



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:51 AM UTC

PDB ID : 9NRS / pdb_00009nrs
Title : Crystal structure of the H5 influenza virus hemagglutinin from A/duck/France/161108h/2016 (H5N8) clade 2.3.4.4b in complex with O-linked glycan 26
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2025-03-14
Resolution : 2.50 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

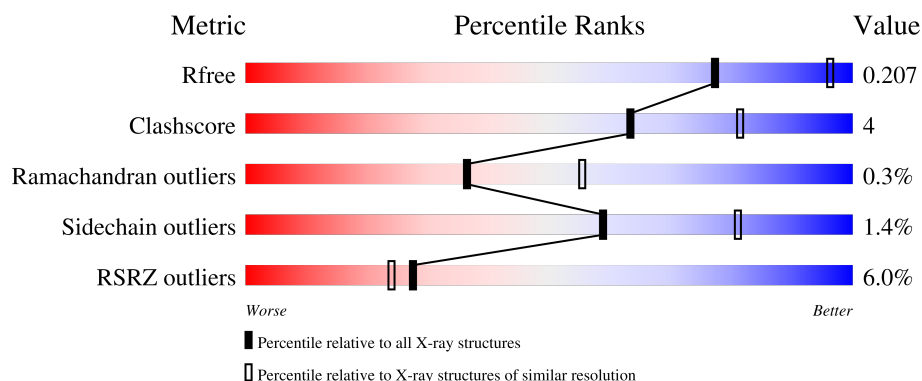
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	329	 4% 87% 10% .
1	C	329	 5% 85% 12% ..
1	E	329	 4% 87% 11% .
2	B	181	 6% 84% 9% 7%
2	D	181	 10% 84% 9% 7%

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Mol	Chain	Length	Quality of chain
2	F	181	
3	G	5	
3	H	5	
3	I	5	
3	l	5	
4	J	5	
4	L	5	
5	K	5	
6	M	2	
6	N	2	
7	O	5	
8	P	5	
9	Q	2	
9	R	2	
9	S	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	SO4	A	609	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 13309 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2548	1614	443	477	14			
1	C	324	Total	C	N	O	S	0	0	0
			2563	1623	445	481	14			
1	E	323	Total	C	N	O	S	0	0	0
			2556	1618	444	480	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	-	expression tag	UNP A0A6M2RJB8
A	9	PRO	-	expression tag	UNP A0A6M2RJB8
A	10	GLY	-	expression tag	UNP A0A6M2RJB8
C	8	ASP	-	expression tag	UNP A0A6M2RJB8
C	9	PRO	-	expression tag	UNP A0A6M2RJB8
C	10	GLY	-	expression tag	UNP A0A6M2RJB8
E	8	ASP	-	expression tag	UNP A0A6M2RJB8
E	9	PRO	-	expression tag	UNP A0A6M2RJB8
E	10	GLY	-	expression tag	UNP A0A6M2RJB8

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1378	855	240	275	8			
2	D	169	Total	C	N	O	S	0	0	0
			1378	855	240	275	8			
2	F	172	Total	C	N	O	S	0	0	0
			1399	866	246	279	8			

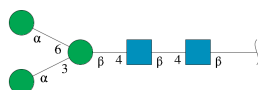
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A6M2RJB8
B	176	GLY	-	expression tag	UNP A0A6M2RJB8
B	177	ARG	-	expression tag	UNP A0A6M2RJB8
B	178	LEU	-	expression tag	UNP A0A6M2RJB8
B	179	VAL	-	expression tag	UNP A0A6M2RJB8
B	180	PRO	-	expression tag	UNP A0A6M2RJB8
B	181	ARG	-	expression tag	UNP A0A6M2RJB8
D	175	SER	-	expression tag	UNP A0A6M2RJB8
D	176	GLY	-	expression tag	UNP A0A6M2RJB8
D	177	ARG	-	expression tag	UNP A0A6M2RJB8
D	178	LEU	-	expression tag	UNP A0A6M2RJB8
D	179	VAL	-	expression tag	UNP A0A6M2RJB8
D	180	PRO	-	expression tag	UNP A0A6M2RJB8
D	181	ARG	-	expression tag	UNP A0A6M2RJB8
F	175	SER	-	expression tag	UNP A0A6M2RJB8
F	176	GLY	-	expression tag	UNP A0A6M2RJB8
F	177	ARG	-	expression tag	UNP A0A6M2RJB8
F	178	LEU	-	expression tag	UNP A0A6M2RJB8
F	179	VAL	-	expression tag	UNP A0A6M2RJB8
F	180	PRO	-	expression tag	UNP A0A6M2RJB8
F	181	ARG	-	expression tag	UNP A0A6M2RJB8

- Molecule 3 is a protein called Peptide linker.

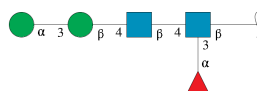
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			26	17	4	5			
3	G	5	Total	C	N	O	0	0	0
			37	26	5	6			
3	H	5	Total	C	N	O	0	0	0
			37	26	5	6			
3	I	5	Total	C	N	O	0	0	0
			37	26	5	6			

- Molecule 4 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
4	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acet amido-2-deoxy-beta-D-glucopyranose.



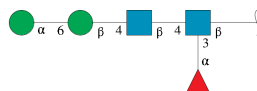
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



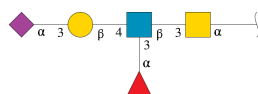
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



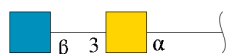
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	O	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 8 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



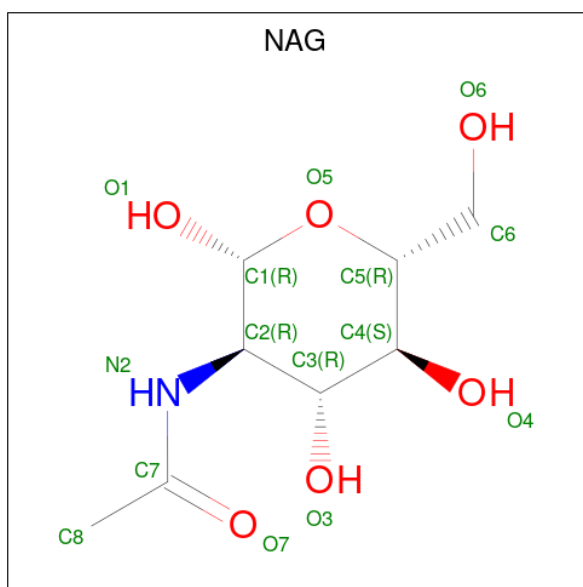
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	P	5	Total	C	N	O	0	0	0
			69	39	3	27			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



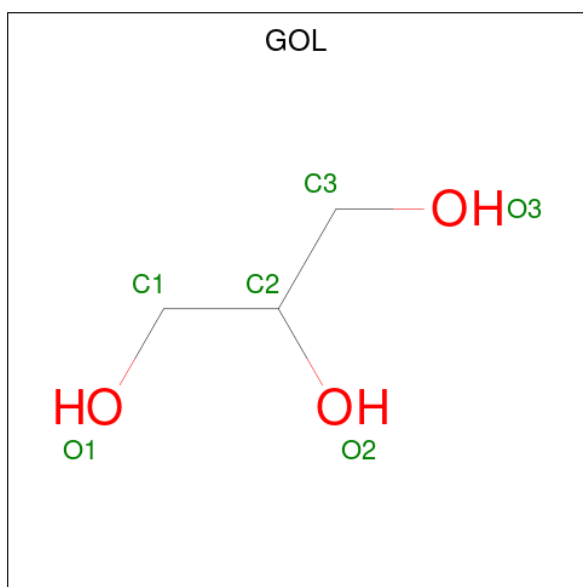
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



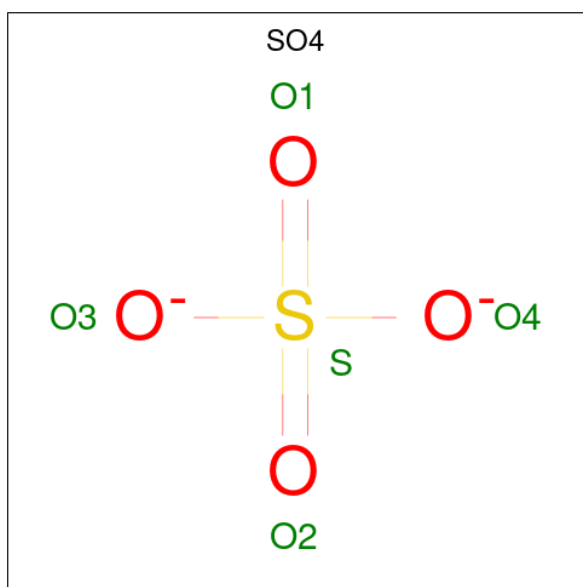
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		
11	C	1	Total	C	O	0	0
			6	3	3		
11	D	1	Total	C	O	0	0
			6	3	3		
11	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	E	1	Total	O	S	0	0
			5	4	1		
12	E	1	Total	O	S	0	0
			5	4	1		
12	E	1	Total	O	S	0	0
			5	4	1		
12	E	1	Total	O	S	0	0
			5	4	1		
12	E	1	Total	O	S	0	0
			5	4	1		

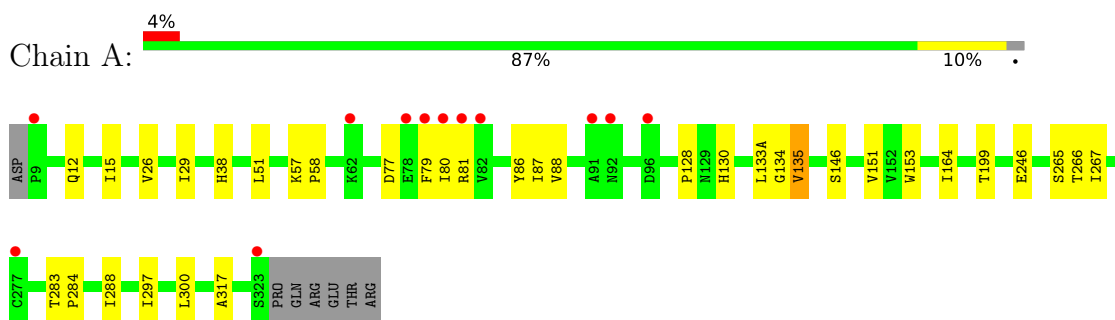
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	159	Total	O	0	0
			159	159		
13	B	58	Total	O	0	0
			58	58		
13	C	150	Total	O	0	0
			150	150		
13	D	35	Total	O	0	0
			35	35		
13	E	186	Total	O	0	0
			186	186		
13	F	76	Total	O	0	0
			76	76		
13	l	1	Total	O	0	0
			1	1		

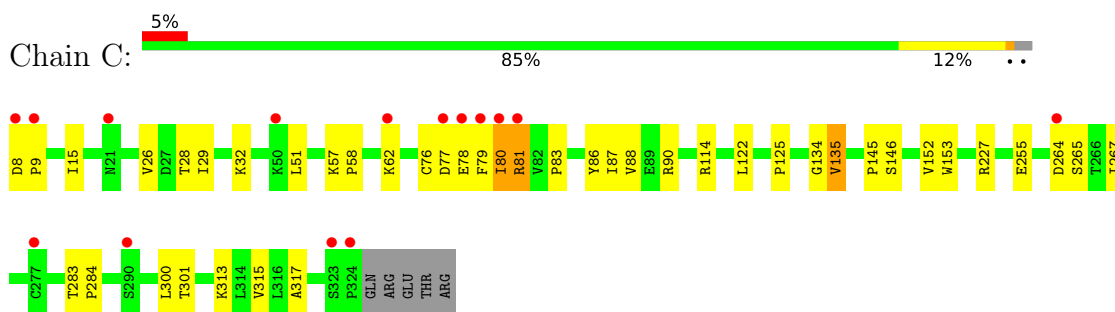
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

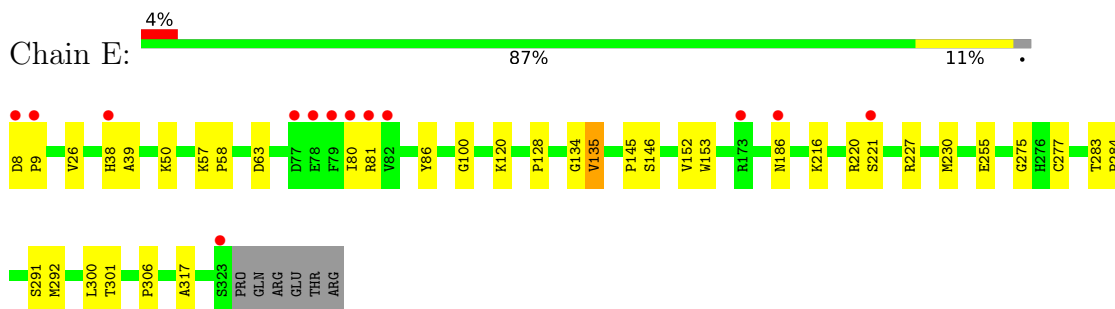
- Molecule 1: Hemagglutinin HA1 chain



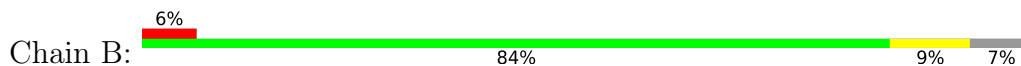
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

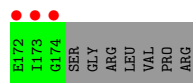
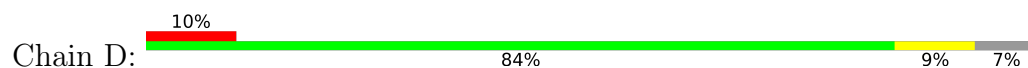


- Molecule 2: Hemagglutinin HA2 chain

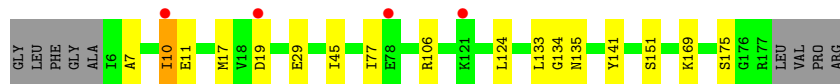
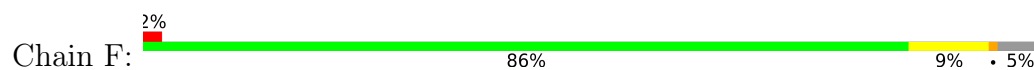




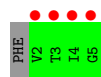
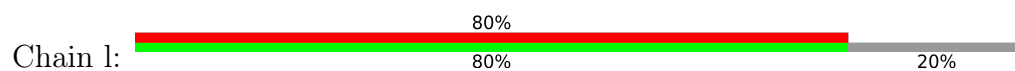
● Molecule 2: Hemagglutinin HA2 chain



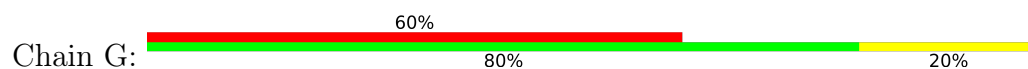
● Molecule 2: Hemagglutinin HA2 chain



● Molecule 3: Peptide linker



● Molecule 3: Peptide linker



● Molecule 3: Peptide linker



● Molecule 3: Peptide linker



- Molecule 4: 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 J:  20% 80%

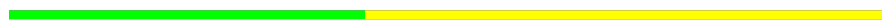
MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 4: 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 L:  20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  40% 60%

MAG1
MAG2
BMA3
MAN4
FUC5

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

Chain M:  100%

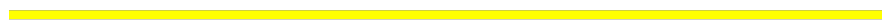
MAG1
MAG2

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

Chain N:  100%

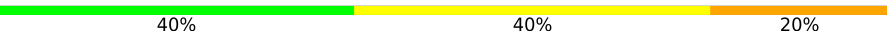
MAG1
MAG2

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

Chain O:  100%

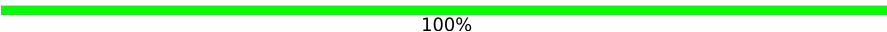
MAG1
MAG2
BMA3
MAN4
FUC5

- Molecule 8: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain P:  40% 40% 20%

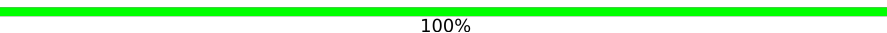
A2G1
NAG2
GAL3
STI4
FUC5

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain Q:  100%

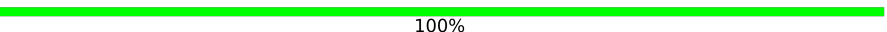
A2G1
NAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain R:  100%

A2G1
NAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain S:  100%

A2G1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.33Å 171.94Å 225.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.50 49.12 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.12-2.50) 99.6 (49.12-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, R_{free}	0.174 , 0.208 0.174 , 0.207	Depositor DCC
R_{free} test set	6355 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13309	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: GAL, NAG, FUC, GOL, BMA, A2G, SIA, SO4, 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	0.11	0/2612	0.31	0/3552
1	C	0.12	0/2628	0.32	0/3576
1	E	0.12	0/2620	0.33	0/3564
2	B	0.11	0/1404	0.28	0/1887
2	D	0.11	0/1404	0.27	0/1887
2	F	0.10	0/1425	0.26	0/1914
3	G	0.09	0/37	0.18	0/49
3	H	0.09	0/37	0.26	0/49
3	I	0.06	0/37	0.21	0/49
3	I	0.08	0/25	0.23	0/33
All	All	0.11	0/12229	0.30	0/16560

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2548	0	2500	19	0
1	C	2563	0	2511	28	0
1	E	2556	0	2504	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1378	0	1282	12	0
2	D	1378	0	1282	13	0
2	F	1399	0	1303	13	0
3	G	37	0	40	1	0
3	H	37	0	40	0	0
3	I	37	0	40	1	0
3	l	26	0	28	0	0
4	J	61	0	52	0	0
4	L	61	0	52	0	0
5	K	60	0	52	0	0
6	M	28	0	25	2	0
6	N	28	0	25	1	0
7	O	60	0	52	1	0
8	P	69	0	58	1	0
9	Q	28	0	24	0	0
9	R	28	0	24	0	0
9	S	28	0	24	0	0
10	A	42	0	39	0	0
10	C	28	0	26	0	0
10	E	28	0	26	0	0
11	A	6	0	8	0	0
11	B	12	0	16	0	0
11	C	6	0	8	0	0
11	D	6	0	8	1	0
11	E	6	0	8	0	0
12	A	25	0	0	3	0
12	B	5	0	0	0	0
12	C	35	0	0	2	0
12	D	5	0	0	0	0
12	E	30	0	0	1	0
13	A	159	0	0	1	0
13	B	58	0	0	1	0
13	C	150	0	0	0	0
13	D	35	0	0	1	0
13	E	186	0	0	3	0
13	F	76	0	0	0	0
13	l	1	0	0	0	0
All	All	13309	0	12057	98	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 4.

