



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:40 AM UTC

PDB ID : 6MYM / pdb_00006mym
Title : Crystal structure of hemagglutinin from influenza virus A/Phillipines/2/1982 (H3N2)
Authors : Dai, Y.N.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2018-11-01
Resolution : 2.45 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

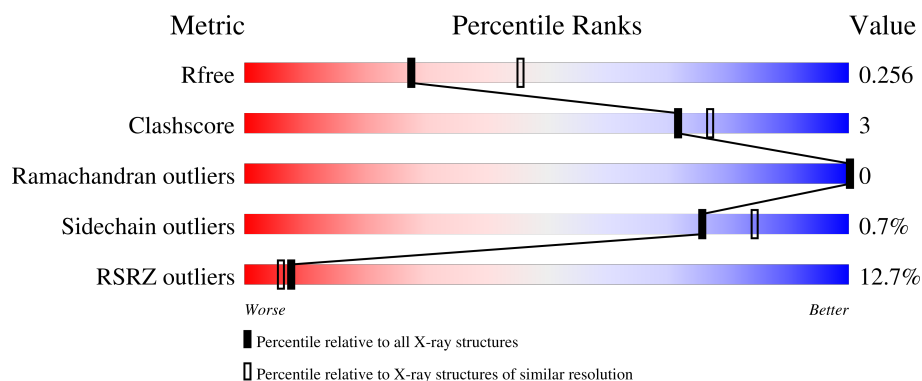
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.



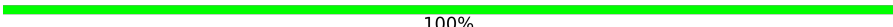
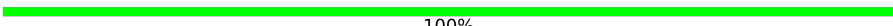
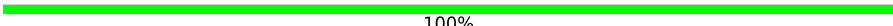
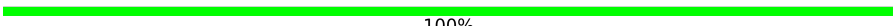
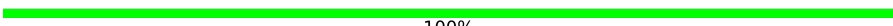
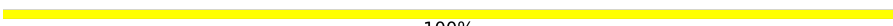
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	497	12% 89% 8%
1	B	497	9% 89% 8%
1	C	497	16% 91% 7%
2	D	2	100%

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Mol	Chain	Length	Quality of chain
2	E	2	 50% 50%
2	H	2	 100%
2	K	2	 100%
2	L	2	 50% 50%
2	N	2	 50% 50%
2	P	2	 50% 50%
3	F	3	 100%
3	G	3	 100%
3	I	3	 67% 33%
3	J	3	 100%
3	M	3	 33% 67%
3	O	3	 100%
3	Q	3	 67% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12267 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3837	2396	678	745	18			
1	B	486	Total	C	N	O	S	0	0	0
			3837	2396	678	745	18			
1	C	487	Total	C	N	O	S	0	0	0
			3841	2398	679	746	18			

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



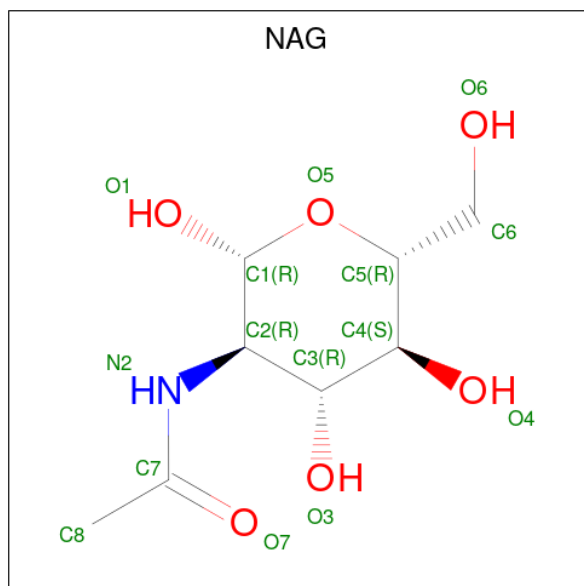
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

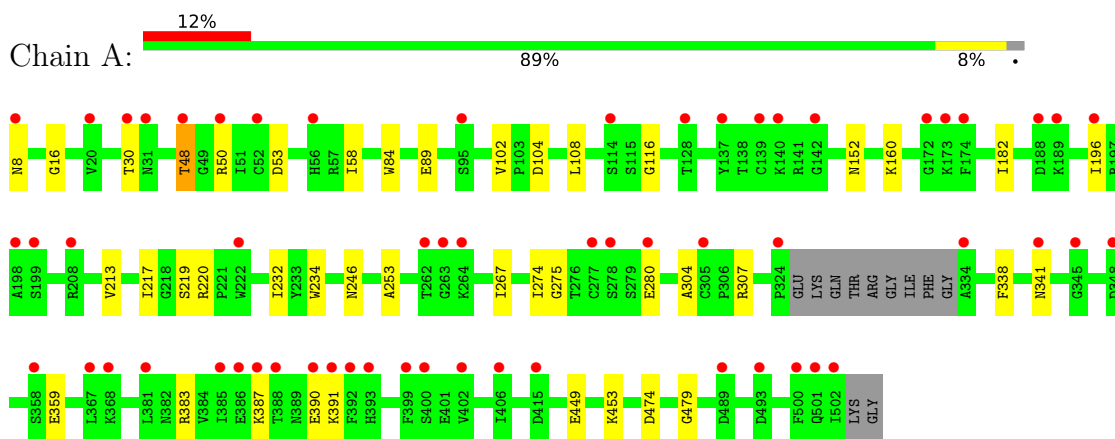
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	B	71	Total	O	0	0
			71	71		
5	C	40	Total	O	0	0
			40	40		

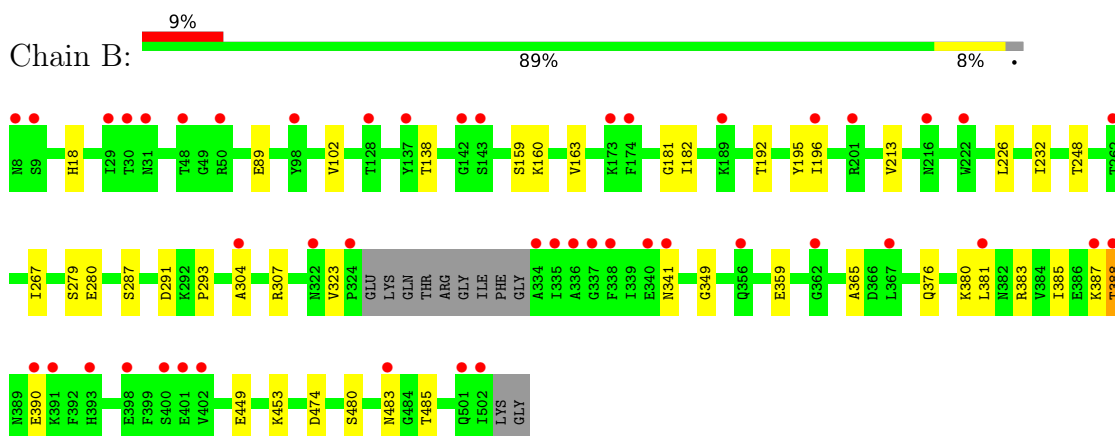
3 Residue-property plots [i](#)

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.

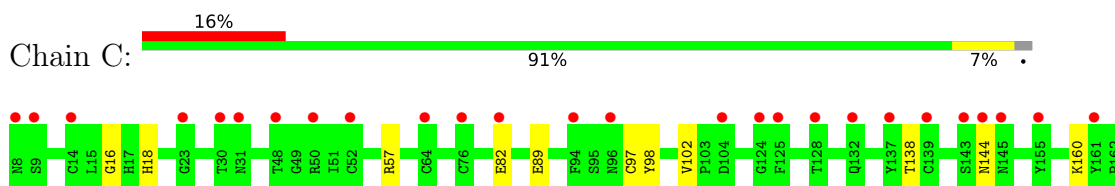
• Molecule 1: Hemagglutinin

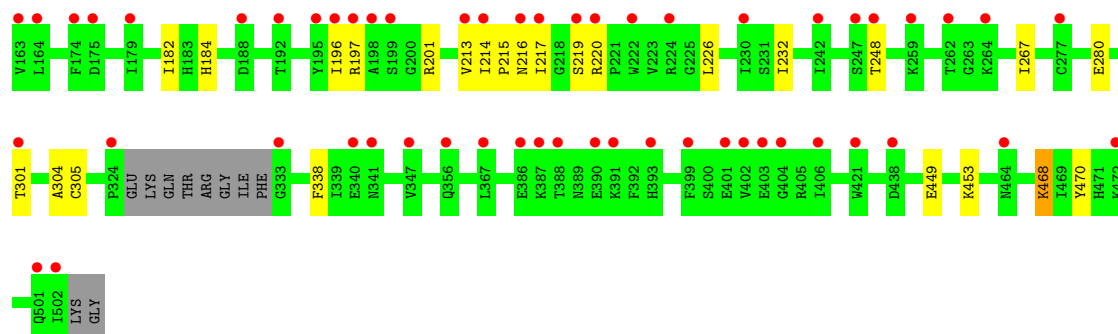


• Molecule 1: Hemagglutinin

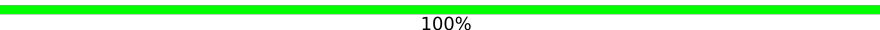


• Molecule 1: Hemagglutinin





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

Chain D:  100%

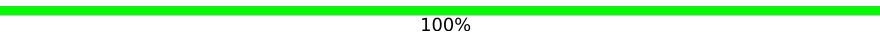


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50%

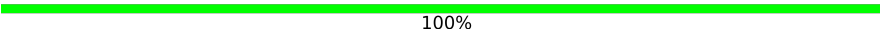


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



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

Chain K:  100%



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

Chain L:  50%



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

Chain N:  50% 50%

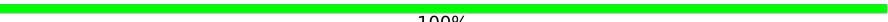
MAG1
MAG2

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

Chain P:  50% 50%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2
BMA3

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

Chain G:  100%

MAG1
MAG2
BMA3

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

Chain I:  67% 33%

MAG1
MAG2
BMA3

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

Chain J:  100%

MAG1
MAG2
BMA3

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

Chain M:  33% 67%



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

Chain O:  100%



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

Chain Q:  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	195.78Å 187.58Å 107.73Å 90.00° 109.82° 90.00°	Depositor
Resolution (Å)	48.58 – 2.45 48.58 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.58-2.45) 99.5 (48.58-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.227 , 0.254 0.230 , 0.256	Depositor DCC
R_{free} test set	6562 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12267	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: BMA, NAG

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	0.28	0/3917	0.49	0/5304
1	B	0.27	0/3917	0.47	0/5304
1	C	0.25	0/3921	0.46	0/5309
All	All	0.26	0/11755	0.47	0/15917

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3837	0	3714	26	0
1	B	3837	0	3713	29	0
1	C	3841	0	3717	20	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	H	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	2	0
2	N	28	0	25	0	0
2	P	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	39	0	34	0	0
3	G	39	0	34	0	0
3	I	39	0	34	2	0
3	J	39	0	34	0	0
3	M	39	0	34	0	0
3	O	39	0	34	0	0
3	Q	39	0	34	0	0
4	A	14	0	13	1	0
4	B	56	0	52	3	0
4	C	42	0	39	0	0
5	A	60	0	0	0	0
5	B	71	0	0	0	0
5	C	40	0	0	0	0
All	All	12267	0	11661	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (79) 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:A:160:LYS:HA	1:A:196:ILE:HD11	1.29	1.14
1:C:57:ARG:NH2	1:C:82:GLU:OE2	2.02	0.90
1:C:160:LYS:HA	1:C:196:ILE:HD11	1.58	0.84
1:C:280:GLU:HG2	1:C:304:ALA:HB3	1.61	0.80
1:B:280:GLU:HG2	1:B:304:ALA:HB3	1.65	0.78
1:B:160:LYS:HA	1:B:196:ILE:HD11	1.68	0.76
1:A:280:GLU:HG2	1:A:304:ALA:HB3	1.68	0.75
1:B:359:GLU:OE2	1:B:474:ASP:HB2	1.92	0.70
1:B:163:VAL:HG12	1:B:248:THR:HG22	1.75	0.68
1:A:160:LYS:HA	1:A:196:ILE:CD1	2.19	0.67
1:B:182:ILE:CD1	1:B:213:VAL:HB	2.23	0.67
1:C:160:LYS:HA	1:C:196:ILE:CD1	2.27	0.65
1:C:160:LYS:CA	1:C:196:ILE:HD11	2.25	0.65
1:C:217:ILE:H	1:C:217:ILE:HD12	1.63	0.64
1:A:48:THR:HG21	1:A:50:ARG:NH2	2.13	0.64
1:A:182:ILE:CD1	1:A:213:VAL:HB	2.28	0.63
1:C:216:ASN:HB2	1:C:220:ARG:HH12	1.64	0.63
2:L:1:NAG:H83	2:L:1:NAG:H3	1.81	0.62
1:A:359:GLU:OE2	1:A:474:ASP:HB2	2.00	0.61
1:B:160:LYS:CA	1:B:196:ILE:HD11	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:702:NAG:H3	4:B:702:NAG:H83	1.84	0.59
1:B:160:LYS:HA	1:B:196:ILE:CD1	2.32	0.58
1:B:182:ILE:HD13	1:B:213:VAL:HB	1.86	0.56
1:C:138:THR:HG21	1:C:226:LEU:HG	1.86	0.56
1:C:219:SER:H	3:I:1:NAG:C8	2.19	0.56
1:C:449:GLU:O	1:C:453:LYS:HG2	2.05	0.56
2:E:2:NAG:H83	2:E:2:NAG:H3	1.87	0.55
1:A:219:SER:O	1:A:220:ARG:NH1	2.40	0.55
1:B:383:ARG:O	1:B:387:LYS:HG2	2.08	0.53
1:A:479:GLY:HA3	4:A:611:NAG:H61	1.91	0.53
1:B:307:ARG:NH1	1:B:390:GLU:OE1	2.41	0.53
1:A:217:ILE:HD12	1:A:217:ILE:H	1.74	0.52
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.92	0.52
1:C:182:ILE:CD1	1:C:213:VAL:HB	2.39	0.52
1:A:449:GLU:O	1:A:453:LYS:HG2	2.10	0.52
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.92	0.51
1:B:449:GLU:O	1:B:453:LYS:HG2	2.10	0.51
1:B:159:SER:C	1:B:196:ILE:HD11	2.36	0.51
1:B:483:ASN:HB3	1:B:485:THR:HG23	1.92	0.51
1:A:48:THR:HG22	1:A:50:ARG:NH1	2.25	0.51
1:A:89:GLU:HG3	1:A:267:ILE:HD11	1.93	0.49
1:A:307:ARG:NH1	1:A:390:GLU:HG3	2.27	0.49
1:C:201:ARG:NH1	1:C:214:ILE:HD11	2.27	0.49
1:A:246:ASN:HD22	3:I:1:NAG:H83	1.78	0.49
1:B:192:THR:HA	1:B:195:TYR:O	2.12	0.48
4:B:708:NAG:H83	4:B:708:NAG:H3	1.95	0.48
1:B:480:SER:HA	1:B:483:ASN:HB2	1.95	0.48
1:C:97:CYS:SG	1:C:98:TYR:N	2.86	0.47
1:B:89:GLU:HG3	1:B:267:ILE:HD11	1.97	0.47
1:B:279:SER:OG	1:B:287:SER:HB3	2.16	0.46
1:A:30:THR:HG21	1:B:376:GLN:HG2	1.98	0.46
1:B:381:LEU:O	1:B:385:ILE:HG12	2.16	0.45
1:A:58:ILE:HG21	1:A:274:ILE:HD12	1.99	0.45
1:B:102:VAL:HG22	1:B:232:ILE:HB	1.99	0.44
1:C:89:GLU:HG3	1:C:267:ILE:HD11	2.00	0.44
1:C:468:LYS:HG2	1:C:470:TYR:CE1	2.53	0.44
1:A:383:ARG:O	1:A:387:LYS:HG2	2.18	0.43
1:A:53:ASP:N	1:A:275:GLY:O	2.44	0.43
1:A:217:ILE:HD12	1:A:217:ILE:N	2.34	0.42
1:A:108:LEU:HB2	1:A:234:TRP:CZ3	2.54	0.42
1:A:152:ASN:HB3	1:A:253:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:709:NAG:O3	2:L:1:NAG:O7	2.26	0.42
1:A:104:ASP:HB3	1:A:234:TRP:CH2	2.54	0.42
1:B:293:PRO:HA	1:B:388:THR:HG22	2.02	0.42
1:B:181:GLY:O	1:B:182:ILE:HG13	2.20	0.41
1:B:291:ASP:OD1	1:B:291:ASP:N	2.53	0.41
1:B:138:THR:HG21	1:B:226:LEU:HG	2.02	0.41
1:A:16:GLY:HA2	1:A:338:PHE:HB3	2.02	0.41
1:C:301:THR:HB	1:C:305:CYS:SG	2.61	0.41
1:A:220:ARG:HA	1:A:220:ARG:HD3	1.95	0.41
1:B:159:SER:O	1:B:196:ILE:HD11	2.21	0.41
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.56	0.41
1:B:380:LYS:HB3	1:B:380:LYS:HE2	1.88	0.41
1:C:16:GLY:HA2	1:C:338:PHE:HB3	2.03	0.41
1:C:184:HIS:CE1	1:C:215:PRO:HA	2.56	0.41
1:C:197:ARG:NH2	1:C:248:THR:O	2.52	0.41
1:B:323:VAL:HG12	1:B:341:ASN:OD1	2.20	0.41
1:B:349:GLY:HA3	1:B:365:ALA:HB1	2.03	0.41
1:B:196:ILE:HG21	1:B:196:ILE:HD13	1.83	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	482/497 (97%)	465 (96%)	17 (4%)	0	100	100
1	B	482/497 (97%)	465 (96%)	17 (4%)	0	100	100
1	C	483/497 (97%)	465 (96%)	18 (4%)	0	100	100
All	All	1447/1491 (97%)	1395 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	425/433 (98%)	421 (99%)	4 (1%)	70	81
1	B	425/433 (98%)	423 (100%)	2 (0%)	81	87
1	C	425/433 (98%)	422 (99%)	3 (1%)	76	84
All	All	1275/1299 (98%)	1266 (99%)	9 (1%)	76	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	48	THR
1	A	341	ASN
1	A	391	LYS
1	B	18	HIS
1	B	388	THR
1	C	18	HIS
1	C	144	ASN
1	C	468	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	GLN
1	A	434	GLN
1	A	488	HIS
1	B	434	GLN
1	B	488	HIS
1	C	56	HIS
1	C	355	HIS
1	C	389	ASN
1	C	393	HIS
1	C	434	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	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.25	0	17,19,21	0.58	0
2	NAG	D	2	2	14,14,15	0.39	0	17,19,21	0.46	0
2	NAG	E	1	2,1	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
2	NAG	E	2	2	14,14,15	0.33	0	17,19,21	1.93	4 (23%)
3	NAG	F	1	3,1	14,14,15	0.20	0	17,19,21	0.47	0
3	NAG	F	2	3	14,14,15	0.21	0	17,19,21	0.65	0
3	BMA	F	3	3	11,11,12	0.63	0	15,15,17	0.76	0
3	NAG	G	1	3,1	14,14,15	0.39	0	17,19,21	0.48	0
3	NAG	G	2	3	14,14,15	0.25	0	17,19,21	0.52	0
3	BMA	G	3	3	11,11,12	0.68	0	15,15,17	0.71	0
2	NAG	H	1	2,1	14,14,15	0.27	0	17,19,21	0.47	0
2	NAG	H	2	2	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	I	1	3,1	14,14,15	0.89	1 (7%)	17,19,21	0.79	1 (5%)
3	NAG	I	2	3	14,14,15	0.45	0	17,19,21	0.56	0
3	BMA	I	3	3	11,11,12	0.60	0	15,15,17	0.78	0
3	NAG	J	1	3,1	14,14,15	0.40	0	17,19,21	0.64	0
3	NAG	J	2	3	14,14,15	0.32	0	17,19,21	0.56	0
3	BMA	J	3	3	11,11,12	0.65	0	15,15,17	0.85	0
2	NAG	K	1	2,1	14,14,15	0.28	0	17,19,21	0.44	0
2	NAG	K	2	2	14,14,15	0.35	0	17,19,21	0.39	0
2	NAG	L	1	2,1	14,14,15	0.60	0	17,19,21	1.40	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	L	2	2	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	M	1	3,1	14,14,15	0.41	0	17,19,21	0.86	1 (5%)
3	NAG	M	2	3	14,14,15	0.69	1 (7%)	17,19,21	0.59	0
3	BMA	M	3	3	11,11,12	0.66	0	15,15,17	0.86	0
2	NAG	N	1	2,1	14,14,15	0.30	0	17,19,21	0.81	1 (5%)
2	NAG	N	2	2	14,14,15	0.38	0	17,19,21	0.55	0
3	NAG	O	1	3,1	14,14,15	1.90	1 (7%)	17,19,21	1.56	3 (17%)
3	NAG	O	2	3	14,14,15	1.08	2 (14%)	17,19,21	0.61	0
3	BMA	O	3	3	11,11,12	0.90	0	15,15,17	0.98	1 (6%)
2	NAG	P	1	2,1	14,14,15	0.56	0	17,19,21	0.63	0
2	NAG	P	2	2	14,14,15	0.23	0	17,19,21	0.79	1 (5%)
3	NAG	Q	1	3,1	14,14,15	0.19	0	17,19,21	0.68	0
3	NAG	Q	2	3	14,14,15	0.53	0	17,19,21	0.58	0
3	BMA	Q	3	3	11,11,12	0.73	0	15,15,17	1.00	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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	1/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1	NAG	O5-C1	6.56	1.54	1.43
3	O	2	NAG	O5-C1	3.20	1.49	1.43
3	I	1	NAG	O5-C1	-3.16	1.38	1.43
3	M	2	NAG	O5-C1	-2.47	1.39	1.43
3	O	2	NAG	C1-C2	-2.05	1.49	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C2-N2-C7	5.28	129.98	122.90
3	O	1	NAG	C1-O5-C5	4.94	118.80	112.19
2	L	1	NAG	C2-N2-C7	4.55	129.00	122.90
2	E	2	NAG	C1-C2-N2	3.41	115.80	110.43
2	P	2	NAG	C1-O5-C5	2.97	116.17	112.19
2	N	1	NAG	C1-O5-C5	2.85	116.01	112.19
3	O	3	BMA	C1-O5-C5	2.78	115.91	112.19
2	E	2	NAG	C3-C4-C5	2.68	115.09	110.23
2	E	2	NAG	C1-O5-C5	2.66	115.76	112.19
3	Q	3	BMA	C1-O5-C5	2.51	115.56	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1	NAG	C2-N2-C7	2.25	125.92	122.90
3	Q	3	BMA	O2-C2-C3	-2.19	105.62	110.15
2	E	1	NAG	C1-O5-C5	2.12	115.03	112.19
3	O	1	NAG	O3-C3-C2	2.09	113.74	109.40
3	I	1	NAG	O4-C4-C5	-2.07	104.23	109.32
3	M	1	NAG	O4-C4-C5	-2.02	104.34	109.32

