



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:13 PM UTC

PDB ID : 8E1P / pdb_00008e1p
Title : Crystal structure of BG505 SOSIP.v4.1-GT1.2 trimer in complex with gl-PGV20 and PGT124 Fabs
Authors : Sarkar, A.; Kumar, S.; Wilson, I.A.
Deposited on : 2022-08-11
Resolution : 3.82 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

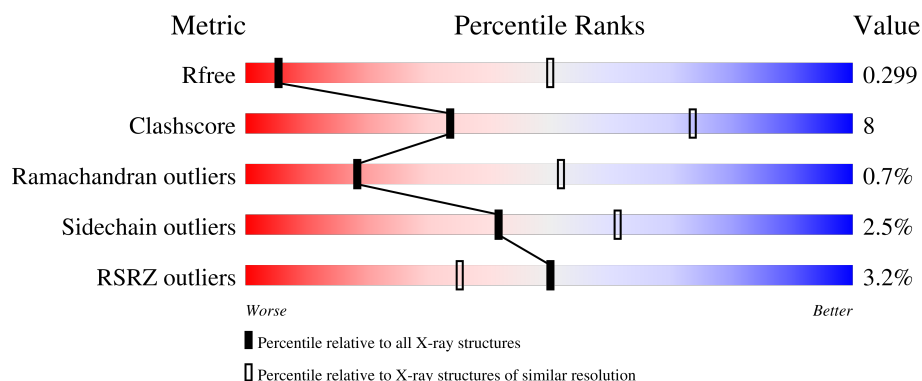
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.82 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1043 (3.98-3.66)
Clashscore	190562	1075 (3.98-3.66)
Ramachandran outliers	187476	1029 (3.98-3.66)
Sidechain outliers	187428	1024 (3.98-3.66)
RSRZ outliers	180081	1042 (3.98-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	F	225	3% 72% 25% ..
1	H	225	2% 81% 17% ..
1	N	225	% 77% 21% .
2	I	210	6% 80% 15% ..
3	L	210	4% 77% 18% ..

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Mol	Chain	Length	Quality of chain
3	O	210	
4	A	214	
4	C	214	
4	J	214	
5	E	474	
5	G	474	
5	M	474	
6	B	236	
6	D	236	
6	K	236	
7	X	153	
7	Y	153	
7	Z	153	
8	P	3	
8	U	3	
8	c	3	
8	e	3	
9	Q	2	
9	S	2	
9	T	2	
9	V	2	
9	W	2	
9	b	2	
9	d	2	
9	f	2	

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Mol	Chain	Length	Quality of chain
9	i	2	 100%
10	R	7	 14% 86%
11	a	9	 11% 56% 33%
12	g	6	 50% 50%
13	h	3	 100%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 34410 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 germline PGV20 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	222	Total	C	N	O	S	0	0	0
			1690	1060	294	326	10			
1	H	222	Total	C	N	O	S	0	0	0
			1690	1060	294	326	10			
1	N	222	Total	C	N	O	S	0	0	0
			1690	1060	294	326	10			

- Molecule 2 is a protein called germline PGV20 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	205	Total	C	N	O	S	0	0	0
			1526	954	250	316	6			

- Molecule 3 is a protein called germline PGV20 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	204	Total	C	N	O	S	0	0	0
			1521	952	249	314	6			
3	O	205	Total	C	N	O	S	0	0	0
			1526	954	250	316	6			

- Molecule 4 is a protein called PGT124 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			
4	C	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			
4	J	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			

- Molecule 5 is a protein called BG505-SOSIP.v4.1-GT1.2gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	447	Total	C	N	O	S	0	0	0
			3526	2219	622	658	27			
5	G	449	Total	C	N	O	S	0	0	0
			3541	2227	625	662	27			
5	M	449	Total	C	N	O	S	0	0	0
			3541	2227	625	662	27			

- Molecule 6 is a protein called PGT124 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	226	Total	C	N	O	S	0	0	0
			1720	1093	287	335	5			
6	D	226	Total	C	N	O	S	0	0	0
			1720	1093	287	335	5			
6	K	226	Total	C	N	O	S	0	0	0
			1720	1093	287	335	5			

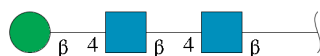
- Molecule 7 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Y	129	Total	C	N	O	S	0	0	0
			1030	655	176	193	6			
7	X	129	Total	C	N	O	S	0	0	0
			1030	655	176	193	6			
7	Z	129	Total	C	N	O	S	0	0	0
			1030	655	176	193	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	559	PRO	ILE	conflict	UNP Q2N0S6
Y	605	CYS	THR	conflict	UNP Q2N0S6
X	559	PRO	ILE	conflict	UNP Q2N0S6
X	605	CYS	THR	conflict	UNP Q2N0S6
Z	559	PRO	ILE	conflict	UNP Q2N0S6
Z	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 8 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.



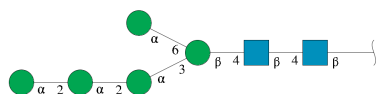
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	U	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	c	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



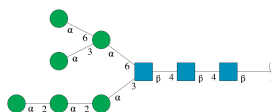
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	b	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	d	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	i	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(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.



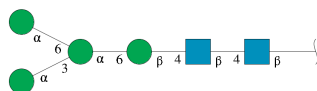
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	R	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(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
11	a	9	Total	C	N	O	0	0	0
			108	60	3	45			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



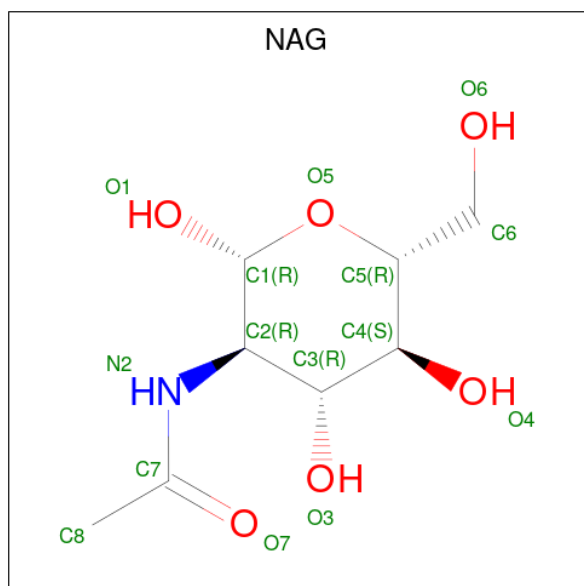
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	g	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	h	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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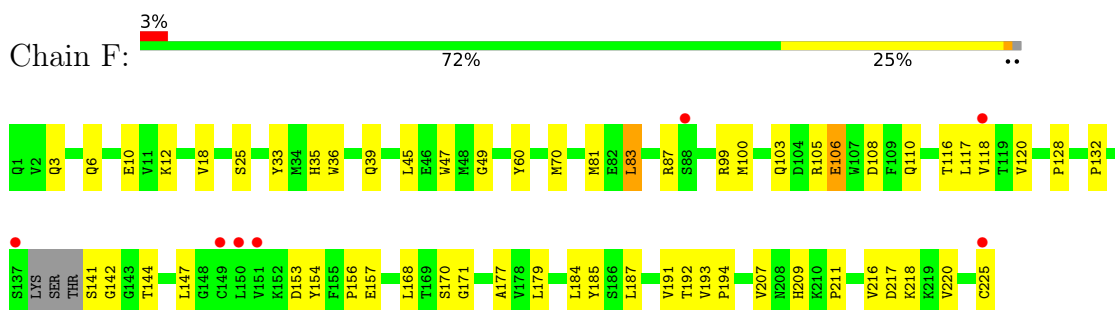
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	M	1	Total	C	N	O	0	0
			14	8	1	5		
14	M	1	Total	C	N	O	0	0
			14	8	1	5		
14	M	1	Total	C	N	O	0	0
			14	8	1	5		
14	M	1	Total	C	N	O	0	0
			14	8	1	5		
14	M	1	Total	C	N	O	0	0
			14	8	1	5		
14	M	1	Total	C	N	O	0	0
			14	8	1	5		
14	M	1	Total	C	N	O	0	0
			14	8	1	5		
14	M	1	Total	C	N	O	0	0
			14	8	1	5		
14	Y	1	Total	C	N	O	0	0
			14	8	1	5		
14	Y	1	Total	C	N	O	0	0
			14	8	1	5		
14	Y	1	Total	C	N	O	0	0
			14	8	1	5		
14	X	1	Total	C	N	O	0	0
			14	8	1	5		
14	X	1	Total	C	N	O	0	0
			14	8	1	5		
14	Z	1	Total	C	N	O	0	0
			14	8	1	5		
14	Z	1	Total	C	N	O	0	0
			14	8	1	5		

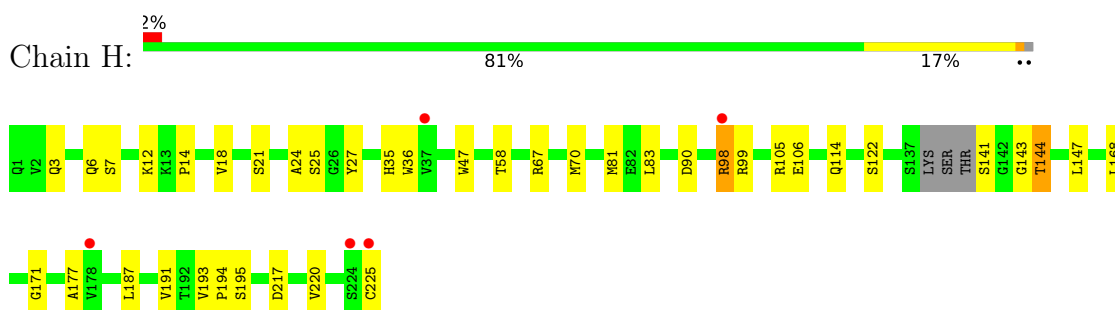
3 Residue-property plots [i](#)

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.

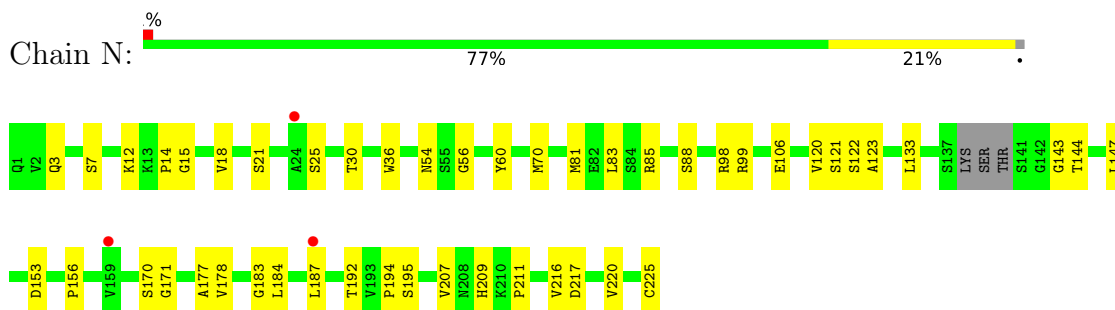
- Molecule 1: germline PGV20 heavy chain



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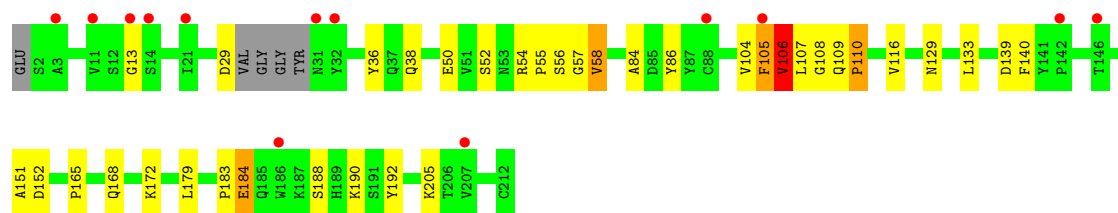


- Molecule 1: germline PGV20 heavy chain

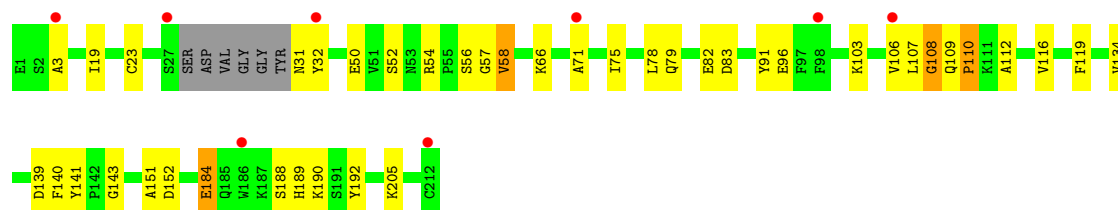
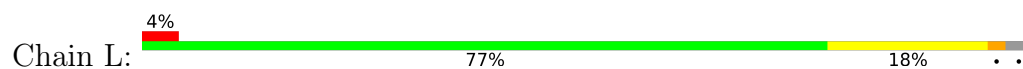


- Molecule 2: germline PGV20 light chain

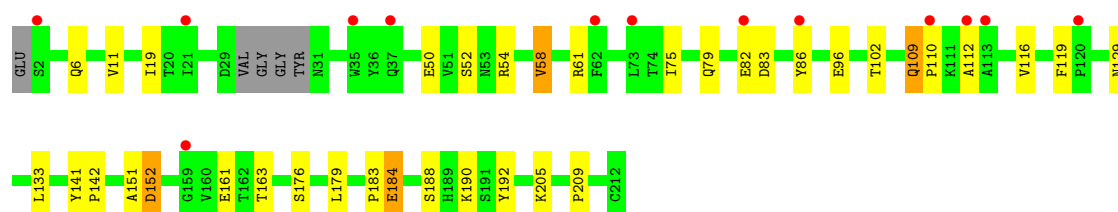
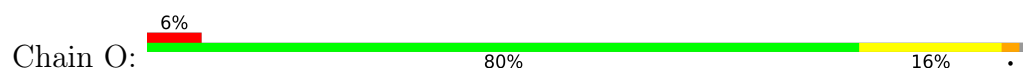




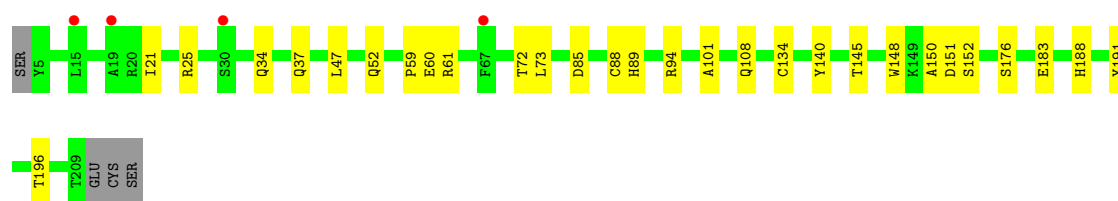
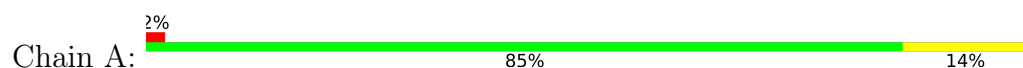
- Molecule 3: germline PGV20 light chain



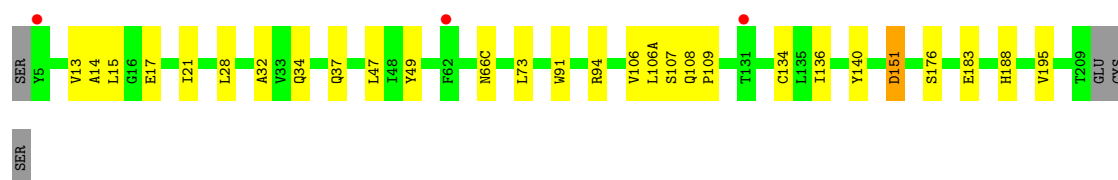
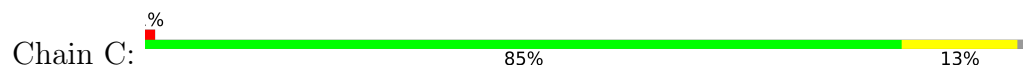
- Molecule 3: germline PGV20 light chain



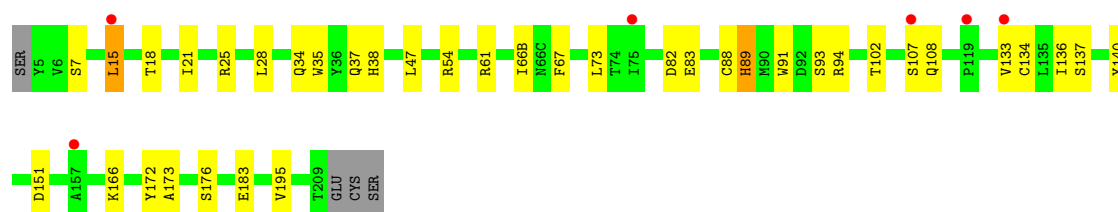
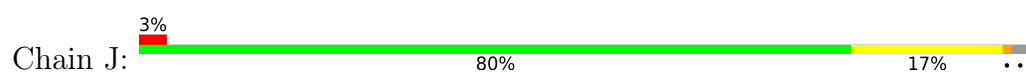
- Molecule 4: PGT124 Fab Light Chain



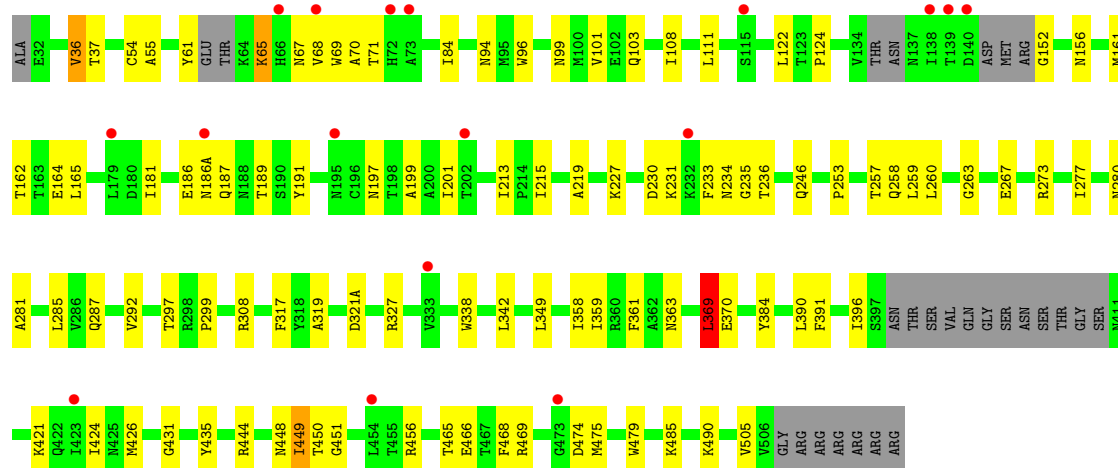
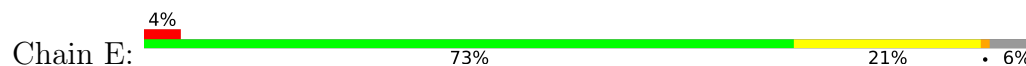
- Molecule 4: PGT124 Fab Light Chain



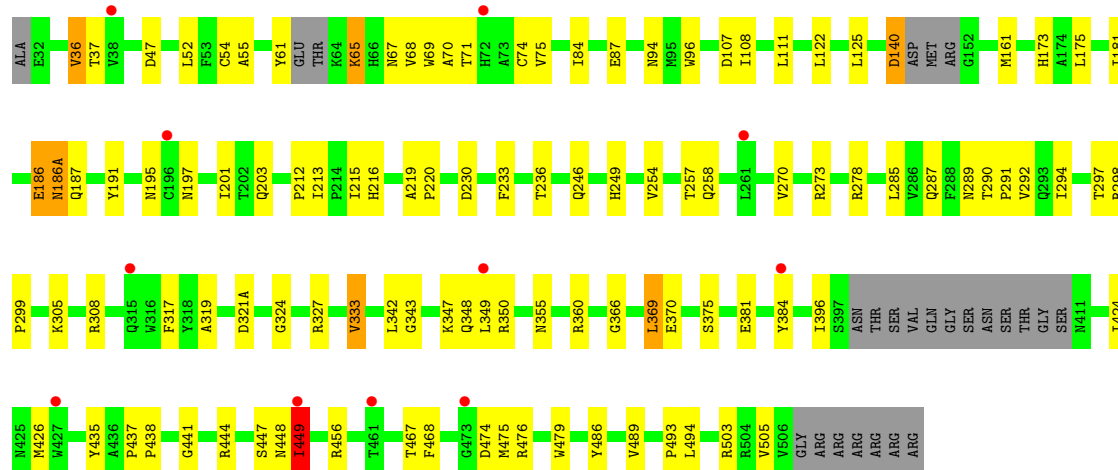
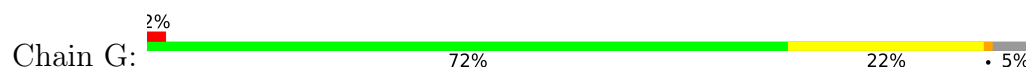
- Molecule 4: PGT124 Fab Light Chain



• Molecule 5: BG505-SOSIP.v4.1-GT1.2gp120

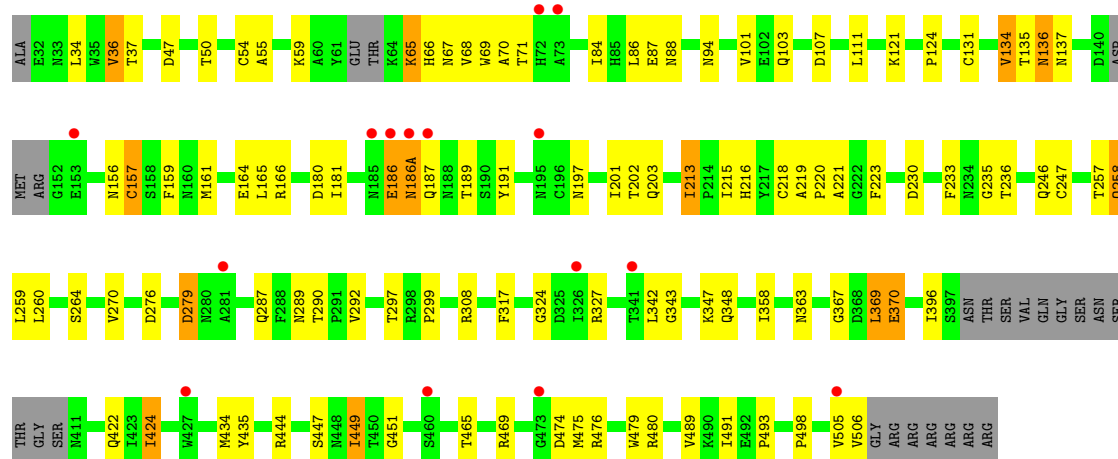


• Molecule 5: BG505-SOSIP.v4.1-GT1.2gp120

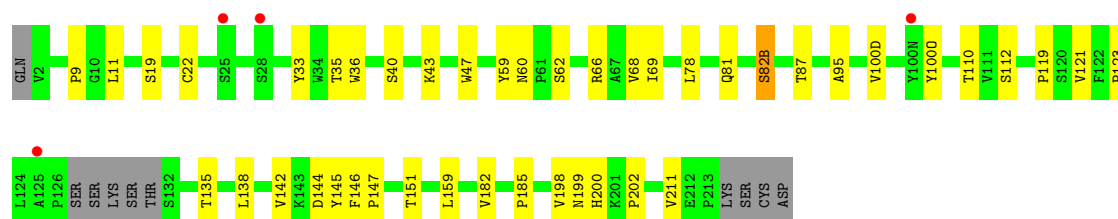
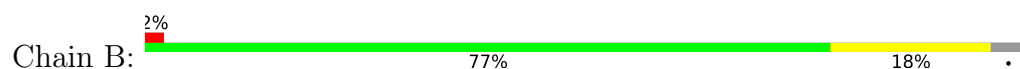


