



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 20, 2026 – 07:06 PM JST

PDB ID : 9W1S / pdb_00009w1s
Title : Crystal structure of AtNUT-AtBAK1-AtSCREW1
Authors : Wan, L.H.
Deposited on : 2025-07-26
Resolution : 3.40 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:

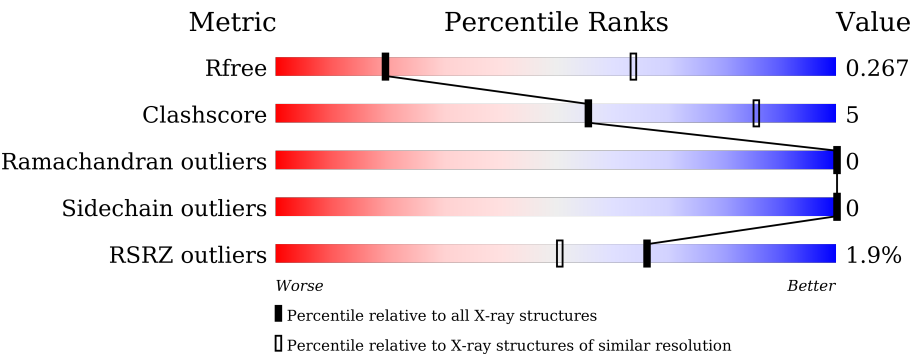
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



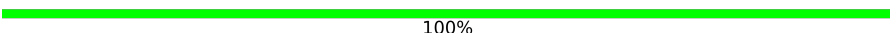
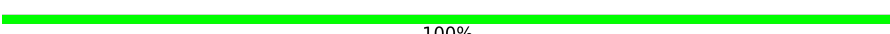
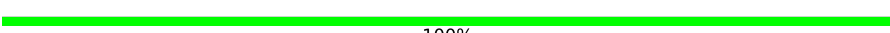
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	634	79%14%7%
1	D	634	81%11%8%
2	B	230	67%10%23%
2	E	230	71%6%23%
3	C	43	9%47%12%42%
3	F	43	7%44%14%42%

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Mol	Chain	Length	Quality of chain
4	G	2	 50%50%
4	H	2	 50%50%
4	I	2	 100%
4	J	2	 50%50%
4	L	2	 100%
4	M	2	 100%
4	N	2	 100%
4	O	2	 100%
5	K	5	 20%60%20%
6	P	6	 67%33%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12776 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 AT5G25930 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	0
			4587	2921	749	905	12			
1	D	586	Total	C	N	O	S	0	0	0
			4558	2906	743	896	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ARG	ASN	conflict	UNP B9DFY2
A	529	ASP	LYS	conflict	UNP B9DFY2
A	531	ASP	LYS	conflict	UNP B9DFY2
A	555	SER	GLN	conflict	UNP B9DFY2
A	629	HIS	-	expression tag	UNP B9DFY2
A	630	HIS	-	expression tag	UNP B9DFY2
A	631	HIS	-	expression tag	UNP B9DFY2
A	632	HIS	-	expression tag	UNP B9DFY2
A	633	HIS	-	expression tag	UNP B9DFY2
A	634	HIS	-	expression tag	UNP B9DFY2
D	25	ARG	ASN	conflict	UNP B9DFY2
D	529	ASP	LYS	conflict	UNP B9DFY2
D	531	ASP	LYS	conflict	UNP B9DFY2
D	555	SER	GLN	conflict	UNP B9DFY2
D	629	HIS	-	expression tag	UNP B9DFY2
D	630	HIS	-	expression tag	UNP B9DFY2
D	631	HIS	-	expression tag	UNP B9DFY2
D	632	HIS	-	expression tag	UNP B9DFY2
D	633	HIS	-	expression tag	UNP B9DFY2
D	634	HIS	-	expression tag	UNP B9DFY2

- Molecule 2 is a protein called BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1354	856	229	266	3			
2	E	178	Total	C	N	O	S	0	0	0
			1354	856	229	266	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	221	HIS	-	expression tag	UNP Q94F62
B	222	HIS	-	expression tag	UNP Q94F62
B	223	HIS	-	expression tag	UNP Q94F62
B	224	HIS	-	expression tag	UNP Q94F62
B	225	HIS	-	expression tag	UNP Q94F62
B	226	HIS	-	expression tag	UNP Q94F62
B	227	HIS	-	expression tag	UNP Q94F62
B	228	HIS	-	expression tag	UNP Q94F62
B	229	HIS	-	expression tag	UNP Q94F62
B	230	HIS	-	expression tag	UNP Q94F62
E	221	HIS	-	expression tag	UNP Q94F62
E	222	HIS	-	expression tag	UNP Q94F62
E	223	HIS	-	expression tag	UNP Q94F62
E	224	HIS	-	expression tag	UNP Q94F62
E	225	HIS	-	expression tag	UNP Q94F62
E	226	HIS	-	expression tag	UNP Q94F62
E	227	HIS	-	expression tag	UNP Q94F62
E	228	HIS	-	expression tag	UNP Q94F62
E	229	HIS	-	expression tag	UNP Q94F62
E	230	HIS	-	expression tag	UNP Q94F62

- Molecule 3 is a protein called Transmembrane protein.

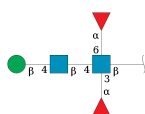
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	S	0	0	0
			174	100	39	33	2			
3	F	25	Total	C	N	O	S	0	0	0
			174	100	39	33	2			

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



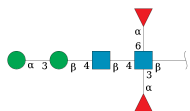
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



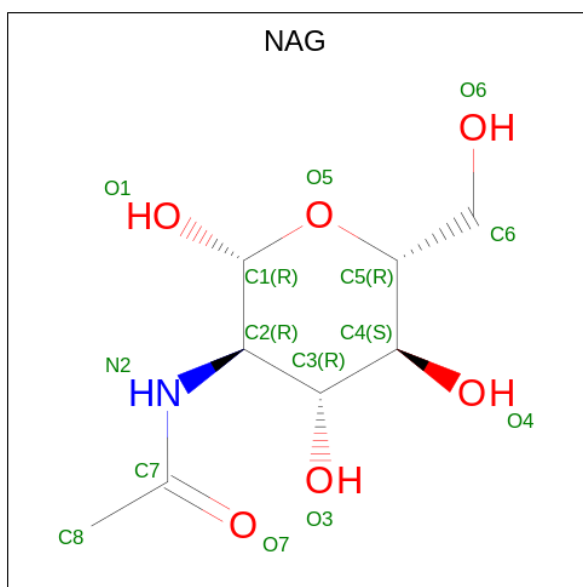
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	5	Total	C	N	O	0	0	0
			59	34	2	23			

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



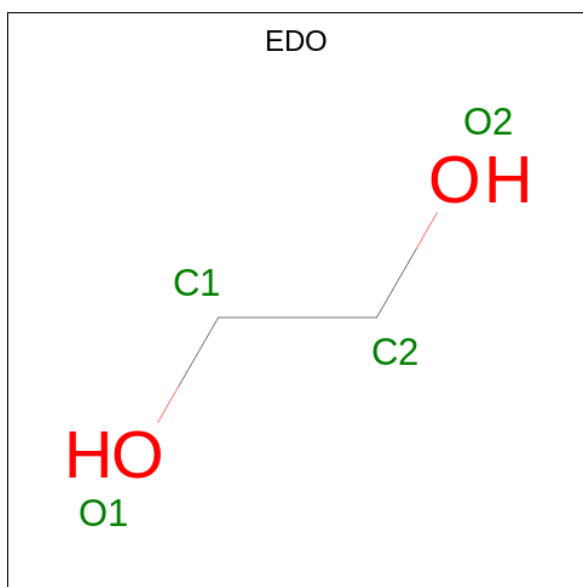
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	P	6	Total	C	N	O	0	0	0
			70	40	2	28			

- Molecule 7 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
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

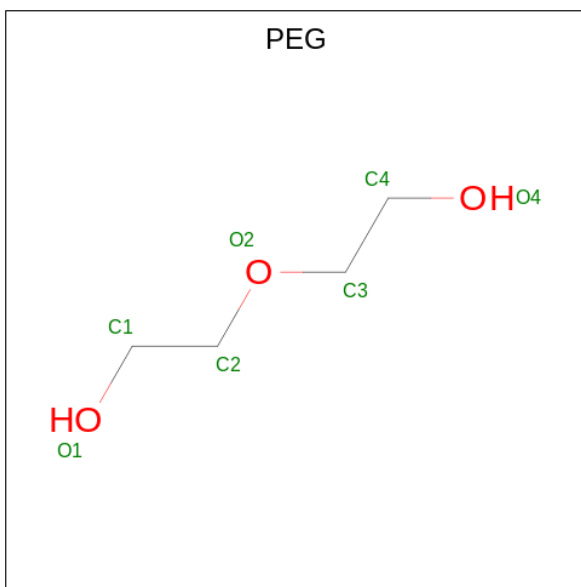


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		
8	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		
9	D	1	Total	Cl	0	0
			1	1		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).

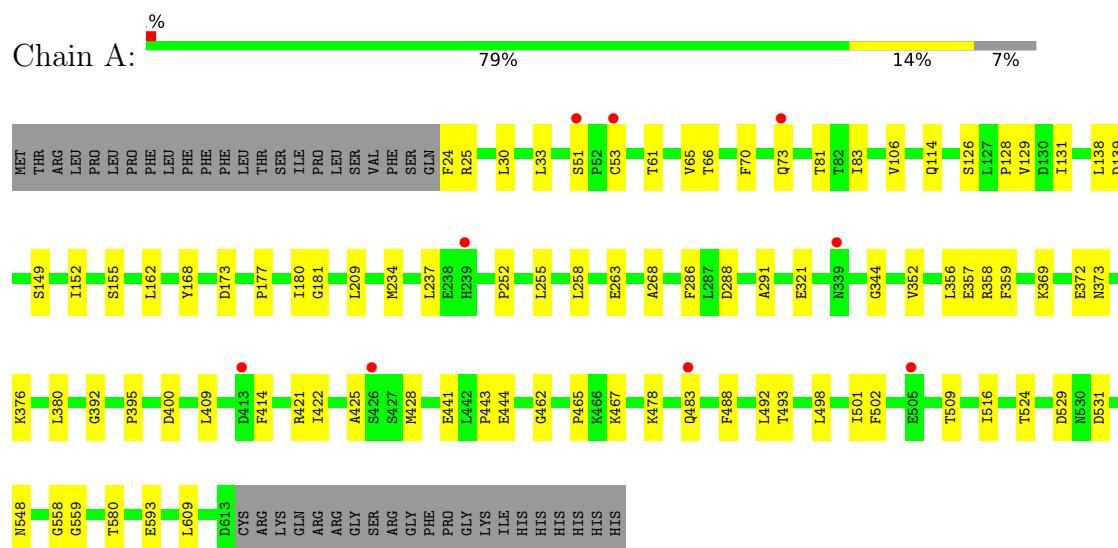


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	C	1	Total	C	O	0	0
			7	4	3		

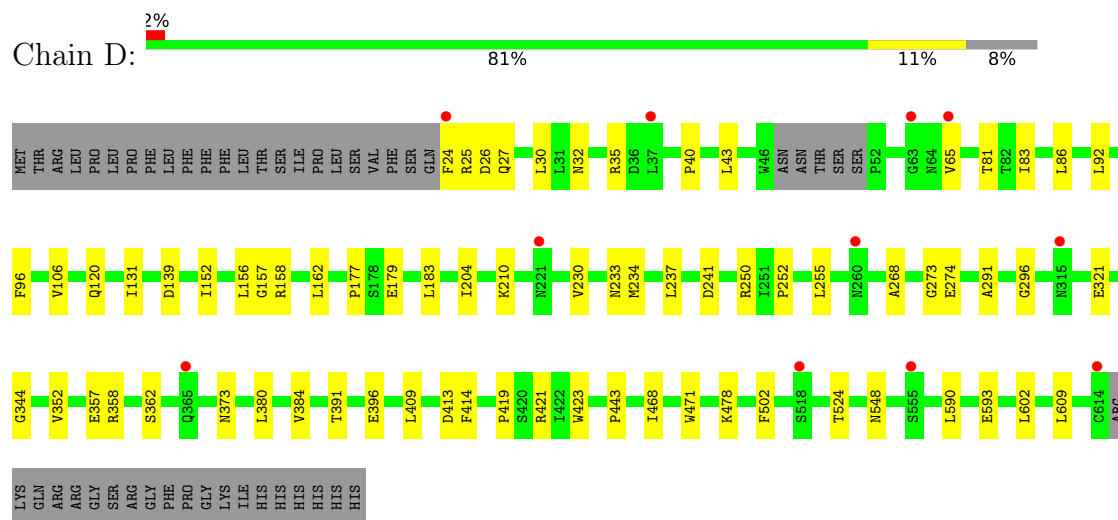
3 Residue-property plots [i](#)

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: AT5G25930 protein

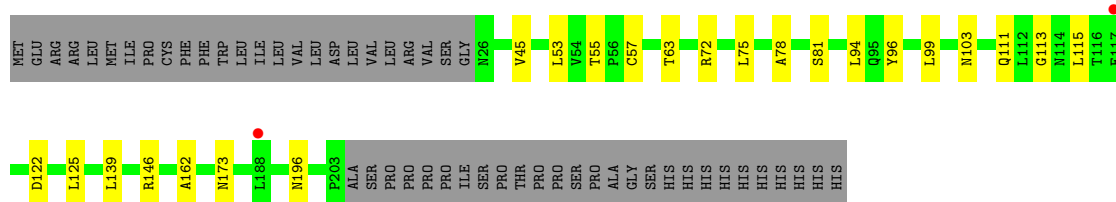


• Molecule 1: AT5G25930 protein



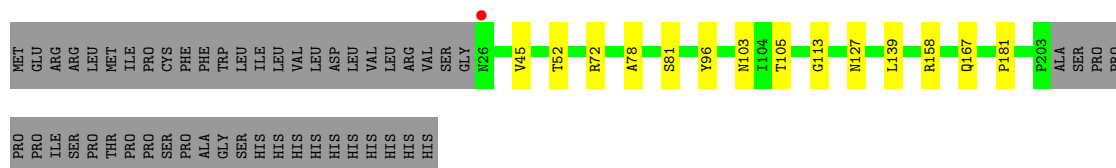
• Molecule 2: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1





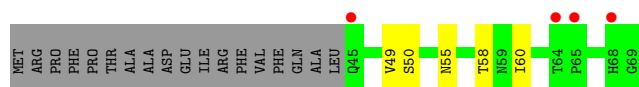
- Molecule 2: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1

Chain E: 71% 6% 23%



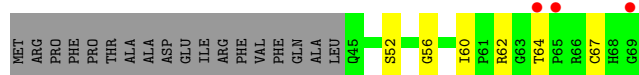
- Molecule 3: Transmembrane protein

Chain C: 9% 47% 12% 42%



- Molecule 3: Transmembrane protein

Chain F: 7% 44% 14% 42%



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

Chain G: 50% 50%



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

Chain H: 50% 50%



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

Chain I:  100%

HA01
HA02

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

Chain J:  50% 50%

HA01
HA02

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

Chain L:  100%

HA01
HA02

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

Chain M:  100%

HA01
HA02

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

Chain N:  100%

HA01
HA02

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

Chain O:  100%

HA01
HA02

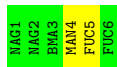
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  20% 60% 20%



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

Chain P:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	64.41Å 136.78Å 298.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.25 – 3.40 25.25 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (25.25-3.40) 99.2 (25.25-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.38Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.229 , 0.268 0.229 , 0.267	Depositor DCC
R_{free} test set	1855 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12776	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: FUC, NAG, BMA, EDO, PEG, CL, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/4677	0.28	0/6356
1	D	0.10	0/4647	0.28	0/6312
2	B	0.08	0/1378	0.28	0/1887
2	E	0.13	0/1378	0.27	0/1887
3	C	0.14	0/178	0.43	0/239
3	F	0.15	0/178	0.52	0/239
All	All	0.10	0/12436	0.29	0/16920

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	4587	0	4559	54	0
1	D	4558	0	4533	41	0
2	B	1354	0	1367	16	0
2	E	1354	0	1368	10	0
3	C	174	0	163	5	0
3	F	174	0	163	5	0
4	G	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	1	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
5	K	59	0	52	1	0
6	P	70	0	61	0	0
7	A	70	0	65	0	0
7	B	28	0	26	1	0
7	D	70	0	65	0	0
7	E	14	0	13	0	0
8	A	4	0	6	0	0
8	B	4	0	6	0	0
8	D	8	0	12	0	0
8	E	8	0	12	1	0
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	A	7	0	10	0	0
10	C	7	0	10	1	0
All	All	12776	0	12691	119	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 5.

The worst 5 of 119 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)
2:B:111:GLN:HG3	7:B:302:NAG:HN2	1.52	0.74
2:B:72:ARG:HG3	2:B:96:TYR:HB2	1.70	0.74
1:A:152:ILE:HB	1:A:177:PRO:HD3	1.75	0.69
1:A:252:PRO:HD2	1:A:255:LEU:HD12	1.77	0.67
1:D:81:THR:HA	1:D:106:VAL:HG21	1.79	0.65

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	588/634 (93%)	586 (100%)	2 (0%)	0	100	100
1	D	582/634 (92%)	579 (100%)	3 (0%)	0	100	100
2	B	176/230 (76%)	176 (100%)	0	0	100	100
2	E	176/230 (76%)	176 (100%)	0	0	100	100
3	C	23/43 (54%)	23 (100%)	0	0	100	100
3	F	23/43 (54%)	22 (96%)	1 (4%)	0	100	100
All	All	1568/1814 (86%)	1562 (100%)	6 (0%)	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	529/570 (93%)	529 (100%)	0	100	100
1	D	525/570 (92%)	525 (100%)	0	100	100
2	B	159/207 (77%)	159 (100%)	0	100	100
2	E	159/207 (77%)	159 (100%)	0	100	100
3	C	19/34 (56%)	19 (100%)	0	100	100
3	F	19/34 (56%)	19 (100%)	0	100	100
All	All	1410/1622 (87%)	1410 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	482	ASN
2	E	47	GLN
3	F	59	ASN
2	E	173	ASN
2	E	196	ASN

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 ⓘ

27 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	G	1	1,4	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	G	2	4	14,14,15	0.34	0	17,19,21	0.54	0
4	NAG	H	1	1,4	14,14,15	0.67	1 (7%)	17,19,21	1.20	1 (5%)
4	NAG	H	2	4	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	I	1	1,4	14,14,15	0.38	0	17,19,21	0.43	0
4	NAG	I	2	4	14,14,15	0.42	0	17,19,21	0.42	0
4	NAG	J	1	2,4	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	J	2	4	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	K	1	2,5	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
5	NAG	K	2	5	14,14,15	0.63	1 (7%)	17,19,21	1.26	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	K	3	5	11,11,12	0.62	0	15,15,17	0.83	0
5	FUC	K	4	5	10,10,11	0.68	0	14,14,16	0.95	1 (7%)
5	FUC	K	5	5	10,10,11	1.07	0	14,14,16	1.04	1 (7%)
4	NAG	L	1	1,4	14,14,15	0.31	0	17,19,21	0.43	0
4	NAG	L	2	4	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	M	1	1,4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	M	2	4	14,14,15	0.26	0	17,19,21	0.36	0
4	NAG	N	1	1,4	14,14,15	0.17	0	17,19,21	0.46	0
4	NAG	N	2	4	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	O	1	2,4	14,14,15	0.31	0	17,19,21	0.48	0
4	NAG	O	2	4	14,14,15	0.26	0	17,19,21	0.39	0
6	NAG	P	1	6,2	14,14,15	0.30	0	17,19,21	0.60	0
6	NAG	P	2	6	14,14,15	0.21	0	17,19,21	0.54	0
6	BMA	P	3	6	11,11,12	0.71	0	15,15,17	0.91	0
6	MAN	P	4	6	11,11,12	1.09	1 (9%)	15,15,17	1.04	0
6	FUC	P	5	6	10,10,11	0.91	0	14,14,16	1.05	1 (7%)
6	FUC	P	6	6	10,10,11	0.93	0	14,14,16	0.93	0

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

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	4	MAN	C1-C2	2.51	1.57	1.52
5	K	2	NAG	O4-C4	-2.18	1.37	1.43
4	H	1	NAG	O5-C1	2.01	1.46	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	2	NAG	O4-C4-C5	4.74	121.06	109.30
4	H	1	NAG	C1-O5-C5	4.61	118.44	112.19
6	P	5	FUC	C1-C2-C3	2.24	112.42	109.67
5	K	5	FUC	O5-C5-C4	2.19	113.44	109.52
5	K	1	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	1	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6

