



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2022 – 02:18 PM JST

PDB ID : 7VPQ  
Title : Structures of a deltacoronavirus spike protein bound to porcine and human receptors indicate the risk of virus adaptation to humans  
Authors : Ji, W.; Xu, Y.; Zhang, S.  
Deposited on : 2021-10-17  
Resolution : 3.10 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

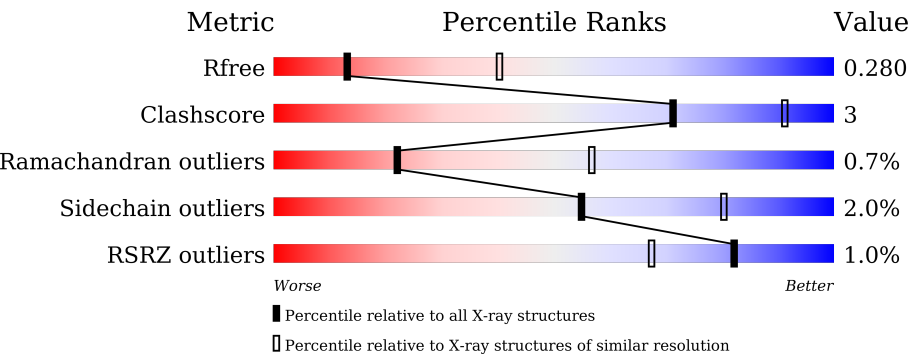
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	909	<div><div></div><div>89%9%</div><div></div></div>
1	C	909	<div><div></div><div>90%8%</div><div></div></div>
1	E	909	<div><div></div><div>89%9%</div><div></div></div>
2	B	127	<div><div>8%</div><div>54%23%</div><div>19%</div></div>
2	D	127	<div><div>5%</div><div>56%20%</div><div>5%19%</div></div>
2	F	127	<div><div>7%</div><div>56%22%</div><div>19%</div></div>

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	H	2	 100%
3	J	2	 50%50%
3	K	2	 100%
3	L	2	 50%50%
4	I	2	 100%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24537 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	895	Total	C	N	O	S	0	0	0
			7223	4609	1217	1373	24			
1	C	895	Total	C	N	O	S	0	0	0
			7223	4609	1217	1373	24			
1	E	892	Total	C	N	O	S	0	0	0
			7211	4603	1214	1370	24			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	964	GLY	-	expression tag	UNP P15144
A	965	HIS	-	expression tag	UNP P15144
A	966	HIS	-	expression tag	UNP P15144
A	967	HIS	-	expression tag	UNP P15144
A	968	HIS	-	expression tag	UNP P15144
A	969	HIS	-	expression tag	UNP P15144
A	970	HIS	-	expression tag	UNP P15144
C	964	GLY	-	expression tag	UNP P15144
C	965	HIS	-	expression tag	UNP P15144
C	966	HIS	-	expression tag	UNP P15144
C	967	HIS	-	expression tag	UNP P15144
C	968	HIS	-	expression tag	UNP P15144
C	969	HIS	-	expression tag	UNP P15144
C	970	HIS	-	expression tag	UNP P15144
E	964	GLY	-	expression tag	UNP P15144
E	965	HIS	-	expression tag	UNP P15144
E	966	HIS	-	expression tag	UNP P15144
E	967	HIS	-	expression tag	UNP P15144
E	968	HIS	-	expression tag	UNP P15144
E	969	HIS	-	expression tag	UNP P15144
E	970	HIS	-	expression tag	UNP P15144

- Molecule 2 is a protein called Spike protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	103	Total	C	N	O	S	0	0	0
			813	511	134	157	11			
2	D	103	Total	C	N	O	S	0	0	0
			813	511	134	157	11			
2	F	103	Total	C	N	O	S	0	0	0
			813	511	134	157	11			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	420	GLY	-	expression tag	UNP A0A4P8D758
B	421	HIS	-	expression tag	UNP A0A4P8D758
B	422	HIS	-	expression tag	UNP A0A4P8D758
B	423	HIS	-	expression tag	UNP A0A4P8D758
B	424	HIS	-	expression tag	UNP A0A4P8D758
B	425	HIS	-	expression tag	UNP A0A4P8D758
B	426	HIS	-	expression tag	UNP A0A4P8D758
D	420	GLY	-	expression tag	UNP A0A4P8D758
D	421	HIS	-	expression tag	UNP A0A4P8D758
D	422	HIS	-	expression tag	UNP A0A4P8D758
D	423	HIS	-	expression tag	UNP A0A4P8D758
D	424	HIS	-	expression tag	UNP A0A4P8D758
D	425	HIS	-	expression tag	UNP A0A4P8D758
D	426	HIS	-	expression tag	UNP A0A4P8D758
F	420	GLY	-	expression tag	UNP A0A4P8D758
F	421	HIS	-	expression tag	UNP A0A4P8D758
F	422	HIS	-	expression tag	UNP A0A4P8D758
F	423	HIS	-	expression tag	UNP A0A4P8D758
F	424	HIS	-	expression tag	UNP A0A4P8D758
F	425	HIS	-	expression tag	UNP A0A4P8D758
F	426	HIS	-	expression tag	UNP A0A4P8D758

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

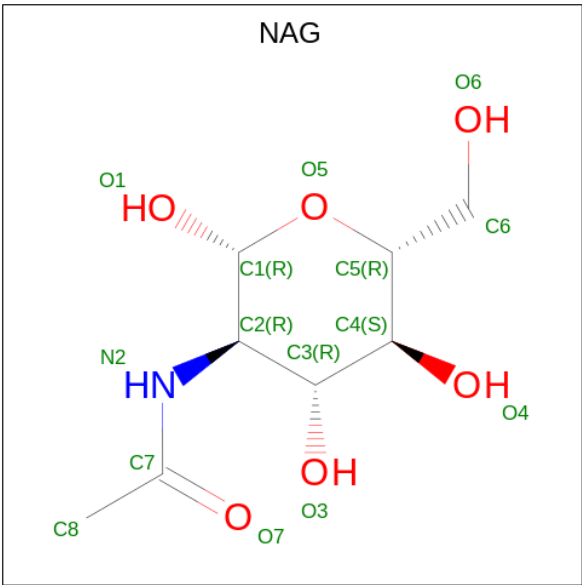


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



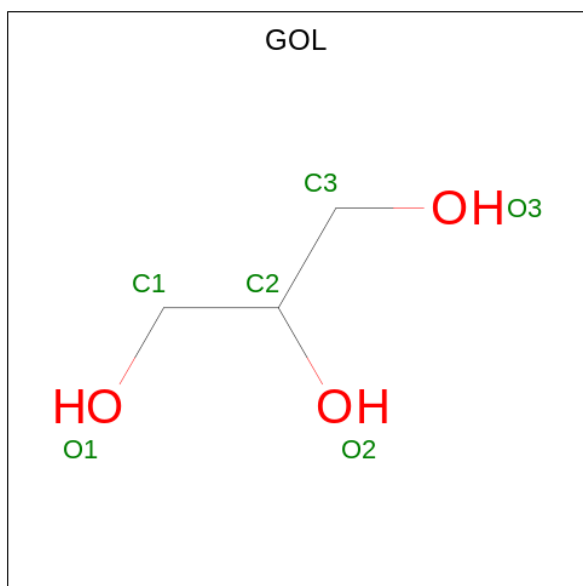
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).

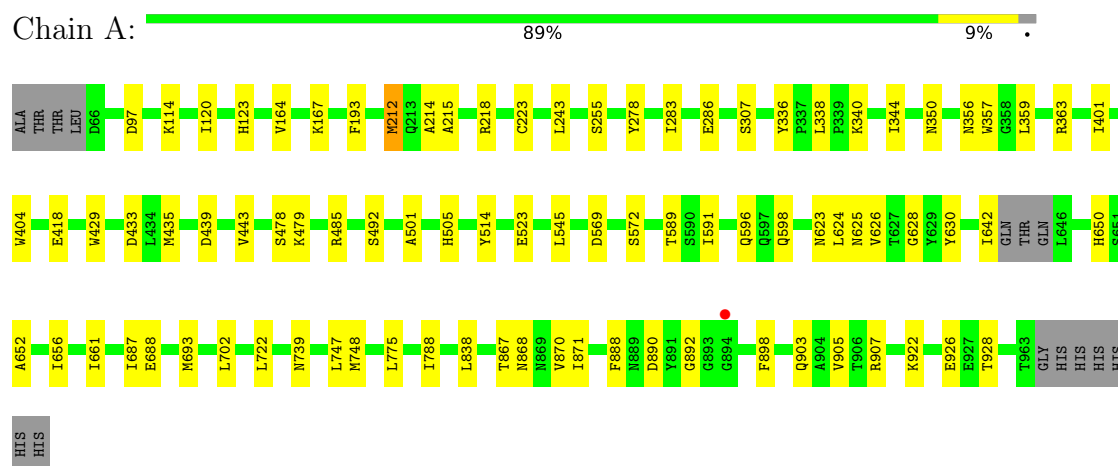


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

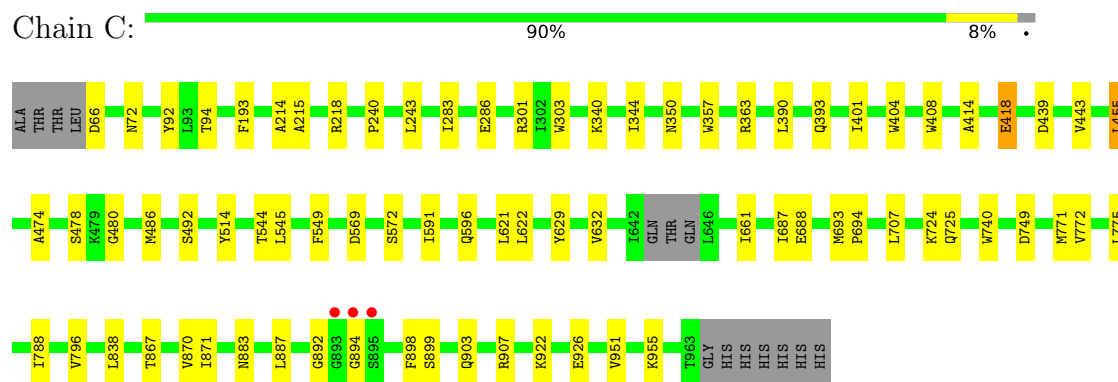
### 3 Residue-property plots

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.

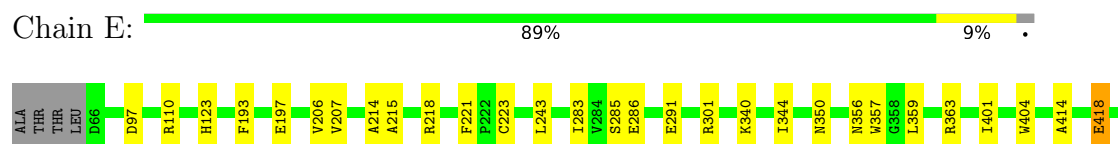
#### • Molecule 1: Aminopeptidase N

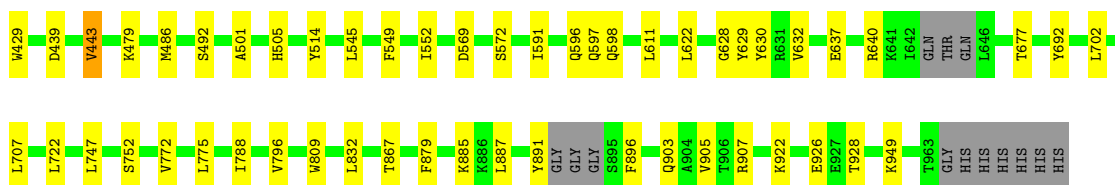


#### • Molecule 1: Aminopeptidase N

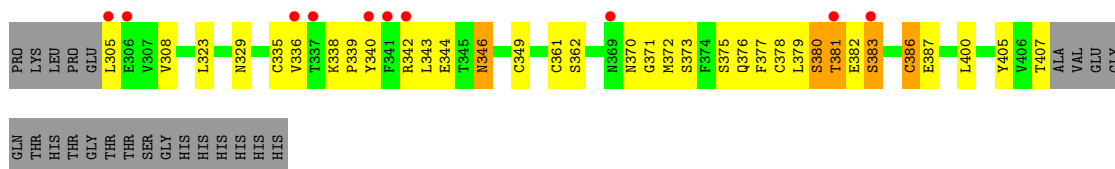


#### • Molecule 1: Aminopeptidase N

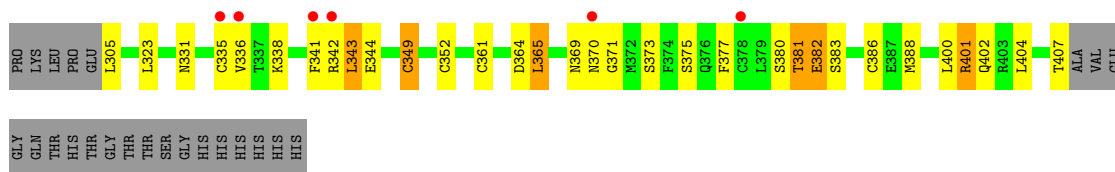




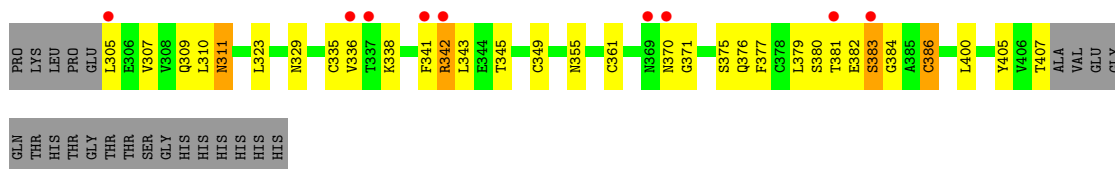
- Molecule 2: Spike protein



- Molecule 2: Spike protein



- Molecule 2: Spike protein



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



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





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

Chain J:  50% 50%



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

Chain K:  100%



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

Chain L:  50% 50%



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

Chain I:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.22Å 347.69Å 255.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 3.10 49.36 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.36-3.10) 99.0 (49.36-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.259 , 0.278 0.262 , 0.280	Depositor DCC
$R_{free}$ test set	8137 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.6	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , -0.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.287 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.328 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	24537	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ZN, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/7410	0.47	0/10093
1	C	0.25	0/7410	0.47	0/10093
1	E	0.25	0/7397	0.47	0/10075
2	B	0.26	0/827	0.54	0/1120
2	D	0.25	0/827	0.53	0/1120
2	F	0.26	0/827	0.56	0/1120
All	All	0.25	0/24698	0.48	0/33621

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7223	0	6985	42	0
1	C	7223	0	6984	43	0
1	E	7211	0	6975	40	0
2	B	813	0	786	18	0
2	D	813	0	786	15	0
2	F	813	0	785	13	0
3	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	1	0
4	I	28	0	25	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	A	70	0	65	1	0
6	B	14	0	13	2	0
6	C	70	0	65	0	0
6	D	14	0	13	0	0
6	E	70	0	65	1	0
6	F	14	0	13	0	0
7	A	6	0	8	0	0
7	C	6	0	8	0	0
7	E	6	0	8	0	0
All	All	24537	0	23709	167	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 (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:LEU:HD11	2:B:383:SER:HB3	1.63	0.79
2:F:377:PHE:HB2	2:F:407:THR:HB	1.72	0.72
2:F:311:ASN:N	2:F:311:ASN:OD1	2.23	0.71
1:C:892:GLY:HA2	1:C:898:PHE:HE2	1.58	0.69
1:E:443:VAL:HG21	1:E:479:LYS:HB2	1.72	0.69
2:F:379:LEU:HD11	2:F:383:SER:HB3	1.75	0.69
1:A:838:LEU:HD23	1:C:870:VAL:HG22	1.76	0.67
2:B:305:LEU:HA	2:B:338:LYS:HG2	1.77	0.67
1:A:892:GLY:HA2	1:A:898:PHE:HE2	1.62	0.65
1:E:637:GLU:OE2	1:E:640:ARG:NH2	2.28	0.64
1:C:443:VAL:HG13	1:C:478:SER:HB2	1.80	0.64
1:A:775:LEU:HG	1:A:788:ILE:HG12	1.81	0.62
1:A:350:ASN:O	1:A:363:ARG:NH1	2.31	0.62
1:C:243:LEU:HD22	1:C:286:GLU:HG3	1.83	0.61
1:A:443:VAL:HG13	1:A:478:SER:HB2	1.82	0.61
2:F:305:LEU:HA	2:F:338:LYS:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:PHE:HB2	2:B:407:THR:HB	1.84	0.60
2:B:380:SER:OG	2:B:381:THR:N	2.34	0.60
1:E:350:ASN:O	1:E:363:ARG:NH1	2.34	0.60
1:A:870:VAL:HG22	1:C:838:LEU:HD23	1.84	0.59
2:D:323:LEU:HB2	2:D:400:LEU:HD13	1.84	0.59
1:C:350:ASN:O	1:C:363:ARG:NH1	2.36	0.58
2:F:380:SER:O	2:F:382:GLU:N	2.33	0.57
2:D:380:SER:O	2:D:382:GLU:N	2.29	0.57
2:F:323:LEU:HB2	2:F:400:LEU:HD13	1.86	0.57
1:C:455:LEU:HD23	1:C:544:THR:HG23	1.87	0.57
1:C:622:LEU:HB2	1:C:632:VAL:HG11	1.87	0.56
2:D:335:CYS:HB3	2:D:377:PHE:CE1	2.41	0.56
1:C:301:ARG:HE	1:C:303:TRP:HE1	1.54	0.55
2:F:309:GLN:N	2:F:329:ASN:OD1	2.29	0.55
1:E:486:MET:HG3	1:E:628:GLY:HA2	1.89	0.55
1:C:514:TYR:CZ	1:C:545:LEU:HD21	2.43	0.54
1:C:621:LEU:HD21	1:C:661:ILE:HD11	1.90	0.53
1:A:626:VAL:HG23	1:A:656:ILE:HG22	1.90	0.53
1:C:215:ALA:HB1	1:C:218:ARG:CZ	2.40	0.52
1:A:255:SER:OG	6:A:1005:NAG:O7	2.24	0.52
1:E:775:LEU:HG	1:E:788:ILE:HG12	1.91	0.52
1:E:591:ILE:HG22	1:E:596:GLN:HA	1.91	0.52
1:C:408:TRP:CD2	1:C:455:LEU:HD21	2.46	0.51
1:C:724:LYS:NZ	1:C:725:GLN:OE1	2.43	0.51
1:A:903:GLN:O	1:A:907:ARG:HG3	2.11	0.50
2:F:310:LEU:HD23	2:F:345:THR:HG22	1.93	0.50
2:F:335:CYS:HB3	2:F:377:PHE:CE1	2.46	0.50
1:A:867:THR:HG21	1:A:905:VAL:HA	1.94	0.49
1:A:215:ALA:HB1	1:A:218:ARG:CZ	2.42	0.49
1:A:501:ALA:O	1:A:505:HIS:ND1	2.44	0.49
1:C:240:PRO:HB2	1:C:243:LEU:HG	1.95	0.49
1:E:215:ALA:HB1	1:E:218:ARG:CZ	2.43	0.49
1:C:687:ILE:HG23	1:C:688:GLU:HG2	1.95	0.49
1:E:891:TYR:HB3	1:E:896:PHE:HB2	1.95	0.48
1:C:455:LEU:HD11	1:C:480:GLY:HA2	1.95	0.48
1:C:903:GLN:O	1:C:907:ARG:HG3	2.13	0.48
1:A:514:TYR:CZ	1:A:545:LEU:HD21	2.48	0.48
2:F:307:VAL:HG13	2:F:342:ARG:HE	1.78	0.48
1:A:439:ASP:O	1:A:443:VAL:HG22	2.14	0.48
1:A:591:ILE:HG22	1:A:596:GLN:HA	1.95	0.47
1:A:283:ILE:HD13	1:A:344:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ASP:HB3	1:A:693:MET:HE1	1.96	0.47
1:A:243:LEU:HD22	1:A:286:GLU:HG3	1.95	0.47
1:E:569:ASP:OD2	1:E:949:LYS:NZ	2.48	0.47
1:A:702:LEU:HD13	1:A:722:LEU:HD21	1.95	0.47
1:E:283:ILE:HD13	1:E:344:ILE:HD13	1.96	0.47
1:E:501:ALA:O	1:E:505:HIS:ND1	2.48	0.47
1:E:549:PHE:HB3	1:E:629:TYR:CE2	2.50	0.47
2:B:308:VAL:HA	2:B:329:ASN:ND2	2.30	0.47
1:E:867:THR:HG21	1:E:905:VAL:HA	1.97	0.47
1:E:514:TYR:CZ	1:E:545:LEU:HD21	2.50	0.47
1:C:443:VAL:HG12	1:C:474:ALA:HB1	1.97	0.46
1:E:243:LEU:HD22	1:E:286:GLU:HG3	1.97	0.46
1:E:414:ALA:O	1:E:418:GLU:HB3	2.16	0.46
1:C:439:ASP:O	1:C:443:VAL:HG22	2.16	0.46
2:D:305:LEU:HA	2:D:338:LYS:HB2	1.97	0.46
1:E:110:ARG:NH2	3:L:1:NAG:O3	2.48	0.46
1:E:885:LYS:HD2	1:E:928:THR:HG21	1.97	0.46
1:C:591:ILE:HG22	1:C:596:GLN:HA	1.96	0.46
2:B:387:GLU:HB3	2:B:405:TYR:CD1	2.50	0.46
1:C:922:LYS:O	1:C:926:GLU:HG2	2.15	0.46
1:C:887:LEU:HD22	1:C:898:PHE:HE1	1.81	0.46
2:D:388:MET:HE2	2:D:404:LEU:HD23	1.97	0.46
2:F:305:LEU:N	2:F:336:VAL:HA	2.31	0.46
2:B:346:ASN:ND2	6:B:501:NAG:H62	2.31	0.45
1:E:922:LYS:O	1:E:926:GLU:HG2	2.17	0.45
1:C:951:VAL:O	1:C:955:LYS:HB2	2.16	0.45
1:C:707:LEU:HD13	1:C:907:ARG:HB3	1.98	0.45
1:C:775:LEU:HG	1:C:788:ILE:HG12	1.98	0.45
1:E:439:ASP:O	1:E:443:VAL:HG12	2.16	0.45
1:E:677:THR:OG1	6:E:1002:NAG:H82	2.17	0.45
1:A:868:ASN:OD1	1:A:907:ARG:NH2	2.50	0.45
2:D:361:CYS:SG	2:D:386:CYS:HB3	2.57	0.45
1:E:569:ASP:HB3	1:E:572:SER:OG	2.17	0.45
1:A:871:ILE:HD12	1:C:871:ILE:HD12	1.99	0.44
1:E:903:GLN:O	1:E:907:ARG:HG3	2.16	0.44
1:A:628:GLY:HA3	1:A:630:TYR:CE1	2.51	0.44
1:A:922:LYS:O	1:A:926:GLU:HG2	2.17	0.44
1:E:291:GLU:HB3	1:E:301:ARG:HG2	1.99	0.44
1:A:435:MET:HE3	1:A:485:ARG:HH11	1.83	0.44
2:B:342:ARG:NH2	2:B:344:GLU:OE1	2.50	0.44
1:E:622:LEU:HB2	1:E:632:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ILE:HG21	1:A:661:ILE:HD13	2.00	0.44
1:A:589:THR:O	1:A:623:ASN:N	2.51	0.44
1:C:66:ASP:O	1:C:72:ASN:ND2	2.41	0.44
2:D:343:LEU:HD12	2:D:343:LEU:HA	1.89	0.44
1:A:429:TRP:CD2	1:A:747:LEU:HD22	2.53	0.44
1:E:429:TRP:CD2	1:E:747:LEU:HD22	2.53	0.44
1:E:702:LEU:HD13	1:E:722:LEU:HD21	2.00	0.44
2:D:342:ARG:O	2:D:343:LEU:HB2	2.18	0.43
1:A:120:ILE:HB	1:A:164:VAL:HB	2.00	0.43
2:B:339:PRO:HG2	2:B:340:TYR:CD1	2.52	0.43
2:B:370:ASN:O	2:B:372:MET:HG2	2.19	0.43
2:B:342:ARG:HH21	2:B:344:GLU:HB2	1.83	0.43
2:D:377:PHE:HB2	2:D:407:THR:HB	2.01	0.43
1:E:597:GLN:HB3	1:E:611:LEU:HD22	1.99	0.43
1:A:598:GLN:H	1:A:598:GLN:HG3	1.57	0.43
1:A:624:LEU:HD12	1:A:625:ASN:H	1.83	0.43
2:B:361:CYS:SG	2:B:386:CYS:HB3	2.58	0.43
2:D:364:ASP:OD1	2:D:365:LEU:N	2.50	0.43
2:B:380:SER:O	2:B:405:TYR:HD2	2.01	0.43
1:E:123:HIS:HB2	1:E:223:CYS:O	2.19	0.43
1:C:486:MET:HB3	1:C:486:MET:HE2	1.90	0.43
1:C:569:ASP:HB3	1:C:572:SER:OG	2.19	0.43
2:D:382:GLU:HB2	2:D:383:SER:H	1.60	0.43
1:A:401:ILE:HD12	1:A:404:TRP:HA	2.01	0.43
2:B:305:LEU:N	2:B:336:VAL:HA	2.33	0.43
2:B:346:ASN:HD22	6:B:501:NAG:H62	1.83	0.43
1:C:772:VAL:HG12	1:C:796:VAL:HG22	2.01	0.42
1:C:693:MET:HB3	1:C:694:PRO:HD3	2.00	0.42
2:F:384:GLY:HA2	2:F:405:TYR:HB3	2.00	0.42
2:D:349:CYS:HB3	2:D:352:CYS:O	2.19	0.42
1:E:197:GLU:HG2	1:E:206:VAL:HG22	2.00	0.42
1:C:749:ASP:OD2	2:D:401:ARG:NH1	2.32	0.42
1:A:569:ASP:HB3	1:A:572:SER:OG	2.20	0.42
2:B:343:LEU:O	2:B:344:GLU:HB3	2.20	0.42
1:E:207:VAL:HG13	1:E:285:SER:HB3	2.01	0.42
1:E:692:TYR:HB2	1:E:752:SER:HB2	2.01	0.42
2:F:361:CYS:HA	2:F:386:CYS:SG	2.60	0.42
1:C:740:TRP:CZ3	1:C:771:MET:HG3	2.55	0.41
1:A:443:VAL:HG11	1:A:479:LYS:N	2.35	0.41
1:C:92:TYR:O	1:C:94:THR:N	2.52	0.41
1:C:401:ILE:HD12	1:C:404:TRP:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:336:VAL:HG11	2:D:341:PHE:CD1	2.56	0.41
1:E:772:VAL:HG12	1:E:796:VAL:HG22	2.03	0.41
1:A:336:TYR:CE2	1:A:338:LEU:HB2	2.56	0.41
1:A:356:ASN:HB2	1:A:359:LEU:O	2.19	0.41
1:C:892:GLY:HA2	1:C:898:PHE:CE2	2.46	0.41
1:E:879:PHE:CE2	1:E:887:LEU:HD11	2.55	0.41
1:C:549:PHE:HB3	1:C:629:TYR:CE2	2.56	0.41
1:E:401:ILE:HD12	1:E:404:TRP:HA	2.03	0.41
1:A:123:HIS:HB2	1:A:223:CYS:O	2.20	0.41
1:E:356:ASN:HB2	1:E:359:LEU:O	2.20	0.41
1:A:212:MET:HB3	1:A:278:TYR:HA	2.02	0.41
1:C:283:ILE:HD13	1:C:344:ILE:HD13	2.02	0.41
1:A:687:ILE:HG23	1:A:688:GLU:HG2	2.02	0.41
2:B:323:LEU:HB2	2:B:400:LEU:HD13	2.03	0.41
1:C:414:ALA:O	1:C:418:GLU:HB3	2.21	0.41
1:C:883:ASN:O	1:C:887:LEU:HB2	2.21	0.41
1:C:892:GLY:C	1:C:894:GLY:H	2.24	0.41
1:E:809:TRP:CE2	1:E:832:LEU:HD22	2.55	0.41
1:A:888:PHE:HA	1:A:898:PHE:CZ	2.56	0.40
1:E:552:ILE:HD12	1:E:630:TYR:CD2	2.56	0.40
1:A:114:LYS:HA	1:A:114:LYS:HD3	1.87	0.40
1:A:167:LYS:HD3	1:A:167:LYS:HA	1.89	0.40
1:C:390:LEU:HA	1:C:393:GLN:HG2	2.03	0.40
2:D:369:ASN:O	2:D:370:ASN:HB2	2.21	0.40
1:E:707:LEU:HD13	1:E:907:ARG:HB3	2.04	0.40
1:A:650:HIS:NE2	1:A:652:ALA:HB2	2.37	0.40
2:B:346:ASN:OD1	2:B:346:ASN:N	2.54	0.40
1:E:221:PHE:CE2	1:E:223:CYS:HB3	2.56	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	891/909 (98%)	853 (96%)	36 (4%)	2 (0%)	47 79
1	C	891/909 (98%)	850 (95%)	38 (4%)	3 (0%)	41 73
1	E	886/909 (98%)	854 (96%)	30 (3%)	2 (0%)	47 79
2	B	101/127 (80%)	82 (81%)	15 (15%)	4 (4%)	3 17
2	D	101/127 (80%)	82 (81%)	14 (14%)	5 (5%)	2 13
2	F	101/127 (80%)	83 (82%)	14 (14%)	4 (4%)	3 17
All	All	2971/3108 (96%)	2804 (94%)	147 (5%)	20 (1%)	22 57

