



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 03:47 PM EDT

PDB ID : 6P6P
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

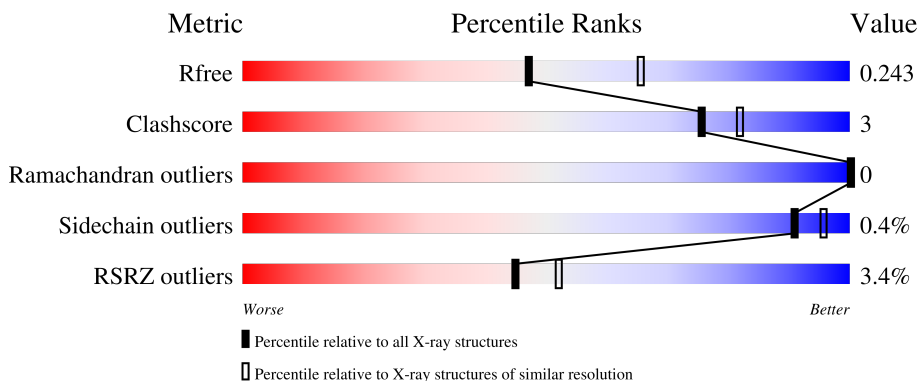
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

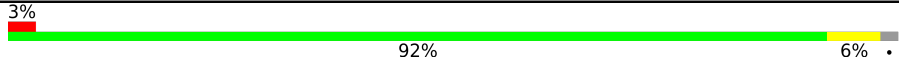

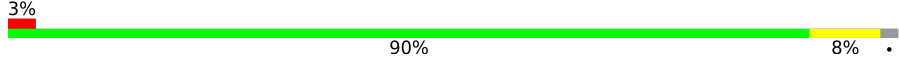
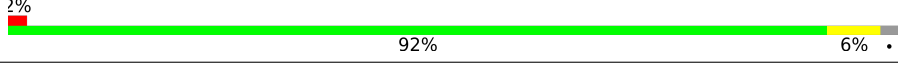
The reported resolution of this entry is 2.31 Å.

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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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	 3% 92% 6%
1	B	497	 4% 89% 9%
1	C	497	 3% 90% 8%
1	D	497	 2% 92% 6%

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Mol	Chain	Length	Quality of chain
1	E	497	 3% 90% 8%
1	F	497	 4% 90% 9%
2	G	3	 100%
2	H	3	 100%
2	I	3	 33% 67%
2	J	3	 100%
2	K	3	 33% 67%
2	L	3	 100%

2 Entry composition [i](#)

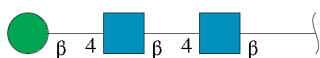
There are 4 unique types of molecules in this entry. The entry contains 24621 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

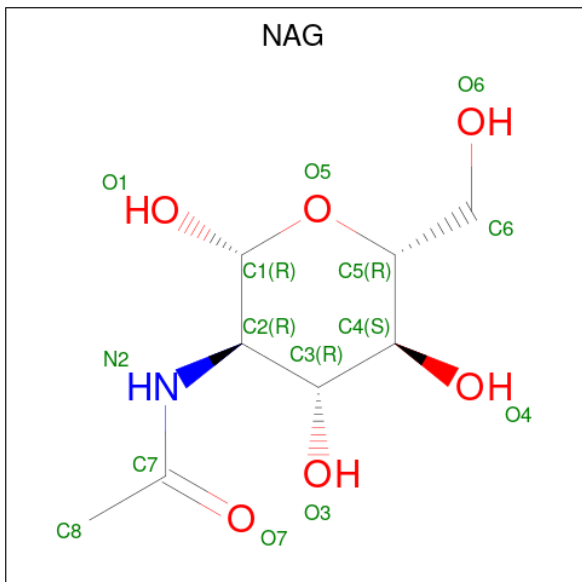
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	Total 3849	C 2401	N 685	O 744	S 19	0	1	0
1	B	488	Total 3873	C 2418	N 688	O 748	S 19	0	3	0
1	C	489	Total 3878	C 2421	N 689	O 749	S 19	0	3	0
1	D	489	Total 3883	C 2424	N 690	O 750	S 19	0	4	0
1	E	489	Total 3883	C 2424	N 690	O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

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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		

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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		

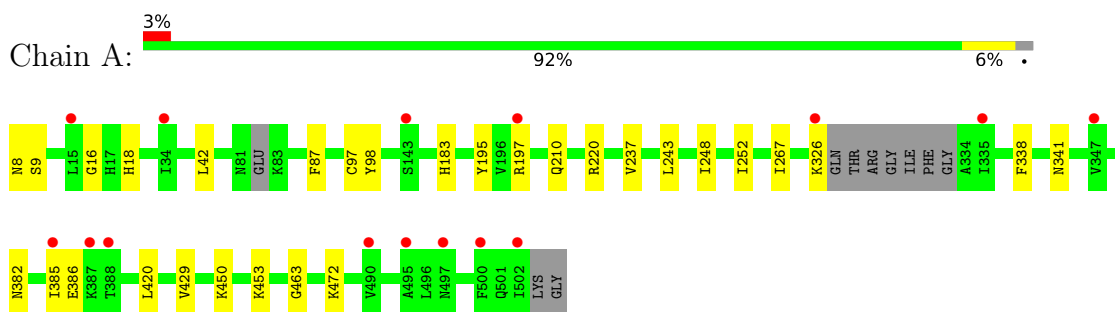
- Molecule 4 is water.

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		

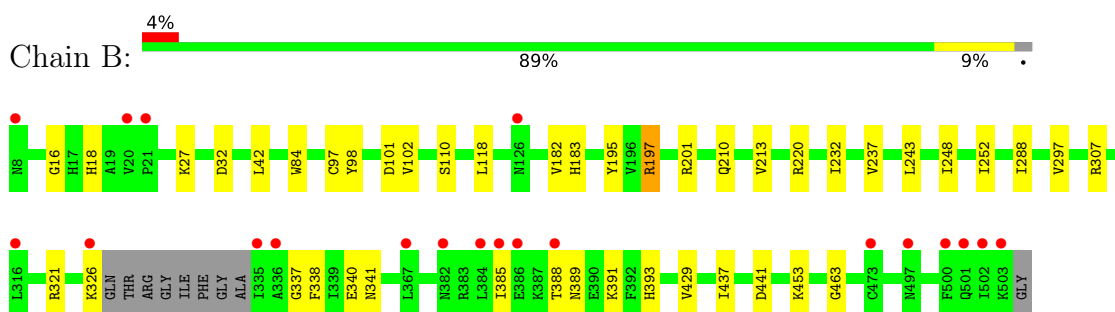
3 Residue-property plots [i](#)

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.

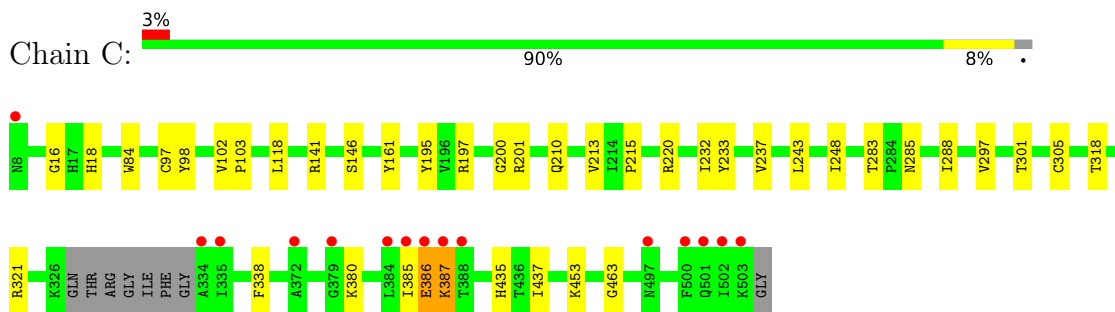
- Molecule 1: Hemagglutinin



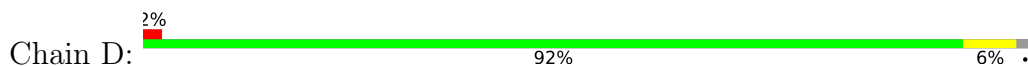
- Molecule 1: Hemagglutinin

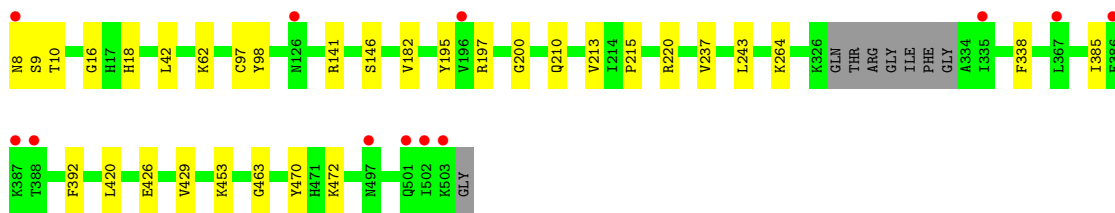


- Molecule 1: Hemagglutinin

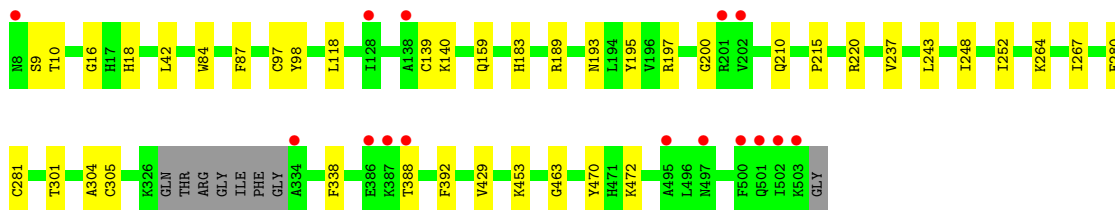
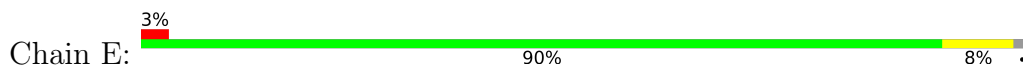


- Molecule 1: Hemagglutinin

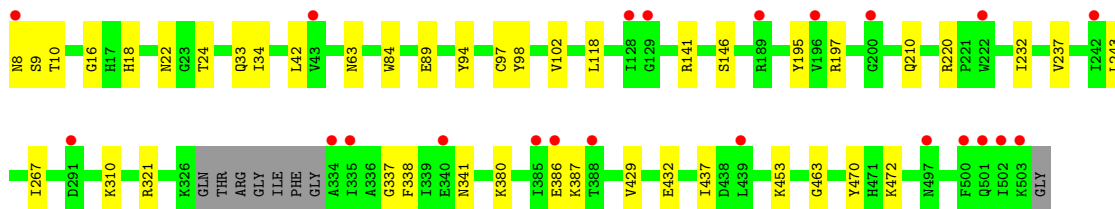
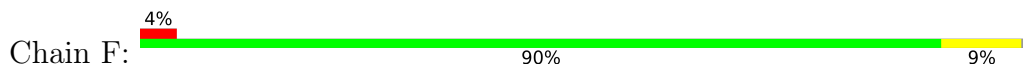




- Molecule 1: Hemagglutinin



- 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



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



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



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) 98.8 (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)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.221 , 0.251 0.224 , 0.243	Depositor DCC
R_{free} test set	7163 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtrriage
Anisotropy	0.186	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.014 for -h-2*k,h+1 0.014 for -h-k-l,l,k 0.017 for -h+k-l,-l,-k 0.022 for -k+1,-h-l,-l 0.021 for k+1,h+1,-l 0.418 for k-l,h+1,-k 0.410 for h+k+1,-l,-h-l 0.408 for -k-l,-h-l,k 0.409 for h-k+1,l,-h-l 0.015 for h,-k,-h-l 0.439 for h+2*k,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24621	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage'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

5.1 Standard geometry

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	0.25	0/3930	0.45	0/5319
1	B	0.26	0/3961	0.45	0/5361
1	C	0.26	0/3966	0.45	0/5368
1	D	0.25	0/3974	0.44	0/5379
1	E	0.30	0/3974	0.45	0/5379
1	F	0.26	0/3974	0.44	0/5379
All	All	0.26	0/23779	0.45	0/32185

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3849	0	3733	20	0
1	B	3873	0	3767	30	0
1	C	3878	0	3772	31	0
1	D	3883	0	3778	20	0
1	E	3883	0	3780	29	0
1	F	3883	0	3778	28	0
2	G	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	142	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 (142) 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: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:A:326:LYS:HZ2	1:A:341:ASN:HB2	1.61	0.66
1:D:62:LYS:HD3	3:D:702:NAG:H82	1.78	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:380:LYS:HZ1	1:C:435:HIS:HB3	1.70	0.56
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: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:F:8:ASN:O	1:F:472:LYS:NZ	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:8:ASN:O	1:A:472:LYS:NZ	2.47	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:THR:HG23	1:F:310:LYS:HZ1	1.86	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 [i](#)

5.3.1 Protein backbone [i](#)

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 [i](#)

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%)	93	97
1	B	430/432 (100%)	428 (100%)	2 (0%)	88	95
1	C	430/432 (100%)	427 (99%)	3 (1%)	84	92
1	D	431/432 (100%)	430 (100%)	1 (0%)	93	97
1	E	431/432 (100%)	429 (100%)	2 (0%)	88	95
1	F	431/432 (100%)	430 (100%)	1 (0%)	93	97
All	All	2579/2592 (100%)	2569 (100%)	10 (0%)	91	96

All (10) 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	18	HIS
1	C	386	GLU
1	C	387	LYS
1	D	18	HIS
1	E	18	HIS
1	E	140	LYS
1	F	18	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	33	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	1.19	2 (14%)	17,19,21	1.03	1 (5%)
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	1.05	2 (11%)
2	BMA	G	3	2	11,11,12	0.97	1 (9%)	15,15,17	0.94	0
2	NAG	H	1	2,1	14,14,15	0.74	0	17,19,21	0.98	1 (5%)
2	NAG	H	2	2	14,14,15	0.58	0	17,19,21	1.14	2 (11%)
2	BMA	H	3	2	11,11,12	1.03	1 (9%)	15,15,17	1.34	2 (13%)
2	NAG	I	1	2,1	14,14,15	0.46	0	17,19,21	1.06	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	1.56	1 (9%)	15,15,17	1.37	4 (26%)
2	NAG	J	1	2,1	14,14,15	0.61	0	17,19,21	1.16	2 (11%)
2	NAG	J	2	2	14,14,15	0.51	0	17,19,21	0.84	1 (5%)
2	BMA	J	3	2	11,11,12	1.40	1 (9%)	15,15,17	1.45	3 (20%)
2	NAG	K	1	2,1	14,14,15	0.34	0	17,19,21	1.26	1 (5%)
2	NAG	K	2	2	14,14,15	0.23	0	17,19,21	0.65	0
2	BMA	K	3	2	11,11,12	1.09	2 (18%)	15,15,17	1.35	2 (13%)
2	NAG	L	1	2,1	14,14,15	0.54	0	17,19,21	1.12	2 (11%)
2	NAG	L	2	2	14,14,15	0.30	0	17,19,21	0.83	1 (5%)
2	BMA	L	3	2	11,11,12	0.64	0	15,15,17	1.66	4 (26%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/2/19/22	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	-4.41	1.36	1.43
2	G	1	NAG	O5-C1	3.30	1.49	1.43
2	H	3	BMA	O5-C1	-3.07	1.38	1.43
2	G	1	NAG	C1-C2	2.65	1.56	1.52
2	G	3	BMA	O5-C1	-2.63	1.39	1.43
2	J	3	BMA	C4-C5	2.49	1.58	1.53
2	K	3	BMA	C1-C2	-2.22	1.47	1.52
2	K	3	BMA	O5-C1	-2.04	1.40	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	3	BMA	O5-C5-C6	4.03	113.53	107.20
2	K	1	NAG	C1-O5-C5	3.87	117.44	112.19
2	H	3	BMA	O5-C5-C6	3.86	113.26	107.20
2	I	1	NAG	C1-O5-C5	3.21	116.54	112.19
2	G	1	NAG	C1-O5-C5	3.17	116.49	112.19
2	J	3	BMA	O5-C5-C6	3.14	112.13	107.20
2	H	1	NAG	C1-O5-C5	3.04	116.31	112.19
2	L	3	BMA	O2-C2-C1	2.99	115.27	109.15
2	J	1	NAG	O4-C4-C5	-2.95	101.96	109.30
2	L	1	NAG	C1-O5-C5	2.82	116.01	112.19
2	H	2	NAG	O3-C3-C2	-2.79	103.70	109.47
2	J	3	BMA	O2-C2-C1	2.75	114.77	109.15
2	I	3	BMA	O2-C2-C3	-2.65	104.84	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	BMA	O2-C2-C3	-2.51	105.10	110.14
2	K	3	BMA	O5-C5-C6	2.49	111.11	107.20
2	H	2	NAG	O4-C4-C3	-2.33	104.96	110.35
2	G	2	NAG	O4-C4-C5	-2.31	103.57	109.30
2	J	1	NAG	C1-O5-C5	2.27	115.27	112.19
2	J	3	BMA	O5-C1-C2	2.24	114.23	110.77
2	I	3	BMA	O5-C5-C6	2.24	110.71	107.20
2	G	2	NAG	O3-C3-C2	-2.19	104.93	109.47
2	L	3	BMA	C1-C2-C3	-2.19	106.97	109.67
2	L	1	NAG	O4-C4-C5	-2.18	103.88	109.30
2	L	2	NAG	O4-C4-C5	-2.17	103.92	109.30
2	L	3	BMA	O4-C4-C3	-2.15	105.38	110.35
2	K	3	BMA	O2-C2-C3	-2.10	105.94	110.14
2	J	2	NAG	O4-C4-C5	-2.04	104.22	109.30
2	I	3	BMA	C3-C4-C5	-2.02	106.63	110.24
2	I	3	BMA	O3-C3-C2	2.01	113.83	109.99

There are no chirality outliers.

All (16) torsion outliers are listed below:

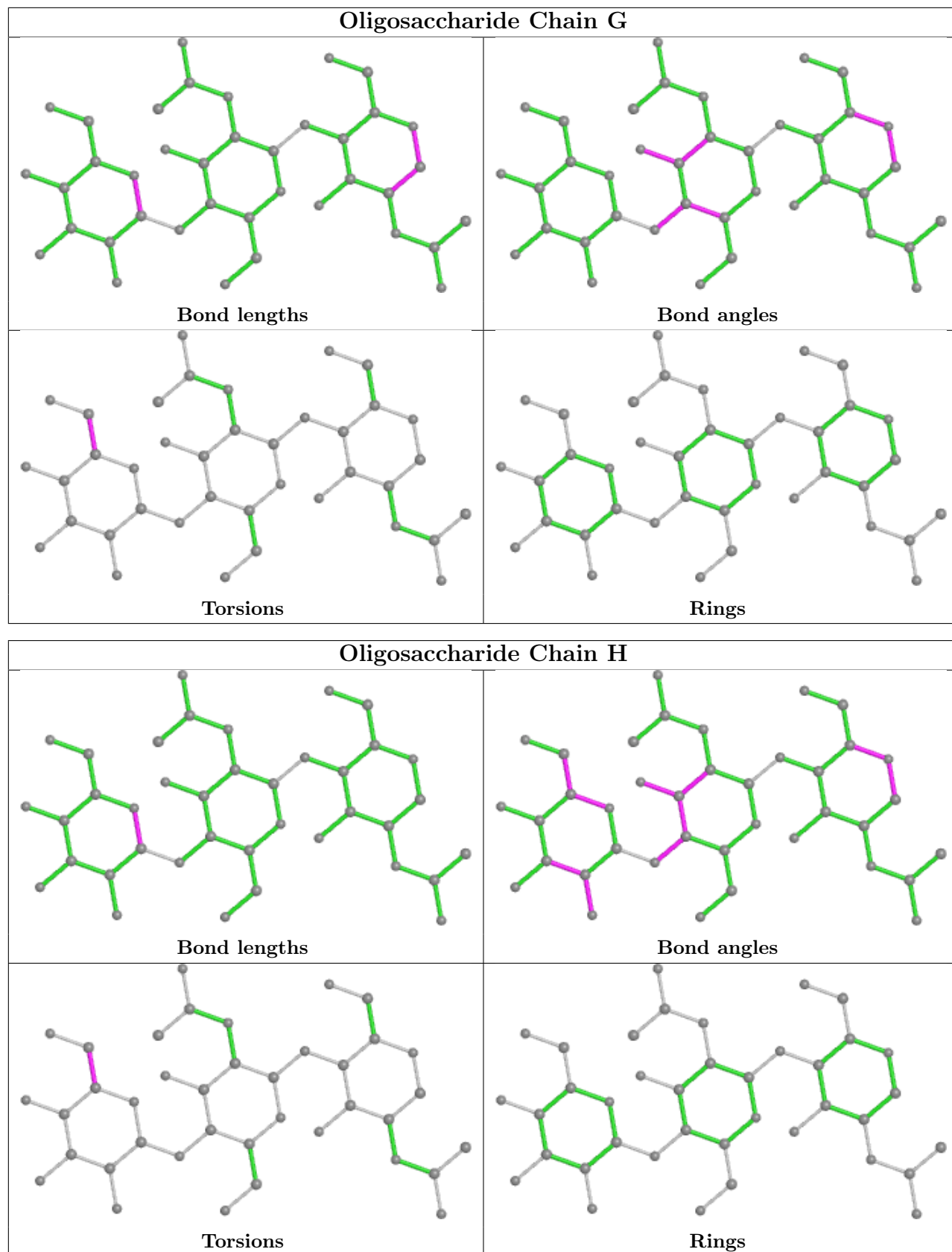
Mol	Chain	Res	Type	Atoms
2	G	3	BMA	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	L	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	H	3	BMA	C4-C5-C6-O6
2	G	3	BMA	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	L	3	BMA	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	I	3	BMA	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	I	3	BMA	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6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

