



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:47 AM UTC

PDB ID : 5U7M / pdb_00005u7m
Title : Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer Bound to Small Molecule HIV-1 Entry Inhibitor BMS-378806 in Complex with Human Antibodies PGT122 and 35O22 at 3.8 Angstrom
Authors : Pancera, M.; Lai, Y.-T.; Kwong, P.D.
Deposited on : 2016-12-12
Resolution : 3.02 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

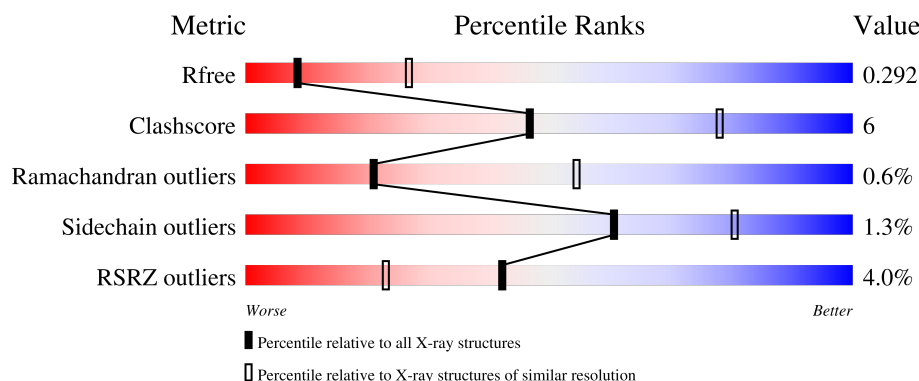
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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.



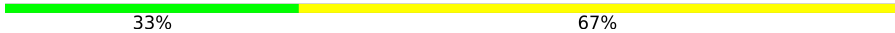
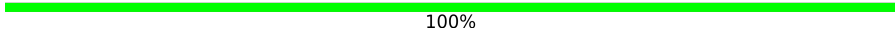
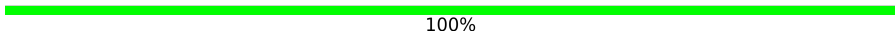
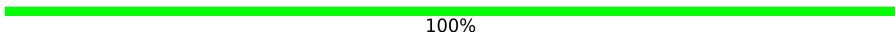
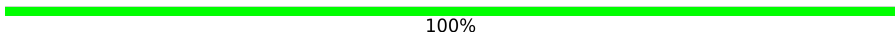
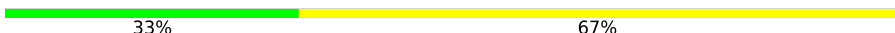
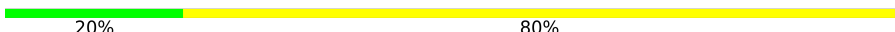
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	B	153	
2	D	243	
3	E	216	
4	G	481	

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Mol	Chain	Length	Quality of chain
5	H	235	
6	L	213	
7	A	7	
8	C	3	
8	S	3	
9	F	5	
10	I	2	
10	J	2	
10	M	2	
10	N	2	
10	P	2	
10	Q	2	
10	R	2	
11	K	6	
12	O	10	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 12026 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S5
B	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 2 is a protein called 35O22 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			

- Molecule 3 is a protein called 35O22 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	442	Total	C	N	O	S	0	0	0
			3472	2183	614	648	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S5
G	501	CYS	ALA	engineered mutation	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	509	ARG	GLU	engineered mutation	UNP Q2N0S5
G	510	ARG	LYS	engineered mutation	UNP Q2N0S5
G	512	ARG	ALA	engineered mutation	UNP Q2N0S5
G	513	ARG	VAL	engineered mutation	UNP Q2N0S5

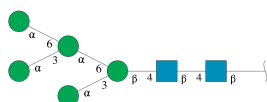
- Molecule 5 is a protein called PGT122 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

- Molecule 6 is a protein called PGT122 FAB LIGHT CHAIN.

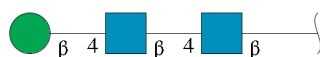
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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
7	A	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 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.



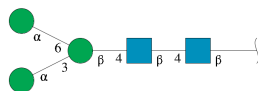
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-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.



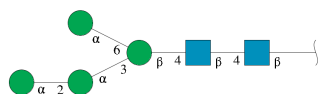
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



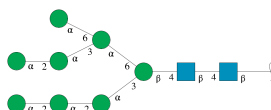
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-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.



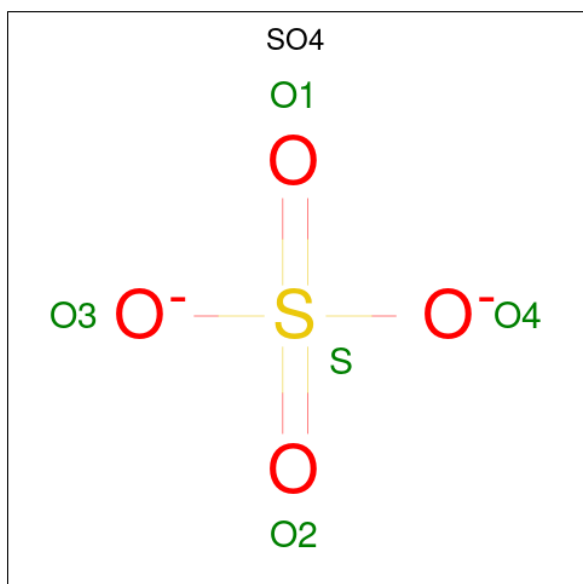
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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
12	O	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 13 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



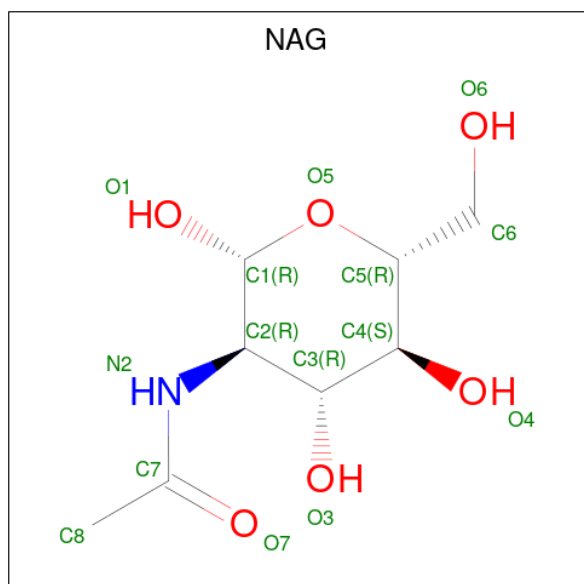
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	G	1	Total	O	S	0	0
			5	4	1		
13	G	1	Total	O	S	0	0
			5	4	1		
13	G	1	Total	O	S	0	0
			5	4	1		
13	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



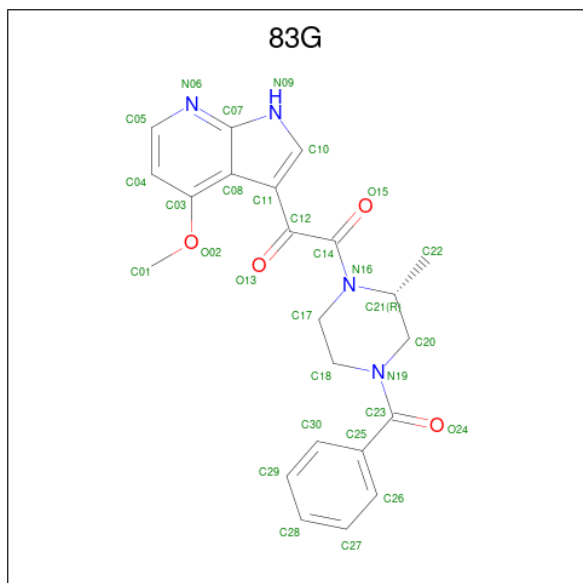
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 15 is 1-[(2R)-4-(benzenecarbonyl)-2-methylpiperazin-1-yl]-2-(4-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)ethane-1,2-dione (CCD ID: 83G) (formula: C₂₂H₂₂N₄O₄).

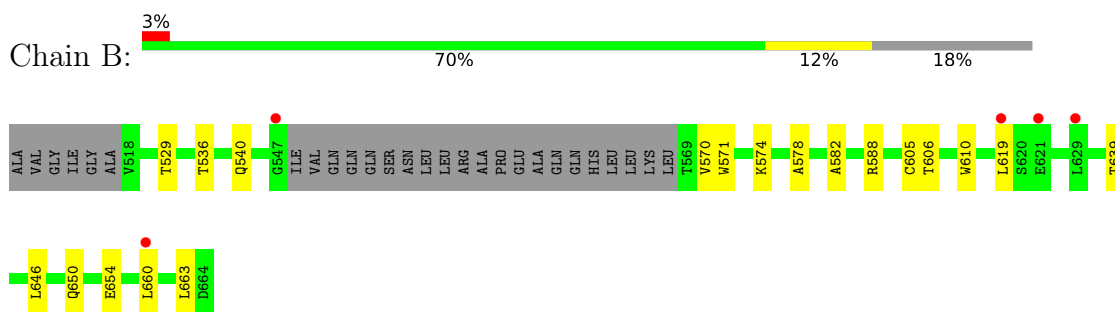


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	G	1	Total	C	N	O	0	0
			30	22	4	4		

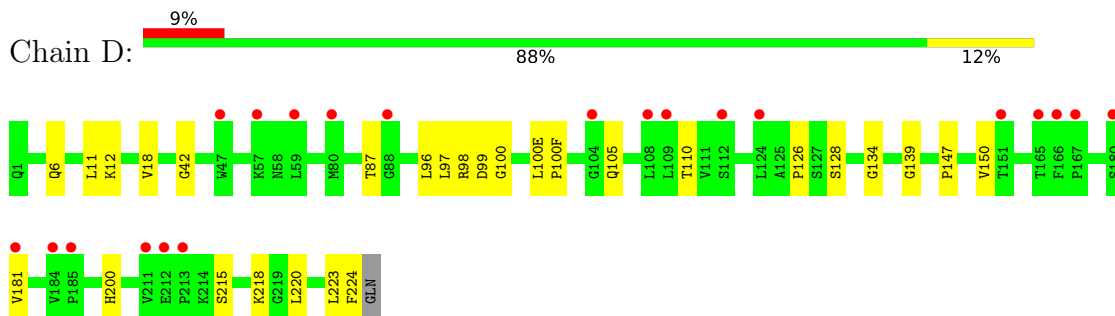
3 Residue-property plots [i](#)

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.

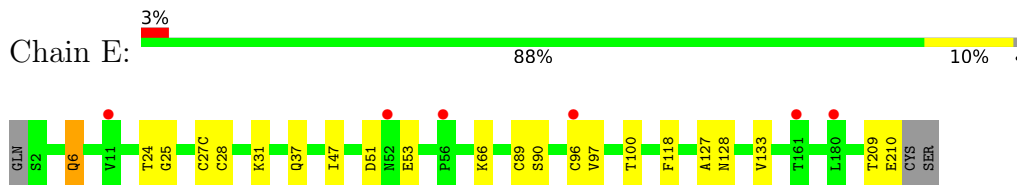
- Molecule 1: Envelope glycoprotein gp160



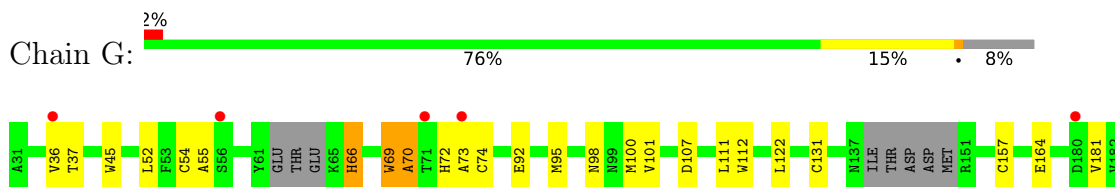
- Molecule 2: 35O22 FAB HEAVY CHAIN

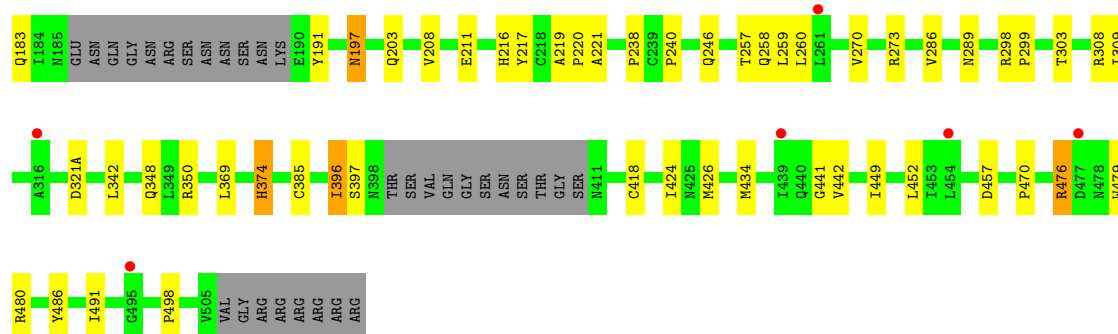


- Molecule 3: 35O22 FAB LIGHT CHAIN

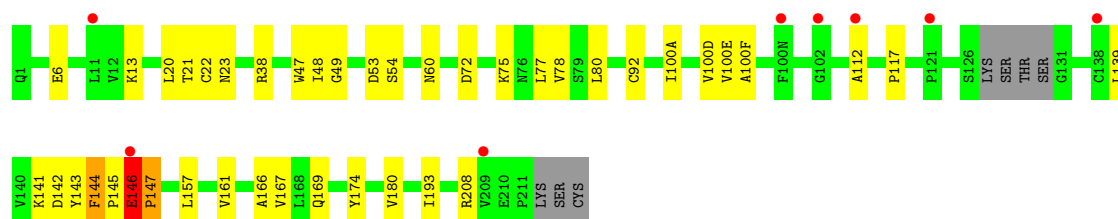
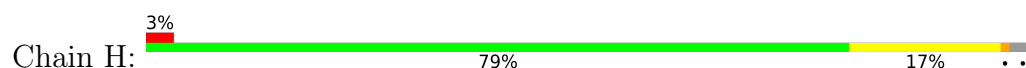


- Molecule 4: Envelope glycoprotein gp160

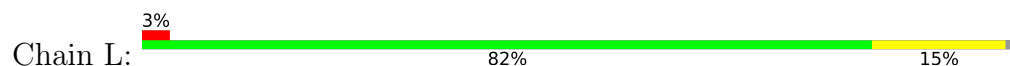




• Molecule 5: PGT122 FAB HEAVY CHAIN



• Molecule 6: PGT122 FAB LIGHT CHAIN



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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



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



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

Chain S:  100%

MAG1
MAG2
EM13

- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-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 F:  60% 40%

MAG1
MAG2
EM13
MAN4
MAN5

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

NAG1
NAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

NAG1
NAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

NAG1
NAG2

- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-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 K:  33% 67%

NAG1
NAG2
BNA3
MAN4
MAN5
MAN6

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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:  20% 80%

NAG1
NAG2
BNA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	129.19Å 129.19Å 312.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.82 – 3.02 40.82 – 3.02	Depositor EDS
% Data completeness (in resolution range)	51.7 (40.82-3.02) 51.7 (40.82-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.245 , 0.289 0.246 , 0.292	Depositor DCC
R_{free} test set	1526 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.096 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12026	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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, NAG, MAN, 83G, SO4

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	B	0.08	0/1019	0.25	0/1382
2	D	0.08	0/1880	0.25	0/2560
3	E	0.09	0/1659	0.29	0/2269
4	G	0.09	0/3544	0.30	0/4811
5	H	0.10	0/1789	0.35	3/2443 (0.1%)
6	L	0.08	0/1619	0.25	0/2217
All	All	0.09	0/11510	0.29	3/15682 (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
5	H	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	146	GLU	C-N-CD	-6.24	106.87	120.60
5	H	146	GLU	CA-C-N	5.67	140.61	127.00
5	H	146	GLU	C-N-CA	5.67	140.61	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	H	144	PHE	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	B	1001	0	975	17	0
2	D	1832	0	1806	15	0
3	E	1615	0	1542	13	0
4	G	3472	0	3404	50	0
5	H	1742	0	1715	27	0
6	L	1577	0	1518	23	0
7	A	83	0	70	1	0
8	C	39	0	34	1	0
8	S	39	0	34	0	0
9	F	61	0	52	0	0
10	I	28	0	25	1	0
10	J	28	0	25	1	0
10	M	28	0	25	0	0
10	N	28	0	25	0	0
10	P	28	0	25	0	0
10	Q	28	0	25	0	0
10	R	28	0	25	0	0
11	K	72	0	61	1	0
12	O	116	0	97	1	0
13	B	5	0	0	1	0
13	G	15	0	0	0	0
13	L	5	0	0	0	0
14	B	42	0	39	1	0
14	G	70	0	65	1	0
14	H	14	0	13	0	0
15	G	30	0	0	1	0
All	All	12026	0	11600	134	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 6.

