



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 08:30 AM UTC

PDB ID : 6XP6 / pdb\_00006xp6  
Title : 3C11-DQ2-glia-a2 complex  
Authors : Petersen, J.; Rossjohn, J.  
Deposited on : 2020-07-08  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

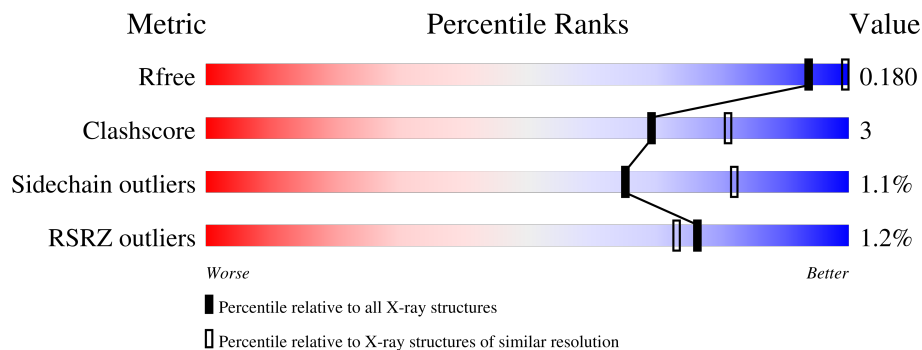
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 of 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	191	 86% 8% 5%
1	D	191	 85% 10% 5%
2	B	201	 79% 11% 10%
2	E	201	 78% 10% 10%
3	H	224	 89% 9% 2%
3	J	224	 88% 7% 5%

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Mol	Chain	Length	Quality of chain
4	G	214	<p>%</p> <p>91% 8% .</p>
4	I	214	<p>3%</p> <p>89% 9% ..</p>
5	C	26	<p>4%</p> <p>38% 12% 50%</p>
5	F	26	<p>50% 50%</p>
6	K	2	<p>100%</p>
6	M	2	<p>50% 50%</p>
6	N	2	<p>50% 50%</p>
7	L	7	<p>43% 29% 29%</p>
8	O	4	<p>50% 50%</p>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 13695 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 MHC class II HLA-DQ-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	181	1459	940	239	277	3	0	2	0
1	D	182	1456	938	237	278	3	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	-	expression tag	UNP O19705
A	183	SER	-	expression tag	UNP O19705
A	184	GLY	-	expression tag	UNP O19705
A	185	ASP	-	expression tag	UNP O19705
A	186	ASP	-	expression tag	UNP O19705
A	187	ASP	-	expression tag	UNP O19705
A	188	ASP	-	expression tag	UNP O19705
A	189	LYS	-	expression tag	UNP O19705
D	182	THR	-	expression tag	UNP O19705
D	183	SER	-	expression tag	UNP O19705
D	184	GLY	-	expression tag	UNP O19705
D	185	ASP	-	expression tag	UNP O19705
D	186	ASP	-	expression tag	UNP O19705
D	187	ASP	-	expression tag	UNP O19705
D	188	ASP	-	expression tag	UNP O19705
D	189	LYS	-	expression tag	UNP O19705

- Molecule 2 is a protein called MHC class II HLA-DQ-beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	181	1499	946	266	280	7	0	2	0
2	E	180	1491	942	265	277	7	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP O19712
B	193	THR	-	expression tag	UNP O19712
B	194	GLY	-	expression tag	UNP O19712
B	195	GLY	-	expression tag	UNP O19712
B	196	ASP	-	expression tag	UNP O19712
B	197	ASP	-	expression tag	UNP O19712
B	198	ASP	-	expression tag	UNP O19712
B	199	ASP	-	expression tag	UNP O19712
B	200	LYS	-	expression tag	UNP O19712
E	0	SER	-	expression tag	UNP O19712
E	193	THR	-	expression tag	UNP O19712
E	194	GLY	-	expression tag	UNP O19712
E	195	GLY	-	expression tag	UNP O19712
E	196	ASP	-	expression tag	UNP O19712
E	197	ASP	-	expression tag	UNP O19712
E	198	ASP	-	expression tag	UNP O19712
E	199	ASP	-	expression tag	UNP O19712
E	200	LYS	-	expression tag	UNP O19712

- Molecule 3 is a protein called 3.C11 IgH Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	220	Total 1638	C 1024	N 285	O 321	S 8	0	2	0
3	J	213	Total 1594	C 1000	N 277	O 309	S 8	0	2	0

- Molecule 4 is a protein called 3.C11 IgK Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	212	Total 1631	C 1021	N 272	O 333	S 5	0	0	0
4	I	212	Total 1639	C 1026	N 272	O 336	S 5	0	2	0

- Molecule 5 is a protein called DQ2-glia-a2 peptide.

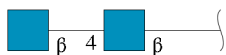
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	13	Total 96	C 63	N 15	O 18	0	0	0

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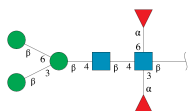
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	13	96	63	15	18	0	0	0

- Molecule 6 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
			Total	C	N	O			
6	K	2	28	16	2	10	0	0	0
6	M	2	28	16	2	10	0	0	0
6	N	2	28	16	2	10	0	0	0

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



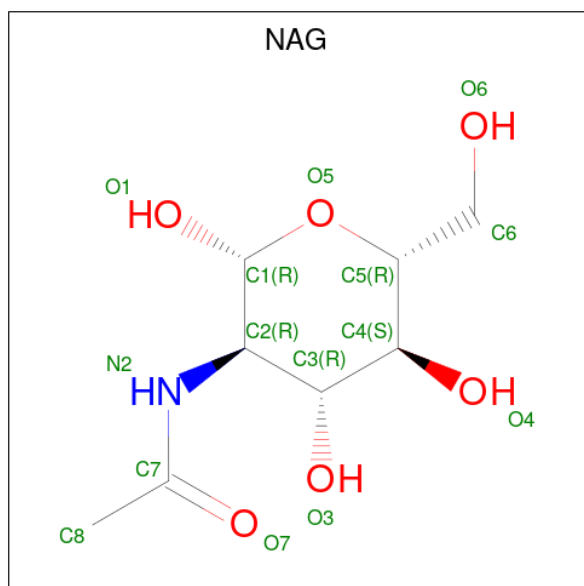
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	L	7	81	46	2	33	0	0	0

