



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2020 – 12:17 PM JST

PDB ID : 6LKS  
Title : Effects of zinc ion on oligomerization and pH stability of influenza virus hemagglutinin  
Authors : Seok, J.; Kim, K.  
Deposited on : 2019-12-20  
Resolution : 3.24 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 : 2.14.6  
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) : 2.14.6

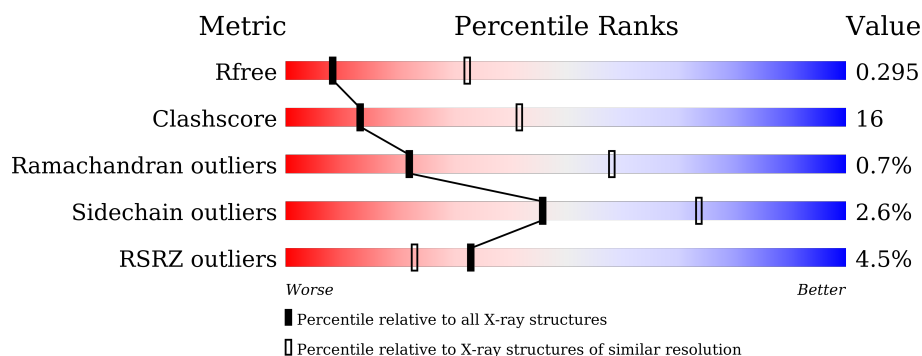
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.24 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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 on 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	330	<div> <div>2%</div> <div>58%</div> <div>37%</div> <div>..</div> </div>
1	C	330	<div> <div>2%</div> <div>66%</div> <div>29%</div> <div>..</div> </div>
1	E	330	<div> <div>61%</div> <div>35%</div> <div>..</div> </div>
1	G	330	<div> <div>62%</div> <div>33%</div> <div>..</div> </div>
1	I	330	<div> <div>3%</div> <div>61%</div> <div>33%</div> <div>..</div> </div>
1	K	330	<div> <div>2%</div> <div>64%</div> <div>31%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	183	
2	D	183	
2	F	183	
2	H	183	
2	J	183	
2	L	183	
3	M	6	
3	S	6	
3	V	6	
4	N	5	
4	P	5	
5	O	4	
5	Q	4	
5	R	4	
5	T	4	
5	U	4	
5	X	4	
6	W	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	M	5	-	-	-	X
3	MAN	S	4	-	-	-	X
3	NAG	V	5	-	-	-	X
7	NAG	A	412	-	-	-	X
7	NAG	I	410	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24413 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 HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	321	Total	C	N	O	S	0	0	0
			2515	1591	436	477	11			
1	A	321	Total	C	N	O	S	0	0	0
			2515	1591	436	477	11			
1	C	321	Total	C	N	O	S	0	0	0
			2515	1591	436	477	11			
1	E	321	Total	C	N	O	S	0	0	0
			2515	1591	436	477	11			
1	G	320	Total	C	N	O	S	0	0	0
			2507	1585	435	476	11			
1	I	320	Total	C	N	O	S	0	0	0
			2507	1585	435	476	11			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	ALA	-	expression tag	UNP A7LI25
K	-2	ASP	-	expression tag	UNP A7LI25
K	-1	PRO	-	expression tag	UNP A7LI25
K	0	GLY	-	expression tag	UNP A7LI25
K	116	ILE	MET	conflict	UNP A7LI25
A	-3	ALA	-	expression tag	UNP A7LI25
A	-2	ASP	-	expression tag	UNP A7LI25
A	-1	PRO	-	expression tag	UNP A7LI25
A	0	GLY	-	expression tag	UNP A7LI25
A	116	ILE	MET	conflict	UNP A7LI25
C	-3	ALA	-	expression tag	UNP A7LI25
C	-2	ASP	-	expression tag	UNP A7LI25
C	-1	PRO	-	expression tag	UNP A7LI25
C	0	GLY	-	expression tag	UNP A7LI25
C	116	ILE	MET	conflict	UNP A7LI25
E	-3	ALA	-	expression tag	UNP A7LI25
E	-2	ASP	-	expression tag	UNP A7LI25

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	PRO	-	expression tag	UNP A7LI25
E	0	GLY	-	expression tag	UNP A7LI25
E	116	ILE	MET	conflict	UNP A7LI25
G	-3	ALA	-	expression tag	UNP A7LI25
G	-2	ASP	-	expression tag	UNP A7LI25
G	-1	PRO	-	expression tag	UNP A7LI25
G	0	GLY	-	expression tag	UNP A7LI25
G	116	ILE	MET	conflict	UNP A7LI25
I	-3	ALA	-	expression tag	UNP A7LI25
I	-2	ASP	-	expression tag	UNP A7LI25
I	-1	PRO	-	expression tag	UNP A7LI25
I	0	GLY	-	expression tag	UNP A7LI25
I	116	ILE	MET	conflict	UNP A7LI25

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			
2	B	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			
2	D	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			
2	F	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			
2	H	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			
2	J	165	Total	C	N	O	S	0	0	0
			1325	831	224	263	7			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	VAL	ILE	conflict	UNP A7LI25
L	169	SER	ASN	conflict	UNP A7LI25
L	177	SER	-	expression tag	UNP A7LI25
L	178	GLY	-	expression tag	UNP A7LI25
L	179	ARG	-	expression tag	UNP A7LI25
L	180	LEU	-	expression tag	UNP A7LI25
L	181	VAL	-	expression tag	UNP A7LI25
L	182	PRO	-	expression tag	UNP A7LI25
L	183	ARG	-	expression tag	UNP A7LI25

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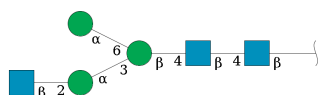
Chain	Residue	Modelled	Actual	Comment	Reference
B	91	VAL	ILE	conflict	UNP A7LI25
B	169	SER	ASN	conflict	UNP A7LI25
B	177	SER	-	expression tag	UNP A7LI25
B	178	GLY	-	expression tag	UNP A7LI25
B	179	ARG	-	expression tag	UNP A7LI25
B	180	LEU	-	expression tag	UNP A7LI25
B	181	VAL	-	expression tag	UNP A7LI25
B	182	PRO	-	expression tag	UNP A7LI25
B	183	ARG	-	expression tag	UNP A7LI25
D	91	VAL	ILE	conflict	UNP A7LI25
D	169	SER	ASN	conflict	UNP A7LI25
D	177	SER	-	expression tag	UNP A7LI25
D	178	GLY	-	expression tag	UNP A7LI25
D	179	ARG	-	expression tag	UNP A7LI25
D	180	LEU	-	expression tag	UNP A7LI25
D	181	VAL	-	expression tag	UNP A7LI25
D	182	PRO	-	expression tag	UNP A7LI25
D	183	ARG	-	expression tag	UNP A7LI25
F	91	VAL	ILE	conflict	UNP A7LI25
F	169	SER	ASN	conflict	UNP A7LI25
F	177	SER	-	expression tag	UNP A7LI25
F	178	GLY	-	expression tag	UNP A7LI25
F	179	ARG	-	expression tag	UNP A7LI25
F	180	LEU	-	expression tag	UNP A7LI25
F	181	VAL	-	expression tag	UNP A7LI25
F	182	PRO	-	expression tag	UNP A7LI25
F	183	ARG	-	expression tag	UNP A7LI25
H	91	VAL	ILE	conflict	UNP A7LI25
H	169	SER	ASN	conflict	UNP A7LI25
H	177	SER	-	expression tag	UNP A7LI25
H	178	GLY	-	expression tag	UNP A7LI25
H	179	ARG	-	expression tag	UNP A7LI25
H	180	LEU	-	expression tag	UNP A7LI25
H	181	VAL	-	expression tag	UNP A7LI25
H	182	PRO	-	expression tag	UNP A7LI25
H	183	ARG	-	expression tag	UNP A7LI25
J	91	VAL	ILE	conflict	UNP A7LI25
J	169	SER	ASN	conflict	UNP A7LI25
J	177	SER	-	expression tag	UNP A7LI25
J	178	GLY	-	expression tag	UNP A7LI25
J	179	ARG	-	expression tag	UNP A7LI25
J	180	LEU	-	expression tag	UNP A7LI25

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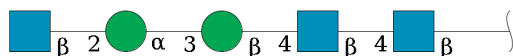
Chain	Residue	Modelled	Actual	Comment	Reference
J	181	VAL	-	expression tag	UNP A7LI25
J	182	PRO	-	expression tag	UNP A7LI25
J	183	ARG	-	expression tag	UNP A7LI25

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	0	0	0
			75	42	3	30			
3	S	6	Total	C	N	O	0	0	0
			75	42	3	30			
3	V	6	Total	C	N	O	0	0	0
			75	42	3	30			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-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
4	N	5	Total	C	N	O	0	0	0
			64	36	3	25			
4	P	5	Total	C	N	O	0	0	0
			64	36	3	25			

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



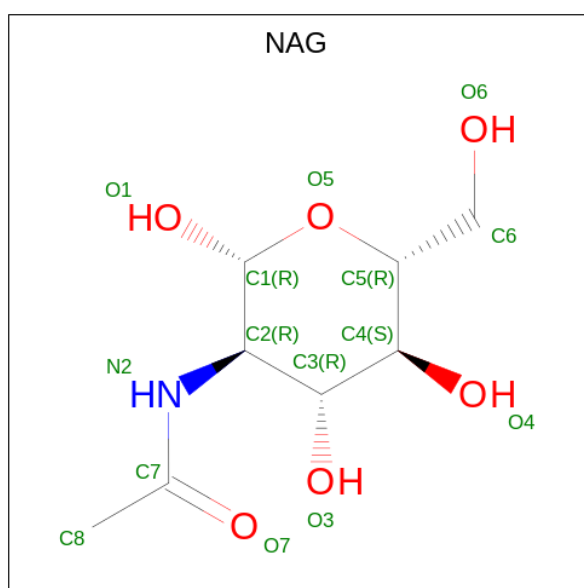
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	R	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	T	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	U	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 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
6	W	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 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 author).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total Zn 1 1	0	0
8	I	1	Total Zn 1 1	0	0
8	K	1	Total Zn 1 1	0	0

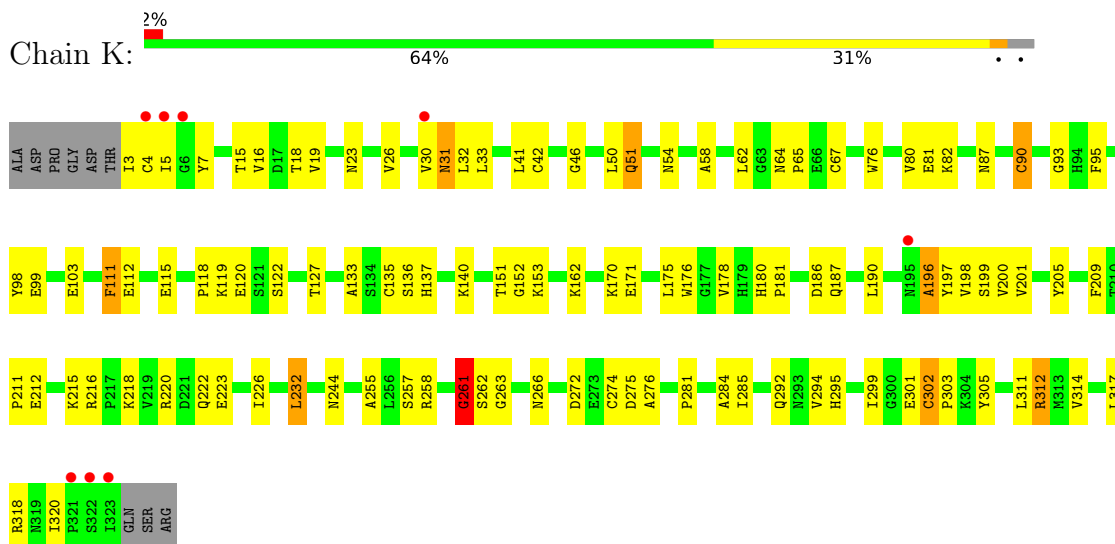
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	K	61	Total O 61 61	0	0
9	L	19	Total O 19 19	0	0
9	A	71	Total O 71 71	0	0
9	B	7	Total O 7 7	0	0
9	C	61	Total O 61 61	0	0
9	D	13	Total O 13 13	0	0
9	E	42	Total O 42 42	0	0
9	F	17	Total O 17 17	0	0
9	G	44	Total O 44 44	0	0
9	H	16	Total O 16 16	0	0
9	I	61	Total O 61 61	0	0
9	J	16	Total O 16 16	0	0

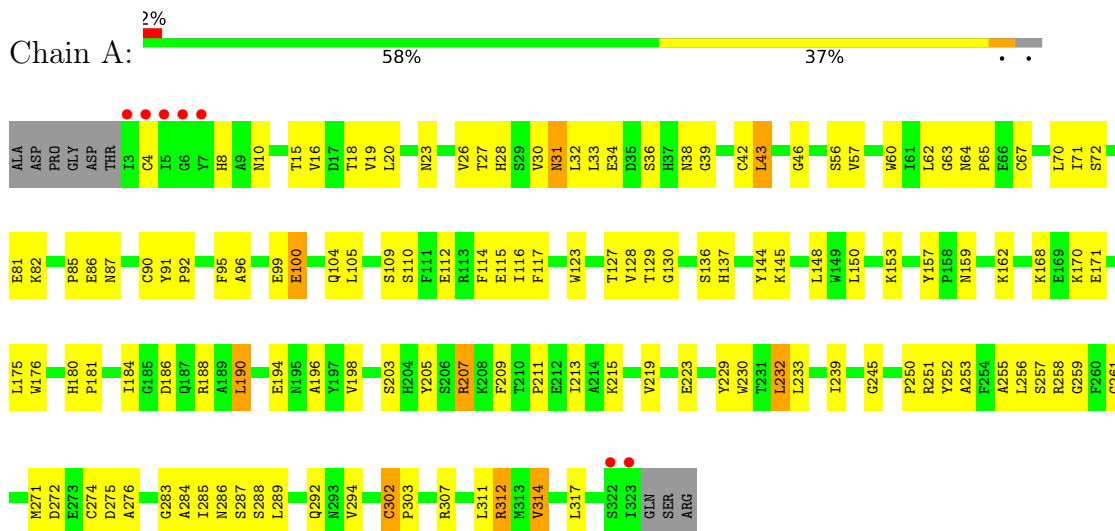
### 3 Residue-property plots [i](#)

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 HA1 chain

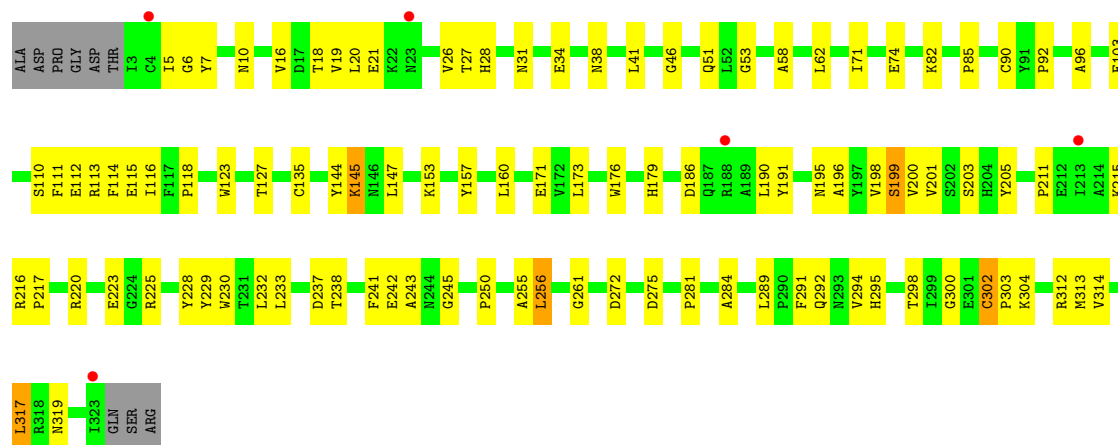


- Molecule 1: Hemagglutinin HA1 chain



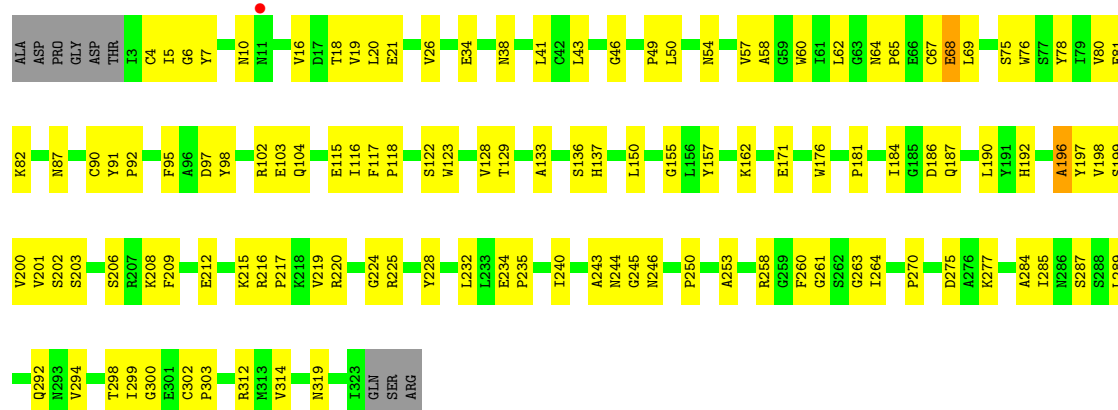
- Molecule 1: Hemagglutinin HA1 chain





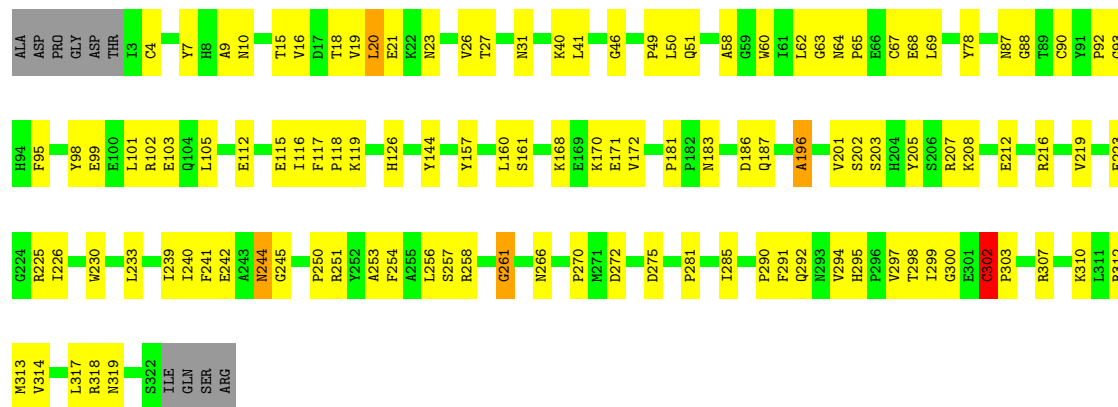
• Molecule 1: Hemagglutinin HA1 chain

Chain E: 61% 35% ..



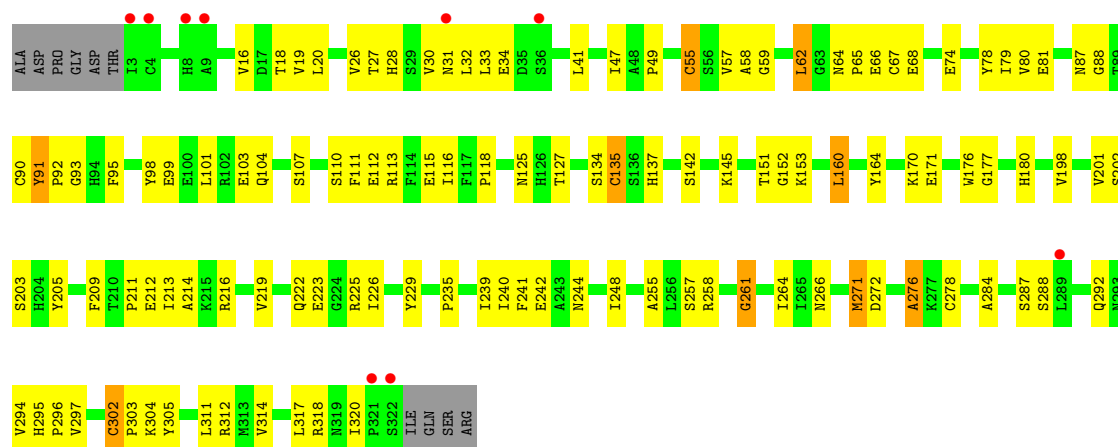
• Molecule 1: Hemagglutinin HA1 chain

Chain G: 62% 33% ..

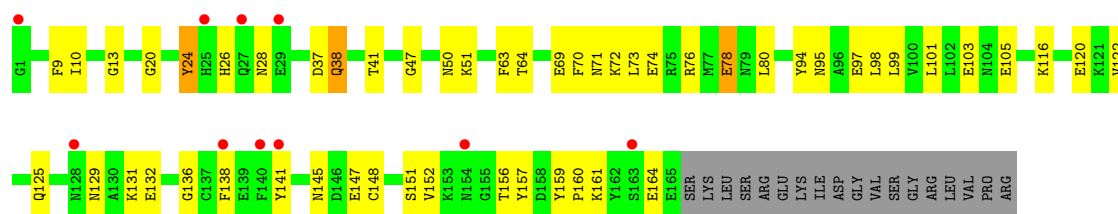


• Molecule 1: Hemagglutinin HA1 chain

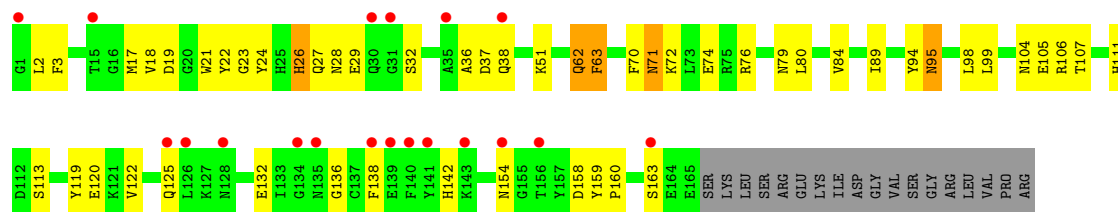
Chain I: 3% 61% 33% ..



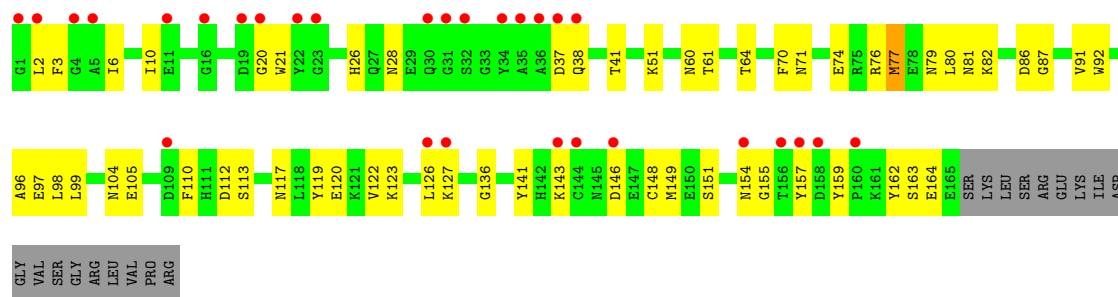
• Molecule 2: Hemagglutinin HA2 chain



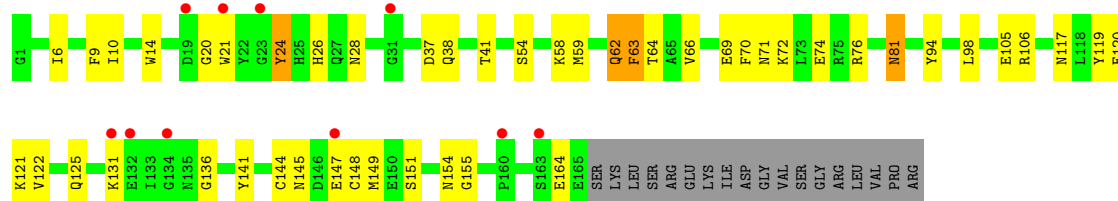
• Molecule 2: Hemagglutinin HA2 chain



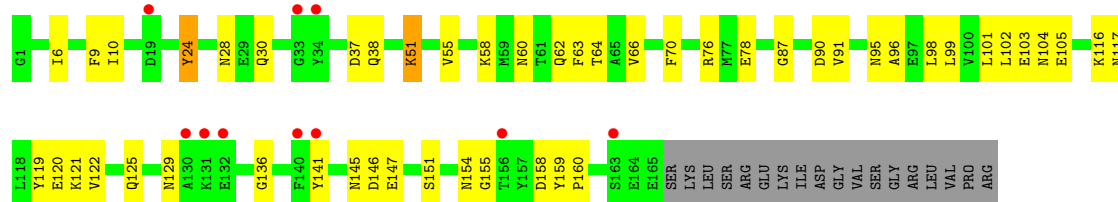
• Molecule 2: Hemagglutinin HA2 chain



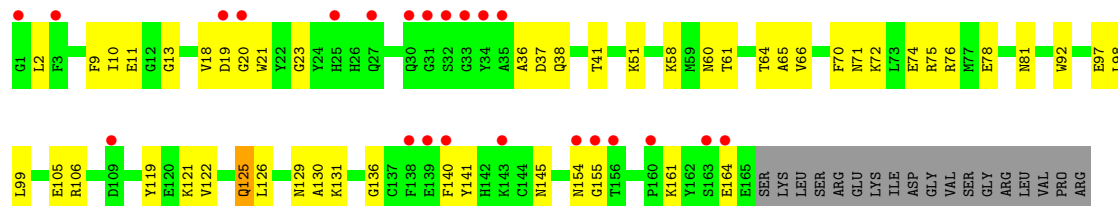
• Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



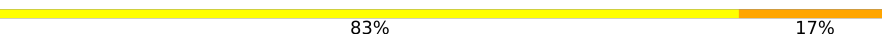
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain V:  83% 17%



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

Chain N:  40% 60%



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

Chain P:  60% 40%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  25% 50% 25%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%

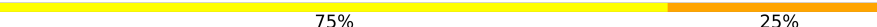


- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  75% 25%

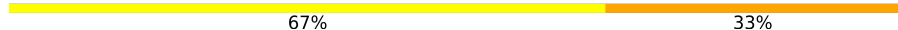
MAG1  
MAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  25% 50% 25%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  67% 33%

MAG1  
MAG2  
BMA3



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	215.71Å 124.27Å 214.53Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	48.75 – 3.24 48.75 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.75-3.24) 94.7 (48.75-3.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.265 , 0.295 0.265 , 0.295	Depositor DCC
$R_{free}$ test set	1999 reflections (2.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 62.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	24413	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6117e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ZN, BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.66	3/2581 (0.1%)	0.90	4/3512 (0.1%)
1	C	0.65	0/2581	0.85	2/3512 (0.1%)
1	E	0.63	1/2581 (0.0%)	0.88	3/3512 (0.1%)
1	G	0.64	1/2573 (0.0%)	0.86	2/3501 (0.1%)
1	I	0.66	3/2573 (0.1%)	0.89	4/3501 (0.1%)
1	K	0.63	1/2581 (0.0%)	0.86	3/3512 (0.1%)
2	B	0.46	0/1352	0.75	0/1819
2	D	0.43	0/1352	0.74	0/1819
2	F	0.52	0/1352	0.76	0/1819
2	H	0.53	0/1352	0.79	0/1819
2	J	0.49	0/1352	0.78	0/1819
2	L	0.55	1/1352 (0.1%)	0.80	1/1819 (0.1%)
All	All	0.60	10/23582 (0.0%)	0.84	19/31964 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	302	CYS	CB-SG	-7.29	1.69	1.82
1	A	100	GLU	CG-CD	6.17	1.61	1.51
1	I	47	ILE	C-N	5.49	1.46	1.34
1	A	100	GLU	CD-OE1	5.45	1.31	1.25
1	E	68	GLU	CG-CD	5.42	1.60	1.51

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	69	LEU	CA-CB-CG	-7.17	98.82	115.30
1	G	20	LEU	CA-CB-CG	6.96	131.31	115.30
1	C	256	LEU	CA-CB-CG	6.26	129.69	115.30
1	E	90	CYS	CA-CB-SG	6.23	125.21	114.00
1	A	190	LEU	CA-CB-CG	6.12	129.36	115.30

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	2515	0	2435	106	0
1	C	2515	0	2440	85	0
1	E	2515	0	2437	105	1
1	G	2507	0	2427	105	0
1	I	2507	0	2427	100	1
1	K	2515	0	2439	89	0
2	B	1325	0	1246	47	0
2	D	1325	0	1246	51	0
2	F	1325	0	1246	52	0
2	H	1325	0	1246	46	0
2	J	1325	0	1246	50	0
2	L	1325	0	1246	49	0
3	M	75	0	64	5	0
3	S	75	0	64	2	0
3	V	75	0	64	5	0
4	N	64	0	55	6	0
4	P	64	0	55	4	0
5	O	50	0	43	1	0
5	Q	50	0	43	0	0
5	R	50	0	43	3	0
5	T	50	0	43	4	0
5	U	50	0	43	1	0
5	X	50	0	43	4	0
6	W	39	0	34	1	0
7	A	70	0	65	4	0
7	C	14	0	13	1	0
7	E	56	0	52	0	0
7	G	42	0	39	1	0
7	I	42	0	39	1	0
7	K	42	0	39	1	0
8	G	1	0	0	0	0
8	I	1	0	0	0	0
8	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	71	0	0	4	0
9	B	7	0	0	1	0
9	C	61	0	0	4	0
9	D	13	0	0	3	0
9	E	42	0	0	3	0
9	F	17	0	0	1	0
9	G	44	0	0	1	0
9	H	16	0	0	0	0
9	I	61	0	0	3	0
9	J	16	0	0	0	0
9	K	61	0	0	4	0
9	L	19	0	0	1	0
All	All	24413	0	22922	759	1

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 16.