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	O	1	NAG	C8-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	I	2	NAG	O5-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6

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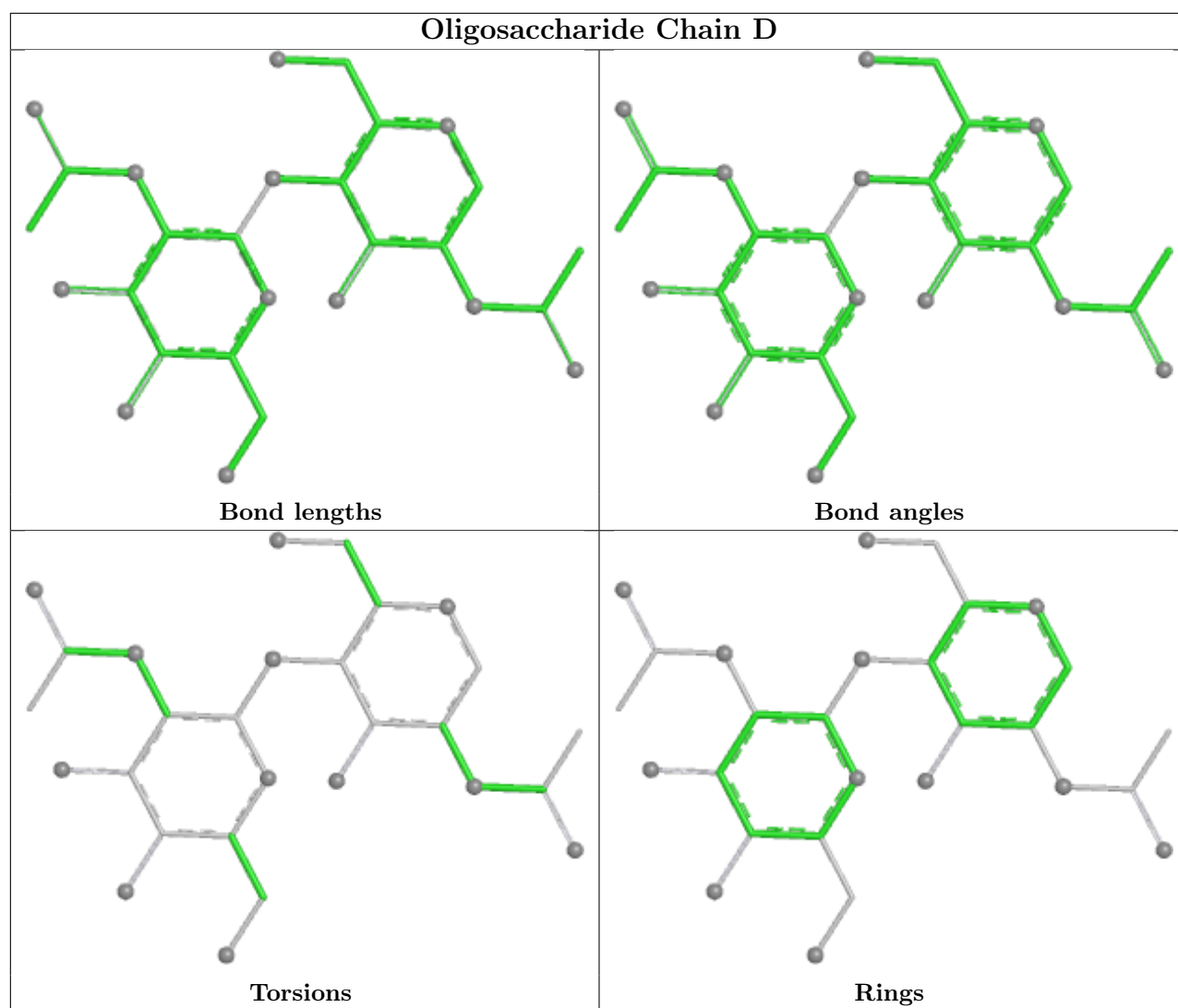
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
3	M	3	BMA	O5-C5-C6-O6
2	L	1	NAG	C1-C2-N2-C7
2	P	1	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6

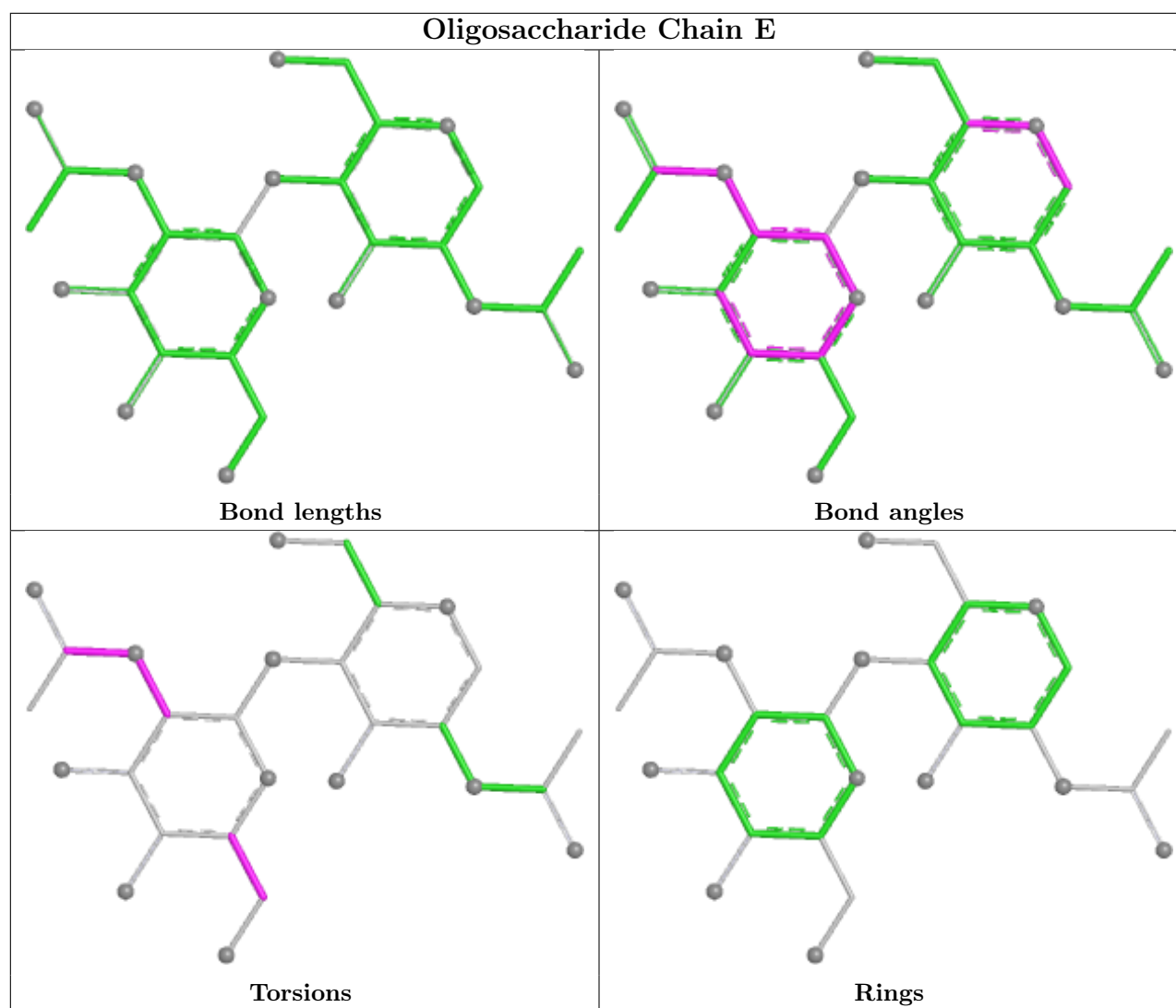
There are no ring outliers.

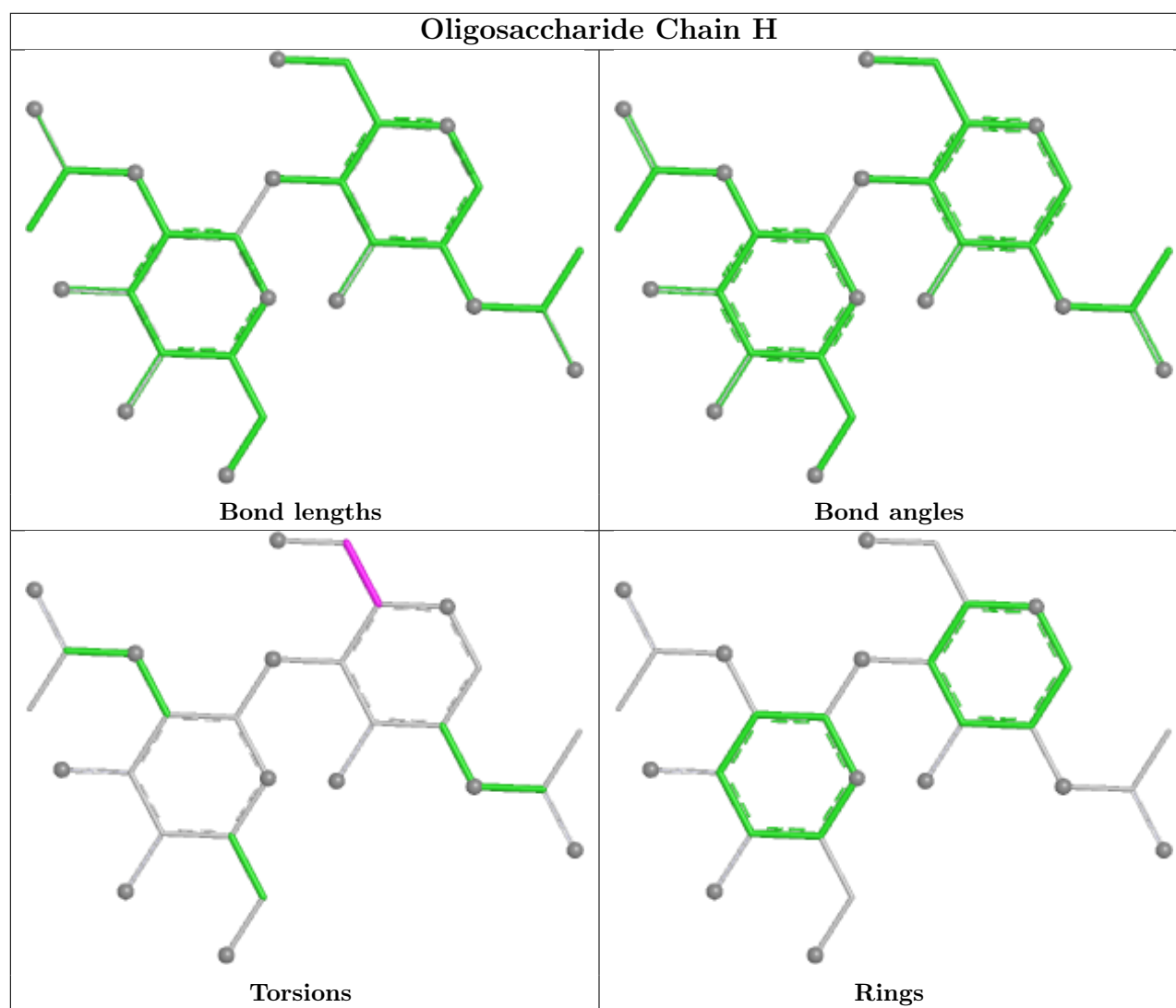
3 monomers are involved in 5 short contacts:

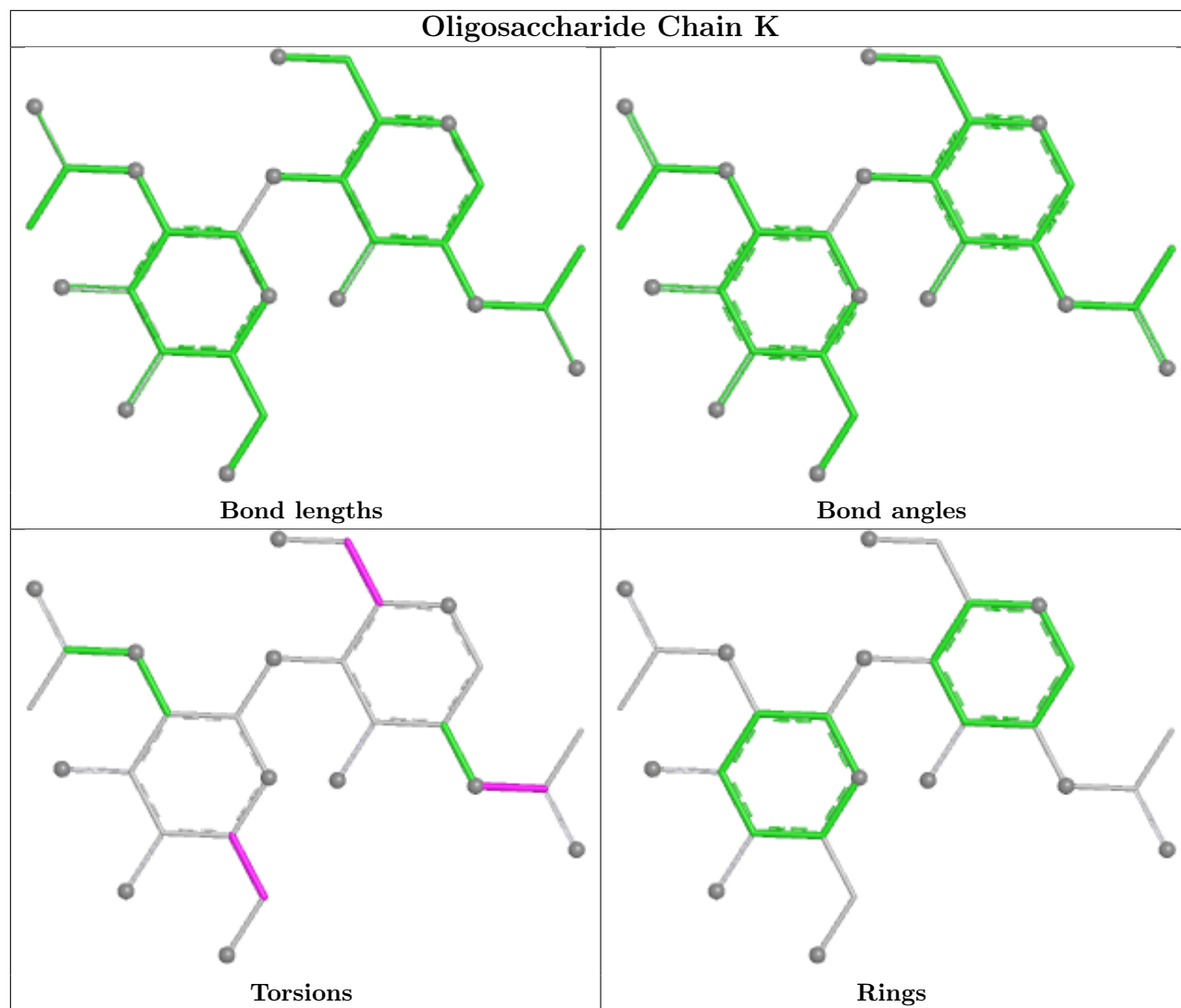
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
3	I	1	NAG	2	0
2	L	1	NAG	2	0