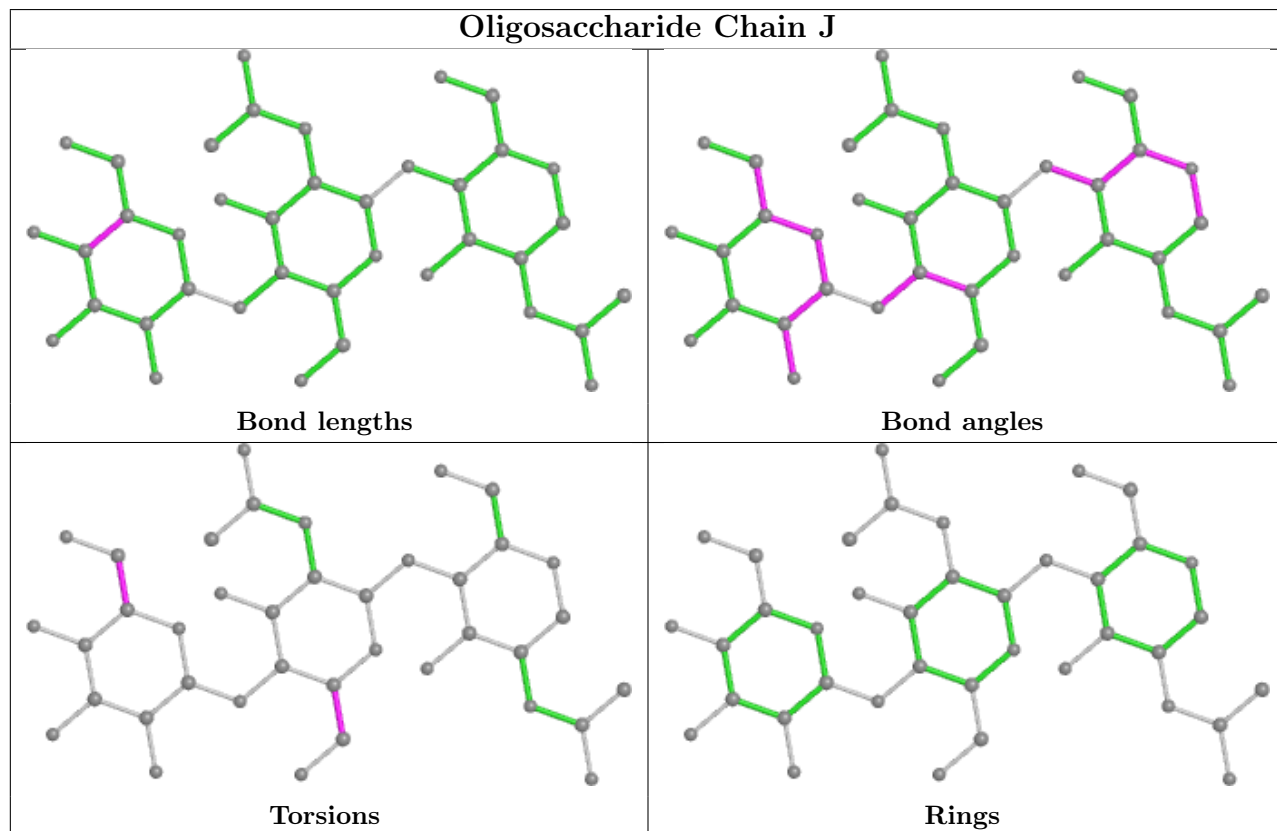
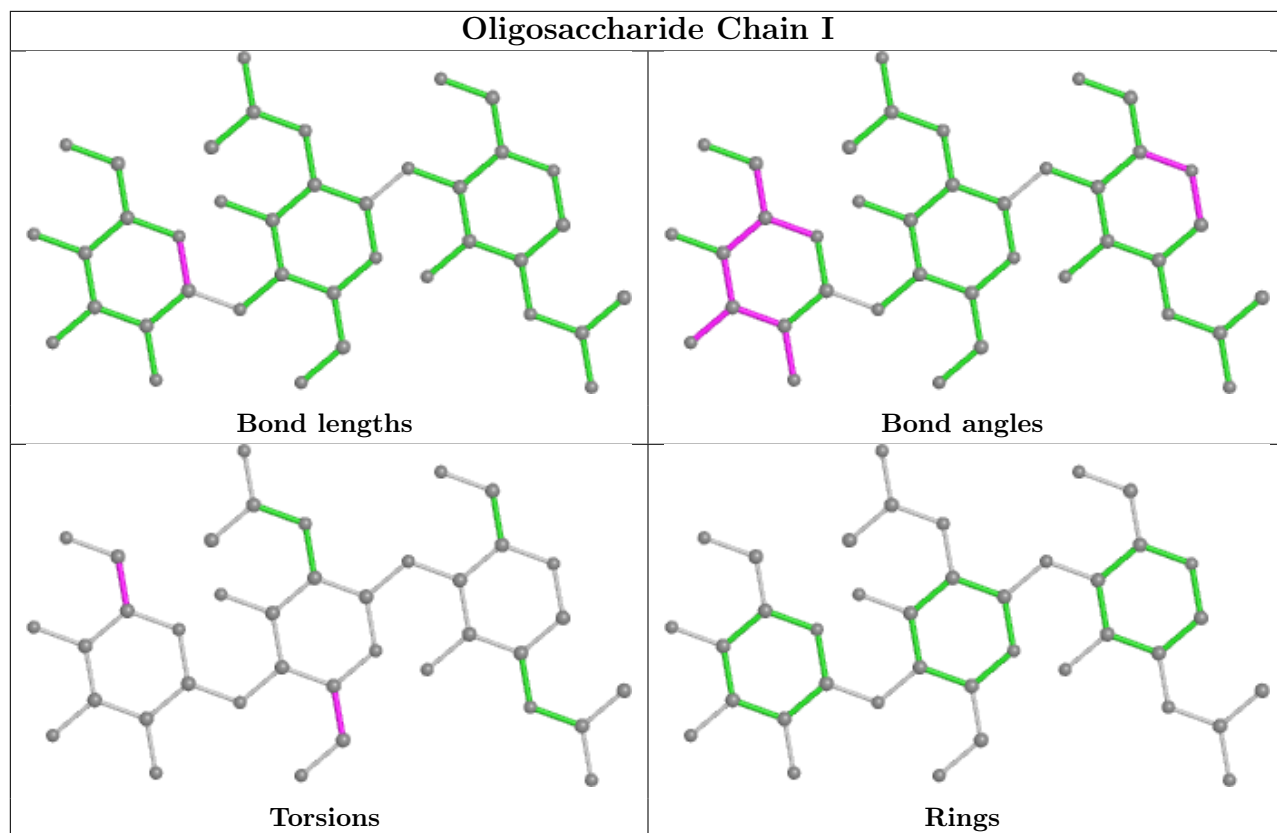
There are no ring outliers.

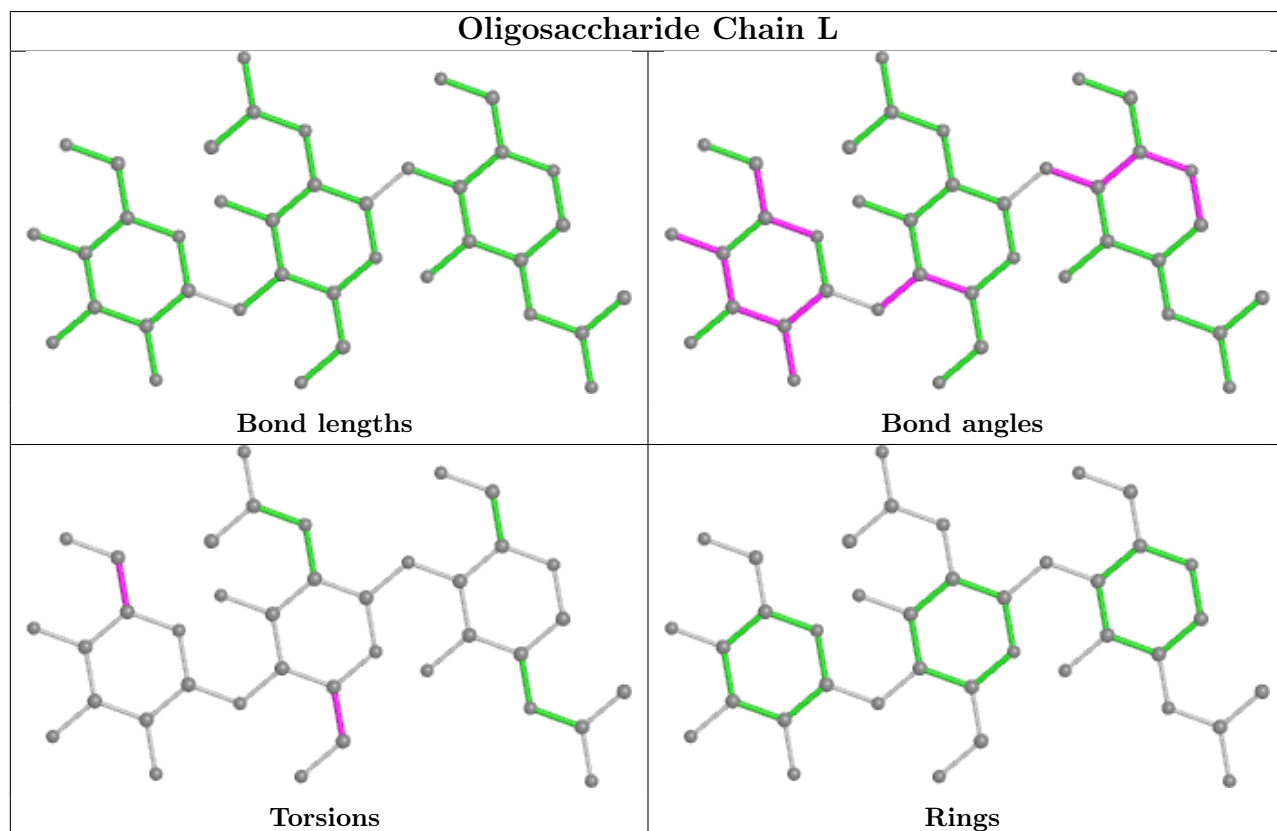
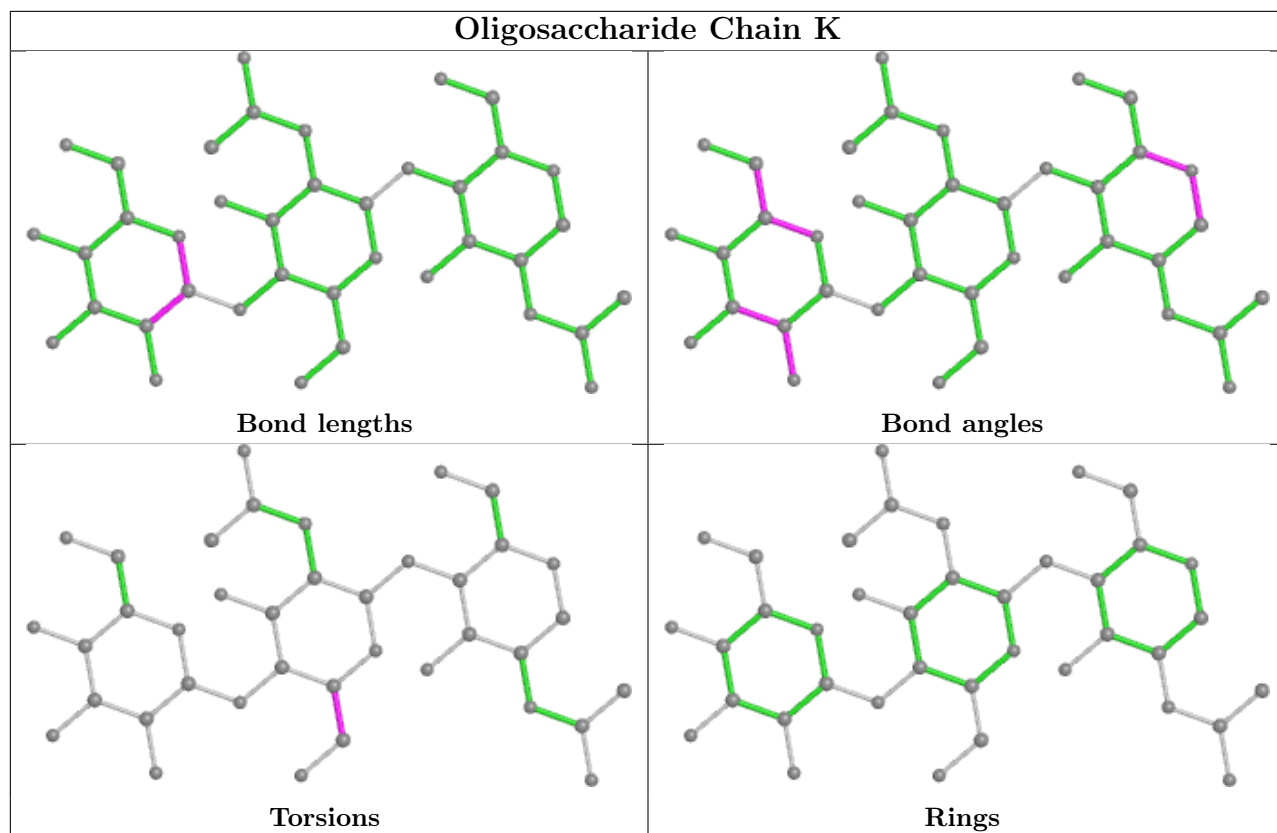
No monomer is involved in short contacts.

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

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	A	700	1	14,14,15	0.94	2 (14%)	17,19,21	0.90	1 (5%)
3	NAG	E	700	1	14,14,15	0.90	2 (14%)	17,19,21	1.34	3 (17%)
3	NAG	C	700	1	14,14,15	2.72	2 (14%)	17,19,21	1.97	4 (23%)
3	NAG	B	702	1	14,14,15	0.40	0	17,19,21	1.09	2 (11%)
3	NAG	F	700	1	14,14,15	0.87	1 (7%)	17,19,21	1.16	2 (11%)
3	NAG	B	700	1	14,14,15	0.79	1 (7%)	17,19,21	0.97	0
3	NAG	E	701	1	14,14,15	1.30	3 (21%)	17,19,21	2.66	4 (23%)
3	NAG	D	706	1	14,14,15	0.82	1 (7%)	17,19,21	1.36	2 (11%)
3	NAG	A	701	1	14,14,15	1.41	2 (14%)	17,19,21	1.20	2 (11%)
3	NAG	A	702	1	14,14,15	0.90	1 (7%)	17,19,21	2.00	4 (23%)
3	NAG	A	706	1	14,14,15	1.58	2 (14%)	17,19,21	1.94	1 (5%)
3	NAG	D	700	1	14,14,15	0.45	0	17,19,21	0.76	1 (5%)
3	NAG	F	701	1	14,14,15	0.76	1 (7%)	17,19,21	1.21	1 (5%)
3	NAG	E	706	1	14,14,15	2.19	2 (14%)	17,19,21	1.50	2 (11%)
3	NAG	F	702	1	14,14,15	0.70	0	17,19,21	1.31	1 (5%)
3	NAG	B	701	1	14,14,15	1.00	1 (7%)	17,19,21	1.94	5 (29%)
3	NAG	C	702	1	14,14,15	1.10	2 (14%)	17,19,21	0.83	0
3	NAG	C	706	1	14,14,15	0.59	0	17,19,21	1.79	3 (17%)
3	NAG	F	706	1	14,14,15	0.65	0	17,19,21	1.61	5 (29%)
3	NAG	D	702	1	14,14,15	1.09	2 (14%)	17,19,21	0.90	1 (5%)
3	NAG	E	702	1	14,14,15	0.84	1 (7%)	17,19,21	1.19	1 (5%)
3	NAG	D	701	1	14,14,15	0.51	0	17,19,21	1.14	1 (5%)
3	NAG	C	701	1	14,14,15	0.83	1 (7%)	17,19,21	2.72	4 (23%)
3	NAG	B	706	1	14,14,15	3.01	3 (21%)	17,19,21	3.95	4 (23%)

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. '2' means no outliers of that kind were identified.

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

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	706	NAG	O5-C1	9.80	1.59	1.43
3	C	700	NAG	O5-C1	9.05	1.58	1.43
3	E	706	NAG	O5-C1	-7.54	1.31	1.43
3	A	706	NAG	O5-C1	5.30	1.52	1.43
3	B	706	NAG	C1-C2	4.94	1.59	1.52
3	A	701	NAG	O5-C1	4.65	1.51	1.43
3	C	700	NAG	C1-C2	4.33	1.58	1.52
3	C	702	NAG	C1-C2	3.42	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	NAG	O5-C1	2.90	1.48	1.43
3	E	706	NAG	C3-C2	2.75	1.58	1.52
3	E	701	NAG	C3-C2	2.67	1.58	1.52
3	F	701	NAG	O5-C1	2.56	1.47	1.43
3	D	702	NAG	C1-C2	2.49	1.56	1.52
3	A	702	NAG	C1-C2	2.49	1.56	1.52
3	A	700	NAG	C1-C2	2.48	1.56	1.52
3	E	700	NAG	O5-C1	2.40	1.47	1.43
3	E	702	NAG	O5-C1	2.40	1.47	1.43
3	E	701	NAG	O5-C1	2.38	1.47	1.43
3	A	701	NAG	C1-C2	2.32	1.55	1.52
3	B	700	NAG	C1-C2	2.31	1.55	1.52
3	B	701	NAG	C3-C2	2.25	1.57	1.52
3	A	706	NAG	C3-C2	2.24	1.57	1.52
3	F	700	NAG	C1-C2	2.23	1.55	1.52
3	C	701	NAG	O5-C1	-2.20	1.40	1.43
3	E	701	NAG	C2-N2	2.14	1.50	1.46
3	B	706	NAG	C3-C2	2.11	1.57	1.52
3	C	702	NAG	O5-C1	2.10	1.47	1.43
3	A	700	NAG	O5-C1	2.09	1.47	1.43
3	D	706	NAG	O5-C1	2.07	1.47	1.43
3	E	700	NAG	C1-C2	2.04	1.55	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	706	NAG	C1-O5-C5	12.78	129.51	112.19
3	C	701	NAG	C2-N2-C7	8.32	134.75	122.90
3	A	706	NAG	C1-O5-C5	7.26	122.03	112.19
3	E	701	NAG	C2-N2-C7	7.23	133.19	122.90
3	B	706	NAG	C4-C3-C2	6.75	120.91	111.02
3	B	706	NAG	C3-C4-C5	6.12	121.16	110.24
3	C	700	NAG	C1-C2-N2	5.59	120.04	110.49
3	A	702	NAG	C1-C2-N2	5.44	119.79	110.49
3	C	706	NAG	C1-O5-C5	5.22	119.27	112.19
3	E	701	NAG	C1-C2-N2	4.97	118.98	110.49
3	C	701	NAG	C1-O5-C5	4.89	118.82	112.19
3	B	701	NAG	O3-C3-C2	4.60	118.99	109.47
3	E	706	NAG	C1-O5-C5	-4.38	106.26	112.19
3	D	706	NAG	C1-O5-C5	4.37	118.11	112.19
3	E	701	NAG	C1-O5-C5	4.36	118.10	112.19
3	B	701	NAG	C1-O5-C5	4.19	117.87	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	700	NAG	C2-N2-C7	4.07	128.70	122.90
3	F	702	NAG	O3-C3-C2	4.05	117.85	109.47
3	F	701	NAG	C1-O5-C5	4.05	117.68	112.19
3	D	701	NAG	C1-O5-C5	3.69	117.19	112.19
3	A	702	NAG	C4-C3-C2	-3.69	105.61	111.02
3	B	701	NAG	C1-C2-N2	-3.61	104.32	110.49
3	A	701	NAG	C1-O5-C5	3.44	116.85	112.19
3	C	701	NAG	C1-C2-N2	-3.21	105.00	110.49
3	E	700	NAG	C1-C2-N2	3.20	115.96	110.49
3	B	706	NAG	C2-N2-C7	3.19	127.45	122.90
3	E	702	NAG	C1-C2-N2	3.18	115.92	110.49
3	A	702	NAG	C2-N2-C7	-3.15	118.41	122.90
3	C	706	NAG	C1-C2-N2	3.14	115.85	110.49
3	F	700	NAG	C1-O5-C5	3.13	116.44	112.19
3	F	706	NAG	C3-C4-C5	3.08	115.74	110.24
3	D	700	NAG	C1-O5-C5	2.93	116.16	112.19
3	E	701	NAG	O4-C4-C5	-2.89	102.13	109.30
3	F	706	NAG	C4-C3-C2	2.86	115.21	111.02
3	E	700	NAG	C1-O5-C5	2.83	116.03	112.19
3	F	706	NAG	C2-N2-C7	2.80	126.89	122.90
3	A	702	NAG	O3-C3-C4	2.71	116.62	110.35
3	C	700	NAG	C1-O5-C5	2.65	115.78	112.19
3	C	700	NAG	O3-C3-C4	2.62	116.41	110.35
3	F	706	NAG	C1-C2-N2	2.59	114.91	110.49
3	A	700	NAG	O3-C3-C2	2.47	114.58	109.47
3	E	700	NAG	O3-C3-C2	2.42	114.48	109.47
3	F	706	NAG	C1-O5-C5	2.37	115.41	112.19
3	C	706	NAG	C2-N2-C7	2.37	126.28	122.90
3	C	701	NAG	O5-C5-C6	-2.32	103.56	107.20
3	D	706	NAG	C1-C2-N2	2.31	114.44	110.49
3	A	701	NAG	C1-C2-N2	2.25	114.33	110.49
3	B	702	NAG	C1-C2-N2	2.25	114.33	110.49
3	D	702	NAG	C2-N2-C7	2.18	126.01	122.90
3	B	702	NAG	O4-C4-C5	-2.17	103.92	109.30
3	B	701	NAG	O4-C4-C3	2.15	115.32	110.35
3	E	706	NAG	C3-C4-C5	2.12	114.02	110.24
3	F	700	NAG	O3-C3-C2	2.10	113.81	109.47
3	B	701	NAG	O5-C5-C6	-2.03	104.02	107.20

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	706	NAG	C3-C2-N2-C7
3	C	700	NAG	C3-C2-N2-C7
3	C	701	NAG	O7-C7-N2-C2
3	E	700	NAG	C3-C2-N2-C7
3	E	701	NAG	C1-C2-N2-C7
3	F	700	NAG	C3-C2-N2-C7
3	E	700	NAG	C4-C5-C6-O6
3	B	701	NAG	O5-C5-C6-O6
3	F	700	NAG	C4-C5-C6-O6
3	E	700	NAG	O5-C5-C6-O6
3	A	706	NAG	O5-C5-C6-O6
3	B	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	701	NAG	O5-C5-C6-O6
3	F	701	NAG	C4-C5-C6-O6
3	F	702	NAG	O5-C5-C6-O6
3	C	706	NAG	C1-C2-N2-C7
3	D	700	NAG	C4-C5-C6-O6
3	F	700	NAG	O5-C5-C6-O6
3	A	701	NAG	C4-C5-C6-O6
3	F	702	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	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	A	702	NAG	C4-C5-C6-O6
3	C	700	NAG	O5-C5-C6-O6
3	E	706	NAG	C3-C2-N2-C7
3	B	700	NAG	O5-C5-C6-O6
3	C	700	NAG	C1-C2-N2-C7
3	E	700	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

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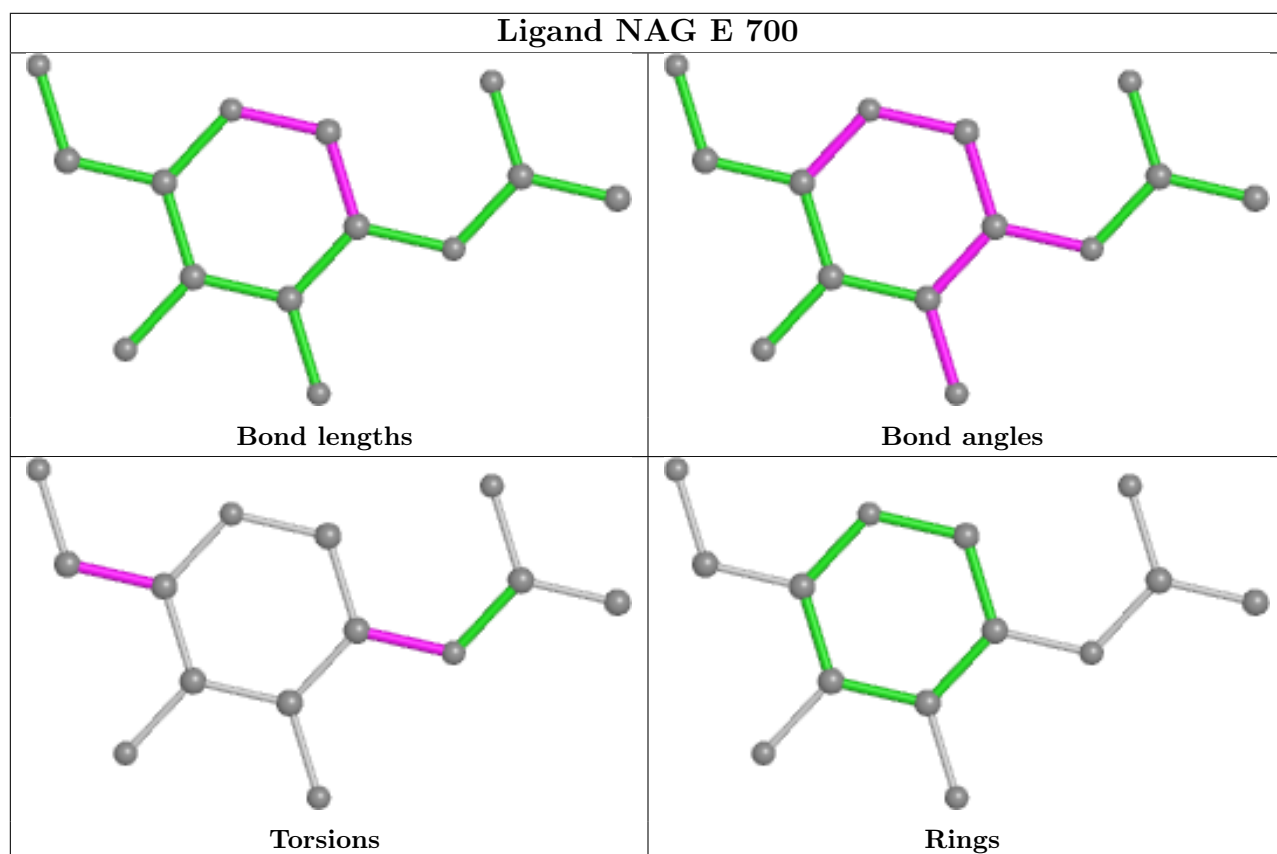
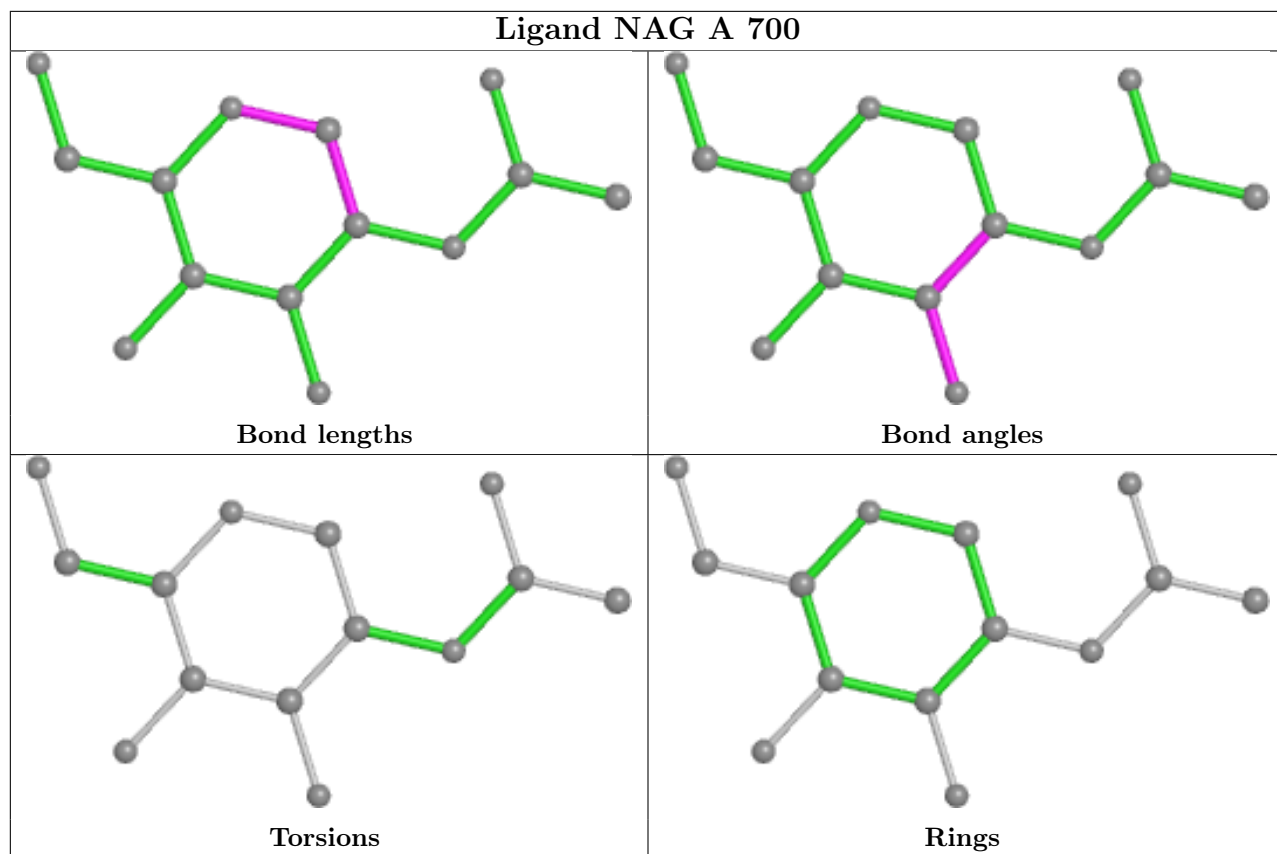
Mol	Chain	Res	Type	Atoms
3	B	700	NAG	C4-C5-C6-O6
3	E	706	NAG	O5-C5-C6-O6
3	F	700	NAG	C1-C2-N2-C7