The worst 5 of 759 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:G:310:LYS:HB3	1:G:312:ARG:HD3	1.41	1.02
1:E:19:VAL:HG12	2:F:105:GLU:HG3	1.36	1.01
2:J:71:ASN:HB3	2:J:74:GLU:HG3	1.41	1.00
1:K:87:ASN:HD22	4:N:1:NAG:H83	1.30	0.96
1:I:202:SER:HB3	1:I:205:TYR:HB3	1.53	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:GLU:OE2	1:I:68:GLU:OE2[3_555]	2.09	0.11

## 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	319/330 (97%)	291 (91%)	24 (8%)	4 (1%)	12	44
1	C	319/330 (97%)	290 (91%)	28 (9%)	1 (0%)	41	73
1	E	319/330 (97%)	291 (91%)	27 (8%)	1 (0%)	41	73
1	G	318/330 (96%)	289 (91%)	27 (8%)	2 (1%)	25	61
1	I	318/330 (96%)	288 (91%)	27 (8%)	3 (1%)	17	52
1	K	319/330 (97%)	290 (91%)	25 (8%)	4 (1%)	12	44
2	B	163/183 (89%)	143 (88%)	18 (11%)	2 (1%)	13	46
2	D	163/183 (89%)	146 (90%)	17 (10%)	0	100	100
2	F	163/183 (89%)	145 (89%)	16 (10%)	2 (1%)	13	46
2	H	163/183 (89%)	149 (91%)	14 (9%)	0	100	100
2	J	163/183 (89%)	146 (90%)	17 (10%)	0	100	100
2	L	163/183 (89%)	147 (90%)	16 (10%)	0	100	100
All	All	2890/3078 (94%)	2615 (90%)	256 (9%)	19 (1%)	22	58

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	32	LEU
1	A	32	LEU
2	B	62	GLN
2	B	63	PHE
2	F	62	GLN

### 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	281/288 (98%)	272 (97%)	9 (3%)	39	69
1	C	281/288 (98%)	271 (96%)	10 (4%)	35	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	281/288 (98%)	278 (99%)	3 (1%)	73	87
1	G	280/288 (97%)	277 (99%)	3 (1%)	73	87
1	I	280/288 (97%)	270 (96%)	10 (4%)	35	66
1	K	281/288 (98%)	273 (97%)	8 (3%)	43	72
2	B	141/157 (90%)	135 (96%)	6 (4%)	29	62
2	D	141/157 (90%)	136 (96%)	5 (4%)	36	67
2	F	141/157 (90%)	138 (98%)	3 (2%)	53	77
2	H	141/157 (90%)	136 (96%)	5 (4%)	36	67
2	J	141/157 (90%)	140 (99%)	1 (1%)	84	92
2	L	141/157 (90%)	138 (98%)	3 (2%)	53	77
All	All	2530/2670 (95%)	2464 (97%)	66 (3%)	46	74

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	135	CYS
2	D	77	MET
1	I	244	ASN
1	C	145	LYS
1	C	272	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	GLN
2	F	26	HIS
2	J	125	GLN
1	E	28	HIS
2	F	117	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

55 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	M	1	1,3	14,14,15	0.40	0	17,19,21	2.46	3 (17%)
3	NAG	M	2	3	14,14,15	1.25	1 (7%)	17,19,21	1.58	2 (11%)
3	BMA	M	3	3	11,11,12	2.19	4 (36%)	15,15,17	1.78	3 (20%)
3	MAN	M	4	3	11,11,12	2.60	3 (27%)	15,15,17	1.82	3 (20%)
3	NAG	M	5	3	14,14,15	0.87	2 (14%)	17,19,21	0.69	0
3	MAN	M	6	3	11,11,12	1.85	3 (27%)	15,15,17	1.66	3 (20%)
4	NAG	N	1	1,4	14,14,15	0.21	0	17,19,21	0.92	1 (5%)
4	NAG	N	2	4	14,14,15	0.82	1 (7%)	17,19,21	1.58	1 (5%)
4	BMA	N	3	4	11,11,12	1.75	3 (27%)	15,15,17	1.40	1 (6%)
4	MAN	N	4	4	11,11,12	2.19	4 (36%)	15,15,17	2.50	5 (33%)
4	NAG	N	5	4	14,14,15	0.76	0	17,19,21	0.89	1 (5%)
5	NAG	O	1	1,5	14,14,15	0.43	0	17,19,21	0.94	0
5	NAG	O	2	5	14,14,15	0.86	1 (7%)	17,19,21	1.68	3 (17%)
5	BMA	O	3	5	11,11,12	2.17	3 (27%)	15,15,17	2.18	3 (20%)
5	MAN	O	4	5	11,11,12	2.00	4 (36%)	15,15,17	1.93	5 (33%)
4	NAG	P	1	1,4	14,14,15	0.97	1 (7%)	17,19,21	0.87	1 (5%)
4	NAG	P	2	4	14,14,15	0.32	0	17,19,21	0.93	1 (5%)
4	BMA	P	3	4	11,11,12	2.66	3 (27%)	15,15,17	1.87	2 (13%)
4	MAN	P	4	4	11,11,12	4.00	7 (63%)	15,15,17	2.74	8 (53%)
4	NAG	P	5	4	14,14,15	1.00	1 (7%)	17,19,21	1.40	3 (17%)
5	NAG	Q	1	1,5	14,14,15	0.26	0	17,19,21	0.80	0
5	NAG	Q	2	5	14,14,15	0.36	0	17,19,21	1.23	0
5	BMA	Q	3	5	11,11,12	2.40	4 (36%)	15,15,17	2.23	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	Q	4	5	11,11,12	1.86	3 (27%)	15,15,17	1.34	3 (20%)
5	NAG	R	1	1,5	14,14,15	0.93	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	R	2	5	14,14,15	0.90	2 (14%)	17,19,21	1.10	1 (5%)
5	BMA	R	3	5	11,11,12	1.93	2 (18%)	15,15,17	2.19	6 (40%)
5	MAN	R	4	5	11,11,12	2.29	4 (36%)	15,15,17	1.50	3 (20%)
3	NAG	S	1	1,3	14,14,15	0.51	0	17,19,21	2.38	2 (11%)
3	NAG	S	2	3	14,14,15	0.91	1 (7%)	17,19,21	1.44	3 (17%)
3	BMA	S	3	3	11,11,12	3.49	7 (63%)	15,15,17	1.92	5 (33%)
3	MAN	S	4	3	11,11,12	3.00	6 (54%)	15,15,17	2.97	5 (33%)
3	NAG	S	5	3	14,14,15	2.78	2 (14%)	17,19,21	3.07	3 (17%)
3	MAN	S	6	3	11,11,12	2.84	7 (63%)	15,15,17	1.84	3 (20%)
5	NAG	T	1	1,5	14,14,15	0.44	0	17,19,21	0.89	1 (5%)
5	NAG	T	2	5	14,14,15	0.69	1 (7%)	17,19,21	1.64	2 (11%)
5	BMA	T	3	5	11,11,12	2.35	4 (36%)	15,15,17	2.59	6 (40%)
5	MAN	T	4	5	11,11,12	2.31	3 (27%)	15,15,17	1.52	4 (26%)
5	NAG	U	1	1,5	14,14,15	1.10	2 (14%)	17,19,21	1.53	2 (11%)
5	NAG	U	2	5	14,14,15	0.72	0	17,19,21	1.28	2 (11%)
5	BMA	U	3	5	11,11,12	2.26	5 (45%)	15,15,17	1.97	4 (26%)
5	MAN	U	4	5	11,11,12	2.33	5 (45%)	15,15,17	2.37	4 (26%)
3	NAG	V	1	1,3	14,14,15	0.35	0	17,19,21	1.13	2 (11%)
3	NAG	V	2	3	14,14,15	0.49	0	17,19,21	1.02	2 (11%)
3	BMA	V	3	3	11,11,12	1.73	1 (9%)	15,15,17	1.52	2 (13%)
3	MAN	V	4	3	11,11,12	3.40	5 (45%)	15,15,17	2.58	7 (46%)
3	NAG	V	5	3	14,14,15	1.90	2 (14%)	17,19,21	1.51	1 (5%)
3	MAN	V	6	3	11,11,12	1.93	3 (27%)	15,15,17	1.26	2 (13%)
6	NAG	W	1	1,6	14,14,15	0.71	1 (7%)	17,19,21	0.57	0
6	NAG	W	2	6	14,14,15	0.34	0	17,19,21	0.69	0
6	BMA	W	3	6	11,11,12	2.08	3 (27%)	15,15,17	2.03	5 (33%)
5	NAG	X	1	1,5	14,14,15	1.15	1 (7%)	17,19,21	1.05	2 (11%)
5	NAG	X	2	5	14,14,15	0.33	0	17,19,21	0.85	0
5	BMA	X	3	5	11,11,12	2.23	3 (27%)	15,15,17	1.74	3 (20%)
5	MAN	X	4	5	11,11,12	1.56	2 (18%)	15,15,17	1.45	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.



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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
5	MAN	T	4	5	-	0/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	U	2	5	-	4/6/23/26	0/1/1/1
5	BMA	U	3	5	-	0/2/19/22	0/1/1/1
5	MAN	U	4	5	-	1/2/19/22	1/1/1/1
3	NAG	V	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	1/6/23/26	0/1/1/1
3	BMA	V	3	3	-	2/2/19/22	0/1/1/1
3	MAN	V	4	3	-	2/2/19/22	0/1/1/1
3	NAG	V	5	3	-	2/6/23/26	0/1/1/1
3	MAN	V	6	3	-	0/2/19/22	0/1/1/1
6	NAG	W	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	BMA	W	3	6	-	1/2/19/22	0/1/1/1
5	NAG	X	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
5	BMA	X	3	5	-	1/2/19/22	1/1/1/1
5	MAN	X	4	5	-	1/2/19/22	1/1/1/1

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	5	NAG	O5-C1	9.78	1.59	1.43
4	P	4	MAN	C2-C3	8.04	1.64	1.52
4	P	4	MAN	O2-C2	6.77	1.57	1.43
3	S	3	BMA	C4-C5	6.67	1.67	1.53
3	V	4	MAN	O2-C2	6.34	1.56	1.43

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	5	NAG	C1-O5-C5	10.99	127.09	112.19
3	M	1	NAG	C1-O5-C5	8.25	123.37	112.19
3	S	1	NAG	C1-O5-C5	8.19	123.29	112.19
3	S	4	MAN	C1-O5-C5	8.10	123.16	112.19
3	V	4	MAN	C1-O5-C5	6.35	120.79	112.19

There are no chirality outliers.

5 of 111 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	1	NAG	C3-C2-N2-C7
3	S	5	NAG	C3-C2-N2-C7
4	P	2	NAG	O5-C5-C6-O6
3	M	5	NAG	C4-C5-C6-O6
5	Q	4	MAN	C4-C5-C6-O6

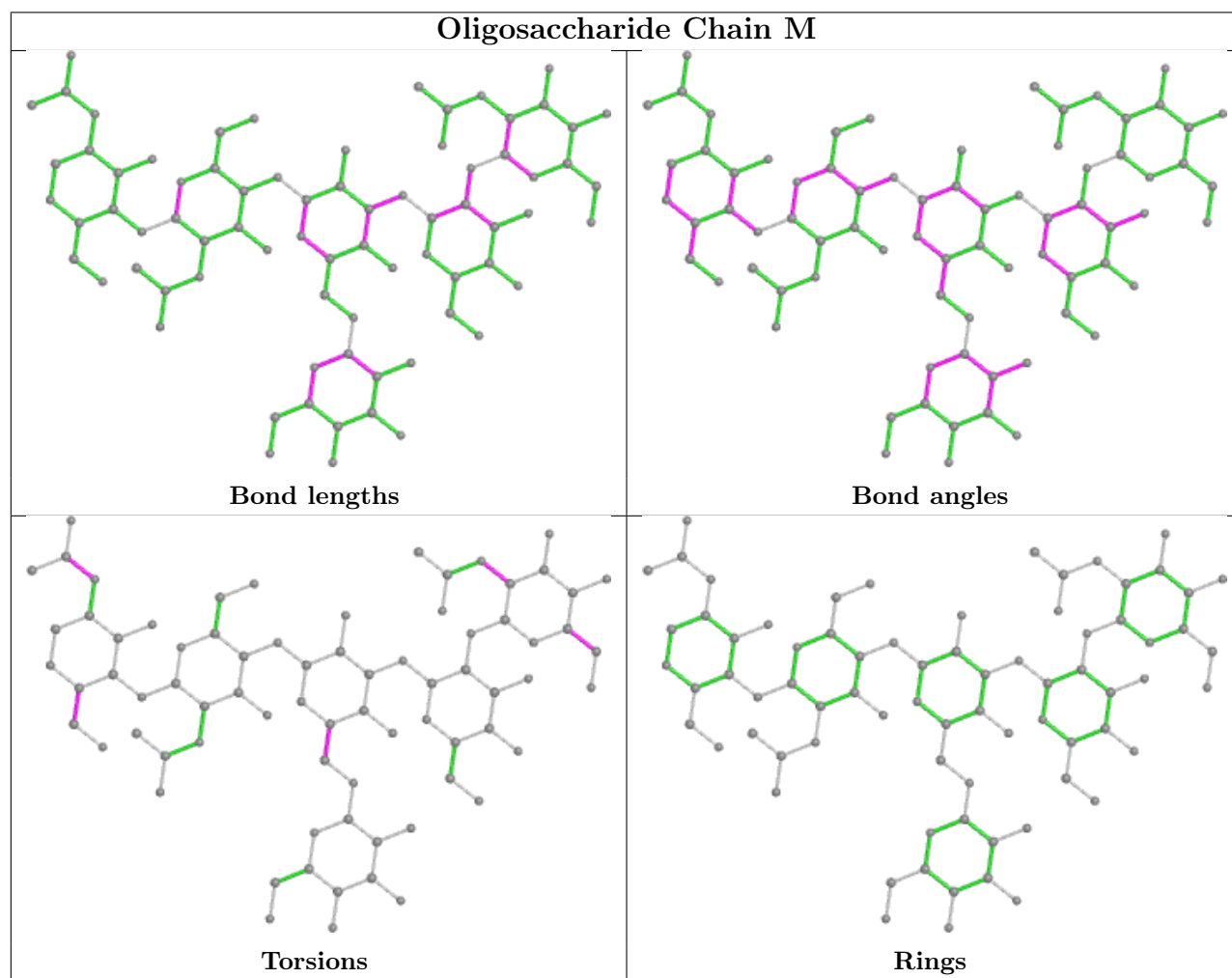
5 of 6 ring outliers are listed below:

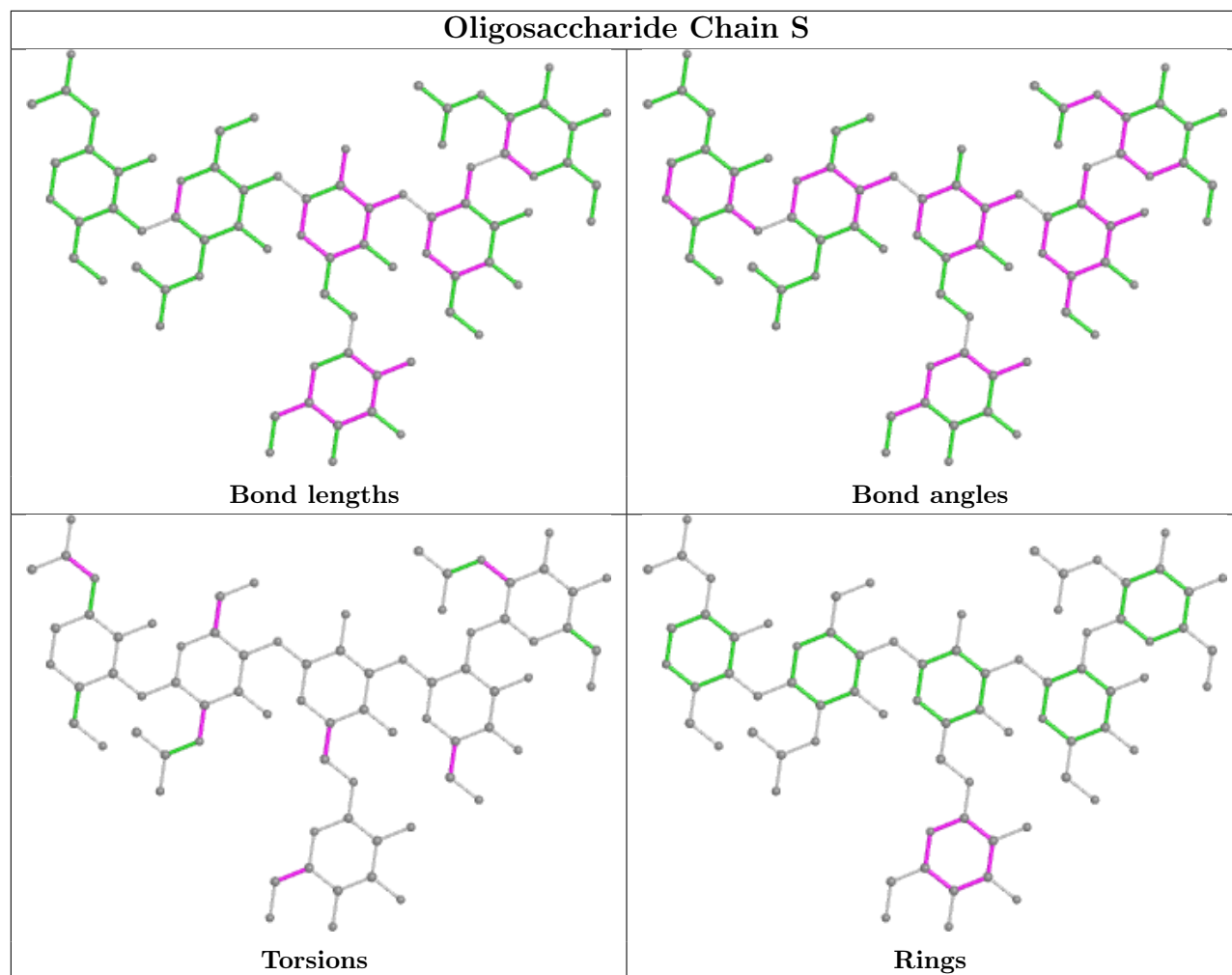
Mol	Chain	Res	Type	Atoms
5	X	3	BMA	C1-C2-C3-C4-C5-O5
3	S	6	MAN	C1-C2-C3-C4-C5-O5
5	U	4	MAN	C1-C2-C3-C4-C5-O5
5	Q	4	MAN	C1-C2-C3-C4-C5-O5
5	X	4	MAN	C1-C2-C3-C4-C5-O5

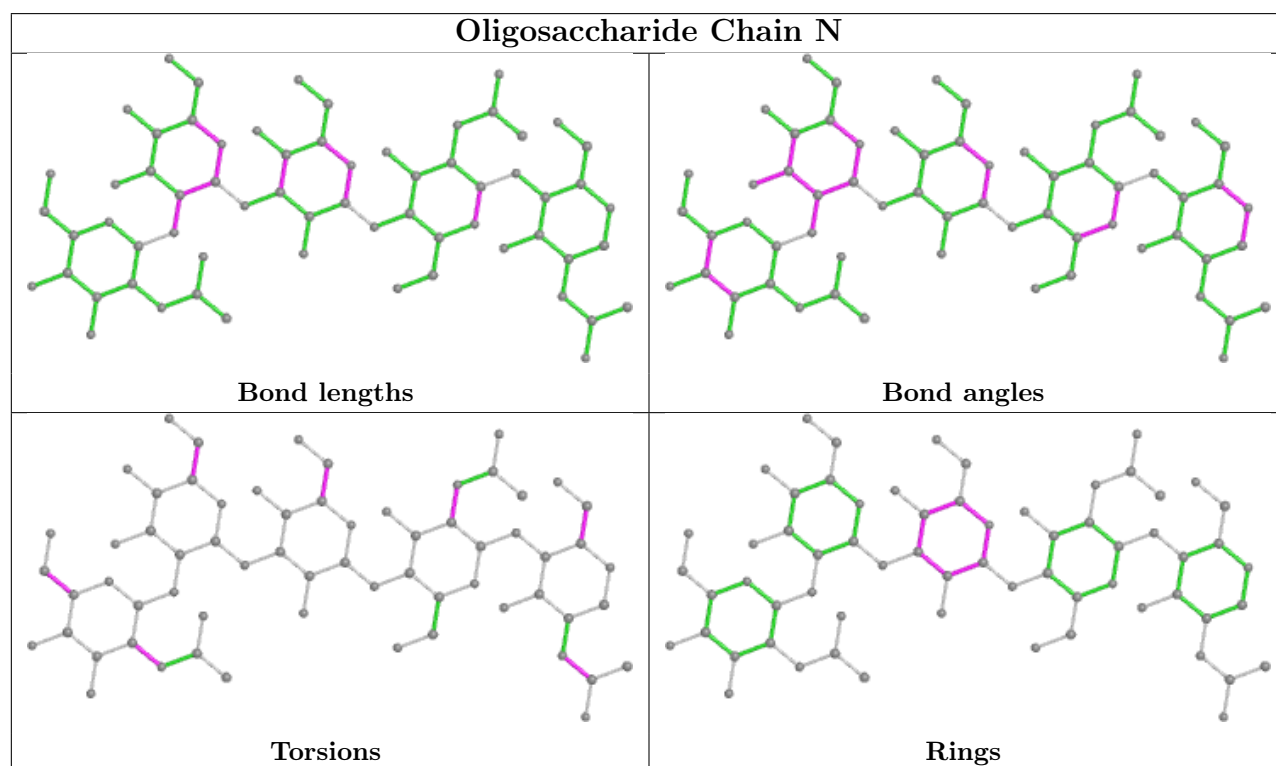
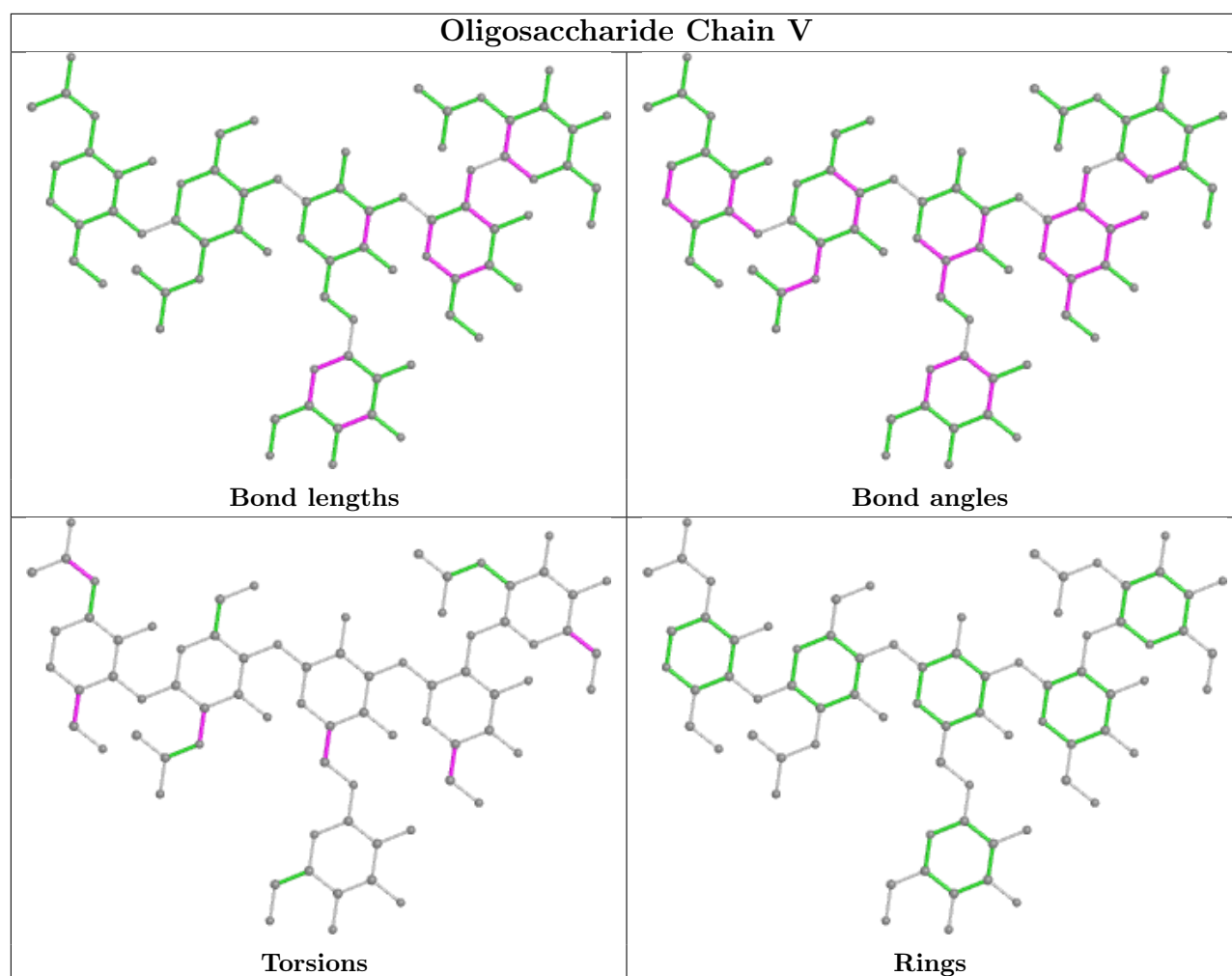
23 monomers are involved in 36 short contacts:

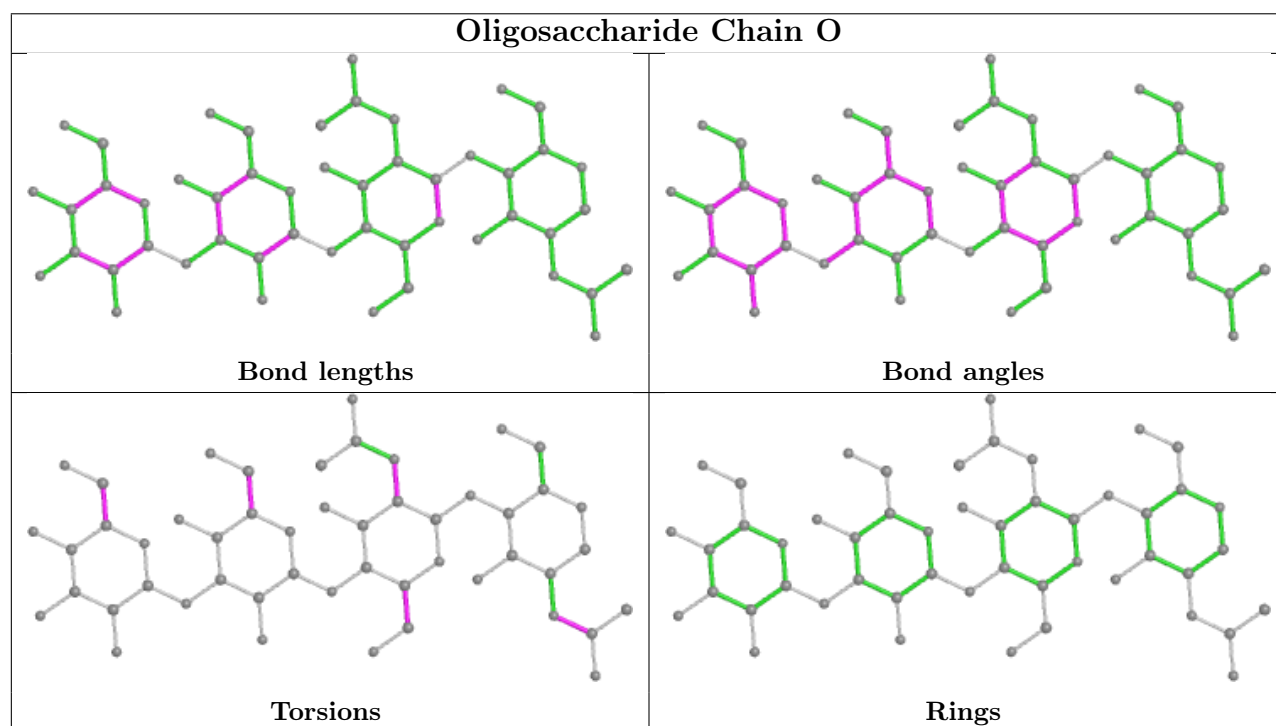
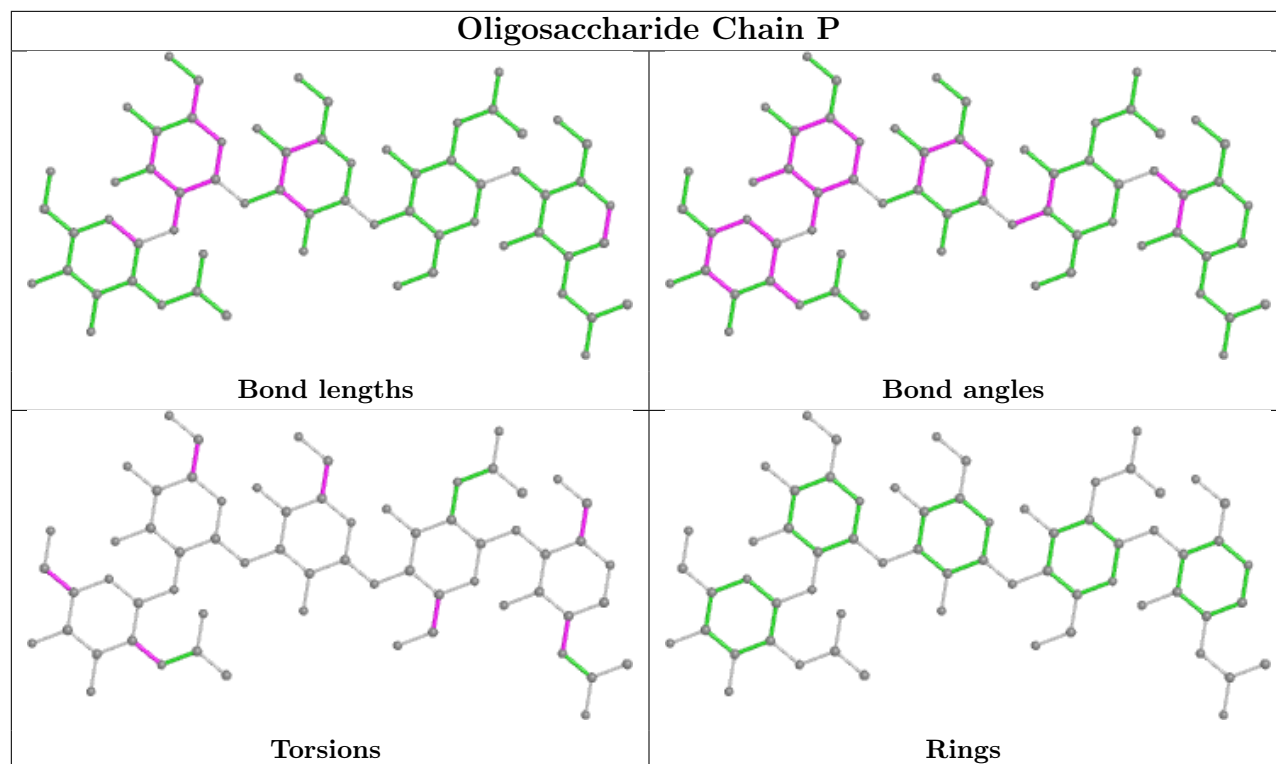
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	6	MAN	1	0
6	W	2	NAG	1	0
3	M	2	NAG	1	0
3	M	6	MAN	3	0
4	P	5	NAG	1	0
3	M	4	MAN	1	0
5	U	4	MAN	1	0
5	T	2	NAG	1	0
5	R	2	NAG	1	0
6	W	3	BMA	1	0
5	R	1	NAG	3	0
3	V	1	NAG	5	0
4	N	1	NAG	5	0
5	T	1	NAG	4	0
3	M	3	BMA	2	0
5	X	1	NAG	4	0
3	S	3	BMA	1	0
4	N	4	MAN	1	0
4	N	3	BMA	1	0
3	M	1	NAG	1	0
5	O	2	NAG	1	0
4	P	1	NAG	3	0
3	S	5	NAG	1	0

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

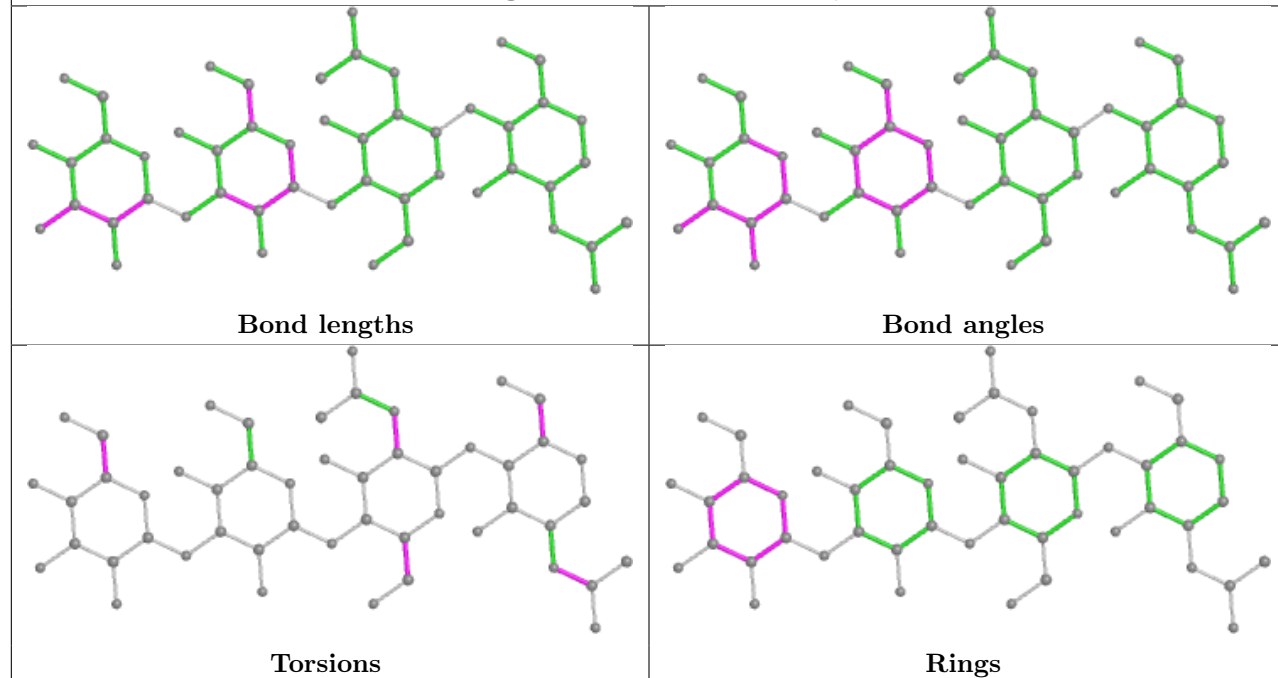




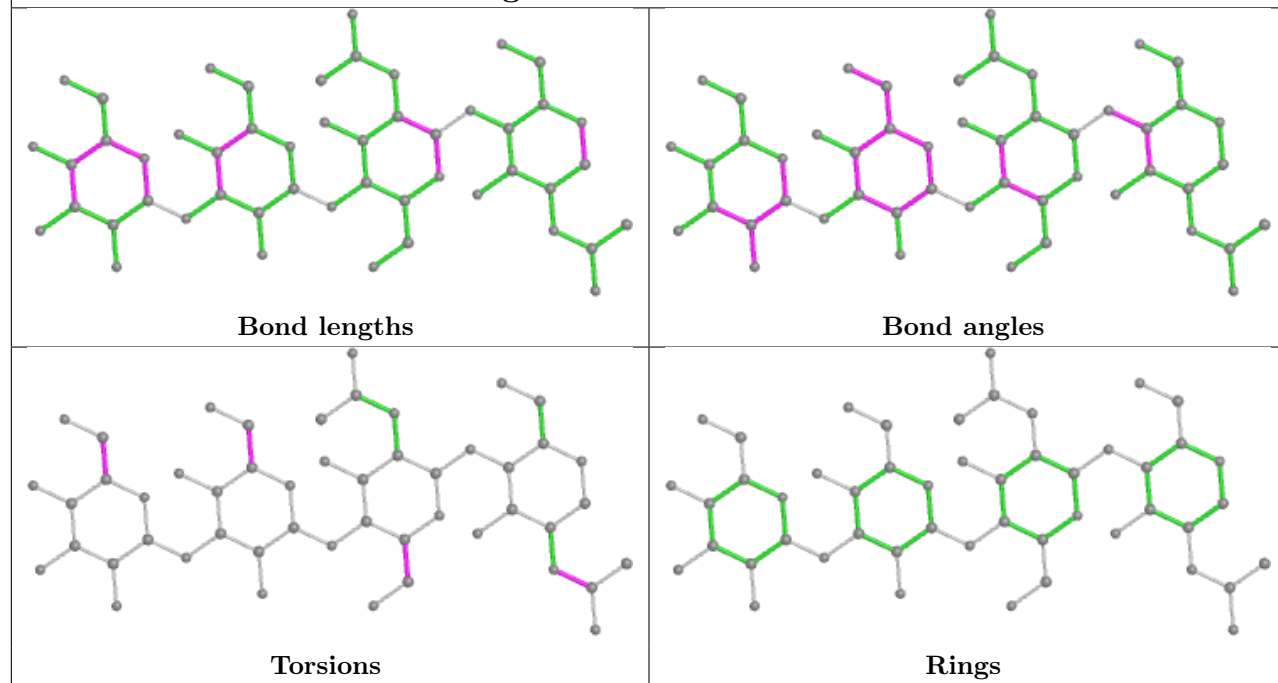




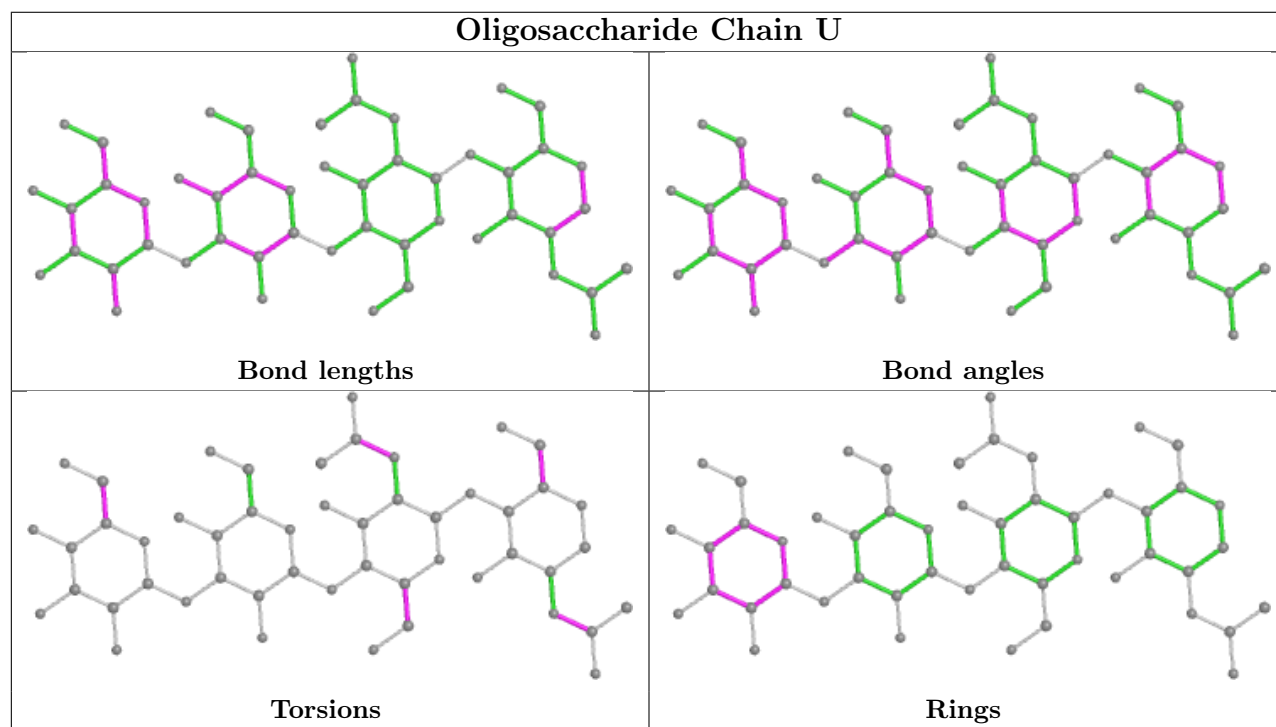
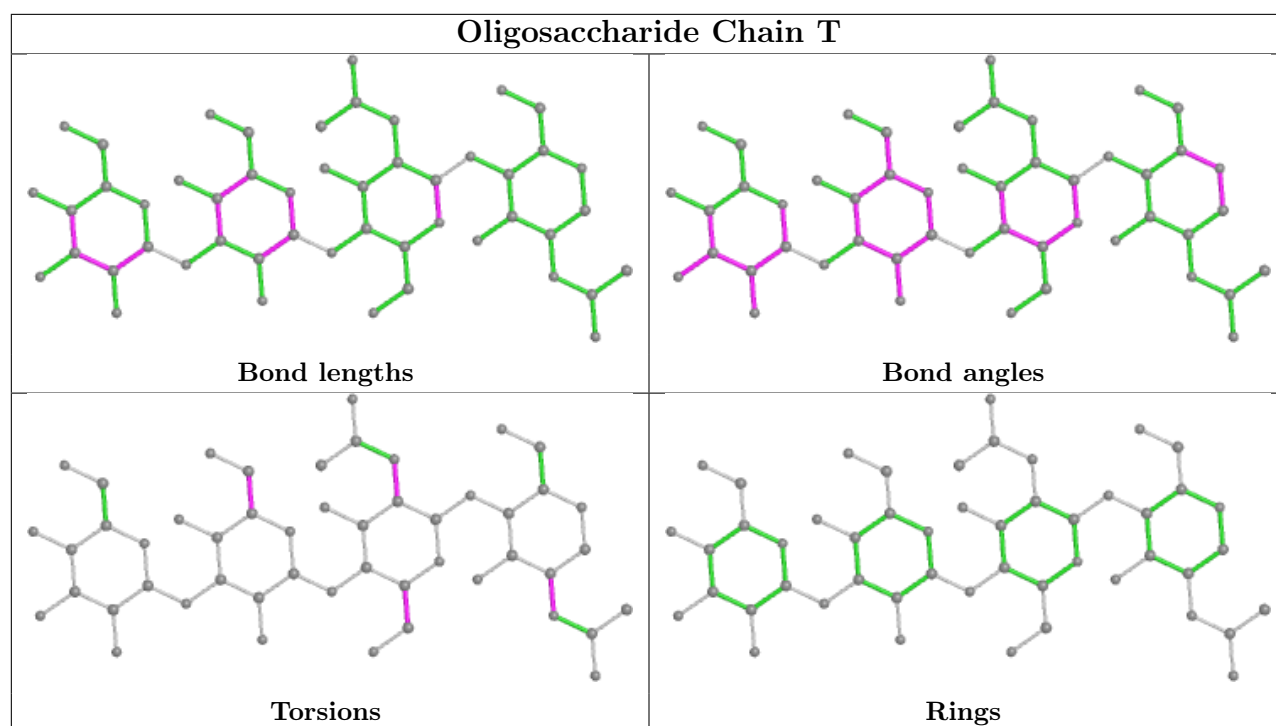
## Oligosaccharide Chain Q

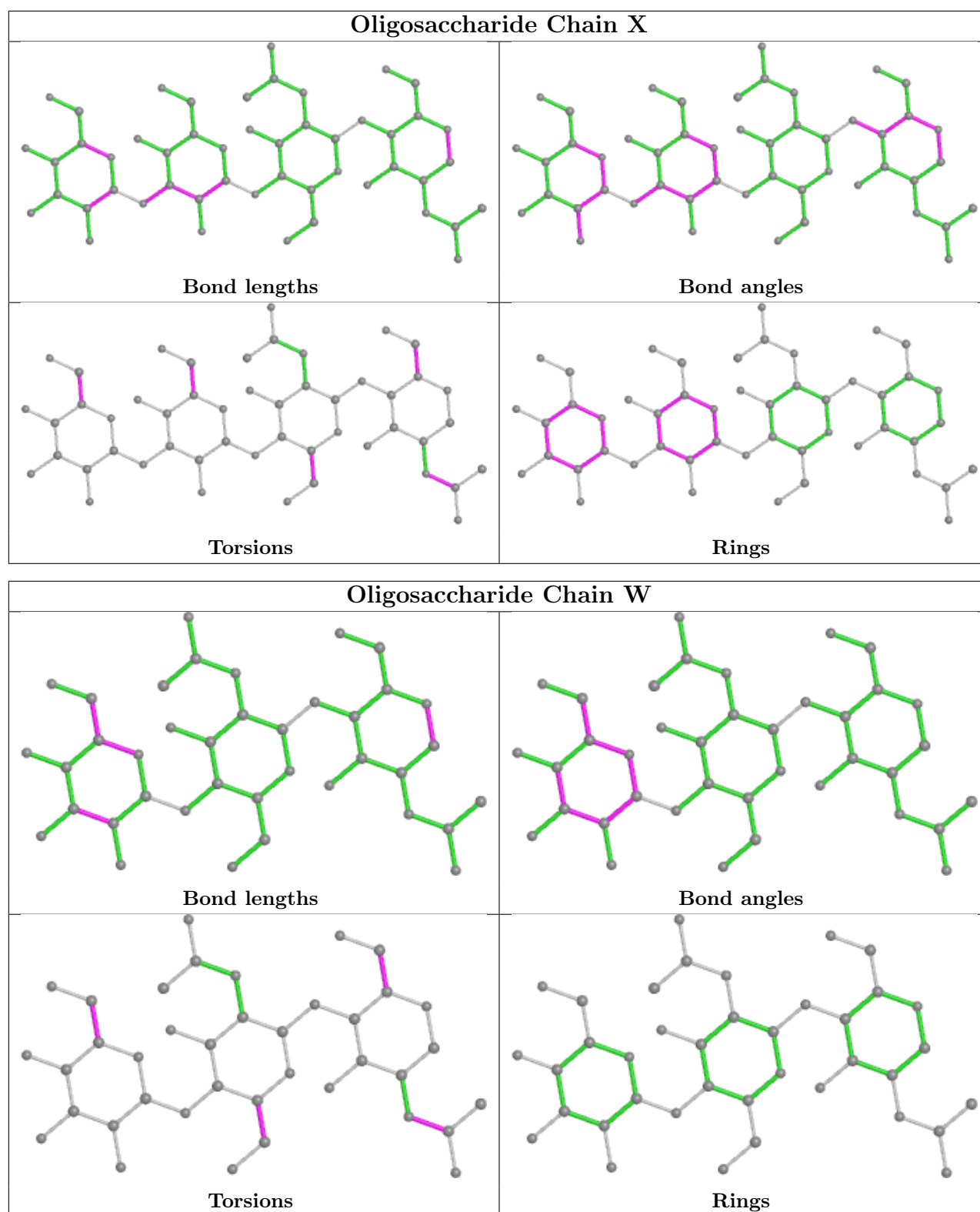


## Oligosaccharide Chain R









## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 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$
7	NAG	G	401	1	14,14,15	1.58	1 (7%)	17,19,21	1.87	1 (5%)
7	NAG	E	401	1	14,14,15	1.12	1 (7%)	17,19,21	0.75	0
7	NAG	G	402	1	14,14,15	0.96	1 (7%)	17,19,21	1.73	1 (5%)
7	NAG	A	402	1	14,14,15	0.78	1 (7%)	17,19,21	2.32	3 (17%)
7	NAG	E	412	1	14,14,15	1.16	1 (7%)	17,19,21	1.04	2 (11%)
7	NAG	I	410	1	14,14,15	0.22	0	17,19,21	0.82	0
7	NAG	K	401	1	14,14,15	0.70	1 (7%)	17,19,21	0.65	0
7	NAG	A	414	1	14,14,15	0.80	1 (7%)	17,19,21	0.64	0
7	NAG	K	413	1	14,14,15	0.43	0	17,19,21	0.66	0
7	NAG	K	414	1	14,14,15	1.08	2 (14%)	17,19,21	1.51	1 (5%)
7	NAG	A	401	1	14,14,15	0.85	1 (7%)	17,19,21	1.30	1 (5%)
7	NAG	E	414	1	14,14,15	2.00	2 (14%)	17,19,21	1.92	1 (5%)
7	NAG	G	413	1	14,14,15	2.14	2 (14%)	17,19,21	2.71	1 (5%)
7	NAG	I	401	1	14,14,15	0.49	0	17,19,21	0.47	0
7	NAG	E	413	1	14,14,15	0.63	1 (7%)	17,19,21	0.86	1 (5%)
7	NAG	A	412	1	14,14,15	1.81	2 (14%)	17,19,21	1.40	1 (5%)
7	NAG	A	413	1	14,14,15	1.72	2 (14%)	17,19,21	1.25	1 (5%)
7	NAG	C	409	1	14,14,15	0.63	0	17,19,21	0.64	0
7	NAG	I	409	1	14,14,15	0.47	0	17,19,21	1.18	1 (5%)

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
7	NAG	G	401	1	-	3/6/23/26	0/1/1/1
7	NAG	E	401	1	-	4/6/23/26	0/1/1/1
7	NAG	G	402	1	-	4/6/23/26	0/1/1/1
7	NAG	A	402	1	-	3/6/23/26	0/1/1/1
7	NAG	E	412	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	I	410	1	-	3/6/23/26	0/1/1/1
7	NAG	K	401	1	-	4/6/23/26	0/1/1/1
7	NAG	A	414	1	-	4/6/23/26	0/1/1/1
7	NAG	K	413	1	-	4/6/23/26	0/1/1/1
7	NAG	K	414	1	-	2/6/23/26	0/1/1/1
7	NAG	A	401	1	-	3/6/23/26	0/1/1/1
7	NAG	E	414	1	-	3/6/23/26	0/1/1/1
7	NAG	G	413	1	-	2/6/23/26	0/1/1/1
7	NAG	I	401	1	-	3/6/23/26	0/1/1/1
7	NAG	E	413	1	-	2/6/23/26	0/1/1/1
7	NAG	A	412	1	-	4/6/23/26	0/1/1/1
7	NAG	A	413	1	-	4/6/23/26	0/1/1/1
7	NAG	C	409	1	-	3/6/23/26	0/1/1/1
7	NAG	I	409	1	-	4/6/23/26	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	413	NAG	O5-C1	7.43	1.55	1.43
7	E	414	NAG	O5-C1	6.54	1.54	1.43
7	G	401	NAG	O5-C1	5.68	1.52	1.43
7	A	412	NAG	O5-C1	5.62	1.52	1.43
7	A	413	NAG	C1-C2	4.67	1.59	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	413	NAG	C1-O5-C5	11.06	127.17	112.19
7	E	414	NAG	C1-O5-C5	7.55	122.42	112.19
7	A	402	NAG	C1-O5-C5	7.29	122.07	112.19
7	G	401	NAG	C1-O5-C5	6.97	121.64	112.19
7	G	402	NAG	C1-O5-C5	6.57	121.09	112.19