All (134) 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)
6:L:39:ARG:NH1	6:L:81:GLY:O	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.69	0.75
1:B:536:THR:O	1:B:540:GLN:NE2	2.27	0.68
6:L:61:ARG:NH1	6:L:77:SER:O	2.28	0.66
6:L:19:ALA:HB3	6:L:75:ILE:HB	1.78	0.66
3:E:37:GLN:HB2	3:E:47:ILE:HD11	1.77	0.65
1:B:574:LYS:NZ	4:G:107:ASP:OD2	2.30	0.65
2:D:6:GLN:H	2:D:105:GLN:HE22	1.46	0.64
4:G:219:ALA:O	4:G:246:GLN:NE2	2.31	0.63
5:H:22:CYS:HB3	5:H:78:VAL:HB	1.81	0.62
1:B:588:ARG:NH2	13:B:701:SO4:O3	2.33	0.61
6:L:150:LYS:HB2	6:L:193:SER:HB2	1.83	0.61
4:G:350:ARG:NH2	4:G:396:ILE:O	2.30	0.60
4:G:66:HIS:HA	4:G:72:HIS:HE1	1.66	0.59
6:L:47:ILE:HG22	6:L:48:ILE:HG13	1.83	0.59
3:E:127:ALA:H	3:E:128:ASN:HA	1.68	0.59
5:H:157:LEU:HD21	5:H:180:VAL:HG11	1.84	0.59
1:B:605:CYS:HA	4:G:37:THR:HG22	1.85	0.58
1:B:650:GLN:NE2	1:B:654:GLU:OE1	2.37	0.58
10:I:2:NAG:H3	10:I:2:NAG:H83	1.85	0.58
7:A:2:NAG:H3	7:A:2:NAG:H83	1.85	0.58
4:G:424:ILE:HD11	4:G:434:MET:HE2	1.86	0.58
6:L:13:VAL:HG21	6:L:19:ALA:HA	1.86	0.57
6:L:181:LEU:HD22	6:L:185:GLN:HG2	1.87	0.57
4:G:270:VAL:HG12	4:G:289:ASN:H	1.69	0.57
4:G:70:ALA:H	4:G:111:LEU:HD22	1.69	0.57
5:H:47:TRP:O	5:H:60:ASN:ND2	2.37	0.57
2:D:87:THR:HG23	2:D:110:THR:HA	1.86	0.56
4:G:101:VAL:HG11	4:G:480:ARG:HG3	1.88	0.56
14:G:631:NAG:H83	14:G:631:NAG:H3	1.87	0.56
4:G:183:GLN:HA	4:G:191:TYR:HA	1.89	0.55
4:G:258:GLN:HG2	4:G:470:PRO:HB2	1.89	0.55
6:L:184:GLU:O	6:L:188:SER:OG	2.21	0.54
5:H:143:TYR:HE1	5:H:146:GLU:HB2	1.71	0.54
2:D:128:SER:HB2	2:D:220:LEU:HB2	1.90	0.54
6:L:139:ASP:H	6:L:172:LYS:HG3	1.72	0.54
3:E:127:ALA:N	3:E:128:ASN:HA	2.23	0.53
5:H:100(D):VAL:HA	12:O:2:NAG:H2	1.90	0.53
2:D:12:LYS:HG3	2:D:18:VAL:HB	1.89	0.53
2:D:99:ASP:OD1	2:D:100:GLY:N	2.41	0.53
4:G:45:TRP:HB3	4:G:491:ILE:HD13	1.91	0.53
1:B:582:ALA:HB1	4:G:221:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:426:MET:HE3	15:G:657:83G:C10	2.38	0.52
4:G:298:ARG:NH2	4:G:441:GLY:O	2.42	0.52
4:G:197:ASN:OD1	10:J:1:NAG:N2	2.43	0.52
4:G:122:LEU:HD11	4:G:203:GLN:HB2	1.92	0.51
5:H:100(D):VAL:O	5:H:100(F):ALA:N	2.40	0.51
4:G:66:HIS:CE1	4:G:208:VAL:HG12	2.46	0.51
2:D:96:LEU:HG	2:D:97:LEU:HG	1.94	0.50
1:B:610:TRP:HE3	4:G:36:VAL:HG22	1.76	0.50
2:D:11:LEU:HB2	2:D:147:PRO:HG3	1.93	0.49
4:G:299:PRO:HA	4:G:442:VAL:HG13	1.94	0.49
1:B:574:LYS:HZ2	4:G:107:ASP:CG	2.20	0.49
4:G:181:VAL:HG22	4:G:191:TYR:HB3	1.93	0.49
1:B:610:TRP:CD2	4:G:498:PRO:HB3	2.48	0.48
5:H:167:VAL:HB	6:L:163:THR:HG22	1.94	0.48
6:L:61:ARG:HD2	6:L:77:SER:HB2	1.94	0.48
2:D:150:VAL:HG22	2:D:200:HIS:HD2	1.78	0.48
4:G:69:TRP:HA	4:G:111:LEU:HD13	1.96	0.48
5:H:21:THR:HG23	5:H:77:LEU:HD13	1.96	0.48
4:G:396:ILE:HG22	4:G:397:SER:H	1.78	0.48
3:E:209:THR:HG23	3:E:210:GLU:HG3	1.96	0.48
4:G:259:LEU:HB2	4:G:374:HIS:CE1	2.48	0.48
5:H:169:GLN:HG2	6:L:161:GLU:HG2	1.95	0.48
4:G:131:CYS:HA	4:G:157:CYS:HA	1.96	0.47
1:B:571:TRP:CZ3	4:G:54:CYS:HB3	2.49	0.47
6:L:138:SER:HB2	6:L:172:LYS:HE2	1.95	0.47
2:D:220:LEU:HG	2:D:224:PHE:HE1	1.80	0.47
4:G:72:HIS:C	4:G:74:CYS:H	2.21	0.47
1:B:570:VAL:O	1:B:574:LYS:HG3	2.14	0.47
1:B:529:THR:HG23	2:D:98:ARG:HD2	1.97	0.47
5:H:193:ILE:HG12	5:H:208:ARG:HA	1.96	0.47
4:G:164:GLU:OE2	4:G:308:ARG:NE	2.48	0.47
4:G:92:GLU:HA	4:G:238:PRO:HA	1.97	0.46
5:H:53:ASP:OD1	5:H:54:SER:N	2.43	0.46
5:H:144:PHE:CG	5:H:145:PRO:HD3	2.50	0.46
3:E:27(C):CYS:HA	3:E:28:CYS:HA	1.58	0.46
14:B:703:NAG:H4	3:E:53:GLU:HG2	1.98	0.46
4:G:457:ASP:OD1	4:G:457:ASP:N	2.47	0.46
1:B:578:ALA:HB1	4:G:220:PRO:HG3	1.97	0.46
6:L:168:GLN:CD	6:L:172:LYS:HZ2	2.23	0.46
2:D:126:PRO:HB2	2:D:215:SER:HB2	1.98	0.46
2:D:139:GLY:HA3	2:D:181:VAL:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:161:VAL:HG22	5:H:180:VAL:HG22	1.98	0.46
2:D:100(E):LEU:HD12	2:D:100(F):PRO:HD2	1.97	0.45
6:L:161:GLU:O	6:L:178:TYR:N	2.40	0.45
5:H:143:TYR:CE1	5:H:146:GLU:HB2	2.52	0.45
4:G:98:ASN:ND2	4:G:486:TYR:O	2.50	0.45
1:B:606:THR:OG1	4:G:36:VAL:O	2.32	0.45
2:D:218:LYS:NZ	3:E:210:GLU:OE1	2.34	0.45
5:H:100(A):ILE:HD13	5:H:100(E):VAL:HG22	1.98	0.45
3:E:24:THR:OG1	3:E:25:GLY:N	2.49	0.44
3:E:96:CYS:SG	3:E:97:VAL:N	2.91	0.43
4:G:66:HIS:NE2	4:G:208:VAL:HG12	2.33	0.43
4:G:286:VAL:HB	4:G:452:LEU:HB2	1.99	0.43
5:H:20:LEU:HD12	5:H:80:LEU:HD22	2.00	0.43
1:B:606:THR:HG21	1:B:646:LEU:HD22	2.00	0.43
6:L:140:PHE:HB2	6:L:198:HIS:CE1	2.53	0.43
5:H:6:GLU:OE2	5:H:92:CYS:N	2.51	0.43
6:L:80:ALA:HA	6:L:106:VAL:HG21	1.99	0.43
4:G:270:VAL:HG23	4:G:348:GLN:HG3	2.00	0.43
5:H:139:LEU:HD21	5:H:141:LYS:HB2	2.01	0.43
1:B:610:TRP:CE3	4:G:36:VAL:HG22	2.54	0.43
3:E:6:GLN:NE2	3:E:100:THR:OG1	2.52	0.42
3:E:89:CYS:SG	3:E:90:SER:N	2.92	0.42
2:D:134:GLY:HA2	2:D:223:LEU:HD13	2.01	0.42
6:L:50:ASN:O	6:L:52:ASN:N	2.48	0.42
5:H:144:PHE:HD1	5:H:144:PHE:HA	1.73	0.42
4:G:66:HIS:HB2	4:G:72:HIS:CE1	2.55	0.42
4:G:385:CYS:HA	4:G:418:CYS:HA	2.02	0.42
5:H:166:ALA:HB1	5:H:174:TYR:HB3	2.01	0.42
5:H:13:LYS:NZ	5:H:112:ALA:O	2.52	0.42
4:G:95:MET:SD	4:G:273:ARG:HD3	2.60	0.42
5:H:117:PRO:HB3	5:H:143:TYR:HB3	2.02	0.42
3:E:118:PHE:HB2	3:E:133:VAL:HB	2.03	0.41
5:H:146:GLU:HA	5:H:147:PRO:C	2.46	0.41
1:B:660:LEU:O	1:B:663:LEU:HG	2.21	0.41
8:C:2:NAG:H61	8:C:3:BMA:H2	2.03	0.41
4:G:260:LEU:HD12	4:G:452:LEU:N	2.35	0.41
4:G:303:THR:OG1	4:G:321(A):ASP:O	2.36	0.41
5:H:38:ARG:HB3	5:H:48:ILE:HD11	2.02	0.41
6:L:133:LEU:HD12	6:L:179:LEU:HD23	2.02	0.41
4:G:52:LEU:HD11	4:G:100:MET:HG2	2.03	0.41
6:L:112:ALA:HB3	6:L:141:TYR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:112:ALA:HB3	5:H:144:PHE:CE2	2.56	0.40
4:G:342:LEU:HD23	4:G:342:LEU:HA	1.87	0.40
6:L:39:ARG:HB3	6:L:42:GLN:HB2	2.03	0.40
5:H:49:GLY:HA2	6:L:96:TRP:HZ3	1.86	0.40
5:H:72:ASP:OD2	5:H:75:LYS:HD2	2.21	0.40
4:G:55:ALA:N	4:G:216:HIS:O	2.54	0.40
4:G:211:GLU:OE2	11:K:2:NAG:O4	2.39	0.40
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.56	0.40
6:L:112:ALA:O	6:L:198:HIS:NE2	2.55	0.40
3:E:31:LYS:O	3:E:66:LYS:NZ	2.43	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	B	122/153 (80%)	116 (95%)	6 (5%)	0	100	100
2	D	240/243 (99%)	227 (95%)	12 (5%)	1 (0%)	30	63
3	E	211/216 (98%)	194 (92%)	16 (8%)	1 (0%)	24	59
4	G	432/481 (90%)	392 (91%)	35 (8%)	5 (1%)	10	38
5	H	224/235 (95%)	211 (94%)	11 (5%)	2 (1%)	14	46
6	L	206/213 (97%)	189 (92%)	17 (8%)	0	100	100
All	All	1435/1541 (93%)	1329 (93%)	97 (7%)	9 (1%)	21	54

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	147	PRO
4	G	70	ALA

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Mol	Chain	Res	Type
4	G	374	HIS
3	E	51	ASP
5	H	142	ASP
4	G	69	TRP
4	G	73	ALA
2	D	42	GLY
4	G	240	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	B	108/129 (84%)	106 (98%)	2 (2%)	50	75
2	D	205/206 (100%)	205 (100%)	0	100	100
3	E	186/189 (98%)	185 (100%)	1 (0%)	81	88
4	G	392/428 (92%)	382 (97%)	10 (3%)	40	71
5	H	198/205 (97%)	196 (99%)	2 (1%)	68	83
6	L	177/181 (98%)	176 (99%)	1 (1%)	78	87
All	All	1266/1338 (95%)	1250 (99%)	16 (1%)	61	80

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	619	LEU
1	B	639	THR
3	E	6	GLN
4	G	66	HIS
4	G	112	TRP
4	G	197	ASN
4	G	217	TYR
4	G	257	THR
4	G	309	ILE
4	G	369	LEU
4	G	396	ILE

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Mol	Chain	Res	Type
4	G	449	ILE
4	G	476	ARG
5	H	23	ASN
5	H	146	GLU
6	L	161	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	543	ASN
1	B	607	ASN
1	B	616	ASN
2	D	58	ASN
3	E	6	GLN
4	G	66	HIS
4	G	72	HIS
4	G	99	ASN
4	G	203	GLN
4	G	258	GLN
4	G	377	ASN
4	G	411	ASN
4	G	425	ASN
4	G	462	ASN
6	L	95(C)	ASN
6	L	189	HIS

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](#)