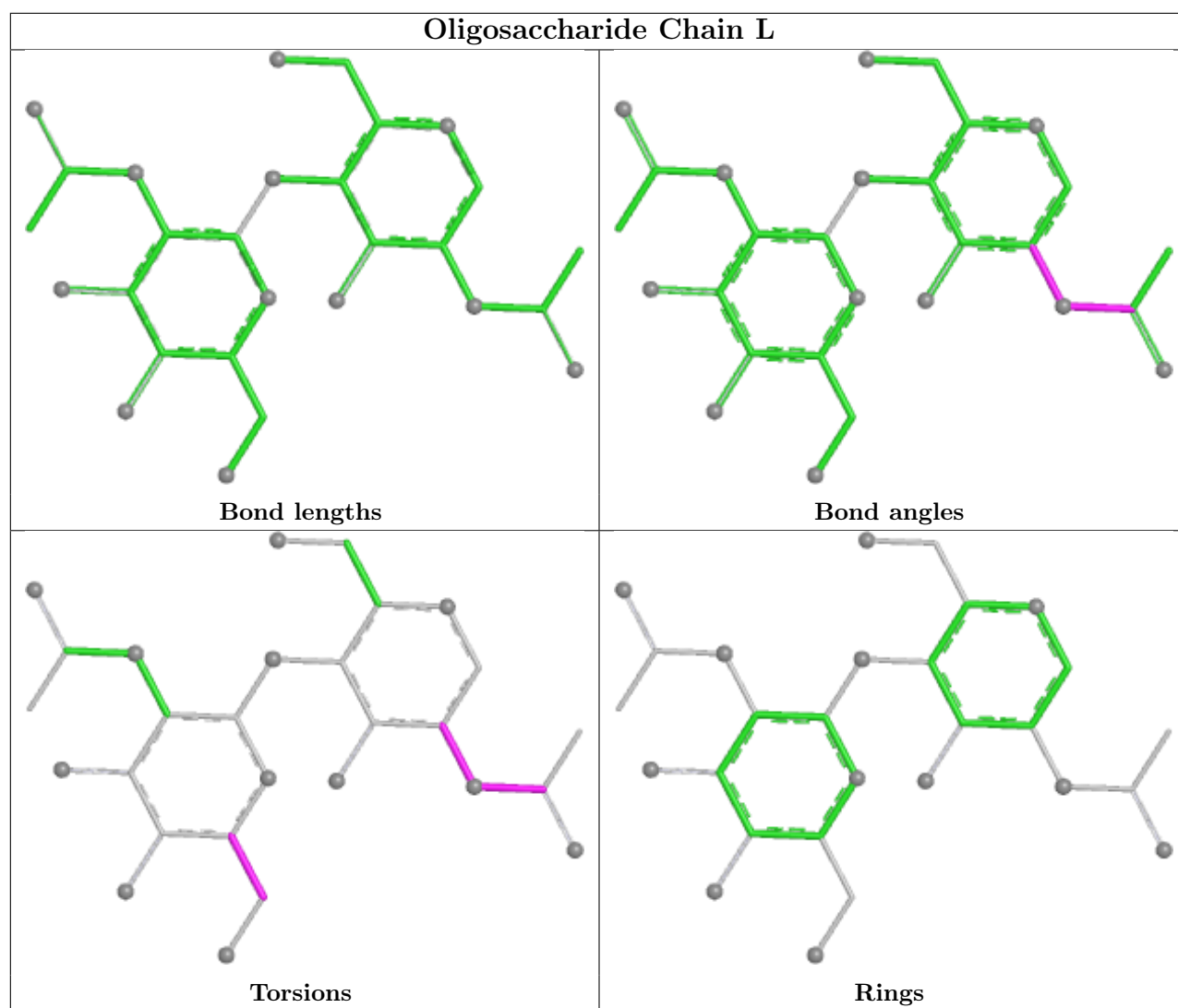
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

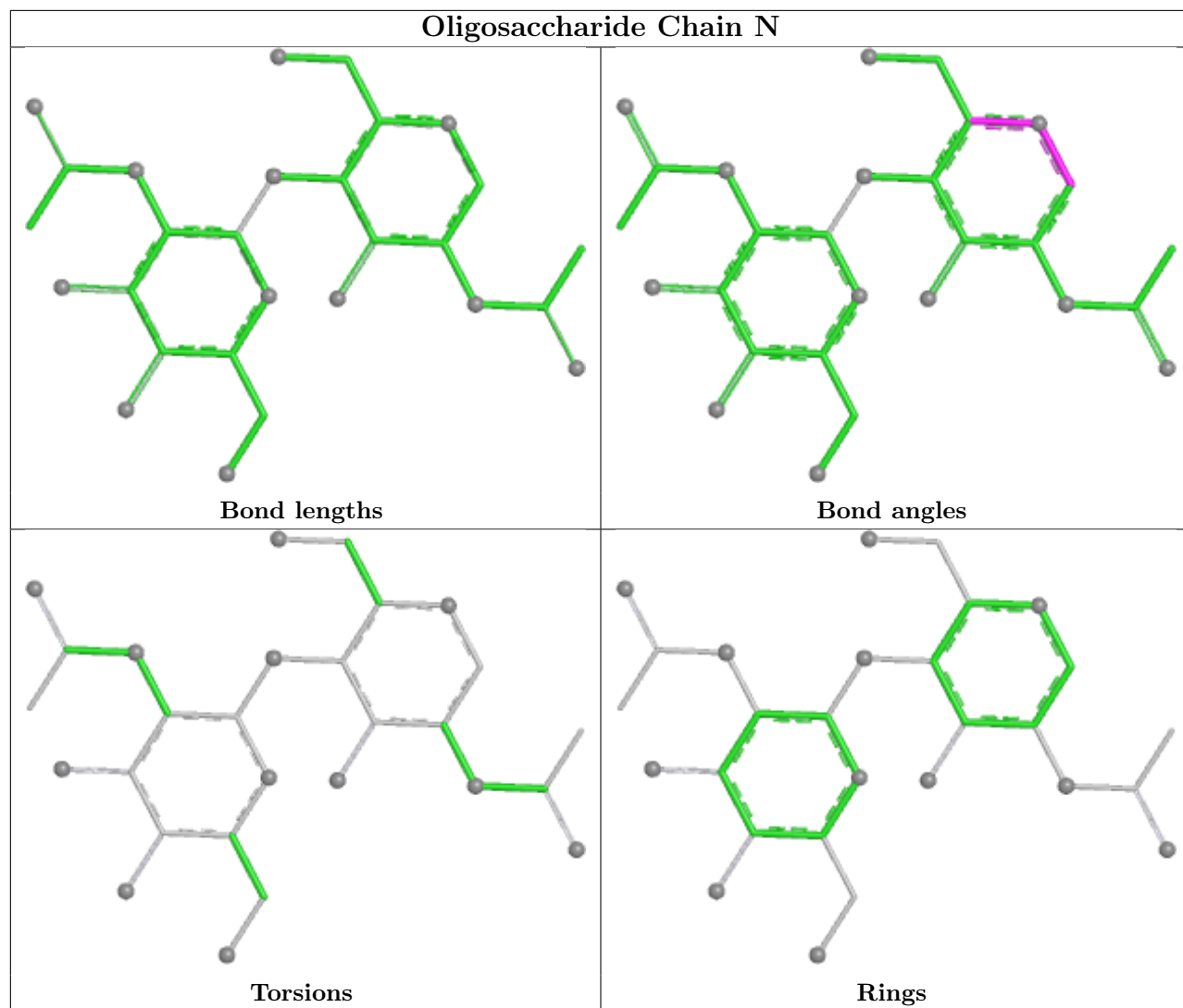


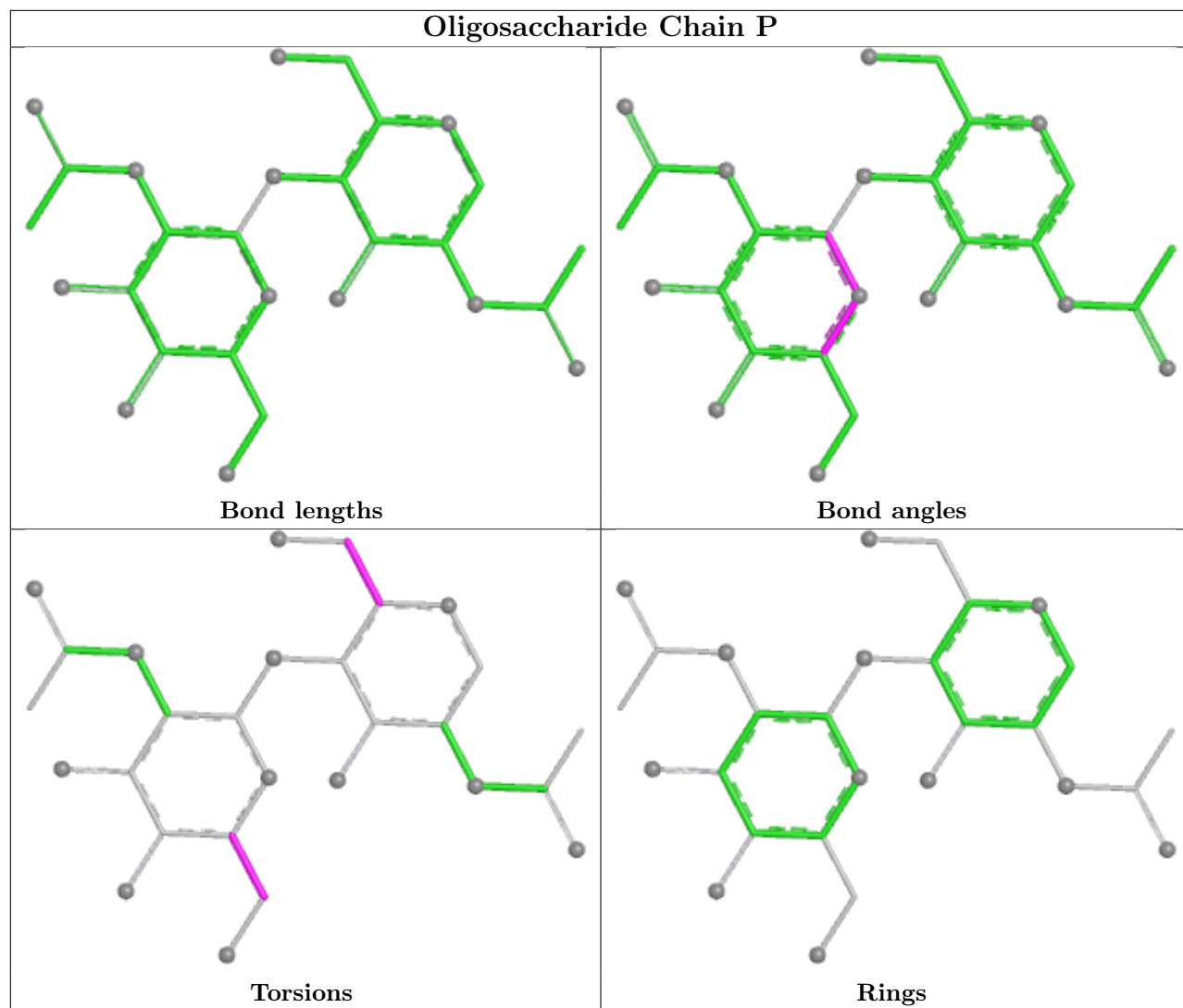


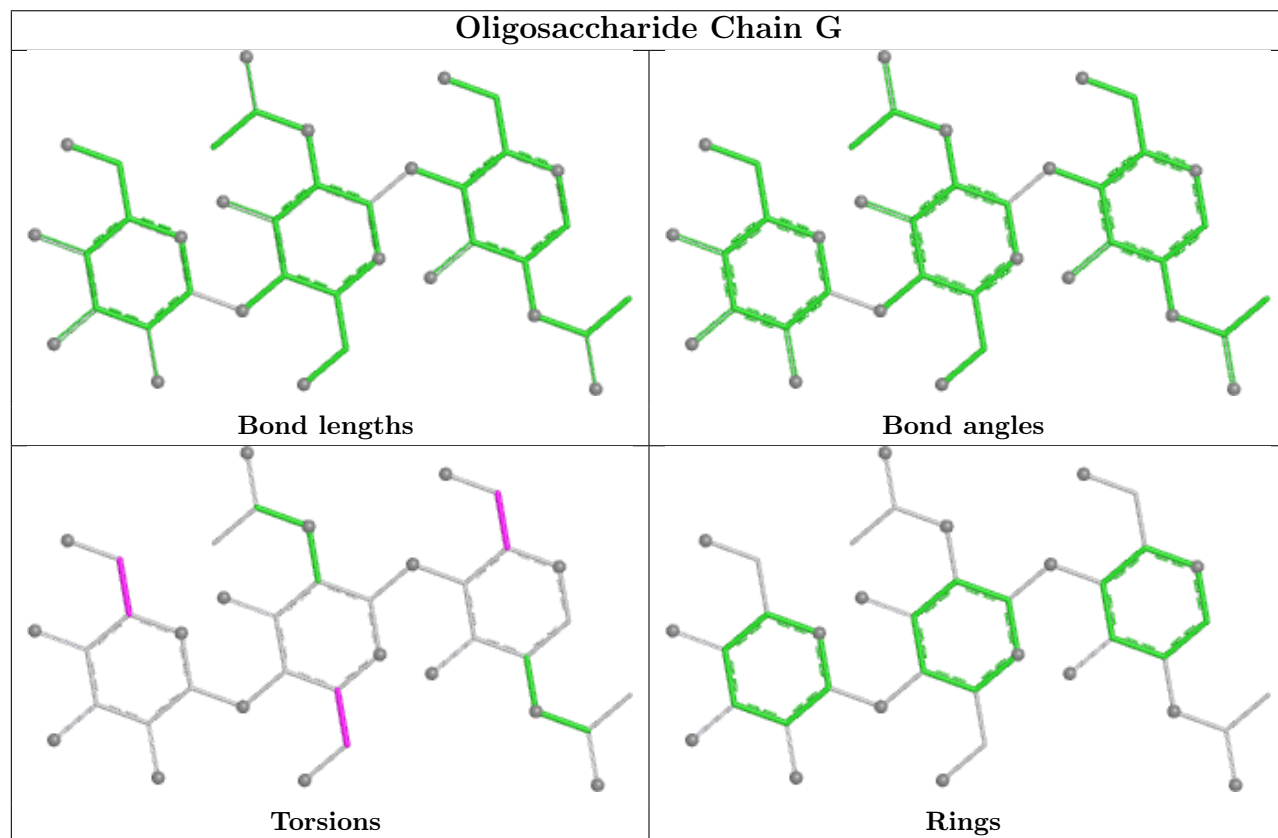
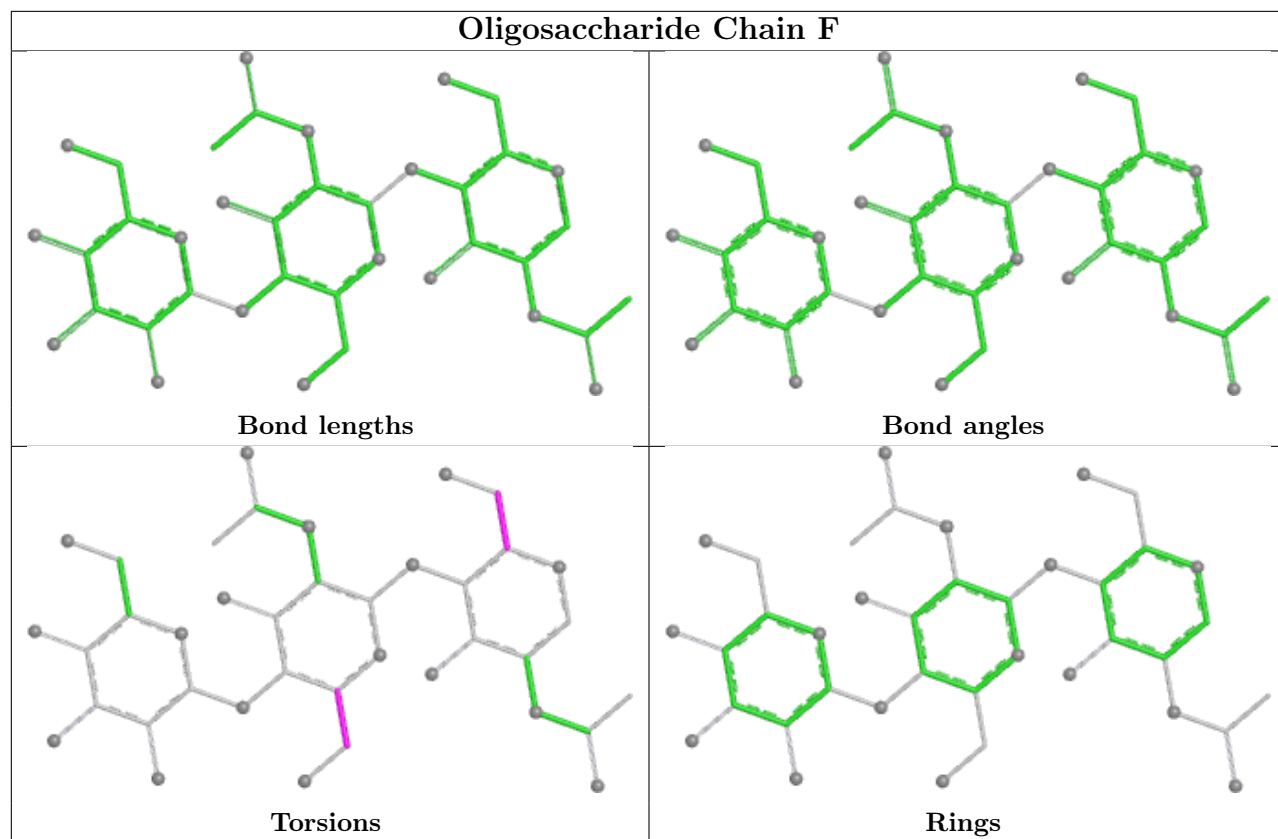


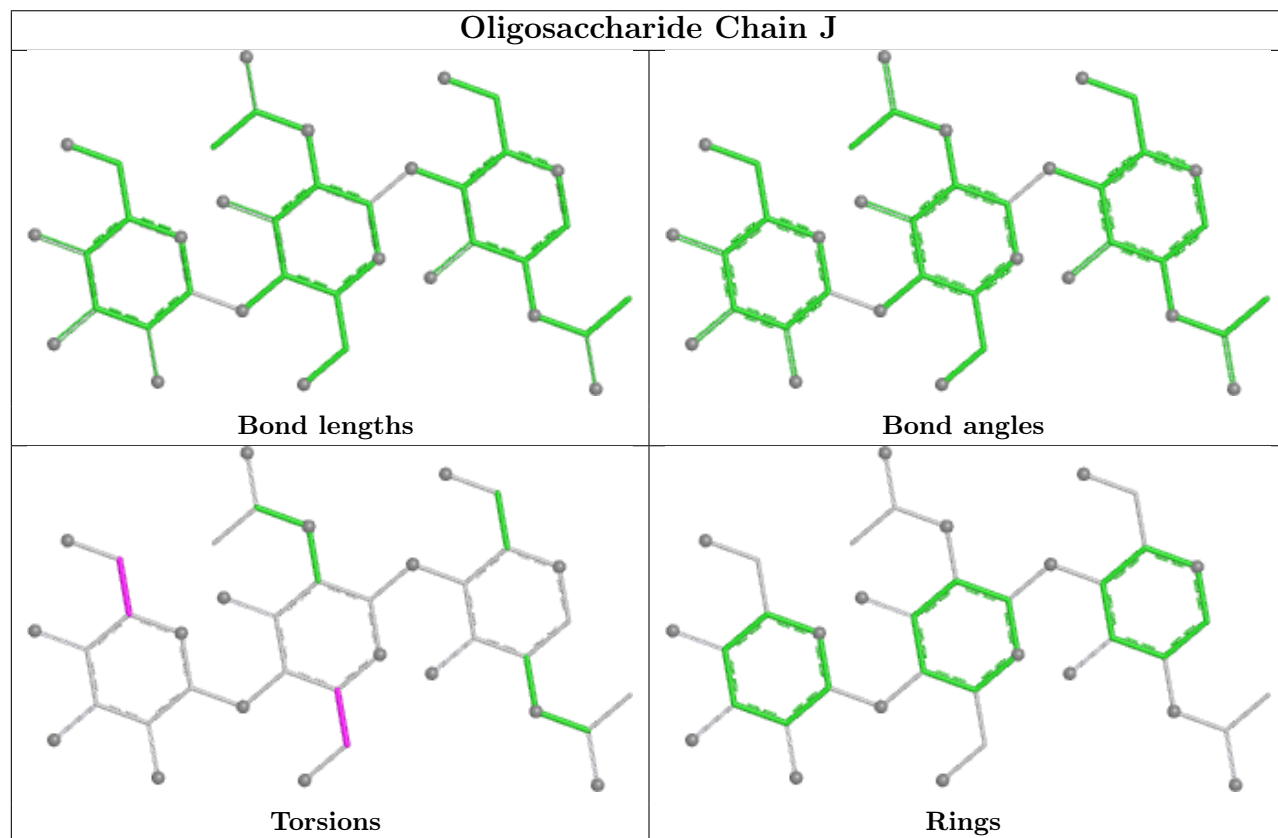
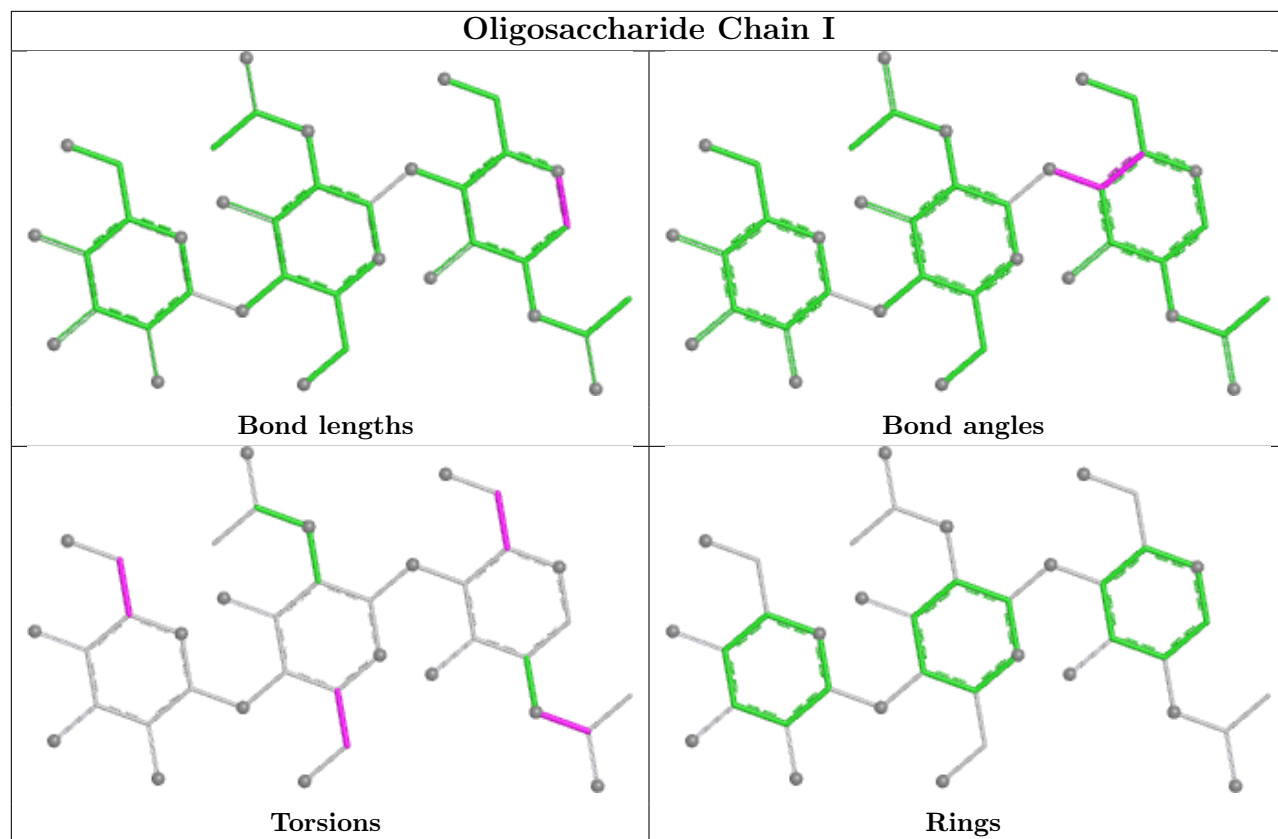


