



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 05:32 PM BST

PDB ID : 5NXB  
Title : Mouse galactocerebrosidase in complex with saposin A  
Authors : Graham, S.C.; Hill, C.H.; Deane, J.E.  
Deposited on : 2017-05-09  
Resolution : 3.60 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](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

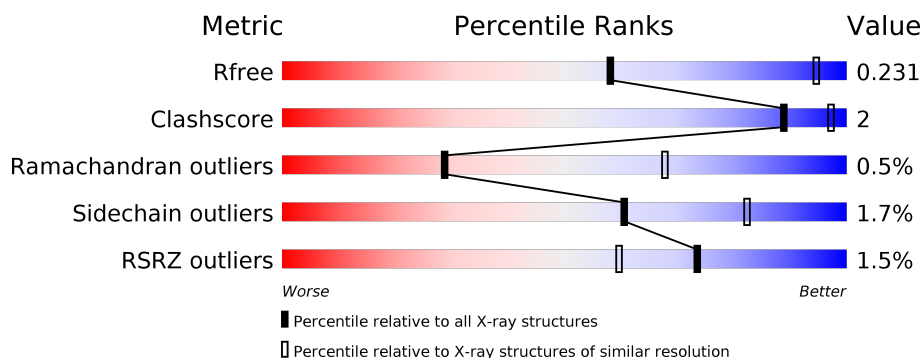
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	654	<div> <div>0%</div> <div>92%</div> <div>7%</div> <div>•</div> </div>
1	B	654	<div> <div>2%</div> <div>92%</div> <div>6%</div> <div>•</div> </div>
2	C	87	<div> <div>5%</div> <div>76%</div> <div>16%</div> <div>8%</div> </div>
2	D	87	<div> <div>2%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
3	E	2	<div> <div>50%</div> <div>50%</div> </div>
3	F	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	2	 50%50%
3	I	2	 100%
4	G	3	 100%
4	J	3	 100%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11742 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 Galactocerebrosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	0	0
			5153	3335	858	945	15			
1	B	644	Total	C	N	O	S	0	0	0
			5153	3335	858	945	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	HIS	-	expression tag	UNP P54818
A	16	HIS	-	expression tag	UNP P54818
A	17	HIS	-	expression tag	UNP P54818
A	18	HIS	-	expression tag	UNP P54818
A	19	HIS	-	expression tag	UNP P54818
A	20	HIS	-	expression tag	UNP P54818
A	21	ILE	-	expression tag	UNP P54818
A	22	GLU	-	expression tag	UNP P54818
A	23	GLY	-	expression tag	UNP P54818
A	24	ARG	-	expression tag	UNP P54818
B	15	HIS	-	expression tag	UNP P54818
B	16	HIS	-	expression tag	UNP P54818
B	17	HIS	-	expression tag	UNP P54818
B	18	HIS	-	expression tag	UNP P54818
B	19	HIS	-	expression tag	UNP P54818
B	20	HIS	-	expression tag	UNP P54818
B	21	ILE	-	expression tag	UNP P54818
B	22	GLU	-	expression tag	UNP P54818
B	23	GLY	-	expression tag	UNP P54818
B	24	ARG	-	expression tag	UNP P54818

- Molecule 2 is a protein called Prosaposin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	80	Total	C	N	O	S	0	0	0
			608	378	96	126	8			
2	D	80	Total	C	N	O	S	0	0	0
			608	378	96	126	8			

There are 4 discrepancies between the modelled and reference sequences:

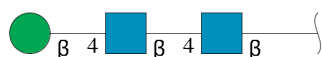
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	MET	-	initiating methionine	UNP Q61207
C	-1	GLY	-	expression tag	UNP Q61207
D	-2	MET	-	initiating methionine	UNP Q61207
D	-1	GLY	-	expression tag	UNP Q61207

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O		0	0	0
			28	16	2	10				
3	F	2	Total	C	N	O		0	0	0
			28	16	2	10				
3	H	2	Total	C	N	O		0	0	0
			28	16	2	10				
3	I	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 4 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
4	G	3	Total	C	N	O		0	0	0
			39	22	2	15				
4	J	3	Total	C	N	O		0	0	0
			39	22	2	15				

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

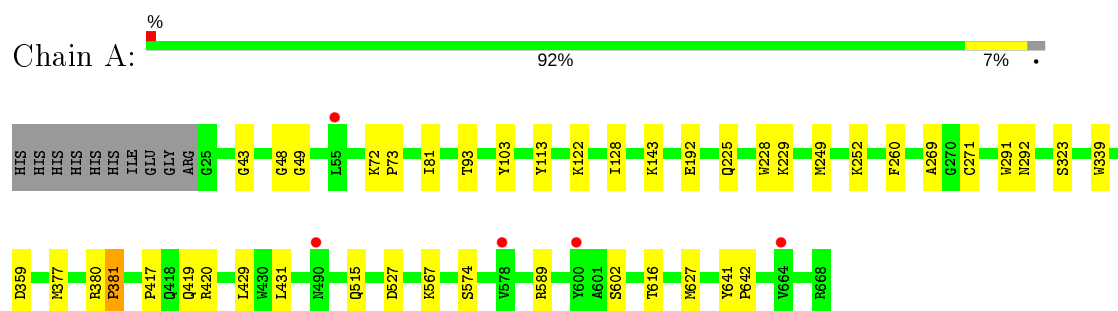
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		

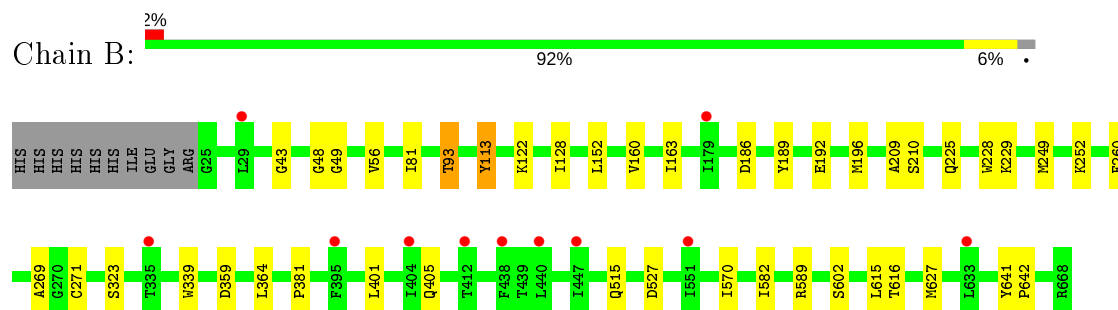
### 3 Residue-property plots

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.