48 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	$\# Z > 2$
7	NAG	A	1	4,7	14,14,15	0.32	0	17,19,21	0.50	0
7	NAG	A	2	7	14,14,15	0.48	0	17,19,21	1.35	2 (11%)
7	BMA	A	3	7	11,11,12	0.63	0	15,15,17	0.71	0
7	MAN	A	4	7	11,11,12	0.82	1 (9%)	15,15,17	1.22	2 (13%)
7	MAN	A	5	7	11,11,12	0.63	0	15,15,17	1.03	2 (13%)
7	MAN	A	6	7	11,11,12	0.63	0	15,15,17	1.11	2 (13%)
7	MAN	A	7	7	11,11,12	0.63	0	15,15,17	1.07	2 (13%)
8	NAG	C	1	4,8	14,14,15	0.30	0	17,19,21	0.43	0
8	NAG	C	2	8	14,14,15	0.23	0	17,19,21	0.40	0
8	BMA	C	3	8	11,11,12	0.53	0	15,15,17	0.82	0
9	NAG	F	1	9,4	14,14,15	0.22	0	17,19,21	0.47	0
9	NAG	F	2	9	14,14,15	0.24	0	17,19,21	0.42	0
9	BMA	F	3	9	11,11,12	0.64	0	15,15,17	0.65	0
9	MAN	F	4	9	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
9	MAN	F	5	9	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
10	NAG	I	1	4,10	14,14,15	0.30	0	17,19,21	0.49	0
10	NAG	I	2	10	14,14,15	0.46	0	17,19,21	1.33	2 (11%)
10	NAG	J	1	4,10	14,14,15	0.38	0	17,19,21	0.60	0
10	NAG	J	2	10	14,14,15	0.25	0	17,19,21	0.49	0
11	NAG	K	1	11,4	14,14,15	0.21	0	17,19,21	0.49	0
11	NAG	K	2	11	14,14,15	0.34	0	17,19,21	0.41	0
11	BMA	K	3	11	11,11,12	0.70	0	15,15,17	0.68	0
11	MAN	K	4	11	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
11	MAN	K	5	11	11,11,12	0.74	0	15,15,17	1.12	2 (13%)
11	MAN	K	6	11	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
10	NAG	M	1	4,10	14,14,15	0.22	0	17,19,21	0.52	0
10	NAG	M	2	10	14,14,15	0.22	0	17,19,21	0.43	0
10	NAG	N	1	4,10	14,14,15	0.20	0	17,19,21	0.42	0
10	NAG	N	2	10	14,14,15	0.23	0	17,19,21	0.45	0
12	NAG	O	1	4,12	14,14,15	0.21	0	17,19,21	0.44	0
12	MAN	O	10	12	11,11,12	0.70	0	15,15,17	0.98	2 (13%)
12	NAG	O	2	12	14,14,15	0.24	0	17,19,21	0.60	0
12	BMA	O	3	12	11,11,12	0.76	0	15,15,17	0.90	0
12	MAN	O	4	12	11,11,12	0.60	0	15,15,17	1.14	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	O	5	12	11,11,12	0.61	0	15,15,17	1.02	2 (13%)
12	MAN	O	6	12	11,11,12	0.63	0	15,15,17	1.30	2 (13%)
12	MAN	O	7	12	11,11,12	0.71	0	15,15,17	0.96	2 (13%)
12	MAN	O	8	12	11,11,12	0.75	0	15,15,17	1.07	1 (6%)
12	MAN	O	9	12	11,11,12	0.79	0	15,15,17	1.12	2 (13%)
10	NAG	P	1	4,10	14,14,15	0.21	0	17,19,21	0.51	0
10	NAG	P	2	10	14,14,15	0.23	0	17,19,21	0.48	0
10	NAG	Q	1	4,10	14,14,15	0.27	0	17,19,21	0.67	0
10	NAG	Q	2	10	14,14,15	0.23	0	17,19,21	0.46	0
10	NAG	R	1	4,10	14,14,15	0.24	0	17,19,21	0.45	0
10	NAG	R	2	10	14,14,15	0.31	0	17,19,21	0.53	0
8	NAG	S	1	4,8	14,14,15	0.22	0	17,19,21	0.60	0
8	NAG	S	2	8	14,14,15	0.20	0	17,19,21	0.41	0
8	BMA	S	3	8	11,11,12	0.58	0	15,15,17	0.77	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
7	NAG	A	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	4/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	0/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
7	MAN	A	7	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	4,8	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	2/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	BMA	F	3	9	-	2/2/19/22	0/1/1/1
9	MAN	F	4	9	-	1/2/19/22	0/1/1/1
9	MAN	F	5	9	-	0/2/19/22	0/1/1/1
10	NAG	I	1	4,10	-	4/6/23/26	0/1/1/1
10	NAG	I	2	10	-	4/6/23/26	0/1/1/1
10	NAG	J	1	4,10	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	J	2	10	-	1/6/23/26	0/1/1/1
11	NAG	K	1	11,4	-	0/6/23/26	0/1/1/1
11	NAG	K	2	11	-	1/6/23/26	0/1/1/1
11	BMA	K	3	11	-	0/2/19/22	0/1/1/1
11	MAN	K	4	11	-	2/2/19/22	0/1/1/1
11	MAN	K	5	11	-	0/2/19/22	1/1/1/1
11	MAN	K	6	11	-	0/2/19/22	0/1/1/1
10	NAG	M	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
10	NAG	N	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	N	2	10	-	2/6/23/26	0/1/1/1
12	NAG	O	1	4,12	-	0/6/23/26	0/1/1/1
12	MAN	O	10	12	-	0/2/19/22	0/1/1/1
12	NAG	O	2	12	-	4/6/23/26	0/1/1/1
12	BMA	O	3	12	-	0/2/19/22	0/1/1/1
12	MAN	O	4	12	-	2/2/19/22	0/1/1/1
12	MAN	O	5	12	-	0/2/19/22	0/1/1/1
12	MAN	O	6	12	-	2/2/19/22	0/1/1/1
12	MAN	O	7	12	-	2/2/19/22	0/1/1/1
12	MAN	O	8	12	-	0/2/19/22	0/1/1/1
12	MAN	O	9	12	-	0/2/19/22	1/1/1/1
10	NAG	P	1	4,10	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	2/6/23/26	0/1/1/1
10	NAG	Q	1	4,10	-	4/6/23/26	0/1/1/1
10	NAG	Q	2	10	-	0/6/23/26	0/1/1/1
10	NAG	R	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	R	2	10	-	2/6/23/26	0/1/1/1
8	NAG	S	1	4,8	-	4/6/23/26	0/1/1/1
8	NAG	S	2	8	-	1/6/23/26	0/1/1/1
8	BMA	S	3	8	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	4	MAN	C1-C2	2.15	1.57	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2	NAG	C2-N2-C7	4.62	129.09	122.90
10	I	2	NAG	C2-N2-C7	4.58	129.04	122.90
12	O	6	MAN	C1-O5-C5	4.09	117.67	112.19
12	O	9	MAN	C1-O5-C5	3.26	116.55	112.19
11	K	5	MAN	C1-O5-C5	3.26	116.55	112.19
12	O	4	MAN	C1-O5-C5	3.23	116.51	112.19
7	A	4	MAN	C1-O5-C5	3.06	116.28	112.19
7	A	6	MAN	C1-O5-C5	2.88	116.04	112.19
12	O	5	MAN	C1-O5-C5	2.82	115.96	112.19
9	F	5	MAN	C1-O5-C5	2.76	115.88	112.19
7	A	7	MAN	C1-O5-C5	2.74	115.86	112.19
7	A	5	MAN	C1-O5-C5	2.58	115.65	112.19
12	O	8	MAN	C1-O5-C5	2.57	115.63	112.19
9	F	4	MAN	C1-O5-C5	2.55	115.61	112.19
11	K	4	MAN	O2-C2-C3	-2.54	104.88	110.15
11	K	6	MAN	C1-O5-C5	2.53	115.58	112.19
11	K	4	MAN	C1-O5-C5	2.48	115.51	112.19
12	O	10	MAN	C1-O5-C5	2.26	115.21	112.19
12	O	5	MAN	O2-C2-C3	-2.20	105.59	110.15
9	F	5	MAN	O2-C2-C3	-2.18	105.64	110.15
11	K	5	MAN	O2-C2-C3	-2.18	105.64	110.15
7	A	7	MAN	O2-C2-C3	-2.17	105.67	110.15
11	K	6	MAN	O2-C2-C3	-2.16	105.67	110.15
7	A	5	MAN	O2-C2-C3	-2.16	105.68	110.15
12	O	6	MAN	O2-C2-C3	-2.16	105.68	110.15
9	F	4	MAN	O2-C2-C3	-2.16	105.68	110.15
12	O	10	MAN	O2-C2-C3	-2.15	105.69	110.15
7	A	4	MAN	O2-C2-C3	-2.15	105.69	110.15
7	A	6	MAN	O2-C2-C3	-2.15	105.69	110.15
12	O	9	MAN	O2-C2-C3	-2.14	105.71	110.15
12	O	7	MAN	O2-C2-C3	-2.11	105.78	110.15
10	I	2	NAG	C1-C2-N2	2.09	113.73	110.43
7	A	2	NAG	C1-C2-N2	2.09	113.72	110.43
12	O	7	MAN	C1-O5-C5	2.05	114.94	112.19

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	N	1	NAG	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
8	C	2	NAG	O5-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	3	BMA	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
12	O	2	NAG	O5-C5-C6-O6
10	M	1	NAG	O5-C5-C6-O6
10	Q	1	NAG	O5-C5-C6-O6
10	R	2	NAG	C4-C5-C6-O6
10	R	2	NAG	O5-C5-C6-O6
10	N	1	NAG	C4-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
10	N	2	NAG	O5-C5-C6-O6
10	R	1	NAG	O5-C5-C6-O6
8	C	2	NAG	C4-C5-C6-O6
8	S	1	NAG	O5-C5-C6-O6
10	P	2	NAG	O5-C5-C6-O6
10	M	1	NAG	C4-C5-C6-O6
10	Q	1	NAG	C4-C5-C6-O6
8	S	1	NAG	C4-C5-C6-O6
10	P	2	NAG	C4-C5-C6-O6
11	K	4	MAN	O5-C5-C6-O6
12	O	2	NAG	C4-C5-C6-O6
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
8	S	1	NAG	C8-C7-N2-C2
8	S	1	NAG	O7-C7-N2-C2
10	I	1	NAG	C8-C7-N2-C2
10	I	1	NAG	O7-C7-N2-C2
10	I	2	NAG	C8-C7-N2-C2
10	I	2	NAG	O7-C7-N2-C2
10	J	1	NAG	C8-C7-N2-C2
10	J	1	NAG	O7-C7-N2-C2
8	S	3	BMA	O5-C5-C6-O6
10	N	2	NAG	C4-C5-C6-O6
10	R	1	NAG	C4-C5-C6-O6
11	K	4	MAN	C4-C5-C6-O6
12	O	6	MAN	O5-C5-C6-O6
10	M	2	NAG	C4-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
10	M	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	S	2	NAG	O5-C5-C6-O6
11	K	2	NAG	O5-C5-C6-O6
9	F	4	MAN	O5-C5-C6-O6
10	I	1	NAG	C4-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6
9	F	3	BMA	C4-C5-C6-O6
10	I	1	NAG	O5-C5-C6-O6
10	Q	1	NAG	C3-C2-N2-C7
12	O	2	NAG	C3-C2-N2-C7
12	O	7	MAN	C4-C5-C6-O6
12	O	7	MAN	O5-C5-C6-O6
9	F	3	BMA	O5-C5-C6-O6
7	A	2	NAG	C1-C2-N2-C7
10	I	2	NAG	C1-C2-N2-C7
10	Q	1	NAG	C1-C2-N2-C7
12	O	2	NAG	C1-C2-N2-C7
7	A	2	NAG	C3-C2-N2-C7
10	I	2	NAG	C3-C2-N2-C7
12	O	6	MAN	C4-C5-C6-O6
12	O	4	MAN	C4-C5-C6-O6
12	O	4	MAN	O5-C5-C6-O6

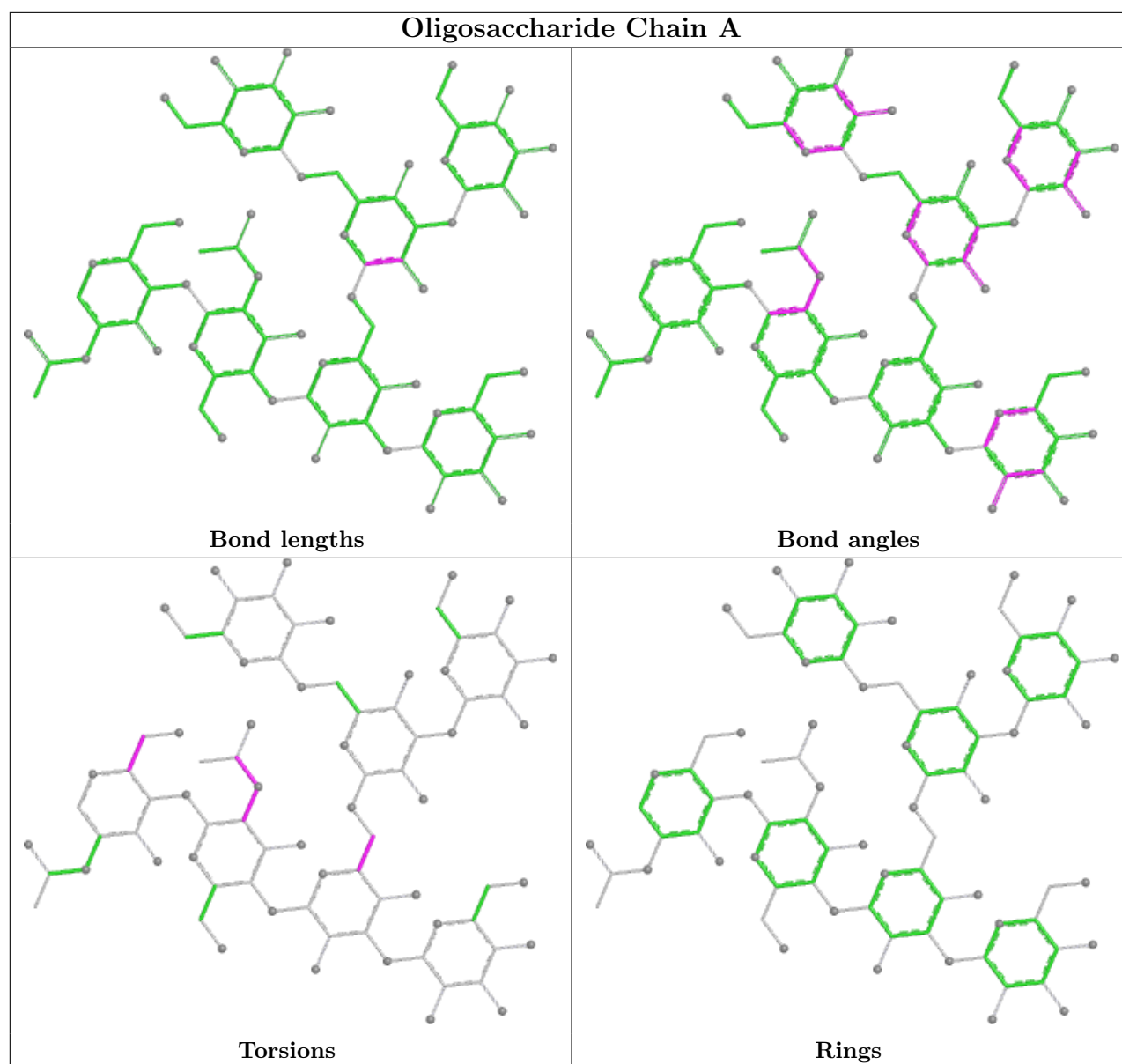
All (2) ring outliers are listed below:

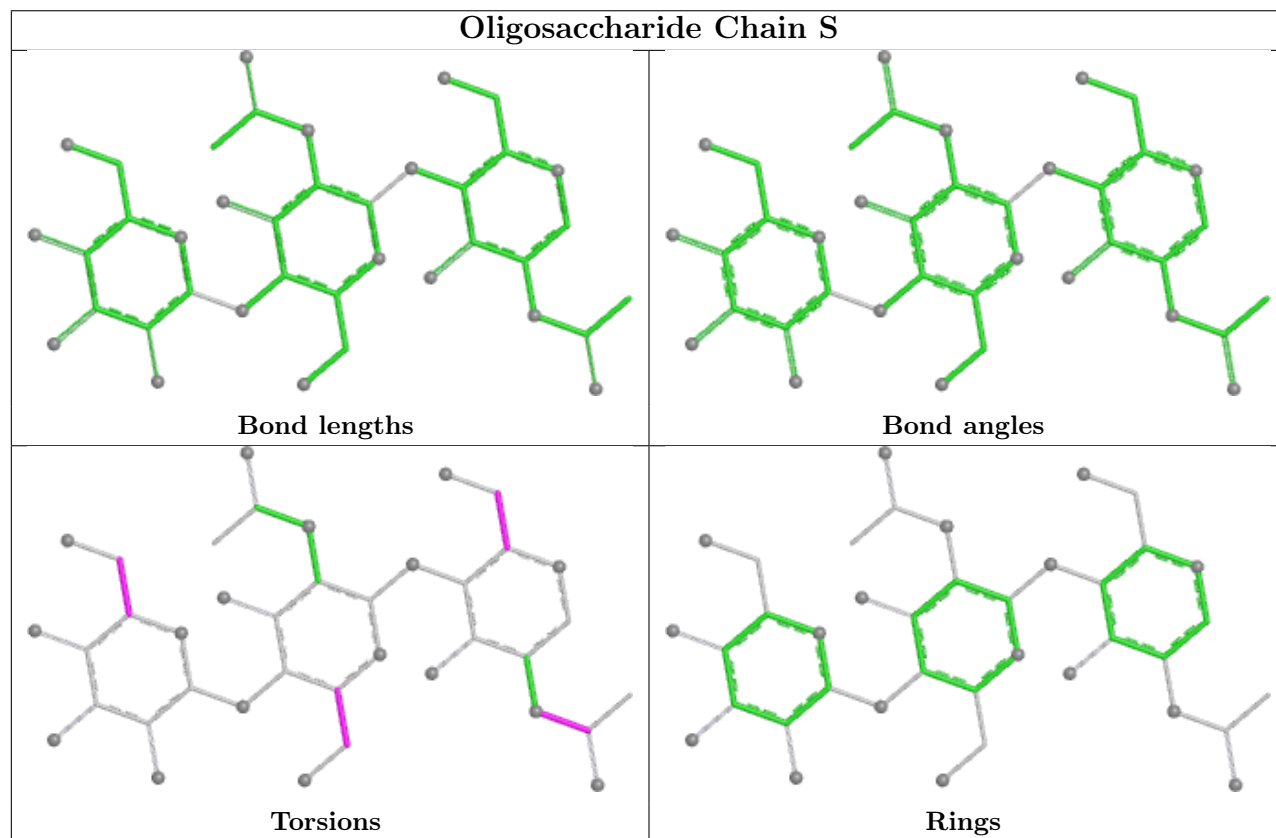
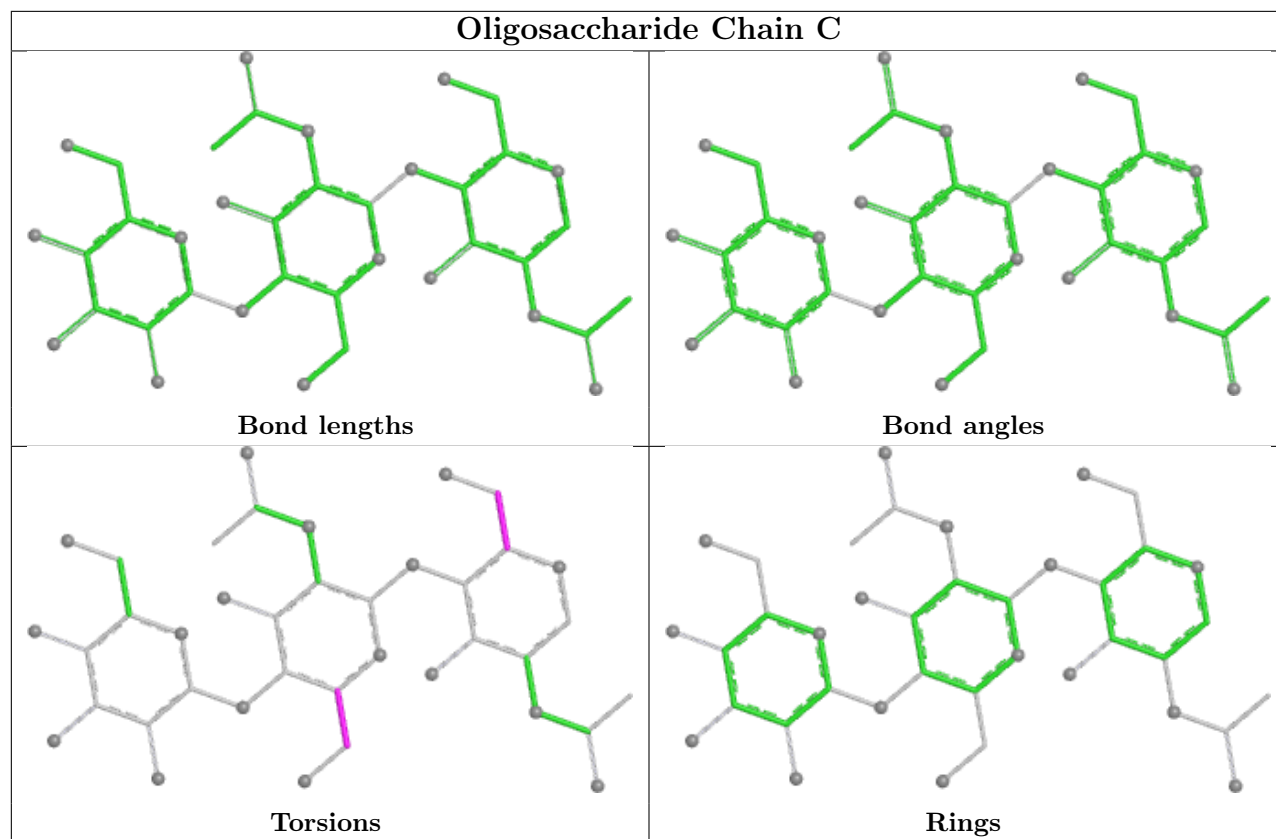
Mol	Chain	Res	Type	Atoms
12	O	9	MAN	C1-C2-C3-C4-C5-O5
11	K	5	MAN	C1-C2-C3-C4-C5-O5