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



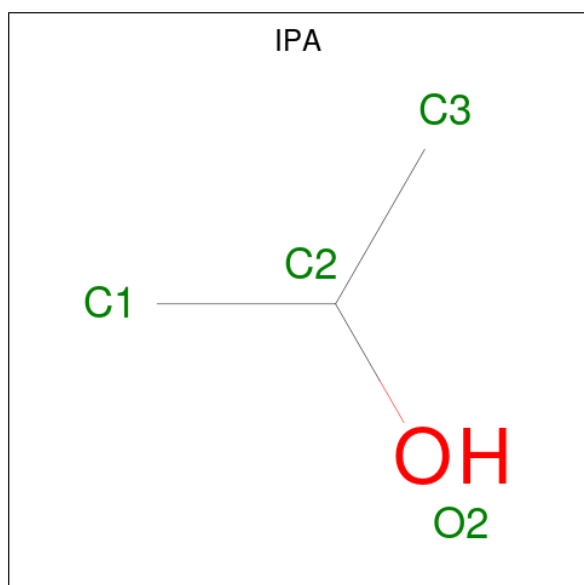
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	O	4	50	28	2	20	0	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 10 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula:  $C_3H_8O$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 3 1	0	0
10	A	1	Total C O 4 3 1	0	0
10	B	1	Total C O 4 3 1	0	0
10	D	1	Total C O 4 3 1	0	0
10	D	1	Total C O 4 3 1	0	0
10	H	1	Total C O 4 3 1	0	0
10	H	1	Total C O 4 3 1	0	0
10	H	1	Total C O 4 3 1	0	0
10	J	1	Total C O 4 3 1	0	0
10	J	1	Total C O 4 3 1	0	0
10	J	1	Total C O 4 3 1	0	0
10	G	1	Total C O 4 3 1	0	0

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	2	Total Cl 2 2	0	0
11	J	1	Total Cl 1 1	0	0
11	G	1	Total Cl 1 1	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	113	Total O 113 113	0	0
12	B	94	Total O 94 94	0	0
12	D	106	Total O 106 106	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
12	E	121	Total 121	O 121	0	0
12	H	86	Total 86	O 86	0	0
12	J	100	Total 100	O 100	0	0
12	G	109	Total 109	O 109	0	0
12	I	77	Total 77	O 77	0	0
12	C	5	Total 5	O 5	0	0
12	F	4	Total 4	O 4	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: MHC class II HLA-DQ-alpha chain

Chain A: 




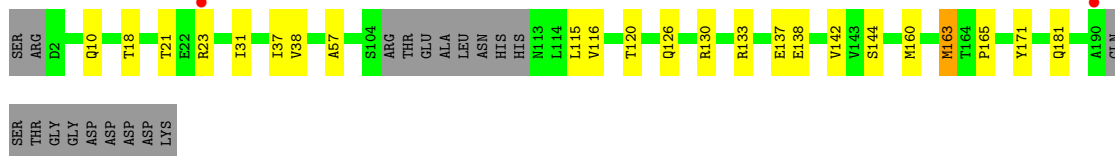
- Molecule 1: MHC class II HLA-DQ-alpha chain

Chain D: 




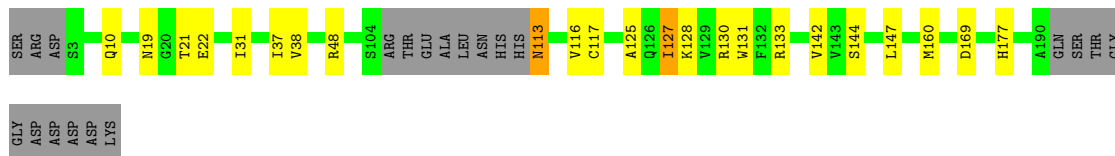
- Molecule 2: MHC class II HLA-DQ-beta-1

Chain B: 



- Molecule 2: MHC class II HLA-DQ-beta-1

Chain E: 

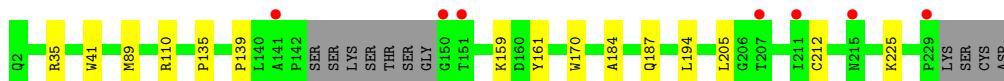
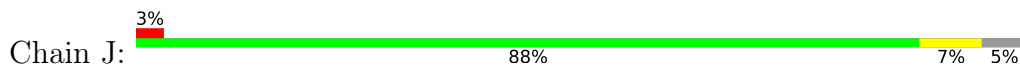


- Molecule 3: 3.C11 IgH Fab

Chain H: 



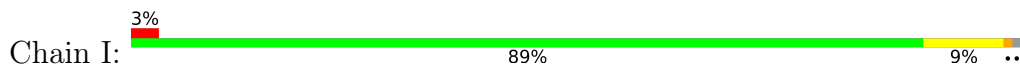
- Molecule 3: 3.C11 IgH Fab



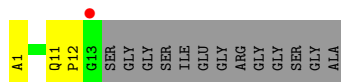
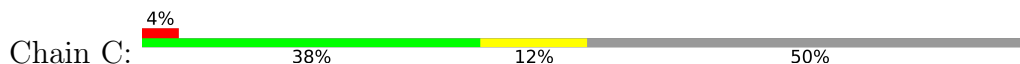
- Molecule 4: 3.C11 IgK Fab



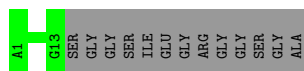
- Molecule 4: 3.C11 IgK Fab



- Molecule 5: DQ2-glia-a2 peptide



- Molecule 5: DQ2-glia-a2 peptide



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%

MAG1  
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

MAG1  
MAG2

- Molecule 7: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  43% 29% 29%

MAG1  
MAG2  
BMA3  
BMA4  
BMA5  
FUC6  
FUC7

- Molecule 8: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%

MAG1  
MAG2  
BMA3  
BMA4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.85Å 143.05Å 170.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.03 – 2.40 47.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.03-2.40) 99.9 (47.03-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.176 , 0.212 (Not available) , 0.180	Depositor DCC
$R_{free}$ test set	1831 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtrriage
Anisotropy	0.629	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: BMA, NAG, IPA, CL, FUC

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	0.27	0/1507	0.44	0/2057
1	D	0.27	0/1501	0.44	0/2050
2	B	0.28	0/1538	0.49	0/2089
2	E	0.29	0/1530	0.49	0/2078
3	H	0.25	0/1678	0.47	0/2282
3	J	0.27	0/1633	0.48	0/2221
4	G	0.26	0/1667	0.50	0/2266
4	I	0.27	0/1681	0.50	0/2286
5	C	0.34	0/101	0.59	0/141
5	F	0.33	0/101	0.60	0/141
All	All	0.27	0/12937	0.48	0/17611

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	1459	0	1415	8	0
1	D	1456	0	1404	9	0
2	B	1499	0	1464	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1491	0	1460	13	0
3	H	1638	0	1636	12	0
3	J	1594	0	1592	9	0
4	G	1631	0	1580	10	0
4	I	1639	0	1583	12	0
5	C	96	0	92	3	0
5	F	96	0	92	0	0
6	K	28	0	25	0	0
6	M	28	0	25	0	0
6	N	28	0	25	0	0
7	L	81	0	70	1	0
8	O	50	0	43	0	0
9	A	14	0	13	0	0
10	A	8	0	16	0	0
10	B	4	0	8	1	0
10	D	8	0	16	1	0
10	G	4	0	8	2	0
10	H	12	0	24	4	0
10	J	12	0	24	0	0
11	G	1	0	0	0	0
11	H	2	0	0	0	0
11	J	1	0	0	0	0
12	A	113	0	0	1	0
12	B	94	0	0	2	0
12	C	5	0	0	1	0
12	D	106	0	0	0	0
12	E	121	0	0	0	0
12	F	4	0	0	0	0
12	G	109	0	0	1	0
12	H	86	0	0	0	0
12	I	77	0	0	0	0
12	J	100	0	0	1	0
All	All	13695	0	12615	89	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 3.