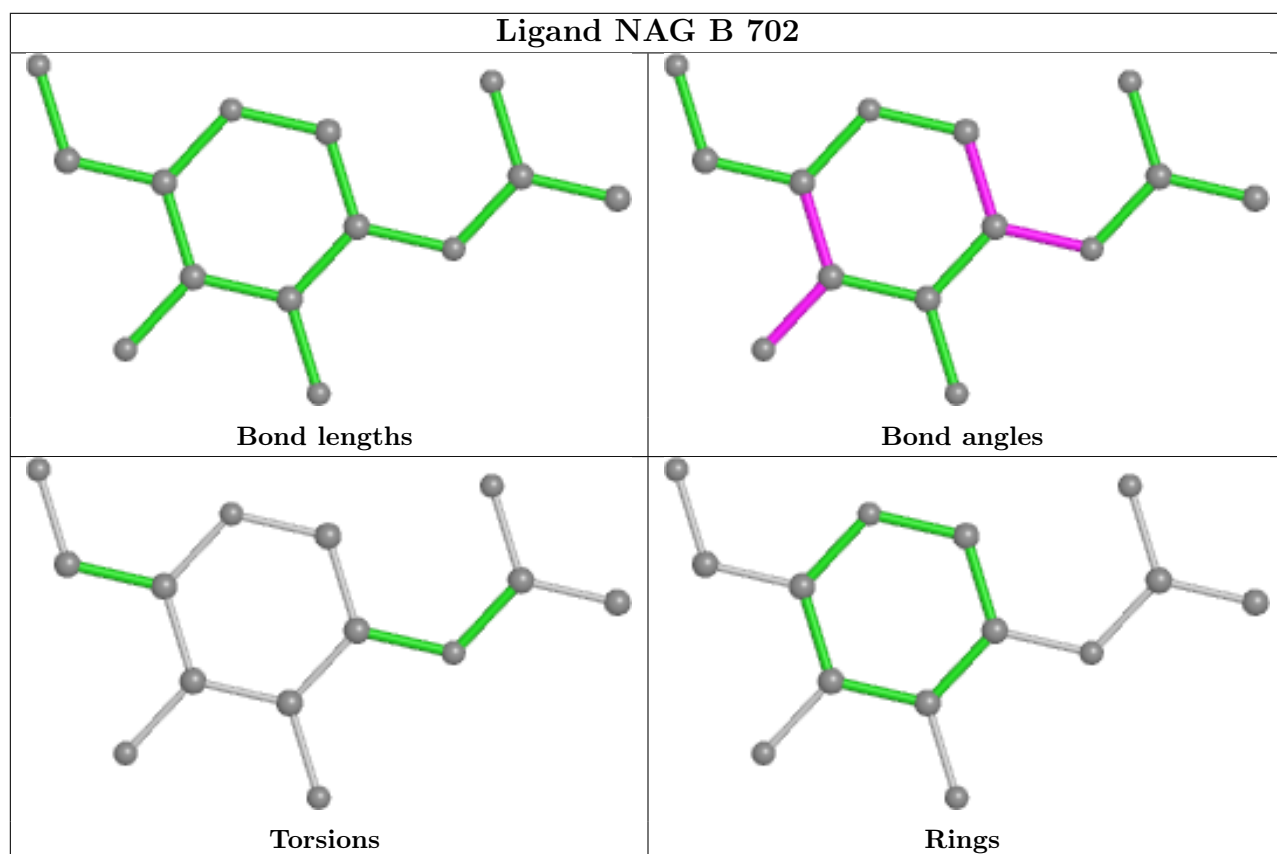
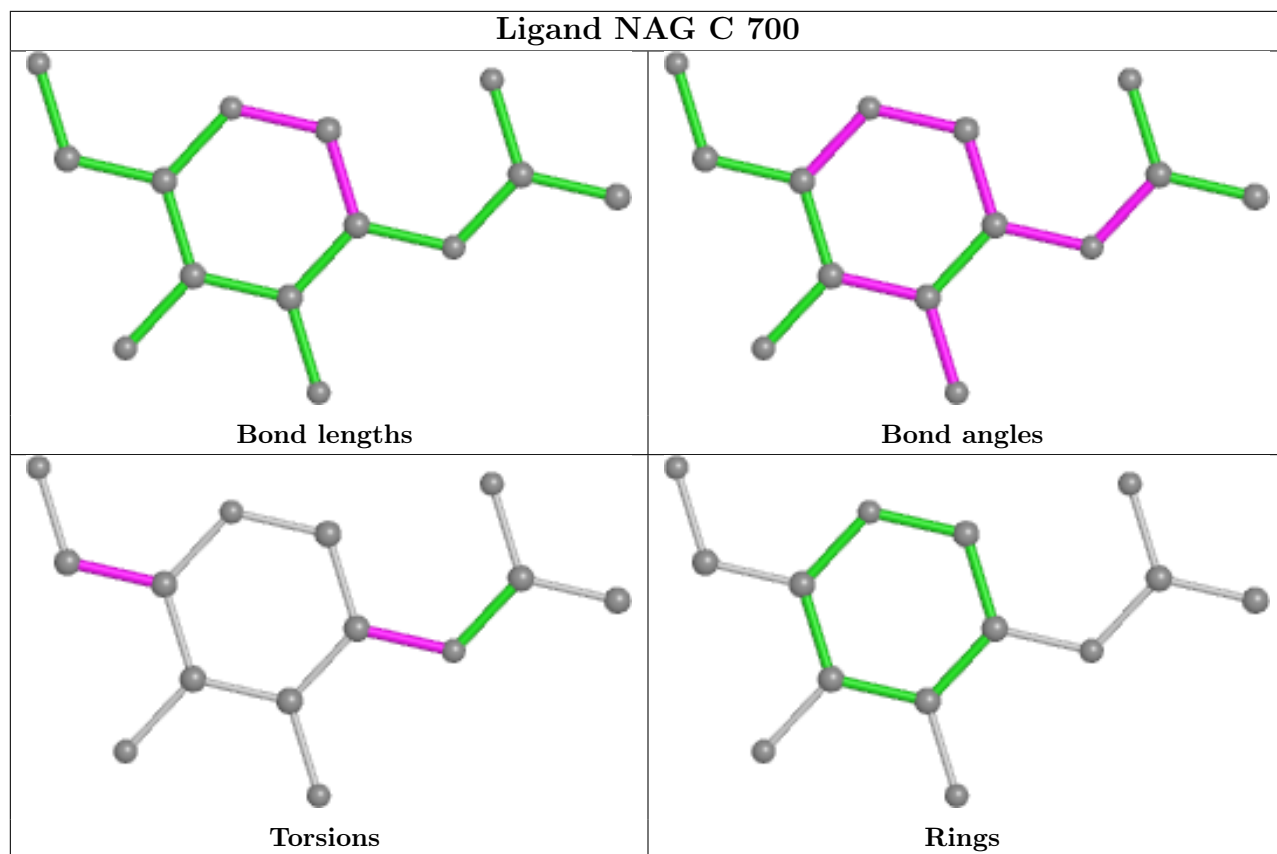
There are no ring outliers.

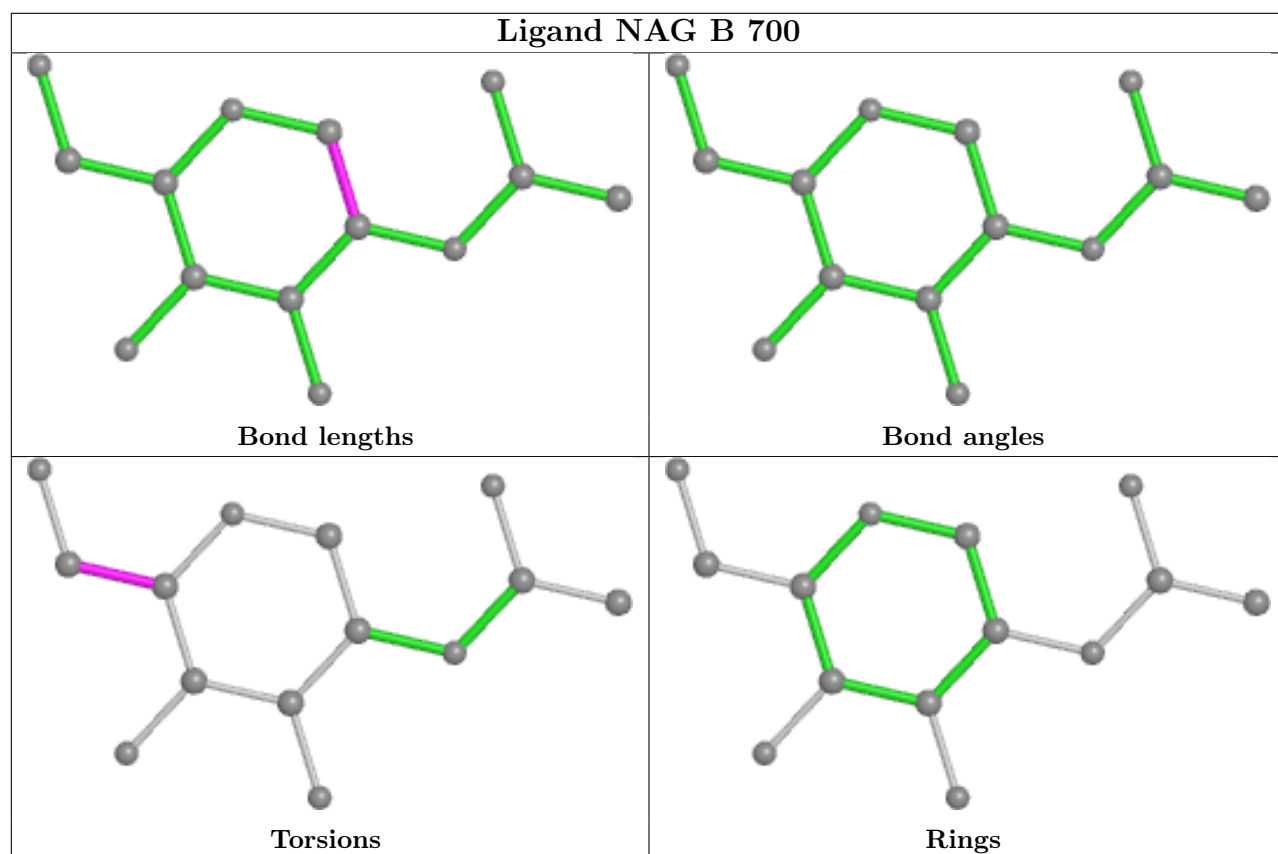
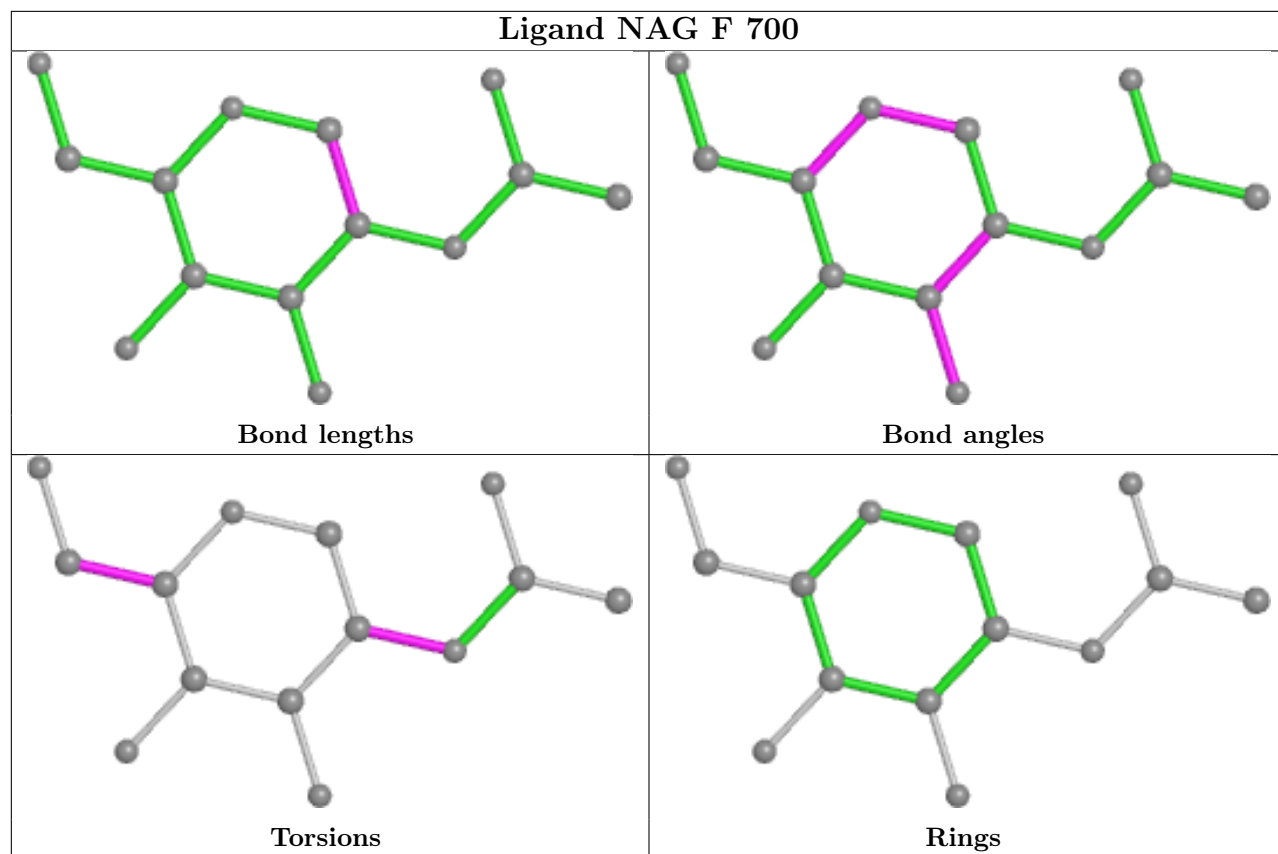
5 monomers are involved in 6 short contacts:

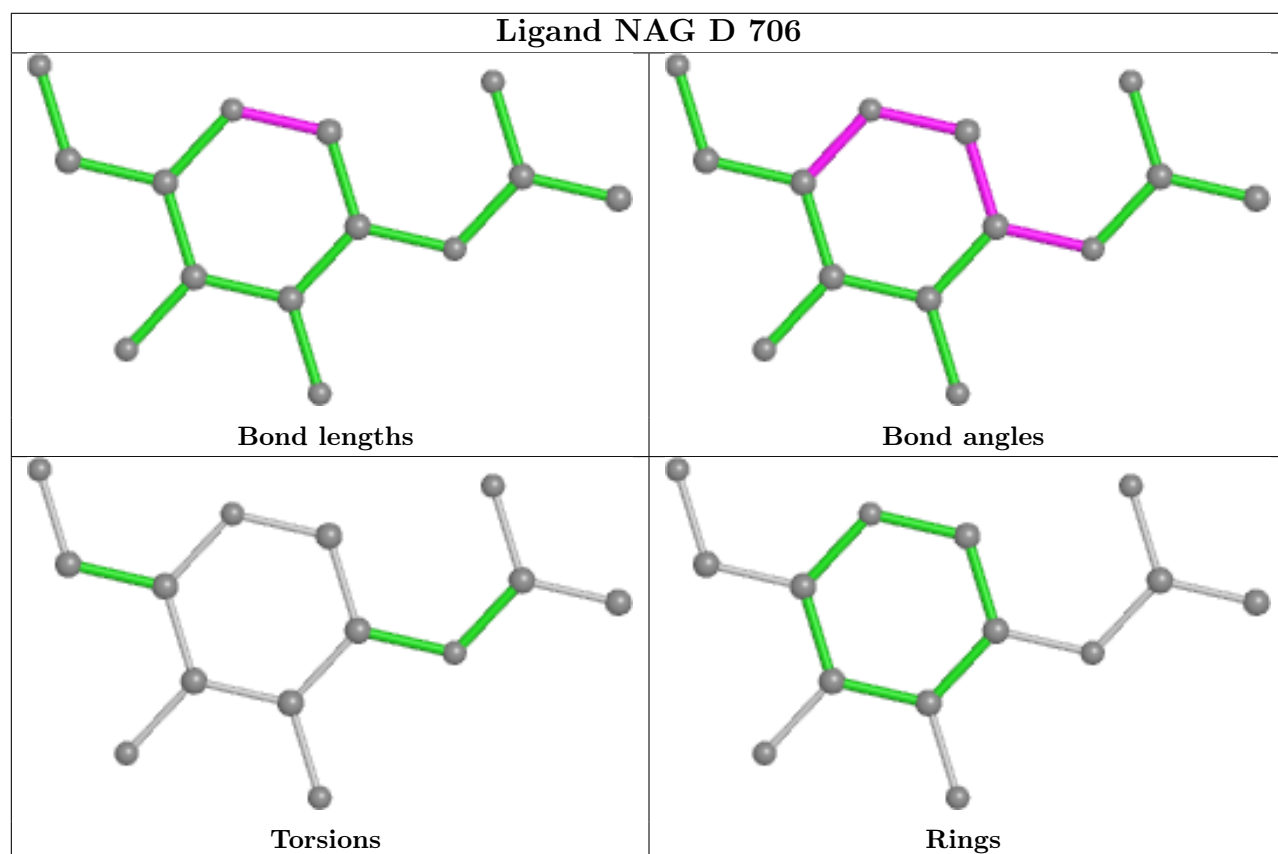
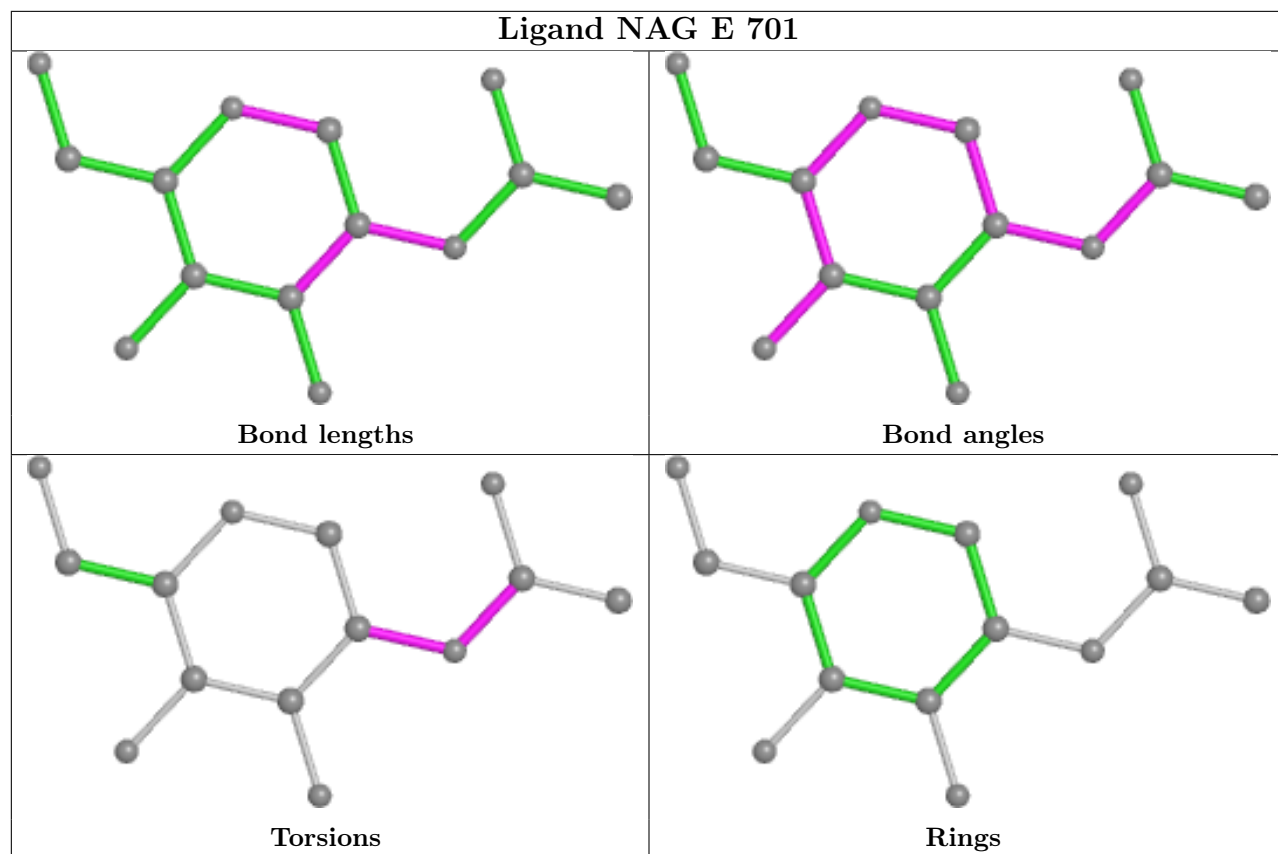
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	700	NAG	2	0
3	C	706	NAG	1	0
3	D	702	NAG	1	0
3	C	701	NAG	1	0
3	B	706	NAG	1	0