• Molecule 5: BG505-SOSIP.v4.1-GT1.2gp120

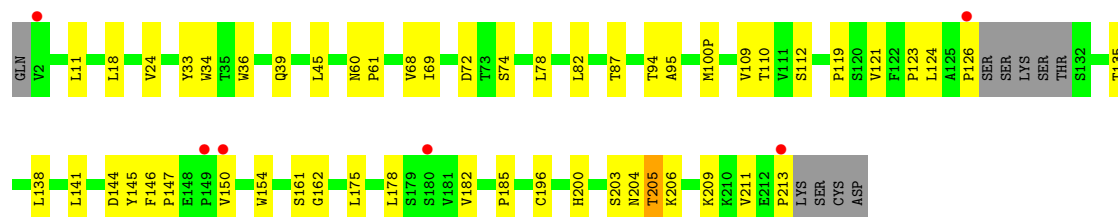
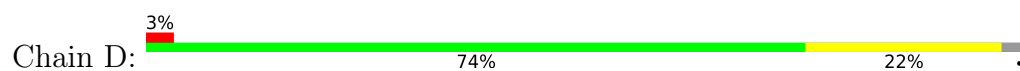




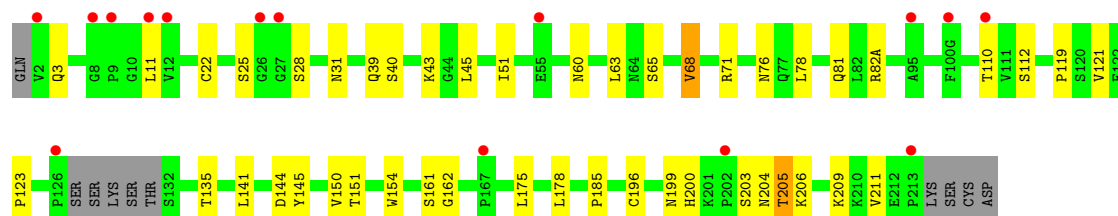
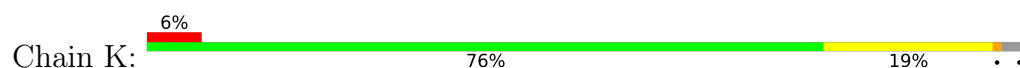
• Molecule 6: PGT124 Fab Heavy Chain



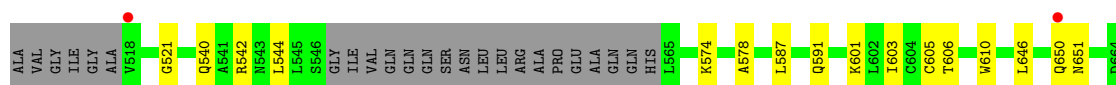
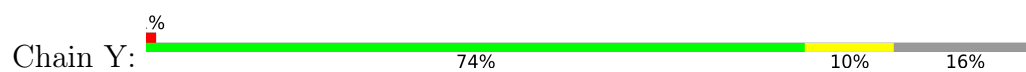
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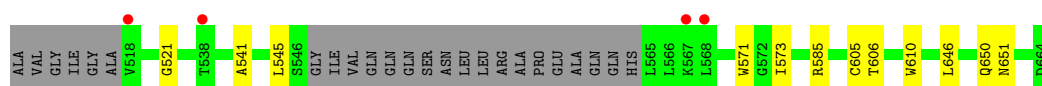
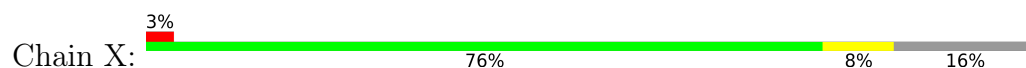
• Molecule 6: PGT124 Fab Heavy Chain



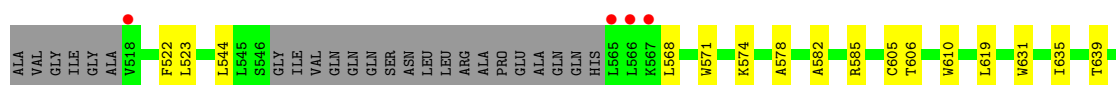
• Molecule 7: Envelope glycoprotein gp41



- Molecule 7: Envelope glycoprotein gp41



- Molecule 7: Envelope glycoprotein gp41



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  33% 67%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%

AG1
AG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  100%

AG1
AG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%

AG1
AG2

- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(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 R:  14% 86%

AG1
AG2
BK3
MAN4
MAN5
MAN6
MAN7

- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  11% 56% 33%

AG1
AG2
AG3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 g:  50% 50%

AG1
AG2
BK3
MAN4
MAN5
MAN6

- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain h:

100%

MAN1
MAN2
MAN3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.06Å 157.67Å 158.56Å 90.00° 102.97° 90.00°	Depositor
Resolution (Å)	49.76 – 3.82 49.76 – 3.83	Depositor EDS
% Data completeness (in resolution range)	94.3 (49.76-3.82) 94.3 (49.76-3.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.271 , 0.301 0.270 , 0.299	Depositor DCC
R_{free} test set	3181 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	104.9	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	34410	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	F	0.14	0/1732	0.33	0/2354
1	H	0.11	0/1732	0.29	0/2354
1	N	0.10	0/1732	0.30	0/2354
2	I	0.13	0/1564	0.33	0/2132
3	L	0.12	0/1558	0.35	0/2122
3	O	0.10	0/1563	0.31	0/2129
4	A	0.09	0/1638	0.25	0/2238
4	C	0.10	0/1638	0.26	0/2238
4	J	0.08	0/1638	0.25	0/2238
5	E	0.11	0/3601	0.28	0/4889
5	G	0.13	0/3618	0.33	1/4916 (0.0%)
5	M	0.12	0/3617	0.30	0/4913
6	B	0.10	0/1763	0.29	0/2407
6	D	0.10	0/1763	0.29	0/2407
6	K	0.11	0/1763	0.29	0/2407
7	X	0.08	0/1048	0.22	0/1421
7	Y	0.09	0/1048	0.22	0/1421
7	Z	0.09	0/1048	0.24	0/1421
All	All	0.11	0/34064	0.29	1/46361 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	140	ASP	N-CA-C	5.29	122.08	110.80

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	F	1690	0	1645	38	0
1	H	1690	0	1645	27	0
1	N	1690	0	1645	27	0
2	I	1526	0	1462	21	0
3	L	1521	0	1461	25	0
3	O	1526	0	1461	24	0
4	A	1595	0	1541	16	0
4	C	1595	0	1541	16	0
4	J	1595	0	1541	24	0
5	E	3526	0	3463	69	0
5	G	3541	0	3478	72	0
5	M	3541	0	3477	75	0
6	B	1720	0	1686	25	0
6	D	1720	0	1686	27	0
6	K	1720	0	1686	27	0
7	X	1030	0	1019	10	0
7	Y	1030	0	1018	16	0
7	Z	1030	0	1019	24	0
8	P	39	0	34	0	0
8	U	39	0	34	1	0
8	c	39	0	34	2	0
8	e	39	0	34	2	0
9	Q	28	0	25	0	0
9	S	28	0	25	1	0
9	T	28	0	25	2	0
9	V	28	0	25	0	0
9	W	28	0	25	0	0
9	b	28	0	25	1	0
9	d	28	0	25	0	0
9	f	28	0	25	0	0
9	i	28	0	25	0	0
10	R	83	0	70	0	0
11	a	108	0	91	3	0
12	g	72	0	61	0	0
13	h	33	0	28	0	0
14	E	112	0	104	3	0
14	G	98	0	91	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	112	0	104	4	0
14	X	28	0	26	0	0
14	Y	42	0	39	0	0
14	Z	28	0	26	0	0
All	All	34410	0	33475	519	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 8.