The worst 5 of 89 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:E:128:LYS:HE3	2:E:130:ARG:HE	1.49	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:133:ARG:NH1	2:E:169:ASP:OD2	2.21	0.73
2:B:116:VAL:HG22	2:B:160:MET:HG3	1.71	0.72
3:H:29:THR:HB	10:H:302:IPA:H13	1.73	0.70
4:G:124:ARG:HG3	4:G:125:THR:H	1.57	0.69

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 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	A	167/174 (96%)	165 (99%)	2 (1%)	63	81
1	D	166/174 (95%)	164 (99%)	2 (1%)	63	81
2	B	168/183 (92%)	165 (98%)	3 (2%)	51	73
2	E	167/183 (91%)	164 (98%)	3 (2%)	51	73
3	H	185/187 (99%)	183 (99%)	2 (1%)	65	82
3	J	179/187 (96%)	178 (99%)	1 (1%)	78	89
4	G	188/190 (99%)	187 (100%)	1 (0%)	81	91
4	I	189/190 (100%)	187 (99%)	2 (1%)	65	82
5	C	10/16 (62%)	10 (100%)	0	100	100
5	F	10/16 (62%)	10 (100%)	0	100	100
All	All	1429/1500 (95%)	1413 (99%)	16 (1%)	65	82

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	I	124	ARG
4	G	139	GLU
2	E	113	ASN
3	J	110	ARG
2	E	21	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	140	GLN
4	I	44	GLN
3	H	48	GLN
4	G	153	ASN
2	E	156	GLN

### 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](#)

17 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	$\# Z  > 2$
6	NAG	K	1	1,6	14,14,15	0.51	0	17,19,21	0.52	0
6	NAG	K	2	6	14,14,15	0.53	0	17,19,21	0.58	0
7	NAG	L	1	2,7	14,14,15	0.35	0	17,19,21	0.60	0
7	NAG	L	2	7	14,14,15	0.25	0	17,19,21	0.65	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	L	3	7	11,11,12	0.96	0	15,15,17	1.45	3 (20%)
7	BMA	L	4	7	11,11,12	0.74	0	15,15,17	0.70	0
7	BMA	L	5	7	11,11,12	1.94	2 (18%)	15,15,17	1.56	3 (20%)
7	FUC	L	6	7	10,10,11	1.03	1 (10%)	14,14,16	1.13	1 (7%)
7	FUC	L	7	7	10,10,11	0.97	0	14,14,16	0.93	0
6	NAG	M	1	1,6	14,14,15	0.56	0	17,19,21	0.91	1 (5%)
6	NAG	M	2	6	14,14,15	0.42	0	17,19,21	0.44	0
6	NAG	N	1	1,6	14,14,15	0.50	0	17,19,21	0.57	0
6	NAG	N	2	6	14,14,15	0.67	1 (7%)	17,19,21	0.45	0
8	NAG	O	1	8,2	14,14,15	0.34	0	17,19,21	0.51	0
8	NAG	O	2	8	14,14,15	0.29	0	17,19,21	0.57	0
8	BMA	O	3	8	11,11,12	1.19	1 (9%)	15,15,17	1.16	1 (6%)
8	BMA	O	4	8	11,11,12	1.80	3 (27%)	15,15,17	1.48	2 (13%)

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
6	NAG	K	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
7	NAG	L	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	0/6/23/26	0/1/1/1
7	BMA	L	3	7	-	2/2/19/22	0/1/1/1
7	BMA	L	4	7	-	0/2/19/22	0/1/1/1
7	BMA	L	5	7	-	2/2/19/22	0/1/1/1
7	FUC	L	6	7	-	-	0/1/1/1
7	FUC	L	7	7	-	-	0/1/1/1
6	NAG	M	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
6	NAG	N	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
8	NAG	O	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	O	2	8	-	0/6/23/26	0/1/1/1
8	BMA	O	3	8	-	2/2/19/22	0/1/1/1
8	BMA	O	4	8	-	2/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	5	BMA	C1-C2	4.85	1.63	1.52
8	O	4	BMA	C1-C2	4.16	1.62	1.52
7	L	5	BMA	C2-C3	3.39	1.57	1.52
8	O	4	BMA	O5-C1	3.27	1.49	1.43
6	N	2	NAG	C1-C2	2.31	1.55	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	3	BMA	O3-C3-C2	3.70	117.60	110.05
8	O	4	BMA	C1-O5-C5	3.49	116.86	112.19
6	M	1	NAG	C1-O5-C5	2.87	116.03	112.19
7	L	5	BMA	C3-C4-C5	-2.86	105.05	110.23
8	O	4	BMA	C1-C2-C3	2.75	113.66	109.64

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

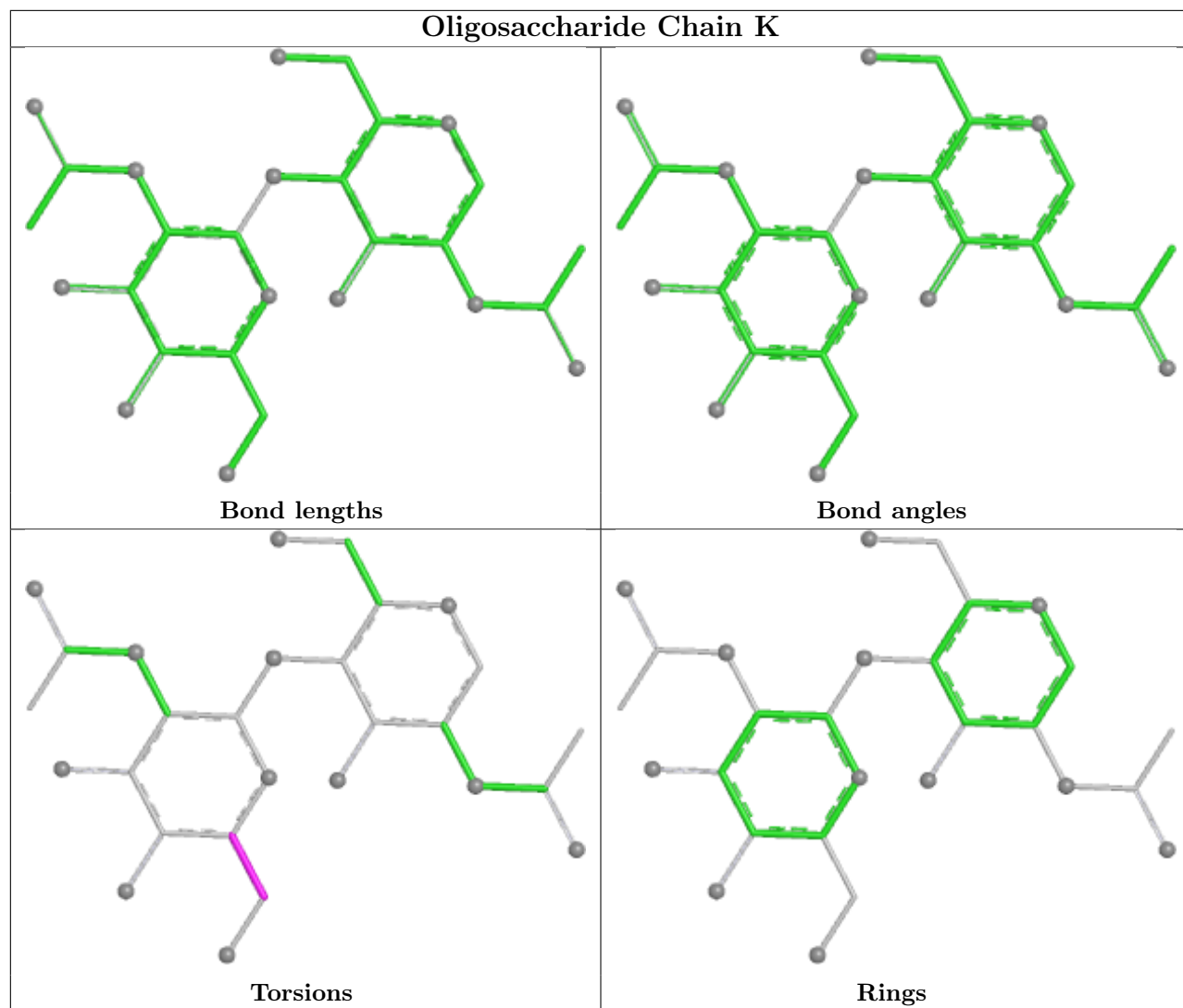
Mol	Chain	Res	Type	Atoms
7	L	3	BMA	O5-C5-C6-O6
8	O	3	BMA	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
7	L	5	BMA	O5-C5-C6-O6