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	412	NAG	C3-C2-N2-C7

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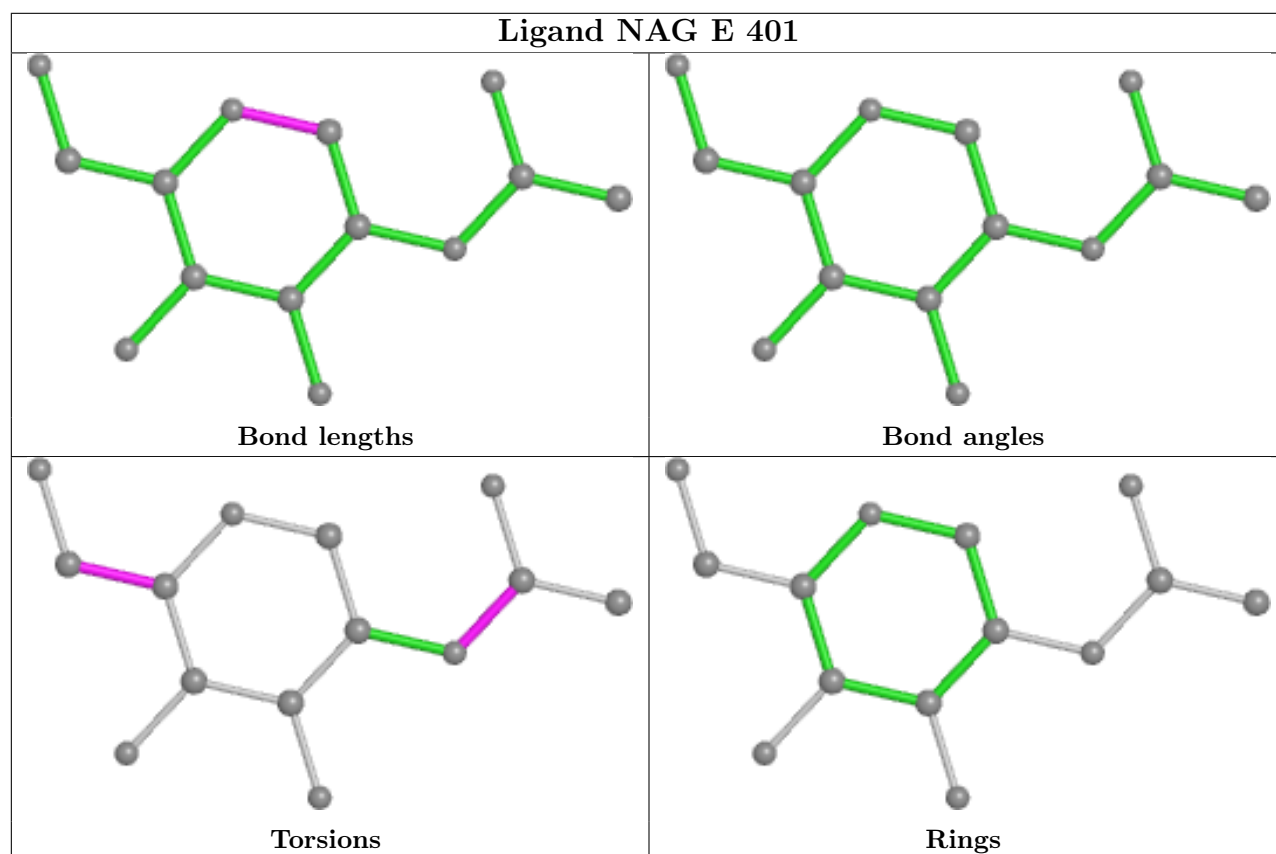
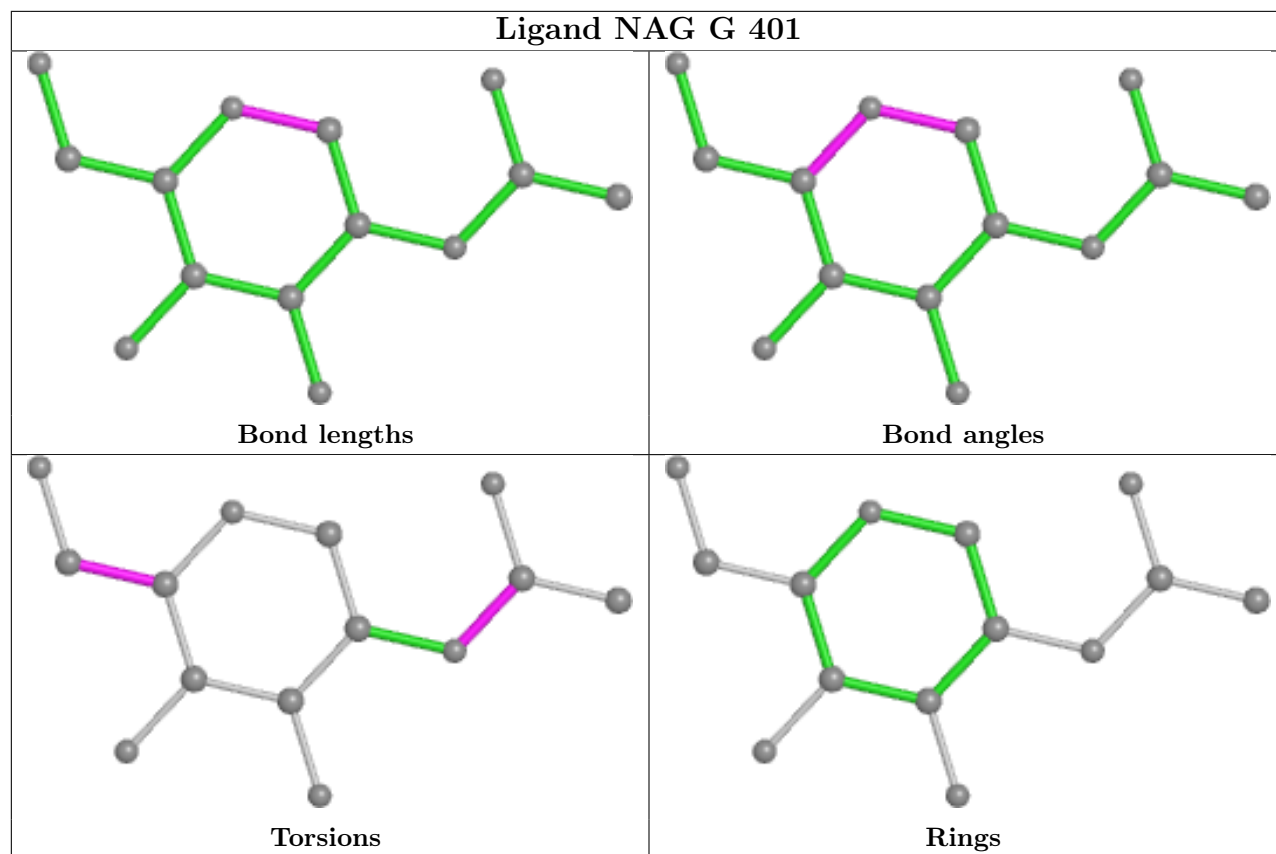
Mol	Chain	Res	Type	Atoms
7	E	401	NAG	O5-C5-C6-O6
7	I	410	NAG	O5-C5-C6-O6
7	A	414	NAG	O5-C5-C6-O6
7	E	413	NAG	O5-C5-C6-O6

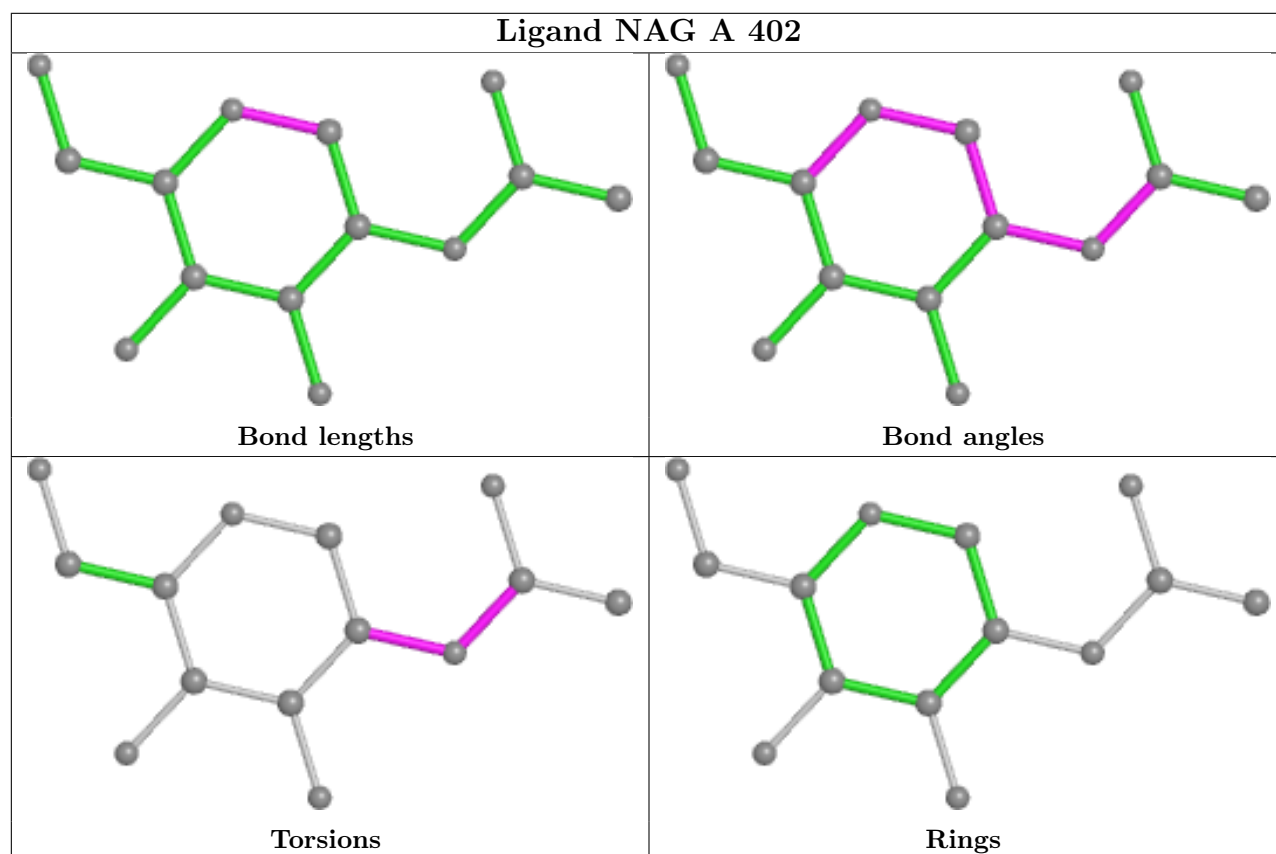
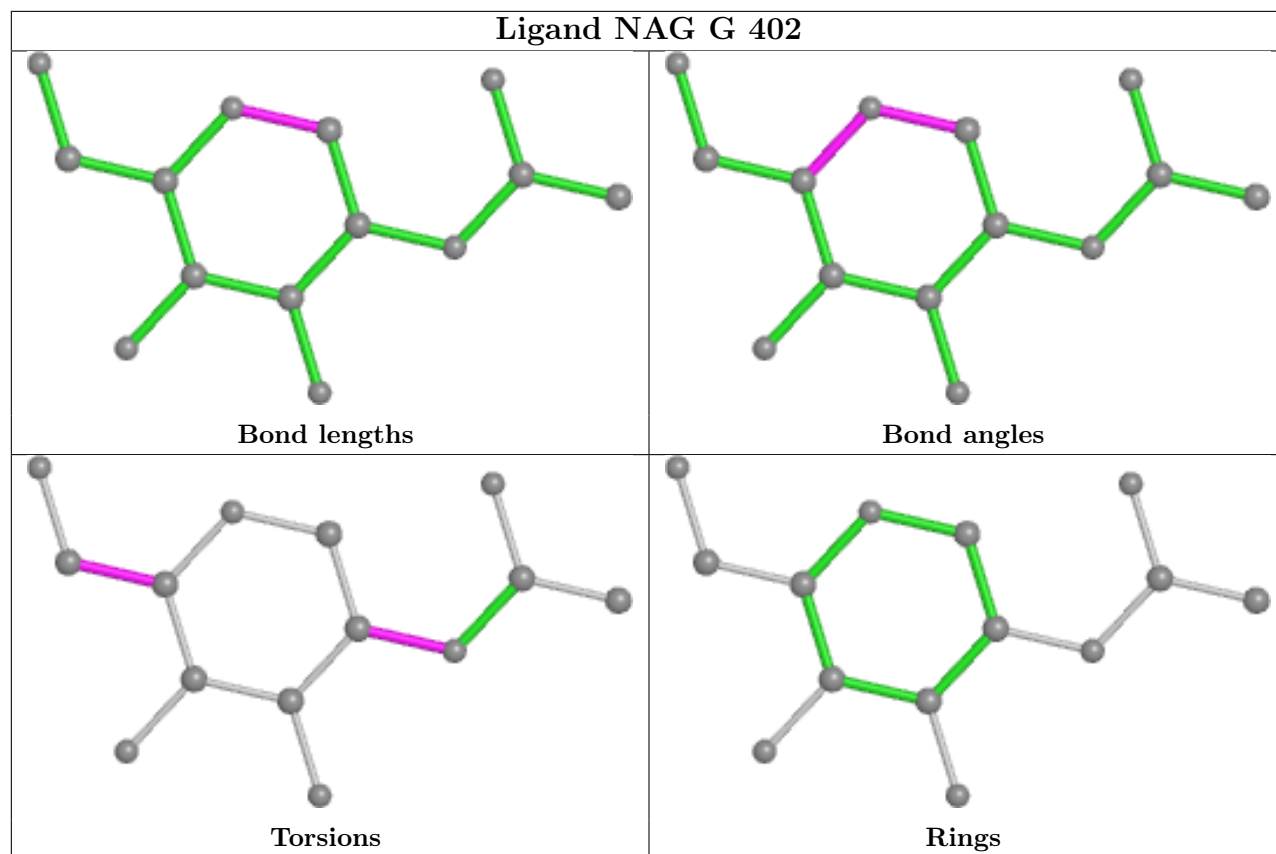
There are no ring outliers.

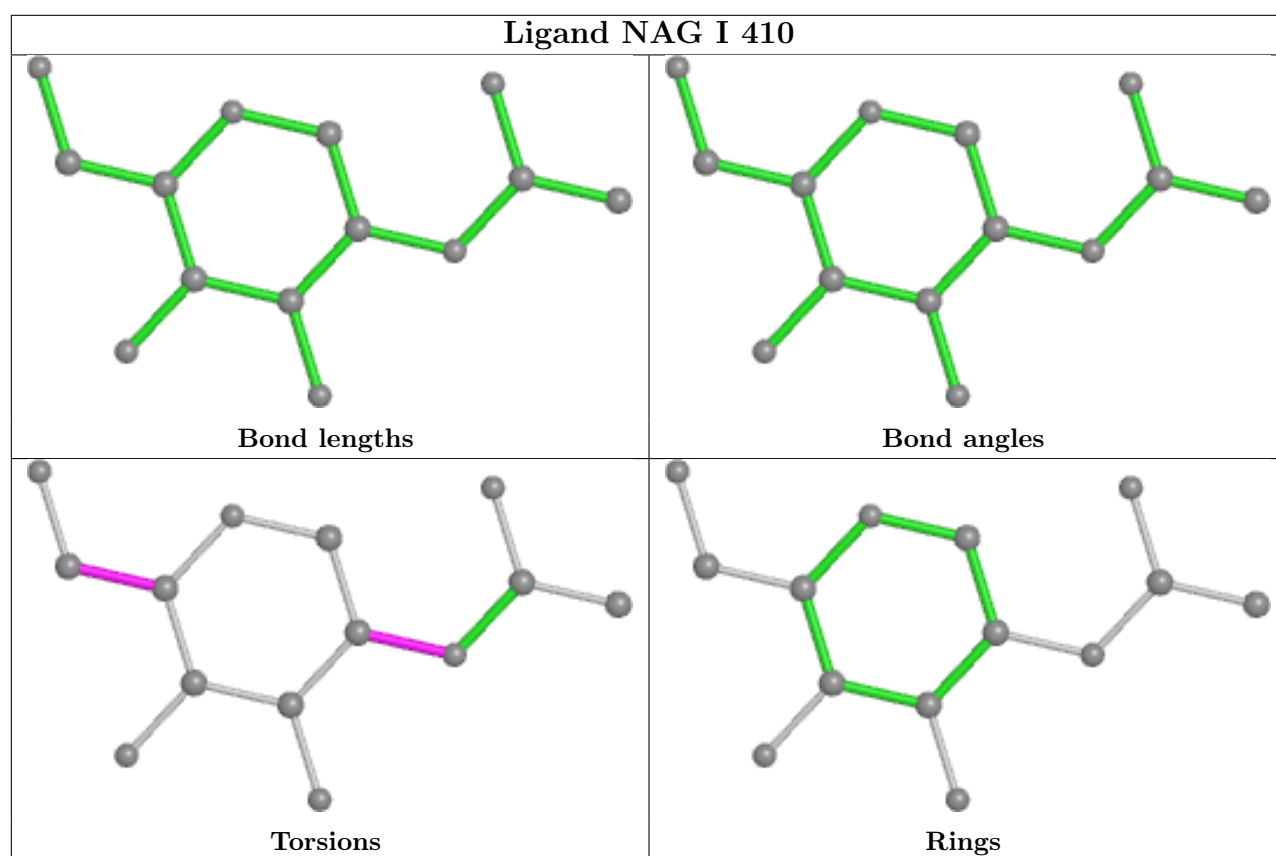
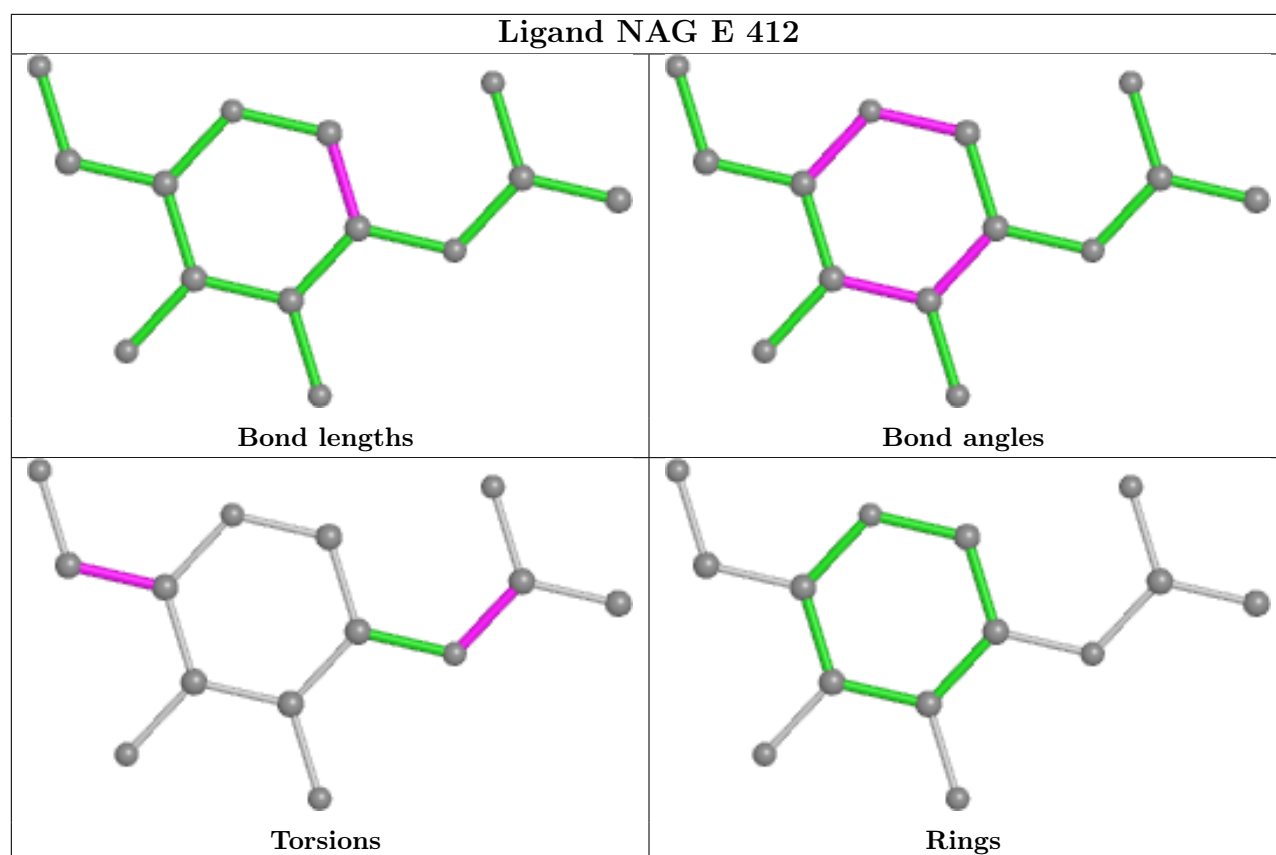
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	402	NAG	1	0
7	A	402	NAG	1	0
7	K	401	NAG	1	0
7	A	414	NAG	2	0
7	A	413	NAG	1	0
7	C	409	NAG	1	0
7	I	409	NAG	1	0

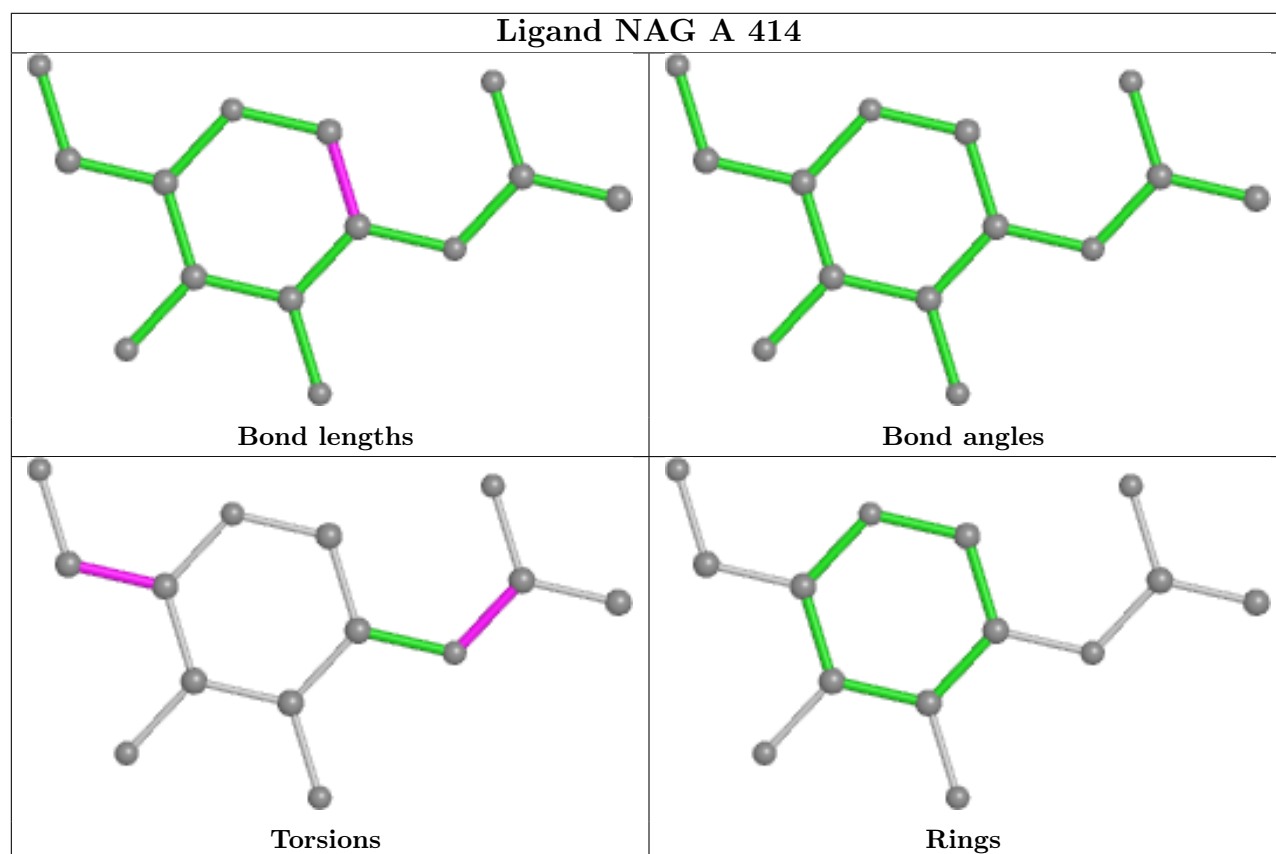
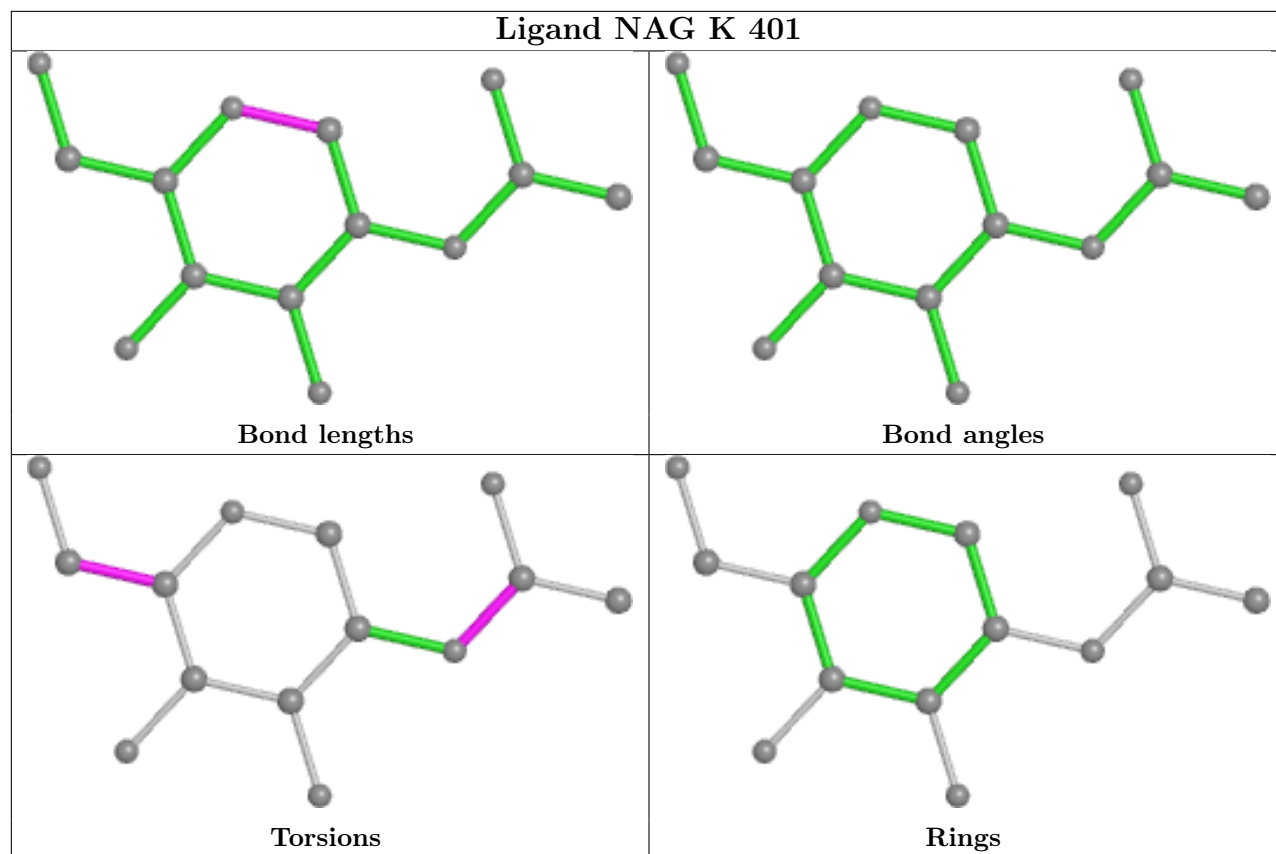
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