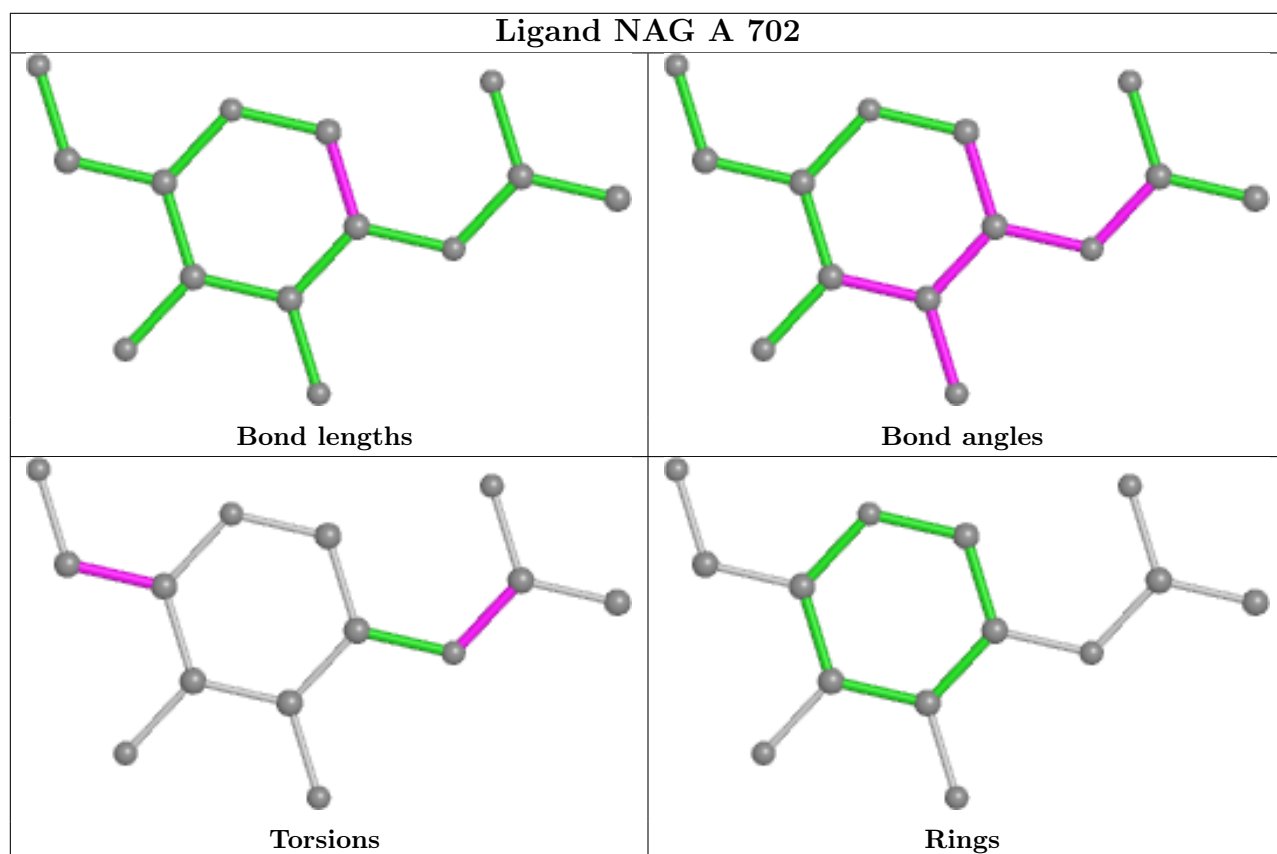
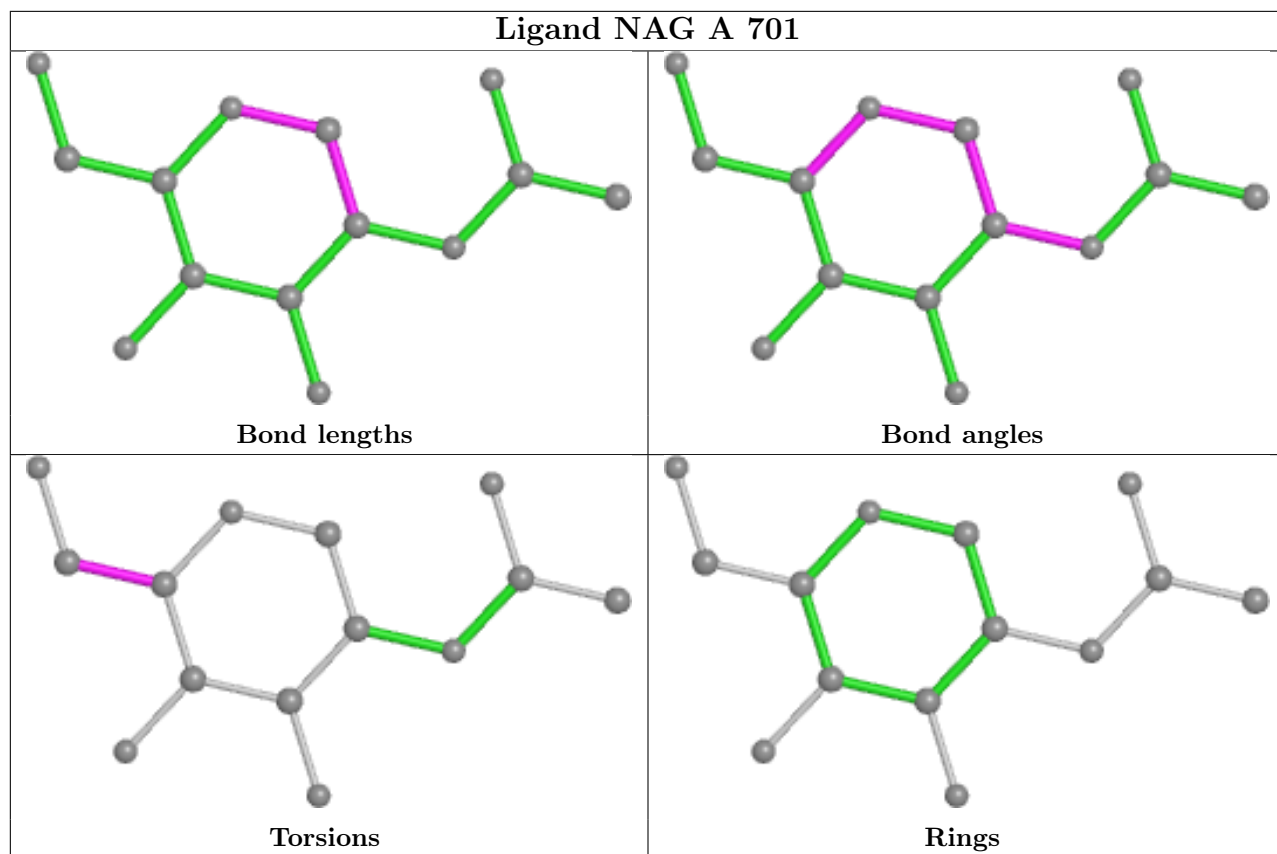
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

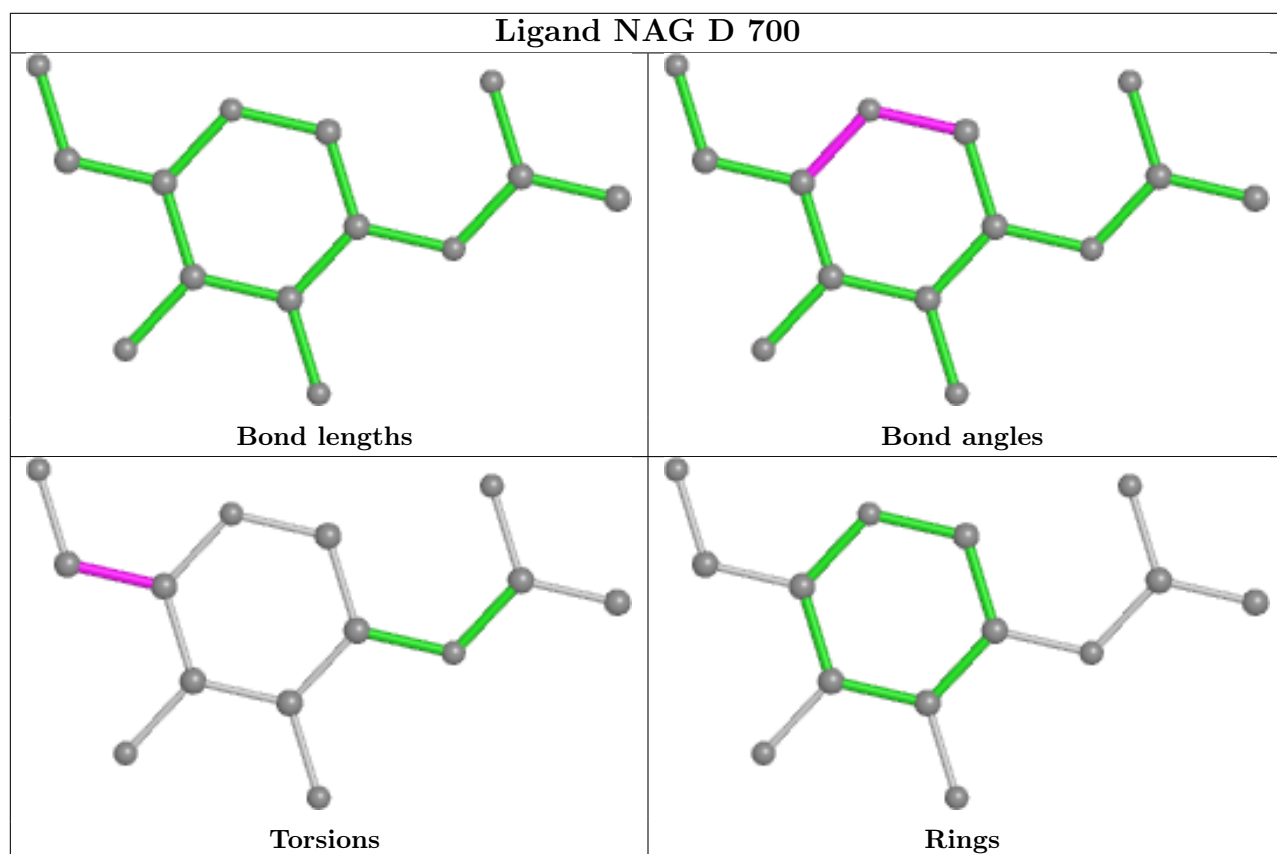
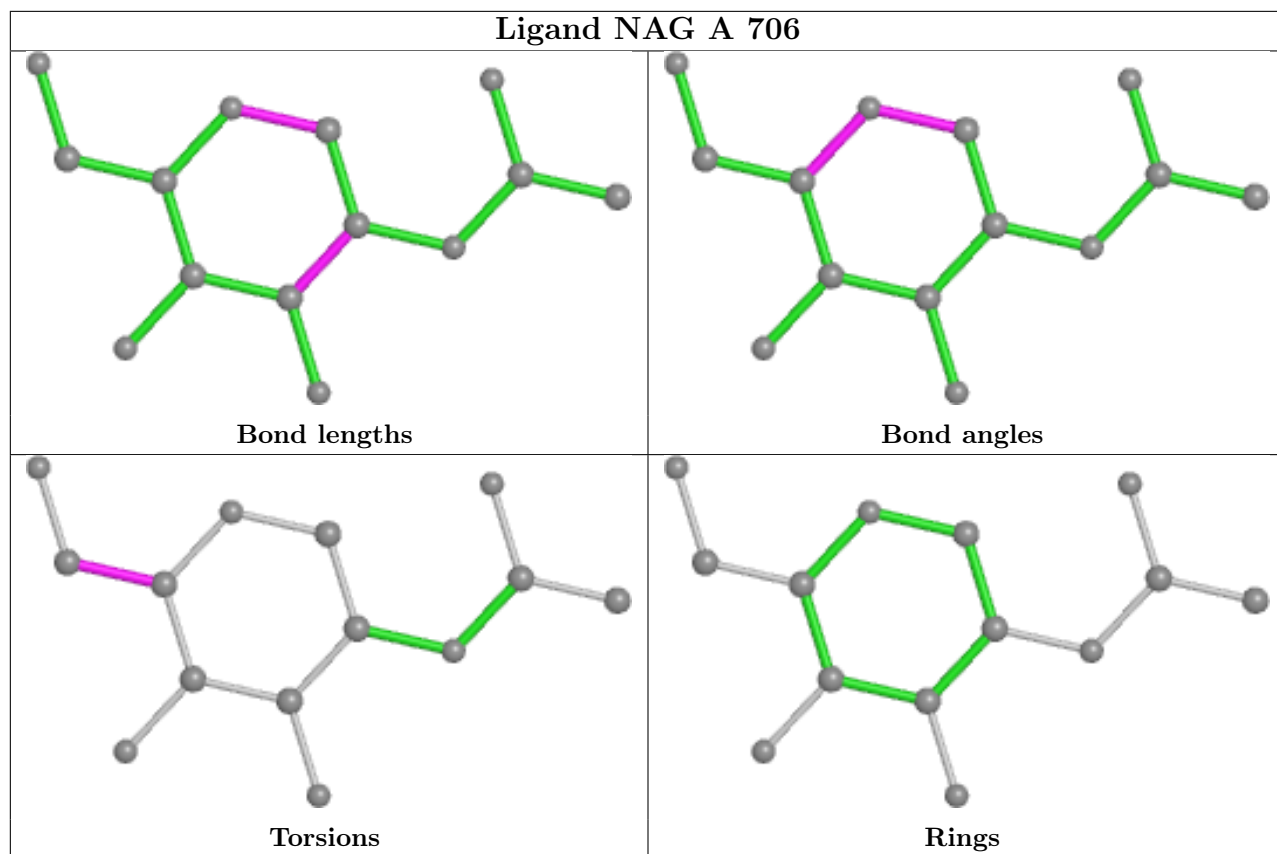


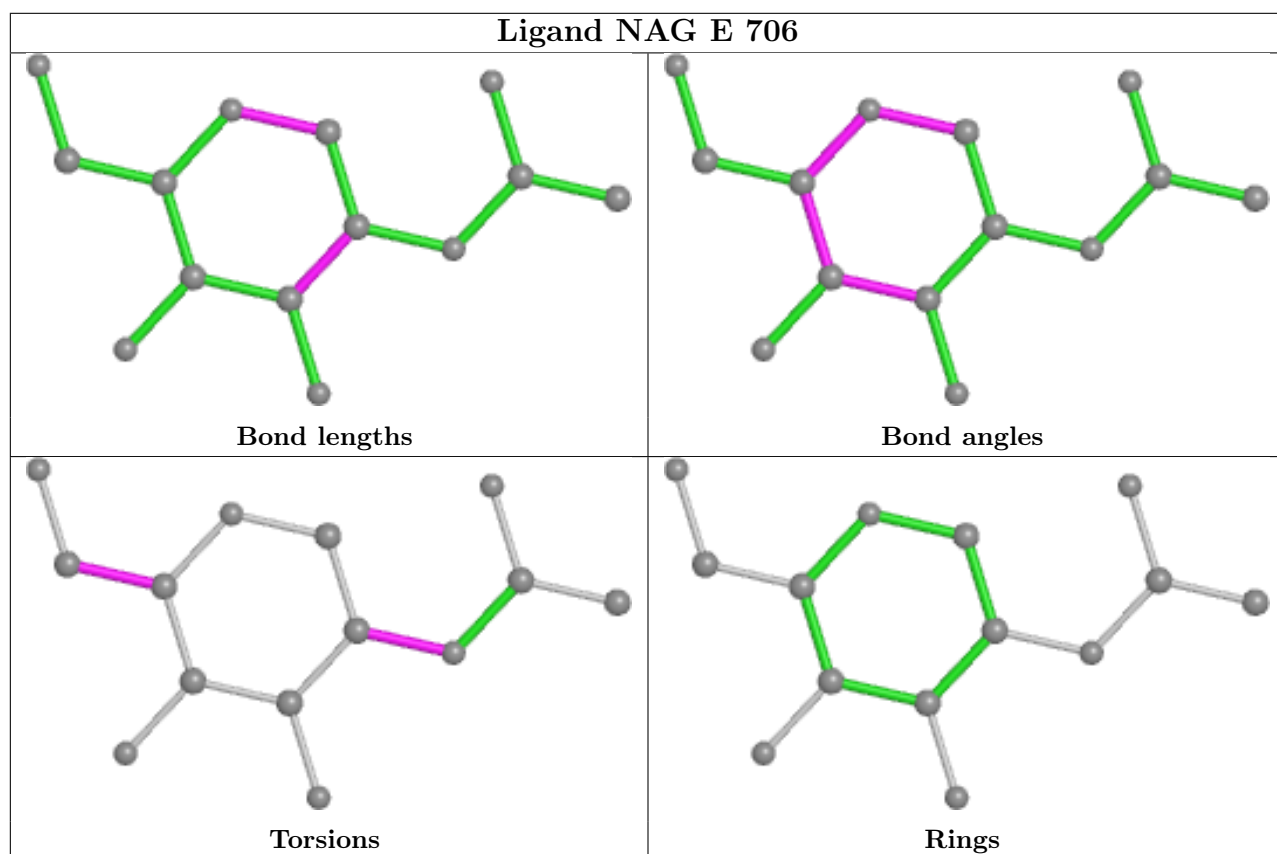
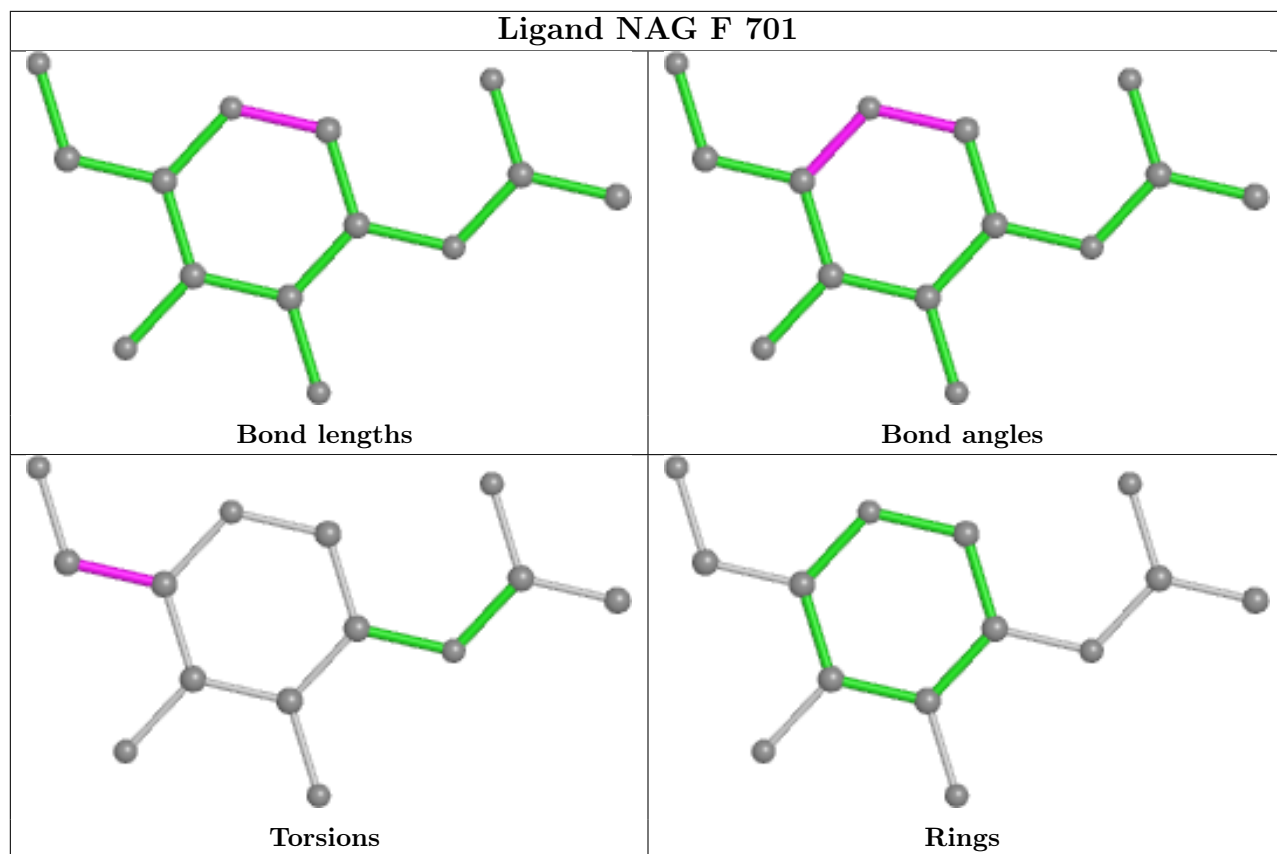


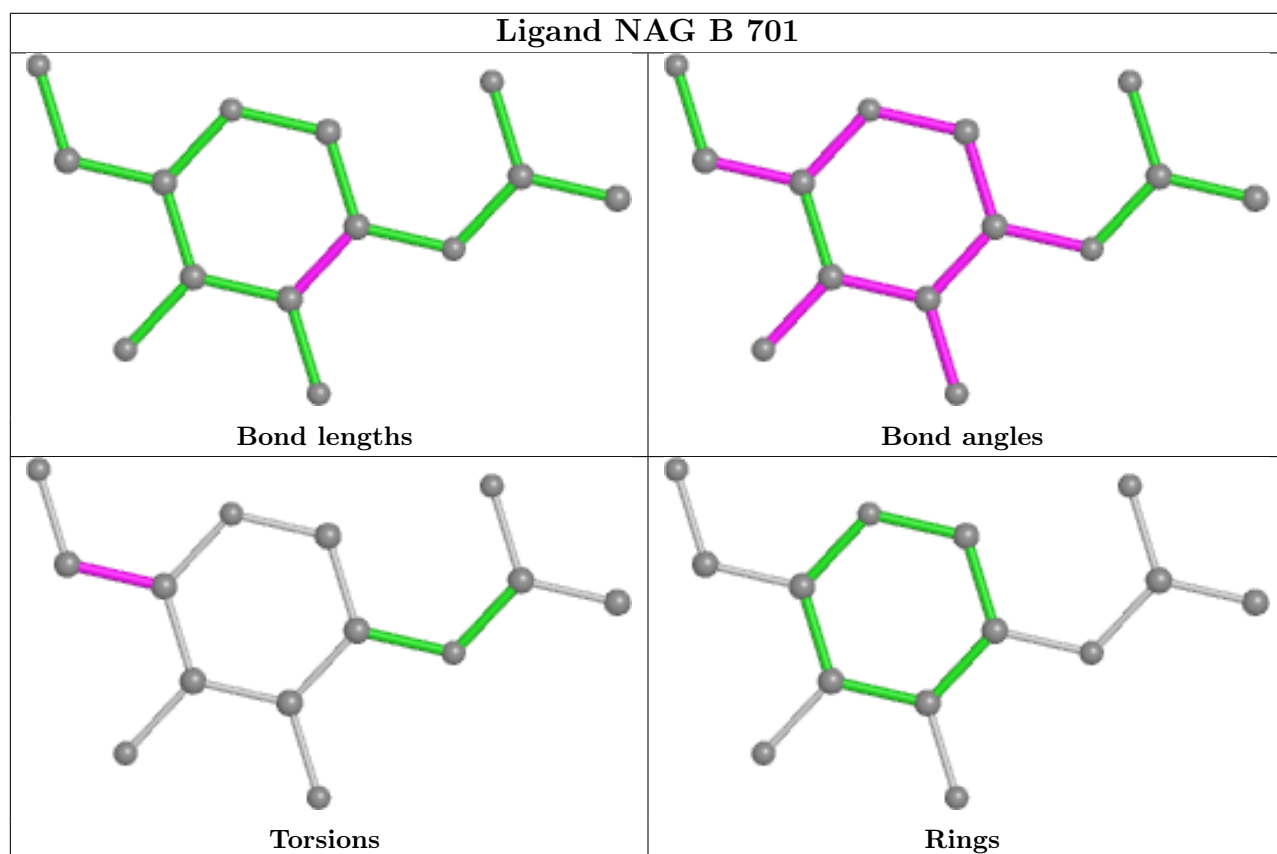
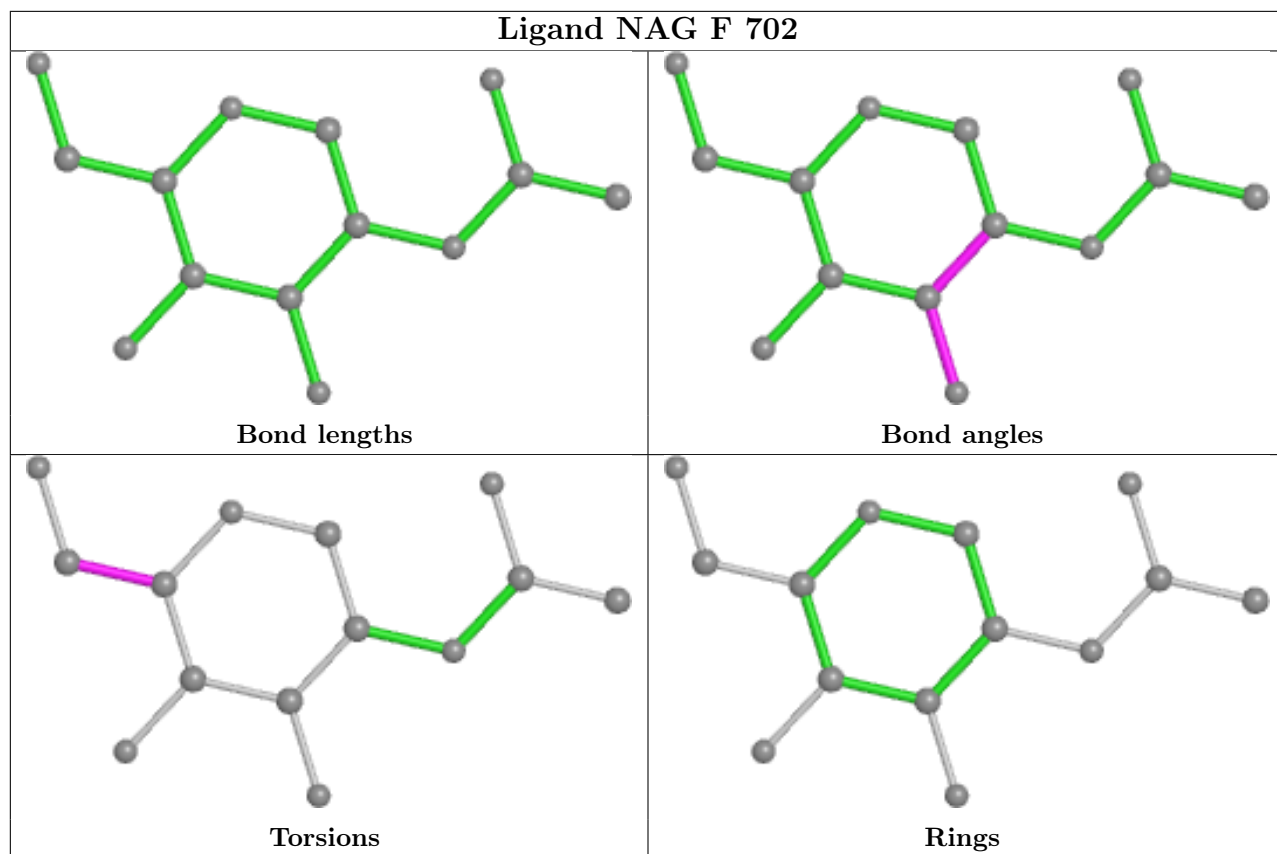