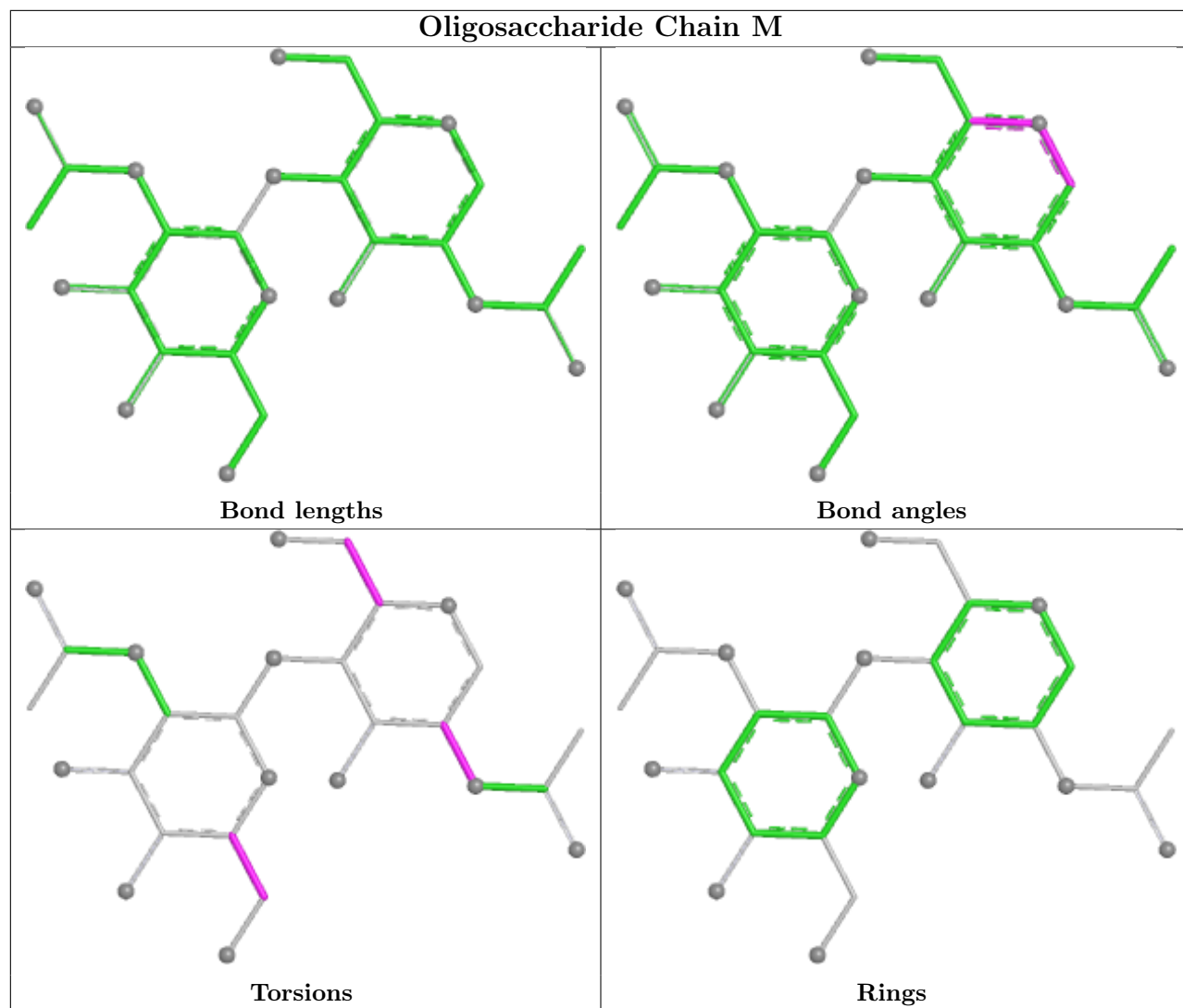
There are no ring outliers.

