



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:34 PM UTC

PDB ID : 6P6P / pdb_00006p6p
Title : Crystal structure of hemagglutinin from influenza virus A/Sichuan/2/1987 (H3N2)
Authors : Dai, Y.N.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2019-06-04
Resolution : 2.31 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:

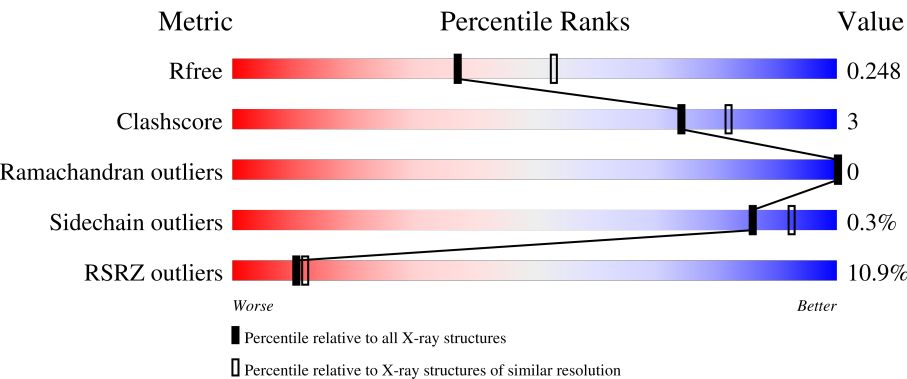
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.31 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.



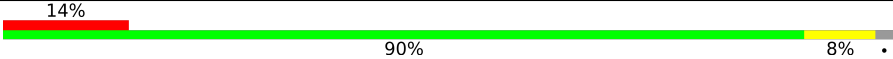
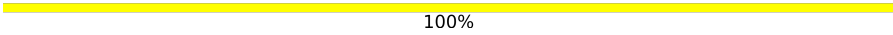
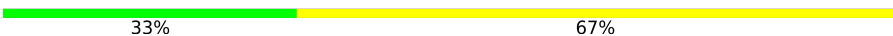
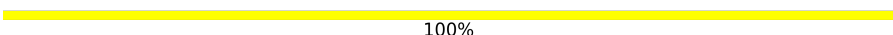
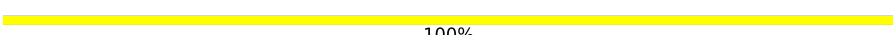
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	10% 92% 6%
1	B	497	12% 89% 9%
1	C	497	8% 90% 8%
1	D	497	9% 92% 6%

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Mol	Chain	Length	Quality of chain
1	E	497	
1	F	497	
2	G	3	
2	H	3	
2	I	3	
2	J	3	
2	K	3	
2	L	3	

2 Entry composition [i](#)

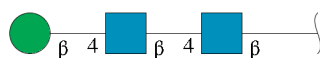
There are 4 unique types of molecules in this entry. The entry contains 24621 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	487	Total	C	N	O	S	0	1	0
			3849	2401	685	744	19			
1	B	488	Total	C	N	O	S	0	3	0
			3873	2418	688	748	19			
1	C	489	Total	C	N	O	S	0	3	0
			3878	2421	689	749	19			
1	D	489	Total	C	N	O	S	0	4	0
			3883	2424	690	750	19			
1	E	489	Total	C	N	O	S	0	4	0
			3883	2424	690	750	19			
1	F	489	Total	C	N	O	S	0	4	0
			3883	2424	690	750	19			

- Molecule 2 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
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

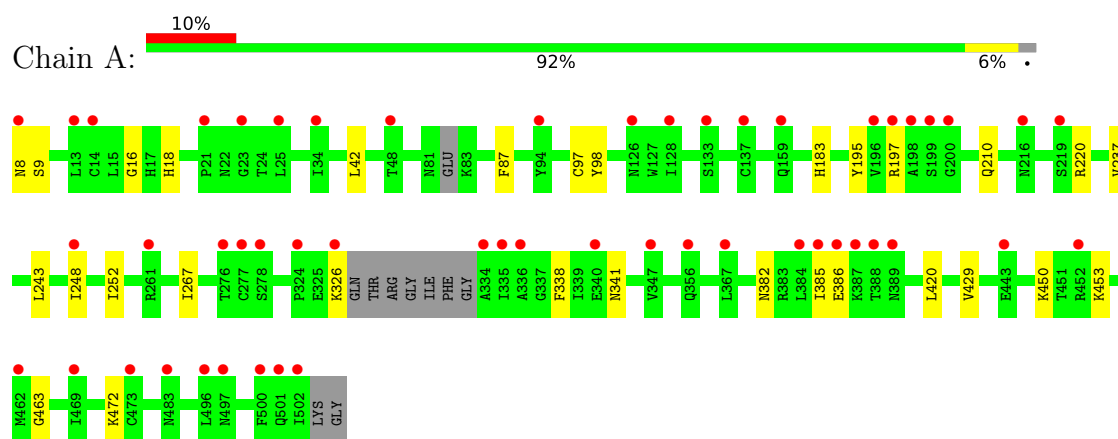
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total	O	0	0
			134	134		
4	B	126	Total	O	0	0
			126	126		
4	C	120	Total	O	0	0
			120	120		
4	D	141	Total	O	0	0
			141	141		
4	E	142	Total	O	0	0
			142	142		
4	F	139	Total	O	0	0
			139	139		

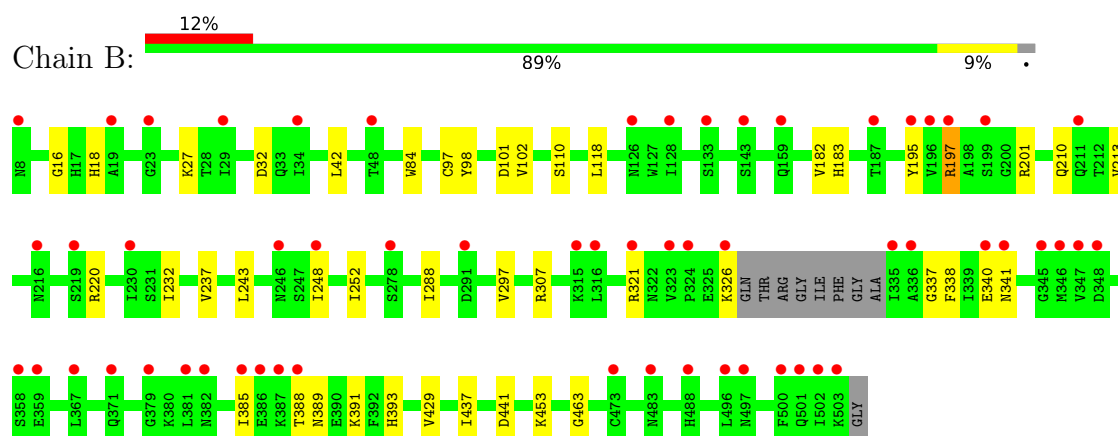
3 Residue-property plots [i](#)

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.

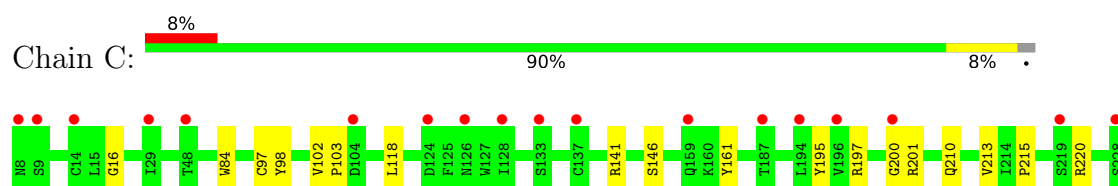
• Molecule 1: Hemagglutinin

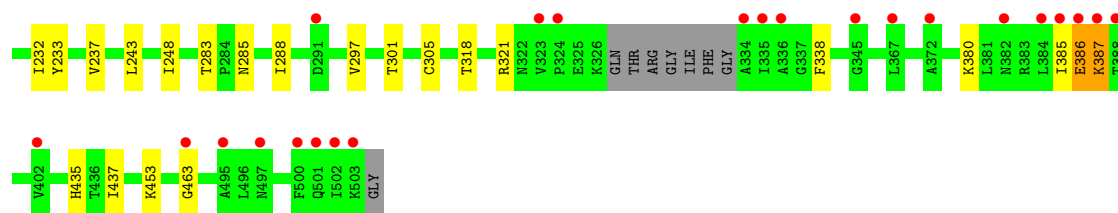


• Molecule 1: Hemagglutinin

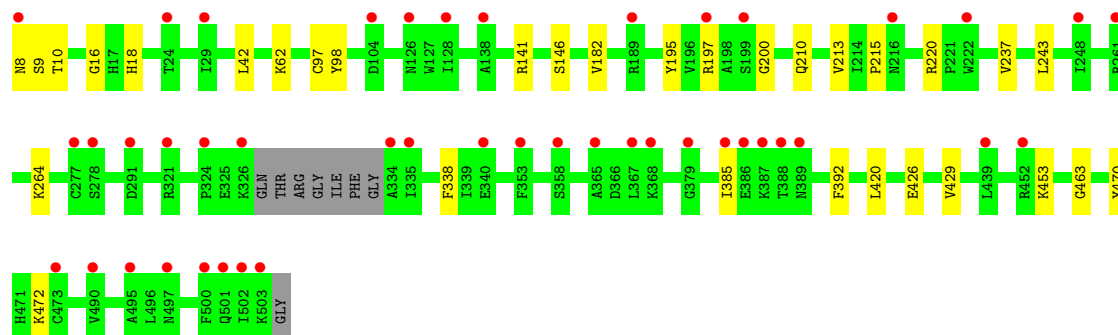
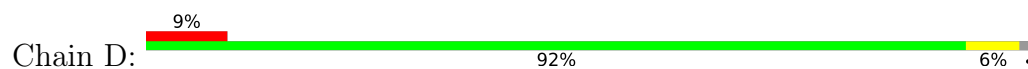


• Molecule 1: Hemagglutinin

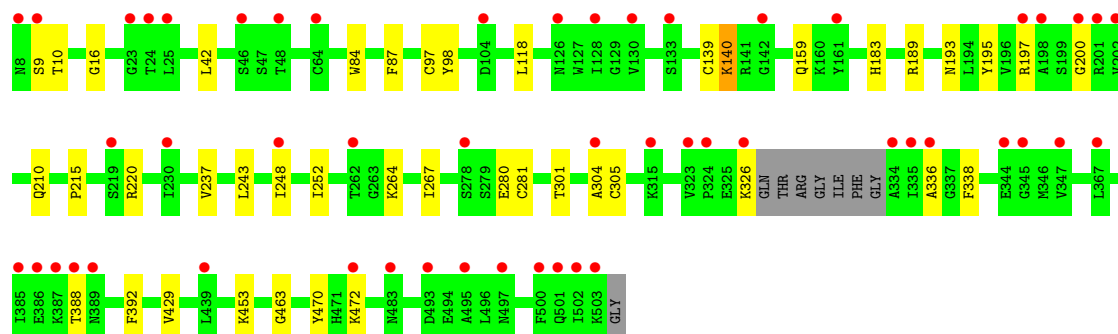
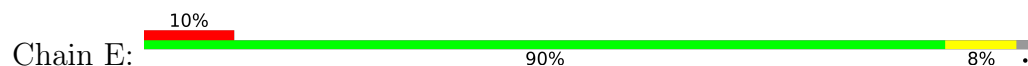




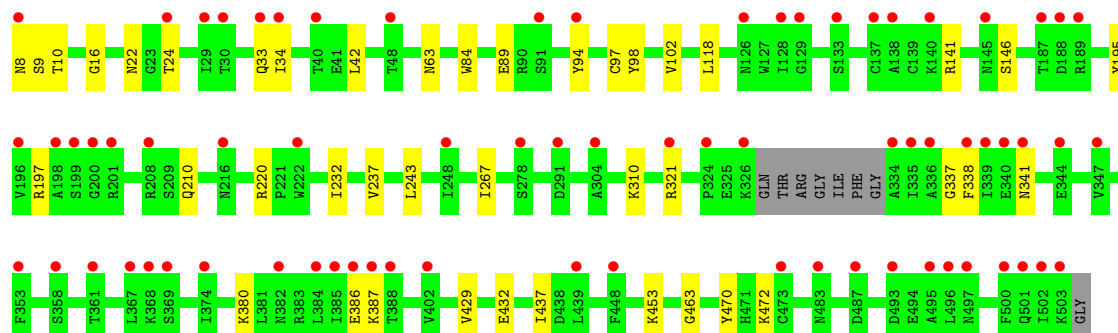
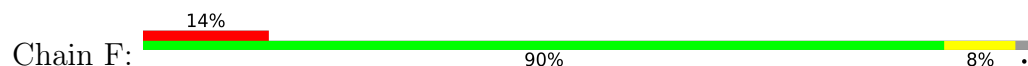
● Molecule 1: Hemagglutinin



● Molecule 1: Hemagglutinin



● Molecule 1: Hemagglutinin



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

Chain H:  100%

MAG1
MAG2
BMA3

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

Chain I:  33%  67%

MAG1
MAG2
BMA3

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

Chain K:  33%  67%

MAG1
MAG2
BMA3

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

Chain L:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.94Å 149.94Å 150.09Å 90.00° 135.01° 90.00°	Depositor
Resolution (Å)	47.47 – 2.31 47.47 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.47-2.31) 98.9 (47.47-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.221 , 0.251 (Not available) , 0.248	Depositor DCC
R_{free} test set	7163 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.014 for -h-2*k,l,h+1 0.014 for -h-k-l,l,k 0.017 for -h+k-l,-l,-k 0.022 for -k+l,-h-l,-l 0.021 for k+l,h+l,-l 0.418 for k-l,h+l,-k 0.410 for h+k+l,-l,-h-l 0.408 for -k-l,-h-l,k 0.409 for h-k+l,l,-h-l 0.015 for h,-k,-h-l 0.439 for h+2*k,l,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24621	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: NAG, BMA

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	0.13	0/3930	0.34	0/5319
1	B	0.14	0/3961	0.34	0/5361
1	C	0.14	0/3966	0.35	0/5368
1	D	0.12	0/3974	0.32	0/5379
1	E	0.25	2/3974 (0.1%)	0.35	0/5379
1	F	0.13	0/3974	0.34	0/5379
All	All	0.16	2/23779 (0.0%)	0.34	0/32185

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140	LYS	C-O	-7.50	1.14	1.23
1	E	140	LYS	CA-C	-7.27	1.43	1.52

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	3849	0	3733	20	0
1	B	3873	0	3767	30	0
1	C	3878	0	3772	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3883	0	3778	20	0
1	E	3883	0	3780	30	0
1	F	3883	0	3778	29	0
2	G	39	0	34	0	0
2	H	39	0	34	0	0
2	I	39	0	34	0	0
2	J	39	0	34	0	0
2	K	39	0	34	0	0
2	L	39	0	34	0	0
3	A	56	0	52	0	0
3	B	56	0	52	1	0
3	C	56	0	52	2	0
3	D	56	0	52	1	0
3	E	56	0	52	0	0
3	F	56	0	52	2	0
4	A	134	0	0	1	0
4	B	126	0	0	1	0
4	C	120	0	0	1	0
4	D	141	0	0	0	0
4	E	142	0	0	1	0
4	F	139	0	0	2	0
All	All	24621	0	23124	144	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 (144) 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:B:326:LYS:NZ	1:B:341:ASN:HB2	1.86	0.90
1:B:326:LYS:HZ3	1:B:341:ASN:HB2	1.41	0.85
1:A:326:LYS:HZ2	1:A:341:ASN:HB2	1.50	0.76
1:B:463:GLY:HA2	1:F:453:LYS:HD2	1.70	0.72
1:B:453:LYS:HD2	1:E:463:GLY:HA2	1.73	0.70
1:C:318:THR:HG21	3:C:701:NAG:H62	1.73	0.70
1:E:453:LYS:HD2	1:F:463:GLY:HA2	1.72	0.70
1:C:453:LYS:HD2	1:D:463:GLY:HA2	1.76	0.68
1:A:463:GLY:HA2	1:D:453:LYS:HD3	1.77	0.67
1:E:197:ARG:HD2	1:E:248:ILE:HG23	1.75	0.67
1:C:285:ASN:ND2	3:C:706:NAG:O7	2.28	0.66
1:D:62:LYS:HD3	3:D:702:NAG:H82	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:CYS:SG	1:E:139:CYS:CB	2.85	0.64
1:B:321:ARG:NH2	1:B:441:ASP:OD2	2.31	0.63
1:C:16:GLY:HA2	1:C:338:PHE:HB3	1.81	0.63
1:B:321:ARG:HH21	1:B:437:ILE:HG22	1.65	0.62
1:A:453:LYS:HD3	1:C:463:GLY:HA2	1.81	0.62
1:B:16:GLY:HA2	1:B:338:PHE:HB3	1.81	0.61
1:B:201:ARG:H	1:B:248:ILE:HB	1.66	0.60
1:D:16:GLY:HA2	1:D:338:PHE:HB3	1.81	0.60
1:B:307:ARG:HE	1:B:388:THR:CG2	2.15	0.60
1:C:380:LYS:HZ1	1:C:435:HIS:HB3	1.66	0.59
1:C:386:GLU:HG2	1:C:387:LYS:N	2.17	0.59
1:A:382:ASN:O	1:A:386:GLU:HG3	2.03	0.59
1:B:195:TYR:O	1:B:197:ARG:N	2.34	0.58
1:F:33:GLN:NE2	4:F:802:HOH:O	2.36	0.58
1:C:161:TYR:O	1:C:197:ARG:NH2	2.37	0.57
1:C:386:GLU:HG2	1:C:387:LYS:H	1.69	0.57
1:F:9:SER:HA	1:F:472:LYS:HD3	1.85	0.57
1:C:210:GLN:OE1	1:D:220:ARG:NE	2.39	0.56
1:B:220:ARG:NE	1:F:210:GLN:OE1	2.37	0.56
1:A:197:ARG:HD2	1:A:248:ILE:HG23	1.89	0.55
1:E:195:TYR:O	1:E:197:ARG:N	2.39	0.54
1:B:307:ARG:HE	1:B:388:THR:HG21	1.72	0.54
1:E:16:GLY:HA2	1:E:338:PHE:HB3	1.89	0.54
1:E:97:CYS:SG	1:E:139:CYS:HB2	2.47	0.54
1:F:8:ASN:O	1:F:472:LYS:NZ	2.39	0.54
1:D:200:GLY:O	1:D:215:PRO:HD2	2.07	0.53
1:B:210:GLN:OE1	1:E:220:ARG:NE	2.37	0.53
1:C:213:VAL:HG21	1:C:233:TYR:CE2	2.43	0.53
1:A:16:GLY:HA2	1:A:338:PHE:HB3	1.90	0.53
1:C:195:TYR:O	1:C:197:ARG:N	2.41	0.53
1:E:97:CYS:HA	1:E:139:CYS:HB2	1.90	0.53
1:A:195:TYR:O	1:A:197:ARG:N	2.42	0.52
1:F:321:ARG:HH21	1:F:437:ILE:HG21	1.74	0.52
1:B:102:VAL:HG22	1:B:232:ILE:HB	1.91	0.52
1:C:200:GLY:O	1:C:215:PRO:HD2	2.09	0.52
1:D:195:TYR:O	1:D:197:ARG:N	2.41	0.52
1:F:195:TYR:O	1:F:197:ARG:N	2.41	0.52
1:C:283:THR:HG22	1:C:301:THR:HG22	1.92	0.51
1:E:237:VAL:HG21	1:E:243:LEU:HB2	1.91	0.51
1:C:197:ARG:HE	1:C:248:ILE:HB	1.76	0.51
1:E:200:GLY:O	1:E:215:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:VAL:HG21	1:F:243:LEU:HB2	1.93	0.51
1:D:9:SER:HA	1:D:472:LYS:HD3	1.93	0.51
1:B:326:LYS:NZ	1:B:340:GLU:O	2.44	0.51
1:F:16:GLY:HA2	1:F:338:PHE:HB3	1.92	0.50
1:D:141:ARG:NH1	1:D:146:SER:OG	2.44	0.50
1:C:380:LYS:NZ	1:C:435:HIS:HB3	2.25	0.50
1:C:237:VAL:HG21	1:C:243:LEU:HB2	1.94	0.49
1:A:87:PHE:HB3	1:A:267:ILE:HG13	1.94	0.49
1:A:385:ILE:HG22	1:A:385:ILE:O	2.12	0.49
1:B:27:LYS:HG2	1:B:32:ASP:O	2.13	0.49
1:A:220:ARG:NE	1:D:210:GLN:OE1	2.41	0.49
1:E:388:THR:HG23	1:F:310:LYS:NZ	2.27	0.49
1:D:237:VAL:HG21	1:D:243:LEU:HB2	1.95	0.48
1:B:42:LEU:HD12	1:B:429:VAL:HG22	1.94	0.48
1:E:326:LYS:HZ1	1:E:336:ALA:HB1	1.79	0.48
1:B:237:VAL:HG21	1:B:243:LEU:HB2	1.94	0.48
1:F:102:VAL:HG22	1:F:232:ILE:HB	1.94	0.48
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.96	0.48
1:E:97:CYS:HG	1:E:139:CYS:HG	0.48	0.48
1:E:183:HIS:HB2	1:E:252:ILE:HD11	1.95	0.48
1:B:337:GLY:O	1:B:341:ASN:HB3	2.14	0.47
1:A:8:ASN:O	1:A:472:LYS:NZ	2.47	0.47
1:A:9:SER:HA	1:A:472:LYS:HD3	1.97	0.47
1:D:385:ILE:HG22	1:D:385:ILE:O	2.15	0.47
1:E:9:SER:HA	1:E:472:LYS:HD3	1.97	0.46
1:D:8:ASN:O	1:D:472:LYS:NZ	2.42	0.46
1:E:388:THR:HG23	1:F:310:LYS:HZ1	1.80	0.46
1:E:280:GLU:HB3	1:E:304:ALA:HB3	1.97	0.46
1:C:285:ASN:HA	4:C:810:HOH:O	2.16	0.46
1:A:237:VAL:HG21	1:A:243:LEU:HB2	1.97	0.46
1:D:10:THR:HG22	1:D:470:TYR:HA	1.98	0.45
1:C:141:ARG:NH1	1:C:146:SER:OG	2.50	0.45
1:C:201:ARG:H	1:C:248:ILE:HG13	1.81	0.45
1:F:141:ARG:NH1	1:F:146:SER:OG	2.49	0.45
1:B:389:ASN:OD1	1:B:391:LYS:HE2	2.17	0.45
1:B:97:CYS:SG	1:B:98:TYR:N	2.88	0.45
1:F:380:LYS:HD3	1:F:432:GLU:OE1	2.17	0.45
1:C:97:CYS:SG	1:C:98:TYR:N	2.89	0.45
1:E:210:GLN:OE1	1:F:220:ARG:NE	2.47	0.45
1:F:10:THR:HG22	1:F:470:TYR:HA	1.99	0.44
1:B:183:HIS:HB2	1:B:252:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ILE:HG22	1:B:385:ILE:O	2.17	0.44
1:A:97:CYS:SG	1:A:98:TYR:N	2.87	0.44
1:A:210:GLN:OE1	1:C:220:ARG:NE	2.46	0.44
1:E:159:GLN:NE2	4:E:808:HOH:O	2.48	0.44
1:B:288:ILE:HG21	1:B:297:VAL:HG21	1.99	0.44
1:C:321:ARG:HH21	1:C:437:ILE:HG21	1.83	0.44
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.98	0.44
1:F:24:THR:OG1	3:F:700:NAG:H81	2.17	0.44
1:F:89:GLU:HG3	1:F:267:ILE:HD11	2.00	0.44
1:E:97:CYS:SG	1:E:98:TYR:N	2.90	0.43
1:F:42:LEU:HD12	1:F:429:VAL:HG22	2.00	0.43
3:B:706:NAG:H62	4:B:883:HOH:O	2.17	0.43
1:C:387:LYS:HE2	1:D:426:GLU:HG2	1.99	0.43
1:F:22:ASN:ND2	3:F:700:NAG:O7	2.52	0.43
1:E:10:THR:HG22	1:E:470:TYR:HA	2.01	0.43
1:D:264:LYS:HD3	1:D:392:PHE:CZ	2.54	0.43
1:C:385:ILE:O	1:C:385:ILE:HG22	2.19	0.43
1:D:182:VAL:HG21	1:D:213:VAL:HB	2.01	0.43
1:A:42:LEU:HD12	1:A:429:VAL:HG22	2.01	0.42
1:E:301:THR:HB	1:E:305:CYS:SG	2.59	0.42
1:C:301:THR:HB	1:C:305:CYS:SG	2.59	0.42
1:E:264:LYS:HD3	1:E:392:PHE:CZ	2.54	0.42
1:F:97:CYS:SG	1:F:98:TYR:N	2.90	0.42
1:C:84:TRP:CZ3	1:C:118:LEU:HG	2.55	0.42
1:E:84:TRP:CZ3	1:E:118:LEU:HG	2.55	0.42
1:F:337:GLY:O	1:F:341:ASN:HB3	2.20	0.42
1:B:101:ASP:OD2	1:F:210:GLN:NE2	2.49	0.42
1:C:84:TRP:HZ3	1:C:118:LEU:HG	1.85	0.42
1:C:103:PRO:HG2	1:C:233:TYR:CE1	2.55	0.42
1:E:281:CYS:HB2	1:E:304:ALA:O	2.19	0.42
1:B:110:SER:OG	1:B:393:HIS:NE2	2.48	0.42
1:F:386:GLU:C	1:F:387:LYS:HG2	2.45	0.42
1:C:288:ILE:HG21	1:C:297:VAL:HG21	2.02	0.41
1:E:42:LEU:HD12	1:E:429:VAL:HG22	2.02	0.41
1:F:84:TRP:CZ3	1:F:118:LEU:HG	2.56	0.41
1:A:197:ARG:HD2	1:A:248:ILE:CG2	2.50	0.41
1:A:420:LEU:HD13	1:D:420:LEU:HD13	2.02	0.41
1:E:87:PHE:HB3	1:E:267:ILE:HG13	2.00	0.41
1:D:42:LEU:HD12	1:D:429:VAL:HG22	2.03	0.41
1:B:84:TRP:CZ3	1:B:118:LEU:HG	2.55	0.41
1:E:189:ARG:HG2	1:E:193:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ILE:HD11	1:F:321:ARG:HE	1.85	0.41
1:F:386:GLU:O	1:F:387:LYS:HG2	2.21	0.41
1:A:450:LYS:NZ	4:A:823:HOH:O	2.53	0.41
1:B:307:ARG:HE	1:B:388:THR:HG22	1.86	0.41
1:D:97:CYS:SG	1:D:98:TYR:N	2.89	0.41
1:E:388:THR:HG21	4:F:873:HOH:O	2.21	0.41
1:B:182:VAL:HG21	1:B:213:VAL:HB	2.02	0.41
1:F:63:ASN:HB3	1:F:94:TYR:CE1	2.57	0.40
1:B:32:ASP:OD1	1:B:32:ASP:N	2.53	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%)	460 (95%)	22 (5%)	0	100	100
1	B	487/497 (98%)	463 (95%)	24 (5%)	0	100	100
1	C	488/497 (98%)	465 (95%)	23 (5%)	0	100	100
1	D	489/497 (98%)	466 (95%)	23 (5%)	0	100	100
1	E	489/497 (98%)	467 (96%)	22 (4%)	0	100	100
1	F	489/497 (98%)	466 (95%)	23 (5%)	0	100	100
All	All	2924/2982 (98%)	2787 (95%)	137 (5%)	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	426/432 (99%)	425 (100%)	1 (0%)	87	94
1	B	430/432 (100%)	428 (100%)	2 (0%)	81	89
1	C	430/432 (100%)	428 (100%)	2 (0%)	81	89
1	D	431/432 (100%)	430 (100%)	1 (0%)	87	94
1	E	431/432 (100%)	430 (100%)	1 (0%)	87	94
1	F	431/432 (100%)	431 (100%)	0	100	100
All	All	2579/2592 (100%)	2572 (100%)	7 (0%)	86	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	B	18	HIS
1	B	197	ARG
1	C	386	GLU
1	C	387	LYS
1	D	18	HIS
1	E	140	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	216	ASN
1	A	296	ASN
1	A	488	HIS
1	B	435	HIS
1	B	488	HIS
1	C	216	ASN
1	C	389	ASN
1	C	488	HIS
1	D	18	HIS
1	E	488	HIS
1	F	18	HIS
1	F	33	GLN
1	F	296	ASN
1	F	355	HIS