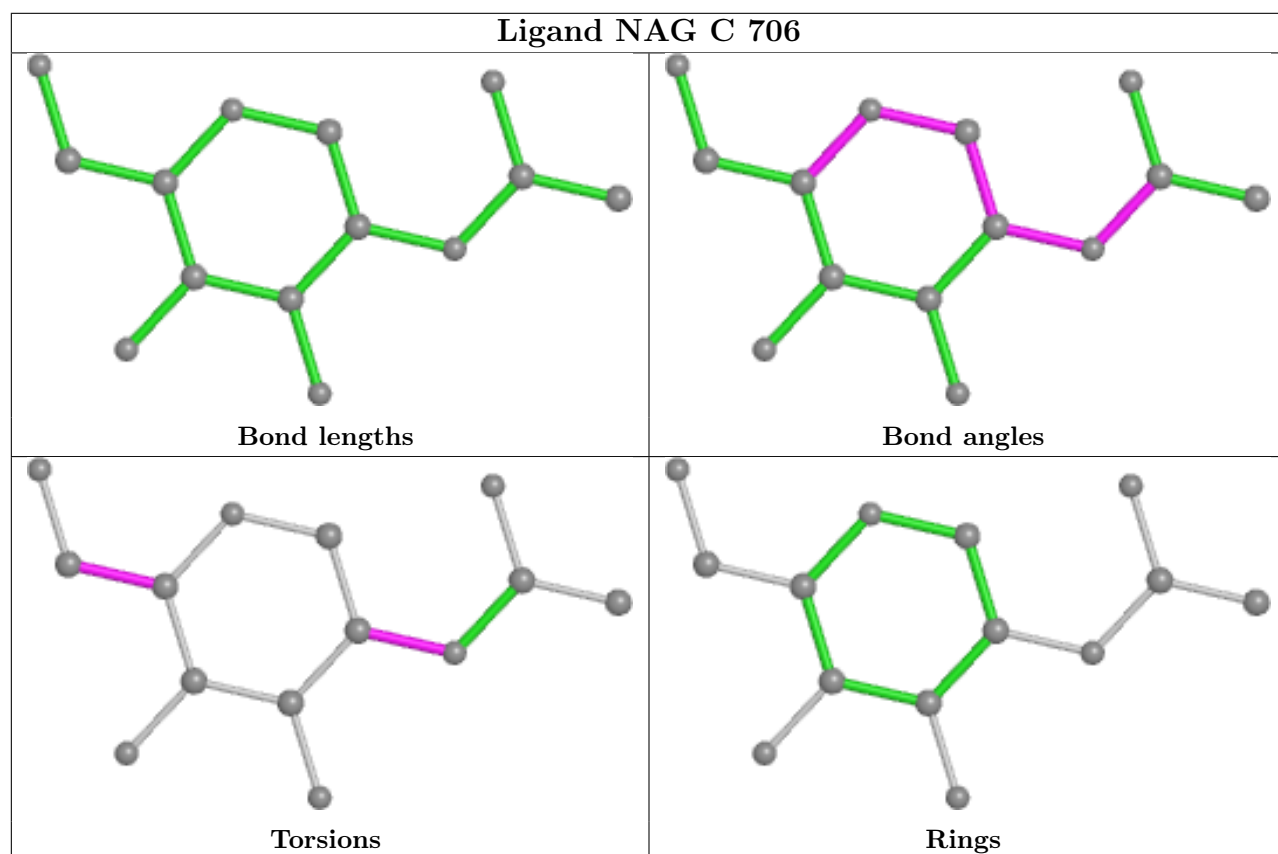
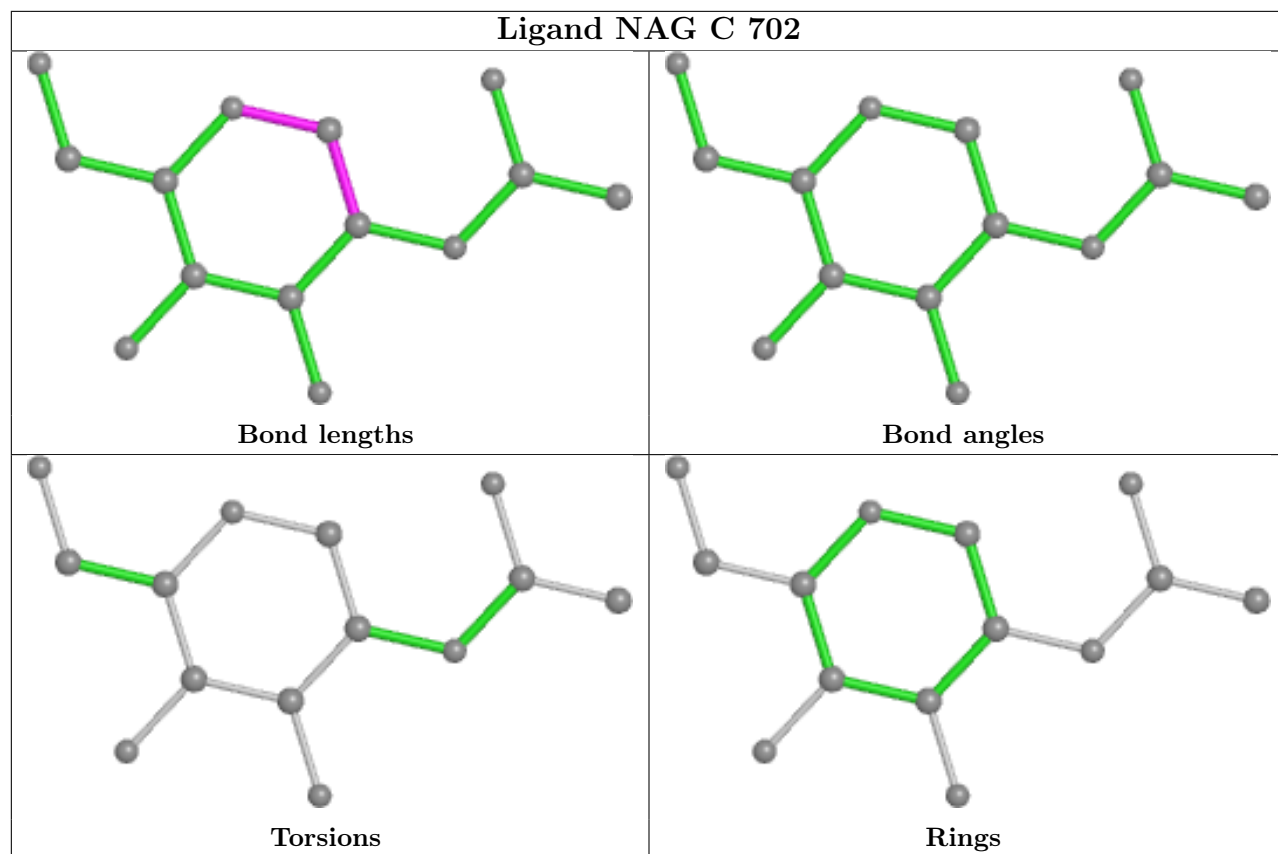


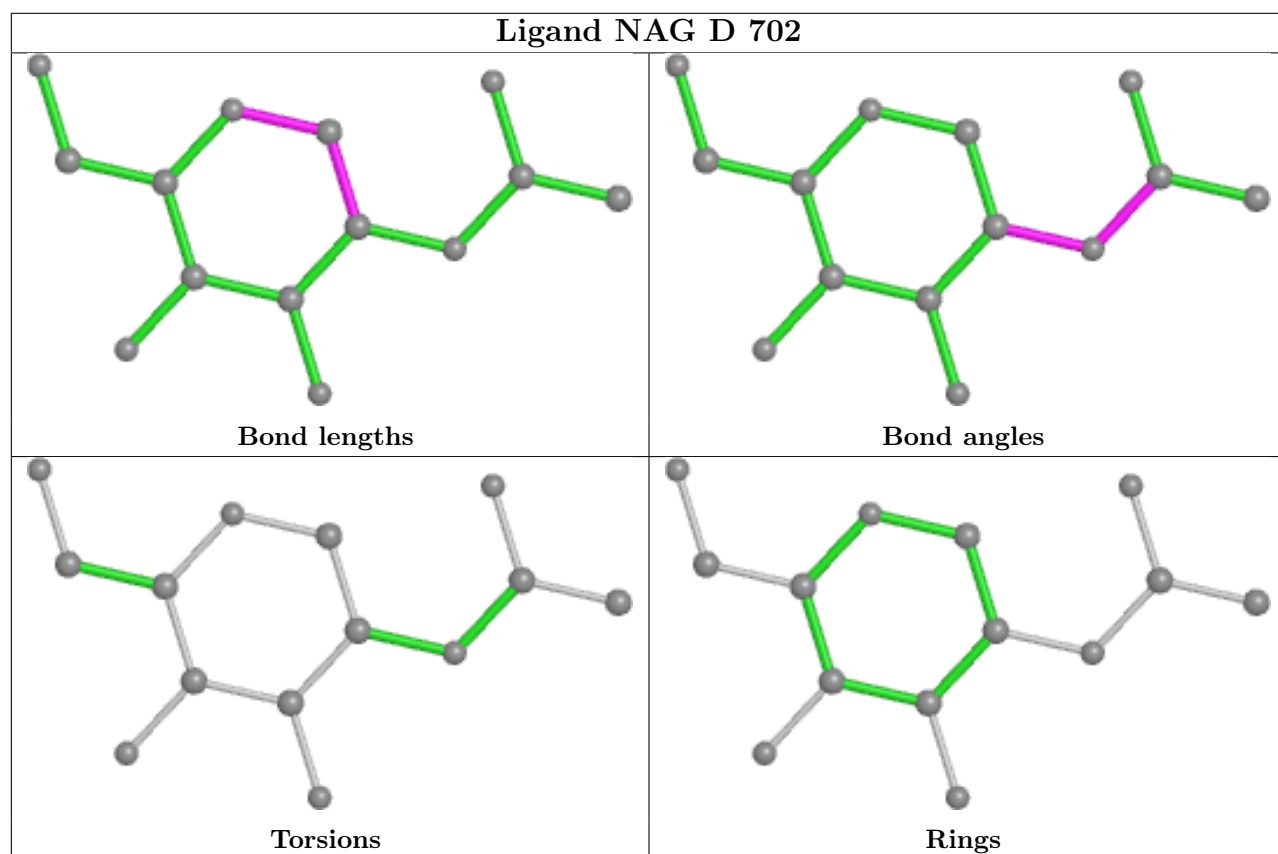
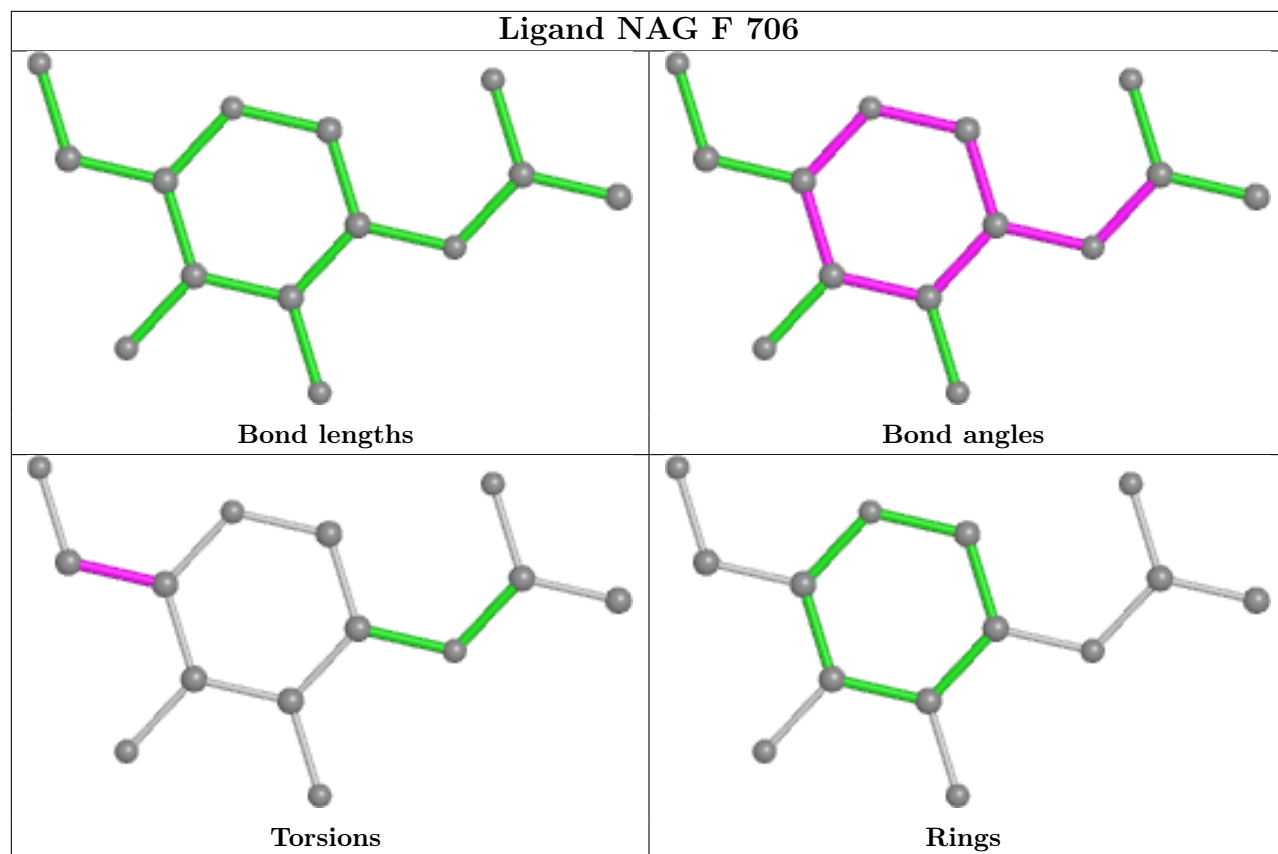


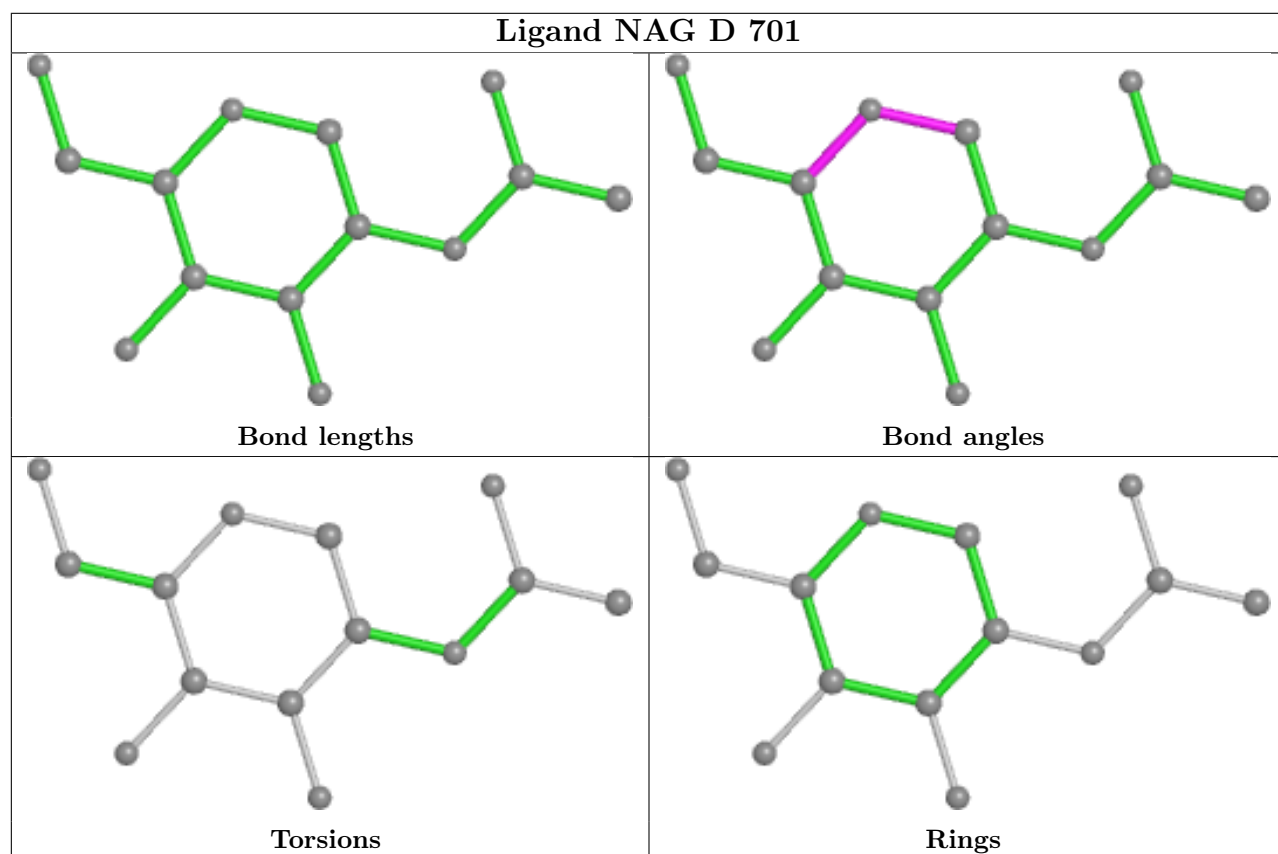
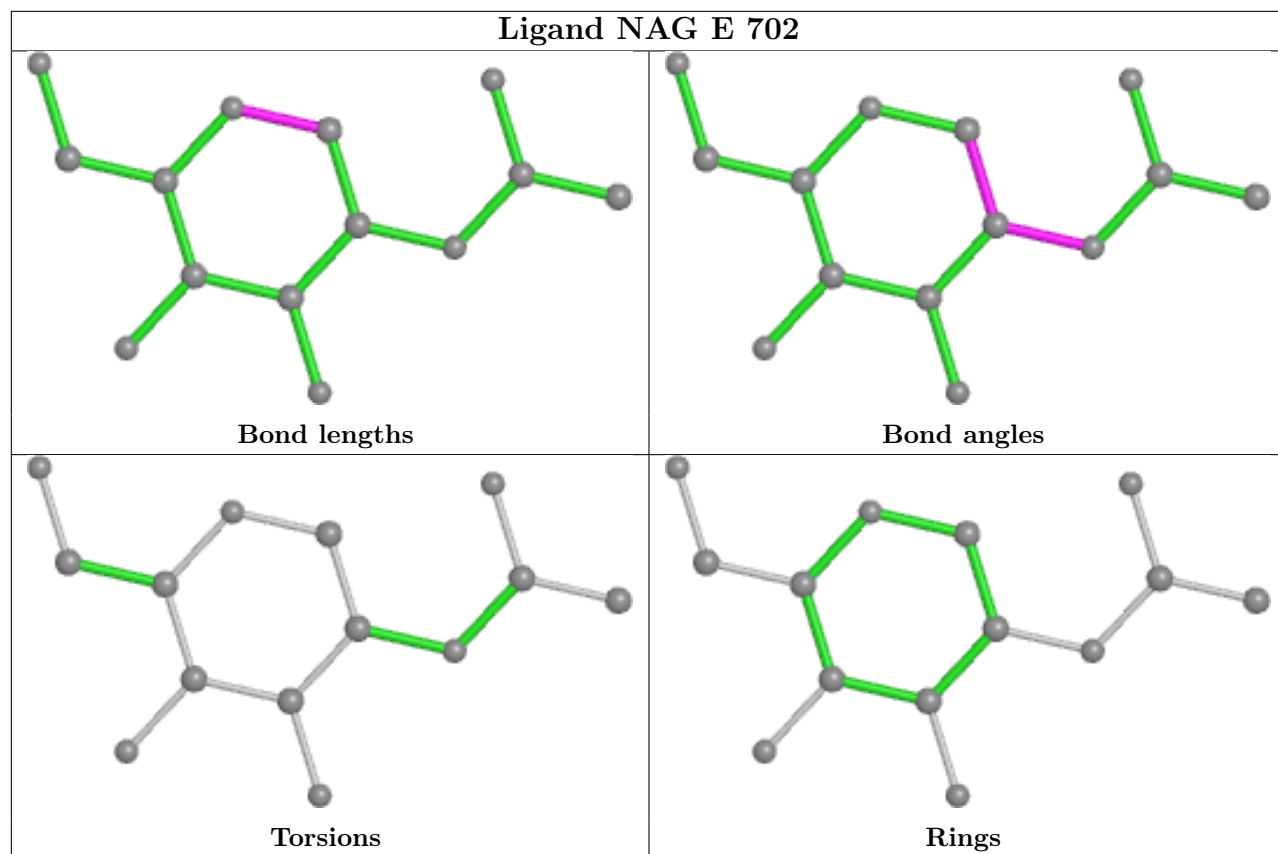