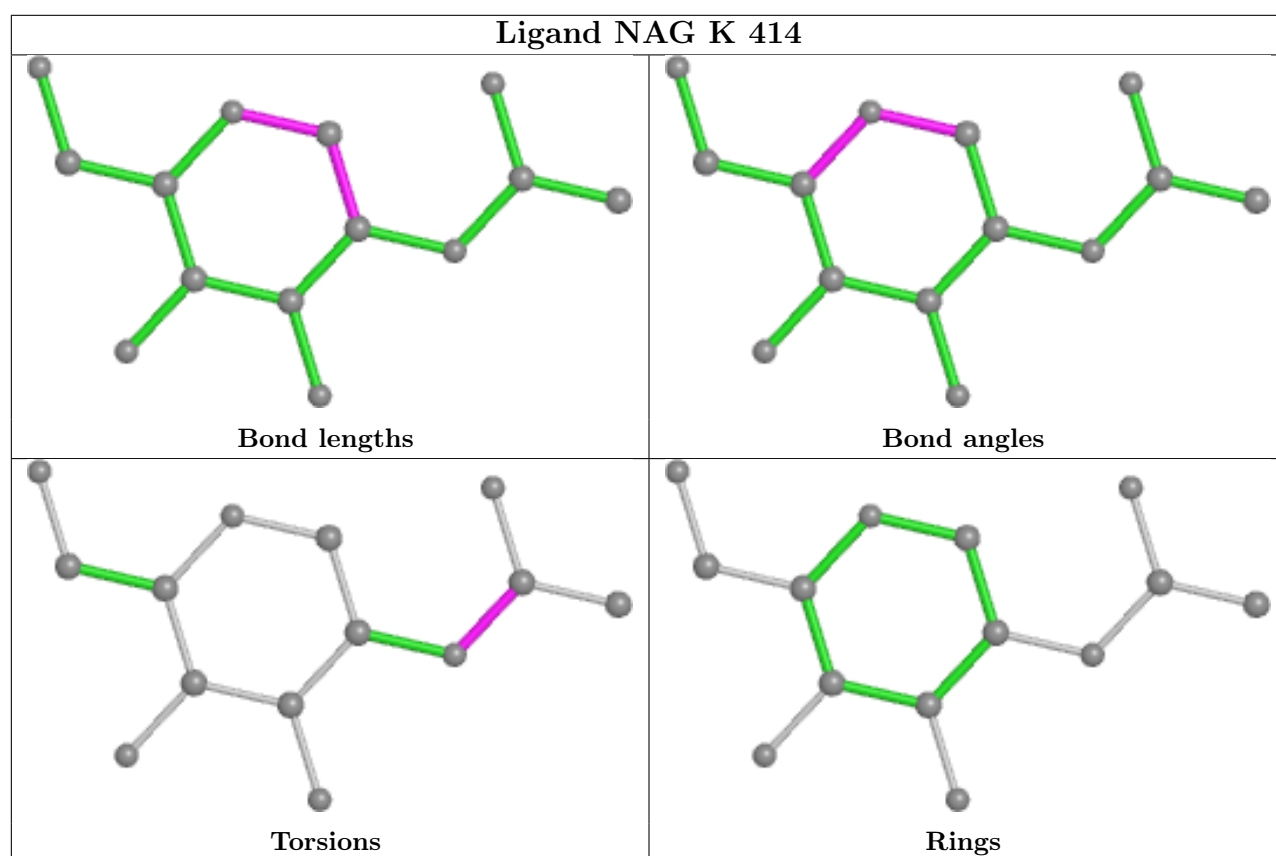
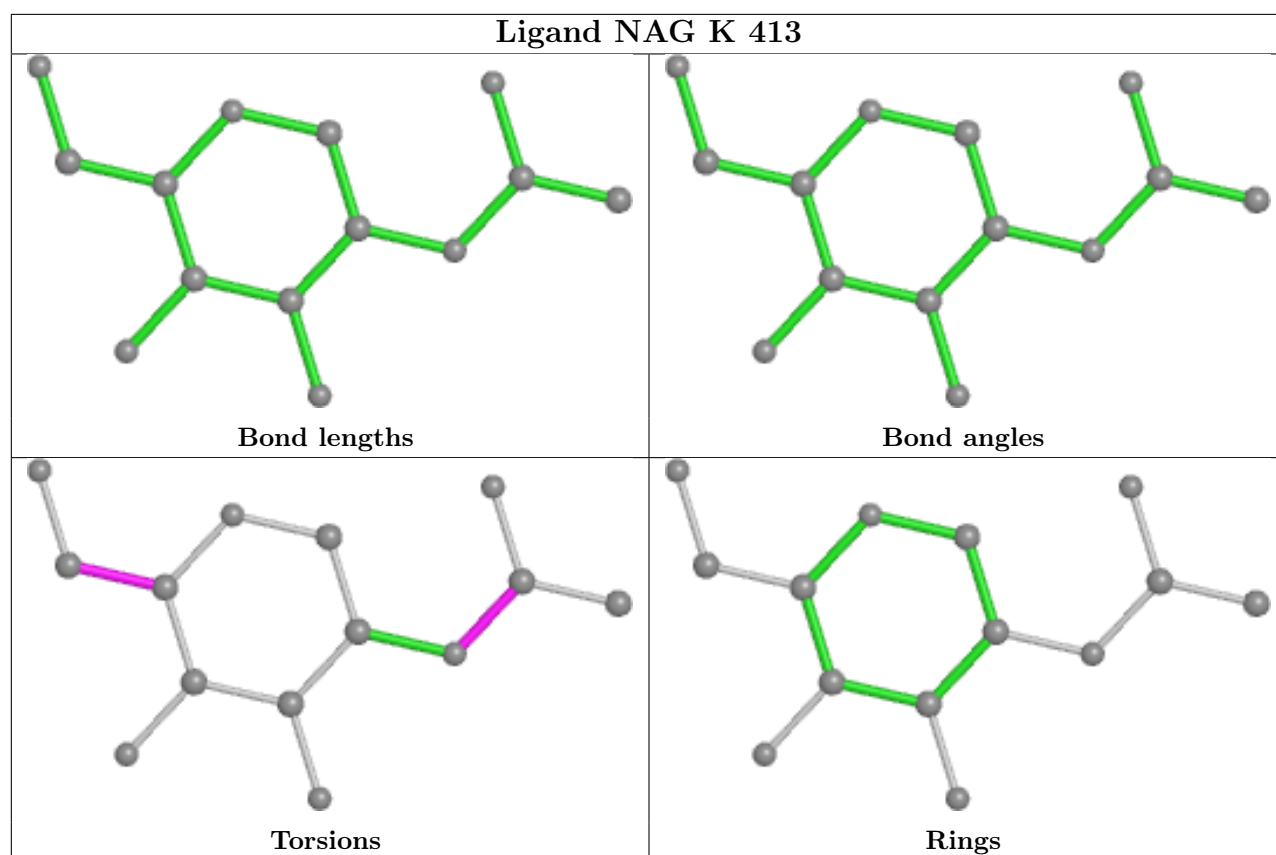


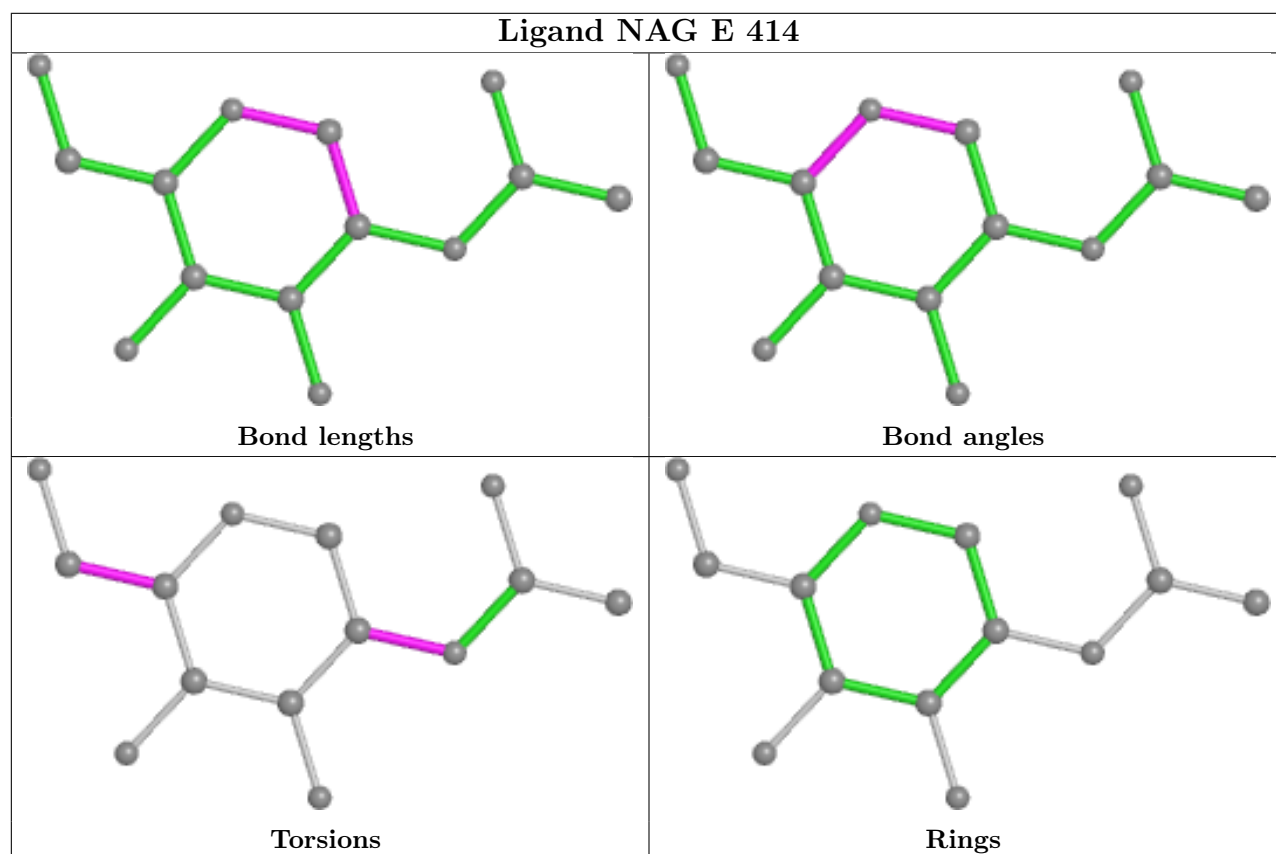
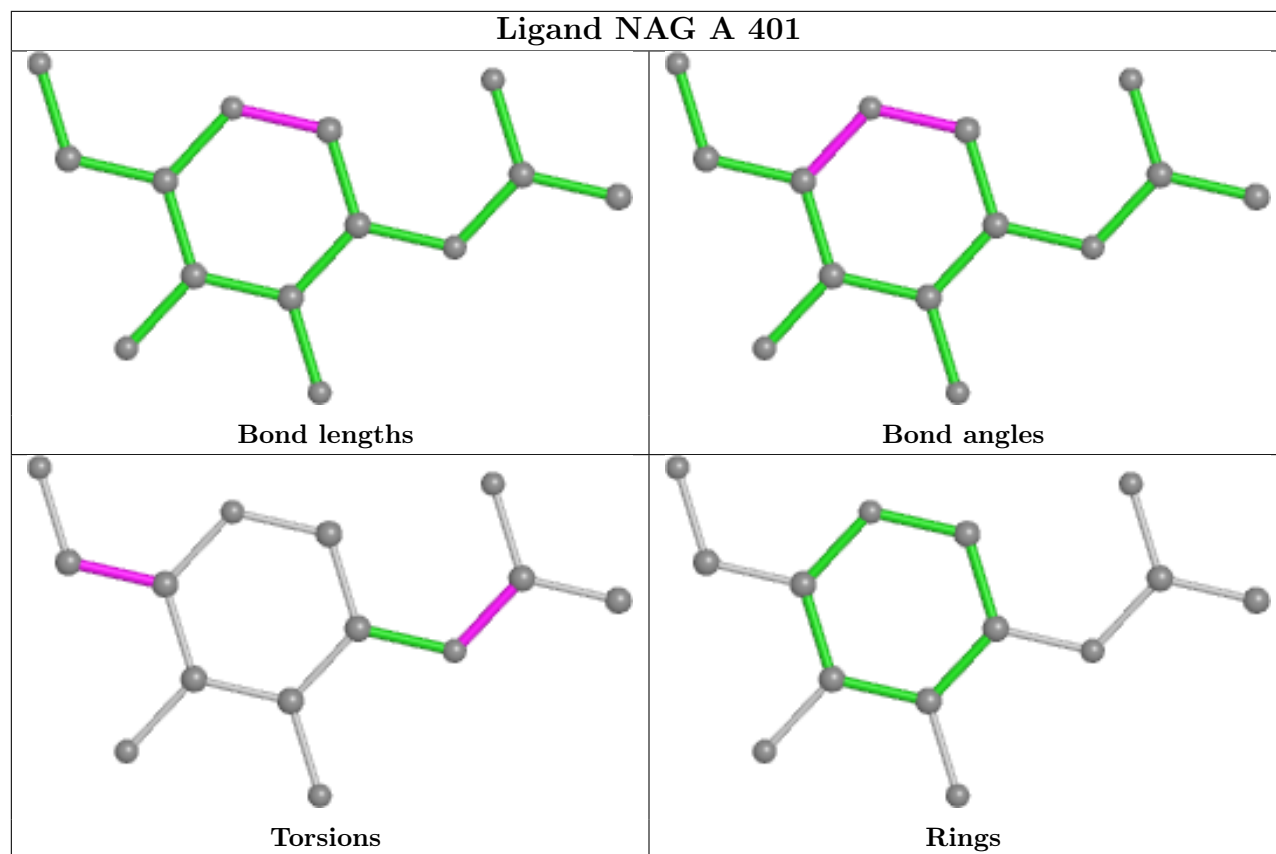


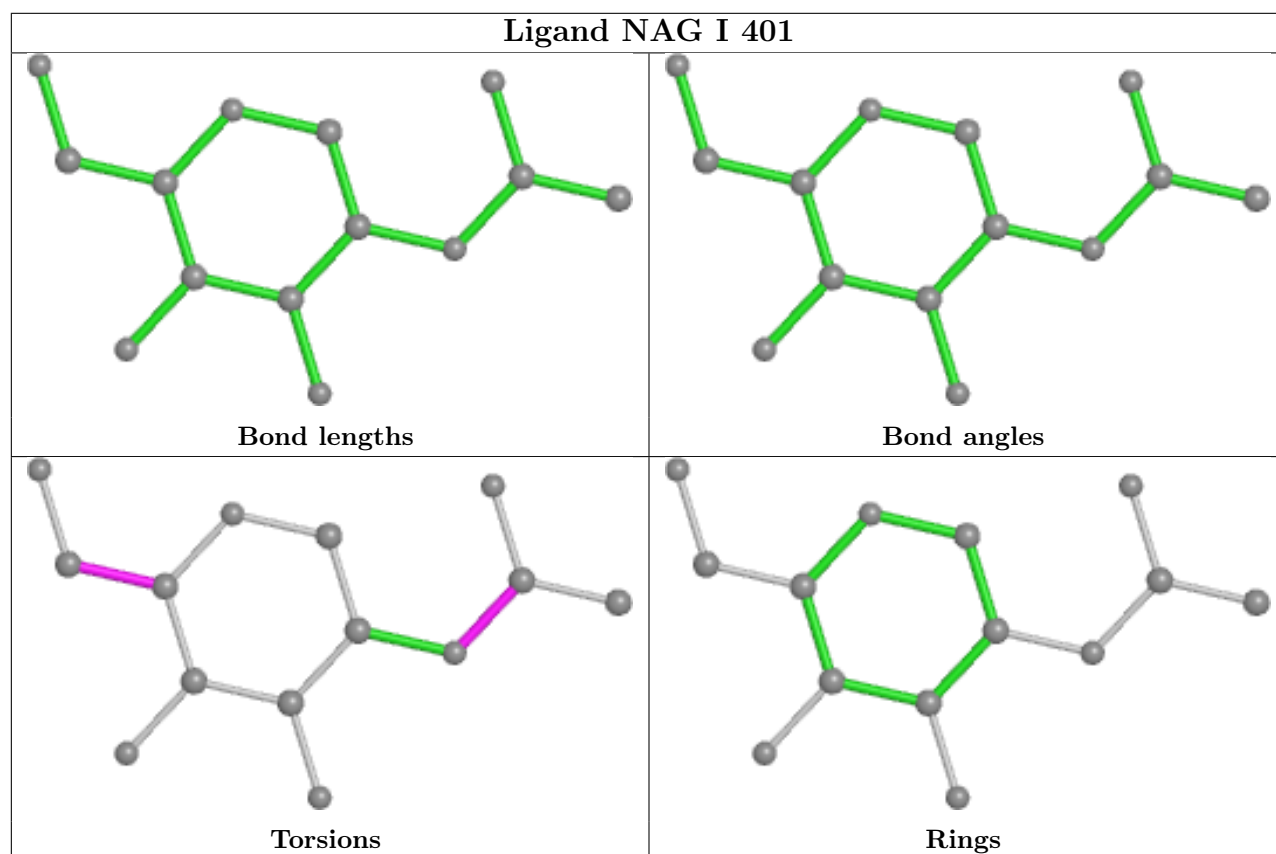
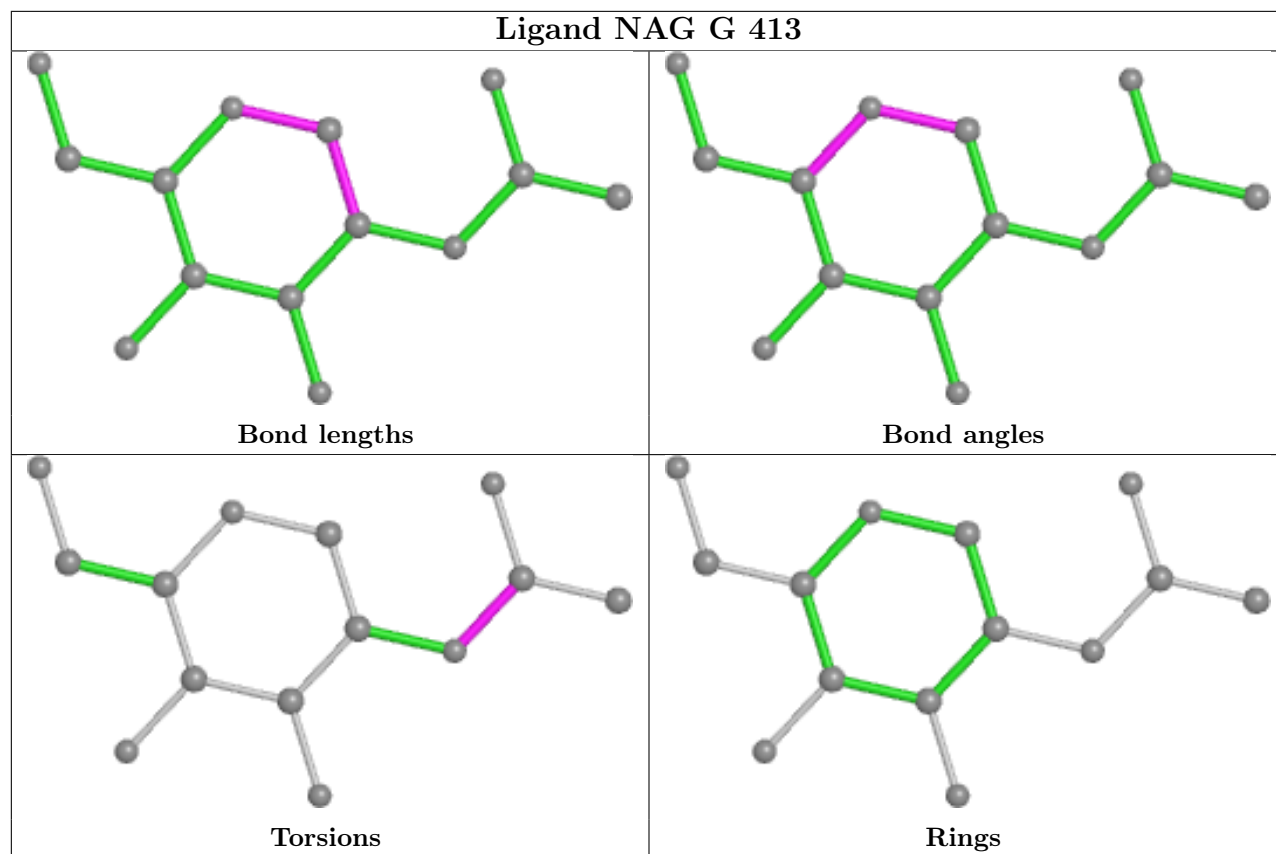


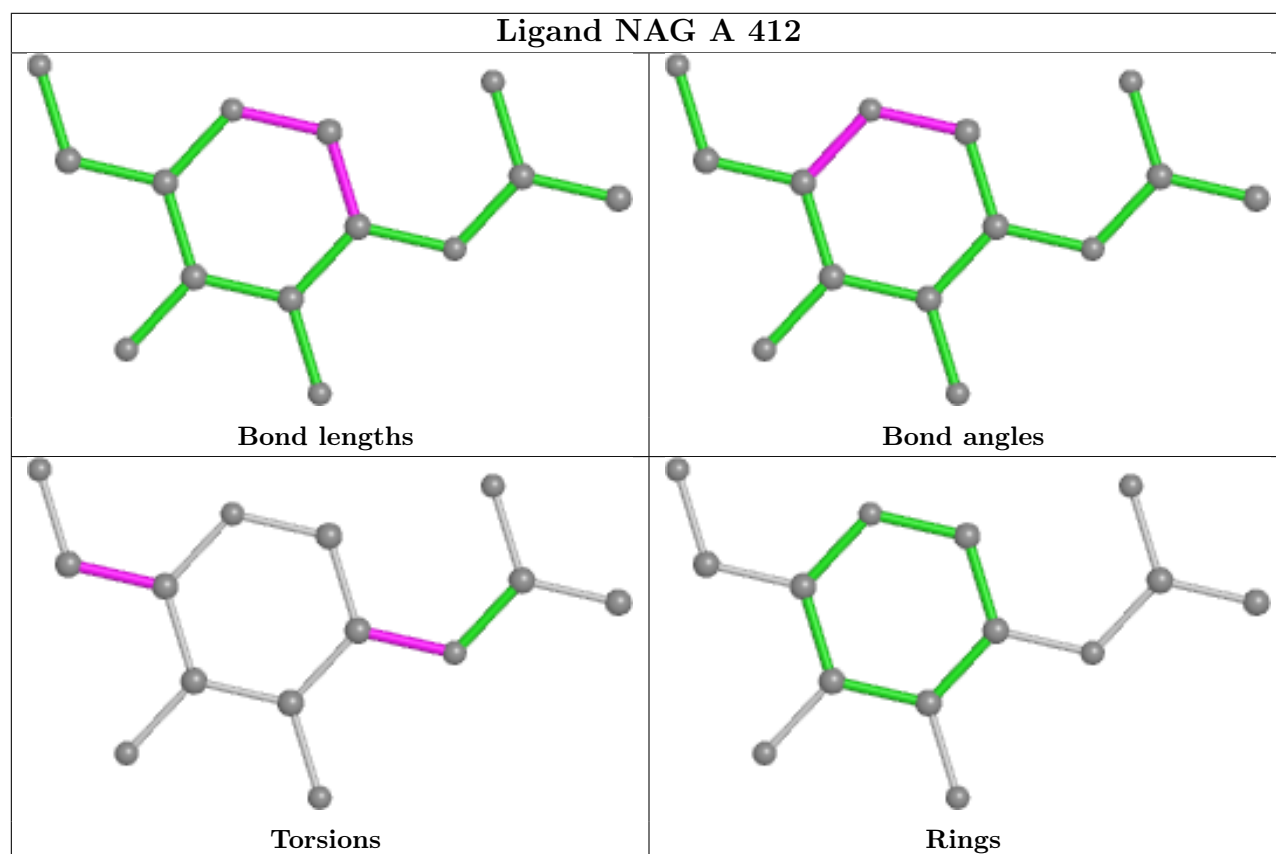
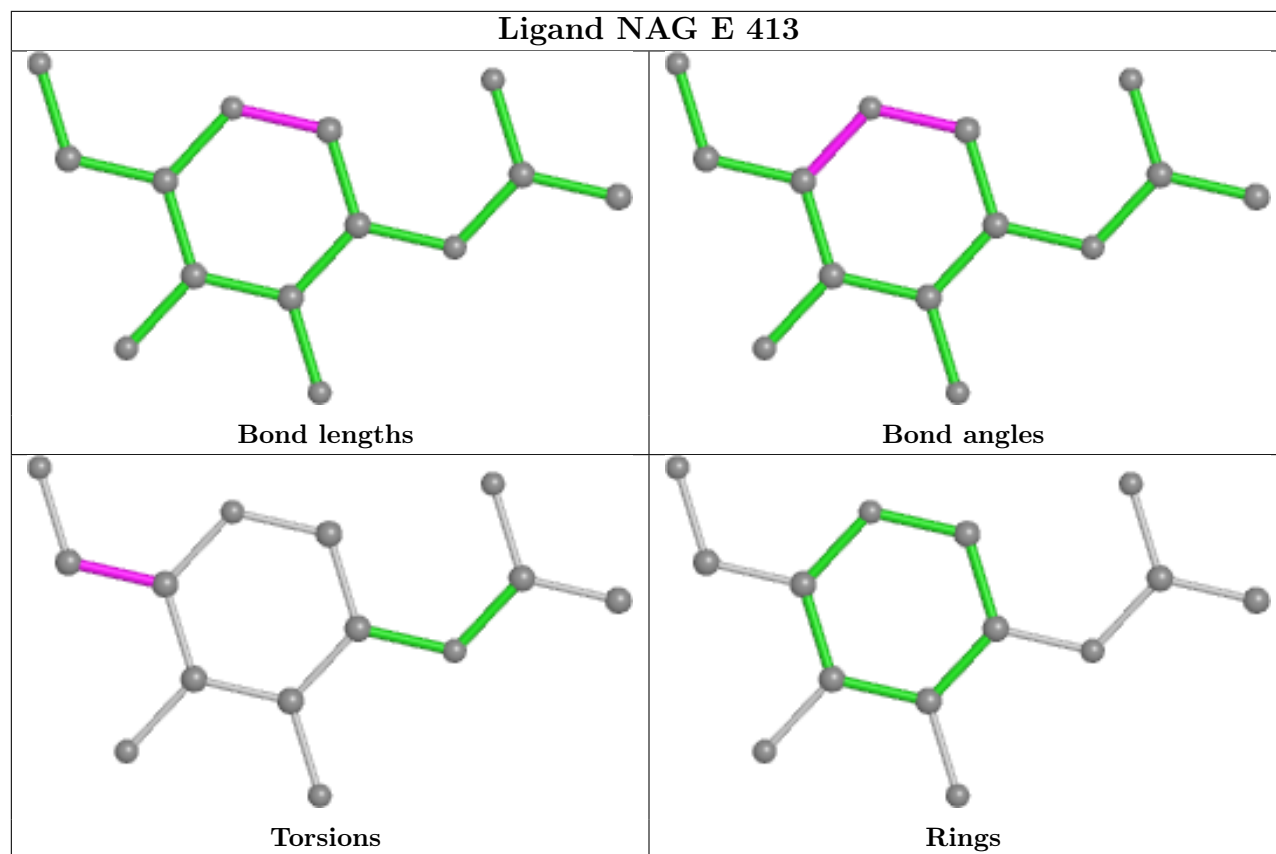


