



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2021 – 12:24 PM EDT

PDB ID : 7KCZ
Title : CRYSTAL STRUCTURE OF RHESUS MACAQUE (MACACA MULATTA)
IGG1 FC FRAGMENT- FC-GAMMA RECEPTOR III COMPLEX V158
MUTANT
Authors : Tolbert, W.D.; Pazgier, M.
Deposited on : 2020-10-07
Resolution : 3.15 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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	:	2.23.2
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)	:	2.23.2

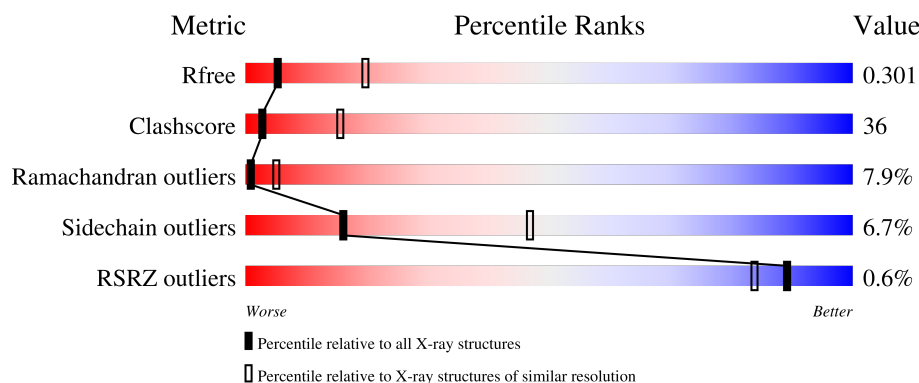
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 ≥ 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	224	<div> <div>%</div> <div> <div></div> <div>43%</div> <div>44%</div> <div>6%</div> <div>7%</div> </div> </div>
1	B	224	<div> <div>39%</div> <div>47%</div> <div>8%</div> <div>5%</div> </div>
1	D	224	<div> <div>44%</div> <div>42%</div> <div>7%</div> <div>7%</div> </div>
1	E	224	<div> <div>%</div> <div>38%</div> <div>48%</div> <div>8%</div> <div>5%</div> </div>
2	C	192	<div> <div>%</div> <div>28%</div> <div>52%</div> <div>7%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	192	 38% 42% 8% 12%
3	G	8	 50% 50%
3	H	8	 25% 62% 12%
3	J	8	 12% 75% 12%
3	K	8	 38% 50% 12%
4	I	4	 25% 50% 25%
5	L	4	 25% 50% 25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10027 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 IgG1 Fc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1666	1058	280	322	6			
1	B	212	Total	C	N	O	S	0	0	0
			1690	1074	283	327	6			
1	D	209	Total	C	N	O	S	0	2	0
			1683	1067	284	326	6			
1	E	212	Total	C	N	O	S	0	0	0
			1690	1074	283	327	6			

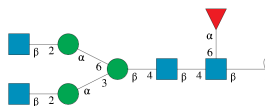
- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	168	Total	C	N	O	S	0	0	0
			1365	869	237	255	4			
2	F	169	Total	C	N	O	S	0	0	0
			1374	874	238	258	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	38	GLN	ASN	engineered mutation	UNP A3RFZ7
C	158	VAL	ILE	engineered mutation	UNP A3RFZ7
C	169	GLN	ASN	engineered mutation	UNP A3RFZ7
F	38	GLN	ASN	engineered mutation	UNP A3RFZ7
F	158	VAL	ILE	engineered mutation	UNP A3RFZ7
F	169	GLN	ASN	engineered mutation	UNP A3RFZ7

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



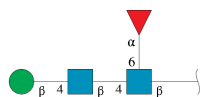
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	8	Total	C	N	O	0	0	0
			99	56	4	39			
3	H	8	Total	C	N	O	0	0	0
			99	56	4	39			
3	J	8	Total	C	N	O	0	0	0
			99	56	4	39			
3	K	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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	I	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	4	Total	C	N	O	0	0	0
			49	28	2	19			

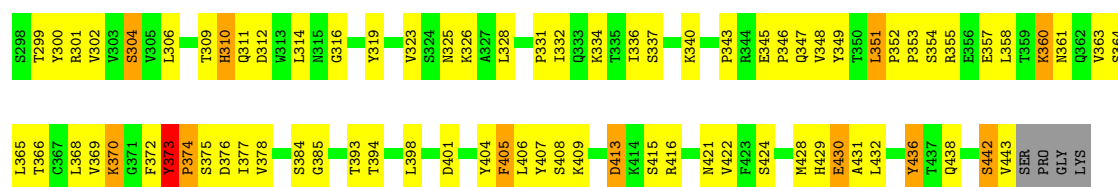
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



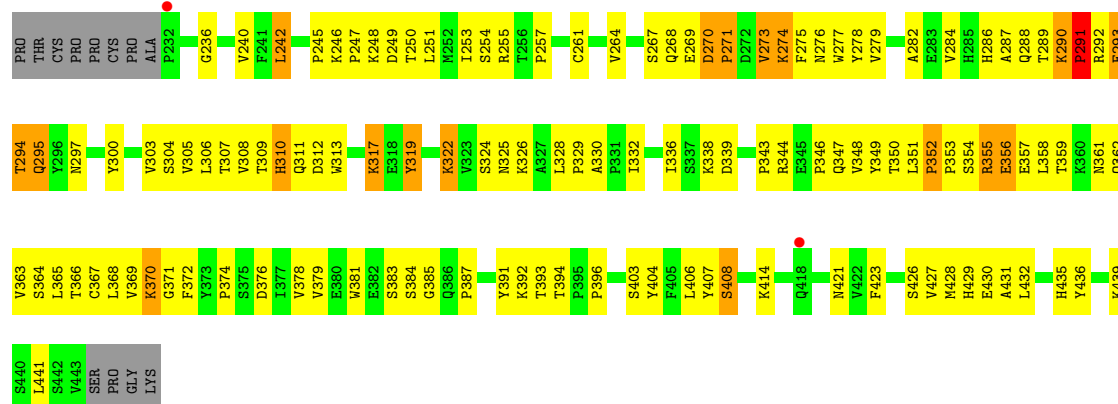
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

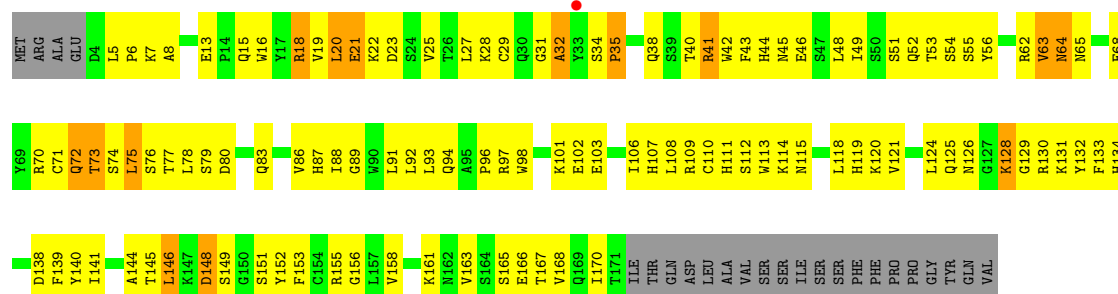
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	O	0	0
			3	3		
7	B	1	Total	O	0	0
			1	1		
7	C	1	Total	O	0	0
			1	1		
7	D	1	Total	O	0	0
			1	1		
7	E	1	Total	O	0	0
			1	1		
7	F	1	Total	O	0	0
			1	1		