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	375	SER
2	B	380	SER
2	D	343	LEU
2	D	375	SER
2	B	371	GLY
1	C	899	SER
2	F	371	GLY
2	F	375	SER
2	F	383	SER
2	B	383	SER
2	D	371	GLY
1	C	214	ALA
1	E	214	ALA
1	A	492	SER
1	C	492	SER
2	F	370	ASN
1	A	214	ALA
2	D	344	GLU
2	D	381	THR
1	E	492	SER

### 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	793/805 (98%)	781 (98%)	12 (2%)	65	85
1	C	793/805 (98%)	787 (99%)	6 (1%)	81	92
1	E	793/805 (98%)	786 (99%)	7 (1%)	78	91
2	B	94/114 (82%)	84 (89%)	10 (11%)	6	26
2	D	94/114 (82%)	86 (92%)	8 (8%)	10	37
2	F	94/114 (82%)	85 (90%)	9 (10%)	8	31
All	All	2661/2757 (96%)	2609 (98%)	52 (2%)	55	80

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ASP
1	A	193	PHE
1	A	212	MET
1	A	307	SER
1	A	340	LYS
1	A	357	TRP
1	A	418	GLU
1	A	523	GLU
1	A	739	ASN
1	A	748	MET
1	A	890	ASP
1	A	928	THR
2	B	335	CYS
2	B	346	ASN
2	B	349	CYS
2	B	362	SER
2	B	373	SER
2	B	376	GLN
2	B	378	CYS
2	B	381	THR
2	B	382	GLU
2	B	386	CYS
1	C	193	PHE
1	C	340	LYS
1	C	357	TRP
1	C	418	GLU
1	C	455	LEU
1	C	867	THR
2	D	331	ASN
2	D	349	CYS

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Mol	Chain	Res	Type
2	D	365	LEU
2	D	373	SER
2	D	381	THR
2	D	382	GLU
2	D	401	ARG
2	D	402	GLN
1	E	97	ASP
1	E	193	PHE
1	E	340	LYS
1	E	357	TRP
1	E	418	GLU
1	E	443	VAL
1	E	598	GLN
2	F	311	ASN
2	F	341	PHE
2	F	342	ARG
2	F	343	LEU
2	F	349	CYS
2	F	355	ASN
2	F	376	GLN
2	F	381	THR
2	F	386	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

12 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
3	NAG	G	1	3,1	14,14,15	0.52	0	17,19,21	0.47	0
3	NAG	G	2	3	14,14,15	0.42	0	17,19,21	0.56	0
3	NAG	H	1	3,1	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	H	2	3	14,14,15	0.24	0	17,19,21	0.40	0
4	NAG	I	1	1,4	14,14,15	1.77	1 (7%)	17,19,21	1.50	3 (17%)
4	NAG	I	2	4	14,14,15	0.96	1 (7%)	17,19,21	0.57	0
3	NAG	J	1	3,1	14,14,15	0.32	0	17,19,21	0.52	0
3	NAG	J	2	3	14,14,15	0.60	1 (7%)	17,19,21	0.54	0
3	NAG	K	1	3,1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	K	2	3	14,14,15	0.19	0	17,19,21	0.47	0
3	NAG	L	1	3,1	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	L	2	3	14,14,15	0.32	0	17,19,21	0.53	0

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	NAG	O5-C1	-6.23	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2	NAG	C1-C2	3.32	1.57	1.52
3	J	2	NAG	C1-C2	2.03	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C3-C4-C5	3.55	116.56	110.24
4	I	1	NAG	C1-O5-C5	-3.33	107.68	112.19
4	I	1	NAG	C4-C3-C2	3.21	115.73	111.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

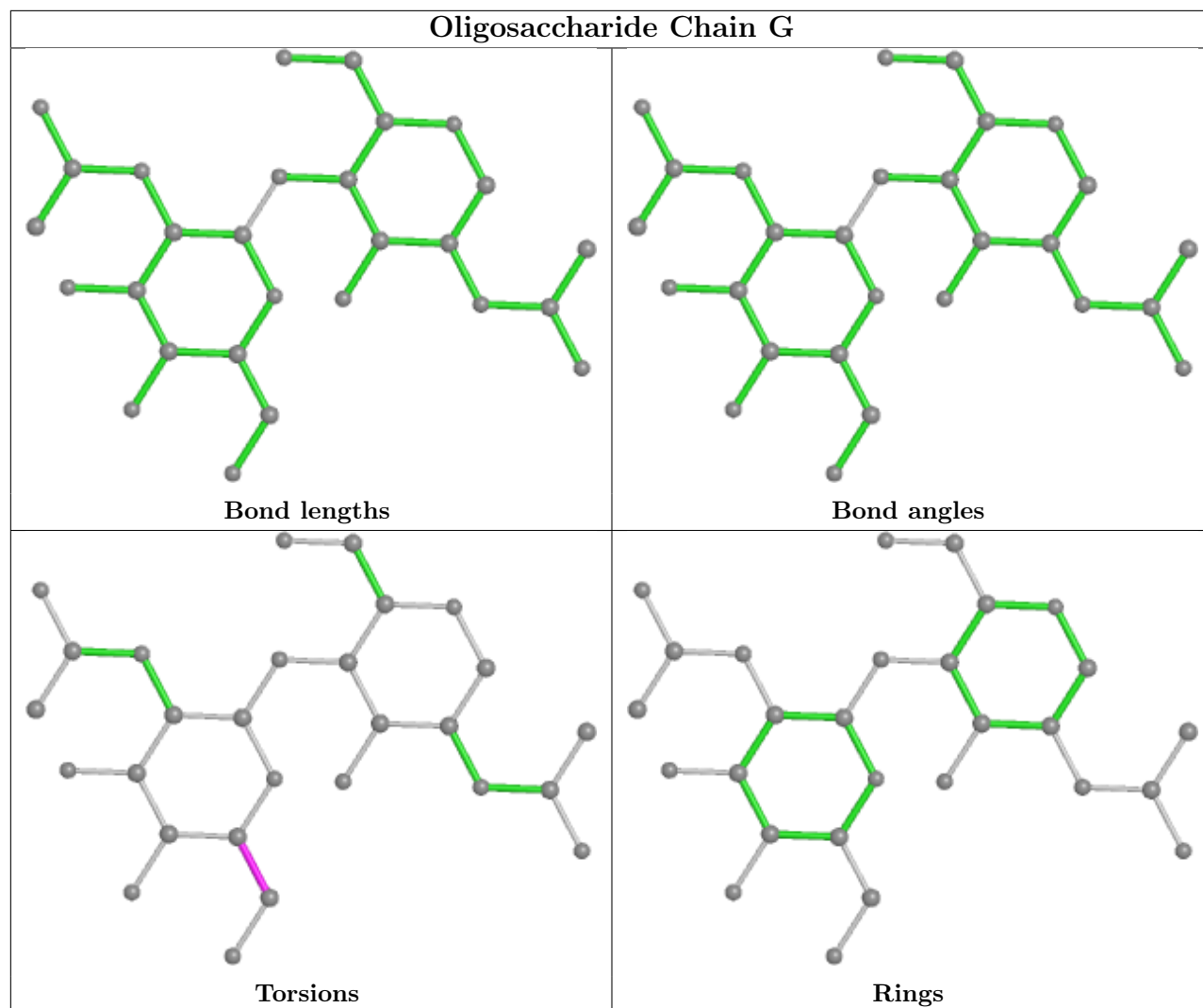
Mol	Chain	Res	Type	Atoms
3	J	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
4	I	2	NAG	C1-C2-N2-C7
3	K	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C3-C2-N2-C7

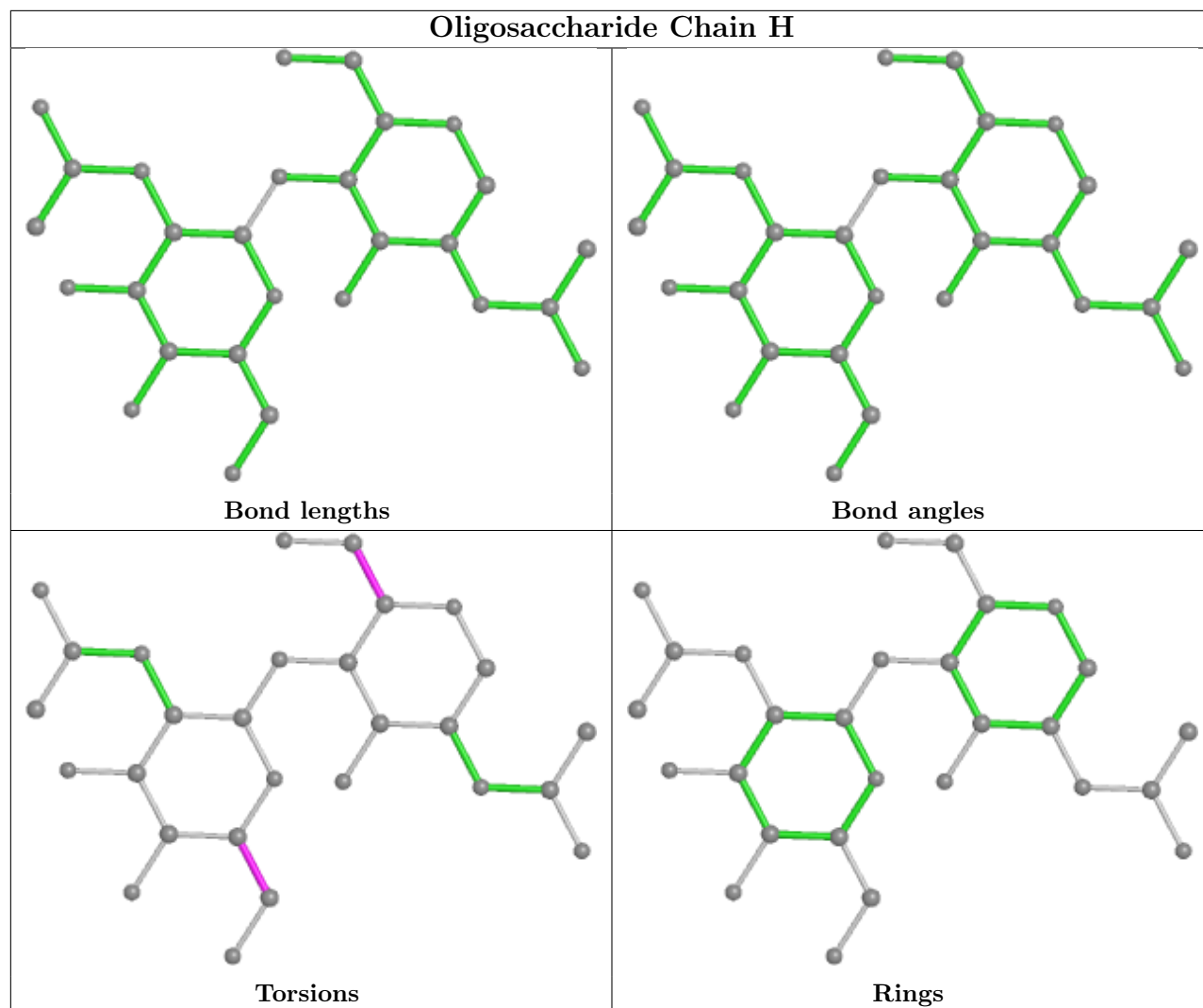
There are no ring outliers.

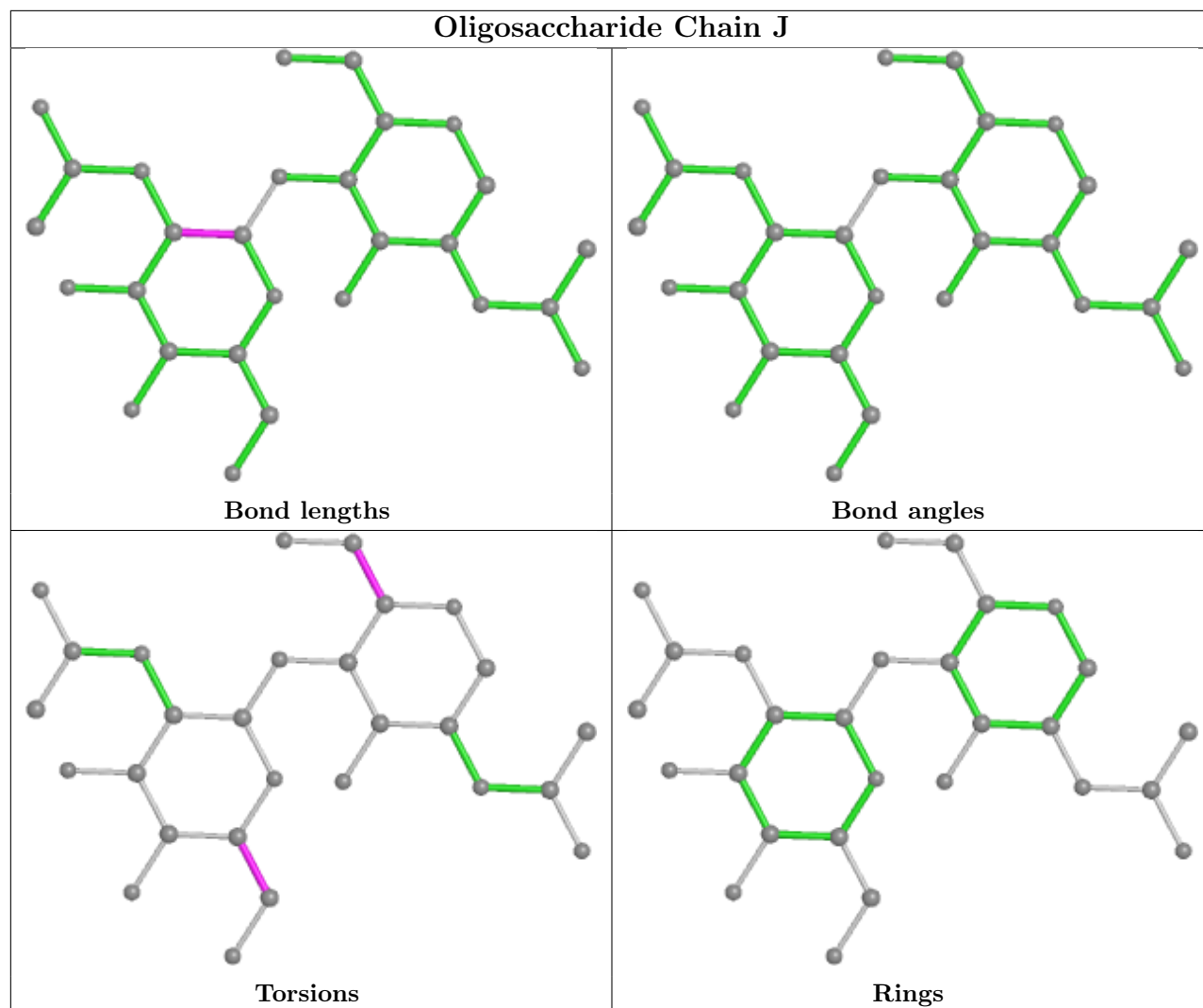
1 monomer is involved in 1 short contact:

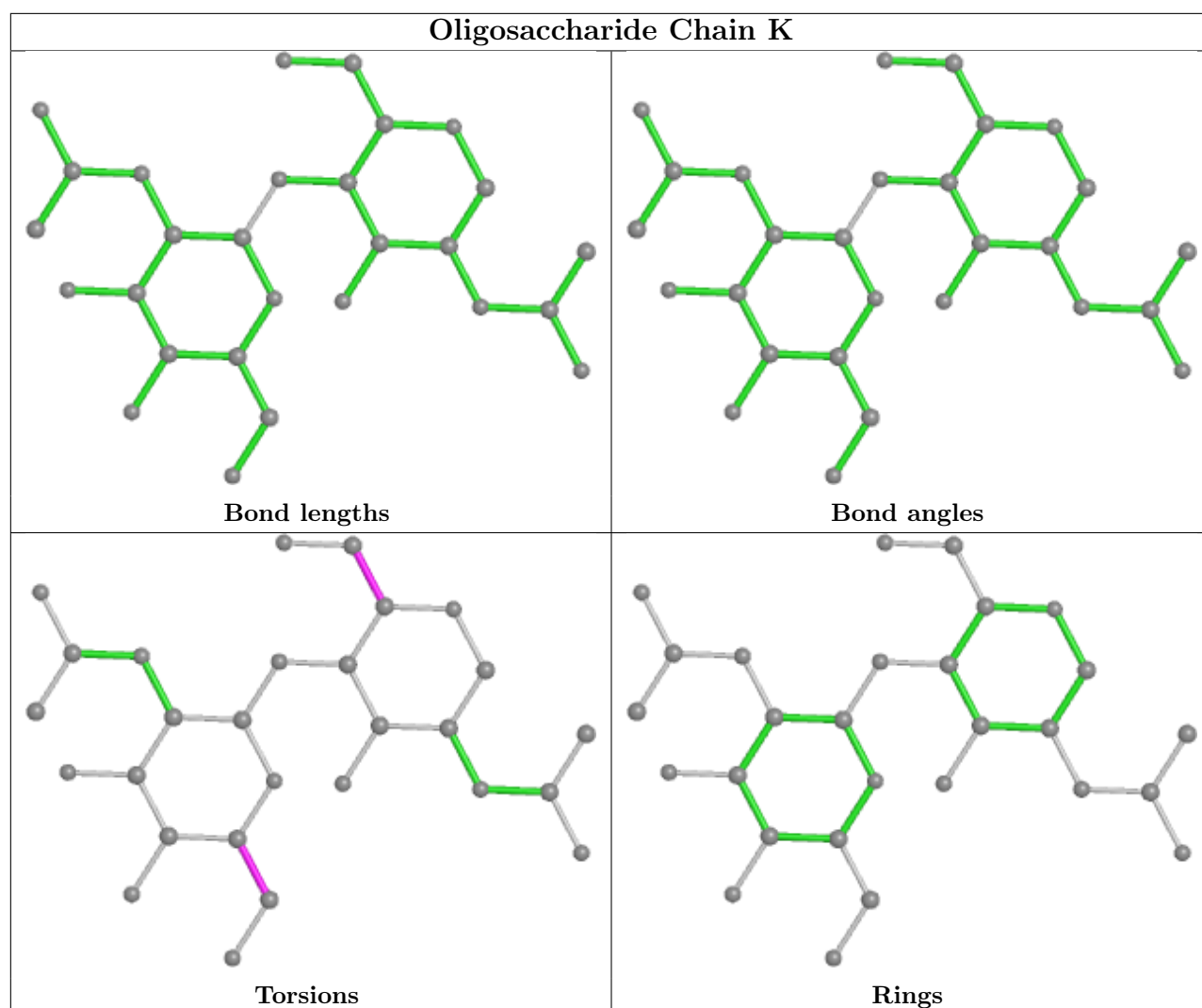
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1	NAG	1	0