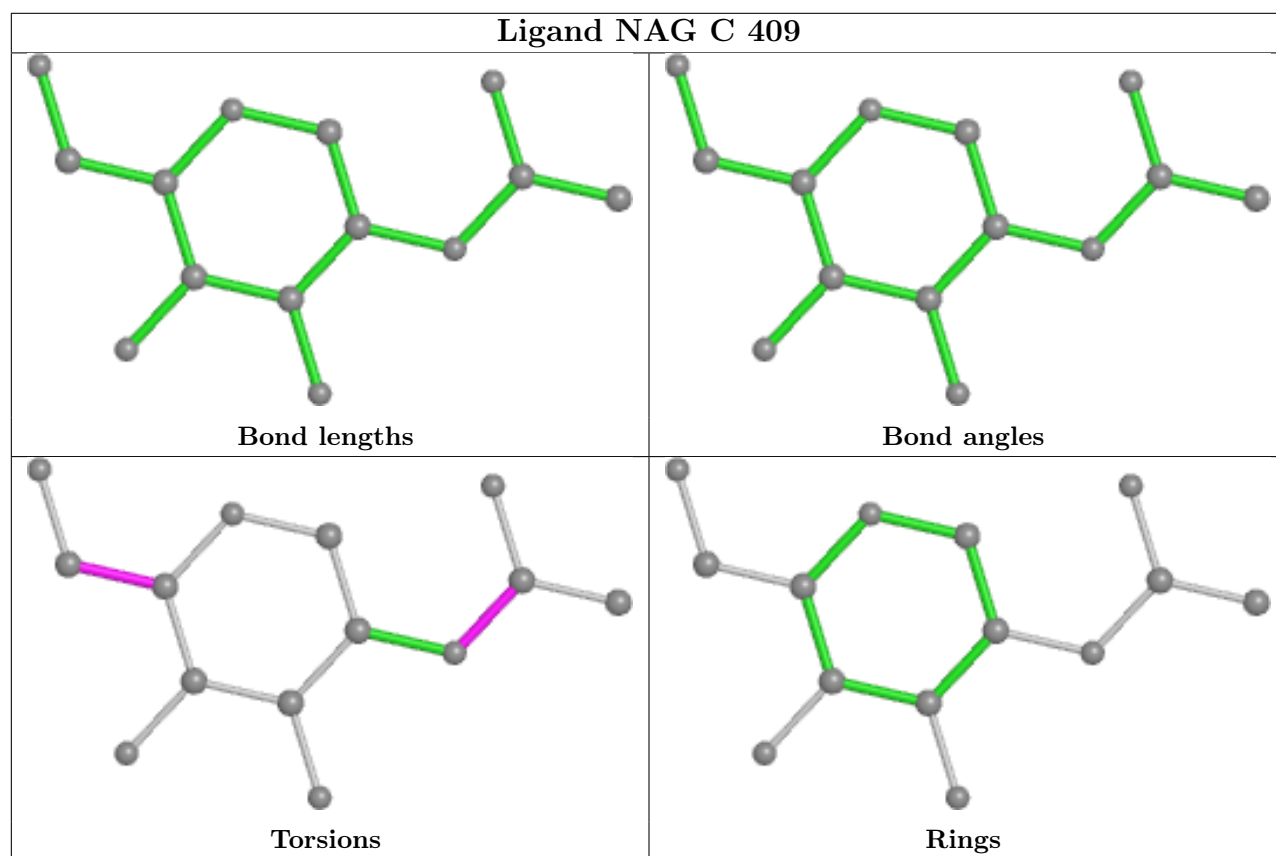
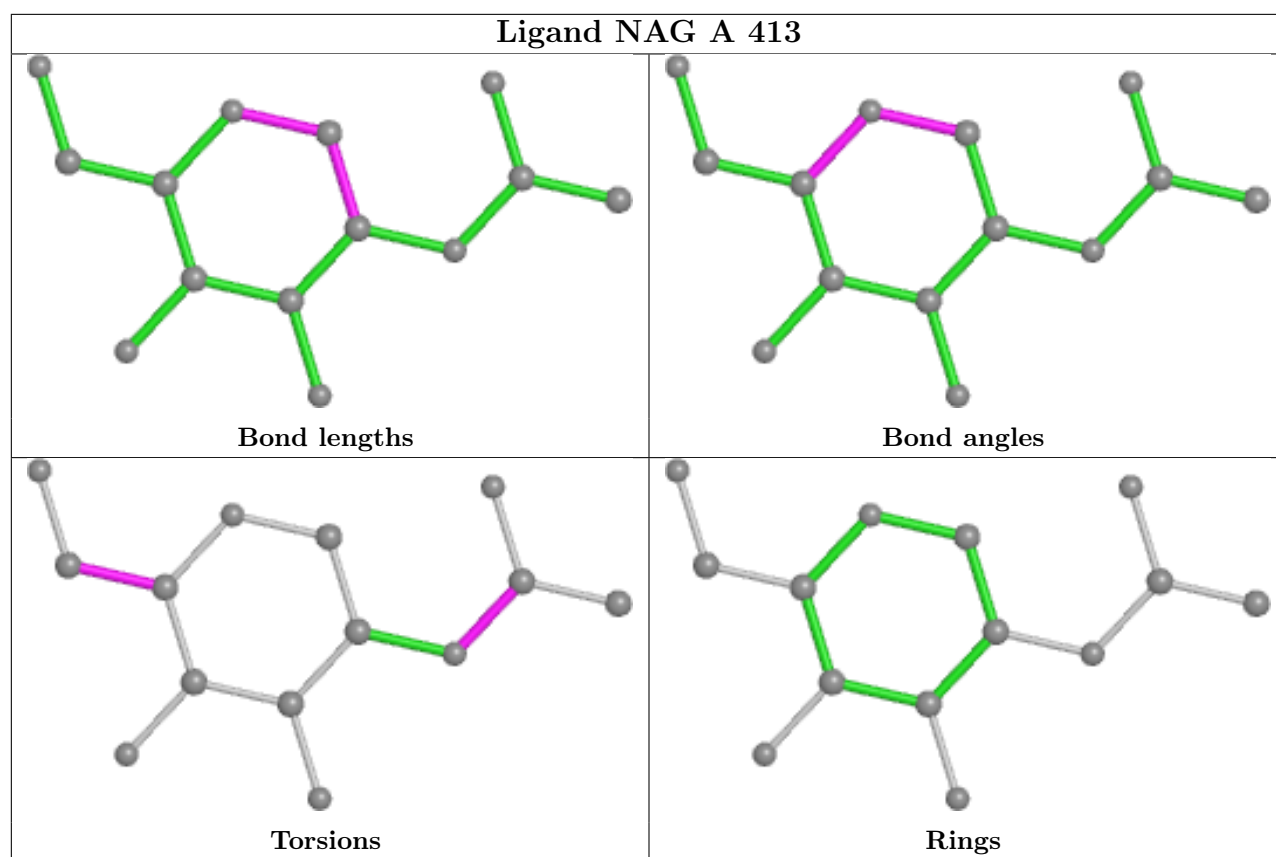


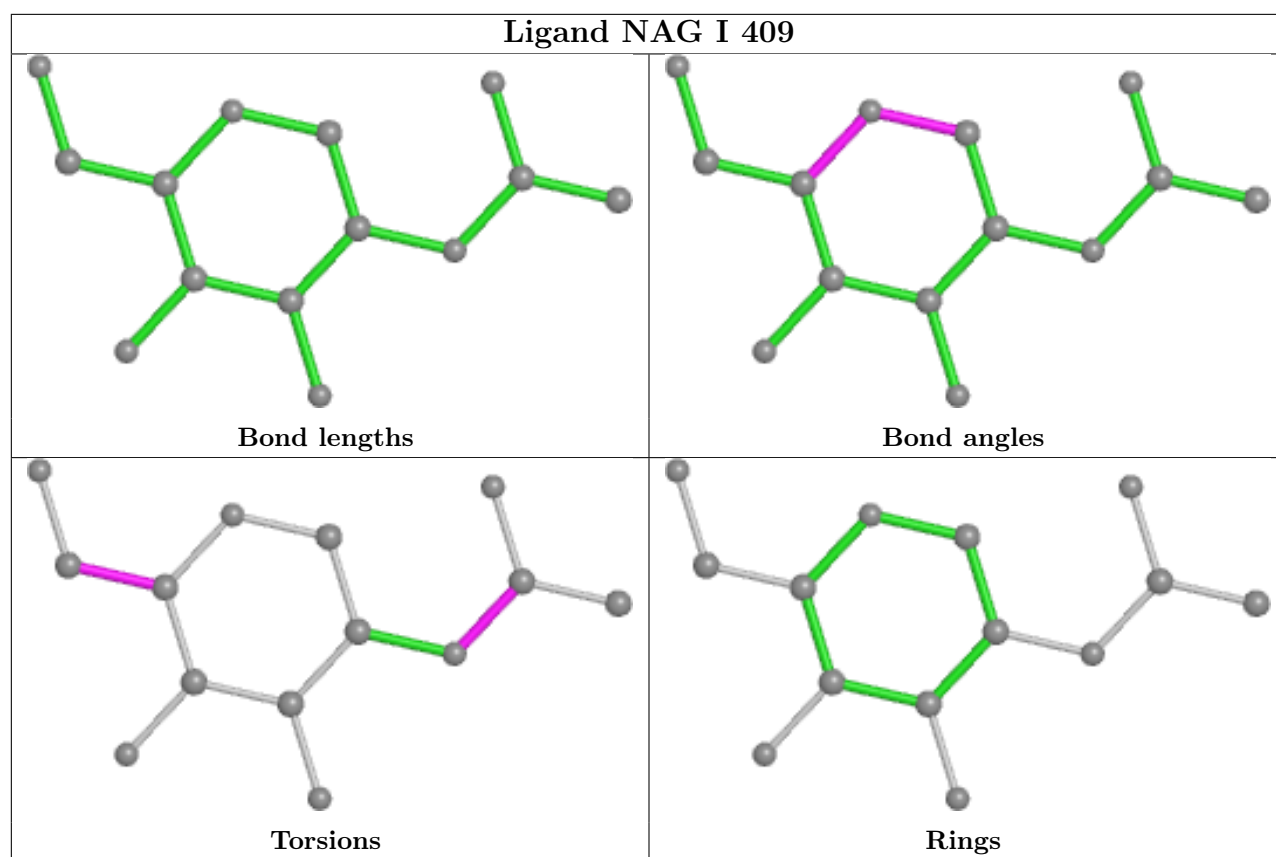












## 5.7 Other polymers [i](#)

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, 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	321/330 (97%)	-0.16	7 (2%) 62 52	20, 54, 117, 244	0
1	C	321/330 (97%)	-0.17	5 (1%) 72 63	26, 54, 108, 183	0
1	E	321/330 (97%)	-0.29	1 (0%) 94 93	19, 57, 93, 133	0
1	G	320/330 (96%)	-0.26	0 100 100	28, 56, 92, 143	0
1	I	320/330 (96%)	-0.13	9 (2%) 53 41	25, 58, 122, 170	0
1	K	321/330 (97%)	-0.23	8 (2%) 57 46	26, 54, 103, 176	0
2	B	165/183 (90%)	0.48	19 (11%) 4 4	37, 117, 172, 201	0
2	D	165/183 (90%)	0.79	29 (17%) 1 1	35, 121, 195, 238	0
2	F	165/183 (90%)	0.21	10 (6%) 21 14	31, 94, 155, 206	0
2	H	165/183 (90%)	0.23	10 (6%) 21 14	31, 82, 131, 177	0
2	J	165/183 (90%)	0.78	23 (13%) 2 2	34, 112, 180, 205	0
2	L	165/183 (90%)	0.34	10 (6%) 21 14	34, 95, 153, 186	0
All	All	2914/3078 (94%)	0.02	131 (4%) 33 23	19, 65, 150, 244	0

The worst 5 of 131 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	GLY	9.5
2	J	156	THR	8.7
2	J	163	SER	8.4
2	B	134	GLY	8.0
2	B	143	LYS	7.3

### 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, 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	MAN	S	4	11/12	0.66	0.47	75,91,111,113	0
3	MAN	V	4	11/12	0.72	0.26	78,108,117,120	0
4	MAN	N	4	11/12	0.72	0.21	82,115,129,130	0
3	MAN	M	4	11/12	0.74	0.26	59,104,113,116	0
3	NAG	V	5	14/15	0.74	0.45	87,108,116,123	0
3	MAN	V	6	11/12	0.74	0.21	56,76,83,86	0
5	BMA	X	3	11/12	0.75	0.30	101,108,114,116	0
3	NAG	M	5	14/15	0.76	0.41	76,102,119,119	0
4	NAG	N	5	14/15	0.78	0.22	73,91,104,110	0
3	BMA	V	3	11/12	0.78	0.23	91,99,104,114	0
5	MAN	T	4	11/12	0.79	0.17	87,109,122,125	0
5	BMA	O	3	11/12	0.79	0.27	85,115,121,131	0
5	MAN	O	4	11/12	0.80	0.29	85,94,108,121	0
4	BMA	N	3	11/12	0.80	0.28	64,92,108,124	0
3	NAG	S	5	14/15	0.80	0.38	58,94,100,100	0
5	NAG	U	2	14/15	0.82	0.33	73,94,99,100	0
3	MAN	M	6	11/12	0.83	0.27	47,69,82,83	0
5	MAN	Q	4	11/12	0.84	0.40	67,80,105,112	0
3	NAG	V	2	14/15	0.84	0.21	46,65,70,71	0
3	BMA	M	3	11/12	0.84	0.23	75,82,103,119	0
5	MAN	R	4	11/12	0.84	0.26	74,98,103,107	0
5	BMA	Q	3	11/12	0.85	0.22	78,91,103,104	0
6	BMA	W	3	11/12	0.85	0.23	79,86,95,97	0
5	BMA	T	3	11/12	0.86	0.20	70,80,86,89	0
3	NAG	S	2	14/15	0.86	0.29	61,83,87,93	0
5	NAG	Q	2	14/15	0.86	0.26	73,83,91,98	0
5	NAG	X	2	14/15	0.87	0.22	68,80,92,98	0
4	MAN	P	4	11/12	0.87	0.23	72,91,95,108	0
5	NAG	U	1	14/15	0.87	0.24	61,71,92,93	0
6	NAG	W	2	14/15	0.88	0.23	53,92,106,115	0
3	BMA	S	3	11/12	0.88	0.42	60,82,98,107	0
5	BMA	U	3	11/12	0.88	0.21	59,68,74,78	0
3	MAN	S	6	11/12	0.88	0.21	35,45,52,52	0
3	NAG	M	2	14/15	0.88	0.28	83,94,106,108	0
5	NAG	O	2	14/15	0.89	0.22	60,84,97,104	0
4	NAG	N	2	14/15	0.89	0.23	47,61,75,88	0
5	NAG	T	2	14/15	0.89	0.23	52,66,72,82	0

*Continued on next page...*

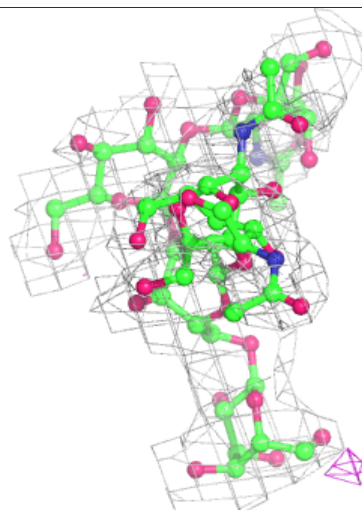
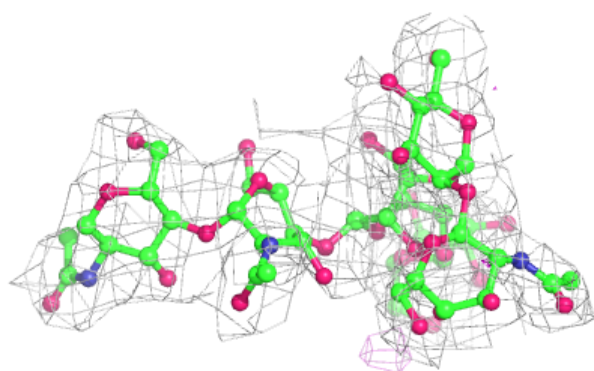
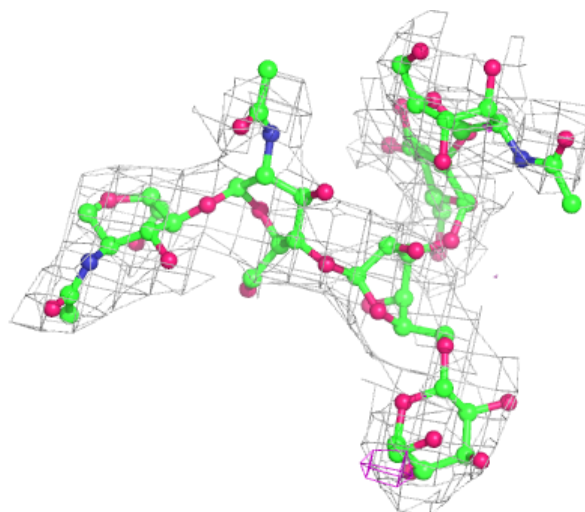
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	Q	1	14/15	0.89	0.21	36,50,56,71	0
4	NAG	P	2	14/15	0.90	0.20	44,52,68,69	0
5	NAG	R	2	14/15	0.90	0.22	57,74,95,102	0
4	BMA	P	3	11/12	0.91	0.21	70,88,95,96	0
3	NAG	S	1	14/15	0.91	0.22	33,62,74,79	0
5	MAN	X	4	11/12	0.92	0.12	56,67,76,78	0
4	NAG	P	5	14/15	0.92	0.16	55,72,77,83	0
5	BMA	R	3	11/12	0.93	0.16	67,73,78,81	0
5	NAG	T	1	14/15	0.93	0.18	34,49,57,63	0
5	MAN	U	4	11/12	0.93	0.20	39,59,70,73	0
5	NAG	R	1	14/15	0.93	0.16	37,40,44,46	0
4	NAG	P	1	14/15	0.93	0.17	34,45,58,67	0
5	NAG	O	1	14/15	0.93	0.22	31,52,63,73	0
3	NAG	V	1	14/15	0.94	0.17	32,37,40,42	0
6	NAG	W	1	14/15	0.94	0.15	53,56,60,65	0
4	NAG	N	1	14/15	0.95	0.18	32,34,36,46	0
3	NAG	M	1	14/15	0.95	0.12	51,54,59,59	0
5	NAG	X	1	14/15	0.95	0.13	32,39,55,58	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.

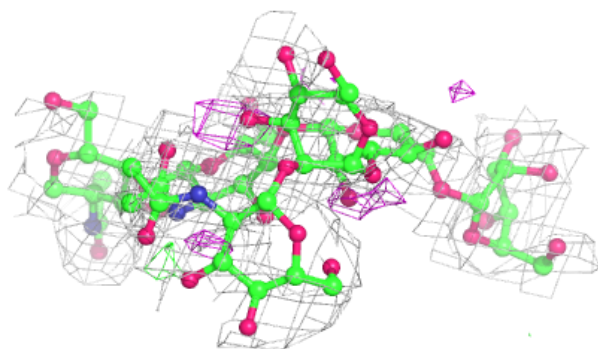
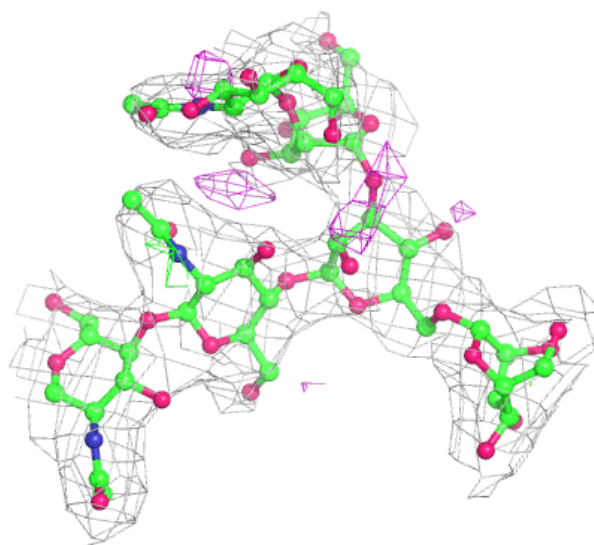
**Electron density around Chain M:**

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



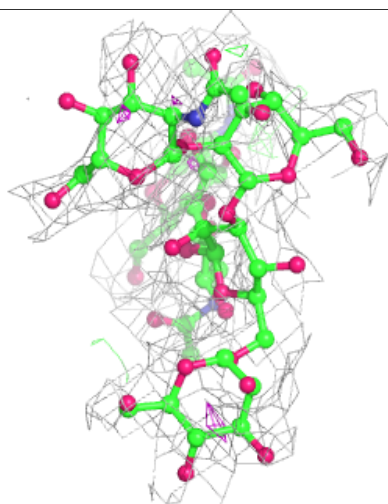
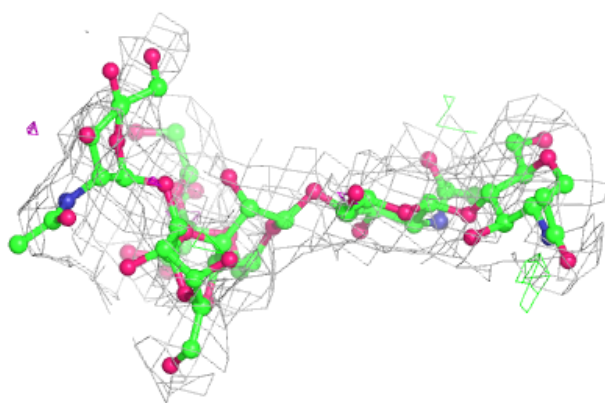
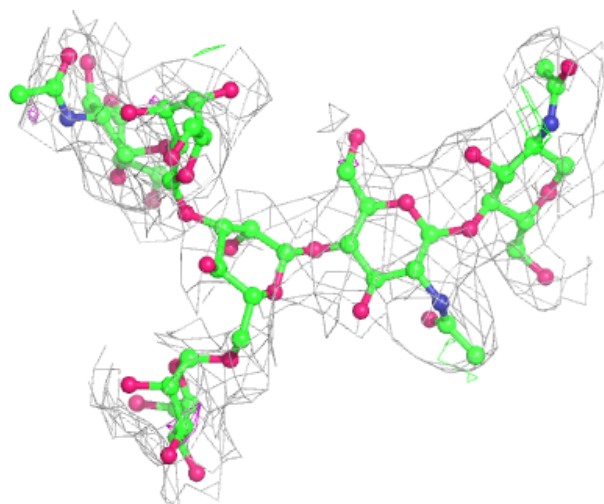
**Electron density around Chain S:**

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



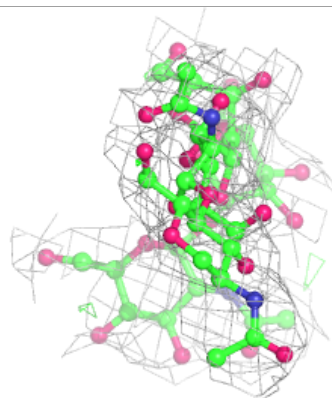
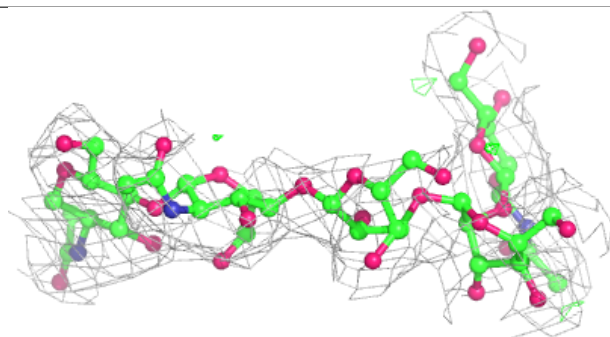
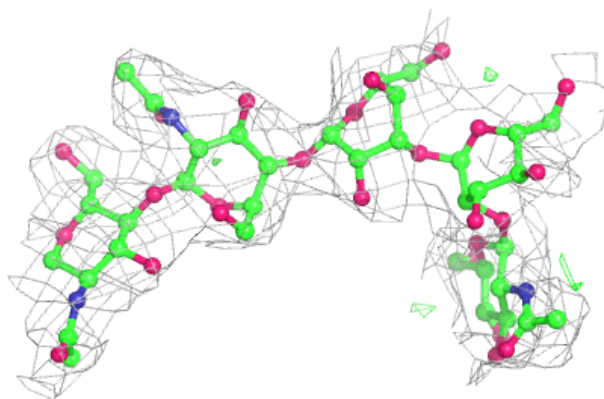
**Electron density around Chain V:**

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

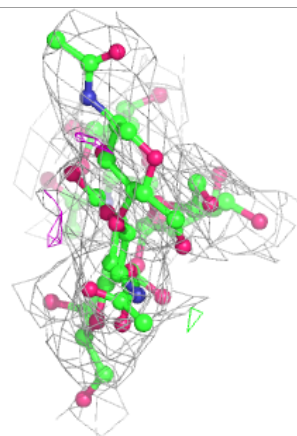
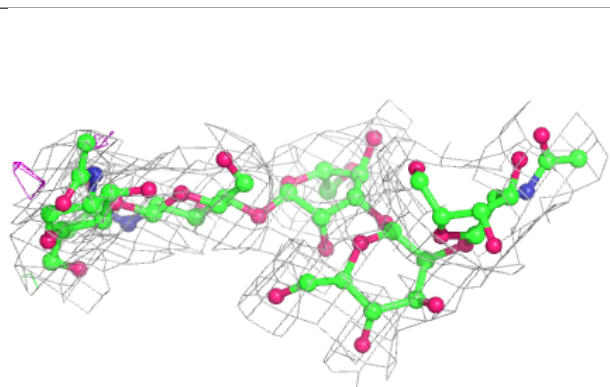
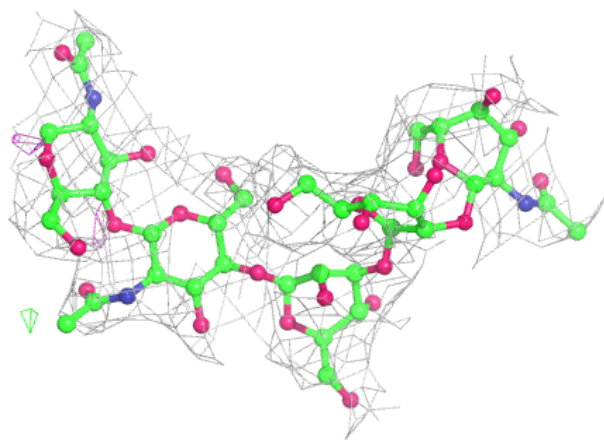


**Electron density around Chain N:**

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

**Electron density around Chain P:**

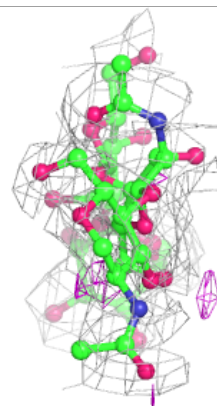
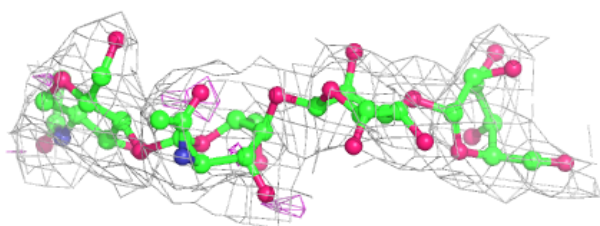
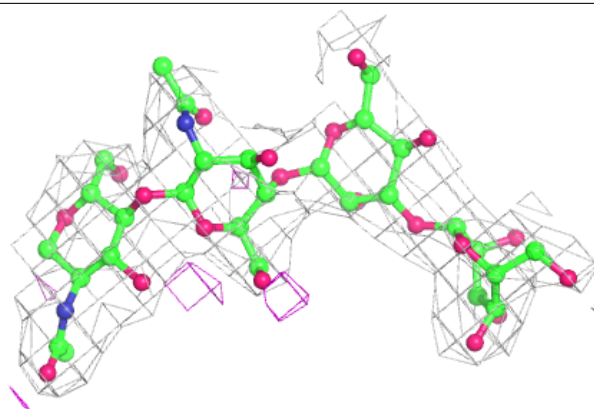
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



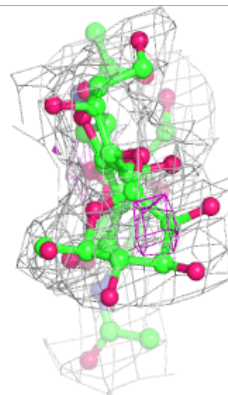
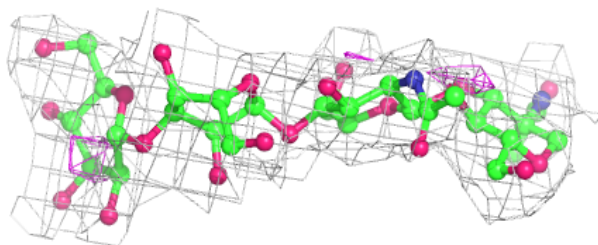
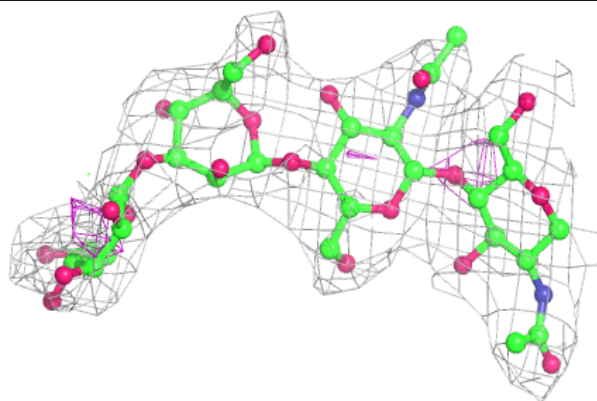