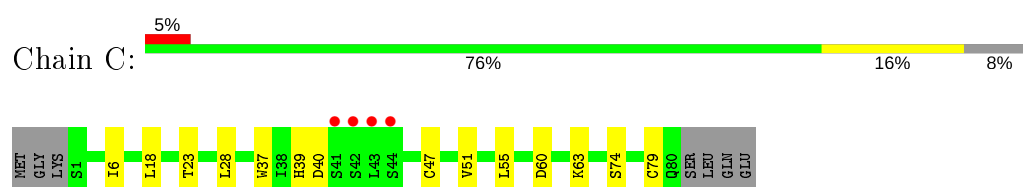
- Molecule 1: Galactocerebrosidase



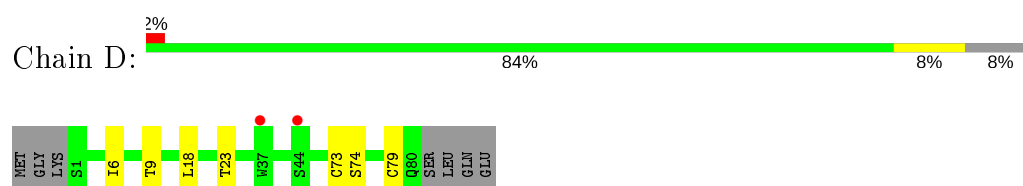
- Molecule 1: Galactocerebrosidase



- Molecule 2: Prosaposin



- Molecule 2: Prosaposin



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

Chain E:  50% 50%

HA01  
HA02

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

Chain F:  100%

HA01  
HA02

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

Chain H:  50% 50%

HA01  
HA02

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

Chain I:  100%

HA01  
HA02

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

Chain G:  100%

HA01  
HA02  
B/A3

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

Chain J:  100%

HA01  
HA02  
B/A3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.18Å 187.18Å 360.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	162.11 – 3.60 162.11 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (162.11-3.60) 99.7 (162.11-3.60)	Depositor EDS
$R_{merge}$	0.39	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 3.58Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.217 , 0.231 0.225 , 0.231	Depositor DCC
$R_{free}$ test set	2138 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	92.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 78.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.38	0/5318	0.56	0/7253
1	B	0.38	0/5318	0.59	0/7253
2	C	0.49	0/616	0.67	0/836
2	D	0.49	0/616	0.68	0/836
All	All	0.39	0/11868	0.59	0/16178

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 [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	5153	0	4904	16	0
1	B	5153	0	4904	19	0
2	C	608	0	596	8	0
2	D	608	0	596	4	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
4	G	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	39	0	34	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	11742	0	11194	44	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 2.

All (44) 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:B:364:LEU:HD22	1:B:401:LEU:HD22	1.60	0.81
2:C:28:LEU:HG	2:C:55:LEU:HD23	1.69	0.75
1:B:152:LEU:HD22	1:B:189:TYR:HB2	1.80	0.62
1:B:122:LYS:HD2	1:B:128:ILE:HG22	1.84	0.58
1:A:122:LYS:HD2	1:A:128:ILE:HG22	1.83	0.58
2:C:74:SER:HA	2:C:79:CYS:O	2.07	0.54
2:D:74:SER:HA	2:D:79:CYS:O	2.08	0.54
1:A:417:PRO:HA	1:A:420:ARG:HG2	1.89	0.53
1:B:160:VAL:HG21	1:B:196:MET:HG3	1.91	0.53
1:A:380:ARG:HG2	2:C:37:TRP:O	2.09	0.51
1:A:339:TRP:CE2	1:A:359:ASP:HB3	2.45	0.51
1:A:616:THR:HB	1:A:627:MET:HB2	1.93	0.51
1:A:48:GLY:N	1:A:49:GLY:HA2	2.25	0.51
1:B:48:GLY:N	1:B:49:GLY:HA2	2.25	0.50
2:C:18:LEU:HA	2:C:23:THR:HG21	1.93	0.50
1:B:269:ALA:HB2	1:B:323:SER:HB2	1.94	0.49
1:A:269:ALA:HB2	1:A:323:SER:HB2	1.95	0.48
1:B:616:THR:HB	1:B:627:MET:HB2	1.94	0.48
2:D:18:LEU:HA	2:D:23:THR:HG21	1.97	0.46
1:A:43:GLY:HA3	1:A:81:ILE:HB	1.98	0.45
1:A:589:ARG:HD3	1:A:602:SER:HB3	1.99	0.45
1:A:567:LYS:HD2	1:A:574:SER:HB2	1.98	0.45
1:B:228:TRP:CE2	1:B:252:LYS:HE2	2.52	0.44
1:B:589:ARG:HD3	1:B:602:SER:HB3	1.99	0.44
1:A:641:TYR:CD1	1:A:642:PRO:HA	2.53	0.43
1:B:160:VAL:HA	1:B:163:ILE:HD12	2.00	0.43
1:A:228:TRP:CE2	1:A:252:LYS:HE2	2.53	0.43
1:B:56:VAL:HG11	1:B:113:TYR:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:PRO:HB3	2:C:37:TRP:HA	2.01	0.43
1:B:43:GLY:HA3	1:B:81:ILE:HB	1.99	0.42
1:A:72:LYS:HA	1:A:73:PRO:HD3	1.92	0.42
1:B:641:TYR:CD1	1:B:642:PRO:HA	2.55	0.42
2:C:47:CYS:O	2:C:51:VAL:HG23	2.20	0.42
1:B:225:GLN:HG2	1:B:229:LYS:HE3	2.02	0.42
1:B:582:ILE:HG12	1:B:615:LEU:HD11	2.02	0.42
1:B:339:TRP:CE2	1:B:359:ASP:HB3	2.54	0.41
1:A:291:TRP:HA	1:A:292:ASN:HA	1.84	0.41
2:D:73:CYS:HB3	2:D:79:CYS:SG	2.61	0.41
1:A:225:GLN:HG2	1:A:229:LYS:HE3	2.01	0.41
1:B:93:THR:HA	1:B:570:ILE:HG23	2.03	0.41
2:C:60:ASP:HA	2:C:63:LYS:HD3	2.03	0.41
2:C:6:ILE:HB	2:D:6:ILE:HG21	2.03	0.41
1:B:209:ALA:HA	1:B:210:SER:HA	1.87	0.40
1:B:186:ASP:HB3	1:B:189:TYR:HB3	2.04	0.40