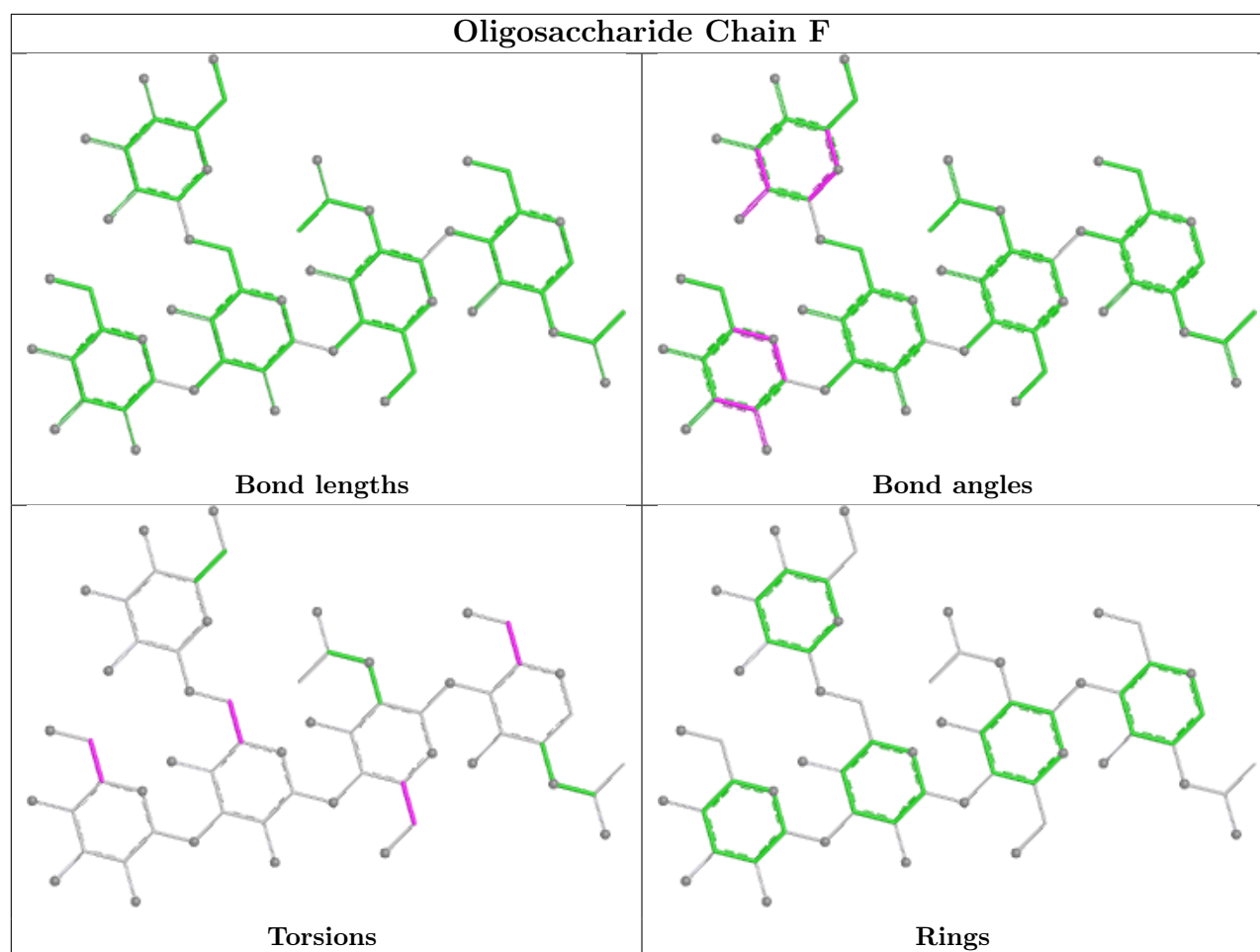
7 monomers are involved in 6 short contacts:

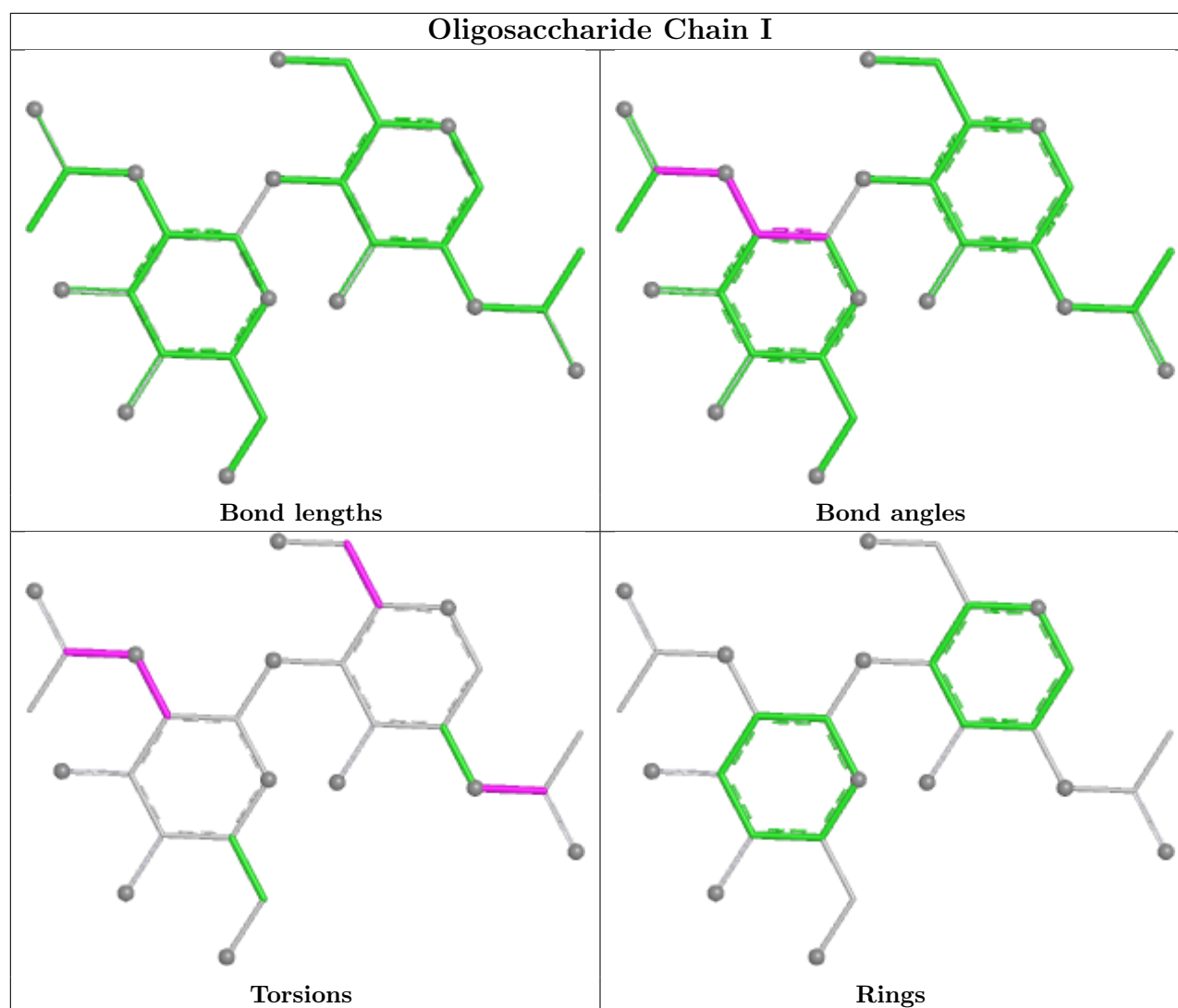
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	1	NAG	1	0
8	C	3	BMA	1	0
7	A	2	NAG	1	0
12	O	2	NAG	1	0
8	C	2	NAG	1	0
10	I	2	NAG	1	0
11	K	2	NAG	1	0

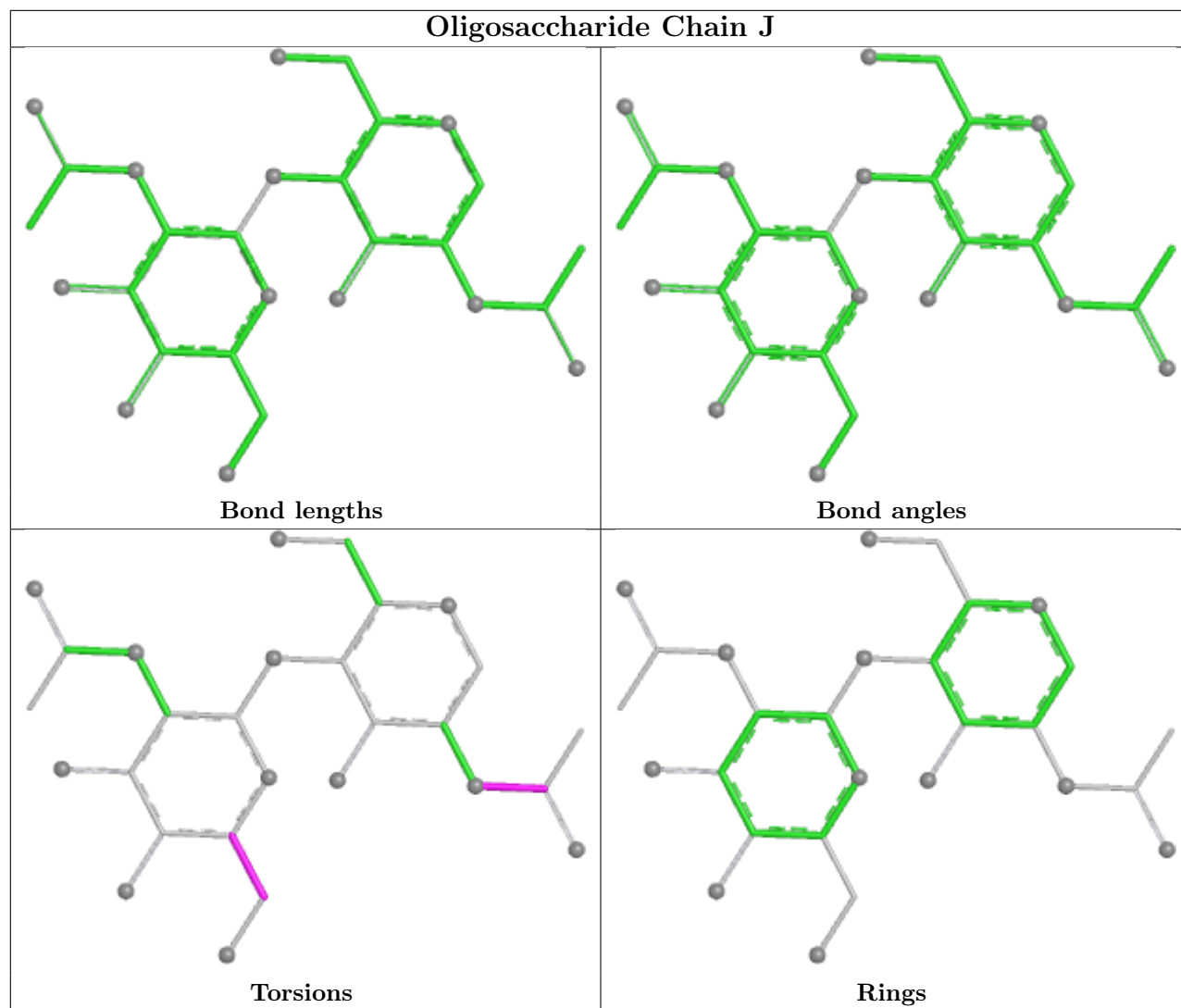
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