All (519) 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)
5:E:186(A):ASN:H	5:E:187:GLN:HA	1.41	0.86
1:N:121:SER:HA	1:N:122:SER:HB3	1.60	0.84
5:M:186(A):ASN:N	5:M:187:GLN:HA	1.94	0.82
5:E:186(A):ASN:N	5:E:187:GLN:HA	1.96	0.81
1:F:144:THR:HA	1:F:194:PRO:HA	1.61	0.80
5:G:186(A):ASN:N	5:G:187:GLN:HA	1.97	0.80
1:F:142:GLY:CA	1:F:144:THR:H	1.96	0.79
5:E:152:GLY:N	14:E:601:NAG:HO6	1.83	0.76
5:G:230:ASP:HB3	5:G:233:PHE:HB2	1.68	0.76
5:M:186(A):ASN:H	5:M:187:GLN:HA	1.50	0.75
7:Y:591:GLN:NE2	7:X:541:ALA:O	2.20	0.74
2:I:13:GLY:H	2:I:105:PHE:HE1	1.35	0.74
5:M:424:ILE:HD11	5:M:434:MET:HE2	1.70	0.74
5:G:291:PRO:HG3	8:c:1:NAG:H61	1.70	0.73
4:C:108:GLN:HG2	4:C:109:PRO:HD2	1.70	0.73
5:E:69:TRP:HB3	5:E:215:ILE:HD11	1.71	0.72
5:E:230:ASP:HB3	5:E:233:PHE:HB2	1.70	0.72
5:M:84:ILE:HD13	7:Z:522:PHE:H	1.53	0.72
6:B:100(D):VAL:HA	11:a:2:NAG:H83	1.72	0.71
5:G:186(A):ASN:H	5:G:187:GLN:HA	1.55	0.71
2:I:54:ARG:HD2	2:I:58:VAL:HG22	1.74	0.69
6:B:22:CYS:HB3	6:B:78:LEU:HB3	1.73	0.69
5:M:219:ALA:O	5:M:246:GLN:NE2	2.26	0.69
6:B:135:THR:HA	6:B:185:PRO:HA	1.75	0.69
5:G:220:PRO:HB3	7:Y:578:ALA:HB1	1.74	0.68
1:F:142:GLY:HA3	1:F:144:THR:H	1.59	0.68
5:M:230:ASP:HB3	5:M:233:PHE:HB2	1.76	0.67
5:G:219:ALA:O	5:G:246:GLN:NE2	2.27	0.67
5:M:37:THR:HG22	7:Z:605:CYS:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:GLN:HB3	1:H:25:SER:HB2	1.77	0.66
5:M:363:ASN:O	5:M:469:ARG:NH1	2.26	0.66
6:D:123:PRO:HG3	6:D:209:LYS:HB3	1.76	0.66
1:H:144:THR:HA	1:H:195:SER:H	1.61	0.65
6:B:121:VAL:HG11	6:B:198:VAL:HG21	1.77	0.65
3:L:54:ARG:HD2	3:L:58:VAL:HG22	1.78	0.65
7:X:573:ILE:HD13	7:Z:568:LEU:HD21	1.79	0.65
7:Y:542:ARG:NH1	7:Z:647:GLU:OE2	2.30	0.65
2:I:152:ASP:OD2	2:I:190:LYS:HG3	1.97	0.65
5:G:308:ARG:NH1	5:M:197:ASN:O	2.30	0.65
5:M:276:ASP:HB3	5:M:279:ASP:HB2	1.78	0.65
4:C:34:GLN:HG3	4:C:49:TYR:HA	1.79	0.64
1:F:105:ARG:HG3	1:F:106:GLU:HB2	1.78	0.64
6:D:135:THR:HA	6:D:185:PRO:HA	1.78	0.64
5:E:156:ASN:ND2	14:E:602:NAG:O7	2.30	0.64
5:M:491:ILE:O	7:Z:585:ARG:NH2	2.31	0.64
1:F:103:GLN:NE2	1:F:108:ASP:OD2	2.29	0.63
5:E:201:ILE:HD11	5:E:435:TYR:HB2	1.80	0.63
9:b:2:NAG:H83	9:b:2:NAG:H3	1.81	0.63
5:E:164:GLU:HG3	5:E:165:LEU:HD12	1.80	0.63
1:F:10:GLU:HB2	1:F:118:VAL:HG12	1.79	0.63
7:Z:606:THR:HG21	7:Z:646:LEU:HD11	1.81	0.63
5:G:70:ALA:HB2	5:G:213:ILE:HD11	1.79	0.62
4:J:21:ILE:HB	4:J:73:LEU:HB3	1.81	0.62
1:H:6:GLN:H	1:H:114:GLN:HE22	1.47	0.62
1:H:7:SER:HB3	1:H:21:SER:HB3	1.81	0.62
5:E:36:VAL:HG12	7:X:610:TRP:HE3	1.64	0.62
14:G:601:NAG:H3	14:G:601:NAG:H83	1.82	0.62
7:X:606:THR:HG21	7:X:646:LEU:HD11	1.81	0.62
5:E:277:ILE:O	5:E:456:ARG:NH1	2.33	0.61
5:G:186(A):ASN:O	5:G:186(A):ASN:ND2	2.33	0.61
5:G:47:ASP:HA	5:G:489:VAL:HG12	1.82	0.61
5:M:36:VAL:HG12	7:Z:610:TRP:HE3	1.64	0.61
5:E:424:ILE:HD12	5:E:426:MET:HE3	1.83	0.61
1:H:144:THR:HG22	1:H:194:PRO:HA	1.83	0.60
5:M:135:THR:O	5:M:137:ASN:N	2.34	0.60
5:E:69:TRP:HA	5:E:111:LEU:HD13	1.82	0.60
5:M:87:GLU:HB2	14:M:601:NAG:H82	1.83	0.60
4:A:134:CYS:HB3	4:A:176:SER:HB3	1.83	0.60
5:M:221:ALA:HB3	7:Z:582:ALA:HB1	1.84	0.60
4:A:25:ARG:NH2	4:A:88:CYS:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:604:NAG:H83	14:G:604:NAG:H3	1.83	0.60
6:B:11:LEU:HD11	6:B:112:SER:HB3	1.84	0.60
5:E:186(A):ASN:O	5:E:186(A):ASN:ND2	2.35	0.59
6:D:87:THR:HG23	6:D:110:THR:HA	1.84	0.59
5:M:94:ASN:HA	5:M:236:THR:HG22	1.84	0.59
5:M:201:ILE:HD11	5:M:435:TYR:HB2	1.84	0.59
5:G:55:ALA:HB3	5:G:216:HIS:HB2	1.84	0.59
6:K:123:PRO:HG3	6:K:209:LYS:HB3	1.85	0.59
2:I:107:LEU:HG	2:I:109:GLN:HA	1.84	0.59
5:M:34:LEU:HD21	7:Z:619:LEU:HD11	1.85	0.59
5:M:292:VAL:HB	5:M:449:ILE:HG23	1.83	0.59
4:J:25:ARG:NH2	4:J:88:CYS:O	2.35	0.59
1:H:168:LEU:HD21	1:H:191:VAL:HG21	1.83	0.59
5:G:122:LEU:HD13	5:G:125:LEU:HD22	1.85	0.59
6:K:65:SER:O	6:K:82(A):ARG:NH1	2.36	0.59
5:M:474:ASP:OD2	5:M:476:ARG:NH1	2.36	0.58
4:C:37:GLN:HB2	4:C:47:LEU:HD11	1.84	0.58
5:E:124:PRO:HA	5:M:166:ARG:HE	1.68	0.58
4:J:7:SER:HB3	4:J:102:THR:HA	1.84	0.58
1:F:144:THR:HG22	1:F:192:THR:HG22	1.86	0.58
5:E:292:VAL:HB	5:E:449:ILE:HG23	1.86	0.58
1:H:171:GLY:O	1:H:191:VAL:HA	2.04	0.58
5:E:308:ARG:NH1	5:G:197:ASN:O	2.37	0.58
1:F:142:GLY:CA	1:F:144:THR:N	2.66	0.58
5:G:299:PRO:HB2	5:G:327:ARG:HB2	1.84	0.58
5:G:321(A):ASP:HB3	14:G:602:NAG:H82	1.85	0.58
6:B:87:THR:HG23	6:B:110:THR:HA	1.84	0.58
3:O:54:ARG:HD2	3:O:58:VAL:HG22	1.84	0.58
5:E:474:ASP:OD1	5:E:475:MET:N	2.37	0.58
1:N:177:ALA:HB2	1:N:187:LEU:HD23	1.86	0.57
1:H:144:THR:HA	1:H:194:PRO:HA	1.84	0.57
1:F:99:ARG:HD2	1:F:105:ARG:HB2	1.87	0.57
3:L:116:VAL:O	3:L:205:LYS:NZ	2.31	0.57
4:C:134:CYS:HB3	4:C:176:SER:HB3	1.87	0.57
9:S:2:NAG:H83	9:S:2:NAG:H3	1.87	0.57
5:G:37:THR:HG22	7:Y:605:CYS:HA	1.87	0.57
1:H:177:ALA:HB2	1:H:187:LEU:HD23	1.87	0.57
4:C:21:ILE:HD12	4:C:73:LEU:HD23	1.87	0.56
5:G:94:ASN:HA	5:G:236:THR:HG22	1.87	0.56
5:G:201:ILE:HD11	5:G:435:TYR:HB2	1.87	0.56
1:F:6:GLN:NE2	1:F:116:THR:OG1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:61:TYR:CD1	5:G:65:LYS:HB3	2.40	0.56
5:G:493:PRO:HG3	7:Y:544:LEU:HD21	1.88	0.56
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.38	0.56
1:N:144:THR:HA	1:N:194:PRO:HA	1.85	0.56
5:M:235:GLY:HA3	14:M:604:NAG:H82	1.86	0.56
5:E:297:THR:HG22	5:E:444:ARG:HG3	1.86	0.56
5:G:84:ILE:HD13	7:Y:521:GLY:HA3	1.88	0.56
6:D:138:LEU:O	6:D:182:VAL:N	2.38	0.56
1:N:14:PRO:HD3	1:N:121:SER:O	2.06	0.56
5:E:448:ASN:HD22	9:T:1:NAG:C7	2.19	0.56
5:E:273:ARG:NH1	5:E:287:GLN:OE1	2.35	0.55
6:K:40:SER:HB2	6:K:43:LYS:HD2	1.87	0.55
6:K:119:PRO:HB3	6:K:145:TYR:HB3	1.87	0.55
6:K:150:VAL:HB	6:K:178:LEU:HD21	1.86	0.55
2:I:116:VAL:O	2:I:205:LYS:NZ	2.30	0.55
6:K:51:ILE:HD13	6:K:71:ARG:HG3	1.88	0.55
1:N:3:GLN:HB3	1:N:25:SER:HB2	1.87	0.55
5:E:299:PRO:HB2	5:E:327:ARG:HB2	1.87	0.55
6:K:135:THR:HA	6:K:185:PRO:HA	1.88	0.55
1:F:177:ALA:HB2	1:F:187:LEU:HD23	1.89	0.55
5:G:173:HIS:CE1	5:G:305:LYS:HE3	2.42	0.55
3:O:109:GLN:NE2	3:O:141:TYR:O	2.40	0.55
3:L:107:LEU:HD11	3:L:110:PRO:HG3	1.89	0.54
3:O:133:LEU:HD12	3:O:179:LEU:HB3	1.89	0.54
5:M:55:ALA:HB3	5:M:216:HIS:HB2	1.90	0.54
5:G:36:VAL:HG12	7:Y:610:TRP:HE3	1.72	0.54
6:D:119:PRO:HB3	6:D:145:TYR:HB3	1.88	0.54
1:F:156:PRO:HD2	1:F:211:PRO:HB2	1.88	0.54
3:L:184:GLU:O	3:L:188:SER:OG	2.24	0.54
5:G:298:ARG:NH2	5:G:441:GLY:O	2.39	0.54
1:H:177:ALA:HA	1:H:187:LEU:HB3	1.90	0.54
1:N:147:LEU:HB2	1:N:220:VAL:HG11	1.89	0.54
5:E:101:VAL:HG13	5:E:479:TRP:HB2	1.90	0.54
1:F:171:GLY:O	1:F:191:VAL:HA	2.08	0.54
1:H:191:VAL:HG22	1:H:193:VAL:HG13	1.90	0.54
5:E:197:ASN:O	5:M:308:ARG:NH1	2.40	0.54
5:G:61:TYR:HD1	5:G:65:LYS:HB3	1.71	0.54
4:A:148:TRP:HE1	4:A:176:SER:HG	1.54	0.54
5:G:173:HIS:ND1	14:G:602:NAG:O7	2.41	0.53
1:F:147:LEU:HB2	1:F:220:VAL:HG11	1.90	0.53
3:L:31:ASN:N	3:L:66:LYS:HZ3	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:264:SER:O	5:M:287:GLN:NE2	2.34	0.53
6:D:126:PRO:HG2	6:D:213:PRO:HB3	1.90	0.53
5:E:84:ILE:HD13	7:X:521:GLY:HA3	1.90	0.53
5:E:490:LYS:HD2	7:X:585:ARG:HH12	1.73	0.53
6:D:11:LEU:HD11	6:D:112:SER:HB3	1.90	0.53
3:L:91:TYR:CE2	5:G:278:ARG:HB3	2.43	0.53
4:J:28:LEU:HB3	4:J:94:ARG:HD3	1.91	0.53
1:F:100:MET:HG2	1:F:110:GLN:HB2	1.91	0.53
6:D:144:ASP:HB3	6:D:175:LEU:HD23	1.91	0.53
5:G:67:ASN:HD21	5:G:70:ALA:H	1.56	0.53
5:M:164:GLU:HG3	5:M:165:LEU:HD12	1.91	0.53
6:K:22:CYS:HB3	6:K:78:LEU:HB3	1.90	0.53
1:N:36:TRP:CE2	1:N:81:MET:HB2	2.44	0.53
5:G:298:ARG:NH1	5:G:381:GLU:OE2	2.41	0.53
1:H:99:ARG:HD3	1:H:106:GLU:HG3	1.92	0.52
3:O:82:GLU:OE2	3:O:86:TYR:OH	2.23	0.52
1:N:178:VAL:HG21	3:O:161:GLU:HB3	1.90	0.52
6:B:200:HIS:CD2	6:B:202:PRO:HD2	2.44	0.52
5:M:159:PHE:HA	14:M:603:NAG:H82	1.91	0.52
5:M:474:ASP:OD1	5:M:475:MET:N	2.41	0.52
3:L:83:ASP:OD1	3:L:83:ASP:N	2.43	0.52
3:O:109:GLN:HG2	3:O:142:PRO:HD3	1.91	0.52
5:E:263:GLY:O	9:T:1:NAG:H81	2.10	0.52
5:E:363:ASN:O	5:E:469:ARG:NH1	2.41	0.52
5:G:474:ASP:OD1	5:G:475:MET:N	2.43	0.52
5:M:257:THR:O	5:M:259:LEU:N	2.40	0.52
6:D:147:PRO:O	6:D:200:HIS:NE2	2.43	0.52
5:E:358:ILE:HB	5:E:465:THR:HA	1.92	0.52
5:G:297:THR:HG22	5:G:444:ARG:HG3	1.92	0.52
3:O:109:GLN:HB2	3:O:141:TYR:HD1	1.75	0.51
5:G:125:LEU:HD12	5:G:161:MET:HE3	1.92	0.51
5:E:37:THR:HG22	7:X:605:CYS:HA	1.93	0.51
5:G:257:THR:HG22	5:G:258:GLN:HG3	1.93	0.51
5:M:476:ARG:HA	5:M:479:TRP:CD1	2.45	0.51
7:Y:587:LEU:HB3	7:X:545:LEU:HD21	1.92	0.51
5:E:67:ASN:ND2	5:E:70:ALA:H	2.08	0.51
5:M:493:PRO:HG3	7:Z:544:LEU:HD21	1.92	0.51
6:B:151:THR:HB	6:B:199:ASN:HB2	1.92	0.51
7:Z:650:GLN:O	7:Z:654:GLU:N	2.31	0.51
2:I:109:GLN:N	2:I:110:PRO:HD2	2.26	0.51
1:H:58:THR:H	5:G:366:GLY:HA3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:LEU:HB2	1:H:220:VAL:HG11	1.93	0.51
3:L:79:GLN:H	3:L:82:GLU:HG3	1.74	0.51
5:E:370:GLU:HG2	5:E:384:TYR:HE2	1.76	0.51
4:J:89:HIS:CD2	4:J:91:TRP:HE1	2.28	0.51
5:M:134:VAL:HG12	5:M:156:ASN:HB2	1.93	0.51
4:A:59:PRO:HB2	4:A:61:ARG:HG3	1.92	0.51
5:G:96:TRP:HH2	5:G:285:LEU:HD23	1.76	0.51
6:D:150:VAL:HB	6:D:178:LEU:HD21	1.92	0.51
5:E:94:ASN:HA	5:E:236:THR:HG22	1.92	0.50
4:C:15:LEU:HB3	4:C:107:SER:HB3	1.93	0.50
6:K:39:GLN:HB2	6:K:45:LEU:HD23	1.93	0.50
5:E:67:ASN:HD21	5:E:70:ALA:H	1.60	0.50
6:K:144:ASP:HB3	6:K:175:LEU:HD23	1.94	0.50
2:I:184:GLU:O	2:I:188:SER:OG	2.29	0.50
5:G:317:PHE:CE2	5:G:319:ALA:HB2	2.47	0.50
5:E:70:ALA:HB2	5:E:213:ILE:HD11	1.92	0.50
4:J:134:CYS:HB3	4:J:176:SER:HB3	1.93	0.50
5:M:161:MET:HE3	5:M:161:MET:HA	1.94	0.50
5:M:260:LEU:HD12	5:M:451:GLY:HA3	1.94	0.50
6:K:11:LEU:HD11	6:K:112:SER:HB3	1.94	0.50
4:J:37:GLN:HB2	4:J:47:LEU:HD11	1.94	0.50
6:K:28:SER:HB3	6:K:31:ASN:HB2	1.93	0.49
1:N:144:THR:HG22	1:N:192:THR:HG22	1.93	0.49
5:E:219:ALA:O	5:E:246:GLN:NE2	2.45	0.49
6:K:3:GLN:HB3	6:K:25:SER:HB2	1.94	0.49
3:O:116:VAL:O	3:O:205:LYS:NZ	2.32	0.49
5:M:131:CYS:HA	5:M:157:CYS:HA	1.93	0.49
5:E:161:MET:HE2	5:E:162:THR:HG22	1.94	0.49
5:G:175:LEU:HD11	14:G:602:NAG:H83	1.94	0.49
7:Y:606:THR:HG21	7:Y:646:LEU:HD11	1.94	0.49
1:N:99:ARG:HD3	1:N:106:GLU:CD	2.38	0.49
1:N:122:SER:OG	1:N:123:ALA:N	2.45	0.49
4:J:34:GLN:HB2	4:J:89:HIS:HB3	1.95	0.49
3:L:108:GLY:HA3	3:L:141:TYR:OH	2.13	0.49
6:B:121:VAL:HG12	6:B:142:VAL:HA	1.94	0.49
5:G:503:ARG:NE	7:Y:605:CYS:O	2.35	0.49
1:F:47:TRP:CZ2	1:F:49:GLY:HA2	2.48	0.49
3:L:23:CYS:N	3:L:71:ALA:O	2.44	0.49
1:N:143:GLY:N	1:N:195:SER:OG	2.46	0.49
5:M:54:CYS:HB2	7:Z:571:TRP:CE3	2.48	0.49
5:M:59:LYS:HD3	5:M:213:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:151:ALA:HB2	3:L:192:TYR:CE1	2.48	0.48
7:Y:603:ILE:HB	7:Z:655:LYS:HB3	1.94	0.48
3:L:19:ILE:HG22	3:L:75:ILE:HB	1.94	0.48
3:O:163:THR:HB	3:O:176:SER:H	1.79	0.48
4:J:93:SER:O	5:M:136:ASN:ND2	2.46	0.48
1:F:33:TYR:HB2	1:F:106:GLU:OE2	2.13	0.48
3:O:110:PRO:HD2	3:O:141:TYR:CE1	2.48	0.48
4:A:108:GLN:HB3	4:A:140:TYR:CE1	2.48	0.48
4:C:28:LEU:HB3	4:C:94:ARG:HD3	1.95	0.48
4:J:94:ARG:HA	5:M:136:ASN:ND2	2.27	0.48
5:M:203:GLN:HE22	5:M:317:PHE:HA	1.78	0.48
4:C:106:VAL:O	4:C:140:TYR:OH	2.27	0.48
5:G:456:ARG:HG2	5:G:468:PHE:HE1	1.78	0.48
1:F:168:LEU:HD21	1:F:191:VAL:HG21	1.94	0.48
6:B:40:SER:HB2	6:B:43:LYS:HD2	1.96	0.48
6:D:33:TYR:HB2	6:D:95:ALA:O	2.13	0.48
6:K:204:ASN:OD1	6:K:205:THR:N	2.47	0.48
1:F:35:HIS:NE2	1:F:106:GLU:OE2	2.39	0.48
2:I:50:GLU:O	2:I:52:SER:N	2.44	0.48
3:L:119:PHE:HB2	3:L:134:VAL:HB	1.95	0.48
5:G:69:TRP:HA	5:G:111:LEU:HD13	1.95	0.48
1:F:3:GLN:HB3	1:F:25:SER:HB2	1.95	0.48
3:O:61:ARG:CZ	3:O:79:GLN:HE22	2.25	0.48
5:E:111:LEU:HD11	7:X:571:TRP:HZ2	1.77	0.48
5:G:212:PRO:HG2	5:G:254:VAL:HG22	1.95	0.48
5:M:186(A):ASN:N	5:M:187:GLN:CA	2.74	0.48
5:E:448:ASN:O	5:E:450:THR:HG23	2.13	0.48
5:E:361:PHE:HB3	5:E:391:PHE:HB3	1.96	0.48
5:M:498:PRO:HB3	7:Z:610:TRP:CD2	2.49	0.48
6:B:119:PRO:HB3	6:B:145:TYR:HB3	1.95	0.48
5:G:257:THR:OG1	5:G:375:SER:OG	2.29	0.47
14:M:608:NAG:H83	8:e:1:NAG:H62	1.96	0.47
6:B:66:ARG:NH1	6:B:82(B):SER:O	2.47	0.47
6:K:123:PRO:HB3	6:K:211:VAL:HG22	1.95	0.47
6:B:35:THR:OG1	6:B:47:TRP:NE1	2.47	0.47
5:E:338:TRP:CZ2	5:E:390:LEU:HB3	2.48	0.47
5:M:257:THR:HG22	5:M:258:GLN:HG3	1.96	0.47
7:Y:601:LYS:HG2	7:Z:655:LYS:NZ	2.30	0.47
1:H:24:ALA:HB1	1:H:27:TYR:HE1	1.80	0.47
2:I:107:LEU:HD11	2:I:109:GLN:HG2	1.95	0.47
3:O:109:GLN:NE2	3:O:110:PRO:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:294:ILE:HB	5:G:333:VAL:HG22	1.96	0.47
6:D:39:GLN:HB2	6:D:45:LEU:HD23	1.95	0.47
1:H:12:LYS:HG3	1:H:18:VAL:HB	1.96	0.47
1:N:15:GLY:HA2	1:N:85:ARG:HA	1.97	0.47
5:M:218:CYS:HA	5:M:247:CYS:HA	1.96	0.47
3:L:19:ILE:HB	3:L:78:LEU:HD11	1.96	0.47
4:A:188:HIS:HD1	4:A:191:TYR:HH	1.56	0.47
4:C:14:ALA:HA	4:C:106(A):LEU:HB2	1.96	0.47
5:E:231:LYS:HD2	5:E:267:GLU:HB3	1.95	0.47
5:G:67:ASN:ND2	5:G:70:ALA:H	2.12	0.47
5:G:107:ASP:OD2	7:Y:574:LYS:NZ	2.48	0.47
5:G:270:VAL:HG23	5:G:348:GLN:HG3	1.95	0.47
5:G:294:ILE:HG23	5:G:447:SER:HB2	1.96	0.47
5:M:299:PRO:HB2	5:M:327:ARG:HB2	1.96	0.47
6:B:60:ASN:ND2	6:B:62:SER:OG	2.47	0.47
2:I:168:GLN:N	2:I:172:LYS:O	2.35	0.47
6:B:68:VAL:HG13	6:B:81:GLN:HB2	1.96	0.47
5:E:257:THR:HG22	5:E:258:GLN:HG3	1.97	0.47
5:M:36:VAL:HG12	7:Z:610:TRP:CE3	2.47	0.47
1:F:191:VAL:HG22	1:F:193:VAL:HG13	1.96	0.47
3:O:83:ASP:OD1	3:O:83:ASP:N	2.47	0.47
4:C:66(C):ASN:ND2	4:C:66(C):ASN:O	2.48	0.46
5:M:358:ILE:HB	5:M:465:THR:HA	1.97	0.46
1:F:207:VAL:HB	1:F:216:VAL:HG23	1.96	0.46
5:M:54:CYS:HB2	7:Z:571:TRP:CD2	2.51	0.46
1:N:88:SER:HA	1:N:120:VAL:HG11	1.97	0.46
1:N:153:ASP:HB3	1:N:184:LEU:HD13	1.97	0.46
5:M:447:SER:OG	8:e:1:NAG:O7	2.18	0.46
1:N:7:SER:HB3	1:N:21:SER:HB3	1.98	0.46
1:N:177:ALA:HA	1:N:187:LEU:HB3	1.98	0.46
5:E:181:ILE:HG23	5:E:191:TYR:HB3	1.97	0.46
6:B:138:LEU:O	6:B:182:VAL:N	2.46	0.46
6:K:60:ASN:HB3	6:K:63:LEU:HD23	1.96	0.46
4:A:150:ALA:O	4:A:152:SER:N	2.49	0.46
5:G:74:CYS:SG	5:G:75:VAL:N	2.88	0.46
5:G:203:GLN:HG3	5:G:435:TYR:HD2	1.81	0.46
4:J:83:GLU:OE1	4:J:166:LYS:NZ	2.32	0.46
6:D:204:ASN:OD1	6:D:205:THR:N	2.48	0.46
7:X:650:GLN:HG3	7:X:651:ASN:H	1.81	0.46
2:I:38:GLN:C	2:I:84:ALA:HB1	2.41	0.46
5:M:65:LYS:HB2	5:M:66:HIS:H	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:GLN:HB2	1:F:45:LEU:HD23	1.97	0.46
1:H:141:SER:HA	1:H:144:THR:O	2.16	0.46
1:N:12:LYS:HG3	1:N:18:VAL:HB	1.97	0.46
5:G:424:ILE:HD12	5:G:426:MET:HE3	1.98	0.46
6:B:146:PHE:HA	6:B:147:PRO:HA	1.78	0.46
5:G:69:TRP:HB3	5:G:215:ILE:HD11	1.97	0.46
4:A:52:GLN:CD	11:a:6:MAN:H2	2.41	0.45
4:J:94:ARG:O	5:M:136:ASN:HB2	2.15	0.45
5:M:180:ASP:OD2	5:M:422:GLN:N	2.43	0.45
5:M:297:THR:HG22	5:M:444:ARG:HG3	1.97	0.45
1:F:87:ARG:O	1:F:120:VAL:HG21	2.16	0.45
5:G:195:ASN:ND2	5:G:201:ILE:HB	2.32	0.45
5:G:343:GLY:O	5:G:347:LYS:HG2	2.16	0.45
5:M:203:GLN:HG3	5:M:435:TYR:HD2	1.81	0.45
5:G:350:ARG:HD3	5:G:355:ASN:O	2.16	0.45
4:J:133:VAL:HG21	6:K:141:LEU:HD13	1.97	0.45
4:J:108:GLN:HB3	4:J:140:TYR:CE1	2.51	0.45
1:F:12:LYS:HG3	1:F:18:VAL:HB	1.98	0.45
2:I:140:PHE:HZ	2:I:165:PRO:HB3	1.82	0.45
1:N:30:THR:OG1	1:N:54:ASN:OD1	2.34	0.45
5:E:99:ASN:OD1	5:E:103:GLN:NE2	2.49	0.45
1:H:6:GLN:H	1:H:114:GLN:NE2	2.14	0.45
5:E:124:PRO:O	5:E:161:MET:HE1	2.15	0.45
4:J:166:LYS:HA	4:J:172:TYR:HA	1.99	0.45
6:D:200:HIS:CE1	6:D:203:SER:HB2	2.51	0.45
1:F:157:GLU:OE2	1:F:177:ALA:HB3	2.17	0.45
1:N:170:SER:HA	1:N:171:GLY:HA2	1.63	0.45
1:F:141:SER:OG	1:F:142:GLY:N	2.48	0.45
3:O:75:ILE:HD13	3:O:82:GLU:OE2	2.17	0.45
5:E:369:LEU:HD22	5:E:370:GLU:HG3	1.98	0.45
6:D:123:PRO:HB3	6:D:211:VAL:HG22	1.98	0.45
4:C:13:VAL:HG13	4:C:17:GLU:HG3	1.98	0.45
5:E:186(A):ASN:N	5:E:187:GLN:CA	2.76	0.45
5:E:234:ASN:OD1	5:E:235:GLY:N	2.50	0.45
1:H:35:HIS:HD1	1:H:47:TRP:HE1	1.65	0.44
4:A:85:ASP:HB3	4:A:101:ALA:HB1	2.00	0.44
5:G:360:ARG:HG2	5:G:467:THR:HG22	1.99	0.44
5:M:107:ASP:OD2	7:Z:574:LYS:NZ	2.49	0.44
5:G:54:CYS:SG	5:G:55:ALA:N	2.90	0.44
5:G:292:VAL:HB	5:G:449:ILE:HG23	1.99	0.44
5:M:47:ASP:HA	5:M:489:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:60:ASN:HD22	6:D:61:PRO:HD2	1.82	0.44
1:F:60:TYR:HE1	1:F:70:MET:HB2	1.82	0.44
1:N:123:ALA:HB2	1:N:183:GLY:HA3	1.98	0.44
5:E:161:MET:HE3	5:E:161:MET:HA	1.99	0.44
3:L:140:PHE:HE2	3:L:143:GLY:HA2	1.82	0.44
1:F:153:ASP:HB3	1:F:184:LEU:HD13	1.98	0.44
2:I:133:LEU:HD12	2:I:179:LEU:HB3	2.00	0.44
7:Z:635:ILE:O	7:Z:639:THR:HG23	2.17	0.44
1:H:144:THR:HA	1:H:195:SER:N	2.29	0.44
4:A:37:GLN:HB2	4:A:47:LEU:HD11	1.99	0.44
5:E:317:PHE:CE2	5:E:319:ALA:HB2	2.53	0.44
5:G:476:ARG:HA	5:G:479:TRP:CD1	2.53	0.44
6:D:72:ASP:OD1	6:D:74:SER:OG	2.24	0.44
6:K:68:VAL:HB	6:K:82(A):ARG:HH21	1.80	0.44
6:K:154:TRP:CZ2	6:K:196:CYS:HB3	2.52	0.44
4:A:94:ARG:HD2	5:G:324:GLY:O	2.18	0.44
5:E:69:TRP:HE1	5:E:108:ILE:HG23	1.82	0.44
5:M:498:PRO:HB3	7:Z:610:TRP:CG	2.53	0.44
1:F:132:PRO:HD3	1:F:218:LYS:HE3	2.00	0.43
3:L:152:ASP:OD2	3:L:190:LYS:HG2	2.18	0.43
3:O:190:LYS:O	3:O:209:PRO:HD2	2.18	0.43
5:E:61:TYR:HD1	5:E:65:LYS:HB3	1.83	0.43
4:J:94:ARG:HD2	5:M:324:GLY:O	2.18	0.43
5:M:220:PRO:HB3	7:Z:578:ALA:HB1	1.98	0.43
2:I:106:VAL:HB	2:I:107:LEU:H	1.43	0.43
5:E:96:TRP:HH2	5:E:285:LEU:HD23	1.83	0.43
5:E:321(A):ASP:HB3	14:E:602:NAG:H82	2.00	0.43
5:E:359:ILE:HD13	5:E:466:GLU:HB3	2.00	0.43
4:J:21:ILE:HD12	4:J:73:LEU:HD23	1.99	0.43
6:B:159:LEU:HD13	6:B:182:VAL:HG11	2.00	0.43
3:L:140:PHE:CE2	3:L:143:GLY:HA2	2.53	0.43
4:A:21:ILE:HD12	4:A:73:LEU:HD23	2.01	0.43
4:C:32:ALA:N	4:C:91:TRP:O	2.51	0.43
6:D:154:TRP:CZ2	6:D:196:CYS:HB3	2.53	0.43
6:K:200:HIS:CE1	6:K:203:SER:HB2	2.53	0.43
2:I:109:GLN:O	2:I:110:PRO:C	2.61	0.43
2:I:129:ASN:HA	2:I:183:PRO:HG2	2.00	0.43
3:L:112:ALA:CB	3:L:141:TYR:HB3	2.48	0.43
1:N:133:LEU:HB3	3:O:119:PHE:CG	2.54	0.43
5:E:227:LYS:HG3	5:E:485:LYS:HD3	2.00	0.43
5:G:249:HIS:ND1	5:G:486:TYR:OH	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:50:THR:O	5:M:103:GLN:NE2	2.32	0.43
1:N:60:TYR:HE1	1:N:70:MET:HB2	1.83	0.43
4:A:59:PRO:C	4:A:61:ARG:H	2.26	0.43
5:E:122:LEU:HB2	5:E:201:ILE:HG23	2.01	0.43
5:E:384:TYR:CE1	5:E:421:LYS:HD3	2.54	0.43
5:G:289:ASN:OD1	5:G:290:THR:N	2.51	0.43
1:H:36:TRP:CE2	1:H:81:MET:HB2	2.54	0.43
5:M:67:ASN:HD21	5:M:70:ALA:HB3	1.83	0.43
3:O:151:ALA:HA	3:O:152:ASP:HA	1.80	0.43
3:O:184:GLU:O	3:O:188:SER:OG	2.33	0.43
5:M:220:PRO:HG2	5:M:223:PHE:CD1	2.53	0.43
4:A:148:TRP:NE1	4:A:176:SER:OG	2.41	0.43
4:C:136:ILE:HG12	4:C:195:VAL:HG11	2.00	0.43
5:M:343:GLY:O	5:M:347:LYS:HG2	2.18	0.43
1:F:179:LEU:HD13	1:F:185:TYR:CE2	2.53	0.43
1:F:209:HIS:CD2	1:F:211:PRO:HD2	2.54	0.43
1:H:143:GLY:O	1:H:144:THR:OG1	2.25	0.43
4:C:13:VAL:O	4:C:106:VAL:HA	2.18	0.43
2:I:56:SER:HA	2:I:57:GLY:HA2	1.51	0.42
6:D:146:PHE:HA	6:D:147:PRO:HA	1.78	0.42
6:D:161:SER:HA	6:D:162:GLY:HA2	1.77	0.42
1:N:209:HIS:CD2	1:N:211:PRO:HD2	2.53	0.42
5:E:253:PRO:HA	5:E:479:TRP:HZ3	1.83	0.42
5:E:456:ARG:HG2	5:E:468:PHE:HE1	1.84	0.42
5:G:52:LEU:O	7:Y:574:LYS:HD3	2.19	0.42
5:G:370:GLU:HG2	5:G:384:TYR:HE2	1.84	0.42
4:A:145:THR:HB	4:A:196:THR:HB	2.01	0.42
5:E:257:THR:O	5:E:259:LEU:N	2.52	0.42
5:E:369:LEU:HB3	5:E:370:GLU:H	1.71	0.42
4:J:136:ILE:HG12	4:J:195:VAL:HG11	2.01	0.42
6:D:124:LEU:HD21	6:D:141:LEU:HB2	2.01	0.42
6:K:145:TYR:HB2	6:K:200:HIS:CE1	2.55	0.42
4:C:151:ASP:OD1	4:C:188:HIS:HB3	2.19	0.42
5:G:456:ARG:HG2	5:G:468:PHE:CE1	2.55	0.42
6:B:123:PRO:HB3	6:B:211:VAL:HG22	2.01	0.42
3:O:11:VAL:HG12	3:O:19:ILE:HD11	2.02	0.42
5:M:101:VAL:HG21	5:M:480:ARG:HG2	2.01	0.42
6:D:94:THR:O	6:D:100(P):MET:HA	2.19	0.42
4:C:21:ILE:HB	4:C:73:LEU:HB3	2.01	0.42
5:G:69:TRP:HE1	5:G:108:ILE:HG23	1.85	0.42
8:U:1:NAG:O6	8:U:2:NAG:N2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:TRP:CE2	1:F:81:MET:HB2	2.54	0.42
3:L:50:GLU:O	3:L:52:SER:N	2.46	0.42
1:N:56:GLY:C	5:M:367:GLY:HA2	2.44	0.42
5:E:384:TYR:CZ	5:E:421:LYS:HD3	2.55	0.42
3:L:32:TYR:HB3	3:L:50:GLU:HA	2.02	0.42
3:L:152:ASP:OD1	3:L:189:HIS:HB3	2.20	0.42
4:A:34:GLN:HG2	6:B:100(O):TYR:HB3	2.00	0.42
5:E:61:TYR:CD1	5:E:65:LYS:HB3	2.55	0.42
5:E:260:LEU:HD12	5:E:451:GLY:HA3	2.01	0.42
6:D:34:TRP:HB3	6:D:78:LEU:HD22	2.02	0.42
6:K:11:LEU:HD12	6:K:110:THR:HB	2.00	0.42
1:F:128:PRO:HB3	1:F:154:TYR:HB3	2.01	0.42
2:I:55:PRO:O	2:I:58:VAL:HG13	2.20	0.42
5:G:125:LEU:HA	5:G:161:MET:HE1	2.01	0.42
6:K:151:THR:HB	6:K:199:ASN:HB2	2.01	0.42
5:G:448:ASN:O	5:G:449:ILE:C	2.63	0.41
4:J:35:TRP:CG	4:J:73:LEU:HD13	2.55	0.41
5:M:121:LYS:HA	5:M:202:THR:HA	2.02	0.41
5:M:124:PRO:O	5:M:161:MET:HE1	2.19	0.41
6:B:33:TYR:HB2	6:B:95:ALA:O	2.20	0.41
6:D:18:LEU:HB3	6:D:82:LEU:HB3	2.02	0.41
6:D:18:LEU:HD11	6:D:109:VAL:HG11	2.01	0.41
3:O:152:ASP:OD1	3:O:152:ASP:N	2.54	0.41
4:J:38:HIS:NE2	6:K:39:GLN:OE1	2.53	0.41
4:J:61:ARG:NH2	4:J:82:ASP:OD1	2.53	0.41
4:J:66(B):ILE:C	4:J:67:PHE:H	2.28	0.41
3:L:151:ALA:HA	3:L:152:ASP:HA	1.71	0.41
1:N:207:VAL:HB	1:N:216:VAL:HG23	2.03	0.41
5:M:369:LEU:HD22	5:M:370:GLU:HG2	2.03	0.41
7:Y:650:GLN:HG3	7:Y:651:ASN:H	1.85	0.41
7:Z:631:TRP:O	7:Z:635:ILE:HG12	2.20	0.41
1:F:177:ALA:HA	1:F:187:LEU:HB3	2.02	0.41
2:I:108:GLY:N	2:I:109:GLN:HA	2.36	0.41
3:L:151:ALA:HB2	3:L:192:TYR:CD1	2.55	0.41
8:c:2:NAG:O3	8:c:3:BMA:O2	2.26	0.41
2:I:151:ALA:HA	2:I:152:ASP:HA	1.86	0.41
5:G:181:ILE:HG23	5:G:191:TYR:HB3	2.02	0.41
5:G:494:LEU:HD23	5:G:494:LEU:HA	1.87	0.41
6:B:22:CYS:HB2	6:B:36:TRP:CH2	2.56	0.41
6:B:59:TYR:HE1	6:B:69:ILE:HG13	1.86	0.41
6:K:161:SER:HA	6:K:162:GLY:HA2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:LEU:HD23	1:F:83:LEU:HA	1.94	0.41
1:H:98:ARG:HB2	1:H:98:ARG:HH11	1.86	0.41
2:I:36:TYR:O	2:I:86:TYR:HA	2.21	0.41
3:L:56:SER:HA	3:L:57:GLY:HA2	1.54	0.41
3:L:107:LEU:HD12	3:L:107:LEU:HA	1.87	0.41
5:G:273:ARG:NH1	5:G:287:GLN:OE1	2.51	0.41
4:J:15:LEU:HB2	4:J:107:SER:HB2	2.02	0.41
1:H:14:PRO:HG3	1:H:122:SER:HB2	2.03	0.41
1:N:156:PRO:HD2	1:N:211:PRO:HB2	2.02	0.41
5:G:437:PRO:HA	5:G:438:PRO:HD3	1.95	0.41
3:O:50:GLU:O	3:O:52:SER:N	2.51	0.41
3:O:129:ASN:HA	3:O:183:PRO:HG2	2.02	0.41
5:E:280:ASN:OD1	5:E:281:ALA:N	2.54	0.41
6:K:200:HIS:O	6:K:204:ASN:HA	2.21	0.41
5:E:199:ALA:HB1	5:E:431:GLY:C	2.46	0.41
4:J:137:SER:HA	4:J:173:ALA:HA	2.03	0.41
6:D:36:TRP:HD1	6:D:69:ILE:HD13	1.86	0.41
7:Y:540:GLN:O	7:Y:544:LEU:HB2	2.20	0.41
1:F:142:GLY:HA2	1:F:144:THR:N	2.36	0.40
1:F:170:SER:HA	1:F:171:GLY:HA2	1.60	0.40
5:E:54:CYS:SG	5:E:55:ALA:N	2.95	0.40
5:M:270:VAL:HG23	5:M:348:GLN:HG3	2.03	0.40
6:B:200:HIS:HD2	6:B:202:PRO:HD2	1.85	0.40
5:M:69:TRP:HB3	5:M:215:ILE:HD11	2.03	0.40
5:M:86:LEU:HD22	7:Z:523:LEU:O	2.21	0.40
5:M:181:ILE:HG23	5:M:191:TYR:HB3	2.03	0.40
5:M:289:ASN:OD1	5:M:290:THR:N	2.55	0.40
1:H:24:ALA:HB1	1:H:27:TYR:CE1	2.57	0.40
1:H:67:ARG:HH22	1:H:90:ASP:CG	2.29	0.40
3:O:19:ILE:HG22	3:O:75:ILE:HB	2.02	0.40
5:E:349:LEU:HD13	5:E:468:PHE:CE2	2.55	0.40
6:K:22:CYS:N	6:K:78:LEU:O	2.53	0.40
5:G:349:LEU:HD13	5:G:468:PHE:CE2	2.55	0.40
5:M:111:LEU:HD11	7:Z:571:TRP:CZ2	2.56	0.40
6:D:200:HIS:O	6:D:204:ASN:HA	2.22	0.40
3:O:6:GLN:HB3	3:O:102:THR:OG1	2.21	0.40
5:M:369:LEU:HB3	5:M:370:GLU:HG2	2.04	0.40
6:B:9:PRO:HD3	6:B:19:SER:O	2.21	0.40
11:a:3:NAG:H62	11:a:7:MAN:H2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	218/225 (97%)	203 (93%)	14 (6%)	1 (0%)	24	58
1	H	218/225 (97%)	202 (93%)	15 (7%)	1 (0%)	24	58
1	N	218/225 (97%)	201 (92%)	17 (8%)	0	100	100
2	I	203/210 (97%)	187 (92%)	12 (6%)	4 (2%)	6	32
3	L	200/210 (95%)	183 (92%)	12 (6%)	5 (2%)	4	28
3	O	201/210 (96%)	183 (91%)	17 (8%)	1 (0%)	24	58
4	A	208/214 (97%)	194 (93%)	12 (6%)	2 (1%)	12	44
4	C	208/214 (97%)	196 (94%)	11 (5%)	1 (0%)	24	58
4	J	208/214 (97%)	196 (94%)	11 (5%)	1 (0%)	24	58
5	E	437/474 (92%)	405 (93%)	30 (7%)	2 (0%)	24	58
5	G	443/474 (94%)	403 (91%)	35 (8%)	5 (1%)	11	42
5	M	441/474 (93%)	406 (92%)	31 (7%)	4 (1%)	14	46
6	B	222/236 (94%)	214 (96%)	6 (3%)	2 (1%)	14	46
6	D	222/236 (94%)	214 (96%)	8 (4%)	0	100	100
6	K	222/236 (94%)	211 (95%)	11 (5%)	0	100	100
7	X	125/153 (82%)	119 (95%)	6 (5%)	0	100	100
7	Y	125/153 (82%)	121 (97%)	4 (3%)	0	100	100
7	Z	125/153 (82%)	120 (96%)	5 (4%)	0	100	100
All	All	4244/4536 (94%)	3958 (93%)	257 (6%)	29 (1%)	18	52