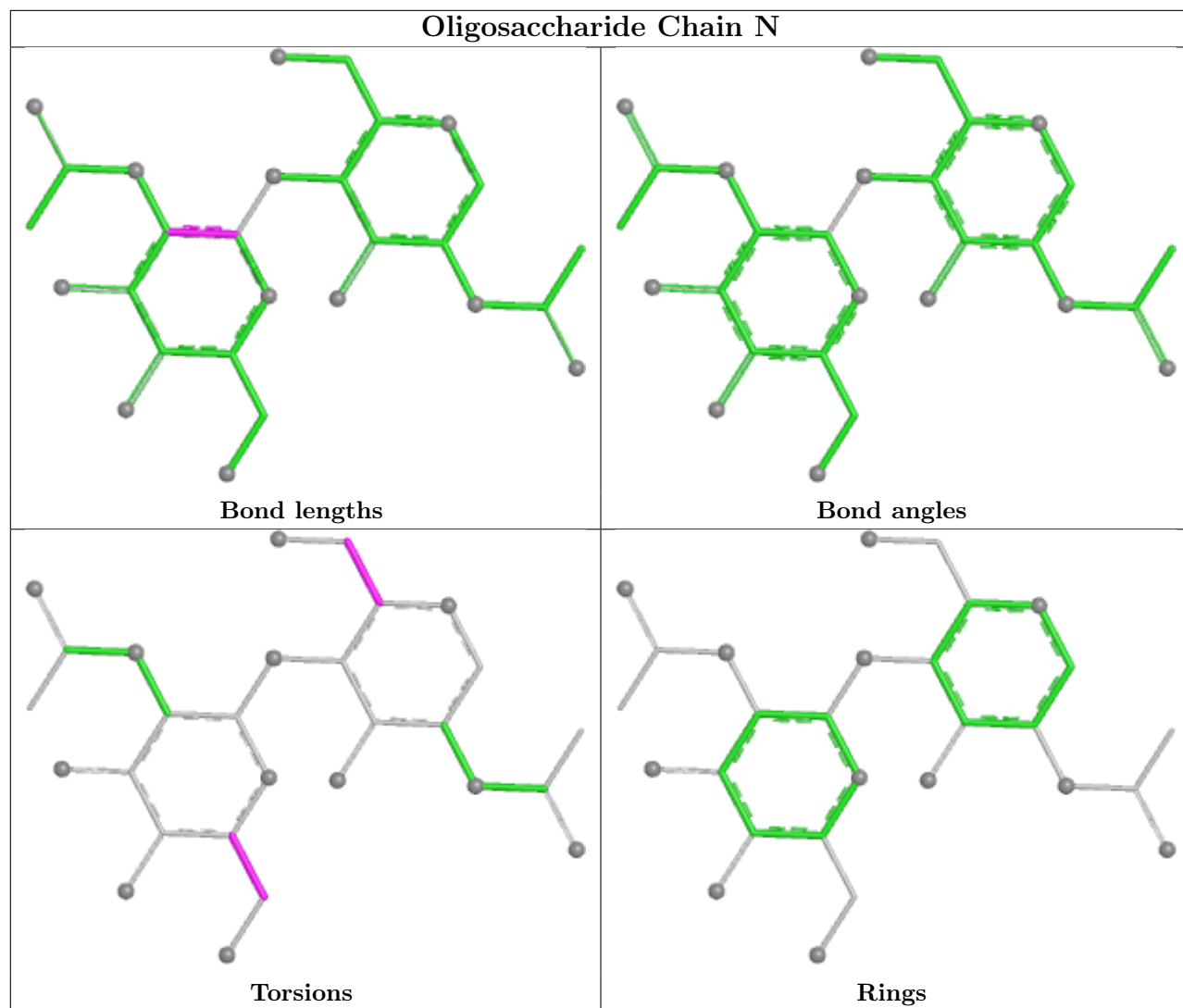
2 monomers are involved in 1 short contact:

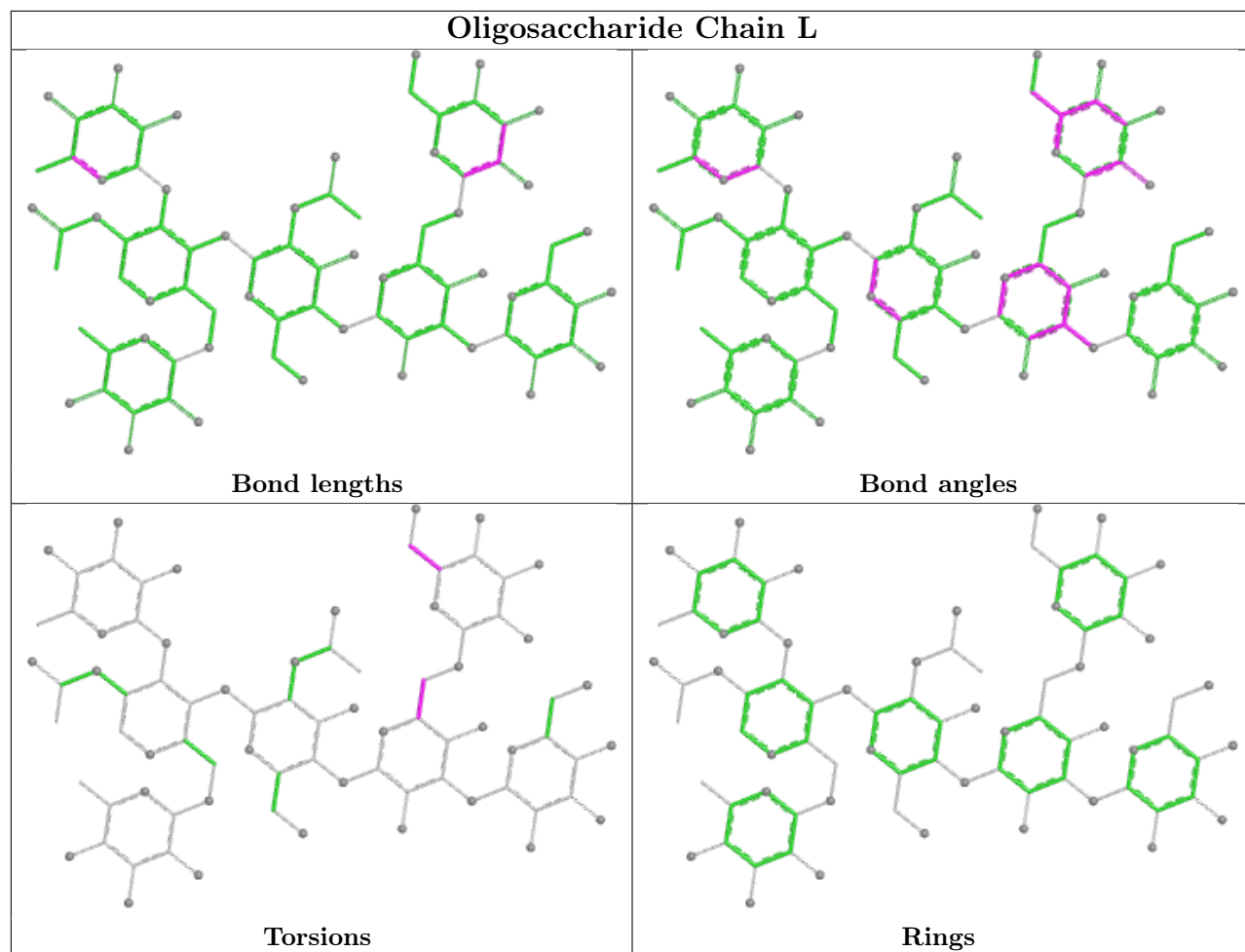
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	6	FUC	1	0
7	L	2	NAG	1	0