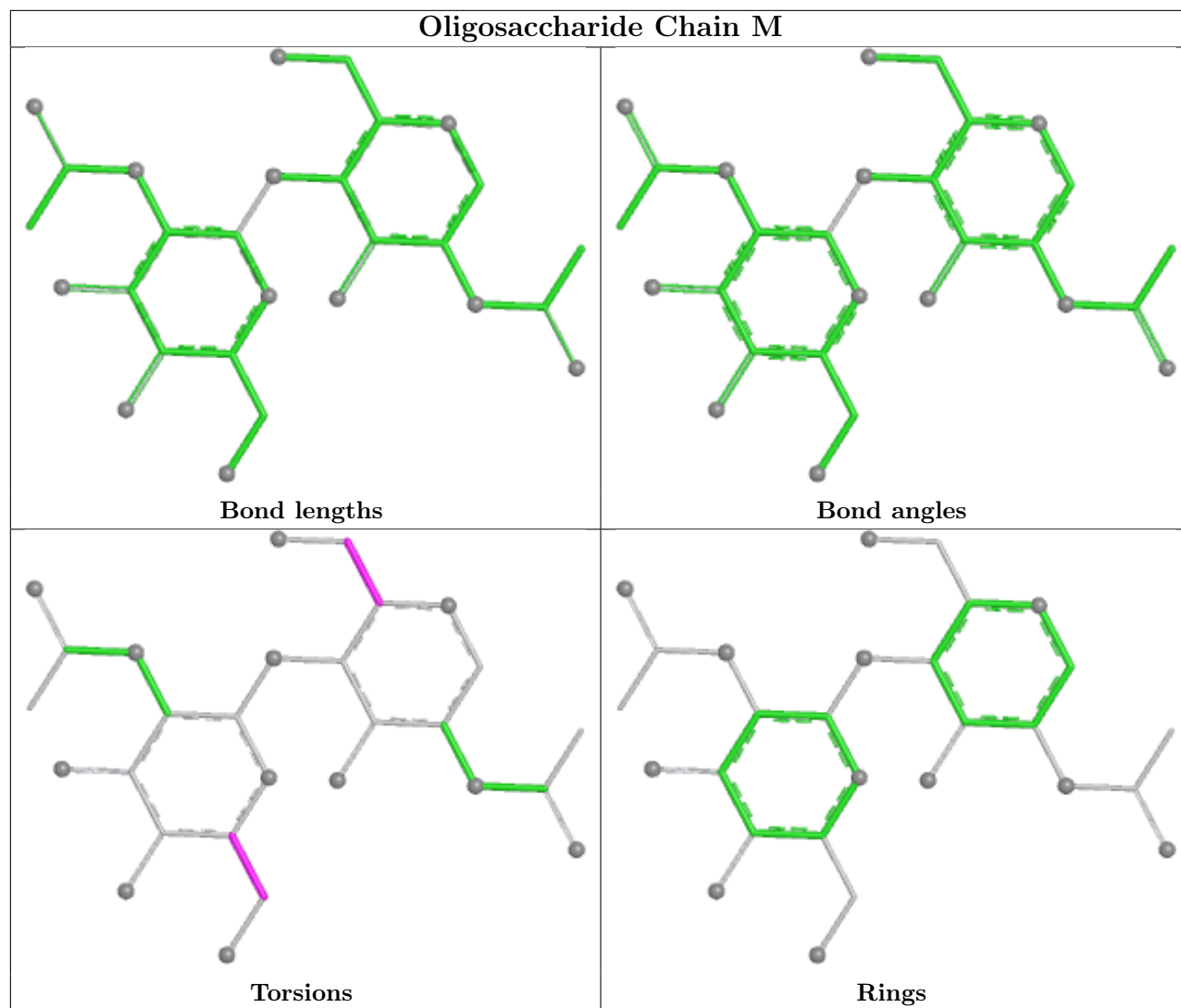


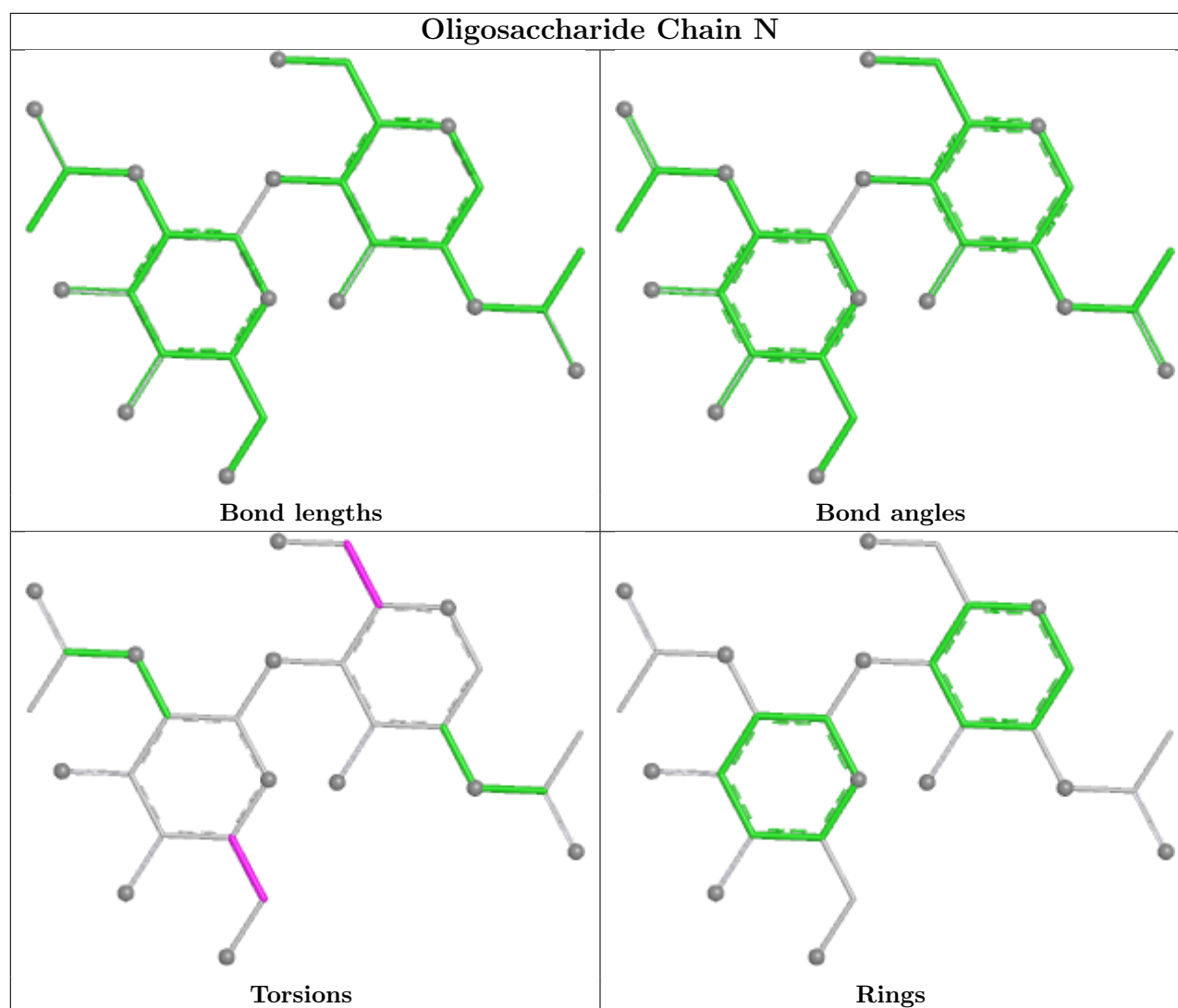


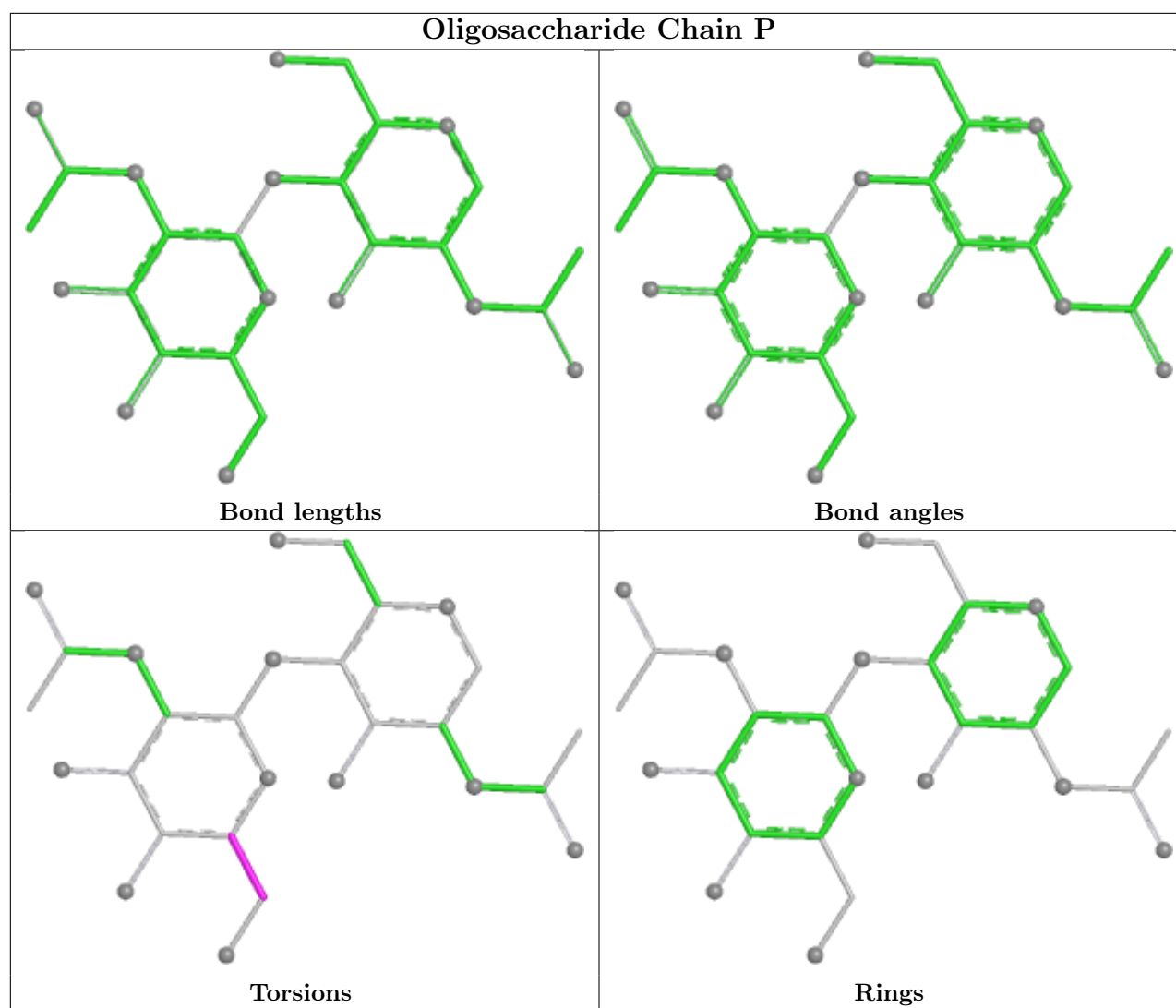


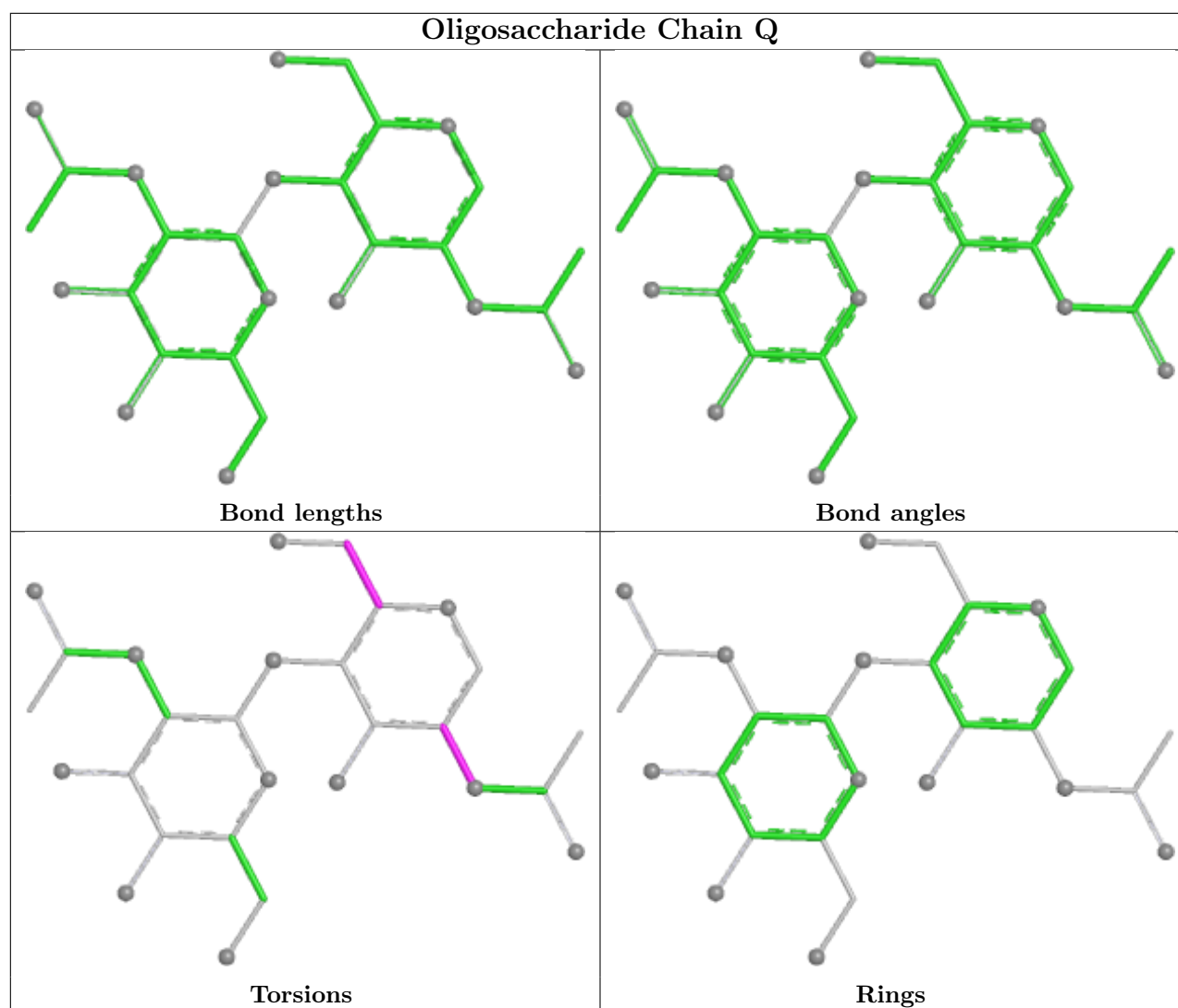


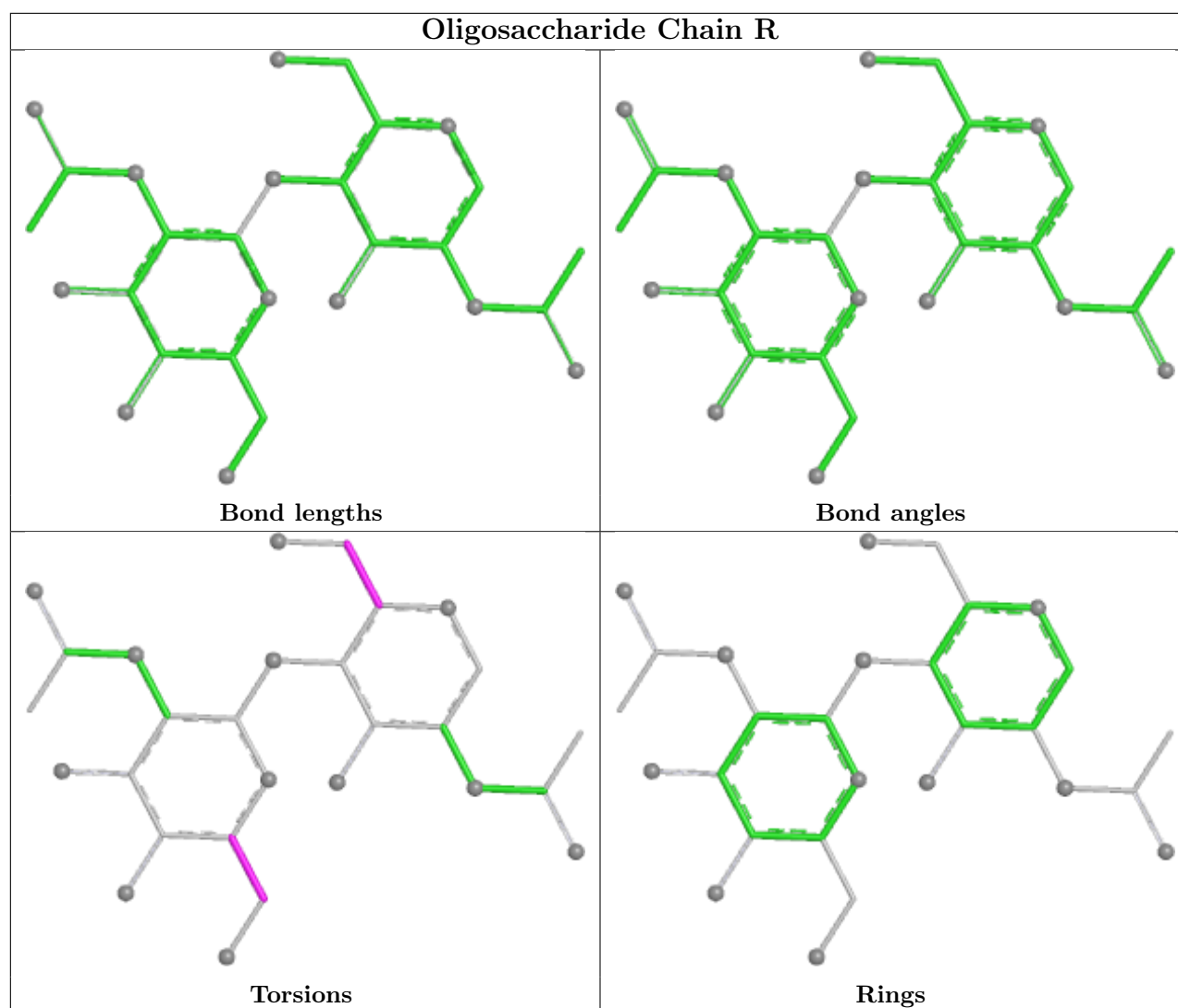




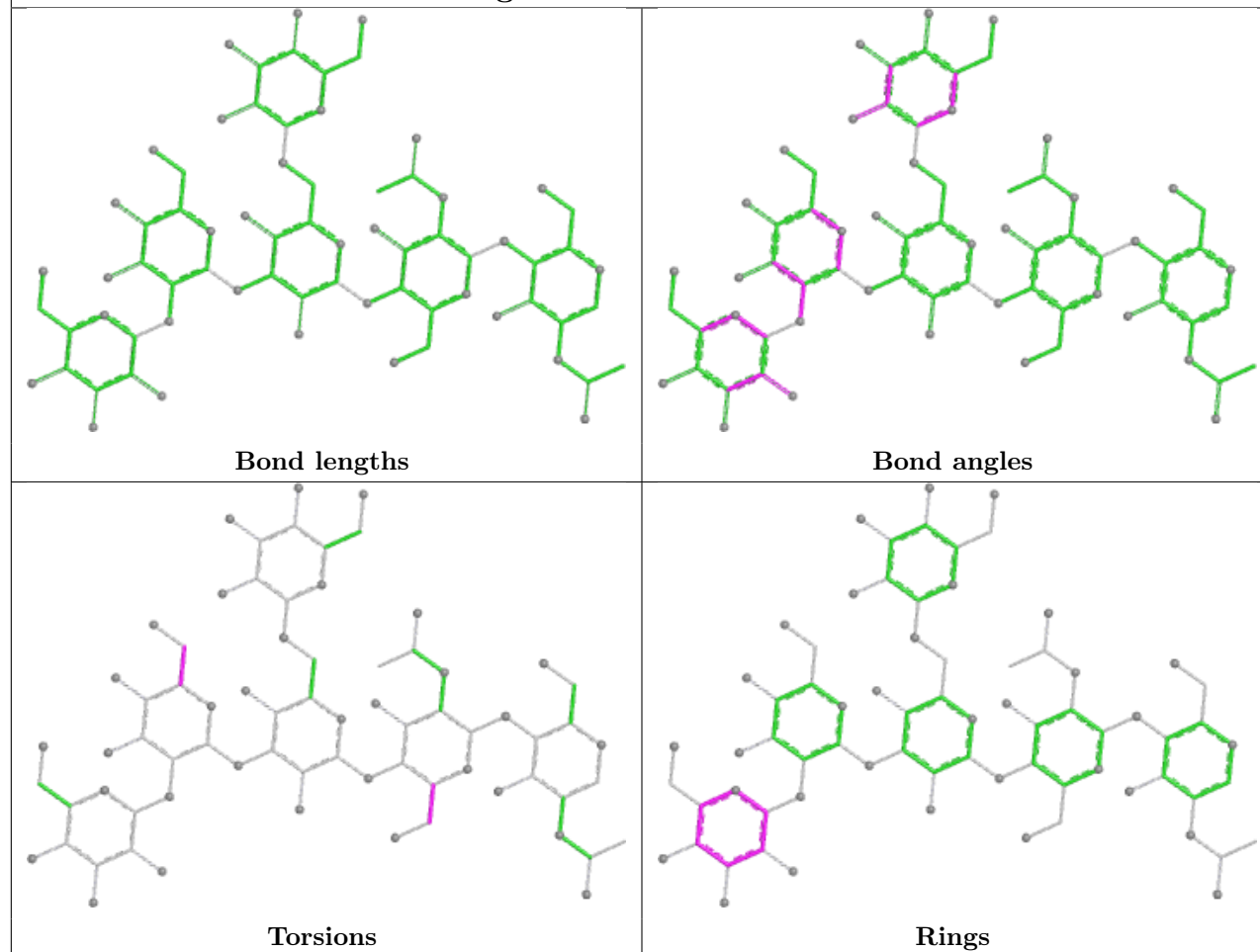


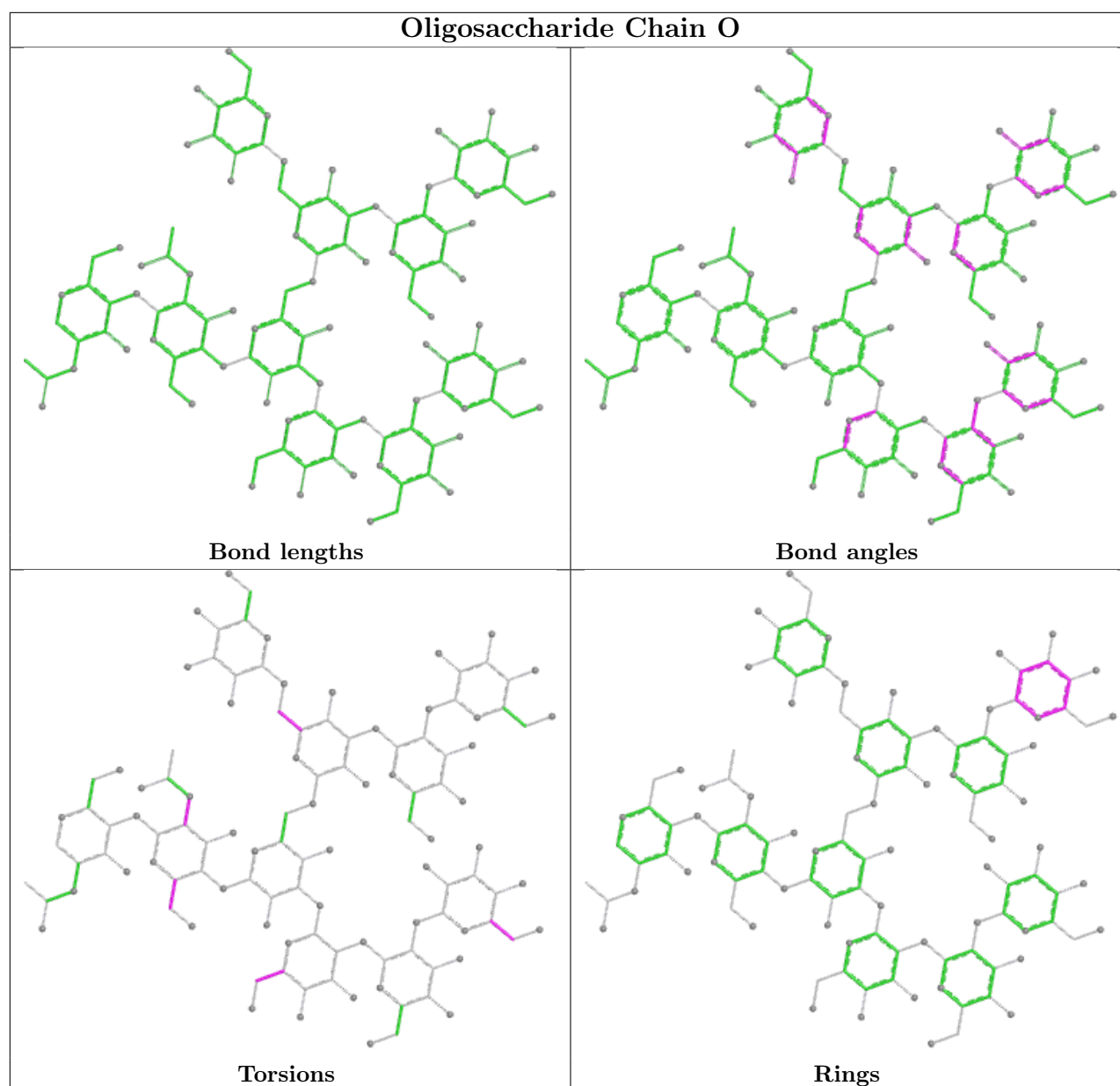






Oligosaccharide Chain K





5.6 Ligand geometry [i](#)

15 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
14	NAG	B	704	1	14,14,15	0.25	0	17,19,21	0.45	0
14	NAG	G	656	4	14,14,15	0.21	0	17,19,21	0.42	0
14	NAG	G	646	4	14,14,15	0.20	0	17,19,21	0.42	0
13	SO4	G	602	-	4,4,4	0.23	0	6,6,6	0.07	0
14	NAG	G	624	4	14,14,15	0.20	0	17,19,21	0.43	0
15	83G	G	657	-	33,33,33	2.56	12 (36%)	44,47,47	2.61	10 (22%)
14	NAG	B	703	1	14,14,15	0.21	0	17,19,21	0.39	0
14	NAG	G	631	4	14,14,15	0.47	0	17,19,21	1.35	2 (11%)
14	NAG	G	611	4	14,14,15	0.23	0	17,19,21	0.46	0
13	SO4	G	603	-	4,4,4	0.24	0	6,6,6	0.08	0
14	NAG	H	301	5	14,14,15	0.25	0	17,19,21	0.43	0
13	SO4	G	601	-	4,4,4	0.24	0	6,6,6	0.08	0
13	SO4	B	701	-	4,4,4	0.23	0	6,6,6	0.07	0
13	SO4	L	301	-	4,4,4	0.23	0	6,6,6	0.07	0
14	NAG	B	702	1	14,14,15	0.25	0	17,19,21	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
14	NAG	B	704	1	-	0/6/23/26	0/1/1/1
14	NAG	G	656	4	-	0/6/23/26	0/1/1/1
14	NAG	G	624	4	-	2/6/23/26	0/1/1/1
15	83G	G	657	-	-	3/22/35/35	0/4/4/4
14	NAG	B	703	1	-	2/6/23/26	0/1/1/1
14	NAG	G	631	4	-	6/6/23/26	0/1/1/1
14	NAG	G	611	4	-	3/6/23/26	0/1/1/1
14	NAG	H	301	5	-	2/6/23/26	0/1/1/1
14	NAG	G	646	4	-	4/6/23/26	0/1/1/1
14	NAG	B	702	1	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	657	83G	C14-N16	7.56	1.45	1.34
15	G	657	83G	C23-N19	5.78	1.47	1.34
15	G	657	83G	C10-N09	-5.24	1.28	1.37
15	G	657	83G	C10-C11	-4.83	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	657	83G	C11-C12	3.77	1.53	1.45
15	G	657	83G	C08-C07	3.49	1.45	1.41
15	G	657	83G	C08-C11	-3.35	1.38	1.45
15	G	657	83G	C25-C23	2.57	1.54	1.50
15	G	657	83G	C21-N16	-2.37	1.45	1.47
15	G	657	83G	O15-C14	-2.11	1.18	1.23
15	G	657	83G	O02-C03	2.08	1.40	1.37
15	G	657	83G	O13-C12	-2.01	1.18	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	657	83G	C07-N09-C10	9.82	113.11	108.48
15	G	657	83G	C08-C11-C10	6.99	113.93	106.10
15	G	657	83G	C21-C20-N19	-5.47	104.74	110.99
15	G	657	83G	C11-C10-N09	-5.36	106.59	110.22
14	G	631	NAG	C2-N2-C7	4.56	129.00	122.90
15	G	657	83G	C17-N16-C21	3.68	120.83	114.75
15	G	657	83G	O02-C03-C08	3.66	121.03	115.84
15	G	657	83G	C03-C08-C11	3.10	143.95	135.25
15	G	657	83G	O02-C03-C04	-2.95	119.33	124.30
15	G	657	83G	C10-C11-C12	-2.91	119.97	126.74
15	G	657	83G	C18-N19-C20	2.81	118.48	113.07