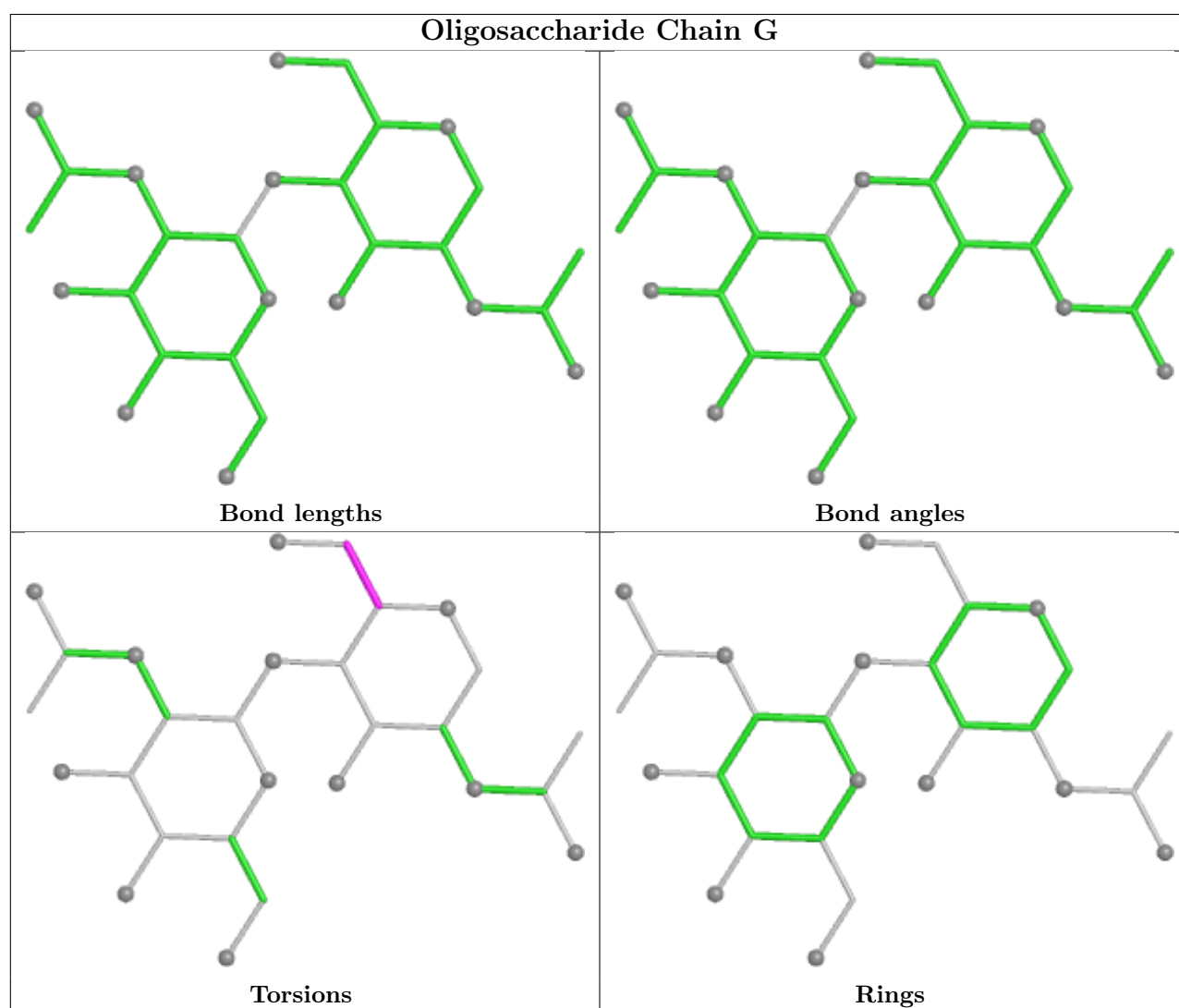
All (2) ring outliers are listed below:

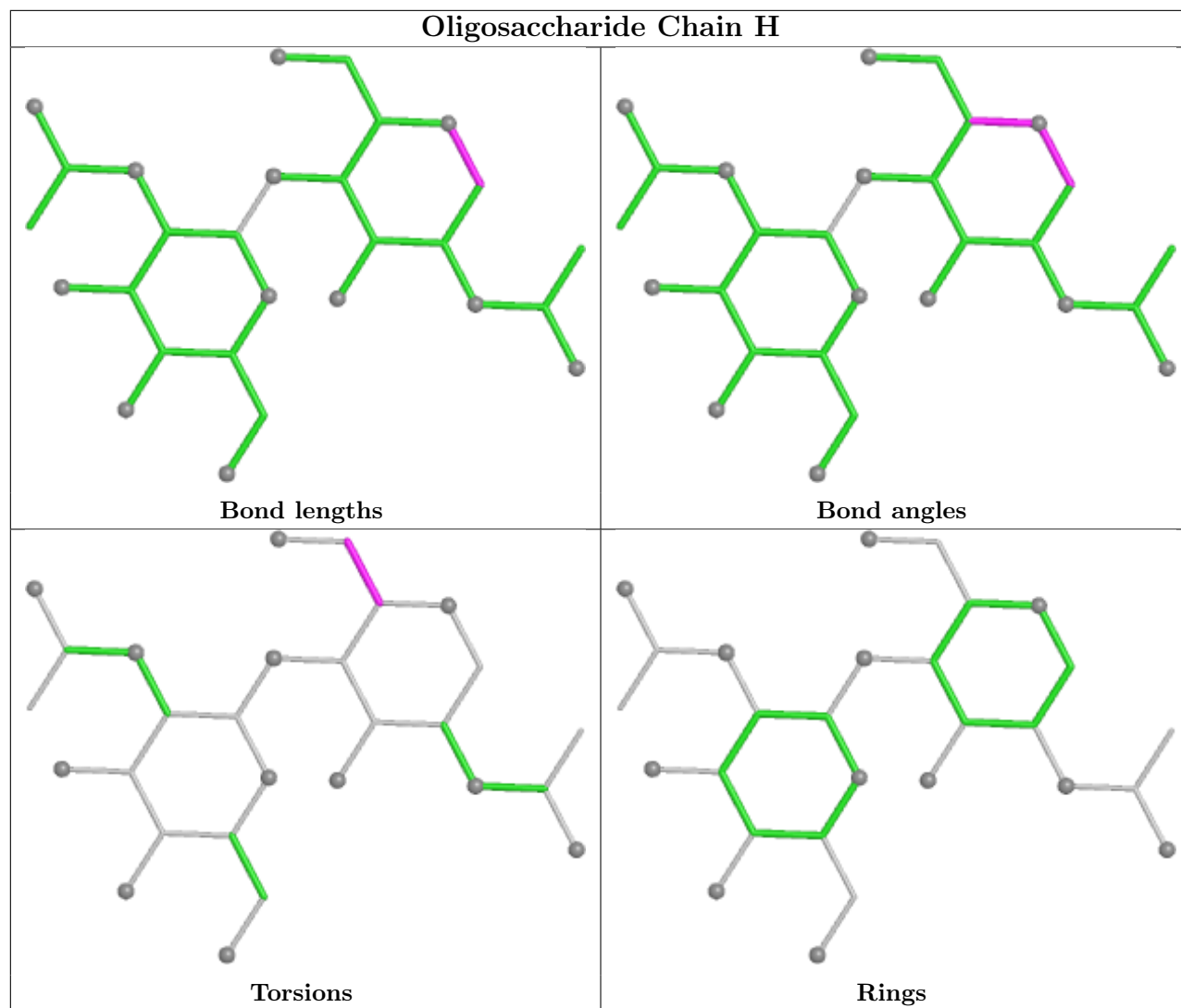
Mol	Chain	Res	Type	Atoms
6	P	3	BMA	C1-C2-C3-C4-C5-O5
6	P	4	MAN	C1-C2-C3-C4-C5-O5

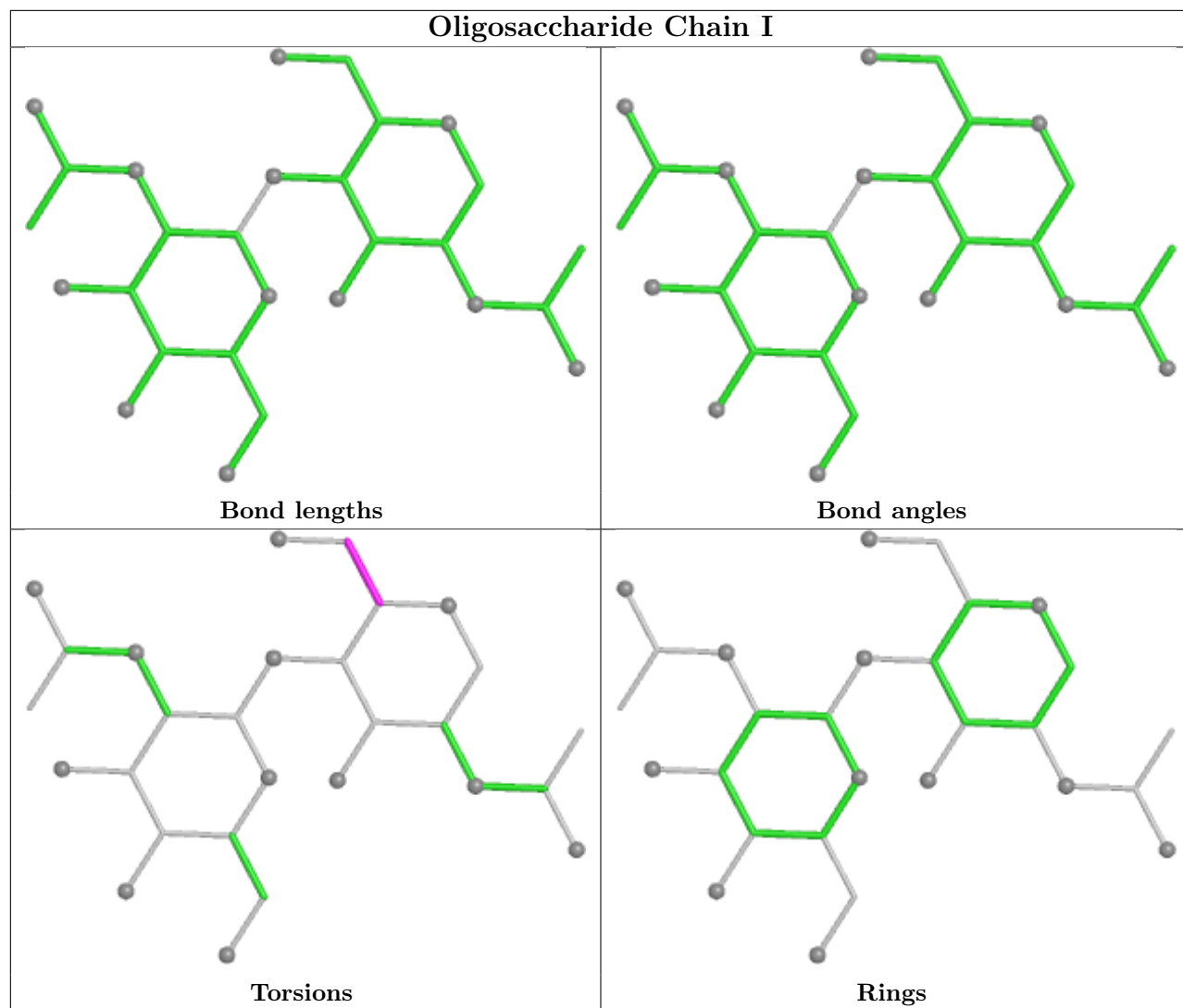
3 monomers are involved in 3 short contacts:

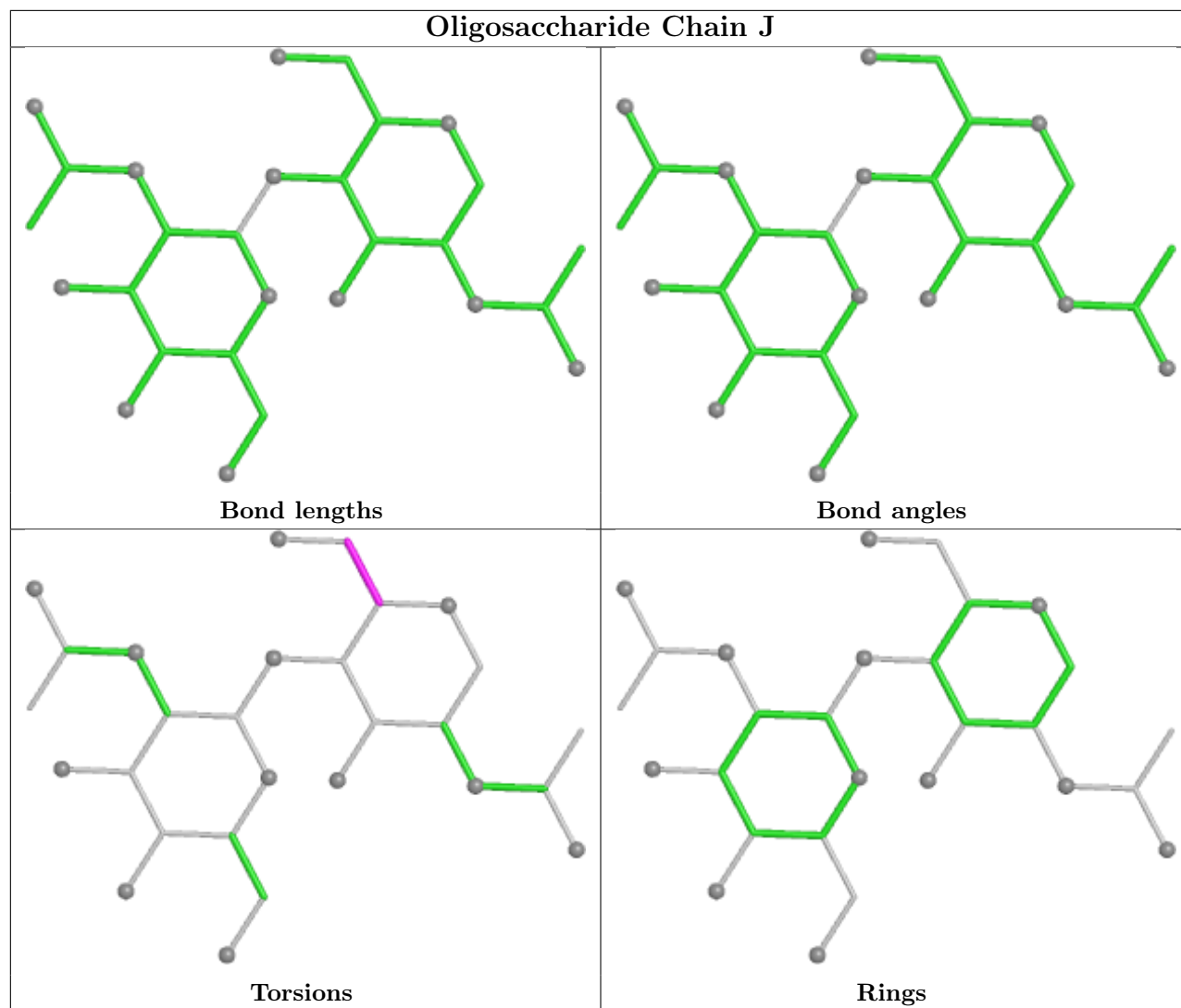
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	1	0
5	K	4	FUC	1	0
4	G	1	NAG	1	0

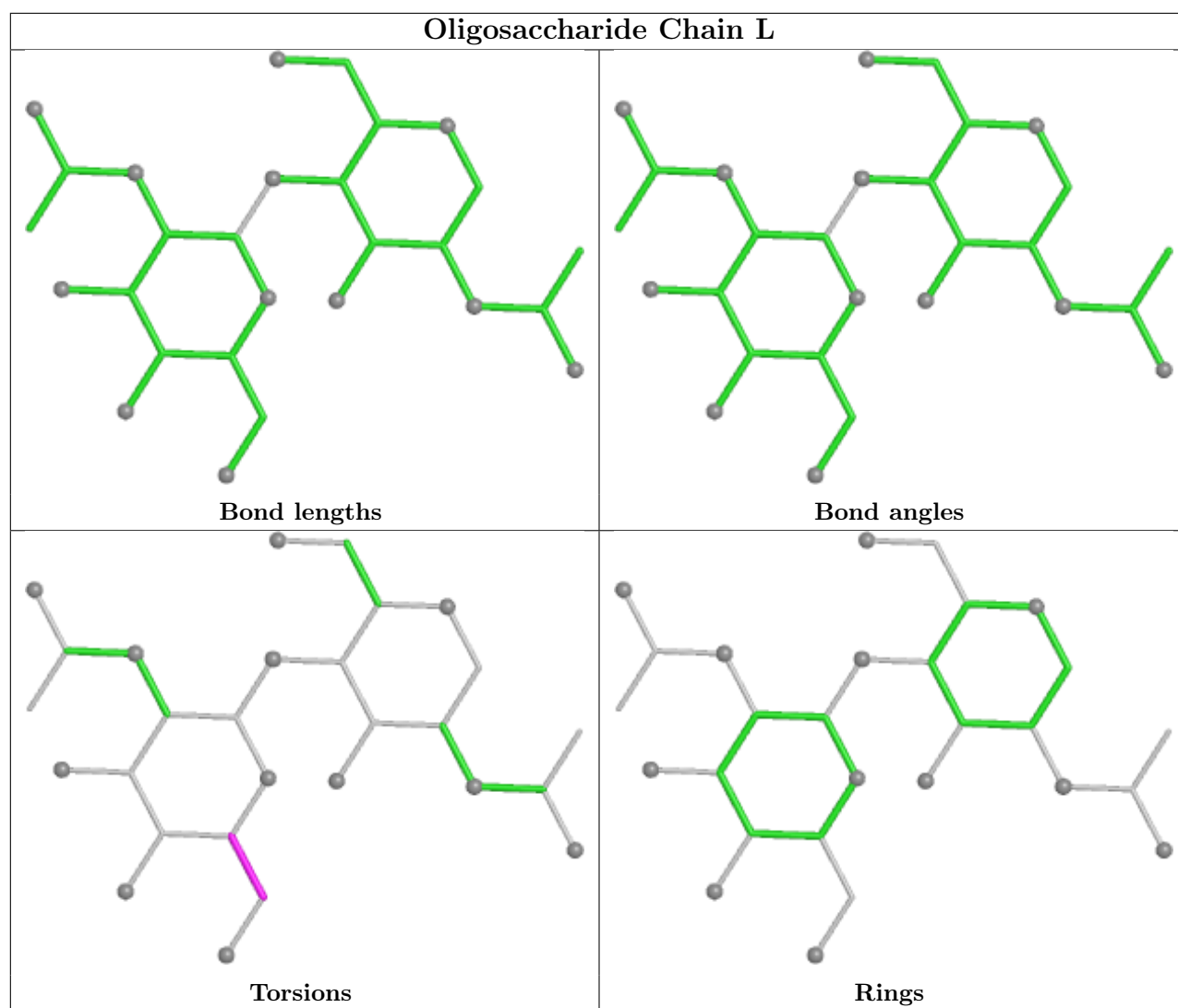
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