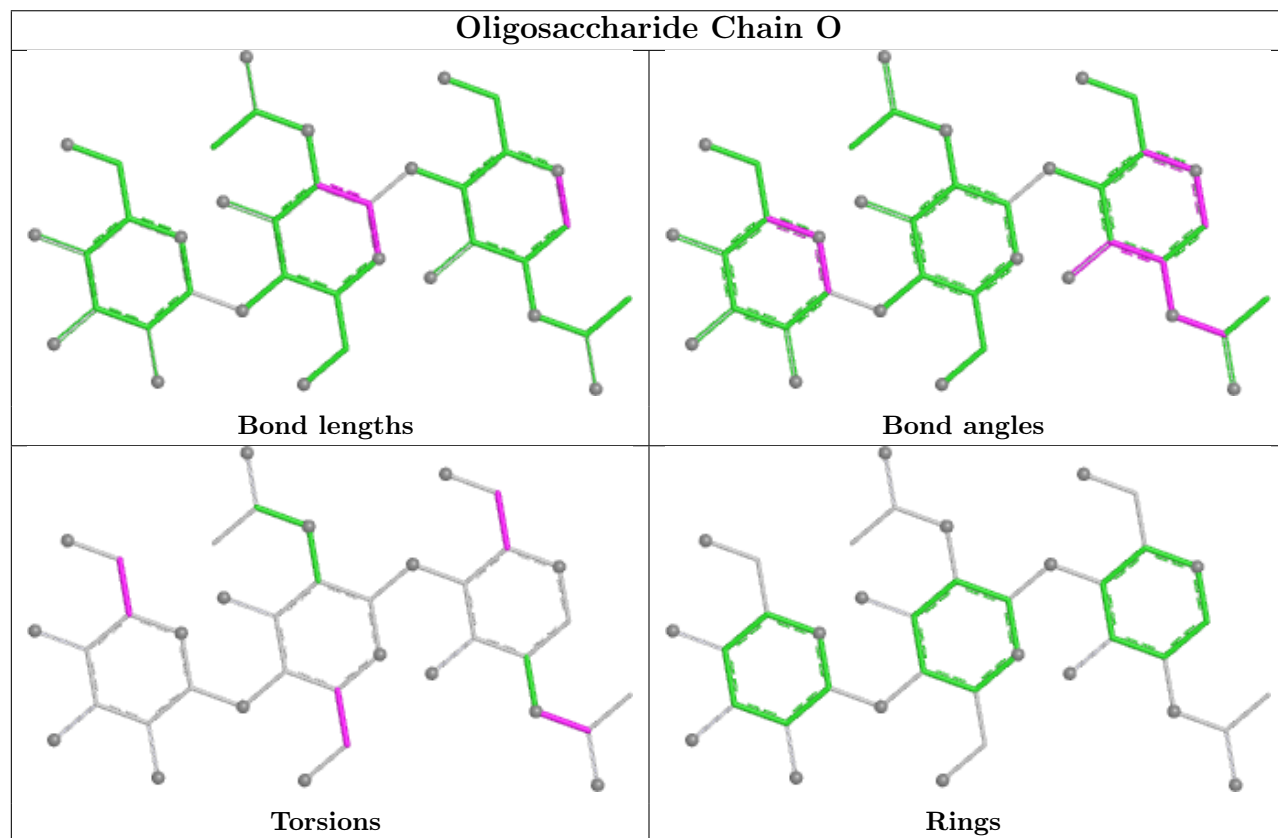
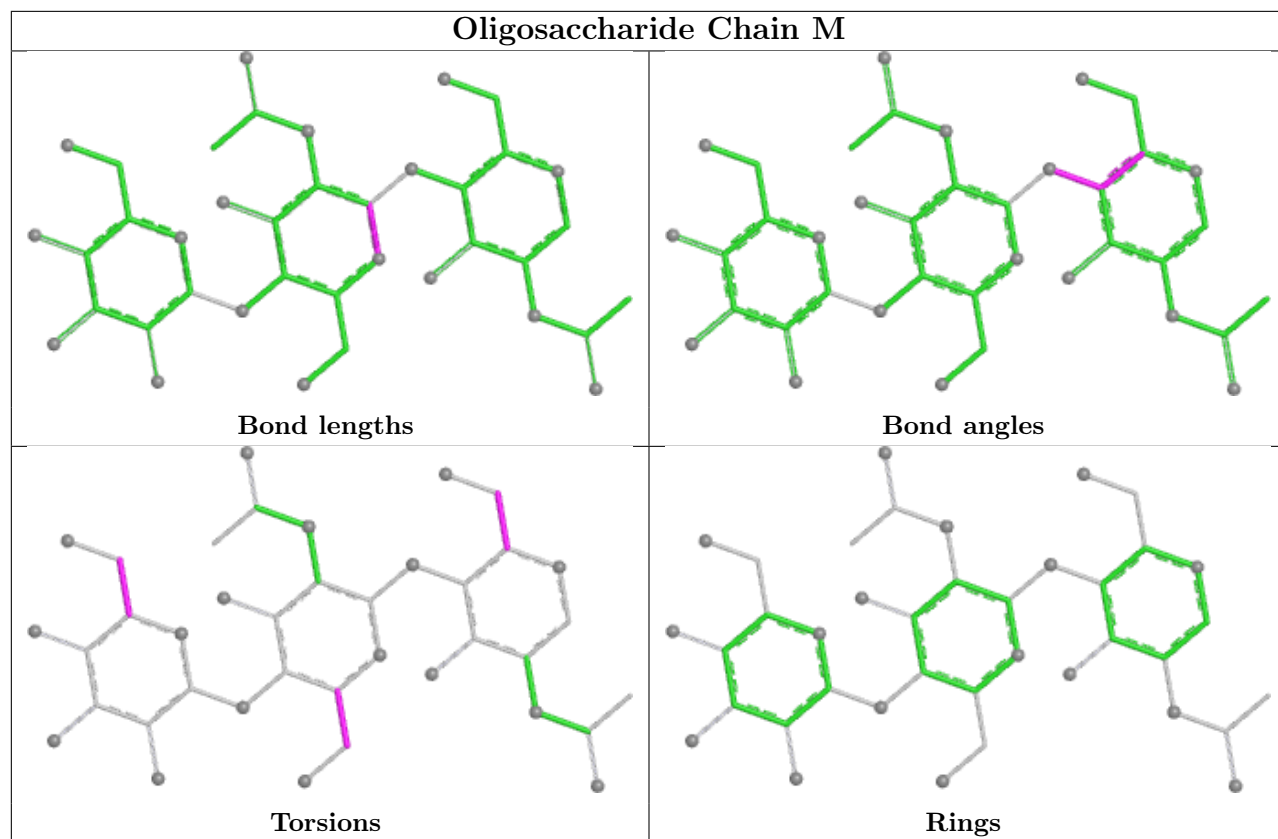


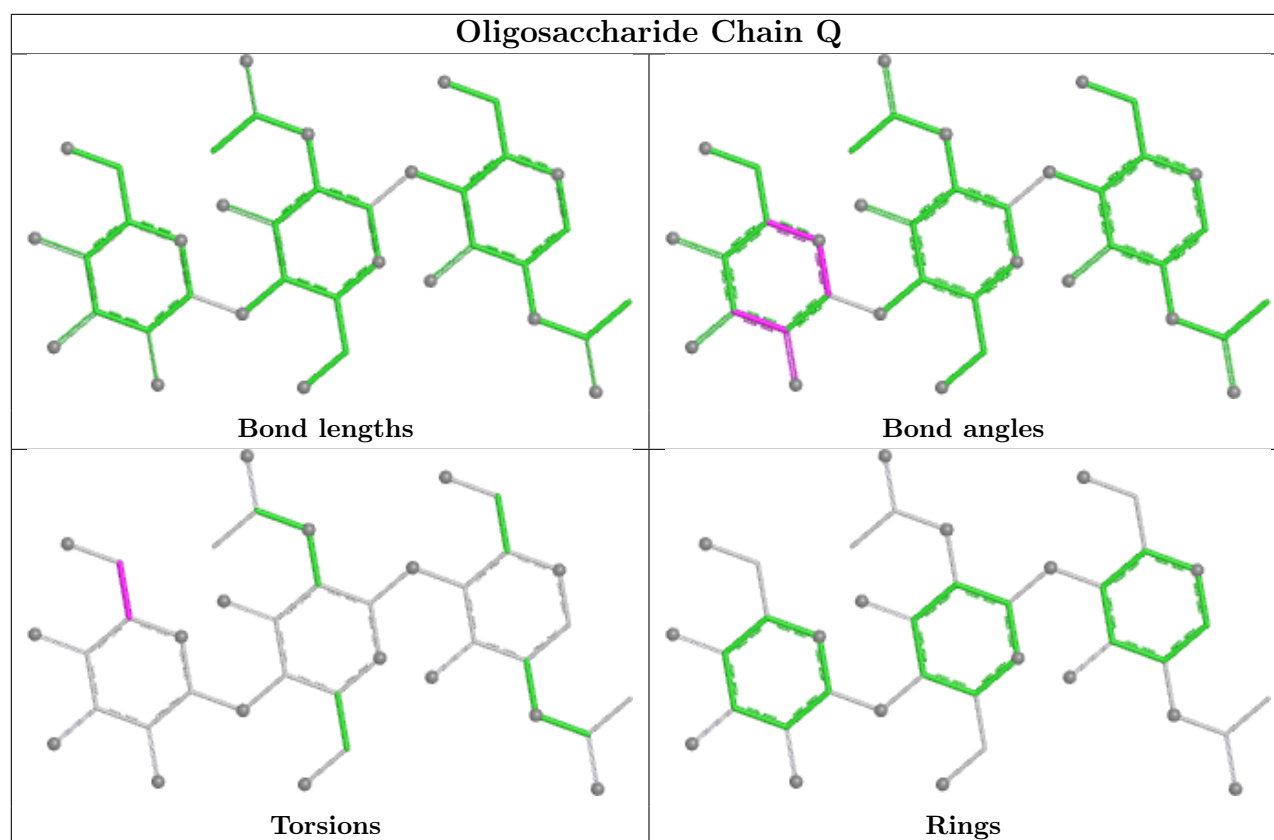












5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
4	NAG	C	610	1	14,14,15	0.69	0	17,19,21	2.28	5 (29%)
4	NAG	C	604	1	14,14,15	0.53	0	17,19,21	0.46	0
4	NAG	A	611	1	14,14,15	0.17	0	17,19,21	0.56	0
4	NAG	B	709	1	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	B	701	1	14,14,15	0.36	0	17,19,21	0.57	0
4	NAG	C	601	1	14,14,15	0.44	0	17,19,21	0.67	1 (5%)
4	NAG	B	702	1	14,14,15	0.72	1 (7%)	17,19,21	1.39	2 (11%)
4	NAG	B	708	1	14,14,15	0.74	0	17,19,21	1.47	3 (17%)

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	C	610	1	-	2/6/23/26	0/1/1/1
4	NAG	C	604	1	-	1/6/23/26	0/1/1/1
4	NAG	A	611	1	-	2/6/23/26	0/1/1/1
4	NAG	B	709	1	-	2/6/23/26	0/1/1/1
4	NAG	B	701	1	-	0/6/23/26	0/1/1/1
4	NAG	C	601	1	-	2/6/23/26	0/1/1/1
4	NAG	B	702	1	-	6/6/23/26	0/1/1/1
4	NAG	B	708	1	-	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	NAG	C1-C2	2.49	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	610	NAG	C1-O5-C5	6.65	121.11	112.19
4	B	708	NAG	C2-N2-C7	4.71	129.21	122.90
4	B	702	NAG	C2-N2-C7	4.64	129.12	122.90
4	C	610	NAG	C2-N2-C7	3.08	127.03	122.90
4	C	610	NAG	C3-C4-C5	2.73	115.19	110.23
4	C	610	NAG	O3-C3-C2	2.72	115.05	109.40
4	C	610	NAG	C1-C2-N2	2.43	114.27	110.43
4	C	601	NAG	C1-O5-C5	2.37	115.36	112.19
4	B	708	NAG	C1-C2-N2	2.29	114.05	110.43
4	B	702	NAG	C1-C2-N2	2.26	114.00	110.43
4	B	708	NAG	C1-O5-C5	2.20	115.13	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	709	NAG	O5-C5-C6-O6
4	A	611	NAG	O5-C5-C6-O6
4	B	709	NAG	C4-C5-C6-O6

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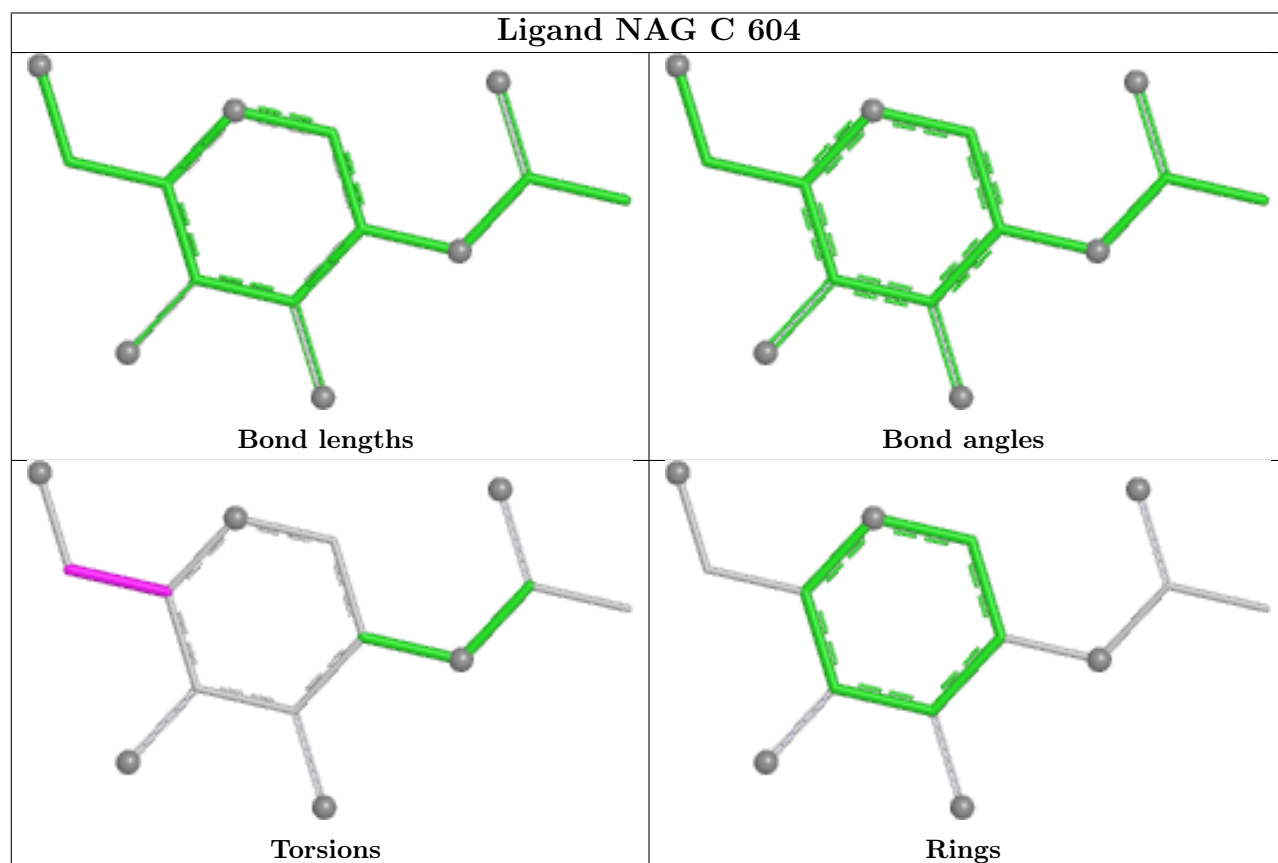
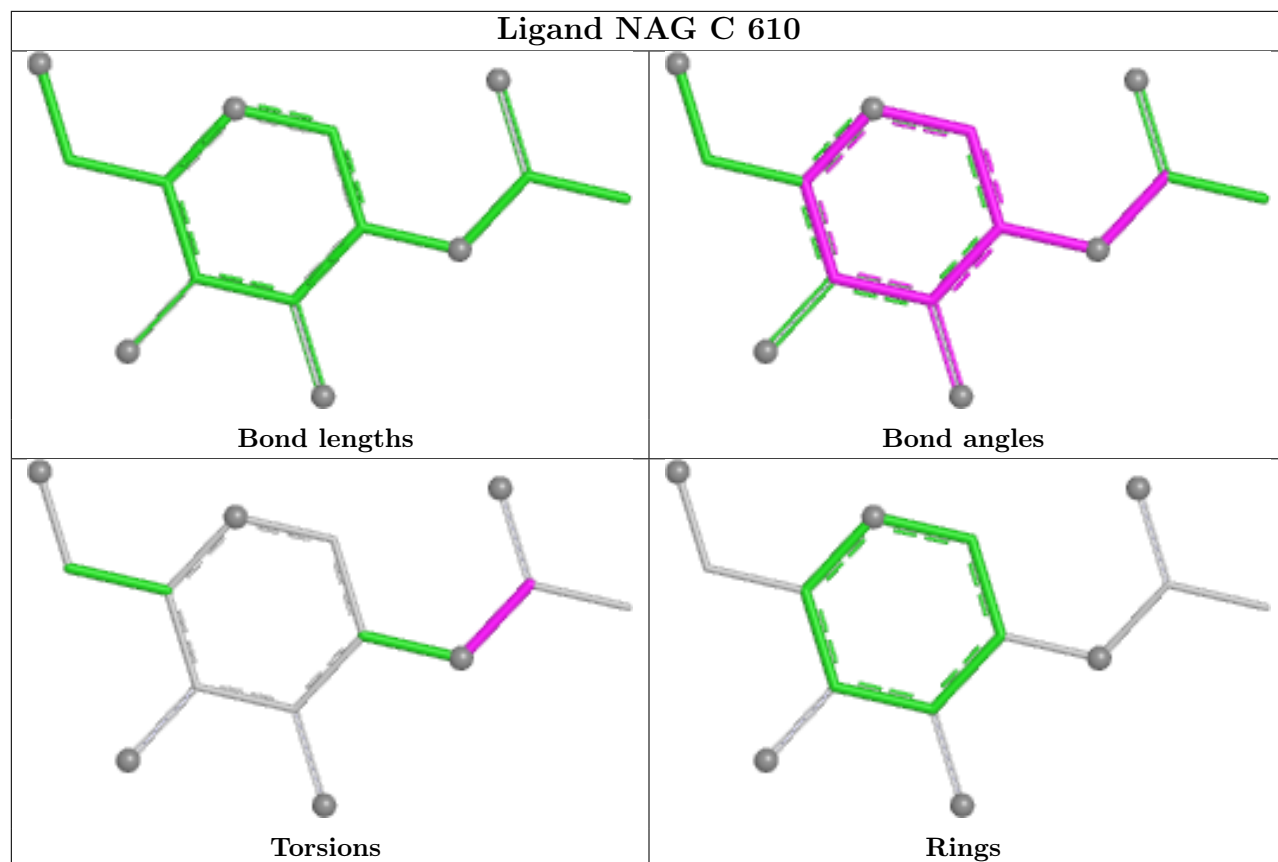
Mol	Chain	Res	Type	Atoms
4	B	702	NAG	C8-C7-N2-C2
4	B	702	NAG	O7-C7-N2-C2
4	B	708	NAG	C8-C7-N2-C2
4	B	708	NAG	O7-C7-N2-C2
4	C	610	NAG	C8-C7-N2-C2
4	C	610	NAG	O7-C7-N2-C2
4	A	611	NAG	C4-C5-C6-O6
4	B	702	NAG	C4-C5-C6-O6
4	B	702	NAG	O5-C5-C6-O6
4	B	708	NAG	O5-C5-C6-O6
4	C	604	NAG	O5-C5-C6-O6
4	C	601	NAG	C4-C5-C6-O6
4	C	601	NAG	O5-C5-C6-O6
4	B	708	NAG	C1-C2-N2-C7
4	B	702	NAG	C3-C2-N2-C7
4	B	702	NAG	C1-C2-N2-C7
4	B	708	NAG	C3-C2-N2-C7

