



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:26 PM UTC

PDB ID : 9O3D / pdb_00009o3d
Title : Crystal structure of broadly neutralizing antibody HEPC108 in complex with Hepatitis C virus envelope glycoprotein E2 ectodomain
Authors : Flyak, A.I.; Wilcox, X.E.
Deposited on : 2025-04-07
Resolution : 2.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

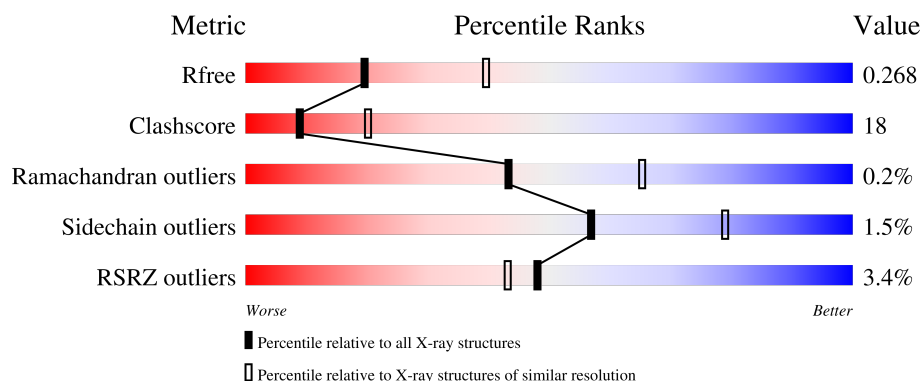
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	237	3% 63% 32% 5%
1	E	237	5% 53% 40% 8%
1	H	237	8% 53% 40% 6%
1	I	237	2% 65% 28% 7%
2	B	216	5% 65% 31% ...

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Mol	Chain	Length	Quality of chain
2	F	216	 65% 34%
2	J	216	 68% 31%
2	L	216	 61% 38%
3	C	262	 63% 25% 11%
3	D	262	 65% 24% 11%
3	G	262	 58% 26% 13%
3	K	262	 66% 22% 11%
4	M	2	 100%
4	P	2	 50% 50%
4	S	2	 100%
4	V	2	 50% 50%
4	W	2	 50% 50%
4	X	2	 100%
5	N	3	 100%
5	R	3	 33% 33% 33%
5	U	3	 67% 33%
6	O	6	 17% 67% 17%
7	Q	4	 50% 50%
7	T	4	 25% 75%
8	Y	6	 67% 33%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 41366 atoms, of which 20138 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 HEPC108 Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	225	Total	C	H	N	O	S	0	0	0
			3330	1055	1660	282	327	6			
1	E	219	Total	C	H	N	O	S	0	0	0
			3253	1034	1620	275	318	6			
1	H	222	Total	C	H	N	O	S	0	0	0
			3275	1039	1630	277	323	6			
1	I	221	Total	C	H	N	O	S	0	0	0
			3280	1041	1635	278	320	6			

- Molecule 2 is a protein called HEPC108 Fab Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	210	Total	C	H	N	O	S	0	0	0
			3183	1014	1565	265	334	5			
2	F	215	Total	C	H	N	O	S	0	0	0
			3264	1040	1603	274	342	5			
2	J	214	Total	C	H	N	O	S	0	0	0
			3248	1035	1596	273	339	5			
2	L	213	Total	C	H	N	O	S	0	0	0
			3241	1033	1593	272	338	5			

- Molecule 3 is a protein called Envelope Glycoprotein E2.

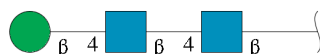
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	232	Total	C	H	N	O	S	0	0	0
			3467	1143	1658	321	326	19			
3	D	233	Total	C	H	N	O	S	0	0	0
			3491	1152	1671	322	327	19			
3	G	227	Total	C	H	N	O	S	0	1	0
			3412	1131	1627	317	318	19			
3	K	232	Total	C	H	N	O	S	0	1	0
			3496	1151	1676	324	326	19			

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



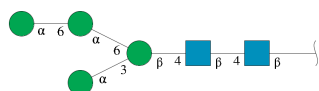
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	2	Total 53	C 16	H 25	N 2	O 10	0	0	0
4	P	2	Total 53	C 16	H 25	N 2	O 10	0	0	0
4	S	2	Total 53	C 16	H 25	N 2	O 10	0	0	0
4	V	2	Total 52	C 16	H 24	N 2	O 10	0	0	0
4	W	2	Total 53	C 16	H 25	N 2	O 10	0	0	0
4	X	2	Total 53	C 16	H 25	N 2	O 10	0	0	0

- Molecule 5 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
5	N	3	Total 63	C 22	H 24	N 2	O 15	0	0	0
5	R	3	Total 63	C 22	H 24	N 2	O 15	0	0	0
5	U	3	Total 73	C 22	H 34	N 2	O 15	0	0	0

- Molecule 6 is an oligosaccharide called 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.



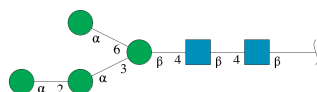
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	6	Total	C	H	N	O	0	0	0
			96	40	24	2	30			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Q	4	Total	C	H	N	O	0	0	0
			74	28	24	2	20			
7	T	4	Total	C	H	N	O	0	0	0
			92	28	42	2	20			

- Molecule 8 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
8	Y	6	Total	C	H	N	O	0	0	0
			133	40	61	2	30			

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	H	O	0	0
			14	3	8	3		
9	D	1	Total	C	H	O	0	0
			14	3	8	3		
9	G	1	Total	C	H	O	0	0
			14	3	8	3		
9	K	1	Total	C	H	O	0	0
			14	3	8	3		
9	K	1	Total	C	H	O	0	0
			14	3	8	3		

- 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	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	D	1	Total	C	N	O		0	0
			14	8	1	5			
10	D	1	Total	C	N	O		0	0
			14	8	1	5			
10	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	G	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	G	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	K	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	K	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	K	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	K	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	K	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

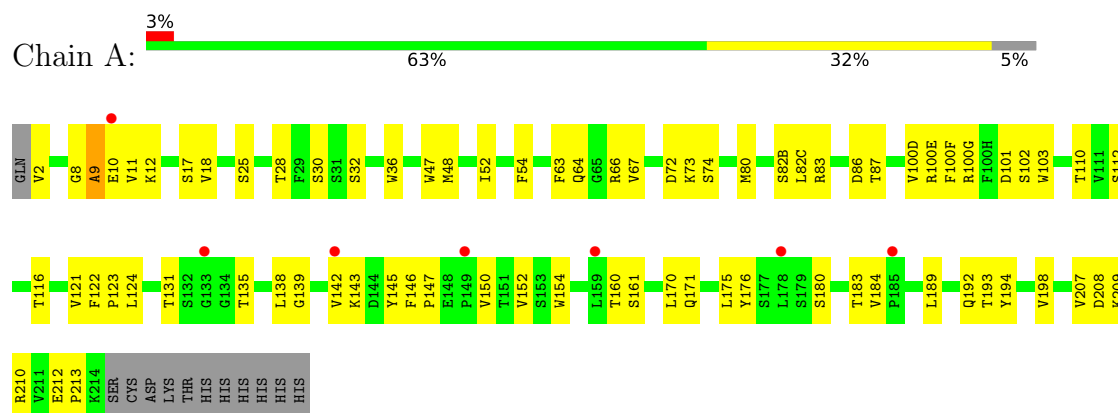
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	3	Total	O	0	0
			3	3		
11	B	2	Total	O	0	0
			2	2		
11	C	5	Total	O	0	0
			5	5		
11	D	1	Total	O	0	0
			1	1		
11	F	4	Total	O	0	0
			4	4		
11	G	9	Total	O	0	0
			9	9		
11	I	6	Total	O	0	0
			6	6		
11	J	1	Total	O	0	0
			1	1		
11	K	8	Total	O	0	0
			8	8		

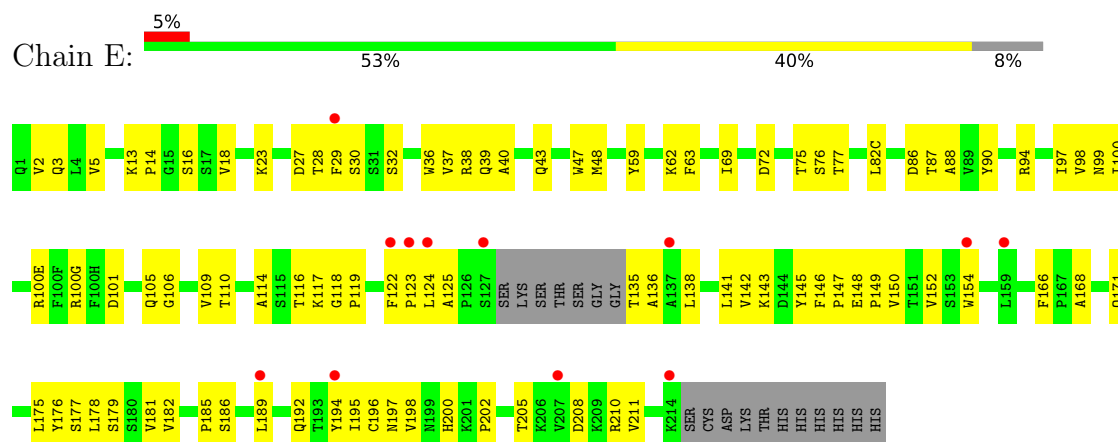
3 Residue-property plots [i](#)

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.

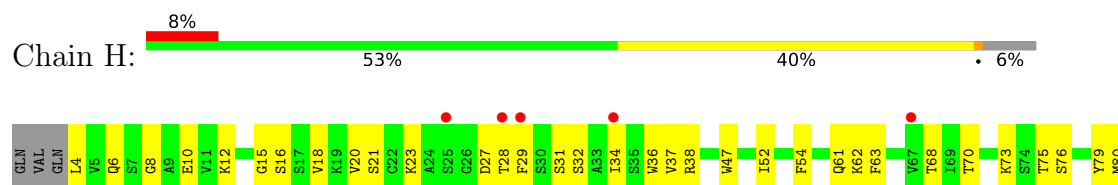
• Molecule 1: HEPC108 Fab Heavy Chain

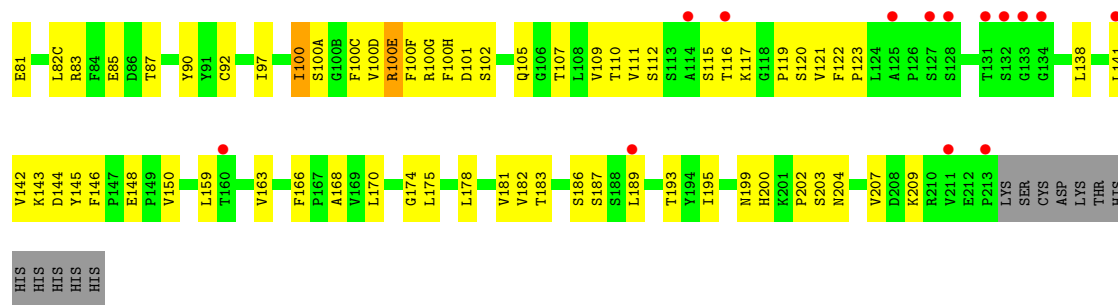


• Molecule 1: HEPC108 Fab Heavy Chain

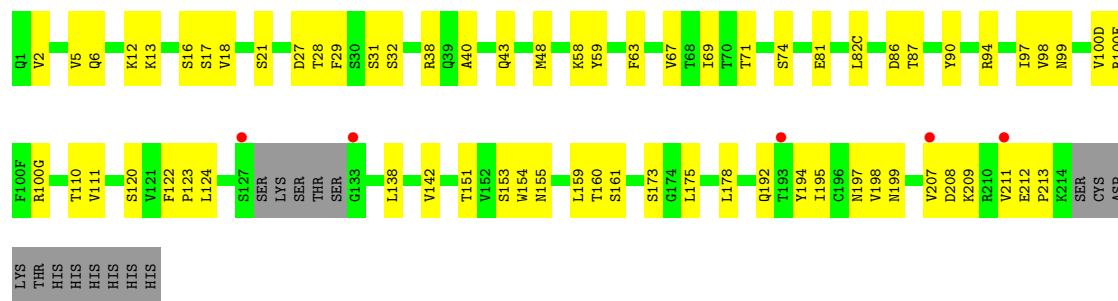


• Molecule 1: HEPC108 Fab Heavy Chain

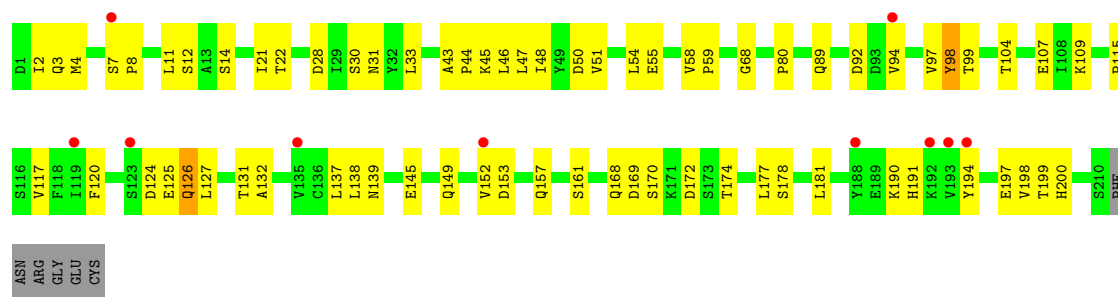




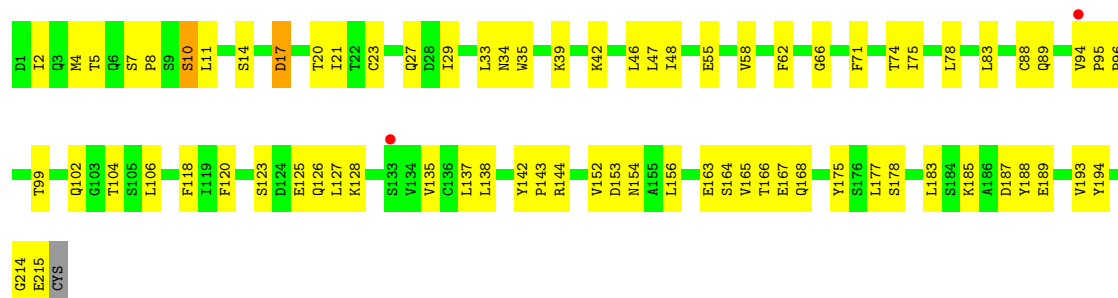
● Molecule 1: HEPC108 Fab Heavy Chain



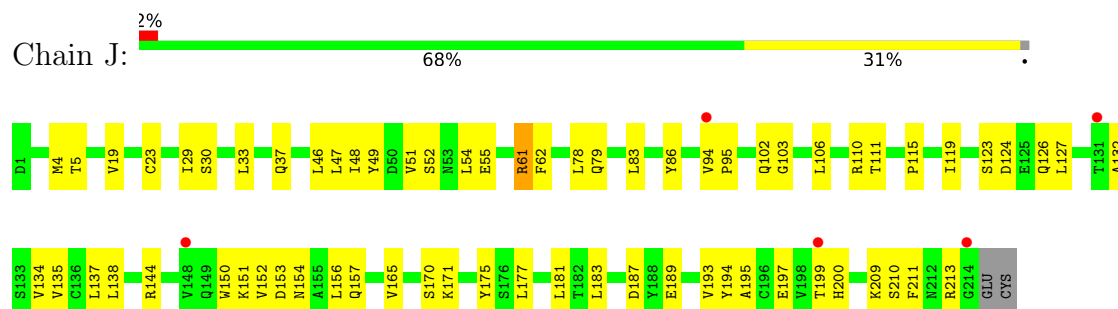
● Molecule 2: HEPC108 Fab Light Chain



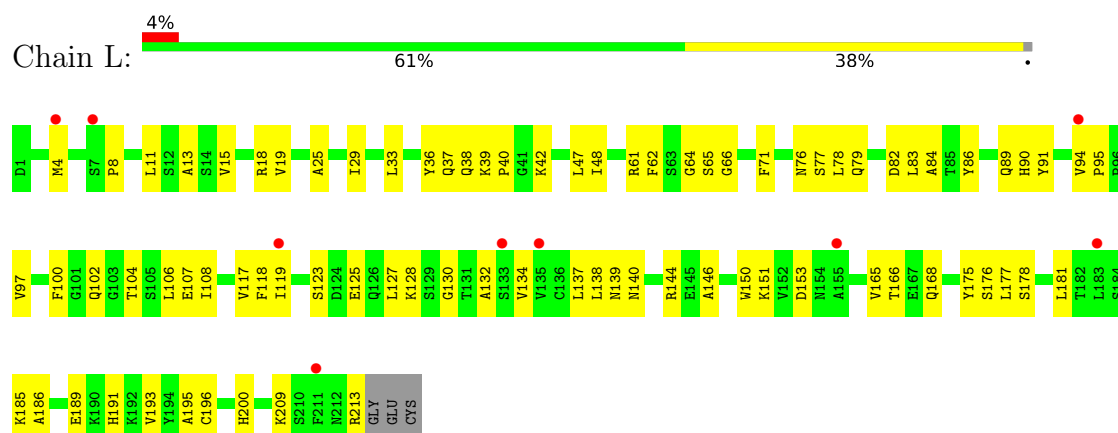
● Molecule 2: HEPC108 Fab Light Chain



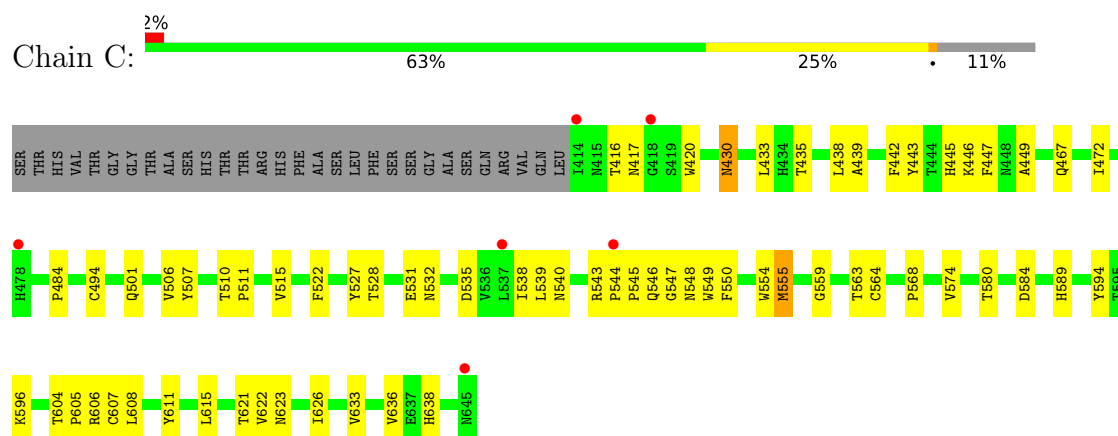
- Molecule 2: HEPC108 Fab Light Chain



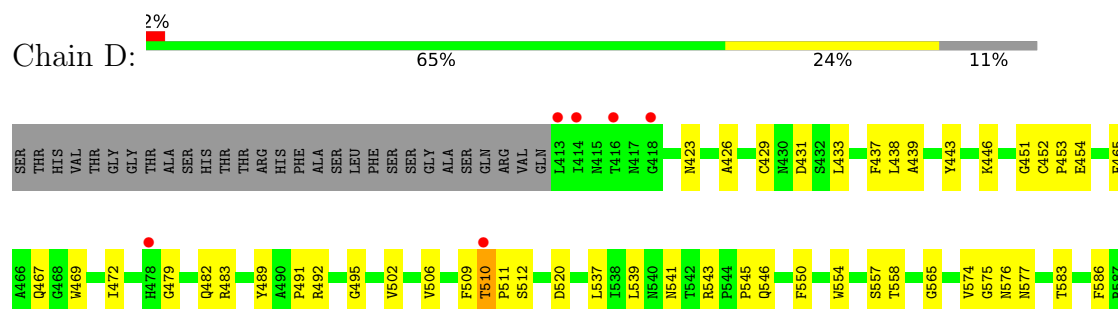
- Molecule 2: HEPC108 Fab Light Chain



- Molecule 3: Envelope Glycoprotein E2

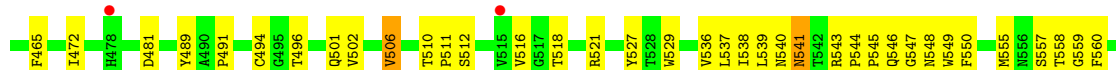
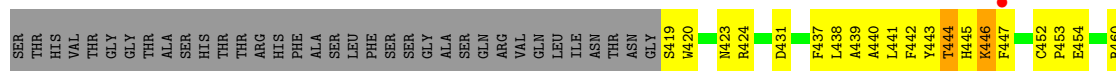


- Molecule 3: Envelope Glycoprotein E2

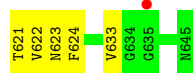
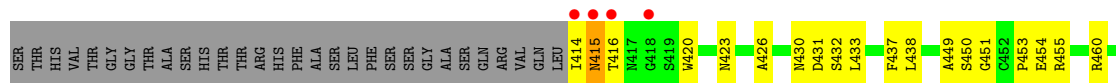




- Molecule 3: Envelope Glycoprotein E2



- Molecule 3: Envelope Glycoprotein E2



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



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



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

Chain S:  100%

NAG1
NAG2

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

Chain V:  50% 50%

NAG1
NAG2

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

Chain W:  50% 50%

NAG1
NAG2

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

Chain X:  100%

NAG1
NAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

NAG1
NAG2
BMA3

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  33% 33% 33%

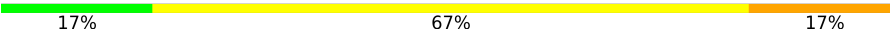
NAG1
NAG2
BMA3

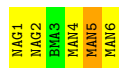
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  67% 33%

NAG1
NAG2
BMA3

- Molecule 6: α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain O:  17% 67% 17%



- Molecule 7: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain Q:  50% 50%



- Molecule 7: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain T:  25% 75%



- Molecule 8: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain Y:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.64Å 78.53Å 227.78Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	52.32 – 2.68 52.32 – 2.68	Depositor EDS
% Data completeness (in resolution range)	96.2 (52.32-2.68) 96.3 (52.32-2.68)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.214 , 0.269 0.212 , 0.268	Depositor DCC
R_{free} test set	5698 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41366	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.01% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/1708	0.63	0/2322
1	E	0.41	0/1670	0.64	0/2272
1	H	0.36	0/1683	0.61	0/2289
1	I	0.42	0/1682	0.59	0/2286
2	B	0.44	0/1653	0.66	0/2251
2	F	0.40	0/1697	0.64	0/2309
2	J	0.40	0/1688	0.63	0/2297
2	L	0.41	0/1684	0.61	0/2292
3	C	0.49	0/1875	0.74	2/2569 (0.1%)
3	D	0.49	0/1886	0.71	0/2584
3	G	0.57	0/1854	0.76	1/2540 (0.0%)
3	K	0.55	0/1889	0.72	0/2588
All	All	0.45	0/20969	0.67	3/28599 (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
3	G	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	510	THR	N-CA-C	6.06	123.21	109.81
3	C	555	MET	CA-C-N	-6.00	110.07	121.54
3	C	555	MET	C-N-CA	-6.00	110.07	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	460[A]	ARG	Sidechain
3	G	460[B]	ARG	Sidechain

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	1670	1660	1660	64	0
1	E	1633	1620	1618	103	0
1	H	1645	1630	1630	83	0
1	I	1645	1635	1635	48	1
2	B	1618	1565	1565	58	0
2	F	1661	1603	1602	71	0
2	J	1652	1596	1596	58	0
2	L	1648	1593	1593	76	1
3	C	1809	1658	1657	75	0
3	D	1820	1671	1676	57	0
3	G	1785	1627	1647	61	0
3	K	1820	1676	1678	50	0
4	M	28	25	25	3	0
4	P	28	25	25	1	0
4	S	28	25	25	0	0
4	V	28	24	25	1	0
4	W	28	25	25	1	0
4	X	28	25	25	0	0
5	N	39	24	34	0	0
5	R	39	24	34	1	0
5	U	39	34	34	0	0
6	O	72	24	61	1	0
7	Q	50	24	43	1	0
7	T	50	42	43	0	0
8	Y	72	61	61	2	0
9	C	6	8	8	0	0
9	D	6	8	8	1	0
9	G	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	12	16	16	1	0
10	C	56	52	52	3	0
10	D	70	39	65	1	0
10	G	28	26	26	0	0
10	K	70	65	65	8	0
11	A	3	0	0	0	0
11	B	2	0	0	0	0
11	C	5	0	0	0	0
11	D	1	0	0	0	0
11	F	4	0	0	1	0
11	G	9	0	0	0	0
11	I	6	0	0	0	0
11	J	1	0	0	0	0
11	K	8	0	0	0	0
All	All	21228	20138	20265	766	1

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 18.