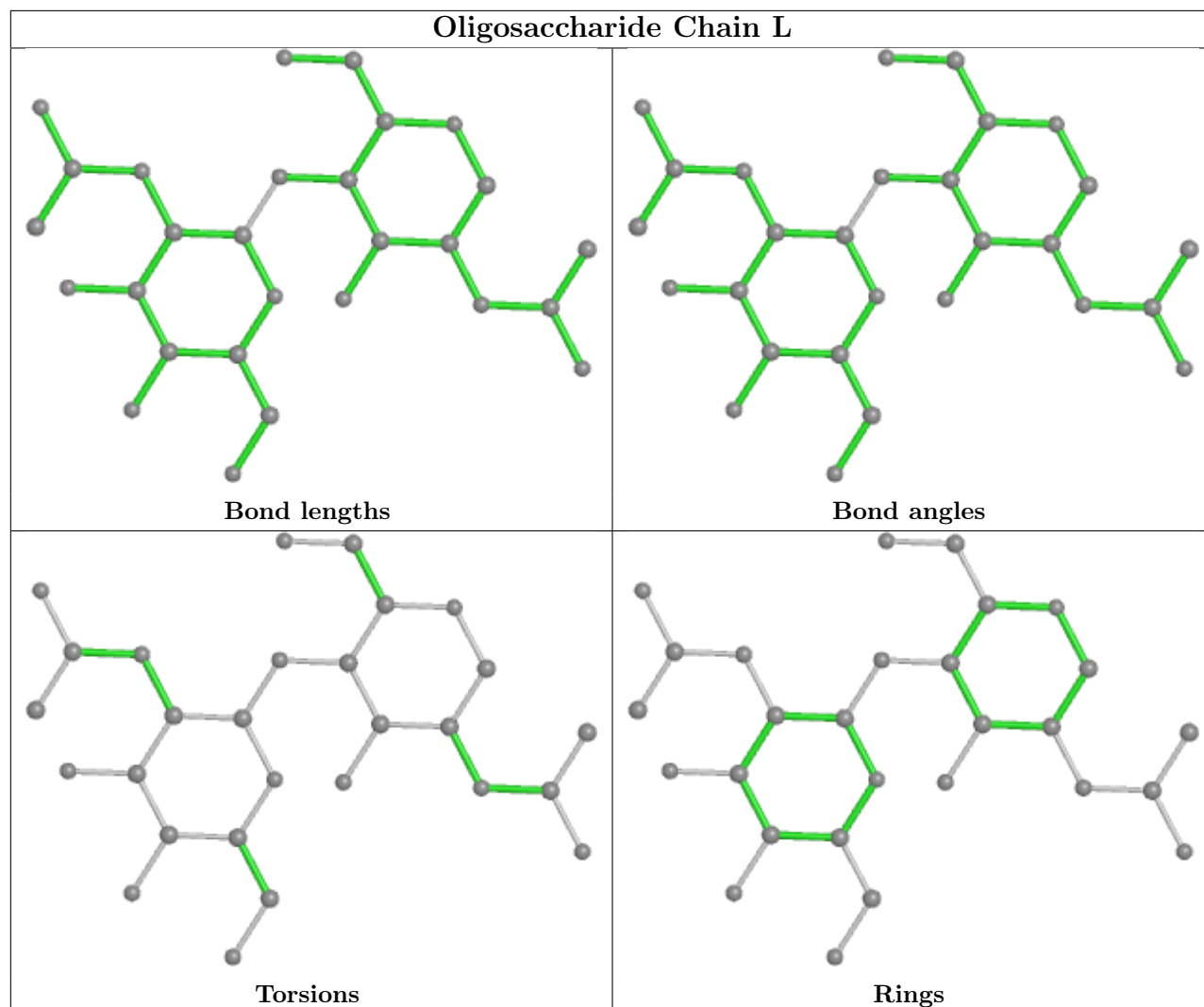
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

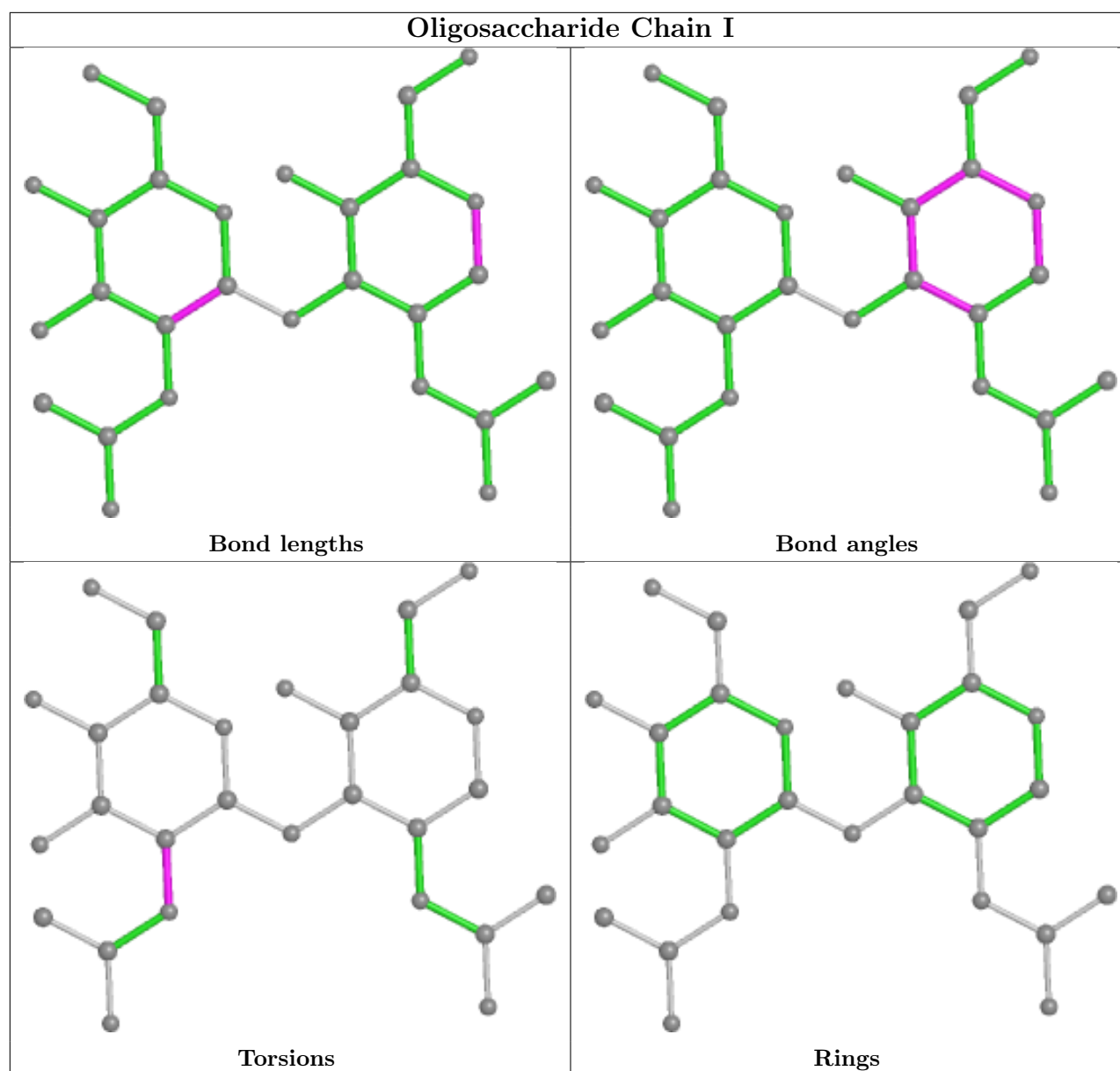












## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	C	1004	1	14,14,15	0.51	0	17,19,21	0.62	0
6	NAG	E	1004	1	14,14,15	0.74	1 (7%)	17,19,21	0.62	0
6	NAG	A	1002	1	14,14,15	0.48	0	17,19,21	0.56	0
6	NAG	A	1005	1	14,14,15	0.46	0	17,19,21	0.42	0
6	NAG	E	1003	1	14,14,15	0.62	1 (7%)	17,19,21	0.56	0
6	NAG	C	1003	1	14,14,15	1.00	2 (14%)	17,19,21	0.82	1 (5%)
6	NAG	D	501	2	14,14,15	0.28	0	17,19,21	0.45	0
6	NAG	C	1005	1	14,14,15	0.32	0	17,19,21	0.47	0
7	GOL	E	1007	-	5,5,5	0.83	0	5,5,5	1.08	0
6	NAG	E	1002	1	14,14,15	0.95	1 (7%)	17,19,21	1.29	1 (5%)
6	NAG	A	1006	1	14,14,15	0.40	0	17,19,21	0.41	0
6	NAG	B	501	2	14,14,15	0.21	0	17,19,21	0.50	0
6	NAG	C	1002	1	14,14,15	0.46	0	17,19,21	0.55	0
6	NAG	C	1006	1	14,14,15	1.19	1 (7%)	17,19,21	1.72	1 (5%)
6	NAG	E	1006	1	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	F	501	2	14,14,15	0.63	1 (7%)	17,19,21	0.68	0
7	GOL	C	1007	-	5,5,5	1.00	0	5,5,5	0.97	0
6	NAG	E	1005	1	14,14,15	0.46	0	17,19,21	0.43	0
6	NAG	A	1004	1	14,14,15	0.55	0	17,19,21	0.43	0
6	NAG	A	1003	1	14,14,15	0.39	0	17,19,21	0.45	0
7	GOL	A	1007	-	5,5,5	0.85	0	5,5,5	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1004	1	-	2/6/23/26	0/1/1/1
6	NAG	E	1004	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
6	NAG	E	1003	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1003	1	-	0/6/23/26	0/1/1/1
6	NAG	D	501	2	-	0/6/23/26	0/1/1/1
6	NAG	C	1005	1	-	2/6/23/26	0/1/1/1
7	GOL	E	1007	-	-	0/4/4/4	-
6	NAG	E	1002	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
6	NAG	B	501	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1002	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1006	1	-	0/6/23/26	0/1/1/1
6	NAG	E	1006	1	-	2/6/23/26	0/1/1/1
6	NAG	F	501	2	-	1/6/23/26	0/1/1/1
7	GOL	C	1007	-	-	0/4/4/4	-
6	NAG	E	1005	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
7	GOL	A	1007	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1006	NAG	O5-C1	4.36	1.50	1.43
6	E	1002	NAG	O5-C1	3.44	1.49	1.43
6	E	1004	NAG	O5-C1	-2.58	1.39	1.43
6	C	1003	NAG	O5-C1	-2.45	1.39	1.43
6	C	1003	NAG	C1-C2	2.37	1.55	1.52
6	F	501	NAG	O5-C1	-2.19	1.40	1.43
6	E	1003	NAG	C1-C2	2.05	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1006	NAG	C1-O5-C5	6.78	121.38	112.19
6	E	1002	NAG	C1-O5-C5	5.07	119.06	112.19
6	C	1003	NAG	C4-C3-C2	2.26	114.33	111.02

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1007	GOL	O1-C1-C2-C3
6	E	1006	NAG	O5-C5-C6-O6
6	C	1004	NAG	O5-C5-C6-O6
6	E	1006	NAG	C4-C5-C6-O6
6	C	1005	NAG	C4-C5-C6-O6
6	C	1004	NAG	C4-C5-C6-O6
6	A	1002	NAG	O5-C5-C6-O6
6	E	1005	NAG	C4-C5-C6-O6

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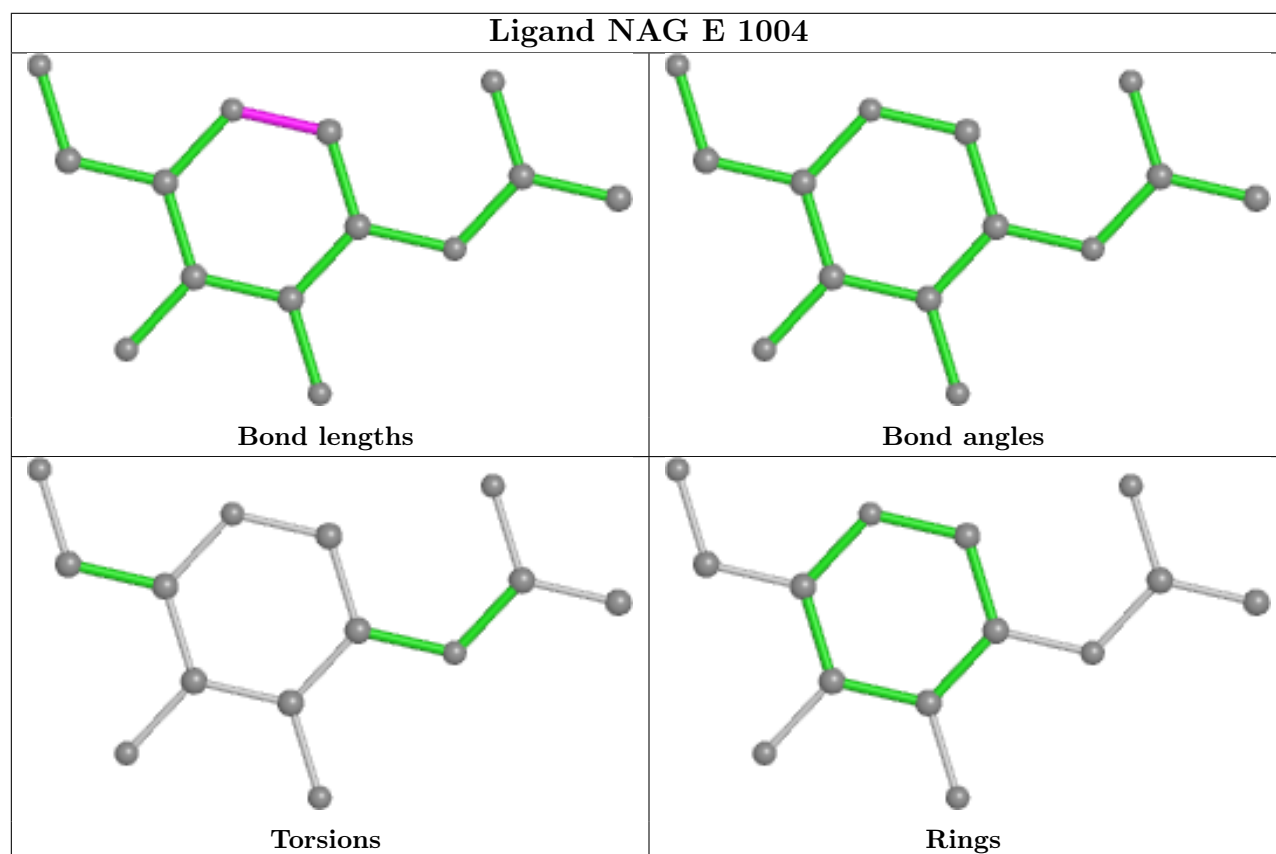
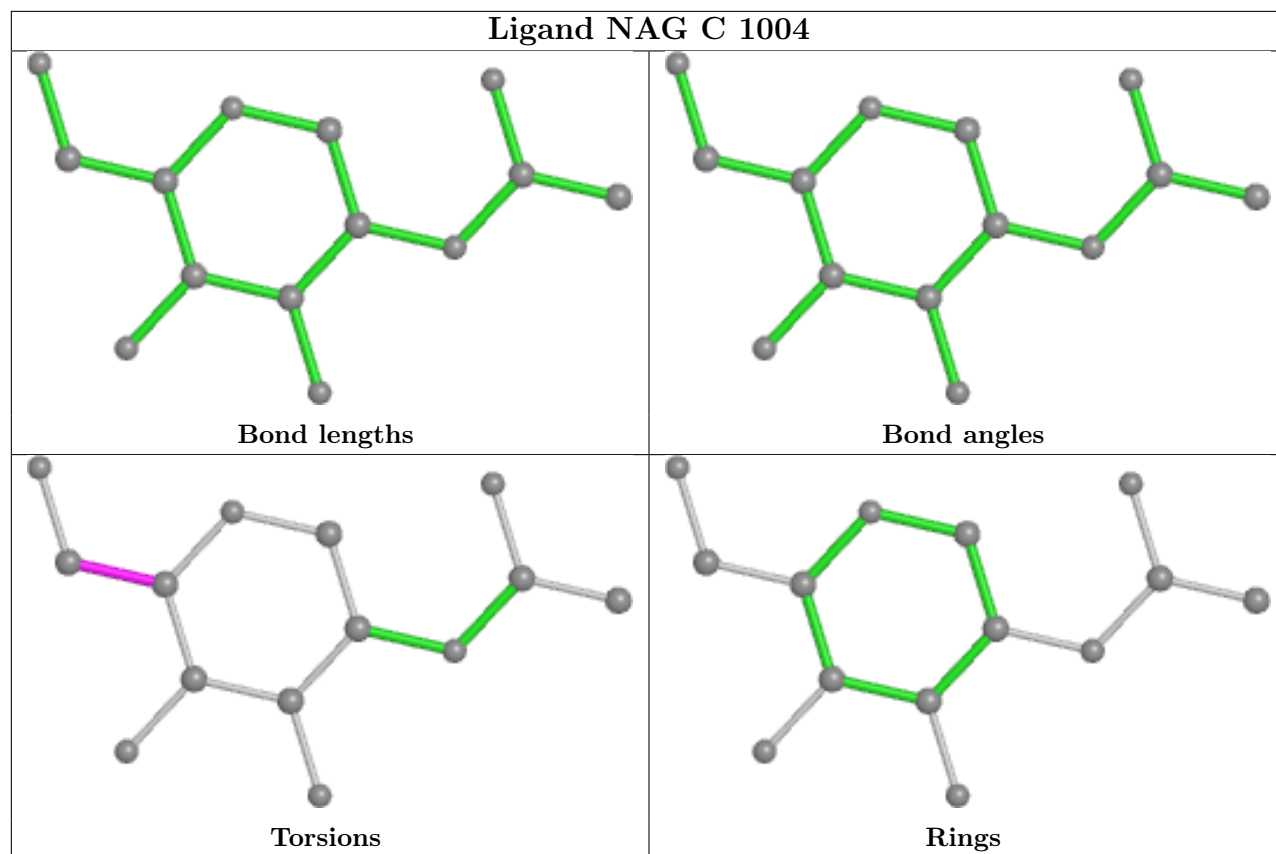
Mol	Chain	Res	Type	Atoms
6	C	1005	NAG	O5-C5-C6-O6
7	A	1007	GOL	O1-C1-C2-O2
6	E	1005	NAG	O5-C5-C6-O6
6	E	1002	NAG	C4-C5-C6-O6
6	A	1002	NAG	C4-C5-C6-O6
6	A	1004	NAG	C4-C5-C6-O6
6	F	501	NAG	C1-C2-N2-C7
6	A	1004	NAG	O5-C5-C6-O6
6	C	1002	NAG	O5-C5-C6-O6
6	E	1002	NAG	O5-C5-C6-O6

There are no ring outliers.

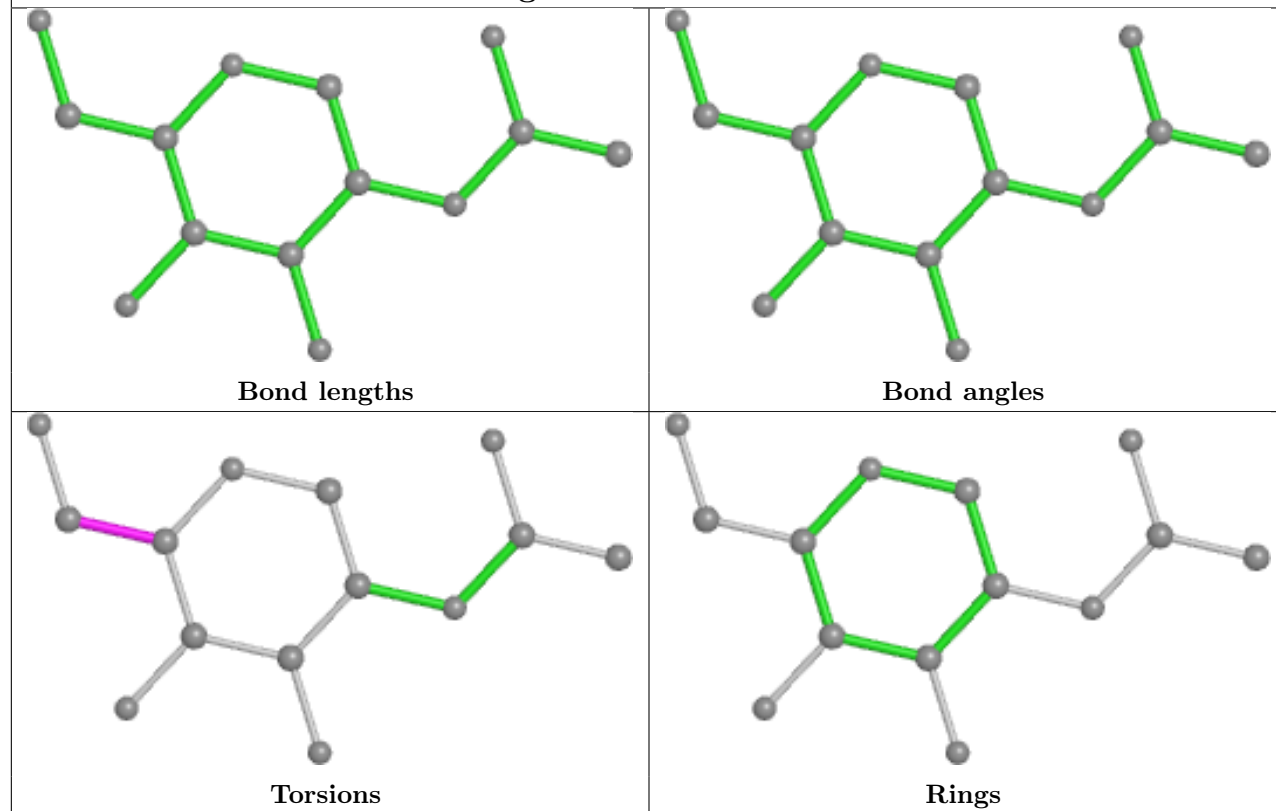
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1005	NAG	1	0
6	E	1002	NAG	1	0
6	B	501	NAG	2	0

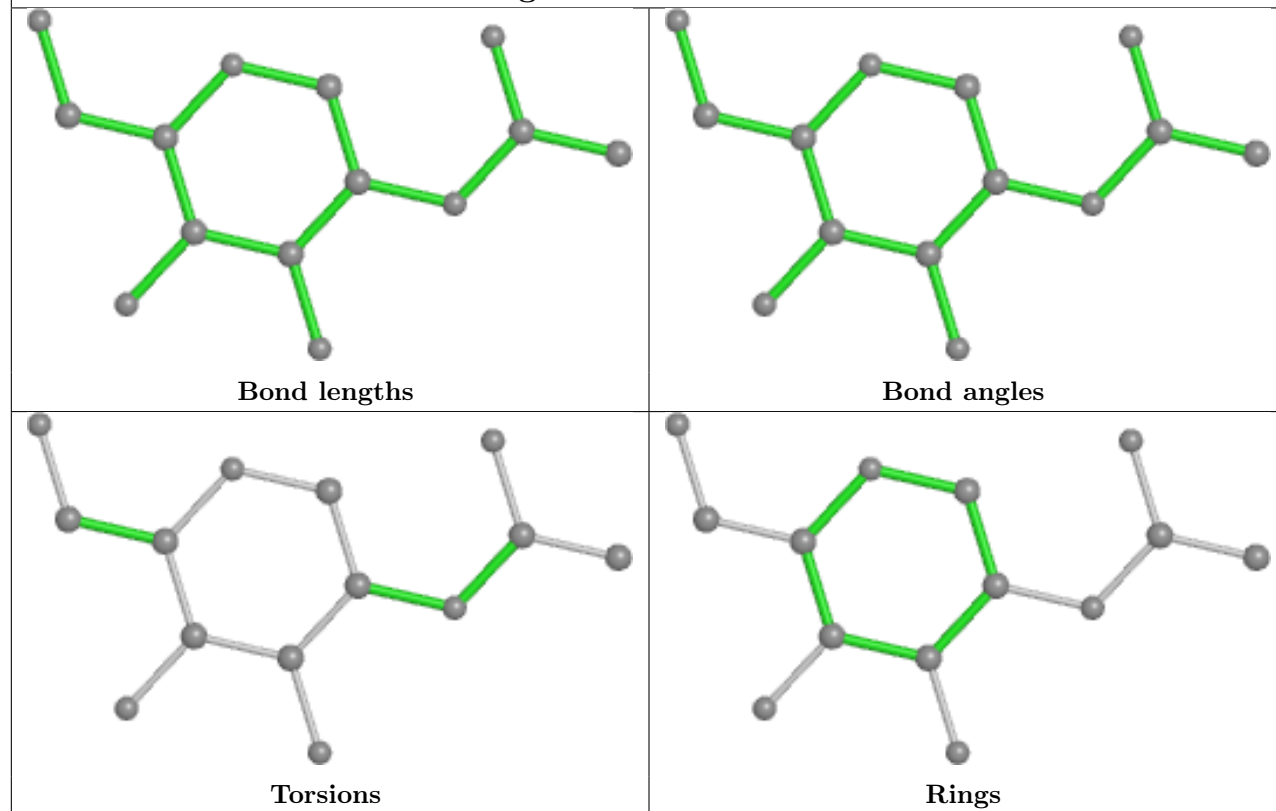
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