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Mol	Chain	Res	Type
1	F	389	ASN
1	F	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 ⓘ

18 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	G	1	2,1	14,14,15	1.20	2 (14%)	17,19,21	1.06	1 (5%)
2	NAG	G	2	2	14,14,15	0.30	0	17,19,21	1.05	2 (11%)
2	BMA	G	3	2	11,11,12	0.92	1 (9%)	15,15,17	0.82	0
2	NAG	H	1	2,1	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
2	NAG	H	2	2	14,14,15	0.56	0	17,19,21	1.14	2 (11%)
2	BMA	H	3	2	11,11,12	0.98	1 (9%)	15,15,17	1.13	2 (13%)
2	NAG	I	1	2,1	14,14,15	0.45	0	17,19,21	1.08	1 (5%)
2	NAG	I	2	2	14,14,15	0.25	0	17,19,21	0.66	0
2	BMA	I	3	2	11,11,12	1.49	1 (9%)	15,15,17	1.25	1 (6%)
2	NAG	J	1	2,1	14,14,15	0.59	0	17,19,21	1.17	2 (11%)
2	NAG	J	2	2	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
2	BMA	J	3	2	11,11,12	1.39	2 (18%)	15,15,17	1.20	2 (13%)
2	NAG	K	1	2,1	14,14,15	0.35	0	17,19,21	1.28	1 (5%)
2	NAG	K	2	2	14,14,15	0.24	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	K	3	2	11,11,12	1.06	1 (9%)	15,15,17	1.21	1 (6%)
2	NAG	L	1	2,1	14,14,15	0.54	0	17,19,21	1.13	2 (11%)
2	NAG	L	2	2	14,14,15	0.29	0	17,19,21	0.84	1 (5%)
2	BMA	L	3	2	11,11,12	0.62	0	15,15,17	1.40	3 (20%)

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	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	2/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	BMA	I	3	2	-	2/2/19/22	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
2	BMA	J	3	2	-	2/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	BMA	L	3	2	-	2/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	BMA	O5-C1	-4.18	1.36	1.43
2	G	1	NAG	O5-C1	3.16	1.49	1.43
2	H	3	BMA	O5-C1	-2.91	1.38	1.43
2	G	1	NAG	C1-C2	2.90	1.56	1.52
2	G	3	BMA	O5-C1	-2.48	1.39	1.43
2	J	3	BMA	C4-C5	2.46	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	3	BMA	C1-C2	-2.12	1.47	1.52
2	J	3	BMA	C6-C5	2.00	1.58	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	NAG	C1-O5-C5	3.92	117.44	112.19
2	I	1	NAG	C1-O5-C5	3.25	116.54	112.19
2	G	1	NAG	C1-O5-C5	3.21	116.49	112.19
2	H	1	NAG	C1-O5-C5	3.08	116.31	112.19
2	L	3	BMA	O5-C5-C6	3.01	113.53	107.66
2	J	1	NAG	O4-C4-C5	-2.99	101.96	109.32
2	H	3	BMA	O5-C5-C6	2.88	113.26	107.66
2	L	1	NAG	C1-O5-C5	2.86	116.01	112.19
2	H	2	NAG	O3-C3-C2	-2.74	103.70	109.40
2	L	3	BMA	O2-C2-C1	2.64	115.27	109.22
2	I	3	BMA	O2-C2-C3	-2.57	104.84	110.15
2	H	3	BMA	O2-C2-C3	-2.44	105.10	110.15
2	J	3	BMA	O2-C2-C1	2.42	114.77	109.22
2	G	2	NAG	O4-C4-C5	-2.34	103.57	109.32
2	J	1	NAG	C1-O5-C5	2.30	115.27	112.19
2	H	2	NAG	O4-C4-C3	-2.30	104.96	110.38
2	J	3	BMA	O5-C5-C6	2.29	112.13	107.66
2	L	1	NAG	O4-C4-C5	-2.21	103.88	109.32
2	L	2	NAG	O4-C4-C5	-2.19	103.92	109.32
2	G	2	NAG	O3-C3-C2	-2.15	104.93	109.40
2	L	3	BMA	O4-C4-C3	-2.12	105.38	110.38
2	J	2	NAG	O4-C4-C5	-2.07	104.22	109.32
2	K	3	BMA	O2-C2-C3	-2.03	105.94	110.15

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	3	BMA	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	L	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	H	3	BMA	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	L	3	BMA	C4-C5-C6-O6

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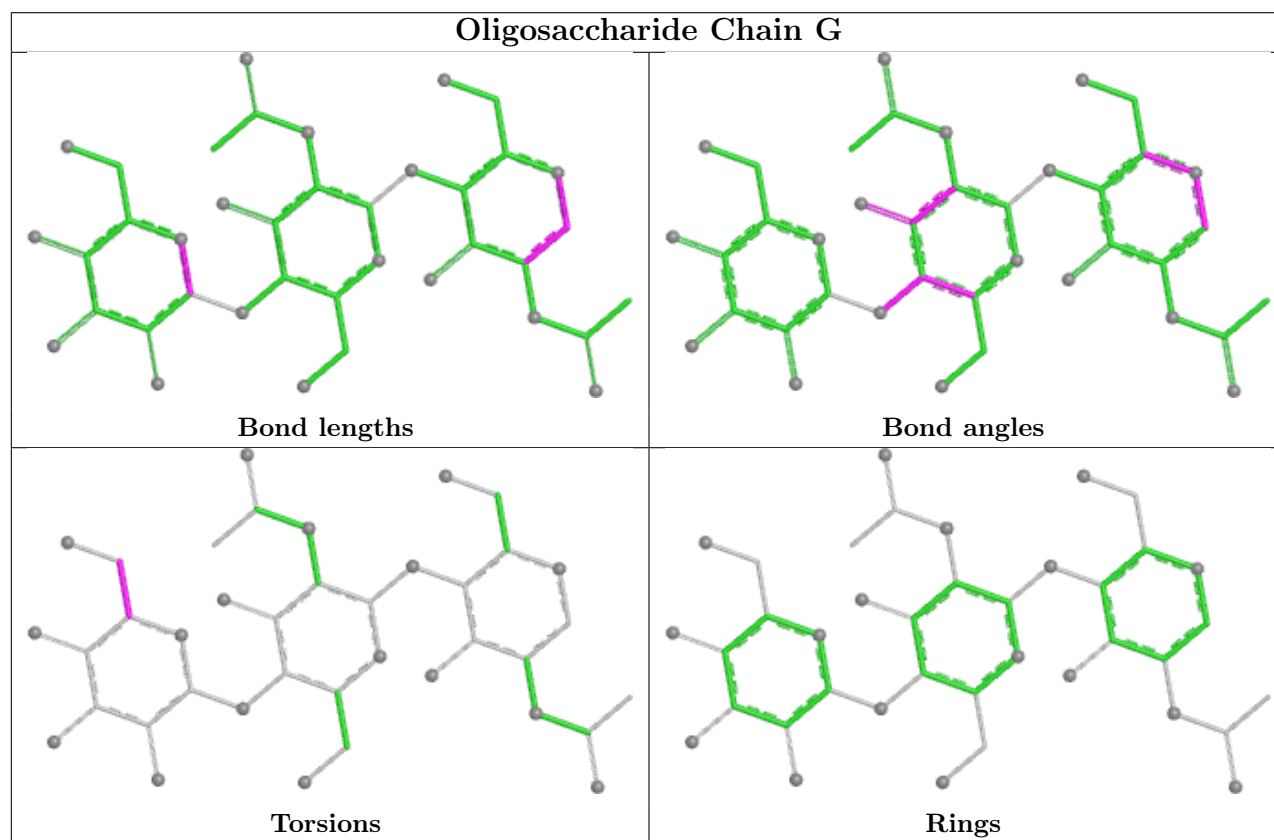
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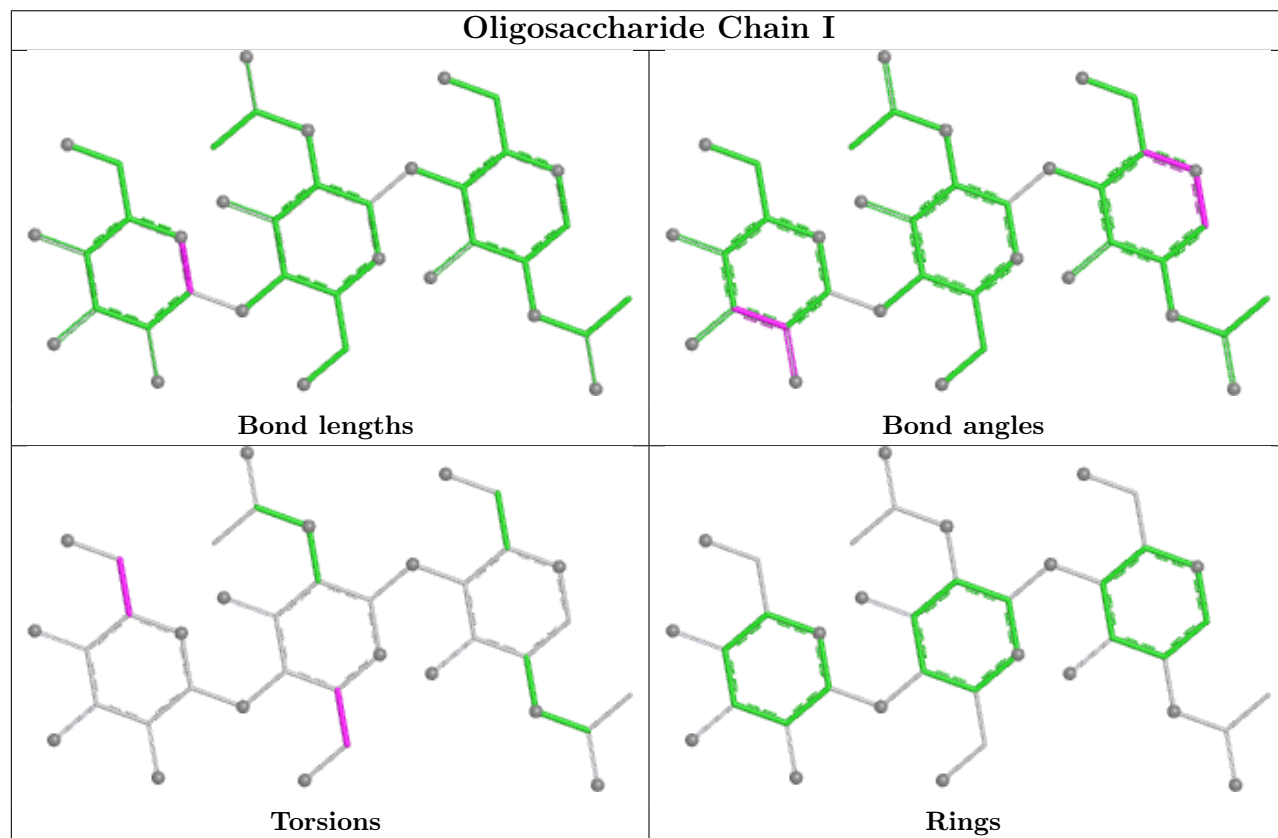
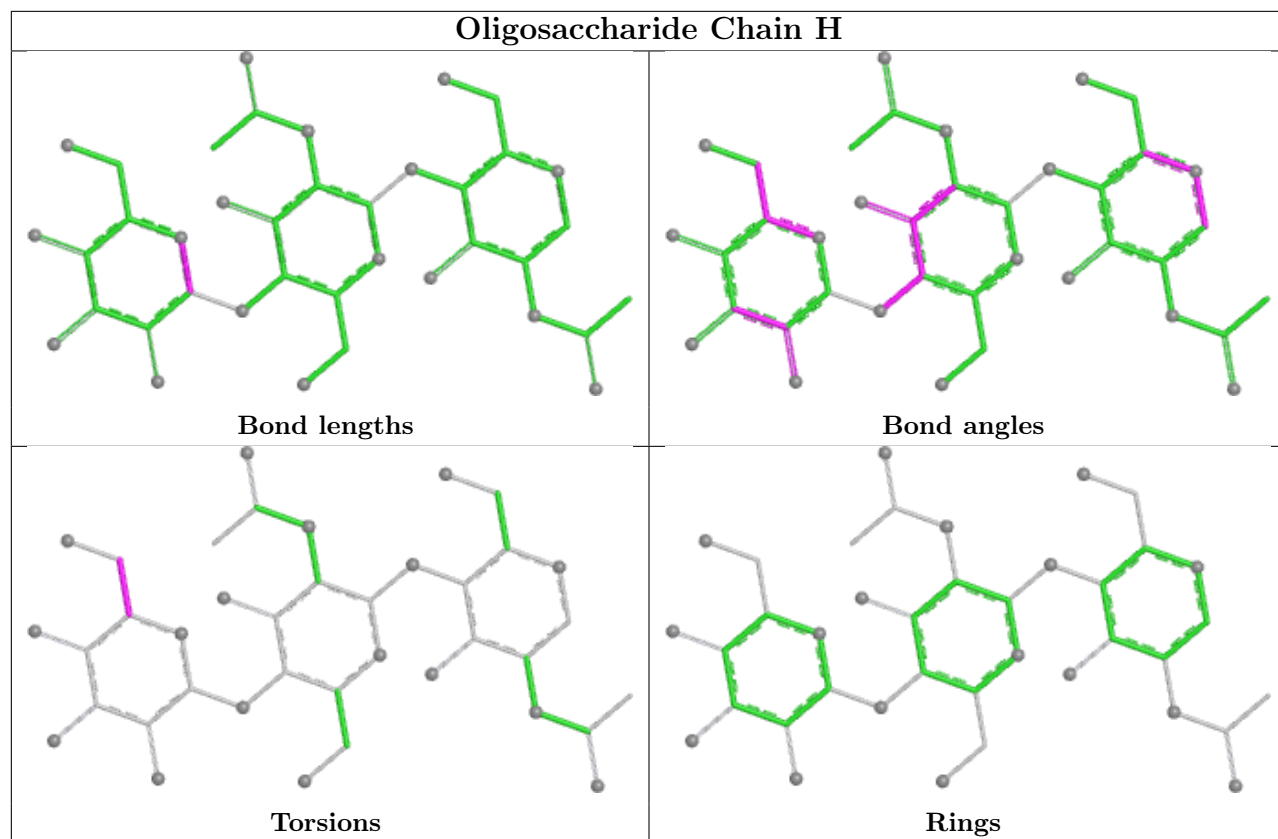
Mol	Chain	Res	Type	Atoms
2	J	2	NAG	O5-C5-C6-O6
2	I	3	BMA	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	I	3	BMA	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6

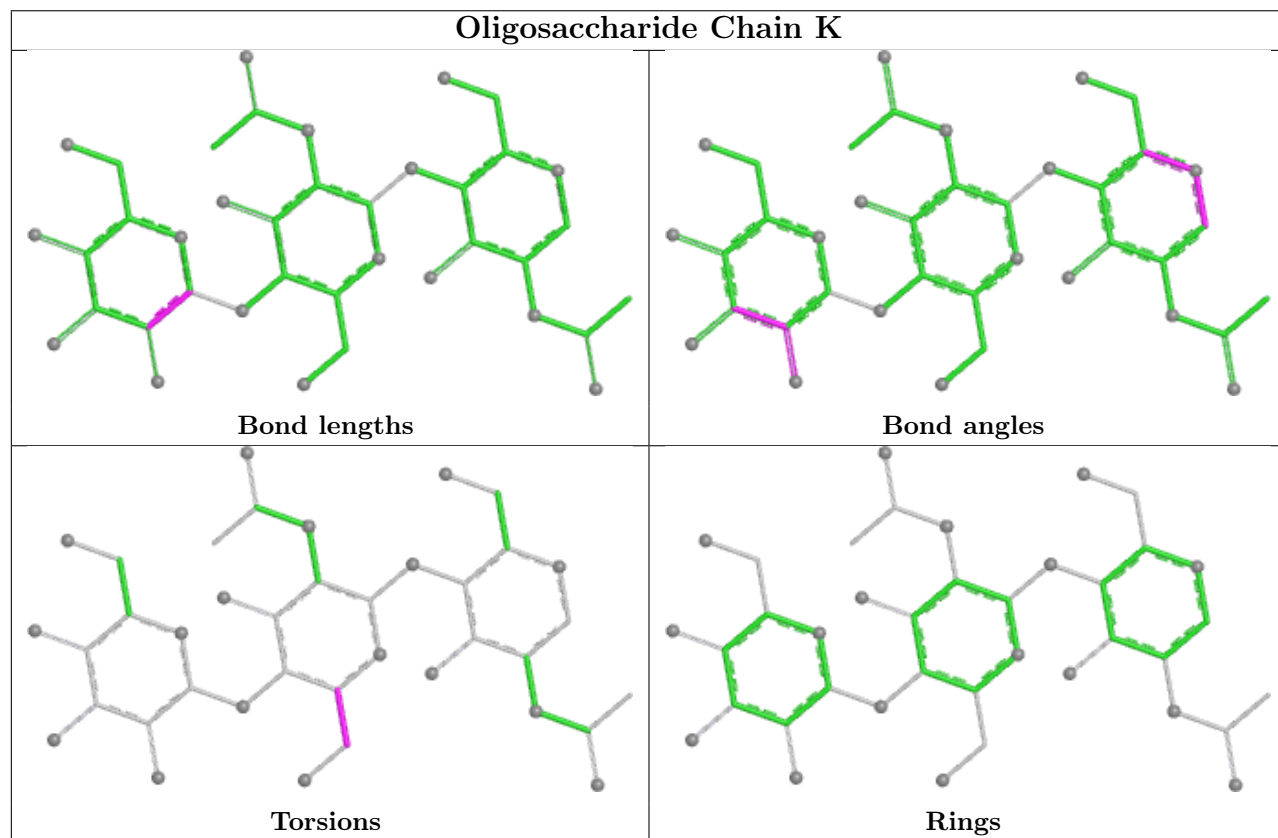
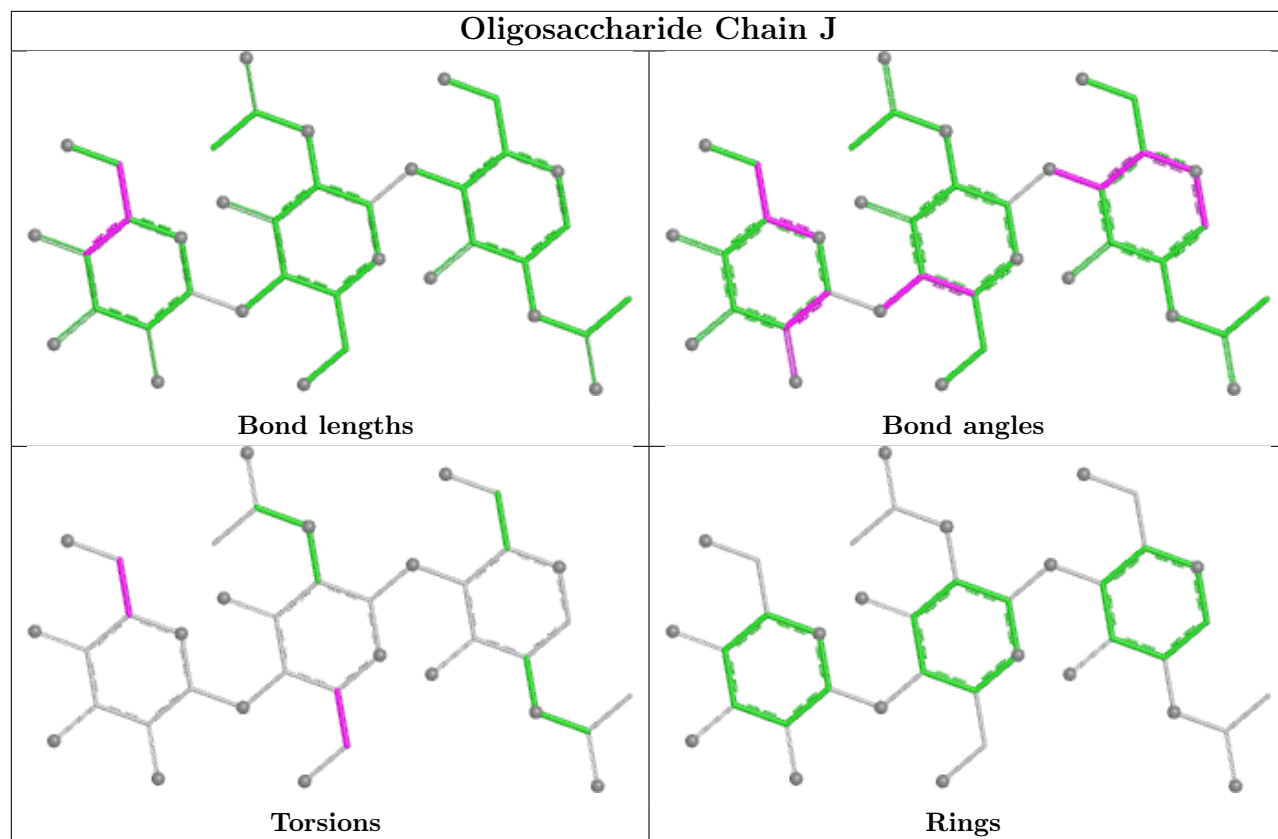
There are no ring outliers.

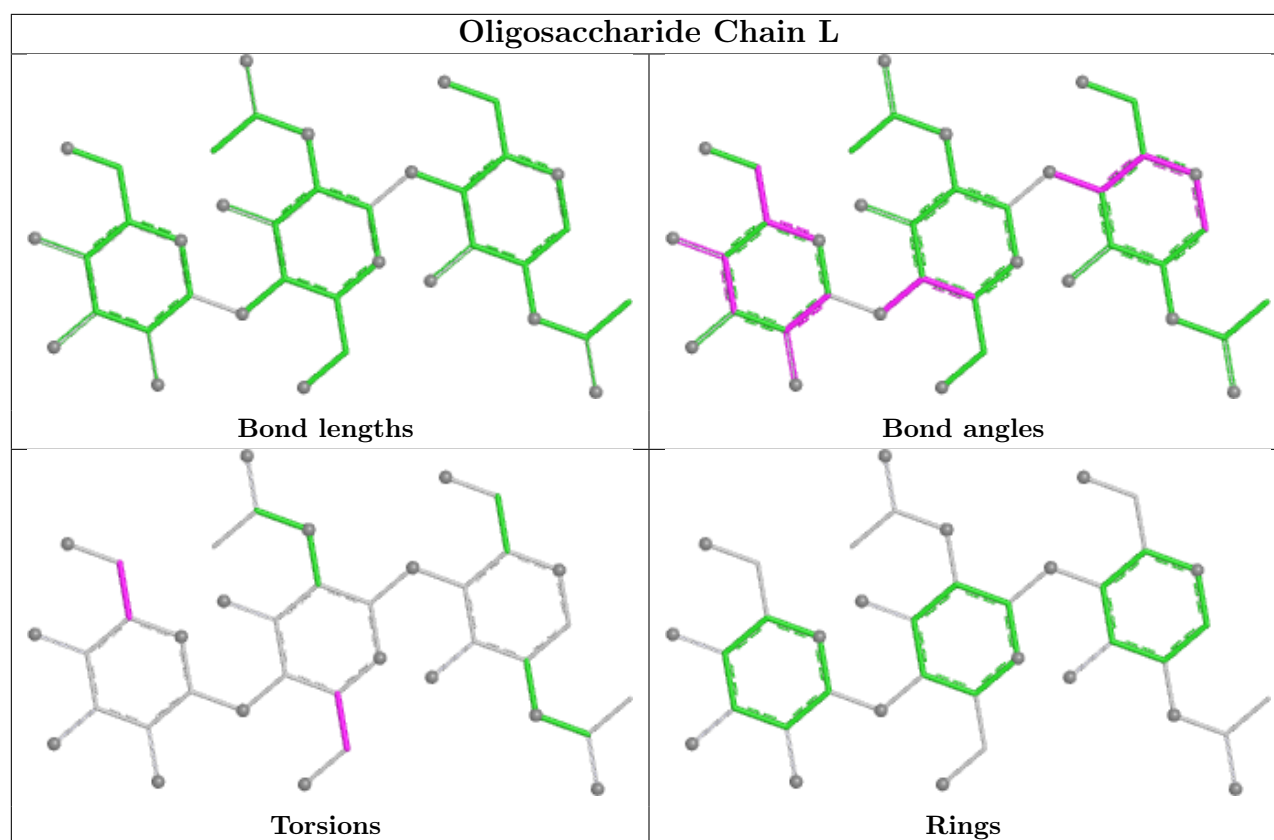
No monomer is involved in short contacts.