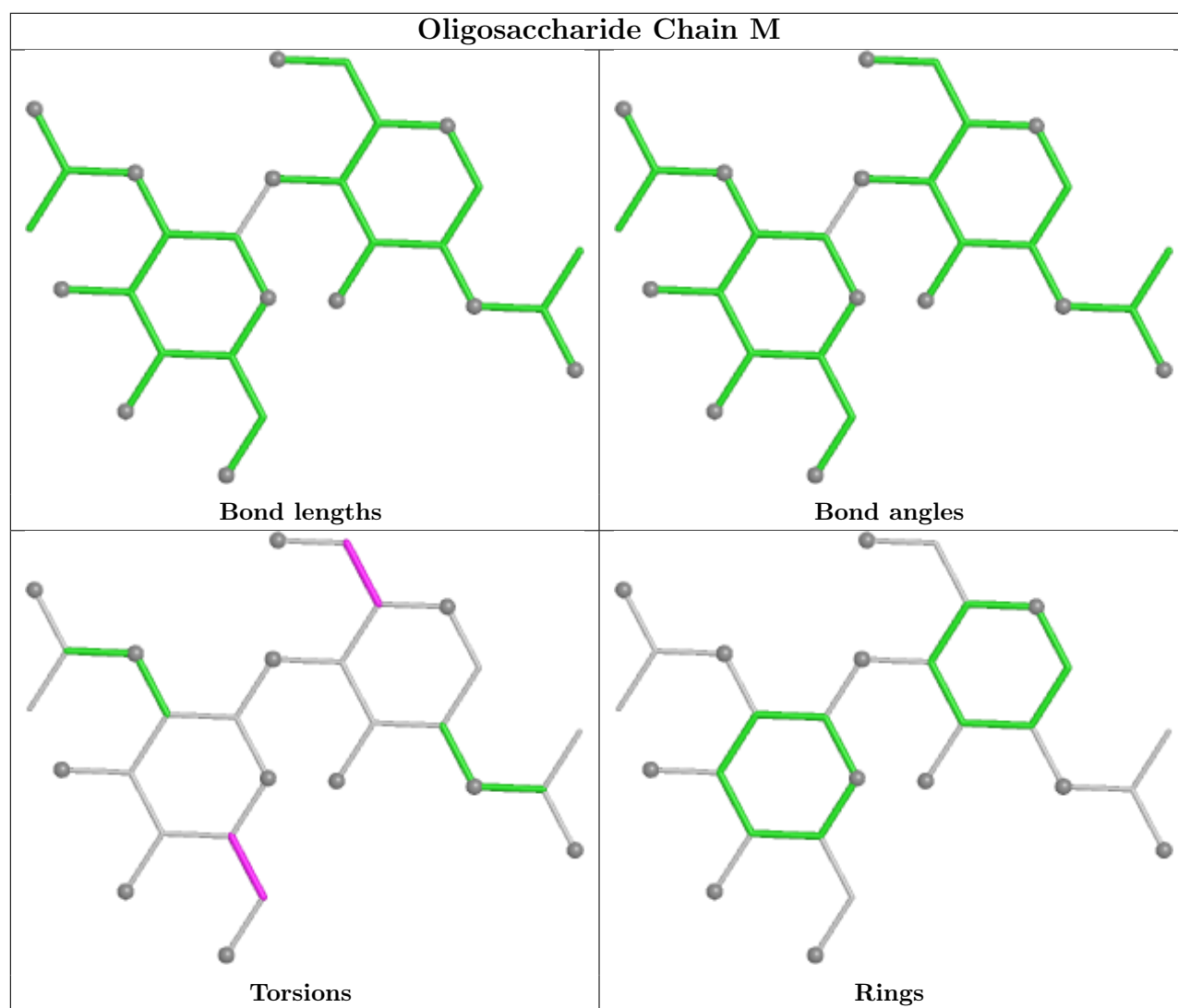


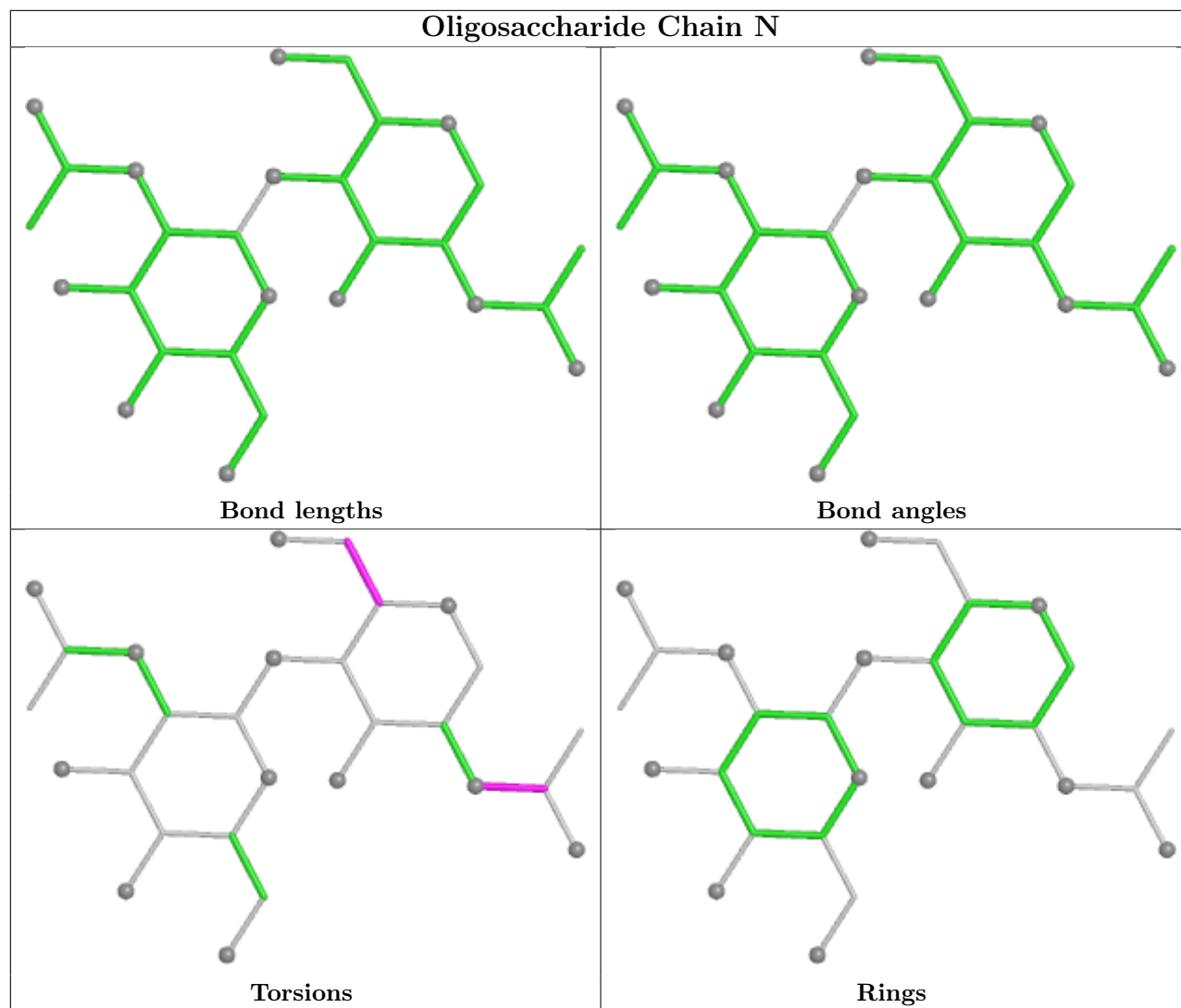


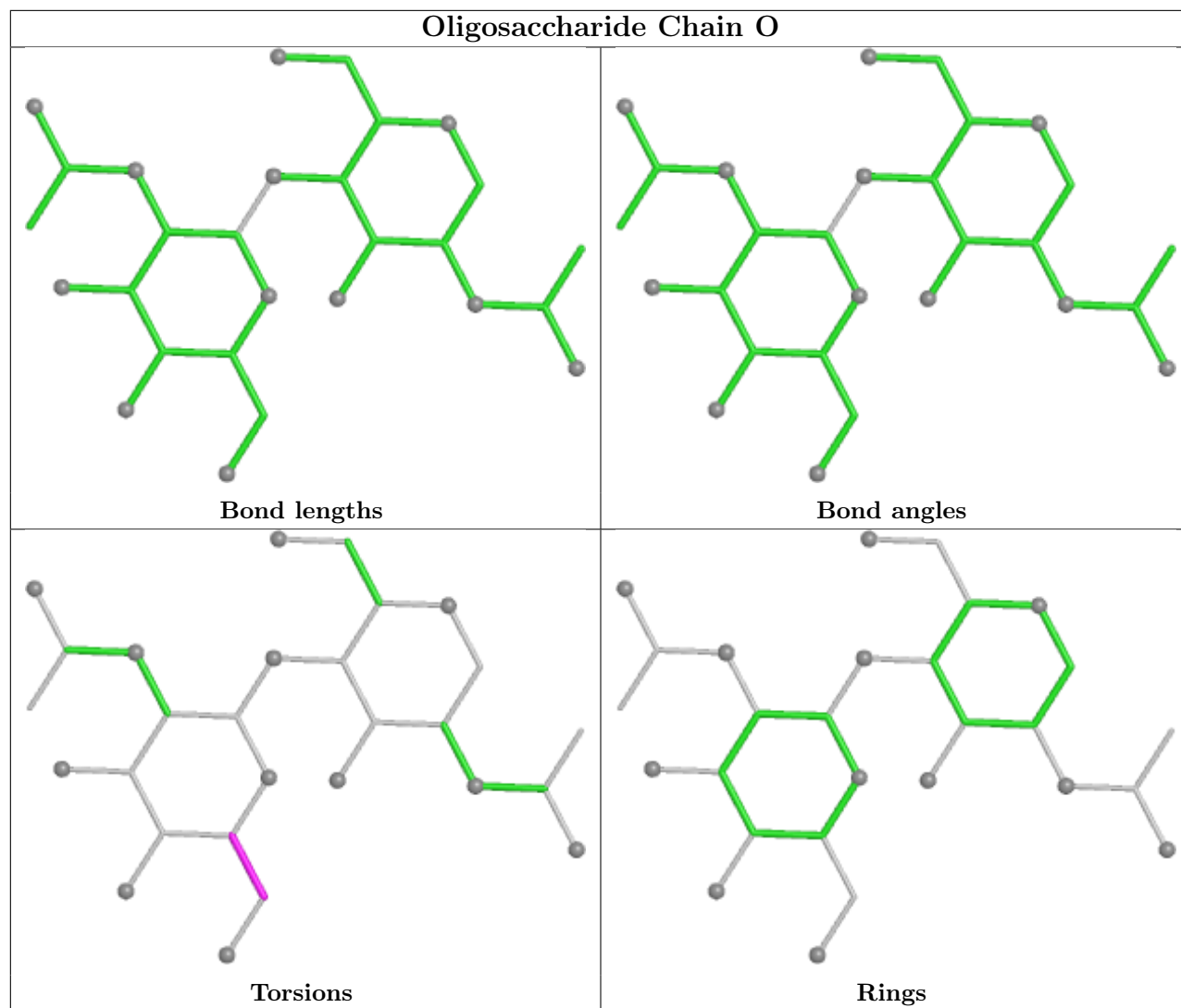




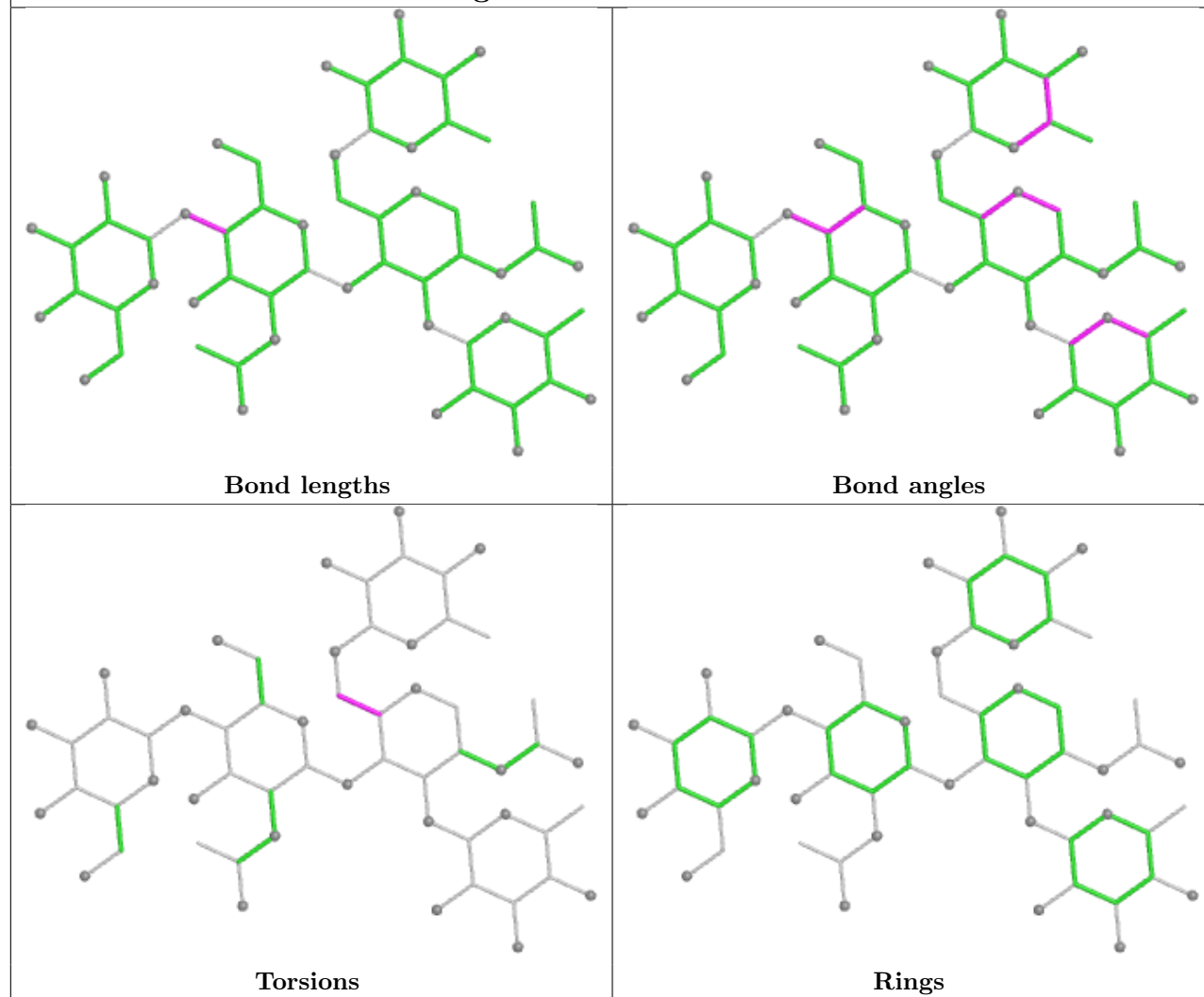


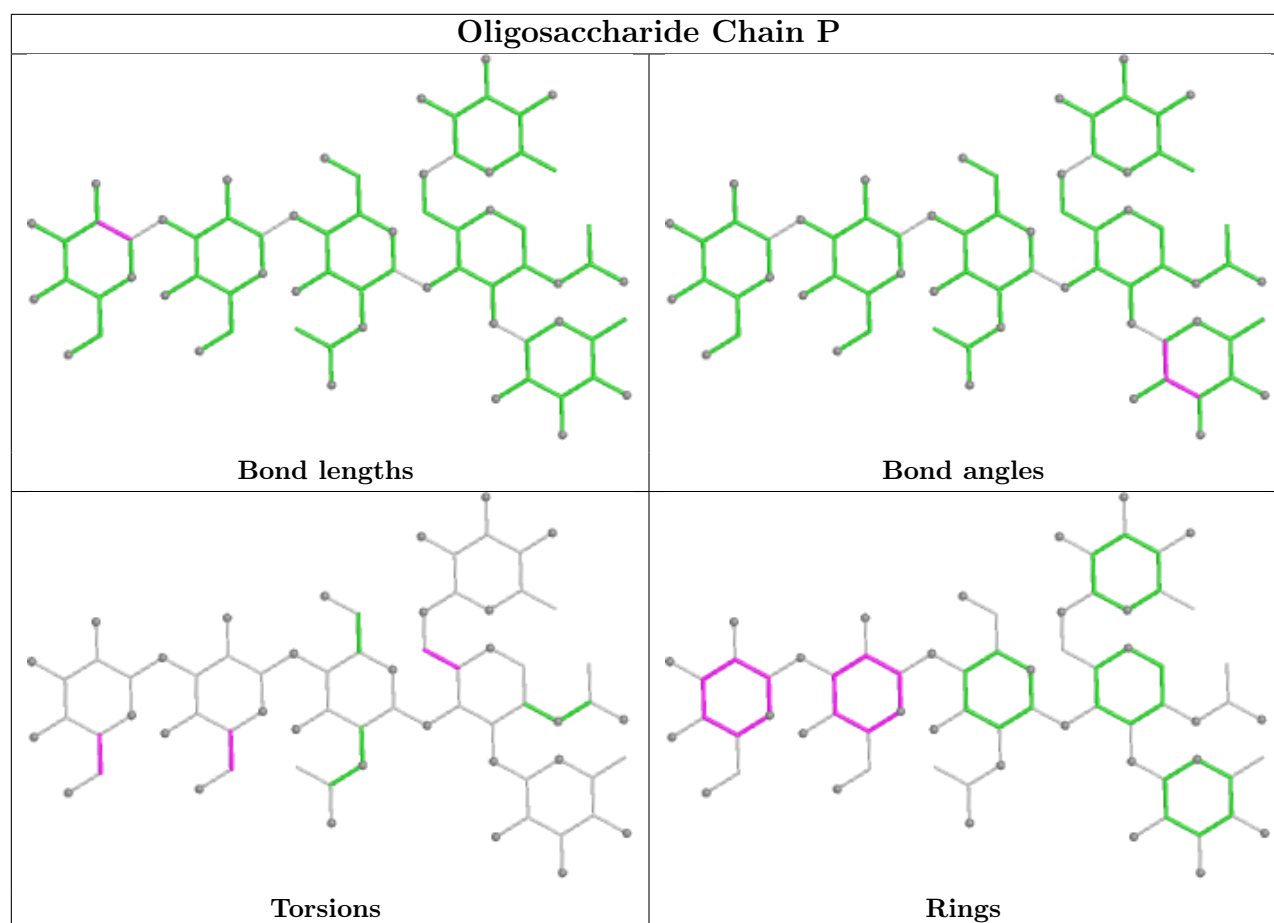






Oligosaccharide Chain K





5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

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	$\# Z > 2$
8	EDO	D	706	-	3,3,3	0.45	0	2,2,2	0.35	0
10	PEG	C	101	-	6,6,6	0.11	0	5,5,5	0.08	0
7	NAG	D	703	1	14,14,15	0.26	0	17,19,21	0.49	0
7	NAG	A	704	1	14,14,15	0.27	0	17,19,21	0.44	0
7	NAG	D	701	1	14,14,15	0.17	0	17,19,21	0.54	0
7	NAG	B	302	2	14,14,15	0.38	0	17,19,21	0.59	0
10	PEG	A	708	-	6,6,6	0.10	0	5,5,5	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	D	702	1	14,14,15	0.29	0	17,19,21	0.41	0
8	EDO	B	303	-	3,3,3	0.45	0	2,2,2	0.34	0
7	NAG	D	705	1	14,14,15	0.46	0	17,19,21	0.60	0
8	EDO	E	303	-	3,3,3	0.46	0	2,2,2	0.32	0
7	NAG	B	301	2	14,14,15	0.25	0	17,19,21	0.46	0
8	EDO	D	708	-	3,3,3	0.45	0	2,2,2	0.35	0
7	NAG	E	301	2	14,14,15	0.25	0	17,19,21	0.47	0
7	NAG	A	703	1	14,14,15	0.28	0	17,19,21	0.46	0
8	EDO	A	706	-	3,3,3	0.46	0	2,2,2	0.34	0
7	NAG	A	702	1	14,14,15	0.87	1 (7%)	17,19,21	1.24	1 (5%)
7	NAG	A	701	1	14,14,15	0.46	0	17,19,21	0.65	1 (5%)
8	EDO	E	302	-	3,3,3	0.45	0	2,2,2	0.32	0
7	NAG	A	705	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
7	NAG	D	704	1	14,14,15	0.28	0	17,19,21	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	D	706	-	-	0/1/1/1	-
10	PEG	C	101	-	-	1/4/4/4	-
7	NAG	D	703	1	-	0/6/23/26	0/1/1/1
7	NAG	A	704	1	-	2/6/23/26	0/1/1/1
7	NAG	D	701	1	-	1/6/23/26	0/1/1/1
7	NAG	B	302	2	-	1/6/23/26	0/1/1/1
10	PEG	A	708	-	-	1/4/4/4	-
7	NAG	D	702	1	-	0/6/23/26	0/1/1/1
8	EDO	B	303	-	-	0/1/1/1	-
7	NAG	D	705	1	-	2/6/23/26	0/1/1/1
8	EDO	E	303	-	-	0/1/1/1	-
7	NAG	B	301	2	-	2/6/23/26	0/1/1/1
8	EDO	D	708	-	-	0/1/1/1	-
7	NAG	E	301	2	-	0/6/23/26	0/1/1/1
7	NAG	A	703	1	-	2/6/23/26	0/1/1/1
8	EDO	A	706	-	-	0/1/1/1	-
7	NAG	A	702	1	-	0/6/23/26	0/1/1/1
7	NAG	A	701	1	-	1/6/23/26	0/1/1/1
8	EDO	E	302	-	-	0/1/1/1	-
7	NAG	A	705	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	704	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	702	NAG	O5-C1	2.56	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	702	NAG	C1-O5-C5	4.82	118.72	112.19
7	A	705	NAG	C2-N2-C7	2.98	127.15	122.90
7	A	701	NAG	C1-O5-C5	2.27	115.27	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	705	NAG	C3-C2-N2-C7
7	A	705	NAG	C8-C7-N2-C2
7	A	705	NAG	O7-C7-N2-C2
7	B	301	NAG	C4-C5-C6-O6
7	A	704	NAG	C4-C5-C6-O6