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	642/654 (98%)	616 (96%)	23 (4%)	3 (0%)	29	68
1	B	642/654 (98%)	612 (95%)	27 (4%)	3 (0%)	29	68
2	C	78/87 (90%)	76 (97%)	1 (1%)	1 (1%)	12	50
2	D	78/87 (90%)	75 (96%)	3 (4%)	0	100	100
All	All	1440/1482 (97%)	1379 (96%)	54 (4%)	7 (0%)	29	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	B	93	THR
2	C	40	ASP
1	A	260	PHE
1	B	260	PHE
1	A	381	PRO
1	B	381	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	537/555 (97%)	525 (98%)	12 (2%)	52	77
1	B	537/555 (97%)	530 (99%)	7 (1%)	69	86
2	C	73/79 (92%)	72 (99%)	1 (1%)	67	85
2	D	73/79 (92%)	72 (99%)	1 (1%)	67	85
All	All	1220/1268 (96%)	1199 (98%)	21 (2%)	60	82

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	TYR
1	A	113	TYR
1	A	143	LYS
1	A	192	GLU
1	A	249	MET
1	A	271	CYS
1	A	377	MET
1	A	419	GLN
1	A	429	LEU
1	A	431	LEU
1	A	515	GLN
1	A	527	ASP
1	B	113	TYR
1	B	192	GLU
1	B	249	MET

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Mol	Chain	Res	Type
1	B	271	CYS
1	B	405	GLN
1	B	515	GLN
1	B	527	ASP
2	C	39	HIS
2	D	9	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

14 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	E	1	1,3	14,14,15	0.37	0	17,19,21	0.91	1 (5%)
3	NAG	E	2	3	14,14,15	0.35	0	17,19,21	0.53	0
3	NAG	F	1	1,3	14,14,15	0.29	0	17,19,21	0.71	0
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	G	1	1,4	14,14,15	0.28	0	17,19,21	0.39	0
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	0.55	0
4	BMA	G	3	4	11,11,12	0.33	0	15,15,17	0.48	0
3	NAG	H	1	1,3	14,14,15	0.34	0	17,19,21	1.05	1 (5%)
3	NAG	H	2	3	14,14,15	0.35	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	I	1	1,3	14,14,15	0.30	0	17,19,21	0.68	0
3	NAG	I	2	3	14,14,15	0.33	0	17,19,21	0.61	0
4	NAG	J	1	1,4	14,14,15	0.28	0	17,19,21	0.42	0
4	NAG	J	2	4	14,14,15	0.29	0	17,19,21	0.65	0
4	BMA	J	3	4	11,11,12	0.33	0	15,15,17	0.46	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	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-C2-N2	-3.43	104.63	110.49
3	E	1	NAG	C1-C2-N2	-2.85	105.62	110.49

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6

*Continued on next page...*

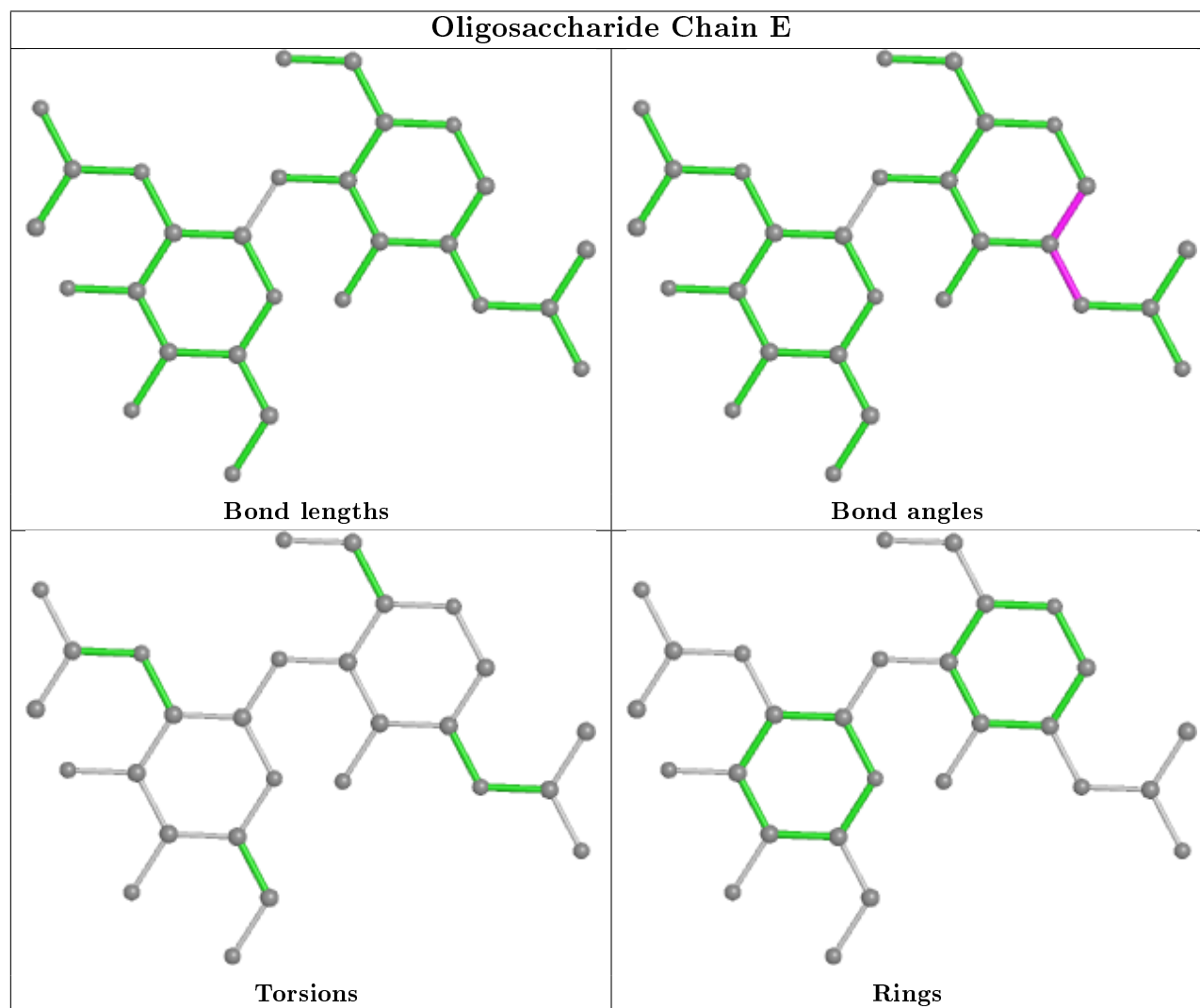
*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	J	2	NAG	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C3-C2-N2-C7
3	F	2	NAG	O5-C5-C6-O6