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](#)

24 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$
3	NAG	F	700	1	14,14,15	0.89	1 (7%)	17,19,21	1.20	2 (11%)
3	NAG	D	706	1	14,14,15	0.84	0	17,19,21	1.40	2 (11%)
3	NAG	B	706	1	14,14,15	2.96	3 (21%)	17,19,21	3.98	4 (23%)
3	NAG	F	706	1	14,14,15	0.68	0	17,19,21	1.65	5 (29%)
3	NAG	C	701	1	14,14,15	0.82	1 (7%)	17,19,21	2.83	4 (23%)
3	NAG	D	700	1	14,14,15	0.47	0	17,19,21	0.77	1 (5%)
3	NAG	B	702	1	14,14,15	0.43	0	17,19,21	1.12	2 (11%)
3	NAG	E	702	1	14,14,15	0.85	1 (7%)	17,19,21	1.24	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	701	1	14,14,15	0.73	1 (7%)	17,19,21	1.24	1 (5%)
3	NAG	A	706	1	14,14,15	1.53	2 (14%)	17,19,21	1.96	1 (5%)
3	NAG	A	700	1	14,14,15	0.98	2 (14%)	17,19,21	0.88	1 (5%)
3	NAG	E	701	1	14,14,15	1.32	3 (21%)	17,19,21	2.79	4 (23%)
3	NAG	B	700	1	14,14,15	0.84	1 (7%)	17,19,21	0.97	0
3	NAG	A	702	1	14,14,15	0.95	1 (7%)	17,19,21	2.10	4 (23%)
3	NAG	C	706	1	14,14,15	0.58	0	17,19,21	1.85	3 (17%)
3	NAG	A	701	1	14,14,15	1.39	2 (14%)	17,19,21	1.23	2 (11%)
3	NAG	E	700	1	14,14,15	0.91	2 (14%)	17,19,21	1.40	3 (17%)
3	NAG	C	700	1	14,14,15	2.67	2 (14%)	17,19,21	2.08	4 (23%)
3	NAG	D	701	1	14,14,15	0.52	0	17,19,21	1.16	1 (5%)
3	NAG	D	702	1	14,14,15	1.11	2 (14%)	17,19,21	0.94	1 (5%)
3	NAG	B	701	1	14,14,15	1.00	1 (7%)	17,19,21	1.97	4 (23%)
3	NAG	C	702	1	14,14,15	1.17	2 (14%)	17,19,21	0.86	0
3	NAG	F	702	1	14,14,15	0.71	0	17,19,21	1.32	1 (5%)
3	NAG	E	706	1	14,14,15	2.10	2 (14%)	17,19,21	1.52	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	700	1	-	4/6/23/26	0/1/1/1
3	NAG	D	706	1	-	0/6/23/26	0/1/1/1
3	NAG	B	706	1	-	4/6/23/26	0/1/1/1
3	NAG	F	706	1	-	2/6/23/26	0/1/1/1
3	NAG	C	701	1	-	2/6/23/26	0/1/1/1
3	NAG	D	700	1	-	2/6/23/26	0/1/1/1
3	NAG	B	702	1	-	0/6/23/26	0/1/1/1
3	NAG	E	702	1	-	0/6/23/26	0/1/1/1
3	NAG	F	701	1	-	2/6/23/26	0/1/1/1
3	NAG	A	706	1	-	3/6/23/26	0/1/1/1
3	NAG	A	700	1	-	0/6/23/26	0/1/1/1
3	NAG	E	701	1	-	3/6/23/26	0/1/1/1
3	NAG	B	700	1	-	2/6/23/26	0/1/1/1
3	NAG	A	702	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	706	1	-	3/6/23/26	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1
3	NAG	E	700	1	-	4/6/23/26	0/1/1/1
3	NAG	C	700	1	-	4/6/23/26	0/1/1/1
3	NAG	D	701	1	-	0/6/23/26	0/1/1/1
3	NAG	D	702	1	-	0/6/23/26	0/1/1/1
3	NAG	B	701	1	-	2/6/23/26	0/1/1/1
3	NAG	C	702	1	-	0/6/23/26	0/1/1/1
3	NAG	F	702	1	-	2/6/23/26	0/1/1/1
3	NAG	E	706	1	-	4/6/23/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	706	NAG	O5-C1	9.33	1.59	1.43
3	C	700	NAG	O5-C1	8.62	1.58	1.43
3	E	706	NAG	O5-C1	-7.16	1.31	1.43
3	B	706	NAG	C1-C2	5.41	1.59	1.52
3	A	706	NAG	O5-C1	5.05	1.52	1.43
3	C	700	NAG	C1-C2	4.75	1.58	1.52
3	A	701	NAG	O5-C1	4.43	1.51	1.43
3	C	702	NAG	C1-C2	3.75	1.57	1.52
3	E	706	NAG	C3-C2	2.79	1.58	1.52
3	D	702	NAG	O5-C1	2.77	1.48	1.43
3	D	702	NAG	C1-C2	2.73	1.56	1.52
3	A	702	NAG	C1-C2	2.73	1.56	1.52
3	A	700	NAG	C1-C2	2.72	1.56	1.52
3	E	701	NAG	C3-C2	2.71	1.58	1.52
3	A	701	NAG	C1-C2	2.54	1.55	1.52
3	B	700	NAG	C1-C2	2.53	1.55	1.52
3	F	701	NAG	O5-C1	2.45	1.47	1.43
3	F	700	NAG	C1-C2	2.44	1.55	1.52
3	E	700	NAG	O5-C1	2.30	1.47	1.43
3	E	702	NAG	O5-C1	2.29	1.47	1.43
3	E	701	NAG	O5-C1	2.28	1.47	1.43
3	B	701	NAG	C3-C2	2.28	1.57	1.52
3	A	706	NAG	C3-C2	2.26	1.57	1.52
3	E	701	NAG	C2-N2	2.24	1.50	1.46
3	E	700	NAG	C1-C2	2.23	1.55	1.52
3	B	706	NAG	C3-C2	2.14	1.57	1.52
3	C	701	NAG	O5-C1	-2.08	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	702	NAG	O5-C1	2.01	1.47	1.43
3	A	700	NAG	O5-C1	2.00	1.47	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	706	NAG	C1-O5-C5	12.93	129.51	112.19
3	C	701	NAG	C2-N2-C7	8.84	134.75	122.90
3	E	701	NAG	C2-N2-C7	7.68	133.19	122.90
3	A	706	NAG	C1-O5-C5	7.35	122.03	112.19
3	B	706	NAG	C4-C3-C2	6.75	120.91	111.02
3	C	700	NAG	C1-C2-N2	6.10	120.04	110.43
3	B	706	NAG	C3-C4-C5	6.03	121.16	110.23
3	A	702	NAG	C1-C2-N2	5.94	119.79	110.43
3	E	701	NAG	C1-C2-N2	5.43	118.98	110.43
3	C	706	NAG	C1-O5-C5	5.28	119.27	112.19
3	C	701	NAG	C1-O5-C5	4.95	118.82	112.19
3	B	701	NAG	O3-C3-C2	4.62	118.99	109.40
3	E	706	NAG	C1-O5-C5	-4.42	106.26	112.19
3	D	706	NAG	C1-O5-C5	4.42	118.11	112.19
3	E	701	NAG	C1-O5-C5	4.41	118.10	112.19
3	C	700	NAG	C2-N2-C7	4.33	128.70	122.90
3	B	701	NAG	C1-O5-C5	4.24	117.87	112.19
3	F	701	NAG	C1-O5-C5	4.10	117.68	112.19
3	F	702	NAG	O3-C3-C2	4.07	117.85	109.40
3	B	701	NAG	C1-C2-N2	-3.88	104.32	110.43
3	D	701	NAG	C1-O5-C5	3.74	117.19	112.19
3	A	702	NAG	C4-C3-C2	-3.69	105.61	111.02
3	E	700	NAG	C1-C2-N2	3.51	115.96	110.43
3	E	702	NAG	C1-C2-N2	3.48	115.92	110.43
3	A	701	NAG	C1-O5-C5	3.48	116.85	112.19
3	C	701	NAG	C1-C2-N2	-3.45	105.00	110.43
3	C	706	NAG	C1-C2-N2	3.44	115.85	110.43
3	B	706	NAG	C2-N2-C7	3.39	127.45	122.90
3	A	702	NAG	C2-N2-C7	-3.35	118.41	122.90
3	F	700	NAG	C1-O5-C5	3.17	116.44	112.19
3	F	706	NAG	C3-C4-C5	3.04	115.74	110.23
3	F	706	NAG	C2-N2-C7	2.98	126.89	122.90
3	D	700	NAG	C1-O5-C5	2.96	116.16	112.19
3	E	701	NAG	O4-C4-C5	-2.92	102.13	109.32
3	E	700	NAG	C1-O5-C5	2.87	116.03	112.19
3	F	706	NAG	C4-C3-C2	2.86	115.21	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	706	NAG	C1-C2-N2	2.84	114.91	110.43
3	C	700	NAG	C1-O5-C5	2.68	115.78	112.19
3	A	702	NAG	O3-C3-C4	2.65	116.62	110.38
3	C	700	NAG	O3-C3-C4	2.56	116.41	110.38
3	D	706	NAG	C1-C2-N2	2.54	114.44	110.43
3	C	706	NAG	C2-N2-C7	2.52	126.28	122.90
3	A	700	NAG	O3-C3-C2	2.49	114.58	109.40
3	A	701	NAG	C1-C2-N2	2.48	114.33	110.43
3	B	702	NAG	C1-C2-N2	2.47	114.33	110.43
3	E	700	NAG	O3-C3-C2	2.45	114.48	109.40
3	F	706	NAG	C1-O5-C5	2.40	115.41	112.19
3	D	702	NAG	C2-N2-C7	2.32	126.01	122.90
3	B	702	NAG	O4-C4-C5	-2.19	103.92	109.32
3	F	700	NAG	O3-C3-C2	2.12	113.81	109.40
3	C	701	NAG	O5-C5-C6	-2.11	103.56	107.66
3	B	701	NAG	O4-C4-C3	2.10	115.32	110.38
3	E	706	NAG	C3-C4-C5	2.09	114.02	110.23

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	706	NAG	C1-C2-N2-C7
3	C	701	NAG	O7-C7-N2-C2
3	C	706	NAG	C1-C2-N2-C7
3	E	701	NAG	C1-C2-N2-C7
3	B	701	NAG	O5-C5-C6-O6
3	E	700	NAG	C4-C5-C6-O6
3	F	700	NAG	C4-C5-C6-O6
3	A	706	NAG	O5-C5-C6-O6
3	E	700	NAG	O5-C5-C6-O6
3	B	701	NAG	C4-C5-C6-O6
3	F	701	NAG	O5-C5-C6-O6
3	F	701	NAG	C4-C5-C6-O6
3	A	702	NAG	C8-C7-N2-C2
3	A	702	NAG	O7-C7-N2-C2
3	C	701	NAG	C8-C7-N2-C2
3	E	701	NAG	C8-C7-N2-C2
3	E	701	NAG	O7-C7-N2-C2
3	F	702	NAG	O5-C5-C6-O6
3	F	700	NAG	O5-C5-C6-O6
3	D	700	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	702	NAG	C4-C5-C6-O6
3	A	701	NAG	C4-C5-C6-O6
3	A	706	NAG	C4-C5-C6-O6
3	A	701	NAG	O5-C5-C6-O6
3	C	706	NAG	O5-C5-C6-O6
3	D	700	NAG	O5-C5-C6-O6
3	B	706	NAG	C3-C2-N2-C7
3	C	700	NAG	C3-C2-N2-C7
3	E	700	NAG	C3-C2-N2-C7
3	F	700	NAG	C3-C2-N2-C7
3	C	700	NAG	C1-C2-N2-C7
3	E	700	NAG	C1-C2-N2-C7
3	F	700	NAG	C1-C2-N2-C7
3	F	706	NAG	C4-C5-C6-O6
3	C	700	NAG	C4-C5-C6-O6
3	E	706	NAG	C4-C5-C6-O6
3	B	706	NAG	O5-C5-C6-O6
3	E	706	NAG	C3-C2-N2-C7
3	A	702	NAG	C4-C5-C6-O6
3	C	700	NAG	O5-C5-C6-O6
3	B	700	NAG	O5-C5-C6-O6
3	A	706	NAG	C1-C2-N2-C7
3	E	706	NAG	C1-C2-N2-C7
3	F	706	NAG	O5-C5-C6-O6
3	B	706	NAG	C4-C5-C6-O6
3	C	706	NAG	C4-C5-C6-O6
3	B	700	NAG	C4-C5-C6-O6
3	E	706	NAG	O5-C5-C6-O6

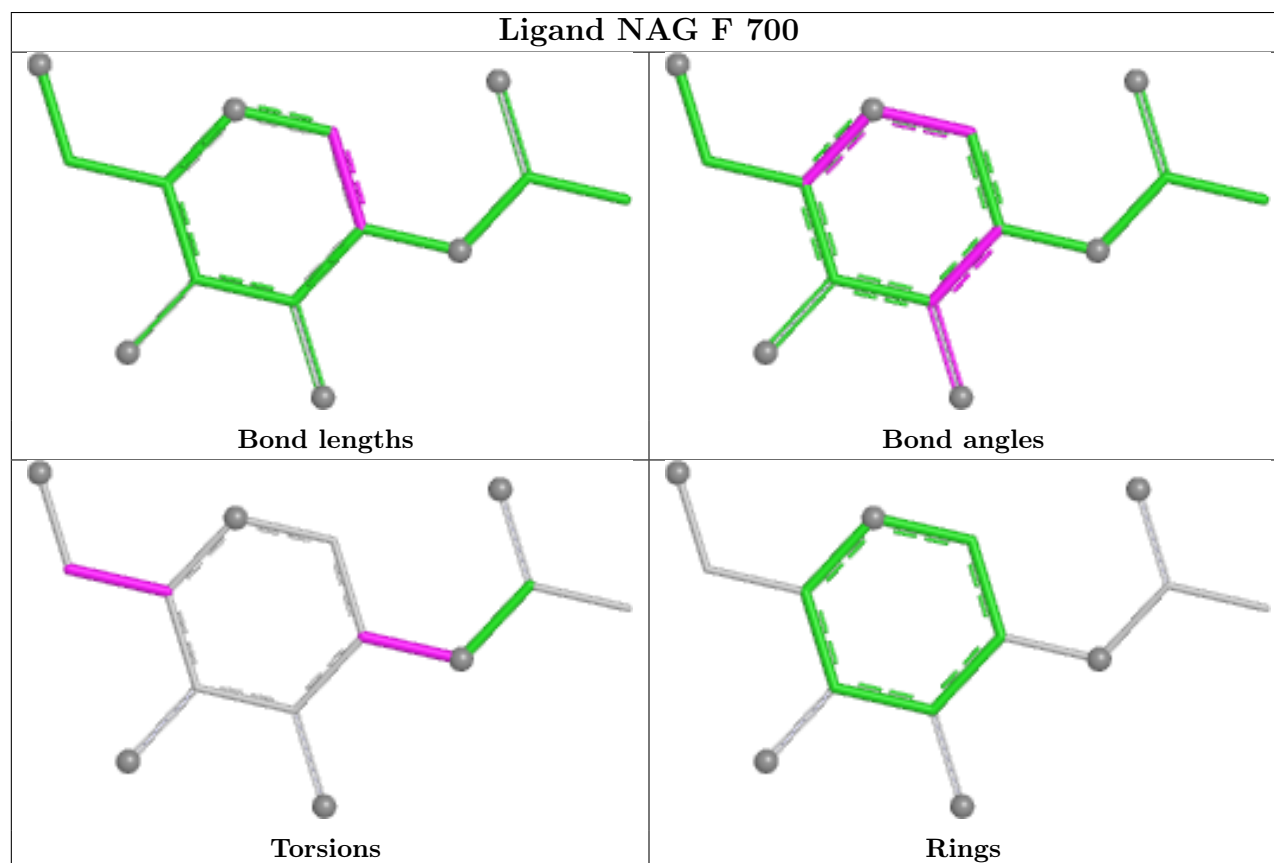
There are no ring outliers.

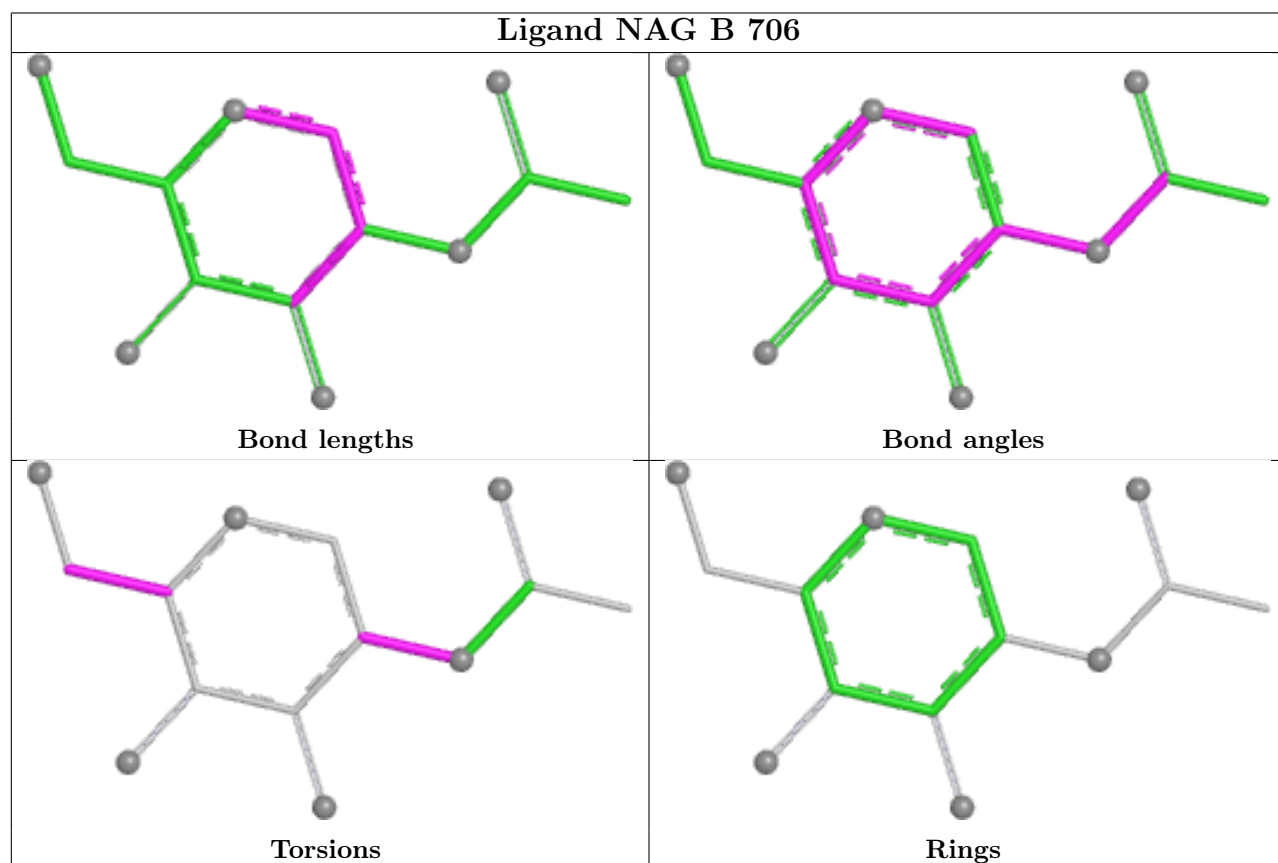
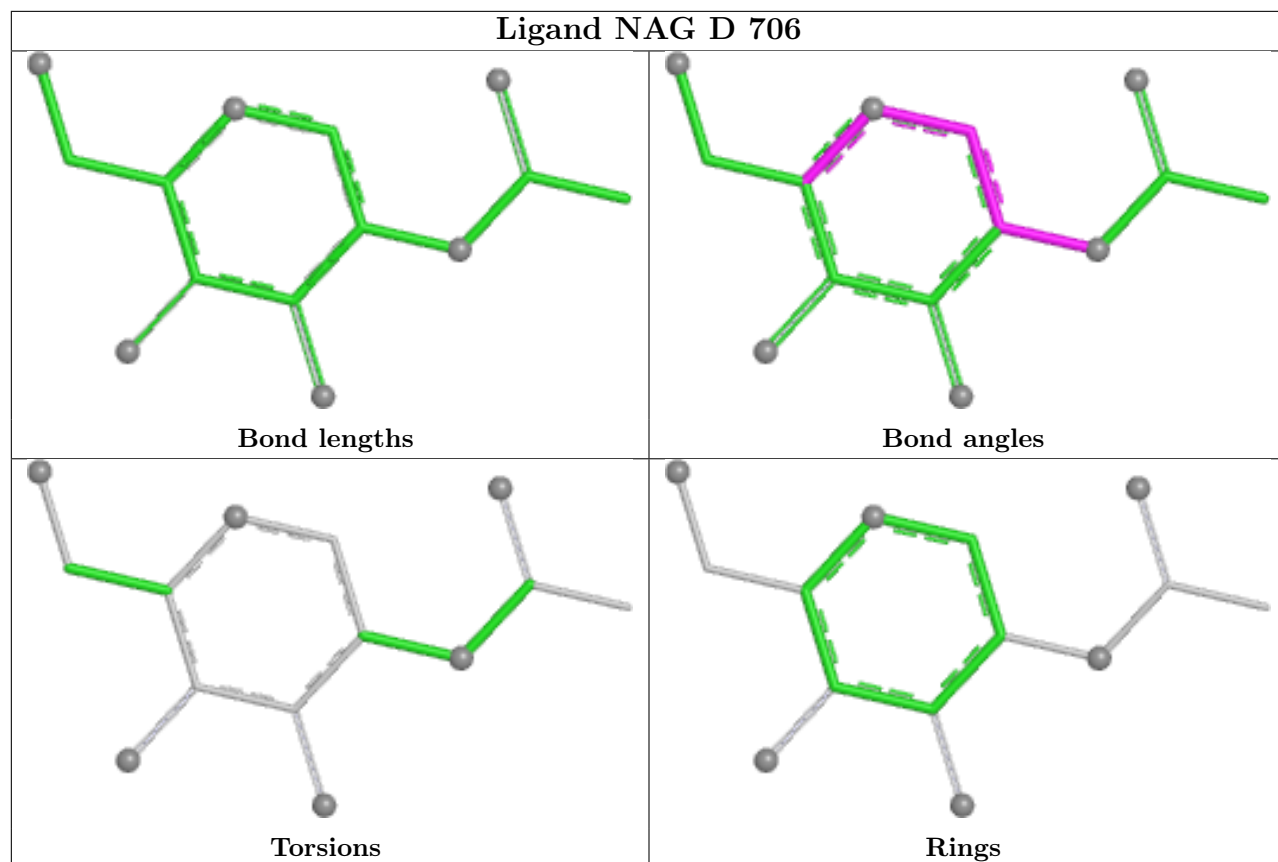
5 monomers are involved in 6 short contacts:

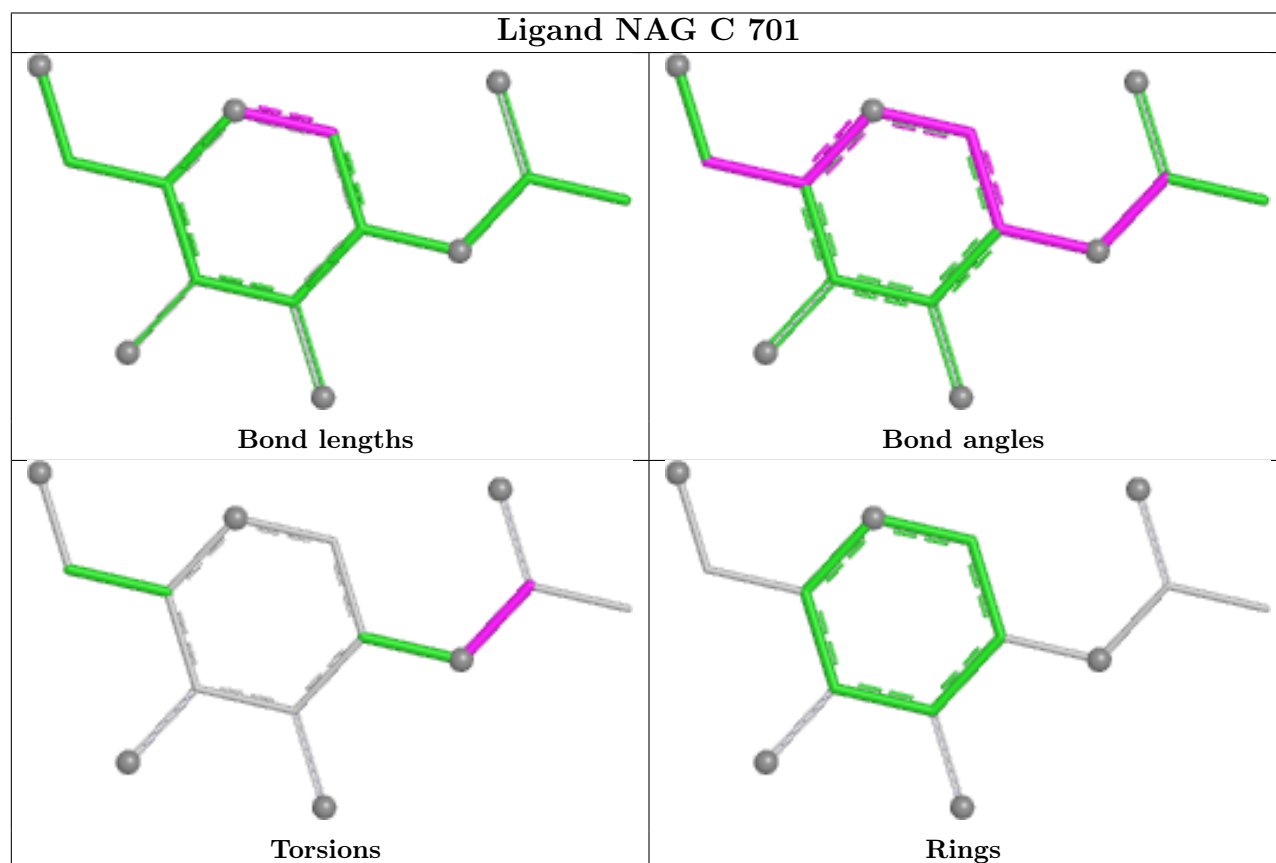
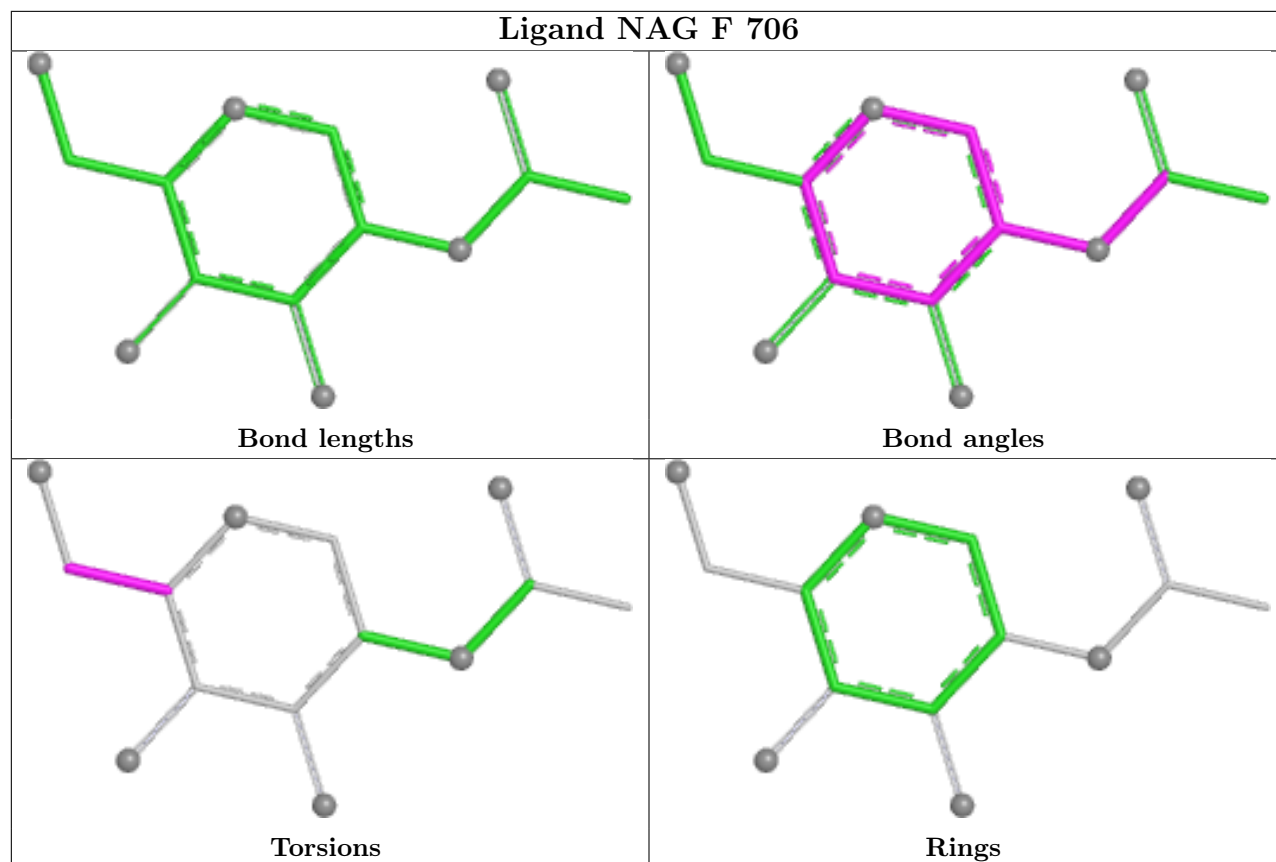
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	700	NAG	2	0
3	B	706	NAG	1	0
3	C	701	NAG	1	0
3	C	706	NAG	1	0
3	D	702	NAG	1	0