The worst 5 of 766 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)
3:G:445:HIS:O	3:G:447:PHE:N	1.88	1.06
1:E:38:ARG:NH2	1:E:90:TYR:OH	1.89	1.05
2:L:83:LEU:HD23	2:L:108:ILE:CD1	1.87	1.05
2:J:189:GLU:OE1	2:J:213:ARG:NH1	1.90	1.04
2:L:83:LEU:HD23	2:L:108:ILE:HD12	1.36	1.03

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:192:GLN:OE1	2:L:102:GLN:NE2[1_565]	2.08	0.12

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	223/237 (94%)	202 (91%)	20 (9%)	1 (0%)	30	51
1	E	215/237 (91%)	197 (92%)	18 (8%)	0	100	100
1	H	220/237 (93%)	192 (87%)	28 (13%)	0	100	100
1	I	217/237 (92%)	208 (96%)	8 (4%)	1 (0%)	24	45
2	B	208/216 (96%)	186 (89%)	22 (11%)	0	100	100
2	F	213/216 (99%)	192 (90%)	21 (10%)	0	100	100
2	J	212/216 (98%)	193 (91%)	19 (9%)	0	100	100
2	L	211/216 (98%)	194 (92%)	17 (8%)	0	100	100
3	C	230/262 (88%)	203 (88%)	27 (12%)	0	100	100
3	D	231/262 (88%)	216 (94%)	14 (6%)	1 (0%)	30	51
3	G	226/262 (86%)	200 (88%)	25 (11%)	1 (0%)	30	51
3	K	231/262 (88%)	215 (93%)	14 (6%)	2 (1%)	14	31
All	All	2637/2860 (92%)	2398 (91%)	233 (9%)	6 (0%)	43	65

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	446	LYS
3	K	415	ASN
1	I	160	THR
3	D	510	THR
1	A	9	ALA

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	189/201 (94%)	189 (100%)	0	100	100
1	E	184/201 (92%)	183 (100%)	1 (0%)	81	91
1	H	186/201 (92%)	175 (94%)	11 (6%)	18	38
1	I	185/201 (92%)	184 (100%)	1 (0%)	81	91
2	B	188/193 (97%)	185 (98%)	3 (2%)	55	78
2	F	192/193 (100%)	189 (98%)	3 (2%)	55	78
2	J	191/193 (99%)	189 (99%)	2 (1%)	68	84
2	L	191/193 (99%)	191 (100%)	0	100	100
3	C	194/219 (89%)	191 (98%)	3 (2%)	57	79
3	D	196/219 (90%)	194 (99%)	2 (1%)	68	84
3	G	192/219 (88%)	187 (97%)	5 (3%)	40	68
3	K	196/219 (90%)	193 (98%)	3 (2%)	57	79
All	All	2284/2452 (93%)	2250 (98%)	34 (2%)	57	79

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	74	SER
2	J	61	ARG
3	K	521	ARG
3	G	444	THR
2	F	17	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	162	GLN
3	K	493	GLN
2	L	140	ASN
2	L	34	ASN
3	K	421	HIS

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 ⓘ

41 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	M	1	4,3	14,14,15	0.72	0	17,19,21	2.28	5 (29%)
4	NAG	M	2	4	14,14,15	0.70	0	17,19,21	1.65	4 (23%)
5	NAG	N	1	5,3	14,14,15	0.93	1 (7%)	17,19,21	1.17	2 (11%)
5	NAG	N	2	5	14,14,15	0.80	0	17,19,21	1.25	2 (11%)
5	BMA	N	3	5	11,11,12	0.86	0	15,15,17	0.95	1 (6%)
6	NAG	O	1	6,3	14,14,15	0.62	0	17,19,21	2.20	6 (35%)
6	NAG	O	2	6	14,14,15	0.77	0	17,19,21	1.79	2 (11%)
6	BMA	O	3	6	11,11,12	0.45	0	15,15,17	0.83	0
6	MAN	O	4	6	11,11,12	0.82	0	15,15,17	0.97	0
6	MAN	O	5	6	11,11,12	0.85	1 (9%)	15,15,17	1.09	1 (6%)
6	MAN	O	6	6	11,11,12	0.75	0	15,15,17	1.31	1 (6%)
4	NAG	P	1	4,3	14,14,15	0.71	0	17,19,21	1.67	4 (23%)
4	NAG	P	2	4	14,14,15	0.79	1 (7%)	17,19,21	1.11	1 (5%)
7	NAG	Q	1	7,3	14,14,15	0.91	1 (7%)	17,19,21	1.34	2 (11%)
7	NAG	Q	2	7	14,14,15	0.83	0	17,19,21	1.52	2 (11%)
7	BMA	Q	3	7	11,11,12	0.79	0	15,15,17	1.01	1 (6%)
7	MAN	Q	4	7	11,11,12	0.59	0	15,15,17	1.66	2 (13%)
5	NAG	R	1	5,3	14,14,15	0.72	0	17,19,21	1.57	3 (17%)
5	NAG	R	2	5	14,14,15	0.98	1 (7%)	17,19,21	1.13	2 (11%)
5	BMA	R	3	5	11,11,12	0.48	0	15,15,17	0.80	0
4	NAG	S	1	4,3	14,14,15	0.71	0	17,19,21	1.83	5 (29%)
4	NAG	S	2	4	14,14,15	0.63	0	17,19,21	1.93	5 (29%)
7	NAG	T	1	7,3	14,14,15	0.83	0	17,19,21	1.33	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	T	2	7	14,14,15	0.75	0	17,19,21	1.19	2 (11%)
7	BMA	T	3	7	11,11,12	0.56	0	15,15,17	0.90	0
7	MAN	T	4	7	11,11,12	0.71	0	15,15,17	1.39	1 (6%)
5	NAG	U	1	5,3	14,14,15	0.66	0	17,19,21	0.95	0
5	NAG	U	2	5	14,14,15	0.81	0	17,19,21	2.07	6 (35%)
5	BMA	U	3	5	11,11,12	0.69	0	15,15,17	0.72	0
4	NAG	V	1	4,3	14,14,15	0.84	0	17,19,21	1.75	4 (23%)
4	NAG	V	2	4	14,14,15	0.66	0	17,19,21	1.57	3 (17%)
4	NAG	W	1	4,3	14,14,15	0.77	0	17,19,21	1.40	3 (17%)
4	NAG	W	2	4	14,14,15	0.66	0	17,19,21	1.23	1 (5%)
4	NAG	X	1	4,3	14,14,15	0.81	0	17,19,21	1.22	1 (5%)
4	NAG	X	2	4	14,14,15	0.83	1 (7%)	17,19,21	1.37	2 (11%)
8	NAG	Y	1	8,3	14,14,15	0.88	0	17,19,21	1.97	6 (35%)
8	NAG	Y	2	8	14,14,15	0.69	0	17,19,21	1.77	5 (29%)
8	BMA	Y	3	8	11,11,12	0.66	0	15,15,17	1.58	3 (20%)
8	MAN	Y	4	8	11,11,12	0.86	1 (9%)	15,15,17	1.05	0
8	MAN	Y	5	8	11,11,12	0.70	0	15,15,17	1.52	3 (20%)
8	MAN	Y	6	8	11,11,12	0.75	0	15,15,17	1.41	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	5/6/23/26	0/1/1/1
5	NAG	N	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	1/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
6	NAG	O	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	1/2/19/22	0/1/1/1
6	MAN	O	5	6	-	2/2/19/22	0/1/1/1
6	MAN	O	6	6	-	1/2/19/22	0/1/1/1
4	NAG	P	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	Q	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
5	NAG	R	1	5,3	-	1/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1
5	BMA	R	3	5	-	1/2/19/22	0/1/1/1
4	NAG	S	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
7	NAG	T	1	7,3	-	0/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	BMA	T	3	7	-	0/2/19/22	0/1/1/1
7	MAN	T	4	7	-	2/2/19/22	0/1/1/1
5	NAG	U	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	3/6/23/26	0/1/1/1
5	BMA	U	3	5	-	1/2/19/22	0/1/1/1
4	NAG	V	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	4/6/23/26	0/1/1/1
4	NAG	W	1	4,3	-	4/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,3	-	1/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
8	NAG	Y	1	8,3	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	4/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	2/2/19/22	0/1/1/1
8	MAN	Y	4	8	-	0/2/19/22	0/1/1/1
8	MAN	Y	5	8	-	2/2/19/22	0/1/1/1
8	MAN	Y	6	8	-	2/2/19/22	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	2	NAG	C1-C2	3.20	1.56	1.52
7	Q	1	NAG	O5-C1	-2.34	1.39	1.43
5	N	1	NAG	O5-C1	-2.21	1.40	1.43
8	Y	4	MAN	O5-C1	-2.16	1.40	1.43
4	P	2	NAG	C1-C2	2.12	1.55	1.52

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1	NAG	C1-C2-N2	5.79	119.56	110.43
4	S	2	NAG	C2-N2-C7	5.12	129.76	122.90
5	U	2	NAG	C4-C3-C2	-5.05	103.62	111.02
6	O	1	NAG	C1-O5-C5	4.84	118.68	112.19
7	Q	4	MAN	C1-O5-C5	4.84	118.67	112.19

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

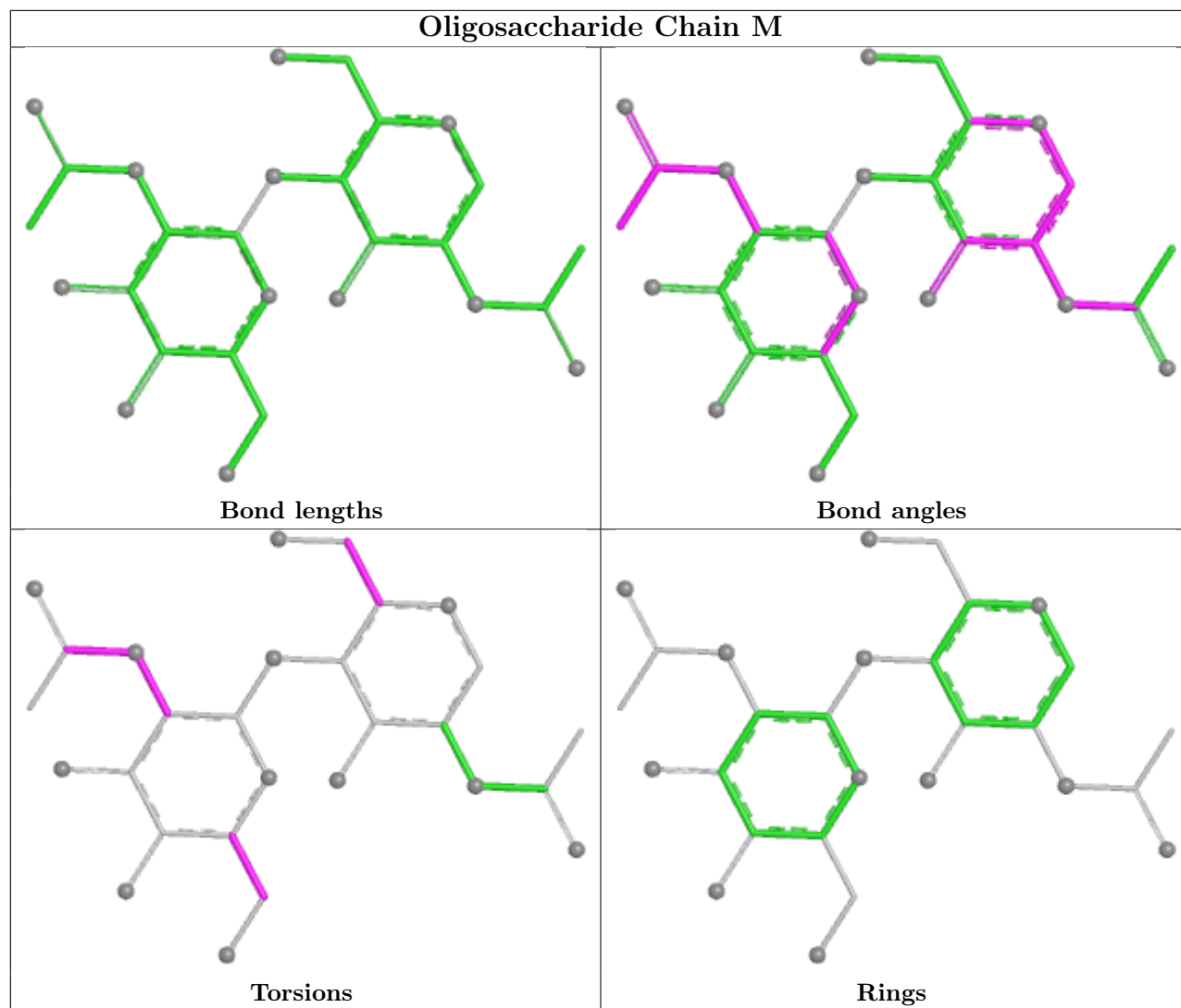
Mol	Chain	Res	Type	Atoms
8	Y	5	MAN	O5-C5-C6-O6
8	Y	5	MAN	C4-C5-C6-O6
8	Y	3	BMA	O5-C5-C6-O6
8	Y	3	BMA	C4-C5-C6-O6
8	Y	6	MAN	C4-C5-C6-O6

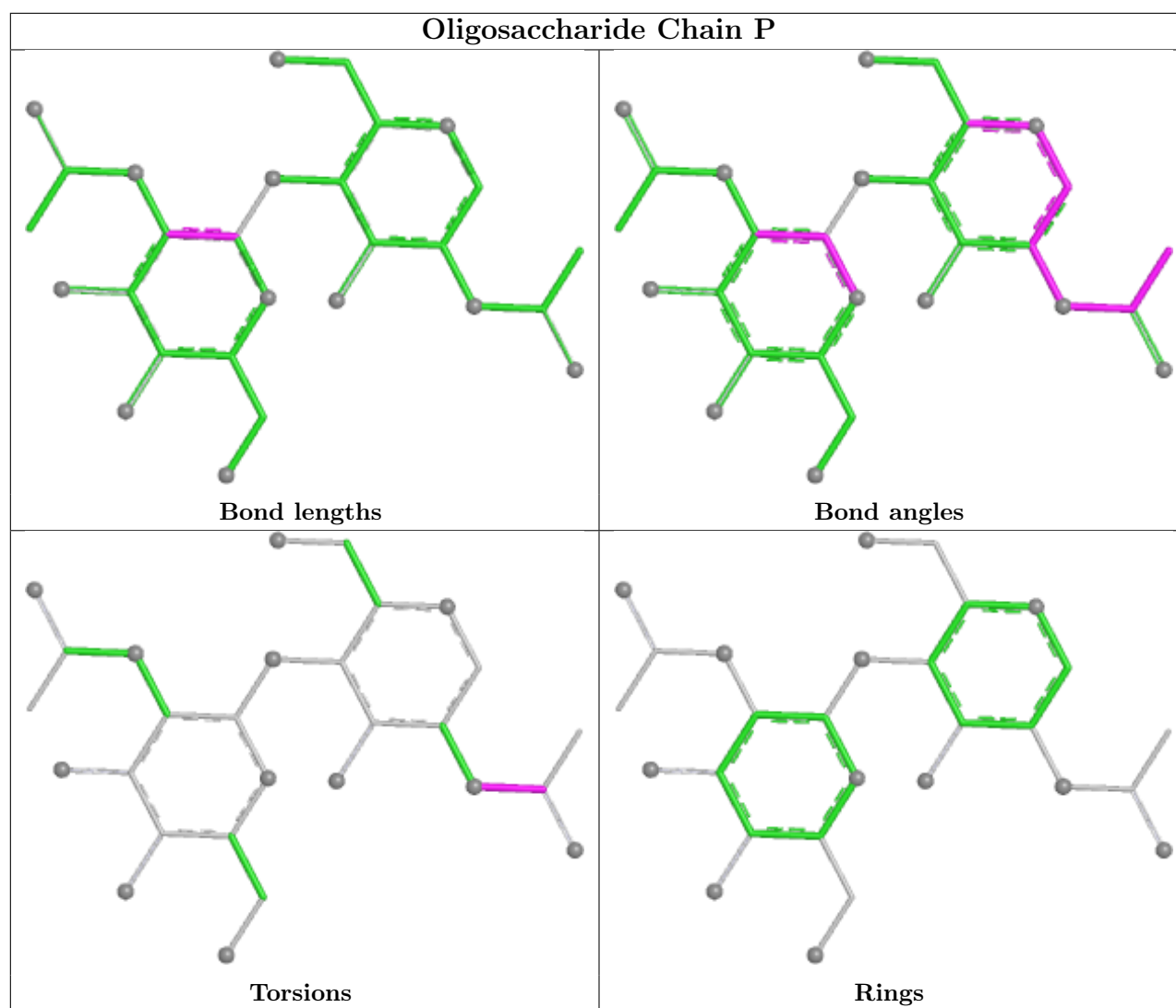
There are no ring outliers.

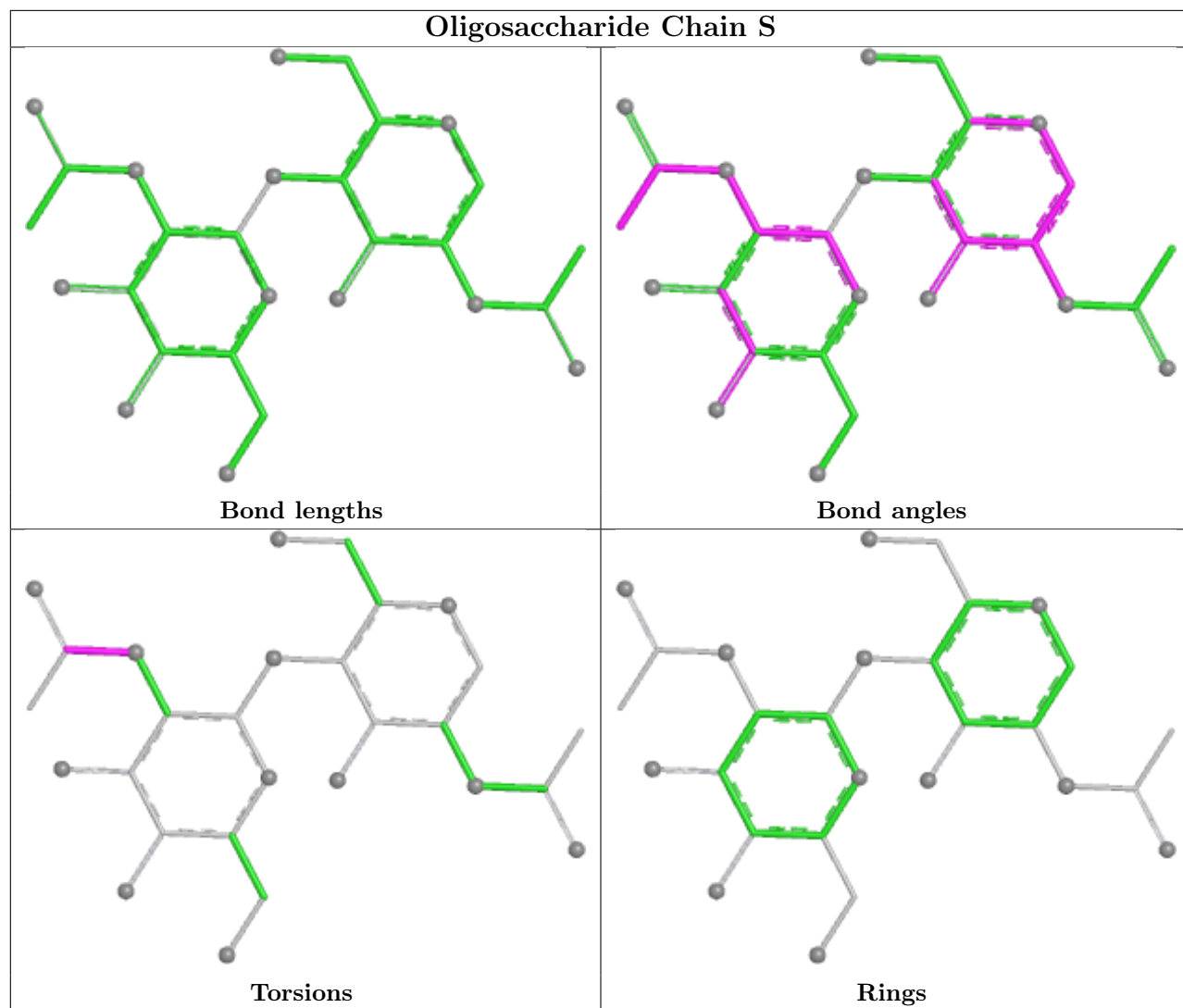
12 monomers are involved in 11 short contacts:

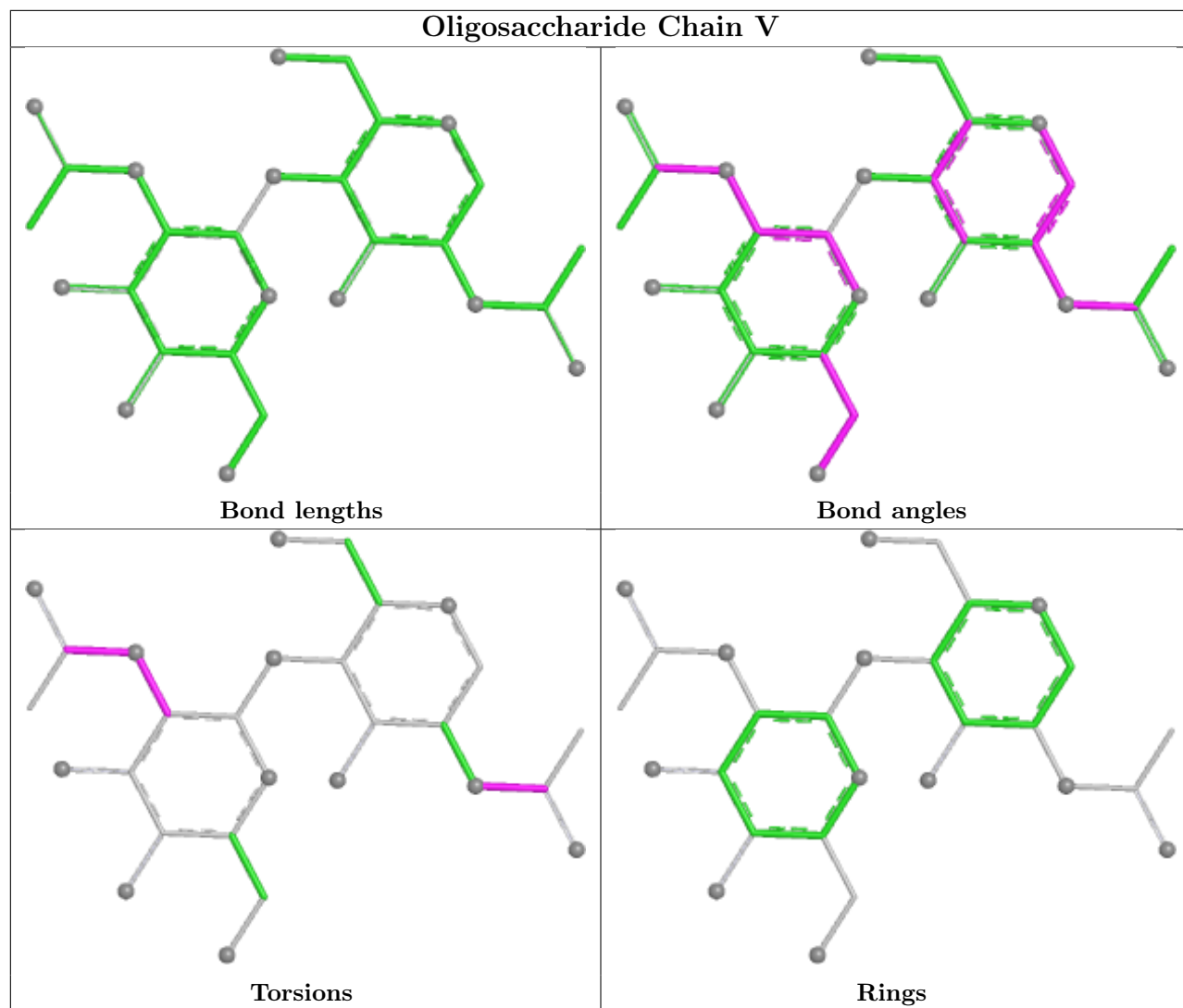
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Q	2	NAG	1	0
8	Y	1	NAG	2	0
6	O	5	MAN	1	0
6	O	4	MAN	1	0
4	P	1	NAG	1	0
4	M	2	NAG	1	0
7	Q	1	NAG	1	0
4	M	1	NAG	2	0
4	W	1	NAG	1	0
8	Y	2	NAG	1	0
4	V	2	NAG	1	0
5	R	1	NAG	1	0