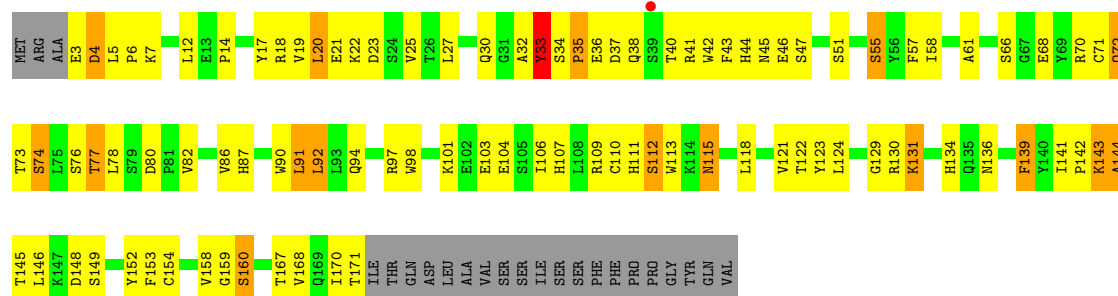
• Molecule 1: IgG1 Fc



• Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III



• Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III



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

Chain G:  50% 50%

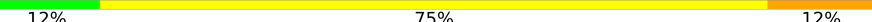


● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  25% 62% 12%



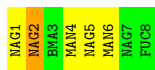
● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  12% 75% 12%



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

Chain K:  38% 50% 12%

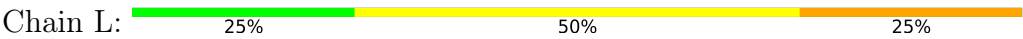


● Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  25% 50% 25%



● Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.69Å 70.11Å 135.41Å 90.00° 119.77° 90.00°	Depositor
Resolution (Å)	60.11 – 3.15 66.94 – 3.15	Depositor EDS
% Data completeness (in resolution range)	93.6 (60.11-3.15) 95.9 (66.94-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???), REFMAC 5.8.0258	Depositor
R, R_{free}	0.269 , 0.303 0.267 , 0.301	Depositor DCC
R_{free} test set	1435 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.832	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	10027	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FUC, NAG, MAN

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	0.47	0/1712	0.71	0/2337
1	B	0.49	0/1737	0.80	0/2371
1	D	0.45	0/1729	0.70	0/2360
1	E	0.45	0/1737	0.82	1/2371 (0.0%)
2	C	0.52	0/1401	0.82	0/1900
2	F	0.43	0/1410	0.78	0/1912
All	All	0.47	0/9726	0.77	1/13251 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	291	PRO	N-CA-CB	-9.67	91.70	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	373	TYR	Peptide

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	1666	0	1628	125	0
1	B	1690	0	1653	126	0
1	D	1683	0	1640	117	0
1	E	1690	0	1653	145	0
2	C	1365	0	1324	126	0
2	F	1374	0	1330	92	0
3	G	99	0	85	0	0
3	H	99	0	85	2	0
3	J	99	0	85	3	0
3	K	99	0	85	2	0
4	I	50	0	43	3	0
5	L	49	0	43	1	0
6	C	28	0	26	1	0
6	F	28	0	26	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
All	All	10027	0	9706	703	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 36.

The worst 5 of 703 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:D:351:LEU:HD12	1:D:352:PRO:CD	1.45	1.46
2:C:20:LEU:HD23	2:C:113:TRP:CD1	1.65	1.30
2:C:20:LEU:CD2	2:C:113:TRP:HD1	1.52	1.22
1:E:242:LEU:CD2	1:E:336:ILE:HB	1.68	1.22
1:B:271:PRO:HB3	1:B:325:ASN:OD1	1.40	1.21

There are no symmetry-related clashes.

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.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/224 (92%)	165 (80%)	29 (14%)	13 (6%)	1	9
1	B	210/224 (94%)	154 (73%)	38 (18%)	18 (9%)	1	4
1	D	209/224 (93%)	174 (83%)	25 (12%)	10 (5%)	2	15
1	E	210/224 (94%)	147 (70%)	40 (19%)	23 (11%)	0	2
2	C	166/192 (86%)	115 (69%)	39 (24%)	12 (7%)	1	6
2	F	167/192 (87%)	122 (73%)	29 (17%)	16 (10%)	0	3
All	All	1169/1280 (91%)	877 (75%)	200 (17%)	92 (8%)	1	5

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	A	271	PRO
1	A	284	VAL
1	A	371	GLY
1	B	273	VAL

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	195/208 (94%)	186 (95%)	9 (5%)	27	60
1	B	198/208 (95%)	182 (92%)	16 (8%)	11	39
1	D	197/208 (95%)	185 (94%)	12 (6%)	18	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	198/208 (95%)	189 (96%)	9 (4%)	27 61
2	C	153/174 (88%)	143 (94%)	10 (6%)	17 48
2	F	154/174 (88%)	137 (89%)	17 (11%)	6 24
All	All	1095/1180 (93%)	1022 (93%)	73 (7%)	16 47

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	20	LEU
2	F	153	PHE
2	F	33	TYR
2	F	91	LEU
1	B	408	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	134	HIS
1	D	429	HIS
2	F	87	HIS
1	E	310	HIS
1	B	347	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](#)