14	G	631	NAG	C1-C2-N2	2.16	113.83	110.43

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	H	301	NAG	O5-C5-C6-O6
14	B	702	NAG	O5-C5-C6-O6
14	G	631	NAG	O5-C5-C6-O6
14	B	702	NAG	C4-C5-C6-O6
14	G	646	NAG	C4-C5-C6-O6
14	B	703	NAG	O5-C5-C6-O6
14	H	301	NAG	C4-C5-C6-O6
14	G	646	NAG	O5-C5-C6-O6
14	G	611	NAG	O5-C5-C6-O6
14	G	631	NAG	C4-C5-C6-O6
14	G	624	NAG	O5-C5-C6-O6
14	G	631	NAG	C8-C7-N2-C2
14	G	631	NAG	O7-C7-N2-C2

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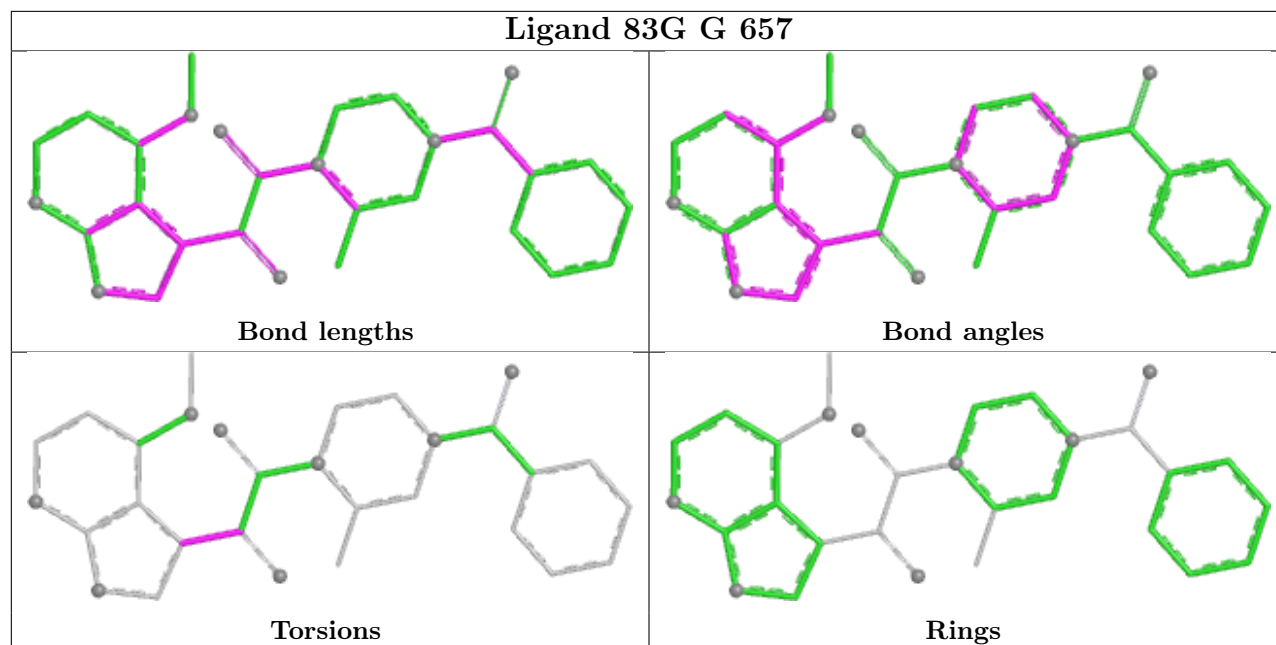
Mol	Chain	Res	Type	Atoms
14	G	646	NAG	C8-C7-N2-C2
14	G	646	NAG	O7-C7-N2-C2
14	B	703	NAG	C4-C5-C6-O6
14	G	624	NAG	C4-C5-C6-O6
14	G	611	NAG	C4-C5-C6-O6
14	G	611	NAG	C1-C2-N2-C7
14	G	631	NAG	C1-C2-N2-C7
14	G	631	NAG	C3-C2-N2-C7
15	G	657	83G	C08-C11-C12-O13
15	G	657	83G	C10-C11-C12-O13
15	G	657	83G	C10-C11-C12-C14

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	G	657	83G	1	0
14	B	703	NAG	1	0
14	G	631	NAG	1	0
13	B	701	SO4	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 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	B	126/153 (82%)	0.42	5 (3%)	42 23	40, 91, 160, 190	0
2	D	242/243 (99%)	0.68	21 (8%)	16 8	93, 197, 320, 379	0
3	E	213/216 (98%)	0.49	6 (2%)	55 32	124, 198, 291, 352	0
4	G	442/481 (91%)	0.27	11 (2%)	58 35	31, 93, 168, 215	0
5	H	228/235 (97%)	0.35	8 (3%)	47 26	83, 136, 198, 261	0
6	L	208/213 (97%)	0.35	7 (3%)	48 27	79, 116, 178, 257	0
All	All	1459/1541 (94%)	0.41	58 (3%)	42 23	31, 129, 265, 379	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	H	138	CYS	6.3
6	L	119	PHE	4.3
2	D	180	SER	3.3
4	G	73	ALA	3.2
4	G	316	ALA	3.2
2	D	181	VAL	3.2
6	L	62	PHE	3.1
3	E	56	PRO	3.1
4	G	71	THR	3.1
2	D	88	GLY	3.0
6	L	120	PRO	3.0
5	H	112	ALA	3.0
3	E	96	CYS	3.0
5	H	121	PRO	2.9
6	L	195	GLN	2.8
2	D	213	PRO	2.8
4	G	180	ASP	2.8
2	D	185	PRO	2.8
6	L	204	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	52	ASN	2.6
2	D	109	LEU	2.6
1	B	619	LEU	2.5
5	H	102	GLY	2.5
2	D	59	LEU	2.4
2	D	112	SER	2.4
2	D	167	PRO	2.3
2	D	151	THR	2.3
2	D	124	LEU	2.3
4	G	56	SER	2.3
2	D	212	GLU	2.3
2	D	165	THR	2.3
1	B	621	GLU	2.2
1	B	547	GLY	2.2
6	L	193	SER	2.2
5	H	146	GLU	2.2
2	D	80	MET	2.2
4	G	495	GLY	2.2
2	D	47	TRP	2.2
2	D	57	LYS	2.2
5	H	11	LEU	2.2
5	H	209	VAL	2.1
1	B	629	LEU	2.1
5	H	100(N)	PHE	2.1
3	E	161	THR	2.1
4	G	439	ILE	2.1
2	D	211	VAL	2.1
1	B	660	LEU	2.1
3	E	180	LEU	2.1
6	L	47	ILE	2.1
4	G	477	ASP	2.1
4	G	36	VAL	2.0
4	G	261	LEU	2.0
4	G	454	LEU	2.0
2	D	104	GLY	2.0
2	D	166	PHE	2.0
3	E	11	VAL	2.0
2	D	108	LEU	2.0
2	D	184	VAL	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, 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.