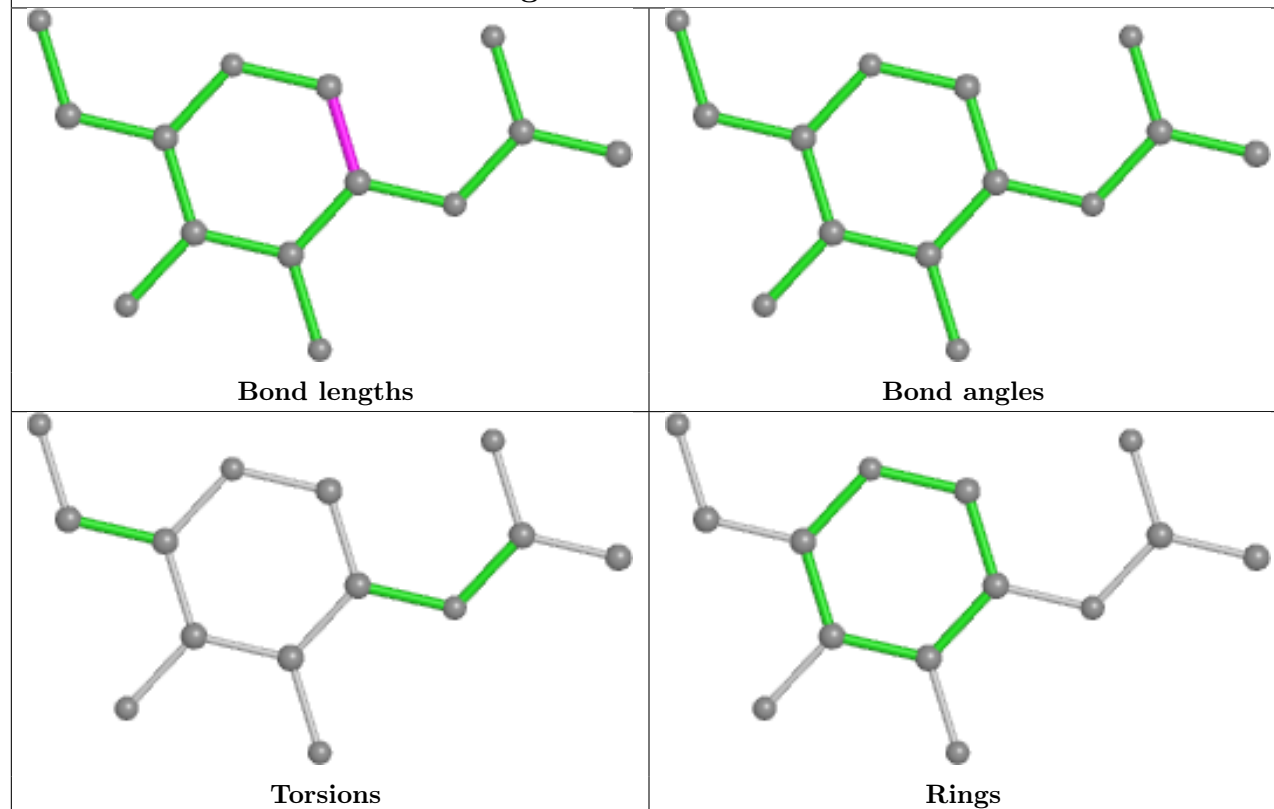
## Ligand NAG A 1002



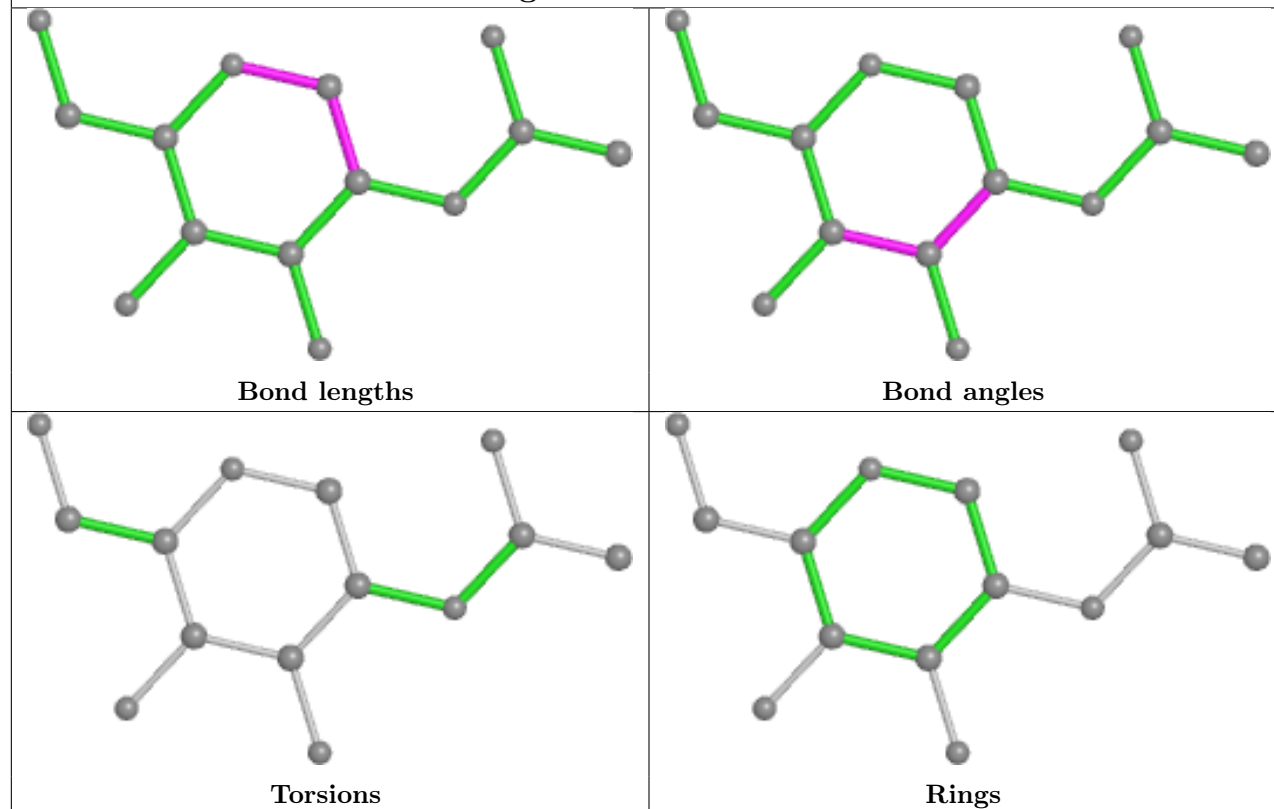
## Ligand NAG A 1005

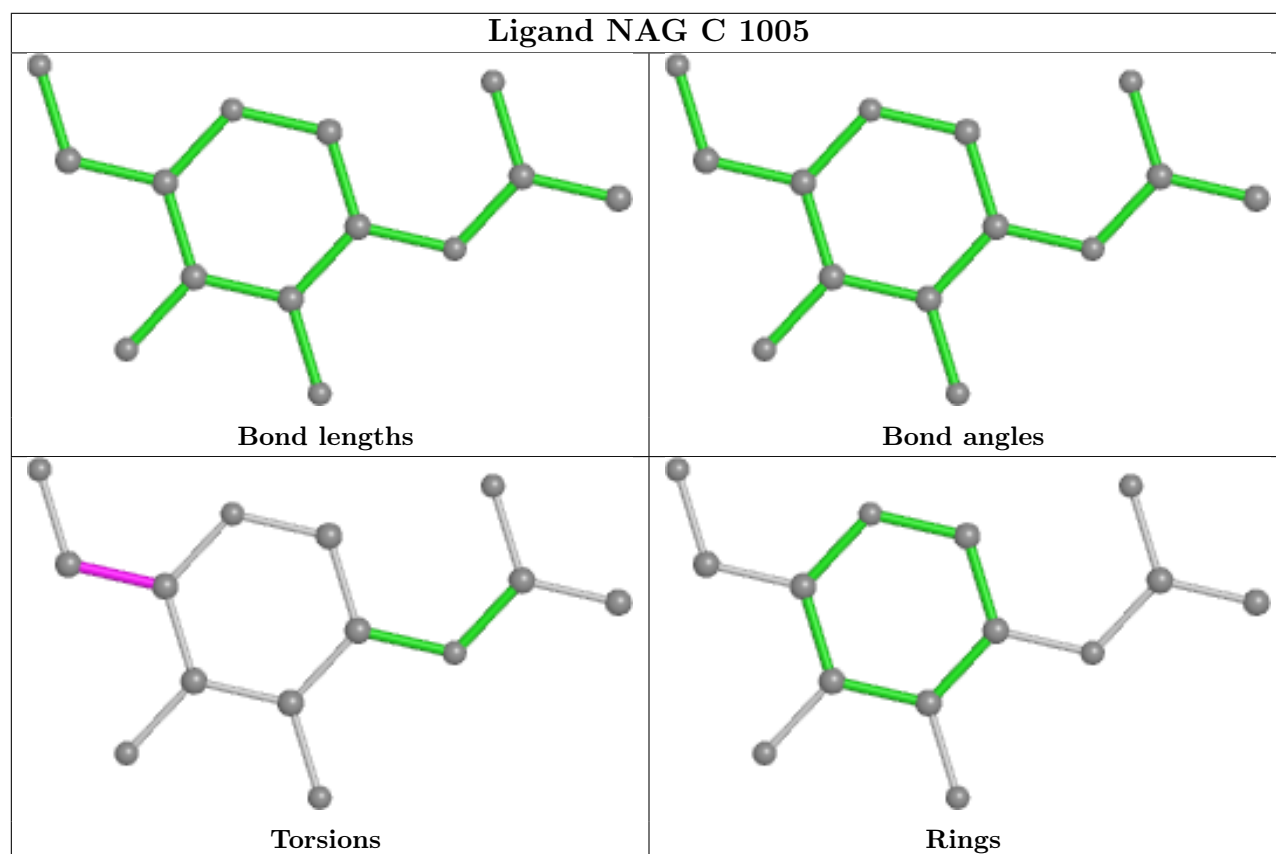
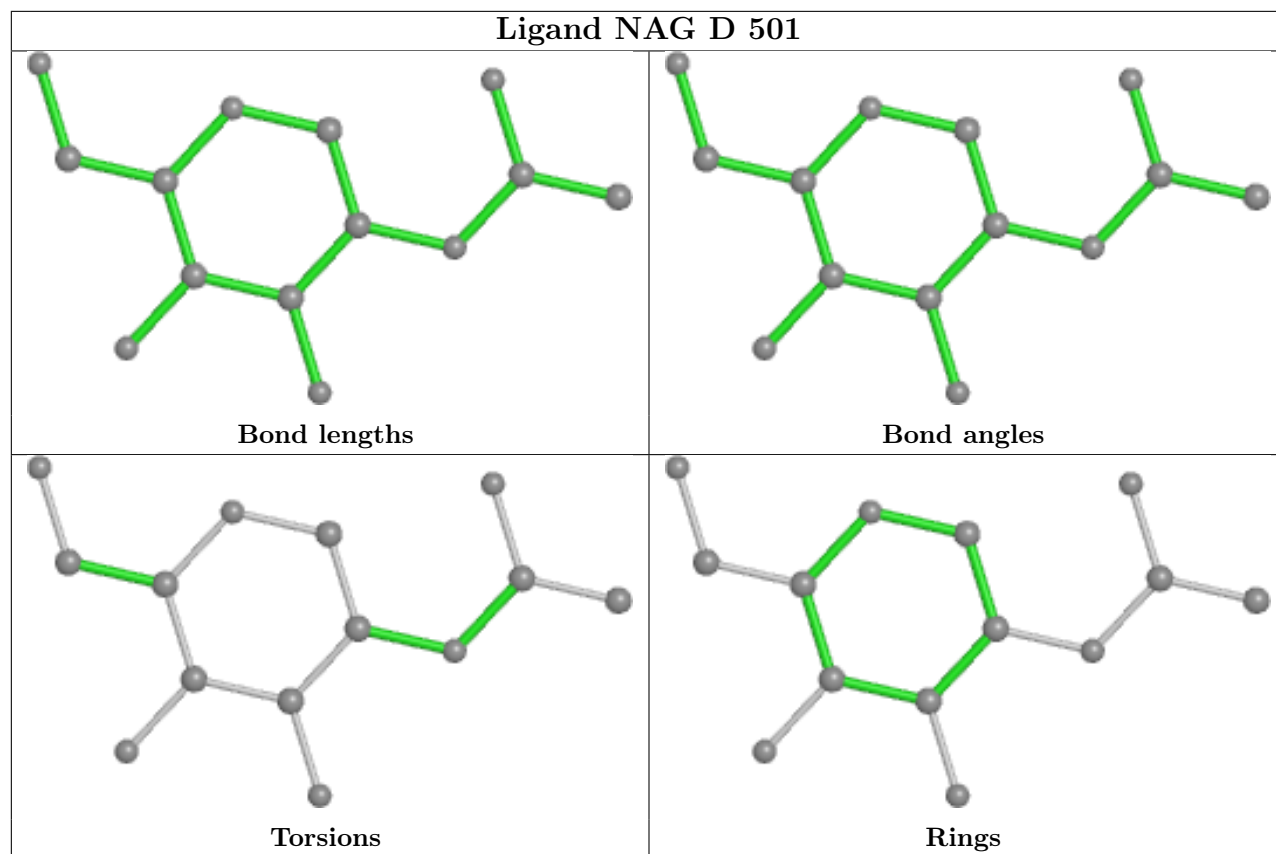


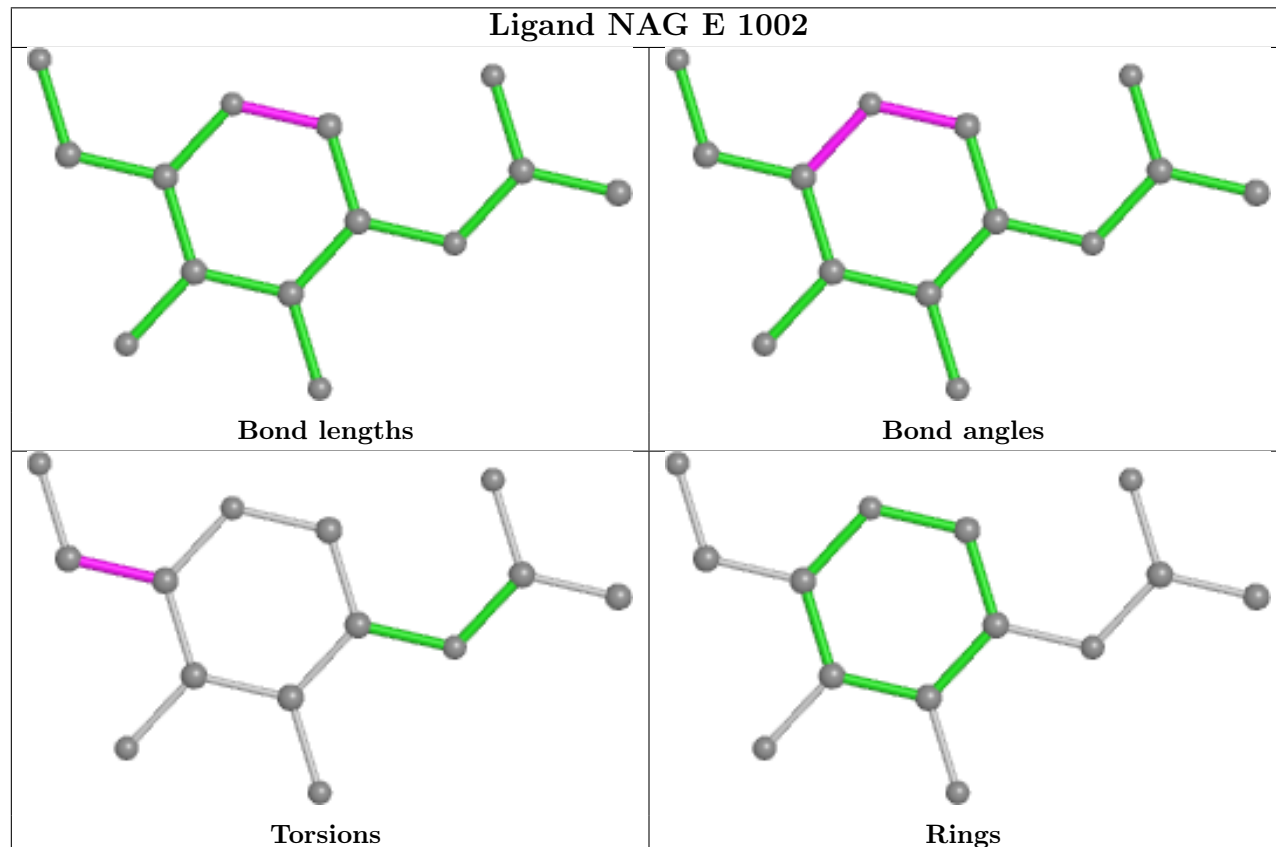
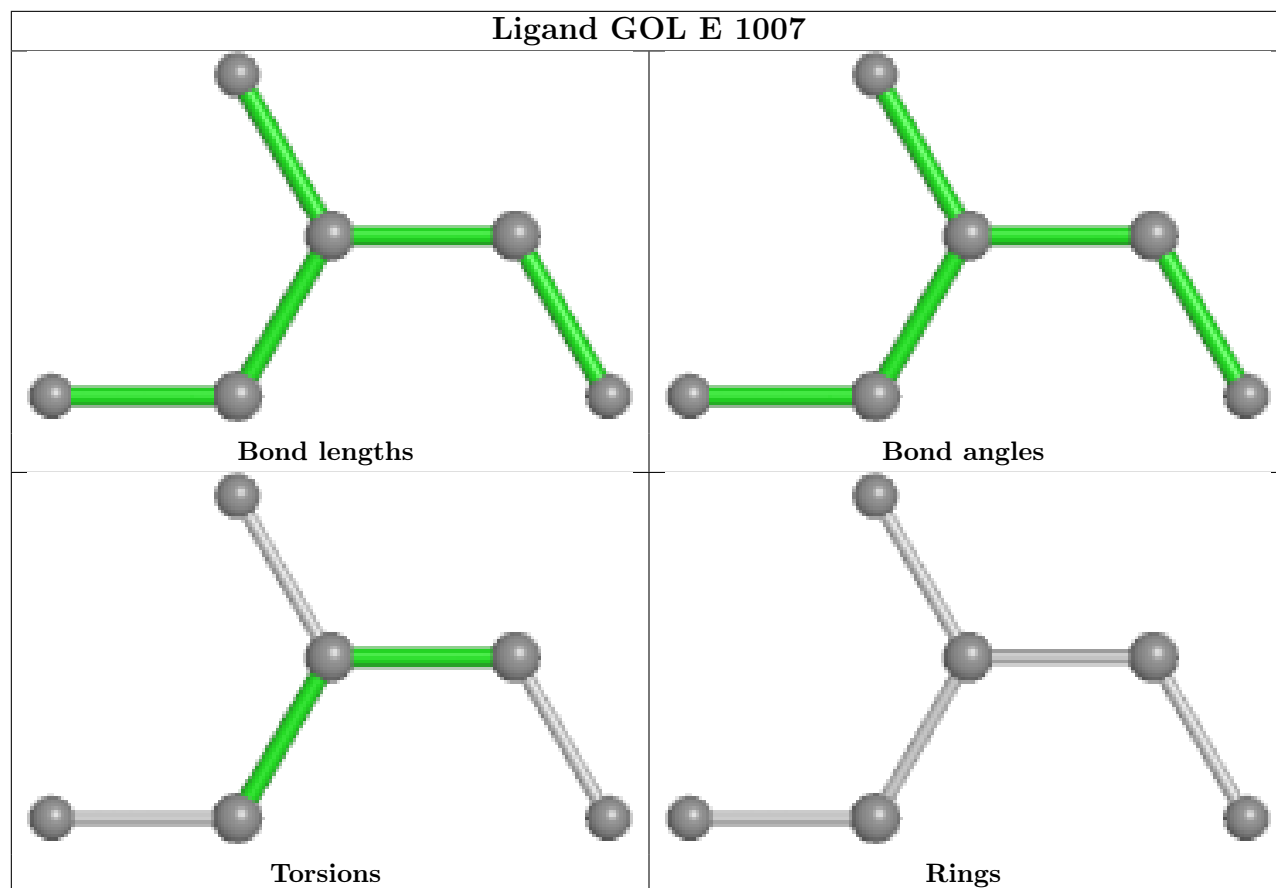
## Ligand NAG E 1003



