

### 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	461/494 (93%)	448 (97%)	13 (3%)	43	70
2	B	609/810 (75%)	585 (96%)	24 (4%)	32	62
All	All	1070/1304 (82%)	1033 (96%)	37 (4%)	36	64

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	123	ARG
2	B	205	ARG
2	B	691	LYS
2	B	137	HIS
2	B	170	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	149	GLN
2	B	253	ASN
2	B	623	GLN
2	B	646	GLN
2	B	700	HIS

### 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 ⓘ

3 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 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
3	NAG	C	1	3,2	14,14,15	0.29	0	17,19,21	0.47	0
3	NAG	C	2	3	14,14,15	0.18	0	17,19,21	0.48	0
3	BMA	C	3	3	11,11,12	0.67	0	15,15,17	0.72	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
3	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

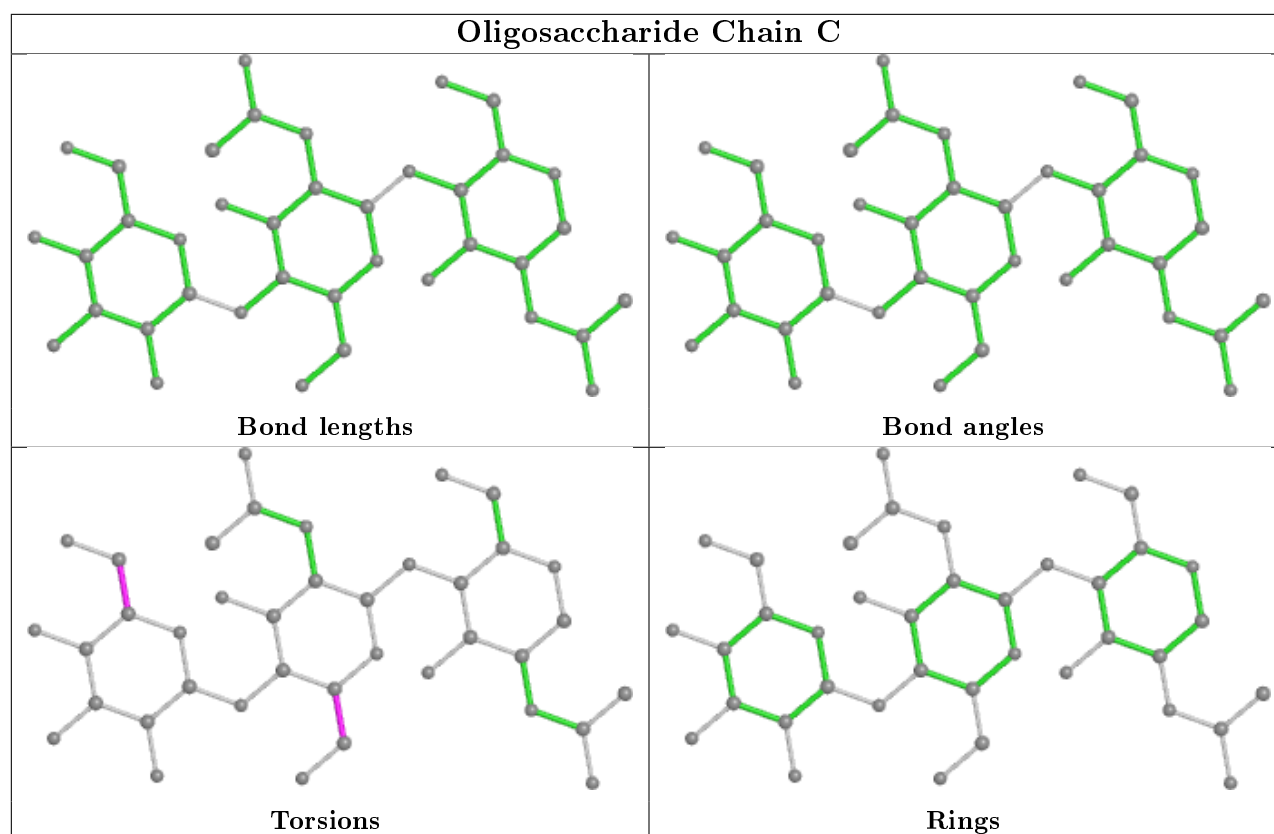
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6

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](#)

8 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	$\# Z  > 2$
4	NAG	B	1007	2	14,14,15	0.24	0	17,19,21	0.35	0
4	NAG	B	1010	2	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	B	1008	2	14,14,15	0.23	0	17,19,21	0.87	1 (5%)
4	NAG	B	1002	2	14,14,15	0.19	0	17,19,21	0.41	0
4	NAG	B	1011	2	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
4	NAG	B	1001	2	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	B	1006	2	14,14,15	0.16	0	17,19,21	0.46	0
4	NAG	B	1009	2	14,14,15	0.35	0	17,19,21	0.60	1 (5%)