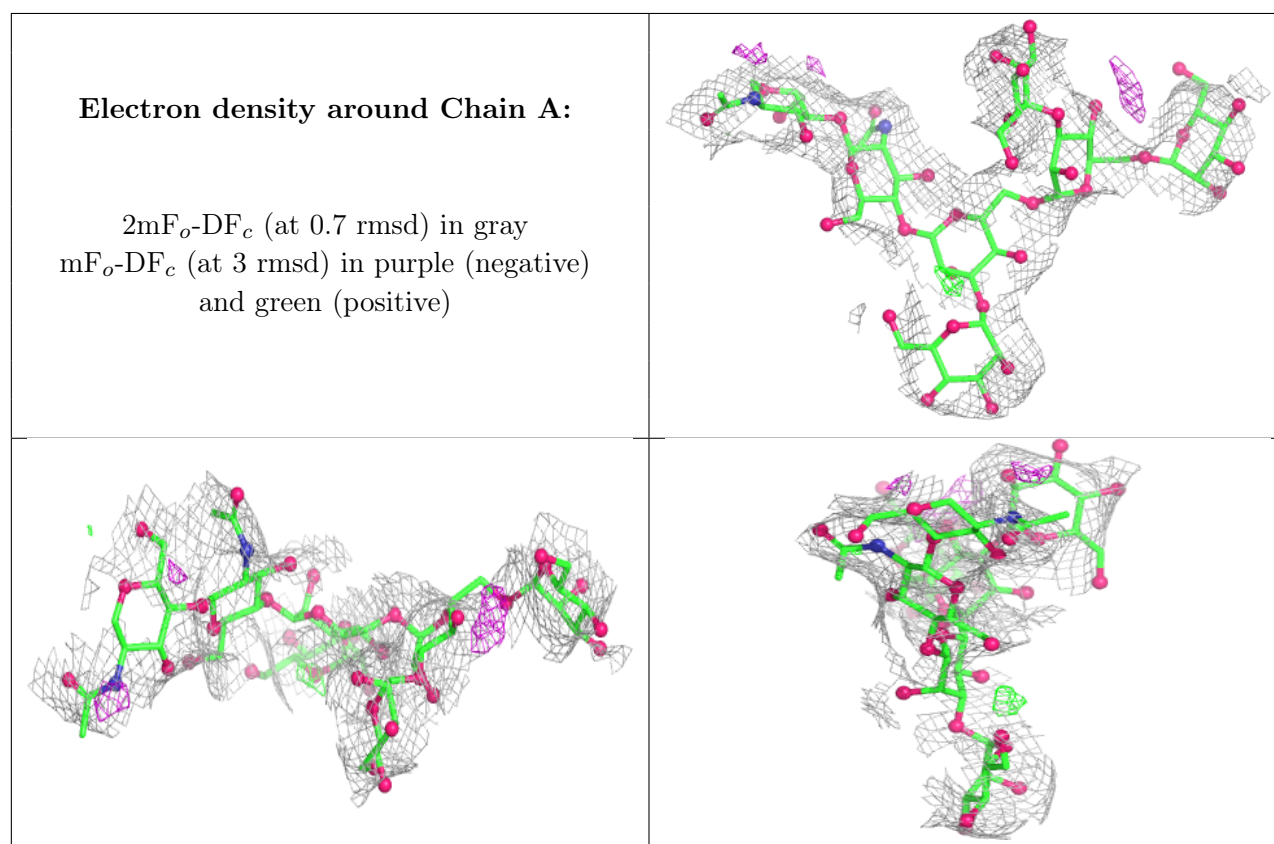
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	1	14/15	-	-	54,95,124,148	0
7	NAG	A	2	14/15	-	-	82,119,131,140	0
7	BMA	A	3	11/12	-	-	82,104,133,136	0
7	MAN	A	4	11/12	-	-	139,184,195,201	0
7	MAN	A	5	11/12	-	-	110,177,184,197	0
7	MAN	A	6	11/12	-	-	160,182,192,192	0
7	MAN	A	7	11/12	-	-	122,135,168,170	0
8	NAG	C	1	14/15	-	-	68,112,132,139	0
8	NAG	C	2	14/15	-	-	90,131,143,153	0
8	BMA	C	3	11/12	-	-	131,139,153,156	0
12	MAN	O	9	11/12	0.37	0.12	114,130,142,144	0
10	NAG	R	2	14/15	0.44	0.12	129,166,178,182	0
8	BMA	S	3	11/12	0.60	0.10	157,176,187,190	0
9	NAG	F	1	14/15	-	-	26,97,119,128	0
9	NAG	F	2	14/15	-	-	79,109,139,151	0
9	BMA	F	3	11/12	-	-	92,138,157,179	0
9	MAN	F	4	11/12	-	-	113,141,152,157	0
9	MAN	F	5	11/12	-	-	149,166,185,194	0
10	NAG	P	2	14/15	0.61	0.09	112,159,179,185	0
10	NAG	Q	2	14/15	0.68	0.10	84,161,179,182	0
10	NAG	J	2	14/15	0.69	0.09	138,164,188,192	0
12	MAN	O	10	11/12	0.71	0.11	122,144,148,151	0
10	NAG	M	2	14/15	0.72	0.11	98,140,152,153	0
10	NAG	N	2	14/15	0.75	0.10	127,156,183,186	0
12	MAN	O	6	11/12	0.77	0.16	97,118,158,181	0
10	NAG	R	1	14/15	0.79	0.10	110,141,158,173	0
10	NAG	J	1	14/15	0.79	0.10	95,123,143,148	0
12	MAN	O	5	11/12	0.79	0.12	52,93,121,154	0
8	NAG	S	1	14/15	0.80	0.10	94,122,139,140	0
10	NAG	I	2	14/15	0.81	0.09	144,164,178,179	0
11	NAG	K	1	14/15	0.81	0.09	11,54,89,89	0
12	MAN	O	8	11/12	0.82	0.07	111,135,157,157	0

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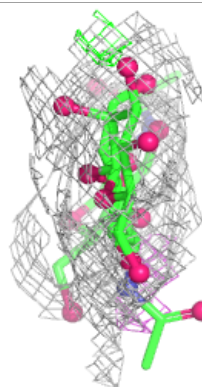
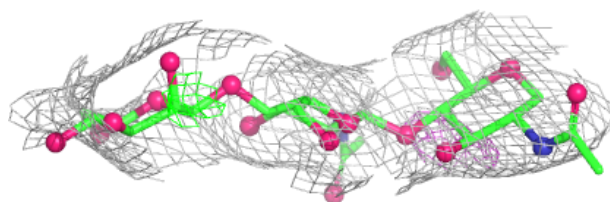
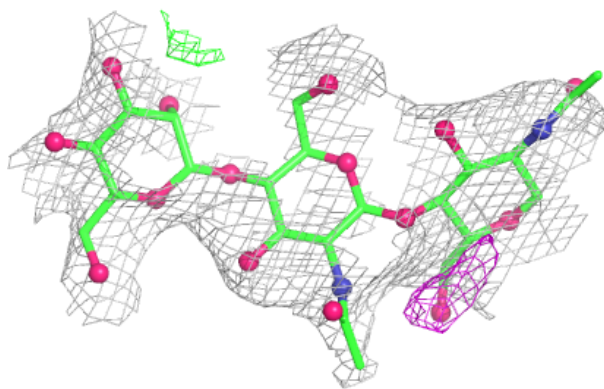
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	K	2	14/15	0.83	0.10	89,113,142,148	0
10	NAG	P	1	14/15	0.83	0.09	88,124,141,162	0
11	BMA	K	3	11/12	-	-	154,166,177,181	0
11	MAN	K	4	11/12	-	-	153,172,183,189	0
11	MAN	K	5	11/12	-	-	149,171,188,197	0
11	MAN	K	6	11/12	-	-	148,169,175,175	0
12	MAN	O	7	11/12	0.84	0.08	106,123,138,139	0
10	NAG	M	1	14/15	0.84	0.10	77,112,131,144	0
10	NAG	Q	1	14/15	0.84	0.11	92,128,138,143	0
8	NAG	S	2	14/15	0.84	0.06	139,159,179,192	0
12	BMA	O	3	11/12	0.86	0.10	84,115,124,124	0
12	NAG	O	2	14/15	0.87	0.11	83,112,127,131	0
12	MAN	O	4	11/12	0.88	0.10	74,83,115,135	0
12	NAG	O	1	14/15	0.89	0.09	82,105,122,128	0
10	NAG	I	1	14/15	0.92	0.07	73,123,159,177	0
10	NAG	N	1	14/15	0.93	0.10	79,98,133,135	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.

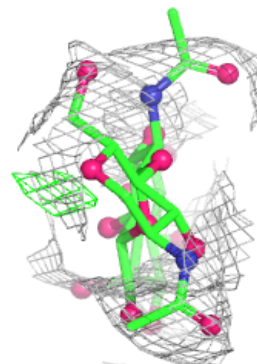
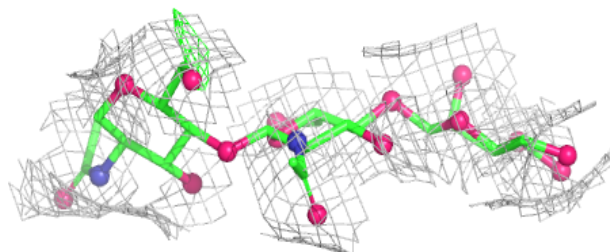
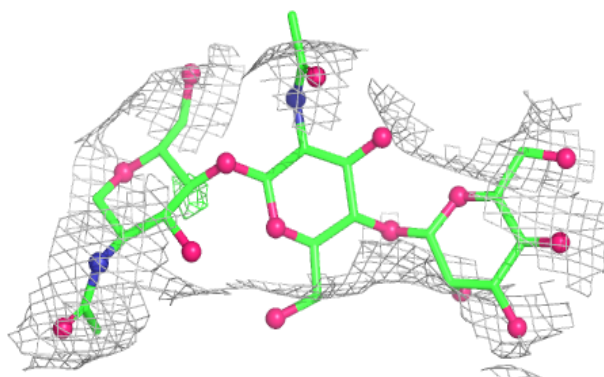


Electron density around Chain C:

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

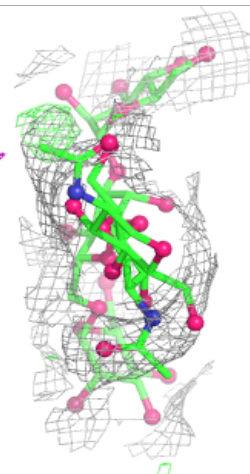
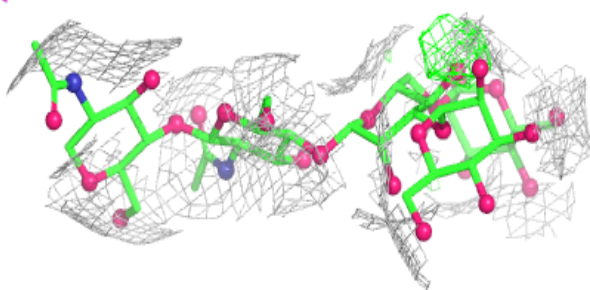
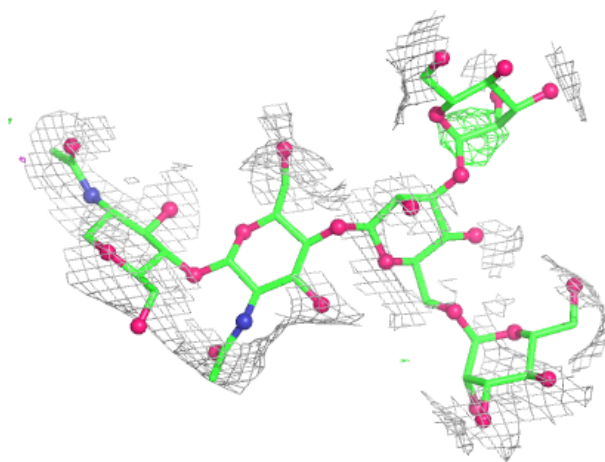
**Electron density around Chain S:**

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



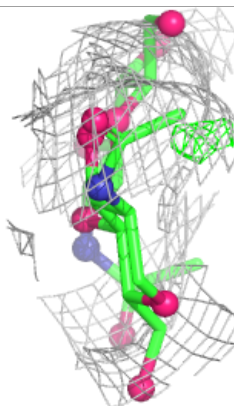
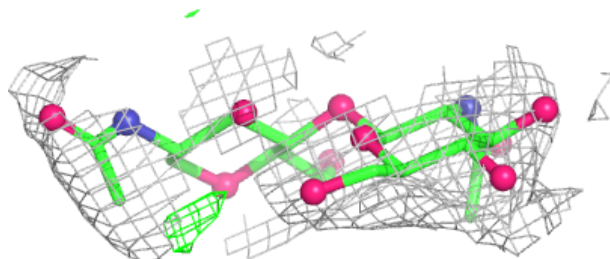
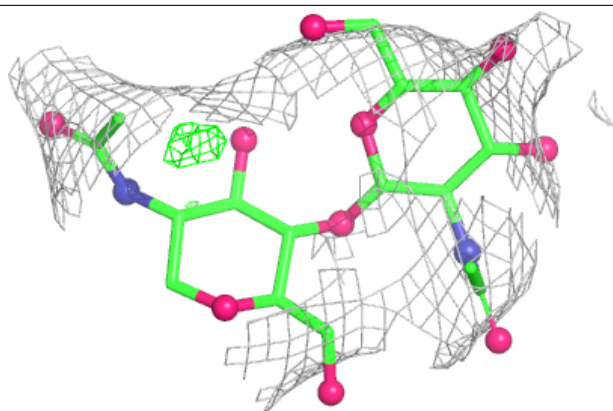
Electron density around Chain F:

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

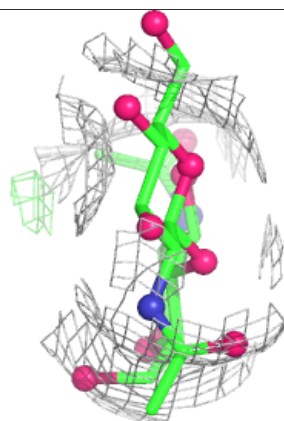
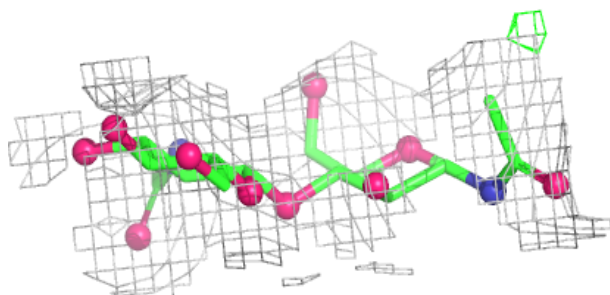
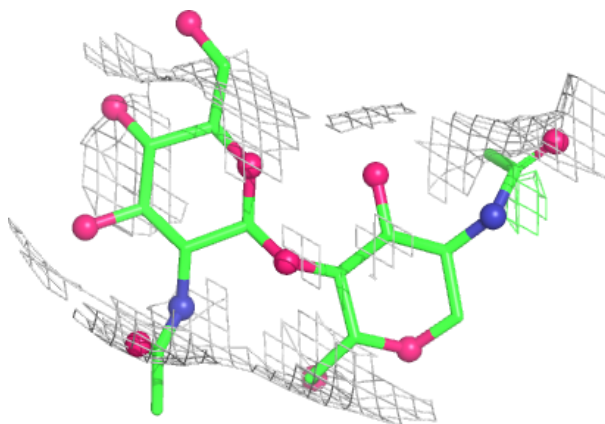


Electron density around Chain I:

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

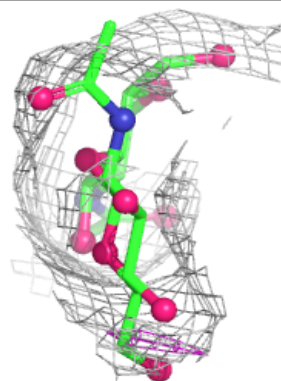
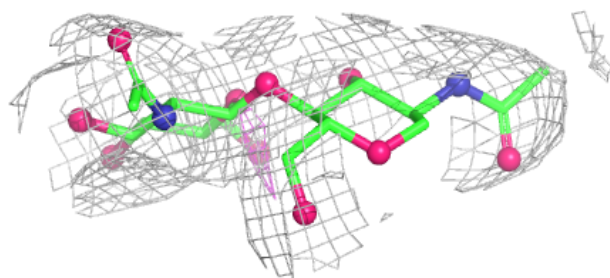
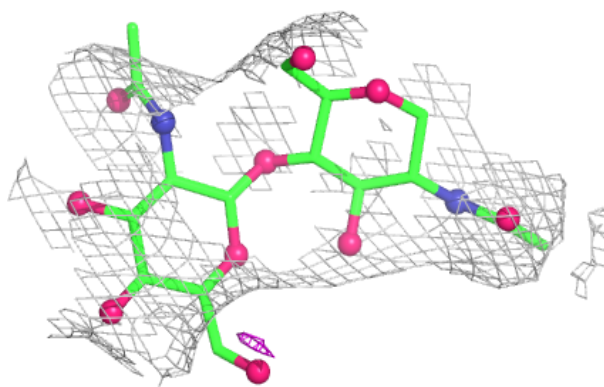
**Electron density around Chain J:**