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	110	PRO
3	O	112	ALA
5	G	140	ASP
5	G	449	ILE

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Mol	Chain	Res	Type
5	M	136	ASN
5	M	157	CYS
1	F	106	GLU
1	H	144	THR
2	I	29	ASP
3	L	106	VAL
4	A	151	ASP
5	G	186	GLU
5	G	333	VAL
2	I	106	VAL
2	I	110	PRO
3	L	3	ALA
3	L	139	ASP
4	C	151	ASP
4	J	151	ASP
5	M	186	GLU
2	I	139	ASP
3	L	108	GLY
5	E	186	GLU
5	M	258	GLN
6	B	82(B)	SER
6	B	144	ASP
4	A	60	GLU
5	E	369	LEU
5	G	369	LEU

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	F	188/191 (98%)	184 (98%)	4 (2%)	47	64
1	H	188/191 (98%)	182 (97%)	6 (3%)	34	56
1	N	188/191 (98%)	184 (98%)	4 (2%)	47	64
2	I	173/176 (98%)	167 (96%)	6 (4%)	32	54
3	L	172/176 (98%)	167 (97%)	5 (3%)	37	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	173/176 (98%)	167 (96%)	6 (4%)	32	54
4	A	176/180 (98%)	173 (98%)	3 (2%)	53	67
4	C	176/180 (98%)	175 (99%)	1 (1%)	78	79
4	J	176/180 (98%)	171 (97%)	5 (3%)	38	58
5	E	399/422 (94%)	389 (98%)	10 (2%)	42	61
5	G	401/422 (95%)	389 (97%)	12 (3%)	36	57
5	M	401/422 (95%)	382 (95%)	19 (5%)	23	48
6	B	194/204 (95%)	194 (100%)	0	100	100
6	D	194/204 (95%)	189 (97%)	5 (3%)	40	60
6	K	194/204 (95%)	188 (97%)	6 (3%)	35	56
7	X	112/129 (87%)	112 (100%)	0	100	100
7	Y	112/129 (87%)	112 (100%)	0	100	100
7	Z	112/129 (87%)	112 (100%)	0	100	100
All	All	3729/3906 (96%)	3637 (98%)	92 (2%)	42	61

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	83	LEU
1	F	117	LEU
1	F	217	ASP
1	F	225	CYS
1	H	70	MET
1	H	83	LEU
1	H	98	ARG
1	H	105	ARG
1	H	217	ASP
1	H	225	CYS
2	I	58	VAL
2	I	104	VAL
2	I	105	PHE
2	I	106	VAL
2	I	184	GLU
2	I	192	TYR
3	L	58	VAL
3	L	96	GLU
3	L	103	LYS

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Mol	Chain	Res	Type
3	L	109	GLN
3	L	184	GLU
1	N	83	LEU
1	N	98	ARG
1	N	217	ASP
1	N	225	CYS
3	O	58	VAL
3	O	96	GLU
3	O	109	GLN
3	O	152	ASP
3	O	184	GLU
3	O	192	TYR
4	A	72	THR
4	A	89	HIS
4	A	183	GLU
4	C	183	GLU
5	E	36	VAL
5	E	65	LYS
5	E	68	VAL
5	E	71	THR
5	E	189	THR
5	E	342	LEU
5	E	369	LEU
5	E	396	ILE
5	E	449	ILE
5	E	505	VAL
5	G	36	VAL
5	G	65	LYS
5	G	68	VAL
5	G	71	THR
5	G	87	GLU
5	G	186	GLU
5	G	186(A)	ASN
5	G	342	LEU
5	G	369	LEU
5	G	396	ILE
5	G	449	ILE
5	G	505	VAL
4	J	15	LEU
4	J	18	THR
4	J	54	ARG
4	J	89	HIS

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Mol	Chain	Res	Type
4	J	183	GLU
5	M	36	VAL
5	M	65	LYS
5	M	68	VAL
5	M	71	THR
5	M	88	ASN
5	M	134	VAL
5	M	186	GLU
5	M	186(A)	ASN
5	M	189	THR
5	M	213	ILE
5	M	279	ASP
5	M	342	LEU
5	M	369	LEU
5	M	370	GLU
5	M	396	ILE
5	M	424	ILE
5	M	449	ILE
5	M	505	VAL
5	M	506	VAL
6	D	24	VAL
6	D	68	VAL
6	D	121	VAL
6	D	205	THR
6	D	206	LYS
6	K	68	VAL
6	K	76	ASN
6	K	81	GLN
6	K	121	VAL
6	K	205	THR
6	K	206	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	208	ASN
2	I	37	GLN
2	I	60	ASN
3	L	17	GLN
3	O	37	GLN
3	O	109	GLN
4	C	50	ASN

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Mol	Chain	Res	Type
4	C	167	GLN
5	E	330	HIS
5	E	478	ASN
5	G	72	HIS
5	G	315	GLN
5	G	478	ASN
4	J	52	GLN
4	J	89	HIS
4	J	167	GLN
4	J	194	GLN
5	M	85	HIS
5	M	425	ASN
5	M	428	GLN
6	B	60	ASN
6	K	5	GLN
7	Y	625	ASN
7	X	651	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	$\# Z > 2$
8	NAG	P	1	5,8	14,14,15	0.19	0	17,19,21	0.56	0
8	NAG	P	2	8	14,14,15	0.39	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	P	3	8	11,11,12	0.74	0	15,15,17	0.72	0
9	NAG	Q	1	9,5	14,14,15	0.34	0	17,19,21	0.48	0
9	NAG	Q	2	9	14,14,15	0.32	0	17,19,21	0.39	0
10	NAG	R	1	10,5	14,14,15	0.37	0	17,19,21	0.47	0
10	NAG	R	2	10	14,14,15	0.44	0	17,19,21	0.85	1 (5%)
10	BMA	R	3	10	11,11,12	1.43	2 (18%)	15,15,17	1.46	3 (20%)
10	MAN	R	4	10	11,11,12	1.25	1 (9%)	15,15,17	2.30	3 (20%)
10	MAN	R	5	10	11,11,12	0.55	0	15,15,17	1.14	2 (13%)
10	MAN	R	6	10	11,11,12	0.71	0	15,15,17	0.91	1 (6%)
10	MAN	R	7	10	11,11,12	0.97	1 (9%)	15,15,17	1.47	2 (13%)
9	NAG	S	1	9,5	14,14,15	0.24	0	17,19,21	0.51	0
9	NAG	S	2	9	14,14,15	0.37	0	17,19,21	1.30	1 (5%)
9	NAG	T	1	9,5	14,14,15	1.00	1 (7%)	17,19,21	1.12	3 (17%)
9	NAG	T	2	9	14,14,15	0.37	0	17,19,21	0.68	0
8	NAG	U	1	5,8	14,14,15	0.36	0	17,19,21	0.44	0
8	NAG	U	2	8	14,14,15	0.42	0	17,19,21	0.70	0
8	BMA	U	3	8	11,11,12	0.64	0	15,15,17	0.66	0
9	NAG	V	1	9,5	14,14,15	0.27	0	17,19,21	0.40	0
9	NAG	V	2	9	14,14,15	0.23	0	17,19,21	0.40	0
9	NAG	W	1	9,5	14,14,15	0.38	0	17,19,21	0.44	0
9	NAG	W	2	9	14,14,15	0.33	0	17,19,21	0.49	0
11	NAG	a	1	5,11	14,14,15	0.27	0	17,19,21	0.44	0
11	NAG	a	2	11	14,14,15	0.34	0	17,19,21	0.50	0
11	NAG	a	3	11	14,14,15	0.16	0	17,19,21	0.76	1 (5%)
11	MAN	a	4	11	11,11,12	1.24	1 (9%)	15,15,17	1.75	2 (13%)
11	MAN	a	5	11	11,11,12	0.75	0	15,15,17	1.04	1 (6%)
11	MAN	a	6	11	11,11,12	0.71	0	15,15,17	1.35	2 (13%)
11	MAN	a	7	11	11,11,12	0.96	1 (9%)	15,15,17	0.83	1 (6%)
11	MAN	a	8	11	11,11,12	0.82	0	15,15,17	0.94	1 (6%)
11	MAN	a	9	11	11,11,12	0.91	1 (9%)	15,15,17	1.35	1 (6%)
9	NAG	b	1	9,5	14,14,15	0.29	0	17,19,21	0.38	0
9	NAG	b	2	9	14,14,15	0.62	1 (7%)	17,19,21	1.38	3 (17%)
8	NAG	c	1	5,8	14,14,15	0.23	0	17,19,21	0.48	0
8	NAG	c	2	8	14,14,15	0.25	0	17,19,21	0.58	0
8	BMA	c	3	8	11,11,12	0.76	0	15,15,17	0.71	0
9	NAG	d	1	9,5	14,14,15	0.14	0	17,19,21	0.58	0
9	NAG	d	2	9	14,14,15	0.27	0	17,19,21	0.60	0
8	NAG	e	1	5,8	14,14,15	0.22	0	17,19,21	0.78	0
8	NAG	e	2	8	14,14,15	0.57	1 (7%)	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	e	3	8	11,11,12	0.77	0	15,15,17	0.69	0
9	NAG	f	1	9,5	14,14,15	0.35	0	17,19,21	0.43	0
9	NAG	f	2	9	14,14,15	0.28	0	17,19,21	0.38	0
12	NAG	g	1	12,5	14,14,15	0.35	0	17,19,21	0.42	0
12	NAG	g	2	12	14,14,15	0.28	0	17,19,21	0.58	0
12	BMA	g	3	12	11,11,12	0.59	0	15,15,17	0.90	0
12	MAN	g	4	12	11,11,12	0.83	0	15,15,17	1.30	2 (13%)
12	MAN	g	5	12	11,11,12	0.74	0	15,15,17	1.23	1 (6%)
12	MAN	g	6	12	11,11,12	0.79	1 (9%)	15,15,17	1.09	2 (13%)
13	MAN	h	1	13	11,11,12	0.96	1 (9%)	15,15,17	1.09	1 (6%)
13	MAN	h	2	13	11,11,12	0.79	0	15,15,17	1.49	2 (13%)
13	MAN	h	3	13	11,11,12	0.67	0	15,15,17	0.90	1 (6%)
9	NAG	i	1	9,5	14,14,15	0.30	0	17,19,21	0.52	0
9	NAG	i	2	9	14,14,15	0.28	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	P	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	P	2	8	-	1/6/23/26	0/1/1/1
8	BMA	P	3	8	-	1/2/19/22	0/1/1/1
9	NAG	Q	1	9,5	-	1/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	0/6/23/26	0/1/1/1
10	NAG	R	1	10,5	-	1/6/23/26	0/1/1/1
10	NAG	R	2	10	-	4/6/23/26	0/1/1/1
10	BMA	R	3	10	-	1/2/19/22	0/1/1/1
10	MAN	R	4	10	-	0/2/19/22	0/1/1/1
10	MAN	R	5	10	-	2/2/19/22	0/1/1/1
10	MAN	R	6	10	-	0/2/19/22	0/1/1/1
10	MAN	R	7	10	-	0/2/19/22	0/1/1/1
9	NAG	S	1	9,5	-	4/6/23/26	0/1/1/1
9	NAG	S	2	9	-	4/6/23/26	0/1/1/1
9	NAG	T	1	9,5	-	1/6/23/26	0/1/1/1
9	NAG	T	2	9	-	2/6/23/26	0/1/1/1
8	NAG	U	1	5,8	-	1/6/23/26	0/1/1/1
8	NAG	U	2	8	-	4/6/23/26	0/1/1/1
8	BMA	U	3	8	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	V	1	9,5	-	2/6/23/26	0/1/1/1
9	NAG	V	2	9	-	1/6/23/26	0/1/1/1
9	NAG	W	1	9,5	-	2/6/23/26	0/1/1/1
9	NAG	W	2	9	-	2/6/23/26	0/1/1/1
11	NAG	a	1	5,11	-	1/6/23/26	0/1/1/1
11	NAG	a	2	11	-	4/6/23/26	0/1/1/1
11	NAG	a	3	11	-	2/6/23/26	0/1/1/1
11	MAN	a	4	11	-	2/2/19/22	0/1/1/1
11	MAN	a	5	11	-	2/2/19/22	0/1/1/1
11	MAN	a	6	11	-	2/2/19/22	0/1/1/1
11	MAN	a	7	11	-	2/2/19/22	0/1/1/1
11	MAN	a	8	11	-	0/2/19/22	0/1/1/1
11	MAN	a	9	11	-	0/2/19/22	0/1/1/1
9	NAG	b	1	9,5	-	2/6/23/26	0/1/1/1
9	NAG	b	2	9	-	6/6/23/26	0/1/1/1
8	NAG	c	1	5,8	-	4/6/23/26	0/1/1/1
8	NAG	c	2	8	-	3/6/23/26	0/1/1/1
8	BMA	c	3	8	-	1/2/19/22	0/1/1/1
9	NAG	d	1	9,5	-	0/6/23/26	0/1/1/1
9	NAG	d	2	9	-	2/6/23/26	0/1/1/1
8	NAG	e	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	e	2	8	-	1/6/23/26	0/1/1/1
8	BMA	e	3	8	-	2/2/19/22	0/1/1/1
9	NAG	f	1	9,5	-	1/6/23/26	0/1/1/1
9	NAG	f	2	9	-	2/6/23/26	0/1/1/1
12	NAG	g	1	12,5	-	2/6/23/26	0/1/1/1
12	NAG	g	2	12	-	2/6/23/26	0/1/1/1
12	BMA	g	3	12	-	0/2/19/22	0/1/1/1
12	MAN	g	4	12	-	0/2/19/22	1/1/1/1
12	MAN	g	5	12	-	0/2/19/22	0/1/1/1
12	MAN	g	6	12	-	0/2/19/22	0/1/1/1
13	MAN	h	1	13	-	0/2/19/22	0/1/1/1
13	MAN	h	2	13	-	1/2/19/22	0/1/1/1
13	MAN	h	3	13	-	2/2/19/22	0/1/1/1
9	NAG	i	1	9,5	-	1/6/23/26	0/1/1/1
9	NAG	i	2	9	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	1	NAG	O5-C1	-3.68	1.37	1.43
11	a	4	MAN	C1-C2	3.20	1.59	1.52
10	R	3	BMA	O5-C1	-3.14	1.38	1.43
10	R	4	MAN	O5-C5	2.95	1.49	1.43
10	R	3	BMA	C4-C5	2.69	1.58	1.53
11	a	9	MAN	C1-C2	2.50	1.58	1.52
13	h	1	MAN	O5-C1	-2.39	1.39	1.43
10	R	7	MAN	O5-C5	2.33	1.48	1.43
11	a	7	MAN	O5-C1	-2.27	1.39	1.43
9	b	2	NAG	C1-C2	2.09	1.55	1.52
12	g	6	MAN	C1-C2	2.06	1.57	1.52
8	e	2	NAG	C1-C2	2.01	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	R	4	MAN	C1-O5-C5	7.58	122.34	112.19
11	a	4	MAN	C1-O5-C5	5.54	119.62	112.19
10	R	7	MAN	C1-O5-C5	4.88	118.72	112.19
9	S	2	NAG	C2-N2-C7	4.52	128.96	122.90
9	b	2	NAG	C2-N2-C7	4.48	128.91	122.90
13	h	2	MAN	C1-O5-C5	4.46	118.17	112.19
11	a	6	MAN	C1-O5-C5	4.06	117.62	112.19
12	g	5	MAN	C1-O5-C5	3.86	117.36	112.19
11	a	9	MAN	C1-O5-C5	3.78	117.25	112.19
12	g	4	MAN	C1-O5-C5	3.61	117.02	112.19
10	R	3	BMA	C3-C4-C5	3.18	116.00	110.23
12	g	6	MAN	C1-O5-C5	3.08	116.31	112.19
13	h	2	MAN	O2-C2-C3	-3.03	103.88	110.15
10	R	5	MAN	C1-O5-C5	2.98	116.18	112.19
11	a	5	MAN	C1-O5-C5	2.93	116.11	112.19
10	R	3	BMA	C1-O5-C5	2.93	116.11	112.19
10	R	4	MAN	C1-C2-C3	2.68	113.55	109.64
10	R	4	MAN	O5-C1-C2	2.61	117.03	110.79
10	R	5	MAN	O2-C2-C3	-2.57	104.83	110.15
11	a	4	MAN	O2-C2-C3	-2.45	105.07	110.15
11	a	3	NAG	C1-O5-C5	2.39	115.39	112.19
12	g	4	MAN	O2-C2-C3	-2.35	105.28	110.15
11	a	8	MAN	O2-C2-C3	-2.26	105.47	110.15
10	R	2	NAG	O4-C4-C5	-2.24	103.81	109.32
11	a	6	MAN	O2-C2-C3	-2.18	105.64	110.15
9	b	2	NAG	C1-C2-N2	2.18	113.86	110.43
13	h	3	MAN	O2-C2-C3	-2.17	105.65	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	T	1	NAG	O4-C4-C3	-2.15	105.30	110.38
10	R	3	BMA	O2-C2-C3	-2.14	105.71	110.15
12	g	6	MAN	O2-C2-C3	-2.14	105.72	110.15
9	T	1	NAG	O4-C4-C5	-2.09	104.17	109.32
9	T	1	NAG	C3-C4-C5	2.07	113.98	110.23
9	b	2	NAG	C1-O5-C5	2.04	114.92	112.19
10	R	7	MAN	O2-C2-C3	-2.03	105.95	110.15
11	a	7	MAN	O2-C2-C3	-2.02	105.97	110.15
13	h	1	MAN	C1-O5-C5	2.00	114.87	112.19
10	R	6	MAN	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	e	1	NAG	C1-C2-N2-C7
9	d	2	NAG	C1-C2-N2-C7
9	T	2	NAG	C4-C5-C6-O6
9	b	2	NAG	C4-C5-C6-O6
11	a	3	NAG	C4-C5-C6-O6
11	a	4	MAN	C4-C5-C6-O6
11	a	7	MAN	O5-C5-C6-O6
9	W	1	NAG	C4-C5-C6-O6
10	R	5	MAN	O5-C5-C6-O6
9	i	2	NAG	C4-C5-C6-O6
9	T	2	NAG	O5-C5-C6-O6
10	R	2	NAG	C4-C5-C6-O6
11	a	7	MAN	C4-C5-C6-O6
10	R	2	NAG	O5-C5-C6-O6
11	a	2	NAG	O5-C5-C6-O6
8	c	1	NAG	O5-C5-C6-O6
11	a	3	NAG	O5-C5-C6-O6
9	b	2	NAG	O5-C5-C6-O6
11	a	4	MAN	O5-C5-C6-O6
11	a	2	NAG	C4-C5-C6-O6
8	e	3	BMA	C4-C5-C6-O6
9	W	1	NAG	O5-C5-C6-O6
9	S	2	NAG	C8-C7-N2-C2
9	S	2	NAG	O7-C7-N2-C2
9	b	2	NAG	C8-C7-N2-C2
9	b	2	NAG	O7-C7-N2-C2
11	a	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
11	a	2	NAG	O7-C7-N2-C2
9	i	2	NAG	O5-C5-C6-O6
9	b	1	NAG	O5-C5-C6-O6
9	f	2	NAG	O5-C5-C6-O6
8	P	3	BMA	O5-C5-C6-O6
9	V	1	NAG	O5-C5-C6-O6
8	e	3	BMA	O5-C5-C6-O6
8	P	1	NAG	O5-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6
10	R	5	MAN	C4-C5-C6-O6
13	h	3	MAN	O5-C5-C6-O6
8	U	3	BMA	O5-C5-C6-O6
8	c	2	NAG	O5-C5-C6-O6
8	c	3	BMA	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
8	c	1	NAG	C4-C5-C6-O6
9	i	1	NAG	O5-C5-C6-O6
9	T	1	NAG	O5-C5-C6-O6
8	P	2	NAG	O5-C5-C6-O6
8	U	1	NAG	O5-C5-C6-O6
10	R	3	BMA	O5-C5-C6-O6
8	c	1	NAG	C1-C2-N2-C7
8	c	2	NAG	C1-C2-N2-C7
9	S	1	NAG	C1-C2-N2-C7
12	g	1	NAG	C1-C2-N2-C7
11	a	6	MAN	C4-C5-C6-O6
9	S	1	NAG	C4-C5-C6-O6
11	a	5	MAN	C4-C5-C6-O6
13	h	2	MAN	O5-C5-C6-O6
8	U	2	NAG	C3-C2-N2-C7
8	c	1	NAG	C3-C2-N2-C7
9	S	1	NAG	C3-C2-N2-C7
9	b	2	NAG	C3-C2-N2-C7
10	R	2	NAG	C3-C2-N2-C7
12	g	1	NAG	C3-C2-N2-C7
12	g	2	NAG	C3-C2-N2-C7
9	b	1	NAG	C4-C5-C6-O6
9	f	2	NAG	C4-C5-C6-O6
10	R	1	NAG	O5-C5-C6-O6
11	a	6	MAN	O5-C5-C6-O6
9	S	1	NAG	O5-C5-C6-O6
11	a	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	V	1	NAG	C4-C5-C6-O6
11	a	5	MAN	O5-C5-C6-O6
8	U	2	NAG	C1-C2-N2-C7
9	S	2	NAG	C1-C2-N2-C7
9	b	2	NAG	C1-C2-N2-C7
10	R	2	NAG	C1-C2-N2-C7
12	g	2	NAG	C1-C2-N2-C7
13	h	3	MAN	C4-C5-C6-O6
8	c	2	NAG	C3-C2-N2-C7
8	e	1	NAG	C3-C2-N2-C7
8	e	2	NAG	C3-C2-N2-C7
9	Q	1	NAG	C3-C2-N2-C7
9	S	2	NAG	C3-C2-N2-C7
9	d	2	NAG	C3-C2-N2-C7
9	f	1	NAG	C3-C2-N2-C7
8	U	2	NAG	C4-C5-C6-O6
9	W	2	NAG	C4-C5-C6-O6
8	P	1	NAG	C4-C5-C6-O6
9	W	2	NAG	O5-C5-C6-O6