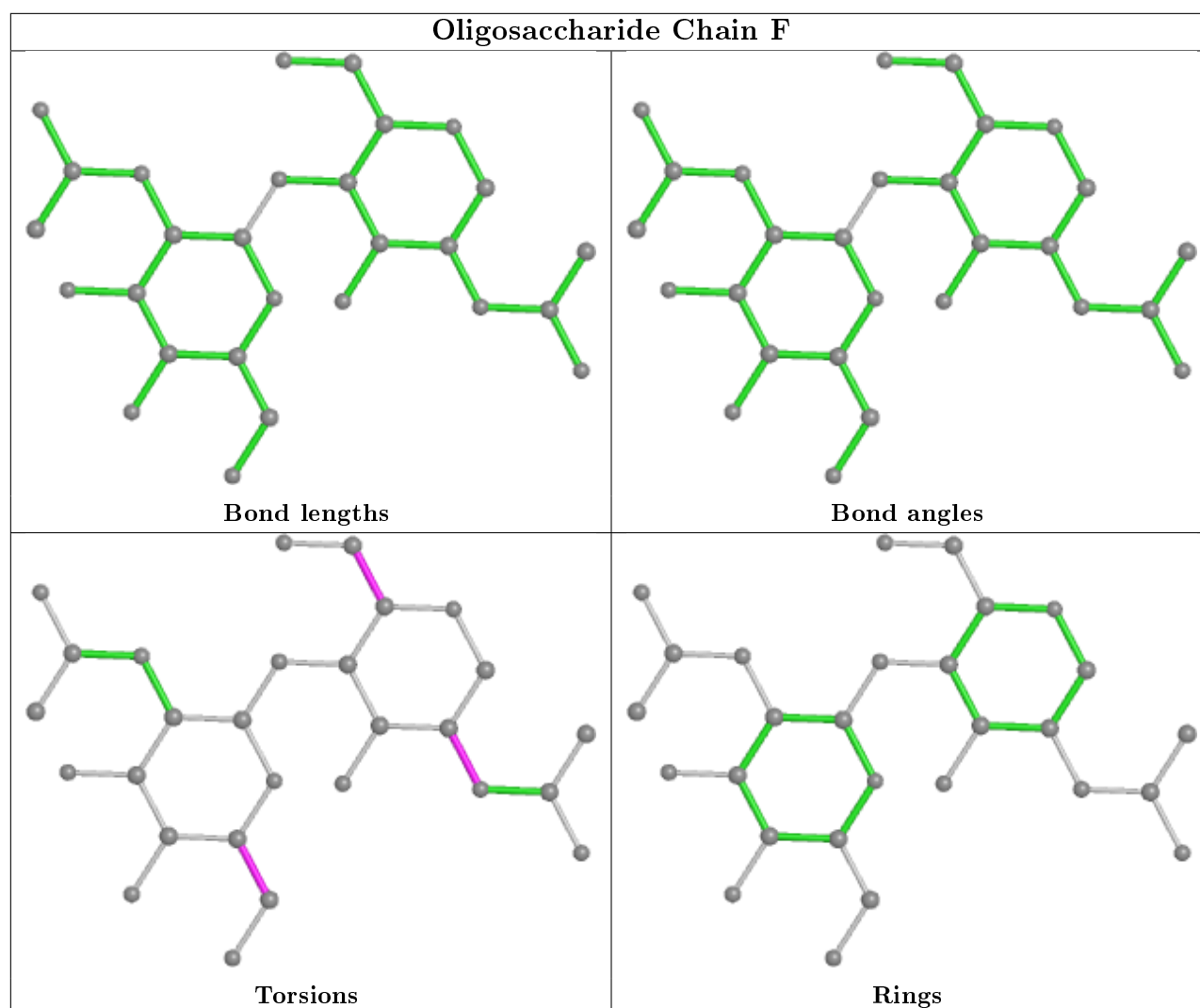
There are no ring outliers.

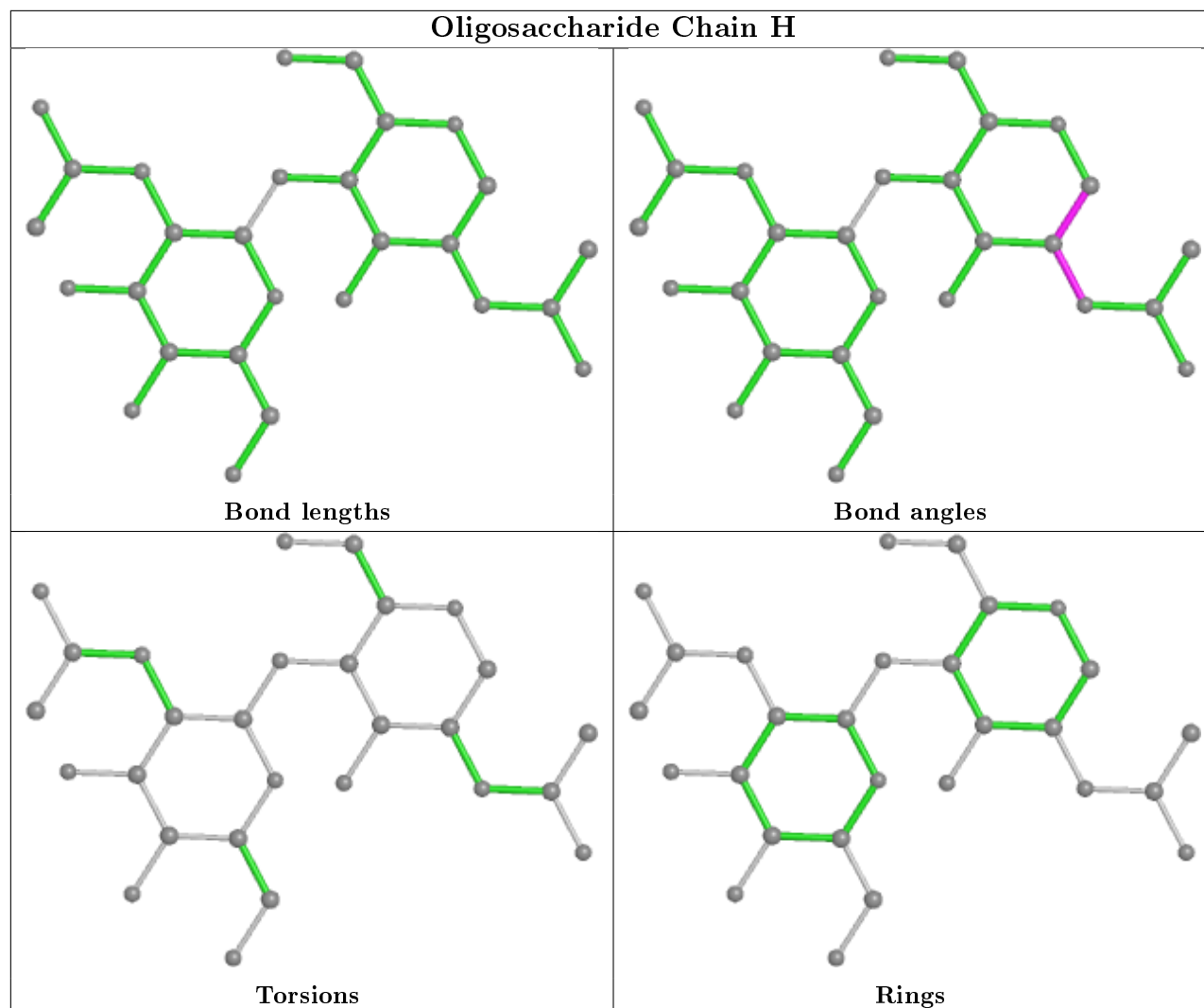
No monomer is involved in short contacts.