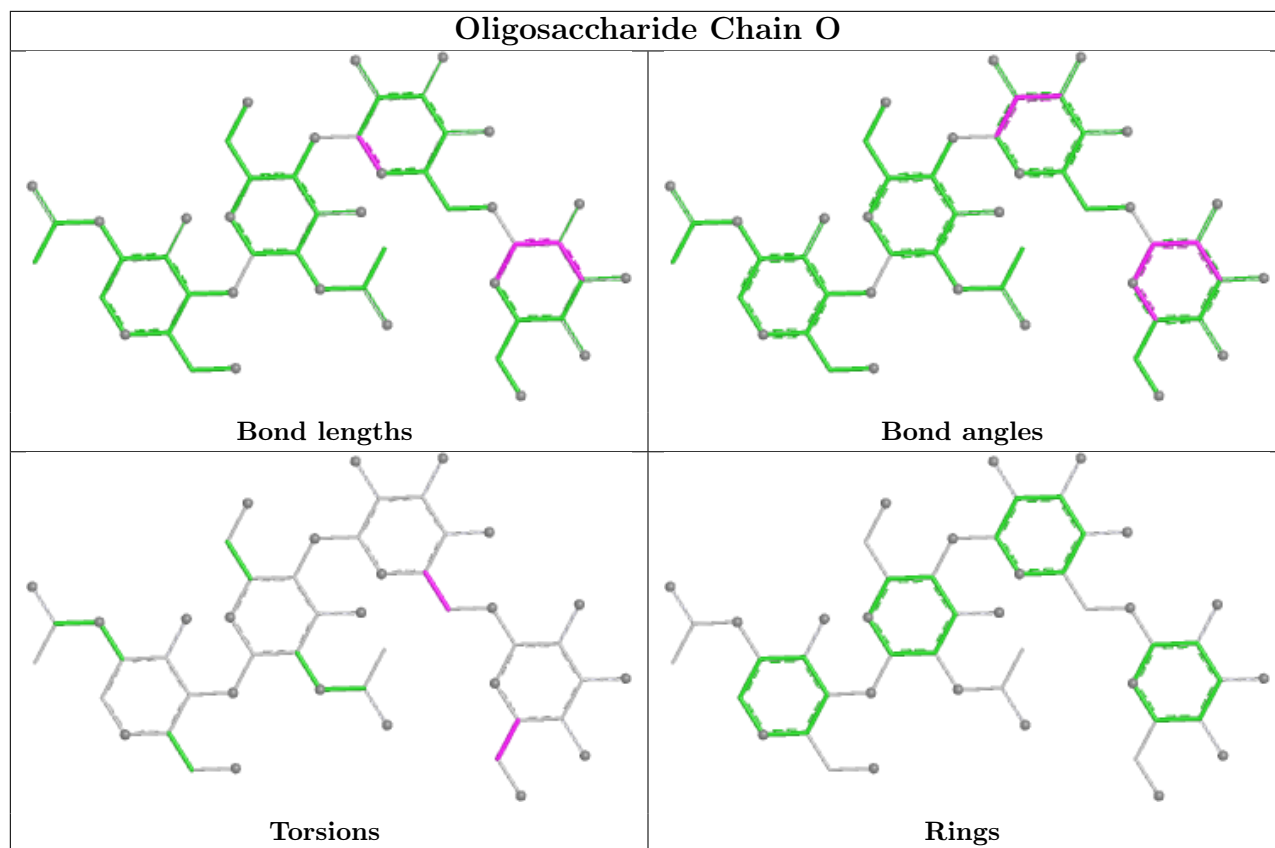
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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
10	IPA	J	301	-	3,3,3	0.61	0	3,3,3	0.37	0
10	IPA	J	302	-	3,3,3	0.59	0	3,3,3	0.31	0
10	IPA	H	301	-	3,3,3	0.57	0	3,3,3	0.11	0
10	IPA	B	1008	-	3,3,3	0.60	0	3,3,3	0.35	0
10	IPA	H	302	-	3,3,3	0.60	0	3,3,3	0.27	0
10	IPA	A	1005	-	3,3,3	0.58	0	3,3,3	0.29	0
10	IPA	A	1004	-	3,3,3	0.59	0	3,3,3	0.32	0
10	IPA	D	206	-	3,3,3	0.66	0	3,3,3	0.29	0
9	NAG	A	1003	1	14,14,15	0.46	0	17,19,21	0.65	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	IPA	G	301	-	3,3,3	0.59	0	3,3,3	0.32	0
10	IPA	J	303	-	3,3,3	0.64	0	3,3,3	0.29	0
10	IPA	H	303	-	3,3,3	0.60	0	3,3,3	0.22	0
10	IPA	D	205	-	3,3,3	0.61	0	3,3,3	0.24	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
9	NAG	A	1003	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1003	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1003	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	301	IPA	1	0
10	B	1008	IPA	1	0
10	H	302	IPA	1	0
10	G	301	IPA	2	0
10	H	303	IPA	2	0
10	D	205	IPA	1	0

## 5.7 Other polymers [i](#)

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 [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	181/191 (94%)	-0.50	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	27, 40, 58, 93	2 (1%)
1	D	182/191 (95%)	-0.44	1 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">85</span>	25, 38, 69, 99	1 (0%)
2	B	181/201 (90%)	-0.43	2 (1%) <span style="border: 1px solid blue; padding: 2px;">78</span> <span style="border: 1px solid blue; padding: 2px;">74</span>	27, 41, 69, 101	2 (1%)
2	E	180/201 (89%)	-0.44	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	24, 38, 71, 105	2 (1%)
3	H	220/224 (98%)	-0.19	1 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">85</span>	22, 48, 77, 98	2 (0%)
3	J	213/224 (95%)	0.04	7 (3%) <span style="border: 1px solid gray; padding: 2px;">49</span> <span style="border: 1px solid gray; padding: 2px;">45</span>	24, 48, 98, 115	2 (0%)
4	G	212/214 (99%)	-0.33	2 (0%) <span style="border: 1px solid blue; padding: 2px;">81</span> <span style="border: 1px solid blue; padding: 2px;">78</span>	27, 44, 70, 82	0
4	I	212/214 (99%)	0.20	6 (2%) <span style="border: 1px solid gray; padding: 2px;">55</span> <span style="border: 1px solid gray; padding: 2px;">51</span>	23, 56, 104, 114	2 (0%)
5	C	13/26 (50%)	-0.21	1 (7%) <span style="border: 1px solid red; padding: 2px;">19</span> <span style="border: 1px solid red; padding: 2px;">16</span>	34, 39, 60, 62	0
5	F	13/26 (50%)	-0.18	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	29, 33, 53, 58	0
All	All	1607/1712 (93%)	-0.24	20 (1%) <span style="border: 1px solid blue; padding: 2px;">76</span> <span style="border: 1px solid blue; padding: 2px;">73</span>	22, 43, 88, 115	13 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	141	ALA	3.5
4	I	124	ARG	3.2
3	J	150	GLY	3.0
1	D	0	ASP	3.0
4	G	228	GLY	2.6