All (98) 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:C:28:THR:HB	2:D:105:GLU:HG2	1.66	0.77
2:D:82:LYS:NZ	2:D:86:ASP:OD2	2.24	0.70
1:E:216:LYS:O	1:E:220:ARG:NH2	2.23	0.70
2:B:80:LEU:HD12	2:D:80:LEU:HD21	1.75	0.69
2:F:10:ILE:HG12	2:F:135:ASN:HA	1.77	0.66
2:D:151:SER:HB3	6:M:1:NAG:H62	1.77	0.65
1:C:227:ARG:NH2	12:C:607:SO4:O2	2.27	0.63
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.81	0.62
1:C:135:VAL:HG22	1:C:146:SER:HA	1.83	0.61
1:A:57:LYS:HG2	1:A:58:PRO:HD2	1.82	0.60
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.81	0.60
1:C:57:LYS:HG2	1:C:58:PRO:HD2	1.82	0.60
2:D:106:ARG:NH1	13:D:301:HOH:O	2.28	0.59
2:B:153:ARG:NH2	13:B:301:HOH:O	2.32	0.58
1:A:288:ILE:HG21	1:A:297:ILE:HD13	1.86	0.57
1:C:313:LYS:HG3	1:C:315:VAL:HG23	1.87	0.56
1:E:283:THR:HG22	1:E:301:THR:HG22	1.88	0.56
1:E:57:LYS:HG2	1:E:58:PRO:HD2	1.86	0.56
6:M:1:NAG:H4	6:M:2:NAG:N2	2.22	0.55
1:C:29:ILE:HG22	2:D:105:GLU:HG3	1.89	0.55
1:E:128:PRO:HD2	12:E:608:SO4:O1	2.07	0.55
1:C:87:ILE:HB	1:C:267:ILE:HD13	1.89	0.54
1:A:135:VAL:HG22	1:A:146:SER:HA	1.87	0.54
1:C:227:ARG:NH1	12:C:606:SO4:O4	2.41	0.54
2:D:124:LEU:HD23	2:F:134:GLY:HA2	1.89	0.54
1:A:38:HIS:CD2	3:I:5:GLY:H	2.26	0.54
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.89	0.53
1:C:283:THR:HG22	1:C:301:THR:HG22	1.91	0.52
1:A:12:GLN:NE2	13:A:707:HOH:O	2.43	0.52
1:C:76:CYS:O	1:C:78:GLU:N	2.42	0.52
2:D:164:GLU:OE1	2:F:175:SER:HA	2.10	0.52
2:B:59:MET:HE3	2:B:59:MET:HA	1.92	0.52
1:A:79:PHE:O	1:A:81:ARG:N	2.41	0.51
2:B:9:PHE:HE1	2:B:116:LYS:HG2	1.75	0.51
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.92	0.51
1:E:135:VAL:HG22	1:E:146:SER:HA	1.91	0.51
2:F:141:TYR:O	2:F:169:LYS:HD2	2.12	0.49
2:F:7:ALA:HB1	2:F:11:GLU:HG3	1.95	0.49
1:C:90:ARG:N	1:C:90:ARG:HD2	2.29	0.48
2:B:77:ILE:HD11	2:F:77:ILE:HD13	1.96	0.48
1:E:186:ASN:ND2	1:E:227:ARG:HB2	2.29	0.48
1:A:130:HIS:ND1	12:A:609:SO4:O1	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LEU:HD13	1:C:88:VAL:HG21	1.95	0.47
2:B:106:ARG:HG2	2:F:106:ARG:NH2	2.29	0.47
1:C:78:GLU:HG2	1:C:80:ILE:H	1.80	0.47
1:E:186:ASN:CG	1:E:227:ARG:HB2	2.40	0.47
2:D:68:ARG:HB3	11:D:201:GOL:H12	1.96	0.46
1:E:152:VAL:HG23	1:E:255:GLU:HB2	1.96	0.46
1:C:15:ILE:HG23	2:D:118:LEU:HD23	1.97	0.46
2:F:151:SER:HB3	7:O:1:NAG:H62	1.97	0.46
1:C:135:VAL:HG13	1:C:145:PRO:HB2	1.97	0.46
1:A:164:ILE:O	1:A:246:GLU:HA	2.15	0.46
2:F:45:ILE:HG23	3:G:4:ILE:HD11	1.97	0.46
1:C:78:GLU:CD	1:C:80:ILE:HG23	2.41	0.46
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.98	0.45
12:A:607:SO4:O1	2:B:71:ASN:ND2	2.49	0.45
1:A:133(A):LEU:O	8:P:4:SIA:H113	2.17	0.45
6:N:1:NAG:H61	6:N:2:NAG:C7	2.46	0.45
2:B:50:ASN:HD21	1:C:32:LYS:HD2	1.82	0.45
1:C:8:ASP:HB3	1:C:9:PRO:HD3	1.99	0.45
1:C:122:LEU:HD21	1:C:125:PRO:HB3	1.98	0.44
1:E:50:LYS:HD3	1:E:275:GLY:HA3	1.98	0.44
1:E:63:ASP:OD1	1:E:63:ASP:N	2.49	0.44
1:C:81:ARG:O	1:C:83:PRO:HD3	2.17	0.44
1:E:292:MET:HA	1:E:292:MET:HE2	2.00	0.44
1:C:114:ARG:HB2	1:C:265:SER:HB2	1.99	0.44
1:E:38:HIS:CD2	1:E:39:ALA:H	2.36	0.44
2:D:59:MET:HE1	2:D:92:TRP:CZ3	2.53	0.43
1:A:26:VAL:HG21	1:A:317:ALA:HB2	2.00	0.43
1:C:284:PRO:HD3	1:C:300:LEU:O	2.18	0.43
1:E:284:PRO:HD3	1:E:300:LEU:O	2.18	0.43
2:F:19:ASP:OD1	2:F:19:ASP:N	2.50	0.43
1:C:114:ARG:NH2	1:C:264:ASP:O	2.52	0.43
1:E:58:PRO:HB3	1:E:86:TYR:CE1	2.54	0.43
1:A:51:LEU:HD13	1:A:88:VAL:HG21	2.00	0.43
1:A:87:ILE:HB	1:A:267:ILE:HD13	2.01	0.42
1:E:8:ASP:HB3	1:E:9:PRO:HD3	2.01	0.42
1:E:26:VAL:HG21	1:E:317:ALA:HB2	2.00	0.42
1:E:100:GLY:HA3	1:E:230:MET:O	2.19	0.42
1:C:58:PRO:HB3	1:C:86:TYR:CE1	2.55	0.42
1:C:79:PHE:HD1	1:C:81:ARG:HG3	1.85	0.42
1:E:135:VAL:HG13	1:E:145:PRO:HB2	2.01	0.42
2:D:123:ARG:HD2	2:D:132:GLU:OE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:GLY:HA2	2:F:124:LEU:HD13	2.03	0.41
2:F:17:MET:HE2	2:F:17:MET:HB3	1.91	0.41
1:C:152:VAL:HG23	1:C:255:GLU:HB2	2.03	0.41
1:E:227:ARG:NH2	13:E:709:HOH:O	2.50	0.41
1:E:291:SER:N	13:E:713:HOH:O	2.52	0.41
1:A:265:SER:OG	1:A:266:THR:N	2.37	0.41
2:B:7:ALA:HB2	2:B:137:CYS:SG	2.61	0.41
13:E:729:HOH:O	2:F:29:GLU:HG3	2.20	0.40
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.56	0.40
1:A:29:ILE:HD12	1:A:29:ILE:HA	1.92	0.40
1:A:284:PRO:HD3	1:A:300:LEU:O	2.22	0.40
2:D:141:TYR:CE2	2:D:170:ARG:HG3	2.56	0.40
1:E:292:MET:O	1:E:306:PRO:HB3	2.22	0.40
1:A:128:PRO:HD2	12:A:609:SO4:O2	2.20	0.40
2:B:83:LYS:HE3	2:B:83:LYS:HB2	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/329 (97%)	303 (95%)	16 (5%)	1 (0%)	36	55
1	C	322/329 (98%)	307 (95%)	14 (4%)	1 (0%)	36	55
1	E	321/329 (98%)	308 (96%)	11 (3%)	2 (1%)	21	38
2	B	167/181 (92%)	164 (98%)	2 (1%)	1 (1%)	21	38
2	D	167/181 (92%)	161 (96%)	6 (4%)	0	100	100
2	F	170/181 (94%)	170 (100%)	0	0	100	100
3	G	3/5 (60%)	3 (100%)	0	0	100	100
3	H	3/5 (60%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	3/5 (60%)	3 (100%)	0	0	100	100
3	l	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1478/1550 (95%)	1424 (96%)	49 (3%)	5 (0%)	36	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	77	ASP
1	E	81	ARG
2	B	8	GLY
1	A	80	ILE
1	E	80	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/294 (98%)	282 (98%)	5 (2%)	53	78
1	C	289/294 (98%)	285 (99%)	4 (1%)	59	81
1	E	288/294 (98%)	284 (99%)	4 (1%)	59	81
2	B	146/154 (95%)	144 (99%)	2 (1%)	59	81
2	D	146/154 (95%)	145 (99%)	1 (1%)	76	89
2	F	148/154 (96%)	146 (99%)	2 (1%)	59	81
3	G	4/4 (100%)	4 (100%)	0	100	100
3	H	4/4 (100%)	4 (100%)	0	100	100
3	I	4/4 (100%)	4 (100%)	0	100	100
3	l	3/4 (75%)	3 (100%)	0	100	100
All	All	1319/1360 (97%)	1301 (99%)	18 (1%)	59	81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	135	VAL
1	A	151	VAL
1	A	199	THR
1	A	283	THR
2	B	22	TYR
2	B	61	THR
1	C	62	LYS
1	C	80	ILE
1	C	81	ARG
1	C	135	VAL
2	D	61	THR
1	E	120	LYS
1	E	135	VAL
1	E	221	SER
1	E	277	CYS
2	F	10	ILE
2	F	133	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	18	HIS
1	A	25	GLN
1	A	38	HIS
1	A	55	ASN
1	A	95	ASN
1	A	117	HIS
1	A	129	ASN
1	A	142	GLN
1	A	172	ASN
1	A	222	GLN
1	C	38	HIS
1	C	240	ASN
1	C	244	HIS
2	D	25	HIS
2	D	95	ASN
1	E	193	ASN
2	F	15	GLN
2	F	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

35 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	$\# Z > 2$
4	NAG	J	1	4,1	14,14,15	0.67	0	17,19,21	0.90	0
4	NAG	J	2	4	14,14,15	0.78	0	17,19,21	1.10	2 (11%)
4	BMA	J	3	4	11,11,12	0.77	0	15,15,17	1.55	2 (13%)
4	MAN	J	4	4	11,11,12	0.62	0	15,15,17	1.37	1 (6%)
4	MAN	J	5	4	11,11,12	0.68	0	15,15,17	1.47	1 (6%)
5	NAG	K	1	2,5	14,14,15	0.74	0	17,19,21	0.90	1 (5%)
5	NAG	K	2	5	14,14,15	0.74	0	17,19,21	0.85	0
5	BMA	K	3	5	11,11,12	0.82	0	15,15,17	1.79	2 (13%)
5	MAN	K	4	5	11,11,12	0.62	0	15,15,17	1.46	1 (6%)
5	FUC	K	5	5	10,10,11	0.75	0	14,14,16	0.94	0
4	NAG	L	1	4,1	14,14,15	0.78	0	17,19,21	1.14	2 (11%)
4	NAG	L	2	4	14,14,15	0.70	0	17,19,21	0.77	0
4	BMA	L	3	4	11,11,12	0.88	0	15,15,17	1.49	2 (13%)
4	MAN	L	4	4	11,11,12	0.63	0	15,15,17	1.35	1 (6%)
4	MAN	L	5	4	11,11,12	0.73	0	15,15,17	1.07	1 (6%)
6	NAG	M	1	2,6	14,14,15	0.70	0	17,19,21	0.96	1 (5%)
6	NAG	M	2	6	14,14,15	0.83	1 (7%)	17,19,21	1.42	3 (17%)
6	NAG	N	1	1,6	14,14,15	0.79	0	17,19,21	1.24	2 (11%)
6	NAG	N	2	6	14,14,15	0.69	0	17,19,21	1.25	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	O	1	7,2	14,14,15	0.70	0	17,19,21	0.86	0
7	NAG	O	2	7	14,14,15	0.72	0	17,19,21	1.00	1 (5%)
7	BMA	O	3	7	11,11,12	0.88	0	15,15,17	1.70	1 (6%)
7	MAN	O	4	7	11,11,12	0.69	0	15,15,17	1.09	1 (6%)
7	FUC	O	5	7	10,10,11	0.72	0	14,14,16	1.26	1 (7%)
8	A2G	P	1	3,8	14,14,15	0.81	0	17,19,21	0.85	0
8	NAG	P	2	8	14,14,15	0.76	0	17,19,21	0.84	0
8	GAL	P	3	8	11,11,12	0.72	0	15,15,17	1.12	1 (6%)
8	SIA	P	4	8	20,20,21	1.61	2 (10%)	21,28,31	1.66	4 (19%)
8	FUC	P	5	8	10,10,11	0.76	0	14,14,16	0.95	1 (7%)
9	A2G	Q	1	9,3	14,14,15	0.80	0	17,19,21	0.76	0
9	NAG	Q	2	9	14,14,15	0.74	0	17,19,21	0.90	0
9	A2G	R	1	9,3	14,14,15	0.80	0	17,19,21	0.80	0
9	NAG	R	2	9	14,14,15	0.73	0	17,19,21	0.87	0
9	A2G	S	1	9,3	14,14,15	0.79	0	17,19,21	0.79	0
9	NAG	S	2	9	14,14,15	0.72	0	17,19,21	0.89	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
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	MAN	J	5	4	-	0/2/19/22	0/1/1/1
5	NAG	K	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	2/2/19/22	0/1/1/1
5	MAN	K	4	5	-	1/2/19/22	0/1/1/1
5	FUC	K	5	5	-	-	0/1/1/1
4	NAG	L	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
4	MAN	L	4	4	-	0/2/19/22	0/1/1/1
4	MAN	L	5	4	-	0/2/19/22	0/1/1/1
6	NAG	M	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	N	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	3/6/23/26	0/1/1/1
7	NAG	O	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
7	BMA	O	3	7	-	1/2/19/22	0/1/1/1
7	MAN	O	4	7	-	0/2/19/22	0/1/1/1
7	FUC	O	5	7	-	-	0/1/1/1
8	A2G	P	1	3,8	-	2/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1
8	GAL	P	3	8	-	0/2/19/22	0/1/1/1
8	SIA	P	4	8	-	1/18/34/38	0/1/1/1
8	FUC	P	5	8	-	-	0/1/1/1
9	A2G	Q	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	0/6/23/26	0/1/1/1
9	A2G	R	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	R	2	9	-	0/6/23/26	0/1/1/1
9	A2G	S	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	S	2	9	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	4	SIA	C2-C1	5.66	1.59	1.52
6	M	2	NAG	C1-C2	2.32	1.55	1.52
8	P	4	SIA	O6-C2	2.09	1.47	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	3	BMA	C1-O5-C5	5.19	119.14	112.19
7	O	3	BMA	C1-O5-C5	5.10	119.02	112.19
5	K	4	MAN	C1-O5-C5	4.82	118.64	112.19
4	J	5	MAN	C1-O5-C5	4.43	118.12	112.19
8	P	4	SIA	O1A-C1-C2	-4.34	113.47	122.85
4	L	4	MAN	C1-O5-C5	4.33	117.99	112.19
4	J	4	MAN	C1-O5-C5	4.30	117.95	112.19
4	J	3	BMA	C1-O5-C5	4.08	117.65	112.19
6	M	2	NAG	C1-O5-C5	4.04	117.61	112.19
4	L	3	BMA	C1-O5-C5	3.70	117.15	112.19
8	P	4	SIA	O6-C2-C3	-3.62	105.69	110.56
6	N	2	NAG	C2-N2-C7	3.48	127.57	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	3	GAL	O3-C3-C2	-3.31	103.31	110.05
7	O	4	MAN	C1-O5-C5	3.17	116.43	112.19
7	O	2	NAG	O5-C1-C2	-2.93	106.76	111.29
4	L	5	MAN	C1-O5-C5	2.65	115.73	112.19
4	J	2	NAG	O4-C4-C3	-2.54	104.39	110.38
5	K	3	BMA	O3-C3-C2	-2.43	105.10	110.05
6	M	1	NAG	O5-C1-C2	-2.41	107.56	111.29
8	P	4	SIA	O1B-C1-O1A	2.40	129.53	124.08
6	M	2	NAG	C2-N2-C7	2.28	125.96	122.90
7	O	5	FUC	C1-O5-C5	2.27	118.31	112.97
4	J	2	NAG	C4-C3-C2	2.25	114.32	111.02
6	N	1	NAG	C1-O5-C5	2.24	115.19	112.19
4	J	3	BMA	O3-C3-C2	-2.22	105.52	110.05
8	P	4	SIA	C6-C5-N5	-2.21	107.38	110.91
6	N	1	NAG	C2-N2-C7	2.20	125.85	122.90
6	M	2	NAG	C1-C2-N2	2.13	113.79	110.43
4	L	1	NAG	C2-N2-C7	2.09	125.70	122.90
5	K	1	NAG	C1-O5-C5	2.02	114.89	112.19
4	L	3	BMA	O3-C3-C2	-2.01	105.95	110.05
8	P	5	FUC	C1-O5-C5	2.00	117.69	112.97
4	L	1	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	S	2	NAG	C4-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
8	P	1	A2G	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
7	O	2	NAG	C4-C5-C6-O6
9	S	2	NAG	O5-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6
6	M	2	NAG	C8-C7-N2-C2
6	M	2	NAG	O7-C7-N2-C2
4	J	2	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	N	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
5	K	3	BMA	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6