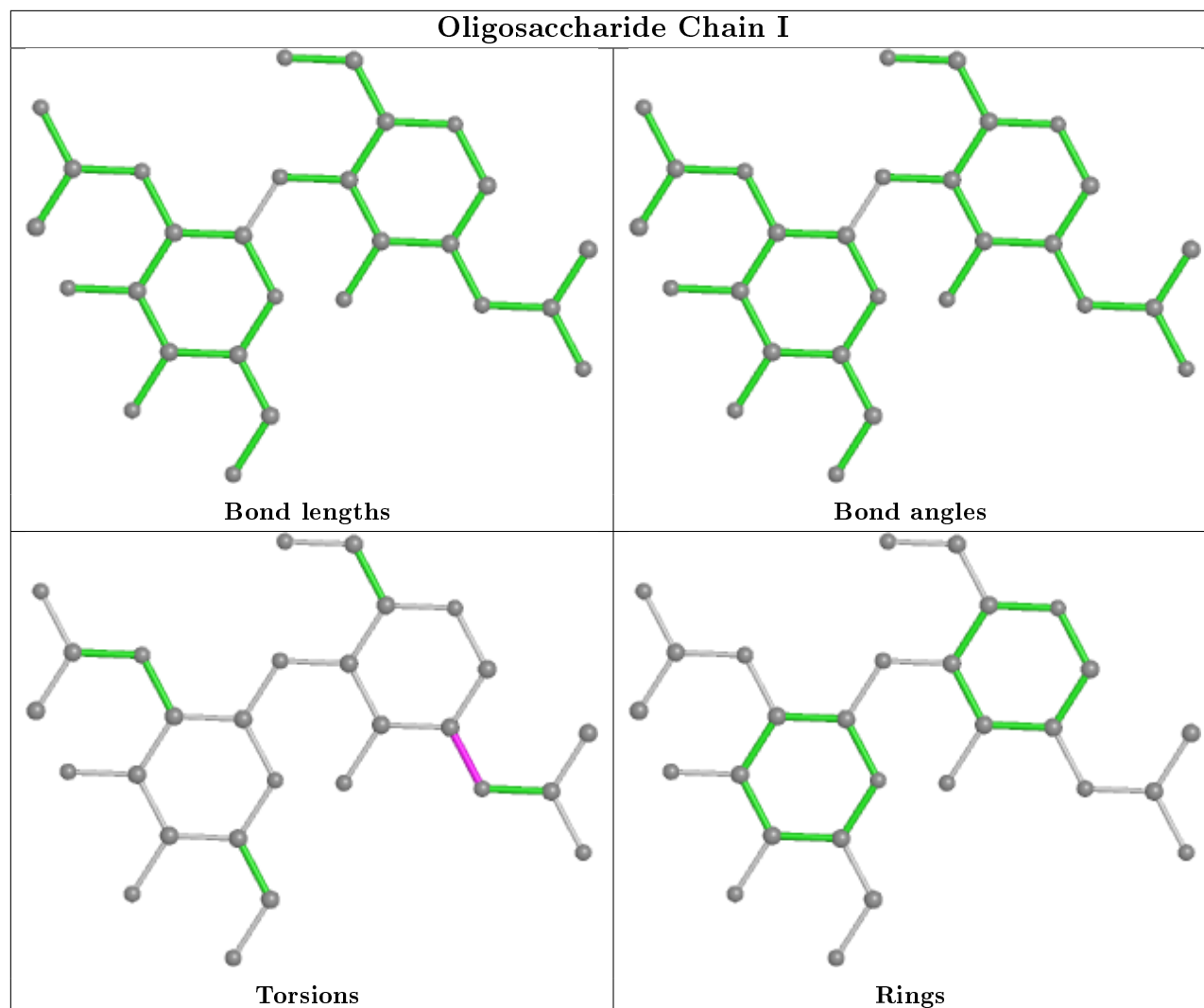
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