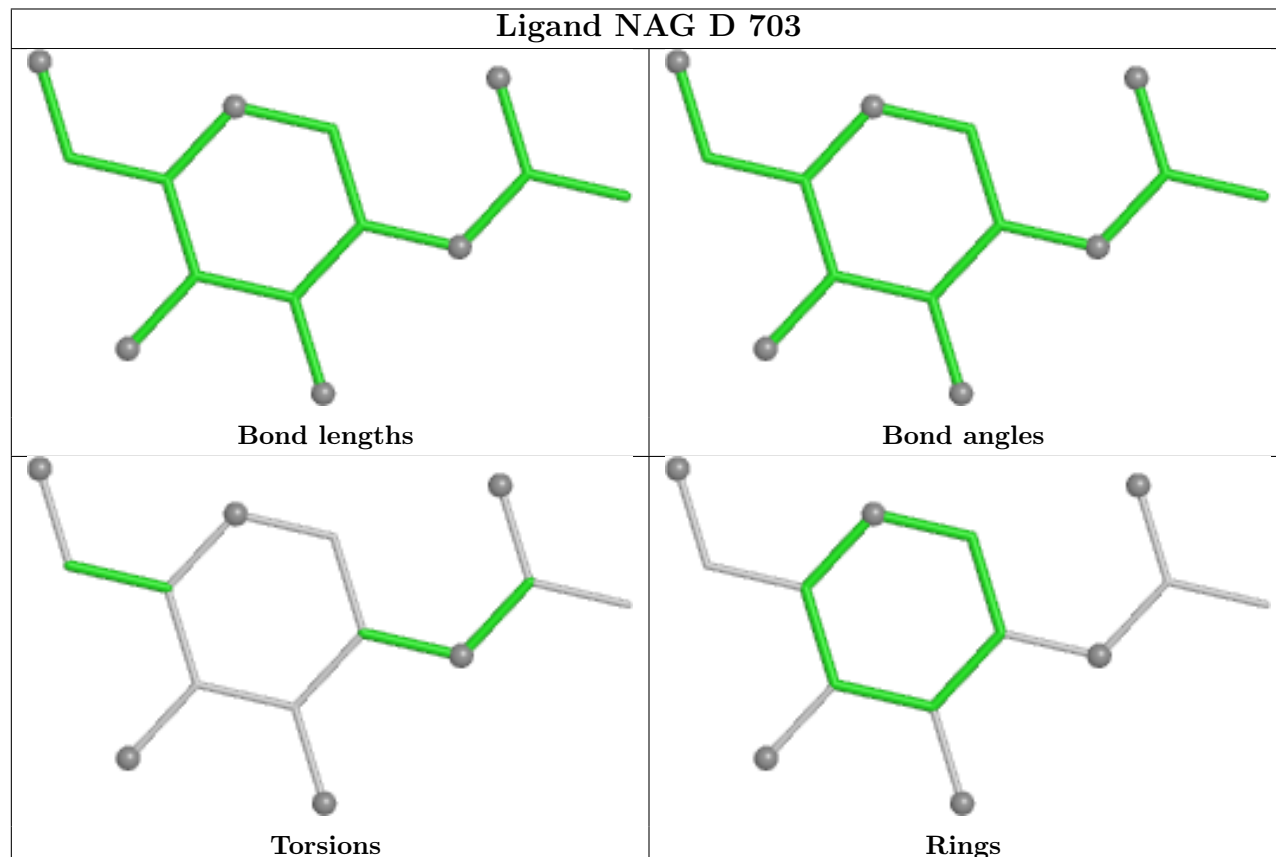
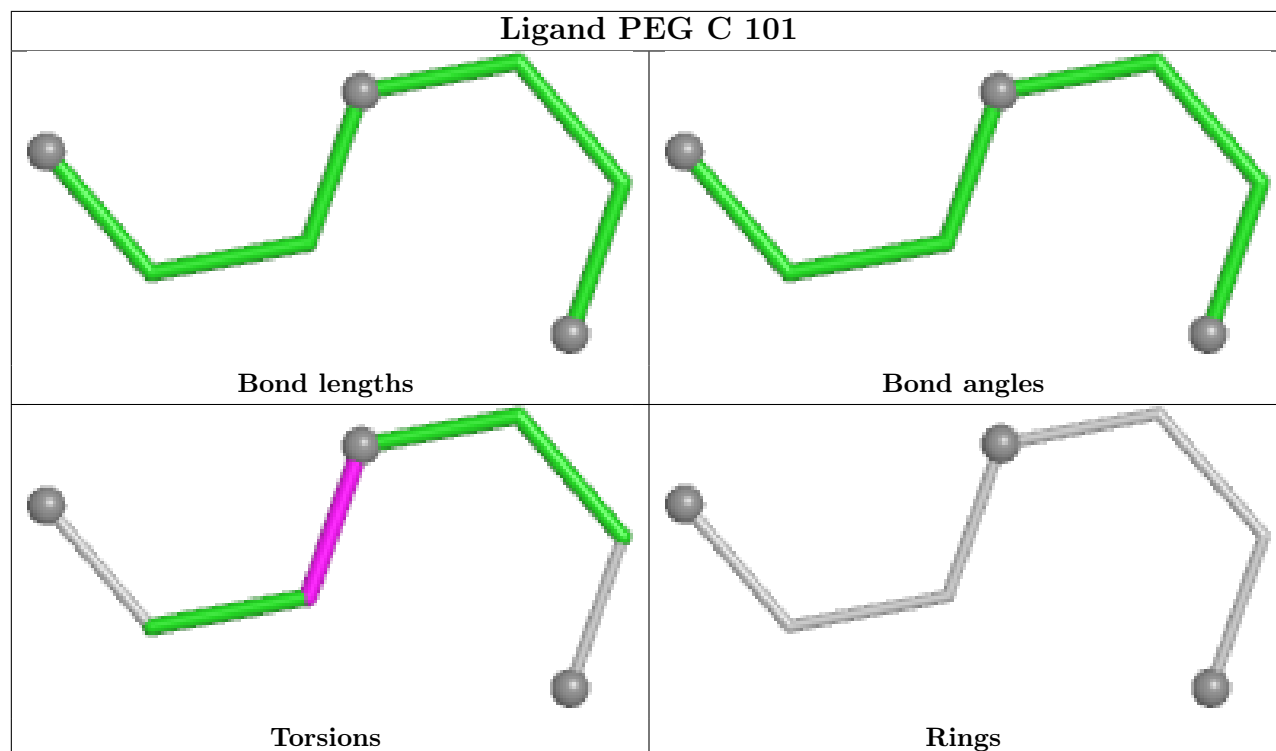
There are no ring outliers.

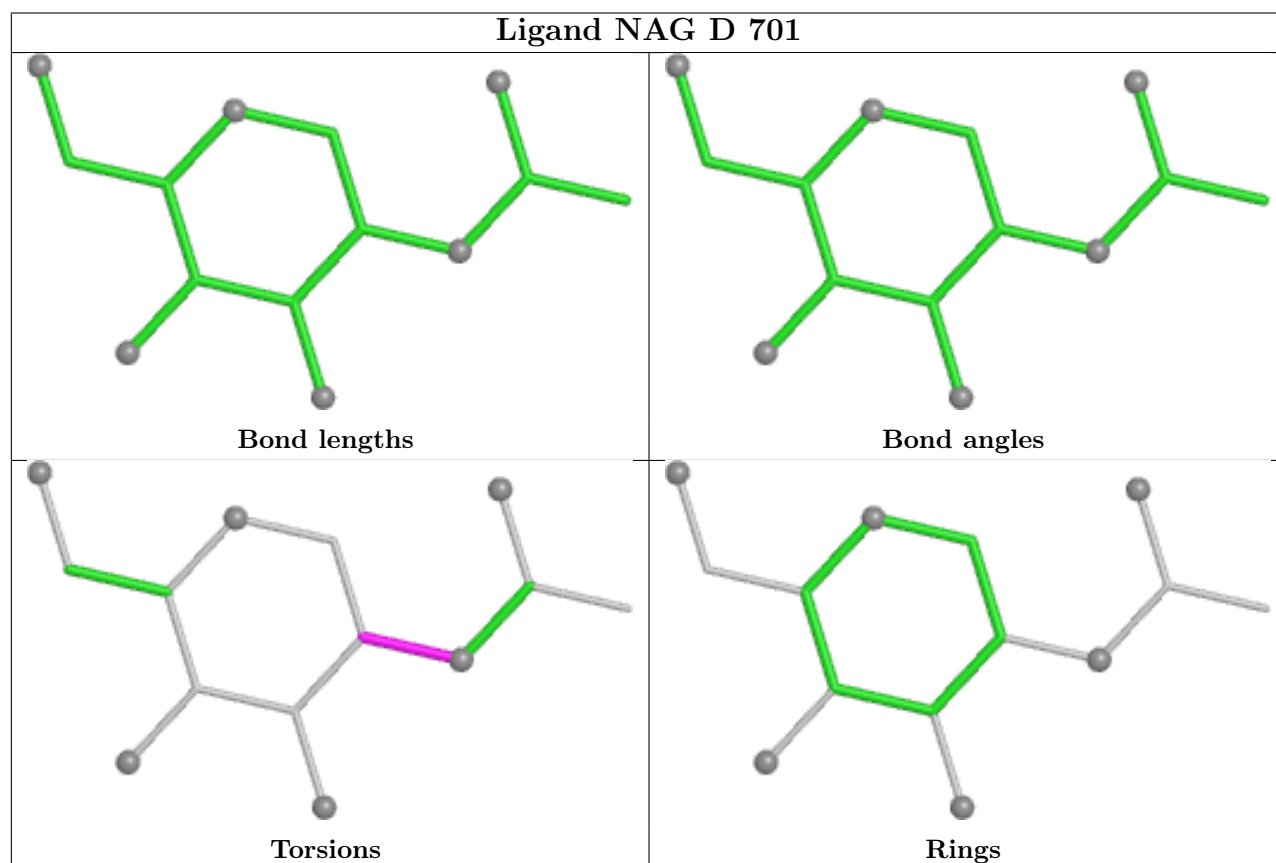
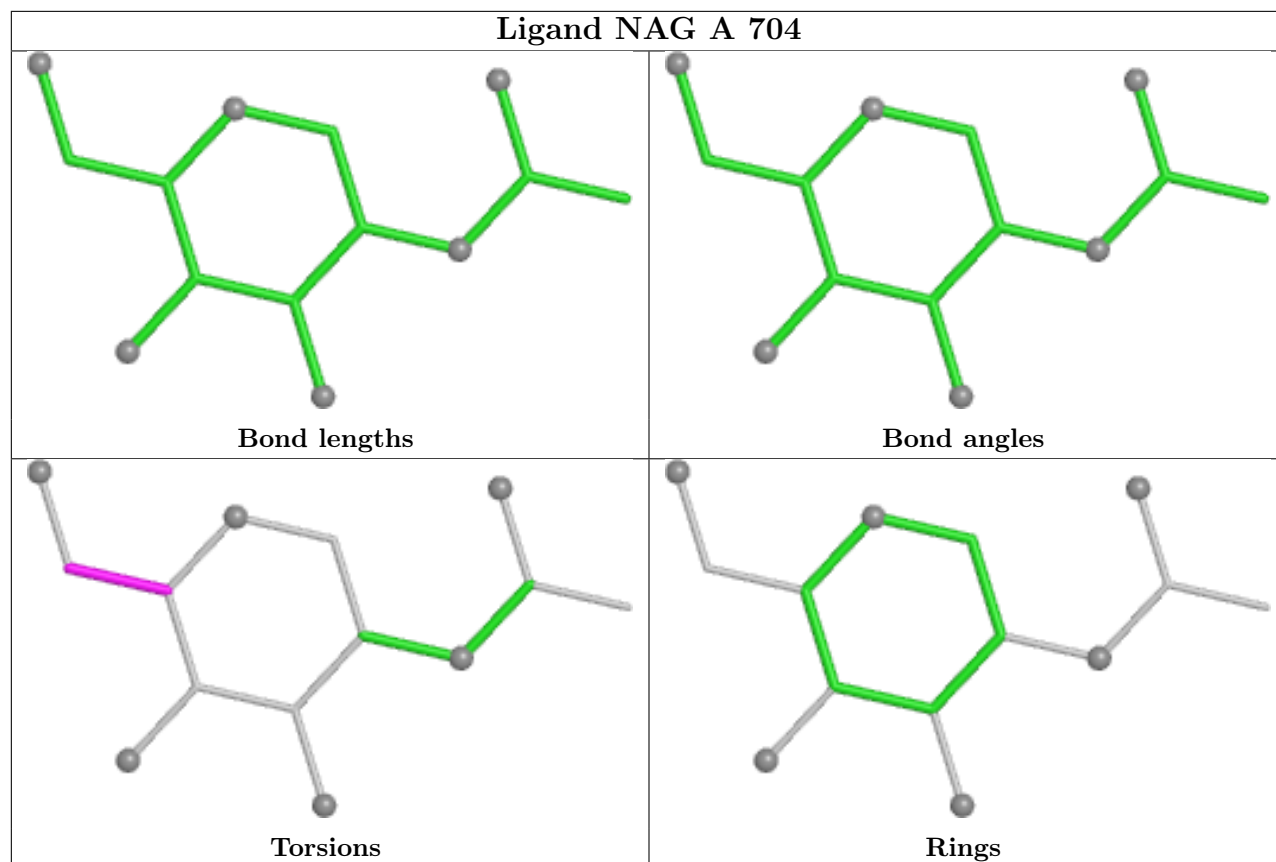
3 monomers are involved in 3 short contacts:

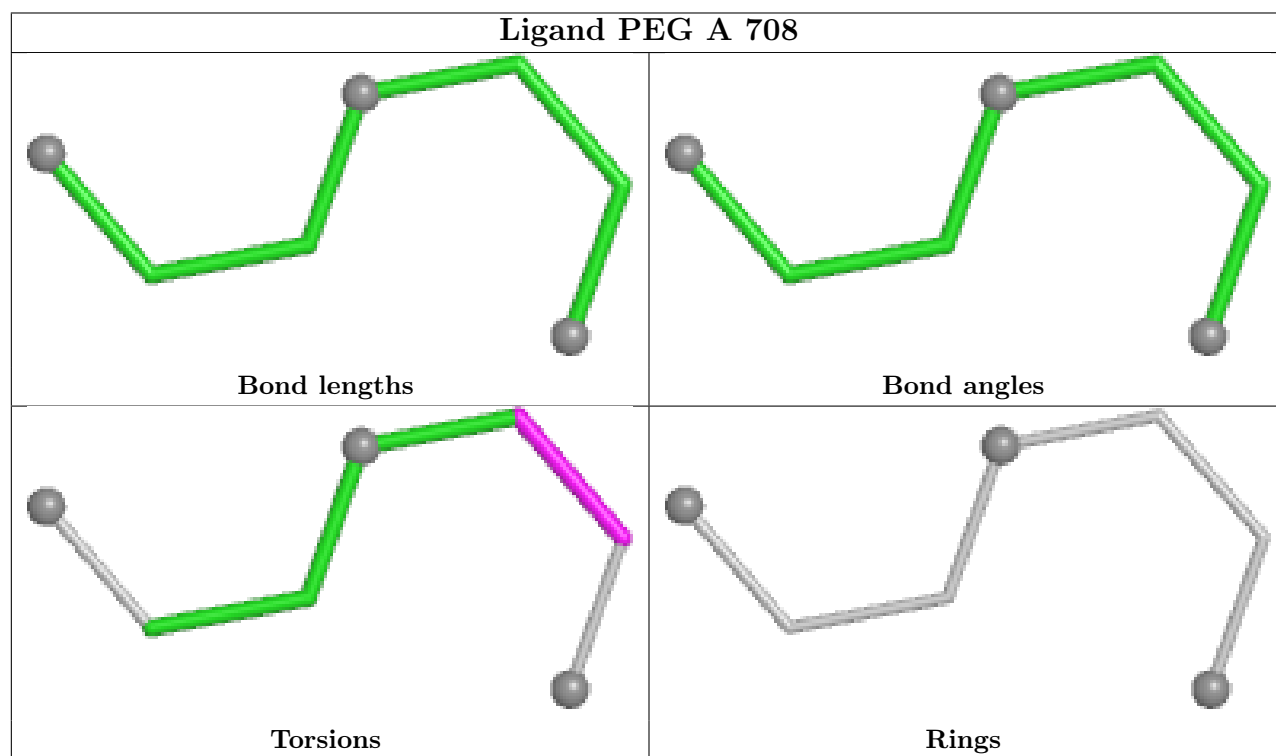
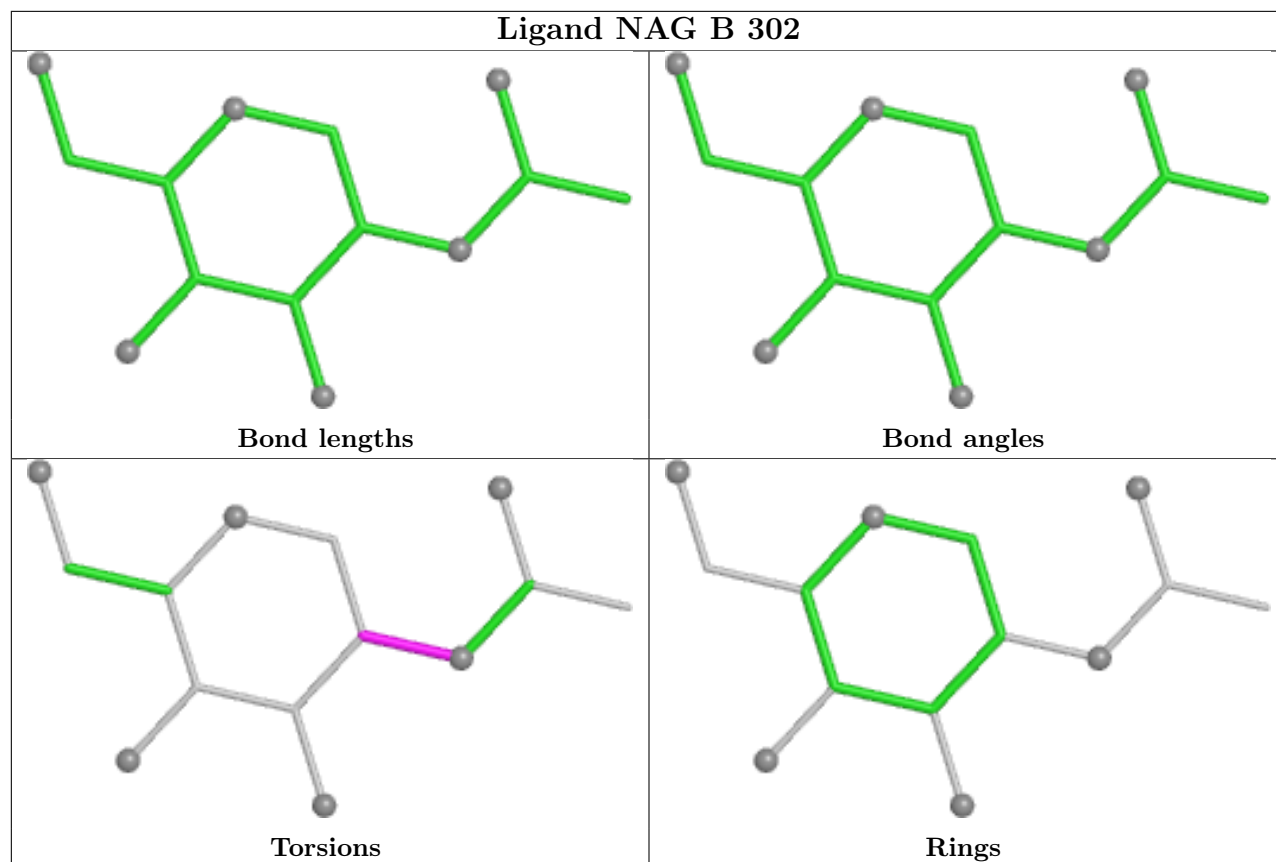
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	101	PEG	1	0
7	B	302	NAG	1	0
8	E	302	EDO	1	0

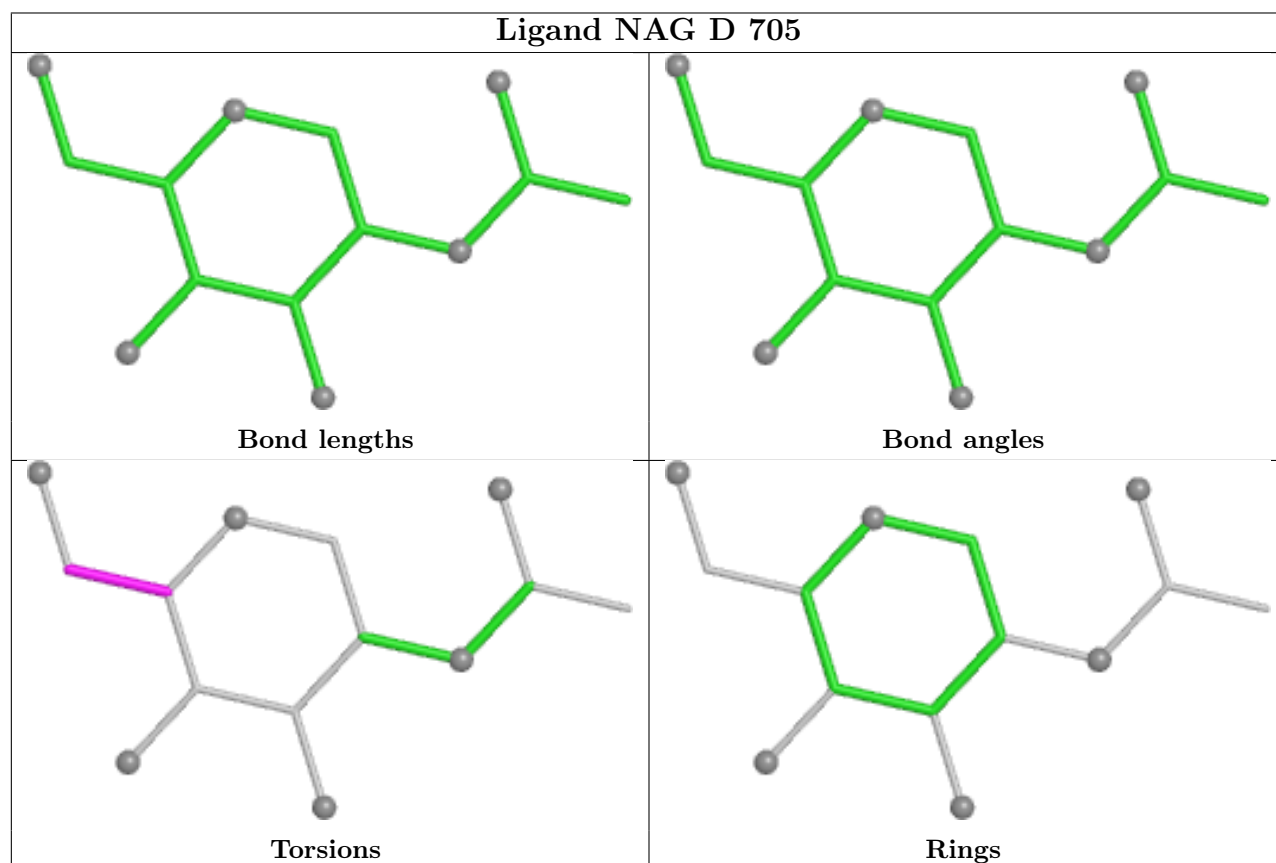
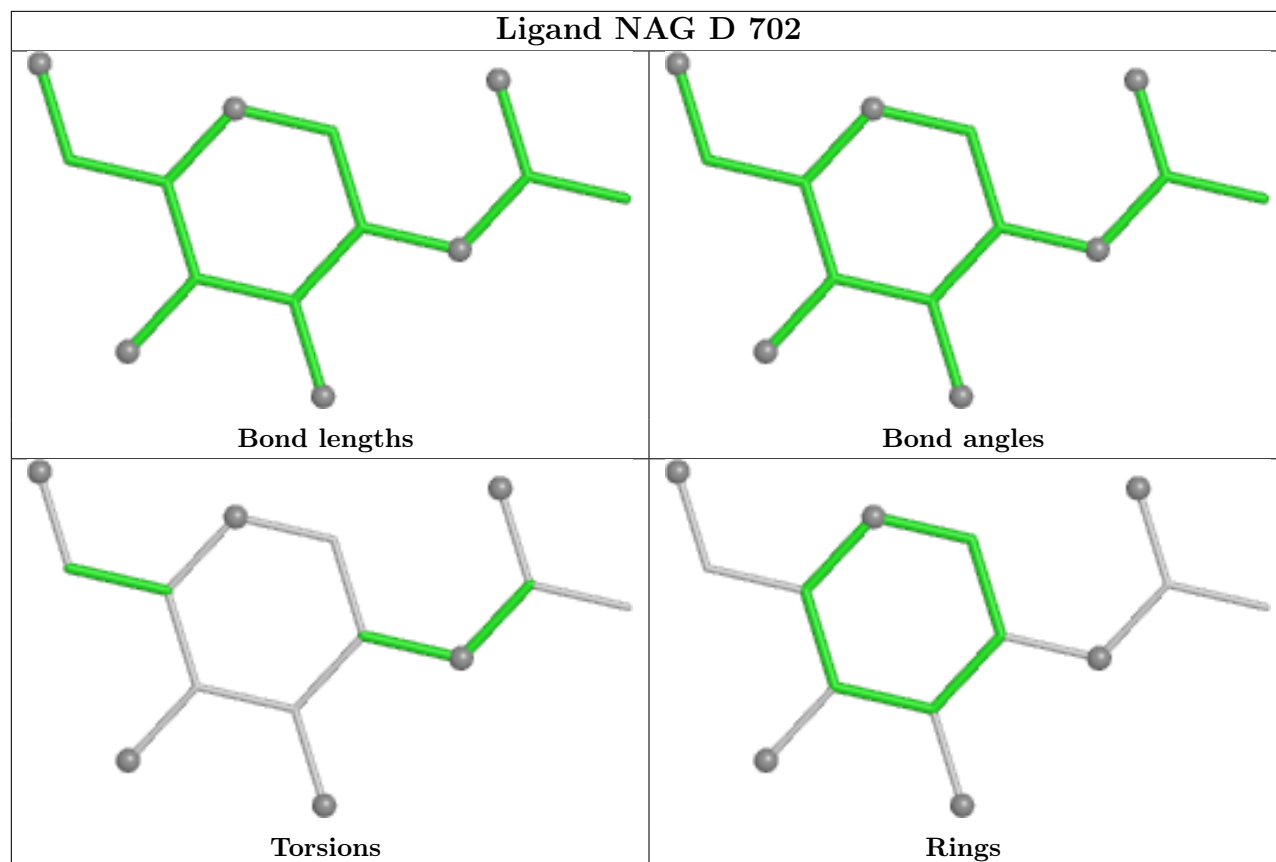
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