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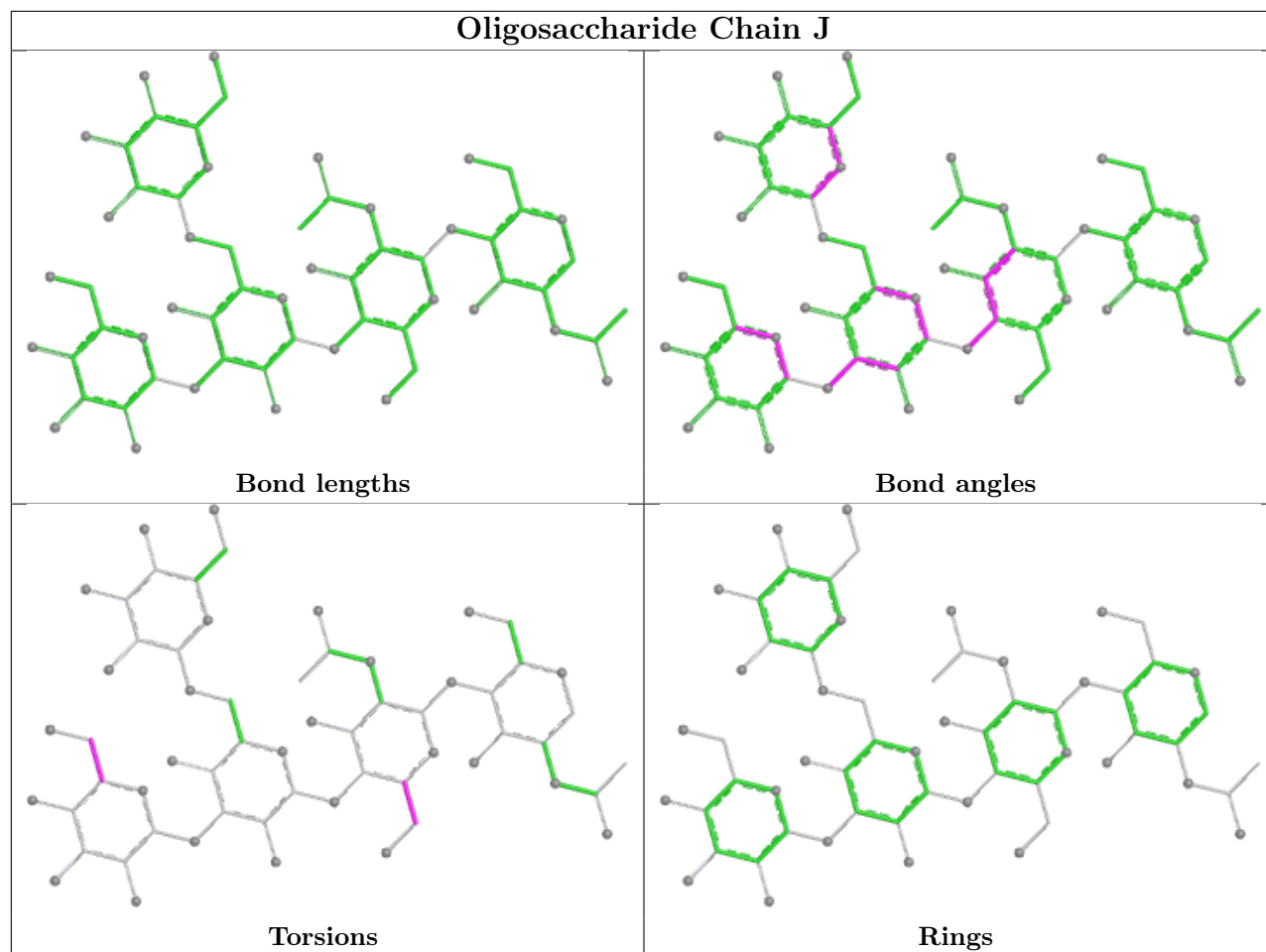
Mol	Chain	Res	Type	Atoms
7	O	3	BMA	O5-C5-C6-O6
8	P	1	A2G	C4-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
8	P	4	SIA	C6-C7-C8-O8
5	K	4	MAN	C4-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
6	N	2	NAG	C3-C2-N2-C7
6	M	2	NAG	O5-C5-C6-O6

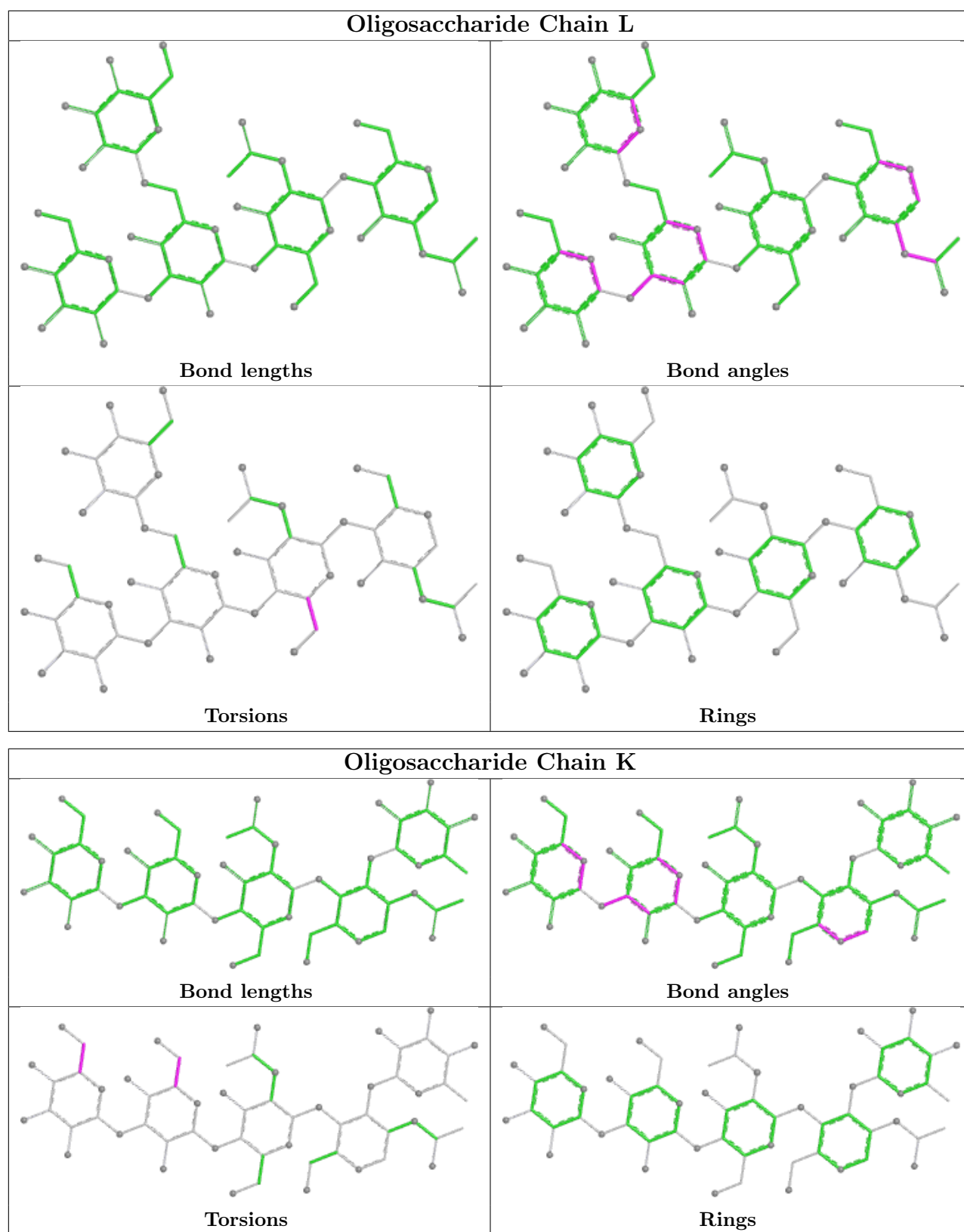
There are no ring outliers.

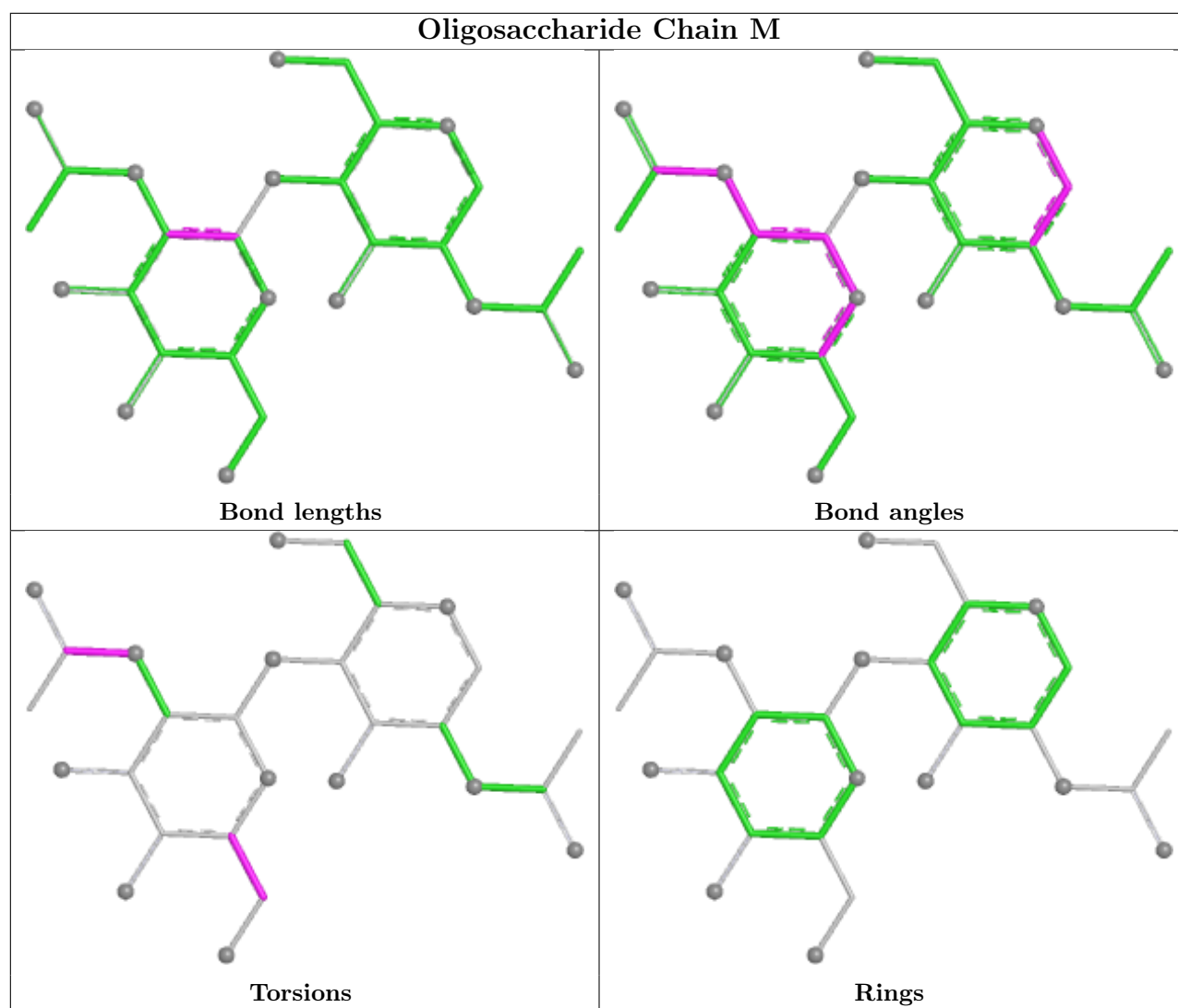
6 monomers are involved in 5 short contacts:

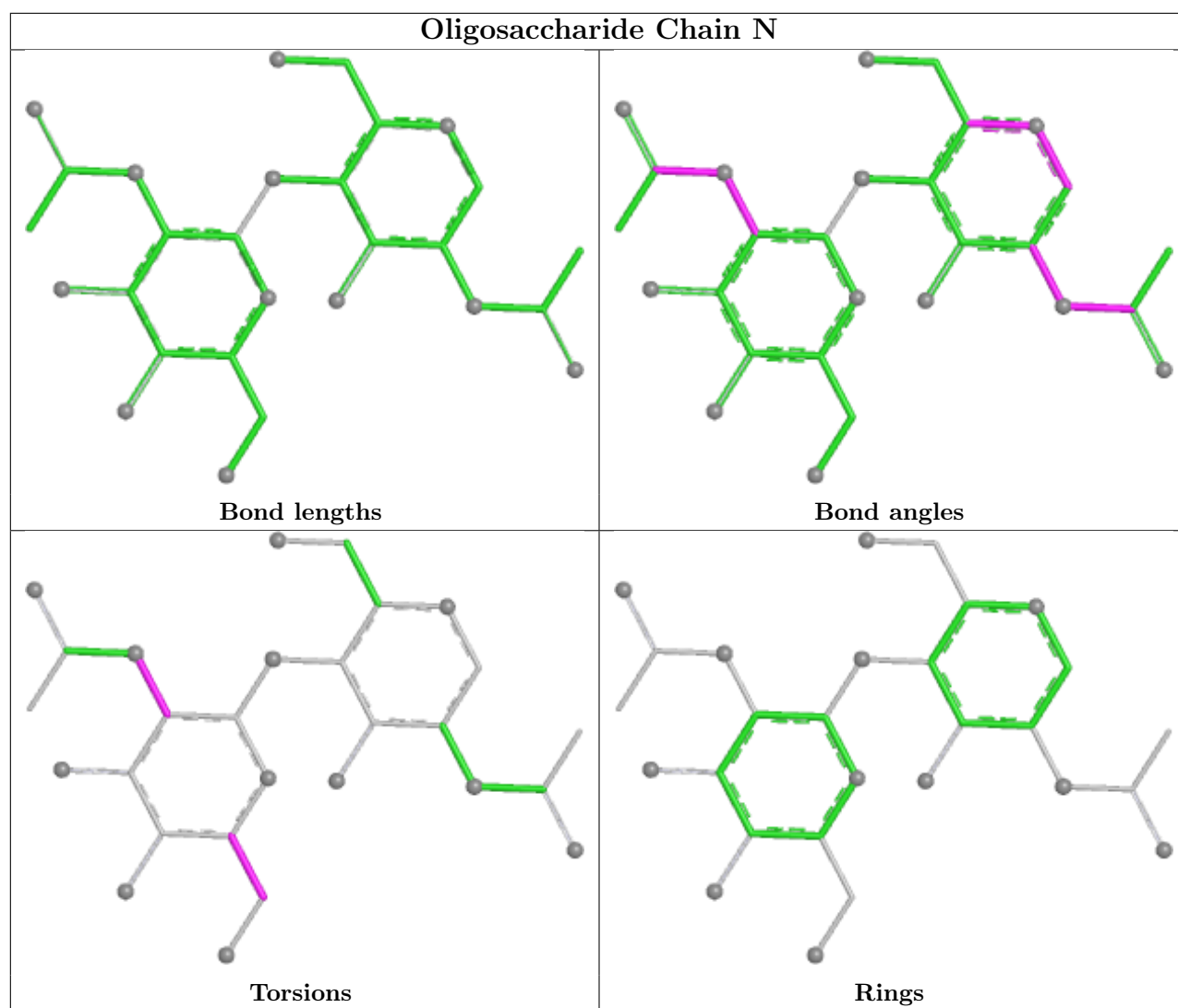
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1	NAG	2	0
6	N	1	NAG	1	0
6	M	2	NAG	1	0
8	P	4	SIA	1	0
7	O	1	NAG	1	0
6	N	2	NAG	1	0

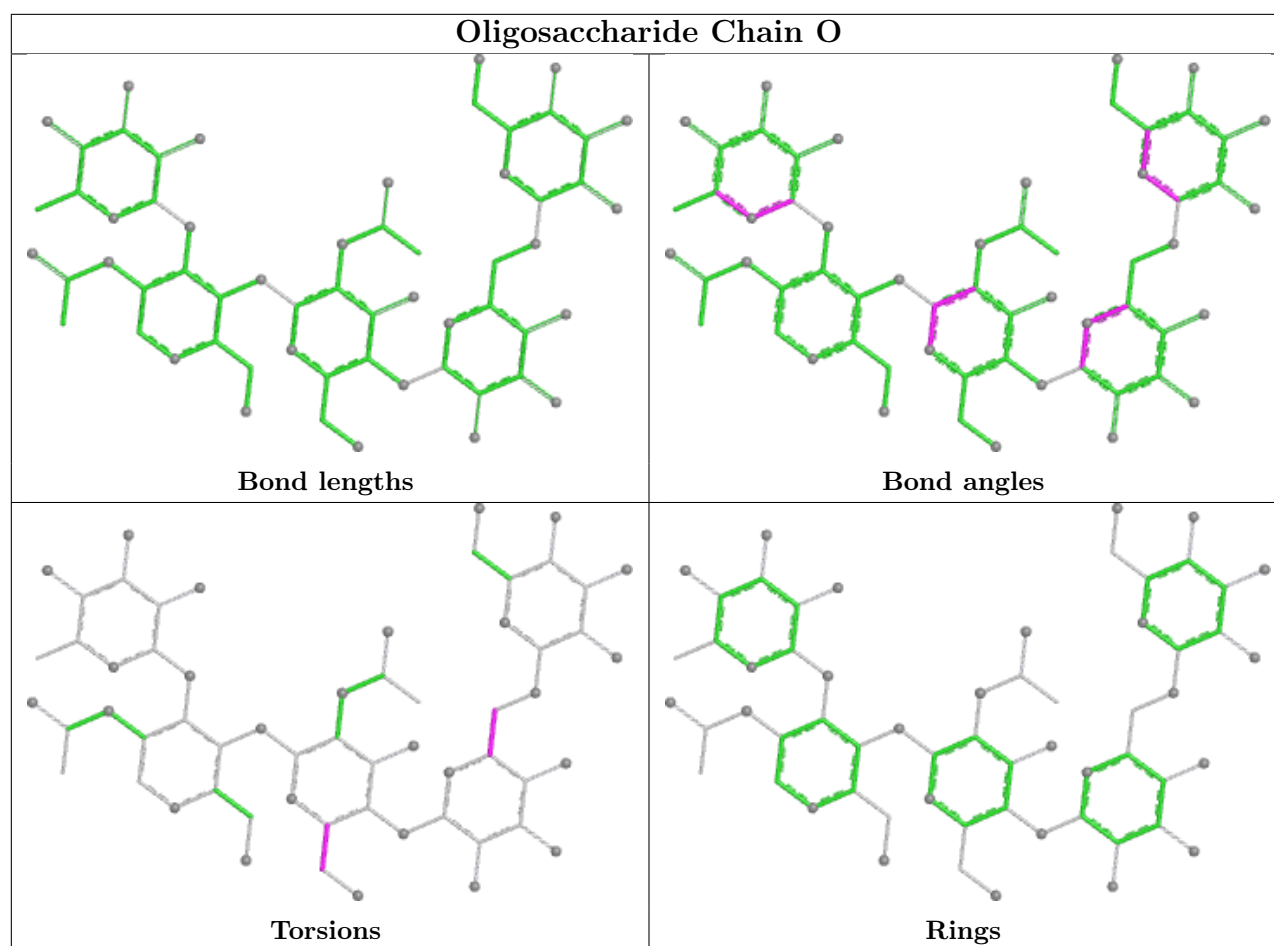
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