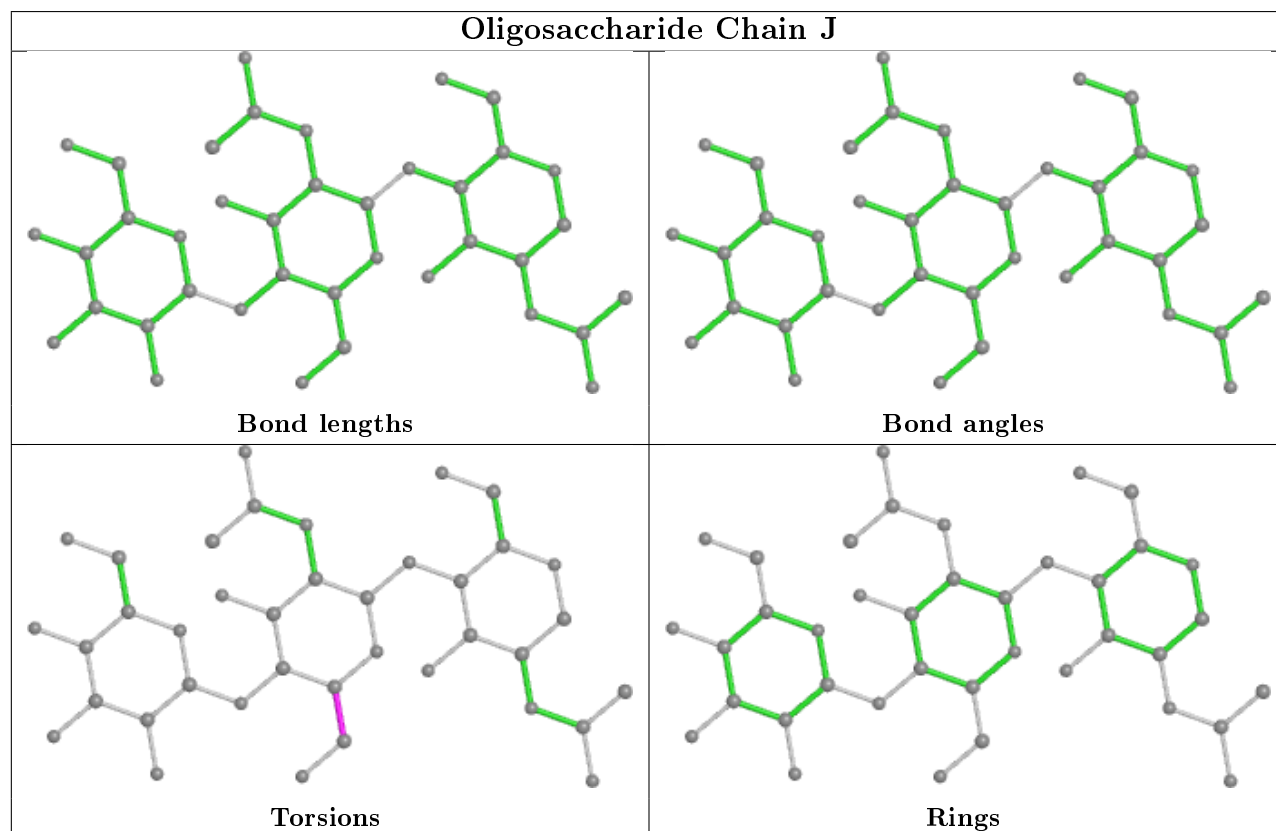
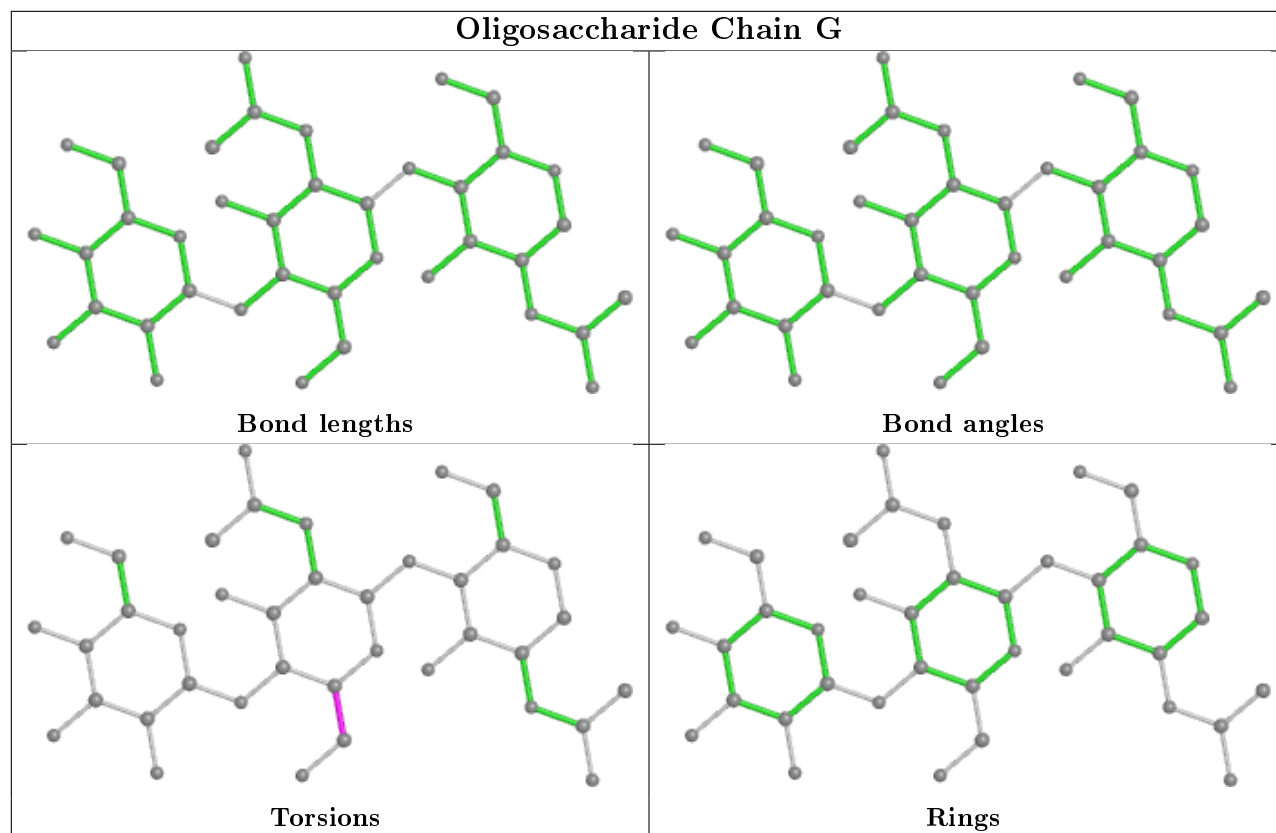












## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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$
5	NAG	B	705	1	14,14,15	0.36	0	17,19,21	0.76	1 (5%)
5	NAG	A	705	1	14,14,15	0.32	0	17,19,21	0.69	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
5	NAG	B	705	1	-	2/6/23/26	0/1/1/1
5	NAG	A	705	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	705	NAG	C1-O5-C5	2.73	115.89	112.19
5	A	705	NAG	C1-O5-C5	2.40	115.44	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	705	NAG	C4-C5-C6-O6
5	A	705	NAG	O5-C5-C6-O6
5	B	705	NAG	C4-C5-C6-O6
5	B	705	NAG	O5-C5-C6-O6

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, 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	644/654 (98%)	0.48	5 (0%) 86 75	66, 94, 133, 161	0
1	B	644/654 (98%)	0.53	11 (1%) 70 55	71, 98, 142, 170	0
2	C	80/87 (91%)	0.46	4 (5%) 28 18	75, 102, 155, 184	0
2	D	80/87 (91%)	0.29	2 (2%) 57 41	75, 99, 151, 165	0
All	All	1448/1482 (97%)	0.49	22 (1%) 73 60	66, 96, 140, 184	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	41	SER	3.8
2	C	42	SER	3.4
2	C	43	LEU	3.0
2	C	44	SER	3.0
1	B	395	PHE	2.9
1	B	438	PHE	2.7
2	D	44	SER	2.4
1	B	440	LEU	2.4
1	B	29	LEU	2.3
2	D	37	TRP	2.3
1	B	404	ILE	2.3
1	B	551	ILE	2.2
1	B	447	ILE	2.2
1	A	578	VAL	2.1
1	B	335	THR	2.1
1	B	412	THR	2.1
1	A	55	LEU	2.1
1	A	664	VAL	2.1
1	A	600	TYR	2.1
1	A	490	ASN	2.0
1	B	179	ILE	2.0
1	B	633	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

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.