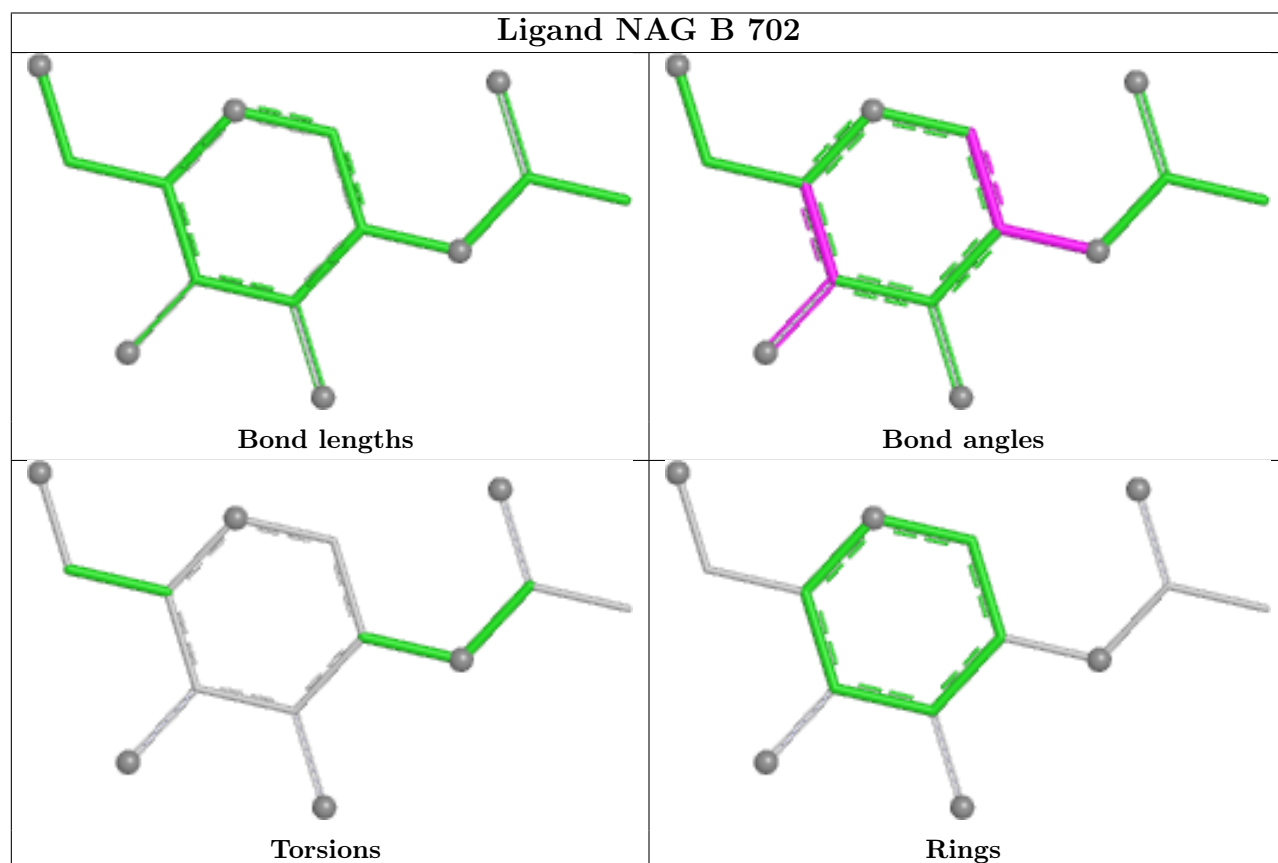
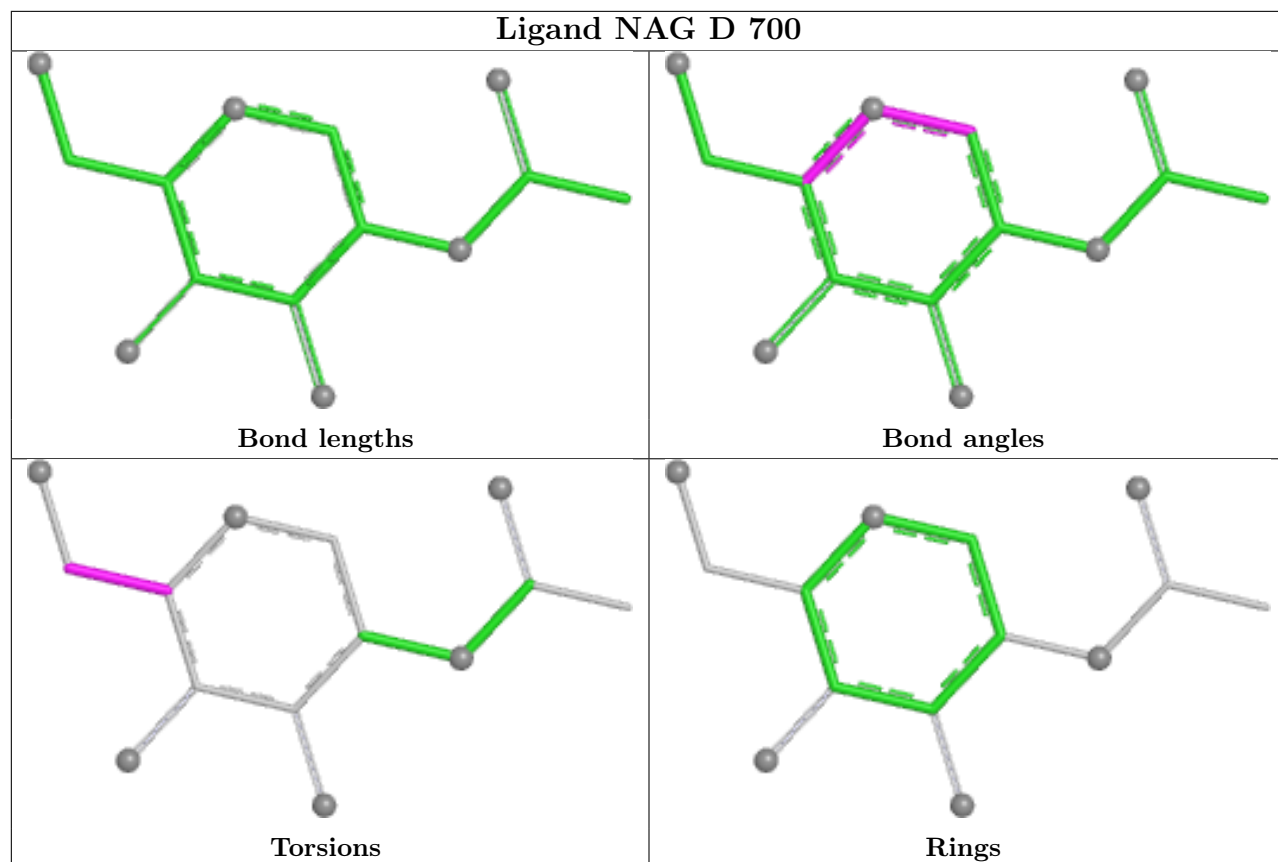
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

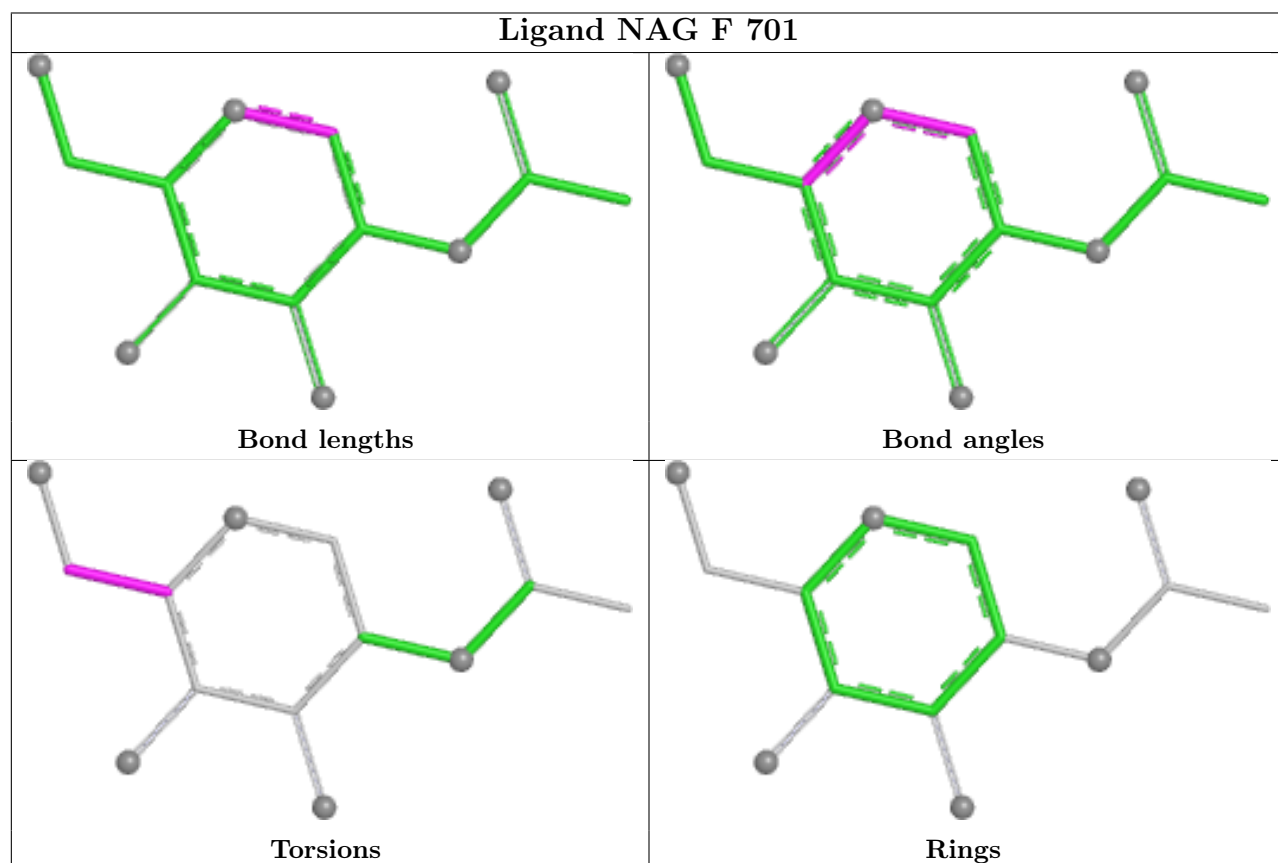
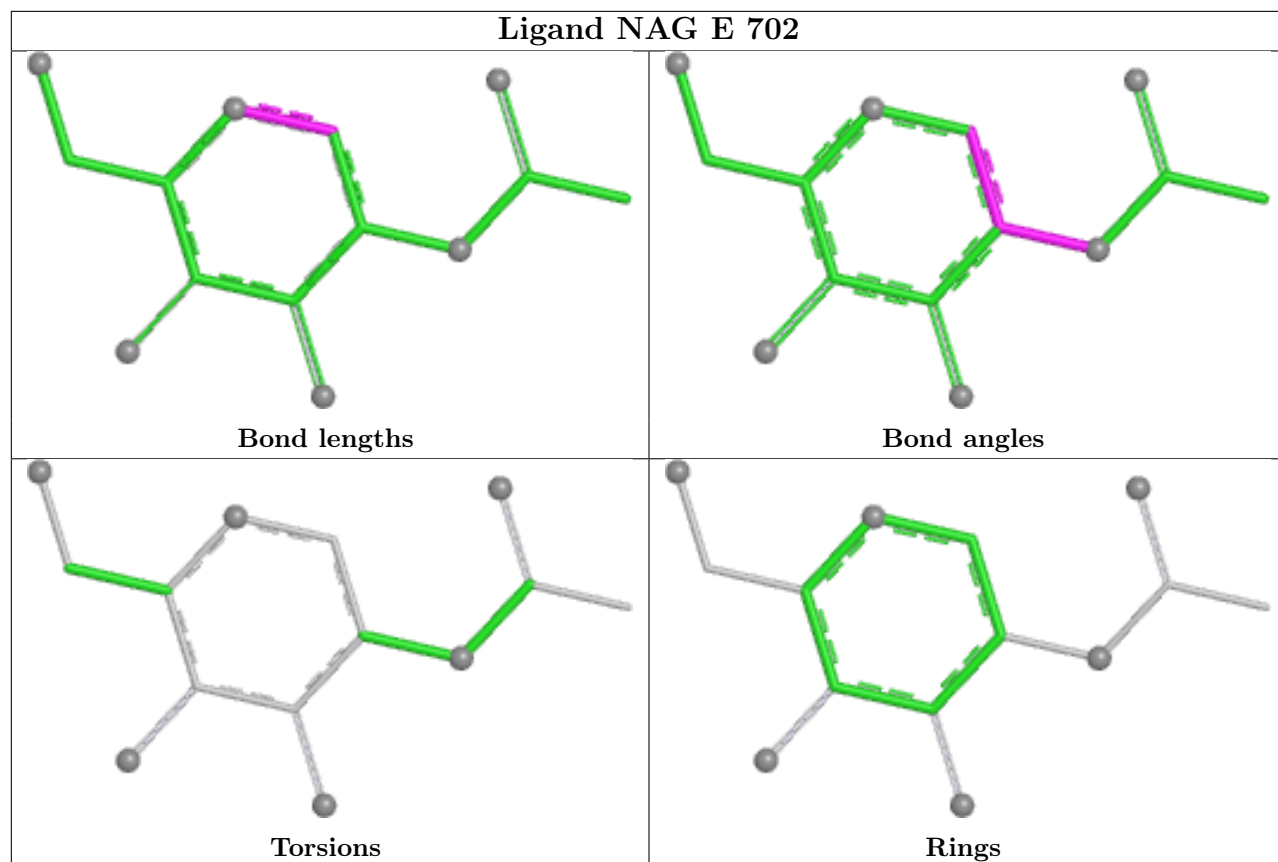
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

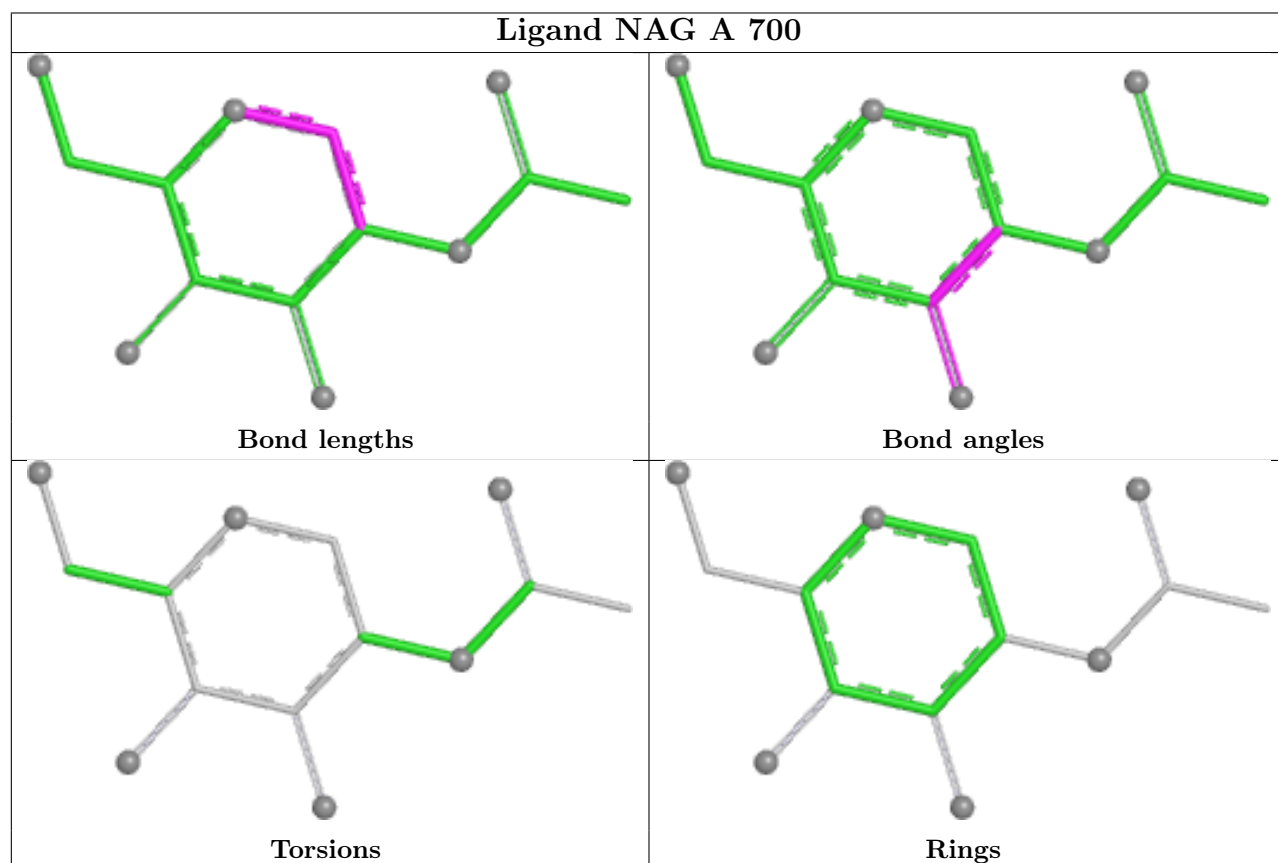
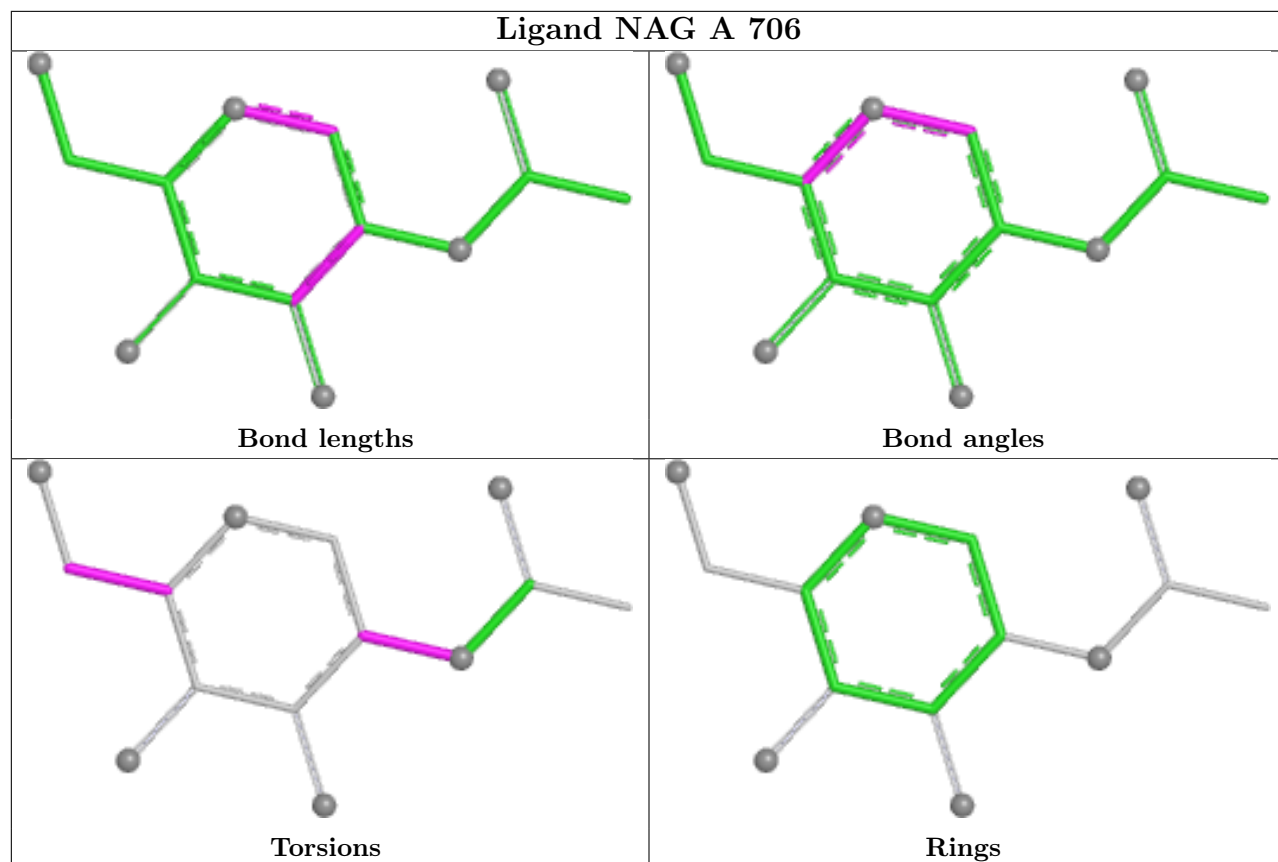


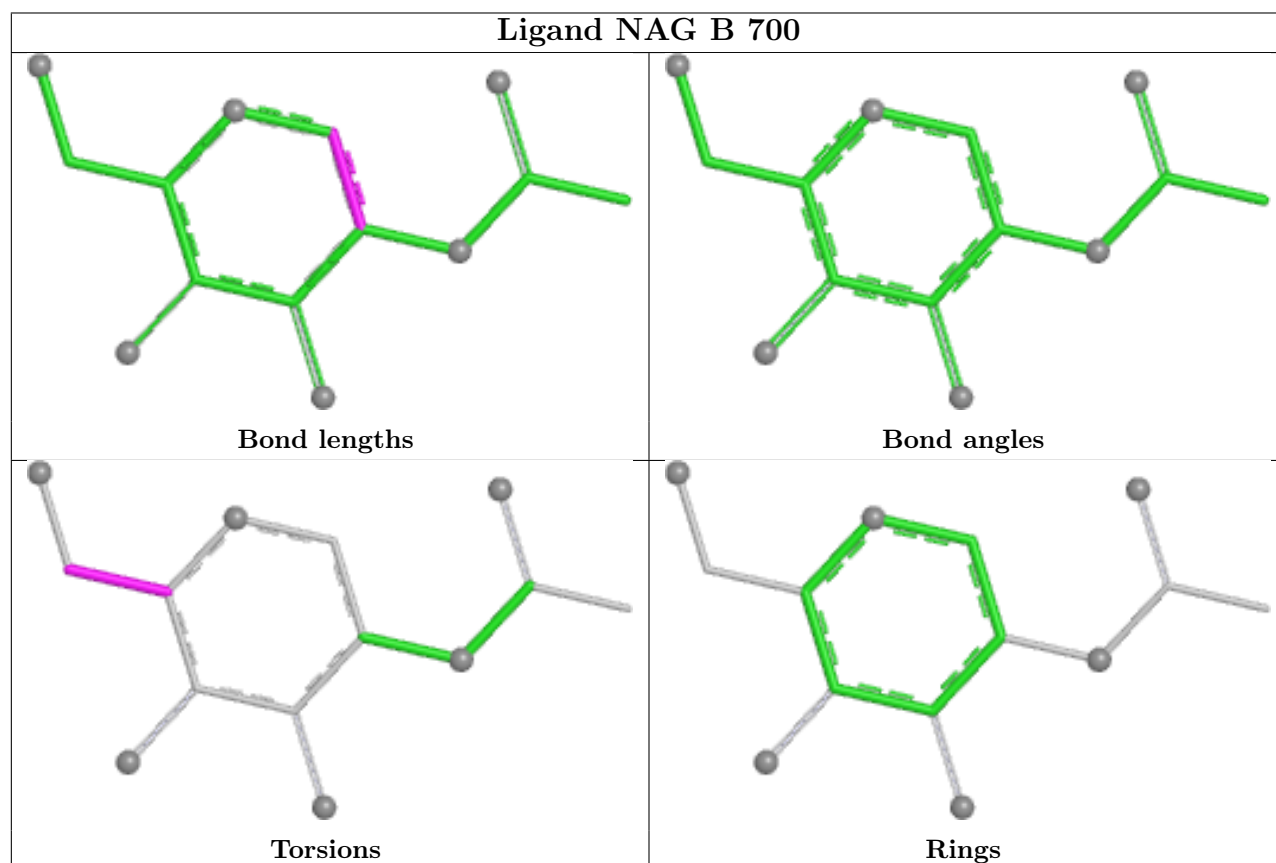
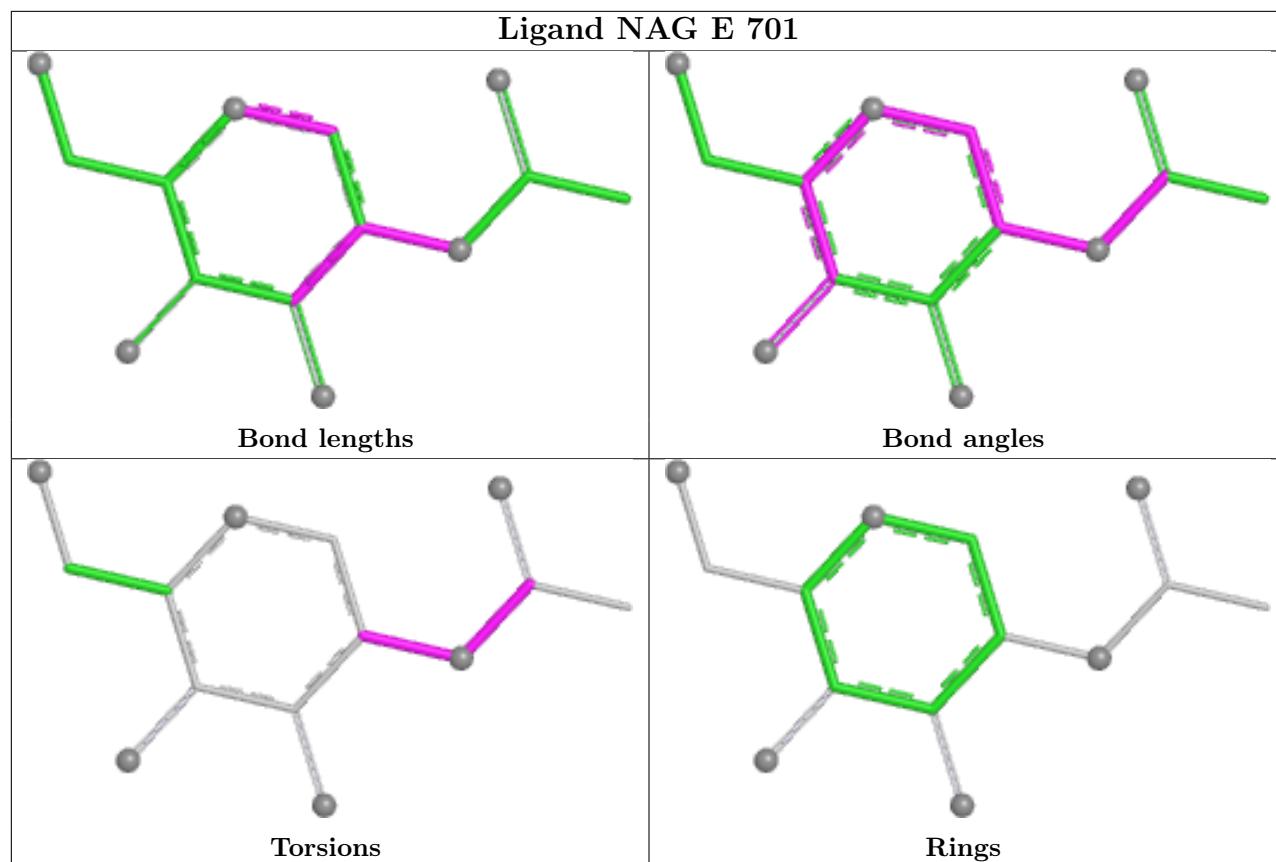