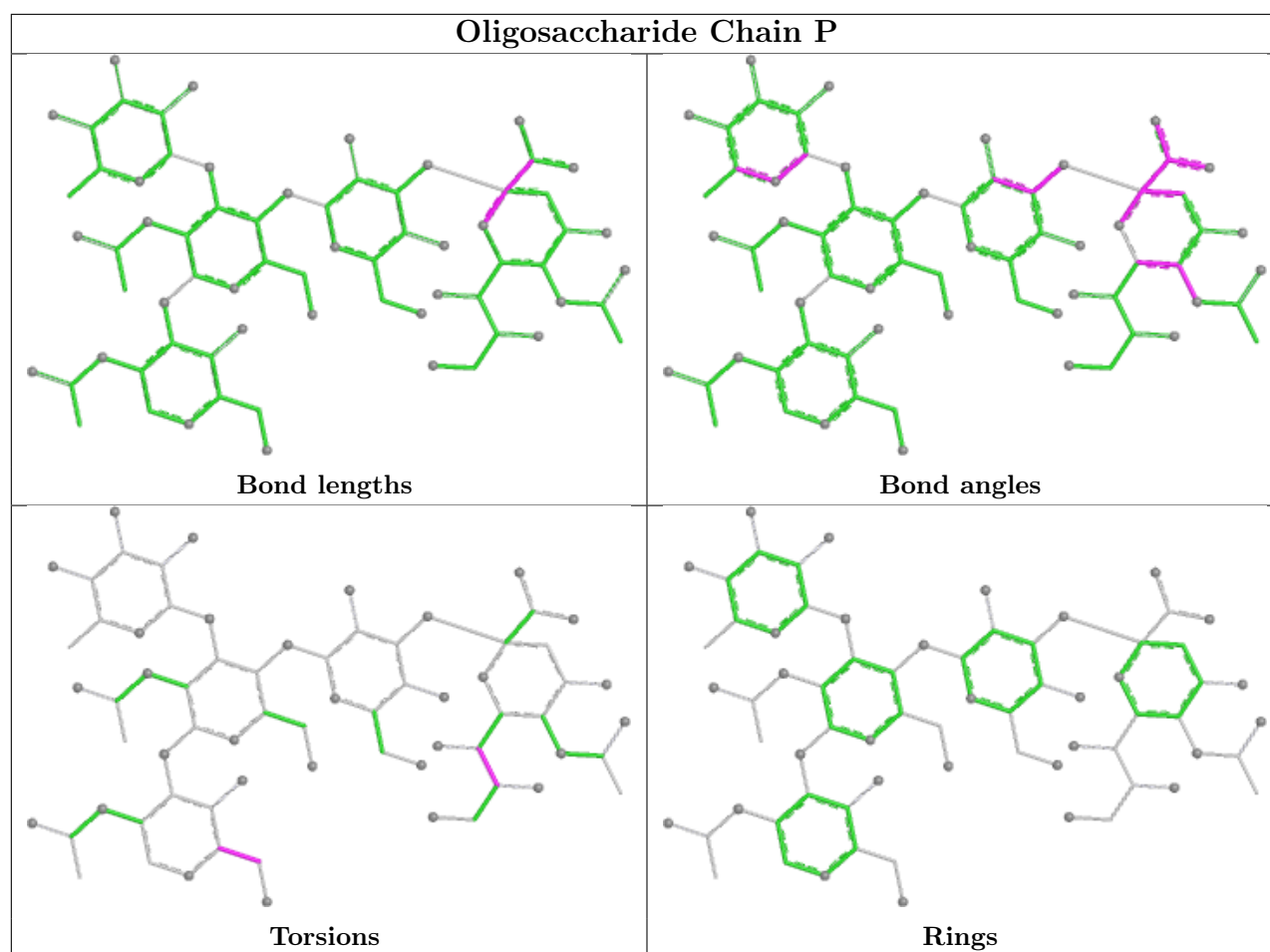


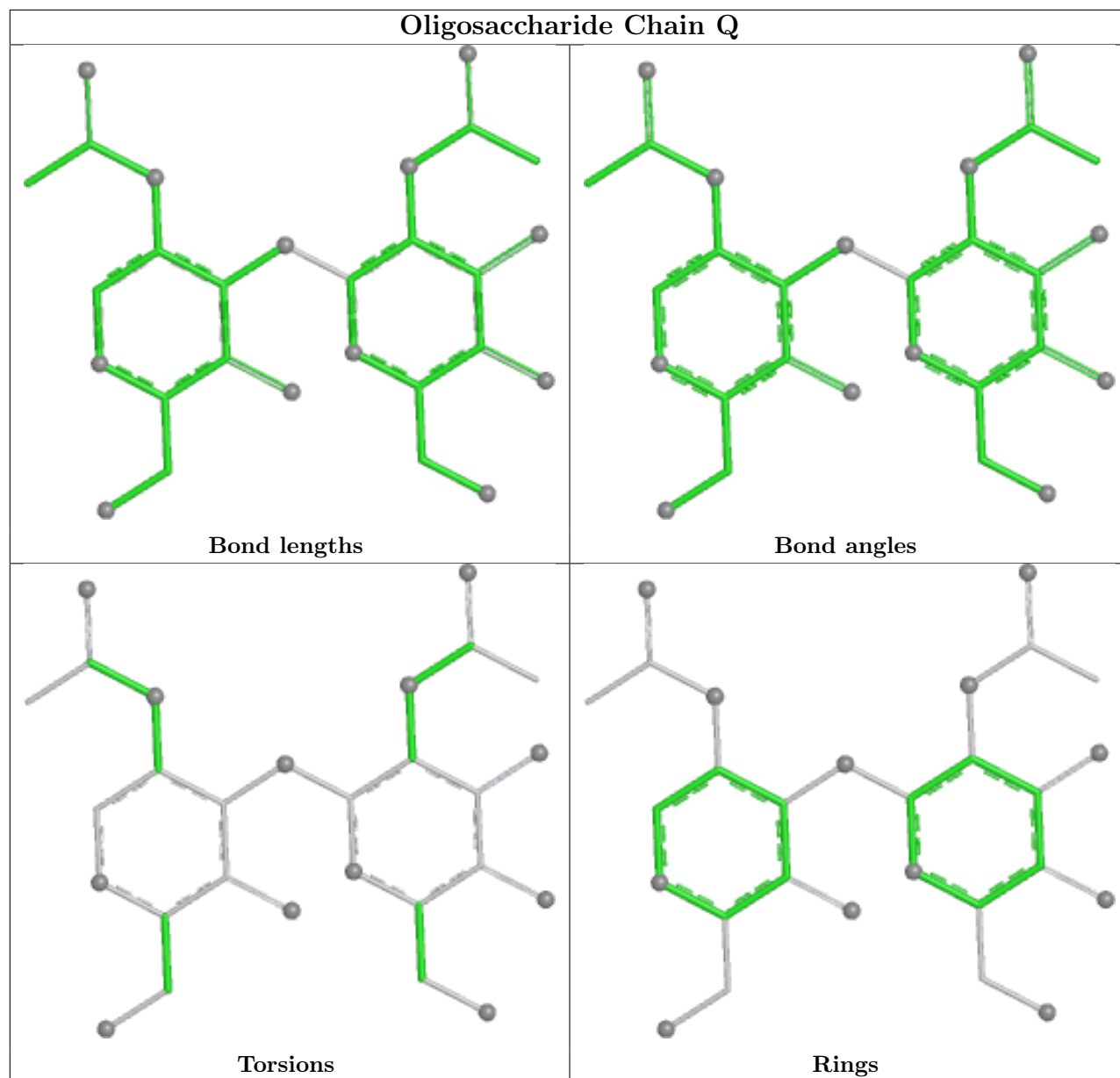


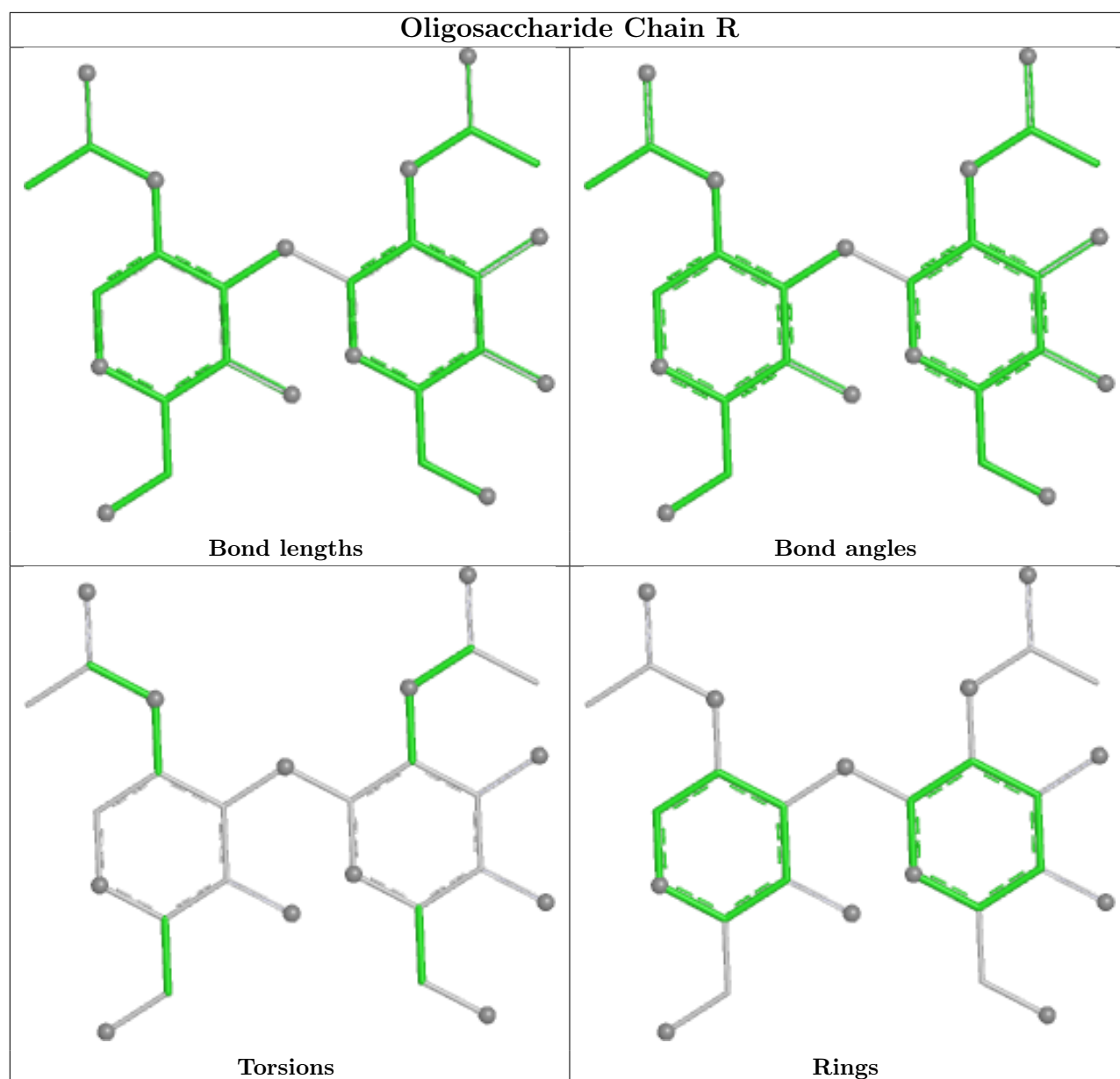


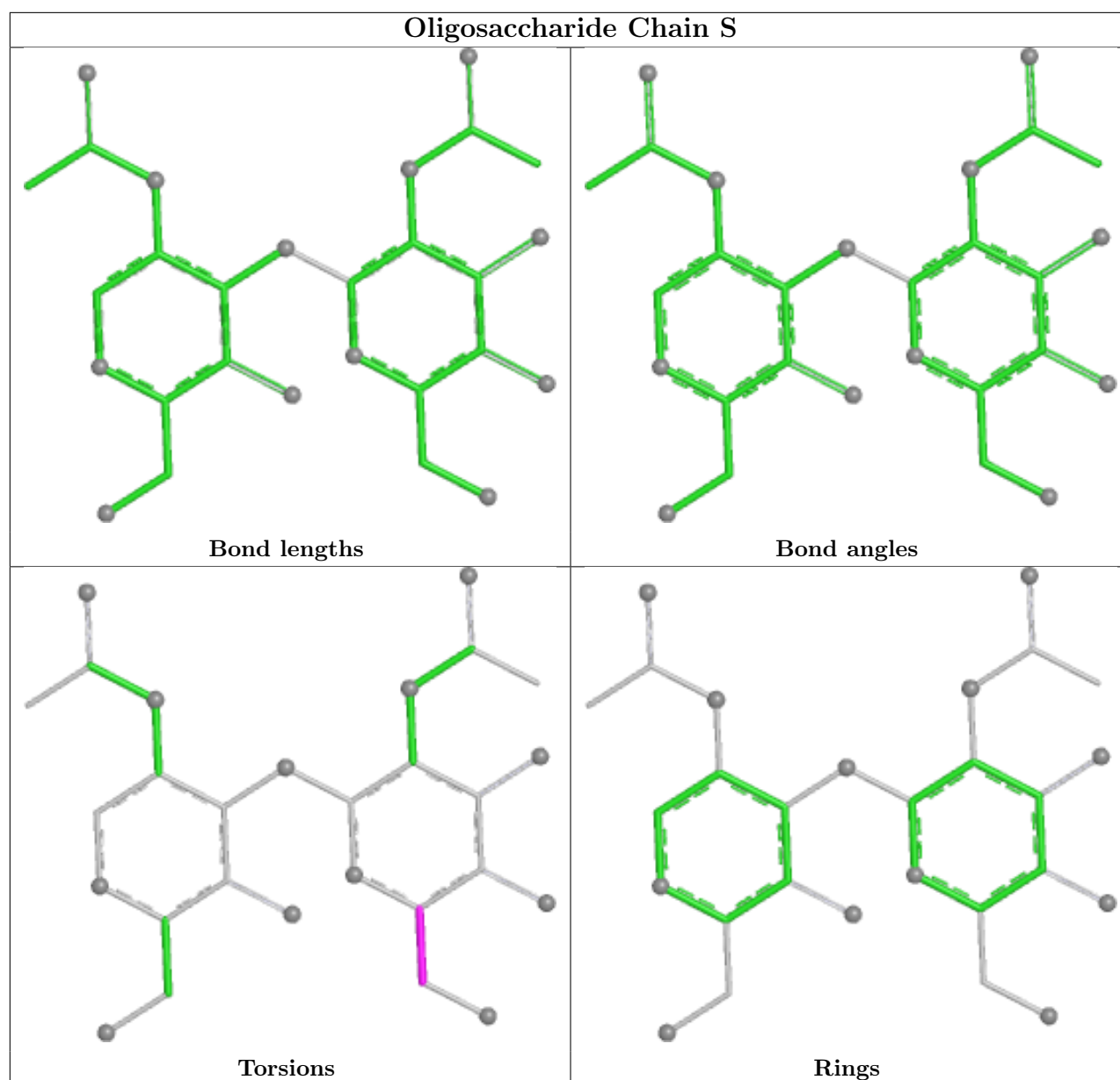












5.6 Ligand geometry [i](#)

33 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
12	SO4	D	202	-	4,4,4	0.68	0	6,6,6	0.09	0
12	SO4	E	604	-	4,4,4	0.68	0	6,6,6	0.08	0
12	SO4	A	606	-	4,4,4	0.67	0	6,6,6	0.09	0
10	NAG	C	602	1	14,14,15	0.71	0	17,19,21	0.90	0
12	SO4	C	604	-	4,4,4	0.66	0	6,6,6	0.10	0
11	GOL	B	201	-	5,5,5	0.34	0	5,5,5	0.48	0
12	SO4	E	606	-	4,4,4	0.69	0	6,6,6	0.10	0
10	NAG	A	604	1	14,14,15	0.67	0	17,19,21	0.94	1 (5%)
12	SO4	C	605	-	4,4,4	0.66	0	6,6,6	0.07	0
10	NAG	A	602	1	14,14,15	0.74	0	17,19,21	2.29	3 (17%)
12	SO4	B	203	-	4,4,4	0.67	0	6,6,6	0.08	0
12	SO4	C	610	-	4,4,4	0.67	0	6,6,6	0.05	0
10	NAG	E	602	1	14,14,15	0.71	0	17,19,21	1.02	1 (5%)
11	GOL	A	603	-	5,5,5	0.33	0	5,5,5	0.46	0
12	SO4	C	607	-	4,4,4	0.68	0	6,6,6	0.11	0
10	NAG	A	601	1	14,14,15	0.69	0	17,19,21	0.90	0
12	SO4	C	606	-	4,4,4	0.67	0	6,6,6	0.09	0
12	SO4	C	609	-	4,4,4	0.69	0	6,6,6	0.08	0
12	SO4	A	607	-	4,4,4	0.68	0	6,6,6	0.09	0
11	GOL	D	201	-	5,5,5	0.35	0	5,5,5	0.40	0
12	SO4	A	605	-	4,4,4	0.65	0	6,6,6	0.25	0
12	SO4	E	607	-	4,4,4	0.68	0	6,6,6	0.07	0
11	GOL	C	603	-	5,5,5	0.34	0	5,5,5	0.43	0
12	SO4	C	608	-	4,4,4	0.68	0	6,6,6	0.09	0
12	SO4	E	609	-	4,4,4	0.68	0	6,6,6	0.08	0
10	NAG	C	601	1	14,14,15	0.68	0	17,19,21	0.93	0
12	SO4	A	608	-	4,4,4	0.68	0	6,6,6	0.08	0
12	SO4	E	605	-	4,4,4	0.68	0	6,6,6	0.07	0
11	GOL	E	603	-	5,5,5	0.33	0	5,5,5	0.42	0
12	SO4	E	608	-	4,4,4	0.65	0	6,6,6	0.11	0
12	SO4	A	609	-	4,4,4	0.66	0	6,6,6	0.11	0
10	NAG	E	601	1	14,14,15	0.68	0	17,19,21	1.16	1 (5%)
11	GOL	B	202	-	5,5,5	0.33	0	5,5,5	0.44	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
11	GOL	D	201	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	A	604	1	-	2/6/23/26	0/1/1/1
11	GOL	E	603	-	-	4/4/4/4	-
10	NAG	A	602	1	-	4/6/23/26	0/1/1/1
11	GOL	C	603	-	-	0/4/4/4	-
10	NAG	E	601	1	-	0/6/23/26	0/1/1/1
10	NAG	E	602	1	-	1/6/23/26	0/1/1/1
11	GOL	A	603	-	-	0/4/4/4	-
10	NAG	C	601	1	-	2/6/23/26	0/1/1/1
10	NAG	A	601	1	-	2/6/23/26	0/1/1/1
10	NAG	C	602	1	-	0/6/23/26	0/1/1/1
11	GOL	B	202	-	-	0/4/4/4	-
11	GOL	B	201	-	-	2/4/4/4	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	602	NAG	C2-N2-C7	8.01	133.63	122.90
10	E	601	NAG	C1-O5-C5	3.72	117.17	112.19
10	E	602	NAG	C1-O5-C5	3.18	116.44	112.19
10	A	602	NAG	C1-C2-N2	2.43	114.27	110.43
10	A	602	NAG	C8-C7-N2	2.40	120.10	116.12
10	A	604	NAG	O5-C1-C2	-2.03	108.14	111.29