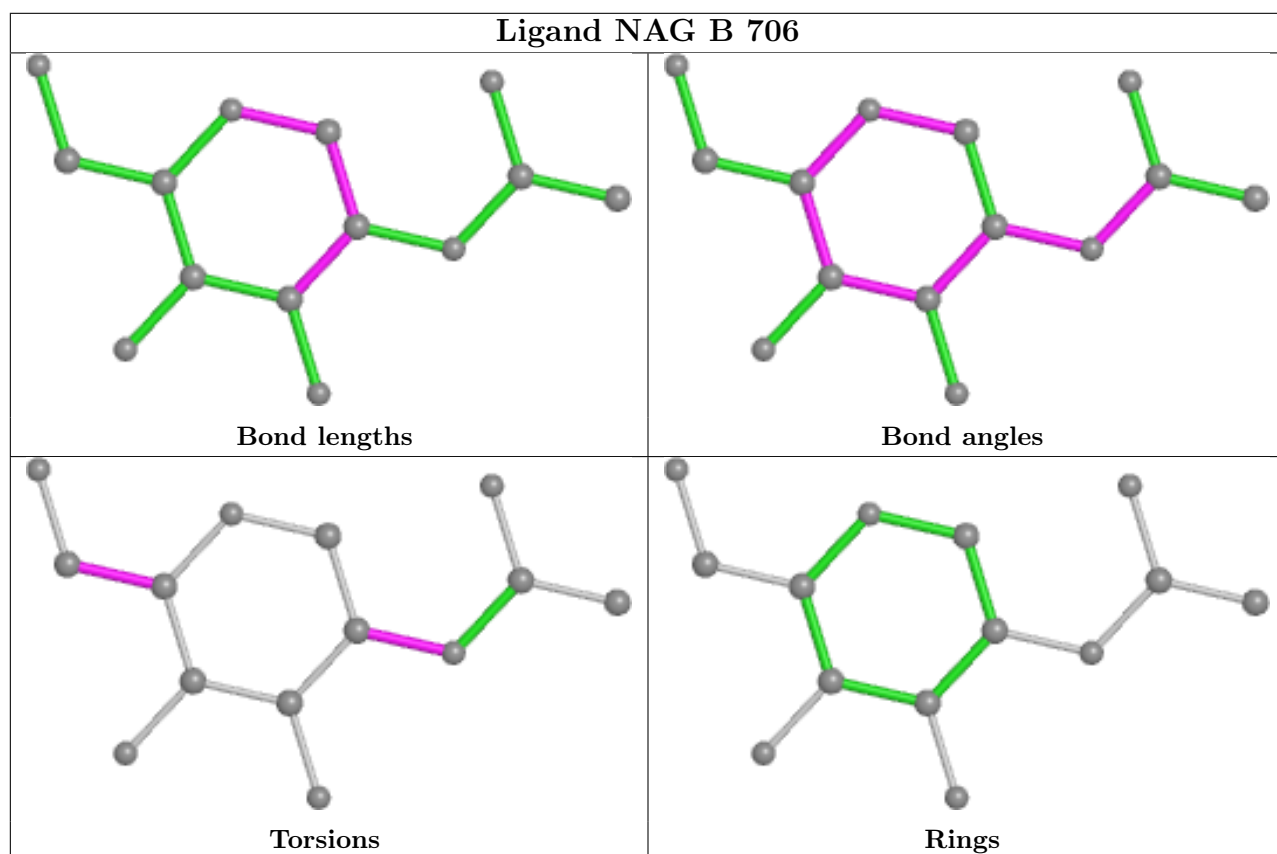
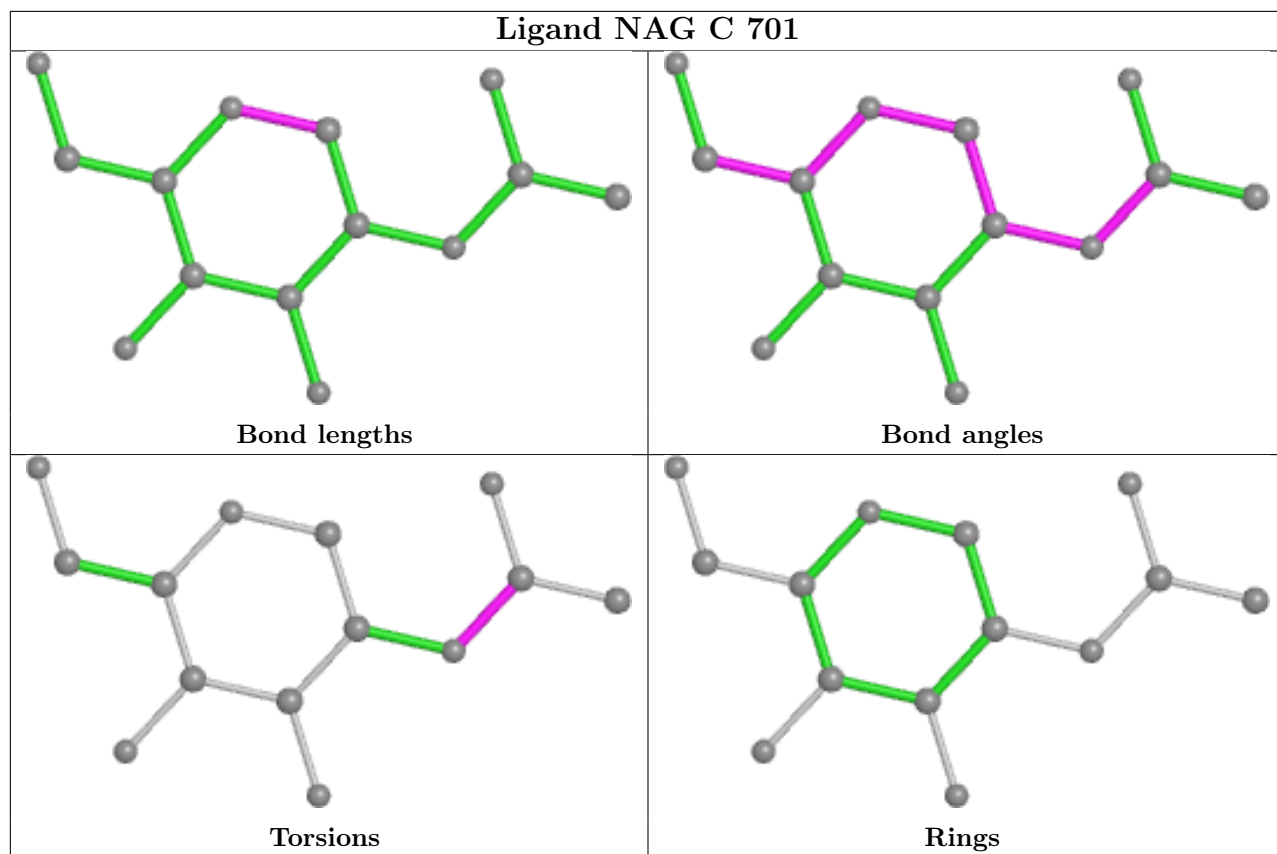












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/497 (97%)	0.39	15 (3%) 49 56	22, 39, 64, 119	0
1	B	488/497 (98%)	0.42	20 (4%) 37 44	15, 39, 67, 130	0
1	C	489/497 (98%)	0.34	15 (3%) 49 56	21, 37, 64, 135	0
1	D	489/497 (98%)	0.32	12 (2%) 57 64	19, 36, 62, 125	0
1	E	489/497 (98%)	0.40	15 (3%) 49 56	20, 38, 65, 108	0
1	F	489/497 (98%)	0.45	22 (4%) 33 40	21, 40, 73, 128	0
All	All	2931/2982 (98%)	0.39	99 (3%) 45 52	15, 38, 66, 135	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	503	LYS	8.2
1	A	502	ILE	7.4
1	D	502	ILE	5.7
1	F	502	ILE	5.6
1	C	502	ILE	5.5
1	E	502	ILE	5.3
1	E	503	LYS	5.3
1	C	503	LYS	5.2
1	C	387	LYS	4.9
1	E	386	GLU	4.8
1	E	388	THR	4.7
1	B	388	THR	4.6
1	B	502	ILE	4.5
1	C	501	GLN	4.4
1	F	335	ILE	4.2
1	F	386	GLU	4.2
1	B	8	ASN	4.1
1	D	503	LYS	4.1
1	F	500	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	8	ASN	4.0
1	B	501	GLN	3.8
1	C	500	PHE	3.7
1	B	473	CYS	3.7
1	F	200	GLY	3.6
1	F	334	ALA	3.5
1	A	500	PHE	3.4
1	C	386	GLU	3.3
1	E	497[A]	ASN	3.3
1	D	386	GLU	3.2
1	E	495	ALA	3.2
1	B	497[A]	ASN	3.2
1	F	8	ASN	3.2
1	D	388	THR	3.1
1	E	334	ALA	3.1
1	D	387	LYS	3.0
1	B	500	PHE	3.0
1	C	385	ILE	2.9
1	D	196	VAL	2.9
1	C	388	THR	2.9
1	F	242	ILE	2.9
1	D	501	GLN	2.9
1	B	20	VAL	2.9
1	E	387	LYS	2.8
1	F	222	TRP	2.8
1	A	387	LYS	2.8
1	D	367	LEU	2.8
1	E	501	GLN	2.8
1	D	126	ASN	2.7
1	B	335	ILE	2.7
1	C	334	ALA	2.7
1	A	495	ALA	2.7
1	E	500	PHE	2.7
1	F	385	ILE	2.6
1	A	197	ARG	2.6
1	F	189	ARG	2.6
1	E	202	VAL	2.6
1	F	439	LEU	2.6
1	F	497[A]	ASN	2.6
1	C	384	LEU	2.6
1	F	128	ILE	2.6
1	F	501	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	143	SER	2.6
1	F	340	GLU	2.6
1	A	388	THR	2.5
1	E	138	ALA	2.5
1	D	8	ASN	2.5
1	D	497[A]	ASN	2.5
1	A	497[A]	ASN	2.5
1	B	385	ILE	2.4
1	B	326	LYS	2.4
1	B	336	ALA	2.4
1	A	490	VAL	2.4
1	F	291	ASP	2.4
1	B	503	LYS	2.3
1	A	15	LEU	2.3
1	A	326	LYS	2.3
1	C	372	ALA	2.3
1	B	126	ASN	2.3
1	E	201	ARG	2.3
1	C	335	ILE	2.3
1	C	379	GLY	2.3
1	A	335	ILE	2.3
1	B	367	LEU	2.2
1	B	382	ASN	2.2
1	A	34	ILE	2.2
1	A	385	ILE	2.2
1	B	384	LEU	2.2
1	C	497[A]	ASN	2.2
1	F	388	THR	2.2
1	F	196	VAL	2.1
1	B	386	GLU	2.1
1	D	335	ILE	2.1
1	F	129	GLY	2.1
1	E	128	ILE	2.1
1	E	8	ASN	2.1
1	A	347	VAL	2.1
1	F	43	VAL	2.1
1	B	21	PRO	2.0
1	B	316	LEU	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

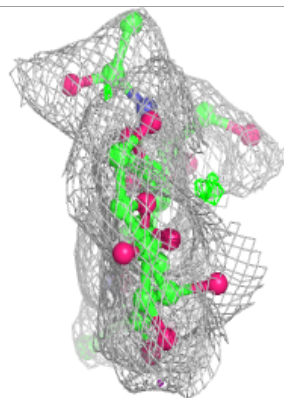
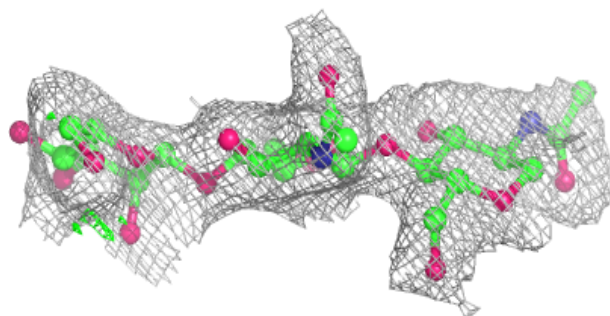
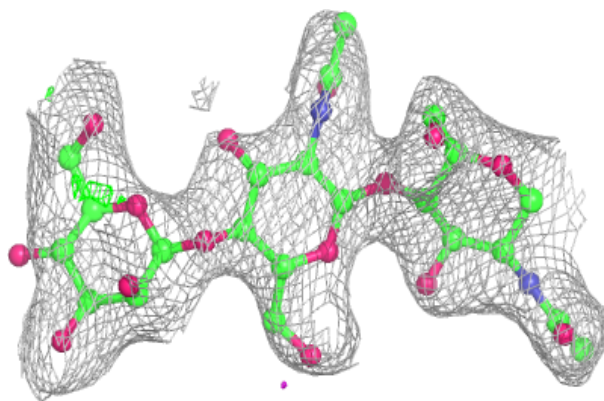
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	G	3	11/12	0.81	0.18	36,49,60,79	0
2	BMA	I	3	11/12	0.81	0.12	43,51,65,67	0
2	NAG	G	2	14/15	0.85	0.15	31,35,43,57	0
2	BMA	K	3	11/12	0.87	0.14	36,54,67,78	0
2	BMA	J	3	11/12	0.88	0.13	46,54,59,62	0
2	NAG	J	1	14/15	0.88	0.16	17,30,39,42	0
2	NAG	L	1	14/15	0.88	0.16	26,40,46,52	0
2	NAG	K	2	14/15	0.89	0.14	15,41,60,61	0
2	BMA	H	3	11/12	0.89	0.14	42,50,60,63	0
2	NAG	G	1	14/15	0.89	0.14	30,45,52,55	0
2	NAG	L	2	14/15	0.90	0.14	35,46,57,59	0
2	BMA	L	3	11/12	0.90	0.11	41,53,66,68	0
2	NAG	H	2	14/15	0.91	0.14	27,37,56,63	0
2	NAG	H	1	14/15	0.91	0.14	25,36,51,52	0
2	NAG	I	1	14/15	0.91	0.12	21,35,45,49	0
2	NAG	I	2	14/15	0.91	0.14	27,37,43,65	0
2	NAG	K	1	14/15	0.92	0.16	21,39,64,66	0
2	NAG	J	2	14/15	0.92	0.19	24,35,49,67	0

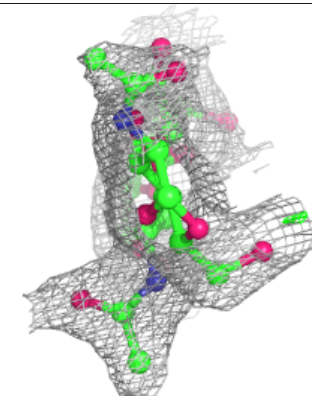
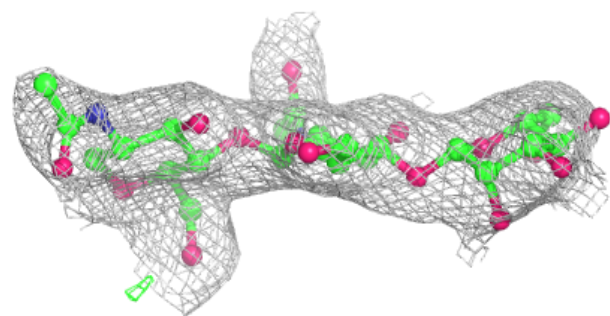
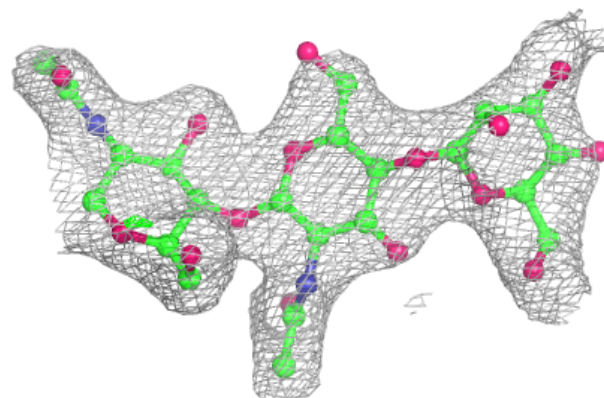
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

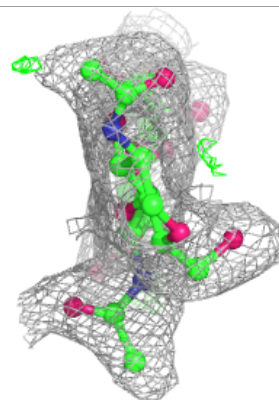
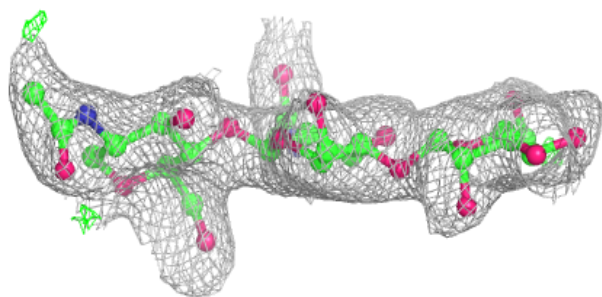
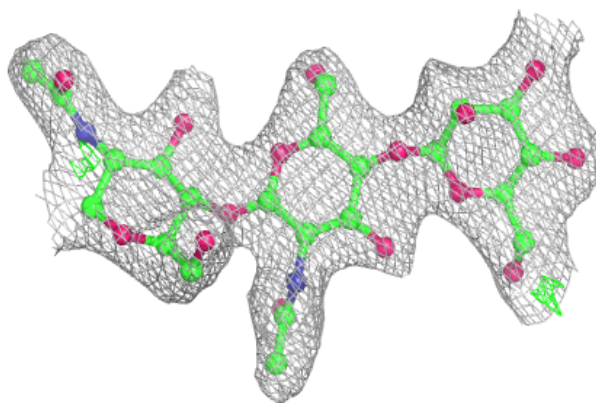
**Electron density around Chain H:**

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

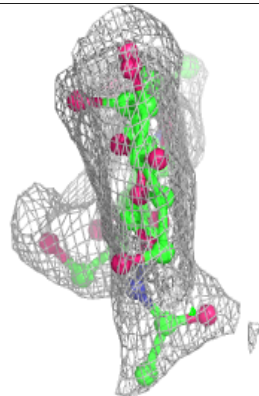
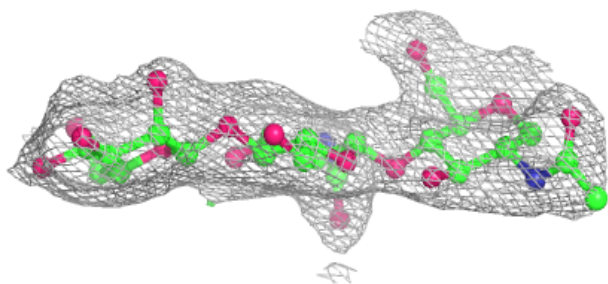
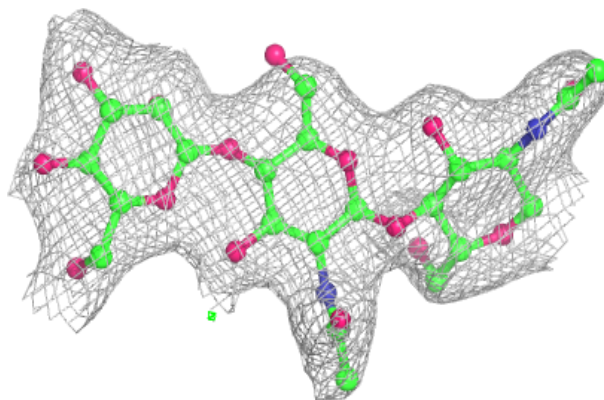


Electron density around Chain I:

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

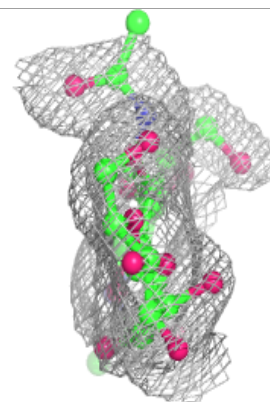
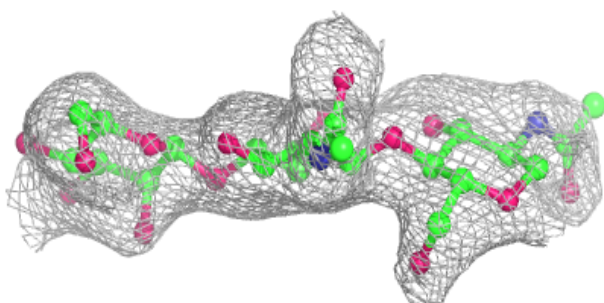
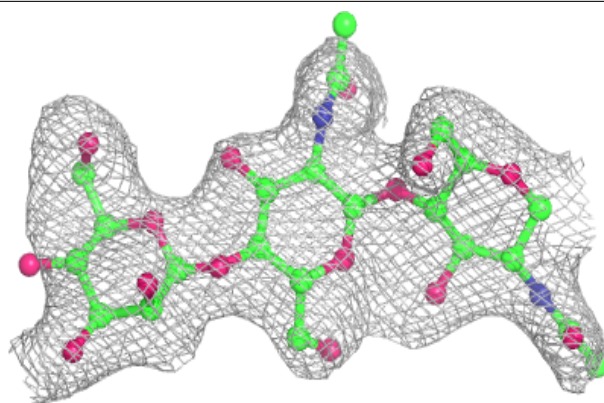
**Electron density around Chain J:**

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

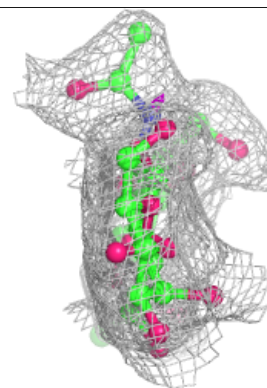
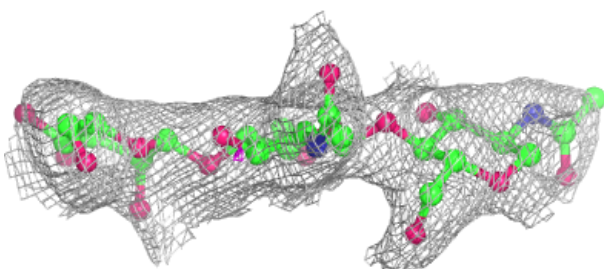
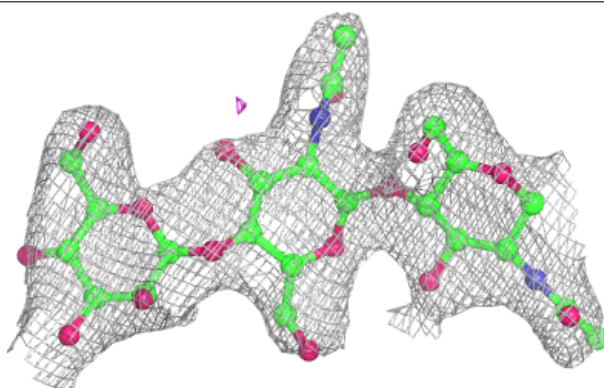


Electron density around Chain K:

$2mF_o-DF_c$ (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

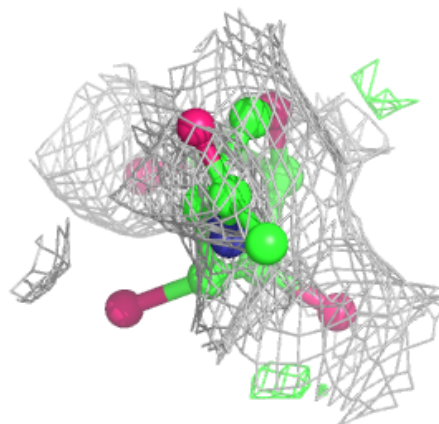
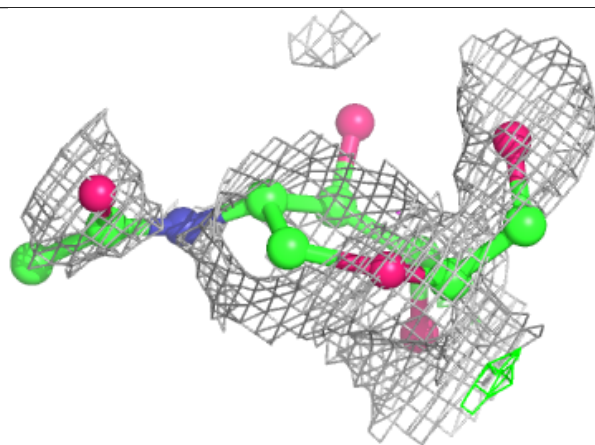
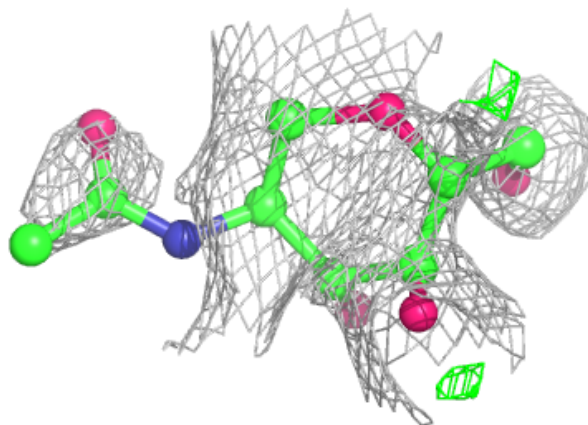
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	706	14/15	0.54	0.40	45,63,71,75	0
3	NAG	A	706	14/15	0.63	0.34	39,60,69,70	0
3	NAG	E	701	14/15	0.66	0.28	39,60,79,81	0
3	NAG	A	702	14/15	0.68	0.37	65,74,84,86	0
3	NAG	F	702	14/15	0.68	0.32	39,58,70,76	0
3	NAG	B	701	14/15	0.69	0.24	58,66,77,79	0
3	NAG	D	706	14/15	0.70	0.29	35,54,66,72	0
3	NAG	A	700	14/15	0.71	0.21	35,41,62,64	0
3	NAG	F	706	14/15	0.71	0.30	50,57,70,76	0
3	NAG	C	702	14/15	0.72	0.28	49,76,102,106	0
3	NAG	D	700	14/15	0.72	0.23	36,60,71,72	0
3	NAG	C	700	14/15	0.72	0.22	45,63,73,82	0
3	NAG	D	702	14/15	0.73	0.29	26,75,92,102	0
3	NAG	E	702	14/15	0.76	0.22	31,45,58,60	0
3	NAG	E	700	14/15	0.76	0.23	47,57,79,79	0
3	NAG	D	701	14/15	0.76	0.24	30,63,74,79	0
3	NAG	B	700	14/15	0.77	0.25	43,54,64,71	0
3	NAG	C	701	14/15	0.78	0.20	32,53,67,76	0
3	NAG	F	700	14/15	0.78	0.22	30,46,62,63	0
3	NAG	A	701	14/15	0.80	0.26	27,45,59,76	0
3	NAG	B	702	14/15	0.81	0.17	46,56,76,78	0
3	NAG	E	706	14/15	0.83	0.24	23,47,74,75	0
3	NAG	C	706	14/15	0.83	0.19	37,46,65,66	0
3	NAG	F	701	14/15	0.86	0.18	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.