40 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	G	1	3,1	14,14,15	0.42	0	17,19,21	0.37	0
3	NAG	G	2	3	14,14,15	0.22	0	17,19,21	0.50	0
3	BMA	G	3	3	11,11,12	0.98	0	15,15,17	1.09	0
3	MAN	G	4	3	11,11,12	1.25	1 (9%)	15,15,17	1.40	1 (6%)
3	NAG	G	5	3	14,14,15	0.73	1 (7%)	17,19,21	1.24	2 (11%)
3	MAN	G	6	3	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
3	NAG	G	7	3	14,14,15	0.28	0	17,19,21	0.49	0
3	FUC	G	8	3	10,10,11	0.97	0	14,14,16	1.09	2 (14%)
3	NAG	H	1	3,1	14,14,15	1.12	1 (7%)	17,19,21	1.58	1 (5%)
3	NAG	H	2	3	14,14,15	0.33	0	17,19,21	1.41	2 (11%)
3	BMA	H	3	3	11,11,12	0.54	0	15,15,17	1.17	1 (6%)
3	MAN	H	4	3	11,11,12	0.54	0	15,15,17	1.21	2 (13%)
3	NAG	H	5	3	14,14,15	0.75	1 (7%)	17,19,21	1.00	2 (11%)
3	MAN	H	6	3	11,11,12	0.73	0	15,15,17	0.89	1 (6%)
3	NAG	H	7	3	14,14,15	0.21	0	17,19,21	0.45	0
3	FUC	H	8	3	10,10,11	0.99	0	14,14,16	1.01	0
4	NAG	I	1	4,2	14,14,15	0.50	0	17,19,21	0.39	0
4	NAG	I	2	4	14,14,15	0.29	0	17,19,21	1.42	2 (11%)
4	BMA	I	3	4	11,11,12	1.16	1 (9%)	15,15,17	1.29	2 (13%)
4	MAN	I	4	4	11,11,12	1.54	3 (27%)	15,15,17	2.79	4 (26%)
3	NAG	J	1	3,1	14,14,15	0.38	0	17,19,21	0.35	0
3	NAG	J	2	3	14,14,15	0.20	0	17,19,21	0.49	0
3	BMA	J	3	3	11,11,12	0.64	0	15,15,17	1.02	1 (6%)
3	MAN	J	4	3	11,11,12	1.17	1 (9%)	15,15,17	1.19	1 (6%)
3	NAG	J	5	3	14,14,15	0.63	1 (7%)	17,19,21	1.10	2 (11%)
3	MAN	J	6	3	11,11,12	0.62	0	15,15,17	1.13	2 (13%)
3	NAG	J	7	3	14,14,15	0.25	0	17,19,21	0.51	0
3	FUC	J	8	3	10,10,11	0.90	0	14,14,16	1.10	2 (14%)
3	NAG	K	1	3,1	14,14,15	1.06	1 (7%)	17,19,21	1.64	1 (5%)
3	NAG	K	2	3	14,14,15	0.26	0	17,19,21	1.41	2 (11%)
3	BMA	K	3	3	11,11,12	0.65	0	15,15,17	0.83	0
3	MAN	K	4	3	11,11,12	0.78	0	15,15,17	1.34	3 (20%)
3	NAG	K	5	3	14,14,15	0.88	1 (7%)	17,19,21	1.04	1 (5%)
3	MAN	K	6	3	11,11,12	1.01	2 (18%)	15,15,17	1.35	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	K	7	3	14,14,15	0.25	0	17,19,21	0.38	0
3	FUC	K	8	3	10,10,11	0.99	0	14,14,16	0.92	0
5	NAG	L	1	5,2	14,14,15	0.52	0	17,19,21	0.43	0
5	NAG	L	2	5	14,14,15	0.36	0	17,19,21	1.79	3 (17%)
5	BMA	L	3	5	11,11,12	1.10	1 (9%)	15,15,17	1.18	2 (13%)
5	FUC	L	4	5	10,10,11	1.14	1 (10%)	14,14,16	1.68	4 (28%)

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	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	NAG	G	5	3	-	2/6/23/26	0/1/1/1
3	MAN	G	6	3	-	2/2/19/22	0/1/1/1
3	NAG	G	7	3	-	1/6/23/26	0/1/1/1
3	FUC	G	8	3	-	-	0/1/1/1
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	5/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
3	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	NAG	H	5	3	-	3/6/23/26	0/1/1/1
3	MAN	H	6	3	-	0/2/19/22	0/1/1/1
3	NAG	H	7	3	-	2/6/23/26	0/1/1/1
3	FUC	H	8	3	-	-	0/1/1/1
4	NAG	I	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	5/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	1/2/19/22	0/1/1/1
3	NAG	J	5	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	J	6	3	-	2/2/19/22	0/1/1/1
3	NAG	J	7	3	-	2/6/23/26	0/1/1/1
3	FUC	J	8	3	-	-	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	5/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	MAN	K	4	3	-	0/2/19/22	0/1/1/1
3	NAG	K	5	3	-	1/6/23/26	0/1/1/1
3	MAN	K	6	3	-	2/2/19/22	0/1/1/1
3	NAG	K	7	3	-	2/6/23/26	0/1/1/1
3	FUC	K	8	3	-	-	0/1/1/1
5	NAG	L	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	L	2	5	-	5/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	FUC	L	4	5	-	-	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	4.08	1.50	1.43
3	K	1	NAG	O5-C1	3.86	1.49	1.43
3	J	4	MAN	O5-C1	-3.15	1.38	1.43
3	K	5	NAG	O5-C1	-3.11	1.38	1.43
3	G	4	MAN	O5-C1	-3.11	1.38	1.43

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	4	MAN	C1-O5-C5	8.96	124.33	112.19
3	K	1	NAG	C1-O5-C5	6.40	120.87	112.19
3	H	1	NAG	C1-O5-C5	6.15	120.53	112.19
5	L	2	NAG	C2-N2-C7	5.44	130.66	122.90
3	G	4	MAN	O2-C2-C3	-4.78	100.56	110.14

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	2	NAG	C4-C5-C6-O6

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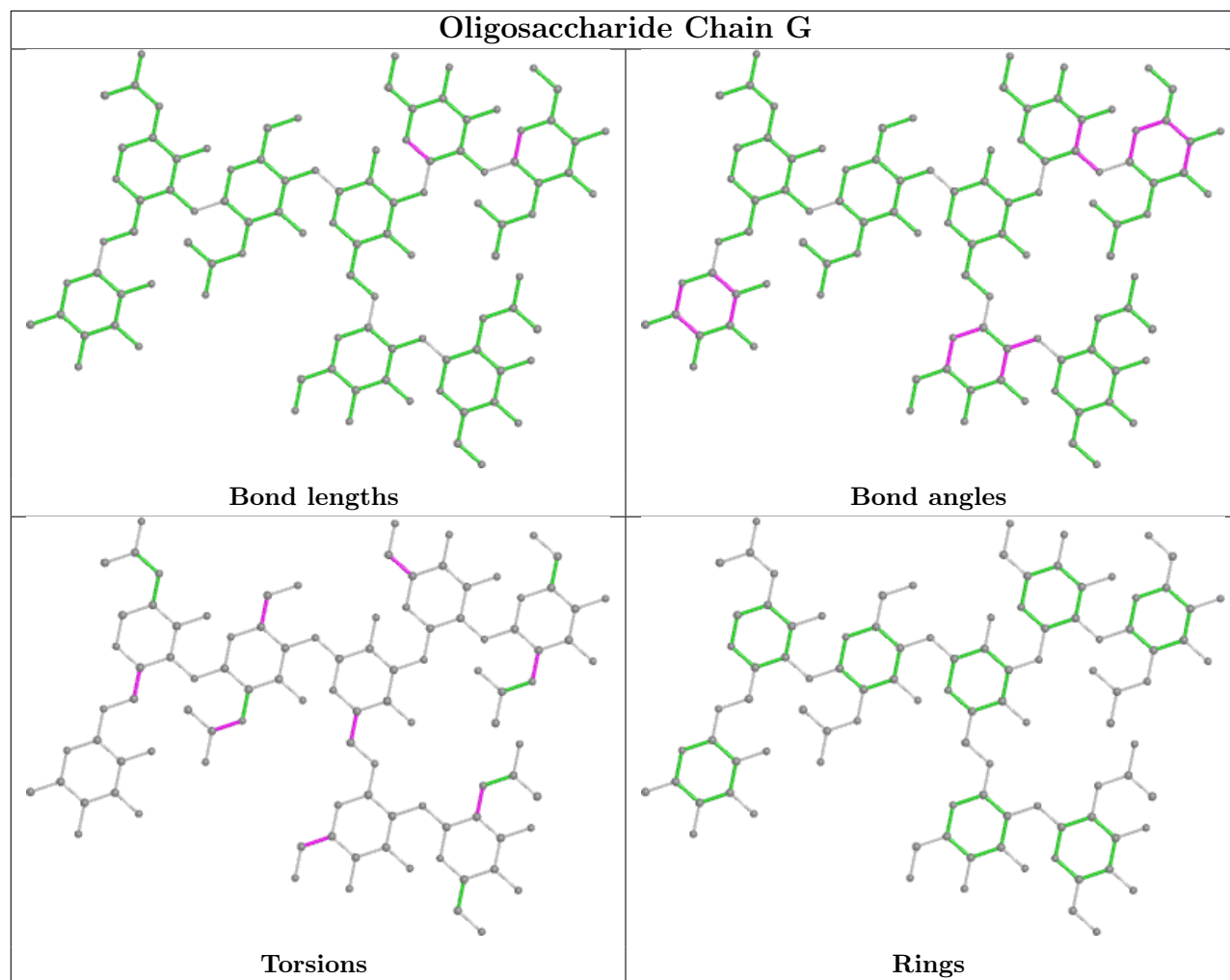
Mol	Chain	Res	Type	Atoms
3	K	2	NAG	C4-C5-C6-O6
3	H	7	NAG	O5-C5-C6-O6
3	J	7	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6