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	201	GOL	O1-C1-C2-C3
11	E	603	GOL	O1-C1-C2-C3
11	E	603	GOL	C1-C2-C3-O3
10	A	601	NAG	O5-C5-C6-O6
10	A	601	NAG	C4-C5-C6-O6
10	A	602	NAG	C8-C7-N2-C2
10	A	602	NAG	O7-C7-N2-C2
10	A	604	NAG	C8-C7-N2-C2
10	A	604	NAG	O7-C7-N2-C2
11	B	201	GOL	C1-C2-C3-O3
10	C	601	NAG	O5-C5-C6-O6
11	D	201	GOL	O1-C1-C2-O2

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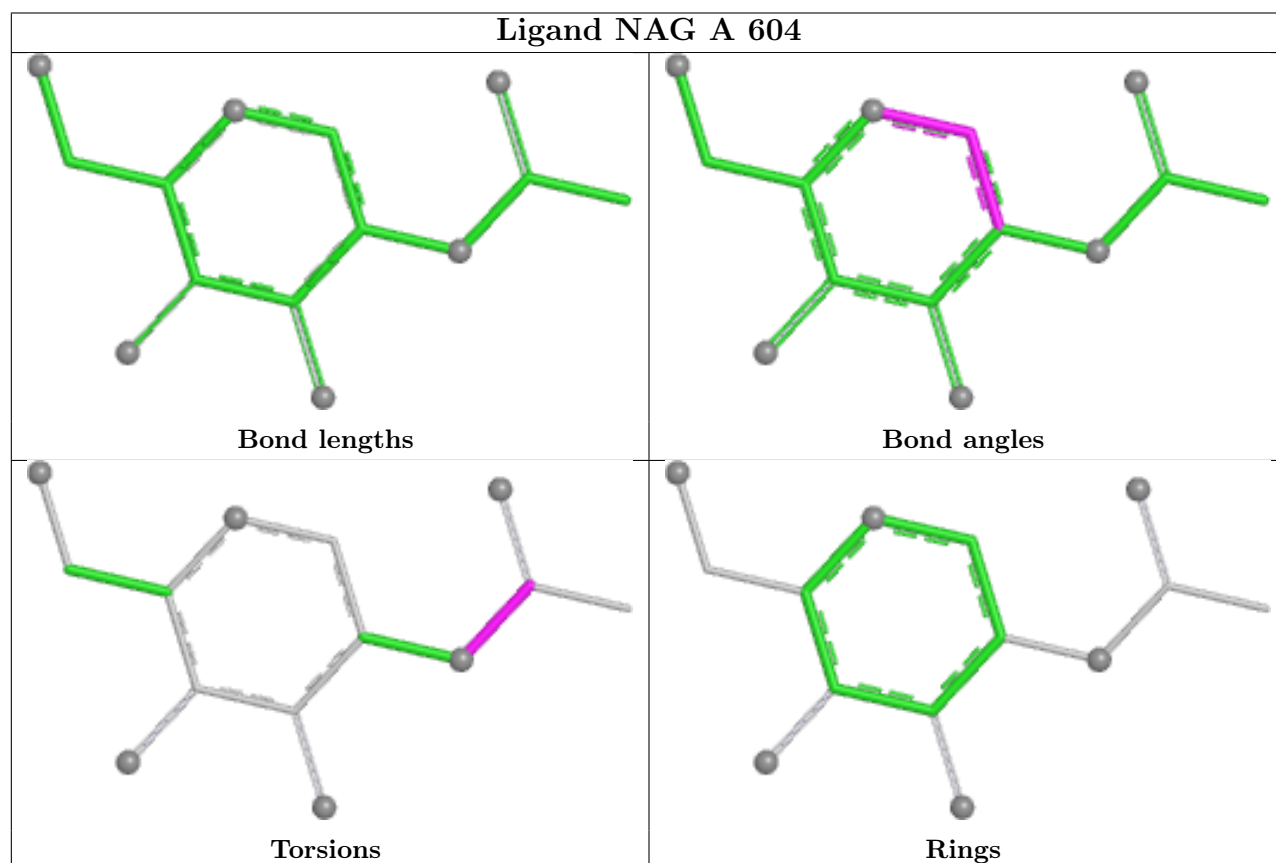
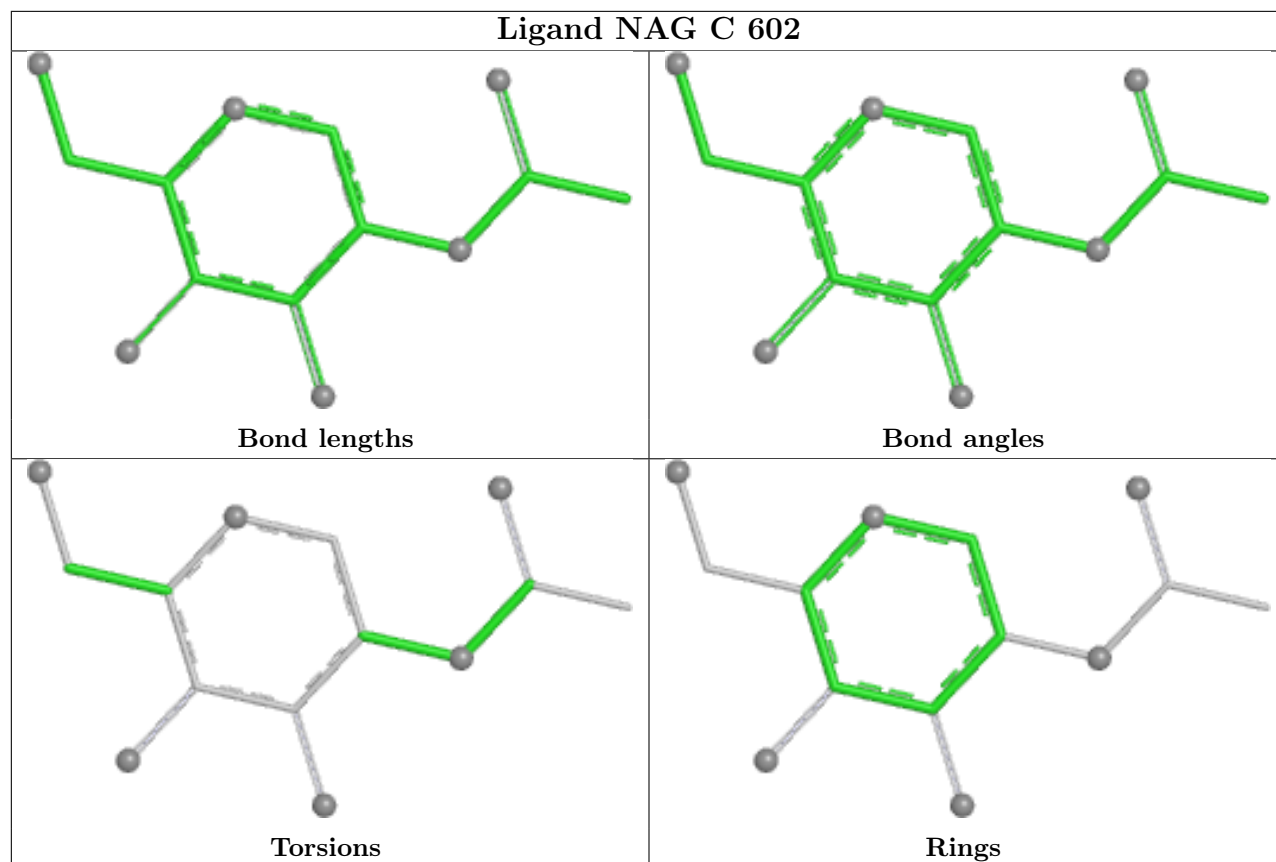
Mol	Chain	Res	Type	Atoms
11	E	603	GOL	O2-C2-C3-O3
11	E	603	GOL	O1-C1-C2-O2
11	B	201	GOL	O2-C2-C3-O3
10	C	601	NAG	C4-C5-C6-O6
10	A	602	NAG	C1-C2-N2-C7
10	A	602	NAG	C3-C2-N2-C7
10	E	602	NAG	O5-C5-C6-O6

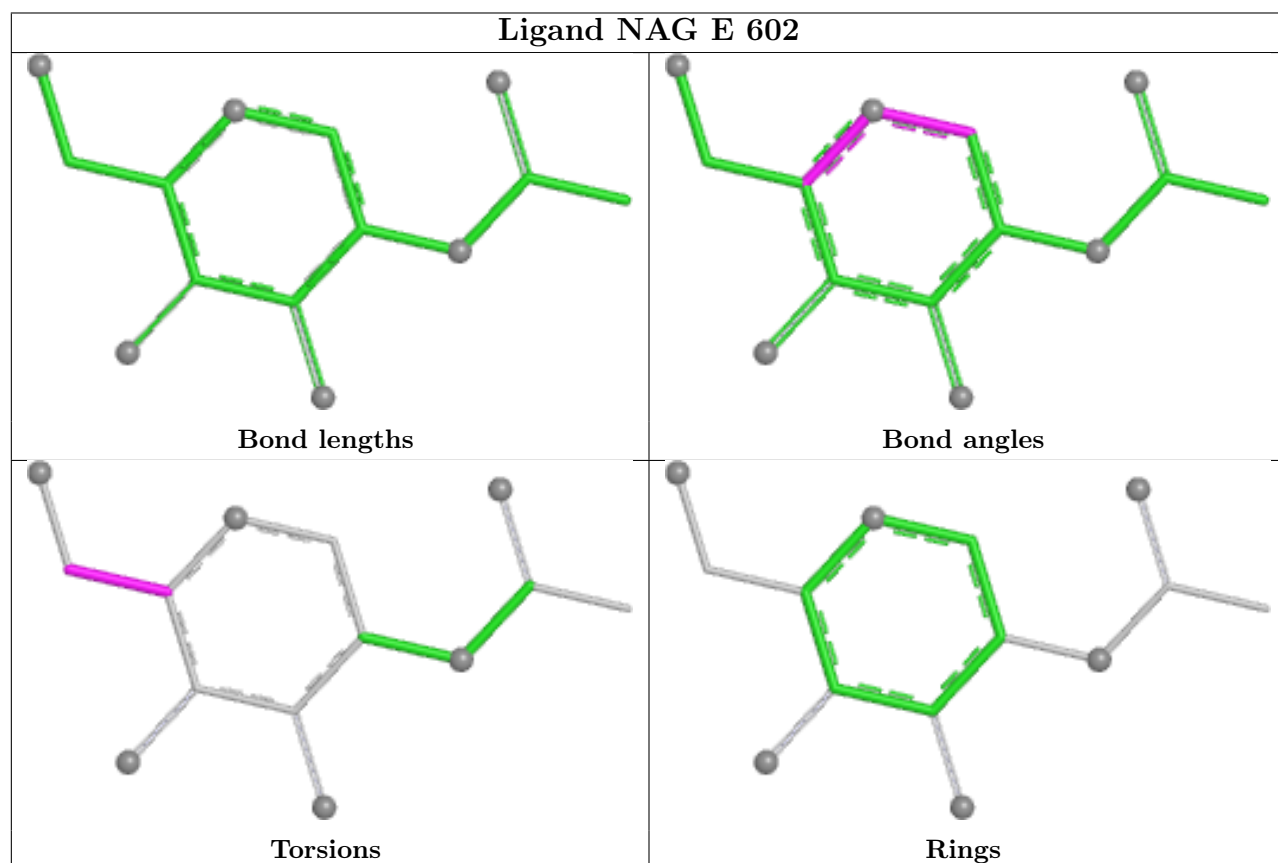
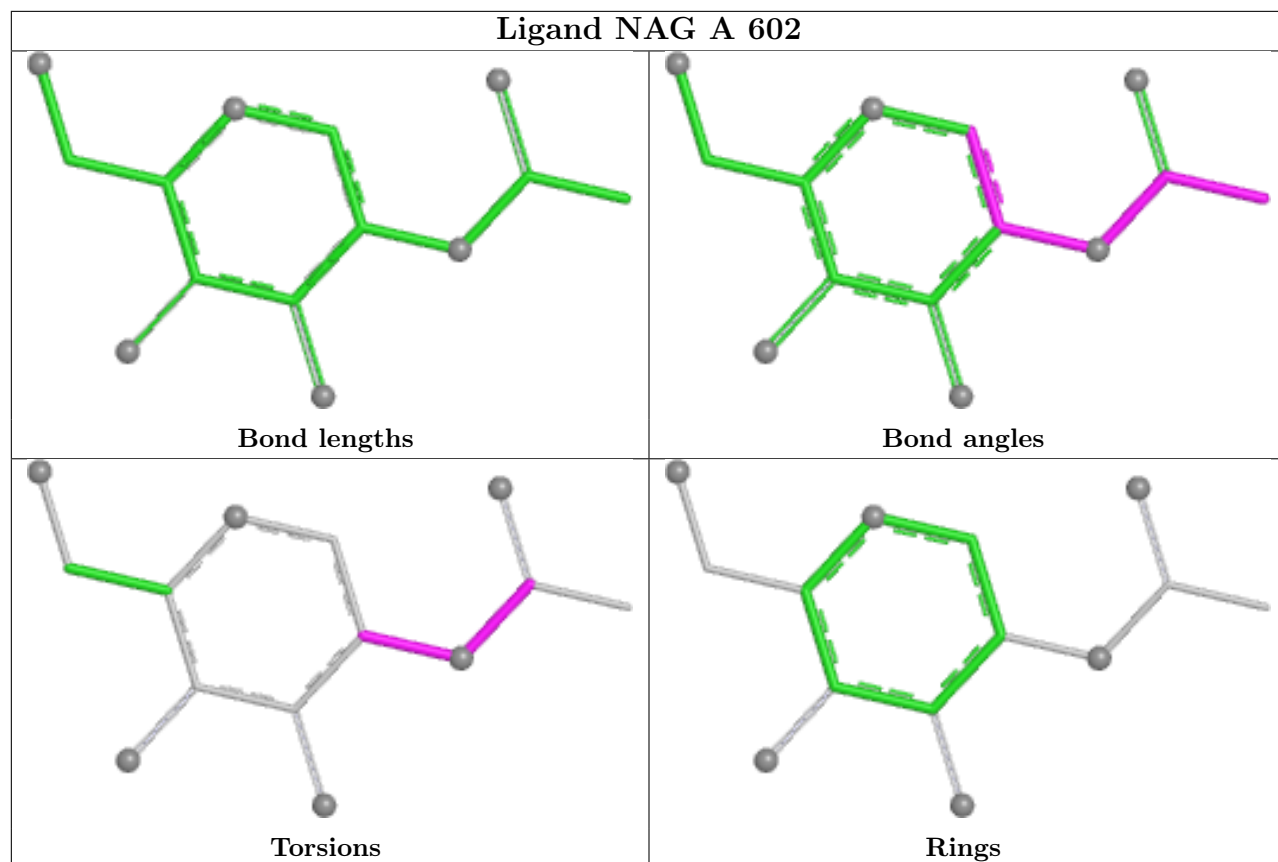
There are no ring outliers.