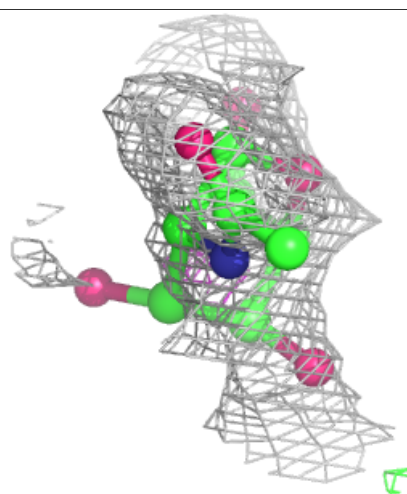
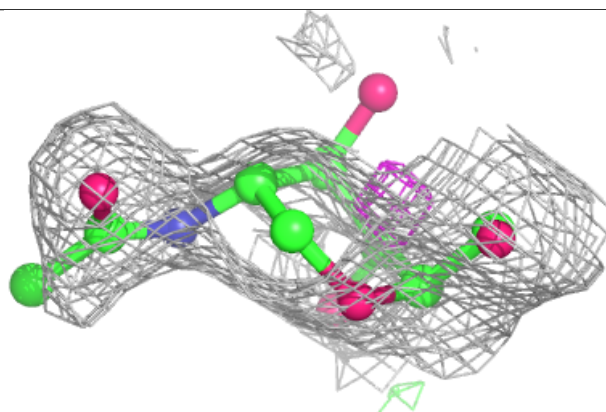
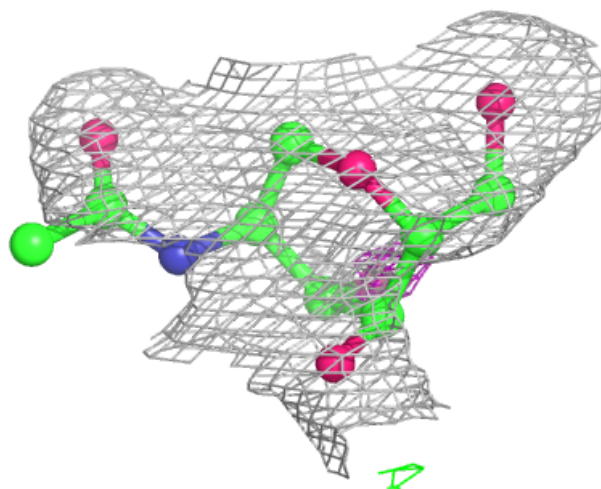
Electron density around NAG B 706:

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



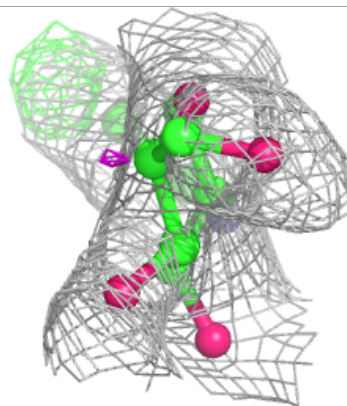
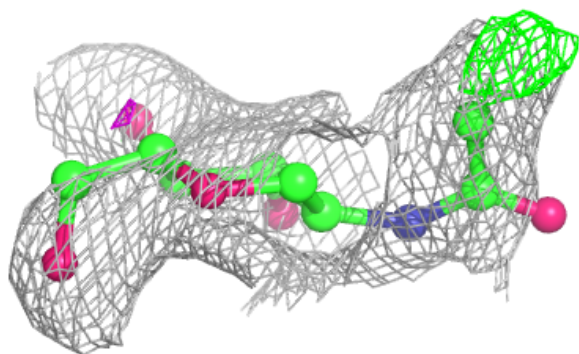
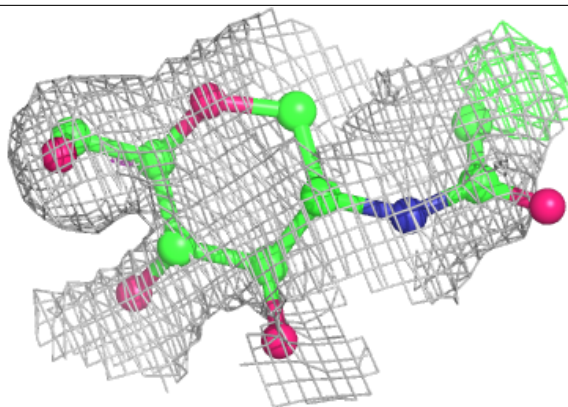
Electron density around NAG A 706:

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

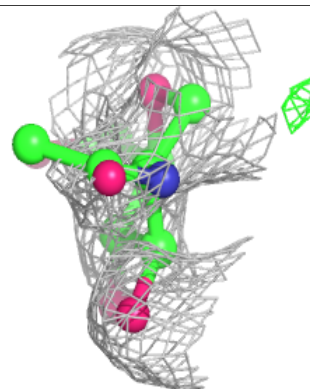
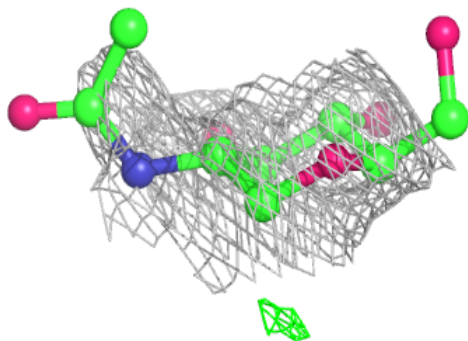
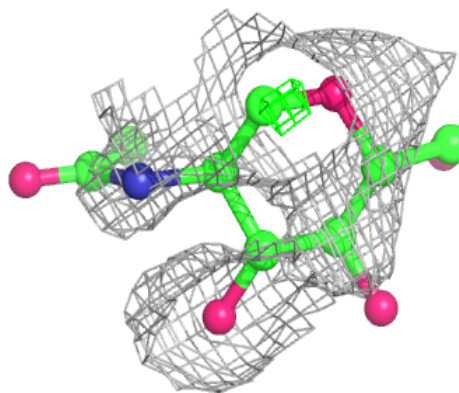


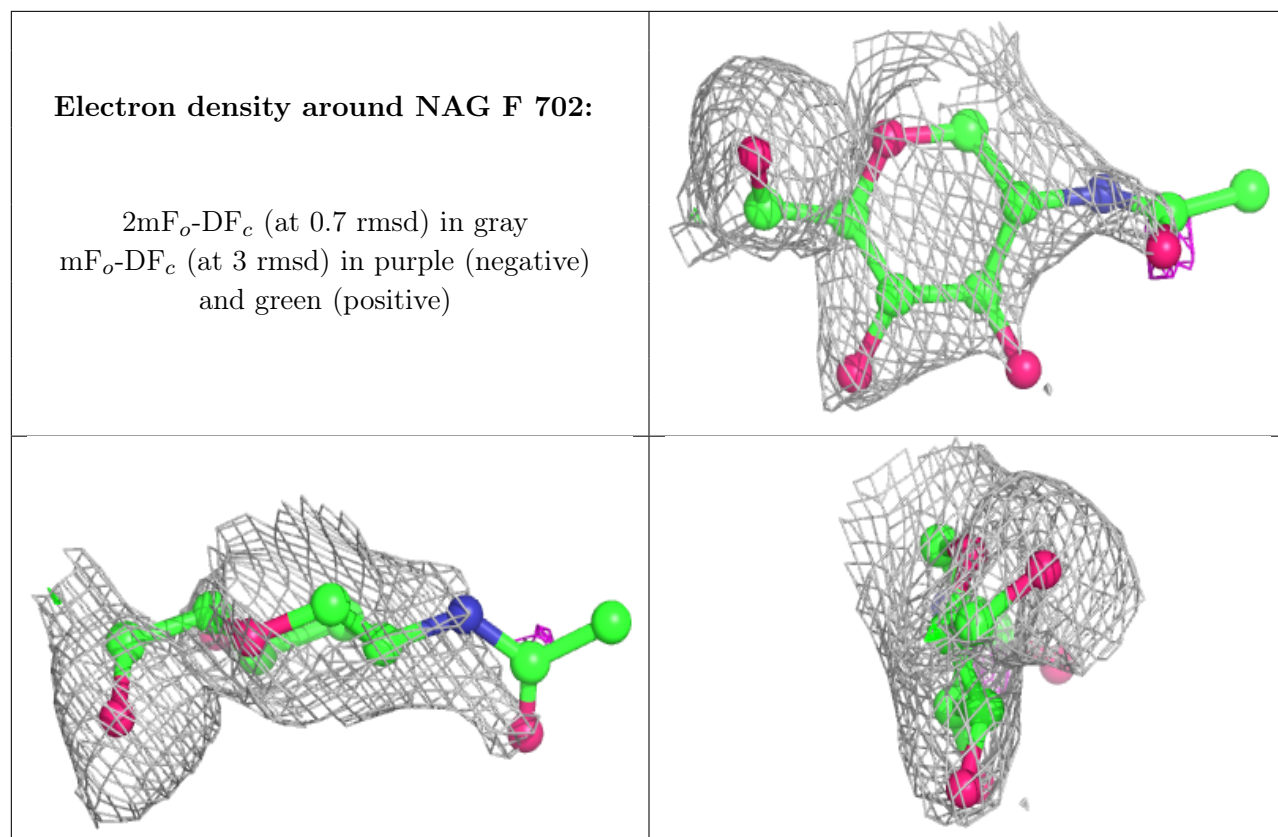
Electron density around NAG E 701:

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

**Electron density around NAG A 702:**

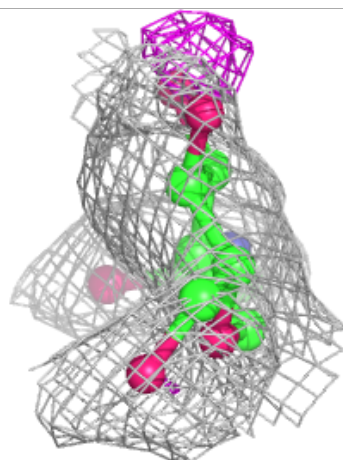
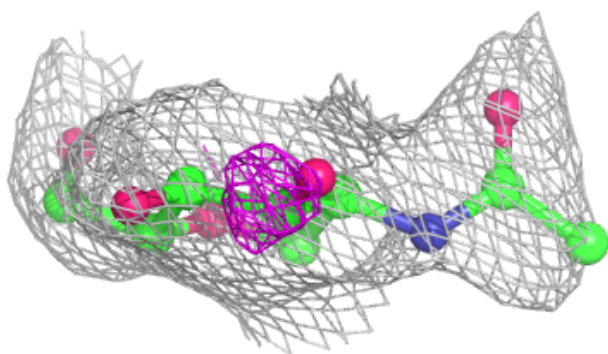
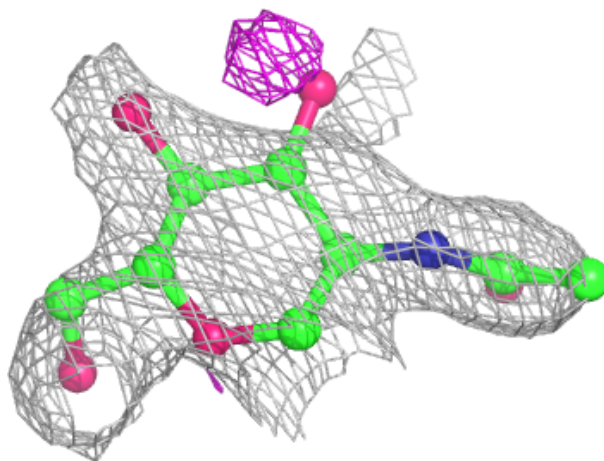
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





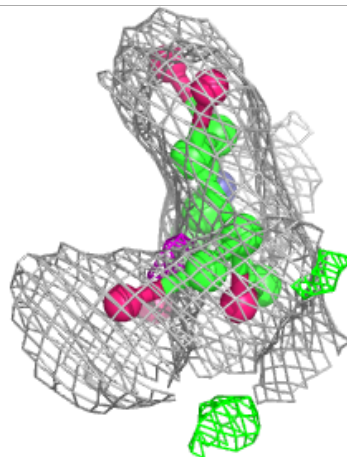
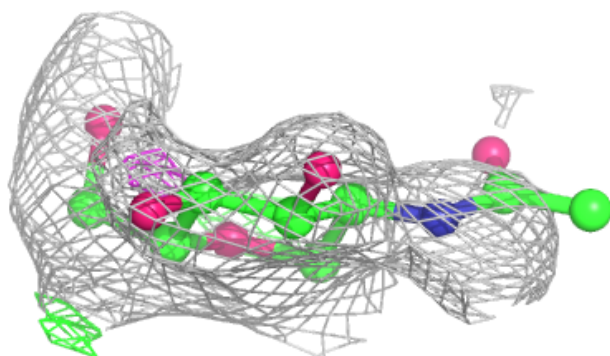
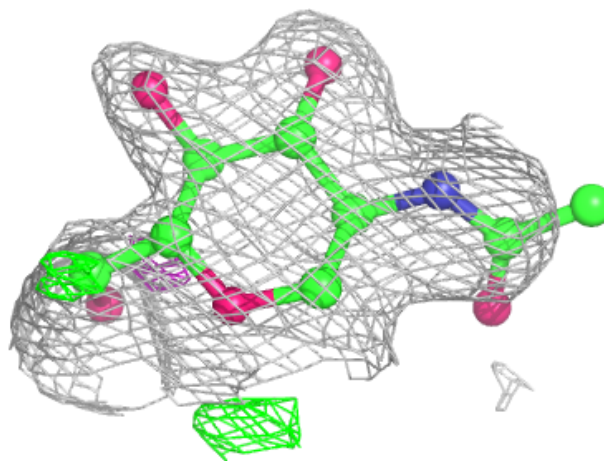
Electron density around NAG B 701:

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



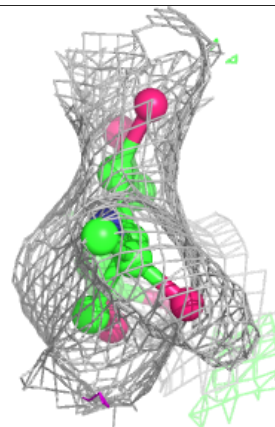
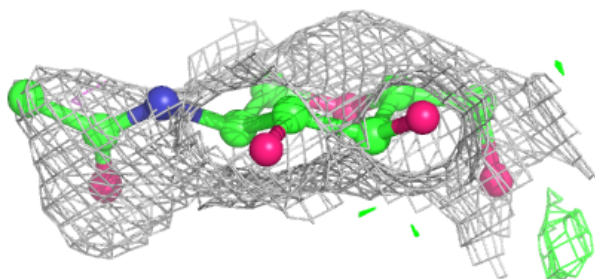
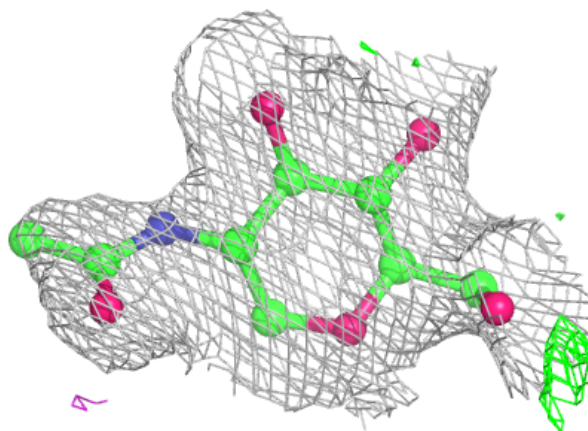
Electron density around NAG D 706:

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



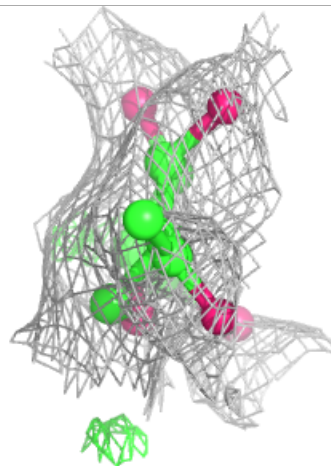
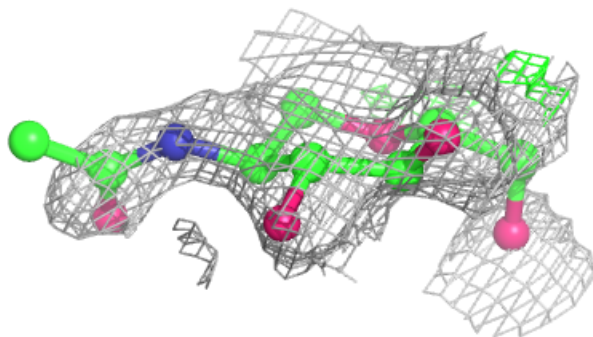
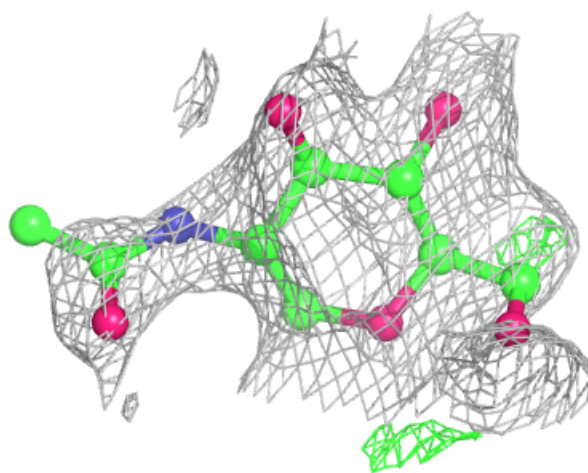
Electron density around NAG A 700:

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



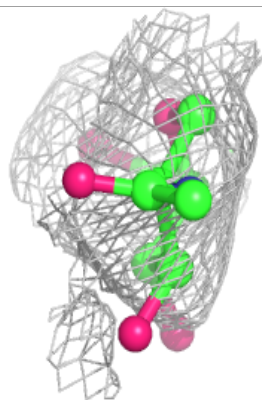
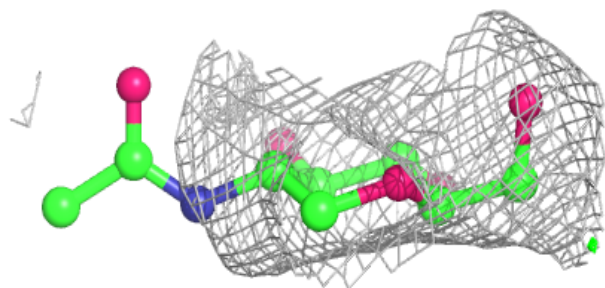
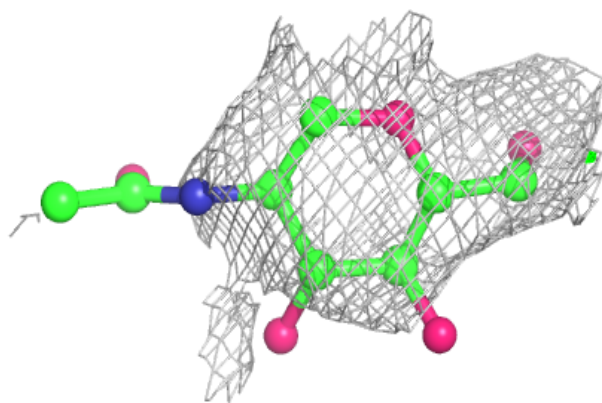
Electron density around NAG F 706:

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

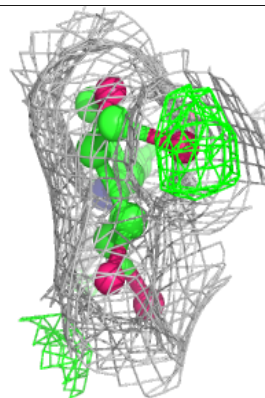
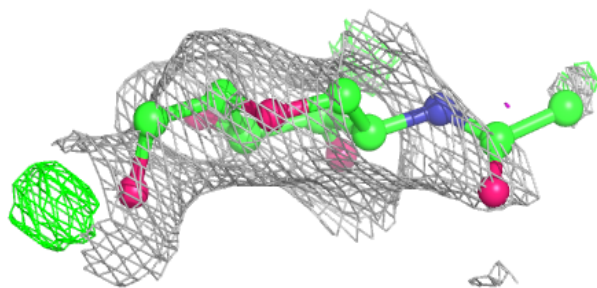
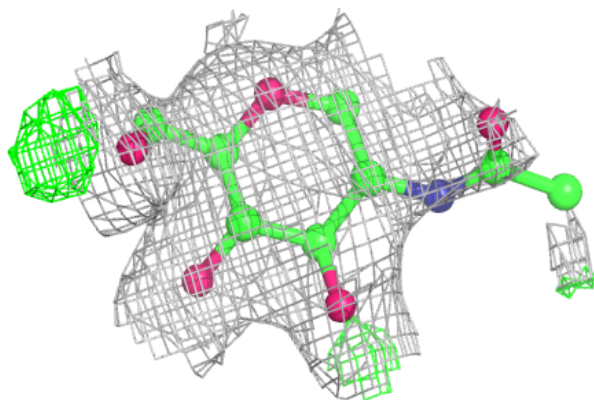


Electron density around NAG C 702:

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

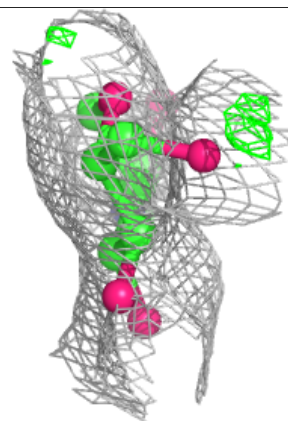
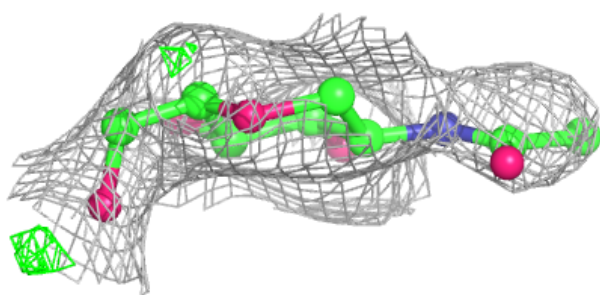
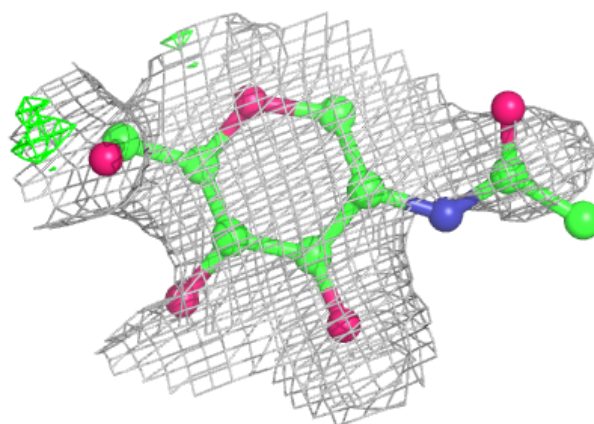
**Electron density around NAG D 700:**