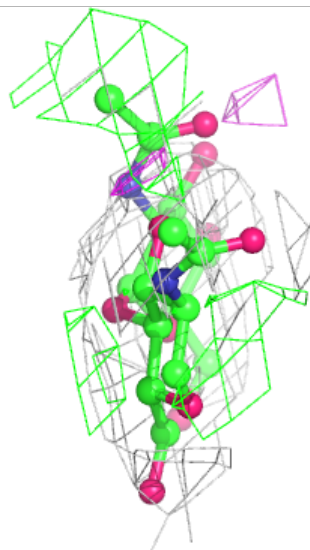
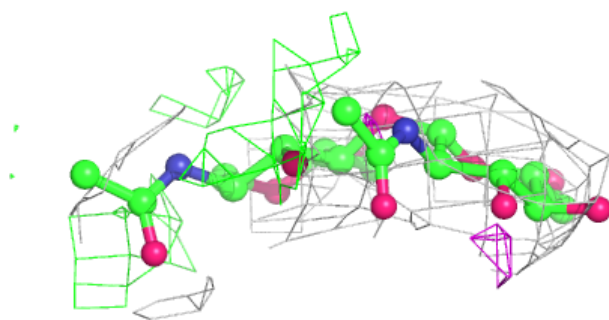
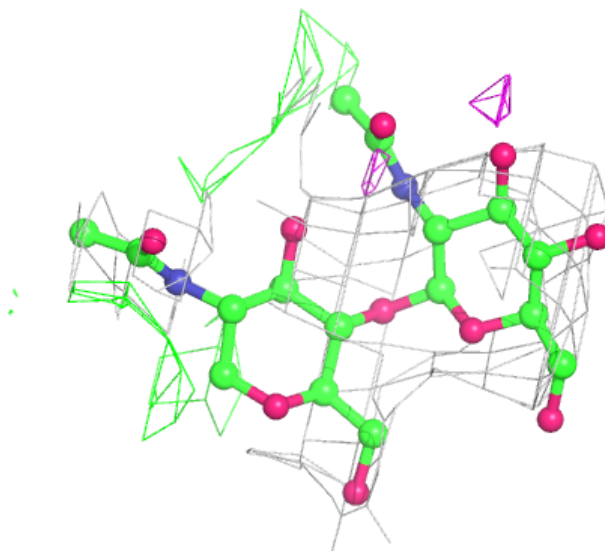
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	G	3	11/12	0.66	0.18	162,163,163,164	0
3	NAG	H	2	14/15	0.68	0.36	155,158,160,160	0
3	NAG	E	2	14/15	0.72	0.35	152,157,164,165	0
3	NAG	I	2	14/15	0.77	0.26	126,130,136,138	0
4	NAG	J	2	14/15	0.78	0.23	152,156,161,167	0
4	BMA	J	3	11/12	0.79	0.18	170,171,172,172	0
3	NAG	H	1	14/15	0.81	0.22	124,134,141,149	0
4	NAG	G	2	14/15	0.81	0.25	152,154,158,161	0
3	NAG	F	2	14/15	0.82	0.22	123,127,132,132	0
4	NAG	G	1	14/15	0.83	0.29	133,137,141,147	0
4	NAG	J	1	14/15	0.86	0.25	132,137,141,147	0
3	NAG	E	1	14/15	0.88	0.25	128,132,139,146	0
3	NAG	F	1	14/15	0.91	0.23	102,104,109,116	0
3	NAG	I	1	14/15	0.92	0.28	106,109,115,121	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.



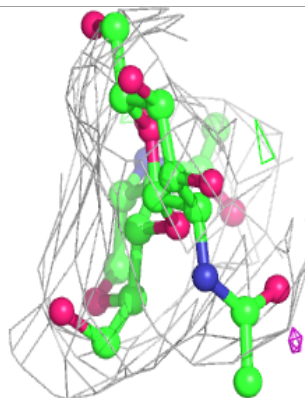
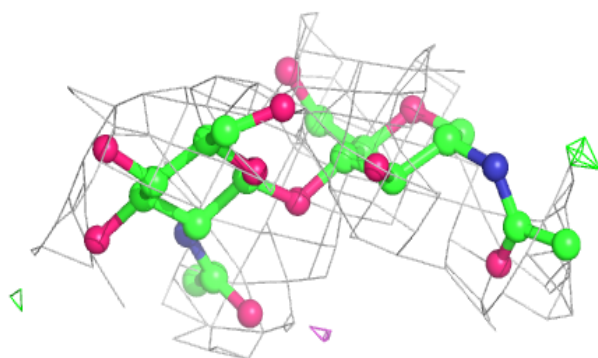
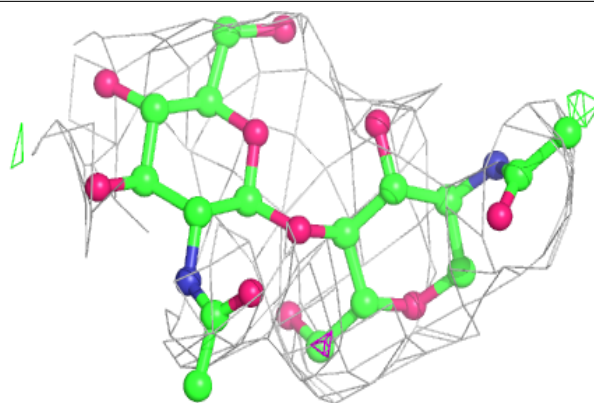
**Electron density around Chain E:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



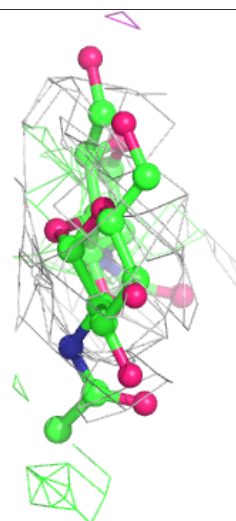
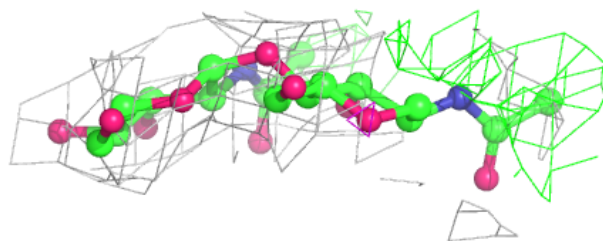
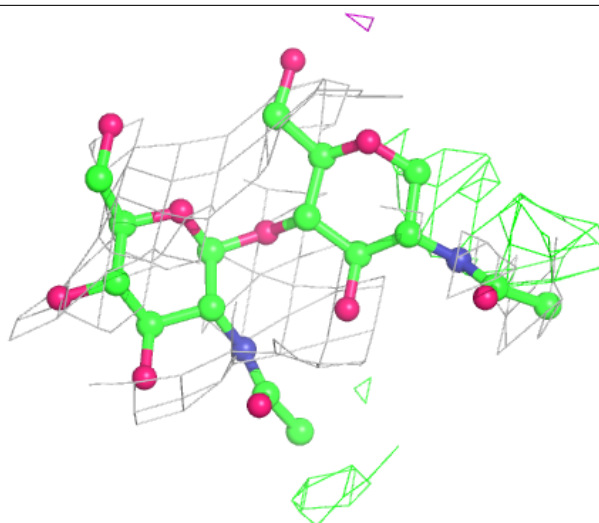
**Electron density around Chain F:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