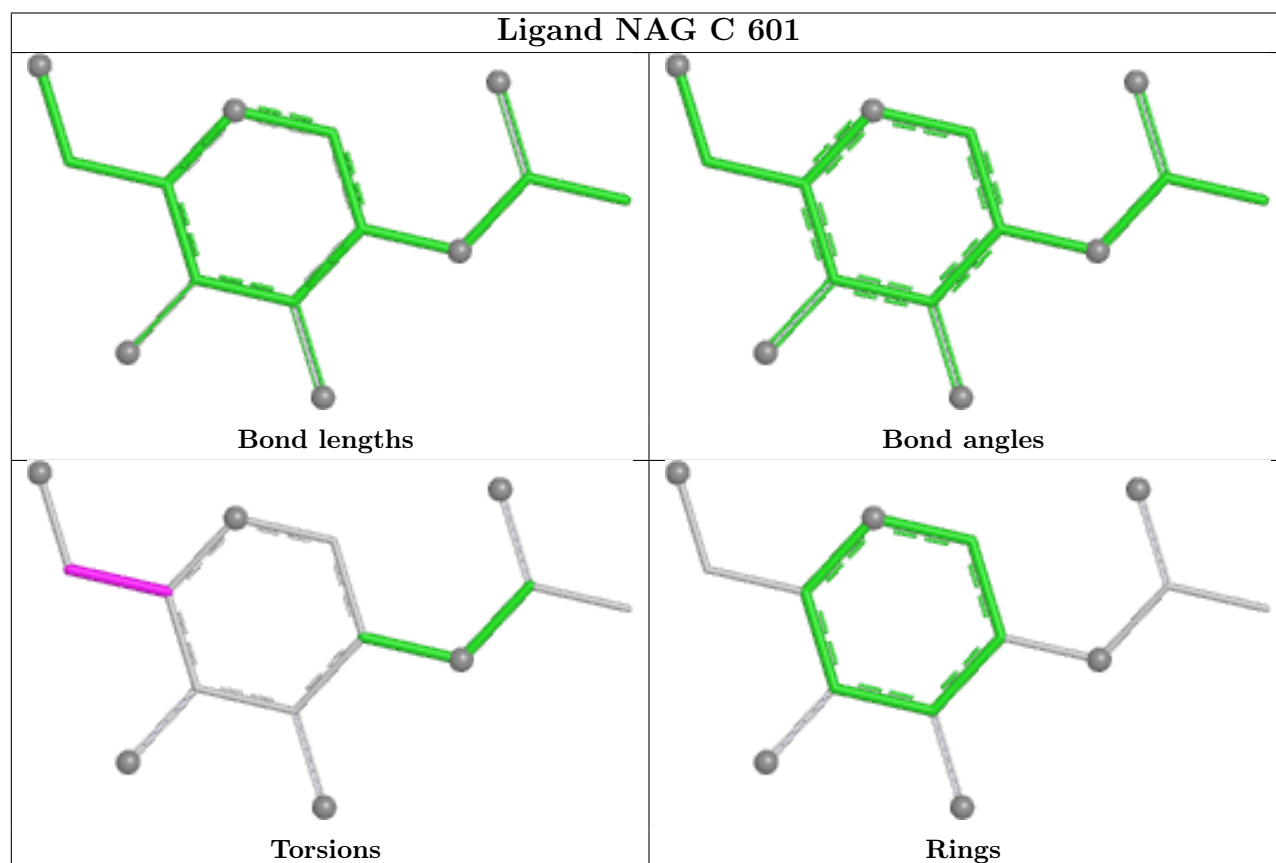
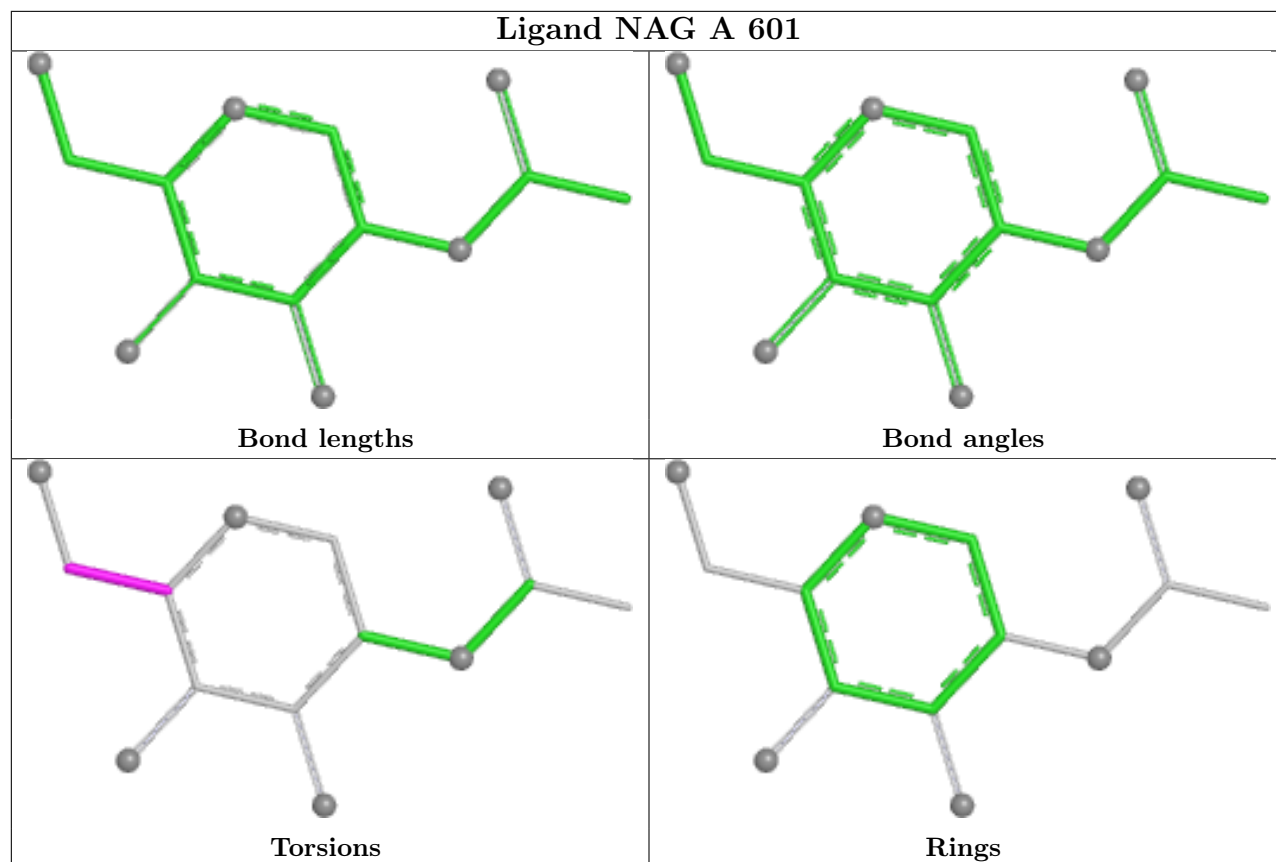
6 monomers are involved in 7 short contacts:

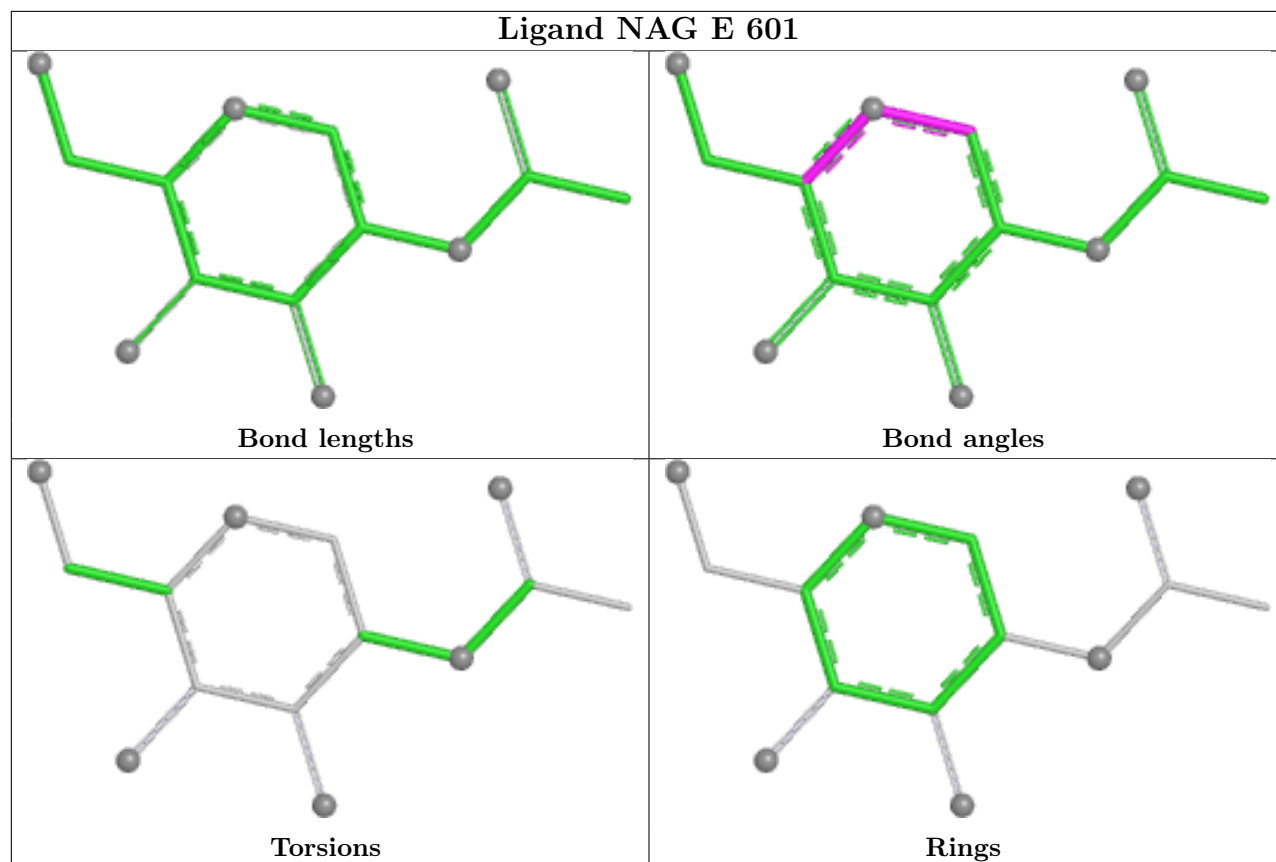
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	607	SO4	1	0
12	C	606	SO4	1	0
12	A	607	SO4	1	0
11	D	201	GOL	1	0
12	E	608	SO4	1	0
12	A	609	SO4	2	0

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	A	322/329 (97%)	-0.11	12 (3%) 45 40	27, 44, 76, 163	0
1	C	324/329 (98%)	-0.10	15 (4%) 37 33	26, 43, 79, 160	0
1	E	323/329 (98%)	-0.18	13 (4%) 42 38	25, 41, 71, 147	0
2	B	169/181 (93%)	0.18	11 (6%) 25 22	34, 51, 86, 141	0
2	D	169/181 (93%)	0.53	18 (10%) 11 9	34, 63, 102, 128	0
2	F	172/181 (95%)	-0.07	4 (2%) 61 57	33, 49, 71, 102	0
3	G	5/5 (100%)	3.07	3 (60%) 0 0	83, 88, 96, 129	0
3	H	5/5 (100%)	4.56	5 (100%) 0 0	109, 113, 130, 132	0
3	I	5/5 (100%)	4.31	5 (100%) 0 0	97, 103, 120, 138	0
3	l	4/5 (80%)	6.80	4 (100%) 0 0	117, 119, 129, 142	0
All	All	1498/1550 (96%)	0.05	90 (6%) 27 24	25, 47, 91, 163	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	l	2	VAL	9.8
2	B	174	GLY	9.5
1	E	80	ILE	9.1
2	B	9	PHE	8.8
1	C	80	ILE	8.8
2	B	6	ILE	8.6
3	l	5	GLY	8.5
2	D	173	ILE	8.4
3	I	1	PHE	7.9
1	E	79	PHE	7.6
1	C	79	PHE	7.5
1	A	80	ILE	7.3
2	D	6	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
3	I	4	ILE	6.4
3	G	1	PHE	6.3
1	A	91	ALA	6.3
3	H	1	PHE	6.1
1	C	324	PRO	5.9
1	E	323	SER	5.9
1	A	79	PHE	5.9
1	A	323	SER	5.6
2	D	174	GLY	5.6
1	C	81	ARG	5.5
1	A	9	PRO	5.4
2	D	7	ALA	5.3
1	E	78	GLU	5.1
1	C	323	SER	5.0
2	B	7	ALA	4.9
2	B	10	ILE	4.9
3	H	2	VAL	4.7
3	H	5	GLY	4.5
2	D	164	GLU	4.4
1	C	8	ASP	4.4
1	C	9	PRO	4.3
3	I	2	VAL	4.2
1	C	78	GLU	4.0
2	F	19	ASP	4.0
1	E	221	SER	3.9
3	I	3	THR	3.9
3	H	4	ILE	3.9
3	H	3	THR	3.6
1	A	78	GLU	3.6
1	C	62	LYS	3.5
3	I	5	GLY	3.4
2	D	171	GLU	3.4
1	A	92	ASN	3.3
1	E	9	PRO	3.3
1	A	82	VAL	3.2
1	E	81	ARG	3.2
3	G	3	THR	3.2
1	E	77	ASP	3.1
2	B	29	GLU	3.0
2	D	19	ASP	3.0
2	B	8	GLY	3.0
2	B	11	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	77	ASP	2.9
1	E	186	ASN	2.9
2	B	173	ILE	2.9
1	A	62	LYS	2.8
2	F	10	ILE	2.8
1	C	21	ASN	2.7
2	D	39	GLU	2.7
1	A	81	ARG	2.6
2	D	168	LEU	2.6
3	I	3	THR	2.5
2	D	29	GLU	2.5
2	D	172	GLU	2.4
3	G	5	GLY	2.4
2	D	143	LYS	2.4
1	C	290	SER	2.3
1	C	264	ASP	2.3
1	C	277	CYS	2.3
2	D	144	CYS	2.3
2	B	17	MET	2.3
1	E	8	ASP	2.3
2	D	78	GLU	2.3
2	D	18	VAL	2.3
2	D	158	ASP	2.2
2	D	27	SER	2.2
2	F	121	LYS	2.2
1	A	277	CYS	2.2
2	B	18	VAL	2.1
3	I	4	ILE	2.1
2	F	78	GLU	2.1
1	E	82	VAL	2.1
1	E	173	ARG	2.1
1	A	96	ASP	2.1
2	D	127	ARG	2.0
1	C	50	LYS	2.0
1	E	38	HIS	2.0

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

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

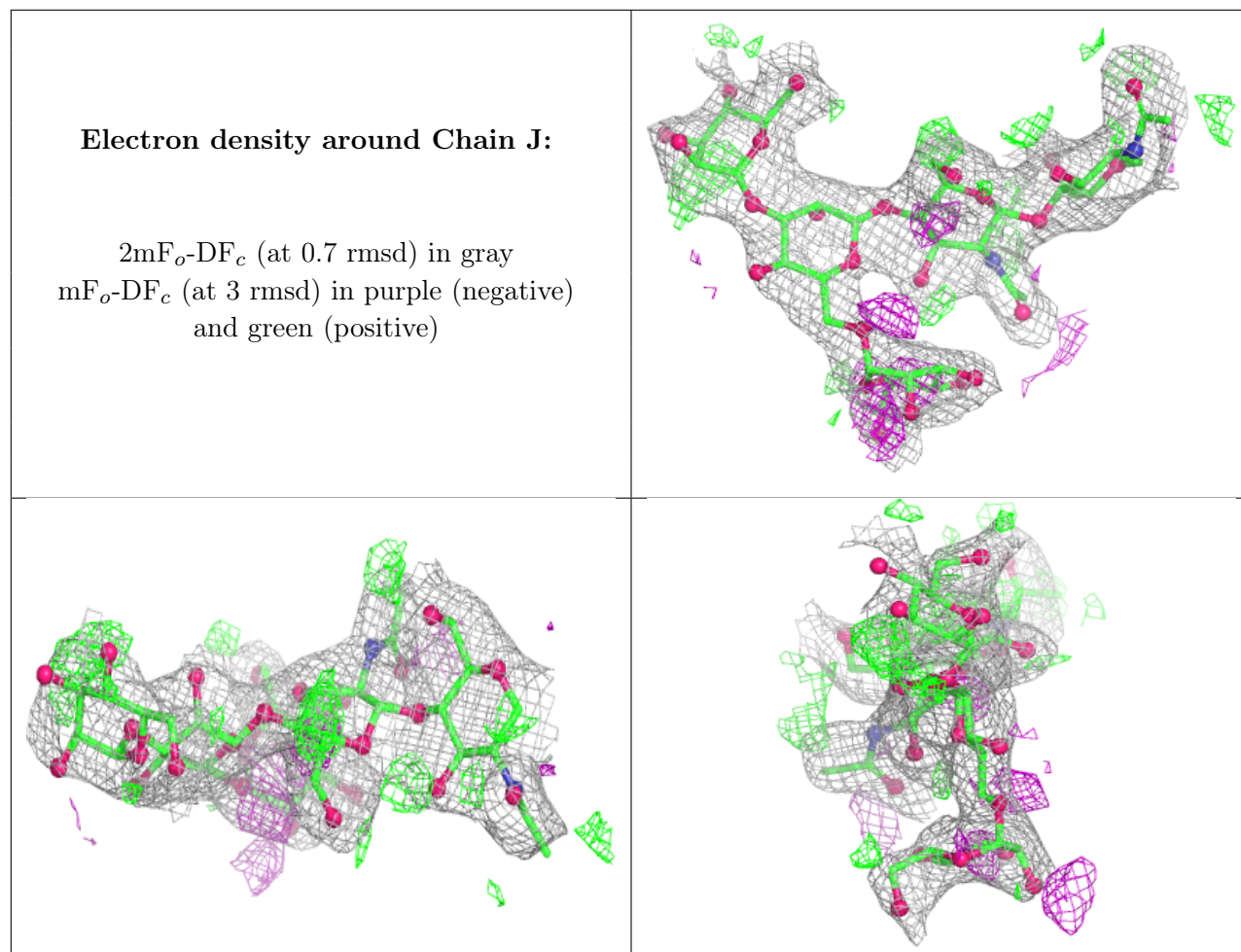
6.3 Carbohydrates

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
4	NAG	J	1	14/15	-	-	51,64,75,79	0
4	NAG	J	2	14/15	-	-	54,78,94,98	0
4	BMA	J	3	11/12	-	-	76,93,108,117	0
4	MAN	J	4	11/12	-	-	84,119,127,133	0
4	MAN	J	5	11/12	-	-	71,85,100,117	0
9	NAG	S	2	14/15	0.40	0.26	135,162,173,176	0
9	NAG	R	2	14/15	0.50	0.26	137,162,170,171	0
9	A2G	S	1	14/15	0.52	0.22	112,136,155,156	0
7	NAG	O	2	14/15	0.56	0.20	64,97,112,127	0
4	MAN	L	5	11/12	-	-	98,126,133,135	0
4	BMA	L	3	11/12	0.65	0.17	64,79,105,130	0
5	MAN	K	4	11/12	0.67	0.21	108,138,145,148	0
4	MAN	L	4	11/12	0.68	0.18	54,62,69,89	0
8	FUC	P	5	10/11	0.69	0.21	38,46,50,55	0
5	FUC	K	5	10/11	-	-	65,86,91,98	0
6	NAG	N	2	14/15	0.71	0.20	73,110,128,129	0
6	NAG	N	1	14/15	0.71	0.21	51,73,83,96	0
9	A2G	Q	1	14/15	0.80	0.18	70,101,118,133	0
5	NAG	K	2	14/15	0.81	0.17	79,92,111,119	0
5	BMA	K	3	11/12	0.84	0.15	102,114,124,124	0
9	A2G	R	1	14/15	0.85	0.18	114,147,162,162	0
7	BMA	O	3	11/12	-	-	107,130,140,160	0
7	MAN	O	4	11/12	-	-	134,165,175,180	0
7	FUC	O	5	10/11	-	-	104,112,124,126	0
8	A2G	P	1	14/15	-	-	69,92,96,98	0
8	NAG	P	2	14/15	0.86	0.14	37,58,69,77	0
8	GAL	P	3	11/12	-	-	34,44,49,50	0
8	SIA	P	4	20/21	-	-	29,36,57,60	0
4	NAG	L	1	14/15	0.88	0.14	45,58,70,73	0
7	NAG	O	1	14/15	0.90	0.12	63,78,96,105	0
6	NAG	M	1	14/15	0.91	0.12	98,120,134,143	0
5	NAG	K	1	14/15	0.91	0.12	55,85,97,97	0
4	NAG	L	2	14/15	0.91	0.13	42,57,68,72	0
6	NAG	M	2	14/15	0.92	0.12	123,135,146,152	0
9	NAG	Q	2	14/15	0.95	0.09	109,131,140,150	0