**Electron density around Chain O:**

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

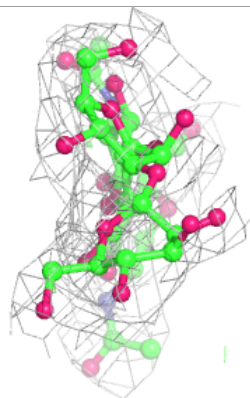
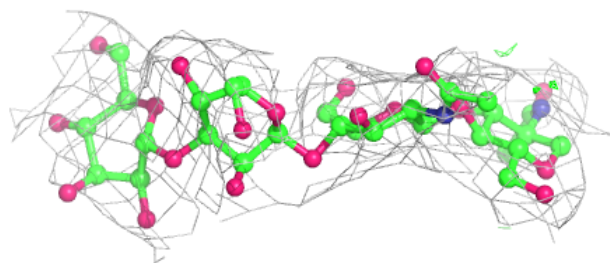
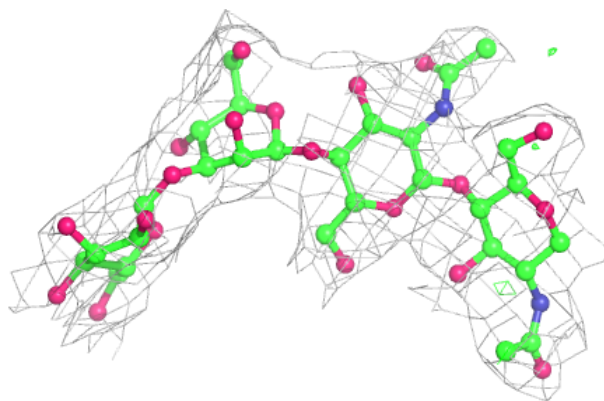
**Electron density around Chain Q:**

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

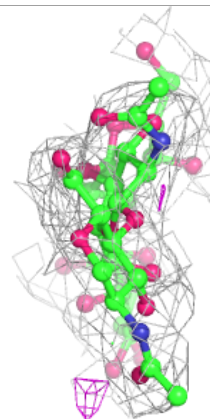
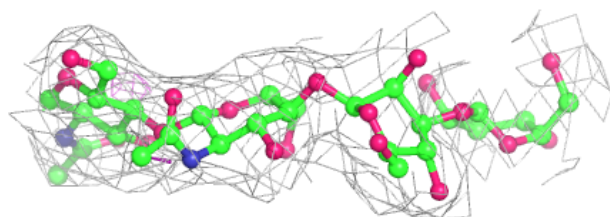
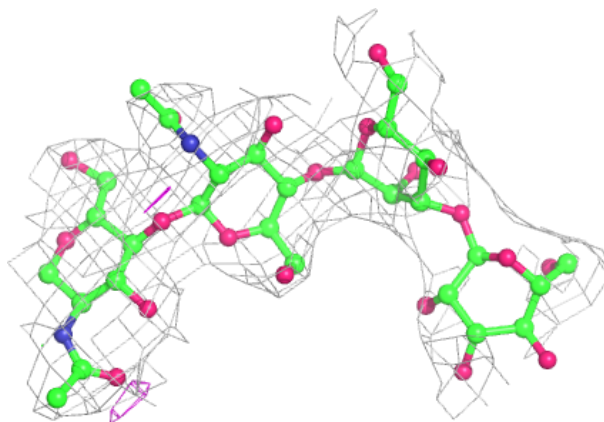


**Electron density around Chain R:**

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

**Electron density around Chain T:**

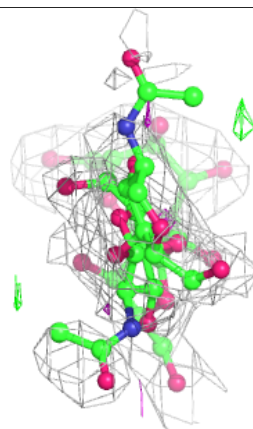
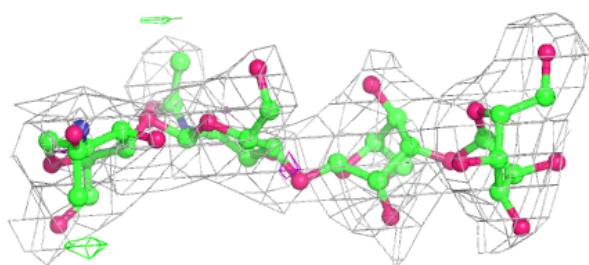
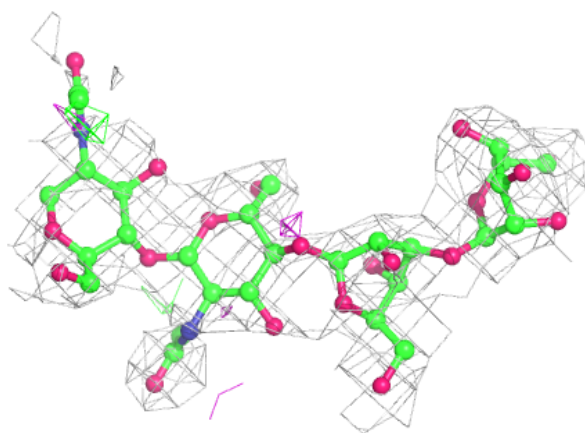
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



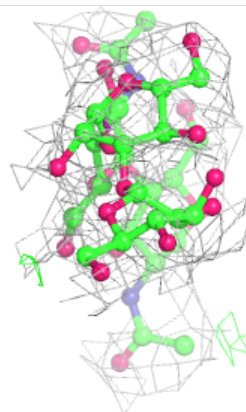
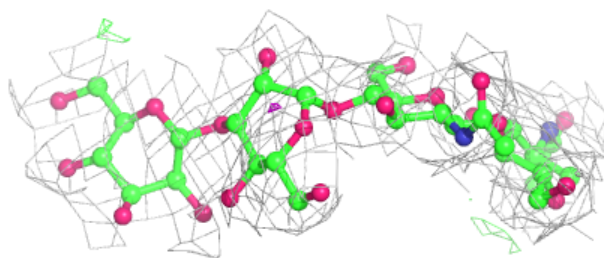
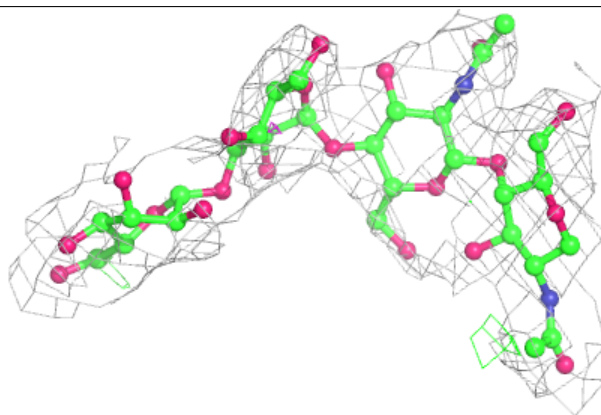


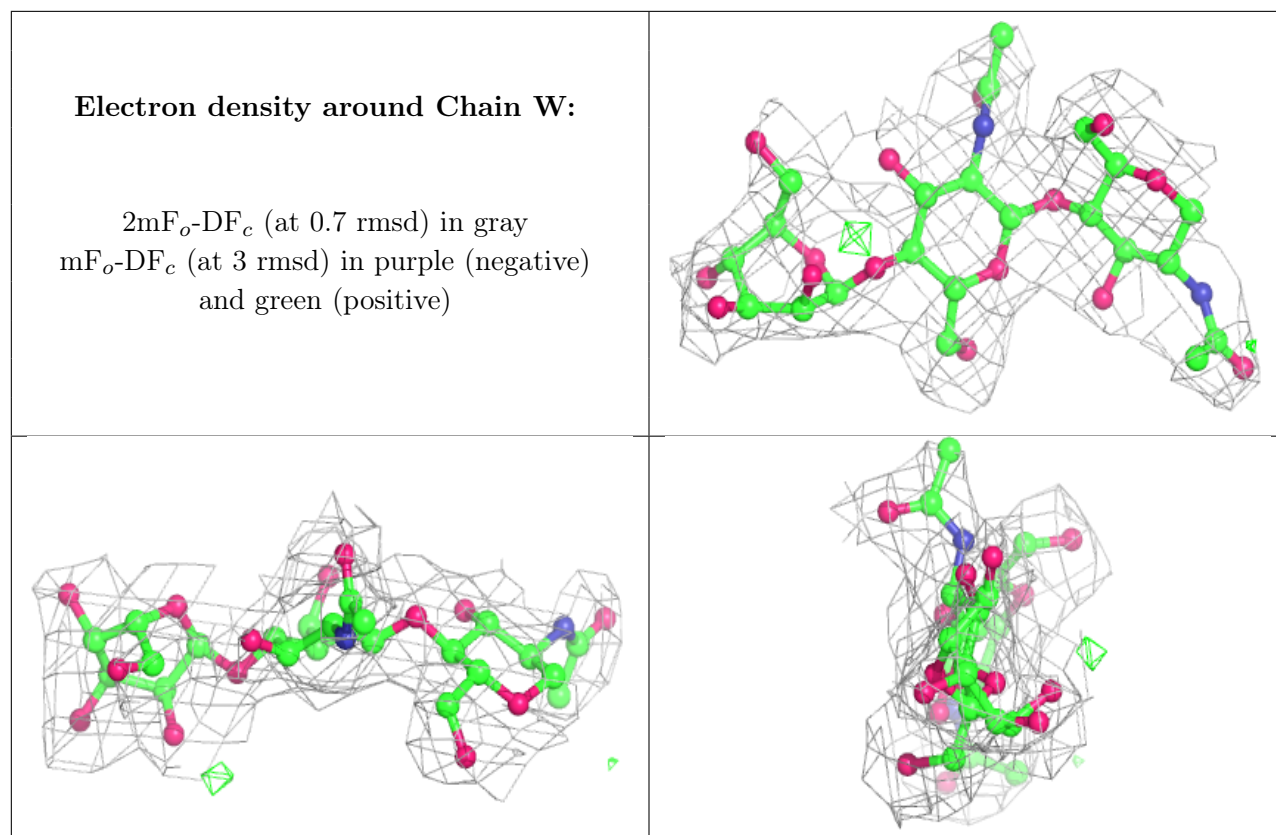
**Electron density around Chain U:**

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

**Electron density around Chain X:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

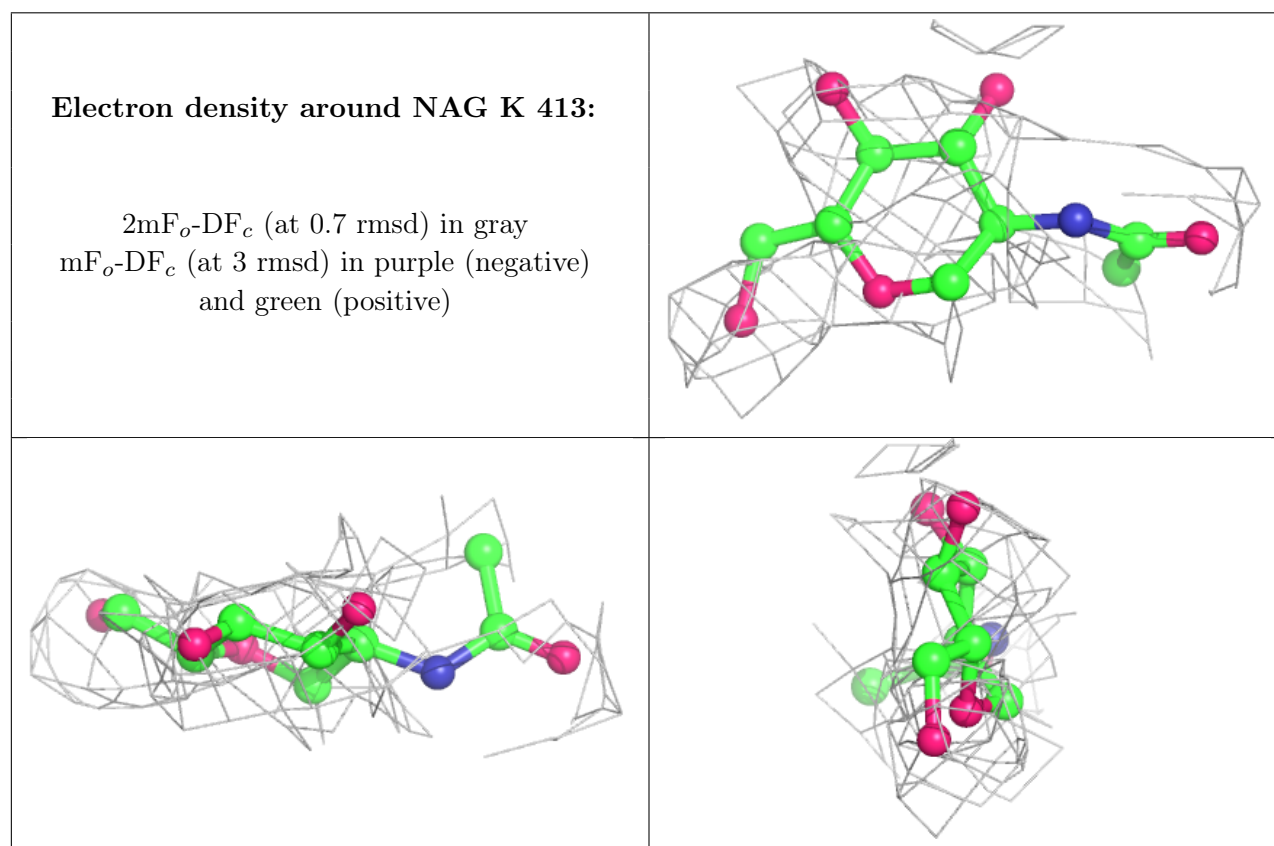
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	K	413	14/15	0.63	0.33	79,112,140,143	0
7	NAG	A	401	14/15	0.69	0.29	108,129,155,157	0
7	NAG	A	413	14/15	0.69	0.32	80,93,100,101	0
7	NAG	E	412	14/15	0.70	0.30	98,123,129,130	0
7	NAG	A	402	14/15	0.71	0.33	118,155,164,170	0
7	NAG	I	410	14/15	0.71	0.44	100,131,137,147	0
7	NAG	I	409	14/15	0.72	0.25	75,90,97,99	0
7	NAG	K	401	14/15	0.72	0.39	102,134,139,140	0
7	NAG	E	414	14/15	0.73	0.34	103,124,132,137	0
7	NAG	A	412	14/15	0.74	0.64	60,112,127,129	0
7	NAG	G	401	14/15	0.76	0.20	71,80,91,92	0
7	NAG	I	401	14/15	0.76	0.28	118,132,146,152	0
7	NAG	G	402	14/15	0.77	0.16	82,107,120,120	0
7	NAG	K	414	14/15	0.81	0.29	103,115,122,122	0

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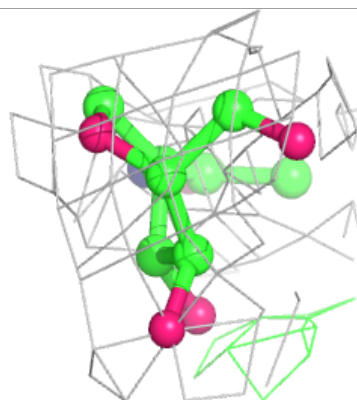
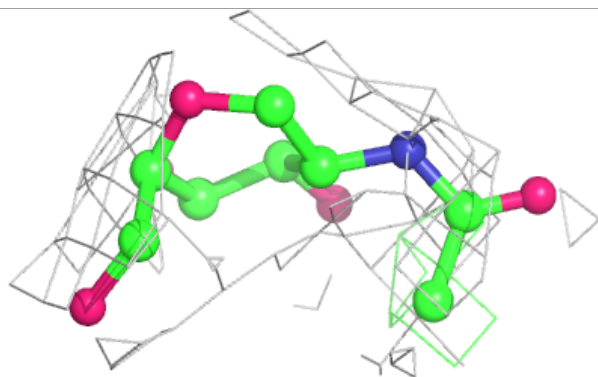
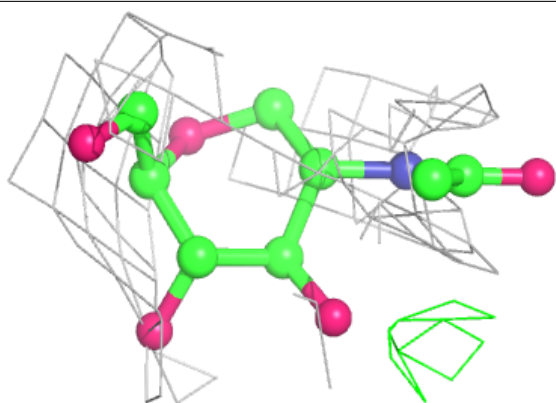
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	C	409	14/15	0.82	0.27	84,91,98,101	0
7	NAG	E	413	14/15	0.82	0.50	75,88,96,98	0
7	NAG	E	401	14/15	0.84	0.22	66,91,109,110	0
7	NAG	A	414	14/15	0.88	0.25	62,80,86,88	0
7	NAG	G	413	14/15	0.88	0.20	57,80,96,97	0
8	ZN	G	414	1/1	0.98	0.06	40,40,40,40	0
8	ZN	I	411	1/1	0.99	0.04	43,43,43,43	0
8	ZN	K	415	1/1	0.99	0.06	47,47,47,47	0

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

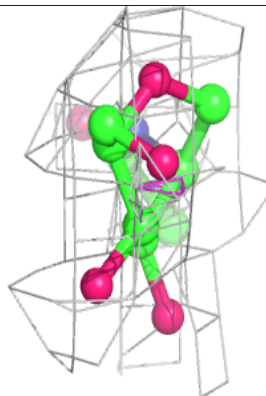
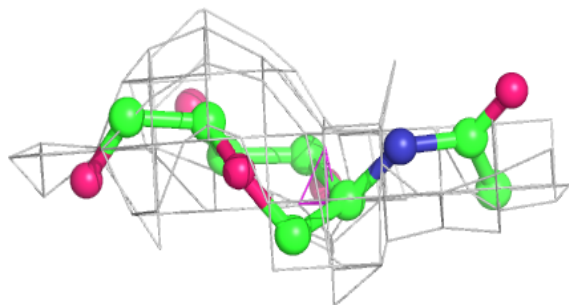
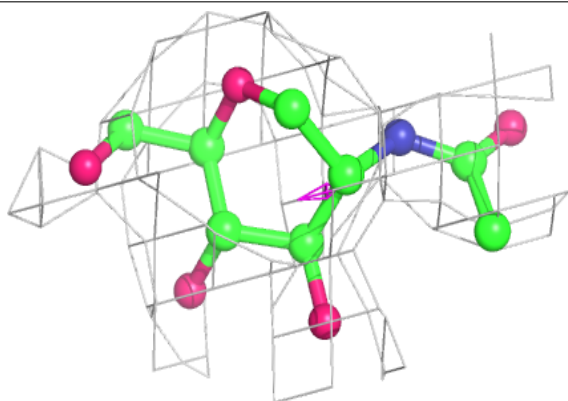


**Electron density around NAG A 401:**

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

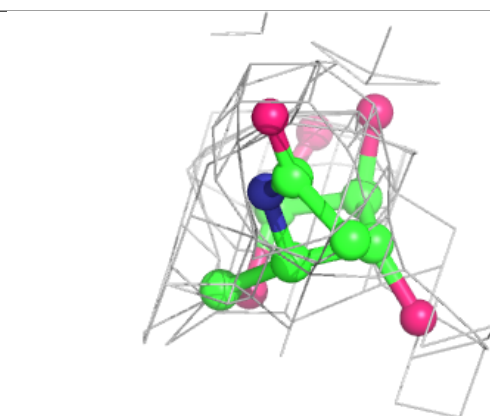
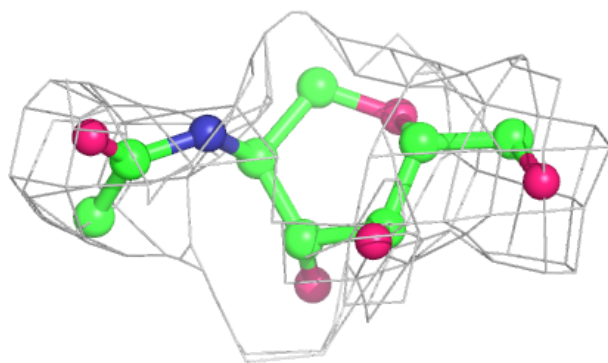
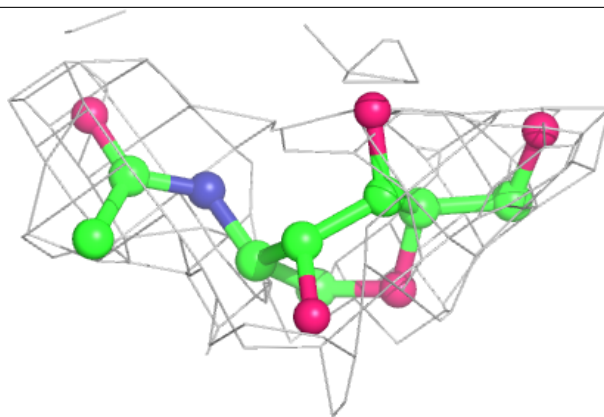
**Electron density around NAG A 413:**

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

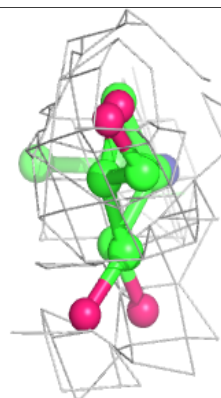
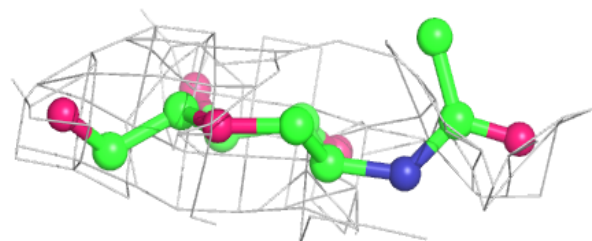
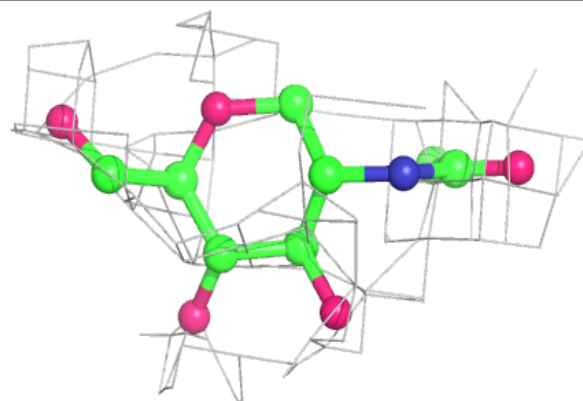


**Electron density around NAG E 412:**

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

**Electron density around NAG A 402:**

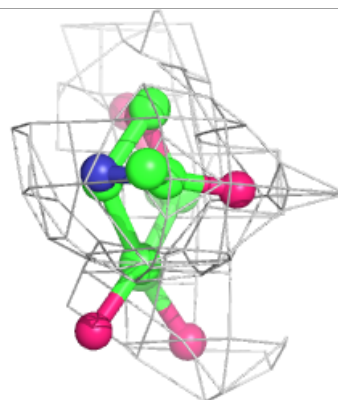
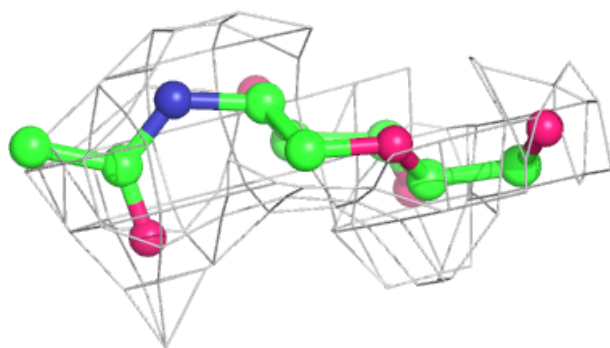
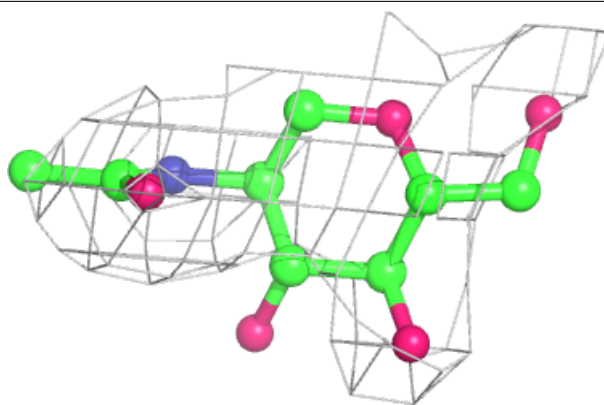
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



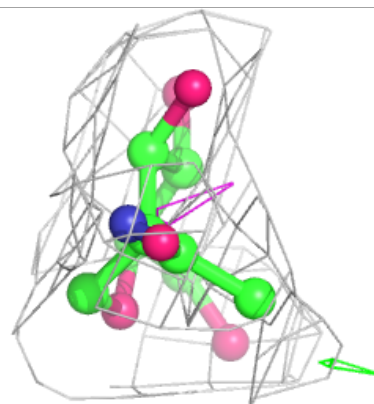
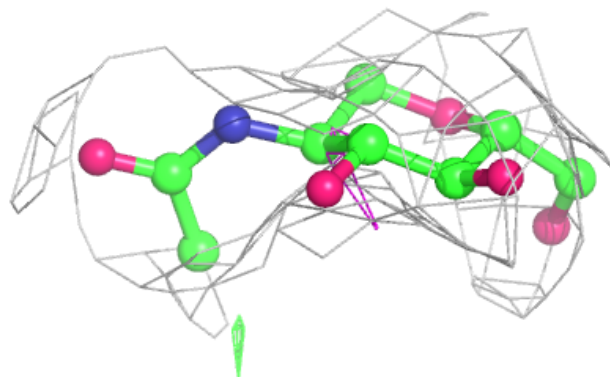
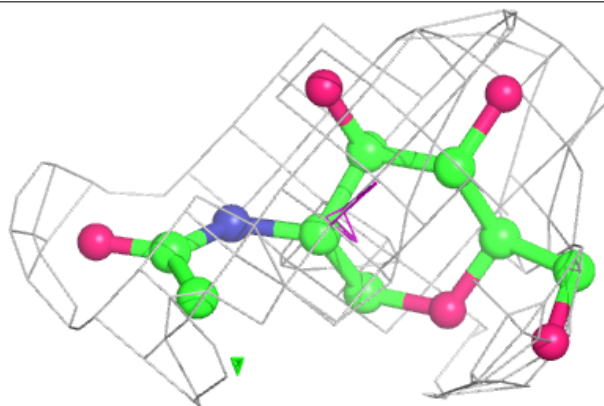