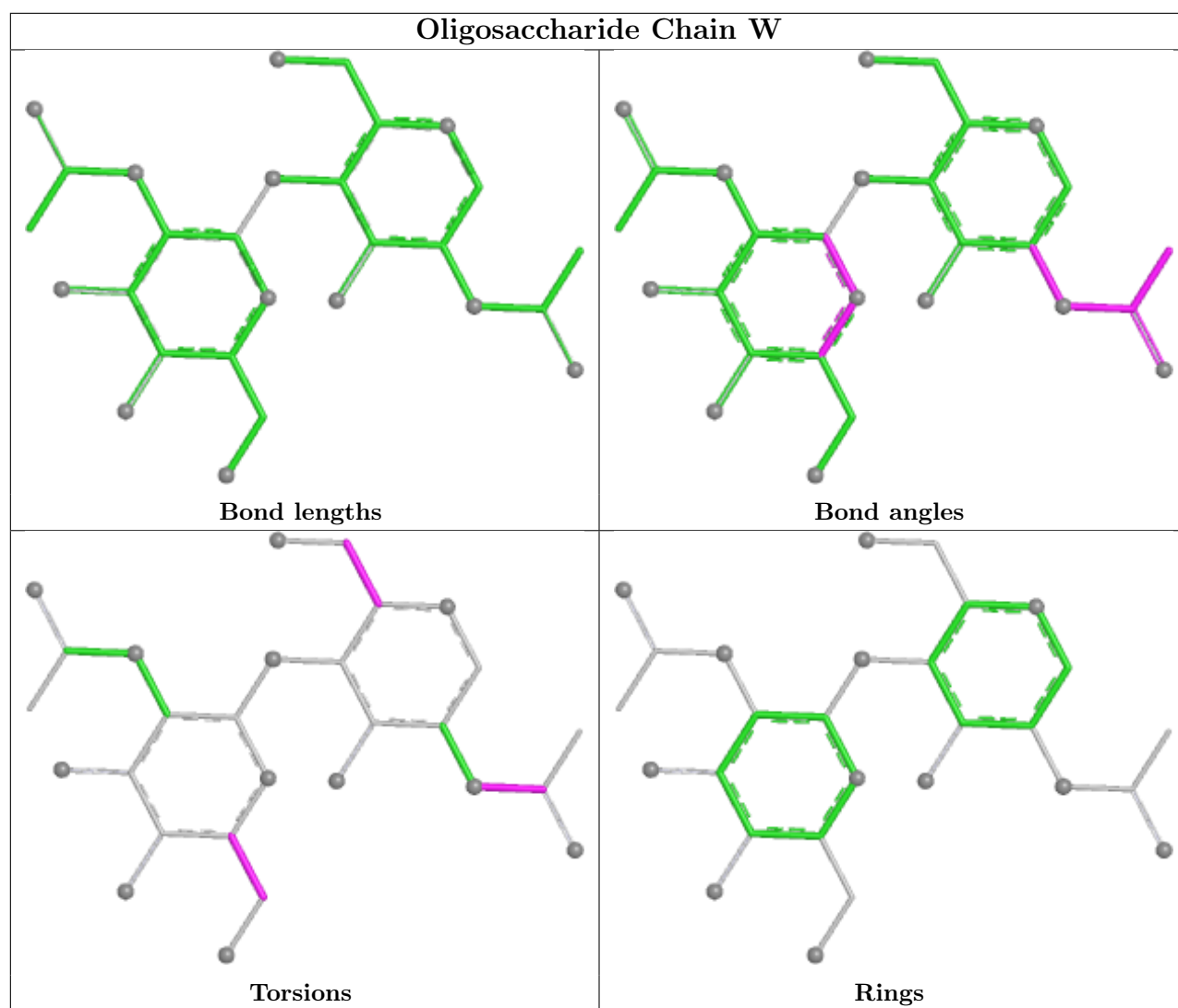
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

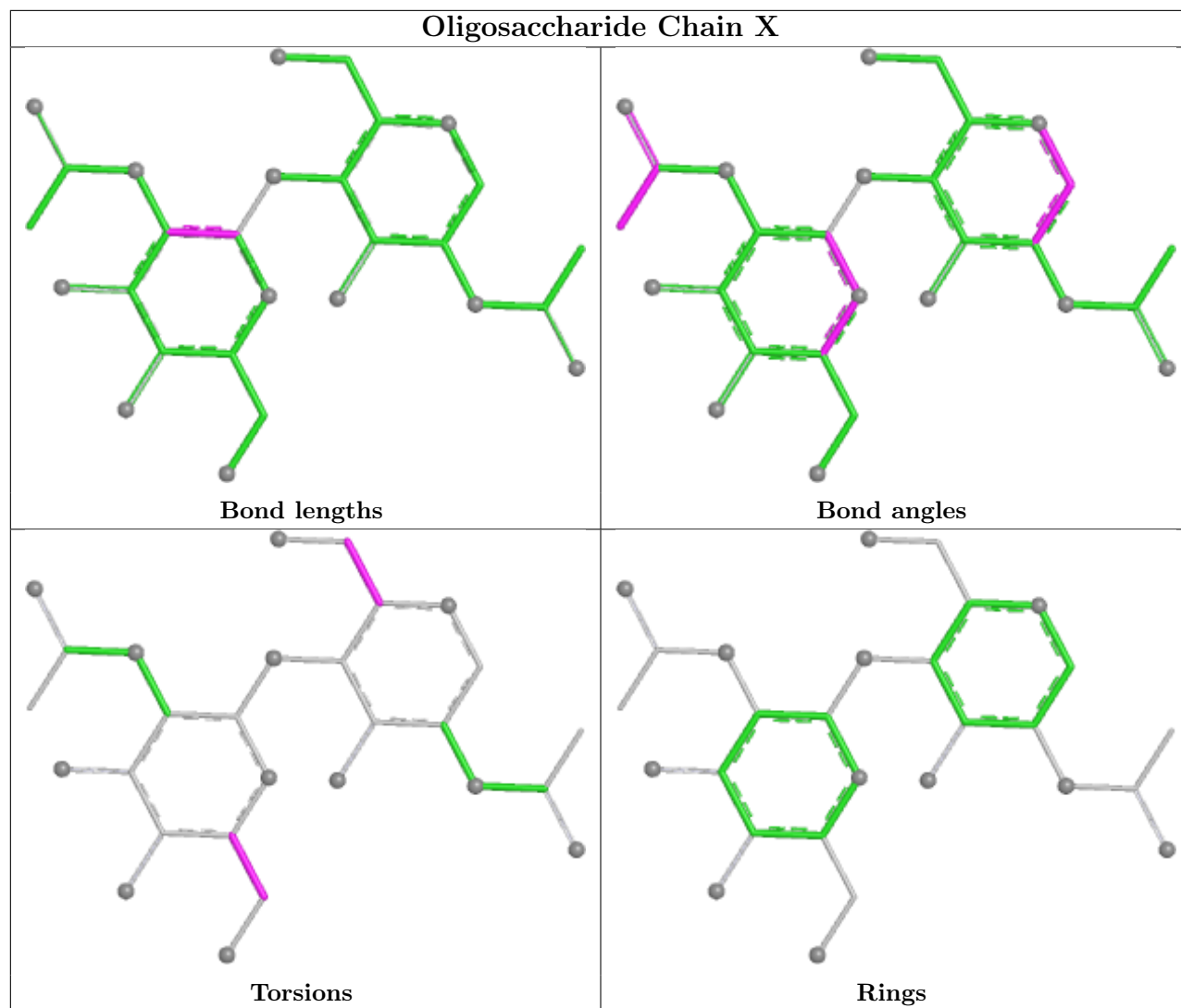


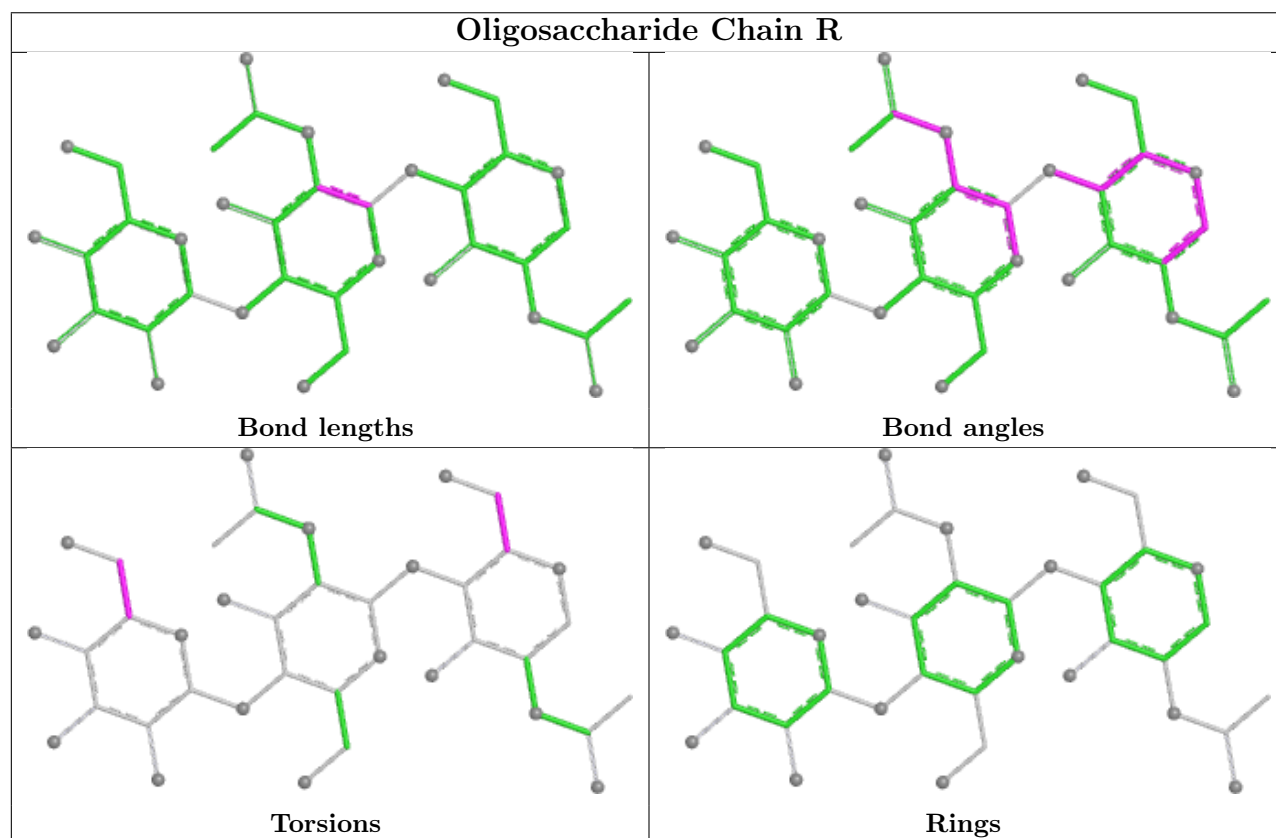
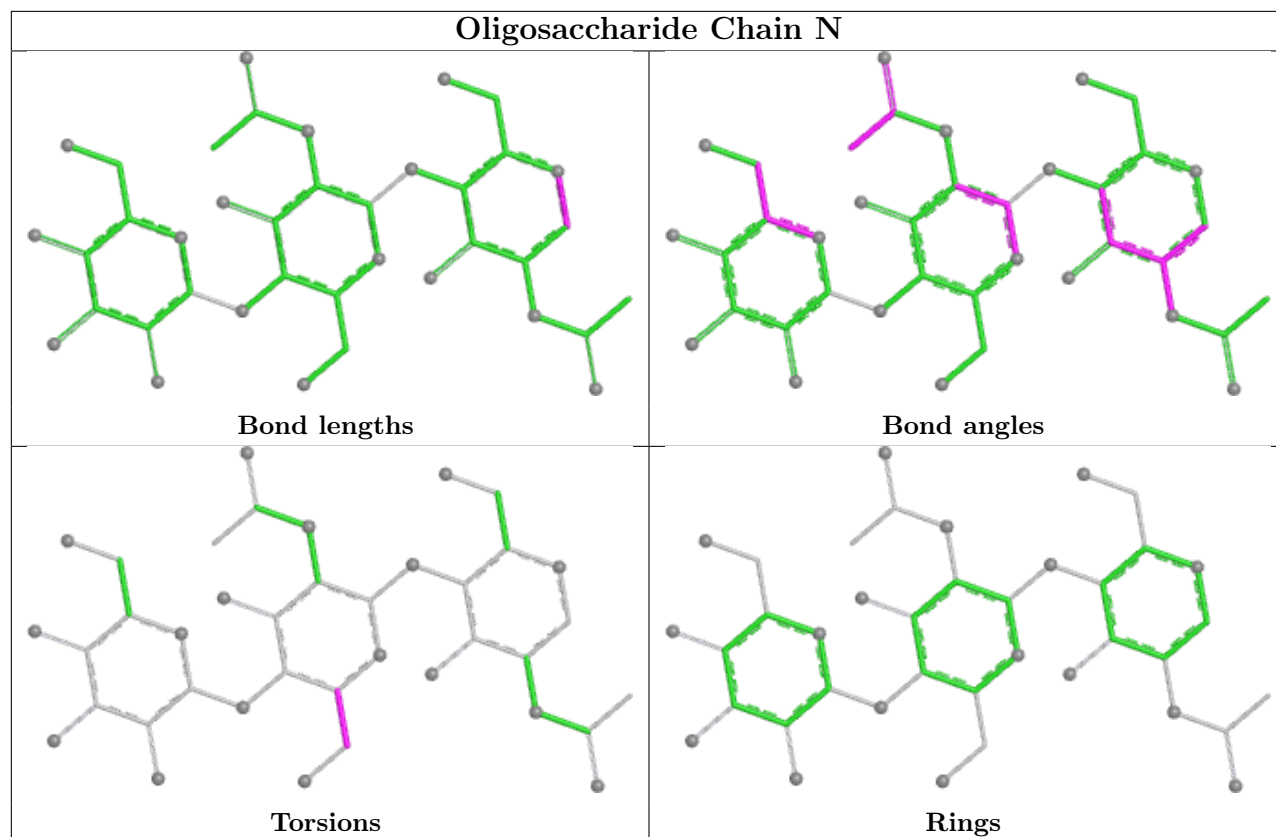