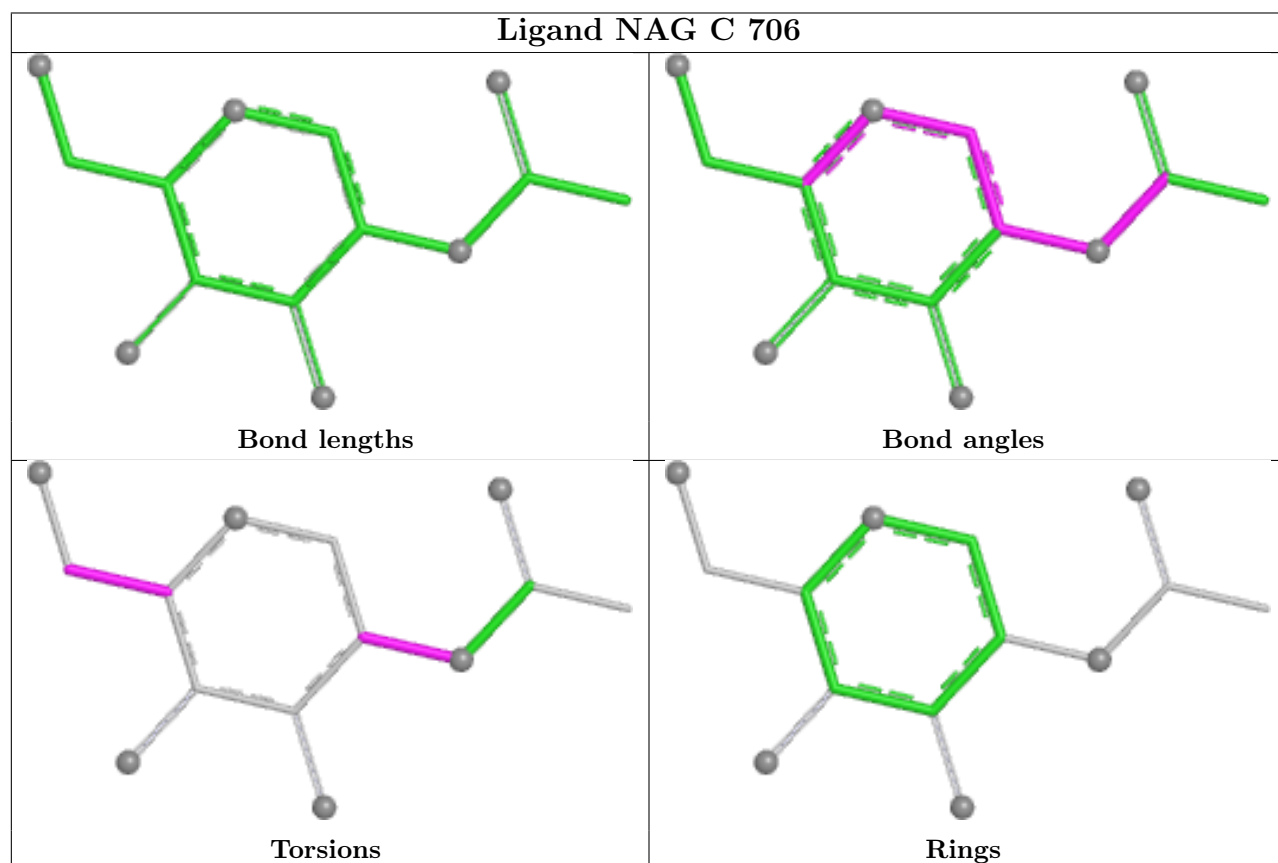
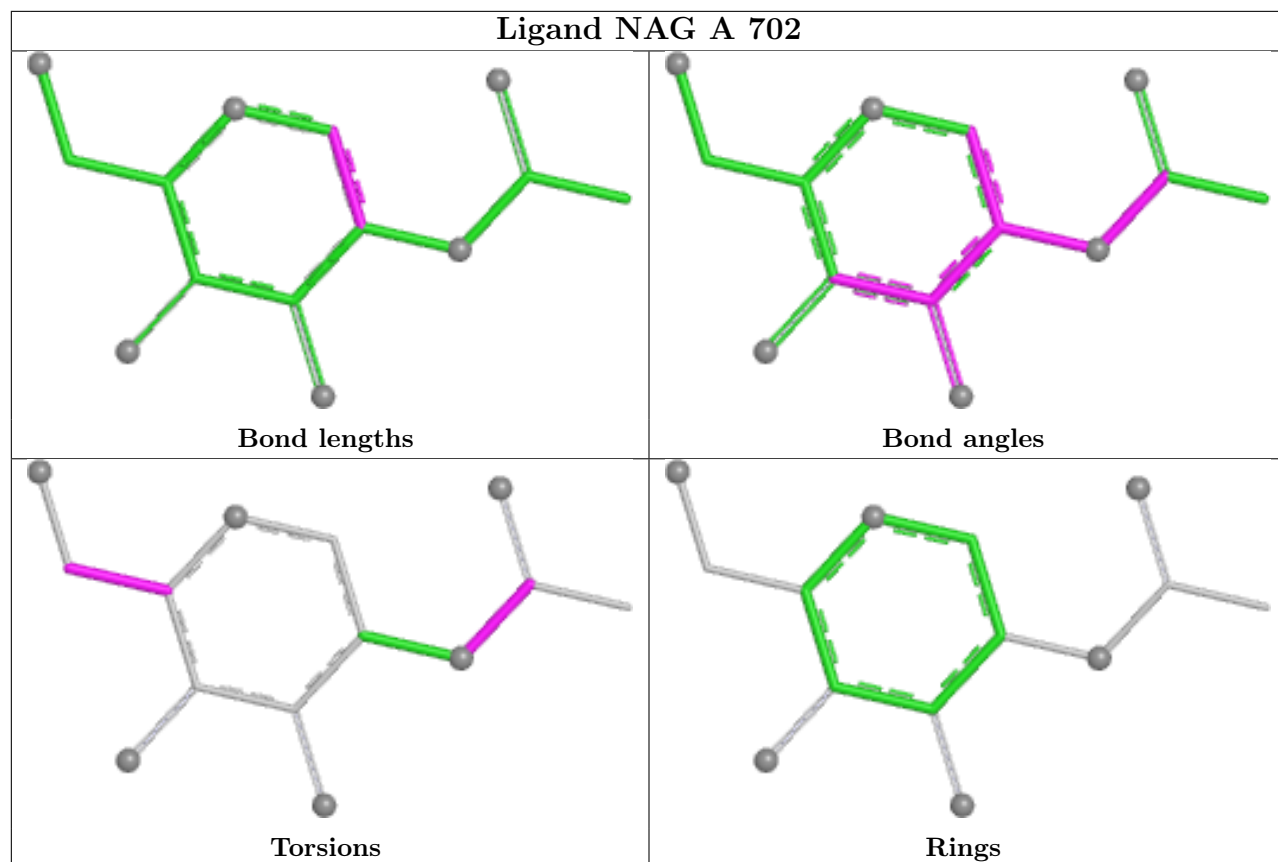


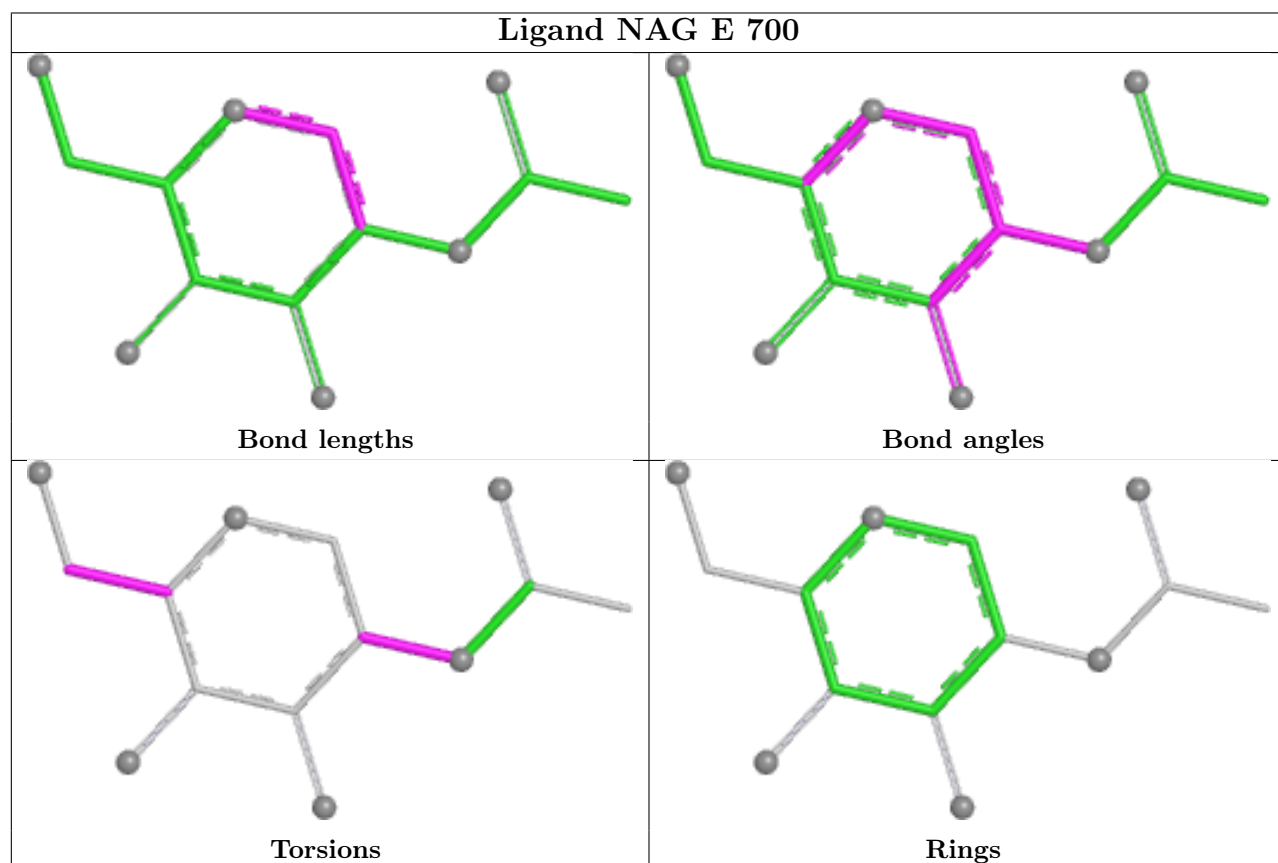
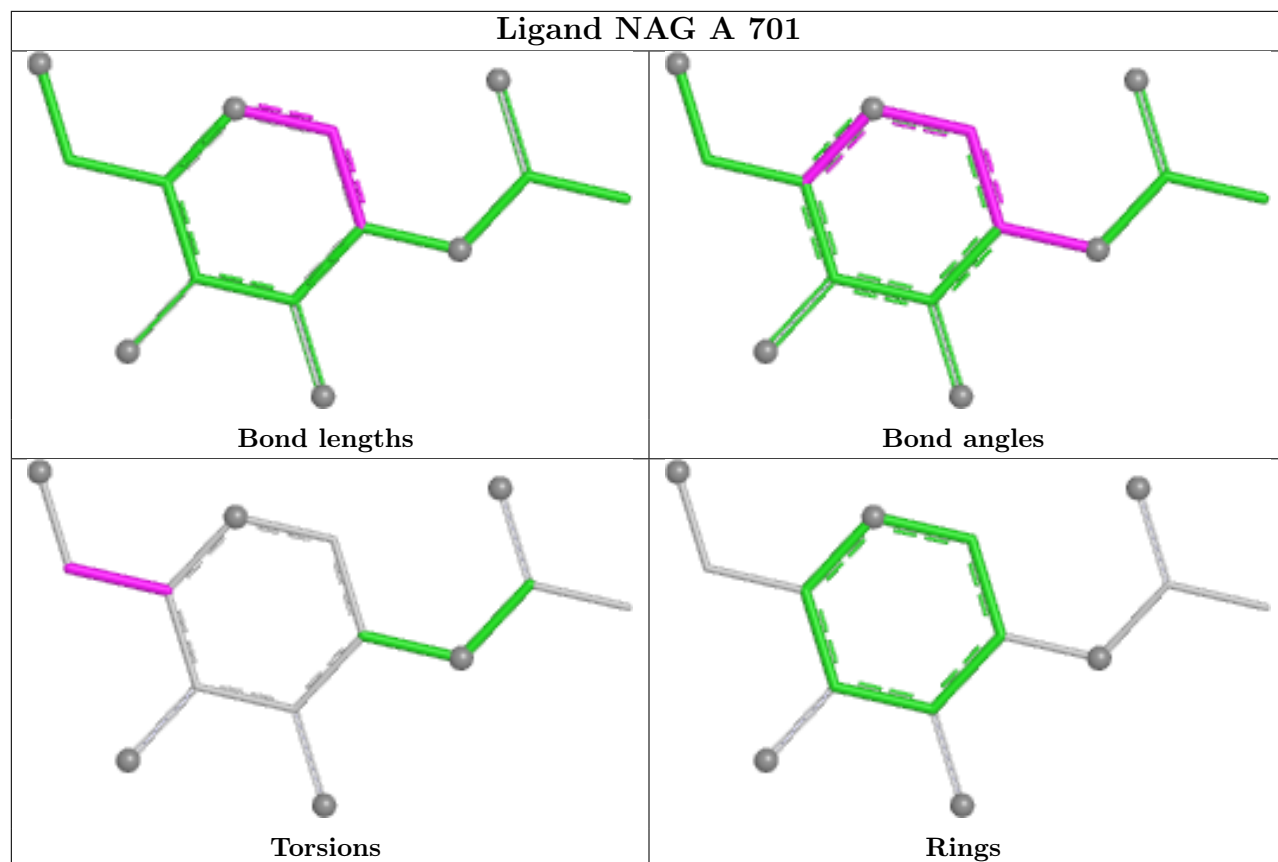


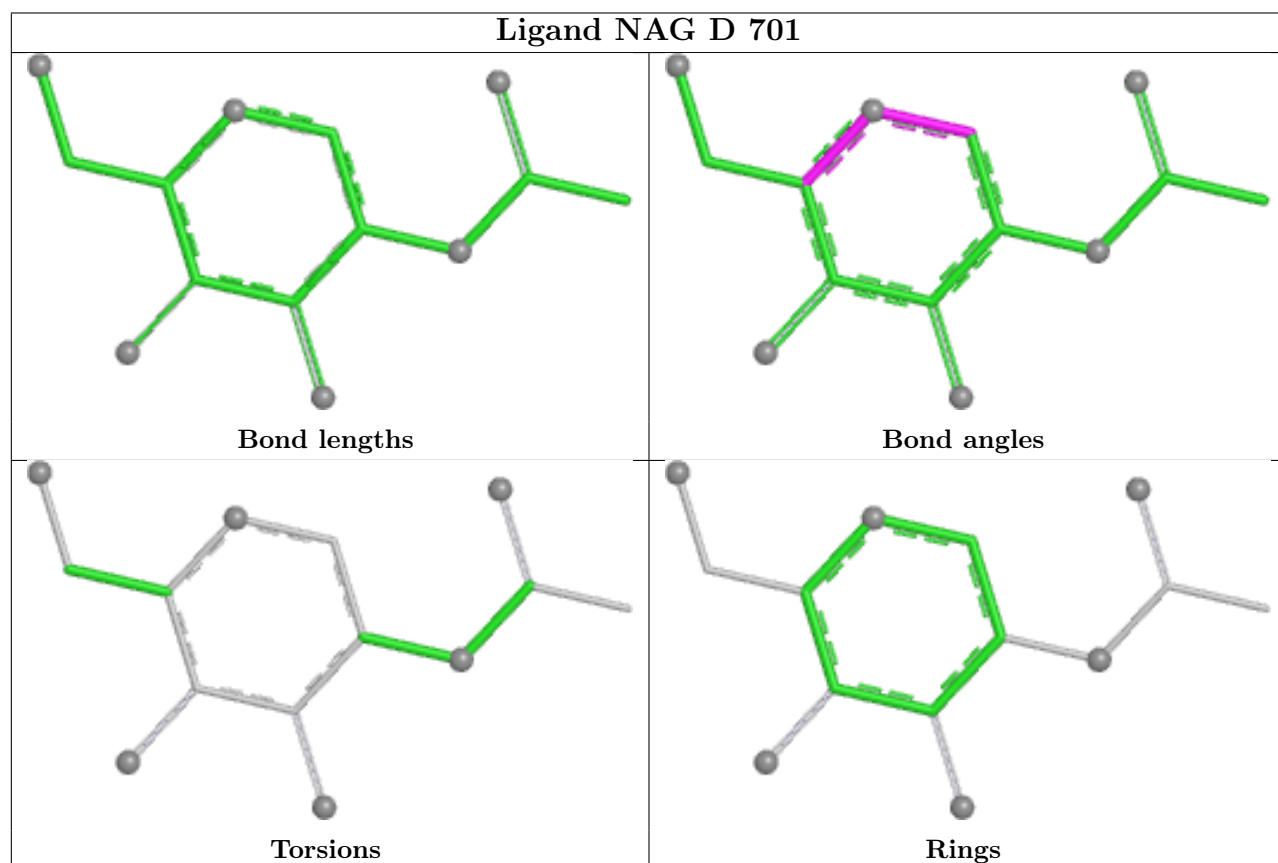
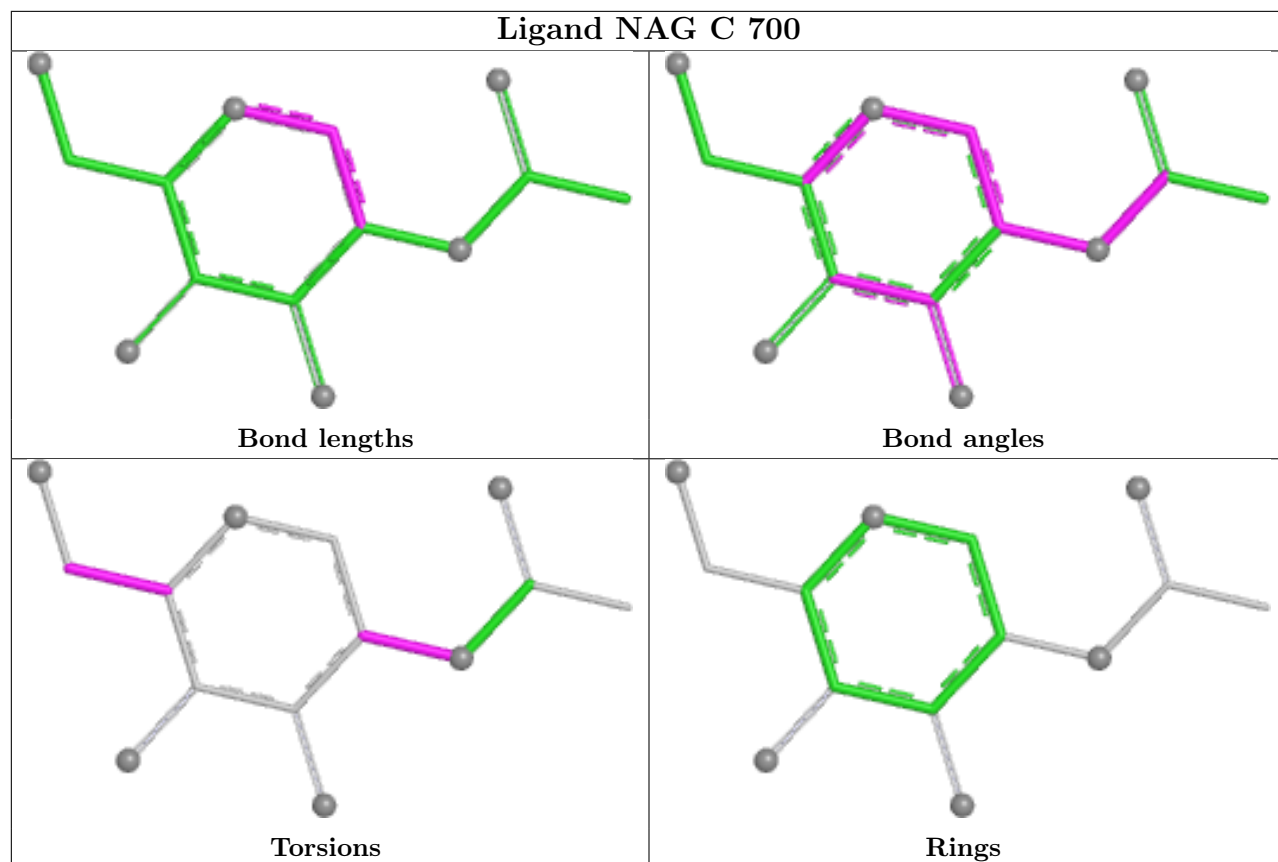


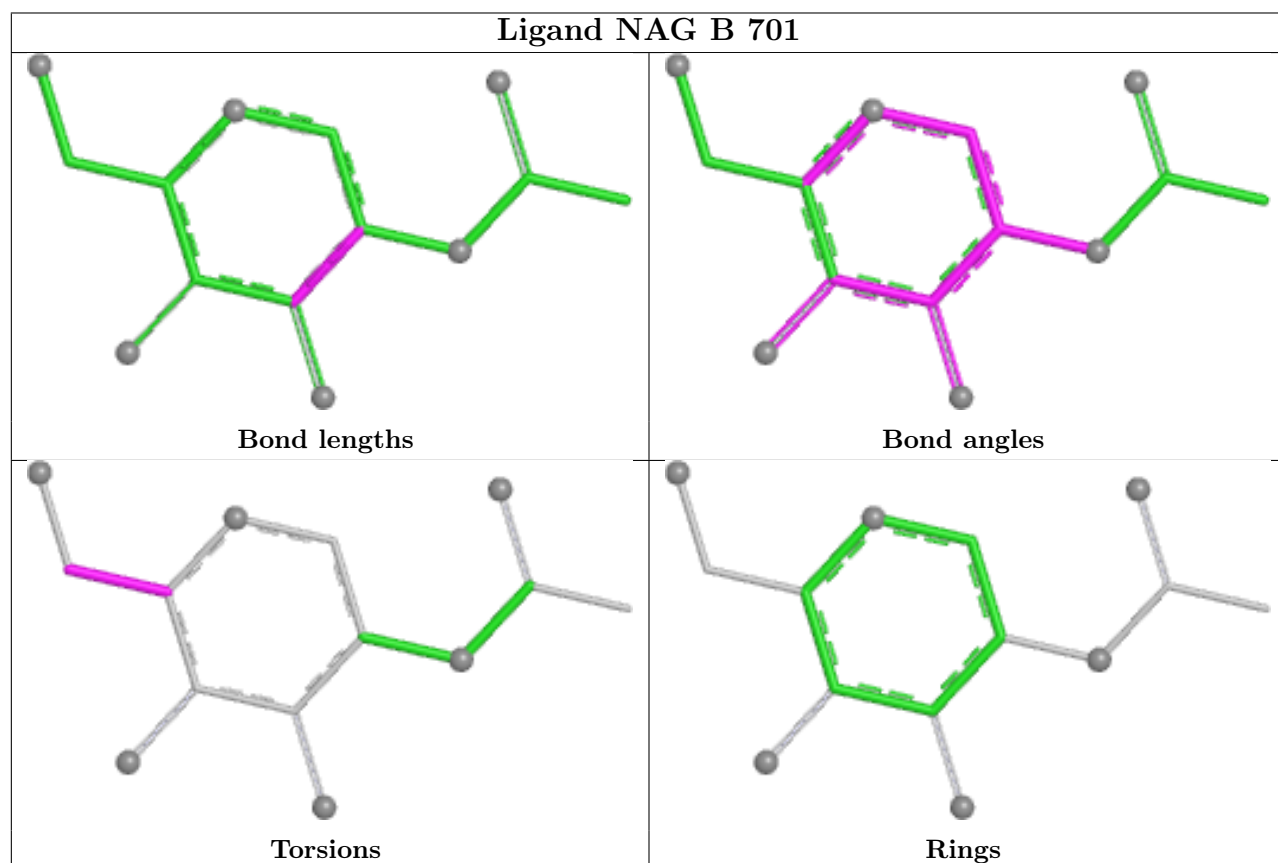
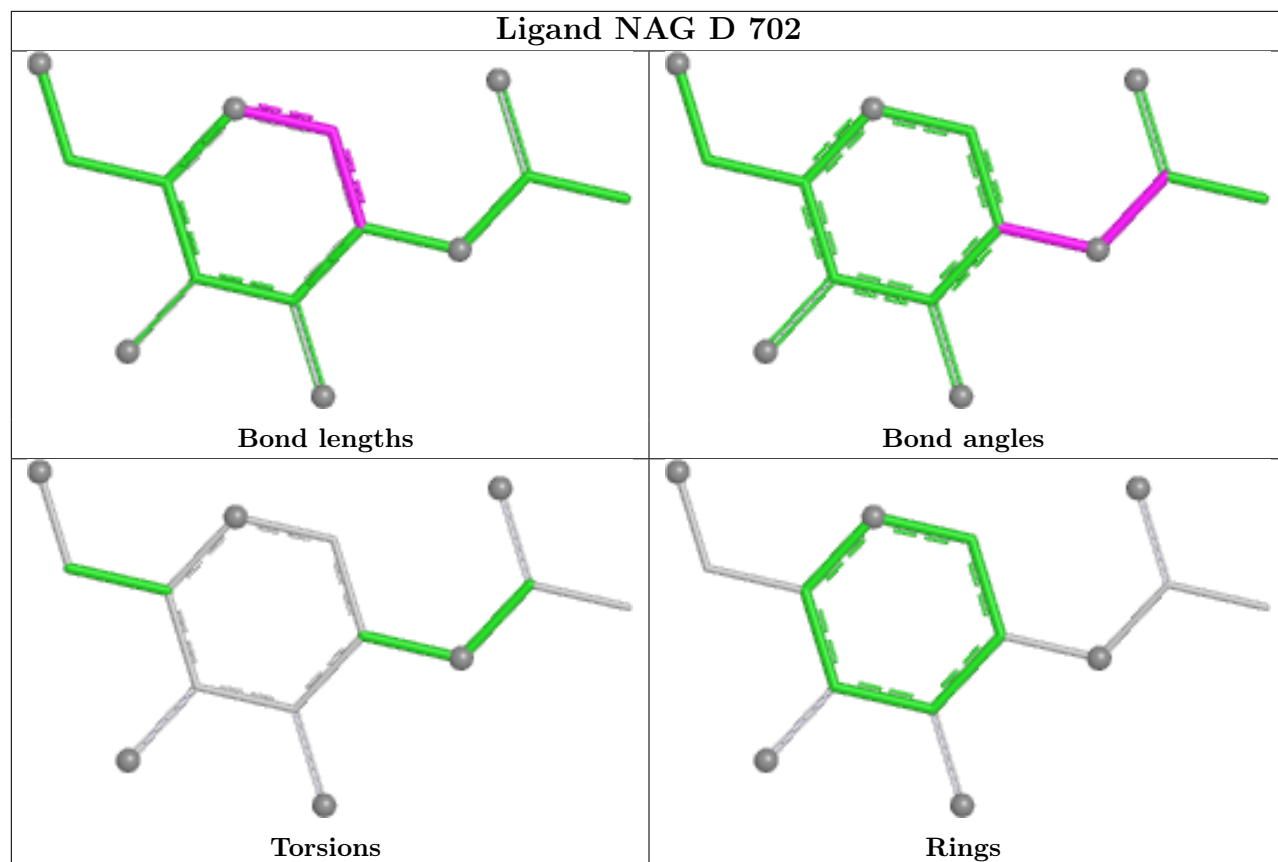