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
4	NAG	B	1007	2	-	3/6/23/26	0/1/1/1
4	NAG	B	1010	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1008	2	-	5/6/23/26	0/1/1/1
4	NAG	B	1002	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1011	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1006	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1009	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1008	NAG	C2-N2-C7	2.75	126.82	122.90
4	B	1011	NAG	C1-O5-C5	2.51	115.59	112.19
4	B	1009	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1010	NAG	O5-C5-C6-O6
4	B	1009	NAG	O5-C5-C6-O6
4	B	1007	NAG	C4-C5-C6-O6
4	B	1010	NAG	C4-C5-C6-O6
4	B	1009	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1008	NAG	3	0
4	B	1001	NAG	0	1
4	B	1009	NAG	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	547/575 (95%)	0.20	10 (1%) 68 67	52, 88, 137, 193	0
2	B	689/910 (75%)	0.53	74 (10%) 6 5	62, 127, 198, 217	0
All	All	1236/1485 (83%)	0.39	84 (6%) 17 17	52, 104, 188, 217	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	530	VAL	7.5
2	B	607	TYR	7.0
1	A	587	PHE	5.1
2	B	581	LEU	5.1
2	B	532	LEU	4.8

### 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](#)

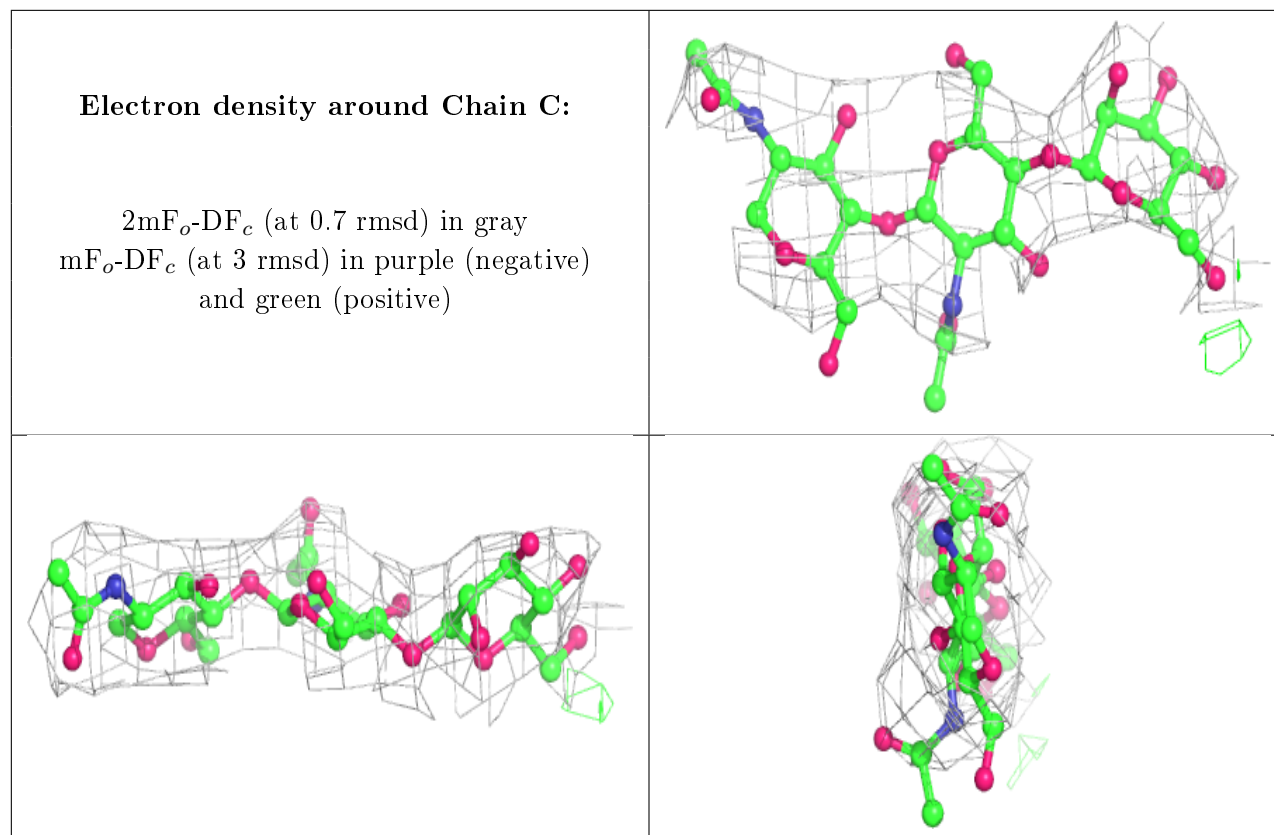
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BMA	C	3	11/12	0.66	0.28	161,187,195,198	0
3	NAG	C	2	14/15	0.85	0.34	139,162,180,183	0
3	NAG	C	1	14/15	0.88	0.25	137,147,165,167	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-



charide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.4 Ligands ⓘ

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<sup>th</sup> 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
4	NAG	B	1006	14/15	0.76	0.17	173,192,197,198	0
4	NAG	B	1009	14/15	0.77	0.25	101,142,149,156	0
4	NAG	B	1010	14/15	0.81	0.72	163,187,195,195	0
4	NAG	B	1008	14/15	0.82	0.28	132,148,165,166	0
4	NAG	B	1001	14/15	0.83	0.25	150,177,186,189	0
4	NAG	B	1002	14/15	0.84	0.23	114,131,136,148	0
4	NAG	B	1007	14/15	0.85	0.38	124,136,148,160	0
4	NAG	B	1011	14/15	0.88	0.21	113,128,139,139	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.