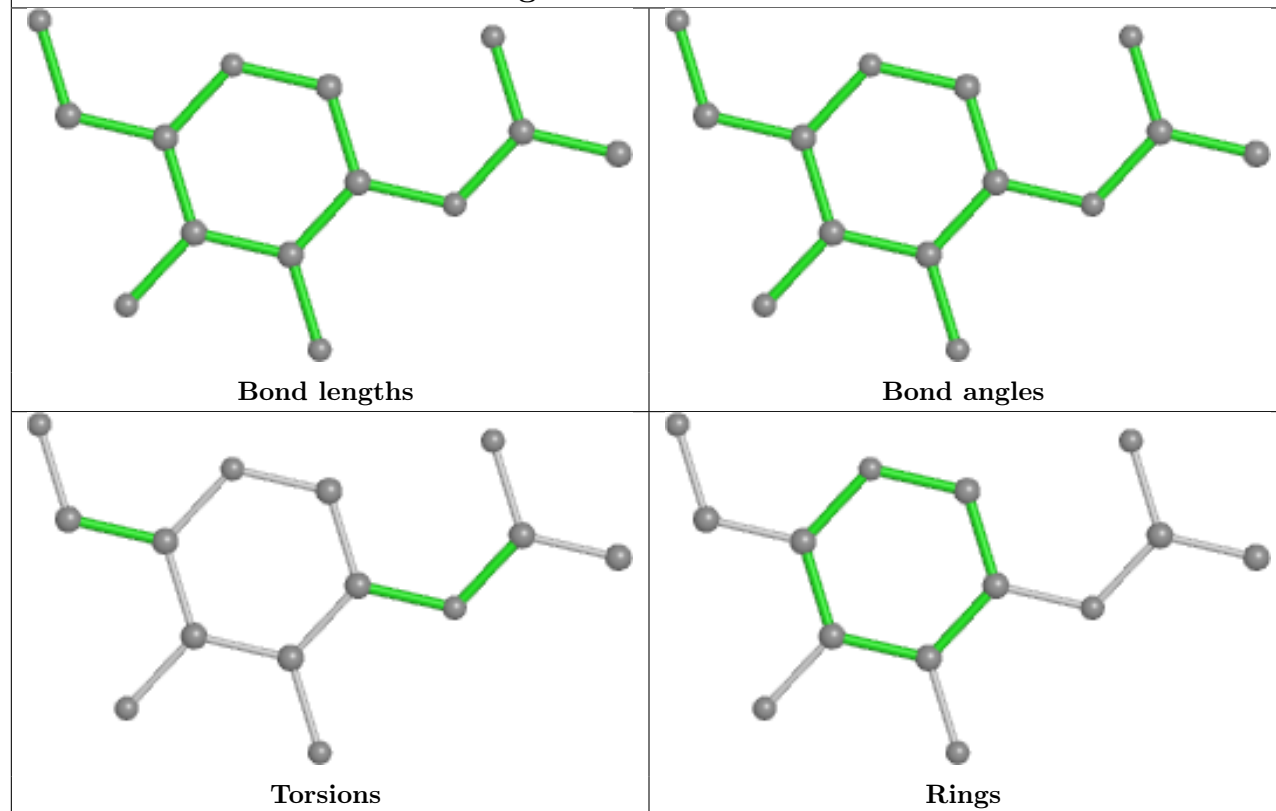
## Ligand NAG C 1003



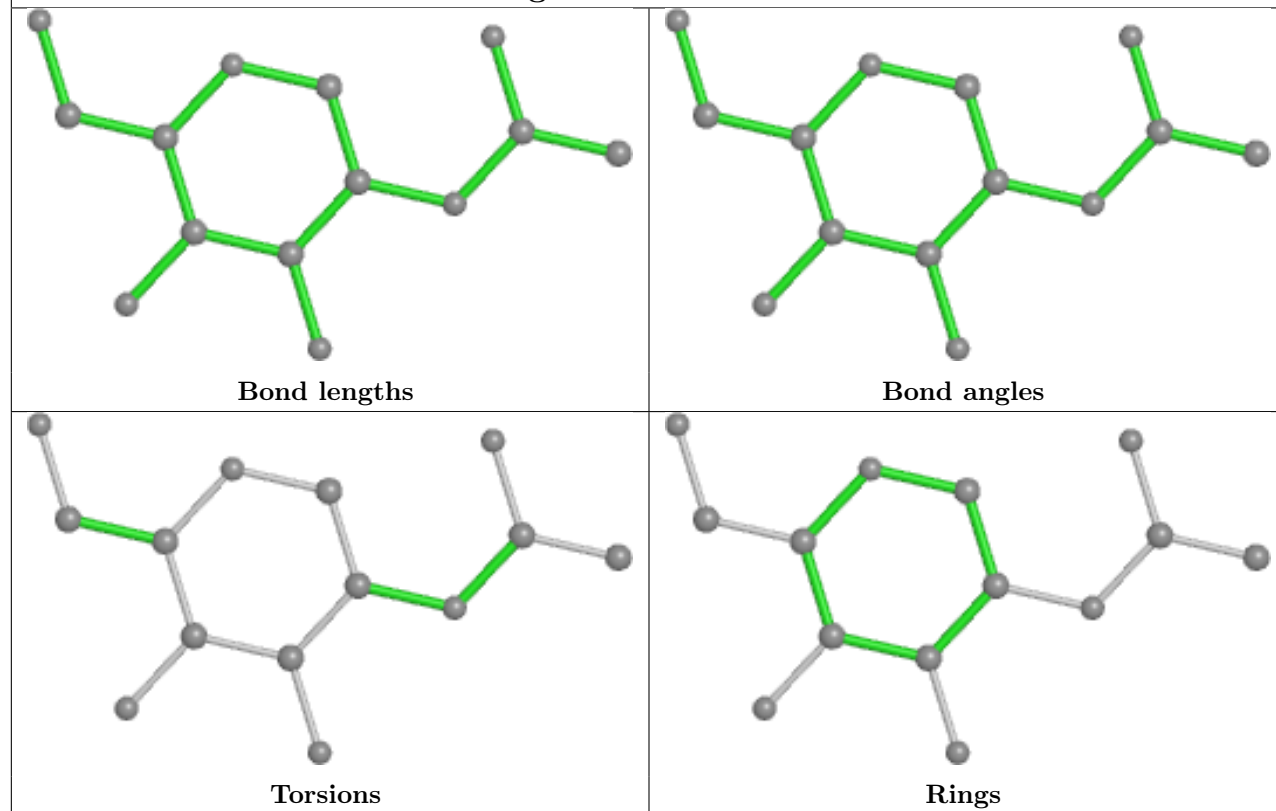




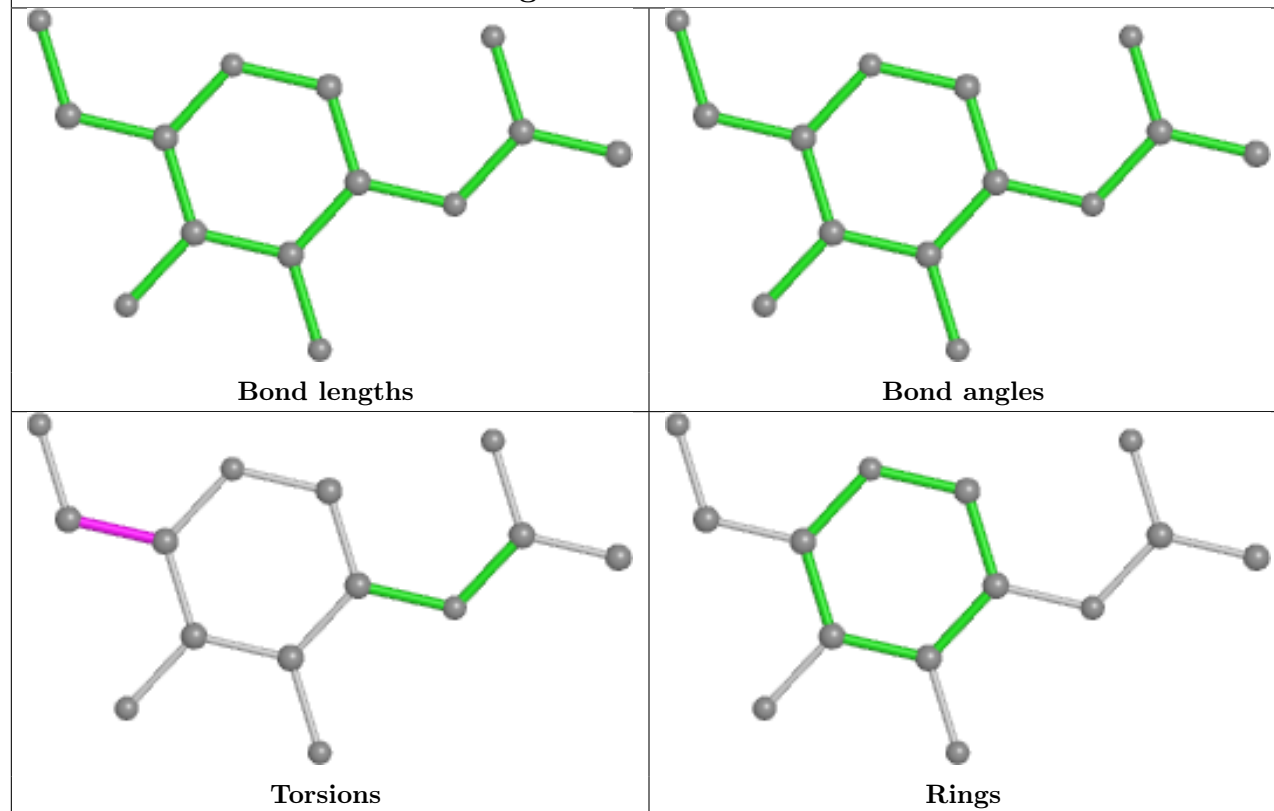
## Ligand NAG A 1006



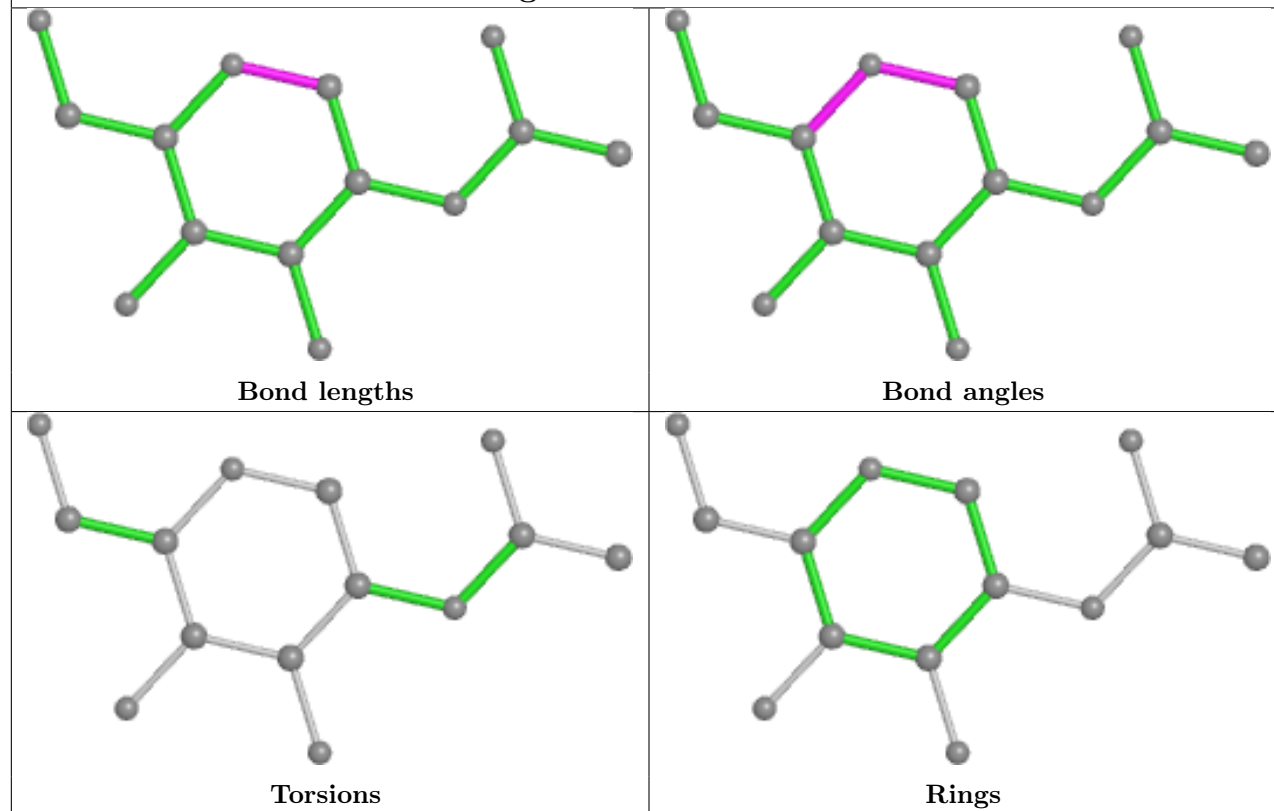
## Ligand NAG B 501



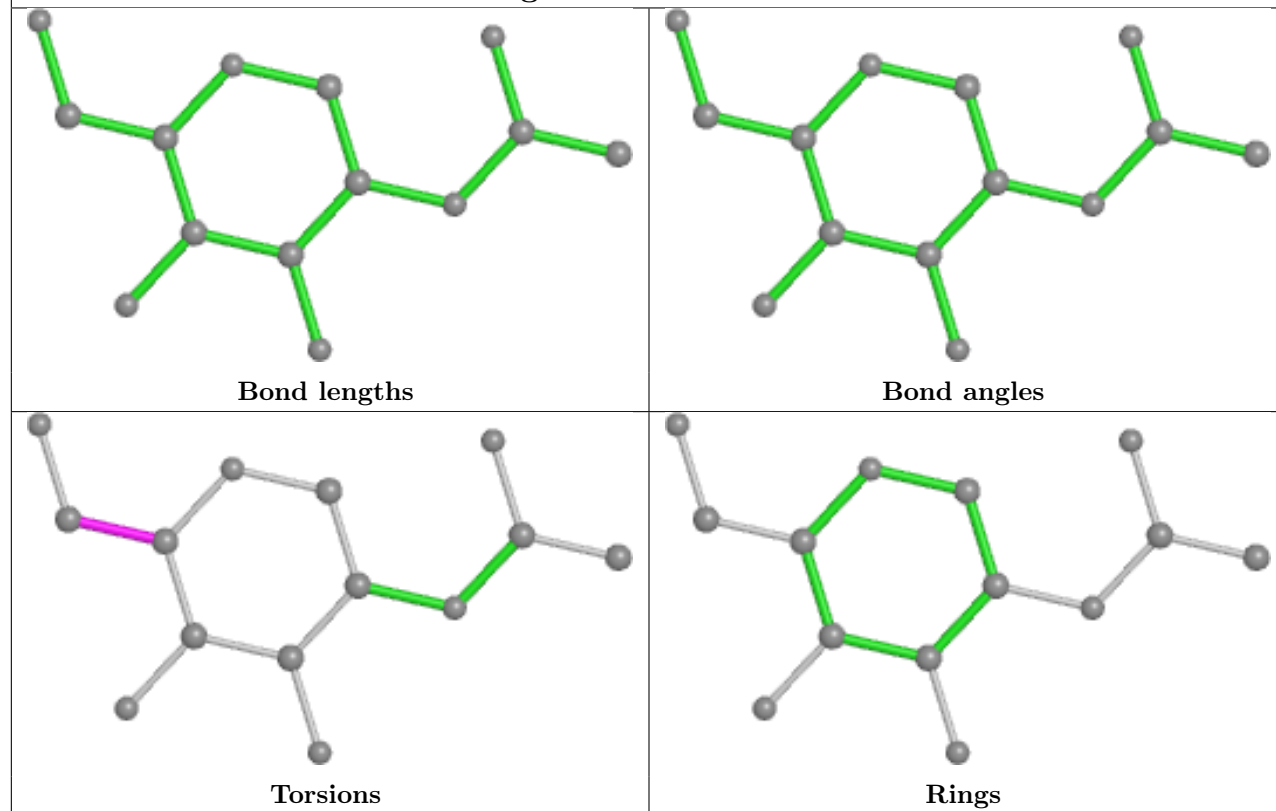
## Ligand NAG C 1002



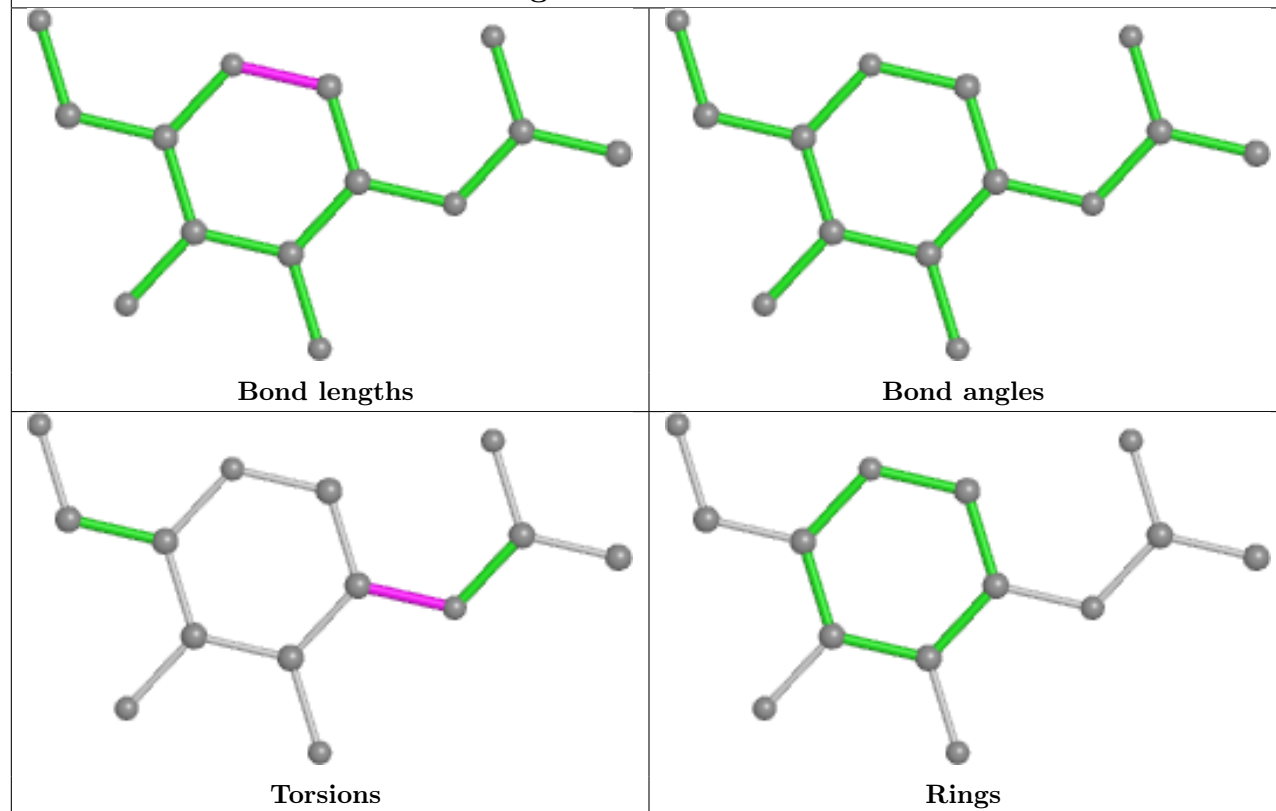
## Ligand NAG C 1006

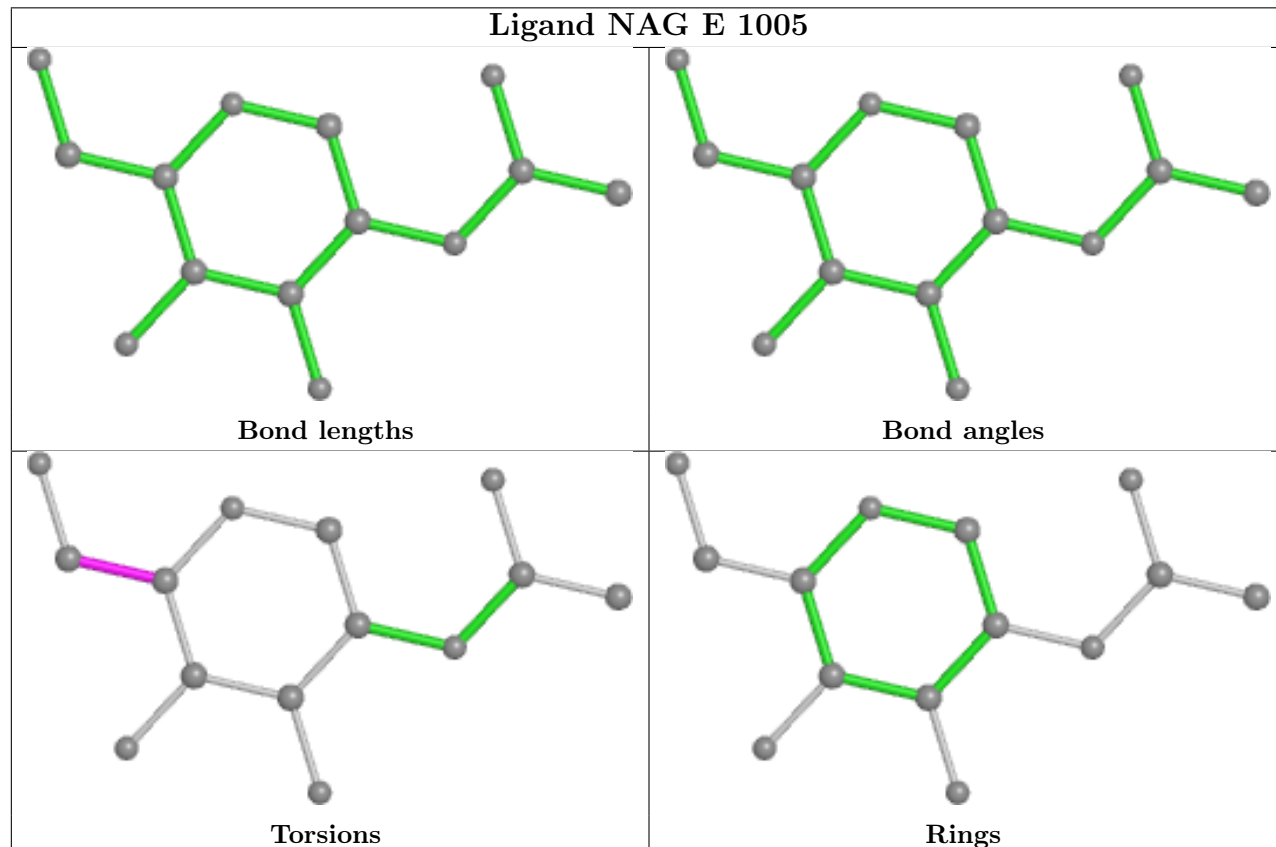
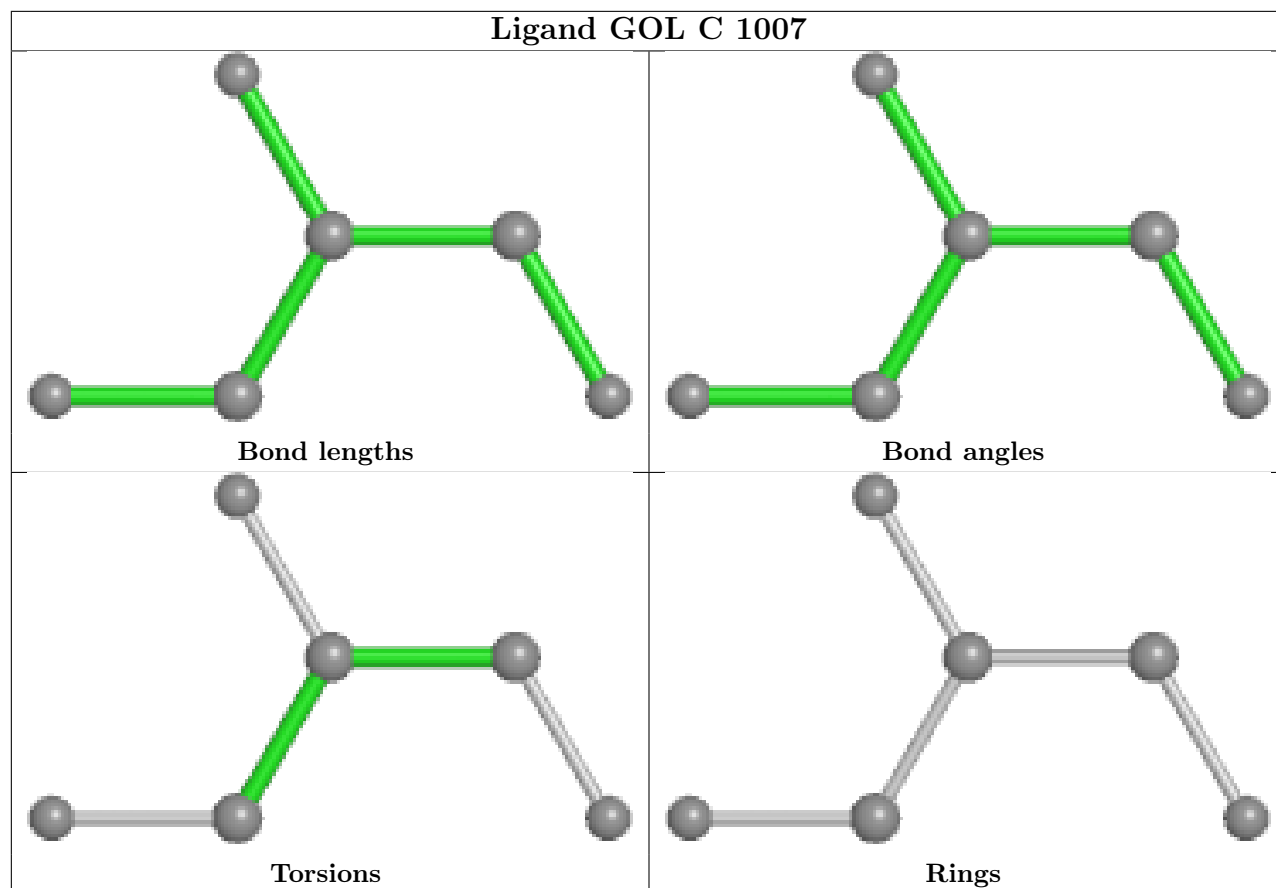