### 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

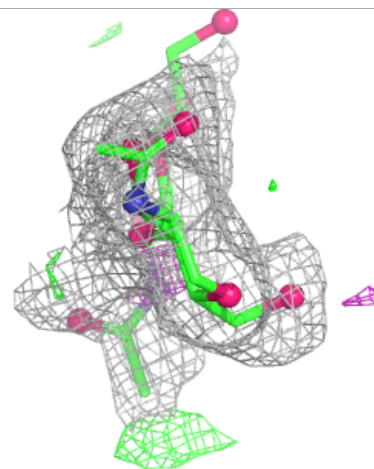
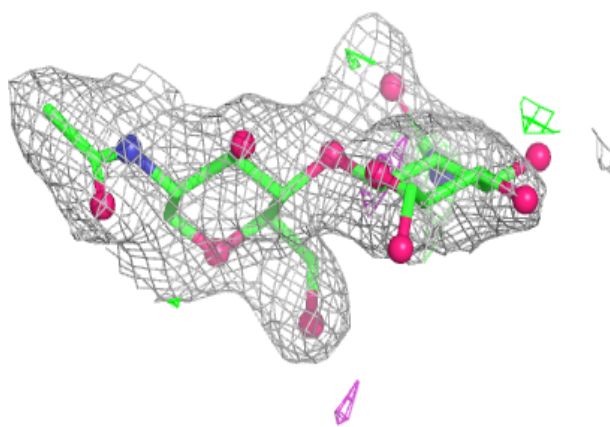
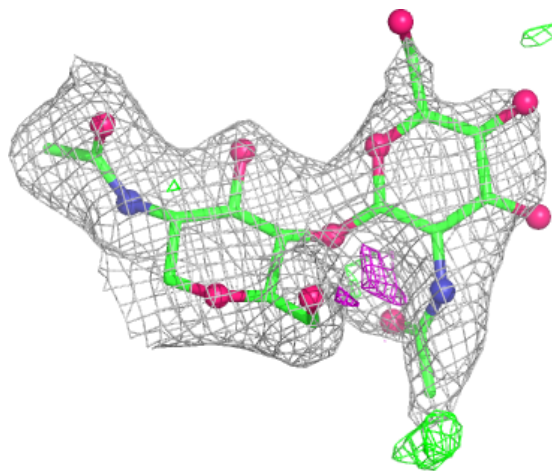
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	FUC	L	7	10/11	0.32	0.22	95,103,106,113	0
6	NAG	N	2	14/15	0.40	0.20	89,116,122,122	0
7	FUC	L	6	10/11	0.47	0.21	89,103,110,114	0
6	NAG	M	2	14/15	0.50	0.17	104,121,124,128	0
6	NAG	K	2	14/15	0.54	0.16	74,91,97,100	0
6	NAG	M	1	14/15	0.59	0.15	92,101,111,112	0
7	NAG	L	2	14/15	0.70	0.16	76,90,96,97	0
8	NAG	O	2	14/15	0.71	0.14	84,90,96,97	0
8	NAG	O	1	14/15	0.72	0.13	64,77,84,89	0
7	NAG	L	1	14/15	0.72	0.14	68,80,93,100	0
7	BMA	L	4	11/12	0.76	0.14	73,81,88,88	0
8	BMA	O	3	11/12	0.79	0.12	78,87,94,97	0
8	BMA	O	4	11/12	0.79	0.16	68,72,84,90	0
6	NAG	N	1	14/15	0.83	0.12	48,87,100,113	0
7	BMA	L	5	11/12	0.84	0.17	46,64,82,83	0
6	NAG	K	1	14/15	0.85	0.11	40,61,79,84	0
7	BMA	L	3	11/12	0.87	0.11	59,69,80,80	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.

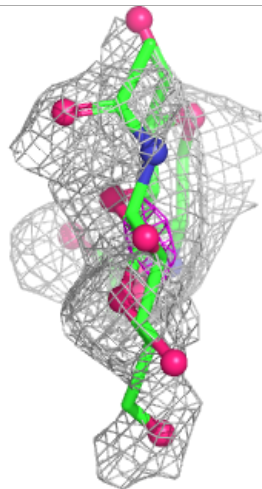
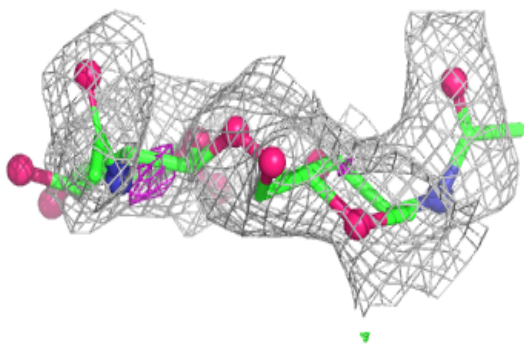
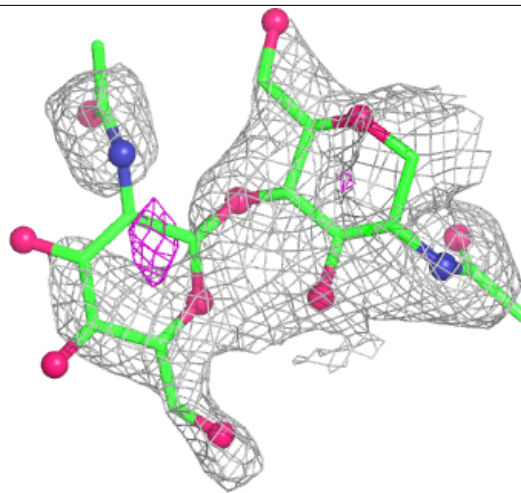
**Electron density around Chain K:**

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



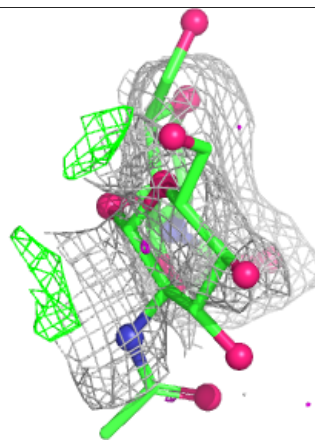
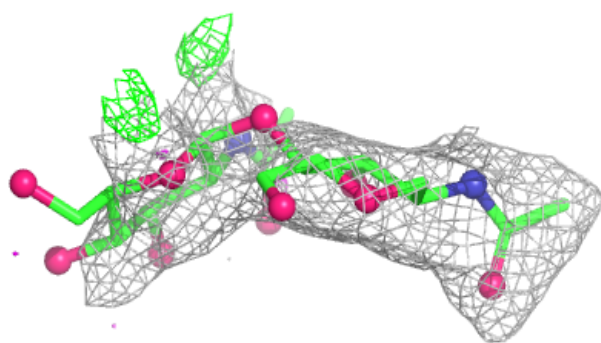
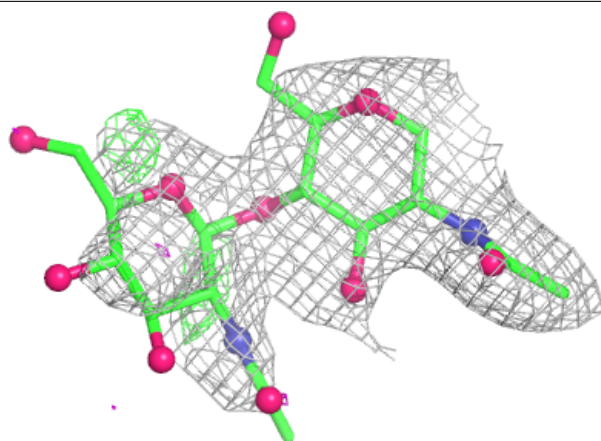
**Electron density around Chain M:**