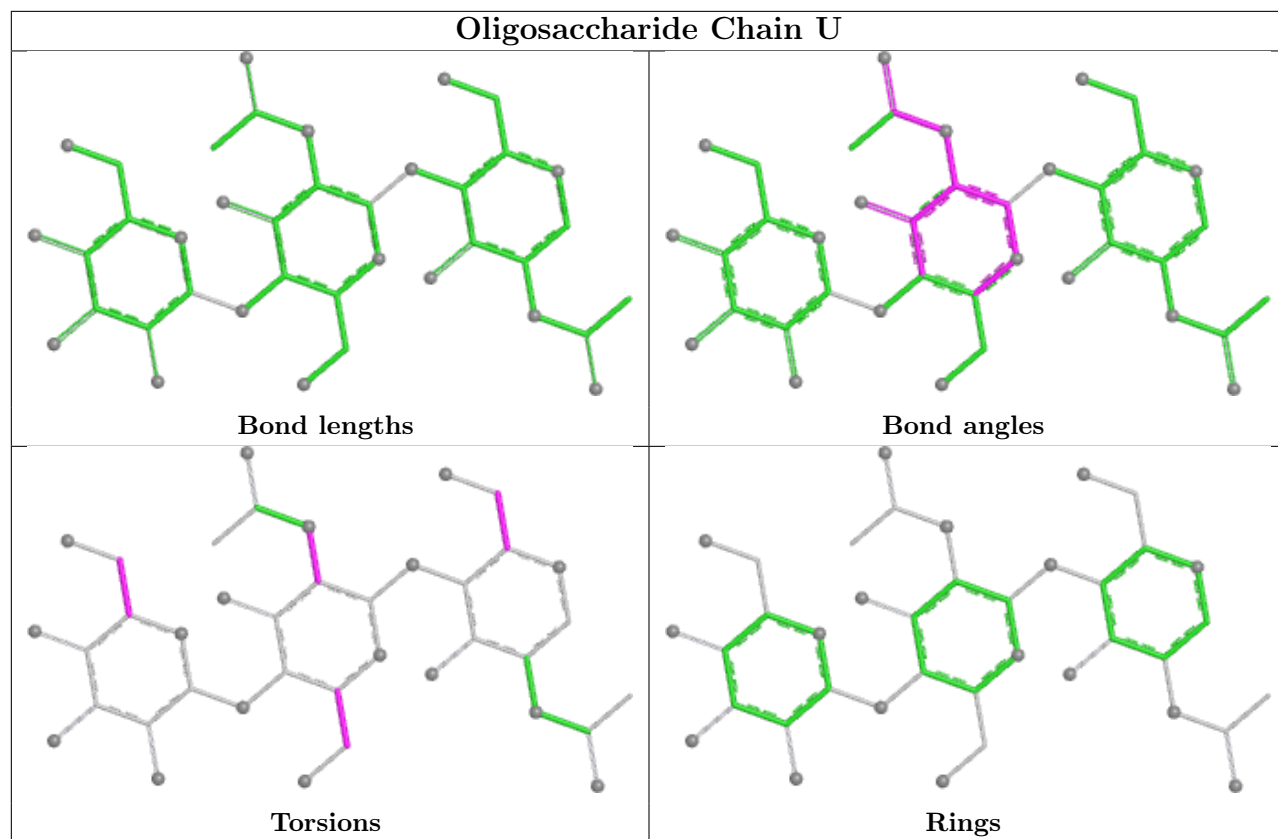


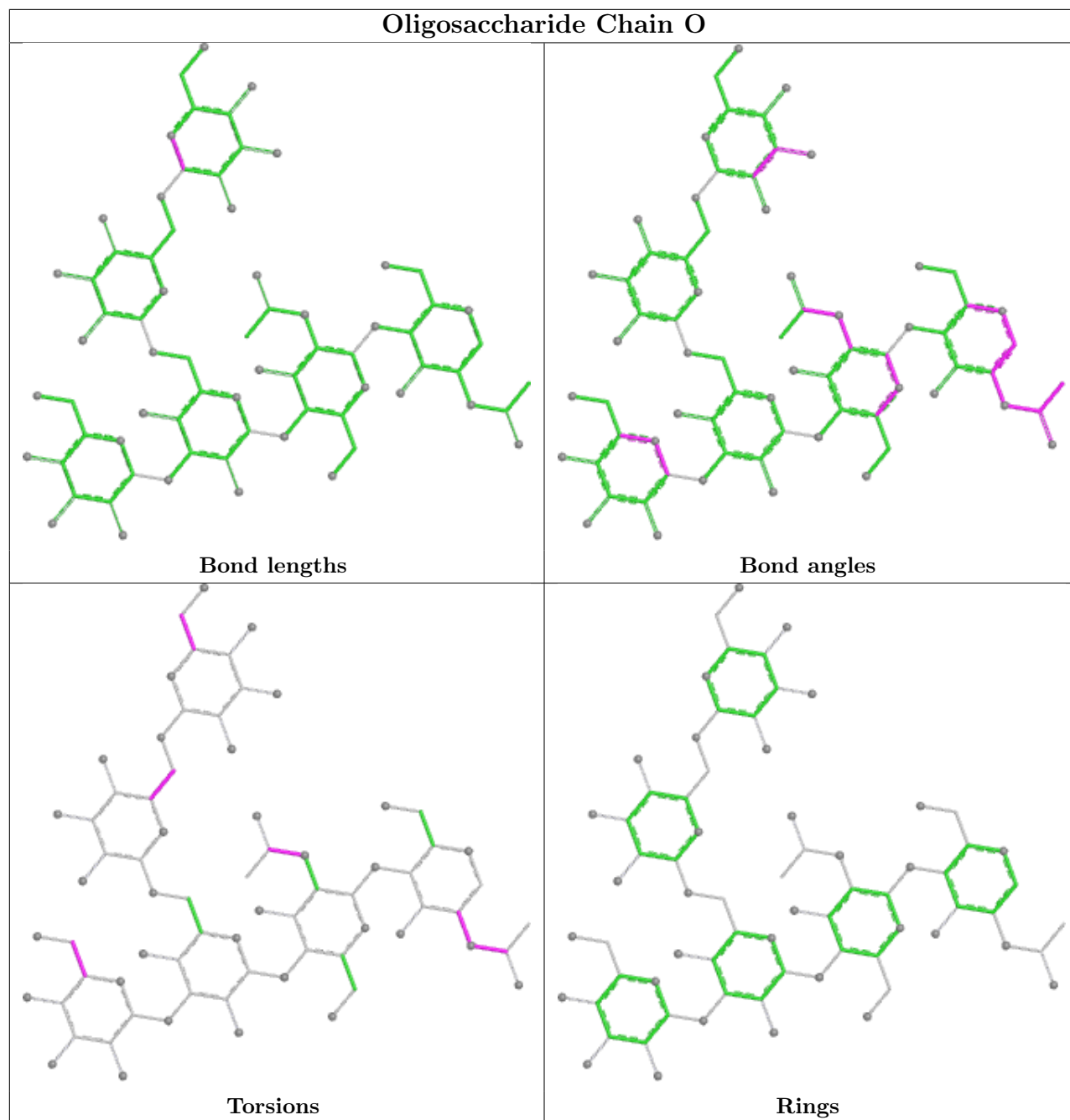




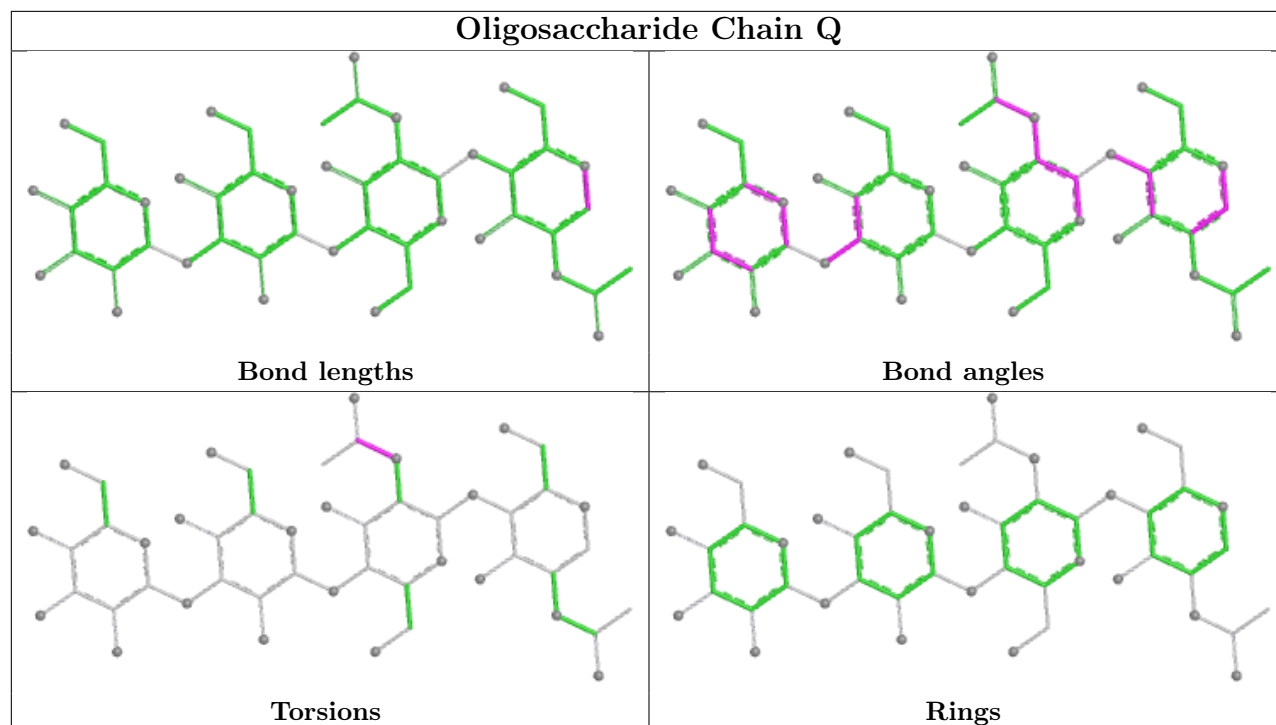




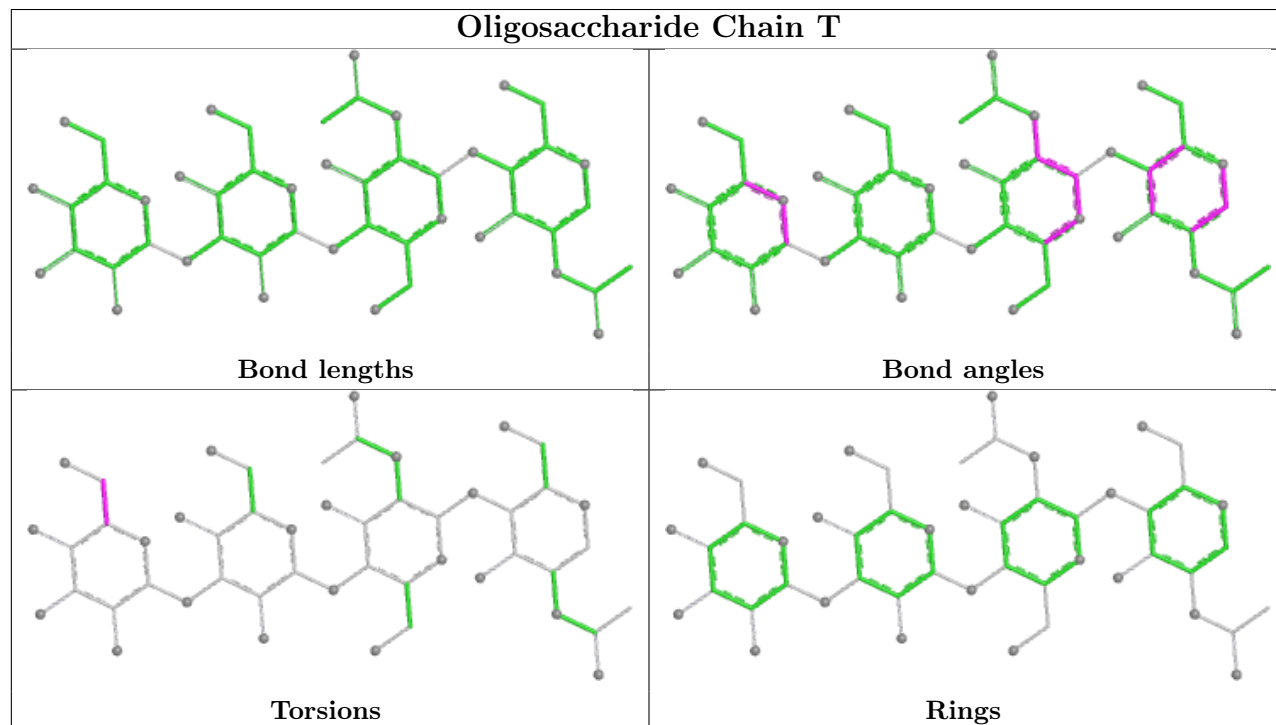


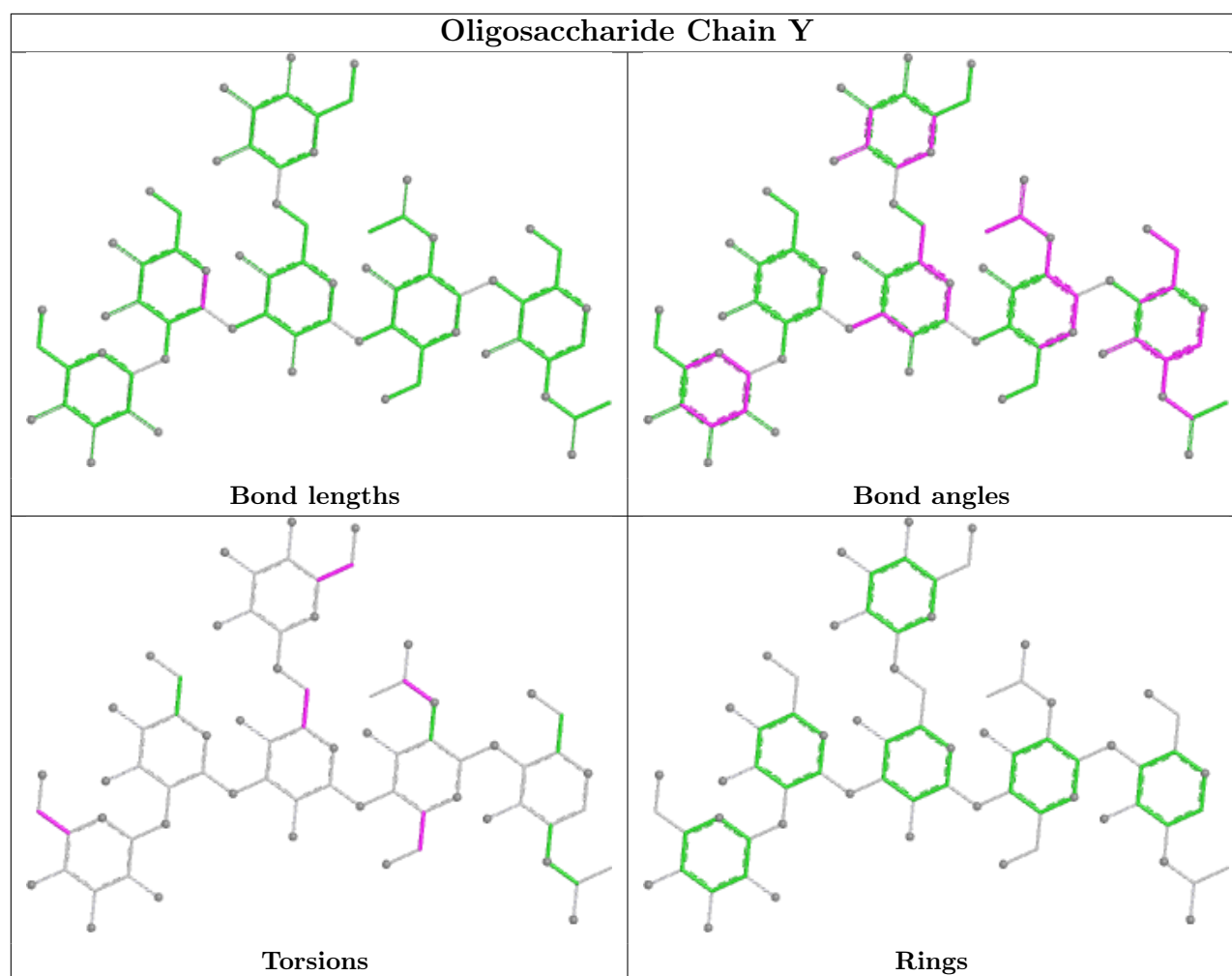


Oligosaccharide Chain Q



Oligosaccharide Chain T





5.6 Ligand geometry [i](#)

21 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	$\# Z > 2$
9	GOL	K	702	-	5,5,5	0.41	0	5,5,5	0.52	0
10	NAG	D	706	3	14,14,15	0.63	0	17,19,21	1.59	2 (11%)
10	NAG	G	703	3	14,14,15	0.91	1 (7%)	17,19,21	1.25	1 (5%)
10	NAG	G	702	3	14,14,15	0.79	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
10	NAG	K	707	3	14,14,15	0.82	1 (7%)	17,19,21	1.30	2 (11%)
9	GOL	G	701	-	5,5,5	0.21	0	5,5,5	0.55	0
9	GOL	D	701	-	5,5,5	0.36	0	5,5,5	0.46	0
10	NAG	C	703	3	14,14,15	0.81	1 (7%)	17,19,21	1.21	1 (5%)
10	NAG	C	702	3	14,14,15	0.71	0	17,19,21	1.44	4 (23%)
9	GOL	K	701	-	5,5,5	0.29	0	5,5,5	0.46	0
10	NAG	D	705	3	14,14,15	0.98	1 (7%)	17,19,21	2.07	3 (17%)
10	NAG	C	704	3	14,14,15	0.90	1 (7%)	17,19,21	3.03	7 (41%)
9	GOL	C	701	-	5,5,5	0.33	0	5,5,5	0.53	0
10	NAG	K	706	3	14,14,15	0.76	0	17,19,21	2.01	4 (23%)
10	NAG	C	705	3	14,14,15	0.63	0	17,19,21	1.15	1 (5%)
10	NAG	K	703	3	14,14,15	0.58	0	17,19,21	1.58	4 (23%)
10	NAG	D	704	3	14,14,15	0.86	0	17,19,21	1.31	2 (11%)
10	NAG	D	702	3	14,14,15	0.81	1 (7%)	17,19,21	1.15	1 (5%)
10	NAG	D	703	3	14,14,15	0.79	1 (7%)	17,19,21	1.46	3 (17%)
10	NAG	K	704	3	14,14,15	0.70	0	17,19,21	1.29	2 (11%)
10	NAG	K	705	3	14,14,15	0.81	1 (7%)	17,19,21	1.11	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	K	702	-	-	2/4/4/4	-
10	NAG	D	706	3	-	2/6/23/26	0/1/1/1
10	NAG	G	703	3	-	1/6/23/26	0/1/1/1
10	NAG	G	702	3	-	1/6/23/26	0/1/1/1
10	NAG	K	707	3	-	0/6/23/26	0/1/1/1
9	GOL	G	701	-	-	1/4/4/4	-
9	GOL	D	701	-	-	4/4/4/4	-
10	NAG	C	703	3	-	2/6/23/26	0/1/1/1
10	NAG	C	702	3	-	0/6/23/26	0/1/1/1
9	GOL	K	701	-	-	2/4/4/4	-
10	NAG	D	705	3	-	2/6/23/26	0/1/1/1
10	NAG	C	704	3	-	2/6/23/26	0/1/1/1
9	GOL	C	701	-	-	2/4/4/4	-
10	NAG	K	706	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	C	705	3	-	0/6/23/26	0/1/1/1
10	NAG	K	703	3	-	3/6/23/26	0/1/1/1
10	NAG	D	704	3	-	1/6/23/26	0/1/1/1
10	NAG	D	702	3	-	2/6/23/26	0/1/1/1
10	NAG	D	703	3	-	2/6/23/26	0/1/1/1
10	NAG	K	704	3	-	2/6/23/26	0/1/1/1
10	NAG	K	705	3	-	4/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	707	NAG	C1-C2	2.62	1.55	1.52
10	D	705	NAG	C1-C2	2.61	1.55	1.52
10	C	703	NAG	C1-C2	2.44	1.55	1.52
10	G	703	NAG	C1-C2	2.41	1.55	1.52
10	C	704	NAG	C1-C2	2.32	1.55	1.52

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	704	NAG	C1-O5-C5	8.87	124.08	112.19
10	K	706	NAG	C2-N2-C7	6.04	130.99	122.90
10	D	705	NAG	C1-O5-C5	-5.63	104.64	112.19
10	D	706	NAG	C2-N2-C7	4.63	129.10	122.90
10	D	705	NAG	C2-N2-C7	4.35	128.73	122.90

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

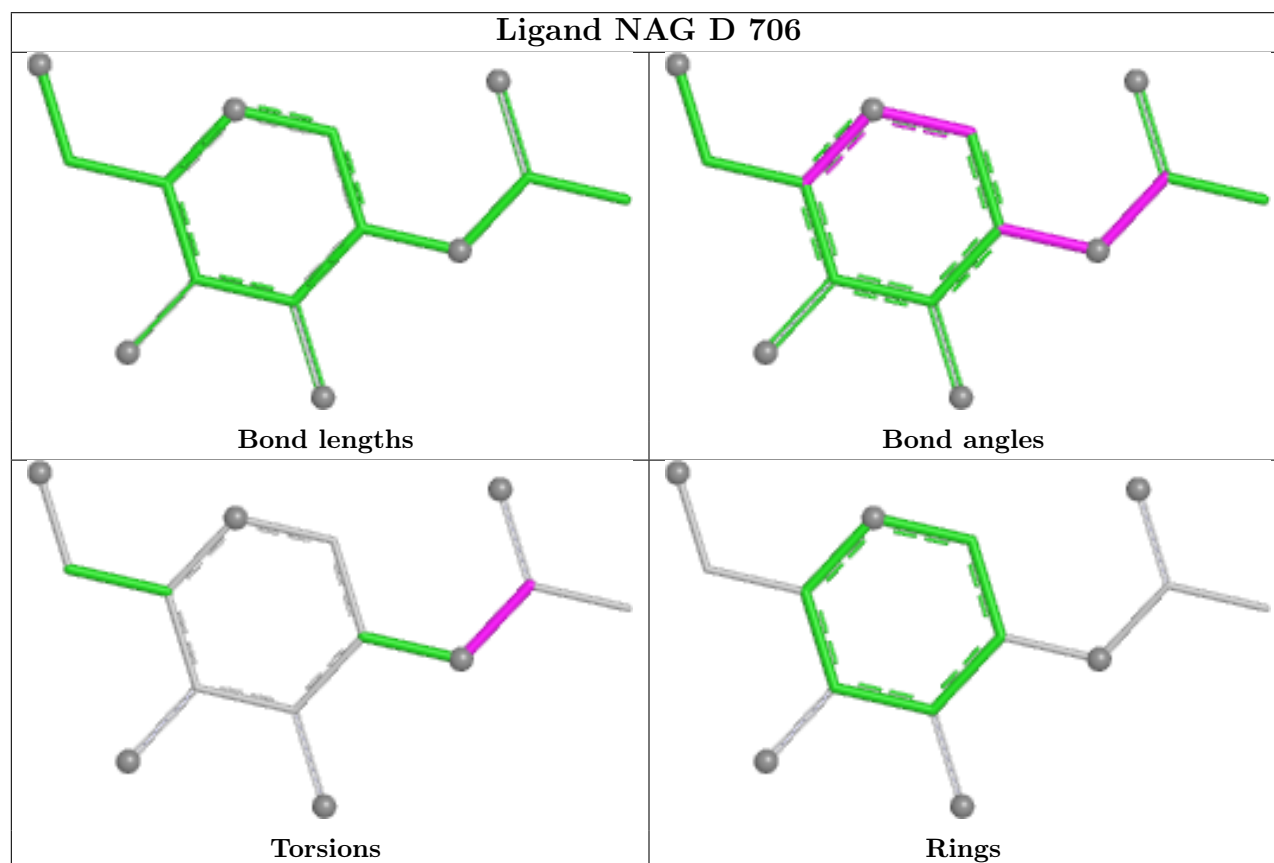
Mol	Chain	Res	Type	Atoms
9	C	701	GOL	C1-C2-C3-O3
9	D	701	GOL	C1-C2-C3-O3
9	K	701	GOL	C1-C2-C3-O3
10	D	705	NAG	C3-C2-N2-C7
10	G	703	NAG	C1-C2-N2-C7

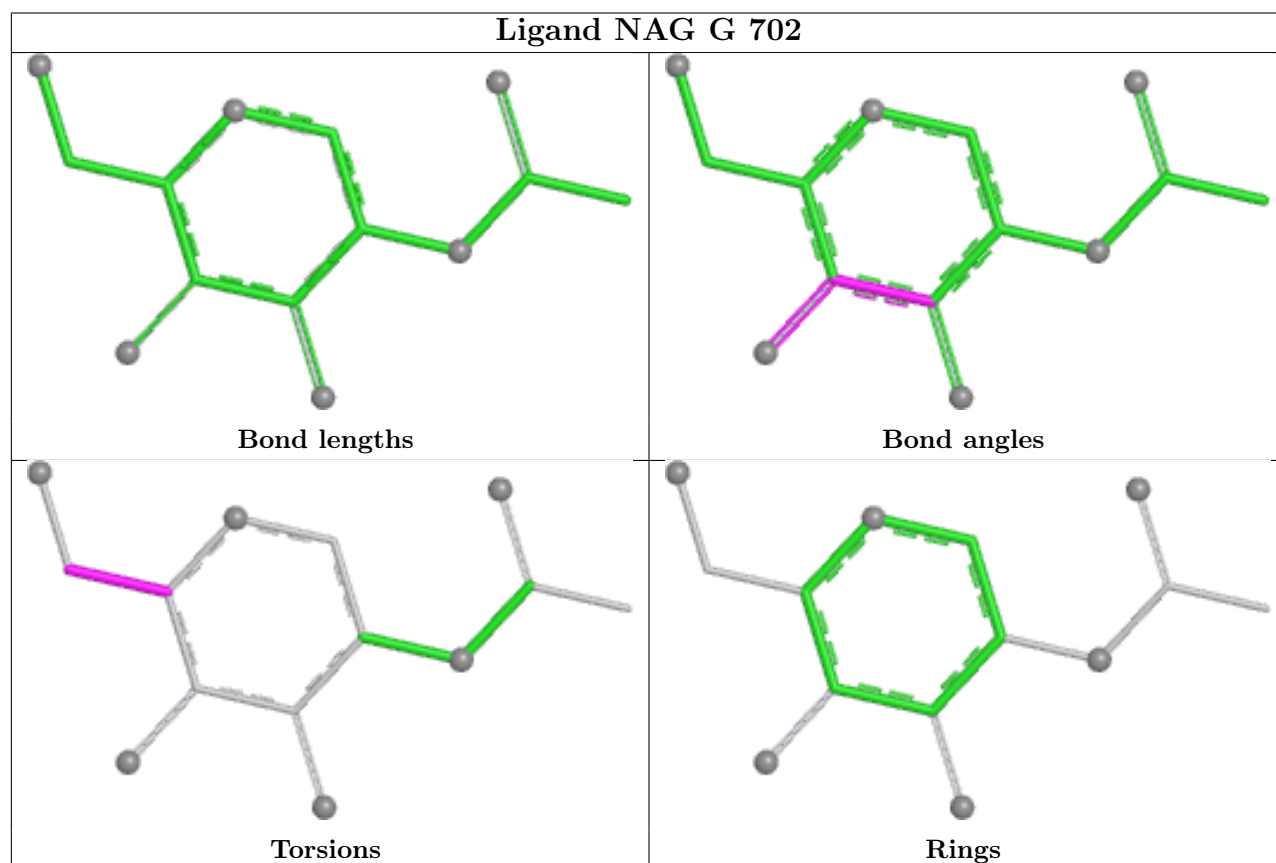
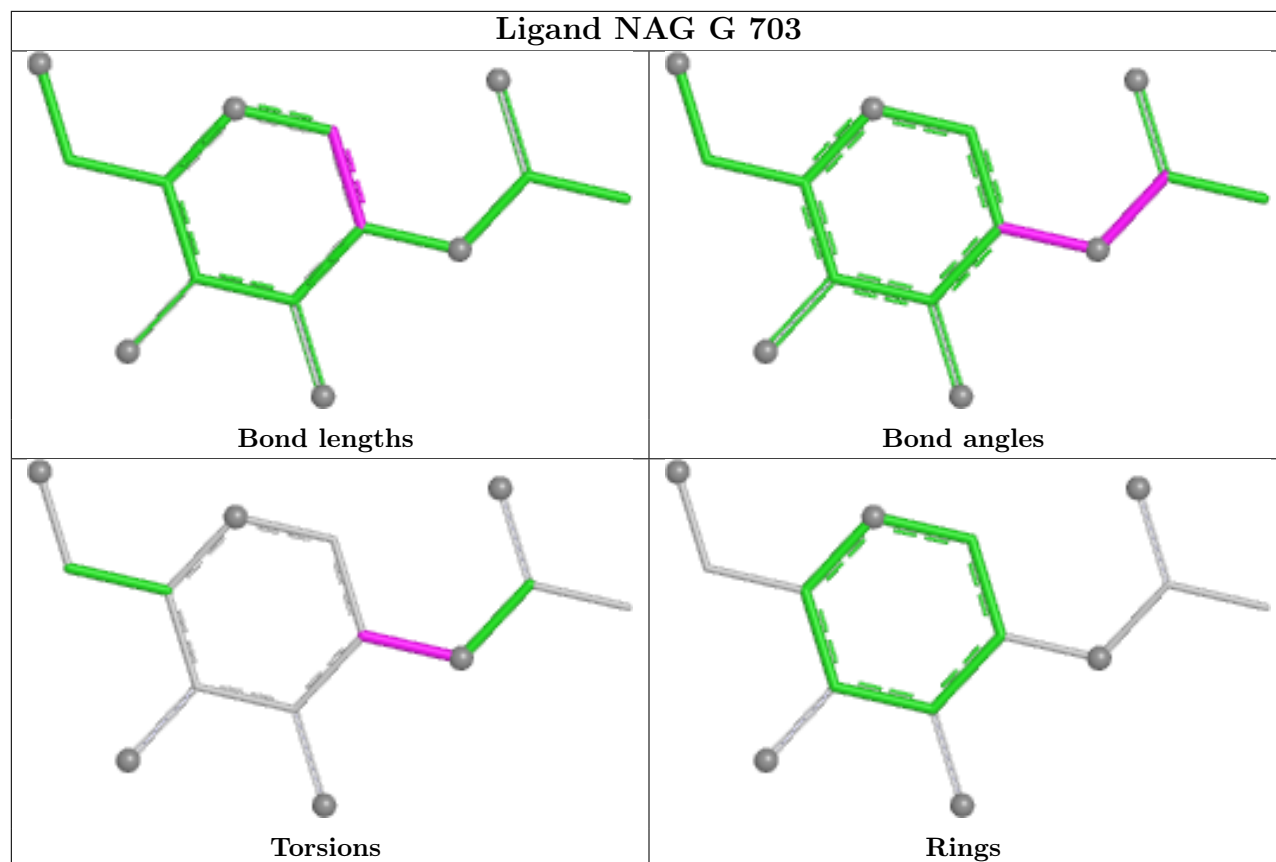
There are no ring outliers.