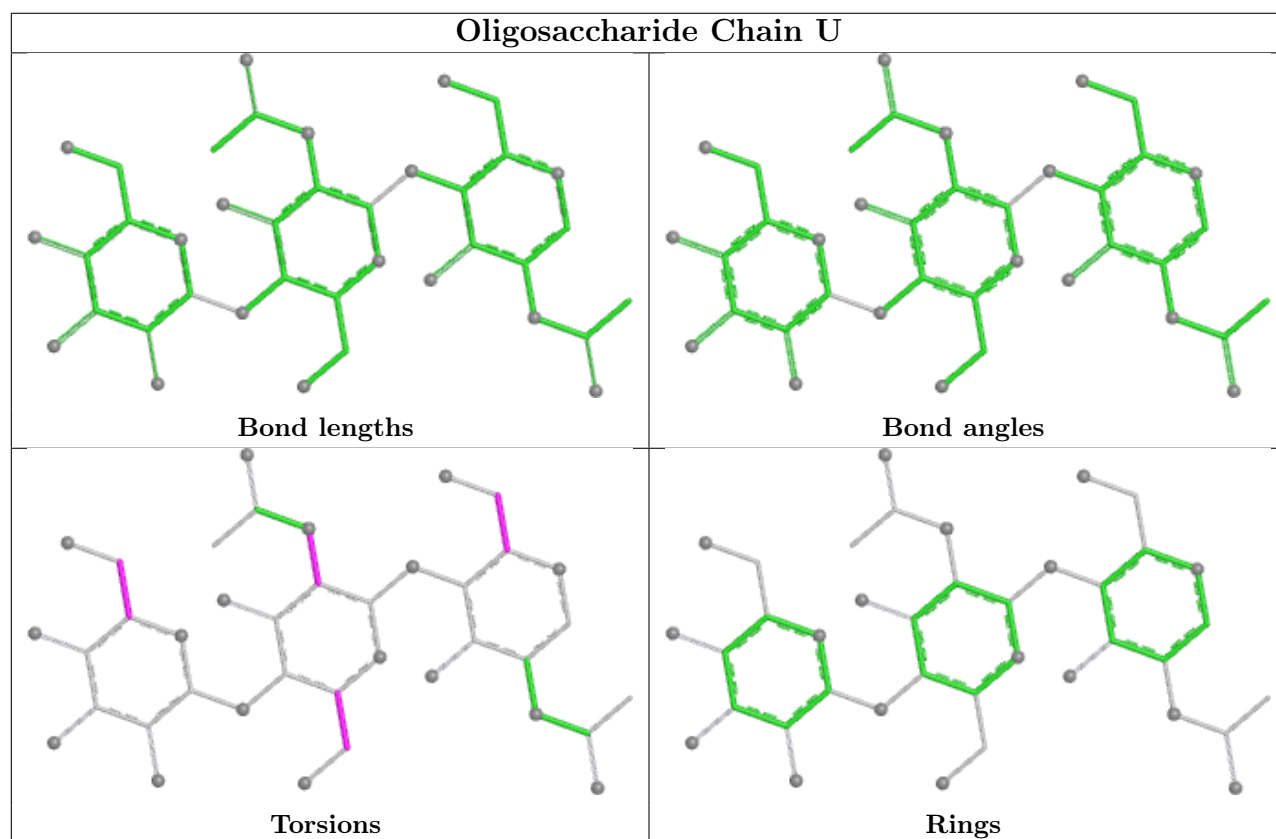
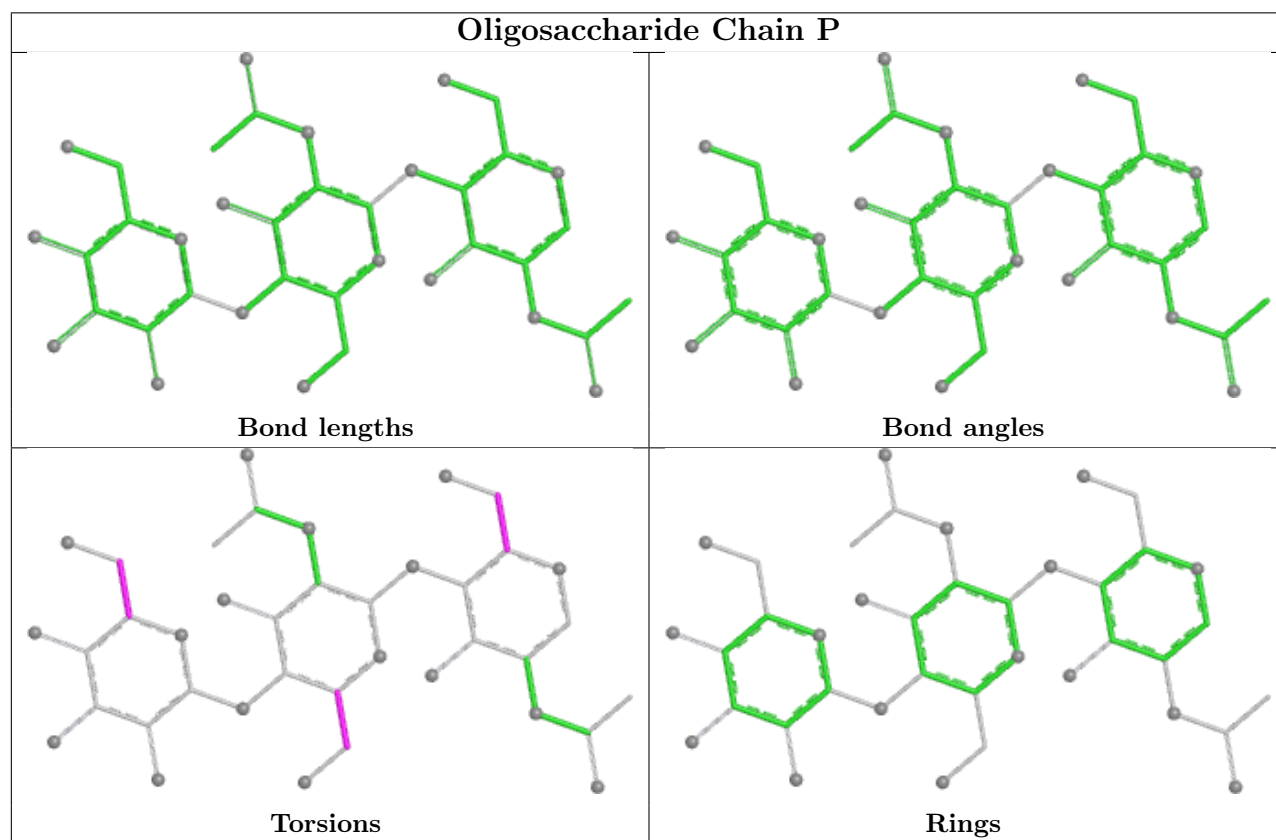
All (1) ring outliers are listed below:

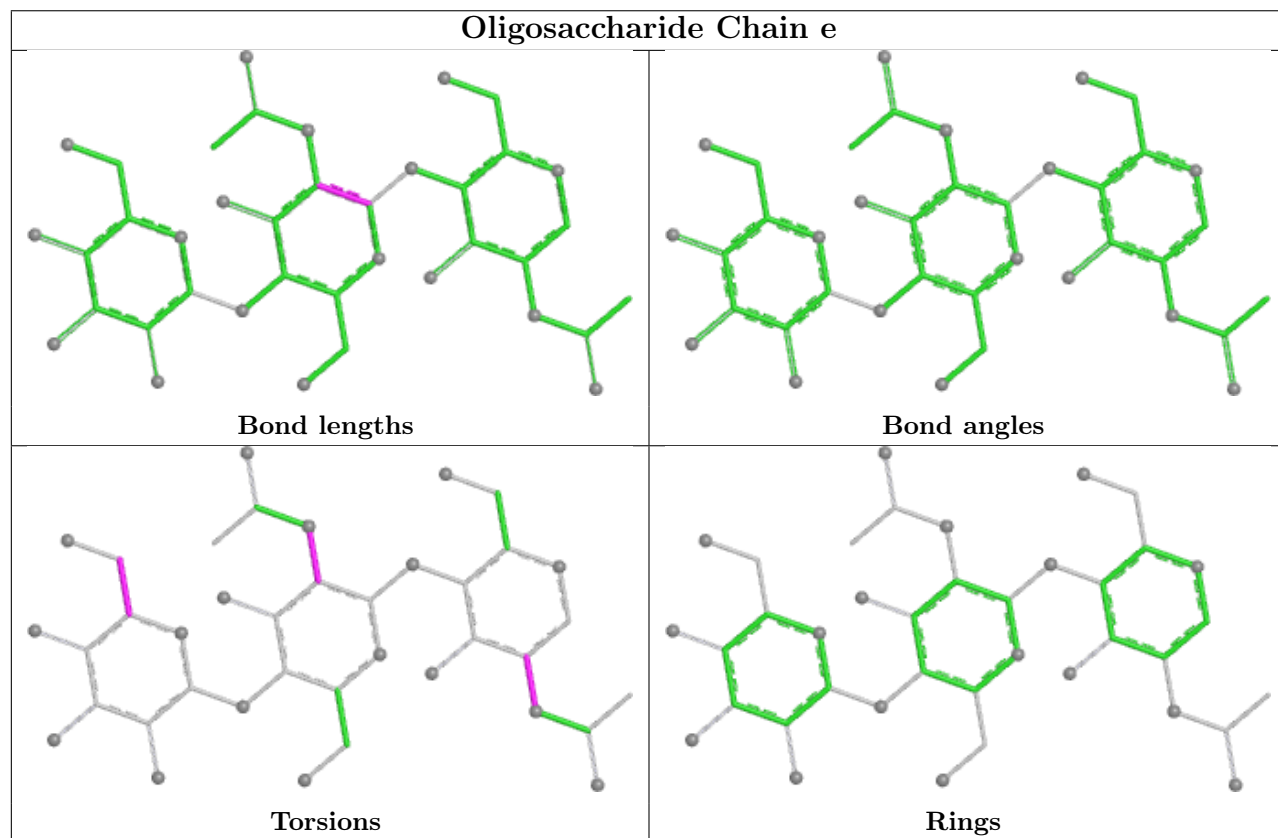
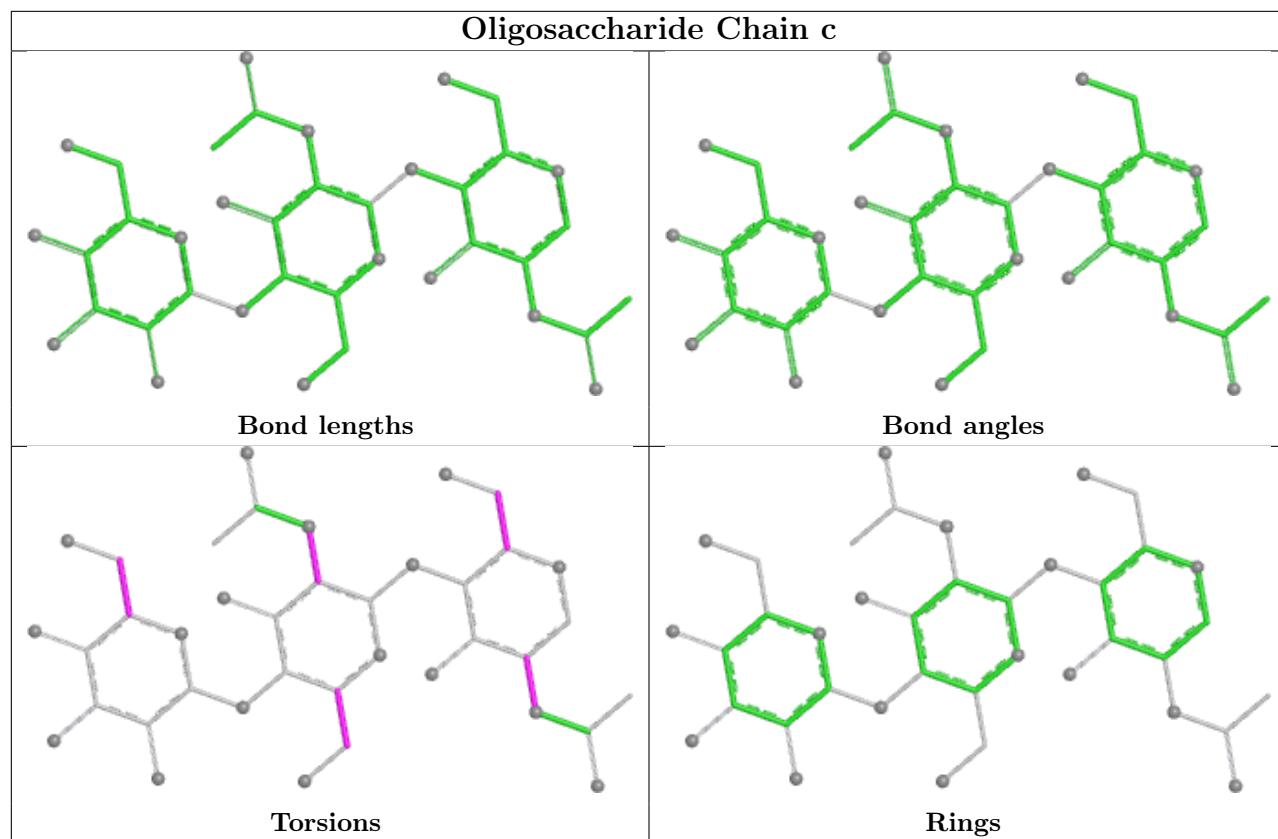
Mol	Chain	Res	Type	Atoms
12	g	4	MAN	C1-C2-C3-C4-C5-O5

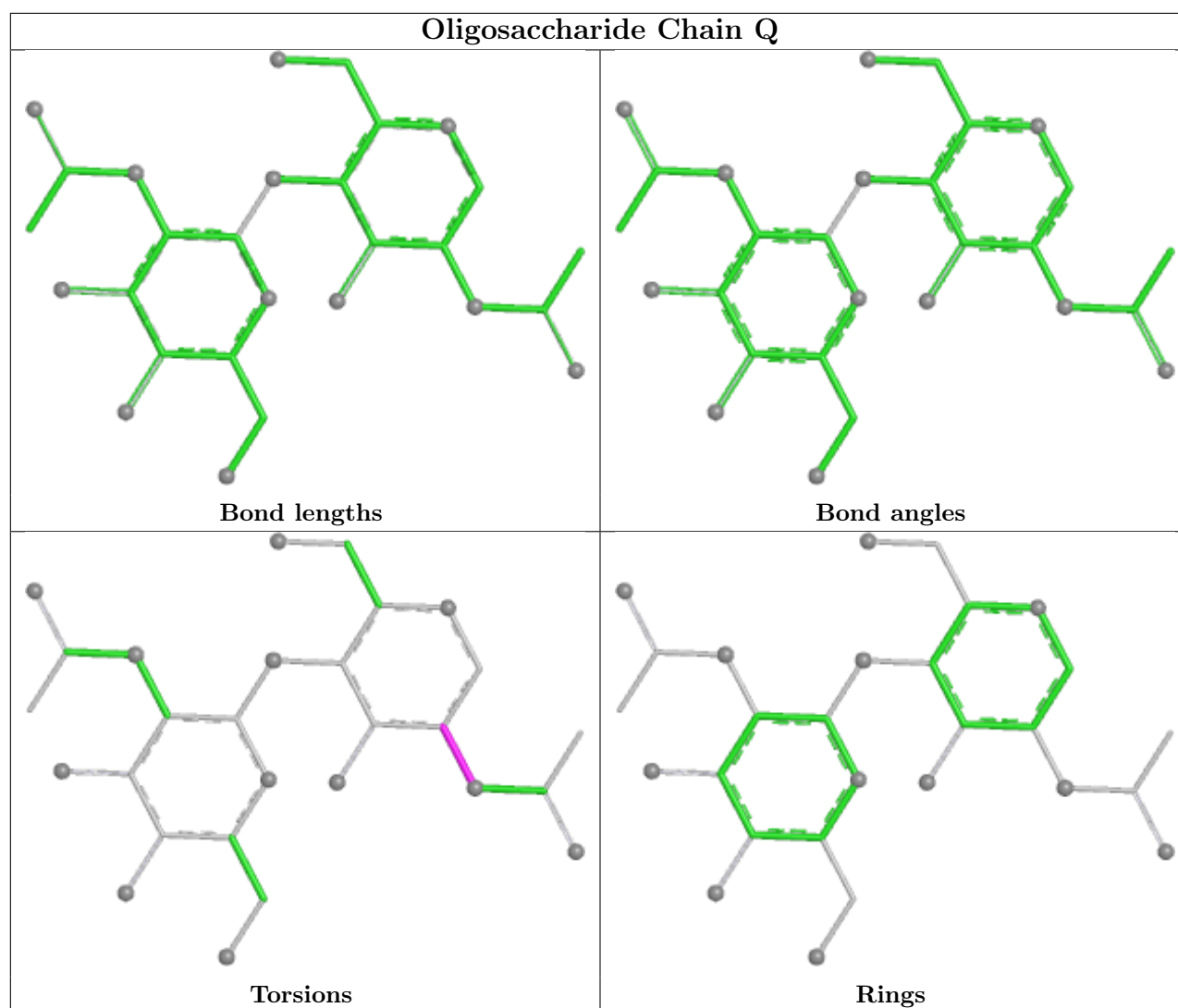
13 monomers are involved in 12 short contacts:

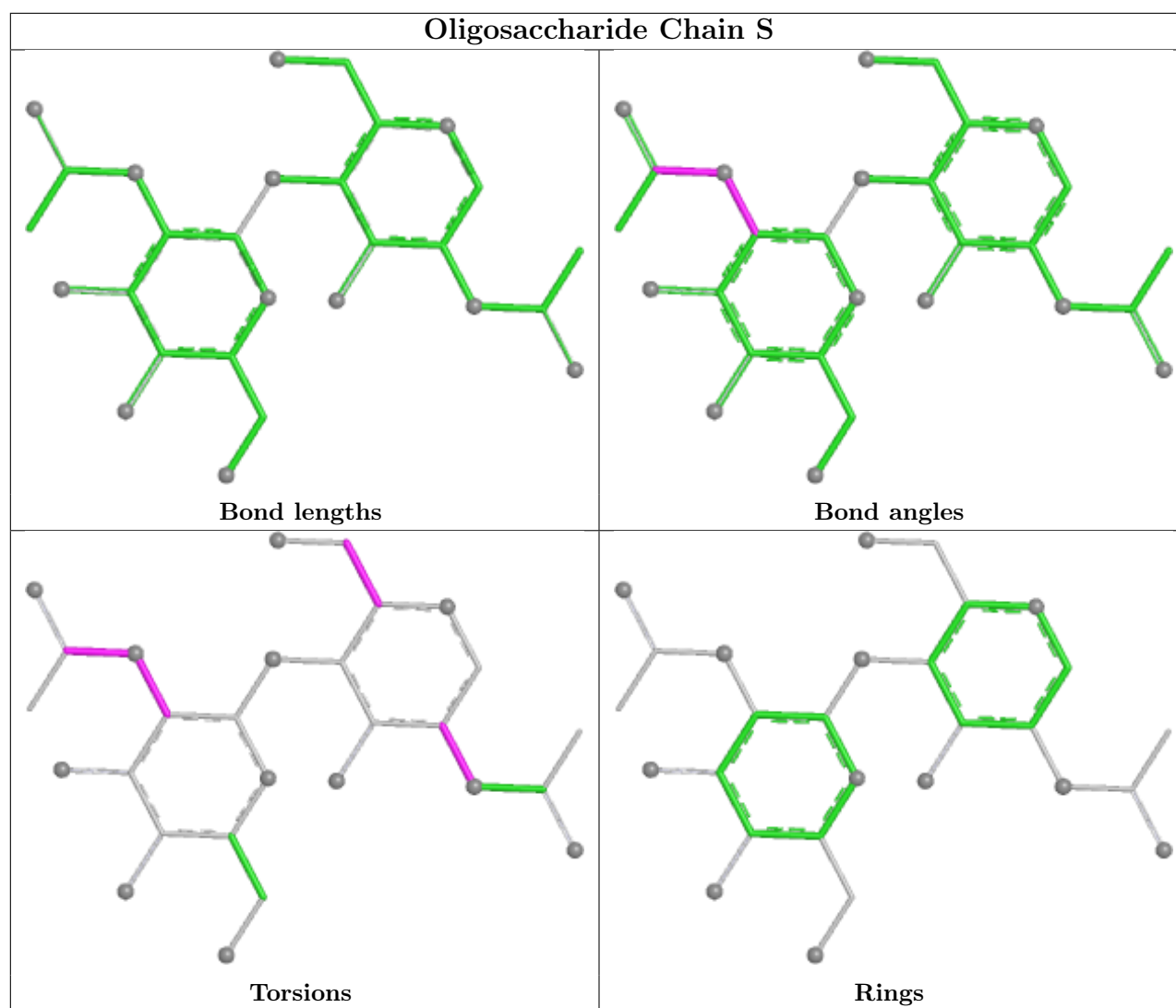
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	a	3	NAG	1	0
8	U	2	NAG	1	0
9	b	2	NAG	1	0
8	c	1	NAG	1	0
8	c	3	BMA	1	0
8	U	1	NAG	1	0
9	S	2	NAG	1	0
11	a	7	MAN	1	0
8	e	1	NAG	2	0
9	T	1	NAG	2	0
11	a	6	MAN	1	0
8	c	2	NAG	1	0
11	a	2	NAG	1	0

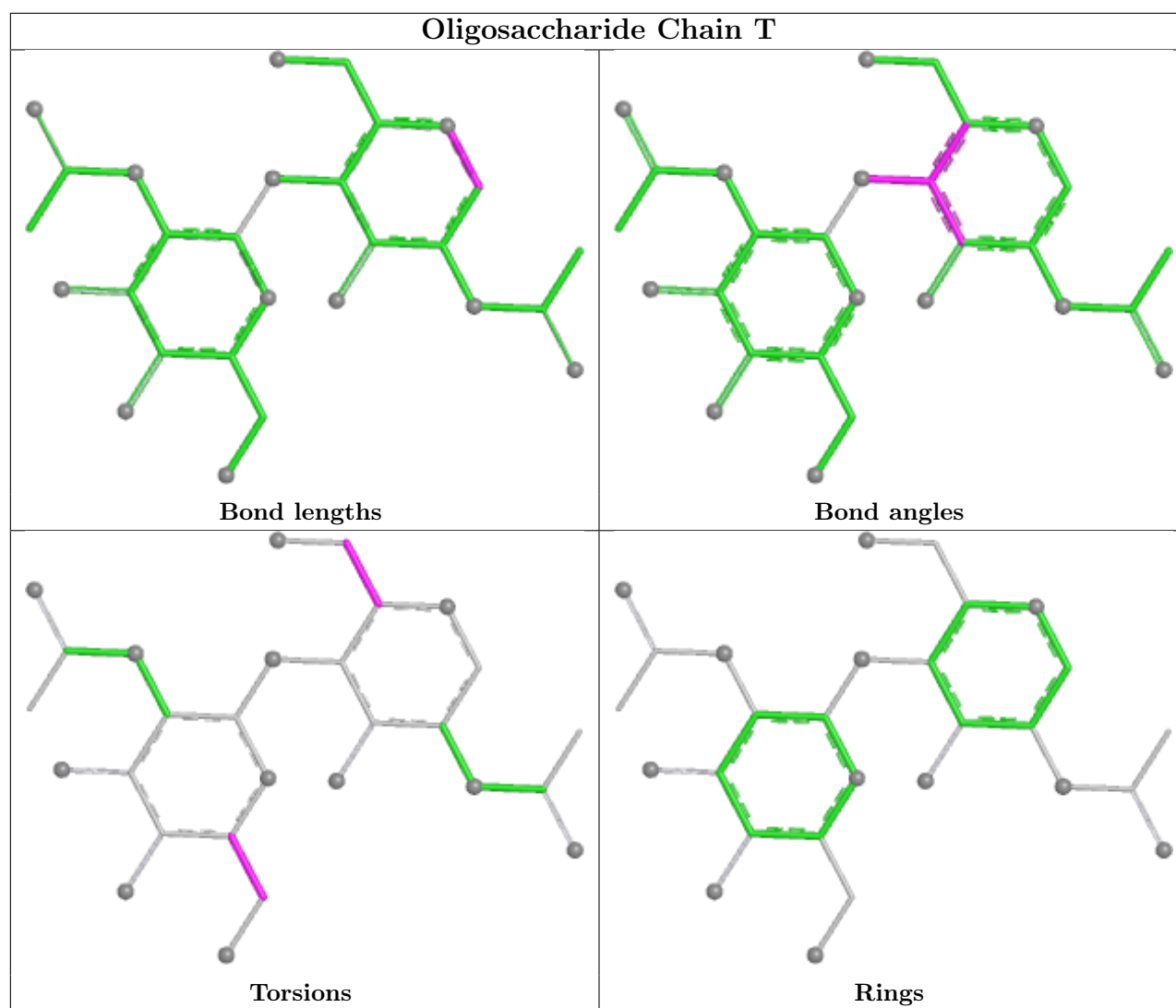
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