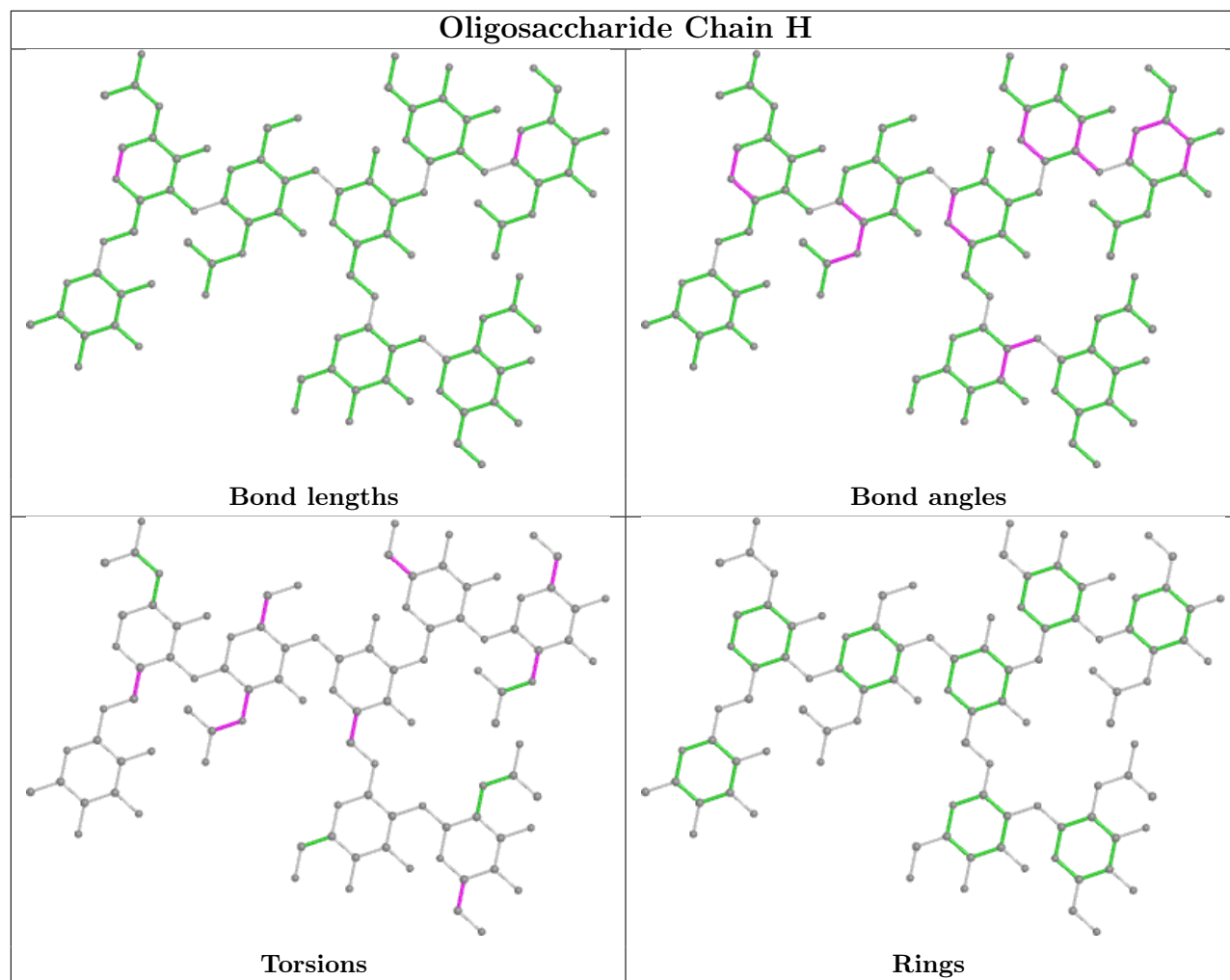
There are no ring outliers.

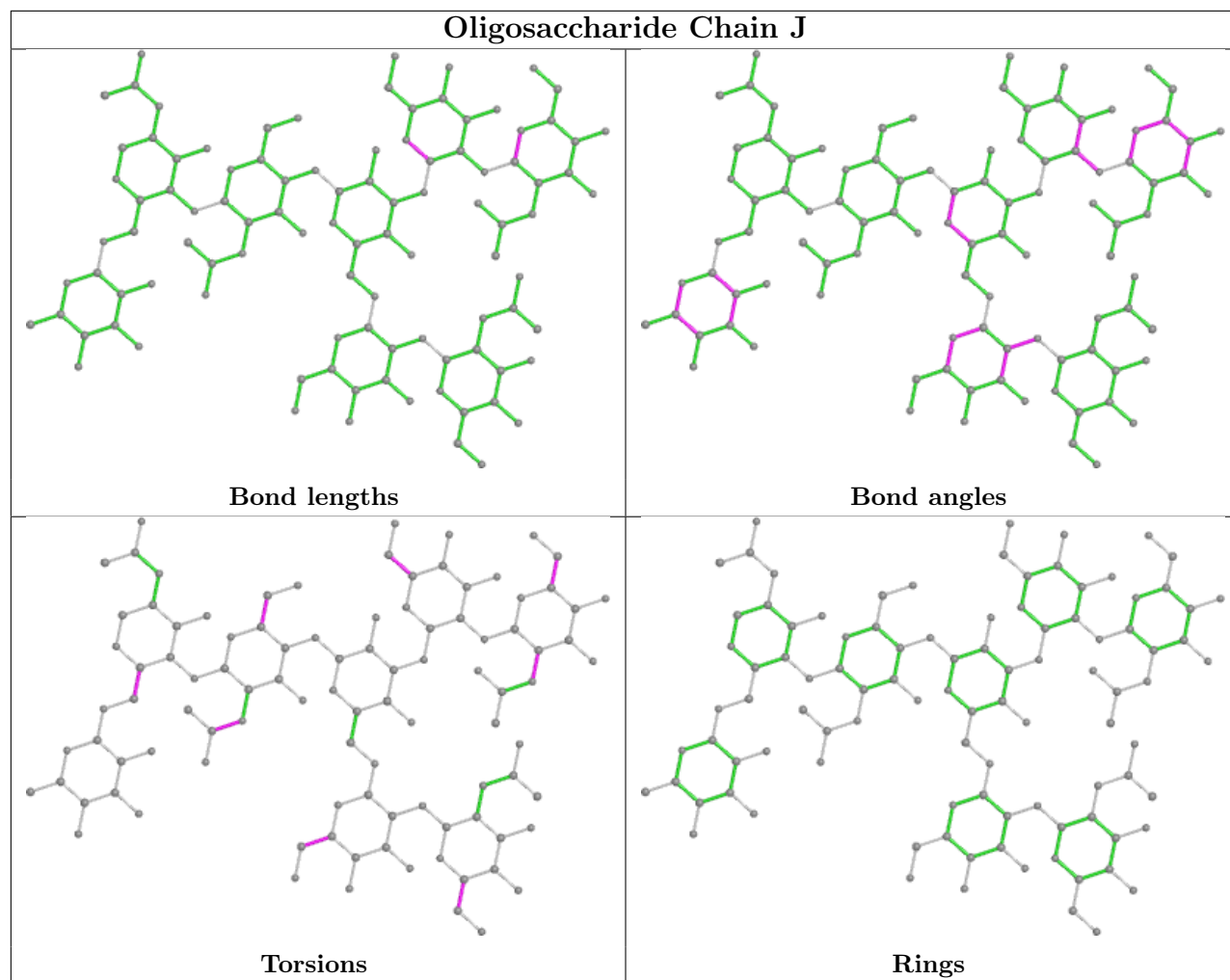
7 monomers are involved in 11 short contacts:

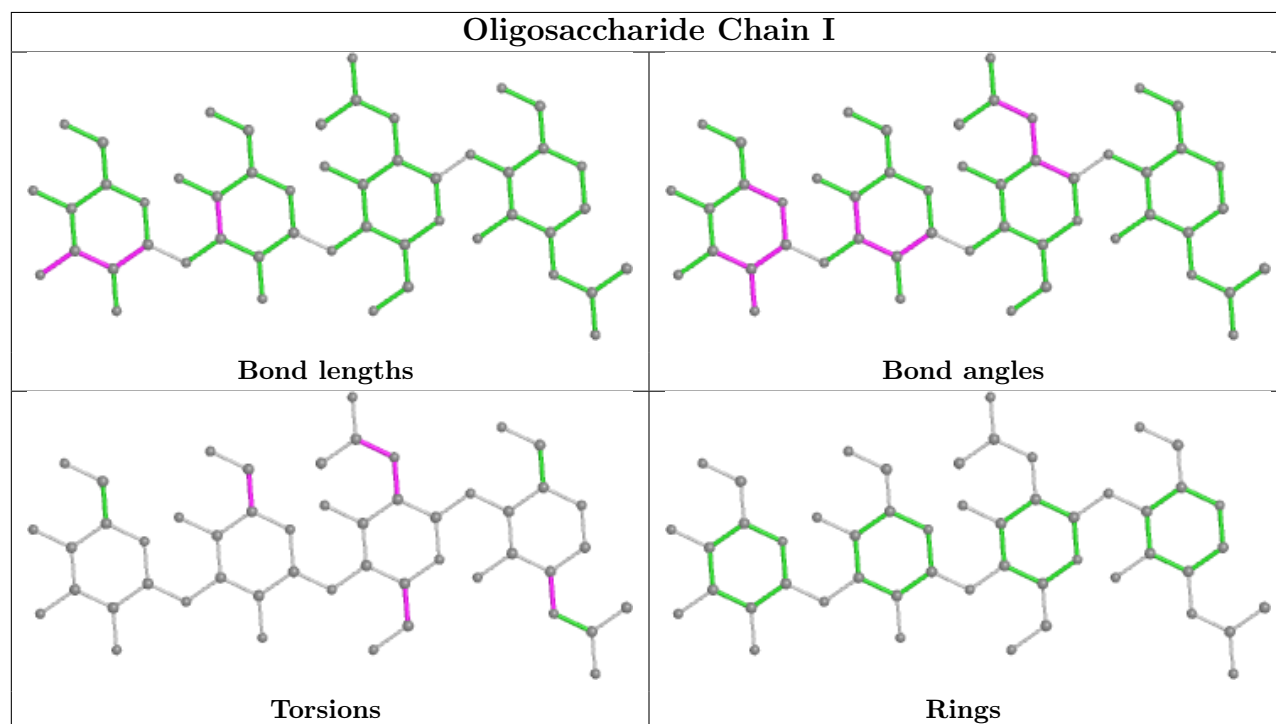
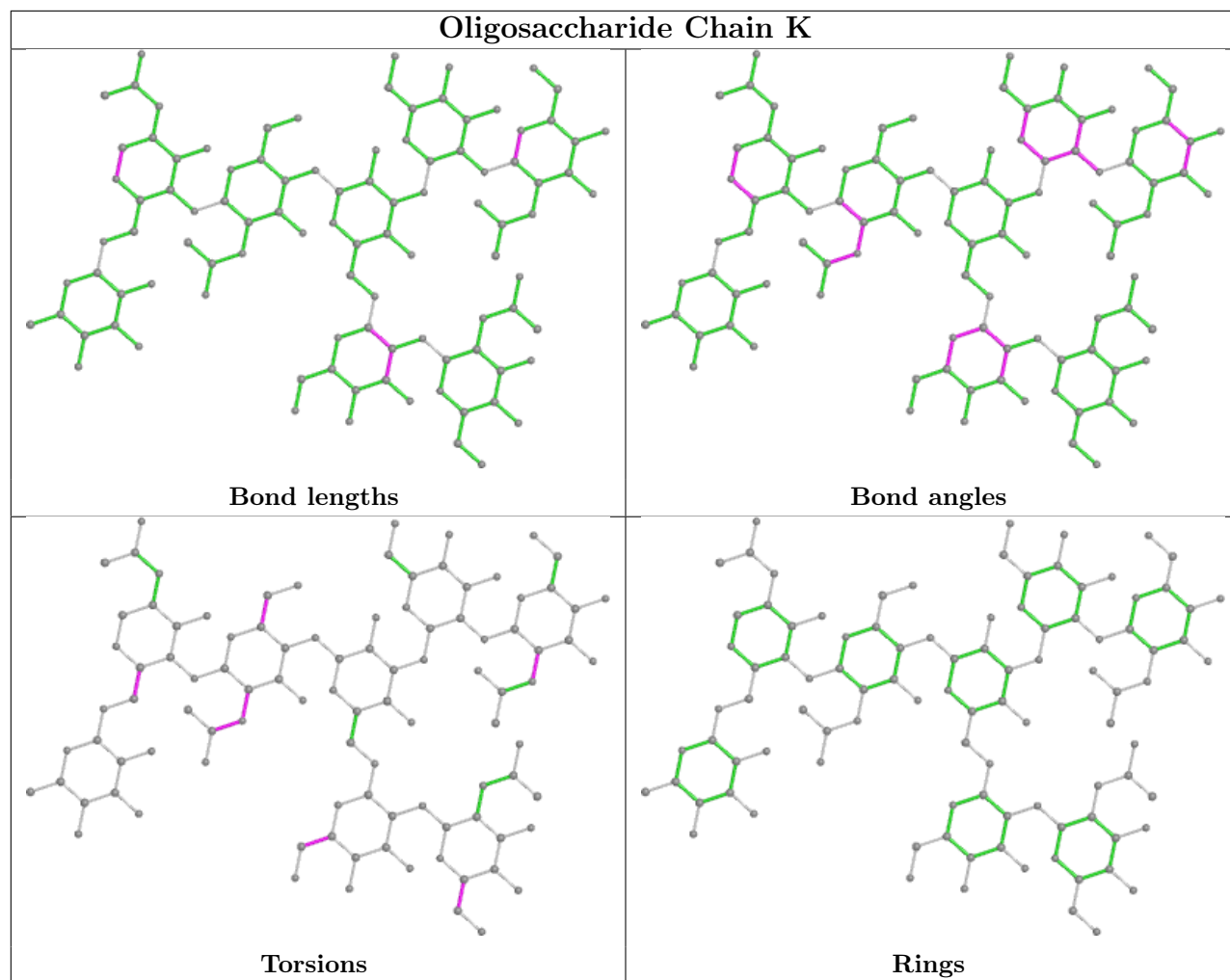
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	2	NAG	1	0
3	H	2	NAG	2	0
3	K	2	NAG	2	0
3	J	2	NAG	1	0
3	J	1	NAG	1	0
3	J	5	NAG	1	0
4	I	2	NAG	3	0