## Ligand NAG E 1006

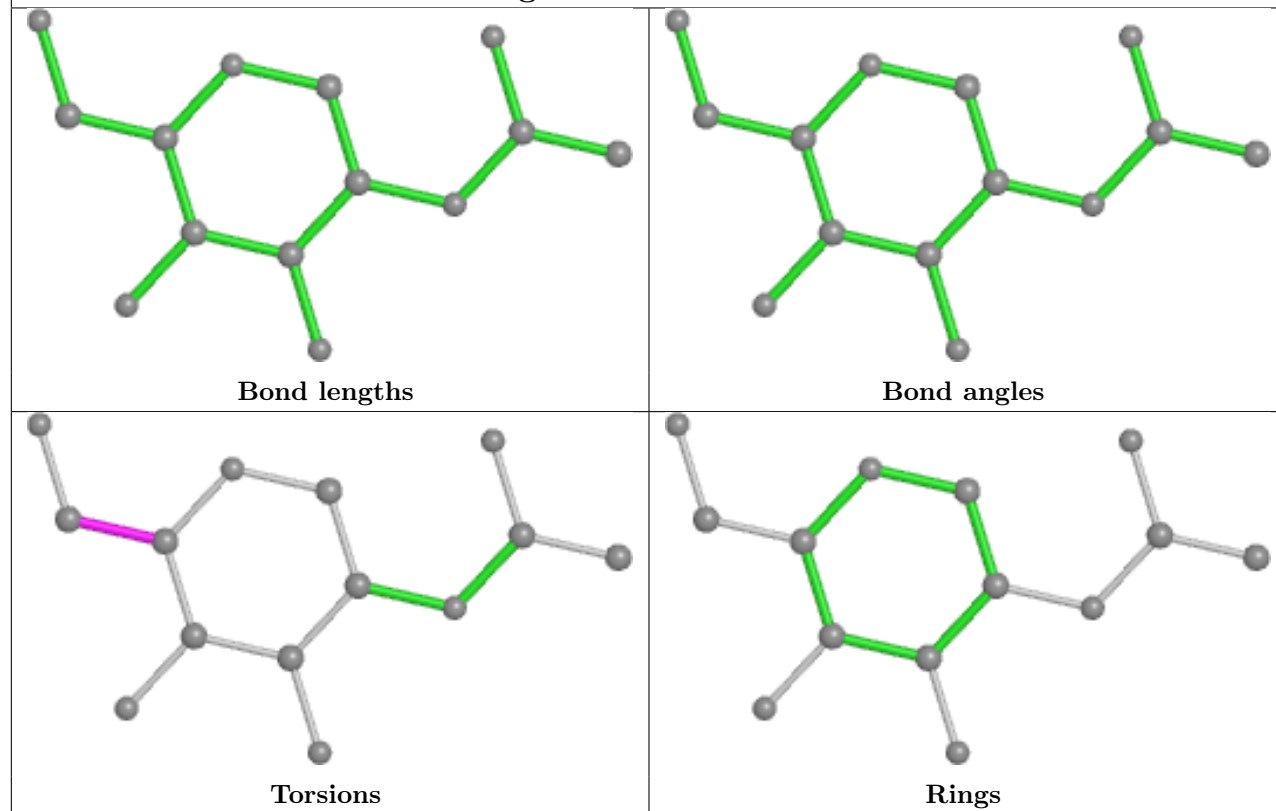


## Ligand NAG F 501

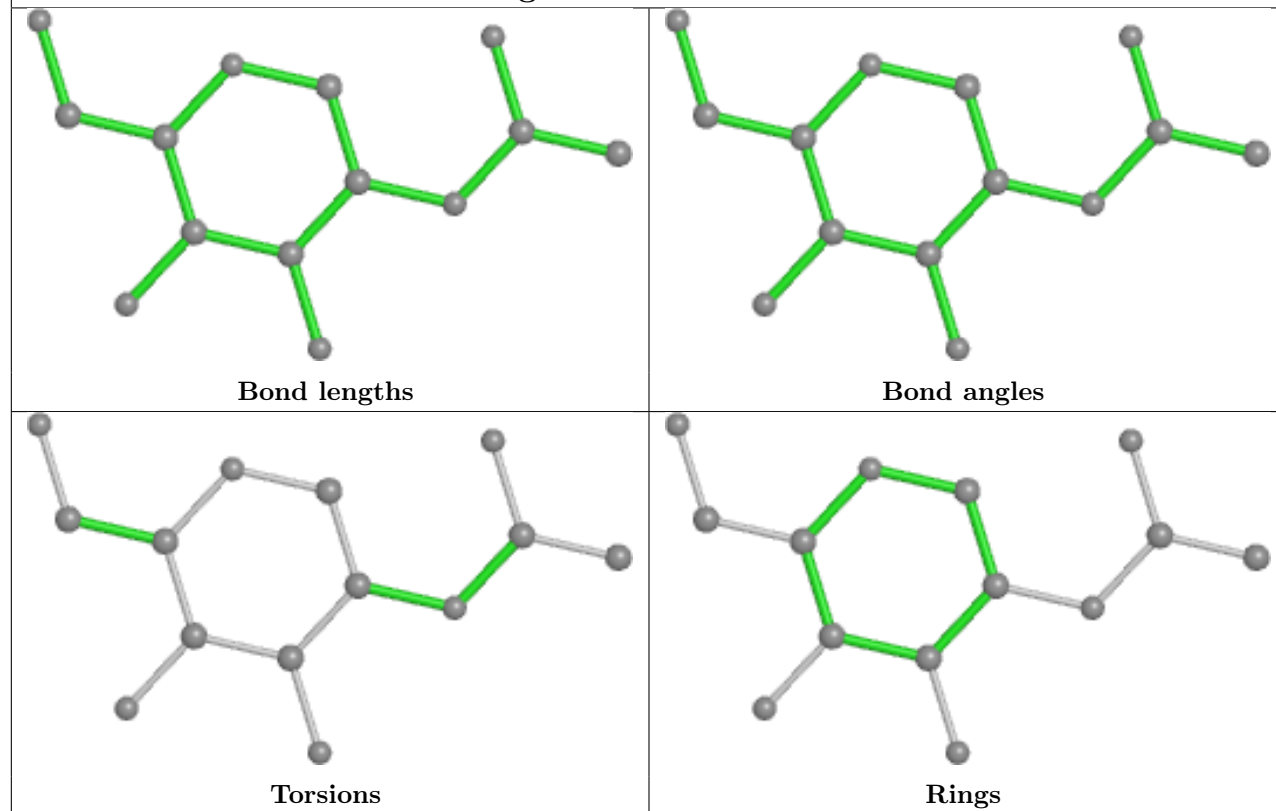


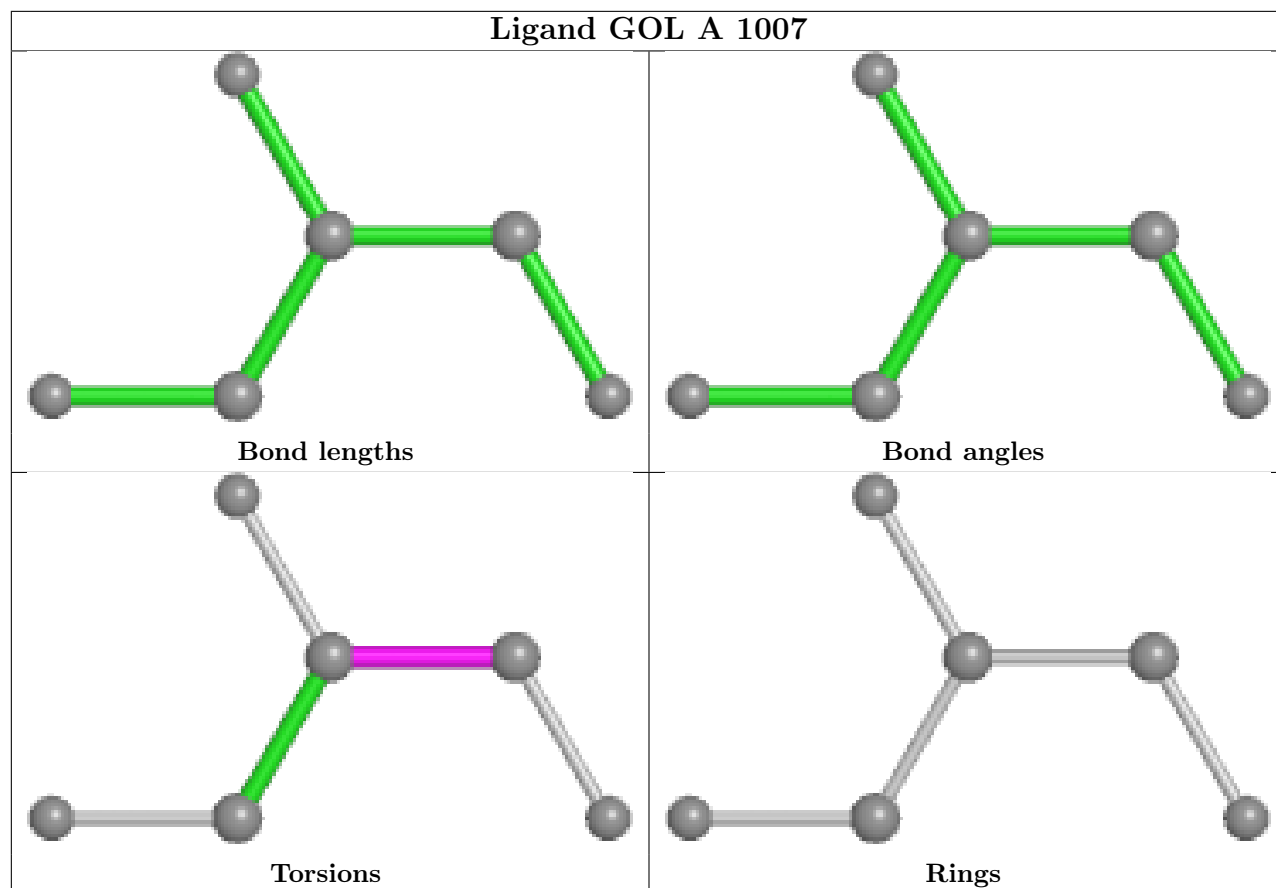


## Ligand NAG A 1004



## Ligand NAG A 1003





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	895/909 (98%)	0.24	1 (0%) 95 92	23, 31, 50, 101	0
1	C	895/909 (98%)	0.24	3 (0%) 94 88	21, 31, 50, 100	0
1	E	892/909 (98%)	0.23	0 100 100	21, 31, 49, 78	0
2	B	103/127 (81%)	0.65	10 (9%) 7 2	27, 66, 94, 107	0
2	D	103/127 (81%)	0.63	6 (5%) 23 10	29, 63, 92, 98	0
2	F	103/127 (81%)	0.68	9 (8%) 10 4	28, 67, 91, 100	0
All	All	2991/3108 (96%)	0.28	29 (0%) 82 67	21, 32, 70, 107	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	305	LEU	3.8
2	F	381	THR	3.7
2	B	369	ASN	3.7
2	B	383	SER	3.4
2	B	341	PHE	3.2
2	F	341	PHE	3.2
2	B	336	VAL	3.1
2	F	336	VAL	3.0
2	D	370	ASN	2.9
2	B	305	LEU	2.6
2	F	369	ASN	2.6
2	B	340	TYR	2.6
1	C	895	SER	2.5
2	D	336	VAL	2.5
1	C	893	GLY	2.4
2	D	335	CYS	2.3
2	F	370	ASN	2.3
2	B	306	GLU	2.3
2	B	381	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	342	ARG	2.1
2	F	383	SER	2.1
2	D	342	ARG	2.1
2	B	337	THR	2.1
2	D	341	PHE	2.1
1	C	894	GLY	2.1
2	B	342	ARG	2.1
2	F	337	THR	2.1
1	A	894	GLY	2.0
2	D	378	CYS	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](#)

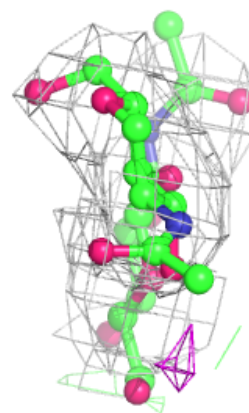
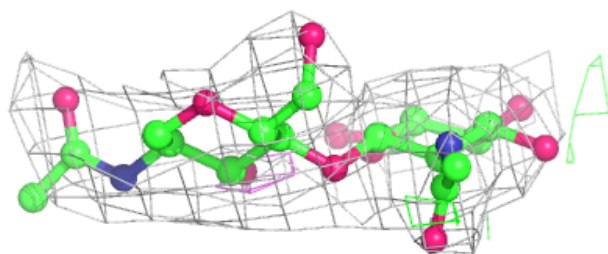
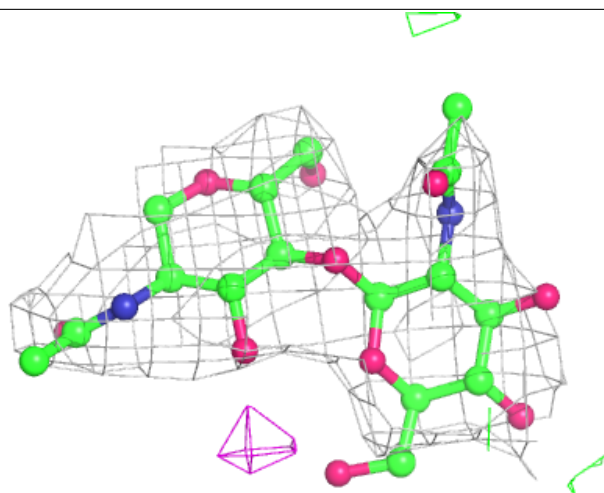
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	L	2	14/15	0.79	0.35	43,72,95,100	0
3	NAG	G	2	14/15	0.83	0.29	60,77,86,87	0
4	NAG	I	2	14/15	0.83	0.32	56,76,84,85	0
3	NAG	H	2	14/15	0.87	0.26	48,71,90,91	0
3	NAG	K	2	14/15	0.87	0.26	61,73,88,90	0
3	NAG	J	2	14/15	0.91	0.24	43,69,81,84	0
4	NAG	I	1	14/15	0.93	0.30	49,55,72,73	0
3	NAG	G	1	14/15	0.94	0.30	40,50,59,59	0
3	NAG	K	1	14/15	0.94	0.25	44,50,57,60	0
3	NAG	J	1	14/15	0.95	0.23	30,37,50,58	0
3	NAG	L	1	14/15	0.96	0.23	33,38,51,55	0
3	NAG	H	1	14/15	0.96	0.21	28,40,49,56	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.

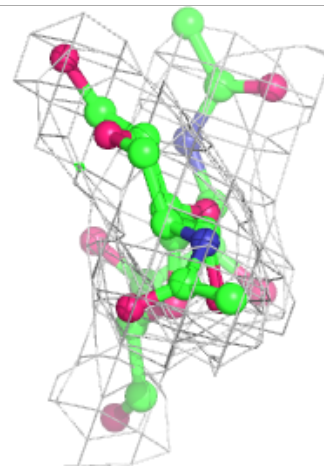
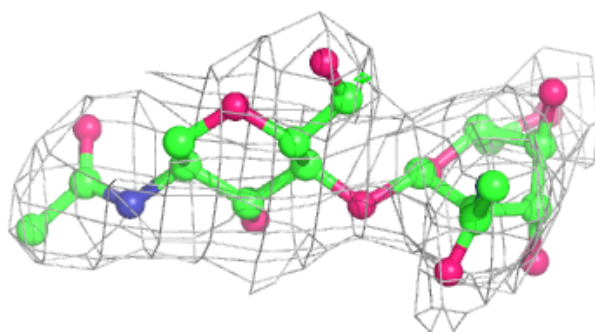
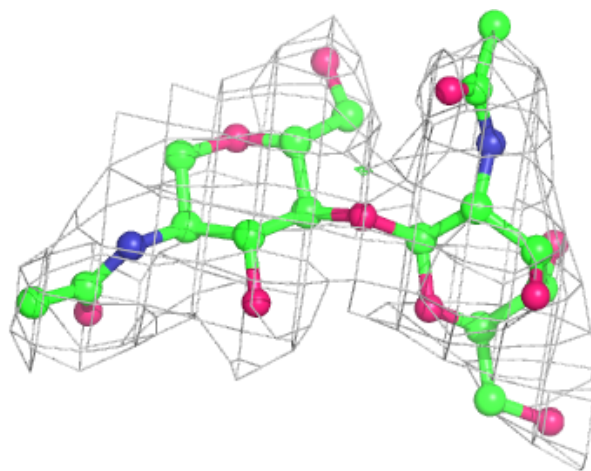
**Electron density around Chain G:**

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



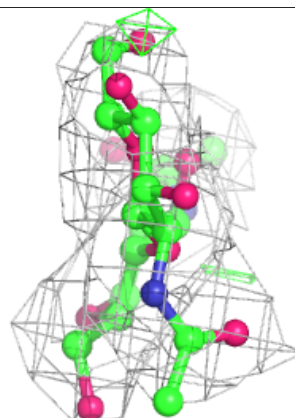
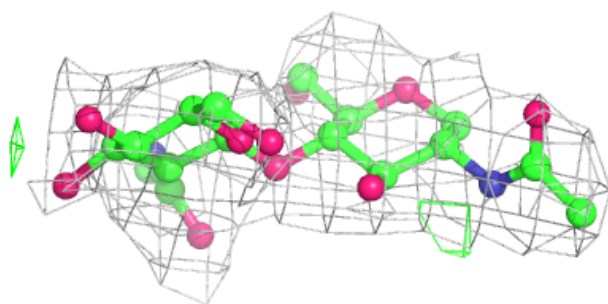
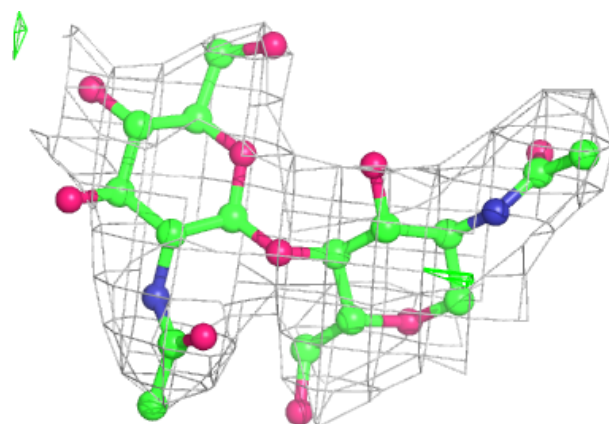
**Electron density around Chain H:**

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



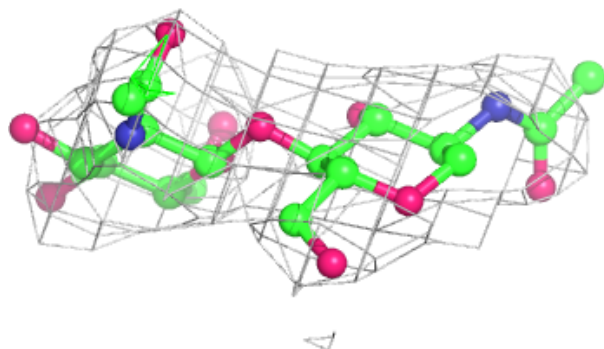
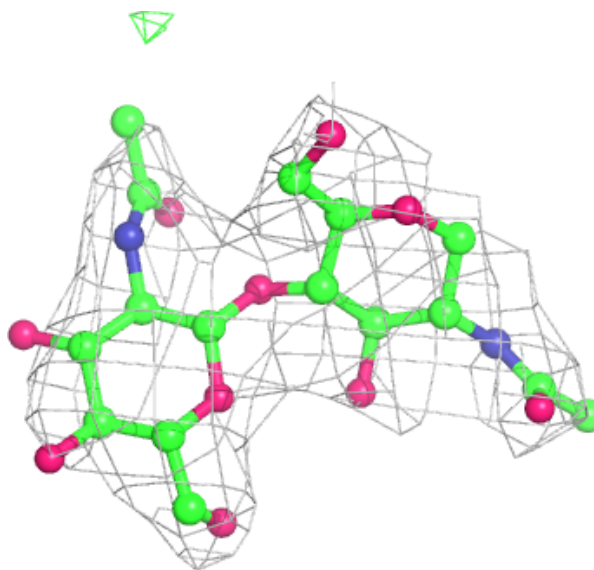
**Electron density around Chain J:**

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



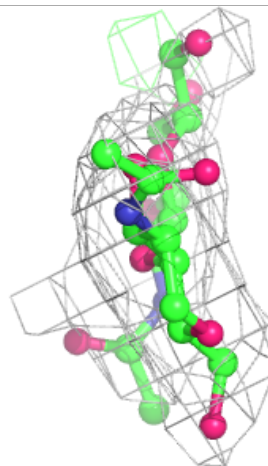
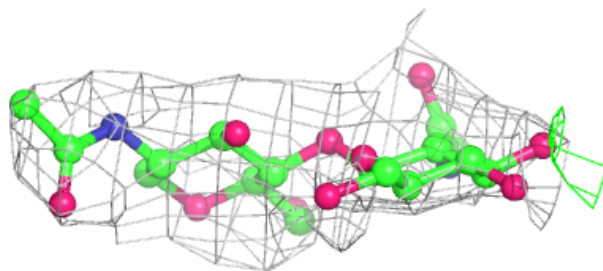
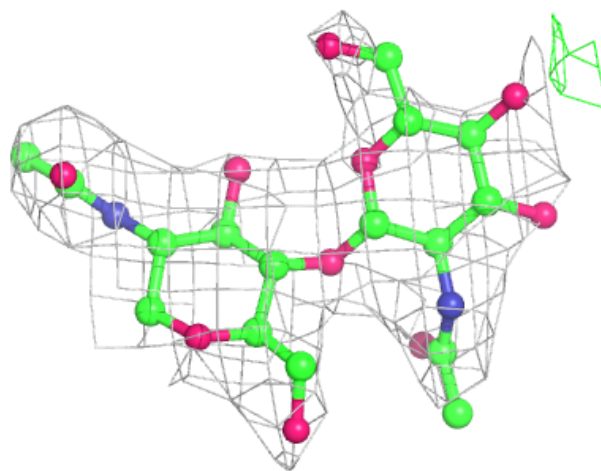
**Electron density around Chain K:**

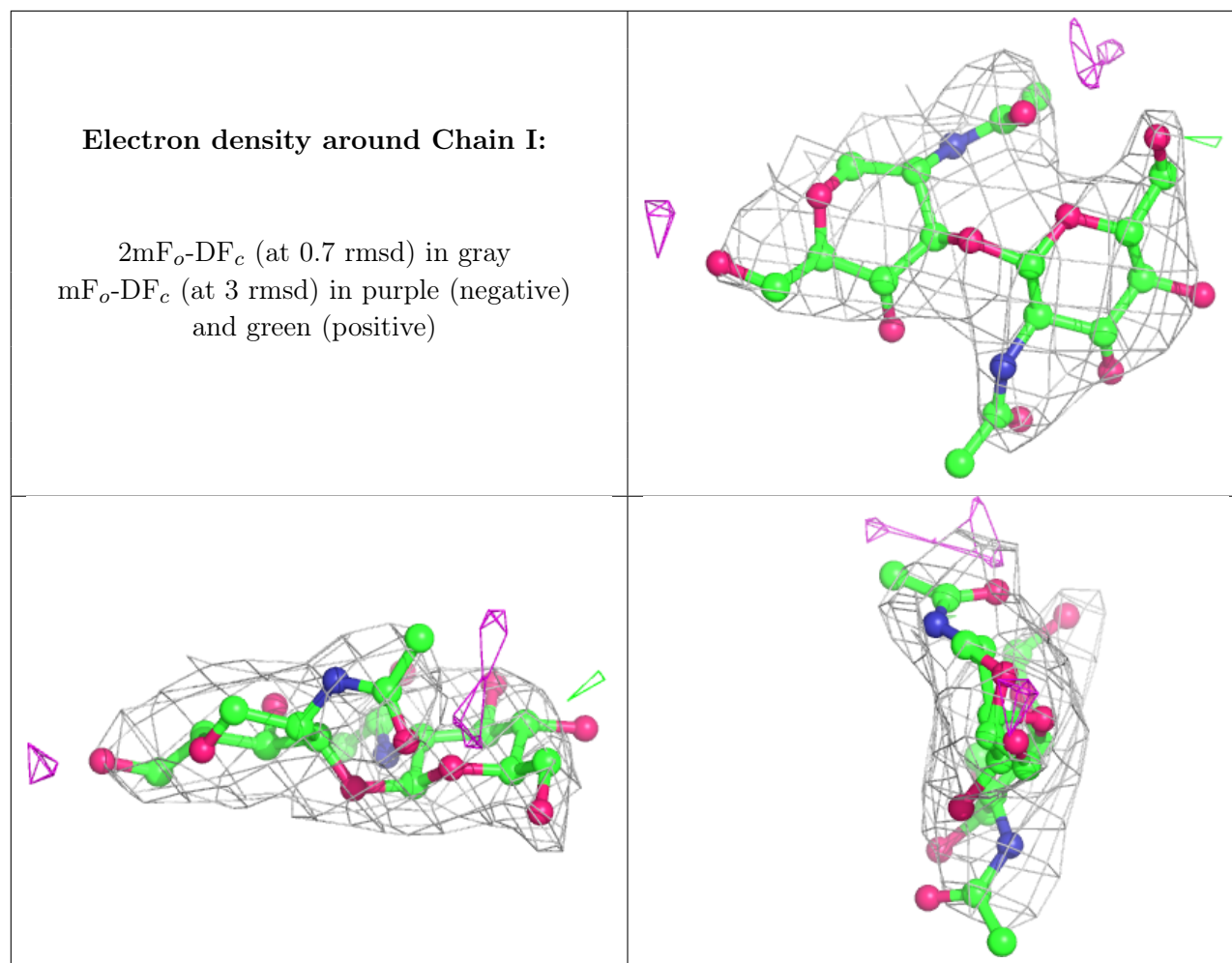
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	C	1003	14/15	0.76	0.28	58,77,87,87	0
6	NAG	E	1003	14/15	0.79	0.30	63,77,88,93	0
6	NAG	E	1005	14/15	0.80	0.28	52,68,78,79	0
6	NAG	A	1005	14/15	0.81	0.23	48,67,76,78	0
6	NAG	F	501	14/15	0.81	0.25	70,75,84,85	0
6	NAG	A	1003	14/15	0.84	0.25	52,74,84,85	0
6	NAG	B	501	14/15	0.85	0.24	56,76,84,85	0
6	NAG	E	1004	14/15	0.87	0.21	53,68,83,87	0
6	NAG	A	1004	14/15	0.88	0.13	63,73,82,84	0
6	NAG	C	1002	14/15	0.88	0.27	35,62,73,77	0

*Continued on next page...*

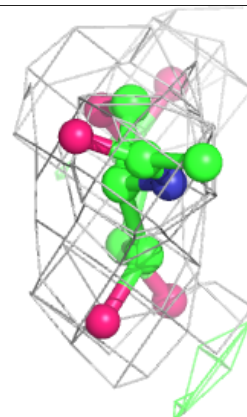
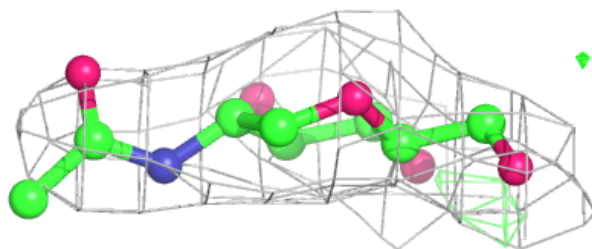
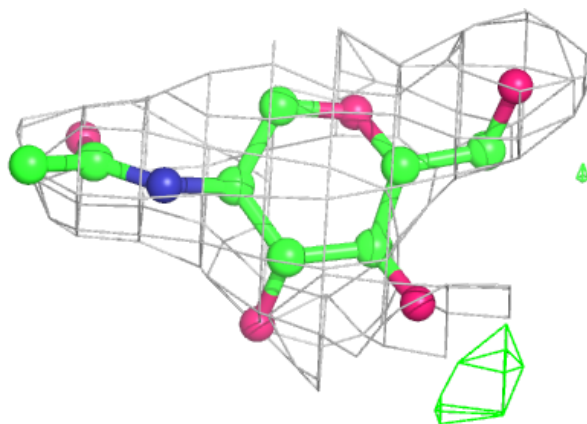
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	A	1006	14/15	0.88	0.25	39,55,65,68	0
6	NAG	C	1005	14/15	0.88	0.27	46,66,73,75	0
6	NAG	C	1006	14/15	0.89	0.26	37,51,65,66	0
6	NAG	C	1004	14/15	0.90	0.16	47,66,75,76	0
6	NAG	D	501	14/15	0.90	0.17	55,68,77,79	0
6	NAG	A	1002	14/15	0.90	0.19	33,59,68,69	0
6	NAG	E	1002	14/15	0.91	0.20	37,61,74,76	0
6	NAG	E	1006	14/15	0.93	0.28	35,51,64,65	0
7	GOL	A	1007	6/6	0.93	0.20	25,31,38,45	0
7	GOL	C	1007	6/6	0.94	0.21	32,43,44,45	0
7	GOL	E	1007	6/6	0.96	0.19	26,27,32,37	0
5	ZN	E	1001	1/1	0.99	0.23	32,32,32,32	0
5	ZN	C	1001	1/1	0.99	0.22	33,33,33,33	0
5	ZN	A	1001	1/1	1.00	0.25	30,30,30,30	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.