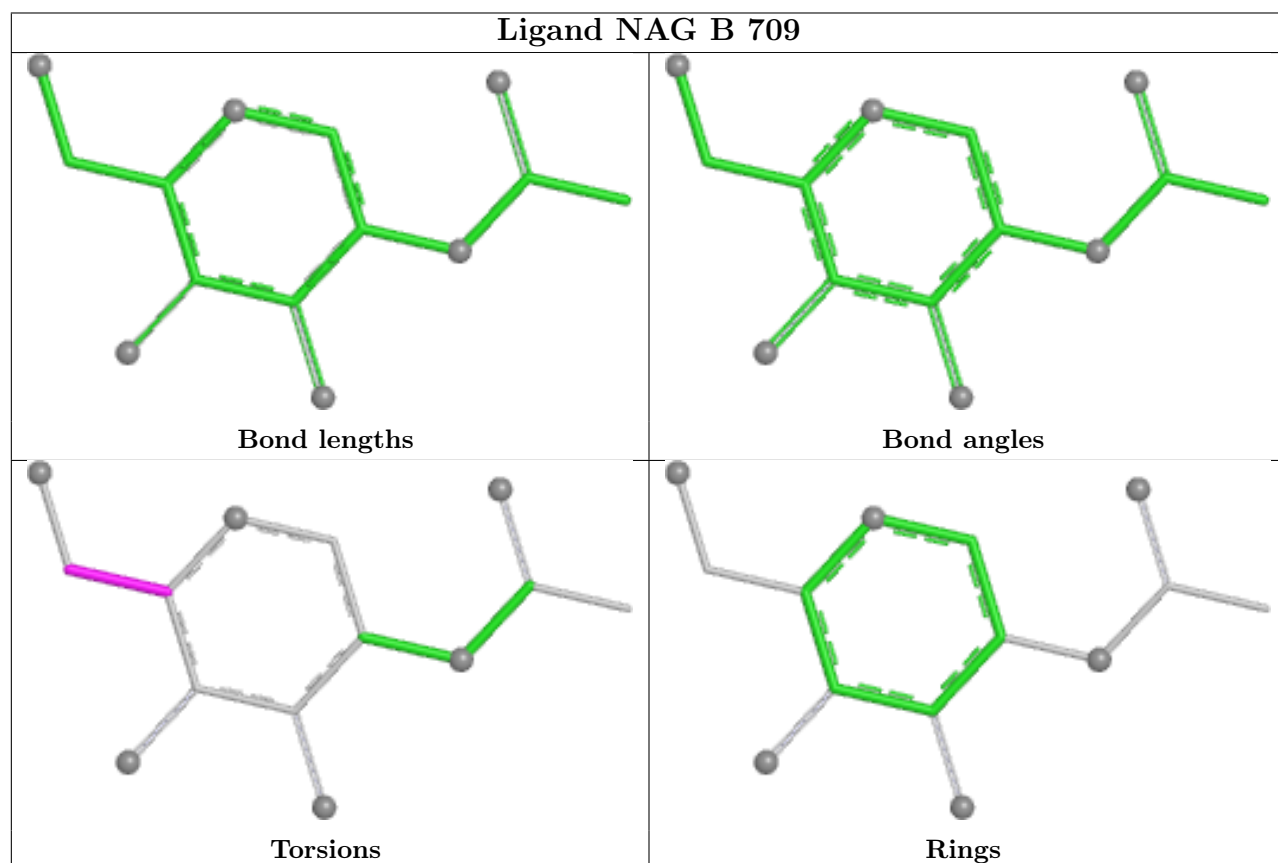
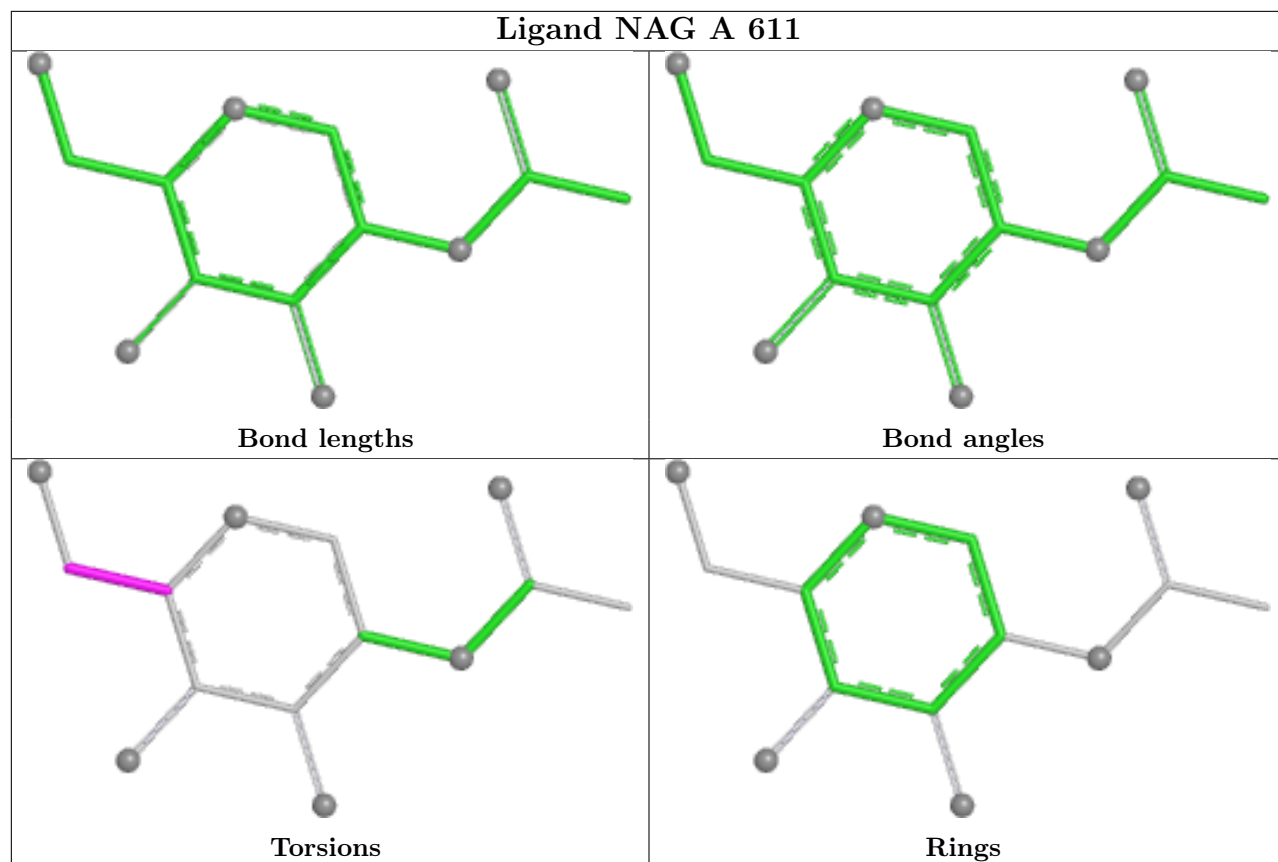
There are no ring outliers.

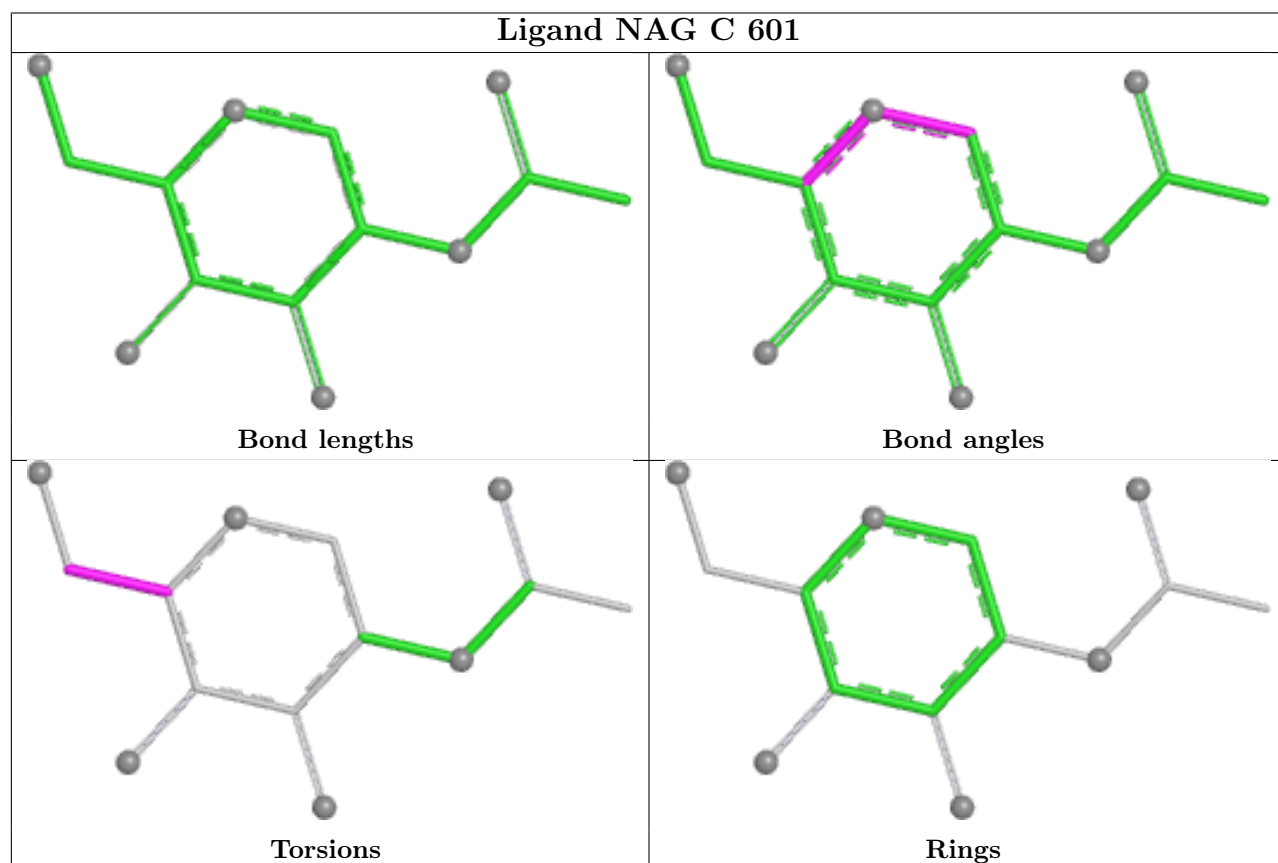
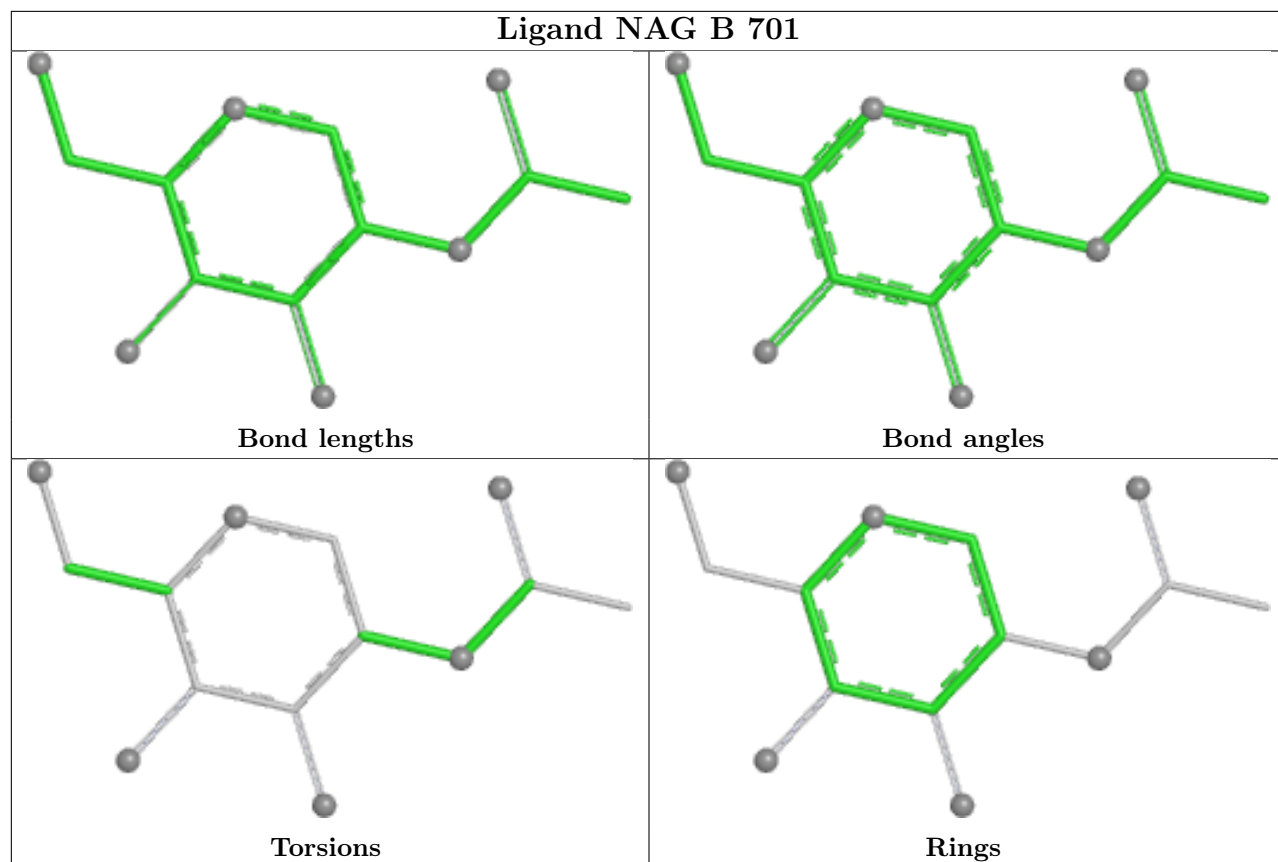
4 monomers are involved in 4 short contacts:

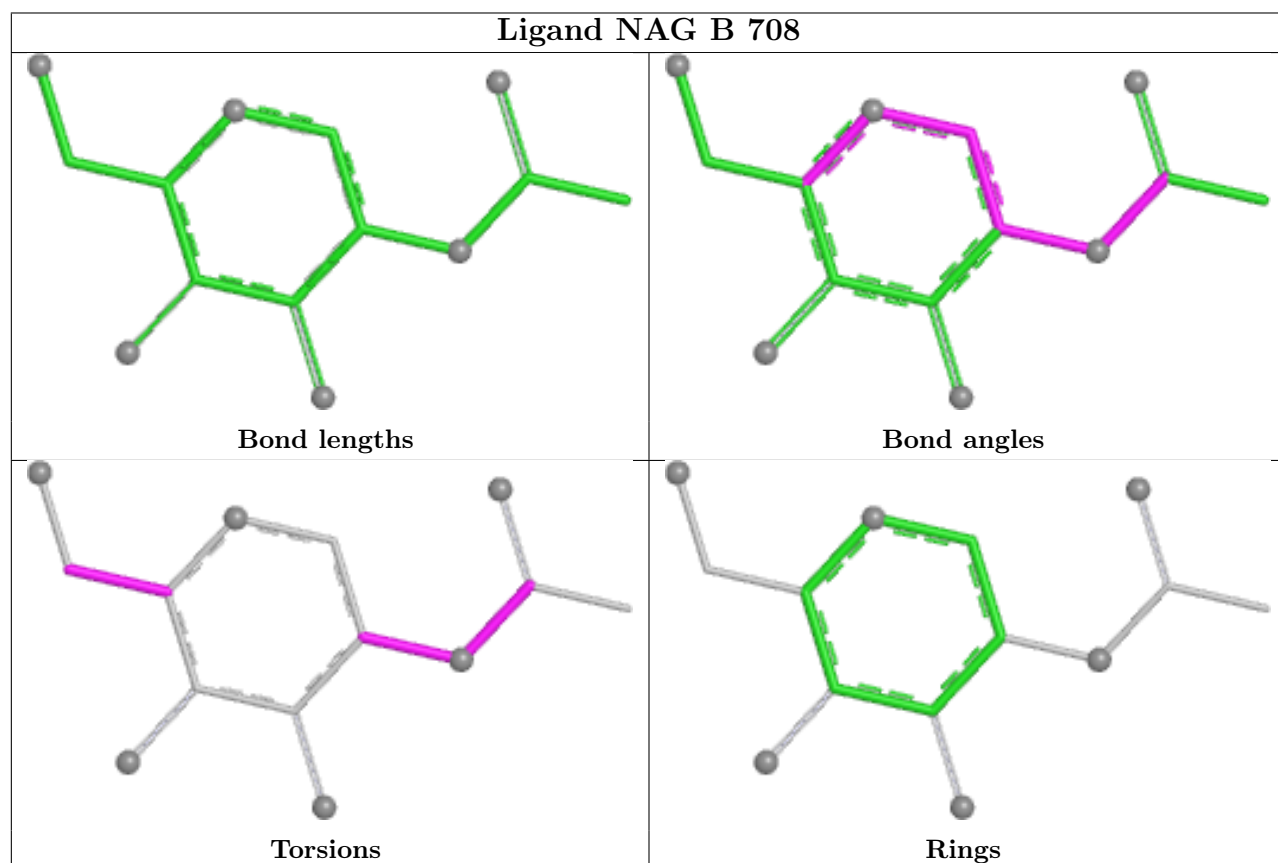
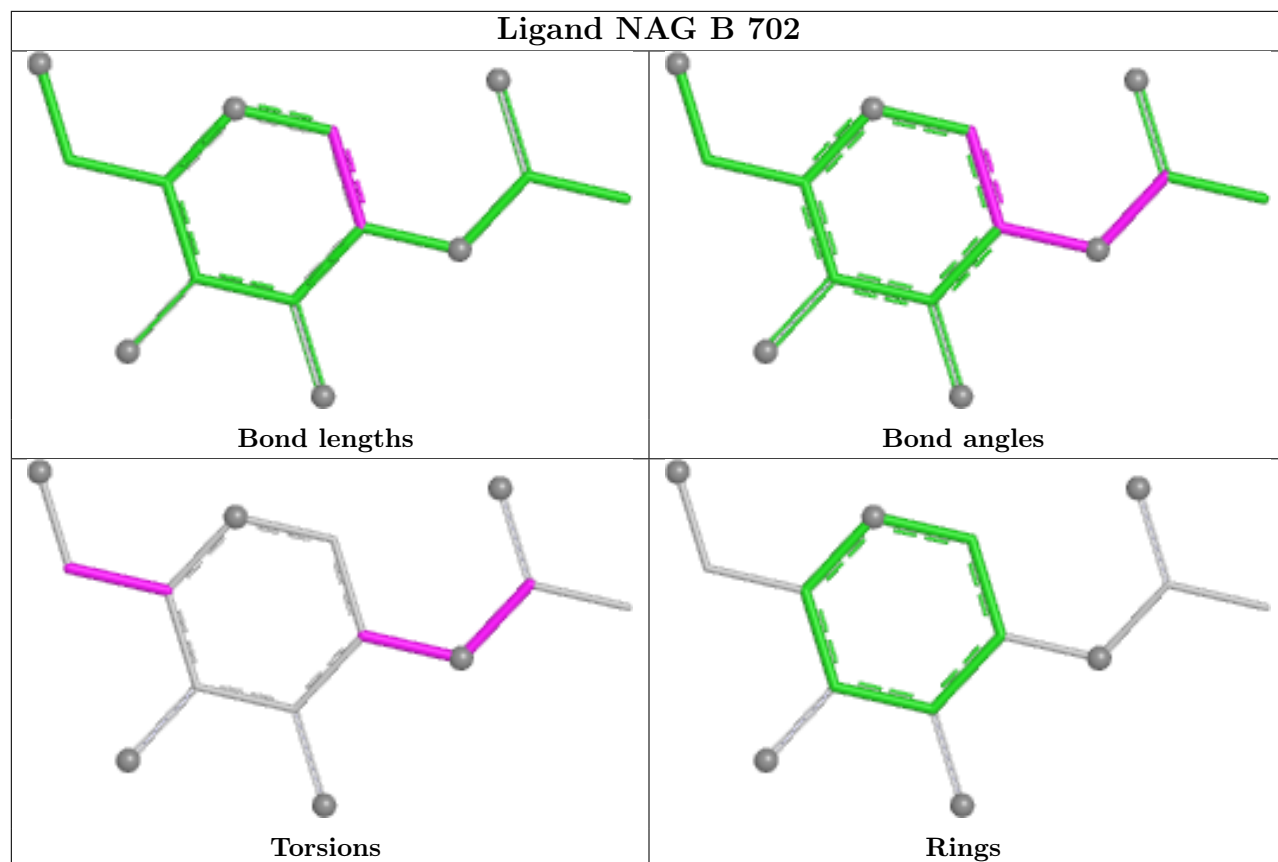
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	611	NAG	1	0
4	B	709	NAG	1	0
4	B	702	NAG	1	0
4	B	708	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	486/497 (97%)	0.85	59 (12%) 8 7	47, 74, 107, 124	0
1	B	486/497 (97%)	0.82	46 (9%) 14 11	47, 74, 107, 131	0
1	C	487/497 (97%)	1.19	80 (16%) 4 3	51, 94, 125, 155	0
All	All	1459/1491 (97%)	0.95	185 (12%) 8 6	47, 78, 118, 155	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	502	ILE	7.6
1	C	402	VAL	7.0
1	B	387	LYS	5.9
1	C	387	LYS	5.5
1	A	502	ILE	5.5
1	C	333	GLY	5.4
1	B	502	ILE	5.4
1	A	387	LYS	5.4
1	B	341	ASN	5.3
1	B	336	ALA	5.2
1	A	324	PRO	4.8
1	C	213	VAL	4.7
1	C	404	GLY	4.7
1	A	196	ILE	4.5
1	C	277	CYS	4.4
1	B	222	TRP	4.4
1	C	341	ASN	4.4
1	B	174	PHE	4.3
1	B	402	VAL	4.3
1	C	199	SER	4.3
1	C	222	TRP	4.3
1	A	30	THR	4.3
1	C	30	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	174	PHE	4.2
1	C	48	THR	4.2
1	C	96	ASN	4.2
1	C	128	THR	4.1
1	A	50	ARG	4.0
1	C	324	PRO	4.0
1	B	334	ALA	4.0
1	C	340	GLU	3.9
1	C	501	GLN	3.9
1	B	388	THR	3.9
1	A	128	THR	3.9
1	C	248	THR	3.9
1	B	324	PRO	3.8
1	B	338	PHE	3.8
1	A	208	ARG	3.8
1	A	222	TRP	3.8
1	B	367	LEU	3.7
1	A	137	TYR	3.7
1	A	385	ILE	3.6
1	B	398	GLU	3.6
1	A	388	THR	3.5
1	C	403	GLU	3.5
1	B	400	SER	3.5
1	A	489	ASP	3.3
1	B	189	LYS	3.3
1	B	8	ASN	3.2
1	B	337	GLY	3.2
1	A	348	ASP	3.1
1	C	155	TYR	3.1
1	A	114	SER	3.1
1	A	31	ASN	3.1
1	C	247	SER	3.1
1	A	277	CYS	3.1
1	C	52	CYS	3.1
1	C	161	TYR	3.0
1	B	48	THR	3.0
1	C	137	TYR	3.0
1	C	144	ASN	3.0
1	A	390	GLU	2.9
1	C	219	SER	2.9
1	B	401	GLU	2.9
1	C	262	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	391	LYS	2.9
1	A	500	PHE	2.9
1	A	188	ASP	2.9
1	A	198	ALA	2.9
1	C	198	ALA	2.9
1	B	340	GLU	2.8
1	C	217	ILE	2.8
1	A	280	GLU	2.8
1	C	391	LYS	2.8
1	B	128	THR	2.8
1	B	137	TYR	2.8
1	B	31	ASN	2.8
1	A	393	HIS	2.8
1	B	196	ILE	2.7
1	C	196	ILE	2.7
1	C	163	VAL	2.7
1	B	262	THR	2.7
1	A	262	THR	2.7
1	C	139	CYS	2.7
1	C	224	ARG	2.7
1	C	143	SER	2.7
1	C	421	TRP	2.7
1	C	264	LYS	2.6
1	C	145	ASN	2.6
1	A	399	PHE	2.6
1	A	501	GLN	2.6
1	B	30	THR	2.6
1	C	192	THR	2.6
1	C	388	THR	2.6
1	B	142	GLY	2.6
1	C	179	ILE	2.6
1	C	50	ARG	2.6
1	C	188	ASP	2.6
1	A	367	LEU	2.6
1	C	367	LEU	2.6
1	C	23	GLY	2.5
1	B	335	ILE	2.5
1	C	390	GLU	2.5
1	C	472	LYS	2.5
1	C	386	GLU	2.5
1	C	301	THR	2.5
1	A	174	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	406	ILE	2.5
1	A	391	LYS	2.5
1	C	464	ASN	2.5
1	A	199	SER	2.5
1	A	172	GLY	2.4
1	C	438	ASP	2.4
1	A	278	SER	2.4
1	A	173	LYS	2.4
1	A	8	ASN	2.4
1	A	341	ASN	2.4
1	A	264	LYS	2.4
1	C	259	LYS	2.4
1	A	263	GLY	2.4
1	C	393	HIS	2.4
1	B	201	ARG	2.4
1	B	143	SER	2.3
1	C	9	SER	2.3
1	A	142	GLY	2.3
1	A	52	CYS	2.3
1	A	334	ALA	2.3
1	C	104	ASP	2.3
1	C	175	ASP	2.3
1	A	189	LYS	2.3
1	B	390	GLU	2.3
1	C	401	GLU	2.3
1	C	197	ARG	2.3
1	C	124	GLY	2.3
1	A	386	GLU	2.3
1	A	392	PHE	2.3
1	A	20	VAL	2.3
1	B	304	ALA	2.2
1	C	31	ASN	2.2
1	B	393	HIS	2.2
1	C	132	GLN	2.2
1	C	214	ILE	2.2
1	C	94	PHE	2.2
1	B	501	GLN	2.2
1	C	230	ILE	2.2
1	C	242	ILE	2.2
1	C	406	ILE	2.2
1	A	402	VAL	2.2
1	A	48	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	195	TYR	2.2
1	C	125	PHE	2.2
1	A	140	LYS	2.2
1	B	356	GLN	2.2
1	A	305	CYS	2.2
1	A	345	GLY	2.2
1	A	95	SER	2.2
1	B	9	SER	2.2
1	B	322	ASN	2.1
1	C	216	ASN	2.1
1	C	356	GLN	2.1
1	B	29	ILE	2.1
1	C	76	CYS	2.1
1	B	216	ASN	2.1
1	B	362	GLY	2.1
1	C	14	CYS	2.1
1	C	8	ASN	2.1
1	C	220	ARG	2.1
1	B	98	TYR	2.1
1	A	358	SER	2.1
1	A	56	HIS	2.1
1	C	347	VAL	2.1
1	C	399	PHE	2.1
1	B	381	LEU	2.1
1	A	368	LYS	2.1
1	B	173	LYS	2.1
1	A	139	CYS	2.1
1	C	64	CYS	2.1
1	A	381	LEU	2.0
1	B	483	ASN	2.0
1	C	164	LEU	2.0
1	A	415	ASP	2.0
1	A	493	ASP	2.0
1	A	400	SER	2.0
1	B	50	ARG	2.0
1	C	82	GLU	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 [i](#)

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

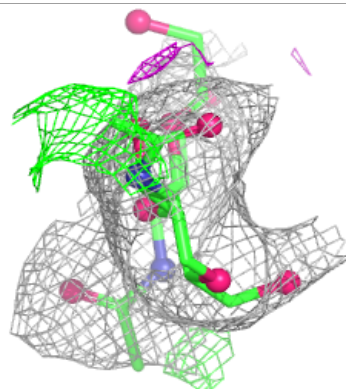
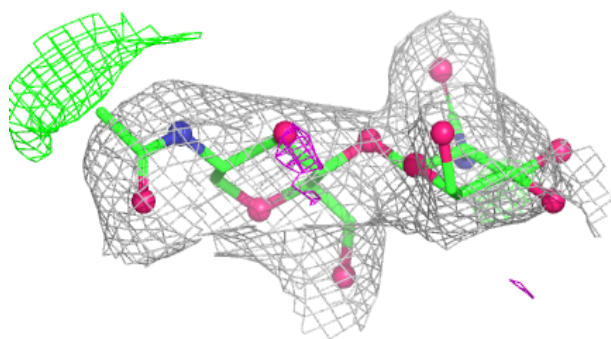
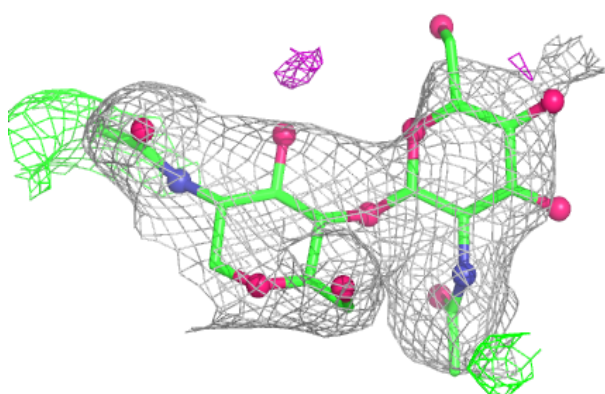
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	G	3	11/12	0.36	0.23	130,165,172,176	0
2	NAG	E	2	14/15	0.38	0.24	164,180,185,186	0
3	BMA	O	3	11/12	0.46	0.25	156,186,215,239	0
3	BMA	M	3	11/12	0.48	0.22	110,121,132,138	0
2	NAG	L	1	14/15	0.48	0.24	92,119,136,143	0
3	BMA	Q	3	11/12	0.49	0.23	137,168,177,180	0
3	BMA	I	3	11/12	0.51	0.21	143,166,169,172	0
3	BMA	F	3	11/12	0.51	0.26	127,161,164,166	0
3	BMA	J	3	11/12	0.58	0.18	130,144,150,155	0
2	NAG	H	2	14/15	0.60	0.19	124,158,169,175	0
2	NAG	K	2	14/15	0.60	0.20	163,176,185,192	0
2	NAG	N	2	14/15	0.62	0.17	129,163,174,177	0
2	NAG	D	2	14/15	0.64	0.17	107,154,167,169	0
2	NAG	L	2	14/15	0.65	0.16	97,144,153,154	0
2	NAG	P	2	14/15	0.68	0.21	172,181,195,199	0
2	NAG	K	1	14/15	0.73	0.21	91,128,144,158	0
3	NAG	I	2	14/15	0.75	0.21	121,142,156,165	0
2	NAG	D	1	14/15	0.76	0.17	92,113,128,145	0
3	NAG	O	1	14/15	0.77	0.20	105,120,137,140	0
3	NAG	Q	2	14/15	0.78	0.16	134,144,150,155	0
2	NAG	P	1	14/15	0.80	0.16	95,111,130,154	0
3	NAG	I	1	14/15	0.81	0.23	91,111,123,124	0
3	NAG	Q	1	14/15	0.83	0.15	103,122,135,136	0
3	NAG	M	2	14/15	0.83	0.17	79,104,122,123	0
3	NAG	F	2	14/15	0.83	0.17	71,128,147,161	0
2	NAG	N	1	14/15	0.86	0.12	109,126,144,159	0
3	NAG	F	1	14/15	0.86	0.16	74,84,95,110	0
3	NAG	O	2	14/15	0.88	0.20	146,157,184,249	0
2	NAG	H	1	14/15	0.89	0.12	72,99,121,138	0
3	NAG	M	1	14/15	0.89	0.17	48,73,99,134	0
2	NAG	E	1	14/15	0.91	0.12	91,113,132,153	0
3	NAG	G	1	14/15	0.92	0.10	63,85,94,99	0
3	NAG	G	2	14/15	0.92	0.15	96,120,147,156	0
3	NAG	J	1	14/15	0.93	0.11	57,70,89,96	0
3	NAG	J	2	14/15	0.95	0.11	77,88,101,109	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.

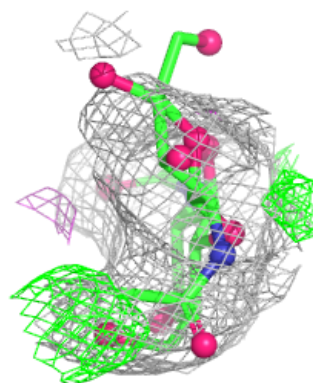
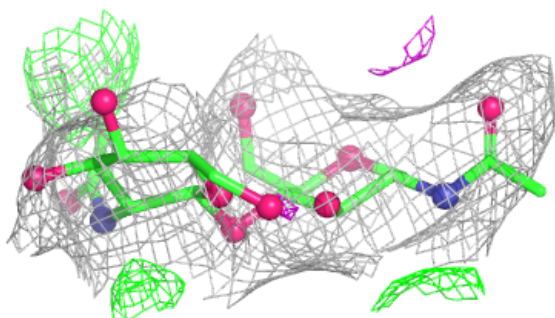
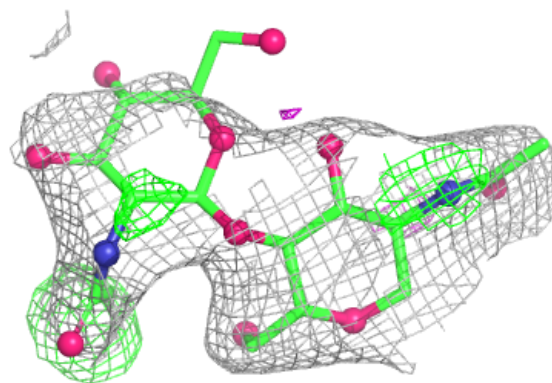
Electron density around Chain D:

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



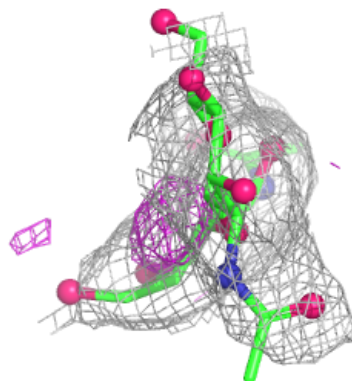
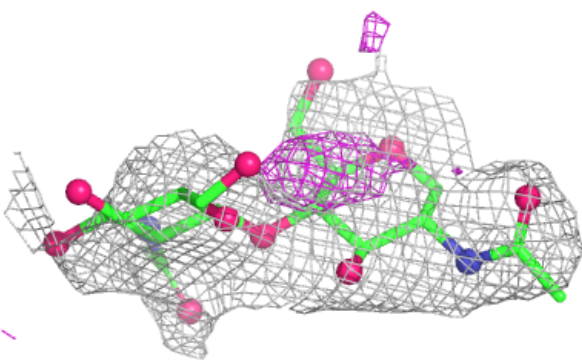
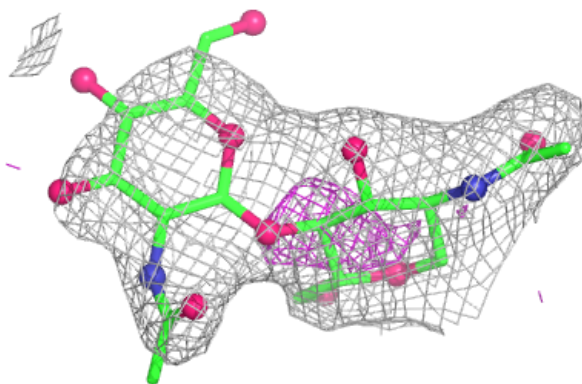
Electron density around Chain E:

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



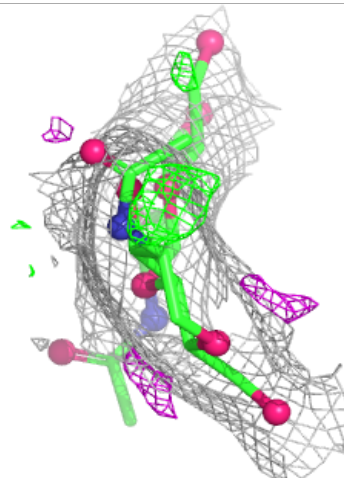
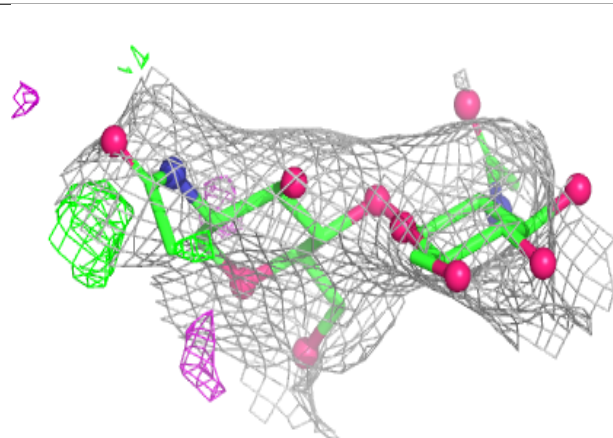
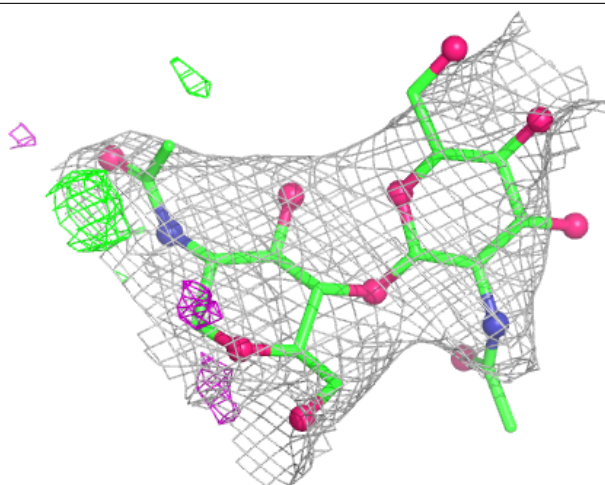
Electron density around Chain H:

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



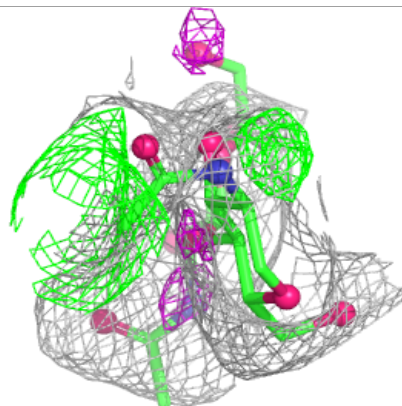
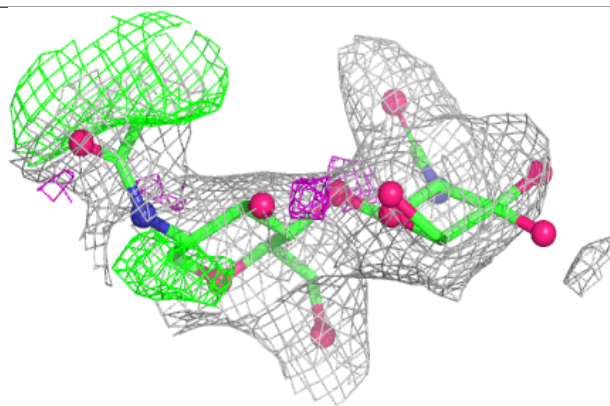
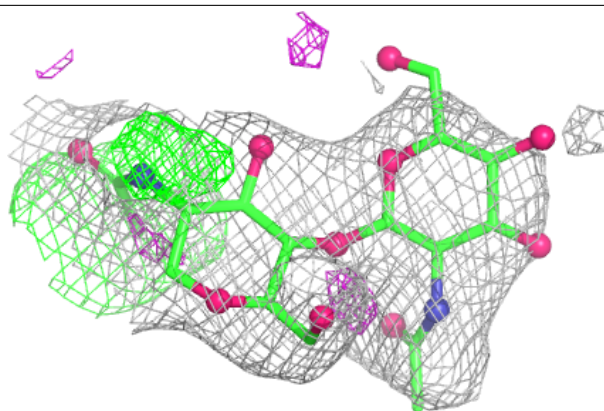
Electron density around Chain K:

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



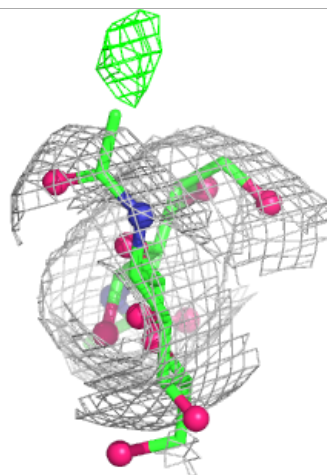
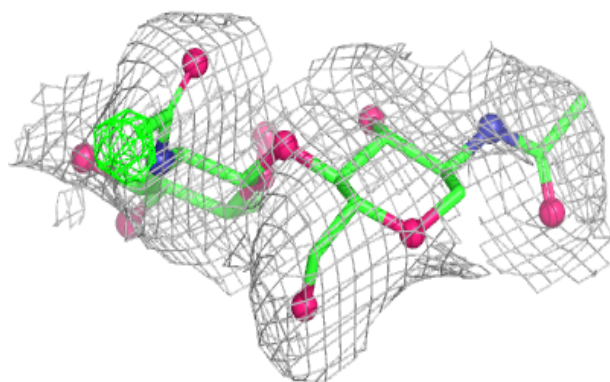
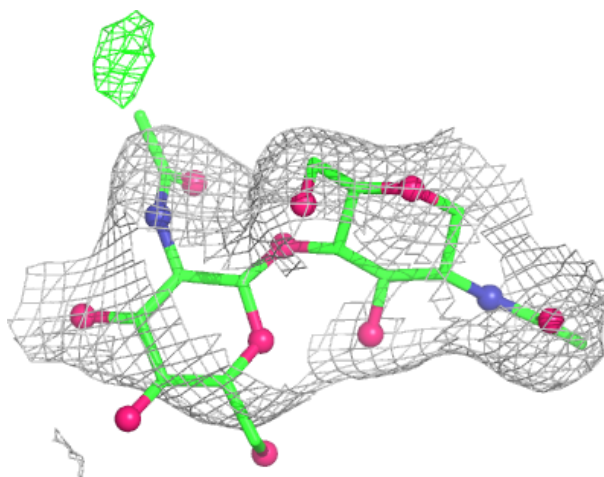
Electron density around Chain L:

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



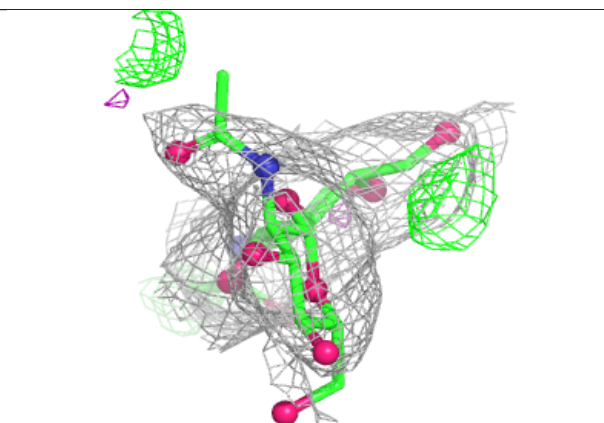
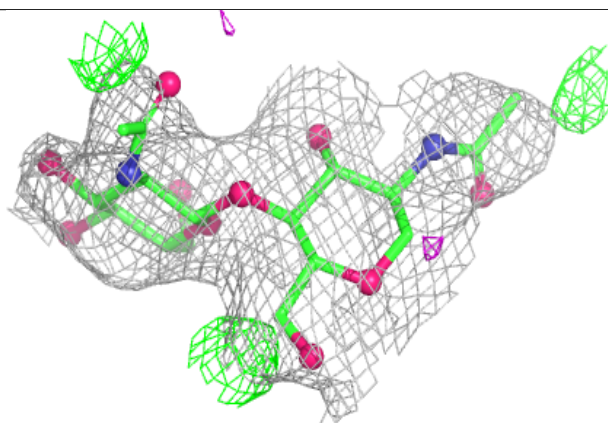
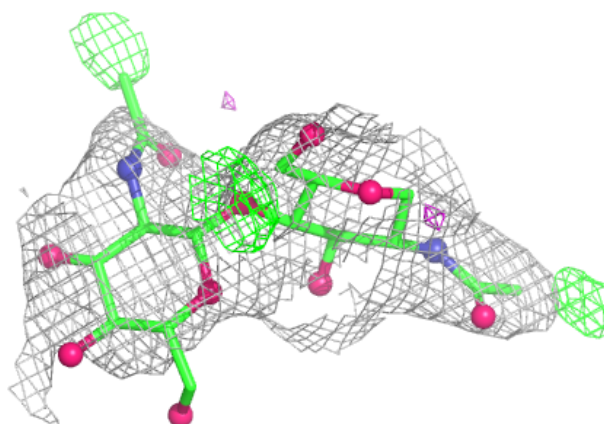
Electron density around Chain N:

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

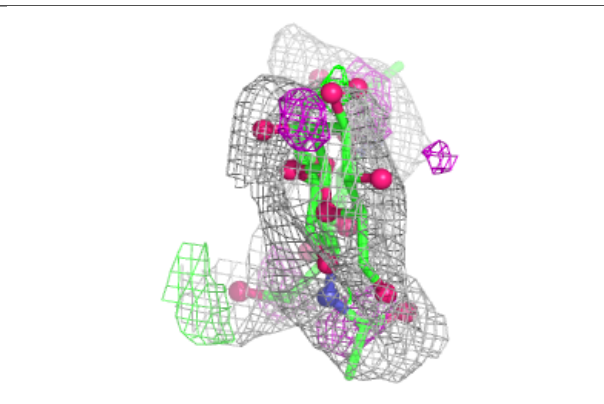
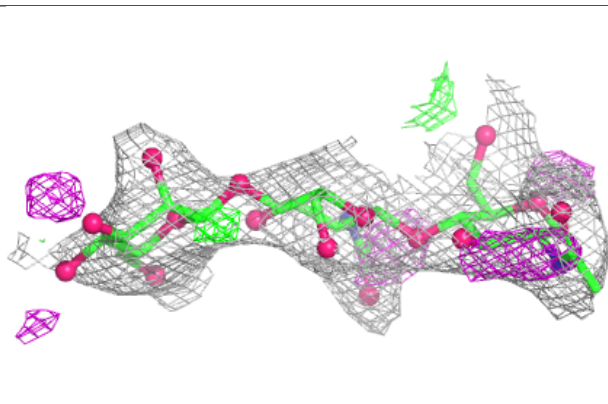
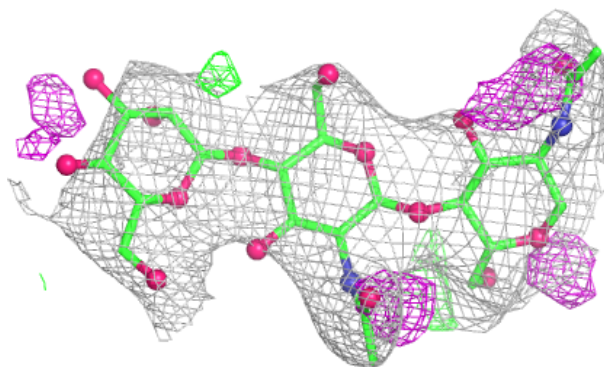


Electron density around Chain P:

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

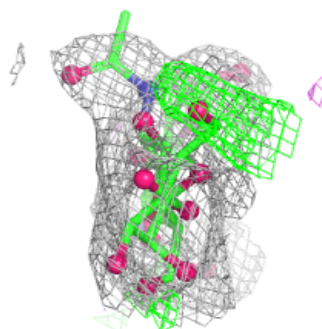
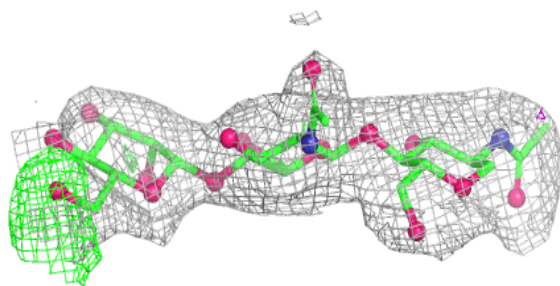
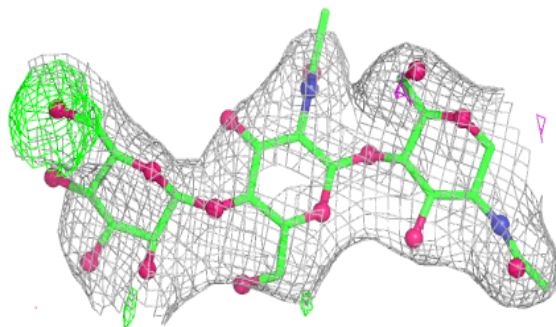
**Electron density around Chain F:**

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

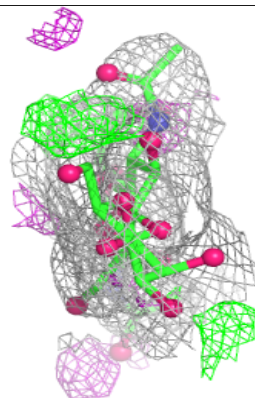
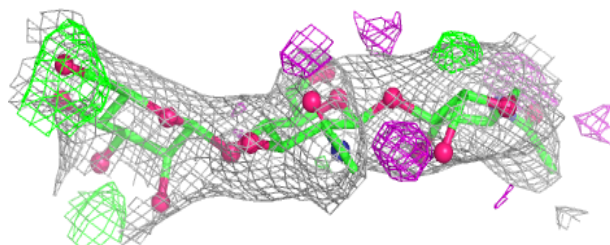
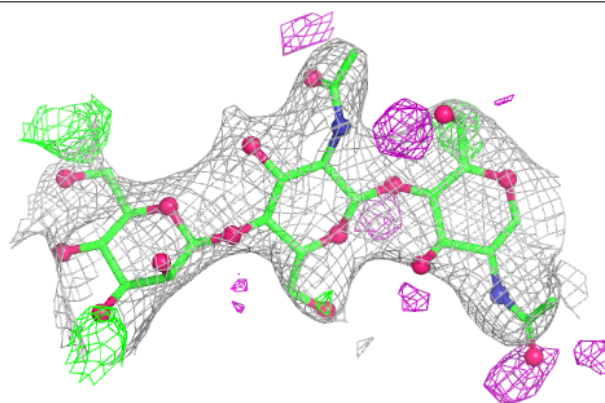


Electron density around Chain G:

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

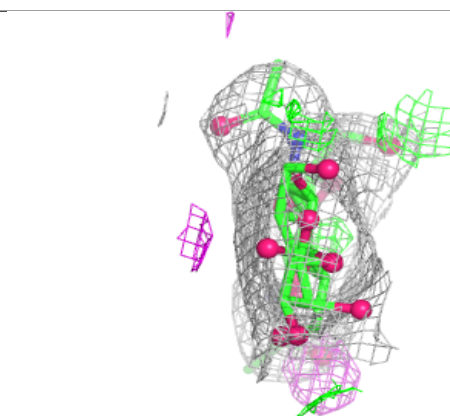
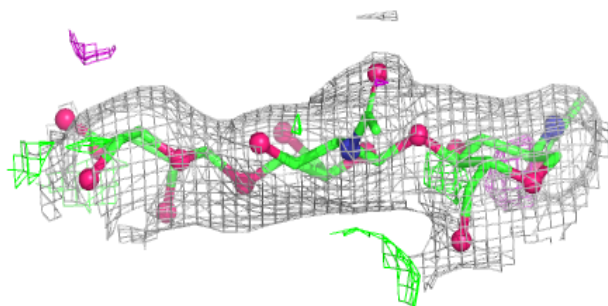
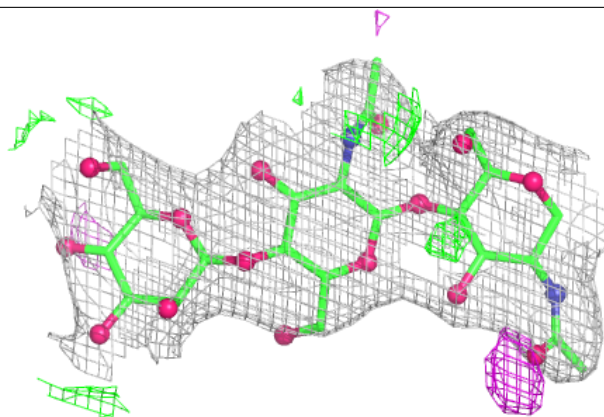
**Electron density around Chain I:**

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

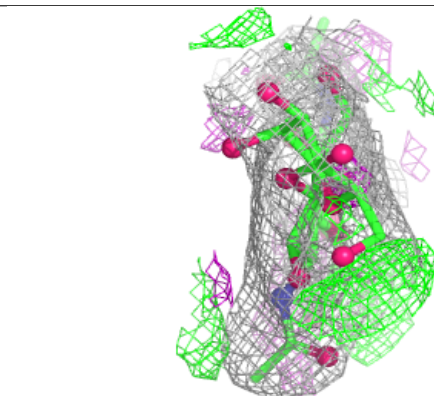
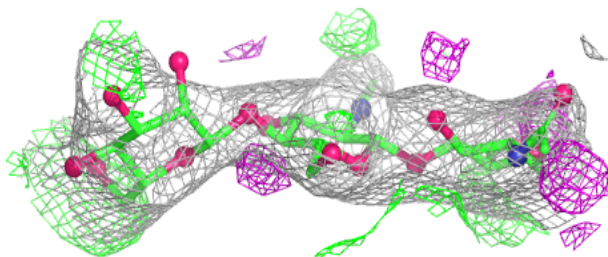
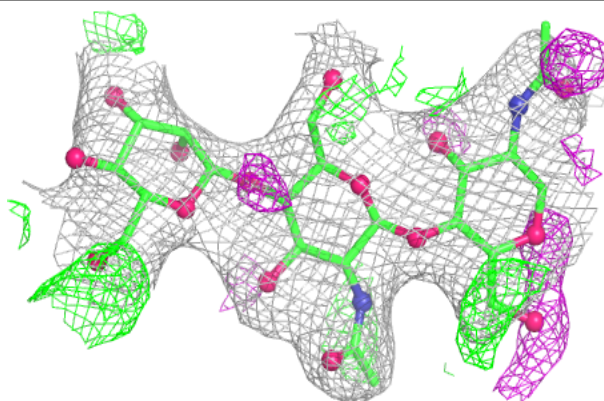


Electron density around Chain J:

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

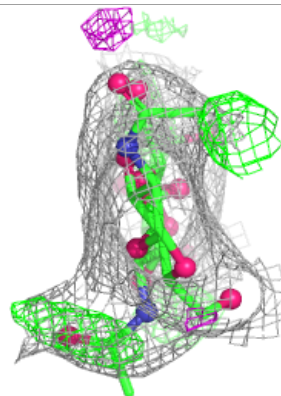
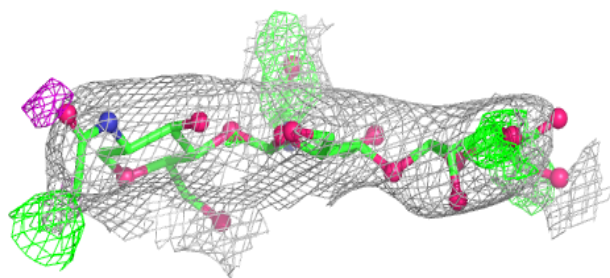
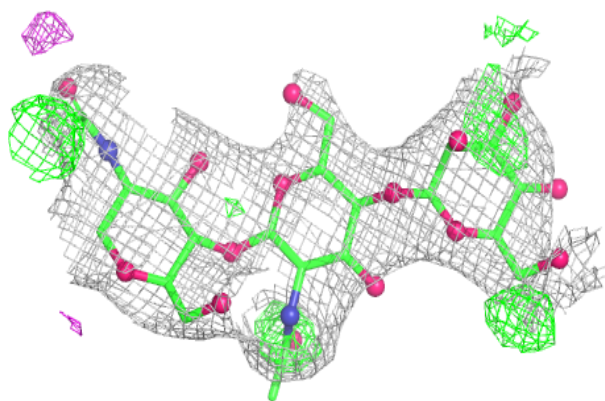
**Electron density around Chain M:**