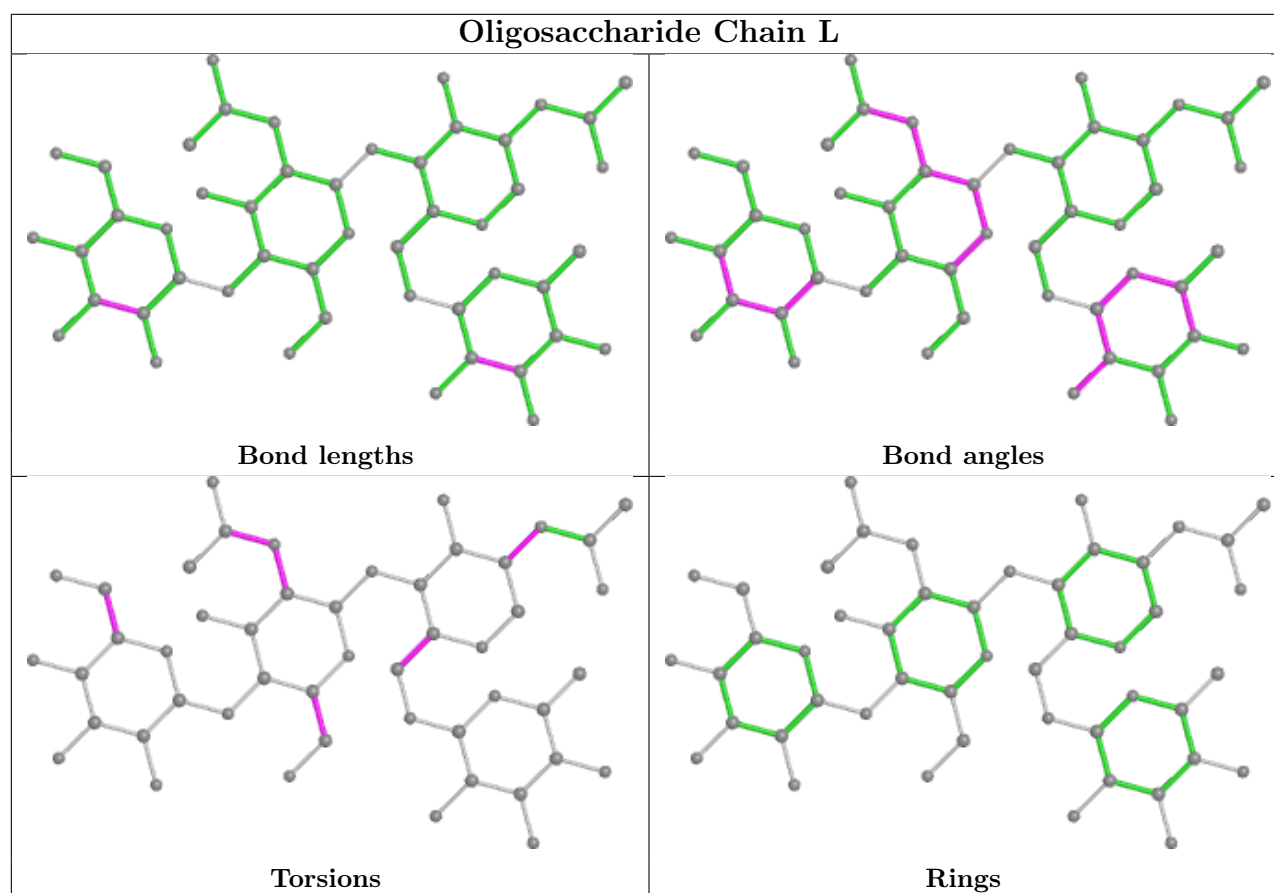
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
6	NAG	F	202	2	14,14,15	0.37	0	17,19,21	0.37	0
6	NAG	C	202	2	14,14,15	0.65	1 (7%)	17,19,21	0.78	1 (5%)
6	NAG	F	201	2	14,14,15	0.46	0	17,19,21	1.76	3 (17%)
6	NAG	C	201	2	14,14,15	0.54	0	17,19,21	1.08	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
6	NAG	F	202	2	-	2/6/23/26	0/1/1/1
6	NAG	C	202	2	-	4/6/23/26	0/1/1/1
6	NAG	F	201	2	-	3/6/23/26	0/1/1/1
6	NAG	C	201	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	202	NAG	C1-C2	2.03	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	201	NAG	C1-O5-C5	5.93	120.23	112.19
6	F	201	NAG	C3-C4-C5	3.01	115.61	110.24
6	C	201	NAG	C1-O5-C5	2.89	116.11	112.19
6	C	202	NAG	C2-N2-C7	2.64	126.67	122.90
6	F	201	NAG	O5-C5-C4	2.29	116.41	110.83

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	202	NAG	C3-C2-N2-C7
6	C	201	NAG	C4-C5-C6-O6
6	F	202	NAG	O5-C5-C6-O6
6	C	201	NAG	O5-C5-C6-O6
6	F	201	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	202	NAG	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, 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	A	209/224 (93%)	-0.16	3 (1%) 75 63	45, 69, 103, 126	0
1	B	212/224 (94%)	-0.11	0 100 100	42, 65, 103, 118	0
1	D	209/224 (93%)	-0.24	0 100 100	53, 68, 89, 98	0
1	E	212/224 (94%)	-0.20	2 (0%) 84 75	49, 80, 120, 133	0
2	C	168/192 (87%)	-0.13	1 (0%) 89 84	67, 80, 109, 128	0
2	F	169/192 (88%)	0.05	1 (0%) 89 84	63, 80, 109, 127	0
All	All	1179/1280 (92%)	-0.14	7 (0%) 89 84	42, 74, 109, 133	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	GLY	3.7
2	C	33	TYR	2.6
1	E	232	PRO	2.5
1	A	337	SER	2.4
1	A	280	ASN	2.3

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](#)