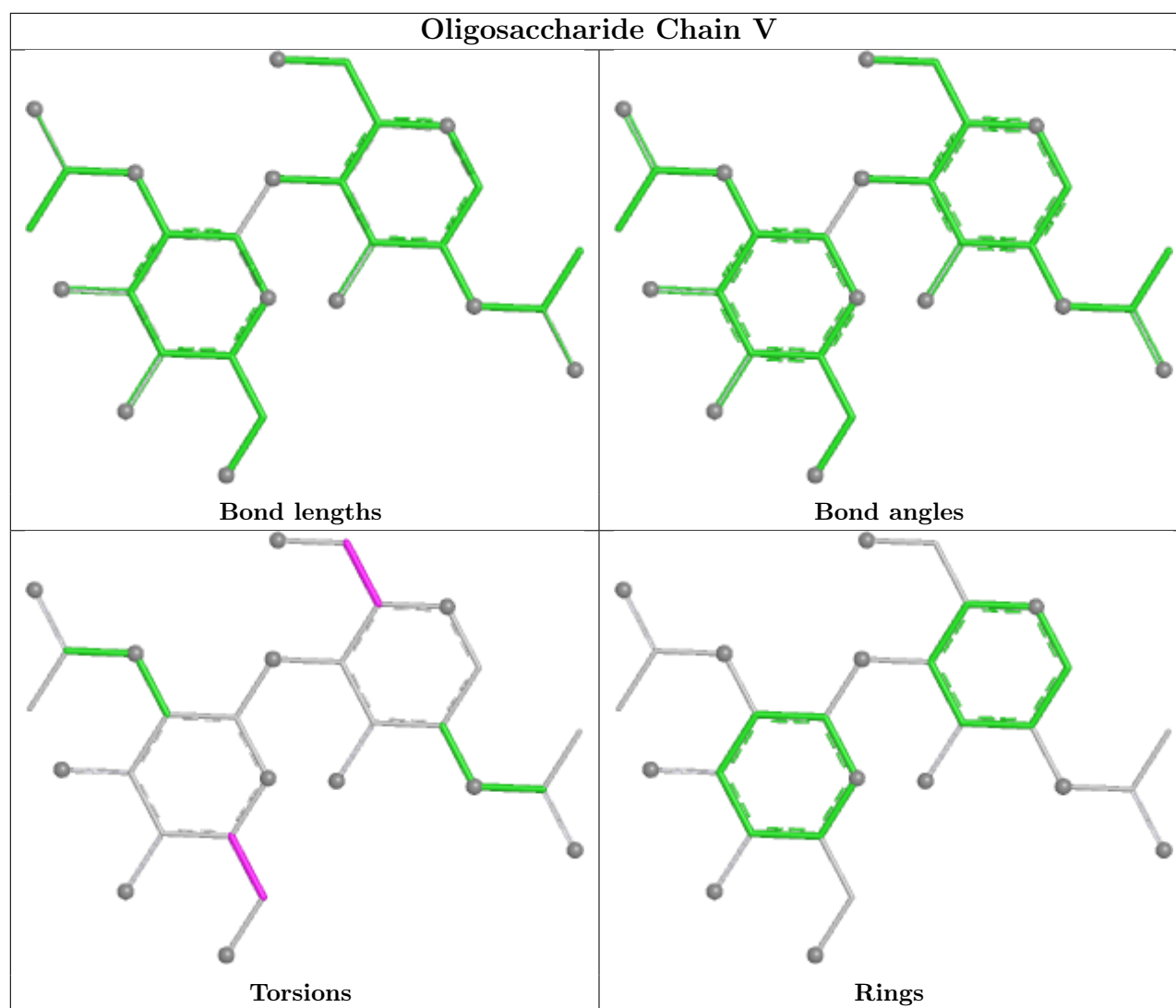


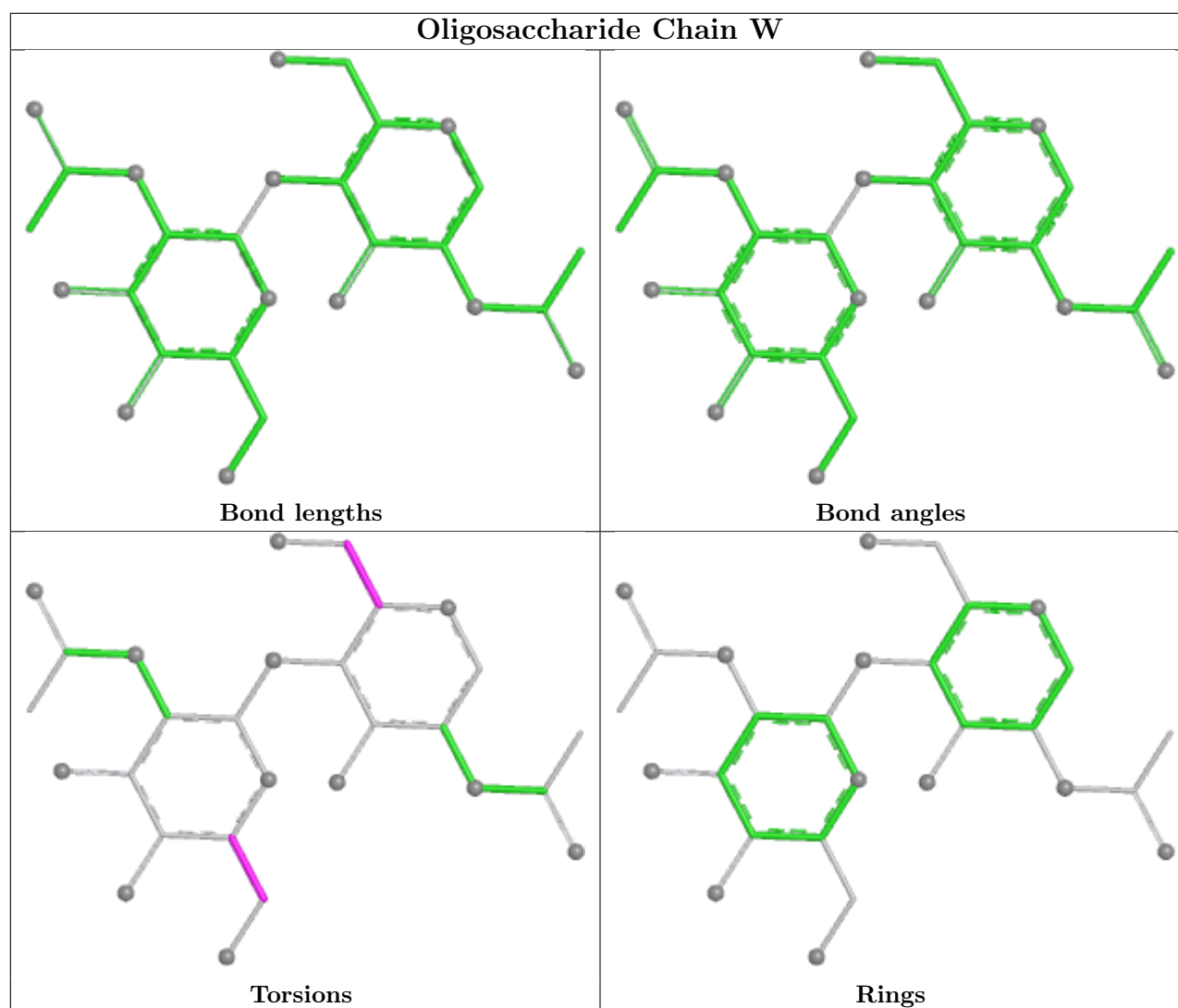


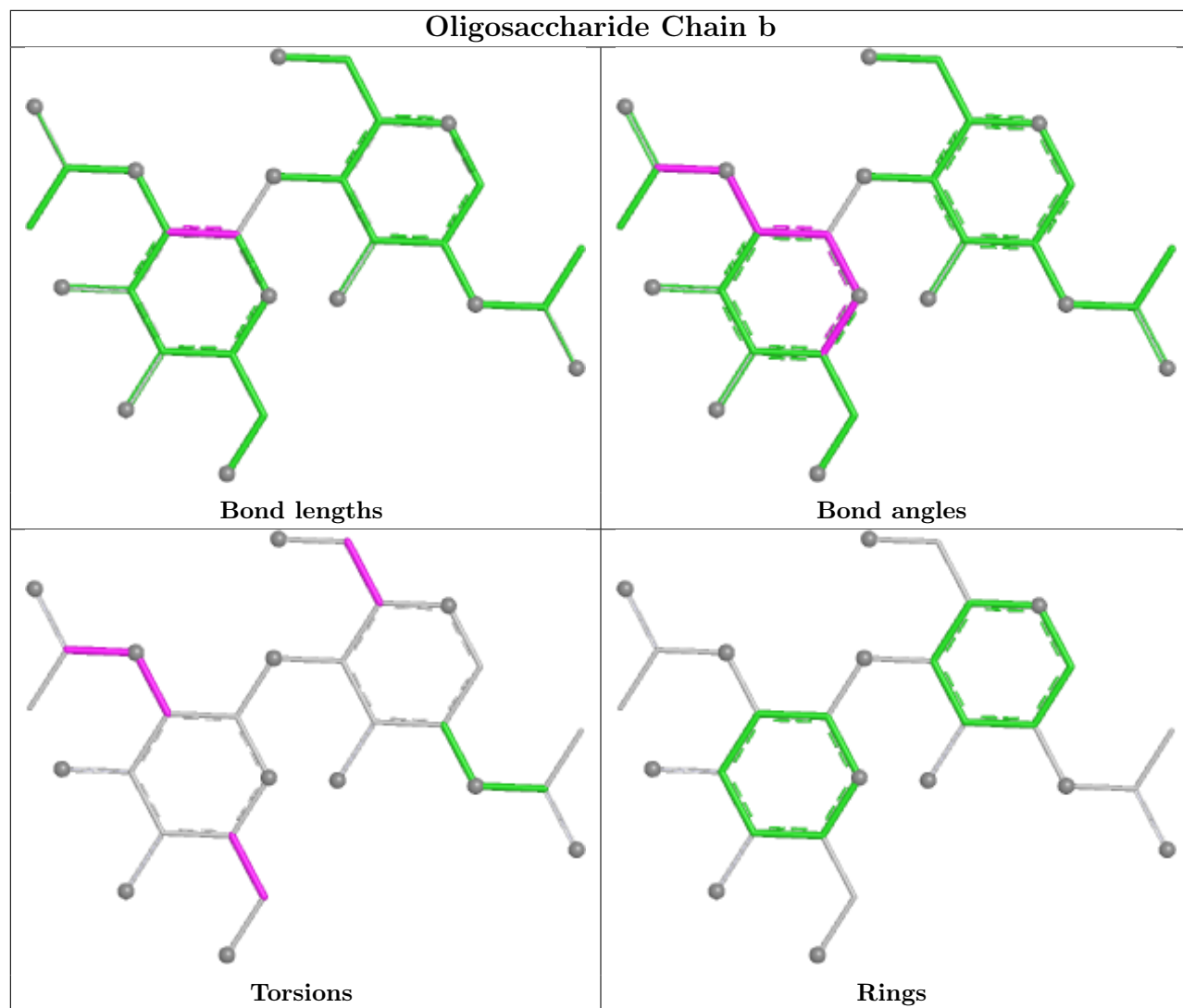


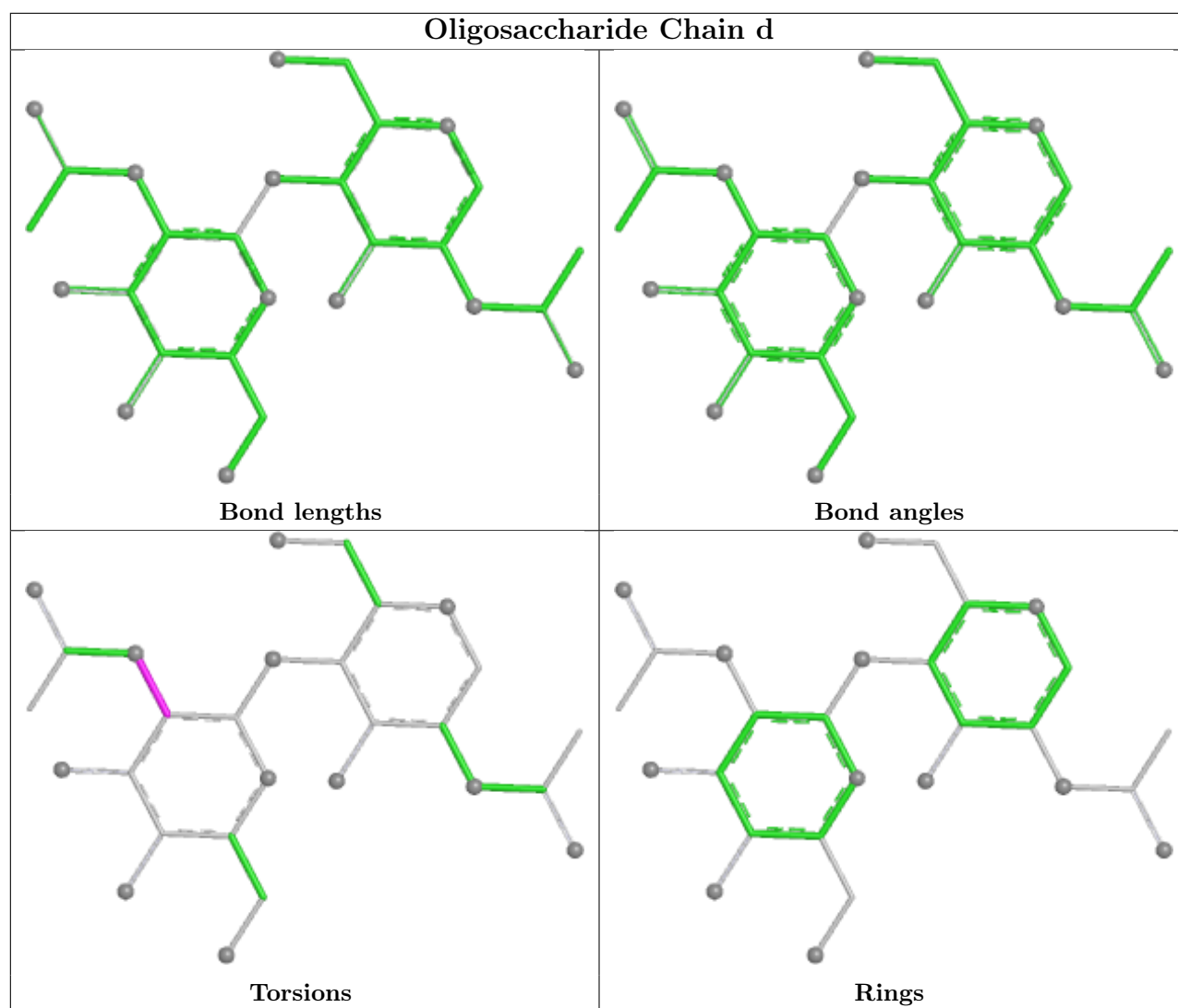


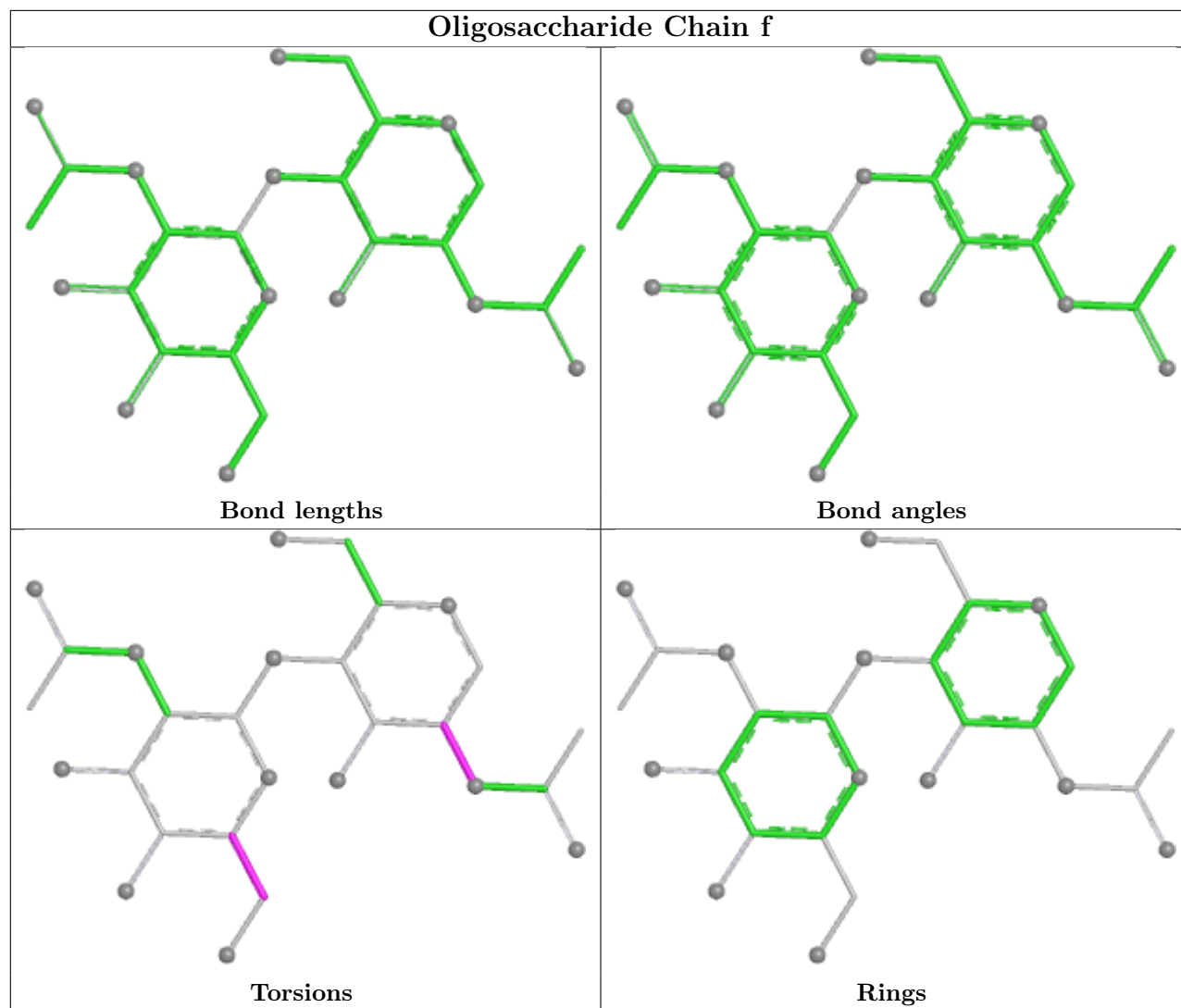


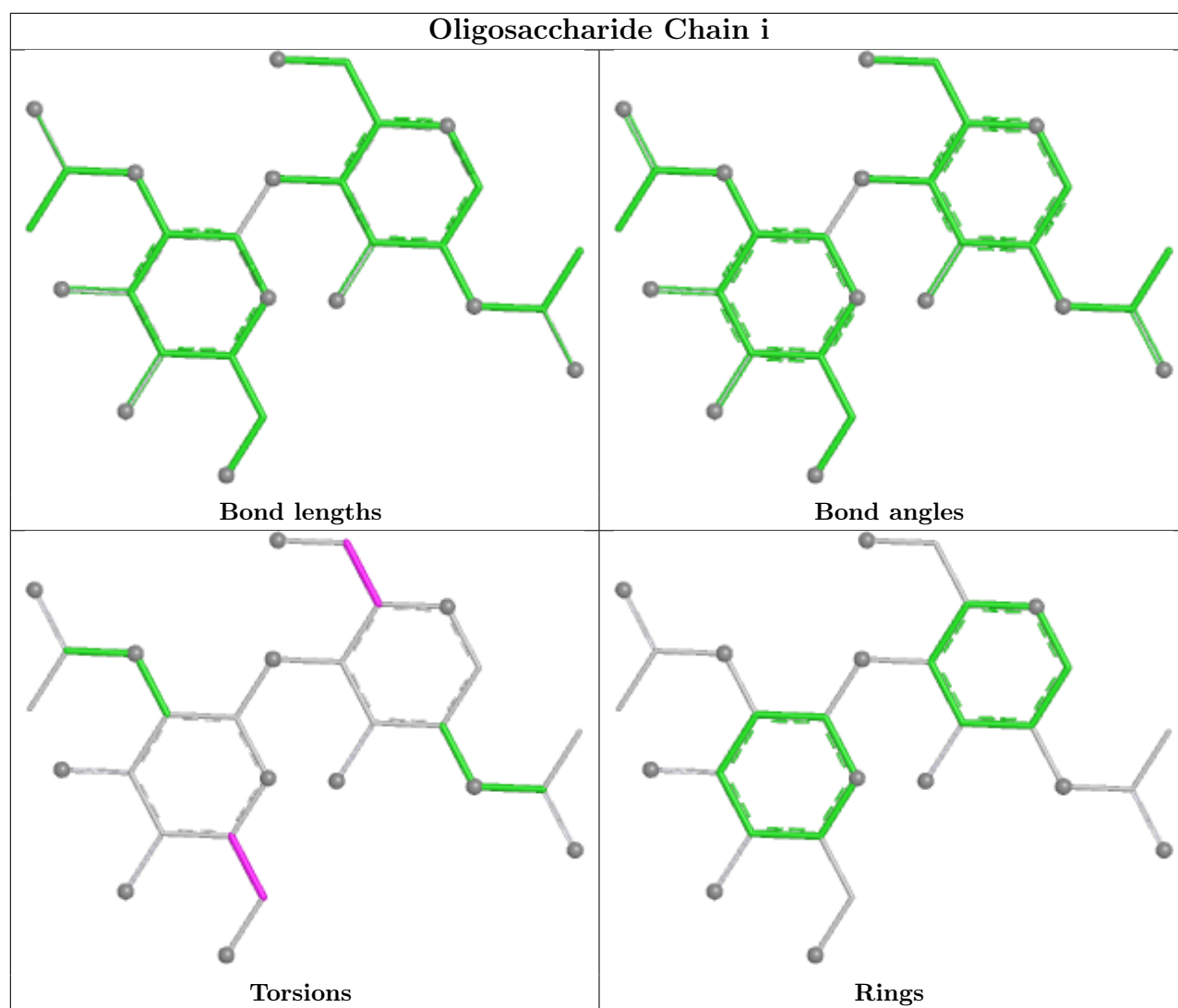


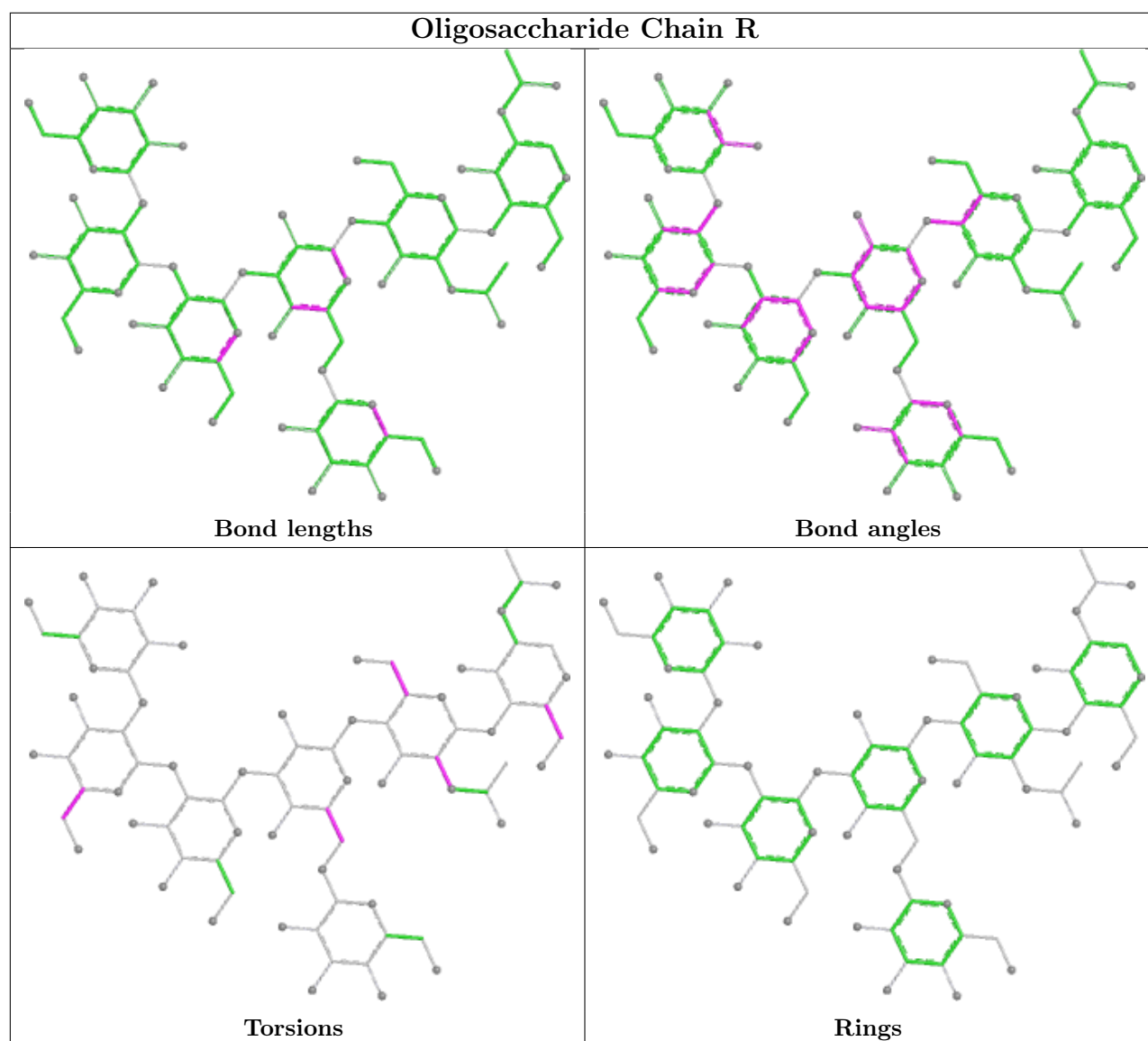


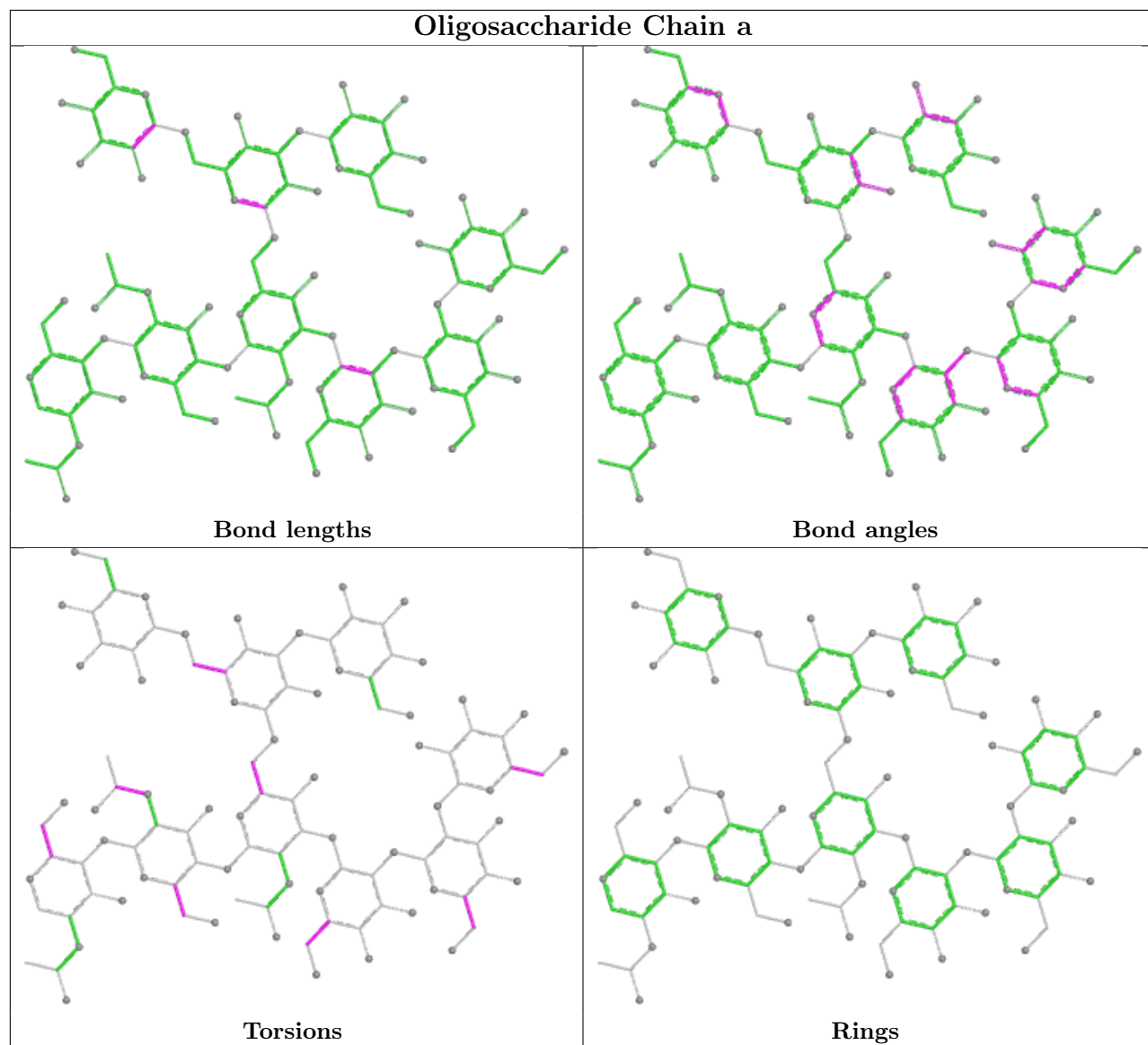


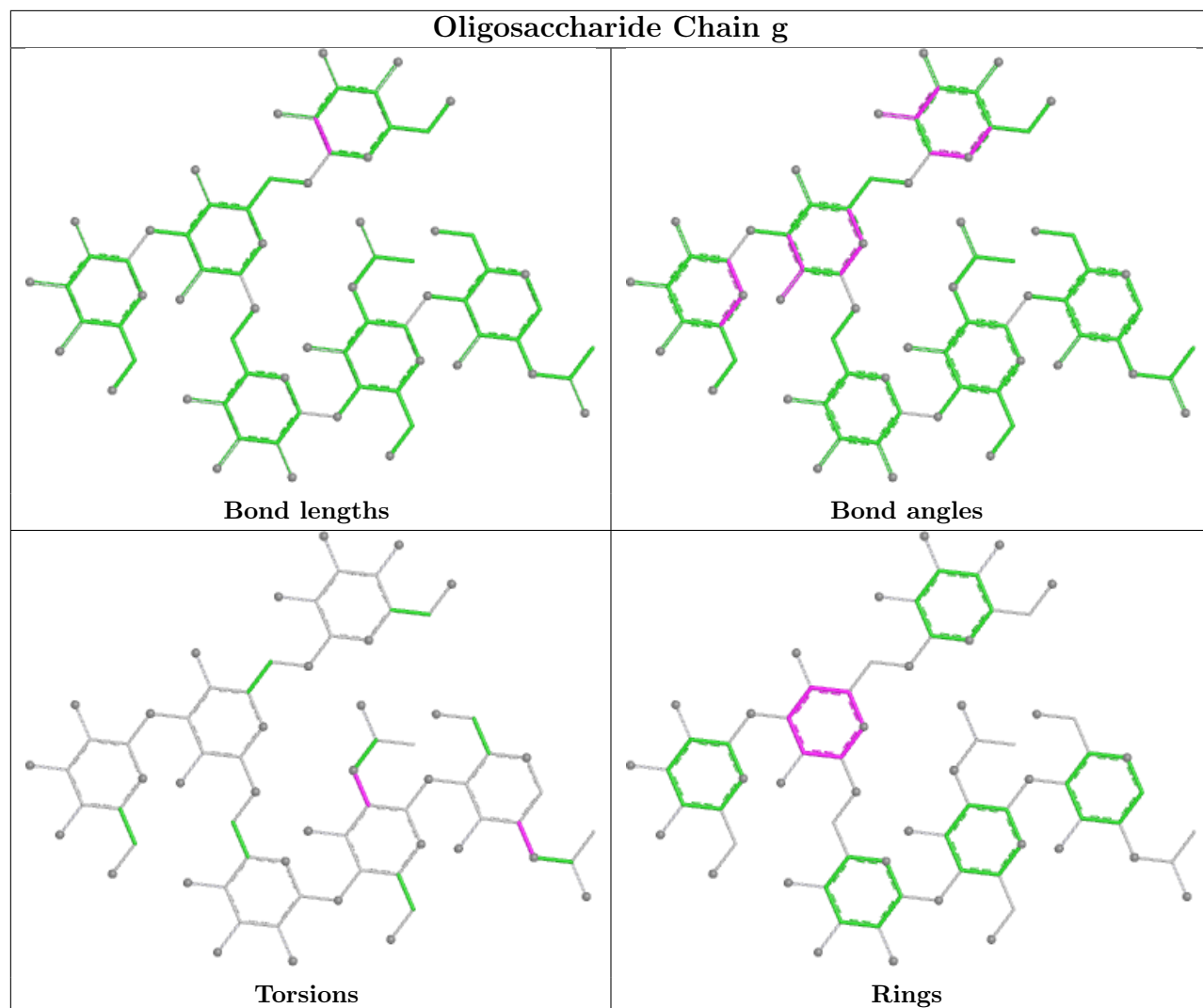


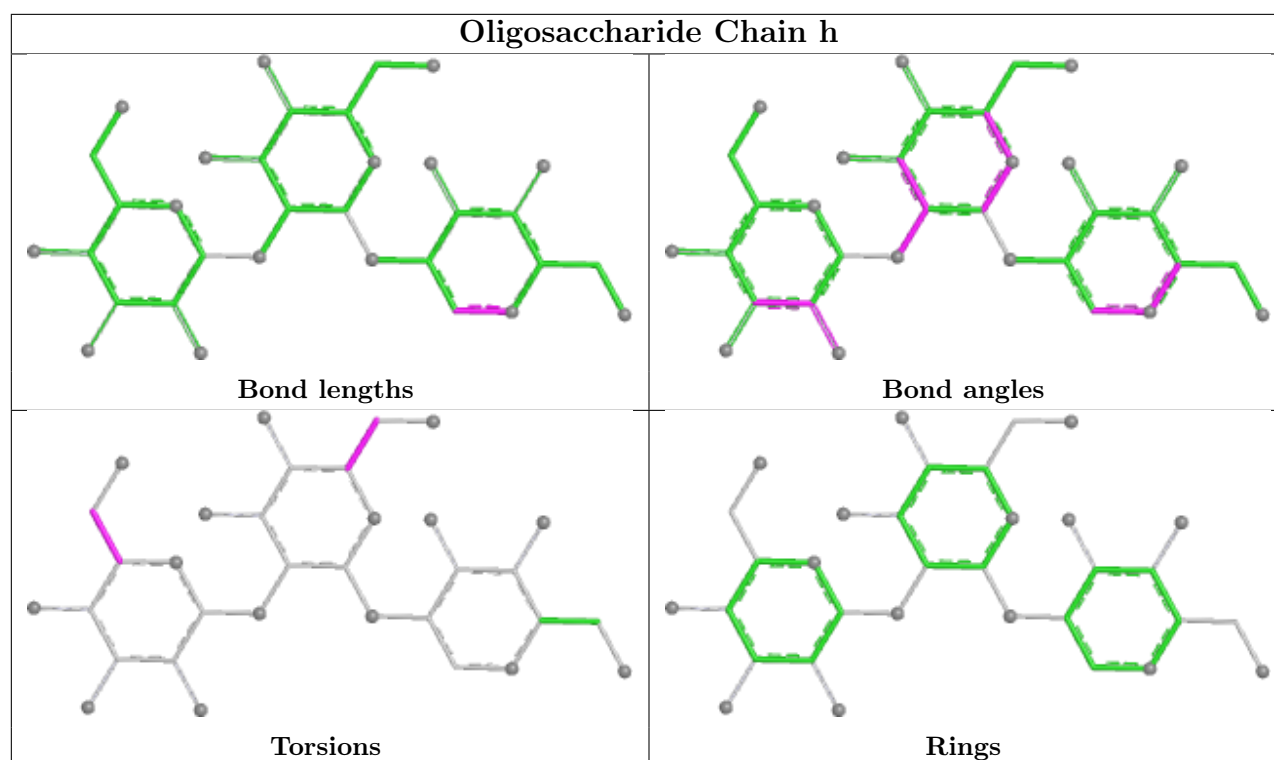












5.6 Ligand geometry [i](#)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	NAG	M	602	5	14,14,15	0.45	0	17,19,21	0.45	0
14	NAG	E	603	5	14,14,15	0.21	0	17,19,21	0.40	0
14	NAG	E	605	5	14,14,15	0.23	0	17,19,21	0.43	0
14	NAG	E	607	5	14,14,15	0.39	0	17,19,21	0.49	0
14	NAG	G	607	5	14,14,15	0.25	0	17,19,21	0.45	0
14	NAG	M	608	5	14,14,15	0.29	0	17,19,21	0.58	0
14	NAG	X	702	7	14,14,15	0.26	0	17,19,21	0.40	0
14	NAG	E	606	5	14,14,15	0.25	0	17,19,21	0.37	0
14	NAG	M	604	5	14,14,15	0.21	0	17,19,21	0.49	0
14	NAG	Y	702	7	14,14,15	0.19	0	17,19,21	0.50	0
14	NAG	E	601	5	14,14,15	0.43	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	Y	703	7	14,14,15	0.31	0	17,19,21	0.52	0
14	NAG	G	606	5	14,14,15	0.24	0	17,19,21	0.41	0
14	NAG	E	608	5	14,14,15	0.22	0	17,19,21	0.42	0
14	NAG	Z	702	7	14,14,15	0.48	0	17,19,21	0.62	0
14	NAG	E	604	5	14,14,15	0.31	0	17,19,21	0.45	0
14	NAG	X	701	7	14,14,15	0.31	0	17,19,21	0.40	0
14	NAG	Z	701	7	14,14,15	0.59	1 (7%)	17,19,21	0.96	1 (5%)
14	NAG	G	603	5	14,14,15	0.33	0	17,19,21	0.52	0
14	NAG	M	606	5	14,14,15	0.31	0	17,19,21	0.42	0
14	NAG	M	603	5	14,14,15	0.26	0	17,19,21	0.51	0
14	NAG	G	605	5	14,14,15	0.23	0	17,19,21	0.43	0
14	NAG	E	602	5	14,14,15	0.60	1 (7%)	17,19,21	0.65	0
14	NAG	G	602	5	14,14,15	0.46	0	17,19,21	0.61	0
14	NAG	M	605	5	14,14,15	0.30	0	17,19,21	0.43	0
14	NAG	G	604	5	14,14,15	0.67	1 (7%)	17,19,21	1.37	2 (11%)
14	NAG	G	601	5	14,14,15	0.53	0	17,19,21	1.30	1 (5%)
14	NAG	Y	701	7	14,14,15	0.39	0	17,19,21	0.39	0
14	NAG	M	601	5	14,14,15	0.36	0	17,19,21	0.50	0
14	NAG	M	607	5	14,14,15	0.41	0	17,19,21	0.54	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
14	NAG	M	602	5	-	2/6/23/26	0/1/1/1
14	NAG	E	603	5	-	0/6/23/26	0/1/1/1
14	NAG	E	605	5	-	0/6/23/26	0/1/1/1
14	NAG	E	607	5	-	0/6/23/26	0/1/1/1
14	NAG	G	607	5	-	2/6/23/26	0/1/1/1
14	NAG	M	608	5	-	1/6/23/26	0/1/1/1
14	NAG	X	702	7	-	1/6/23/26	0/1/1/1
14	NAG	E	606	5	-	2/6/23/26	0/1/1/1
14	NAG	M	604	5	-	2/6/23/26	0/1/1/1
14	NAG	Y	702	7	-	4/6/23/26	0/1/1/1
14	NAG	E	601	5	-	3/6/23/26	0/1/1/1
14	NAG	Y	703	7	-	0/6/23/26	0/1/1/1
14	NAG	G	606	5	-	2/6/23/26	0/1/1/1
14	NAG	E	608	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	Z	702	7	-	2/6/23/26	0/1/1/1
14	NAG	E	604	5	-	1/6/23/26	0/1/1/1
14	NAG	X	701	7	-	0/6/23/26	0/1/1/1
14	NAG	Z	701	7	-	2/6/23/26	0/1/1/1
14	NAG	G	603	5	-	0/6/23/26	0/1/1/1
14	NAG	M	606	5	-	0/6/23/26	0/1/1/1
14	NAG	M	603	5	-	0/6/23/26	0/1/1/1
14	NAG	G	605	5	-	2/6/23/26	0/1/1/1
14	NAG	E	602	5	-	4/6/23/26	0/1/1/1
14	NAG	G	602	5	-	3/6/23/26	0/1/1/1
14	NAG	M	605	5	-	1/6/23/26	0/1/1/1
14	NAG	G	604	5	-	6/6/23/26	0/1/1/1
14	NAG	G	601	5	-	5/6/23/26	0/1/1/1
14	NAG	Y	701	7	-	0/6/23/26	0/1/1/1
14	NAG	M	601	5	-	0/6/23/26	0/1/1/1
14	NAG	M	607	5	-	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)
14	G	604	NAG	C1-C2	2.26	1.55	1.52
14	E	602	NAG	C1-C2	2.11	1.55	1.52
14	Z	701	NAG	C1-C2	2.01	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	604	NAG	C2-N2-C7	4.62	129.09	122.90
14	G	601	NAG	C2-N2-C7	4.49	128.91	122.90
14	Z	701	NAG	C1-O5-C5	3.55	116.95	112.19
14	G	604	NAG	C1-C2-N2	2.49	114.36	110.43