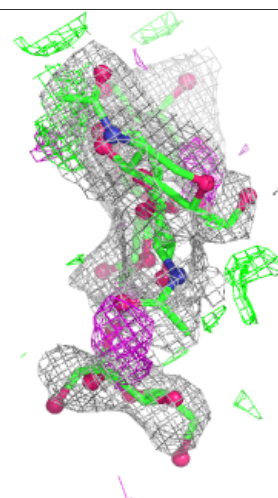
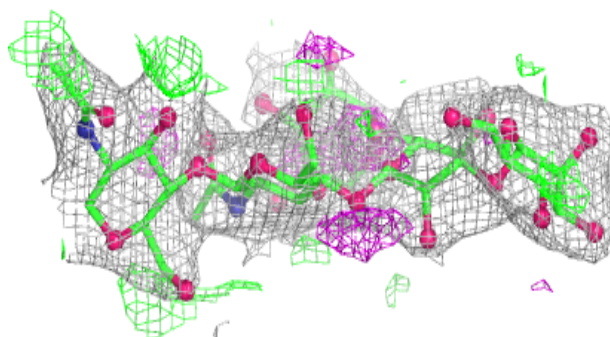
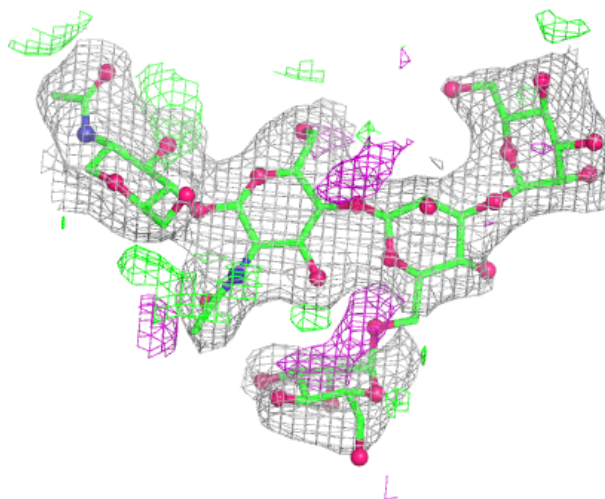
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

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



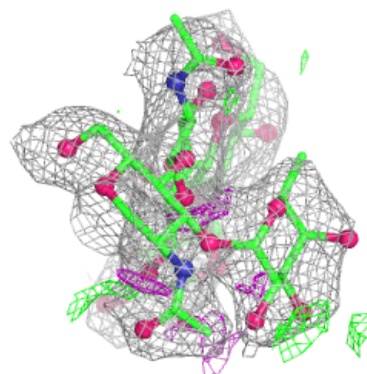
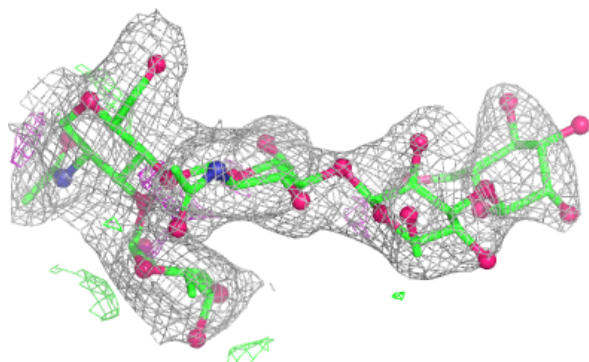
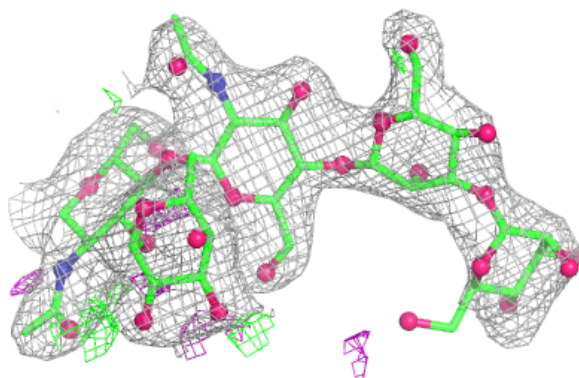
Electron density around Chain L:

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

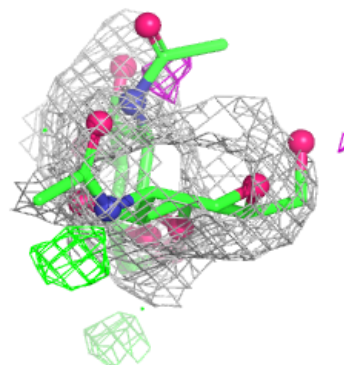
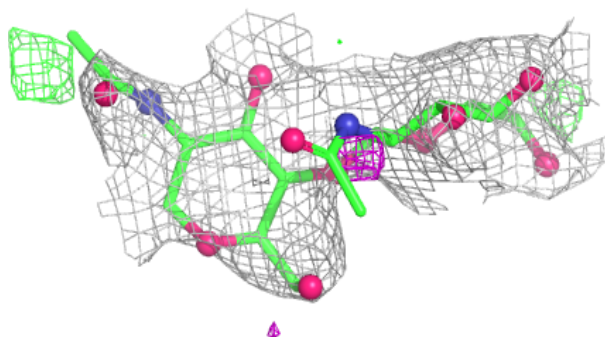
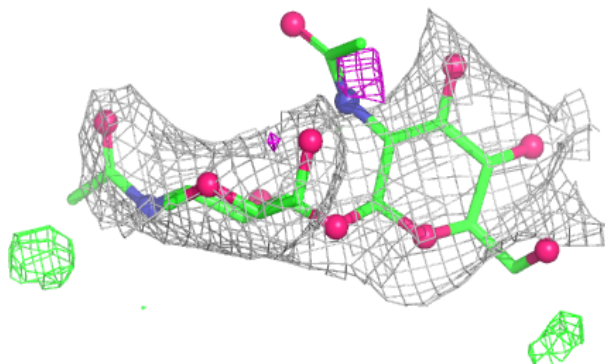


Electron density around Chain K:

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

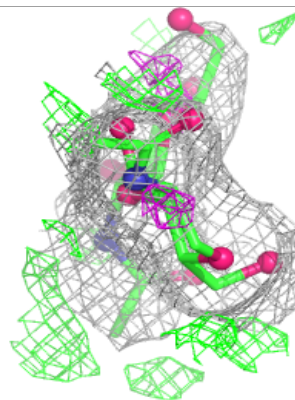
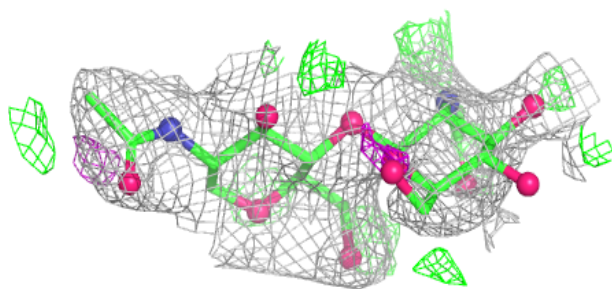
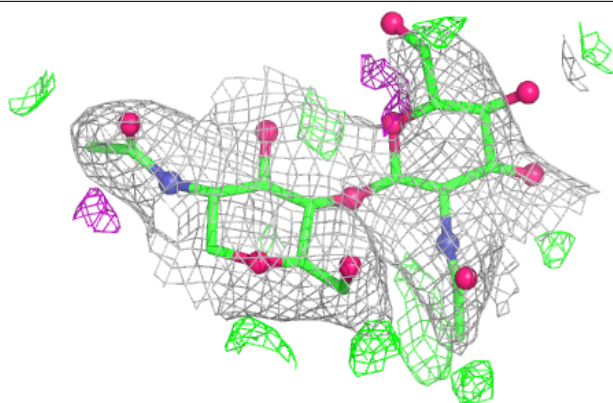
**Electron density around Chain M:**

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

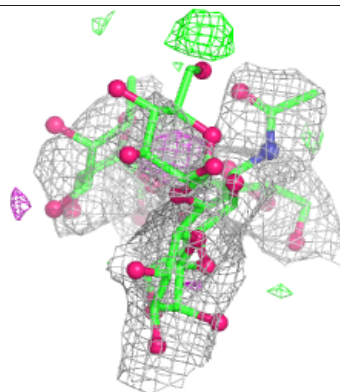
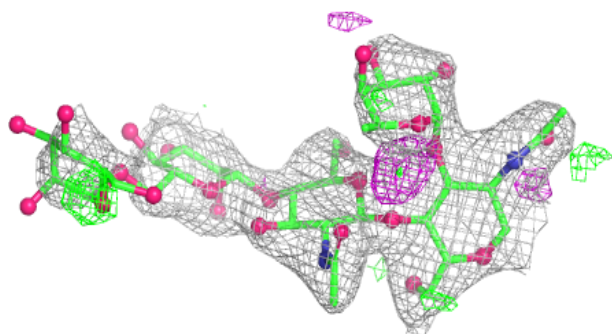
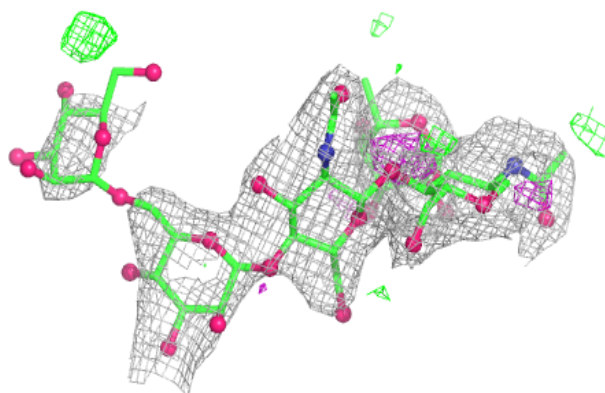


Electron density around Chain N:

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

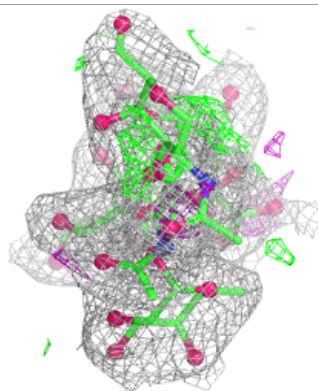
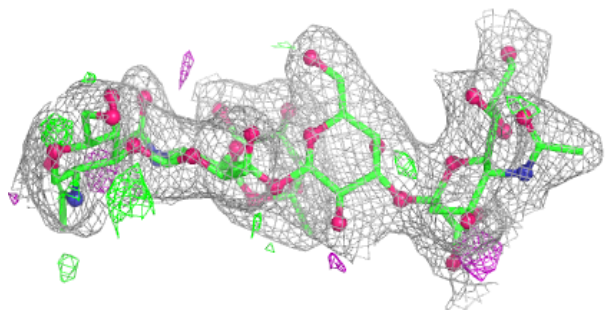
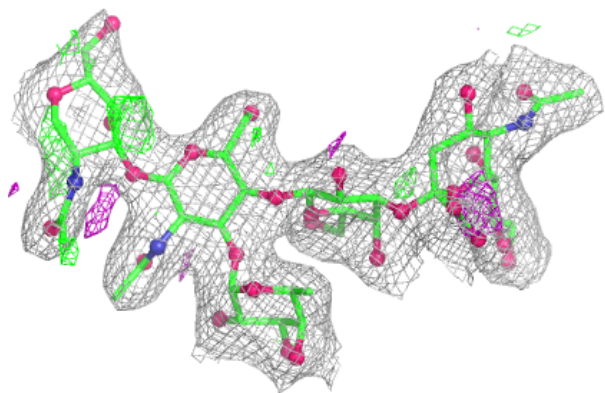
**Electron density around Chain O:**

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



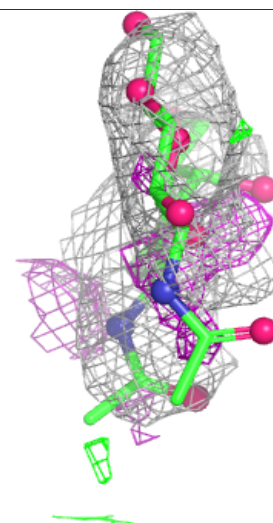
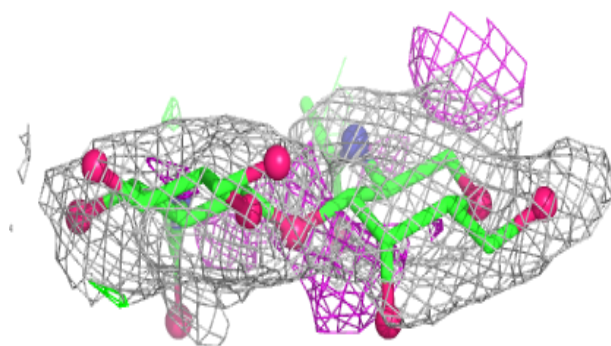
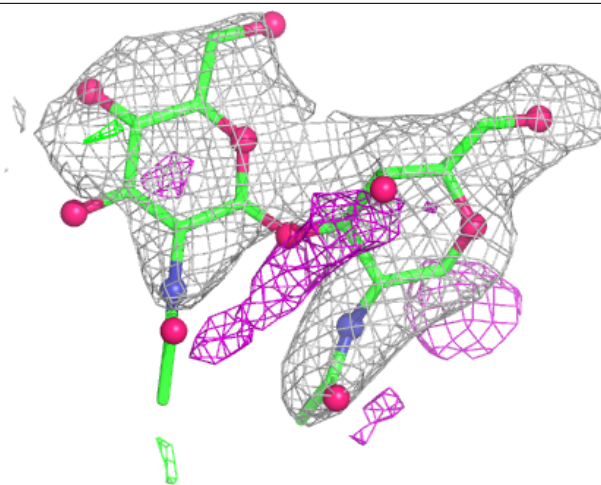
Electron density around Chain P:

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



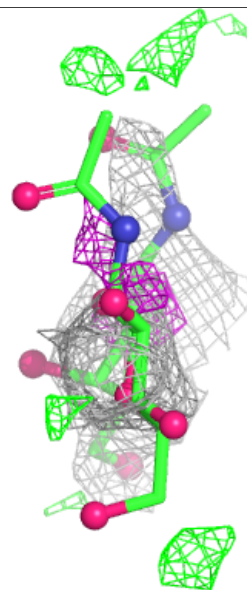
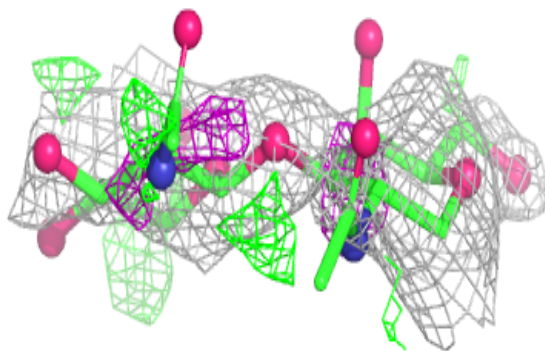
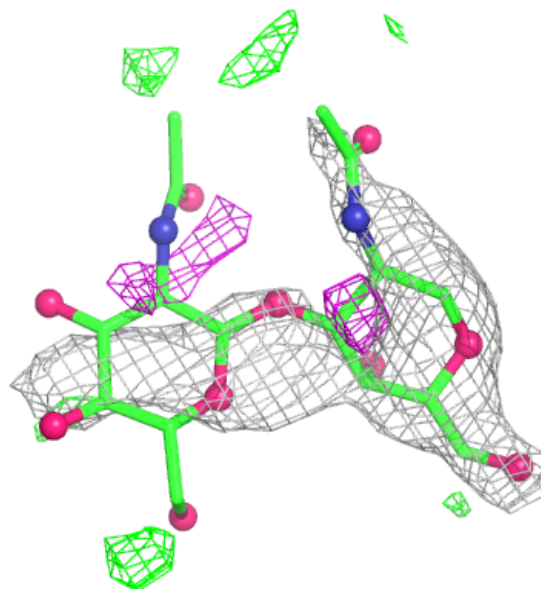
Electron density around Chain Q:

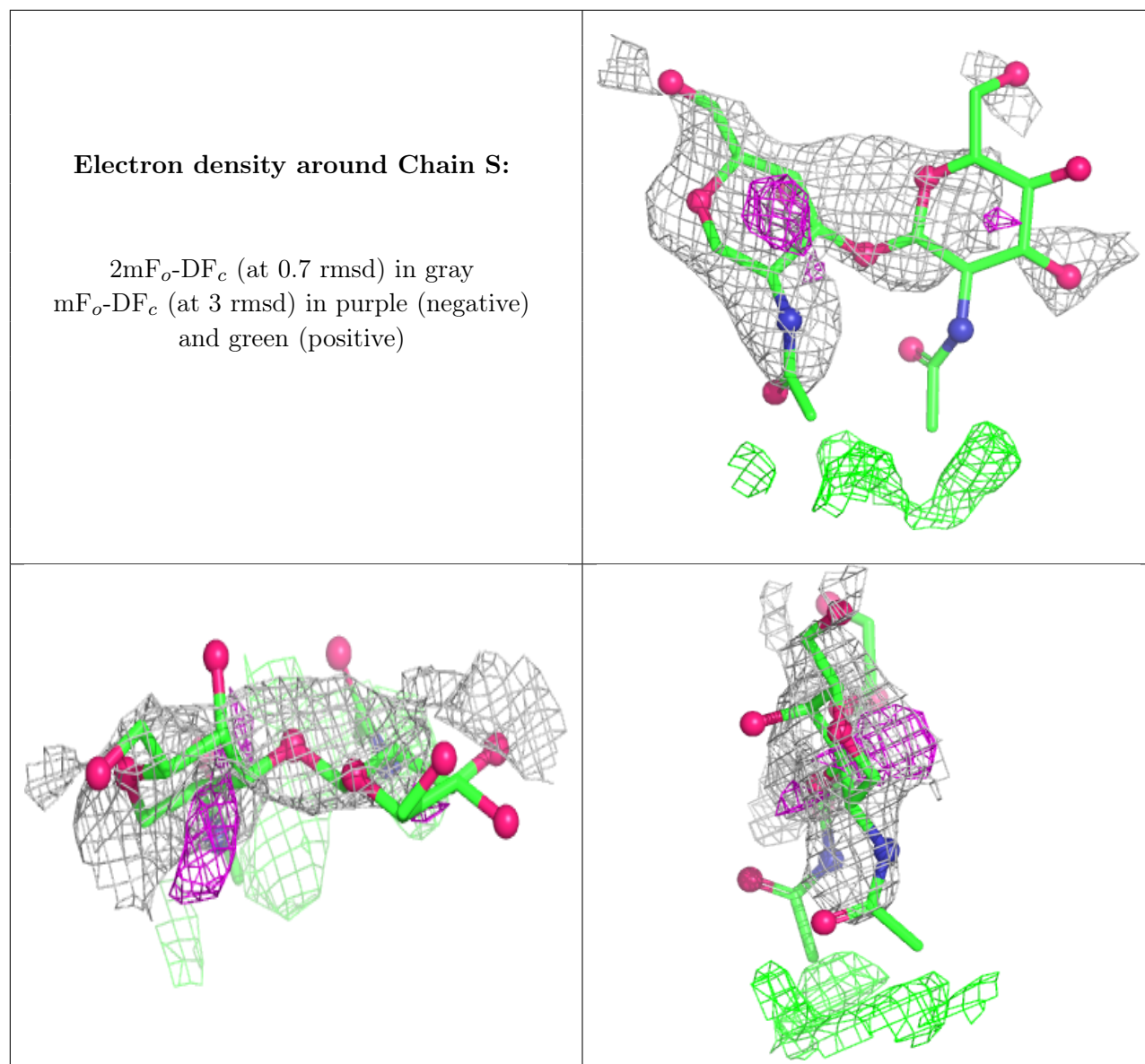
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain R:

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





6.4 Ligands ⓘ

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
10	NAG	A	604	14/15	0.55	0.24	108,125,138,142	0
12	SO4	C	605	5/5	0.63	0.13	104,122,142,152	0
12	SO4	A	606	5/5	0.66	0.13	105,106,117,122	0
10	NAG	E	601	14/15	0.67	0.19	77,101,111,114	0
10	NAG	A	602	14/15	0.68	0.22	97,117,130,141	0

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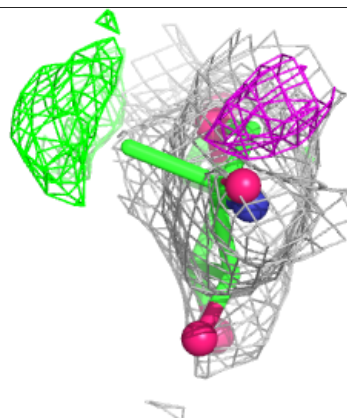
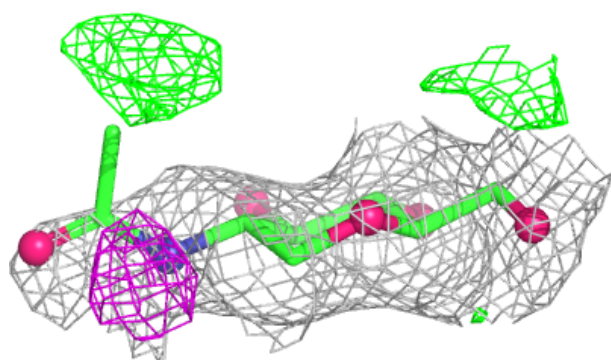
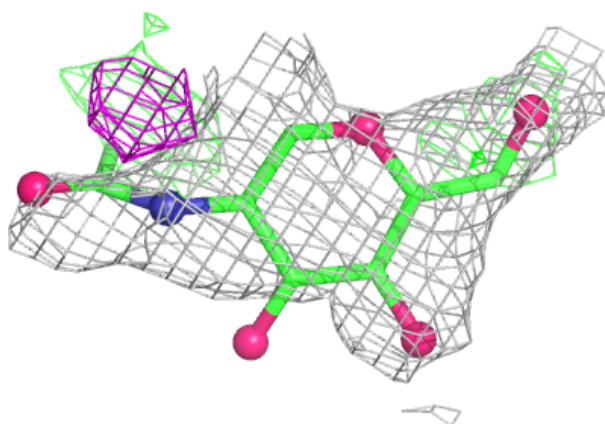
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	SO4	E	609	5/5	0.71	0.15	67,78,138,165	0
10	NAG	C	602	14/15	0.74	0.19	82,113,127,132	0
10	NAG	C	601	14/15	0.78	0.16	82,95,112,116	0
10	NAG	A	601	14/15	0.78	0.15	82,106,121,127	0
10	NAG	E	602	14/15	0.79	0.16	68,100,111,114	0
12	SO4	B	203	5/5	0.81	0.14	101,104,111,114	0
11	GOL	D	201	6/6	0.83	0.22	77,78,85,89	0
11	GOL	B	202	6/6	0.85	0.21	77,93,97,109	0
12	SO4	A	608	5/5	0.85	0.15	67,77,135,146	0
12	SO4	A	609	5/5	0.85	0.21	91,107,120,135	0
12	SO4	D	202	5/5	0.86	0.16	91,105,116,162	0
11	GOL	C	603	6/6	0.88	0.18	51,58,66,72	0
12	SO4	E	606	5/5	0.88	0.15	54,57,102,129	0
12	SO4	C	607	5/5	0.88	0.20	60,63,96,100	0
12	SO4	E	607	5/5	0.89	0.19	68,79,101,139	0
12	SO4	C	609	5/5	0.90	0.15	64,65,109,135	0
12	SO4	C	606	5/5	0.90	0.12	57,60,90,104	0
12	SO4	E	604	5/5	0.90	0.10	79,82,102,121	0
11	GOL	B	201	6/6	0.91	0.15	72,83,85,90	0
12	SO4	A	605	5/5	0.91	0.12	78,84,109,110	0
12	SO4	C	604	5/5	0.91	0.12	73,110,114,123	0
12	SO4	C	610	5/5	0.93	0.17	59,74,76,83	0
11	GOL	A	603	6/6	0.93	0.14	61,66,68,77	0
12	SO4	E	608	5/5	0.94	0.23	56,75,85,89	0
12	SO4	A	607	5/5	0.94	0.17	51,63,77,87	0
11	GOL	E	603	6/6	0.95	0.14	54,67,76,78	0
12	SO4	C	608	5/5	0.96	0.16	51,53,69,69	0
12	SO4	E	605	5/5	0.96	0.14	48,51,65,65	0

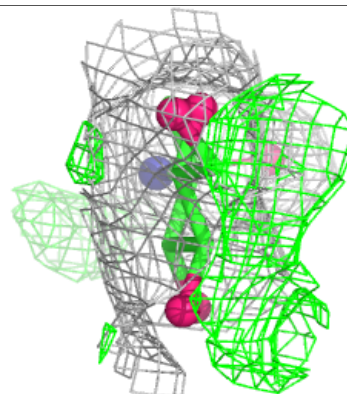
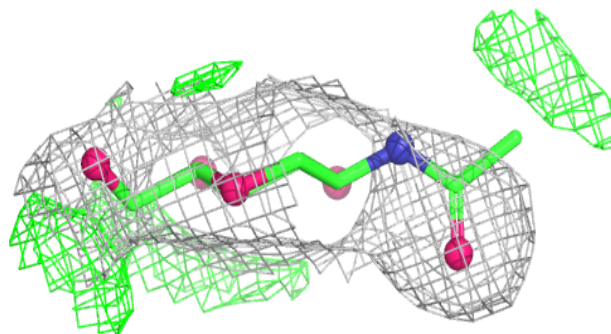
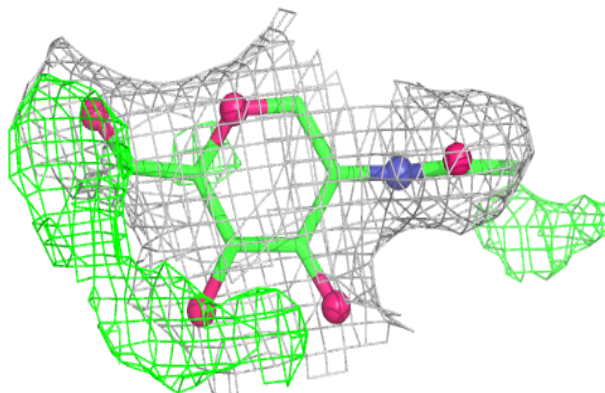
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 604:

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

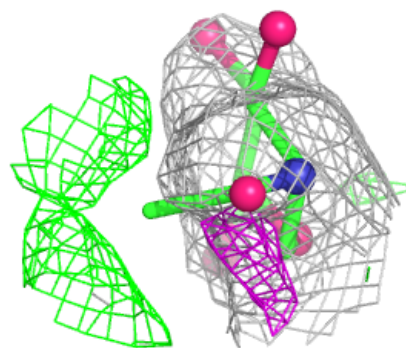
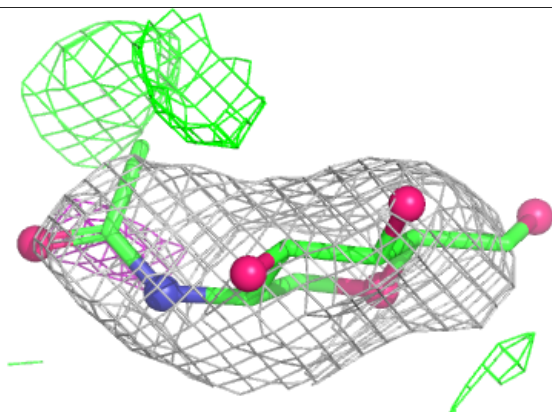
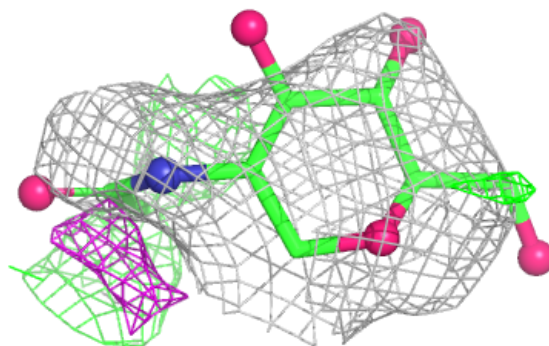
**Electron density around NAG E 601:**

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

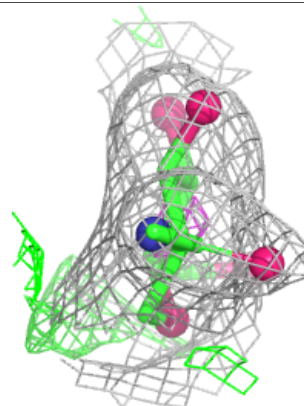
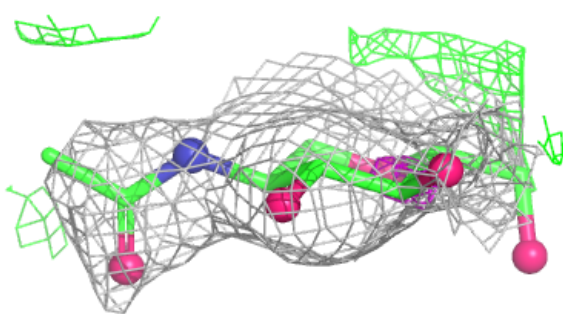
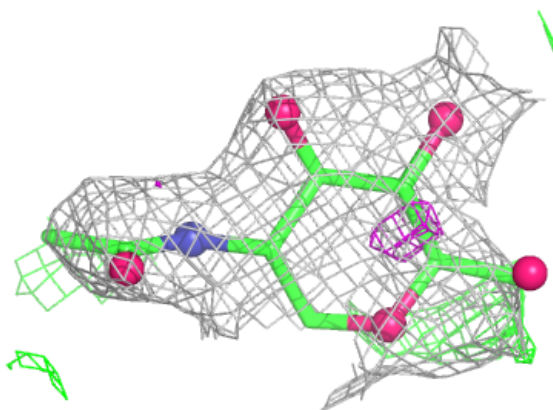


Electron density around NAG A 602:

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

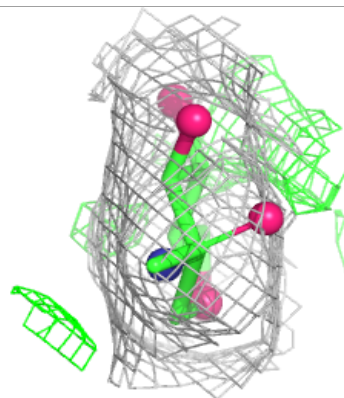
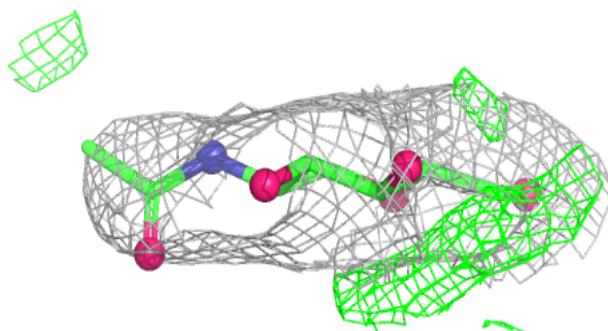
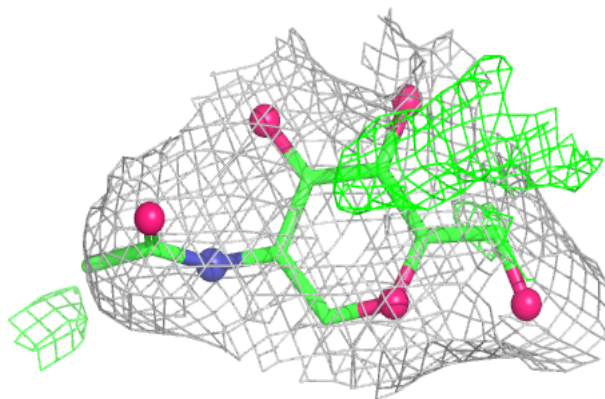
**Electron density around NAG C 602:**

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

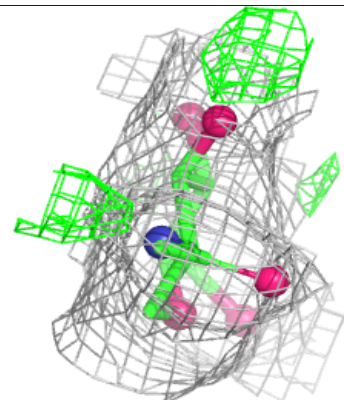
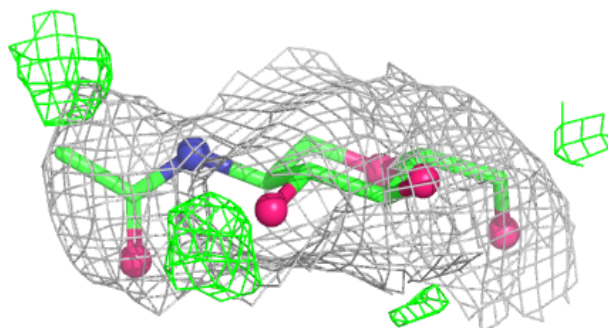
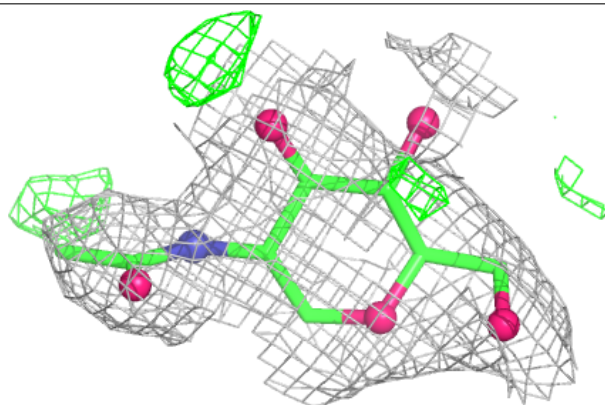


Electron density around NAG C 601:

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

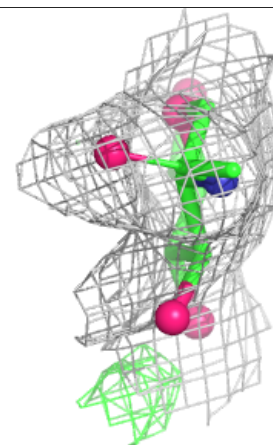
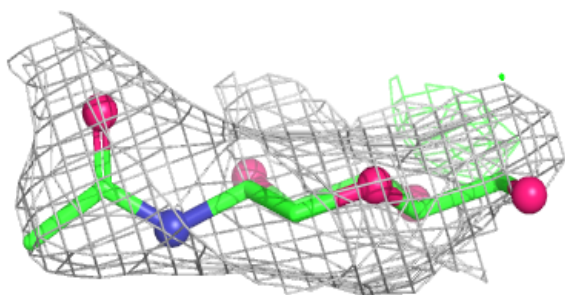
**Electron density around NAG A 601:**

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



Electron density around NAG E 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.