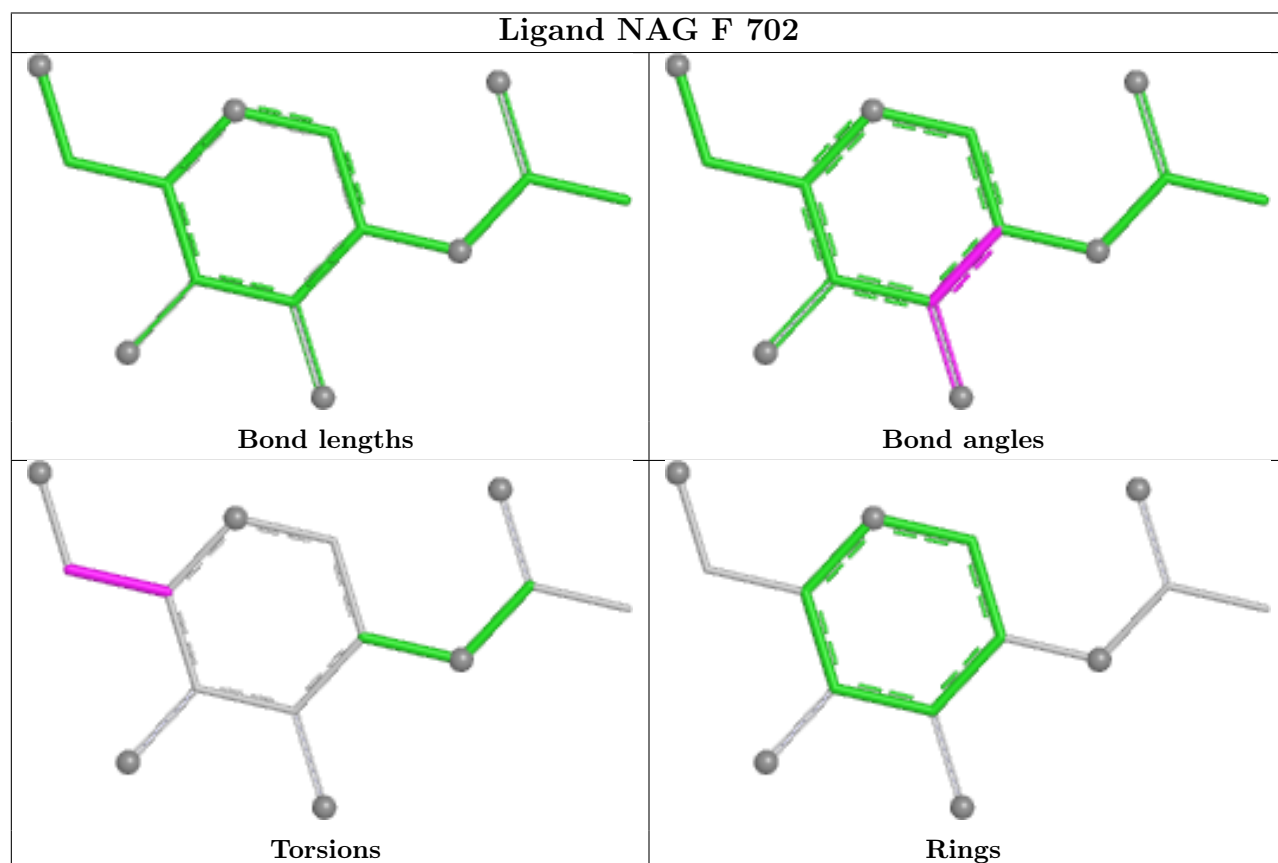
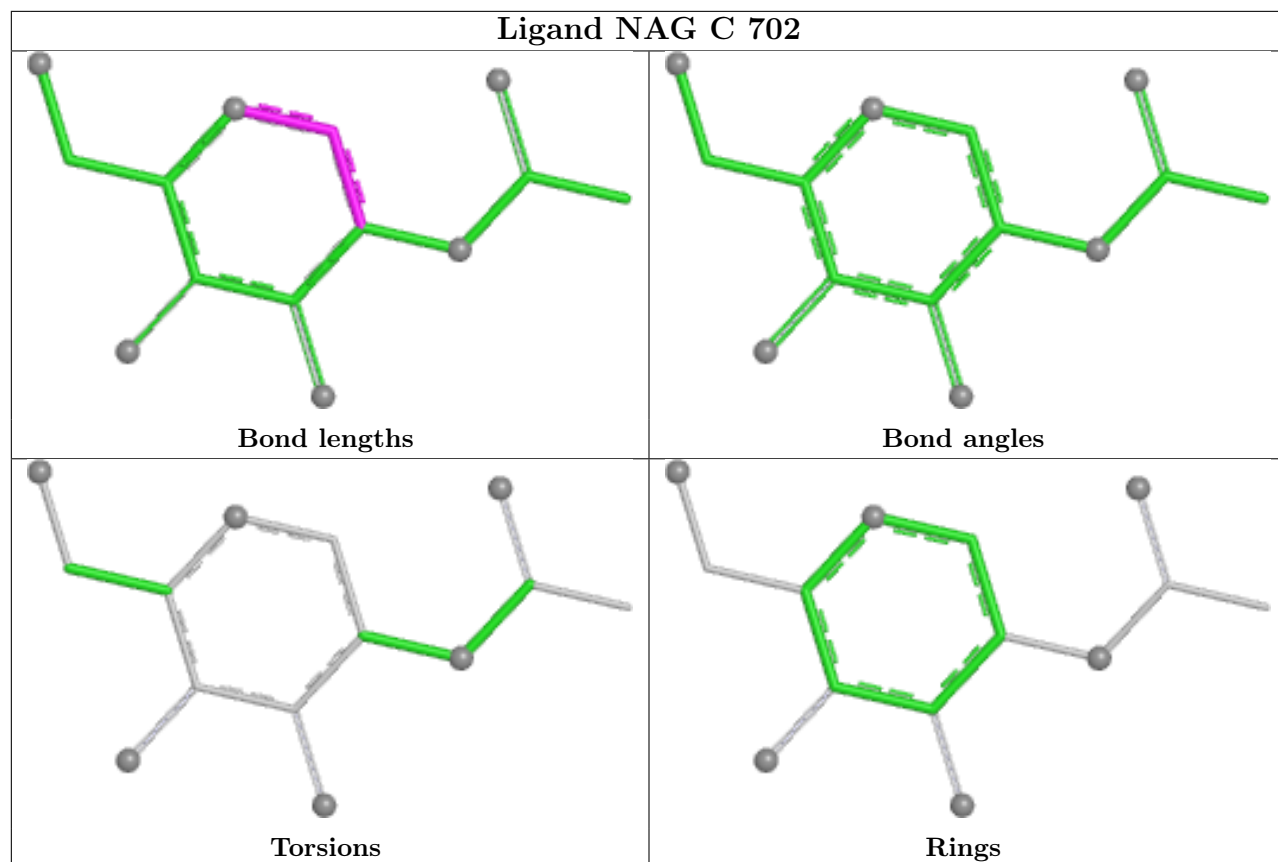


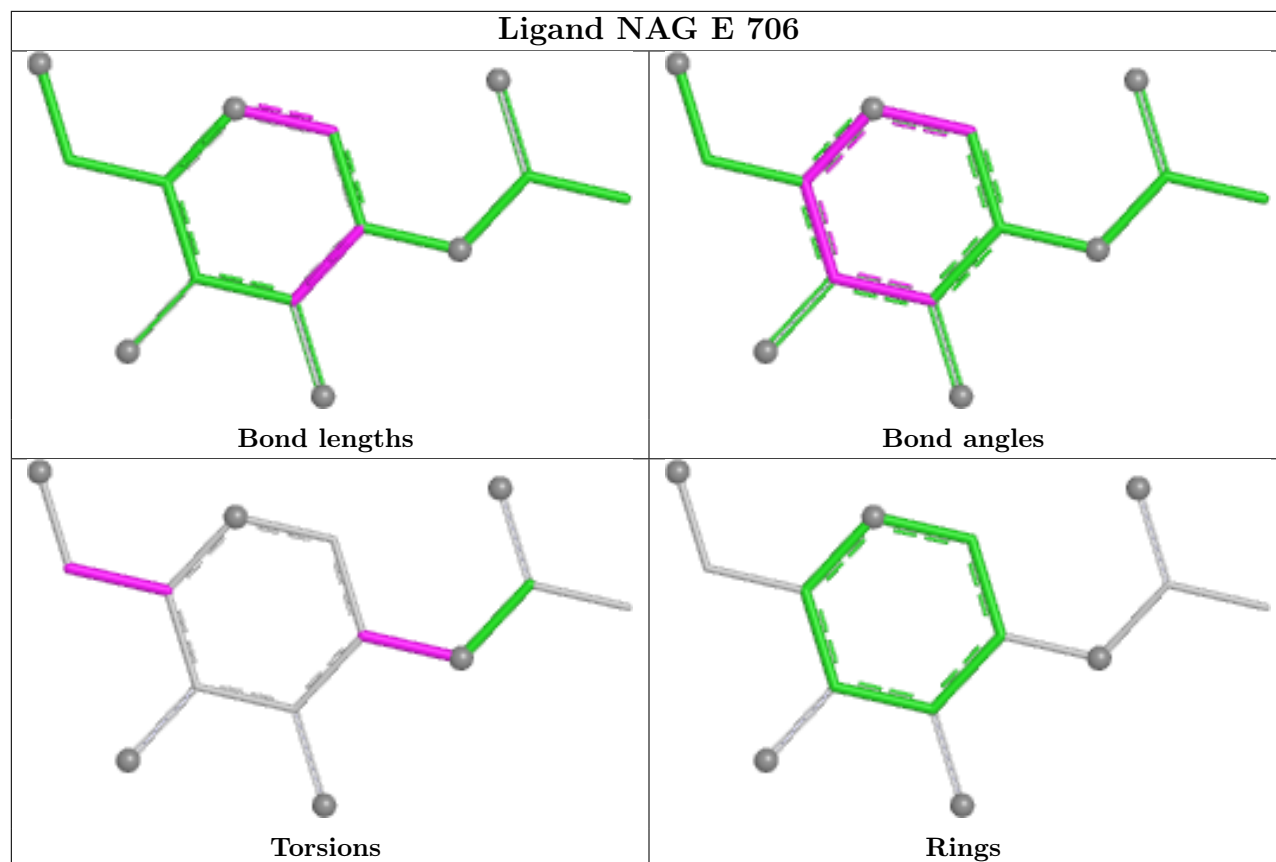












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/497 (97%)	0.93	52 (10%) 11 12	22, 39, 64, 119	1 (0%)
1	B	488/497 (98%)	0.95	58 (11%) 9 10	15, 39, 67, 130	3 (0%)
1	C	489/497 (98%)	0.83	41 (8%) 17 19	19, 37, 64, 135	3 (0%)
1	D	489/497 (98%)	0.78	44 (8%) 15 17	19, 36, 62, 125	4 (0%)
1	E	489/497 (98%)	0.95	52 (10%) 11 13	20, 38, 65, 108	4 (0%)
1	F	489/497 (98%)	1.02	72 (14%) 6 6	17, 40, 73, 128	4 (0%)
All	All	2931/2982 (98%)	0.91	319 (10%) 10 12	15, 38, 66, 135	19 (0%)

All (319) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	ILE	10.5
1	F	200	GLY	6.8
1	E	502	ILE	6.7
1	F	502	ILE	6.4
1	B	473	CYS	6.4
1	B	502	ILE	6.3
1	B	388	THR	6.1
1	D	502	ILE	5.5
1	C	345	GLY	5.5
1	A	335	ILE	5.5
1	C	385	ILE	5.5
1	D	388	THR	5.2
1	F	385	ILE	5.1
1	B	133	SER	5.0
1	C	388	THR	4.9
1	F	335	ILE	4.8
1	A	324	PRO	4.7
1	B	501	GLN	4.7
1	A	388	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	493	ASP	4.6
1	E	388	THR	4.6
1	C	502	ILE	4.5
1	C	324	PRO	4.5
1	E	497[A]	ASN	4.5
1	F	387	LYS	4.4
1	B	324	PRO	4.3
1	C	387	LYS	4.3
1	C	503	LYS	4.3
1	B	199	SER	4.2
1	F	347	VAL	4.2
1	B	335	ILE	4.1
1	A	334	ALA	4.0
1	C	133	SER	4.0
1	A	385	ILE	4.0
1	F	196	VAL	4.0
1	C	367	LEU	4.0
1	B	345	GLY	3.9
1	F	291	ASP	3.9
1	E	334	ALA	3.9
1	B	385	ILE	3.9
1	E	386	GLU	3.8
1	D	389	ASN	3.8
1	F	8	ASN	3.8
1	A	386	GLU	3.8
1	F	388	THR	3.8
1	C	382	ASN	3.8
1	B	8	ASN	3.7
1	A	387	LYS	3.7
1	C	334	ALA	3.7
1	F	500	PHE	3.7
1	D	367	LEU	3.7
1	B	340	GLU	3.6
1	E	48	THR	3.6
1	C	8	ASN	3.6
1	F	503	LYS	3.5
1	D	248	ILE	3.5
1	D	497[A]	ASN	3.5
1	F	199	SER	3.5
1	C	497[A]	ASN	3.5
1	A	501	GLN	3.5
1	F	248	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	8	ASN	3.5
1	F	439	LEU	3.4
1	D	387	LYS	3.4
1	F	386	GLU	3.4
1	D	503	LYS	3.4
1	F	336	ALA	3.4
1	A	497[A]	ASN	3.4
1	F	324	PRO	3.4
1	E	9	SER	3.4
1	D	334	ALA	3.3
1	F	334	ALA	3.3
1	F	495	ALA	3.3
1	E	128	ILE	3.3
1	B	386	GLU	3.3
1	D	8	ASN	3.3
1	B	367	LEU	3.3
1	A	278	SER	3.3
1	A	8	ASN	3.2
1	A	94	TYR	3.2
1	D	126	ASN	3.2
1	C	335	ILE	3.2
1	E	219	SER	3.2
1	F	137	CYS	3.2
1	E	500	PHE	3.2
1	D	324	PRO	3.2
1	B	128	ILE	3.2
1	E	385	ILE	3.2
1	B	341	ASN	3.1
1	E	202	VAL	3.1
1	E	347	VAL	3.1
1	E	161	TYR	3.1
1	F	222	TRP	3.1
1	B	503	LYS	3.1
1	C	124	ASP	3.1
1	E	198	ALA	3.1
1	F	128	ILE	3.1
1	E	133	SER	3.1
1	E	104	ASP	3.1
1	B	323	VAL	3.1
1	E	130	VAL	3.1
1	B	488	HIS	3.0
1	F	278	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	159	GLN	3.0
1	C	501	GLN	3.0
1	B	382	ASN	3.0
1	E	387	LYS	3.0
1	B	29	ILE	3.0
1	F	201	ARG	3.0
1	A	23	GLY	3.0
1	E	324	PRO	3.0
1	A	25	LEU	3.0
1	D	386	GLU	3.0
1	A	48	THR	3.0
1	F	369	SER	3.0
1	F	126	ASN	3.0
1	A	443	GLU	3.0
1	D	291	ASP	3.0
1	E	200	GLY	3.0
1	F	34	ILE	2.9
1	E	46	SER	2.9
1	C	386	GLU	2.9
1	A	367	LEU	2.9
1	E	439	LEU	2.9
1	E	503	LYS	2.9
1	B	23	GLY	2.9
1	D	379	GLY	2.9
1	B	336	ALA	2.9
1	D	500	PHE	2.9
1	A	128	ILE	2.9
1	E	24	THR	2.9
1	B	497[A]	ASN	2.9
1	C	291	ASP	2.9
1	D	29	ILE	2.9
1	C	323	VAL	2.8
1	E	278	SER	2.8
1	A	500	PHE	2.8
1	B	326	LYS	2.8
1	A	196	VAL	2.8
1	F	361	THR	2.8
1	F	497[A]	ASN	2.8
1	B	316	LEU	2.8
1	A	248	ILE	2.7
1	F	339	ILE	2.7
1	A	473	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	216	ASN	2.7
1	F	129	GLY	2.7
1	C	128	ILE	2.7
1	A	133	SER	2.7
1	B	48	THR	2.7
1	B	126	ASN	2.7
1	F	145	ASN	2.7
1	F	483	ASN	2.7
1	E	142	GLY	2.7
1	A	199	SER	2.7
1	E	336	ALA	2.6
1	F	501	GLN	2.6
1	D	326	LYS	2.6
1	D	353	PHE	2.6
1	F	358	SER	2.6
1	F	367	LEU	2.6
1	E	501	GLN	2.6
1	D	321	ARG	2.6
1	F	384	LEU	2.6
1	D	368	LYS	2.6
1	E	389	ASN	2.6
1	F	187	THR	2.6
1	F	29	ILE	2.6
1	C	495	ALA	2.6
1	F	48	THR	2.6
1	F	340	GLU	2.5
1	B	291	ASP	2.5
1	A	347	VAL	2.5
1	D	452	ARG	2.5
1	A	496	LEU	2.5
1	F	24	THR	2.5
1	E	248	ILE	2.5
1	D	439	LEU	2.5
1	F	140	LYS	2.5
1	F	493	ASP	2.5
1	C	9	SER	2.5
1	C	500	PHE	2.5
1	E	197	ARG	2.5
1	E	344	GLU	2.5
1	C	29	ILE	2.5
1	B	315	LYS	2.5
1	B	321	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	30	THR	2.4
1	B	143	SER	2.4
1	B	159	GLN	2.4
1	B	197	ARG	2.4
1	C	336	ALA	2.4
1	F	208	ARG	2.4
1	C	187	THR	2.4
1	D	473	CYS	2.4
1	D	128	ILE	2.4
1	D	385	ILE	2.4
1	B	496	LEU	2.4
1	A	159	GLN	2.4
1	D	24	THR	2.4
1	F	374	ILE	2.4
1	B	211	GLN	2.4
1	D	261	ARG	2.4
1	A	126	ASN	2.4
1	B	196	VAL	2.4
1	B	348	ASP	2.3
1	F	188	ASP	2.3
1	E	23	GLY	2.3
1	D	138	ALA	2.3
1	C	48	THR	2.3
1	B	278	SER	2.3
1	F	448	PHE	2.3
1	D	189	ARG	2.3
1	F	321	ARG	2.3
1	E	126	ASN	2.3
1	A	21	PRO	2.3
1	C	463	GLY	2.3
1	C	372	ALA	2.3
1	B	248	ILE	2.3
1	A	340	GLU	2.3
1	D	501	GLN	2.3
1	F	496	LEU	2.3
1	A	483	ASN	2.3
1	A	469	ILE	2.3
1	E	315	LYS	2.3
1	E	64	CYS	2.3
1	C	126	ASN	2.3
1	D	216	ASN	2.3
1	A	200	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	387	LYS	2.3
1	E	230	ILE	2.3
1	C	402	VAL	2.3
1	E	367	LEU	2.2
1	F	353	PHE	2.2
1	C	104	ASP	2.2
1	C	137	CYS	2.2
1	B	359	GLU	2.2
1	D	340	GLU	2.2
1	F	198	ALA	2.2
1	A	219	SER	2.2
1	B	230	ILE	2.2
1	A	216	ASN	2.2
1	E	483	ASN	2.2
1	A	14	CYS	2.2
1	A	137	CYS	2.2
1	B	19	ALA	2.2
1	F	133	SER	2.2
1	C	194	LEU	2.2
1	E	323	VAL	2.2
1	D	104	ASP	2.2
1	D	197	ARG	2.2
1	A	277	CYS	2.2
1	D	277	CYS	2.2
1	A	384	LEU	2.2
1	C	384	LEU	2.2
1	D	335	ILE	2.2
1	F	338	PHE	2.2
1	E	326	LYS	2.2
1	C	14	CYS	2.2
1	F	473	CYS	2.2
1	B	219	SER	2.2
1	D	358	SER	2.2
1	D	495	ALA	2.2
1	E	304	ALA	2.2
1	F	91	SER	2.2
1	E	201	ARG	2.1
1	E	335	ILE	2.1
1	D	222	TRP	2.1
1	E	472	LYS	2.1
1	A	336	ALA	2.1
1	C	219	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	278	SER	2.1
1	B	195	TYR	2.1
1	F	94	TYR	2.1
1	A	326	LYS	2.1
1	F	368	LYS	2.1
1	A	389	ASN	2.1
1	C	196	VAL	2.1
1	B	371	GLN	2.1
1	B	500	PHE	2.1
1	A	261	ARG	2.1
1	A	276	THR	2.1
1	A	198	ALA	2.1
1	F	304	ALA	2.1
1	F	326	LYS	2.1
1	A	34	ILE	2.1
1	B	34	ILE	2.1
1	F	487	ASP	2.1
1	D	490	VAL	2.1
1	B	379	GLY	2.1
1	C	200	GLY	2.1
1	E	345	GLY	2.1
1	A	197	ARG	2.1
1	A	452	ARG	2.1
1	C	228	SER	2.1
1	D	199	SER	2.1
1	E	495	ALA	2.1
1	A	13	LEU	2.1
1	A	356	GLN	2.1
1	B	381	LEU	2.1
1	B	216	ASN	2.1
1	F	33	GLN	2.1
1	F	402	VAL	2.1
1	F	189	ARG	2.1
1	B	358	SER	2.0
1	B	346	MET	2.0
1	F	138	ALA	2.0
1	F	344	GLU	2.0
1	E	25	LEU	2.0
1	F	382[A]	ASN	2.0
1	B	347	VAL	2.0
1	A	462	MET	2.0
1	B	187	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	262	THR	2.0
1	F	40	THR	2.0
1	D	365	ALA	2.0
1	B	246	ASN	2.0
1	B	483	ASN	2.0
1	F	341	ASN	2.0

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](#)

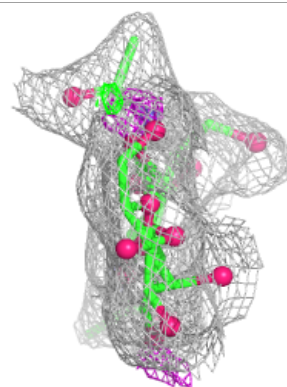
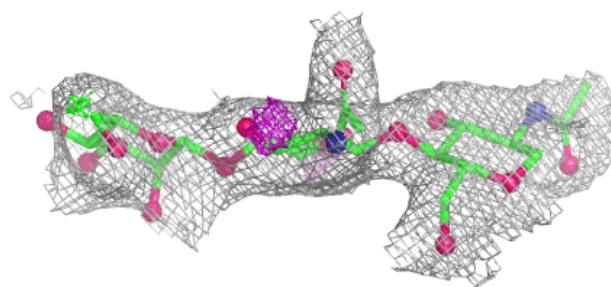
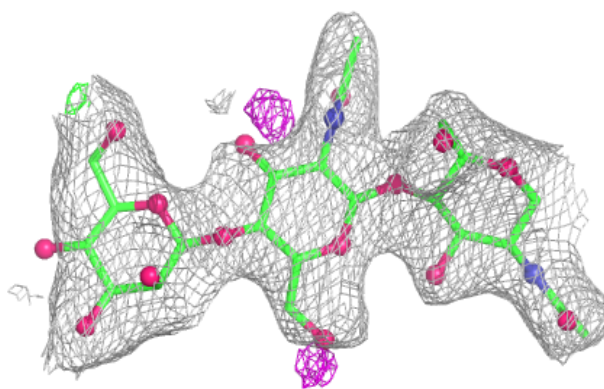
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	I	3	11/12	0.62	0.14	43,51,65,67	0
2	BMA	G	3	11/12	0.67	0.15	36,49,60,79	0
2	BMA	J	3	11/12	0.72	0.11	46,54,59,62	0
2	BMA	K	3	11/12	0.73	0.12	36,54,67,78	0
2	BMA	H	3	11/12	0.74	0.12	42,50,60,63	0
2	BMA	L	3	11/12	0.75	0.11	41,53,66,68	0
2	NAG	G	2	14/15	0.82	0.12	31,35,43,57	0
2	NAG	L	2	14/15	0.84	0.13	35,46,57,59	0
2	NAG	I	2	14/15	0.84	0.10	27,37,43,65	0
2	NAG	J	2	14/15	0.86	0.11	24,35,49,67	0
2	NAG	K	2	14/15	0.87	0.12	15,41,60,61	0
2	NAG	H	2	14/15	0.88	0.10	27,37,56,63	0
2	NAG	J	1	14/15	0.88	0.09	17,30,39,42	0
2	NAG	H	1	14/15	0.89	0.10	25,36,51,52	0
2	NAG	L	1	14/15	0.90	0.09	26,40,46,52	0
2	NAG	G	1	14/15	0.91	0.10	30,45,52,55	0
2	NAG	I	1	14/15	0.91	0.08	21,35,45,49	0
2	NAG	K	1	14/15	0.92	0.09	21,39,64,66	0

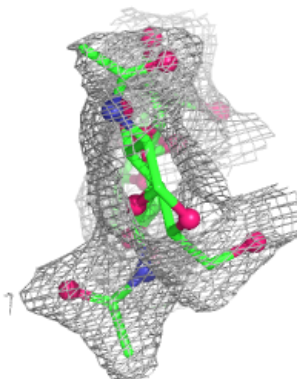
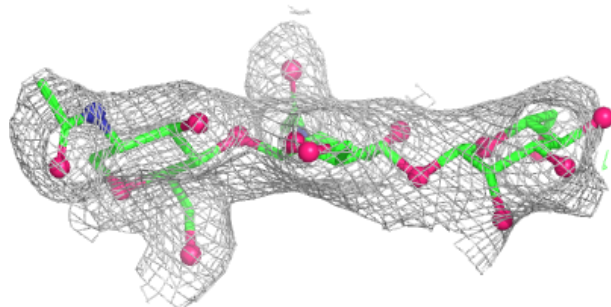
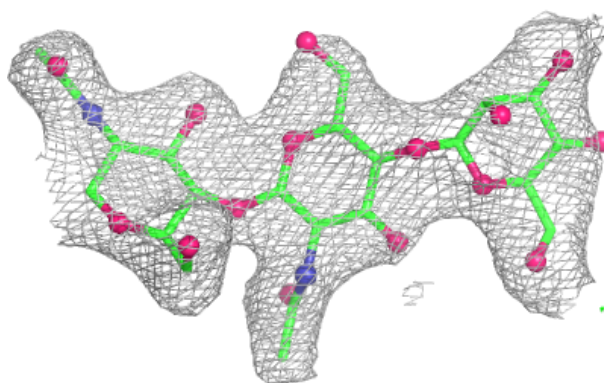
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