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

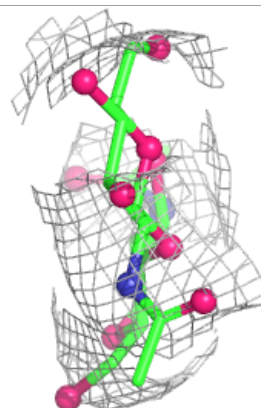
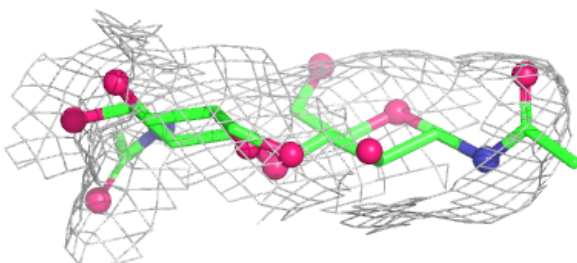
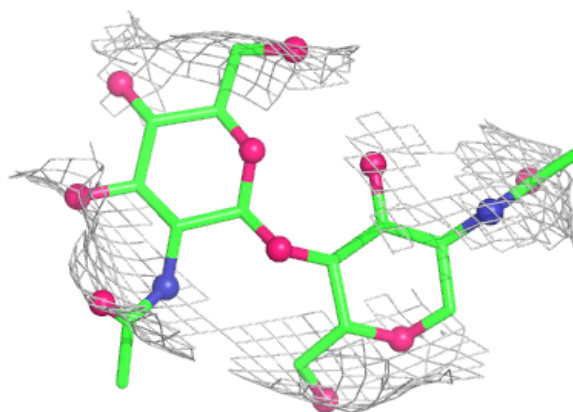


Electron density around Chain M:

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

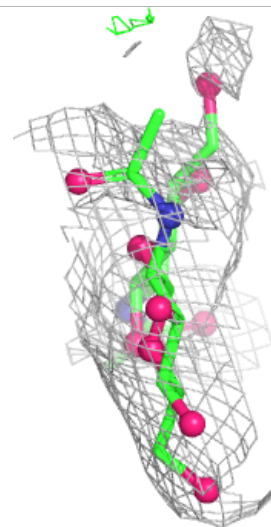
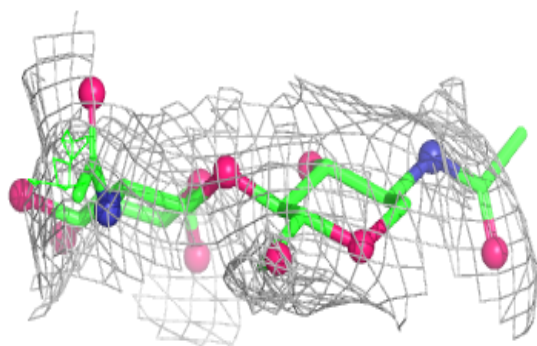
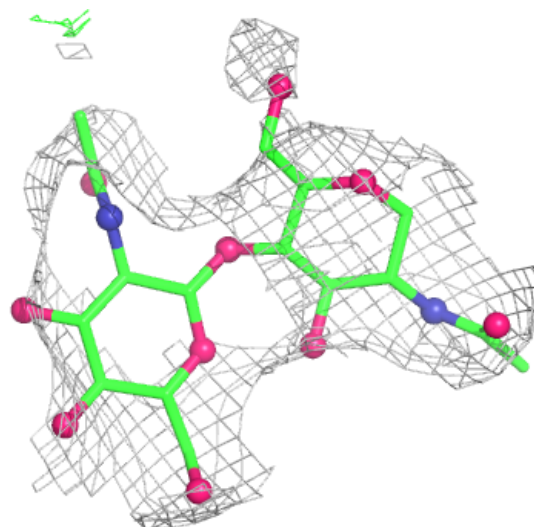
**Electron density around Chain N:**

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



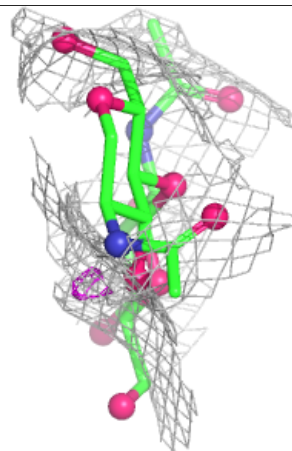
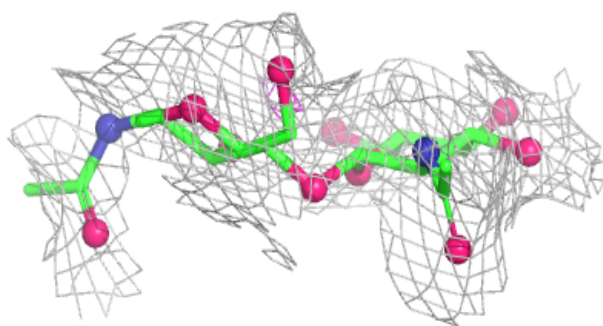
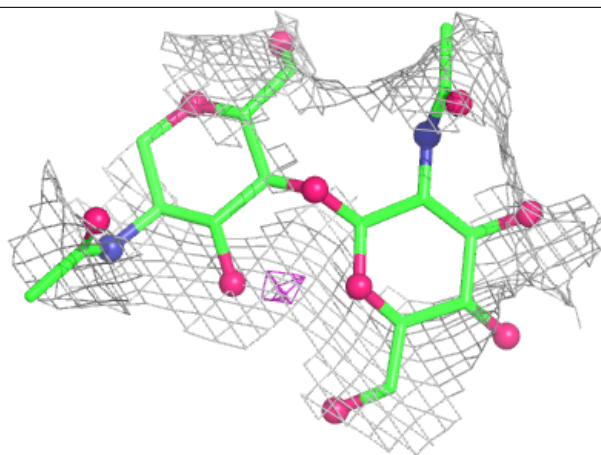
Electron density around Chain P:

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



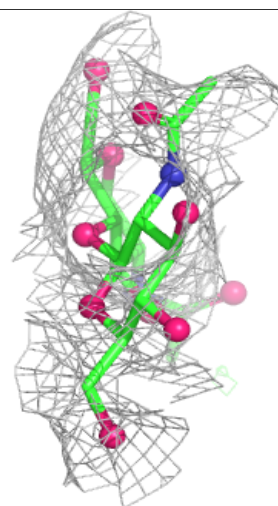
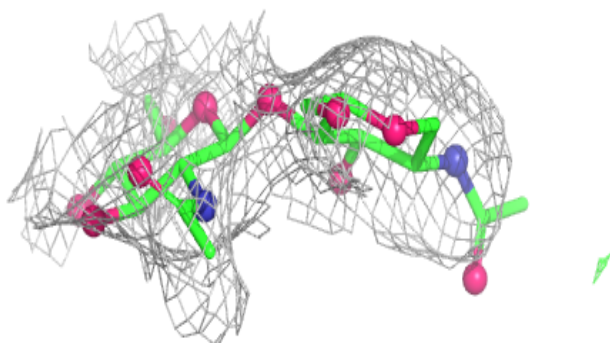
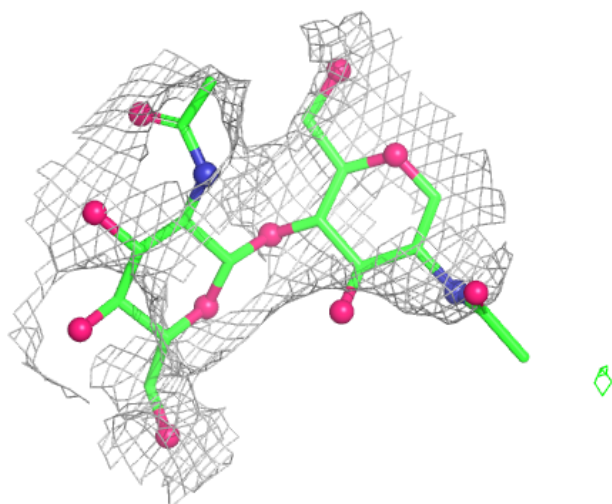
Electron density around Chain Q:

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



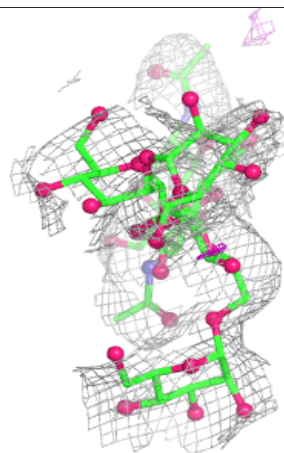
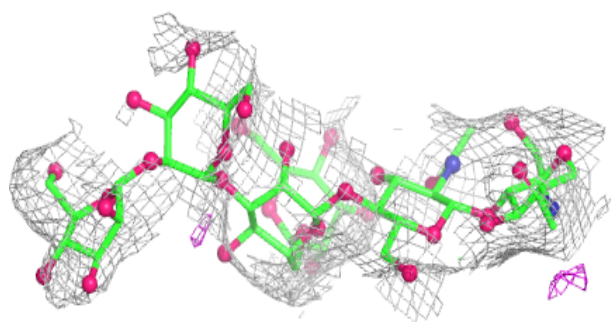
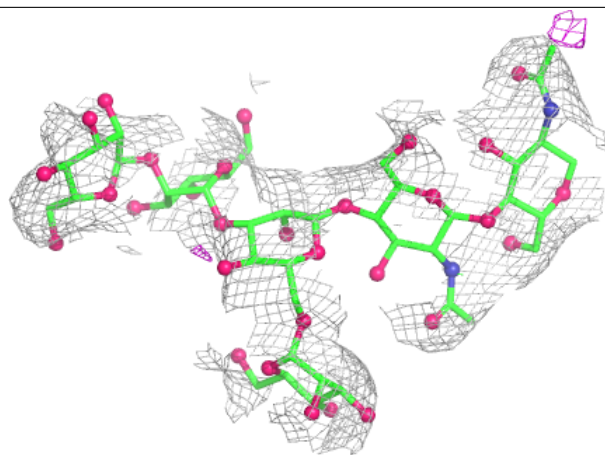
Electron density around Chain R:

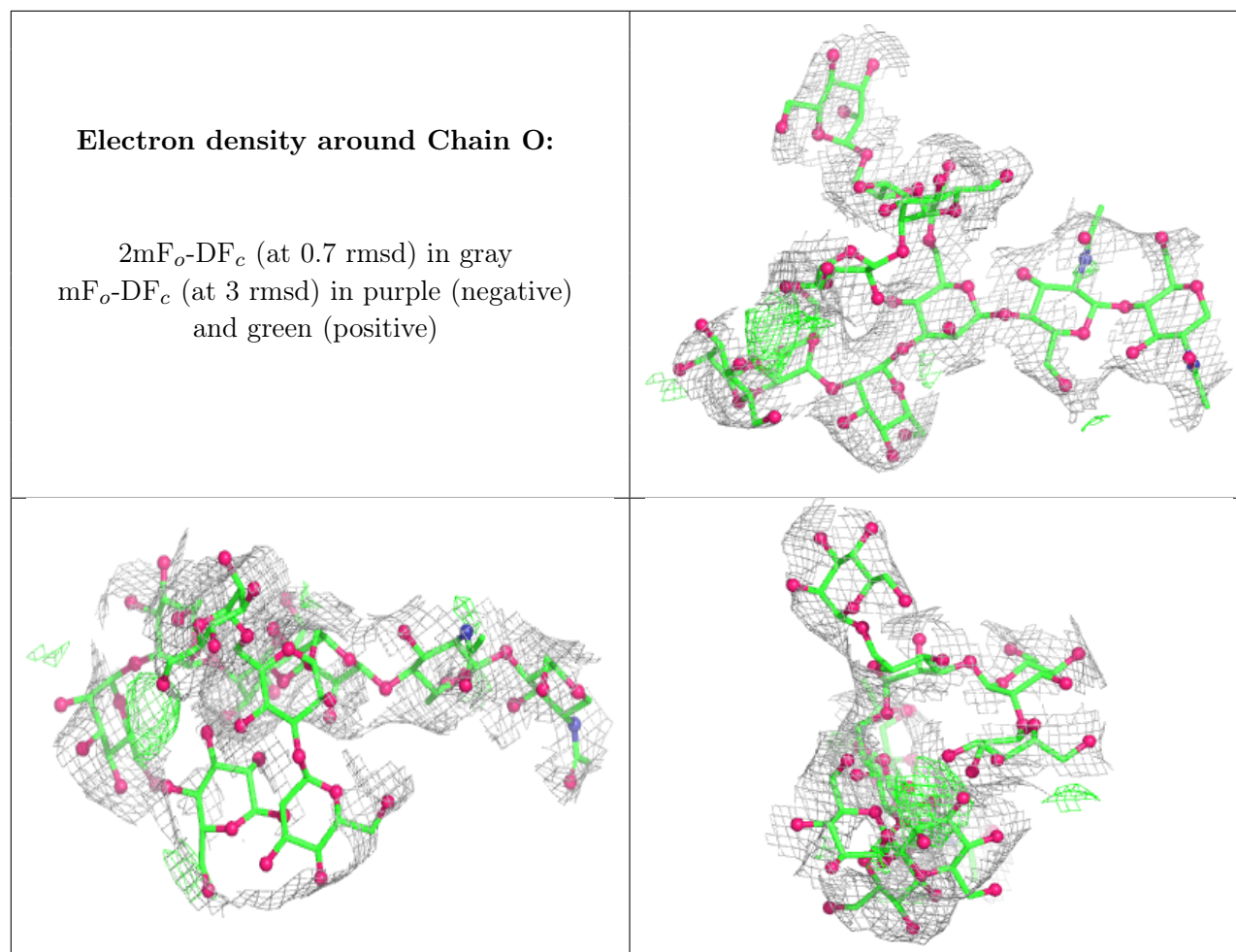
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
14	NAG	G	646	14/15	0.43	0.14	127,168,179,187	0
14	NAG	H	301	14/15	0.47	0.11	113,133,168,188	0
14	NAG	G	656	14/15	0.53	0.10	80,146,160,173	0
14	NAG	B	703	14/15	0.66	0.13	156,162,180,181	0
13	SO4	G	602	5/5	0.66	0.12	154,157,158,166	0
14	NAG	B	702	14/15	0.69	0.10	116,165,178,179	0
14	NAG	G	611	14/15	0.70	0.12	131,146,156,156	0
14	NAG	G	631	14/15	0.71	0.09	140,159,168,176	0
13	SO4	G	601	5/5	0.72	0.08	161,174,180,183	0
14	NAG	B	704	14/15	0.78	0.10	110,130,155,159	0
13	SO4	B	701	5/5	0.81	0.08	108,131,132,152	0

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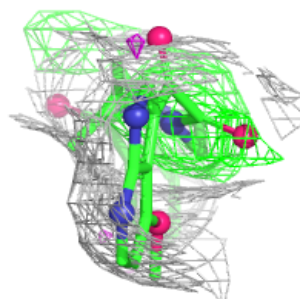
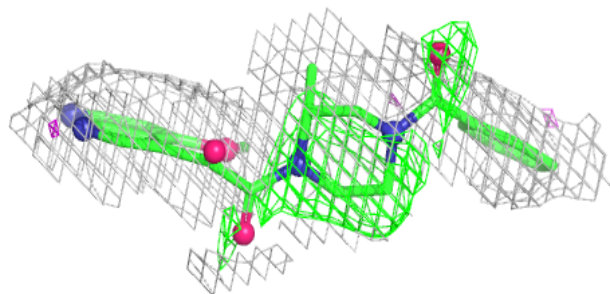
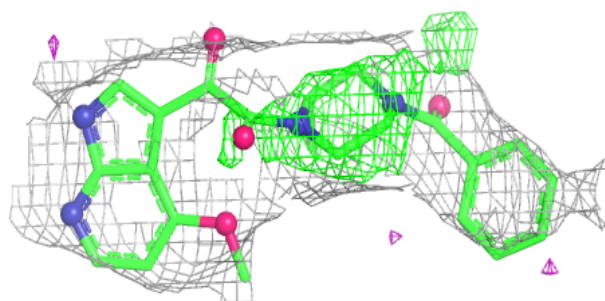
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	SO4	G	603	5/5	0.87	0.12	201,202,204,207	5
14	NAG	G	624	14/15	0.87	0.12	90,123,134,147	0
13	SO4	L	301	5/5	0.89	0.10	192,200,209,229	5
15	83G	G	657	30/30	0.92	0.18	26,74,138,232	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 83G G 657:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.