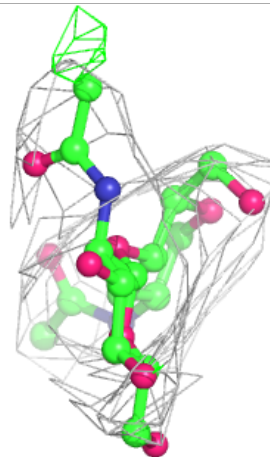
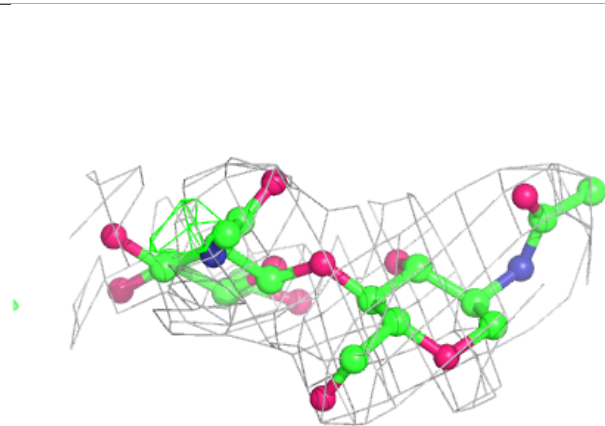
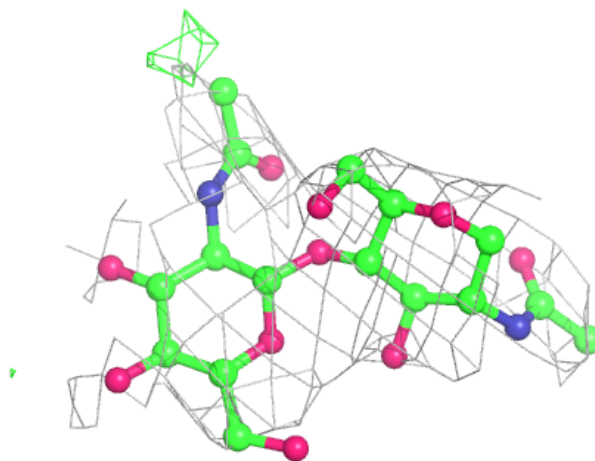
**Electron density around Chain H:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



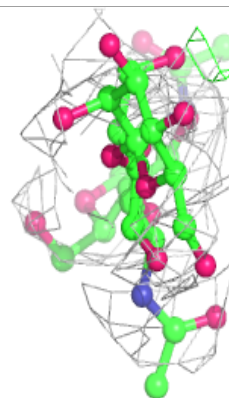
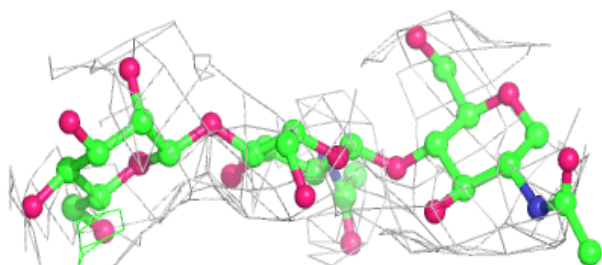
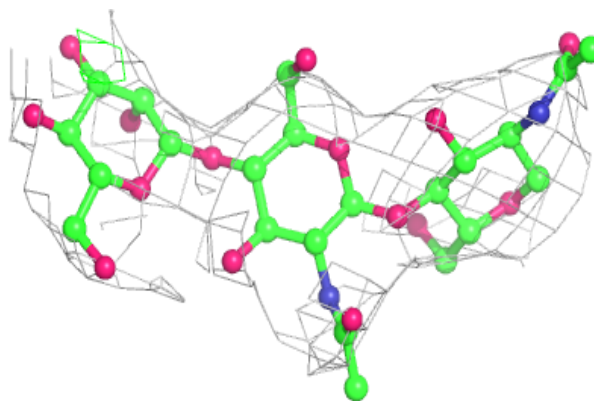
**Electron density around Chain I:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

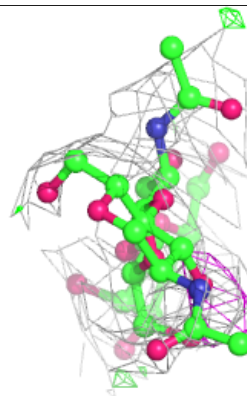
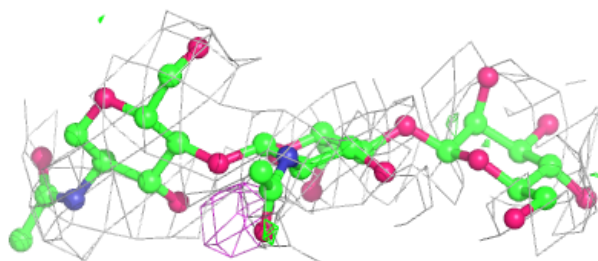
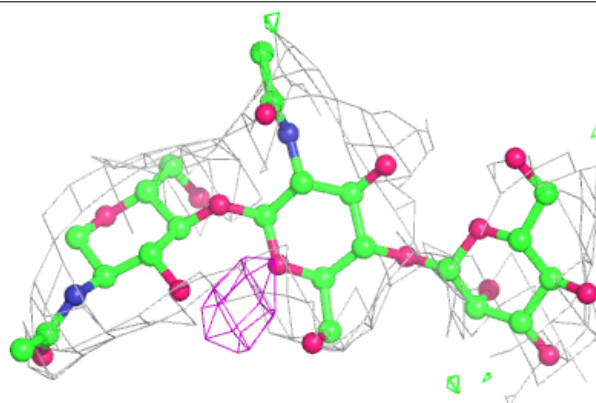


**Electron density around Chain G:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain J:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 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, 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
6	CA	A	709	1/1	0.41	0.14	184,184,184,184	0
5	NAG	A	705	14/15	0.65	0.23	143,146,151,152	0
5	NAG	B	705	14/15	0.67	0.20	124,132,133,134	0
6	CA	B	709	1/1	0.92	0.10	150,150,150,150	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.