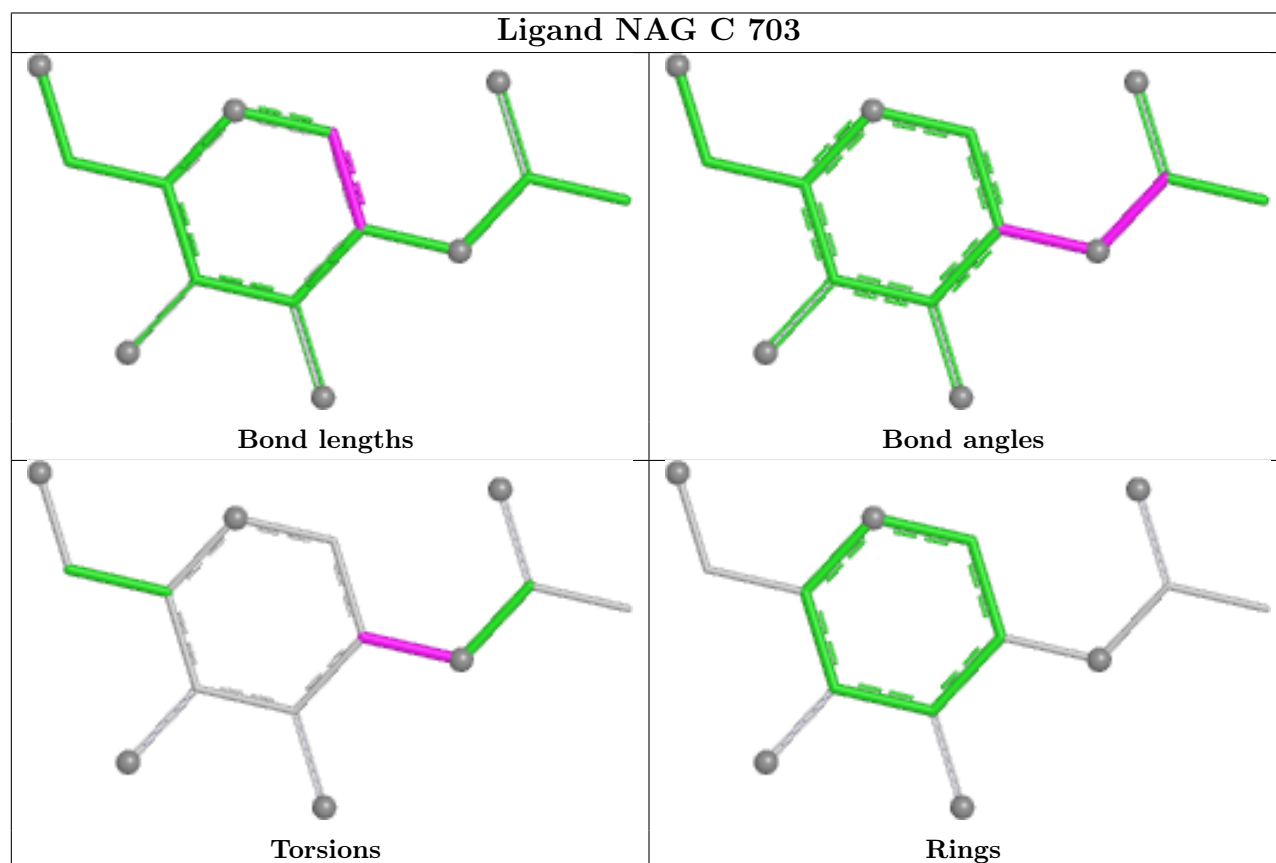
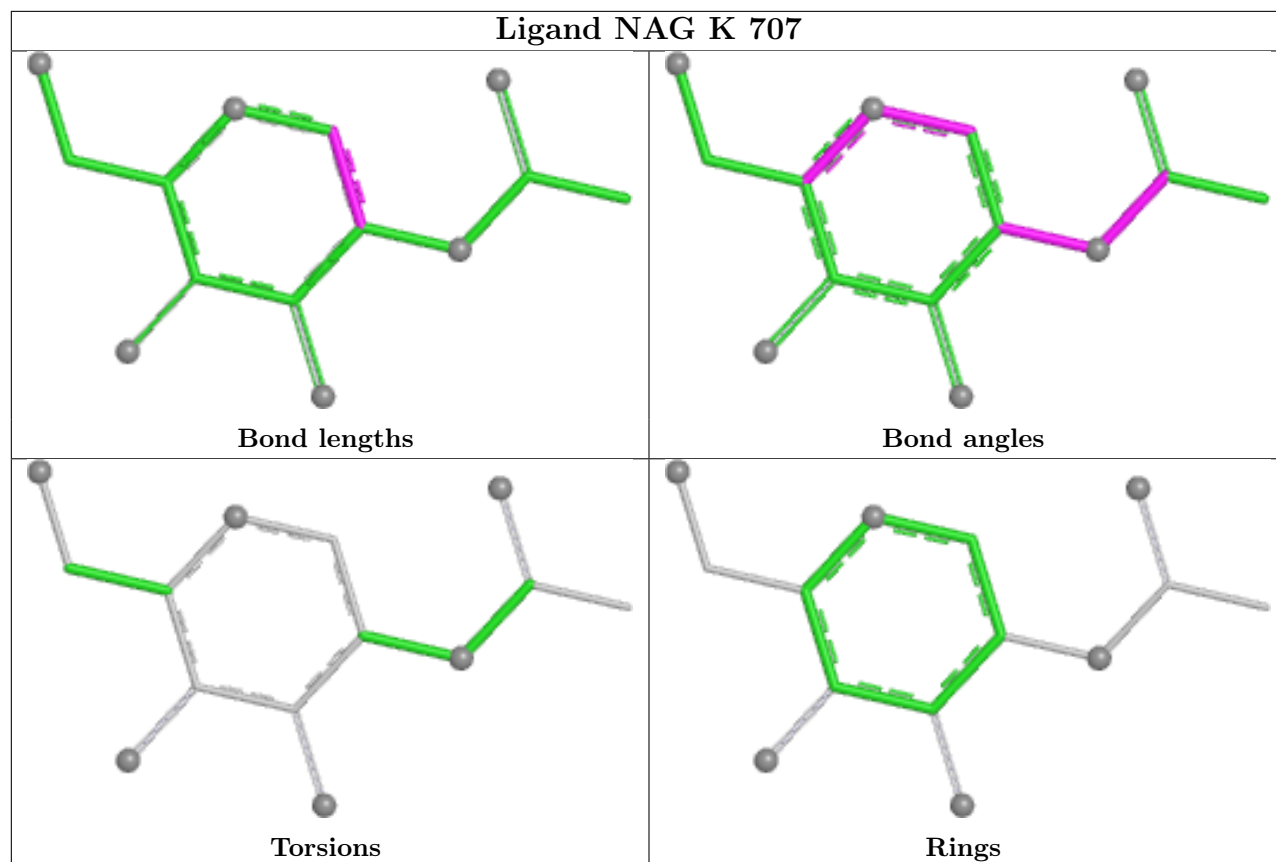
7 monomers are involved in 14 short contacts:

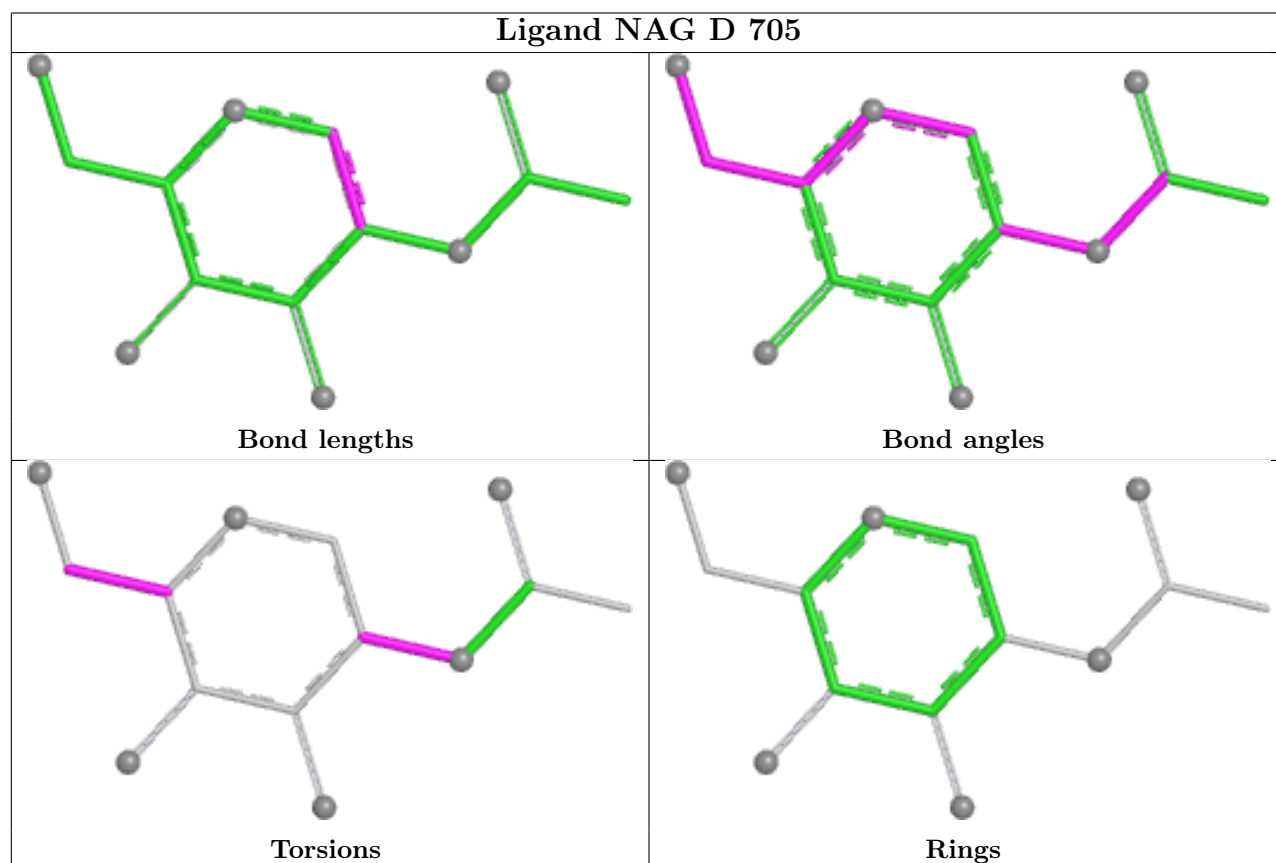
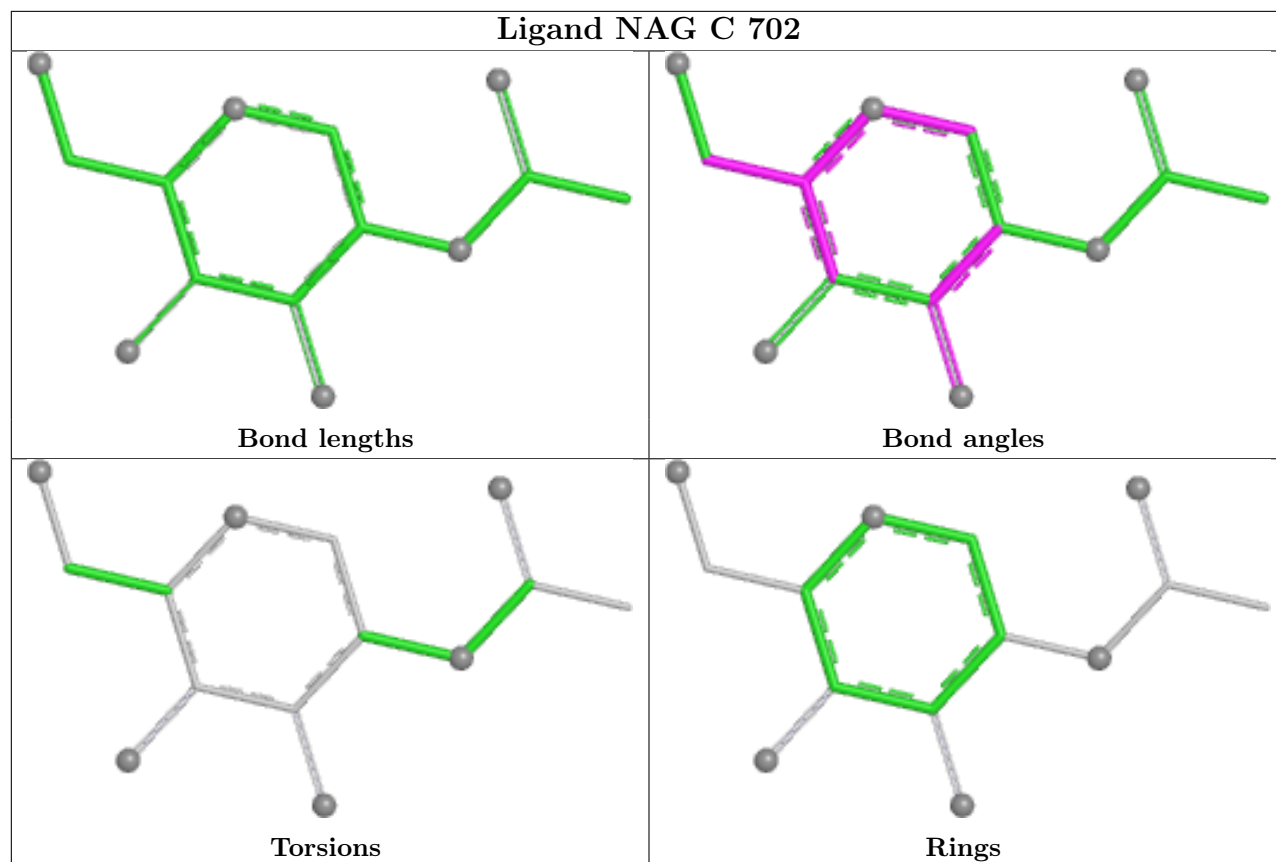
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	K	702	GOL	1	0
10	K	707	NAG	2	0
9	D	701	GOL	1	0
10	C	703	NAG	2	0
10	C	702	NAG	1	0
10	D	705	NAG	1	0
10	K	706	NAG	6	0

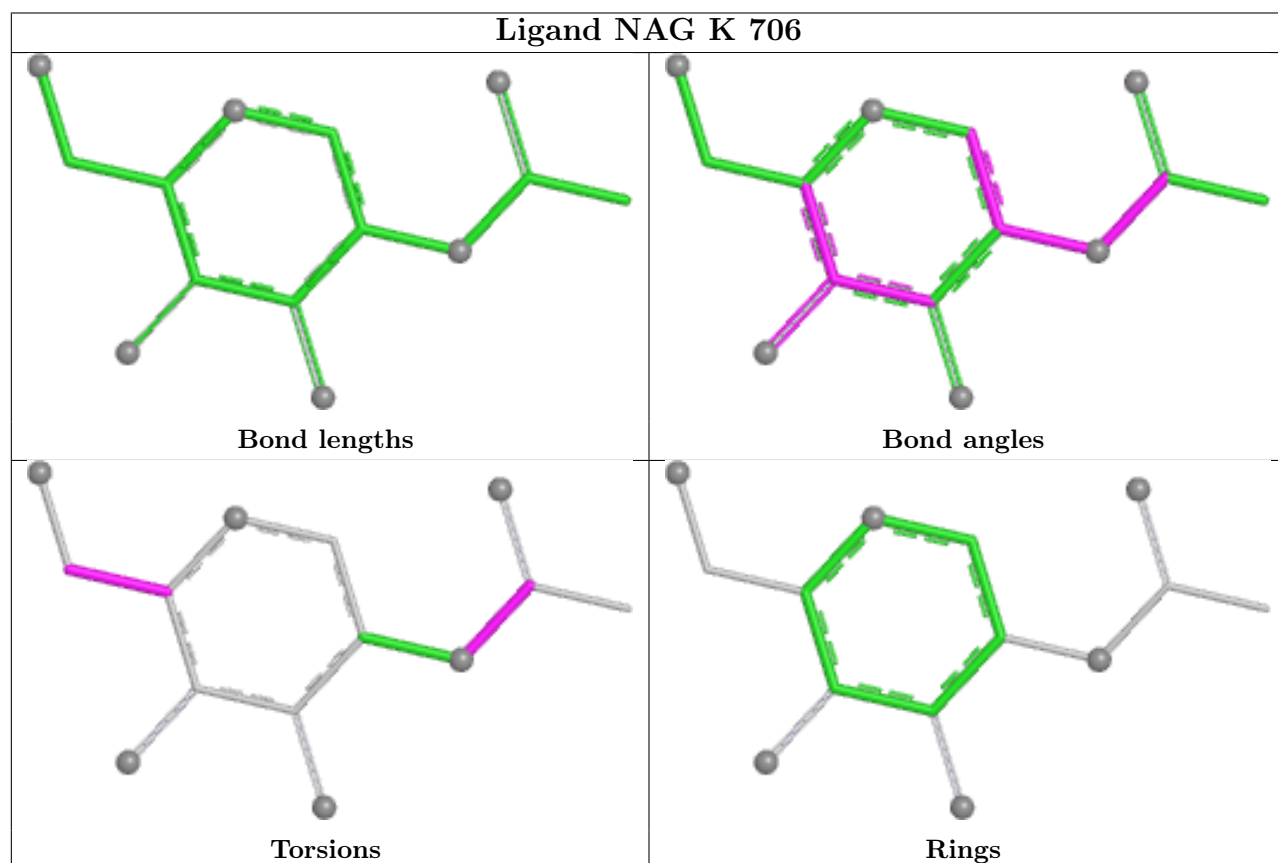
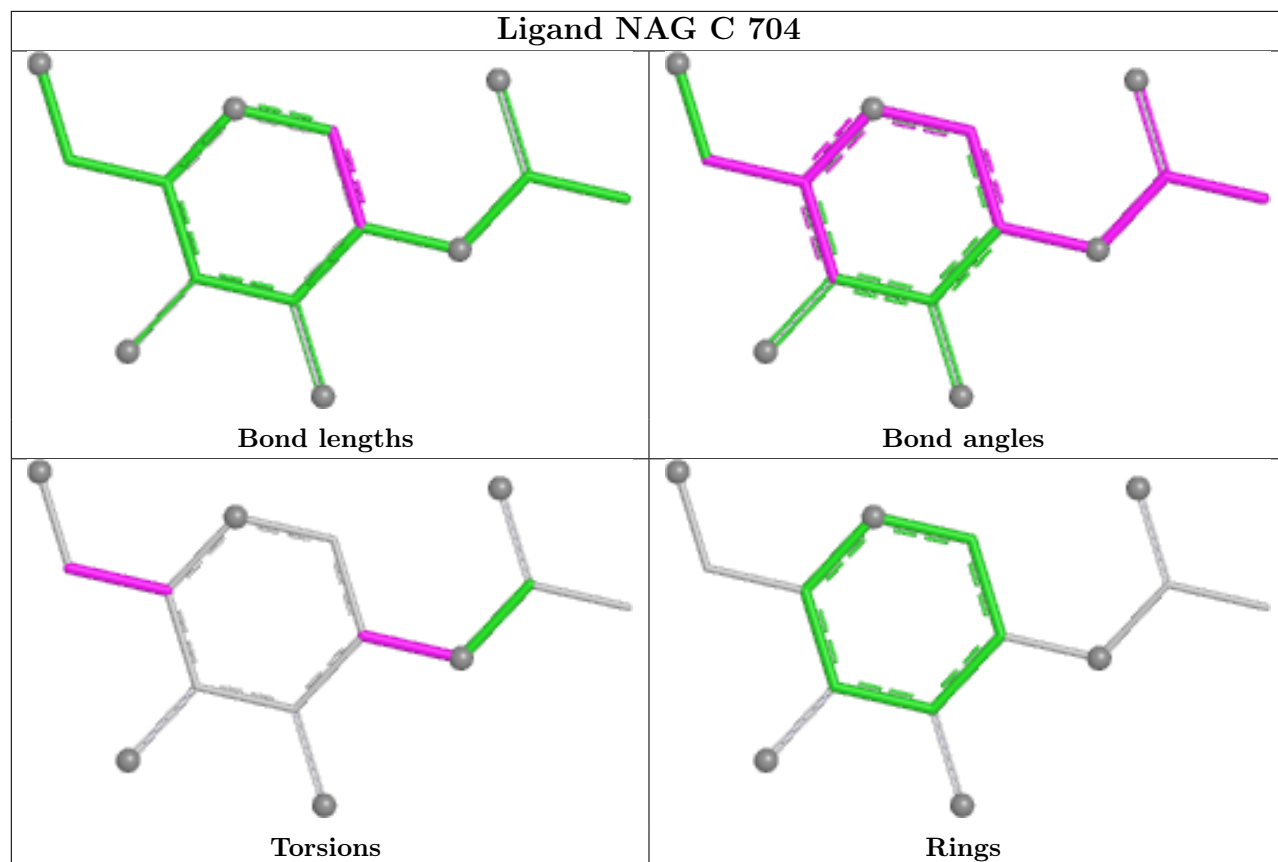
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

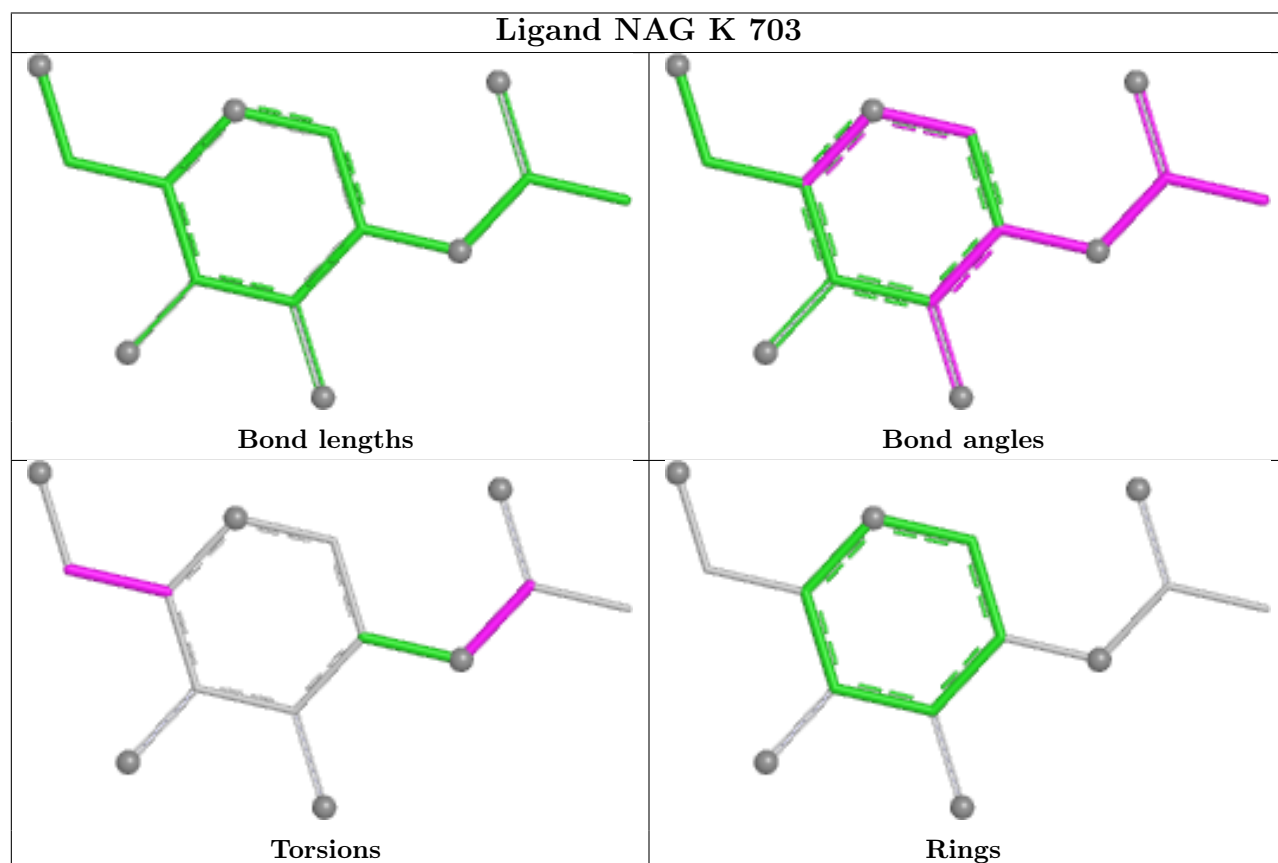
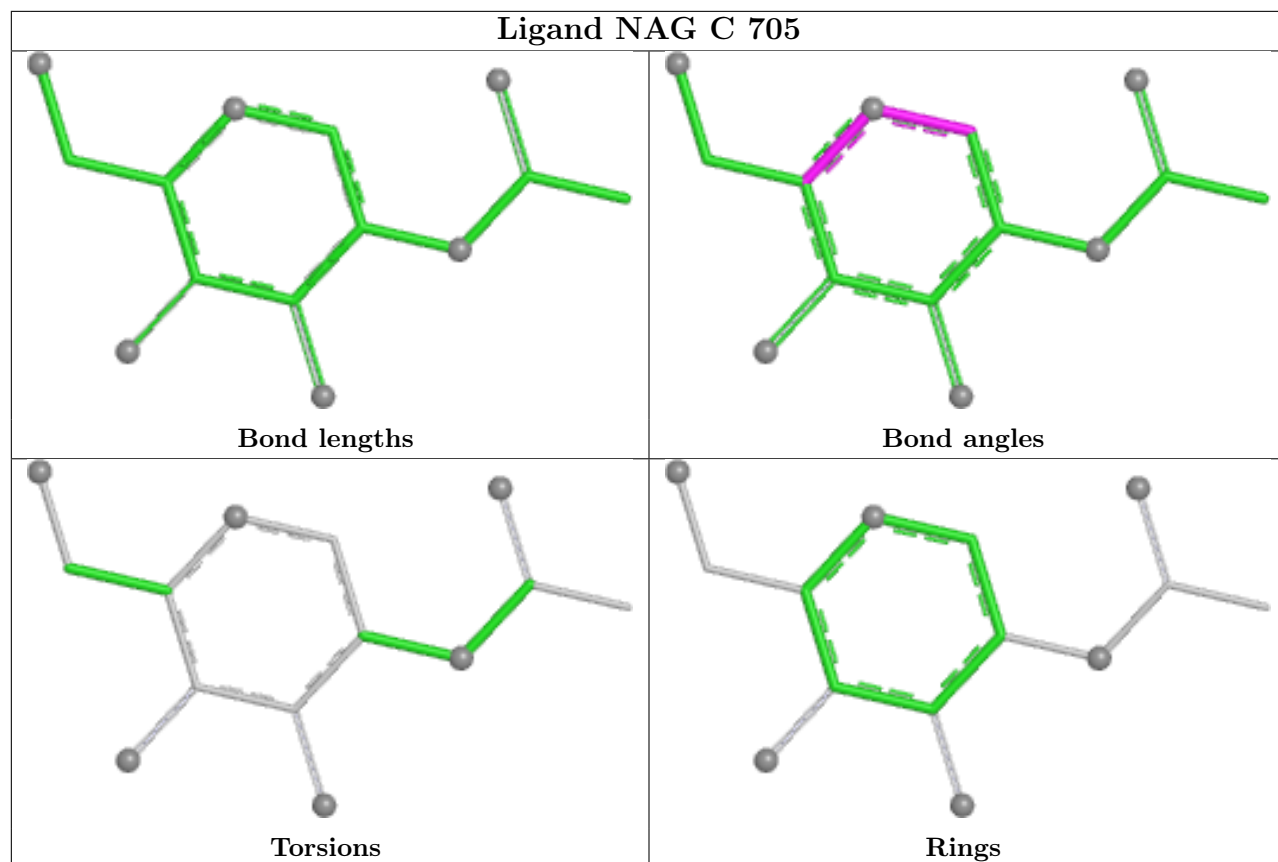