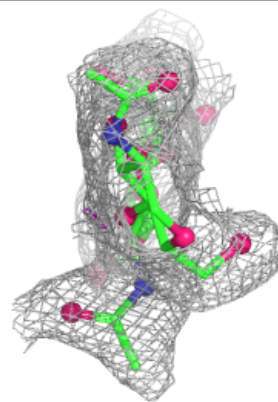
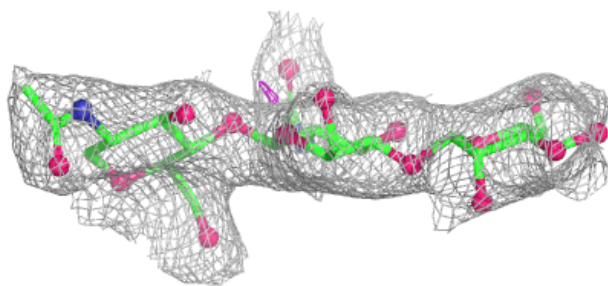
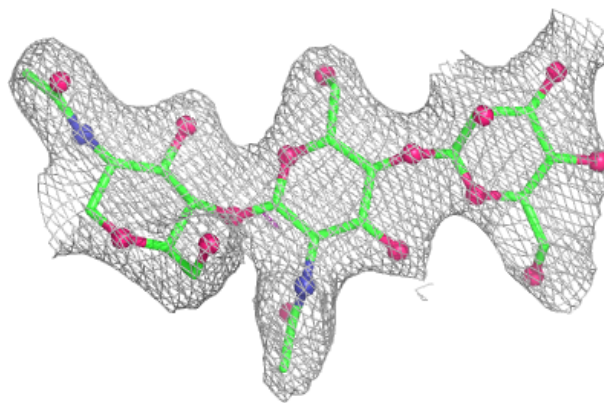
**Electron density around Chain H:**

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

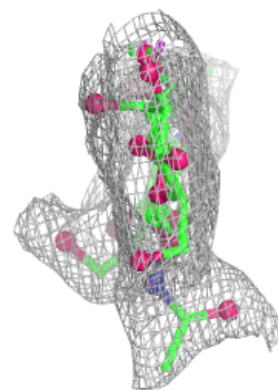
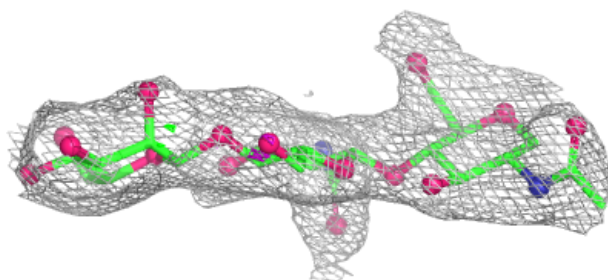
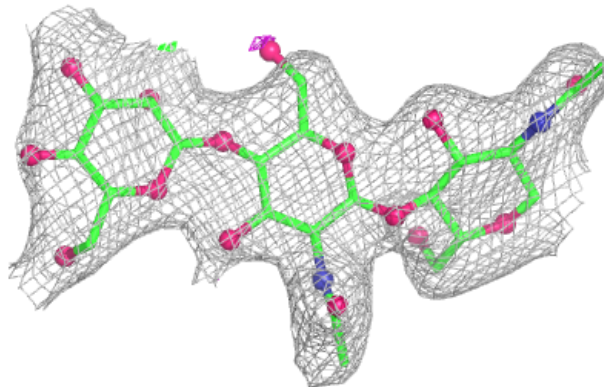


Electron density around Chain I:

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

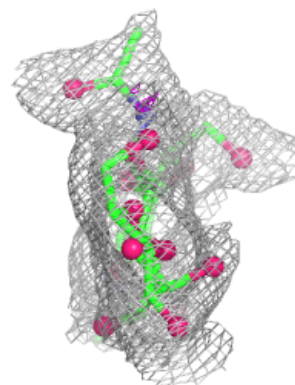
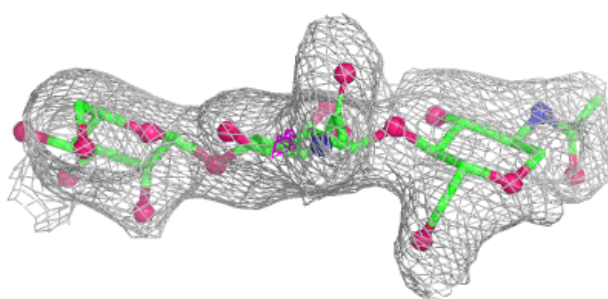
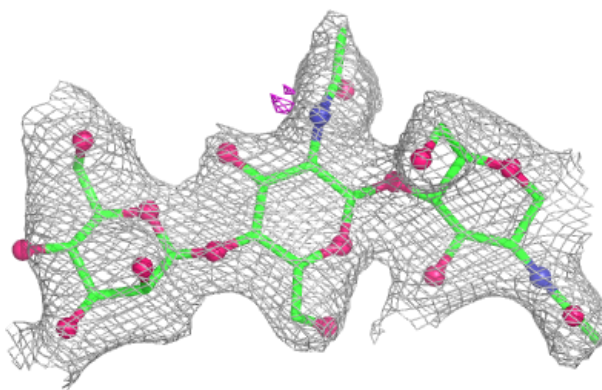
**Electron density around Chain J:**

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

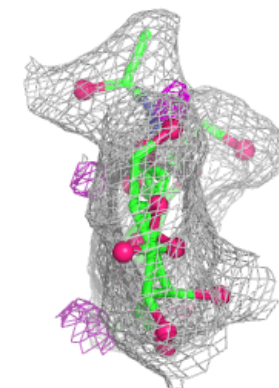
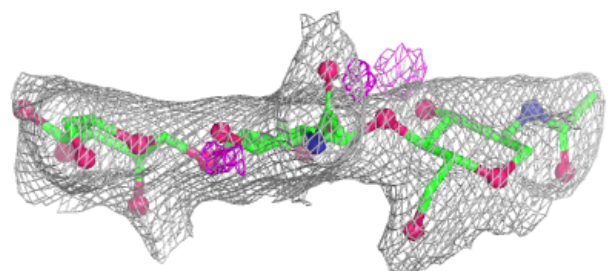
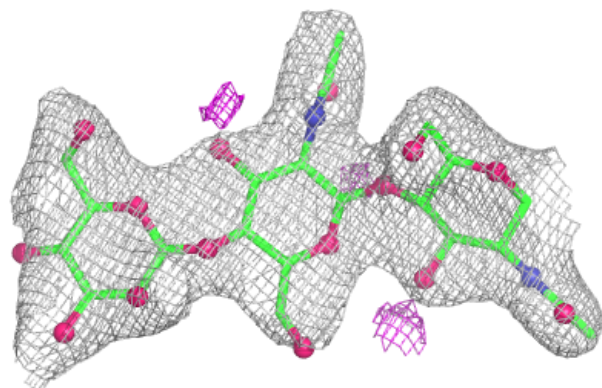


Electron density around Chain K:

$2mF_o-DF_c$ (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)



6.4 Ligands

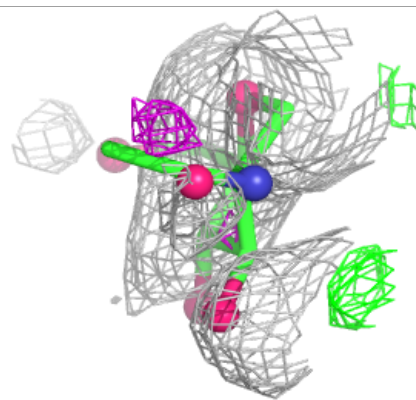
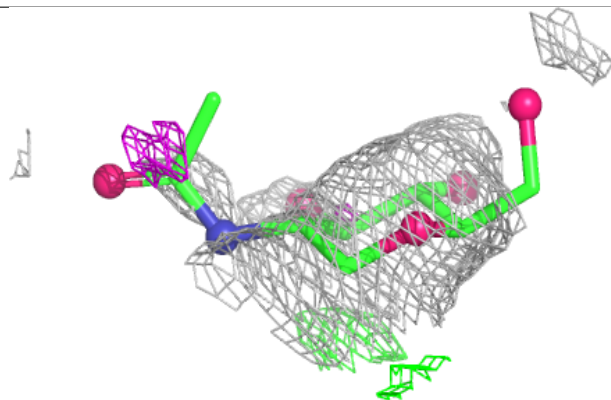
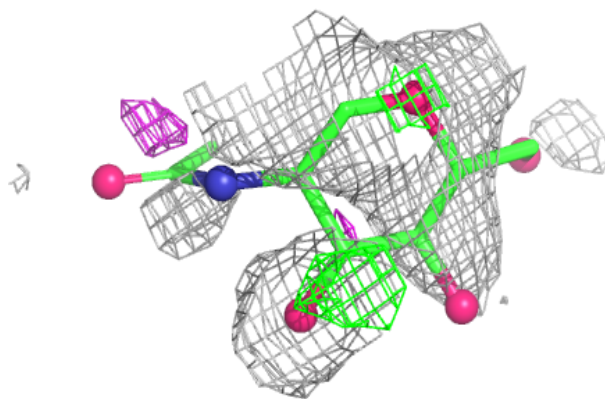
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	702	14/15	0.42	0.20	65,74,84,86	0
3	NAG	E	702	14/15	0.49	0.16	31,45,58,60	0
3	NAG	F	706	14/15	0.49	0.20	50,57,70,76	0
3	NAG	F	702	14/15	0.51	0.19	39,58,70,76	0
3	NAG	B	706	14/15	0.51	0.20	45,63,71,75	0
3	NAG	E	700	14/15	0.53	0.18	47,57,79,79	0
3	NAG	C	702	14/15	0.53	0.19	49,76,102,106	0
3	NAG	D	702	14/15	0.57	0.20	26,75,92,102	0
3	NAG	C	706	14/15	0.59	0.17	37,46,65,66	0
3	NAG	A	706	14/15	0.60	0.19	39,60,69,70	0
3	NAG	E	706	14/15	0.60	0.17	23,47,74,75	0
3	NAG	B	701	14/15	0.61	0.20	58,66,77,79	0
3	NAG	B	702	14/15	0.63	0.16	46,56,76,78	0
3	NAG	C	701	14/15	0.65	0.16	32,53,67,76	0
3	NAG	B	700	14/15	0.67	0.16	43,54,64,71	0
3	NAG	E	701	14/15	0.67	0.16	39,60,79,81	0
3	NAG	D	706	14/15	0.67	0.15	35,54,66,72	0
3	NAG	F	700	14/15	0.68	0.14	30,46,62,63	0
3	NAG	D	700	14/15	0.71	0.15	36,60,71,72	0
3	NAG	C	700	14/15	0.71	0.15	45,63,73,82	0
3	NAG	A	701	14/15	0.72	0.15	27,45,59,76	0
3	NAG	A	700	14/15	0.72	0.13	35,41,62,64	0
3	NAG	D	701	14/15	0.72	0.16	30,63,74,79	0
3	NAG	F	701	14/15	0.73	0.14	38,44,61,65	0

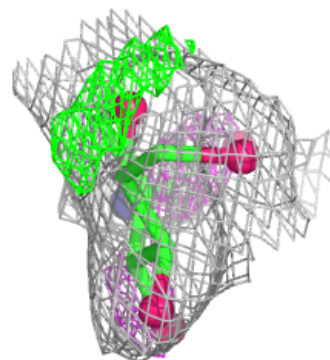
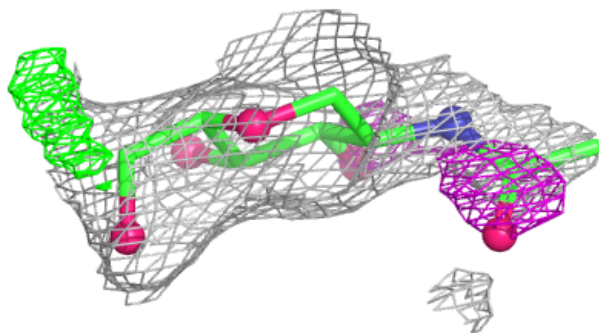
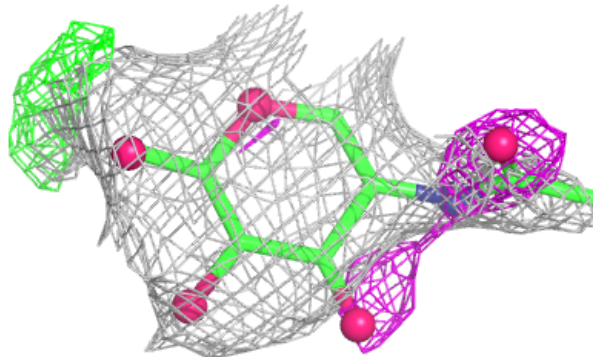
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 702:

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

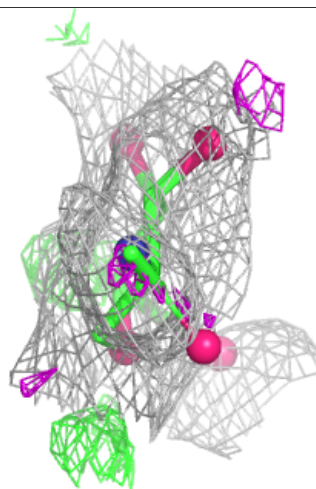
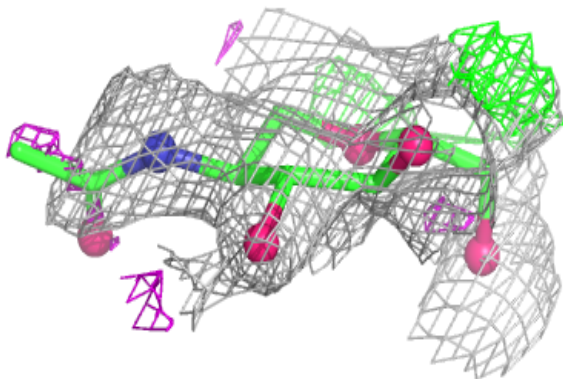
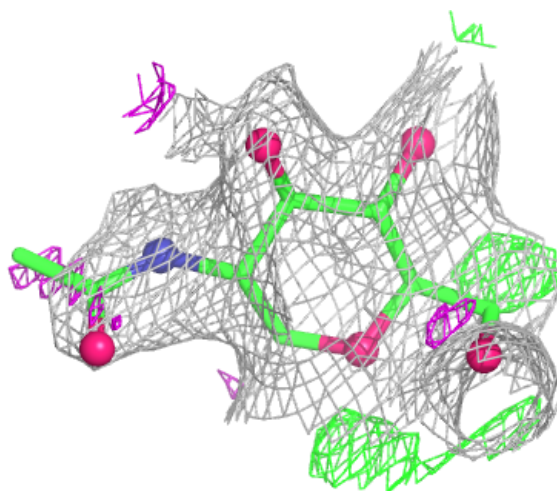
**Electron density around NAG E 702:**

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



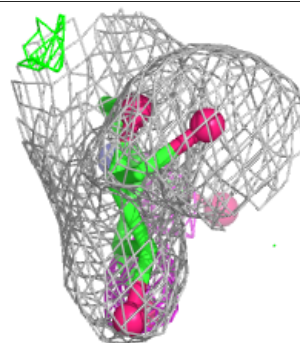
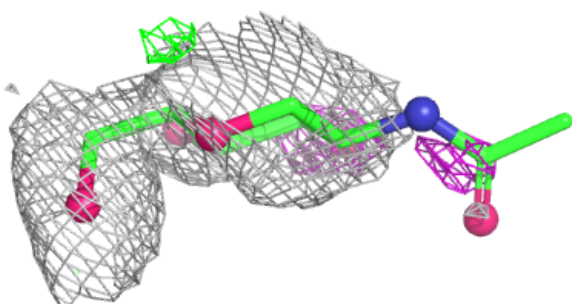
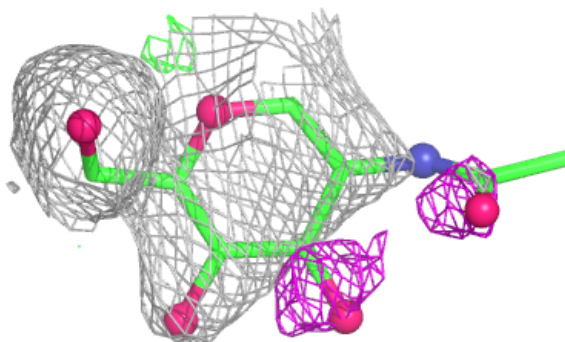
Electron density around NAG F 706:

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

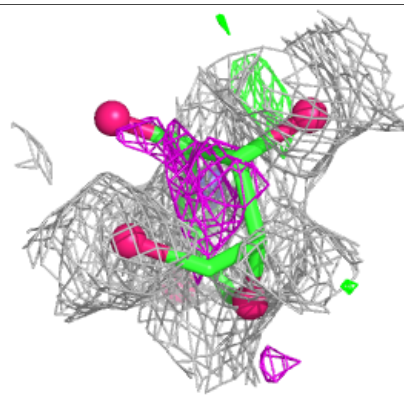
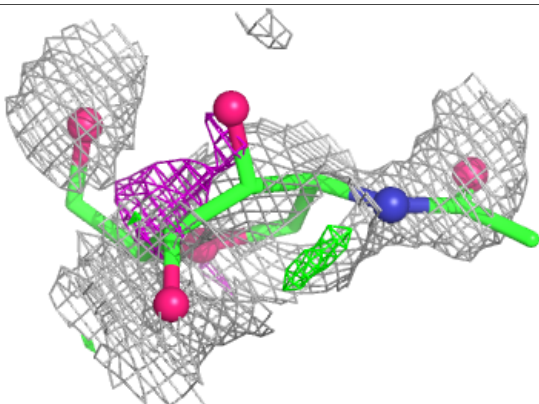
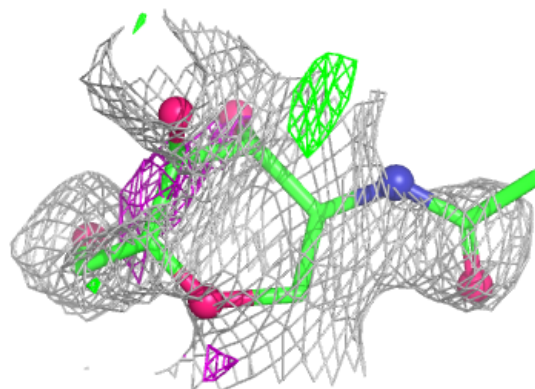


Electron density around NAG F 702:

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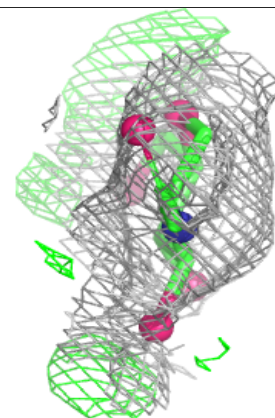
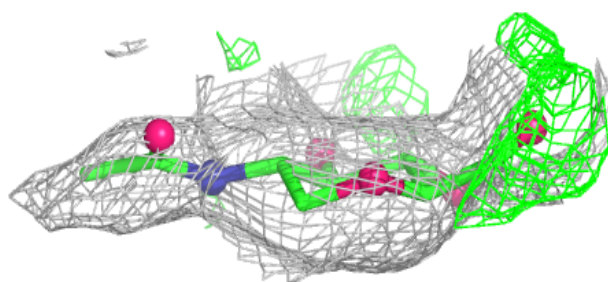
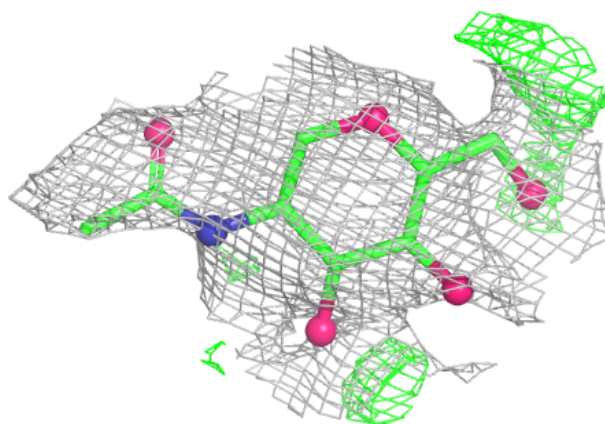
**Electron density around NAG B 706:**

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

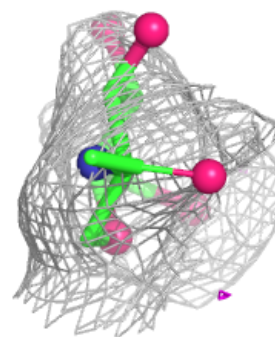
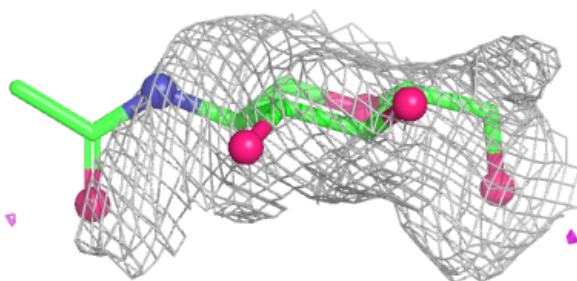
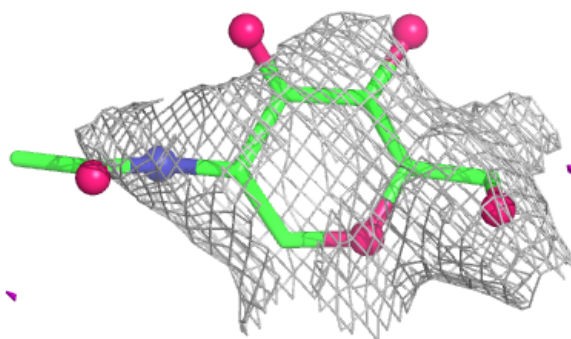


Electron density around NAG E 700:

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and green (positive)

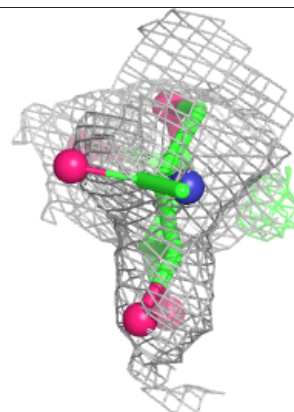
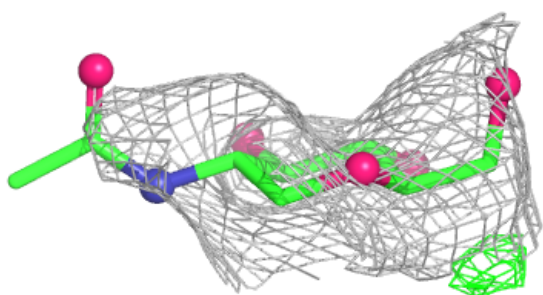
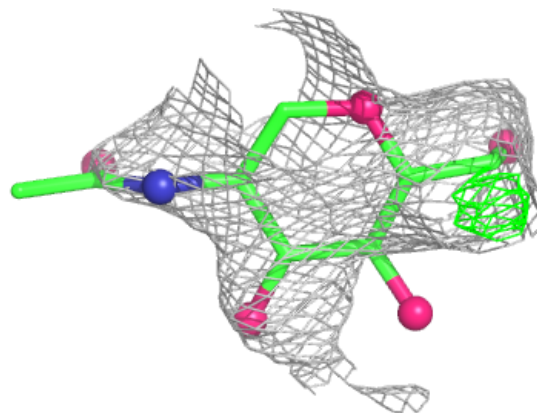
**Electron density around NAG C 702:**

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and green (positive)

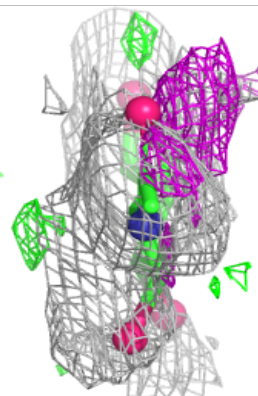
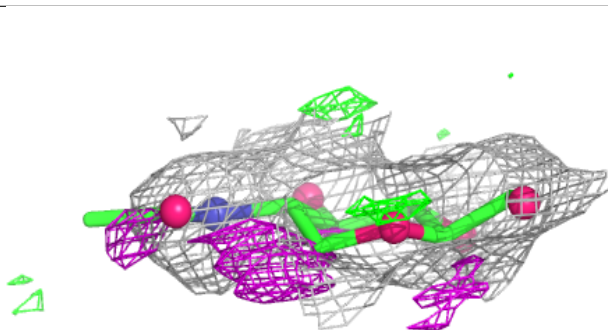
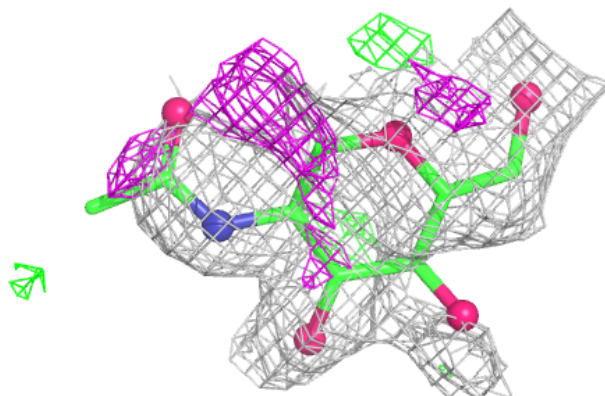


Electron density around NAG D 702:

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

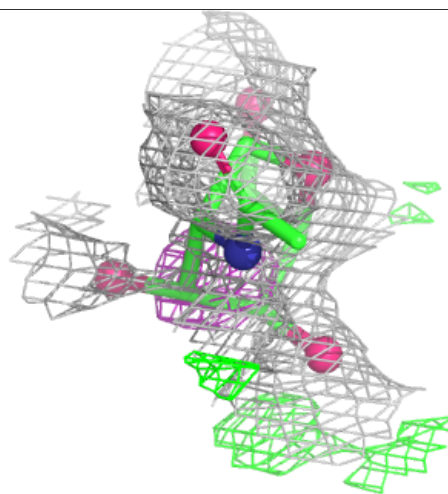
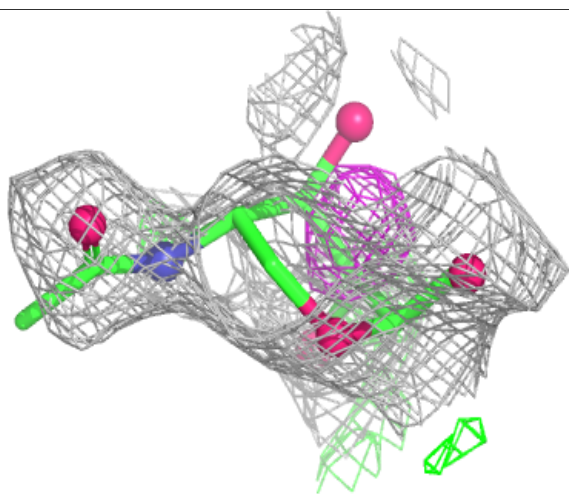
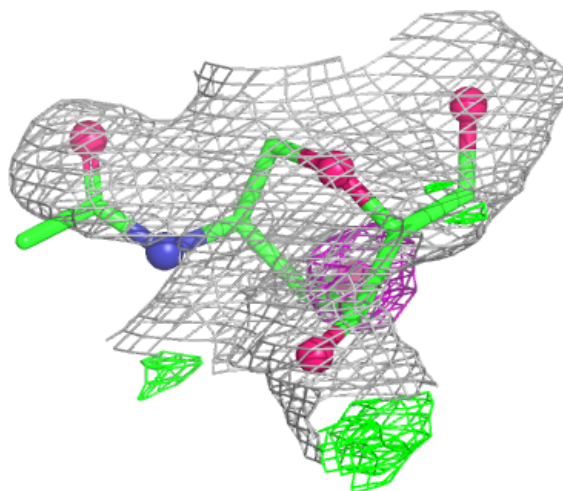
**Electron density around NAG C 706:**

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



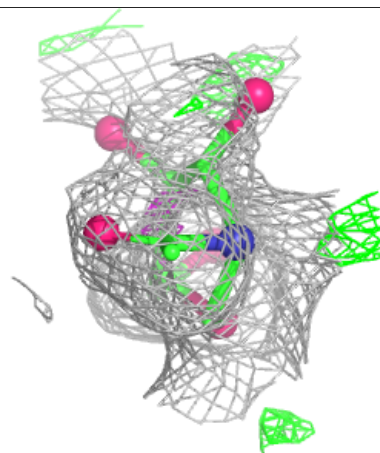
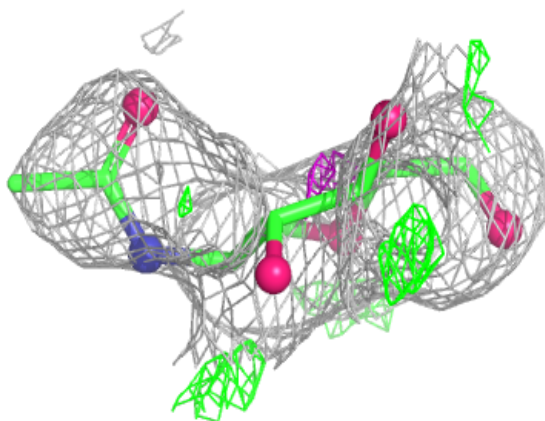
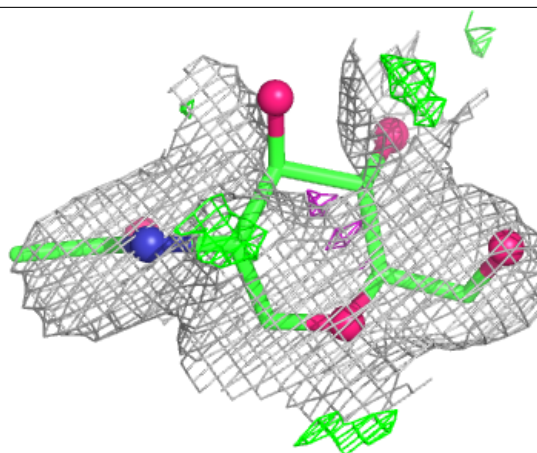
Electron density around NAG A 706:

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and green (positive)



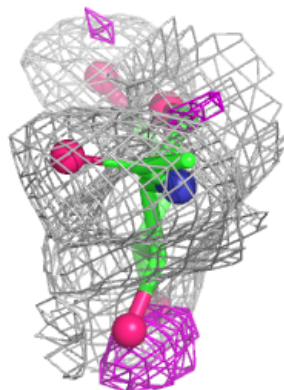
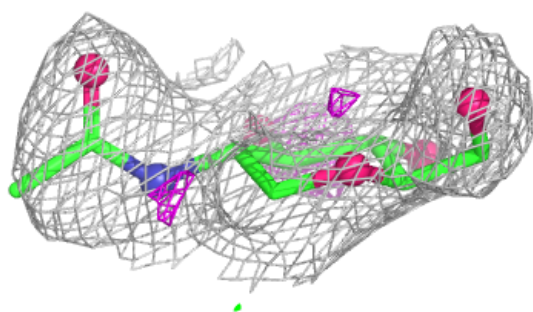
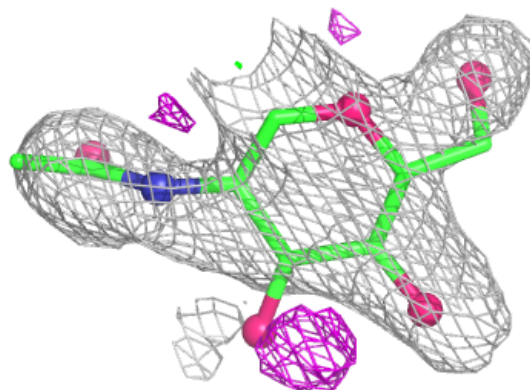
Electron density around NAG E 706:

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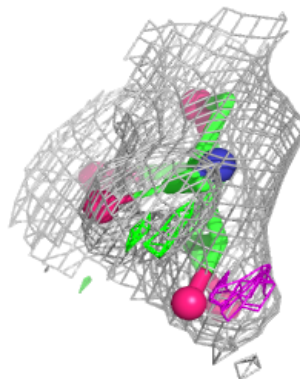
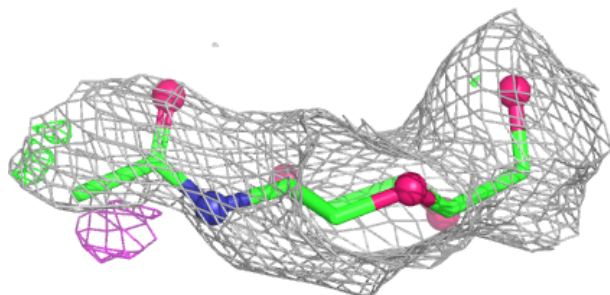
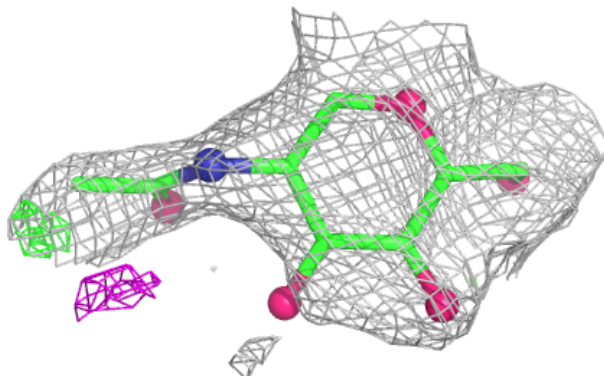


Electron density around NAG B 701:

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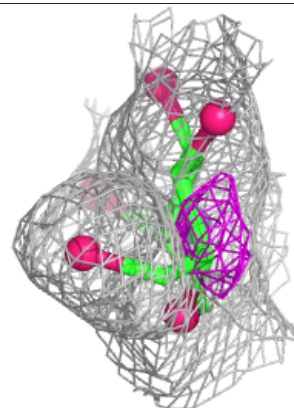
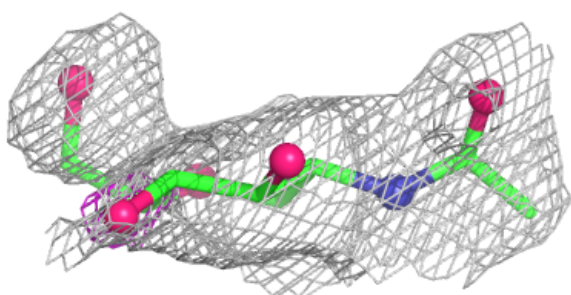
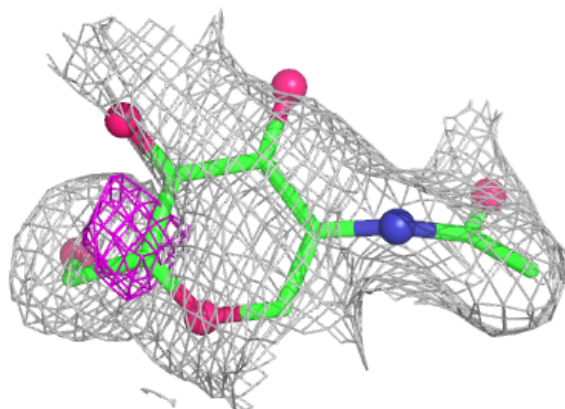
**Electron density around NAG B 702:**

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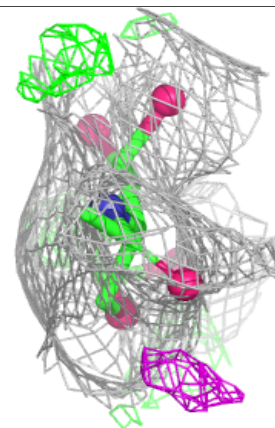
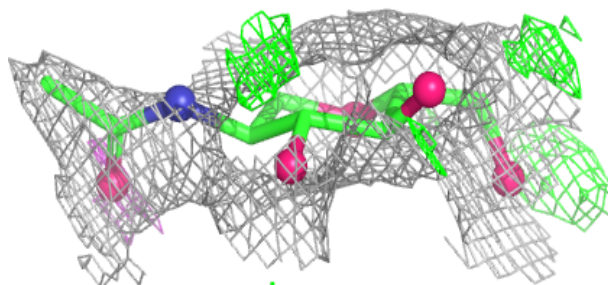
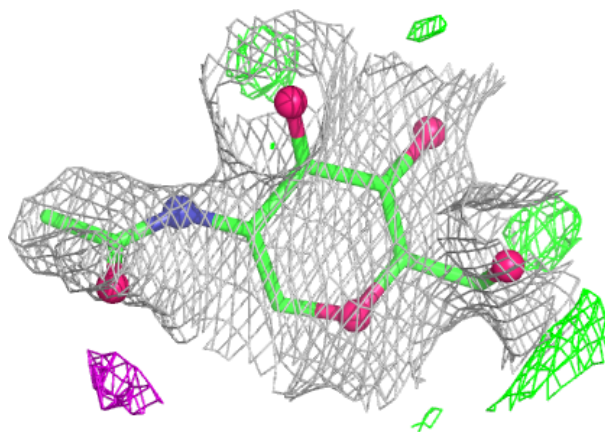


Electron density around NAG C 701:

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and green (positive)

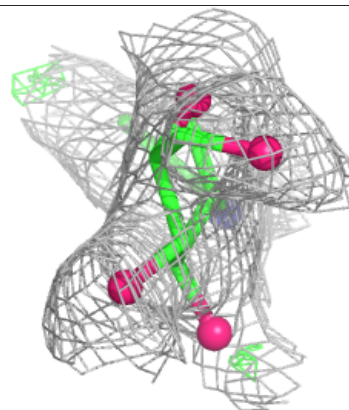
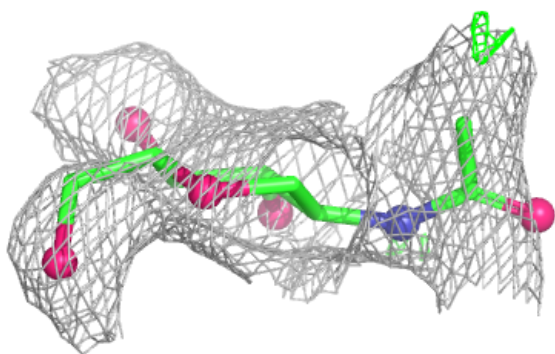
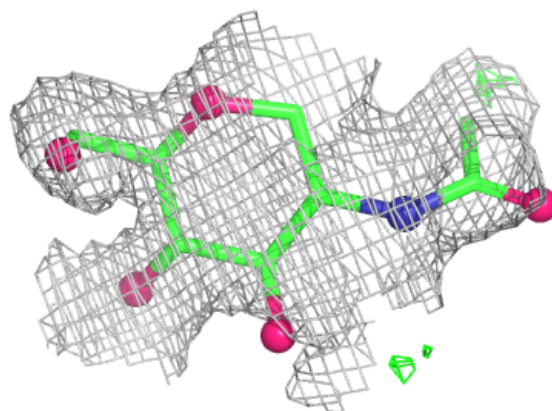
**Electron density around NAG B 700:**

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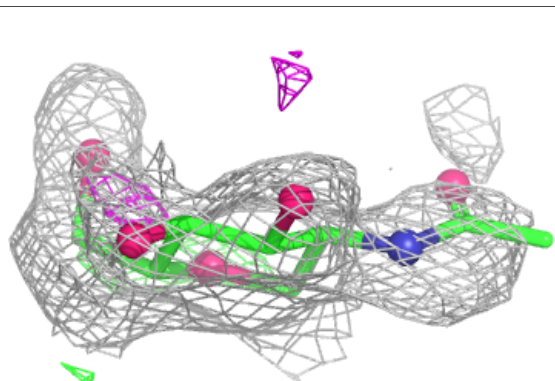
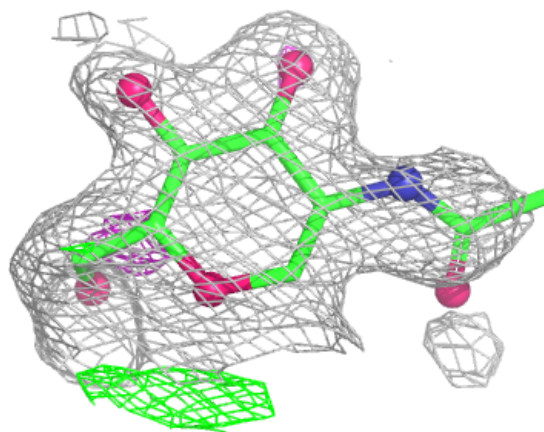


Electron density around NAG E 701:

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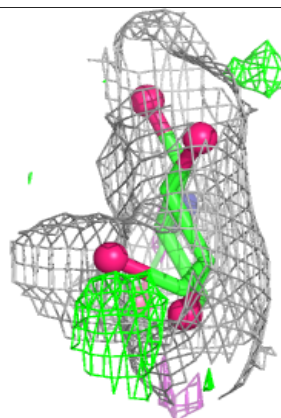
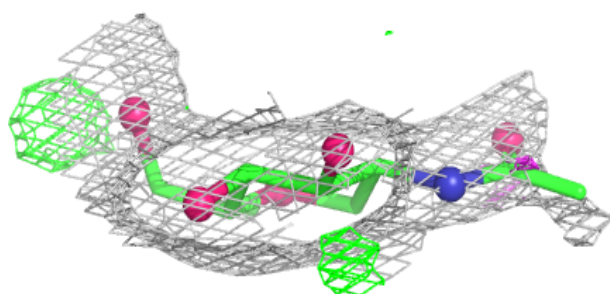
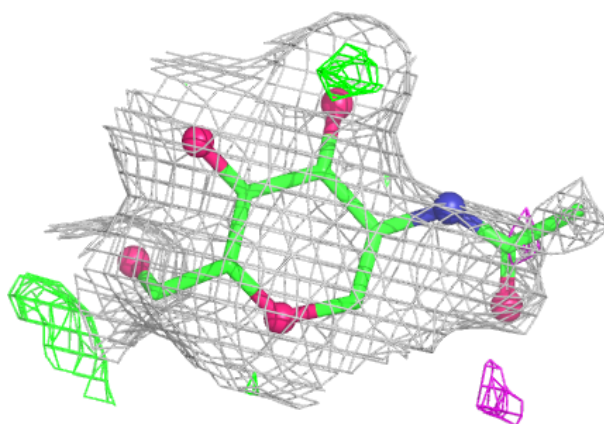
**Electron density around NAG D 706:**

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and green (positive)



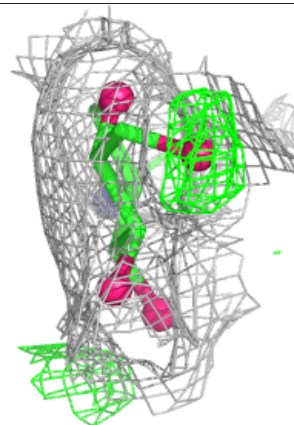
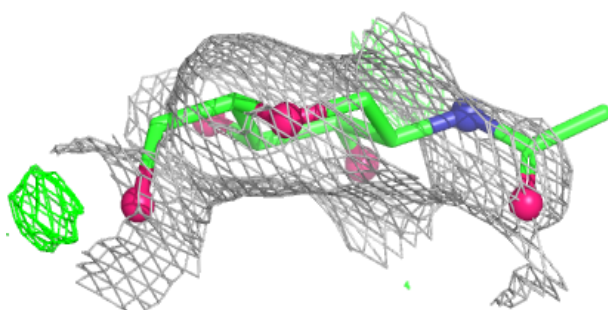
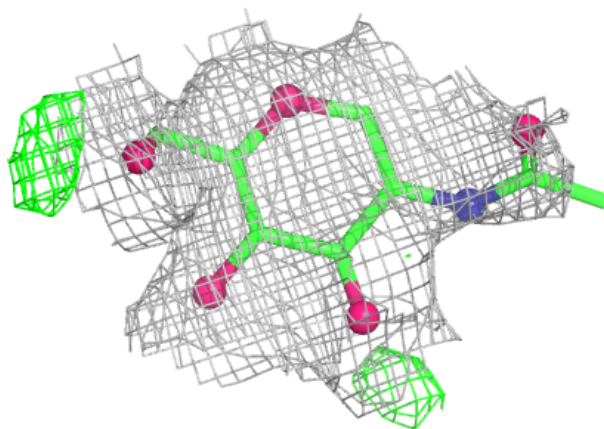
Electron density around NAG F 700:

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and green (positive)

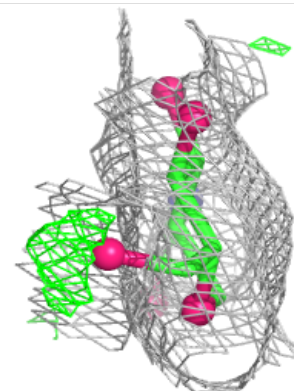
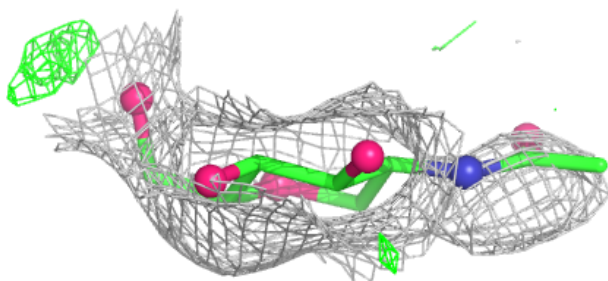
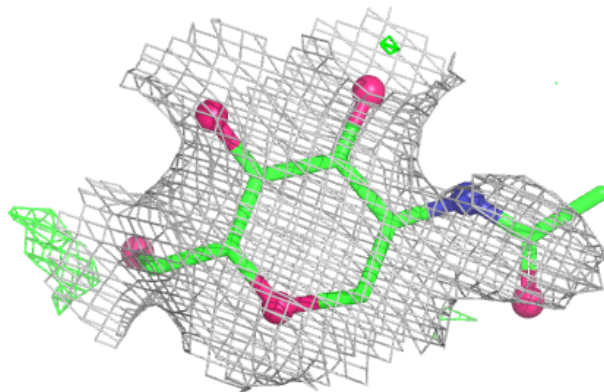


Electron density around NAG D 700:

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

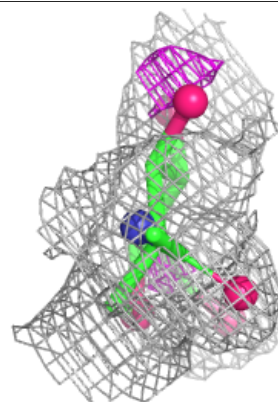
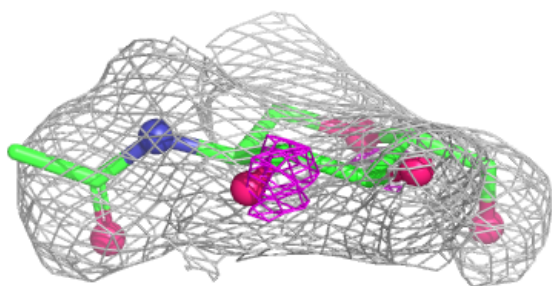
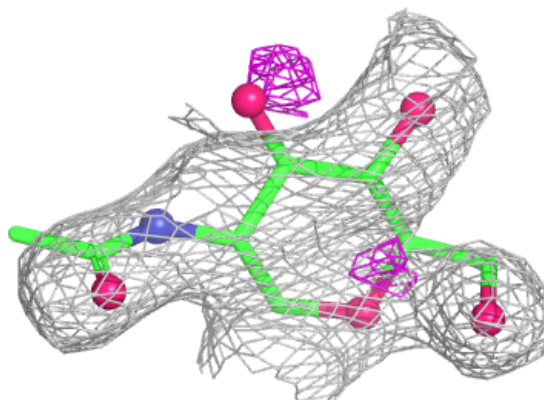
**Electron density around NAG C 700:**

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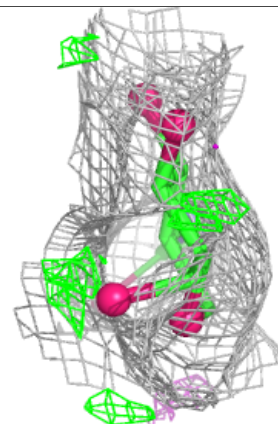
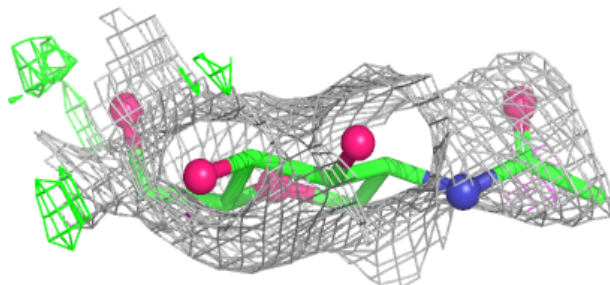
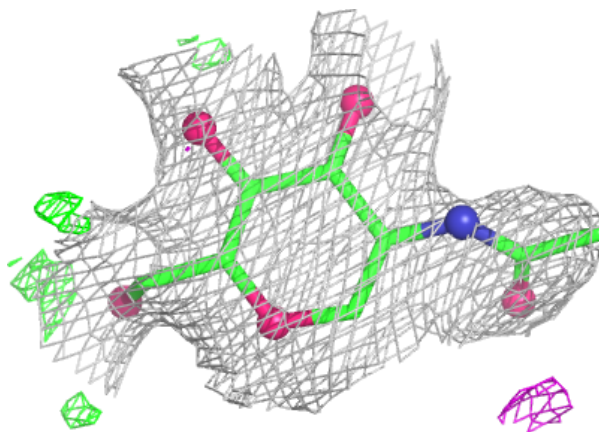


Electron density around NAG A 701:

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and green (positive)

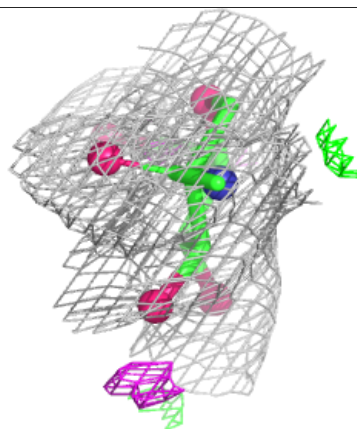
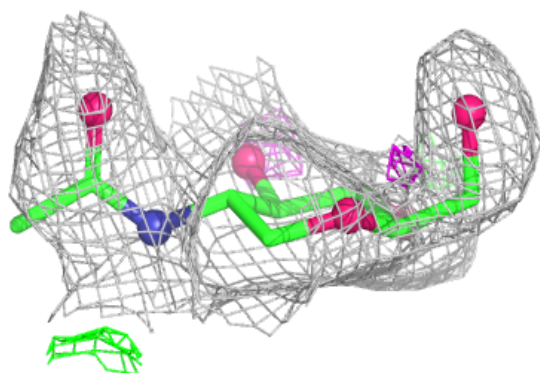
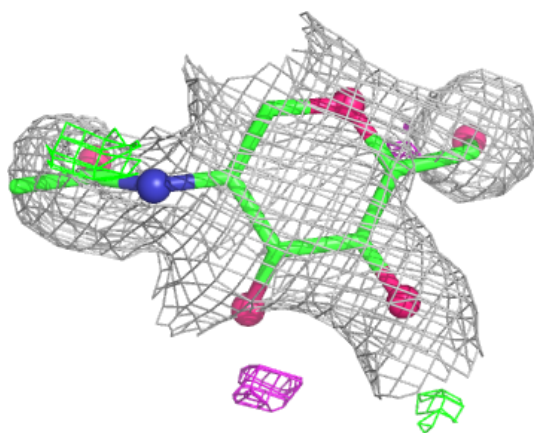
**Electron density around NAG A 700:**

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



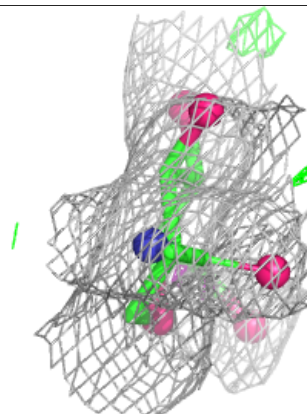
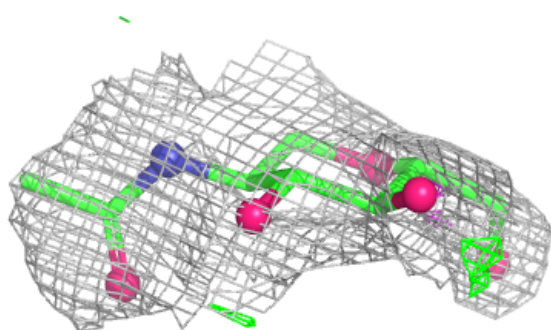
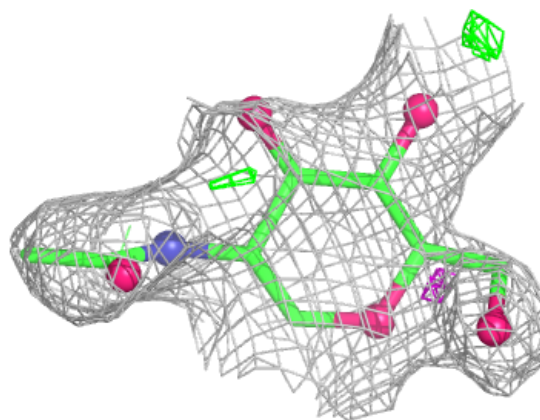
Electron density around NAG D 701:

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



Electron density around NAG F 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 ⓘ

There are no such residues in this entry.