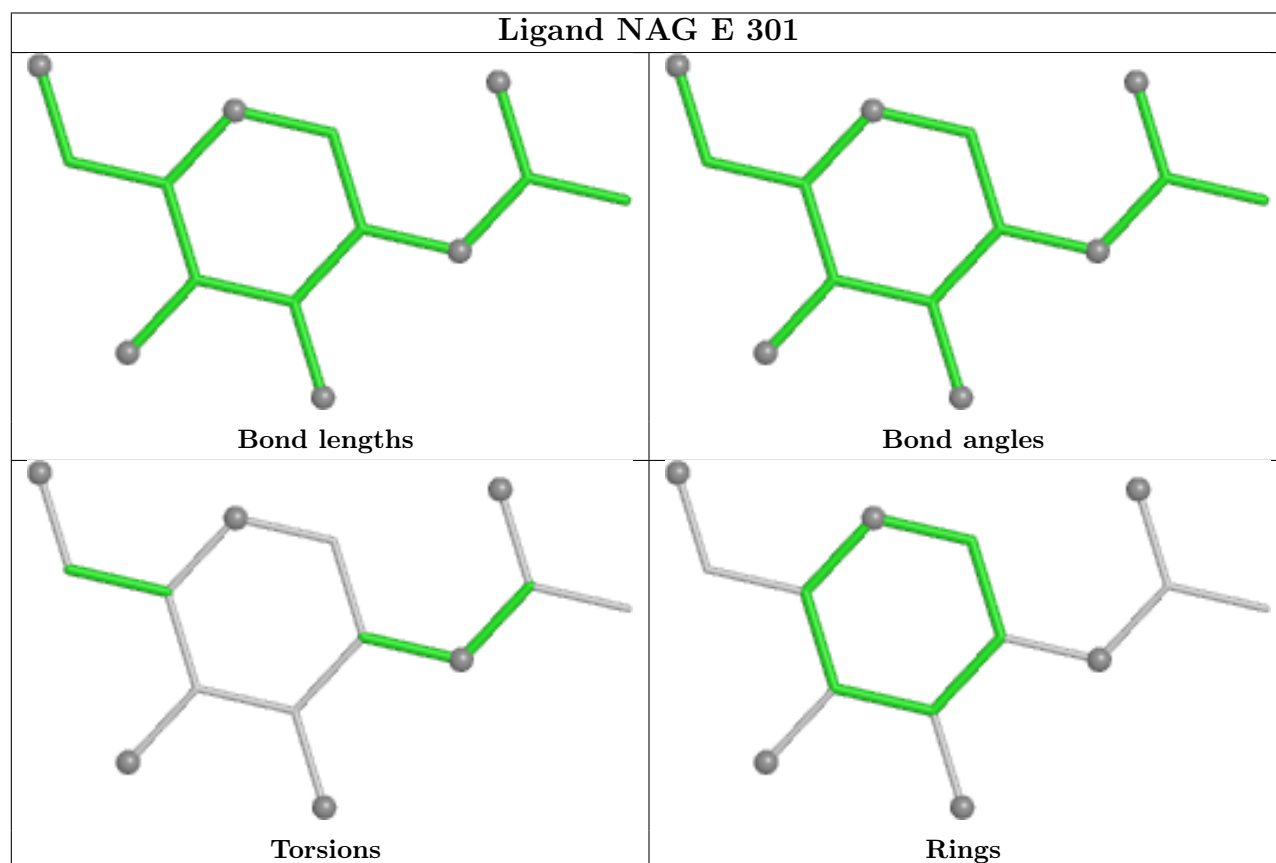
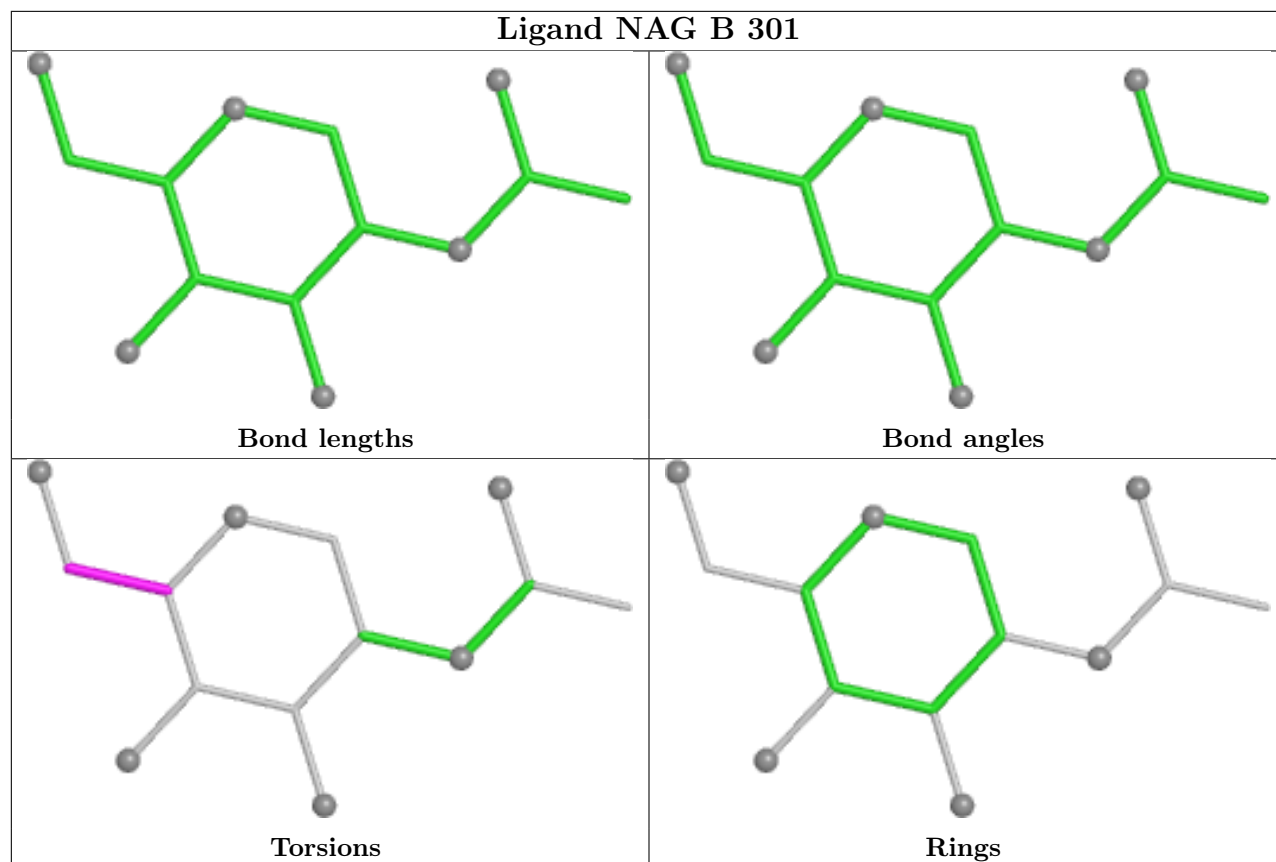
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

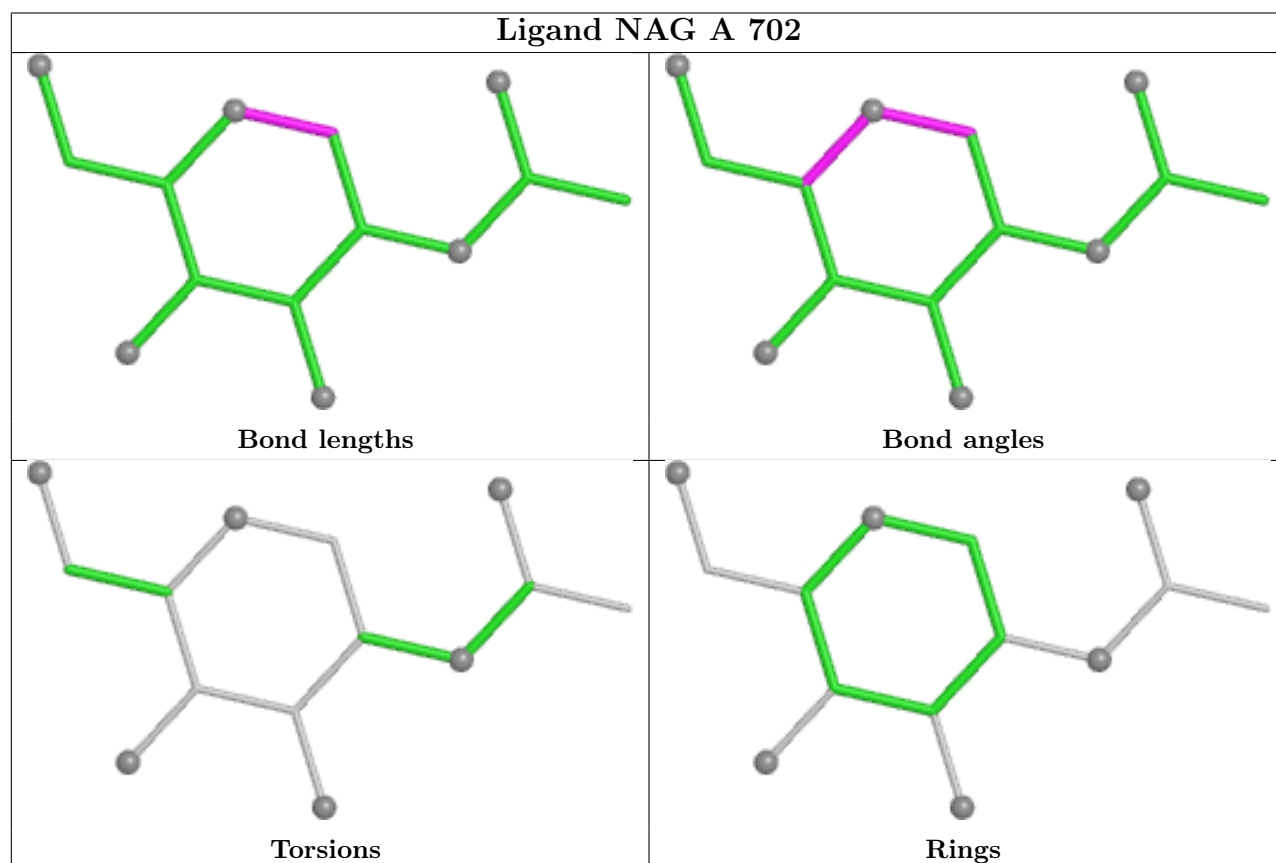
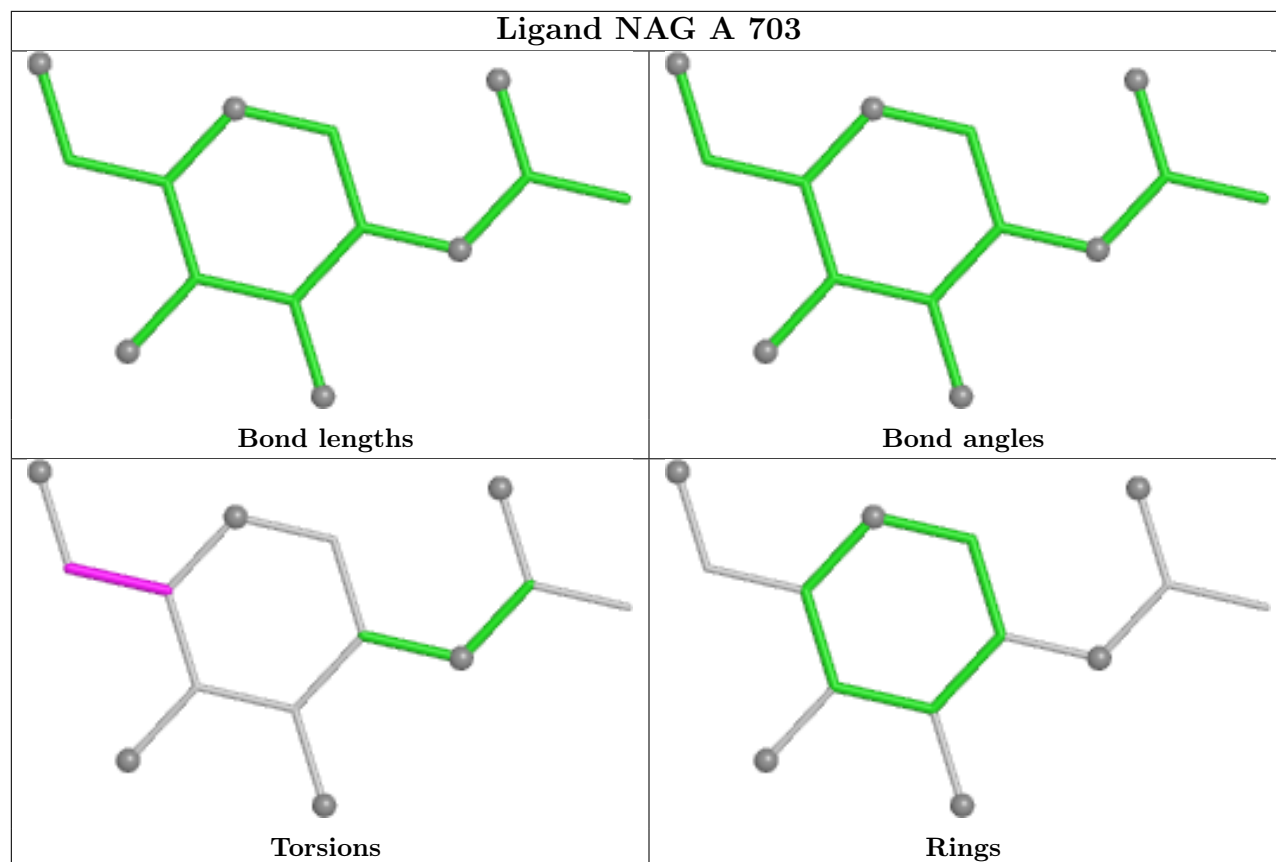


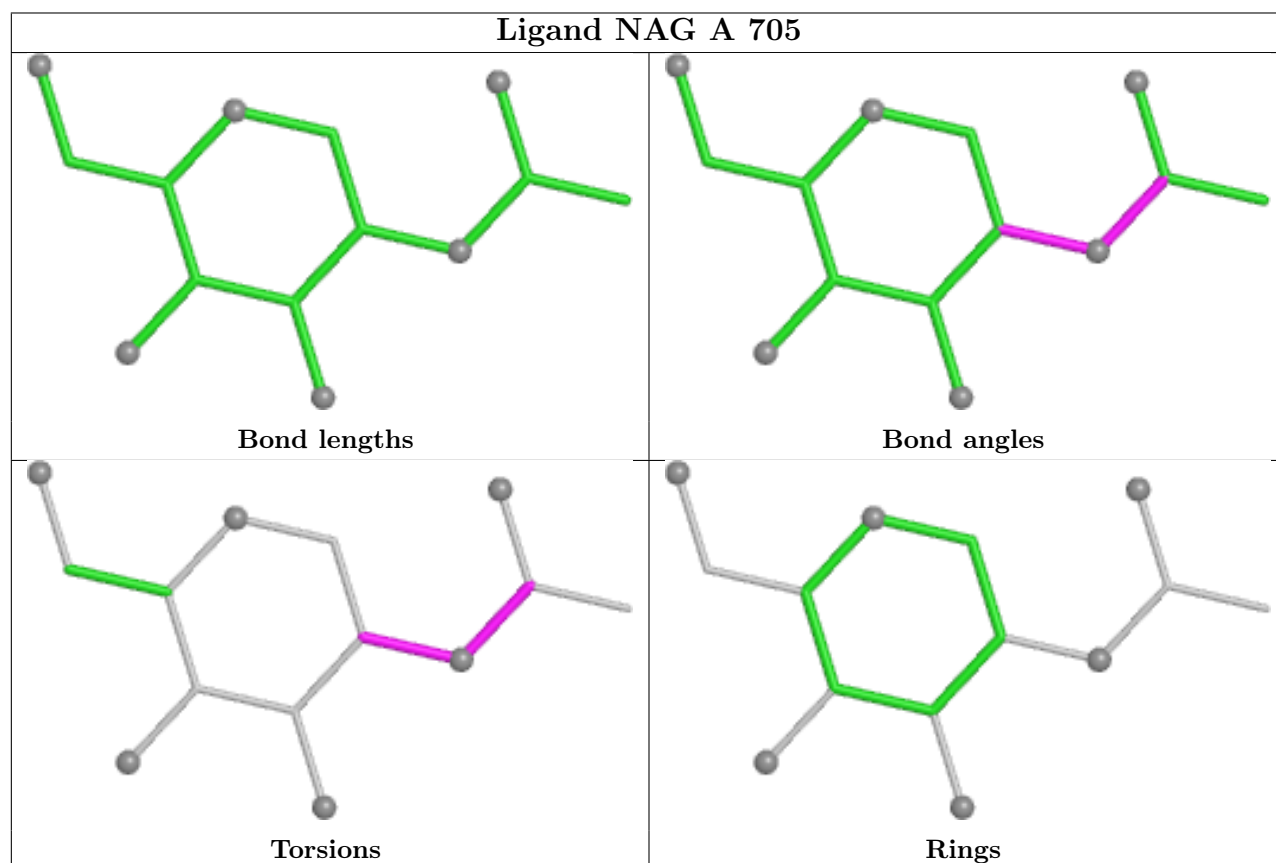
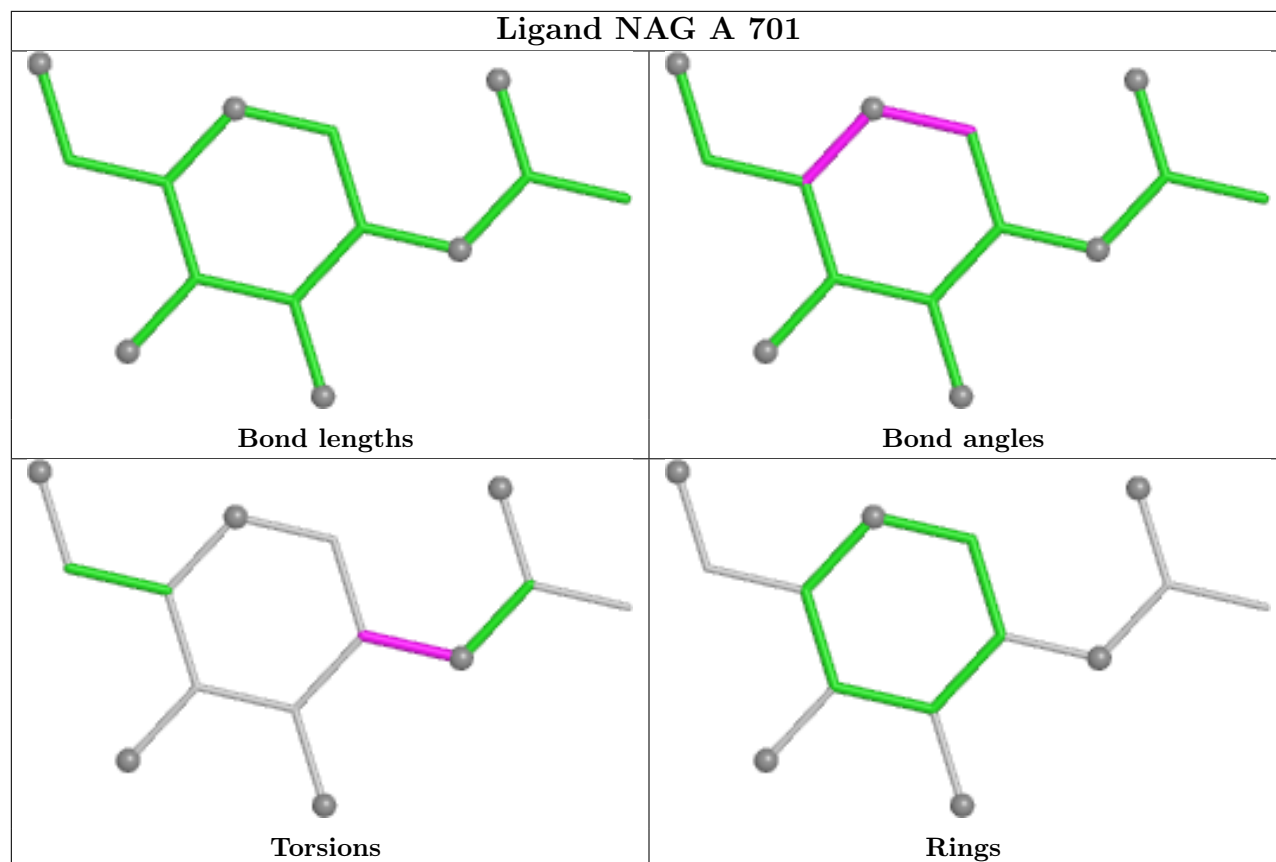