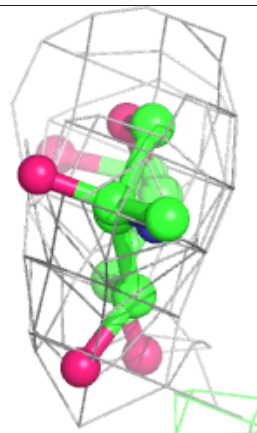
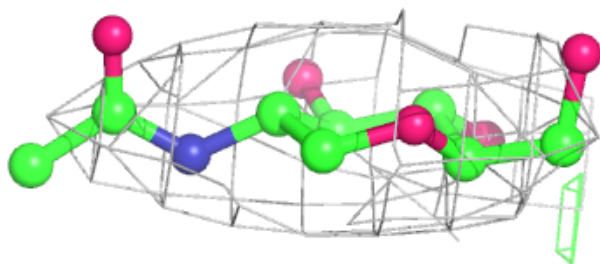
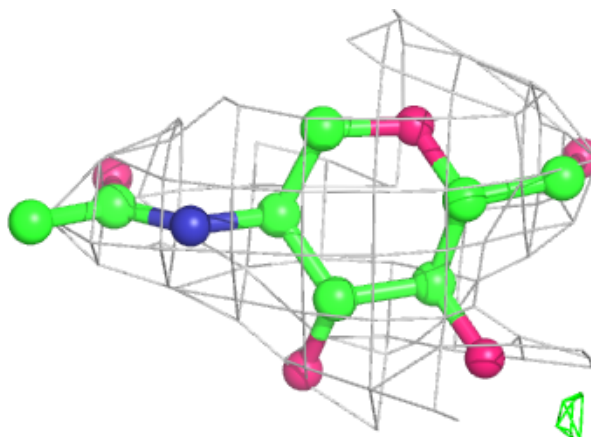
**Electron density around NAG C 1003:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

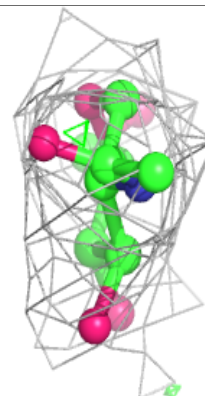
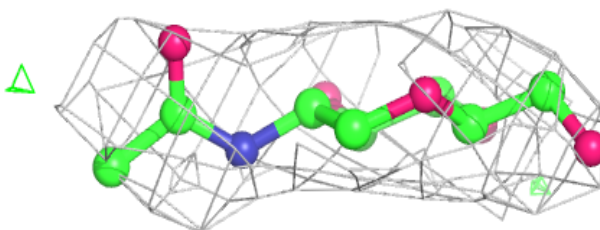
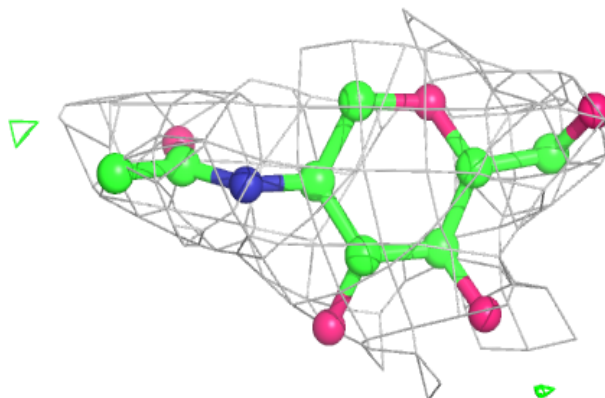


**Electron density around NAG E 1003:**

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

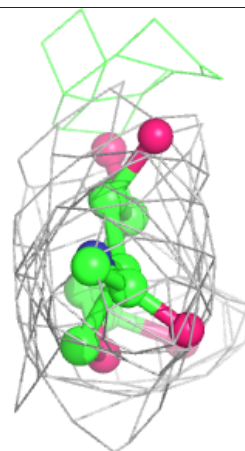
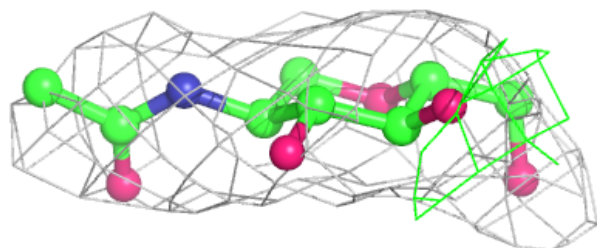
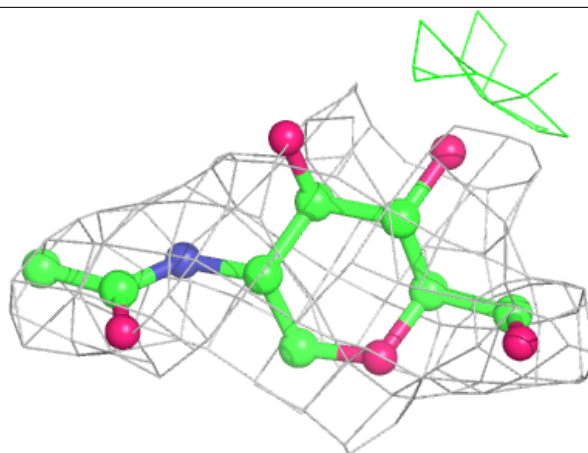
**Electron density around NAG E 1005:**

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

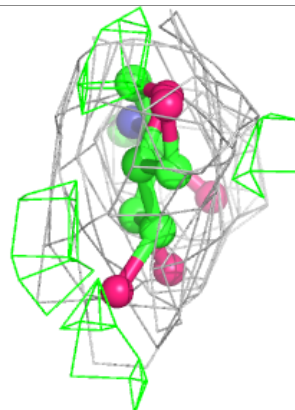
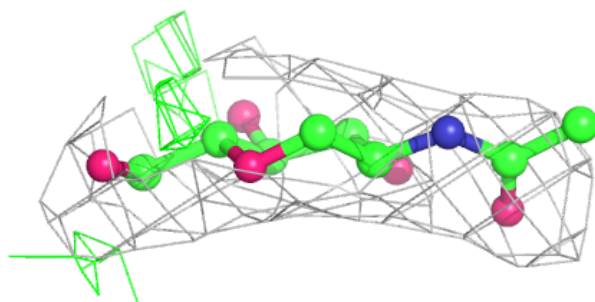
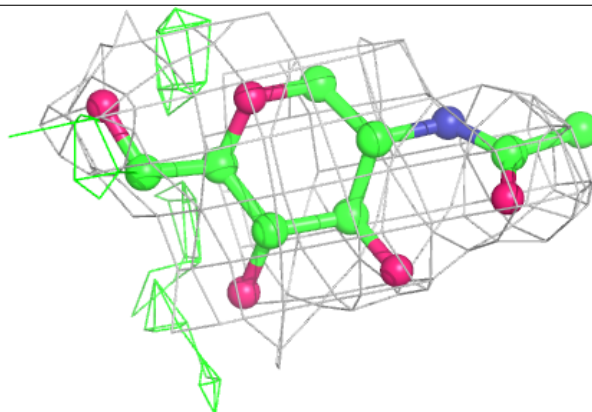


**Electron density around NAG A 1005:**

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

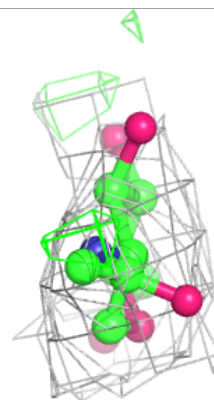
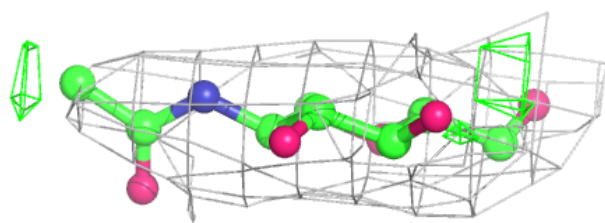
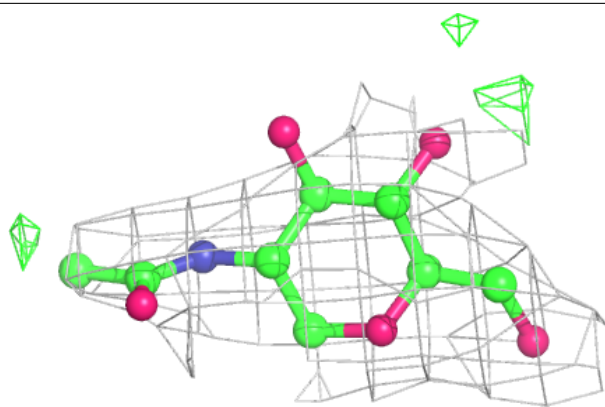
**Electron density around NAG F 501:**

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



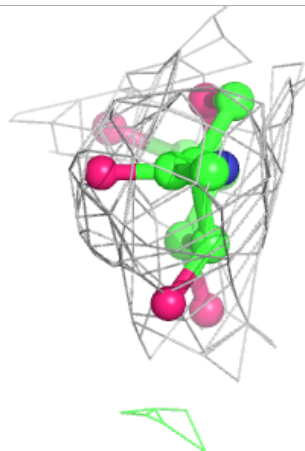
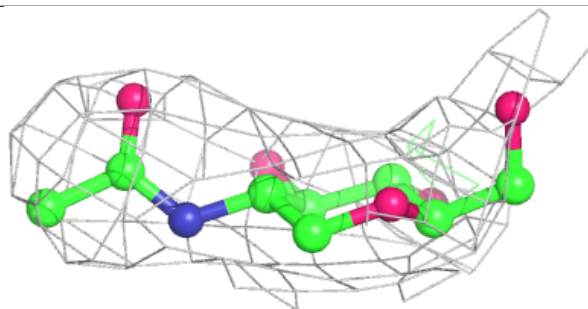
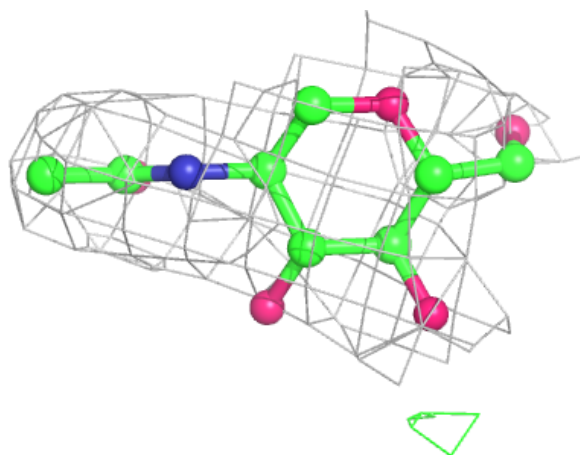
**Electron density around NAG A 1003:**

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



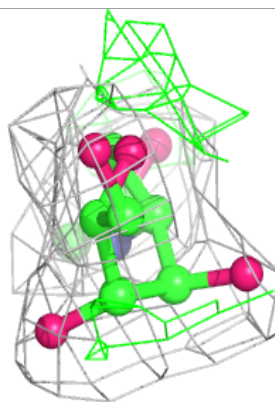
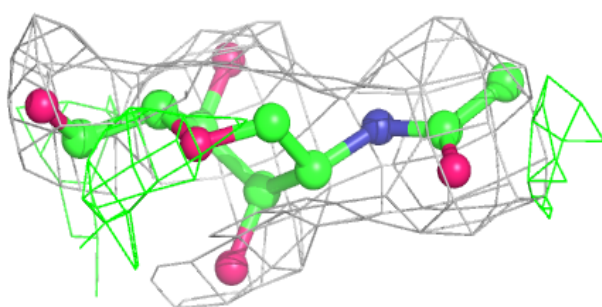
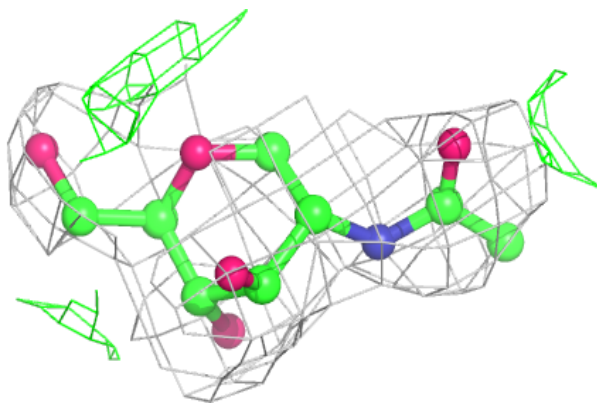
**Electron density around NAG B 501:**

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and green (positive)

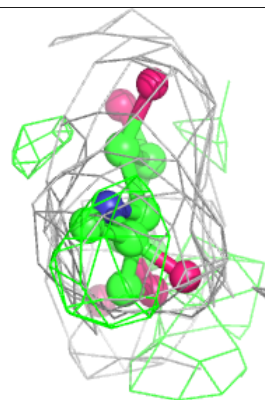
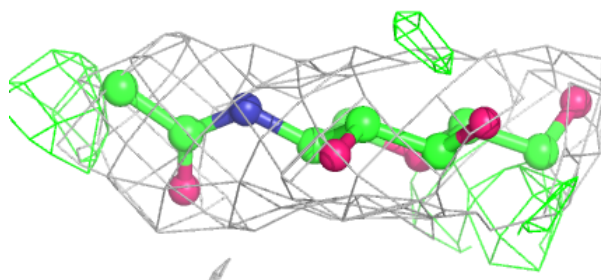
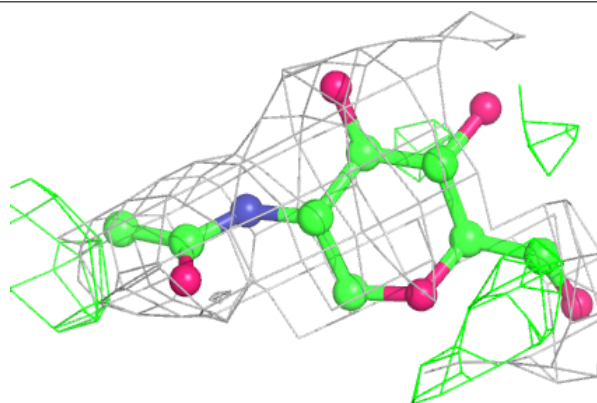


**Electron density around NAG E 1004:**

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and green (positive)

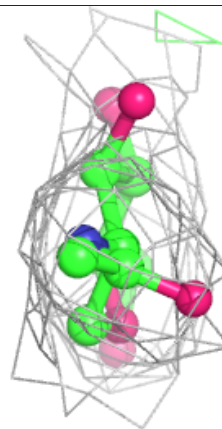
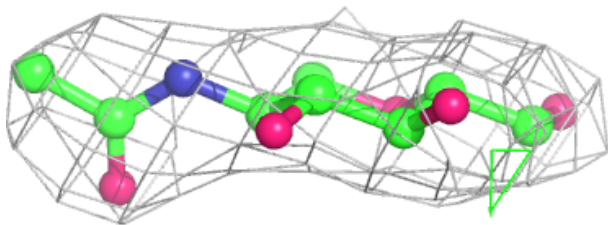
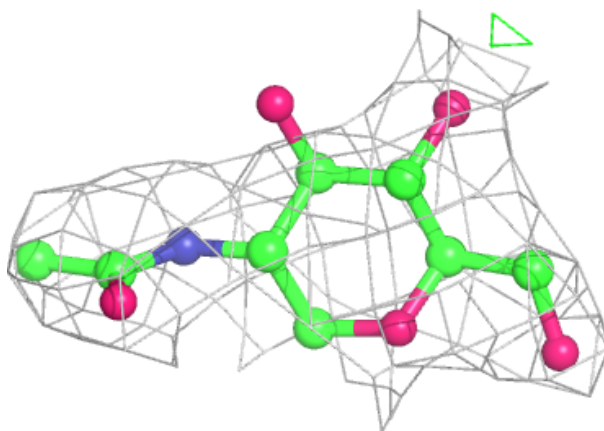
**Electron density around NAG A 1004:**

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and green (positive)



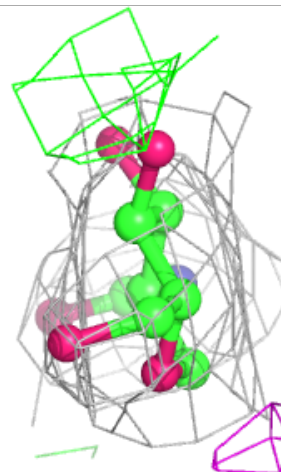
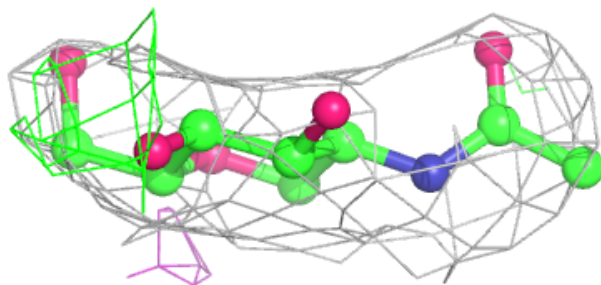
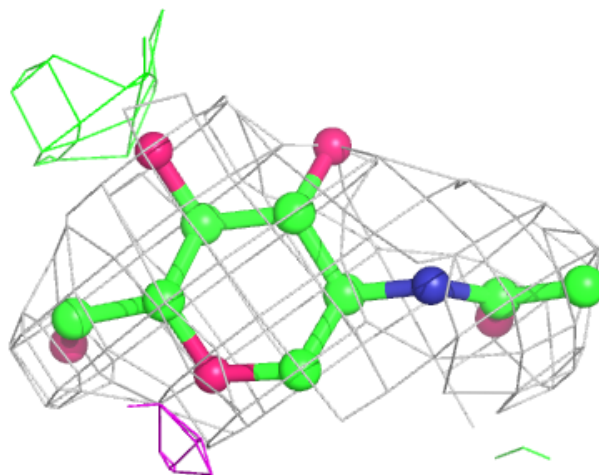
**Electron density around NAG C 1002:**

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



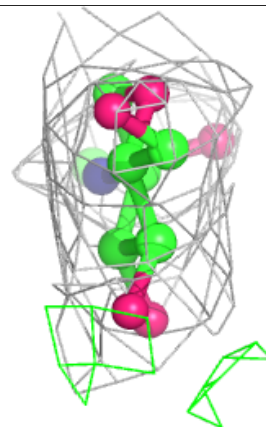
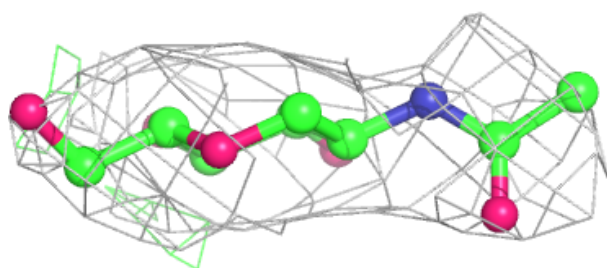
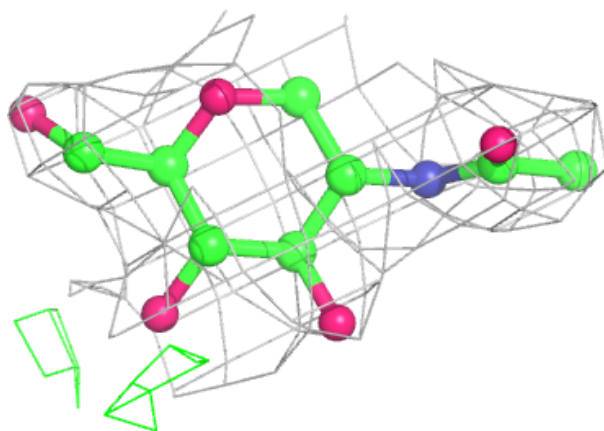
**Electron density around NAG A 1006:**

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and green (positive)



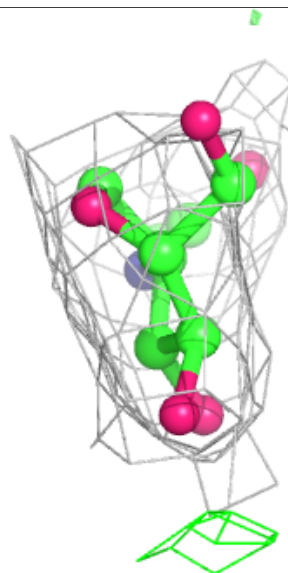
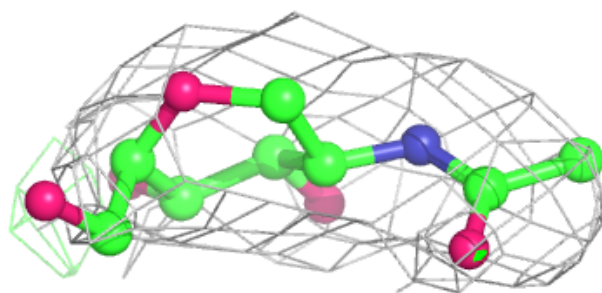
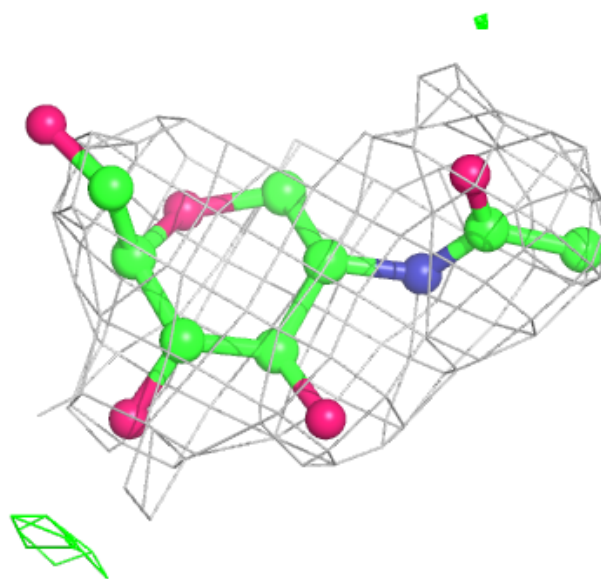
**Electron density around NAG C 1005:**

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and green (positive)