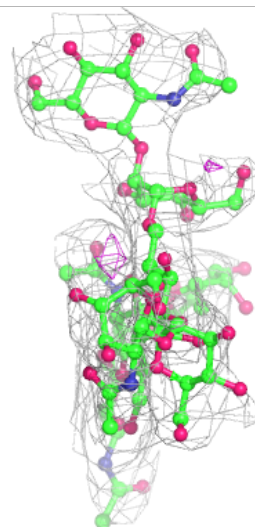
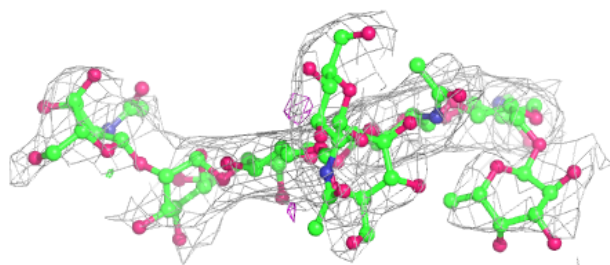
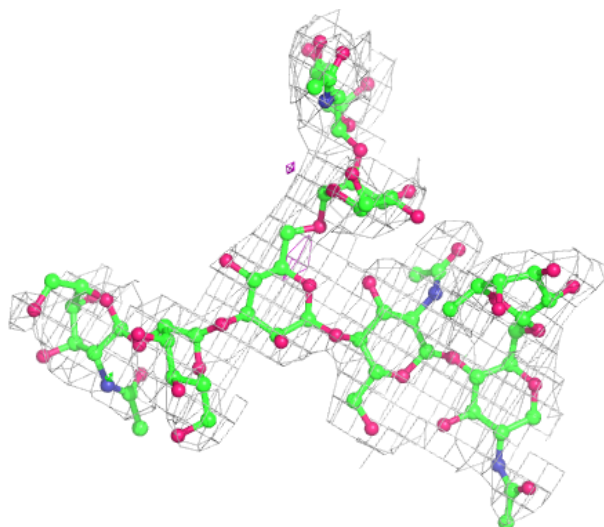
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	I	4	11/12	0.65	0.21	89,105,115,118	0
3	NAG	K	5	14/15	0.74	0.26	105,112,116,121	0
3	NAG	G	5	14/15	0.75	0.29	99,103,106,109	0
5	FUC	L	4	10/11	0.78	0.34	85,99,109,112	0
3	NAG	J	5	14/15	0.79	0.34	111,116,123,124	0
3	FUC	G	8	10/11	0.79	0.30	85,92,97,99	0
3	NAG	H	5	14/15	0.79	0.31	85,101,106,106	0
3	FUC	H	8	10/11	0.79	0.27	85,91,97,99	0
3	MAN	K	4	11/12	0.82	0.30	94,100,101,108	0
5	BMA	L	3	11/12	0.83	0.17	99,101,102,103	0
4	BMA	I	3	11/12	0.84	0.13	68,79,86,98	0
3	NAG	K	7	14/15	0.85	0.21	85,88,91,92	0
3	FUC	K	8	10/11	0.85	0.30	92,96,98,103	0
5	NAG	L	1	14/15	0.86	0.16	68,83,91,94	0
3	MAN	G	4	11/12	0.86	0.20	92,98,101,102	0
3	NAG	G	7	14/15	0.86	0.18	77,85,91,91	0
3	NAG	J	7	14/15	0.87	0.26	61,62,65,65	0
3	NAG	J	1	14/15	0.87	0.20	56,70,83,85	0
3	FUC	J	8	10/11	0.88	0.24	79,88,99,101	0
3	MAN	G	6	11/12	0.88	0.21	68,81,82,87	0
3	NAG	H	1	14/15	0.89	0.18	49,61,77,81	0
3	NAG	G	1	14/15	0.89	0.19	28,50,75,77	0
4	NAG	I	2	14/15	0.90	0.16	58,70,75,78	0
5	NAG	L	2	14/15	0.90	0.16	80,88,90,93	0
3	MAN	H	4	11/12	0.90	0.15	66,76,84,84	0
3	NAG	K	1	14/15	0.90	0.18	55,63,79,88	0
3	MAN	J	4	11/12	0.91	0.18	92,94,100,107	0
3	NAG	G	2	14/15	0.91	0.16	42,49,54,67	0
3	MAN	K	6	11/12	0.91	0.18	76,83,92,93	0
3	MAN	J	6	11/12	0.91	0.32	54,57,63,69	0
3	NAG	H	2	14/15	0.92	0.16	43,46,68,69	0
3	NAG	K	2	14/15	0.92	0.20	41,50,64,65	0
3	BMA	K	3	11/12	0.93	0.15	57,64,78,83	0
3	BMA	H	3	11/12	0.93	0.13	50,58,66,69	0
4	NAG	I	1	14/15	0.93	0.18	15,23,49,56	0
3	BMA	J	3	11/12	0.93	0.16	66,74,84,92	0
3	BMA	G	3	11/12	0.93	0.16	60,68,77,80	0
3	NAG	H	7	14/15	0.94	0.19	43,51,72,75	0
3	NAG	J	2	14/15	0.94	0.20	66,72,80,82	0
3	MAN	H	6	11/12	0.94	0.14	38,43,54,58	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.

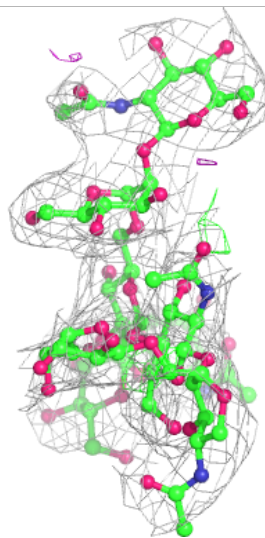
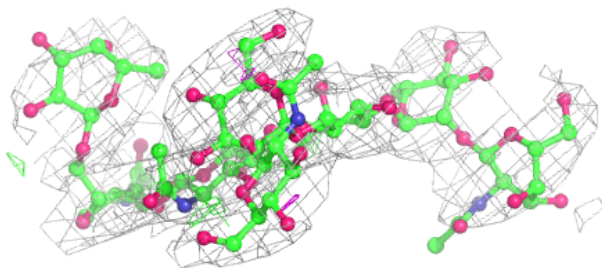
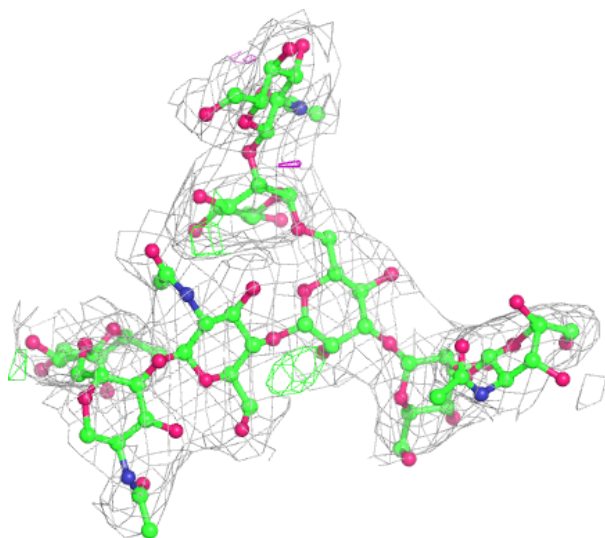
Electron density around Chain G:

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



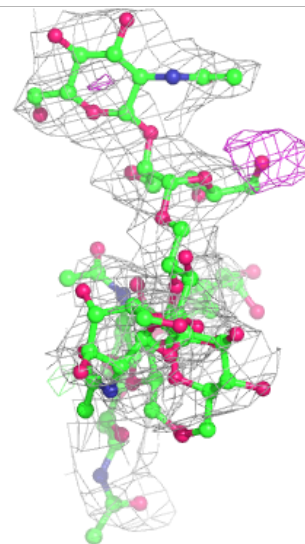
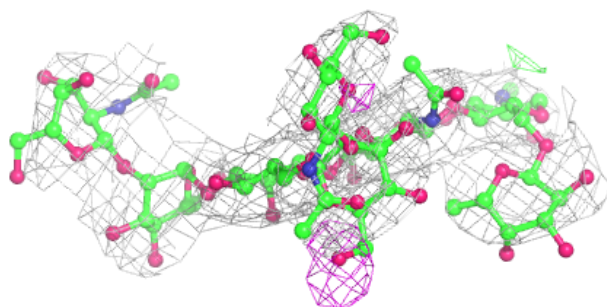
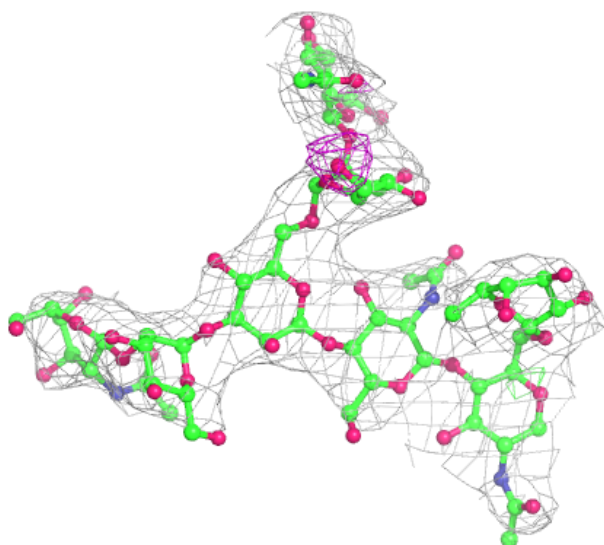
Electron density around Chain H:

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



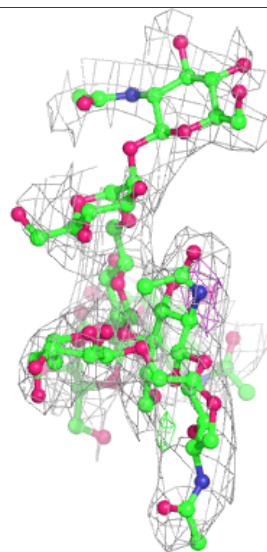
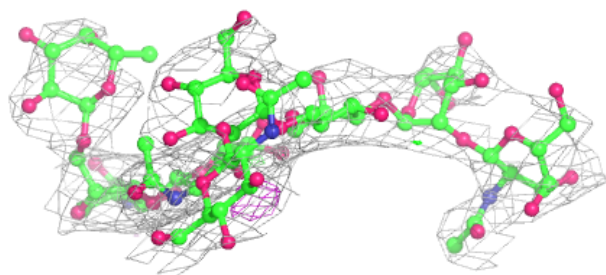
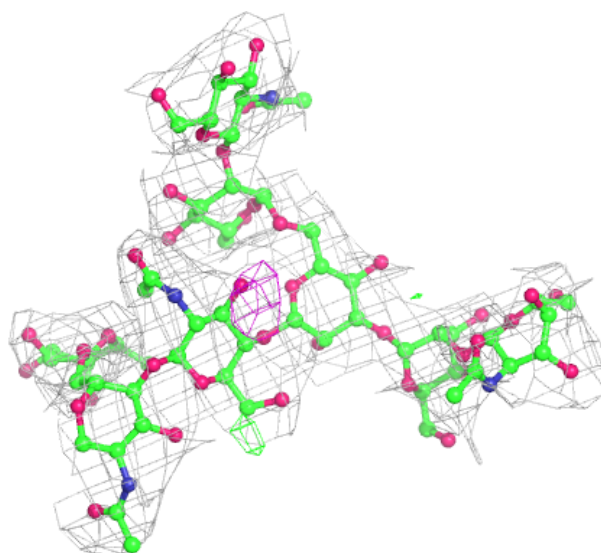
Electron density around Chain J:

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and green (positive)



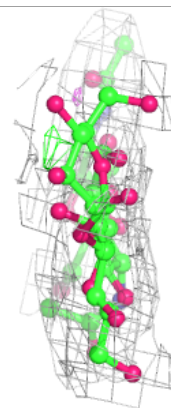
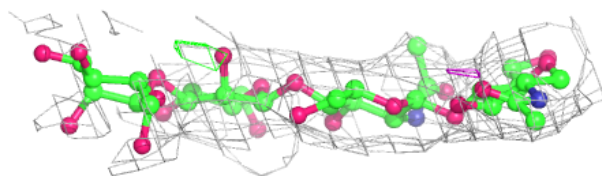
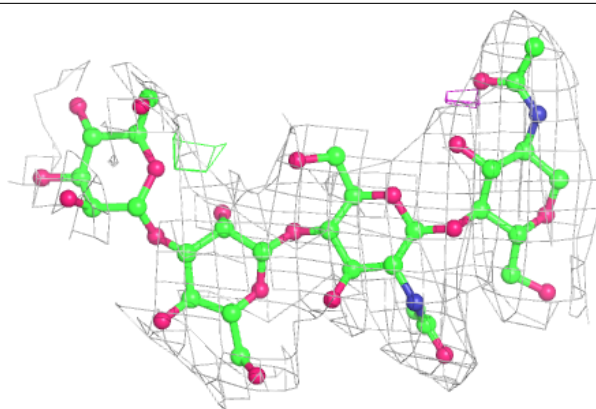
Electron density around Chain K:

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and green (positive)

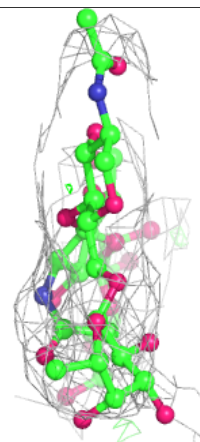
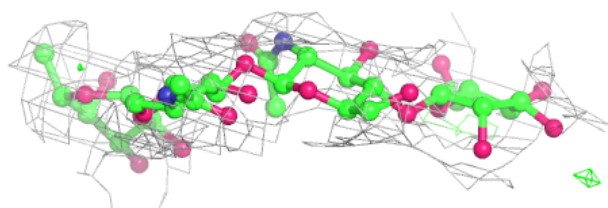
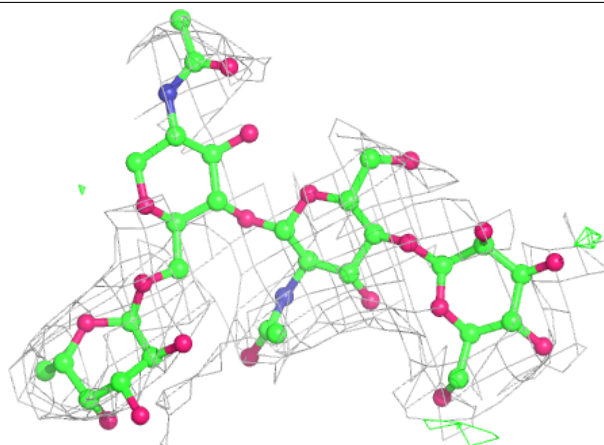


Electron density around Chain I:

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

**Electron density around Chain 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, 95th 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 ²)	Q<0.9
6	NAG	C	201	14/15	0.56	0.37	86,97,114,119	0
6	NAG	F	202	14/15	0.65	0.30	73,90,106,110	0
6	NAG	C	202	14/15	0.72	0.28	69,79,90,92	0
6	NAG	F	201	14/15	0.76	0.24	91,102,117,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.