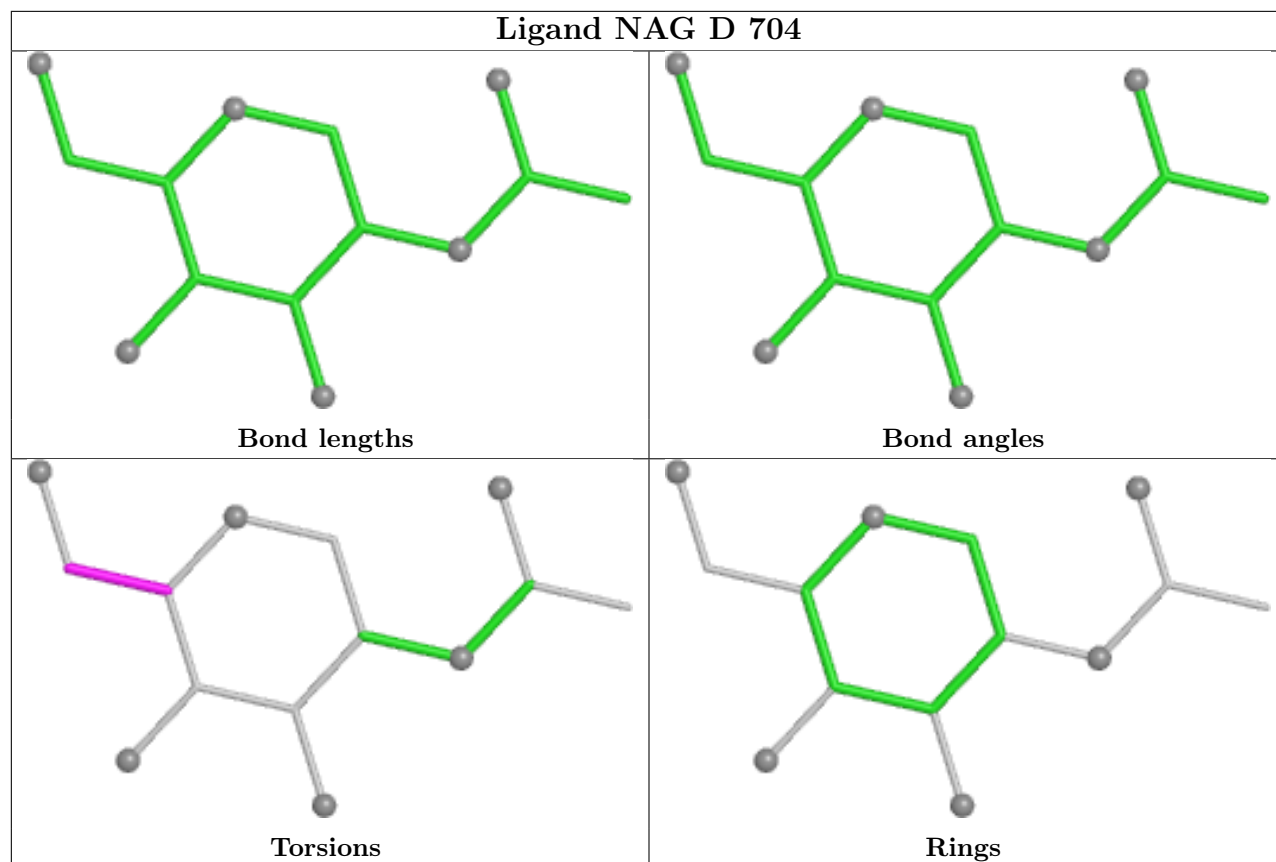












5.7 Other polymers [i](#)

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	590/634 (93%)	0.16	9 (1%) 72 57	74, 97, 147, 164	0
1	D	586/634 (92%)	0.19	11 (1%) 66 51	63, 91, 157, 194	0
2	B	178/230 (77%)	-0.08	2 (1%) 78 65	69, 80, 90, 95	0
2	E	178/230 (77%)	-0.03	1 (0%) 85 75	60, 72, 84, 158	0
3	C	25/43 (58%)	0.89	4 (16%) 5 6	83, 93, 110, 117	0
3	F	25/43 (58%)	0.58	3 (12%) 9 9	76, 85, 108, 119	0
All	All	1582/1814 (87%)	0.14	30 (1%) 66 51	60, 90, 142, 194	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	614	CYS	5.6
2	E	26	ASN	4.0
1	A	413	ASP	3.3
1	D	24	PHE	3.2
3	C	64	THR	3.2

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

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

6.3 Carbohydrates [i](#)

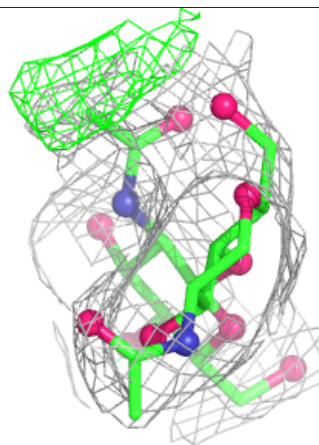
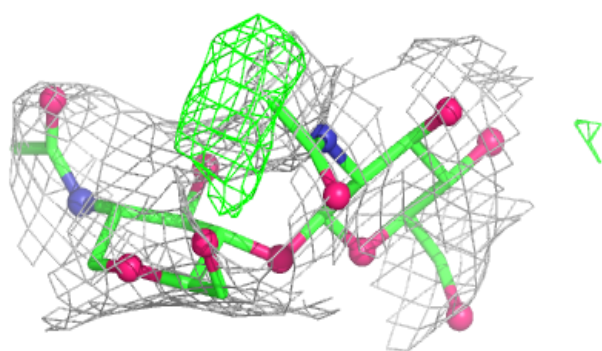
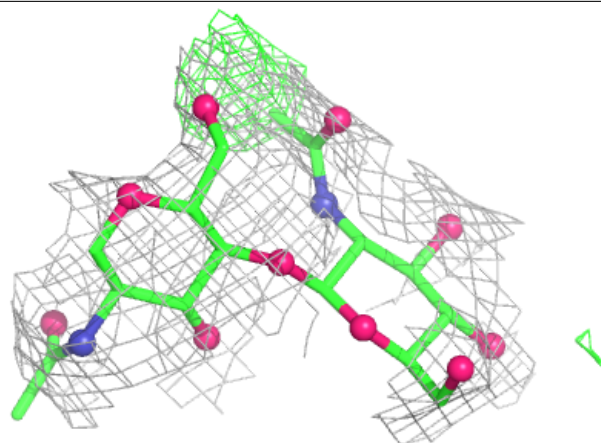
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	M	2	14/15	-0.03	0.15	122,122,122,122	0
4	NAG	G	2	14/15	0.29	0.14	134,134,134,134	0
4	NAG	L	2	14/15	0.41	0.18	141,141,141,141	0
4	NAG	I	2	14/15	0.47	0.13	124,124,124,124	0
5	BMA	K	3	11/12	0.48	0.14	104,104,104,104	0
4	NAG	L	1	14/15	0.52	0.18	125,125,125,125	0
4	NAG	H	2	14/15	0.56	0.14	141,141,141,141	0
4	NAG	H	1	14/15	0.56	0.18	130,130,130,130	0
4	NAG	I	1	14/15	0.60	0.14	118,118,118,118	0
4	NAG	O	2	14/15	0.69	0.13	99,99,99,99	0
6	MAN	P	4	11/12	0.69	0.18	92,92,92,92	0
4	NAG	G	1	14/15	0.75	0.15	125,125,125,125	0
4	NAG	J	2	14/15	0.77	0.12	108,108,108,108	0
5	FUC	K	5	10/11	0.78	0.16	108,108,108,108	0
4	NAG	N	2	14/15	0.78	0.11	104,104,104,104	0
6	BMA	P	3	11/12	0.80	0.12	94,94,94,94	0
4	NAG	M	1	14/15	0.80	0.12	113,113,113,113	0
4	NAG	N	1	14/15	0.81	0.14	94,94,94,94	0
6	FUC	P	5	10/11	0.82	0.13	78,78,78,78	0
5	NAG	K	2	14/15	0.87	0.12	99,99,99,104	0
4	NAG	J	1	14/15	0.89	0.08	97,97,97,97	0
6	NAG	P	2	14/15	0.90	0.12	82,82,82,82	0
6	FUC	P	6	10/11	0.90	0.11	90,90,90,90	0
6	NAG	P	1	14/15	0.91	0.11	81,81,81,81	0
4	NAG	O	1	14/15	0.91	0.08	86,86,86,86	0
5	NAG	K	1	14/15	0.93	0.08	94,94,94,94	0
5	FUC	K	4	10/11	0.97	0.06	93,93,93,93	0

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

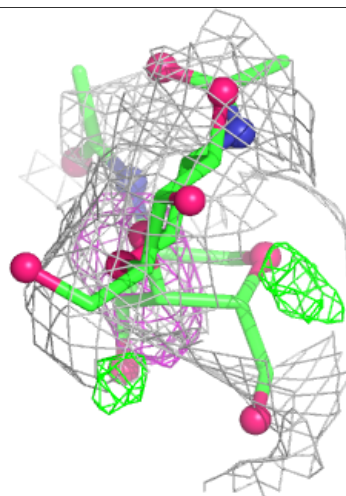
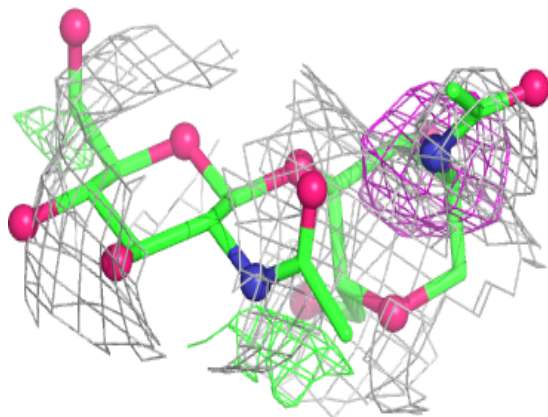
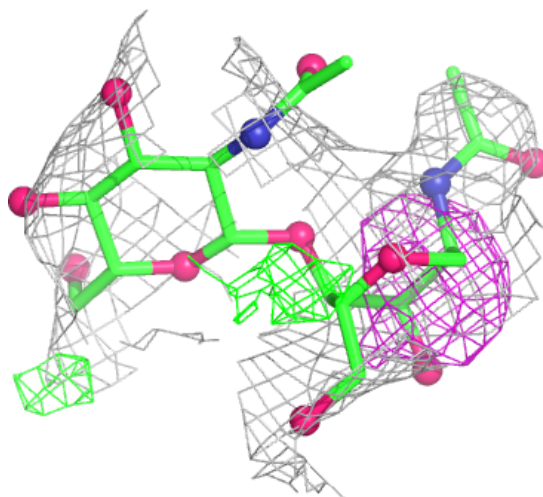
Electron density around Chain G:

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



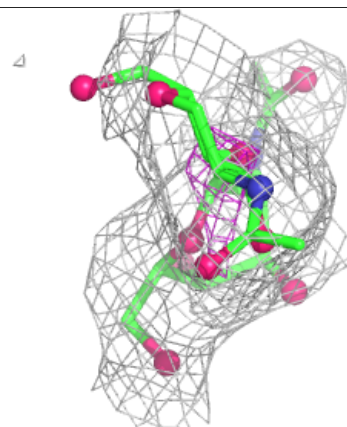
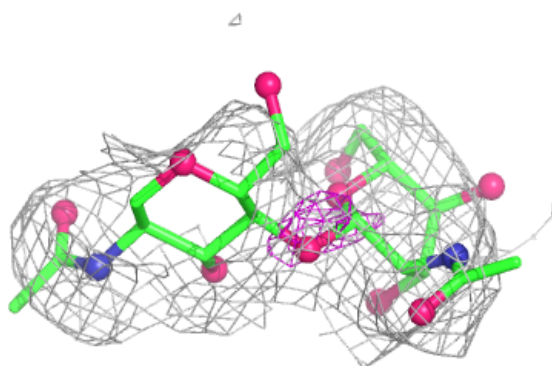
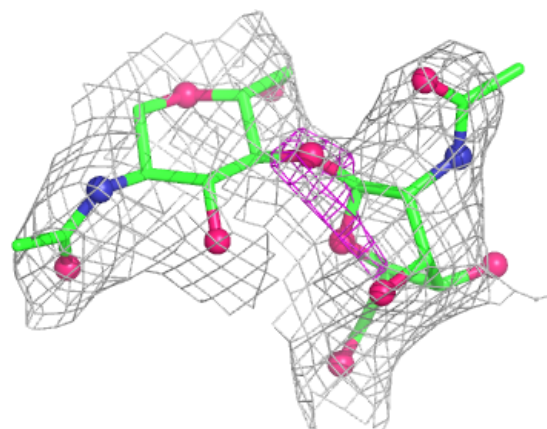
Electron density around Chain H:

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and green (positive)

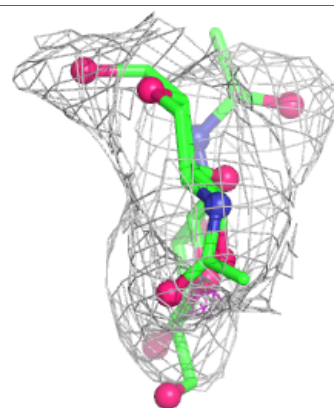
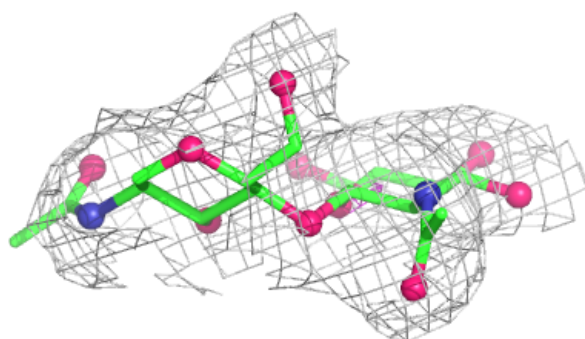
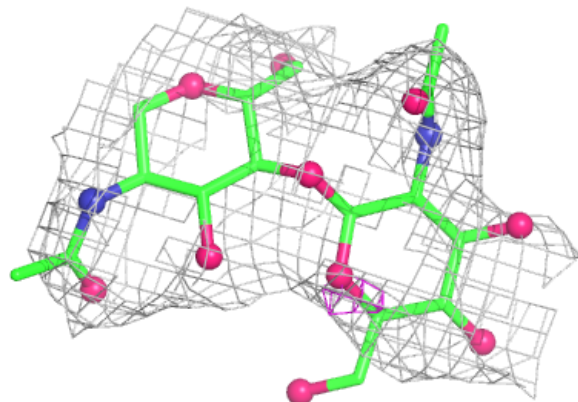


Electron density around Chain I:

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

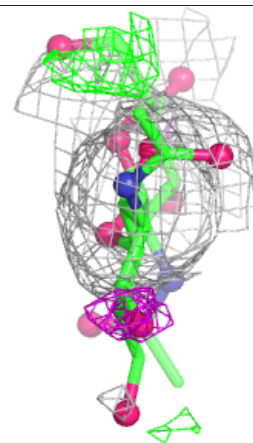
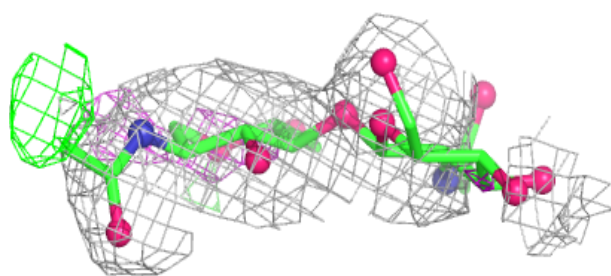
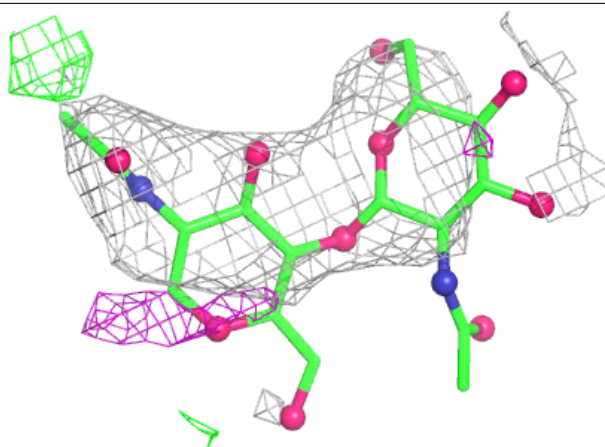
**Electron density around Chain J:**

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



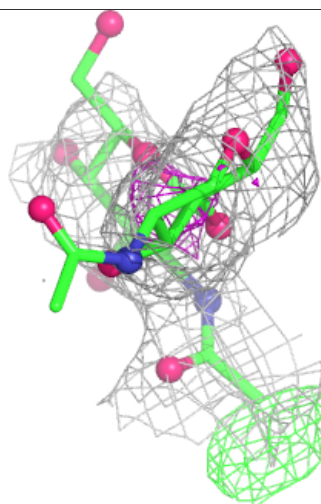
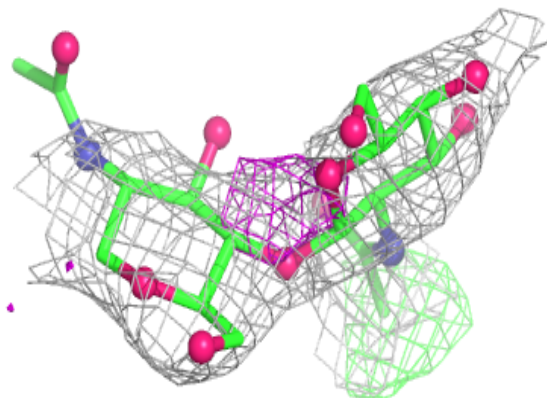
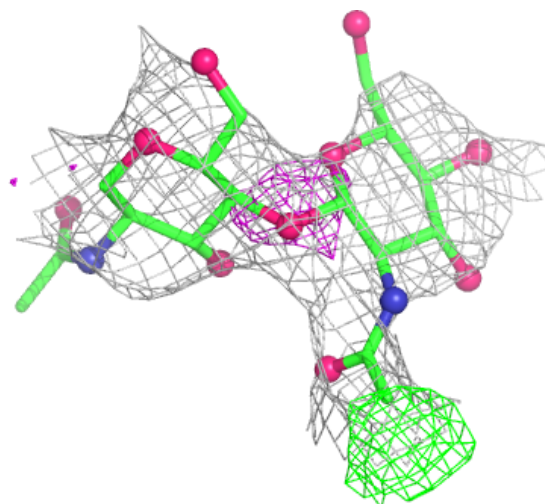
Electron density around Chain L:

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



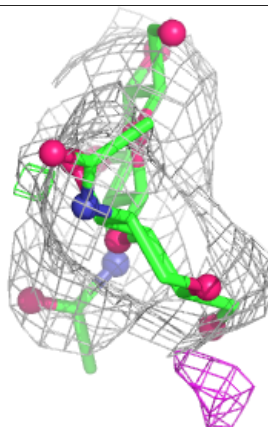
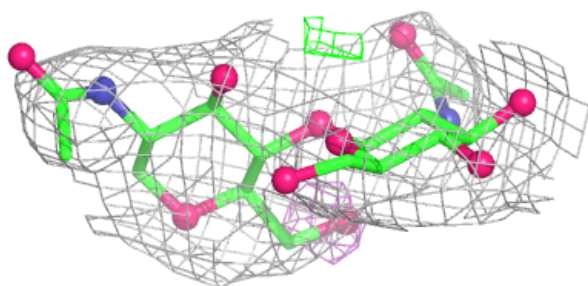
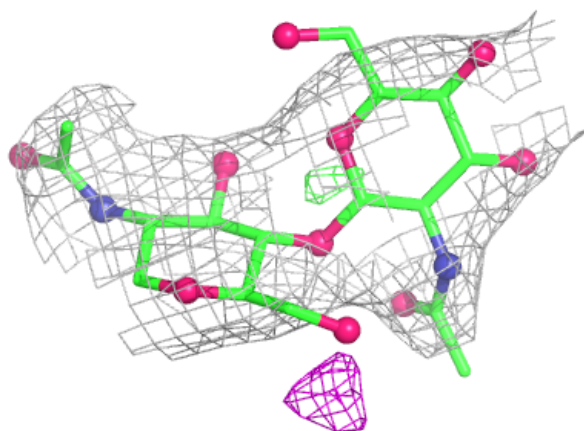
Electron density around Chain M:

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

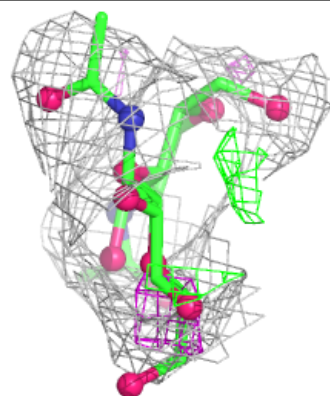
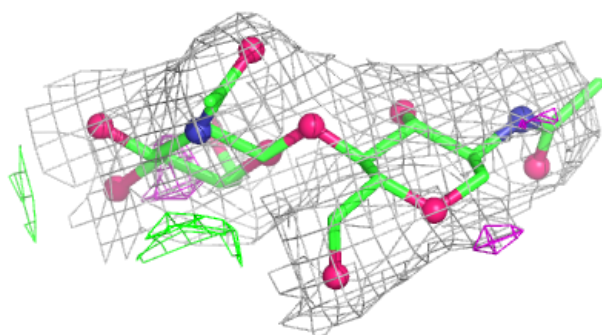
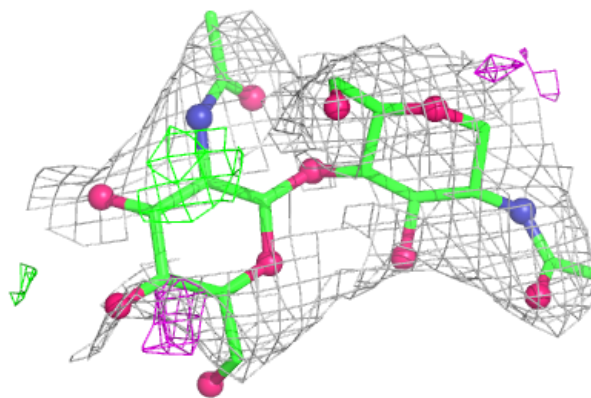


Electron density around Chain N:

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

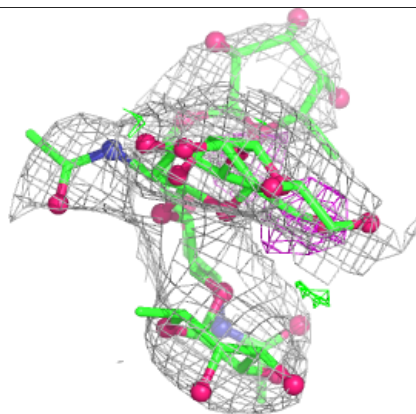
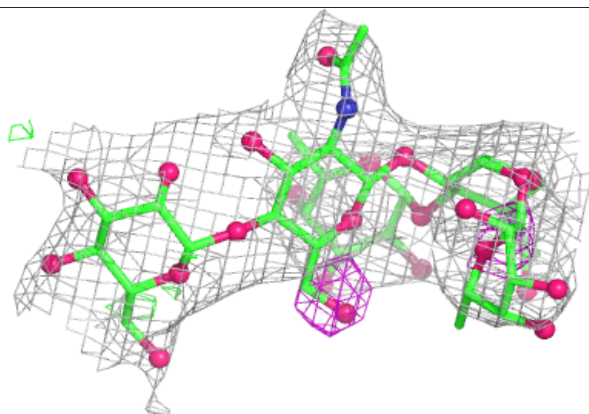
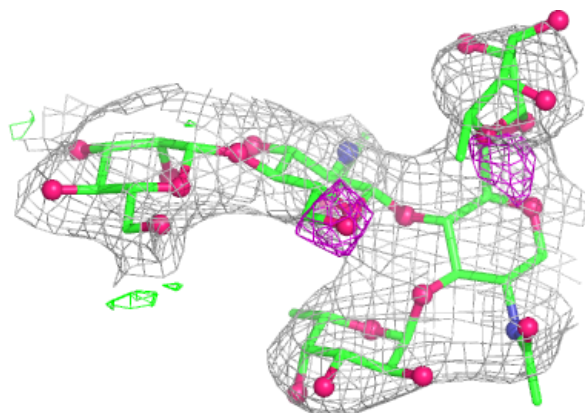
**Electron density around Chain O:**

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

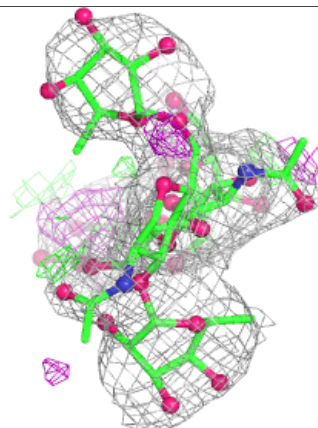
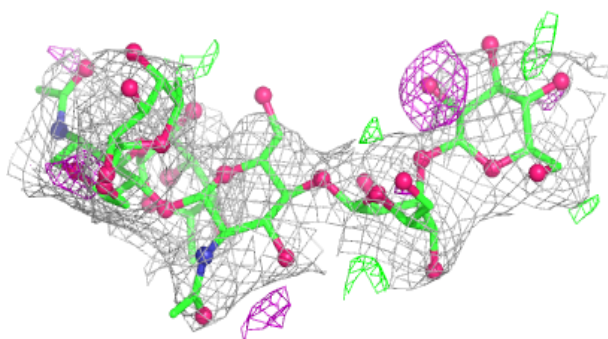
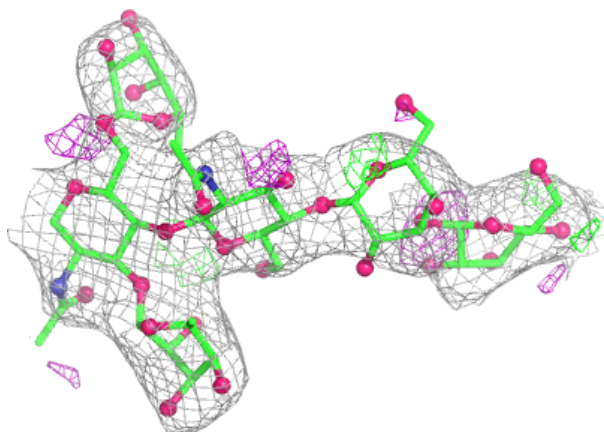


Electron density around Chain K:

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

**Electron density around Chain P:**

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



6.4 Ligands ⓘ

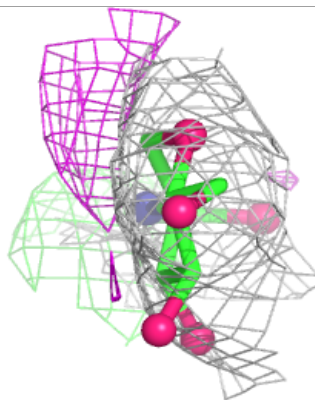
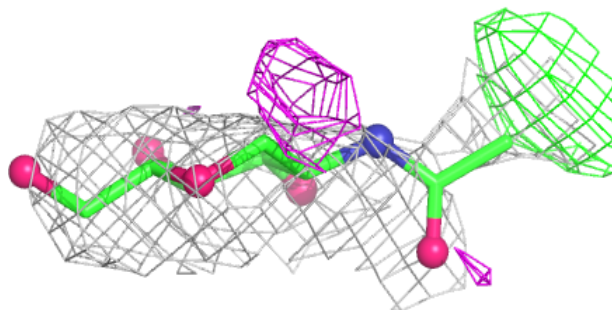
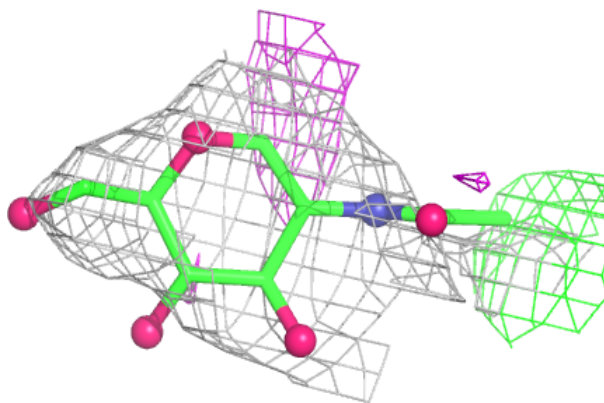
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	EDO	A	706	4/4	-0.01	0.22	107,107,107,107	0
7	NAG	D	705	14/15	0.32	0.18	108,108,108,108	0
10	PEG	C	101	7/7	0.41	0.22	109,109,109,109	0
8	EDO	D	706	4/4	0.45	0.18	97,97,97,97	0
7	NAG	A	705	14/15	0.47	0.19	157,157,157,157	0
7	NAG	E	301	14/15	0.55	0.14	101,101,101,101	0
7	NAG	B	302	14/15	0.56	0.14	105,105,105,105	0
10	PEG	A	708	7/7	0.57	0.18	102,102,102,102	0
7	NAG	D	701	14/15	0.63	0.19	141,141,141,141	0
7	NAG	D	704	14/15	0.66	0.13	101,101,101,101	0
8	EDO	B	303	4/4	0.67	0.15	89,89,89,89	0
8	EDO	D	708	4/4	0.67	0.19	89,89,89,89	0
7	NAG	A	702	14/15	0.68	0.15	115,115,115,115	0
7	NAG	D	702	14/15	0.71	0.13	132,132,132,132	0
7	NAG	B	301	14/15	0.71	0.11	98,98,98,98	0
7	NAG	A	701	14/15	0.72	0.15	130,130,130,130	0
7	NAG	A	703	14/15	0.73	0.14	102,102,102,102	0
7	NAG	D	703	14/15	0.74	0.15	123,123,123,123	0
8	EDO	E	302	4/4	0.78	0.17	83,83,83,83	0
7	NAG	A	704	14/15	0.83	0.15	98,98,98,98	0
8	EDO	E	303	4/4	0.85	0.16	76,76,76,76	0
9	CL	A	707	1/1	0.90	0.10	91,91,91,91	0
9	CL	D	707	1/1	0.91	0.14	70,70,70,70	0

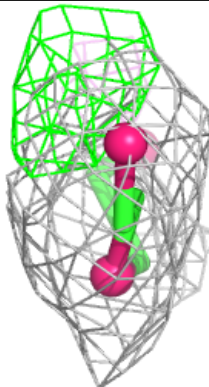
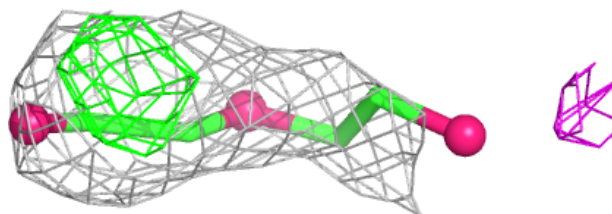
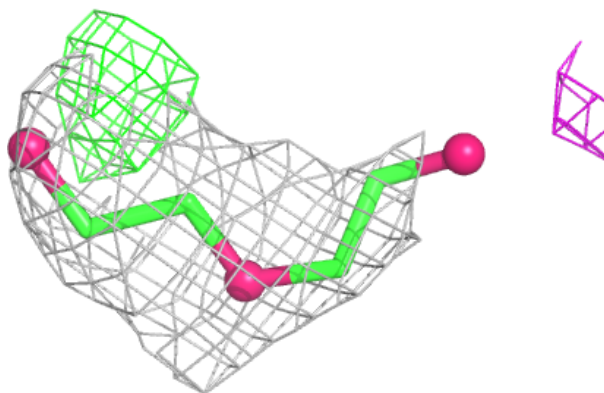
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG D 705:

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

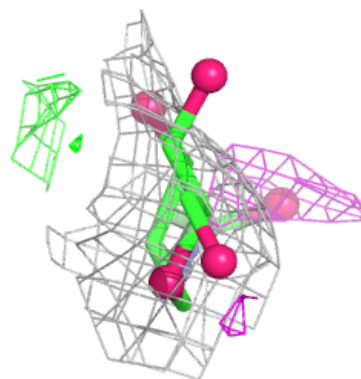
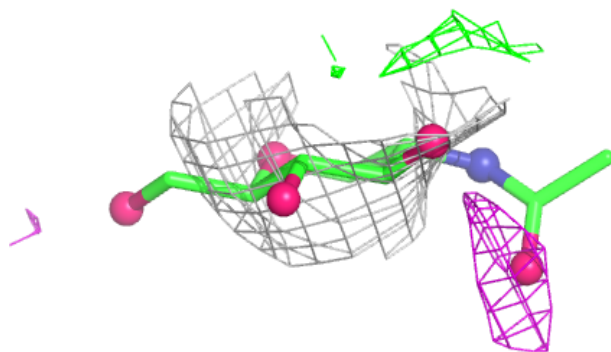
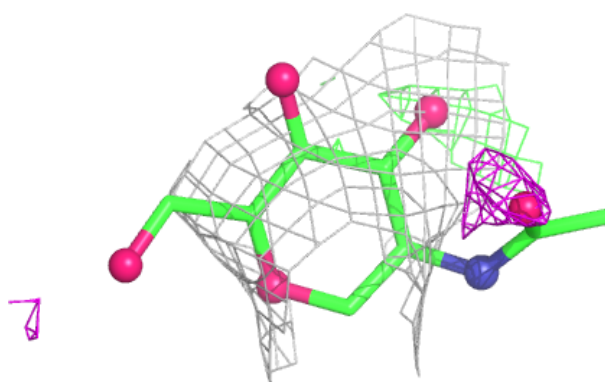
**Electron density around PEG C 101:**

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

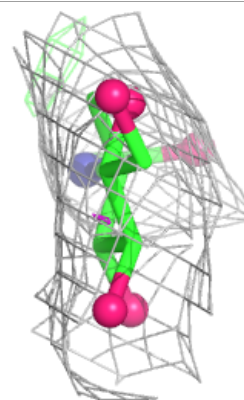
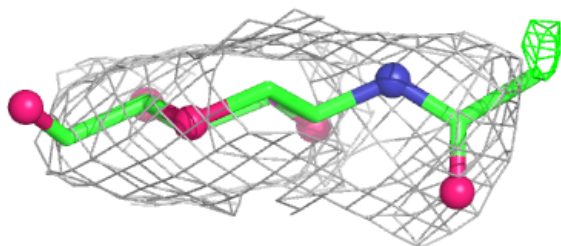
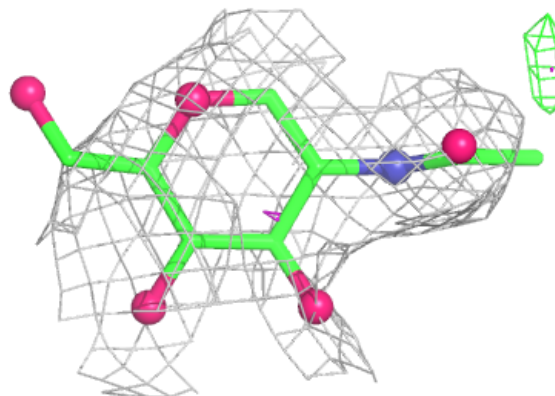


Electron density around NAG A 705:

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

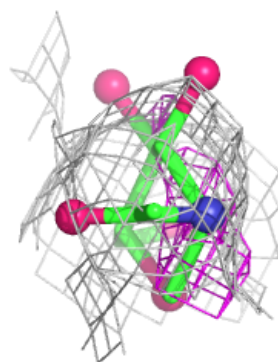
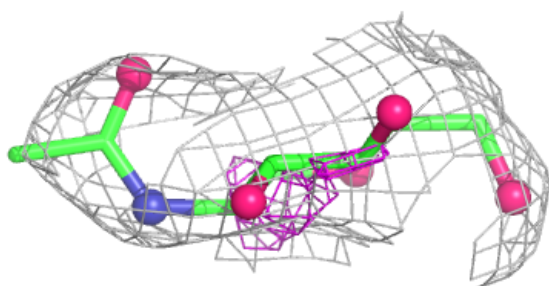
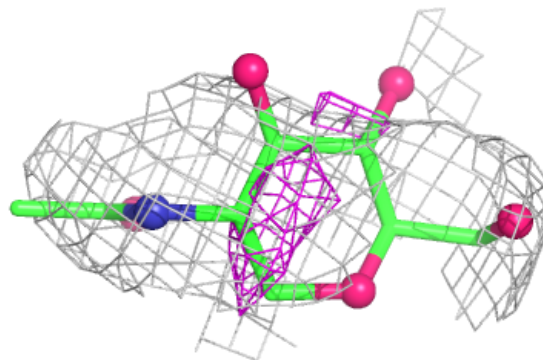
**Electron density around NAG E 301:**

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

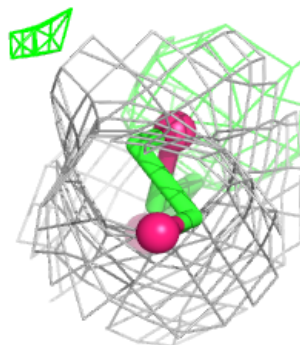
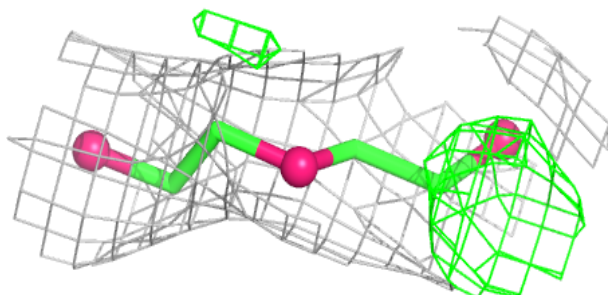
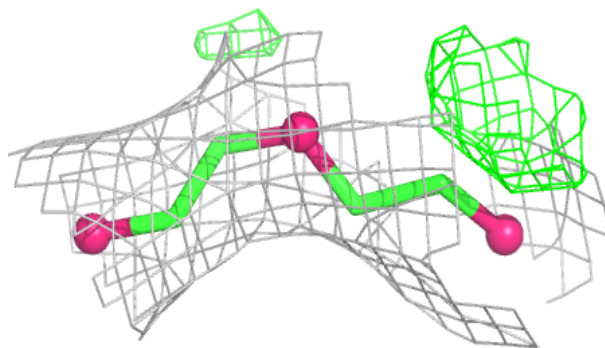


Electron density around NAG B 302:

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

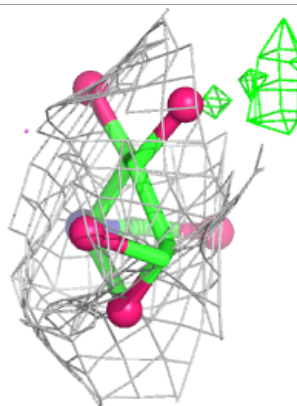
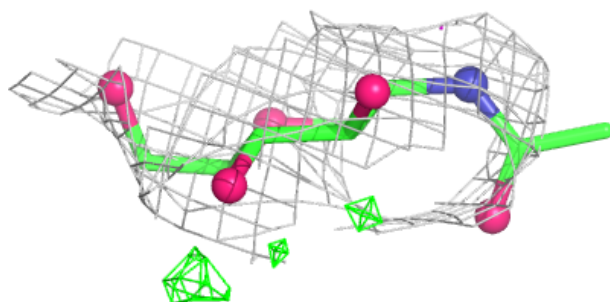
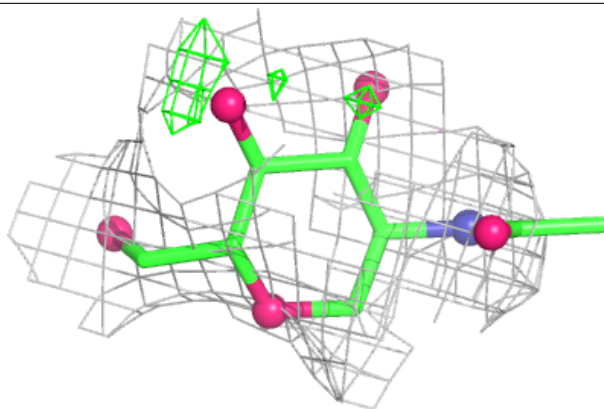
**Electron density around PEG A 708:**

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



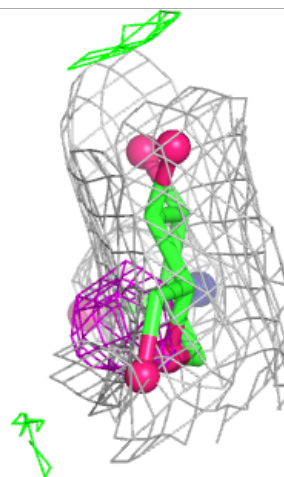
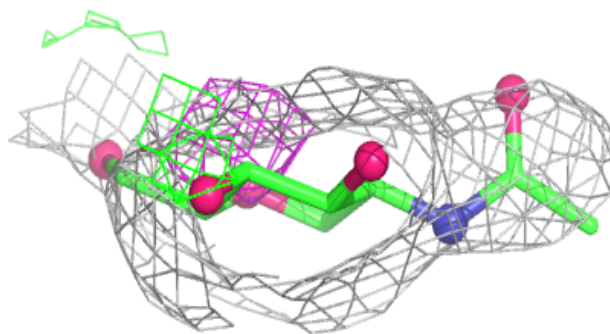
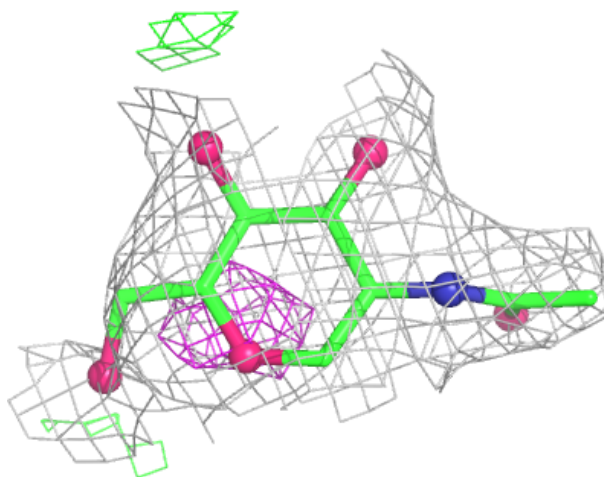
Electron density around NAG D 701:

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



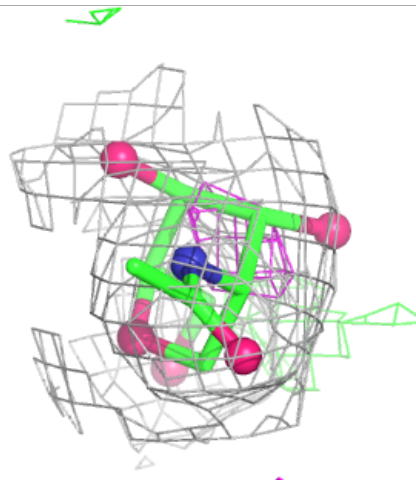
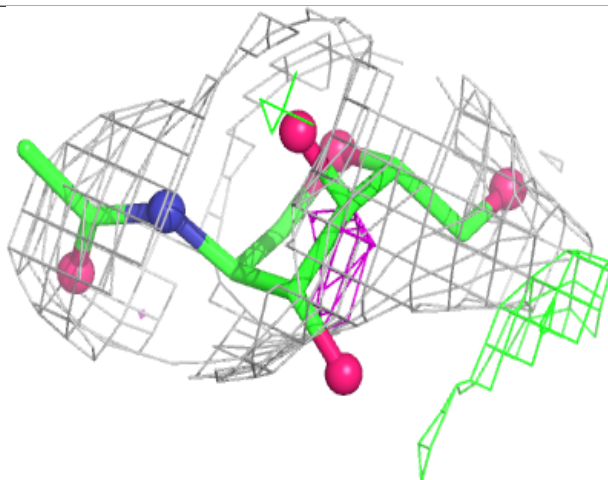
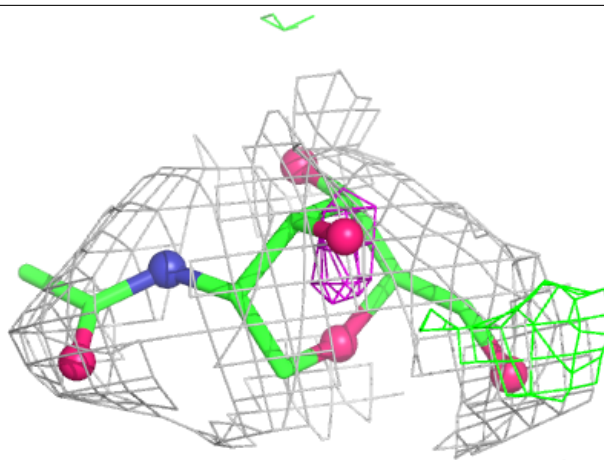
Electron density around NAG D 704:

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



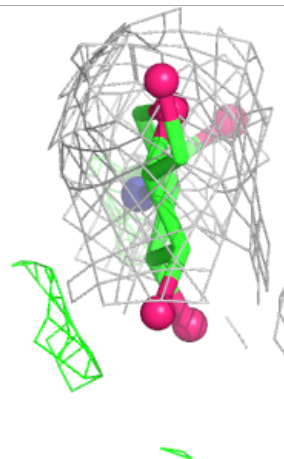
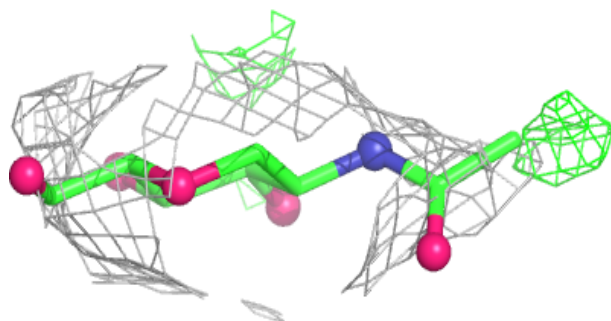
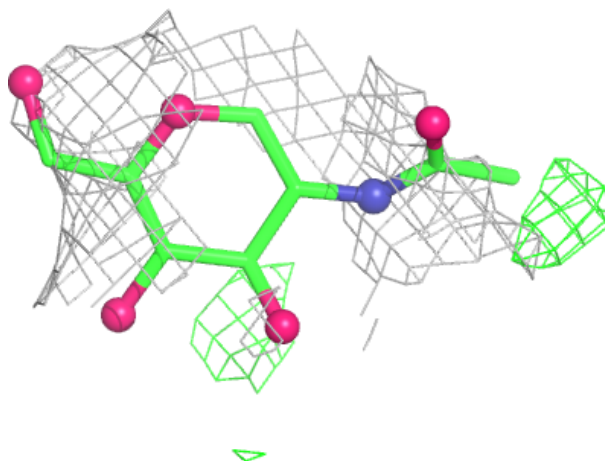
Electron density around NAG A 702:

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



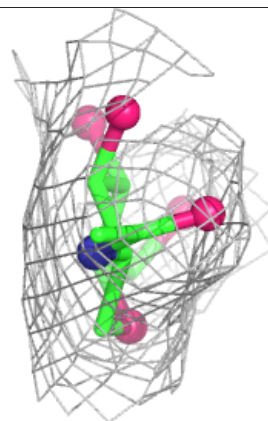
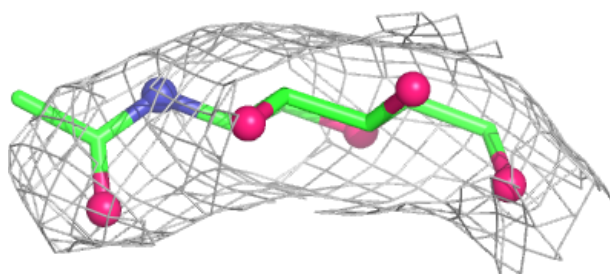
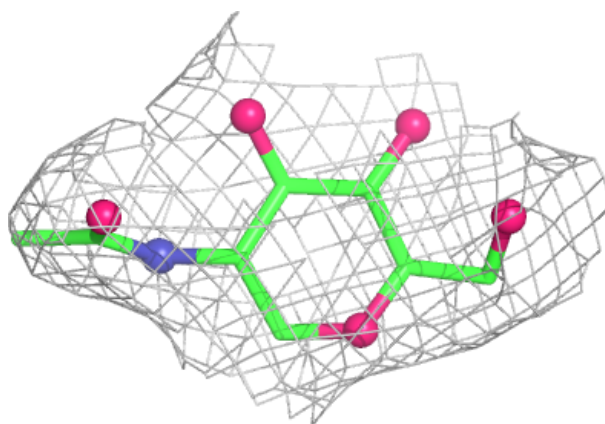
Electron density around NAG D 702:

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

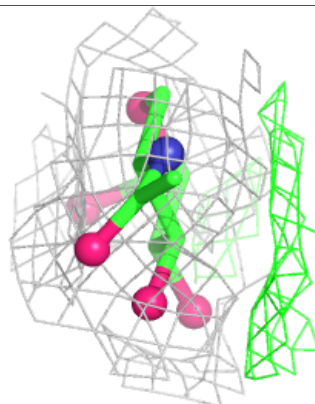
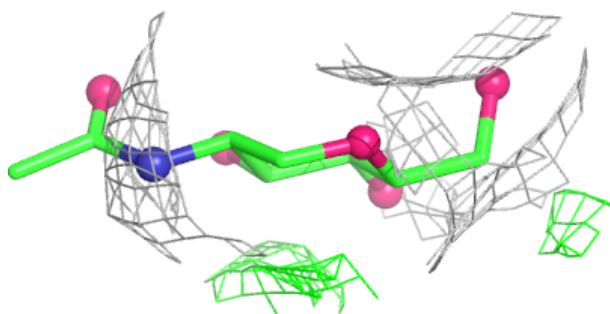
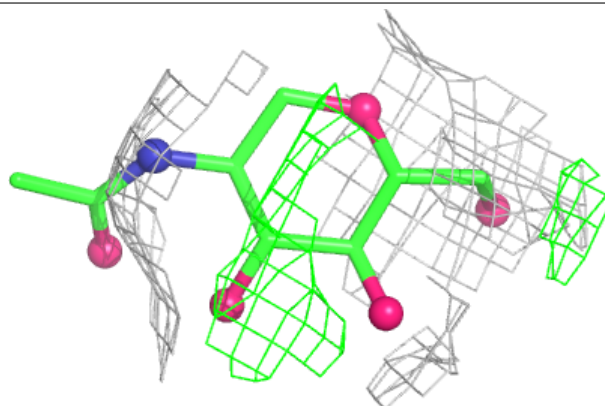


Electron density around NAG B 301:

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

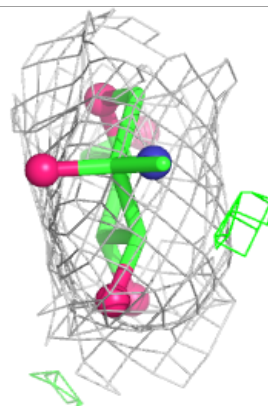
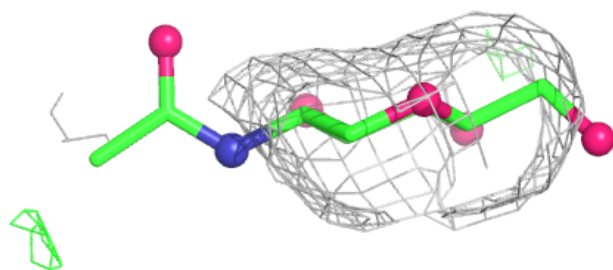
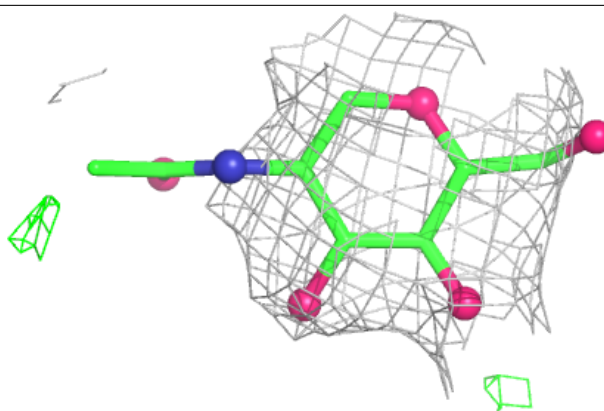
**Electron density around NAG A 701:**

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

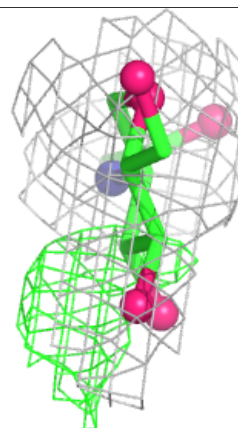
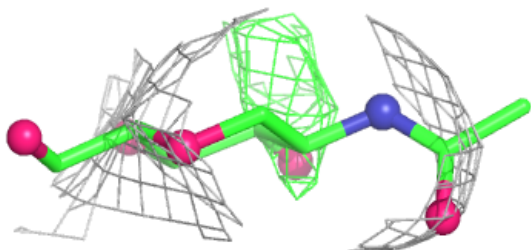
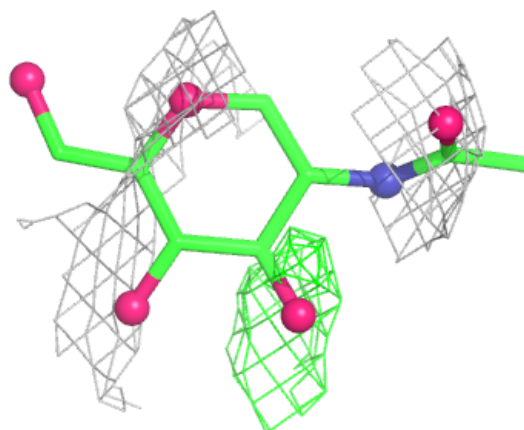


Electron density around NAG A 703:

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

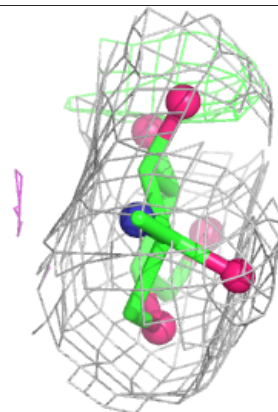
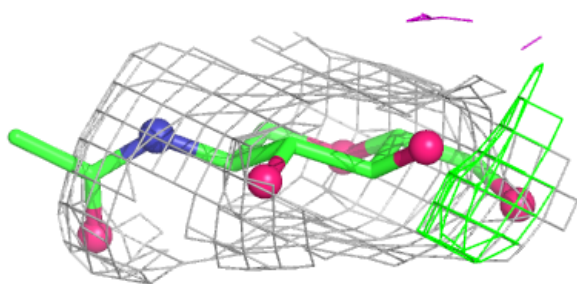
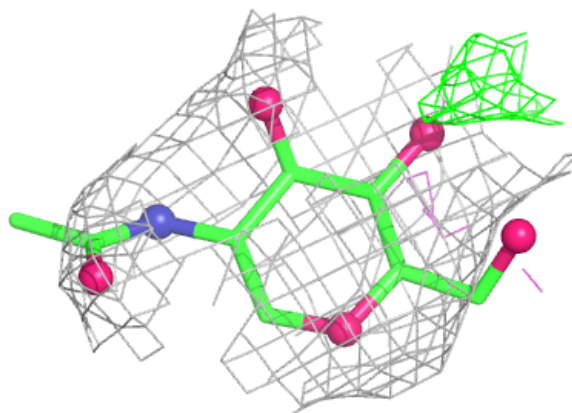
**Electron density around NAG D 703:**

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



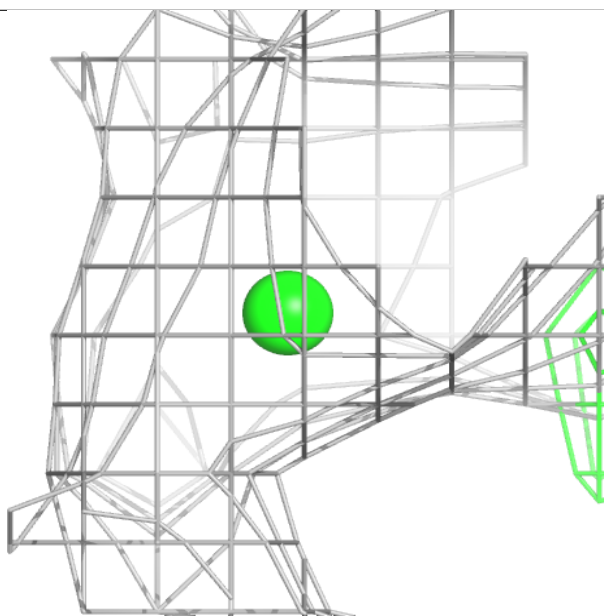
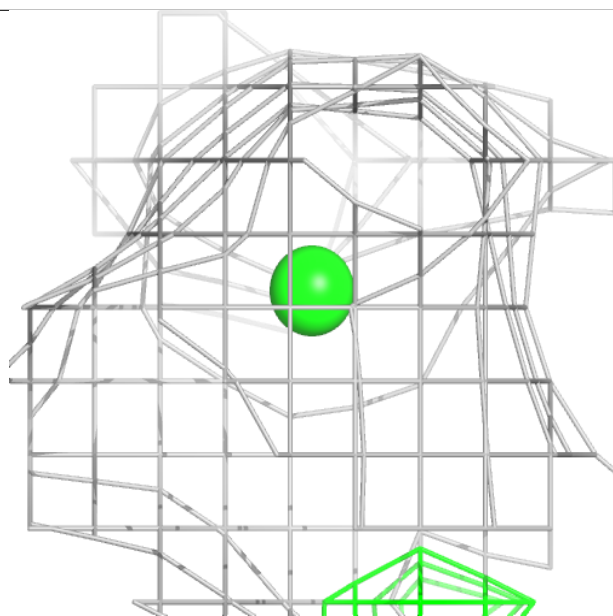
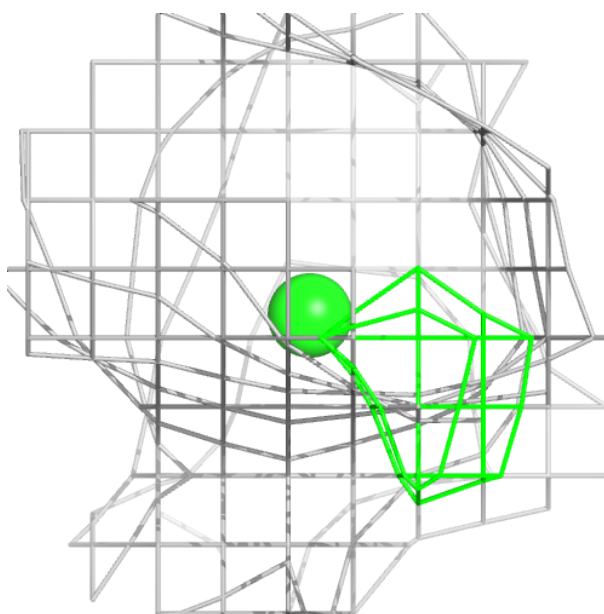
Electron density around NAG A 704:

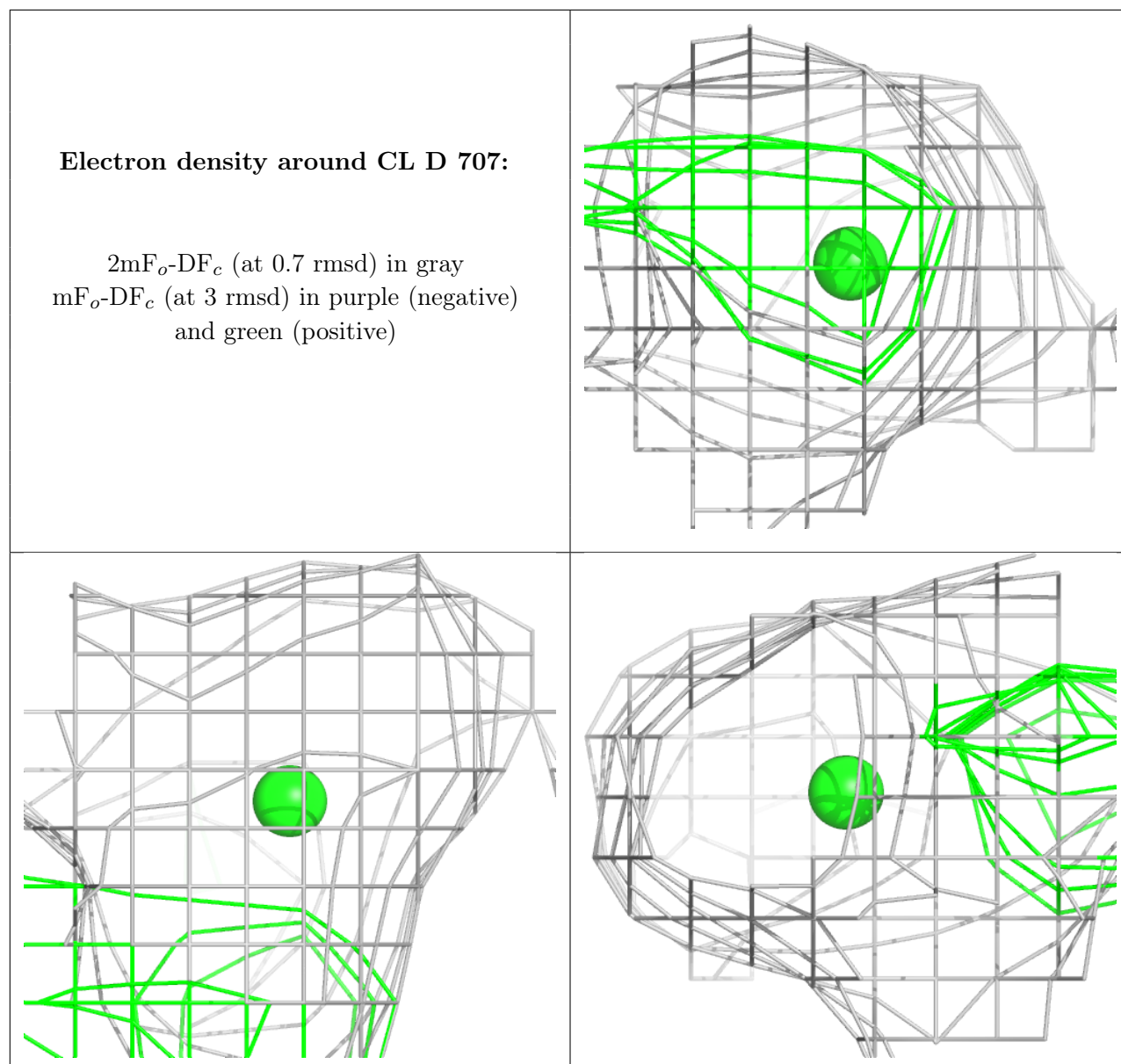
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL A 707:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.