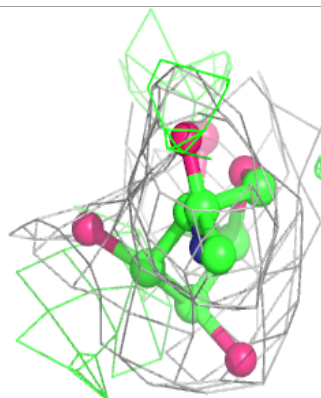
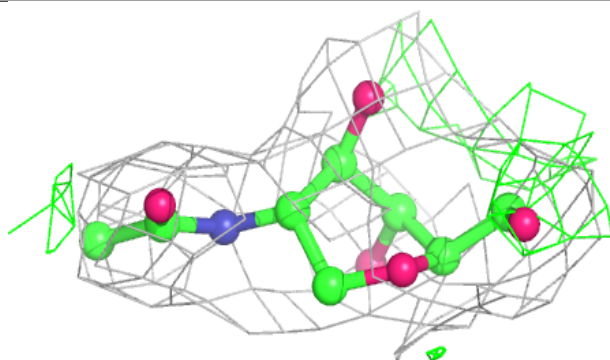
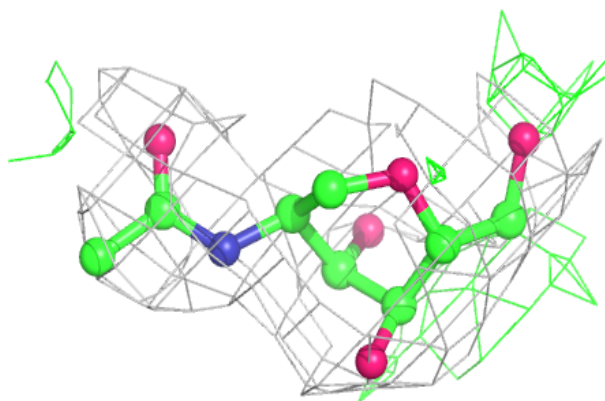
**Electron density around NAG C 1006:**

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and green (positive)

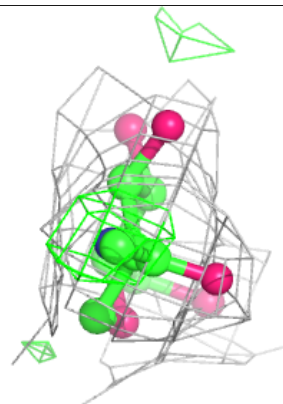
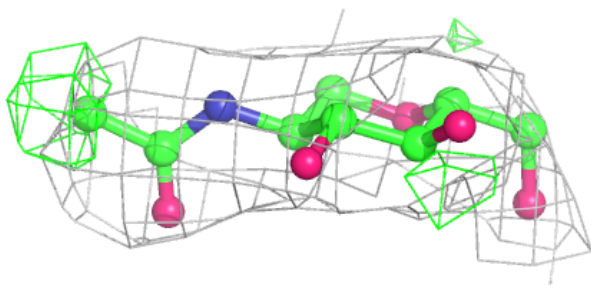
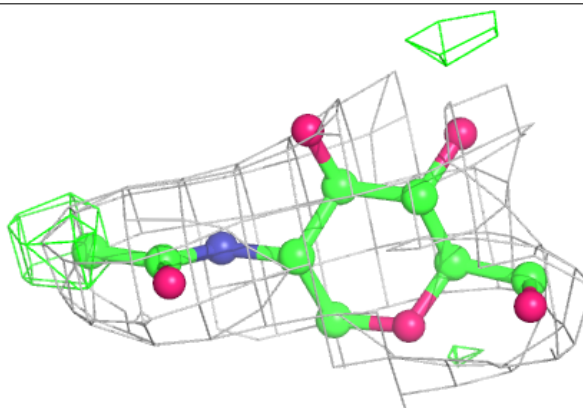


**Electron density around NAG C 1004:**

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and green (positive)

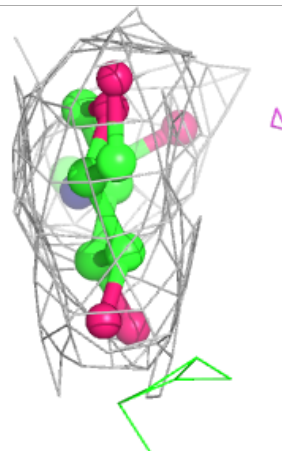
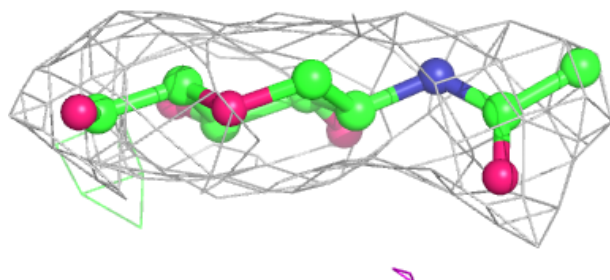
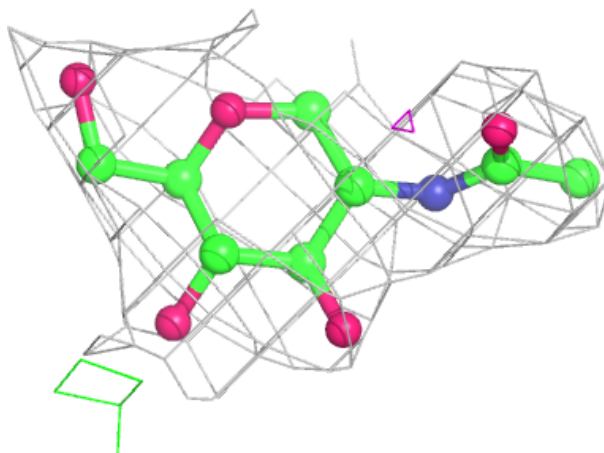
**Electron density around NAG D 501:**

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and green (positive)



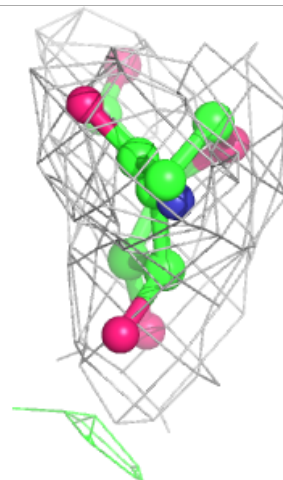
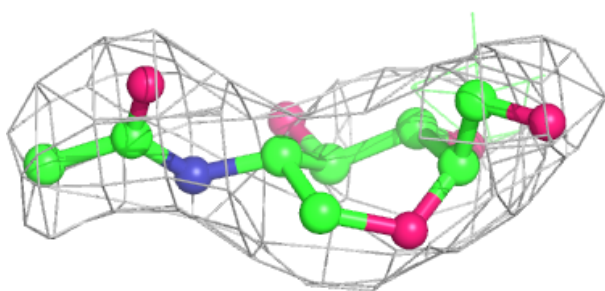
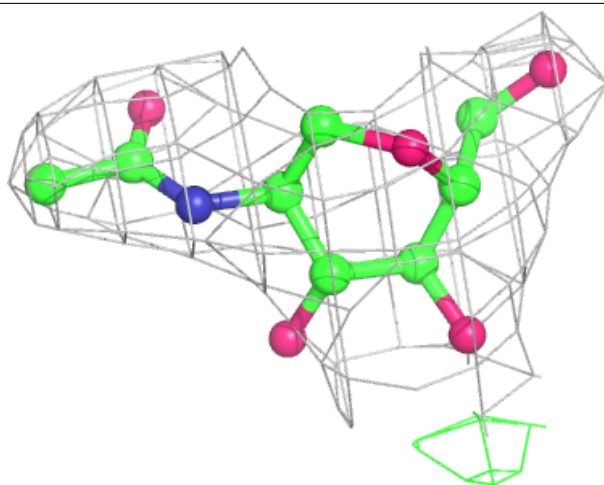
**Electron density around NAG A 1002:**

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and green (positive)



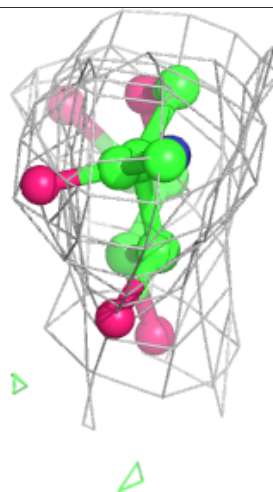
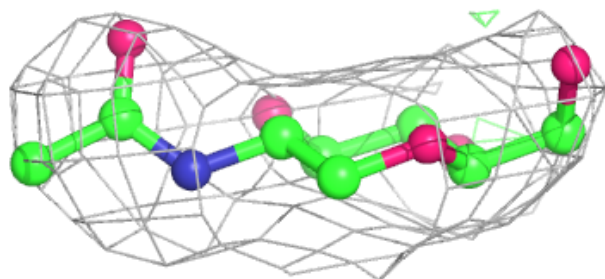
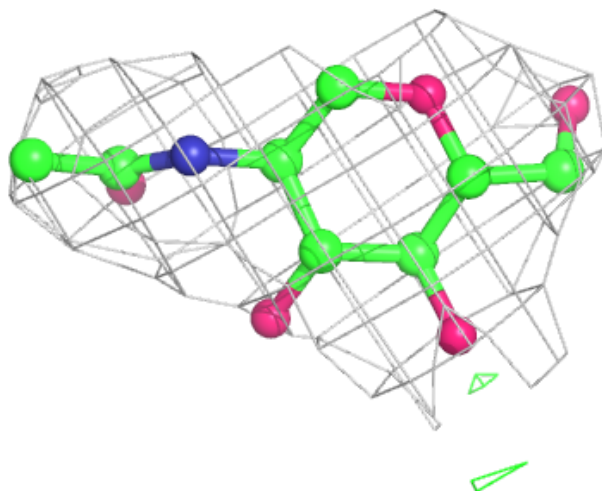
**Electron density around NAG E 1002:**

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



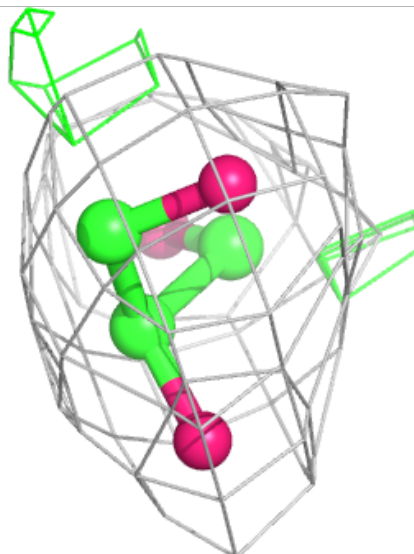
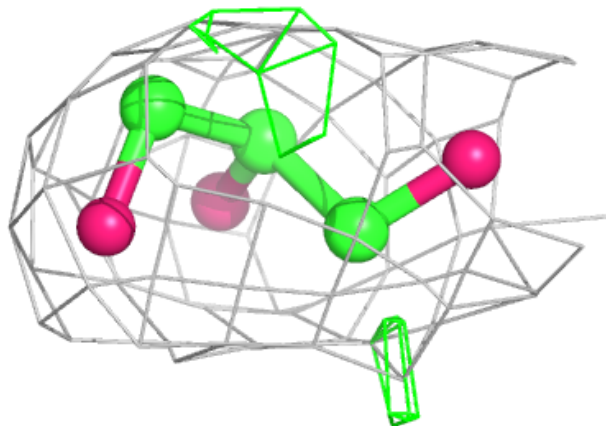
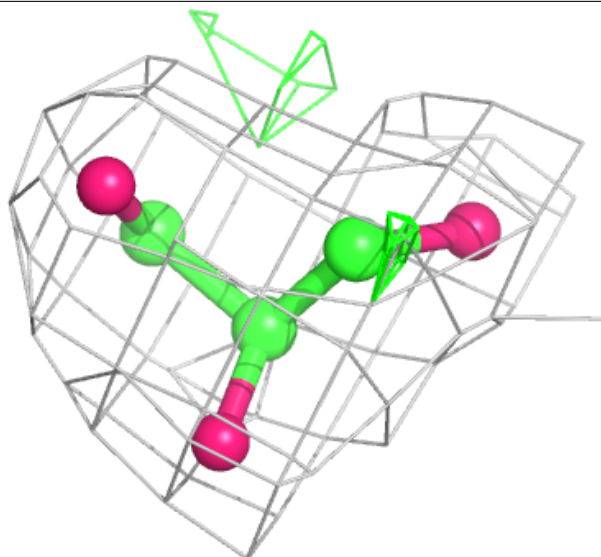
**Electron density around NAG E 1006:**

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and green (positive)



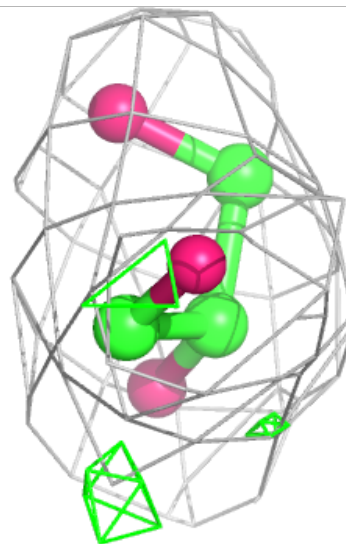
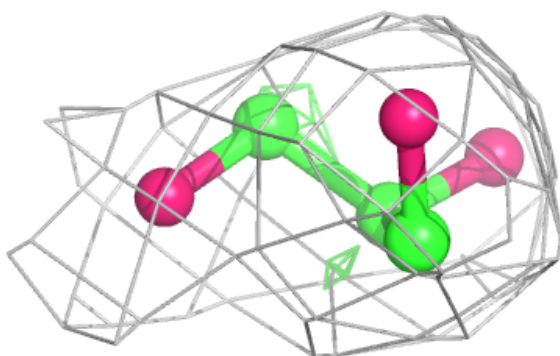
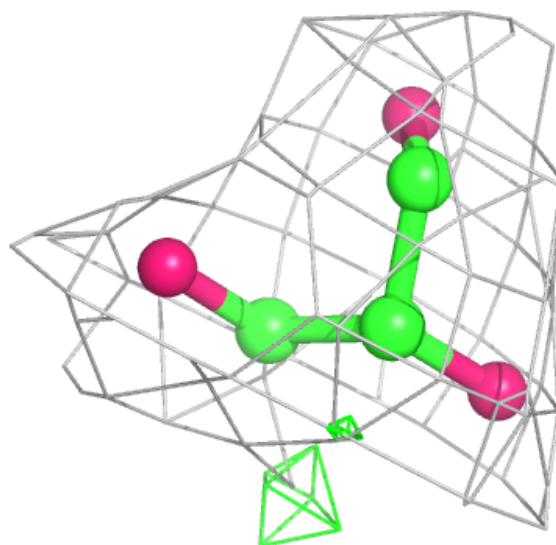
**Electron density around GOL A 1007:**

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



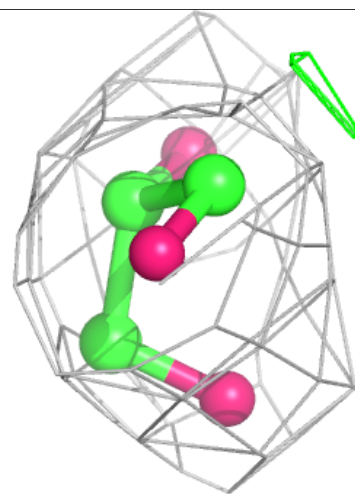
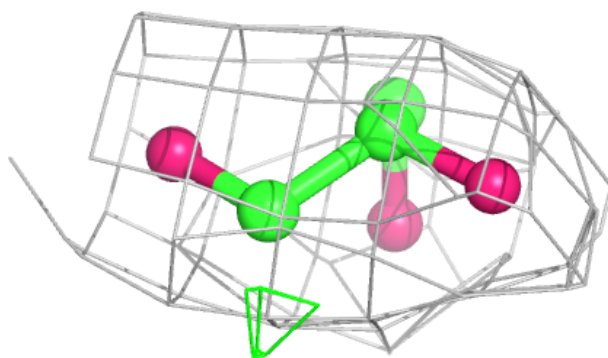
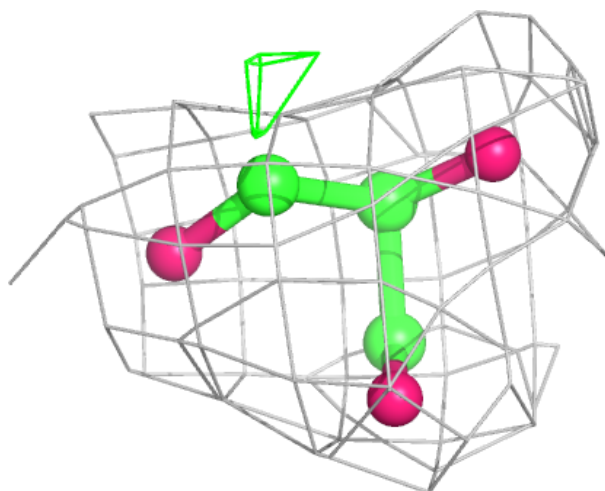
**Electron density around GOL C 1007:**

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



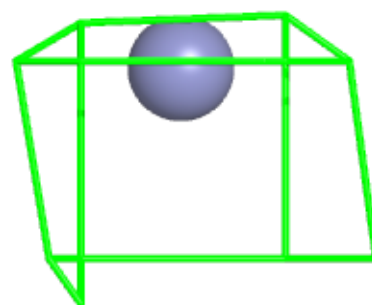
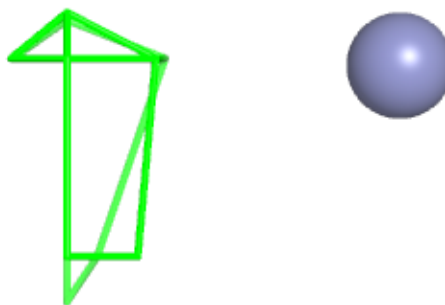
**Electron density around GOL E 1007:**

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and green (positive)



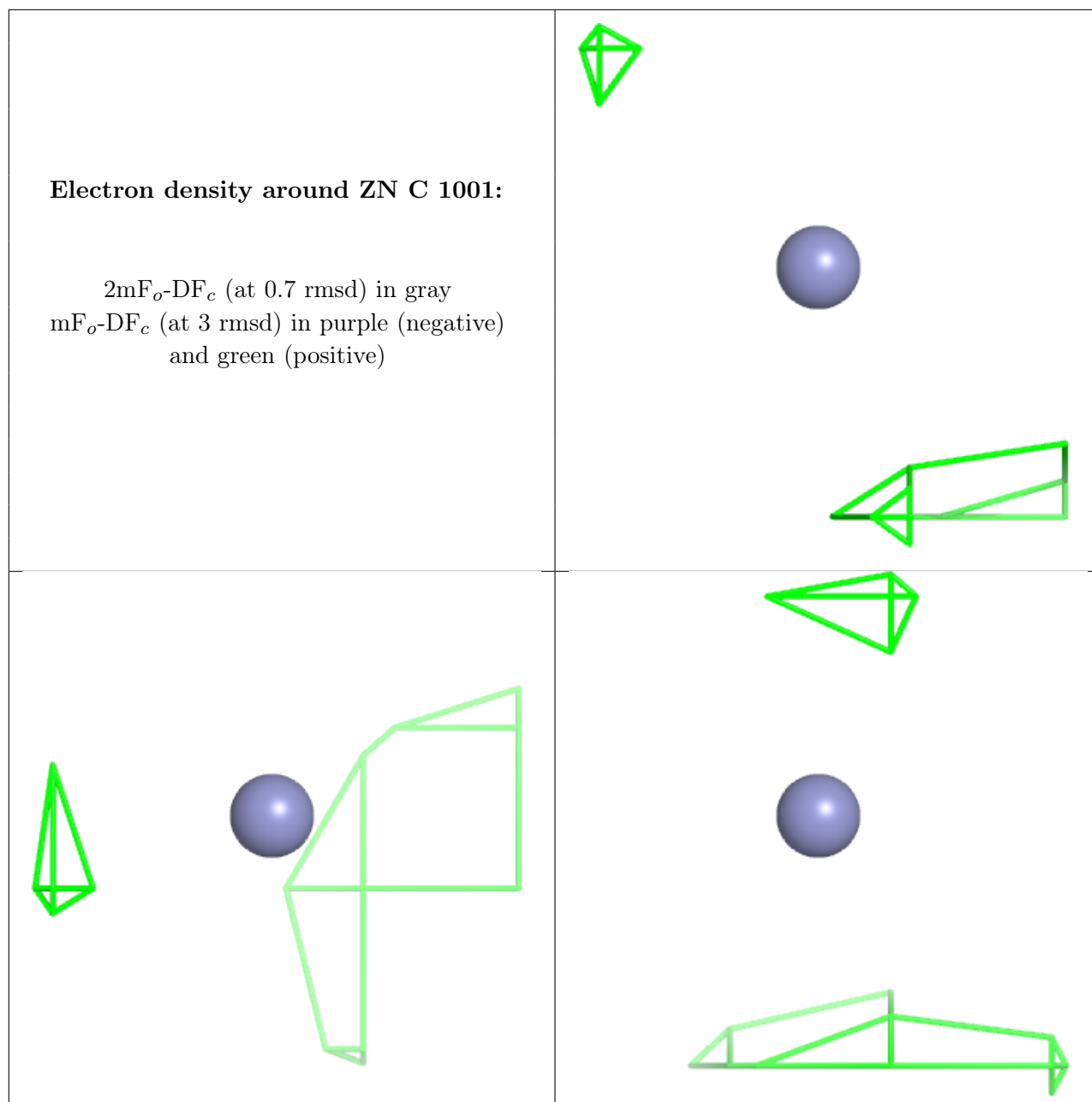
**Electron density around ZN E 1001:**

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and green (positive)



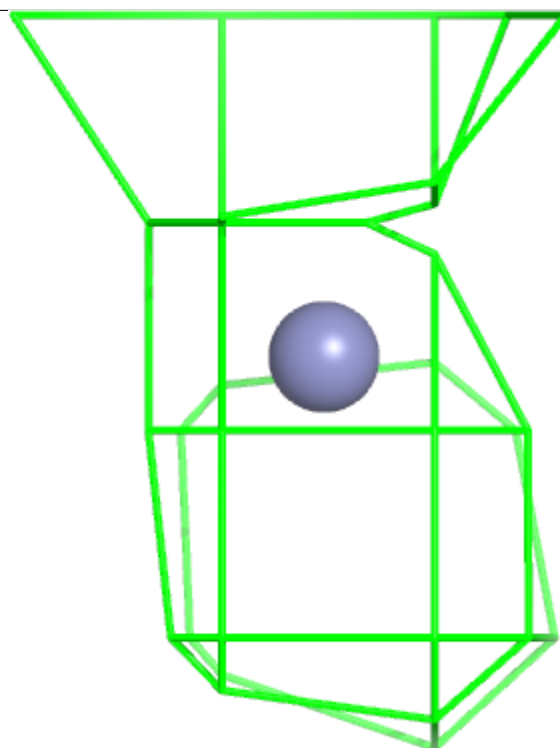
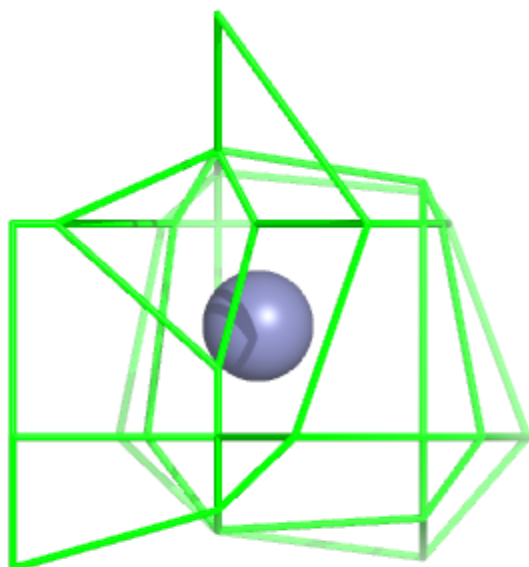
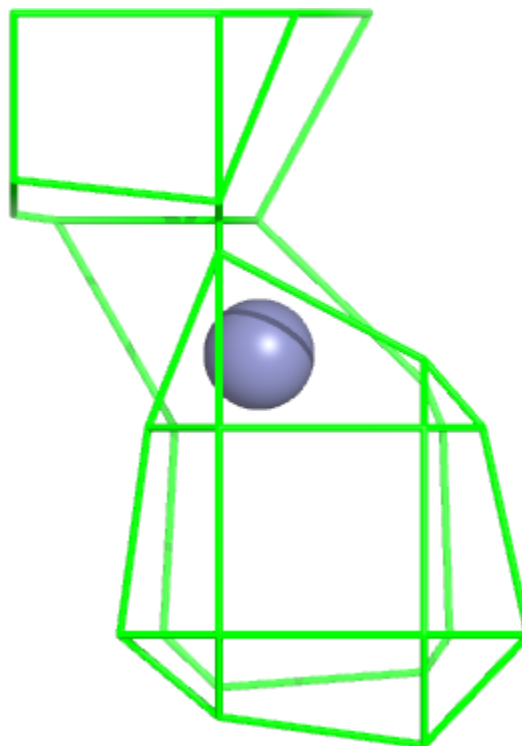
**Electron density around ZN C 1001:**

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



**Electron density around ZN A 1001:**

$2mF_o-DF_c$  (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.