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



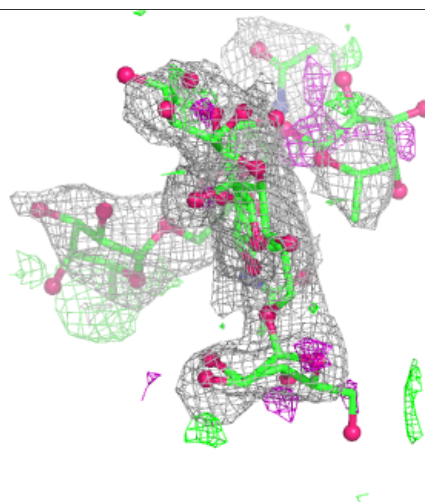
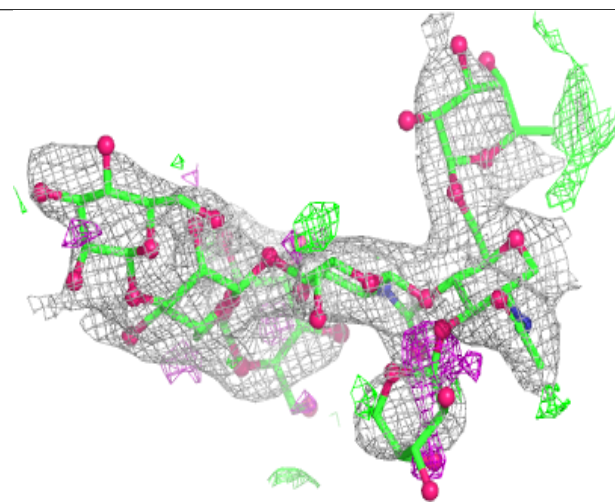
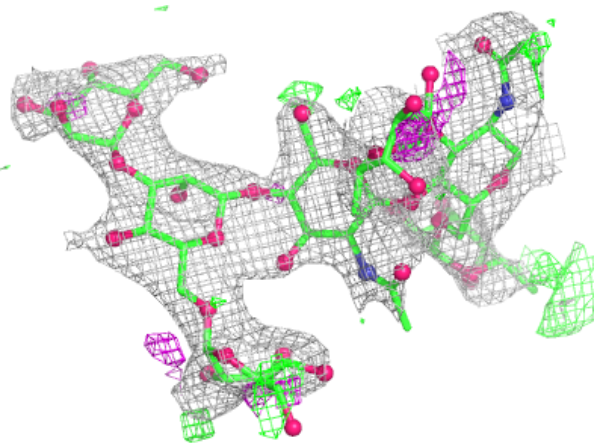
**Electron density around Chain N:**

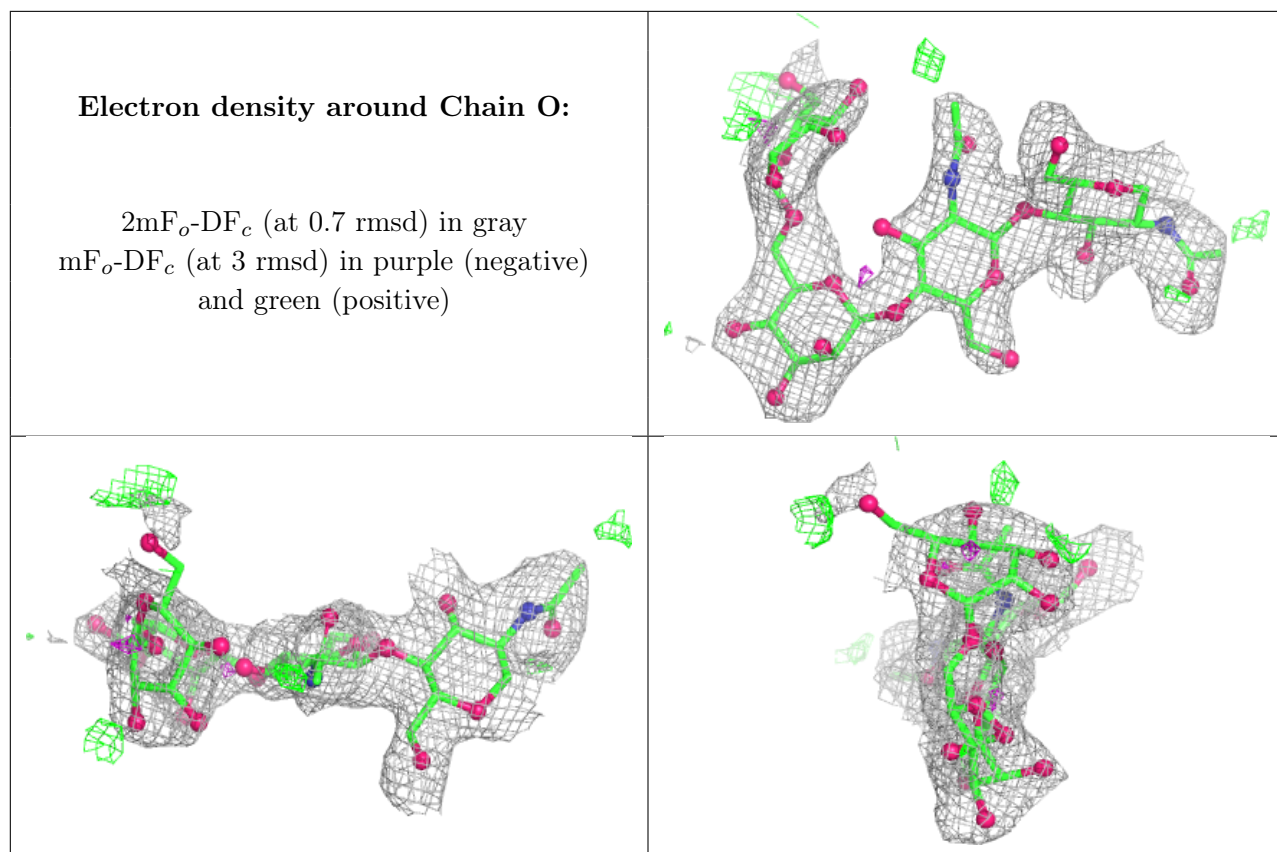
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain L:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
9	NAG	A	1003	14/15	0.73	0.14	82,92,97,98	0
10	IPA	H	302	4/4	0.74	0.21	49,57,61,66	0
10	IPA	B	1008	4/4	0.78	0.23	55,57,59,64	0
10	IPA	G	301	4/4	0.79	0.17	49,54,60,64	0
10	IPA	J	303	4/4	0.85	0.17	36,38,51,53	0
10	IPA	A	1004	4/4	0.87	0.16	31,42,44,45	0
10	IPA	D	205	4/4	0.88	0.16	38,42,43,60	0
10	IPA	D	206	4/4	0.89	0.14	33,38,49,54	0
10	IPA	H	303	4/4	0.92	0.26	43,52,59,65	0
11	CL	H	305	1/1	0.93	0.09	76,76,76,76	0
10	IPA	A	1005	4/4	0.94	0.14	36,45,50,50	0
10	IPA	H	301	4/4	0.95	0.12	42,42,45,52	0
11	CL	G	302	1/1	0.95	0.08	65,65,65,65	0
10	IPA	J	302	4/4	0.96	0.09	39,42,42,47	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	CL	J	304	1/1	0.98	0.04	36,36,36,36	0
10	IPA	J	301	4/4	0.98	0.06	29,33,37,38	0
11	CL	H	304	1/1	0.99	0.03	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.