**Electron density around NAG I 410:**

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

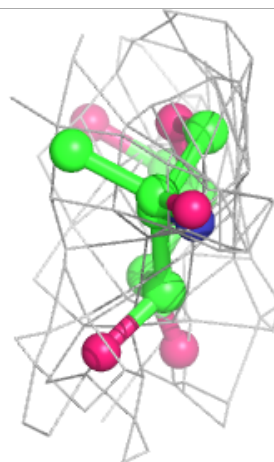
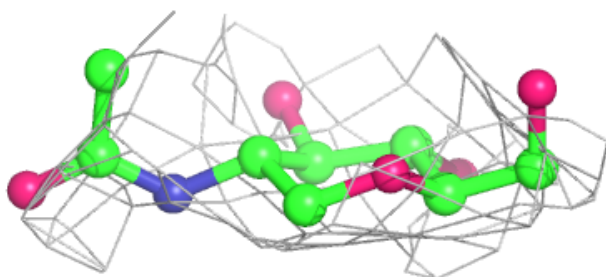
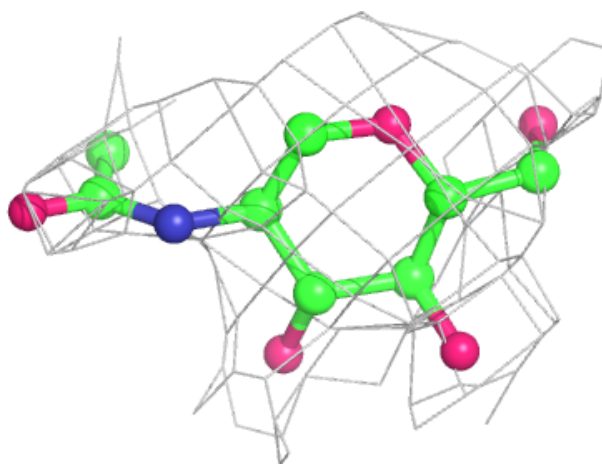
**Electron density around NAG I 409:**

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



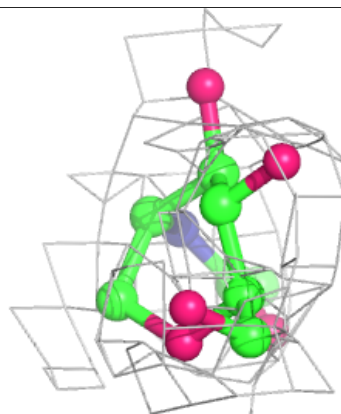
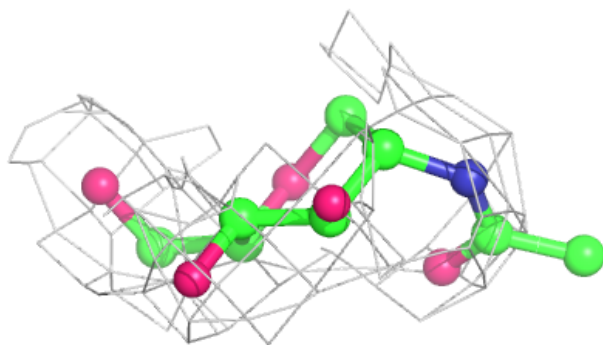
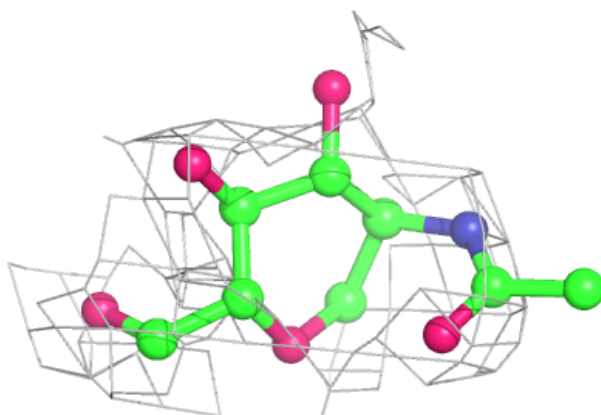
**Electron density around NAG K 401:**

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

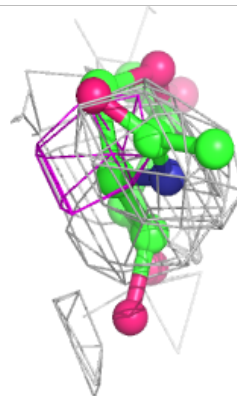
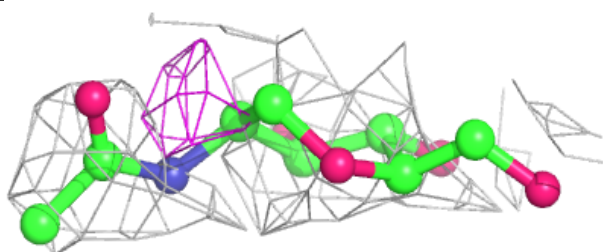
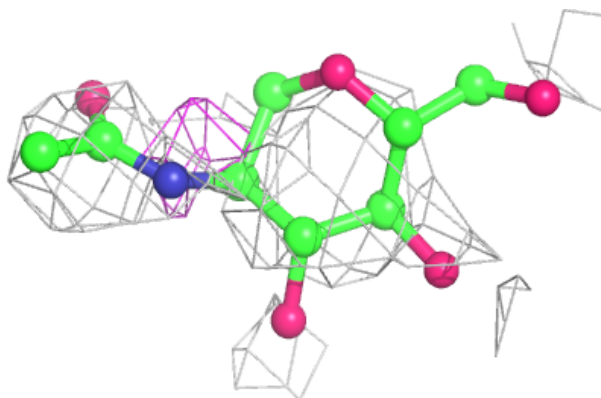


**Electron density around NAG E 414:**

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

**Electron density around NAG A 412:**

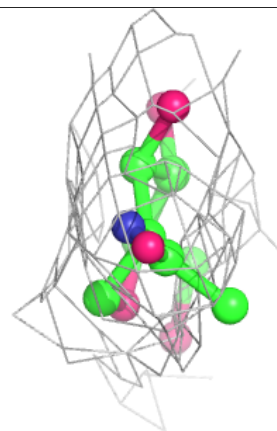
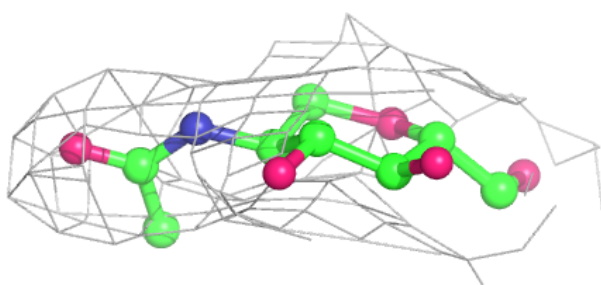
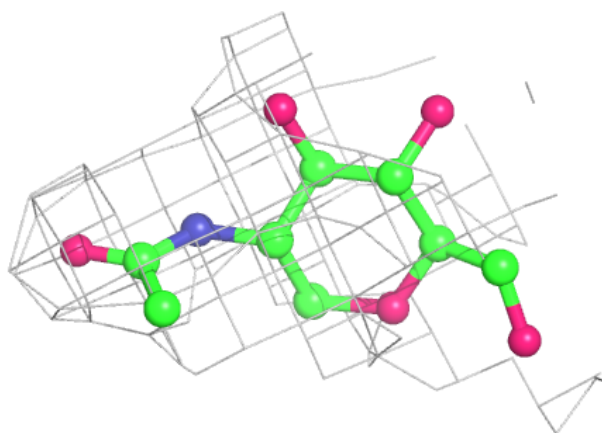
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



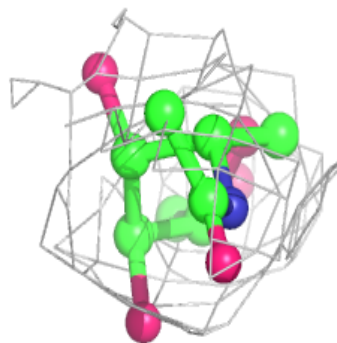
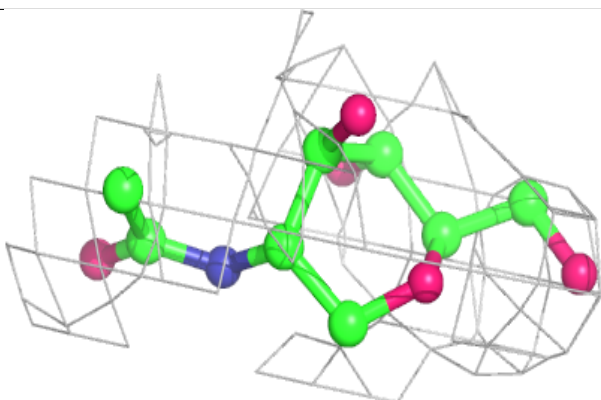
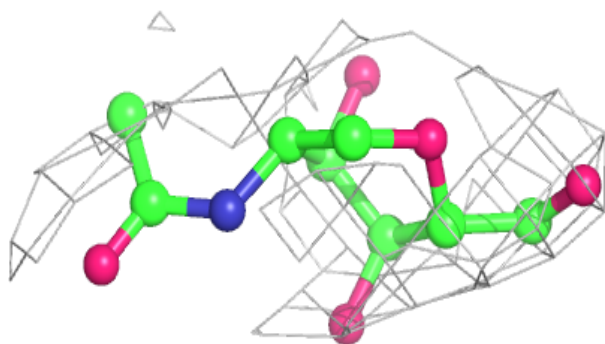


**Electron density around NAG G 401:**

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

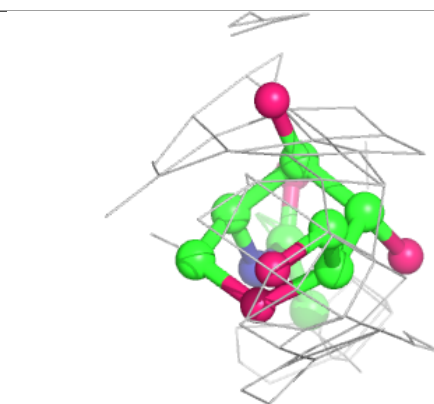
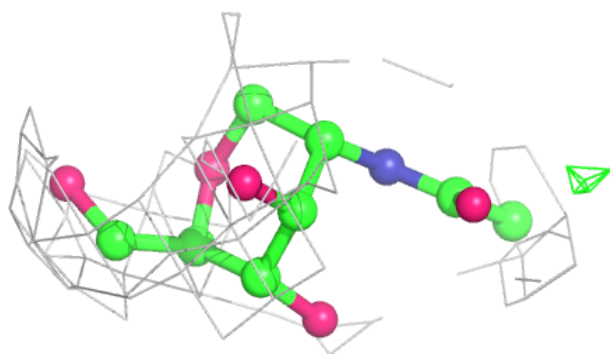
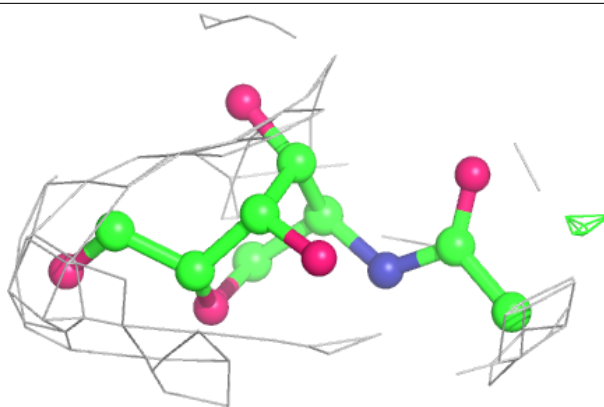
**Electron density around NAG I 401:**

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

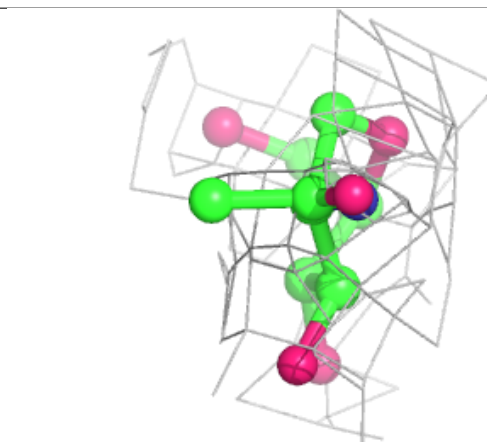
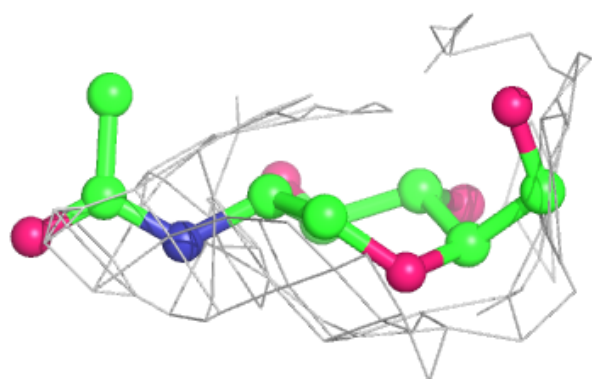
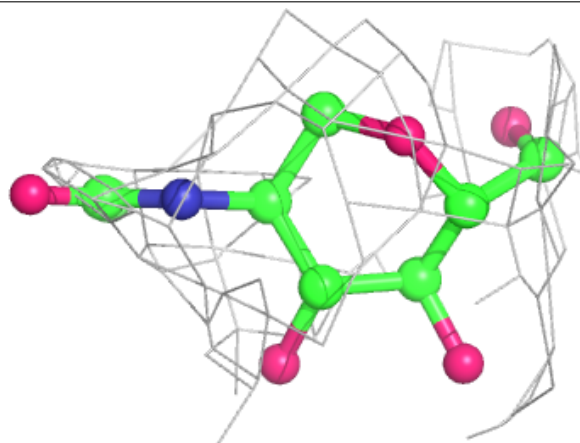


**Electron density around NAG G 402:**

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

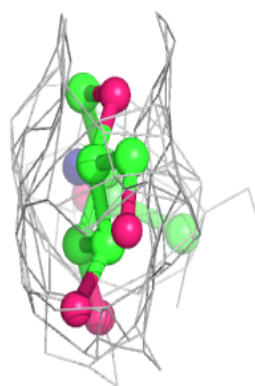
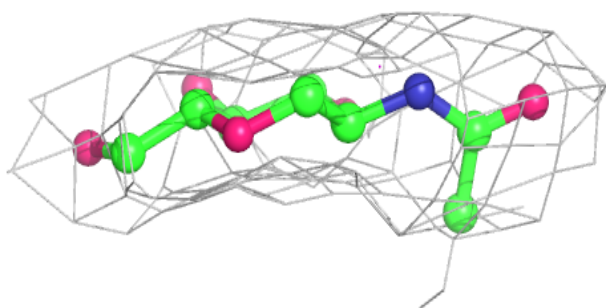
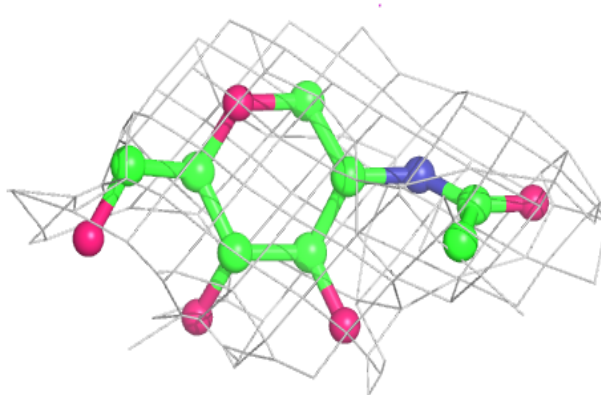
**Electron density around NAG K 414:**

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

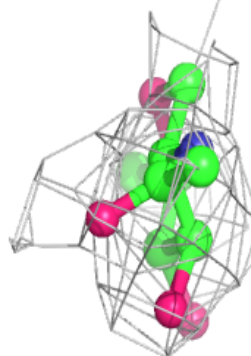
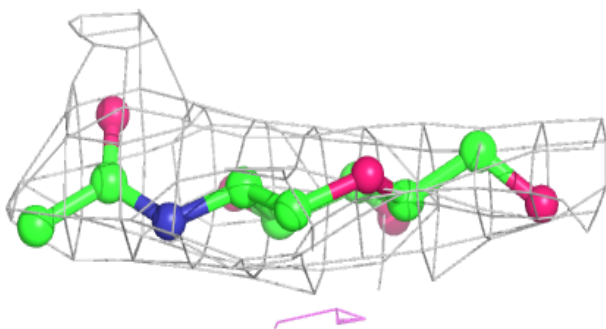
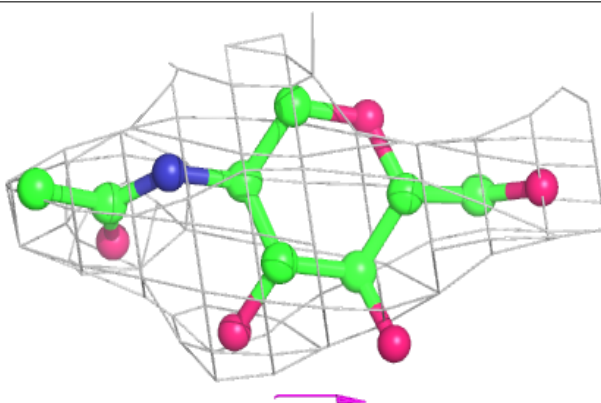


**Electron density around NAG C 409:**

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

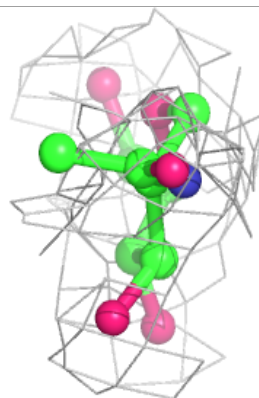
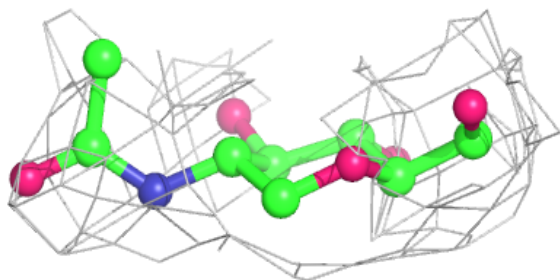
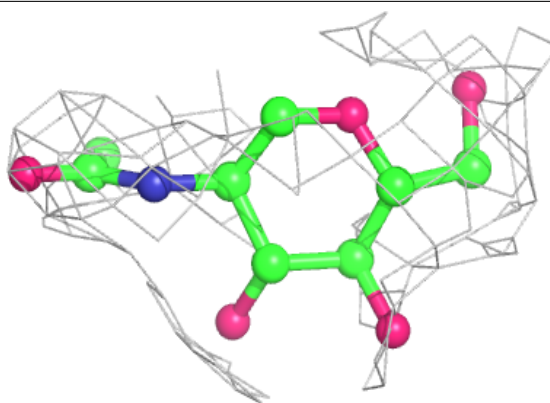
**Electron density around NAG E 413:**

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

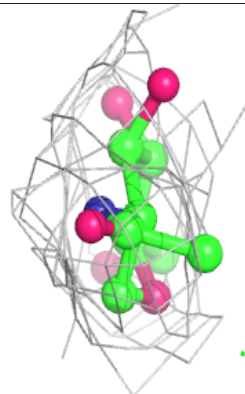
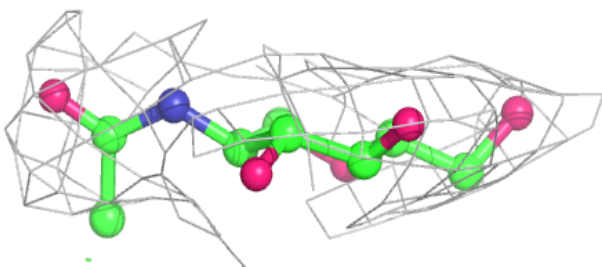
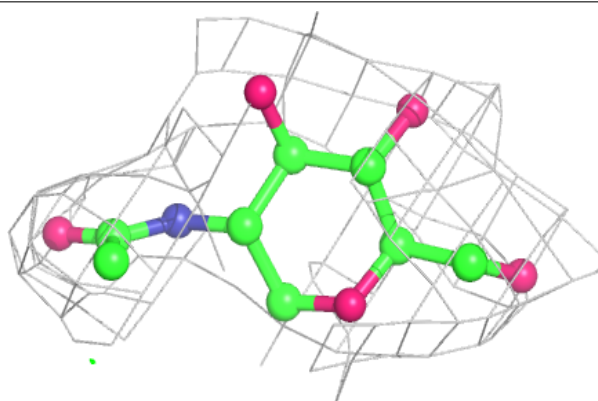


**Electron density around NAG E 401:**

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

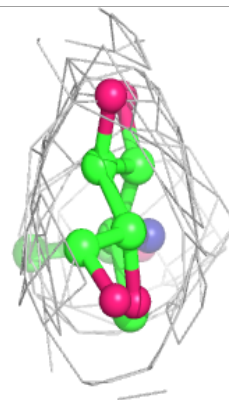
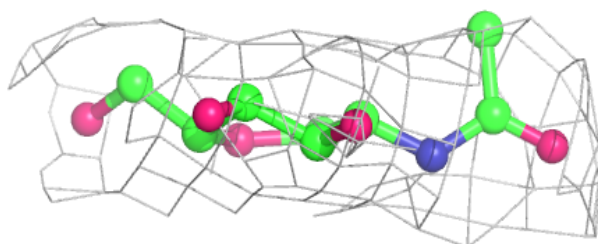
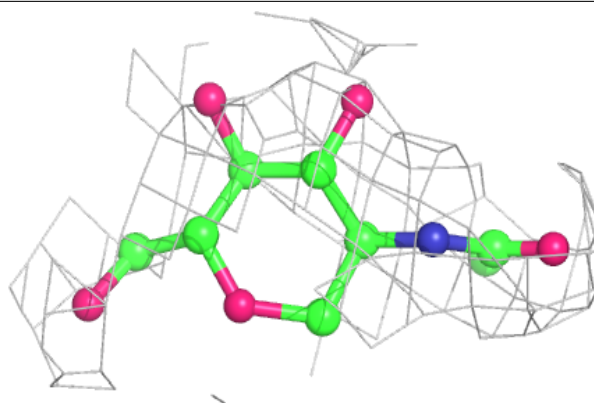
**Electron density around NAG A 414:**

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



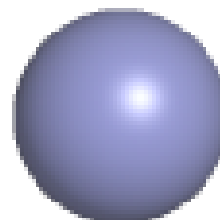
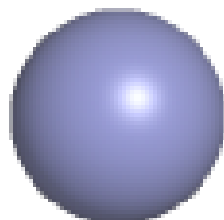
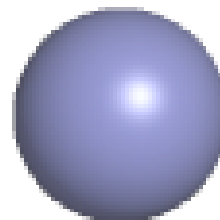
**Electron density around NAG G 413:**

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



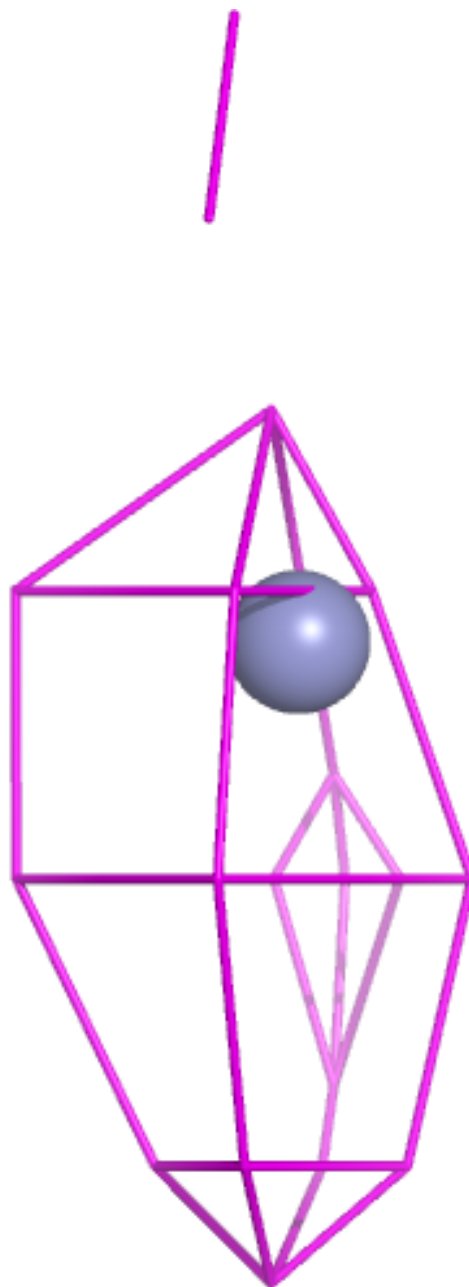
**Electron density around ZN G 414:**

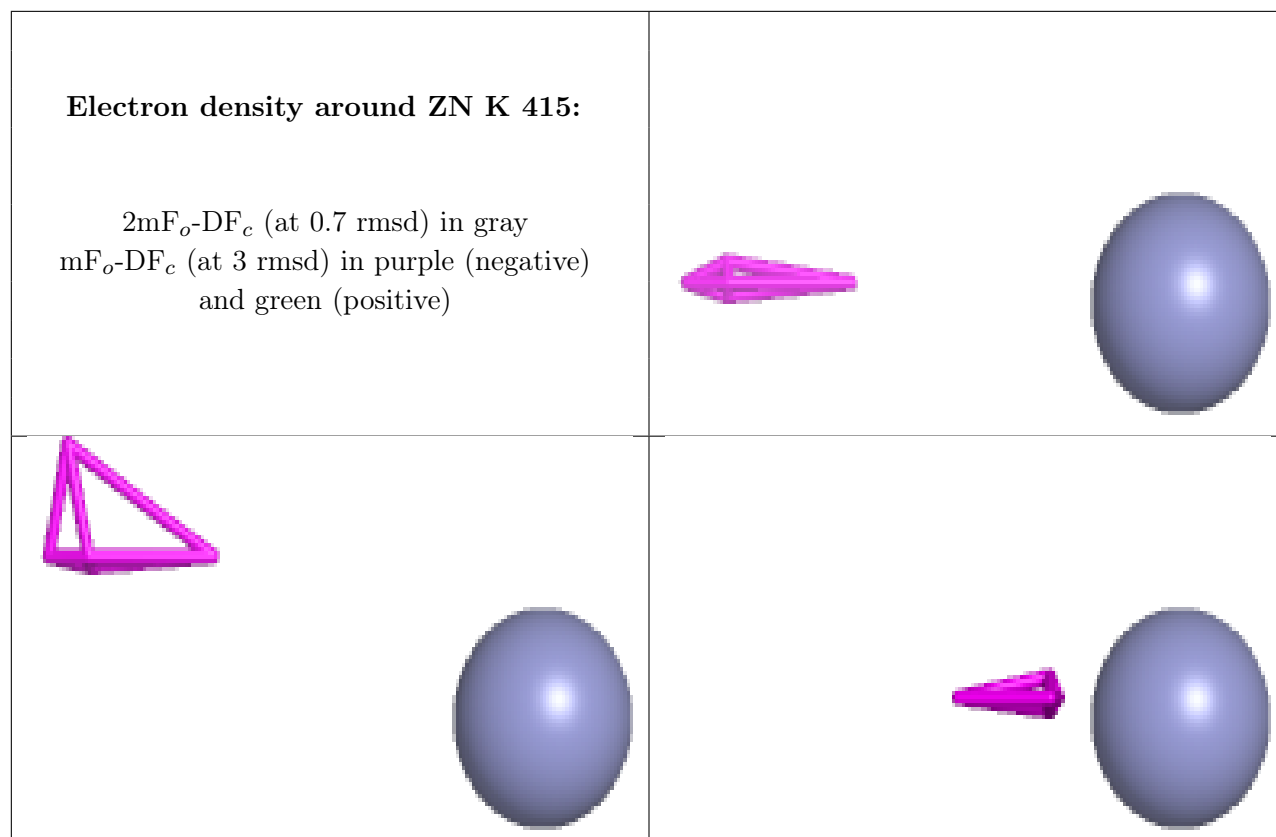
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN I 411:**

$2mF_o - DF_c$  (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.