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

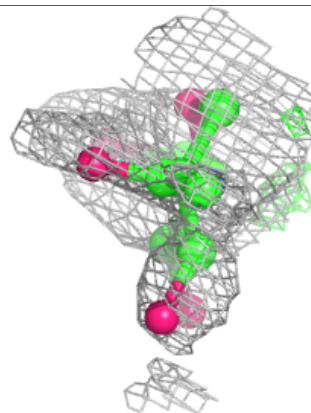
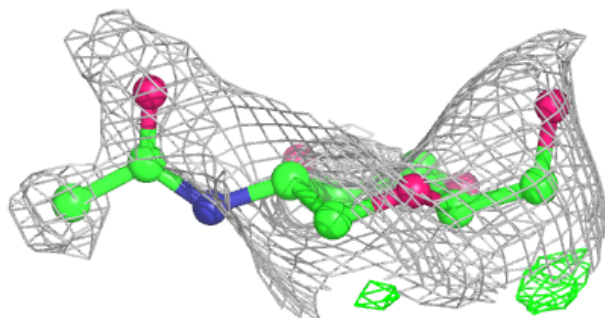
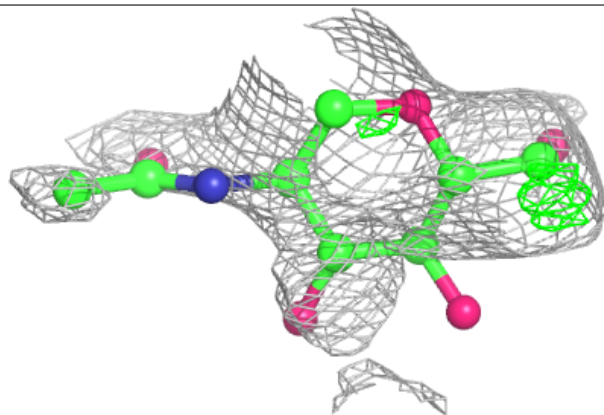


Electron density around NAG C 700:

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

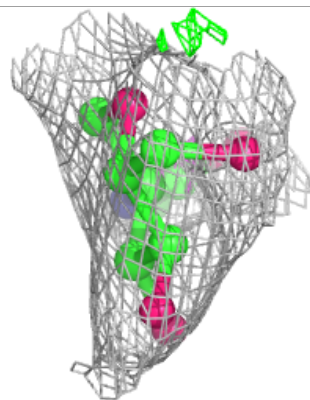
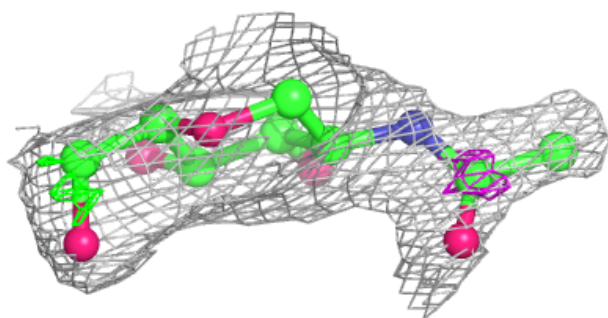
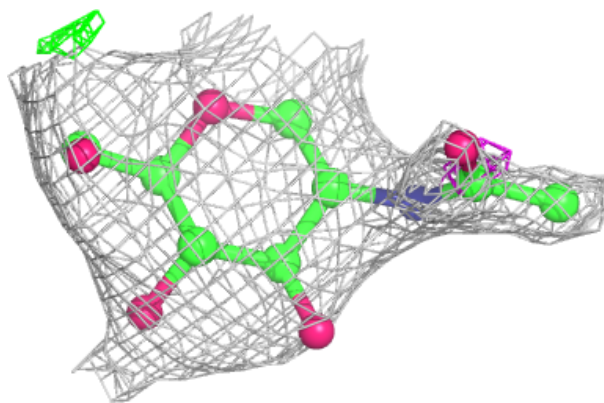
**Electron density around NAG D 702:**

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

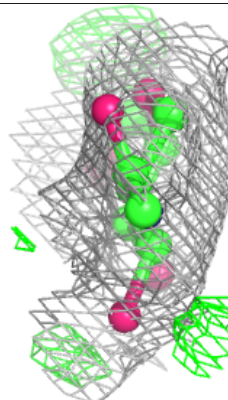
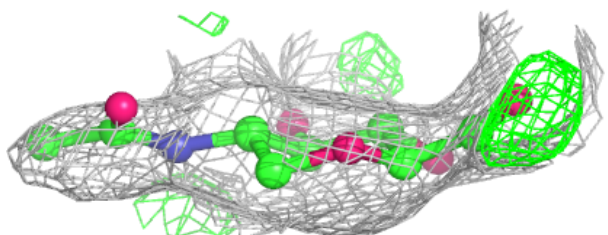
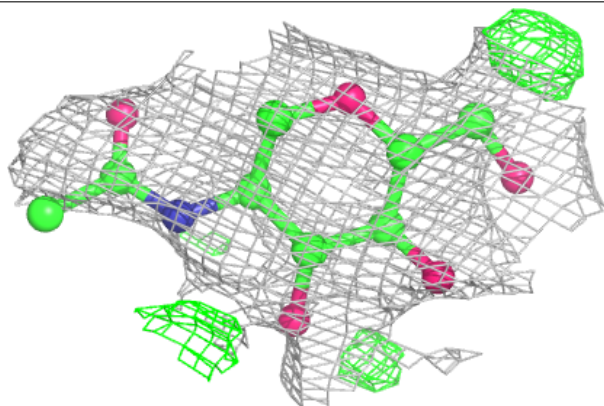


Electron density around NAG E 702:

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

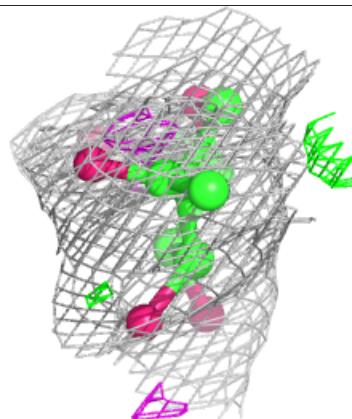
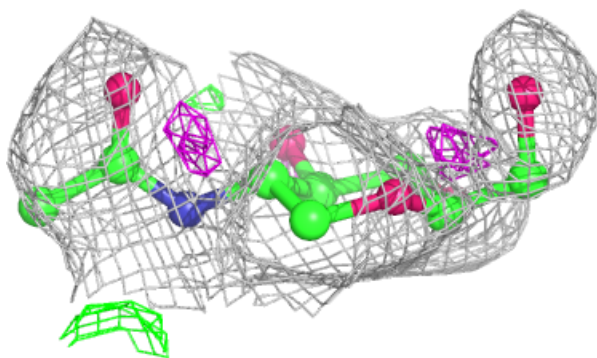
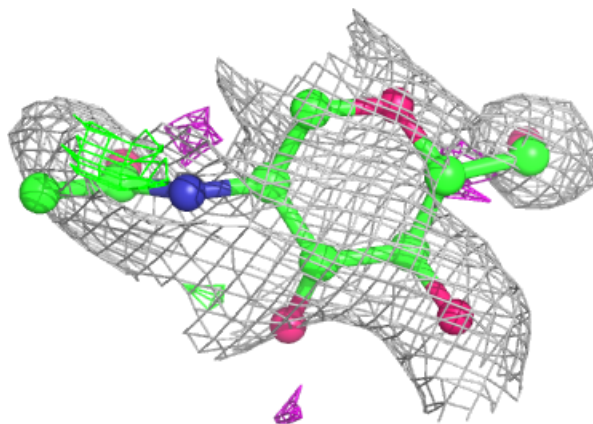
**Electron density around NAG E 700:**

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

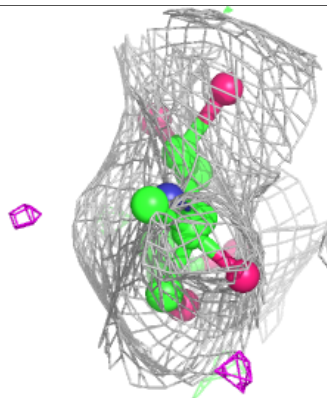
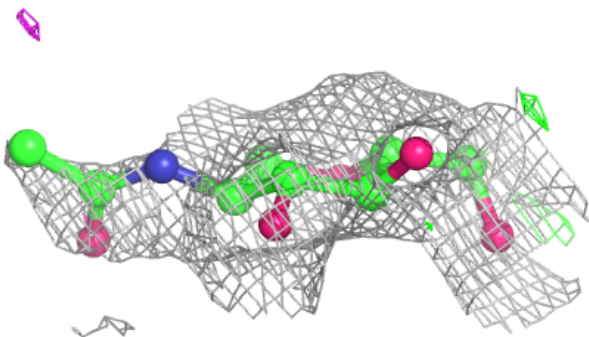
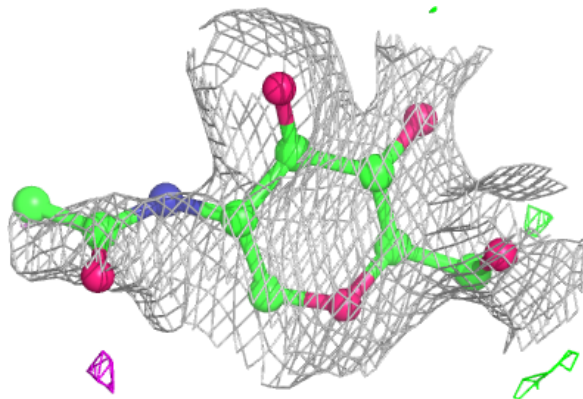


Electron density around NAG D 701:

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

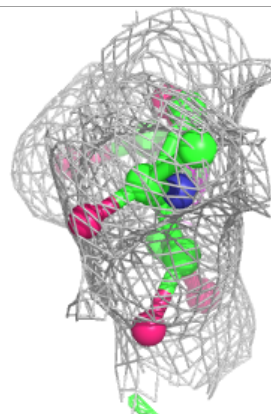
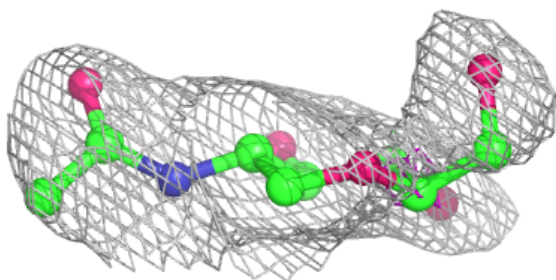
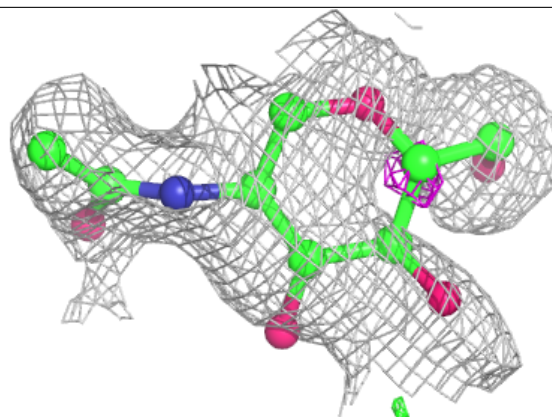
**Electron density around NAG B 700:**

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

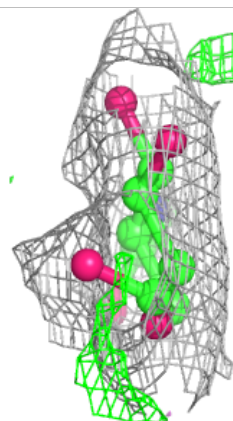
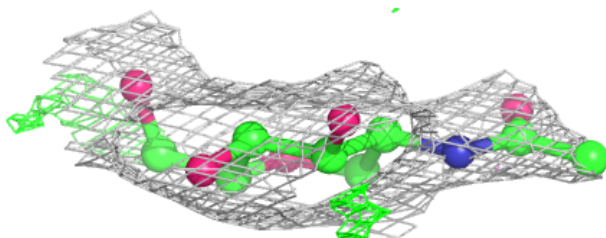
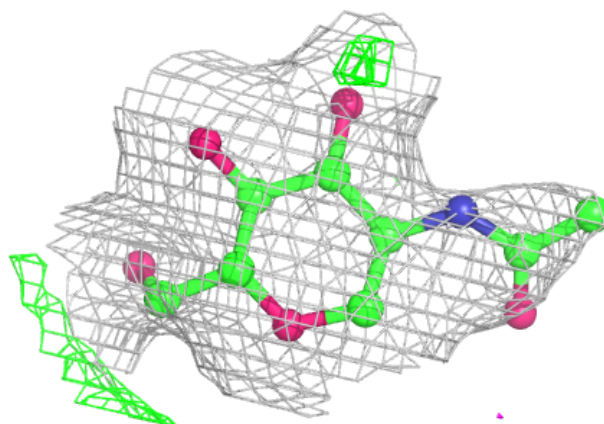


Electron density around NAG C 701:

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

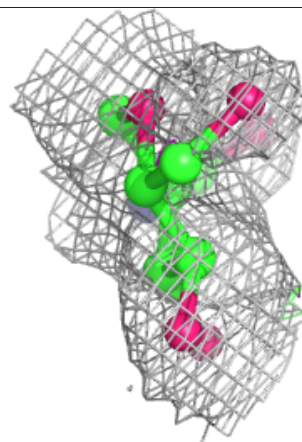
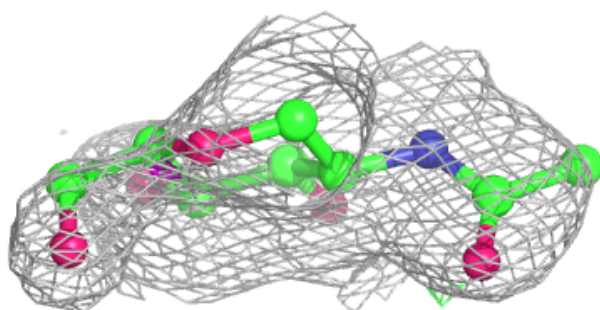
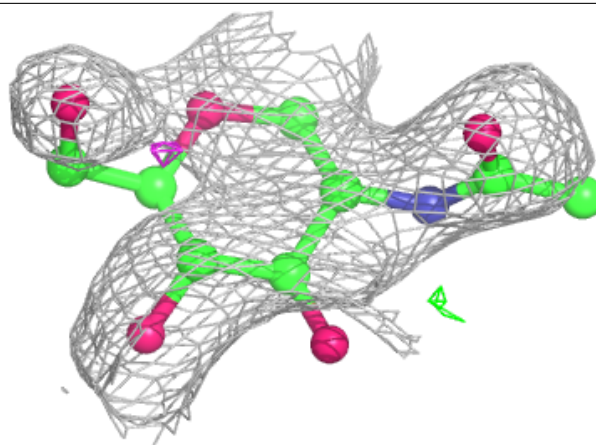
**Electron density around NAG F 700:**

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

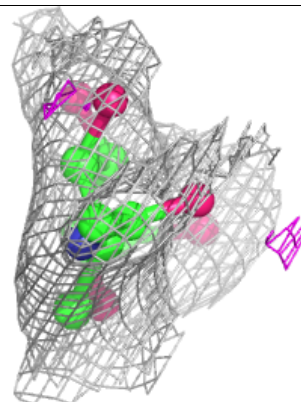
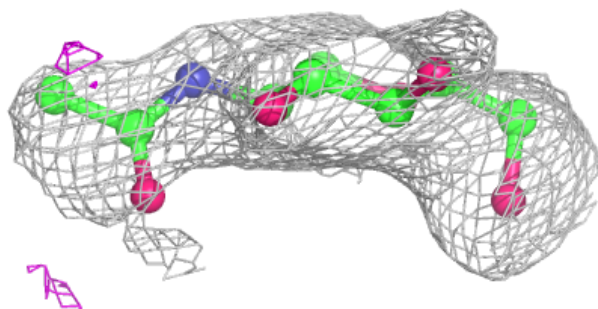
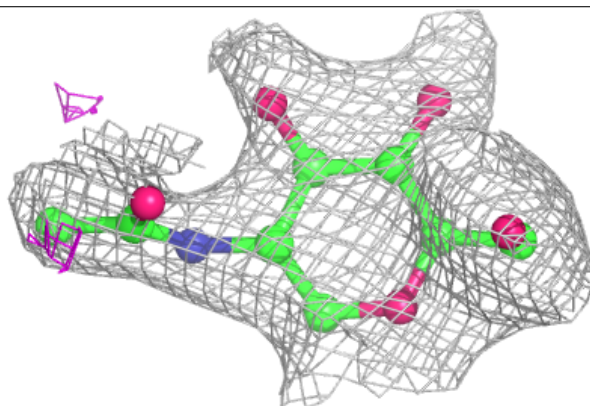


Electron density around NAG A 701:

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

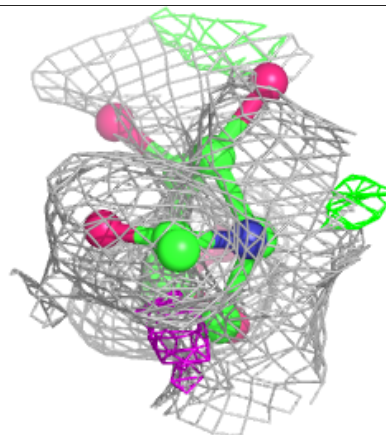
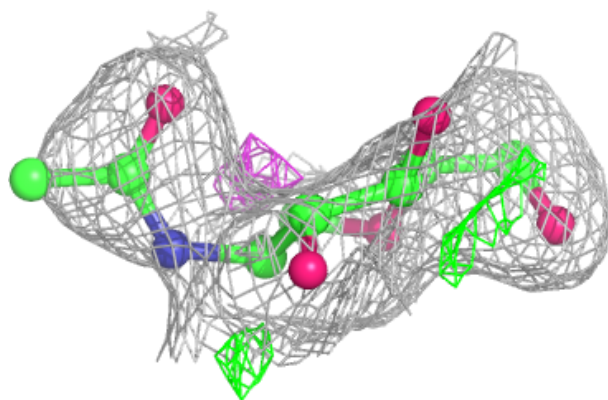
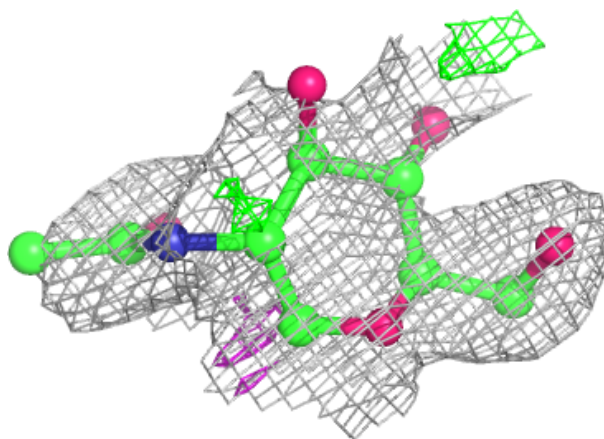
**Electron density around NAG B 702:**

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



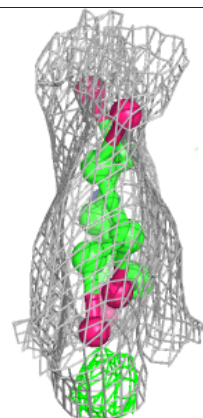
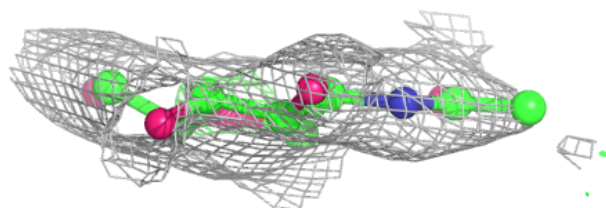
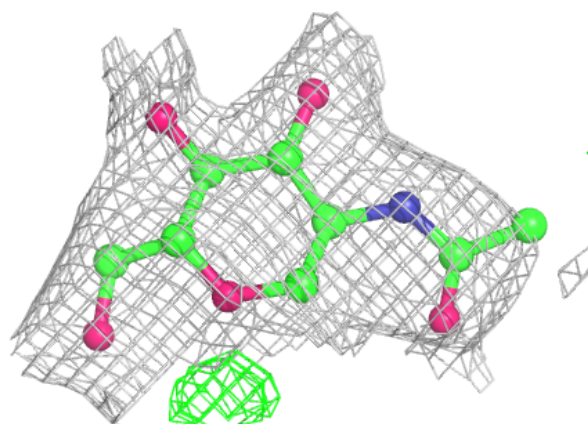
Electron density around NAG E 706:

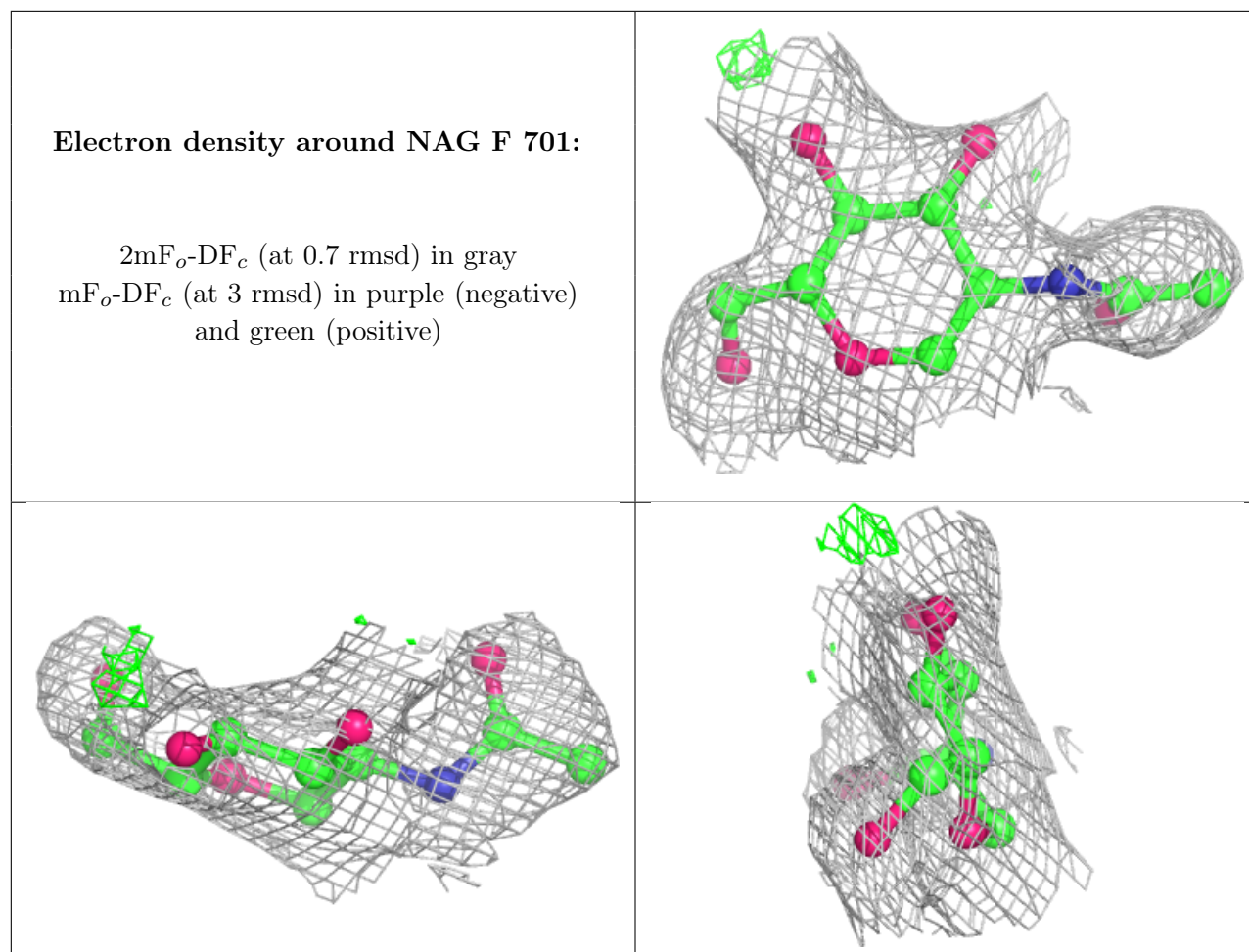
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAG C 706:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.