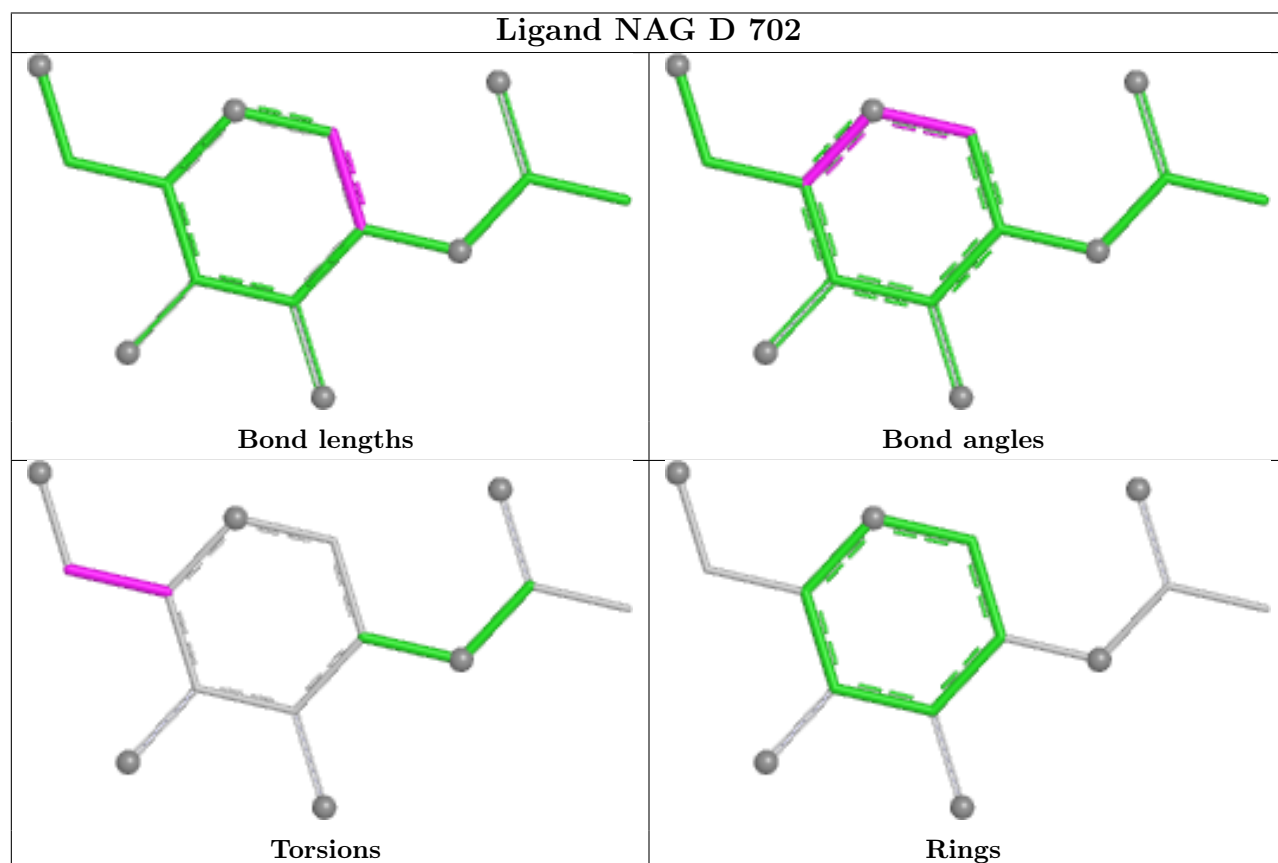
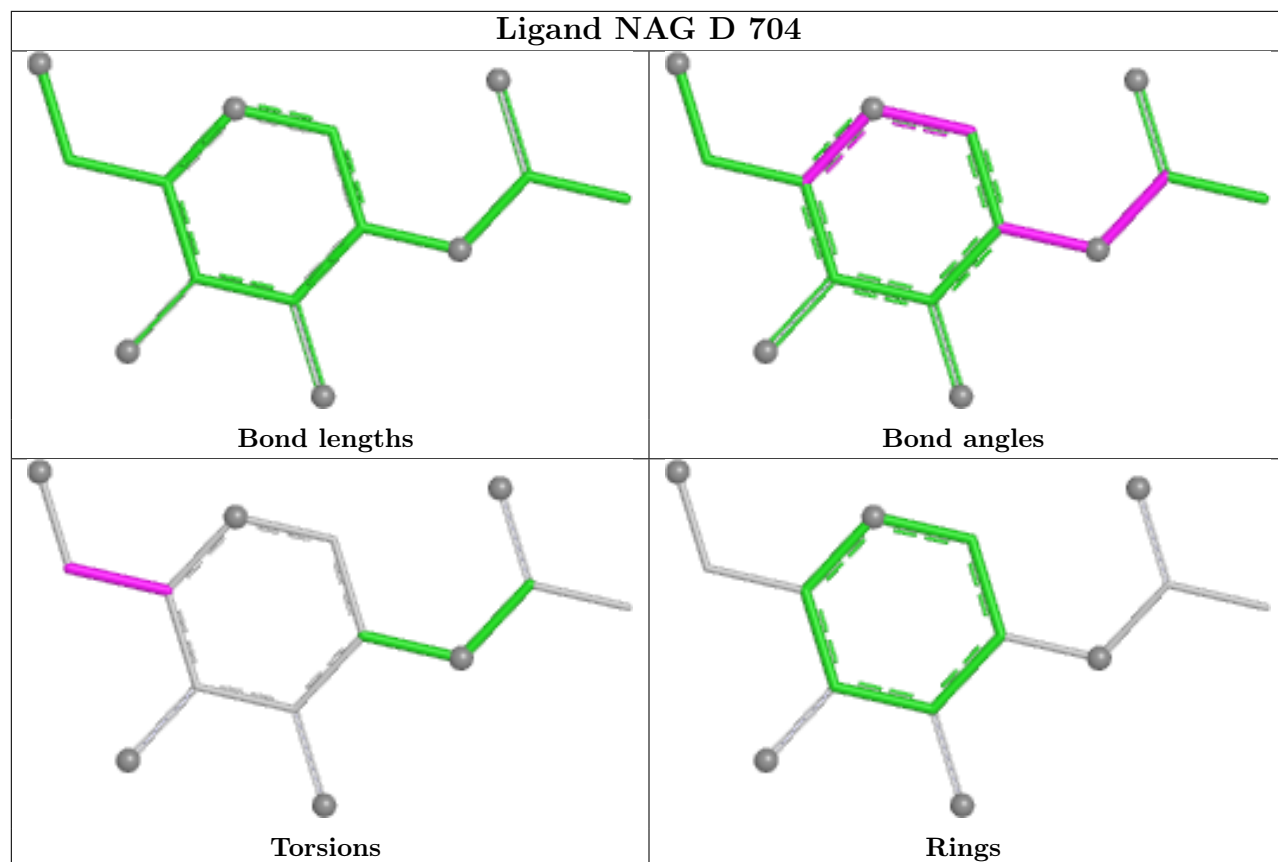


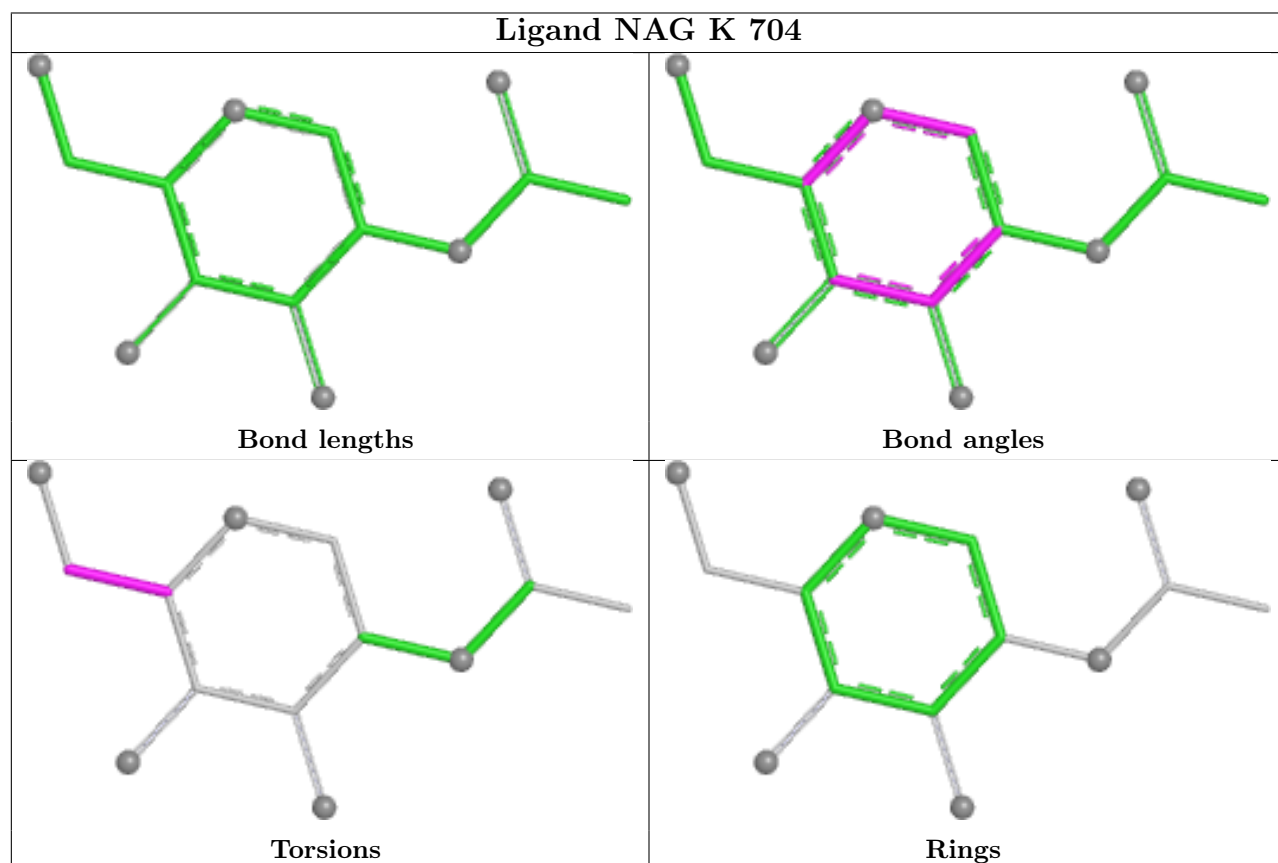
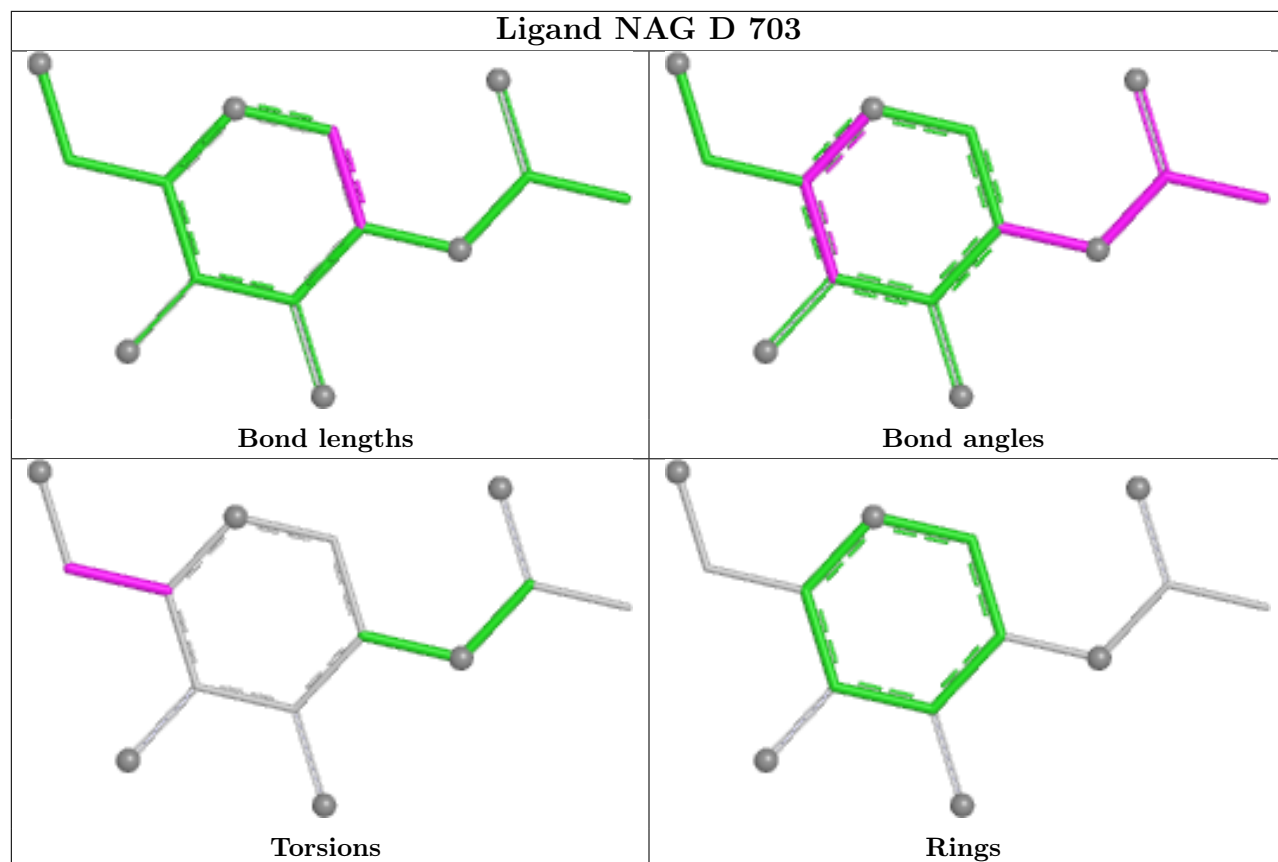


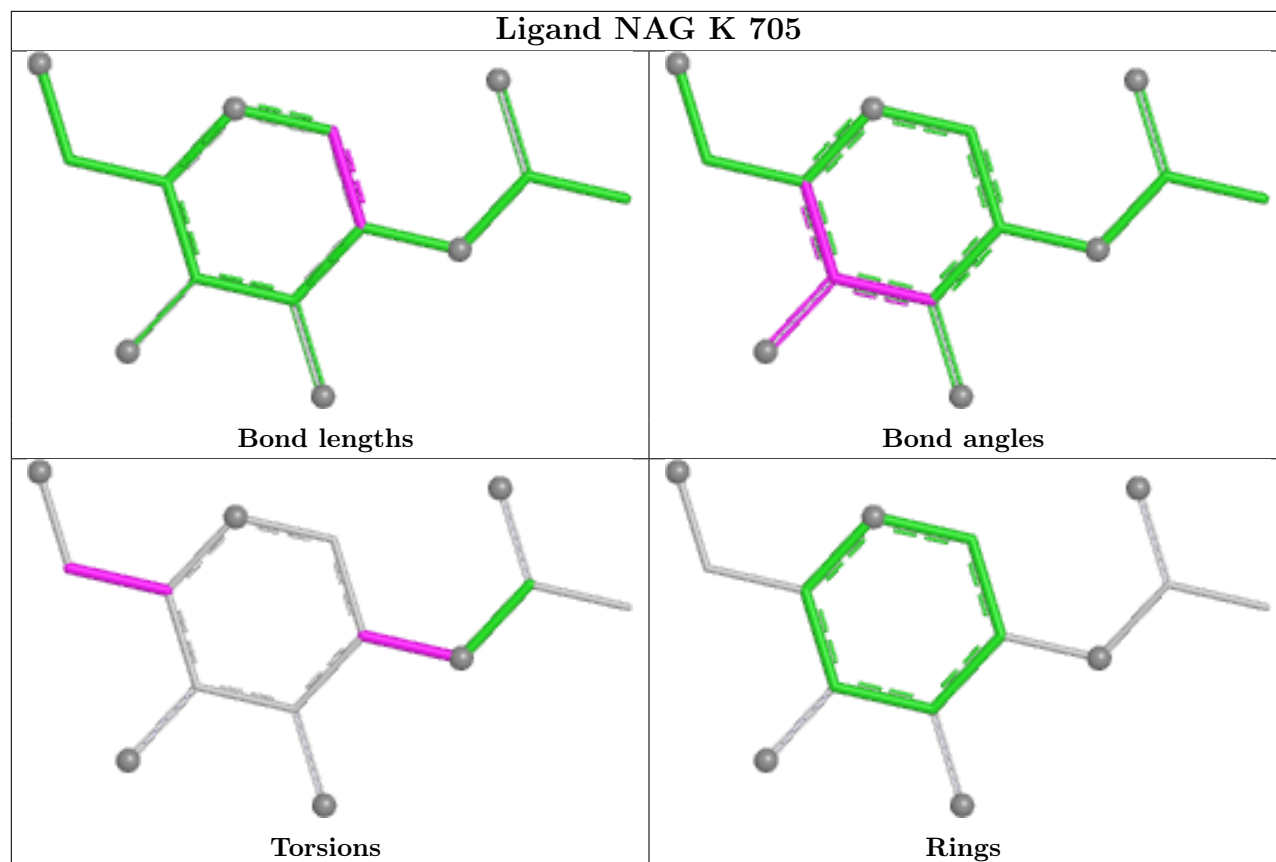












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	225/237 (94%)	0.41	7 (3%) 51 47	57, 98, 154, 174	0
1	E	219/237 (92%)	0.50	12 (5%) 30 26	53, 114, 166, 199	0
1	H	222/237 (93%)	0.72	19 (8%) 16 13	73, 124, 167, 224	0
1	I	221/237 (93%)	0.21	5 (2%) 61 57	45, 91, 155, 177	0
2	B	210/216 (97%)	0.38	10 (4%) 35 31	60, 95, 152, 184	0
2	F	215/216 (99%)	0.42	2 (0%) 81 79	63, 114, 152, 175	0
2	J	214/216 (99%)	0.32	5 (2%) 61 57	51, 96, 162, 179	0
2	L	213/216 (98%)	0.53	9 (4%) 40 36	81, 114, 157, 210	0
3	C	232/262 (88%)	0.29	6 (2%) 57 53	59, 80, 129, 163	0
3	D	233/262 (88%)	0.20	6 (2%) 57 53	57, 76, 124, 179	0
3	G	227/262 (86%)	0.08	3 (1%) 75 73	46, 68, 108, 146	1 (0%)
3	K	232/262 (88%)	0.04	7 (3%) 52 48	46, 66, 109, 176	1 (0%)
All	All	2663/2860 (93%)	0.34	91 (3%) 48 43	45, 94, 154, 224	2 (0%)

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	94	VAL	5.8
2	B	152	VAL	4.6
2	L	94	VAL	4.2
2	F	94	VAL	4.2
3	K	415	ASN	4.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	MAN	Q	4	11/12	0.17	0.19	119,125,127,127	0
7	BMA	T	3	11/12	0.41	0.13	125,131,155,161	0
4	NAG	S	2	14/15	0.45	0.14	110,124,149,150	0
5	BMA	N	3	11/12	0.45	0.14	98,108,119,120	0
7	BMA	Q	3	11/12	0.52	0.14	106,112,122,123	0
5	BMA	U	3	11/12	0.57	0.12	109,125,149,151	0
5	BMA	R	3	11/12	0.60	0.13	98,108,113,114	0
7	MAN	T	4	11/12	0.63	0.12	120,128,149,151	0
6	MAN	O	6	11/12	0.66	0.13	98,105,109,110	0
8	BMA	Y	3	11/12	0.66	0.11	102,110,133,135	0
4	NAG	P	2	14/15	0.67	0.13	96,115,139,147	0
4	NAG	W	2	14/15	0.68	0.13	103,121,144,155	0
7	NAG	T	2	14/15	0.70	0.12	108,130,156,159	0
6	MAN	O	5	11/12	0.72	0.16	108,118,121,126	0
7	NAG	Q	2	14/15	0.72	0.14	78,102,125,130	0
4	NAG	M	2	14/15	0.73	0.10	106,119,143,144	0
7	NAG	T	1	14/15	0.74	0.12	66,107,126,128	0
8	MAN	Y	6	11/12	0.75	0.10	105,115,138,140	0
8	MAN	Y	5	11/12	0.76	0.11	109,119,142,145	0
8	MAN	Y	4	11/12	0.78	0.10	105,113,136,138	0
5	NAG	N	2	14/15	0.79	0.12	96,109,127,136	0
6	MAN	O	4	11/12	0.79	0.10	101,110,114,117	0
5	NAG	U	2	14/15	0.79	0.12	91,108,127,130	0
4	NAG	X	2	14/15	0.81	0.10	85,103,122,137	0
4	NAG	V	2	14/15	0.81	0.11	73,91,109,120	0
6	NAG	O	2	14/15	0.82	0.13	76,93,113,116	0
4	NAG	S	1	14/15	0.83	0.12	77,96,116,117	0
8	NAG	Y	2	14/15	0.85	0.11	73,91,112,112	0
6	BMA	O	3	11/12	0.86	0.08	95,100,106,109	0
4	NAG	M	1	14/15	0.86	0.11	78,95,121,122	0
4	NAG	W	1	14/15	0.89	0.09	72,90,103,111	0
5	NAG	N	1	14/15	0.89	0.11	74,92,116,116	0
7	NAG	Q	1	14/15	0.89	0.11	76,93,114,114	0
4	NAG	P	1	14/15	0.90	0.09	72,92,111,115	0
5	NAG	U	1	14/15	0.90	0.09	66,88,100,105	0
6	NAG	O	1	14/15	0.90	0.10	69,80,97,97	0
4	NAG	X	1	14/15	0.91	0.09	73,89,111,111	0

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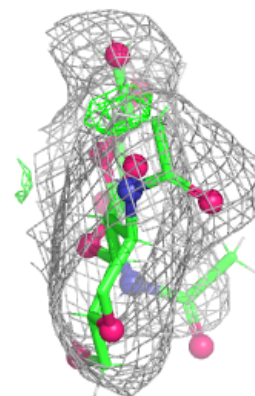
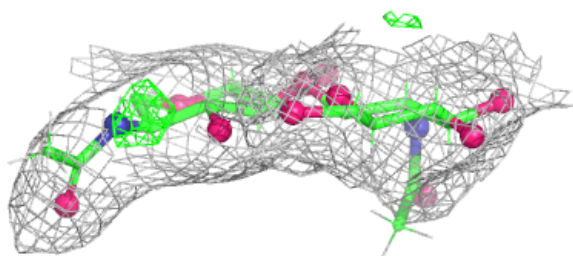
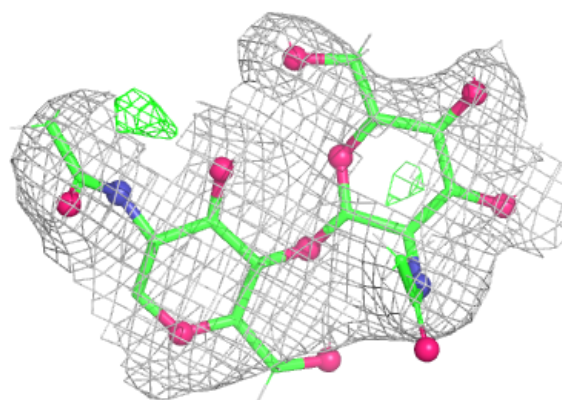
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	V	1	14/15	0.91	0.10	69,83,94,109	0
8	NAG	Y	1	14/15	0.92	0.09	57,73,85,89	0
5	NAG	R	1	14/15	0.92	0.07	69,83,99,101	0
5	NAG	R	2	14/15	0.92	0.09	87,101,116,121	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