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

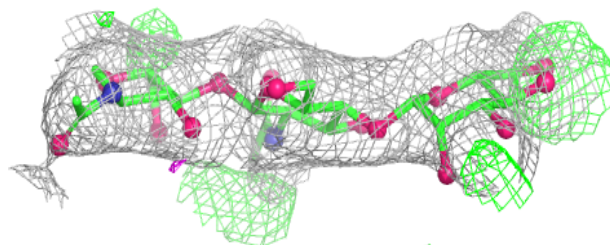
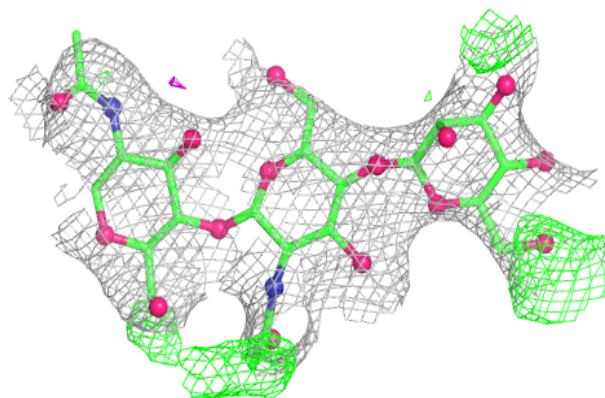


Electron density around Chain O:

$2mF_o-DF_c$ (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)

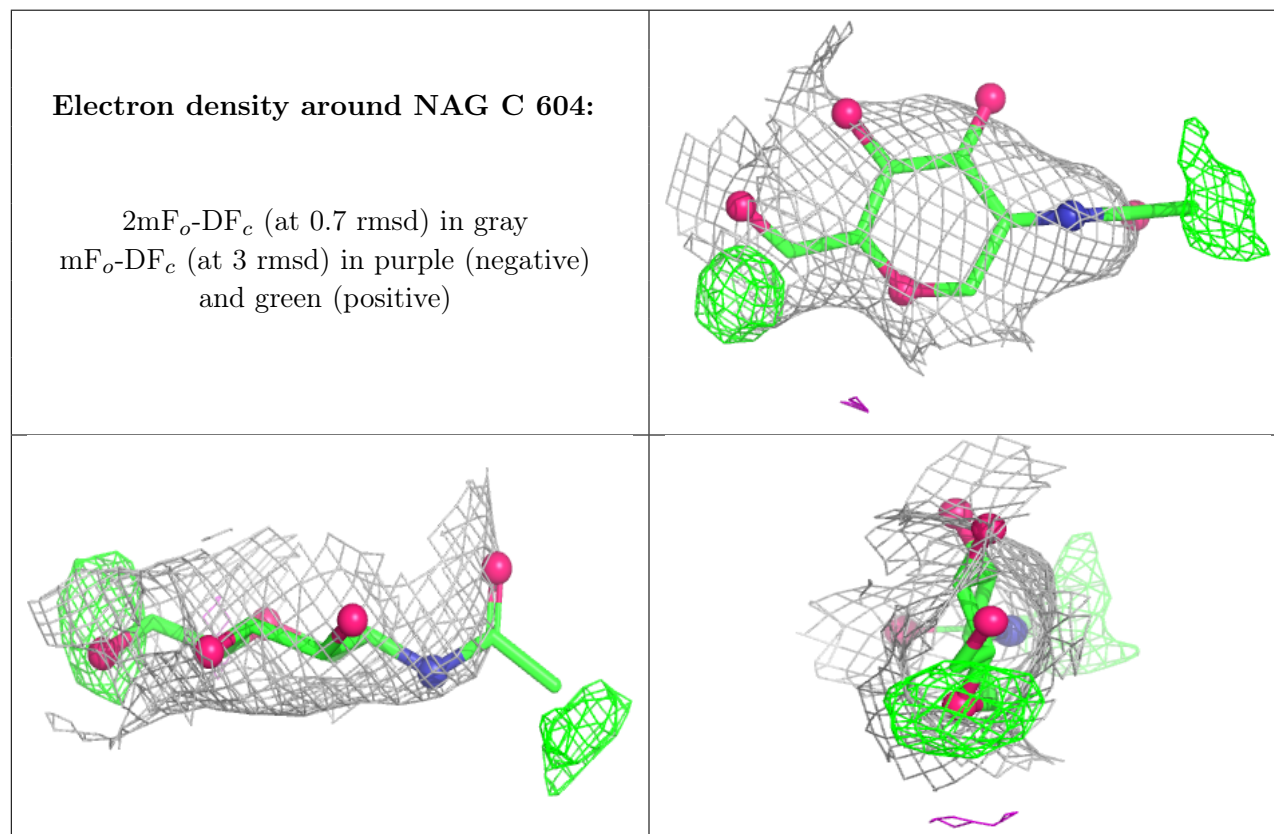


6.4 Ligands [i](#)

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

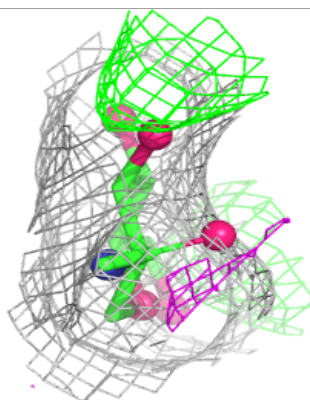
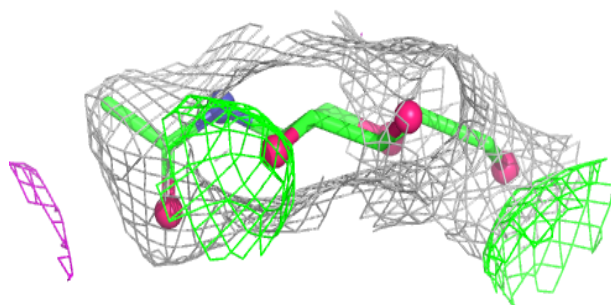
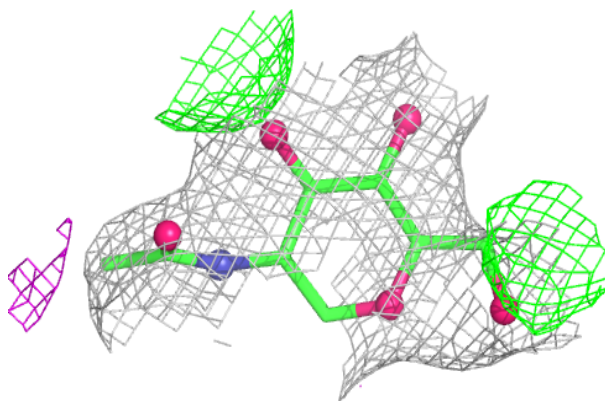
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	604	14/15	0.37	0.21	154,165,176,179	0
4	NAG	B	709	14/15	0.50	0.19	103,136,142,143	0
4	NAG	B	702	14/15	0.58	0.21	104,139,156,158	0
4	NAG	C	601	14/15	0.68	0.22	97,125,133,134	0
4	NAG	B	708	14/15	0.68	0.23	116,134,153,157	0
4	NAG	A	611	14/15	0.74	0.21	106,120,130,132	0
4	NAG	C	610	14/15	0.77	0.24	138,169,174,180	0
4	NAG	B	701	14/15	0.87	0.13	66,93,103,106	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.

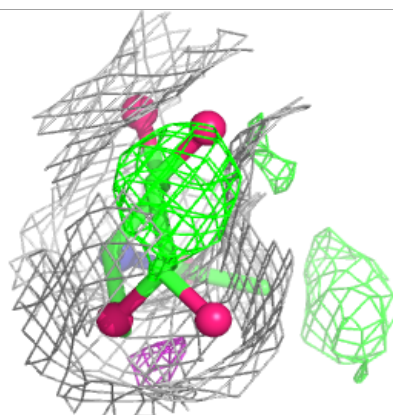
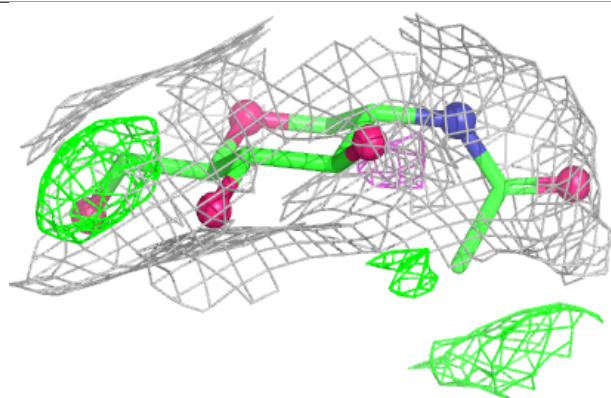
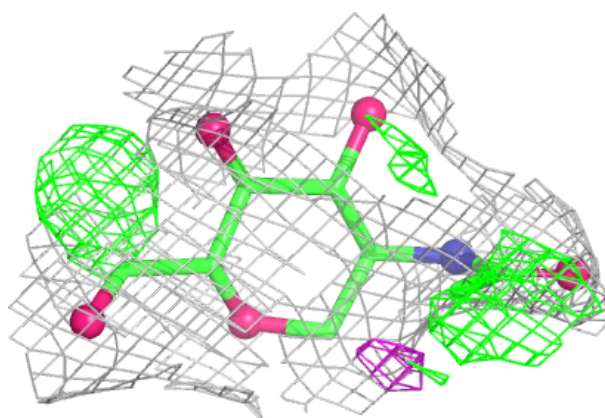


Electron density around NAG B 709:

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

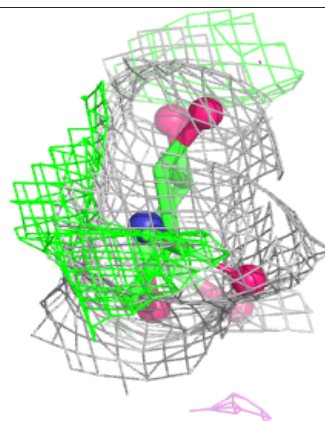
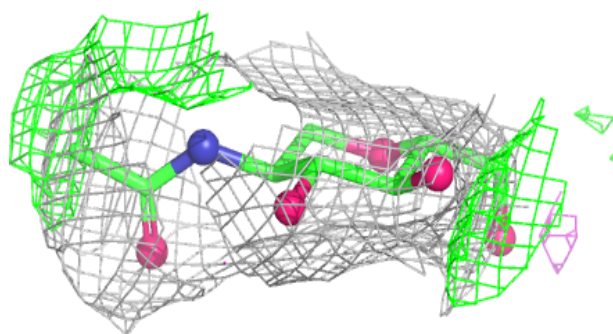
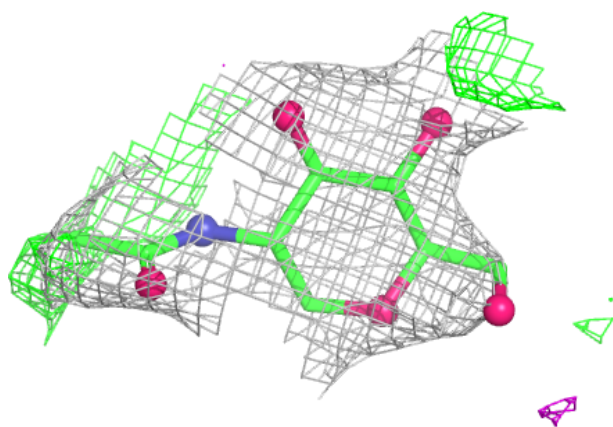
**Electron density around NAG B 702:**

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

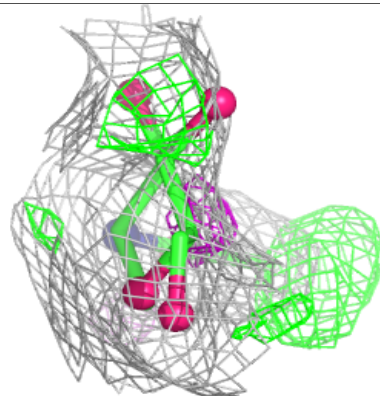
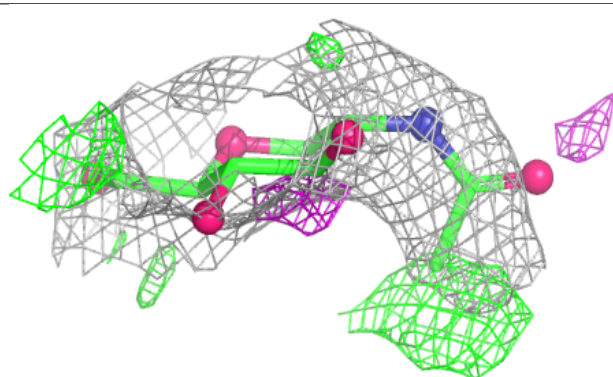
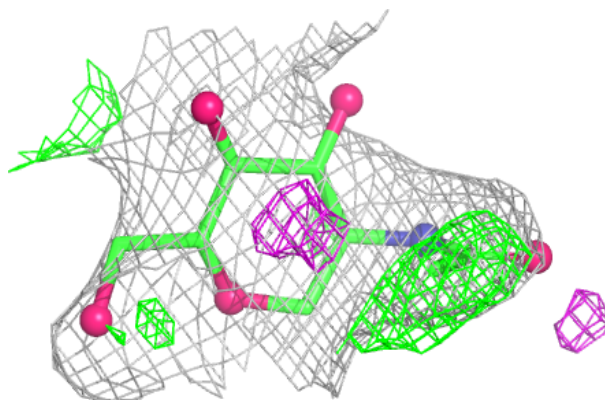


Electron density around NAG C 601:

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

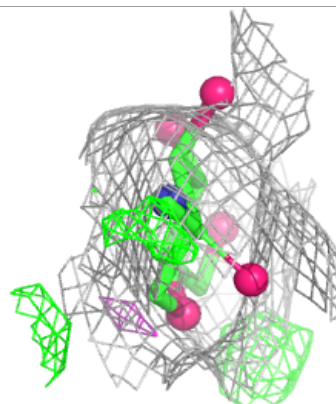
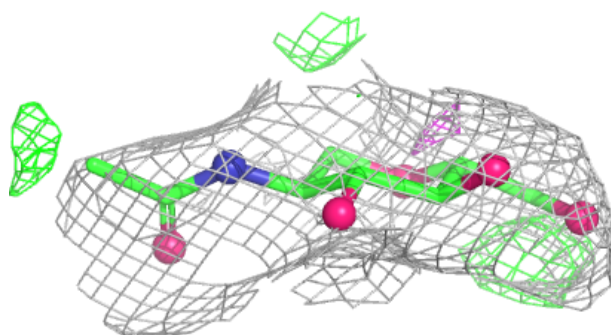
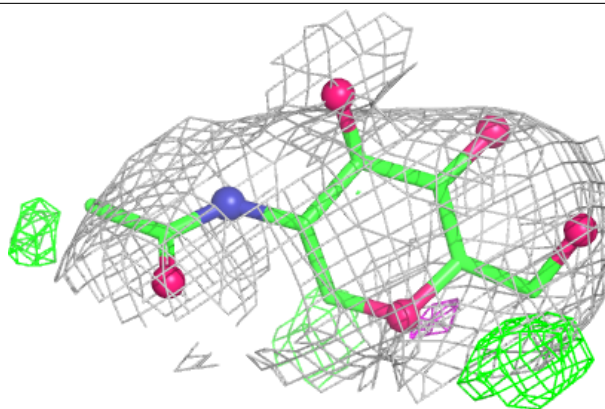
**Electron density around NAG B 708:**

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

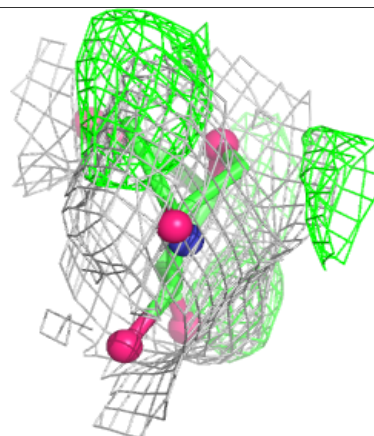
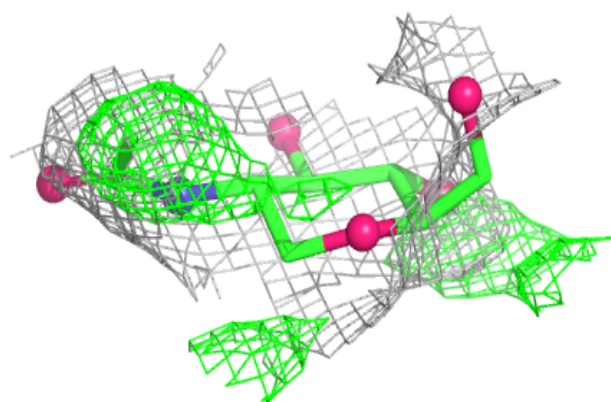
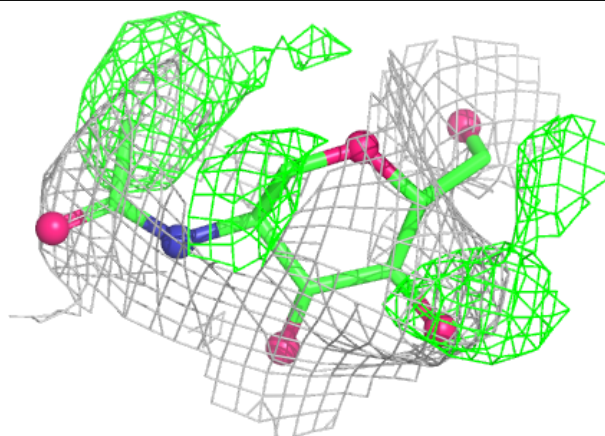


Electron density around NAG A 611:

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

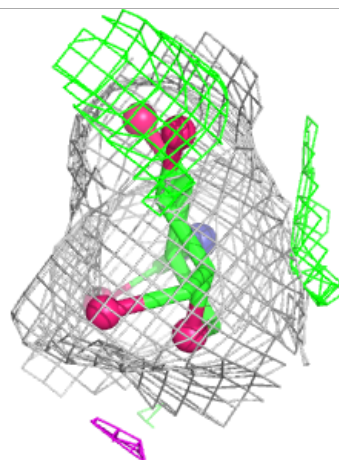
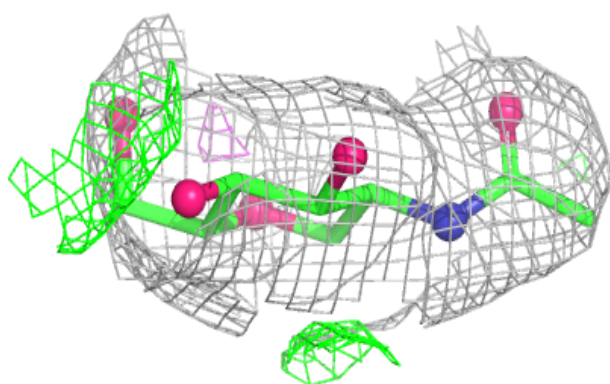
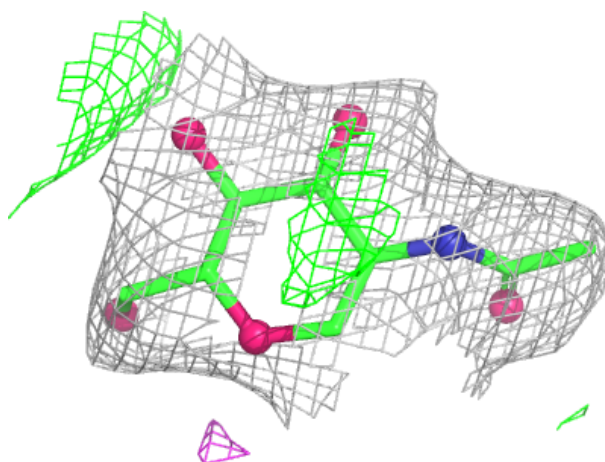
**Electron density around NAG C 610:**

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



Electron density around NAG B 701:

$2mF_o-DF_c$ (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.