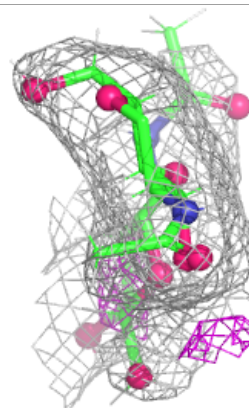
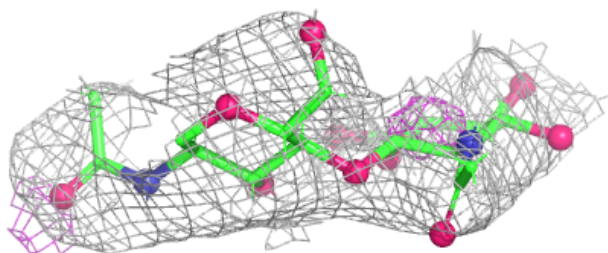
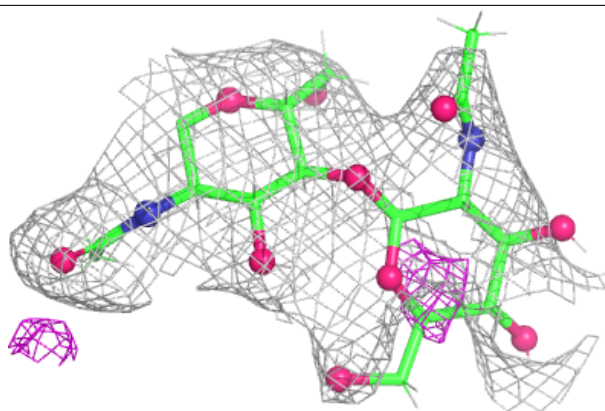
Electron density around Chain M:

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

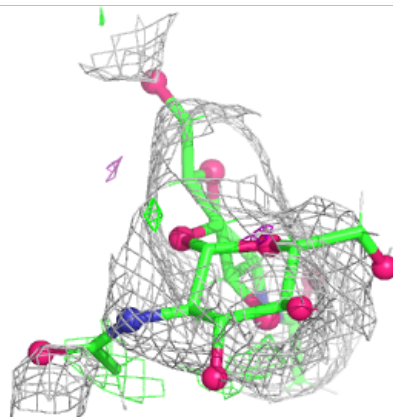
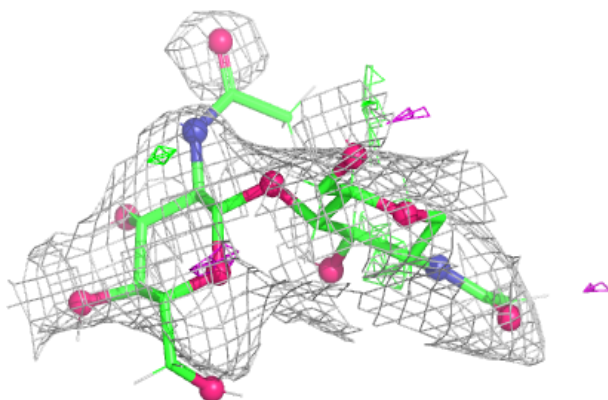
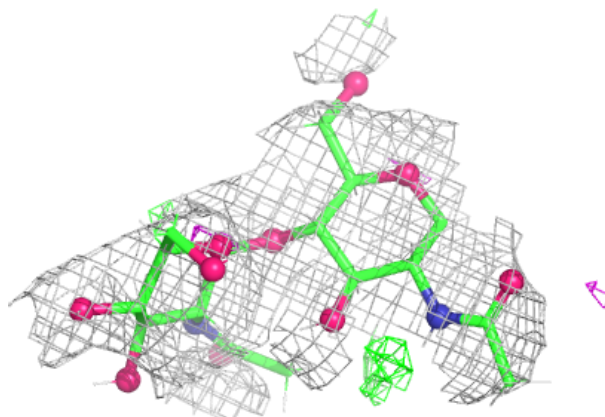


Electron density around Chain P:

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

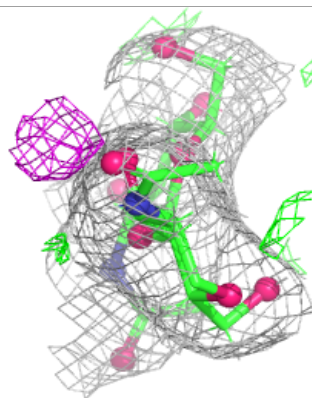
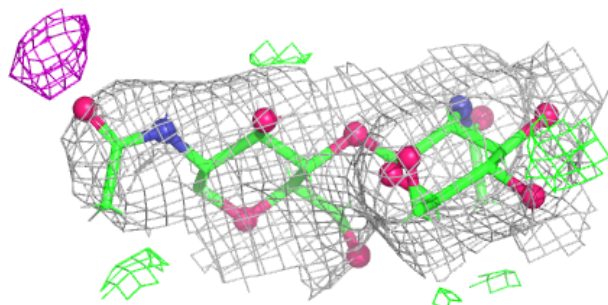
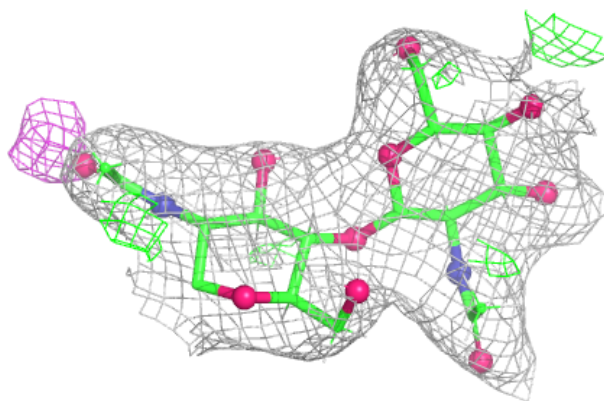
**Electron density around Chain S:**

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

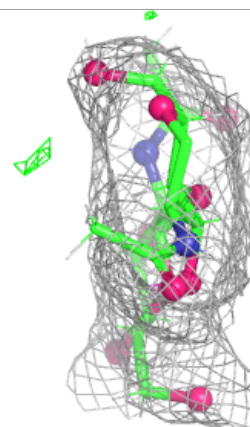
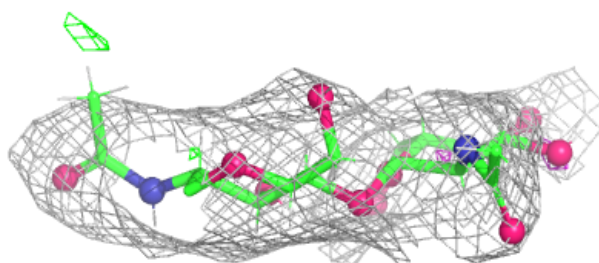
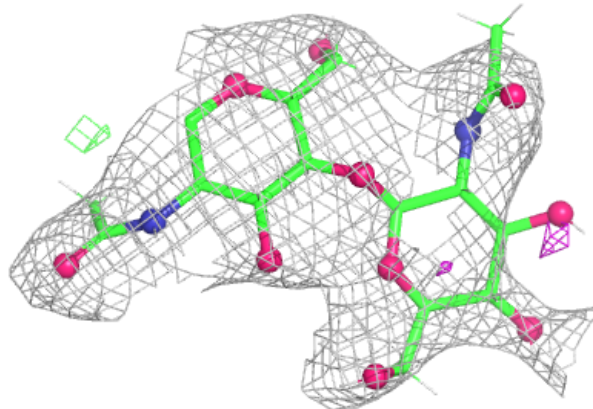


Electron density around Chain V:

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and green (positive)

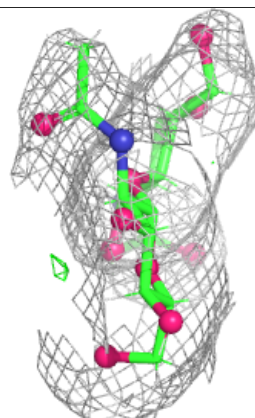
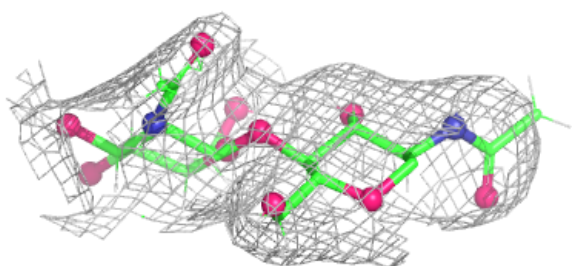
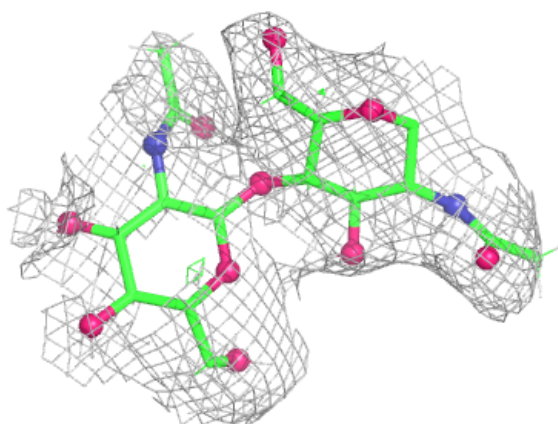
**Electron density around Chain W:**

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

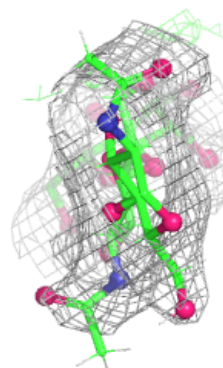
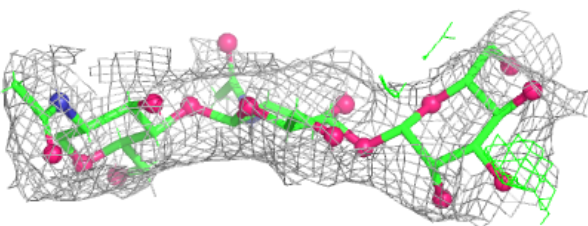
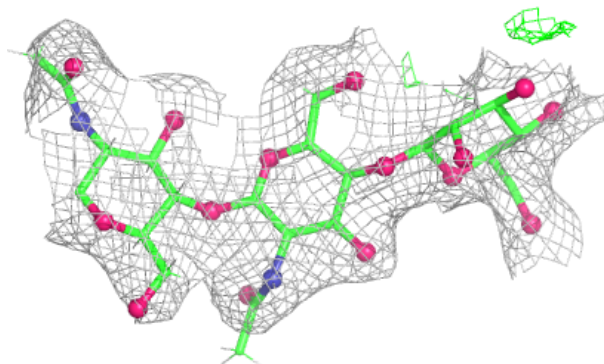


Electron density around Chain X:

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

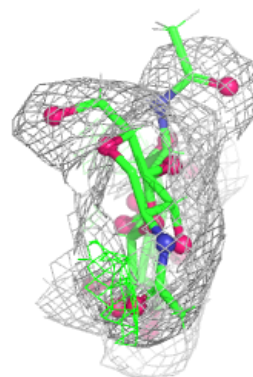
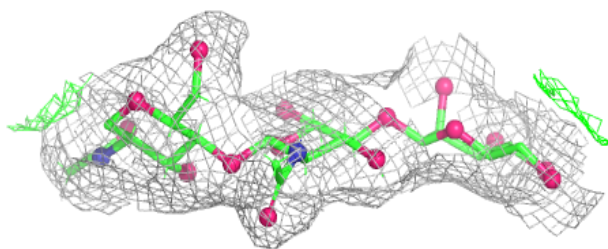
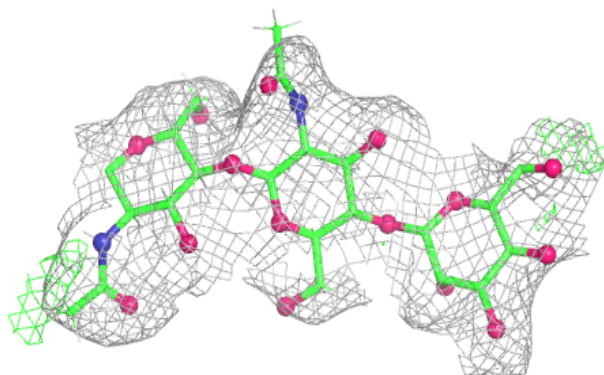
**Electron density around Chain N:**

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

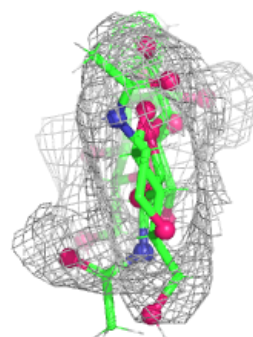
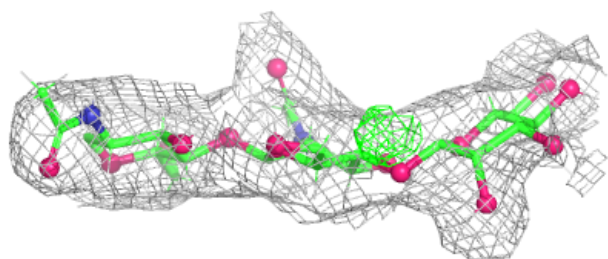
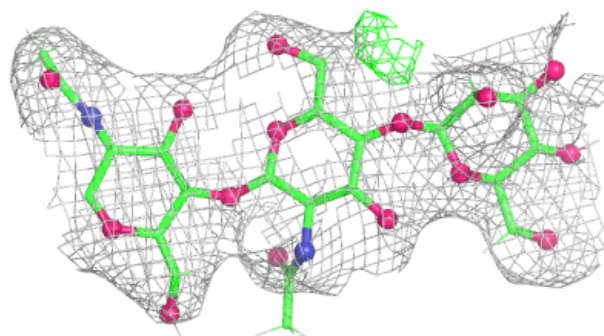


Electron density around Chain R:

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

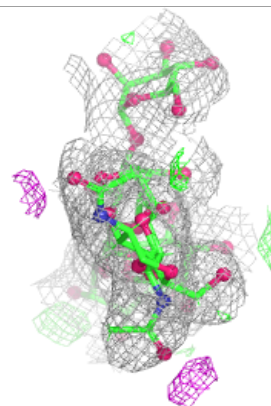
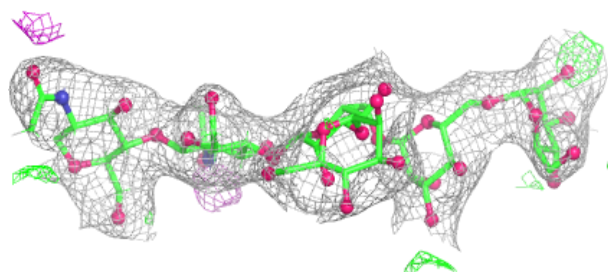
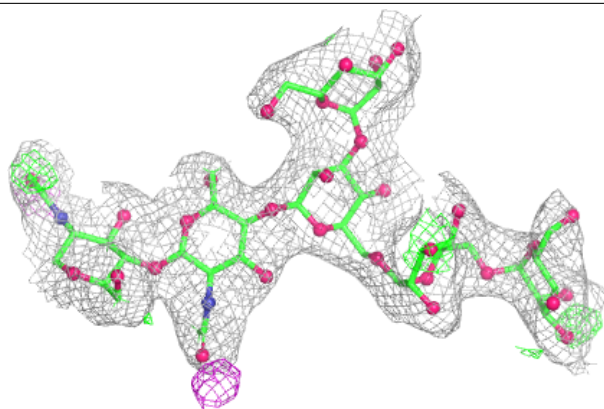
**Electron density around Chain U:**

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

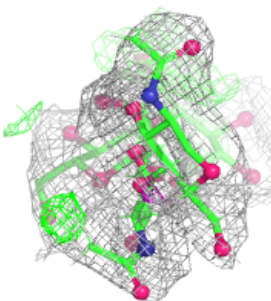
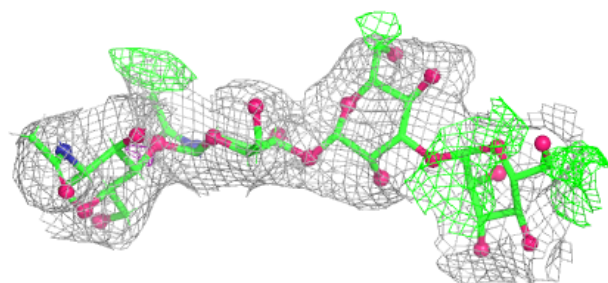
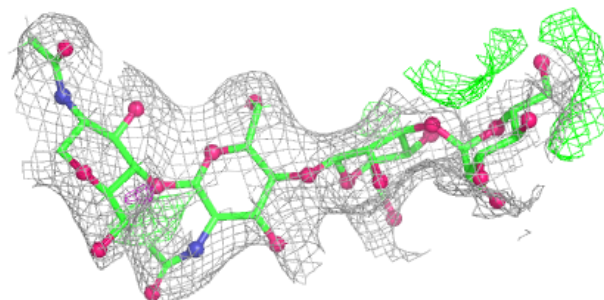


Electron density around Chain O:

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

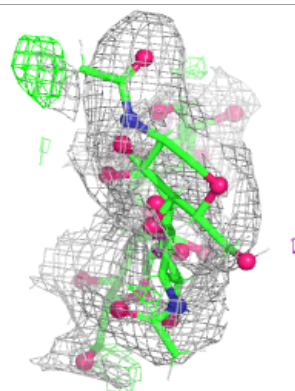
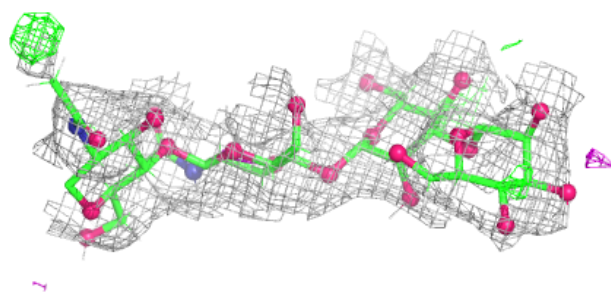
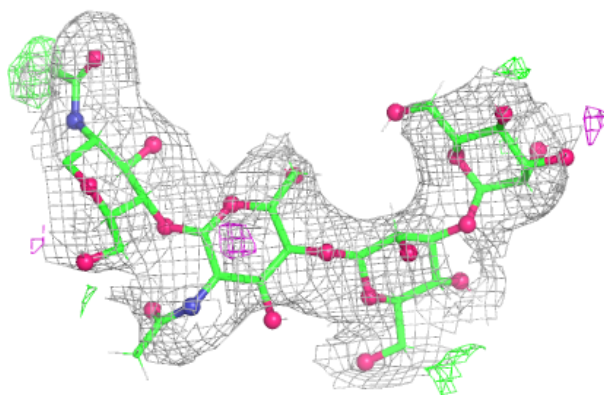
**Electron density around Chain Q:**

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

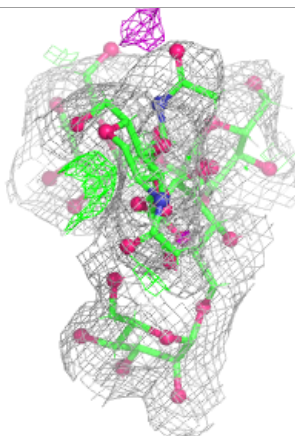
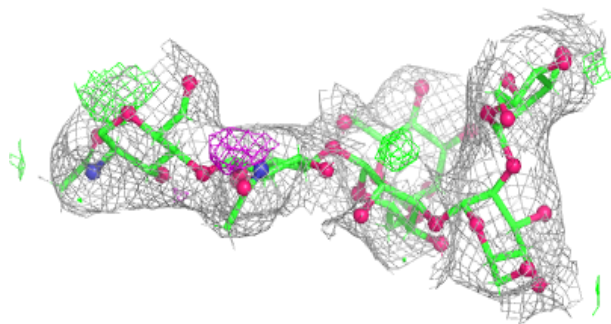
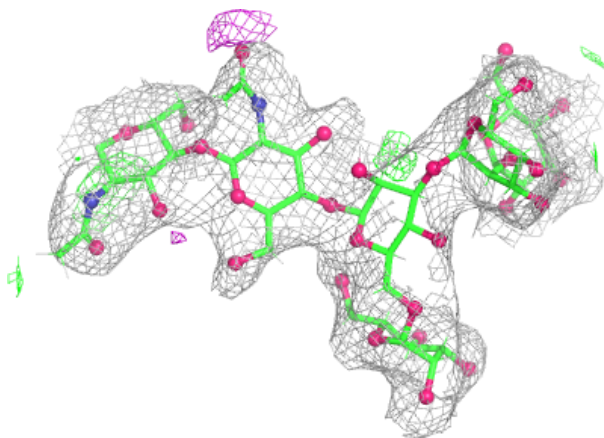


Electron density around Chain T:

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

**Electron density around Chain Y:**

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



6.4 Ligands

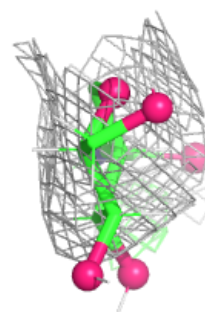
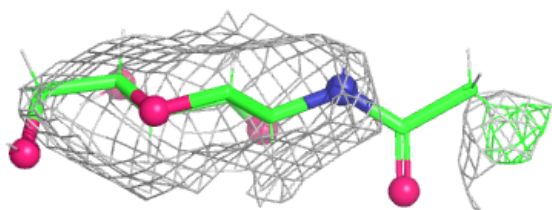
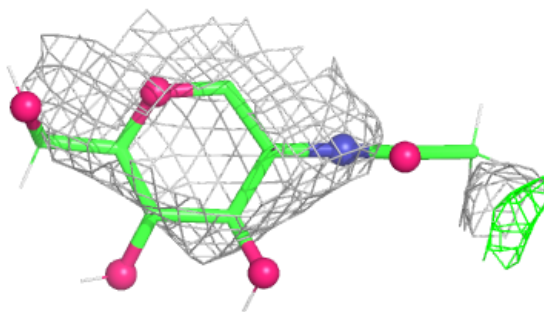
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	D	703	14/15	0.35	0.17	115,132,155,163	0
9	GOL	G	701	6/6	0.47	0.17	93,112,120,122	0
10	NAG	D	704	14/15	0.59	0.17	86,110,117,120	0
10	NAG	K	704	14/15	0.66	0.14	99,119,142,152	0
10	NAG	C	703	14/15	0.70	0.14	106,116,139,147	0
10	NAG	K	705	14/15	0.76	0.10	94,116,140,146	0
10	NAG	D	702	14/15	0.77	0.12	81,104,125,133	0
10	NAG	K	703	14/15	0.77	0.13	81,99,119,120	0
9	GOL	C	701	6/6	0.79	0.12	73,93,102,111	0
10	NAG	C	702	14/15	0.80	0.12	92,108,126,131	0
10	NAG	G	703	14/15	0.81	0.12	64,98,120,123	0
10	NAG	D	706	14/15	0.83	0.10	96,116,142,143	0
9	GOL	K	701	6/6	0.86	0.16	68,82,90,98	0
10	NAG	C	705	14/15	0.87	0.10	99,116,139,146	0
10	NAG	K	707	14/15	0.87	0.09	73,100,128,137	0
10	NAG	D	705	14/15	0.88	0.16	76,86,104,106	0
10	NAG	C	704	14/15	0.89	0.12	65,91,110,110	0
10	NAG	G	702	14/15	0.93	0.09	61,69,83,83	0
9	GOL	K	702	6/6	0.93	0.13	54,65,74,77	0
10	NAG	K	706	14/15	0.93	0.10	58,70,84,86	0
9	GOL	D	701	6/6	0.93	0.12	73,88,96,97	0

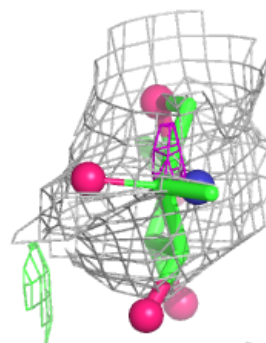
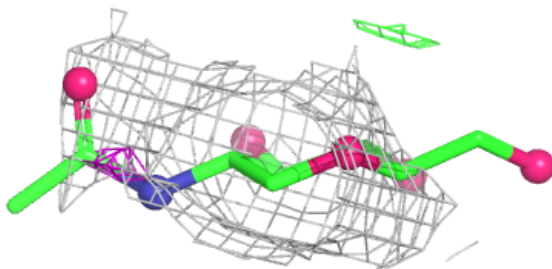
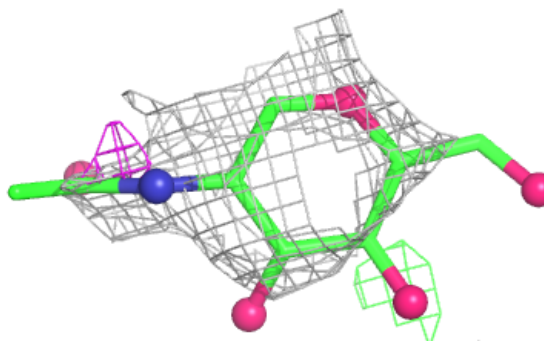
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG D 703:

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

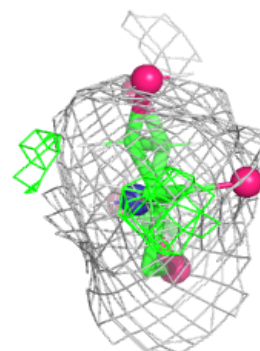
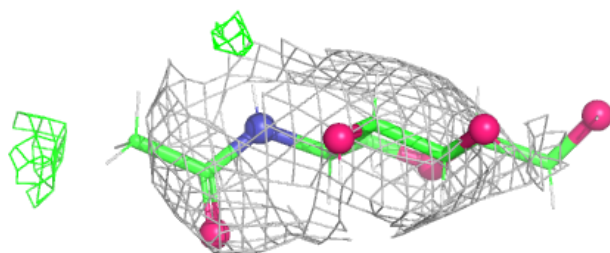
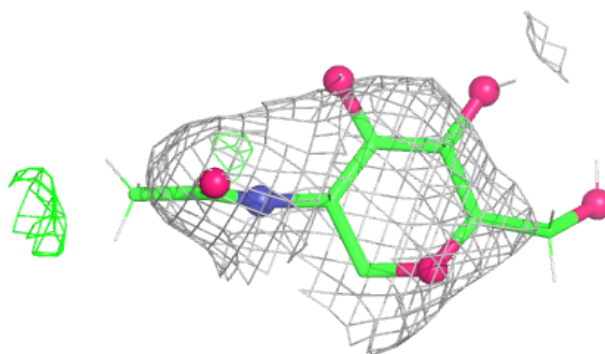
**Electron density around NAG D 704:**

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

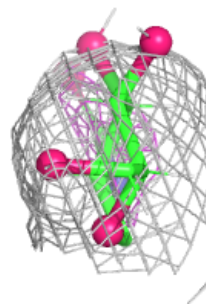
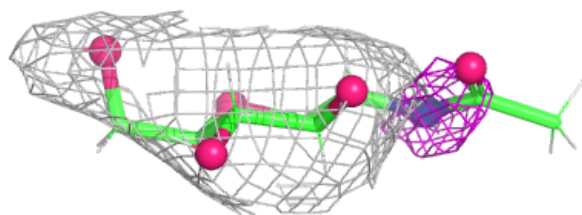
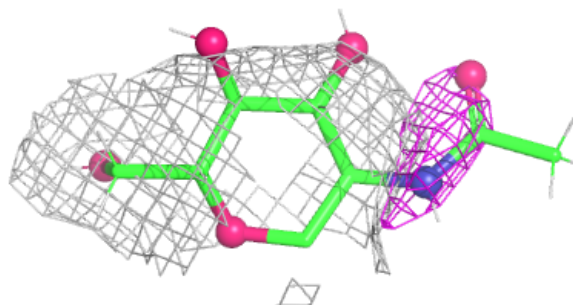


Electron density around NAG K 704:

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

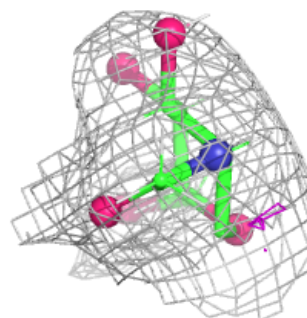
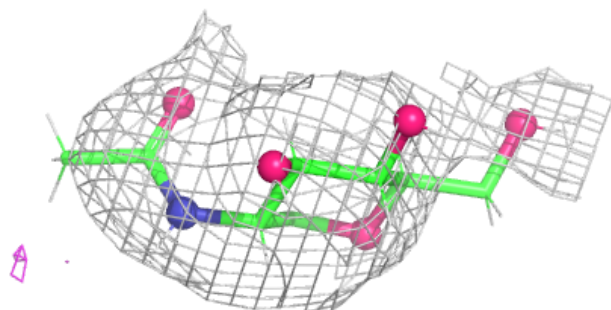
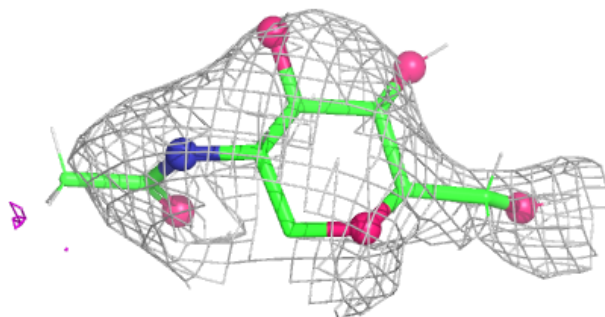
**Electron density around NAG C 703:**

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

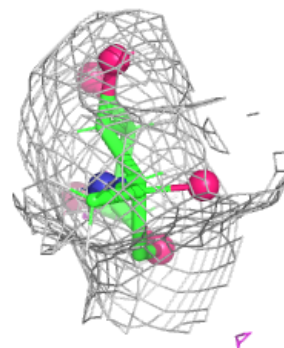
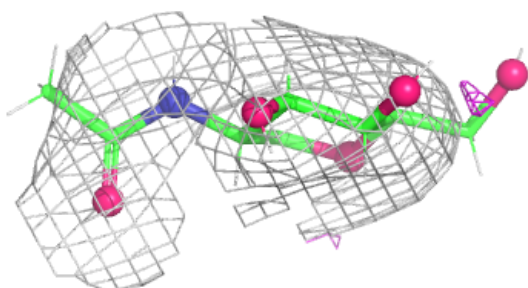
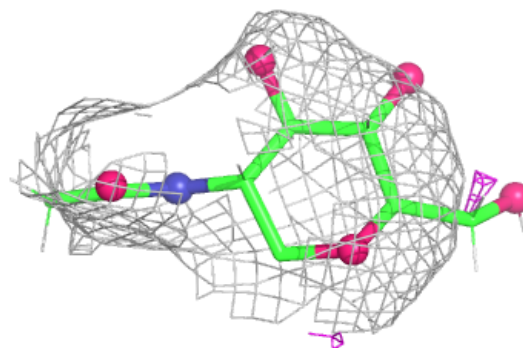


Electron density around NAG K 705:

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

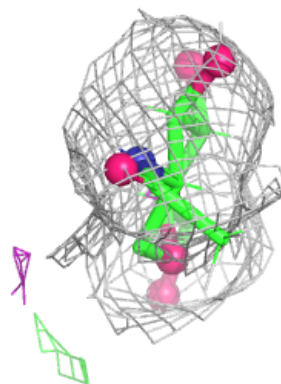
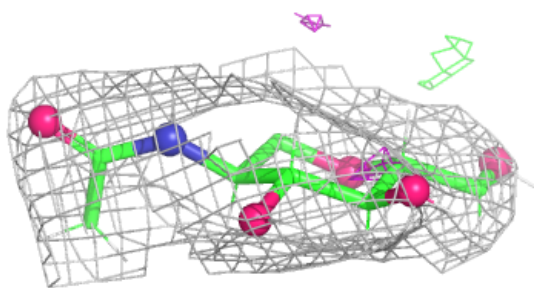
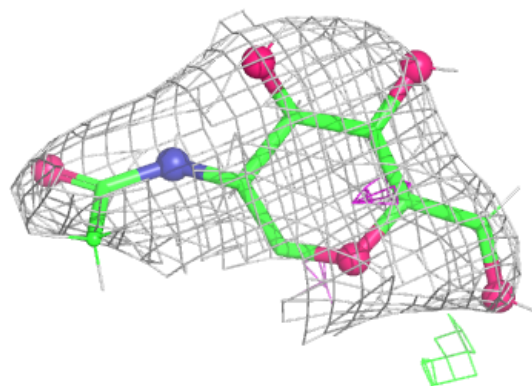
**Electron density around NAG D 702:**

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

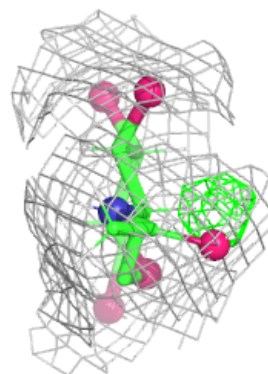
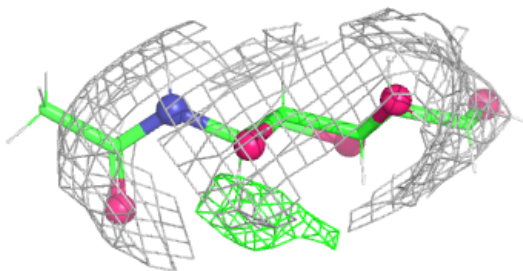
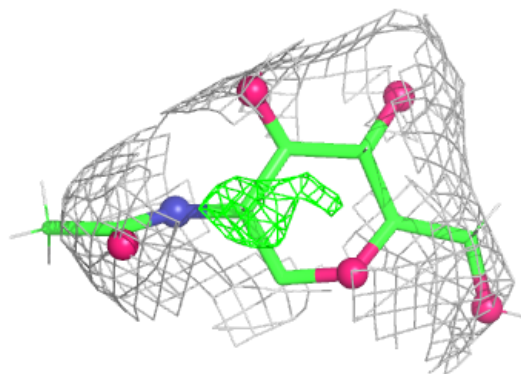


Electron density around NAG K 703:

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

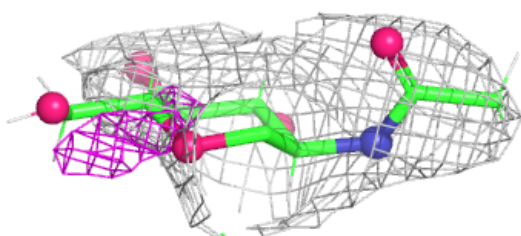
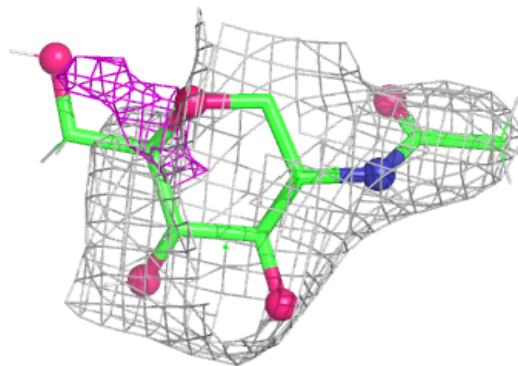
**Electron density around NAG C 702:**

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

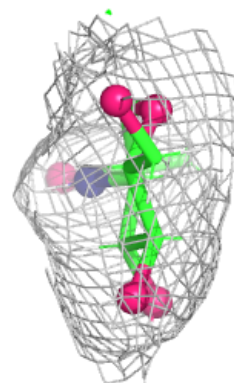
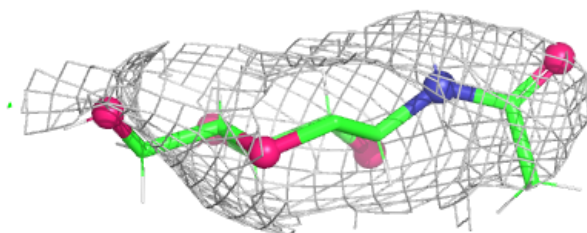
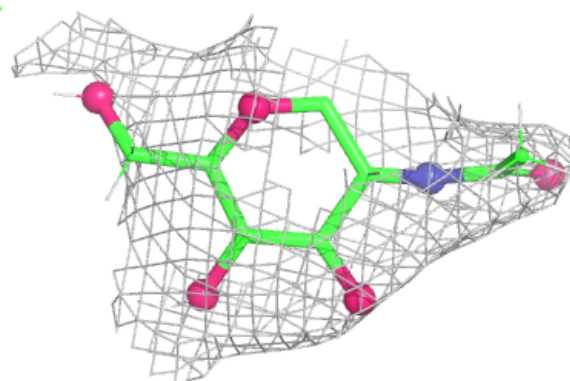


Electron density around NAG G 703:

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

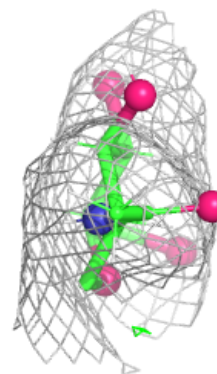
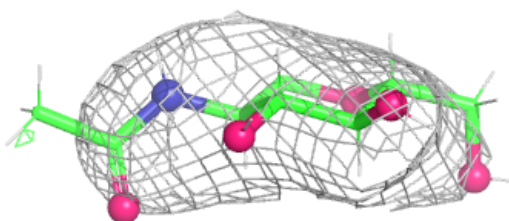
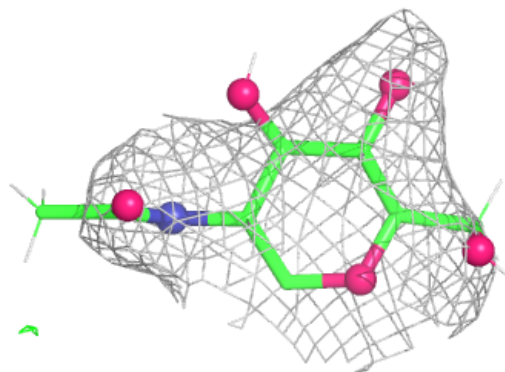
**Electron density around NAG D 706:**

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

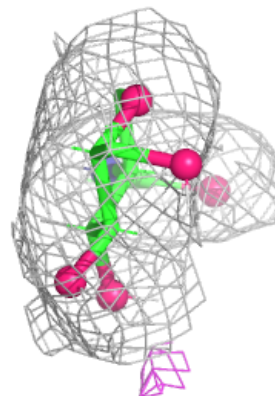
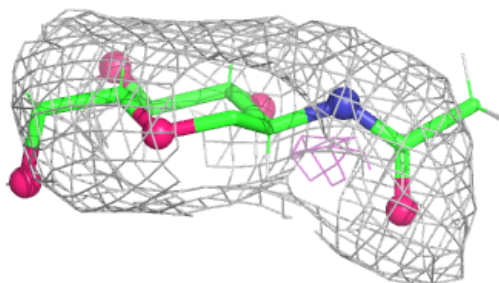
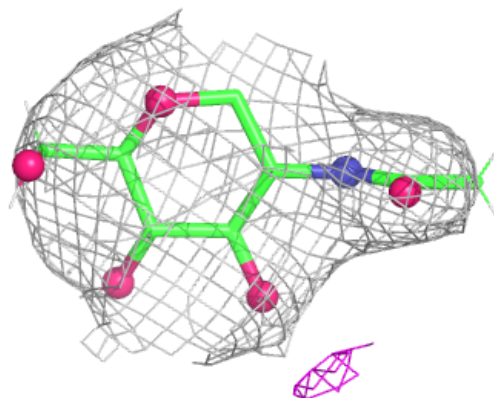


Electron density around NAG C 705:

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

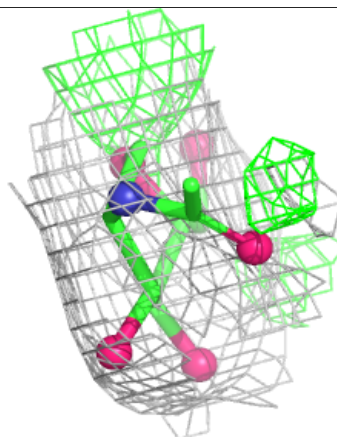
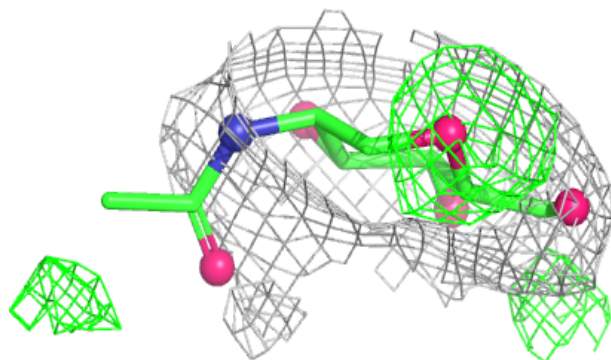
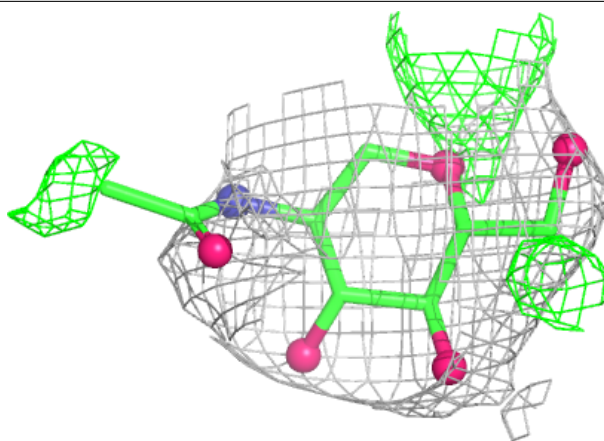
**Electron density around NAG K 707:**

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



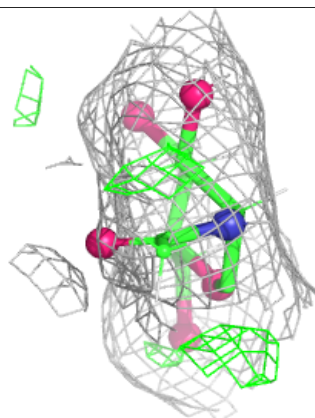
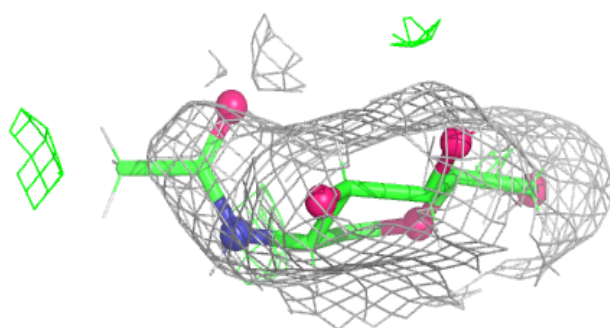
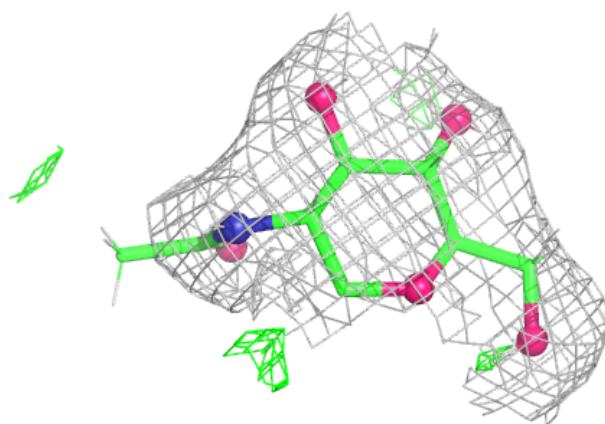
Electron density around NAG D 705:

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



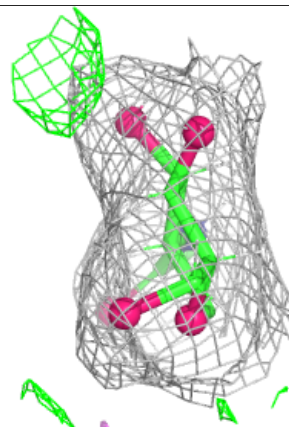
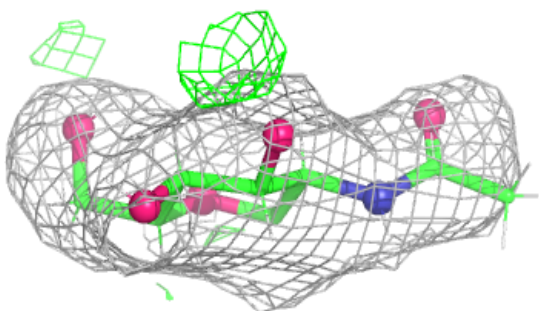
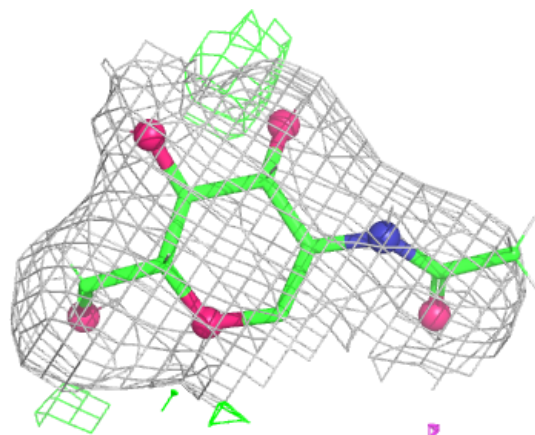
Electron density around NAG C 704:

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



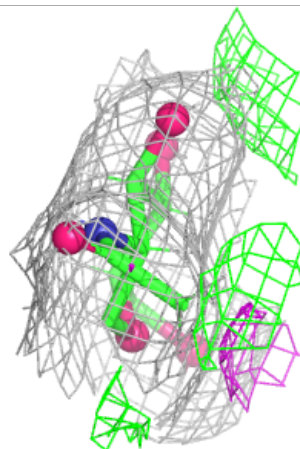
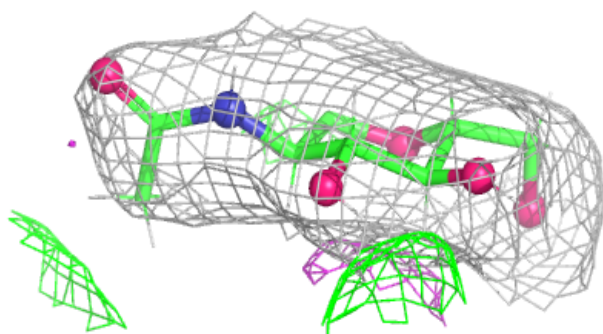
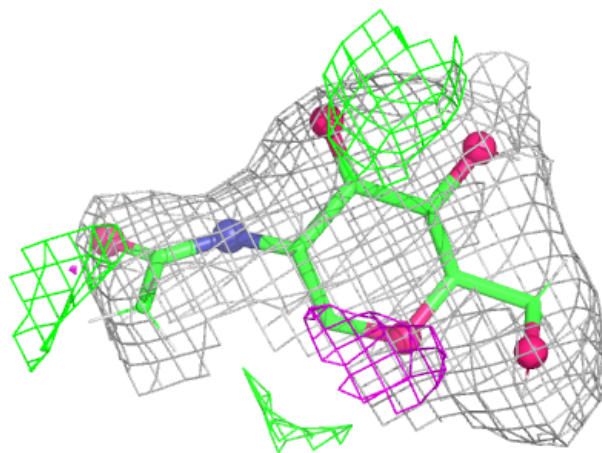
Electron density around NAG G 702:

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



Electron density around NAG K 706:

$2mF_o-DF_c$ (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.