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	M	602	NAG	C4-C5-C6-O6
14	M	602	NAG	O5-C5-C6-O6
14	G	604	NAG	O5-C5-C6-O6
14	G	601	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
14	G	601	NAG	O7-C7-N2-C2
14	G	604	NAG	C8-C7-N2-C2
14	G	604	NAG	O7-C7-N2-C2
14	Z	702	NAG	C8-C7-N2-C2
14	Z	702	NAG	O7-C7-N2-C2
14	G	605	NAG	O5-C5-C6-O6
14	G	605	NAG	C4-C5-C6-O6
14	M	604	NAG	C4-C5-C6-O6
14	E	606	NAG	C4-C5-C6-O6
14	E	604	NAG	O5-C5-C6-O6
14	Z	701	NAG	O5-C5-C6-O6
14	M	604	NAG	O5-C5-C6-O6
14	X	702	NAG	O5-C5-C6-O6
14	E	606	NAG	O5-C5-C6-O6
14	G	604	NAG	C4-C5-C6-O6
14	G	601	NAG	O5-C5-C6-O6
14	M	605	NAG	O5-C5-C6-O6
14	E	602	NAG	C3-C2-N2-C7
14	G	602	NAG	O5-C5-C6-O6
14	G	606	NAG	O5-C5-C6-O6
14	Z	701	NAG	C4-C5-C6-O6
14	Y	702	NAG	C4-C5-C6-O6
14	E	602	NAG	C1-C2-N2-C7
14	G	602	NAG	C1-C2-N2-C7
14	E	608	NAG	C4-C5-C6-O6
14	Y	702	NAG	O5-C5-C6-O6
14	G	601	NAG	C3-C2-N2-C7
14	G	604	NAG	C3-C2-N2-C7
14	Y	702	NAG	C3-C2-N2-C7
14	E	608	NAG	O5-C5-C6-O6
14	G	607	NAG	C4-C5-C6-O6
14	E	601	NAG	C4-C5-C6-O6
14	E	601	NAG	O5-C5-C6-O6
14	G	601	NAG	C1-C2-N2-C7
14	G	604	NAG	C1-C2-N2-C7
14	G	606	NAG	C1-C2-N2-C7
14	M	608	NAG	C1-C2-N2-C7
14	Y	702	NAG	C1-C2-N2-C7
14	E	602	NAG	C4-C5-C6-O6
14	E	602	NAG	O5-C5-C6-O6
14	E	601	NAG	C3-C2-N2-C7
14	G	602	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
14	G	607	NAG	O5-C5-C6-O6

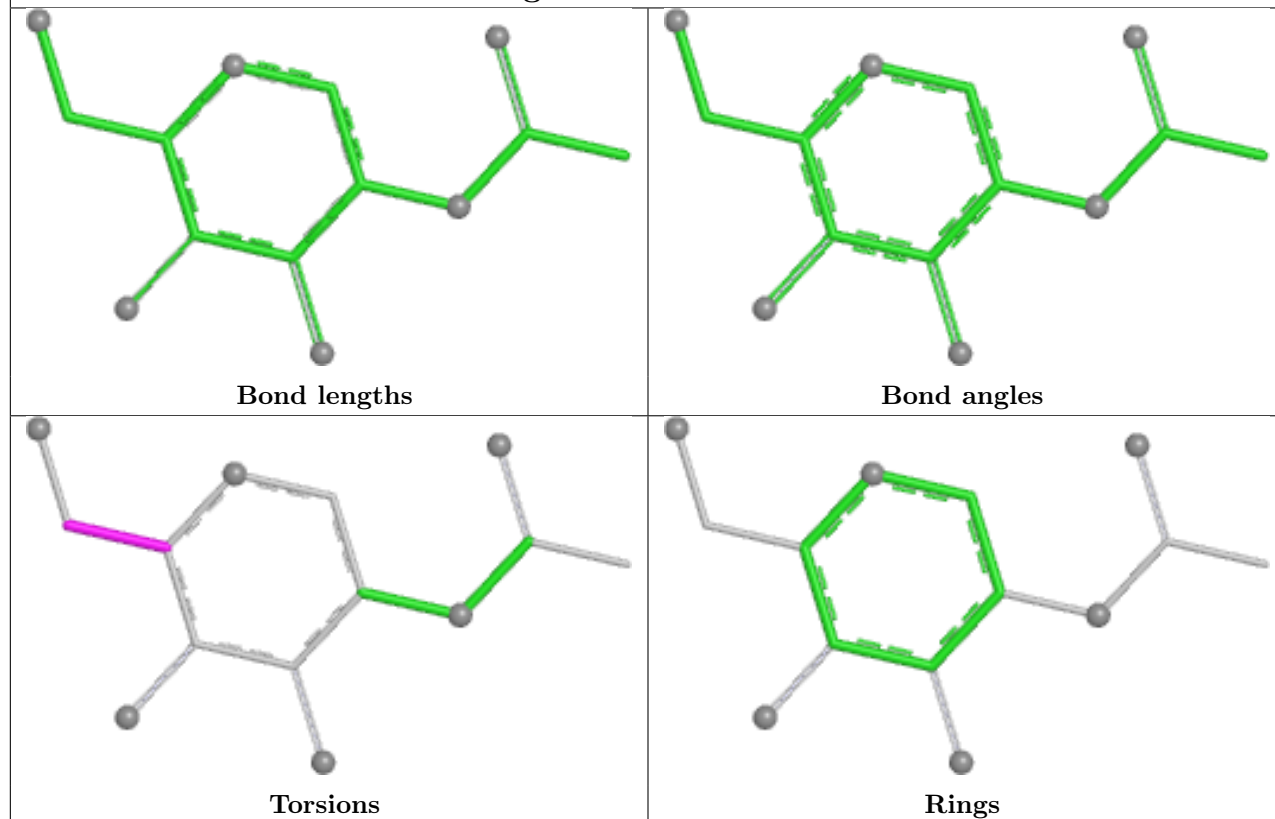
There are no ring outliers.

9 monomers are involved in 12 short contacts:

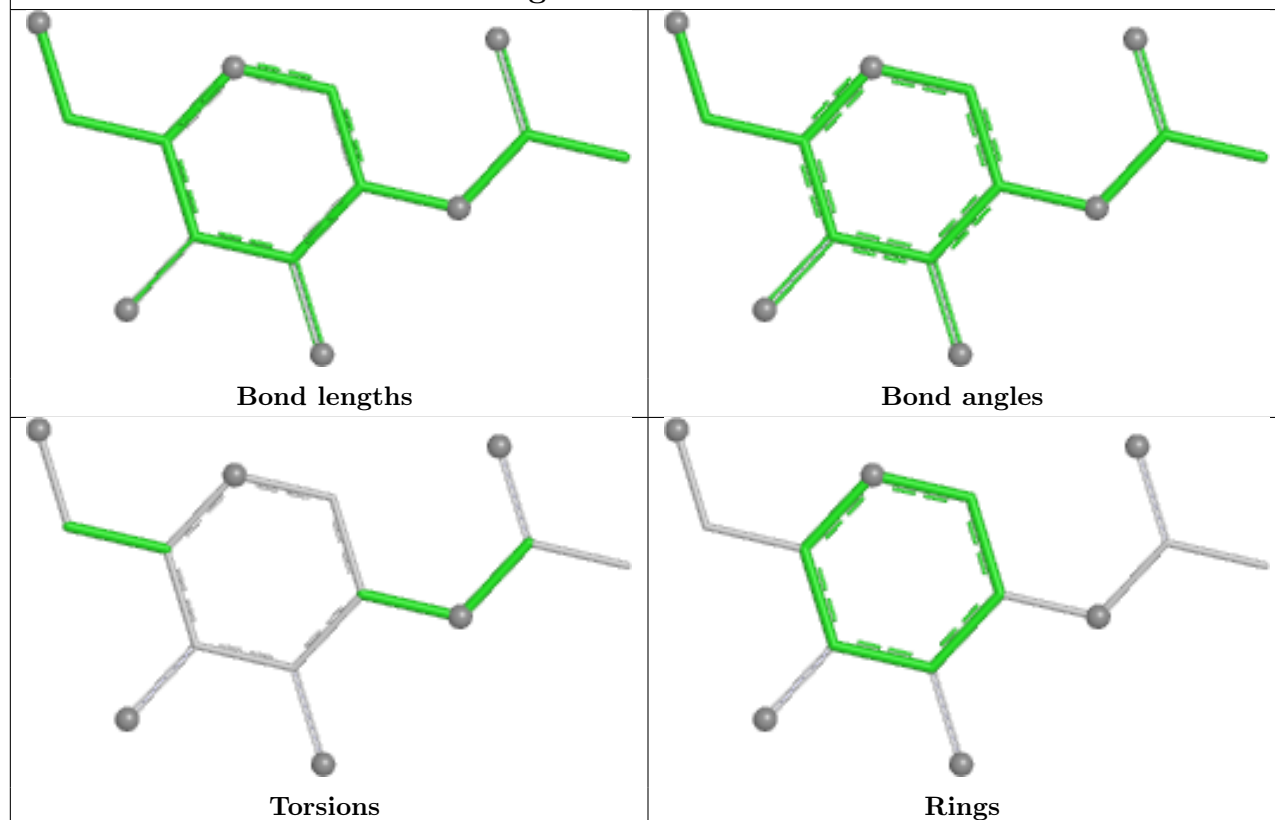
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	M	608	NAG	1	0
14	M	604	NAG	1	0
14	E	601	NAG	1	0
14	M	603	NAG	1	0
14	E	602	NAG	2	0
14	G	602	NAG	3	0
14	G	604	NAG	1	0
14	G	601	NAG	1	0
14	M	601	NAG	1	0

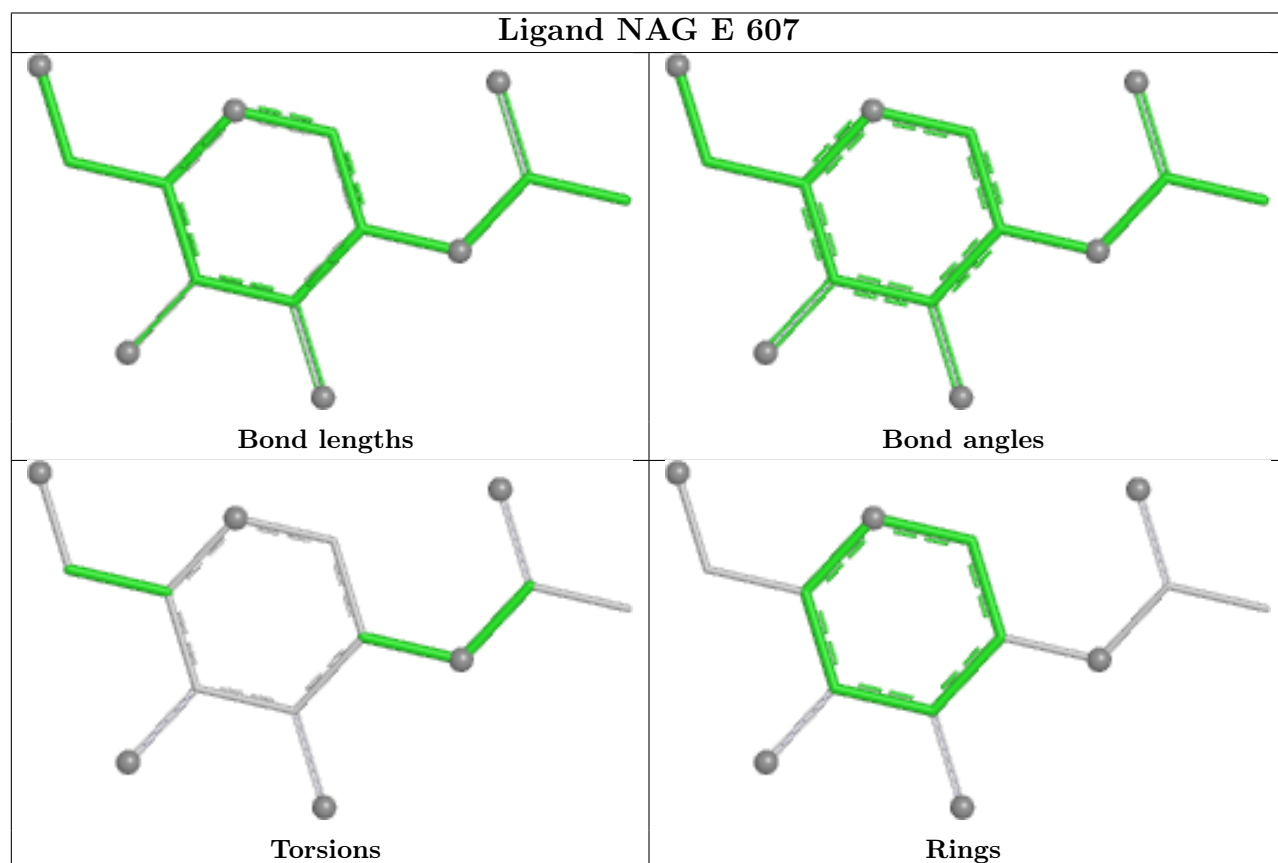
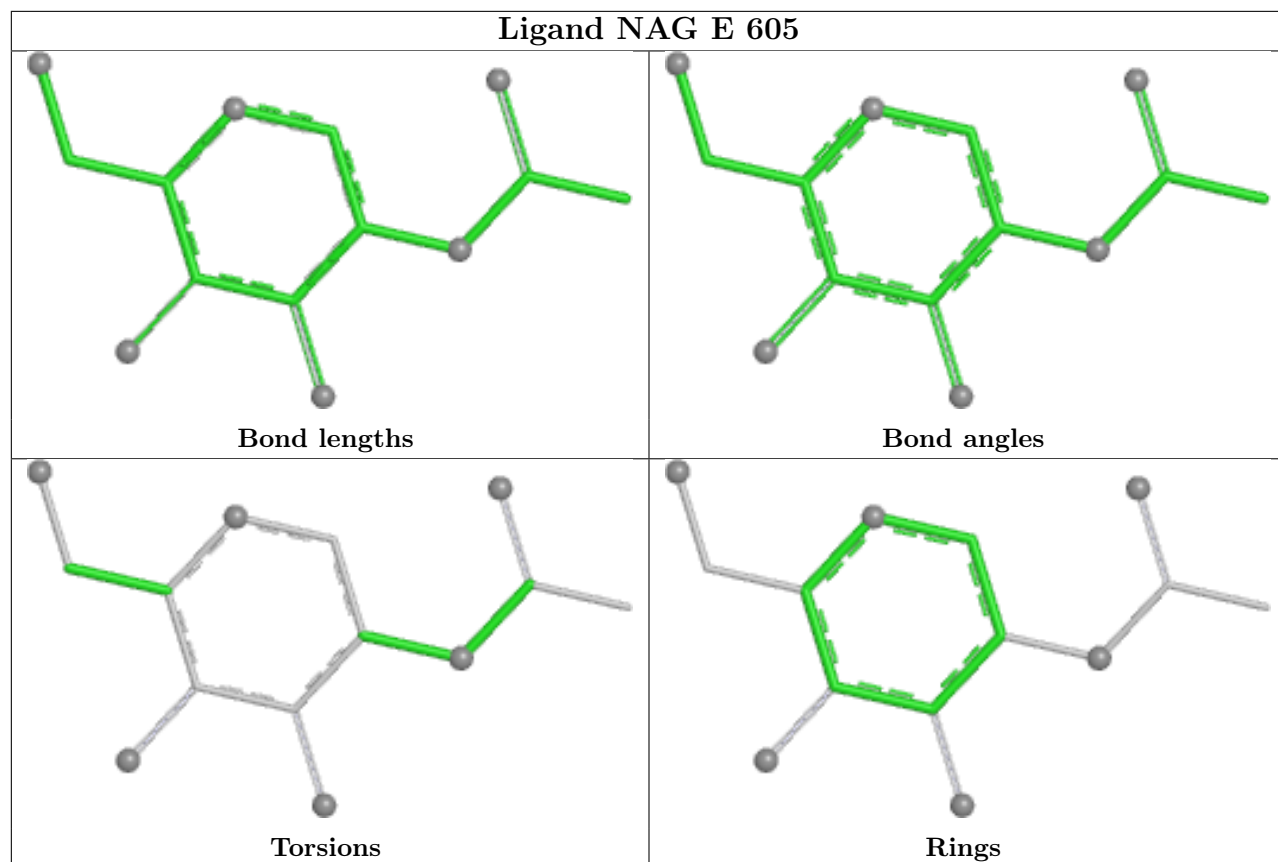
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

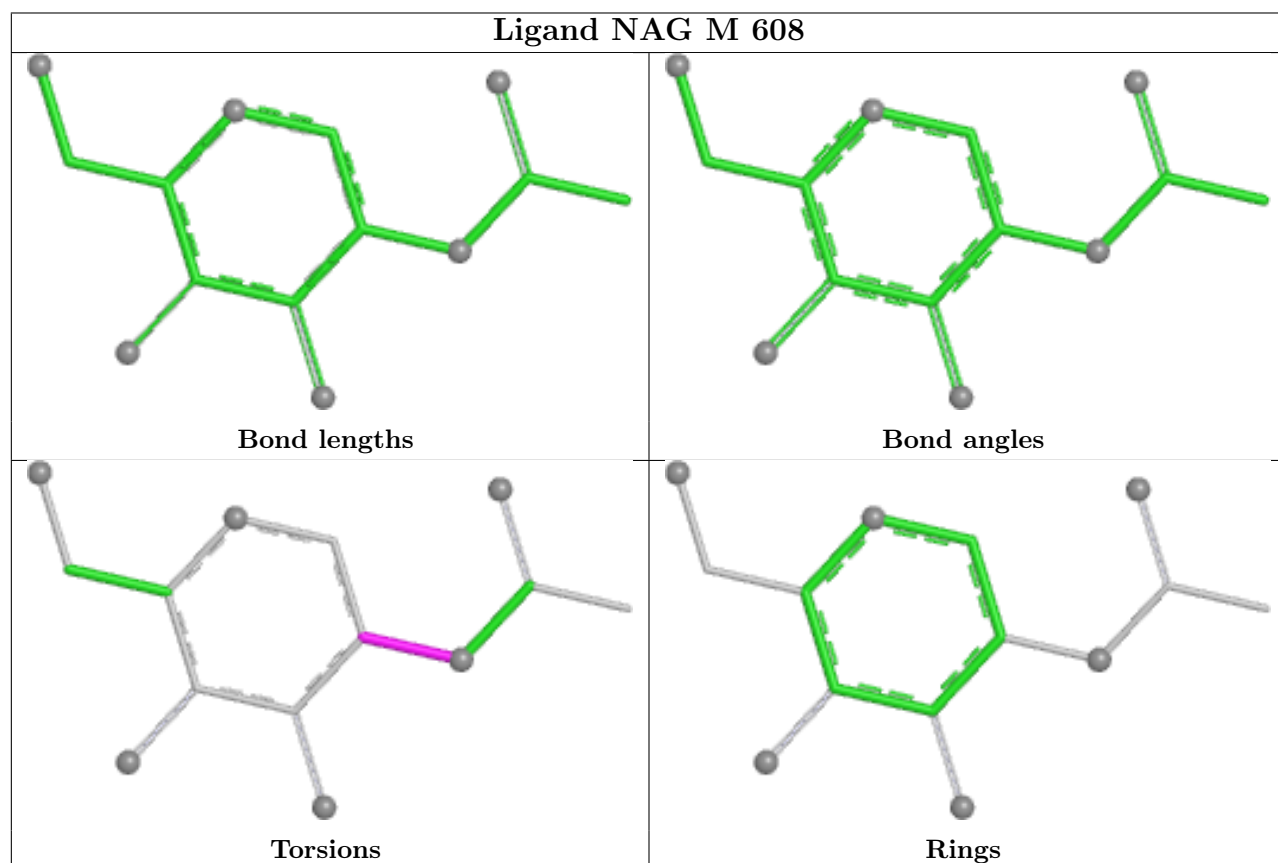
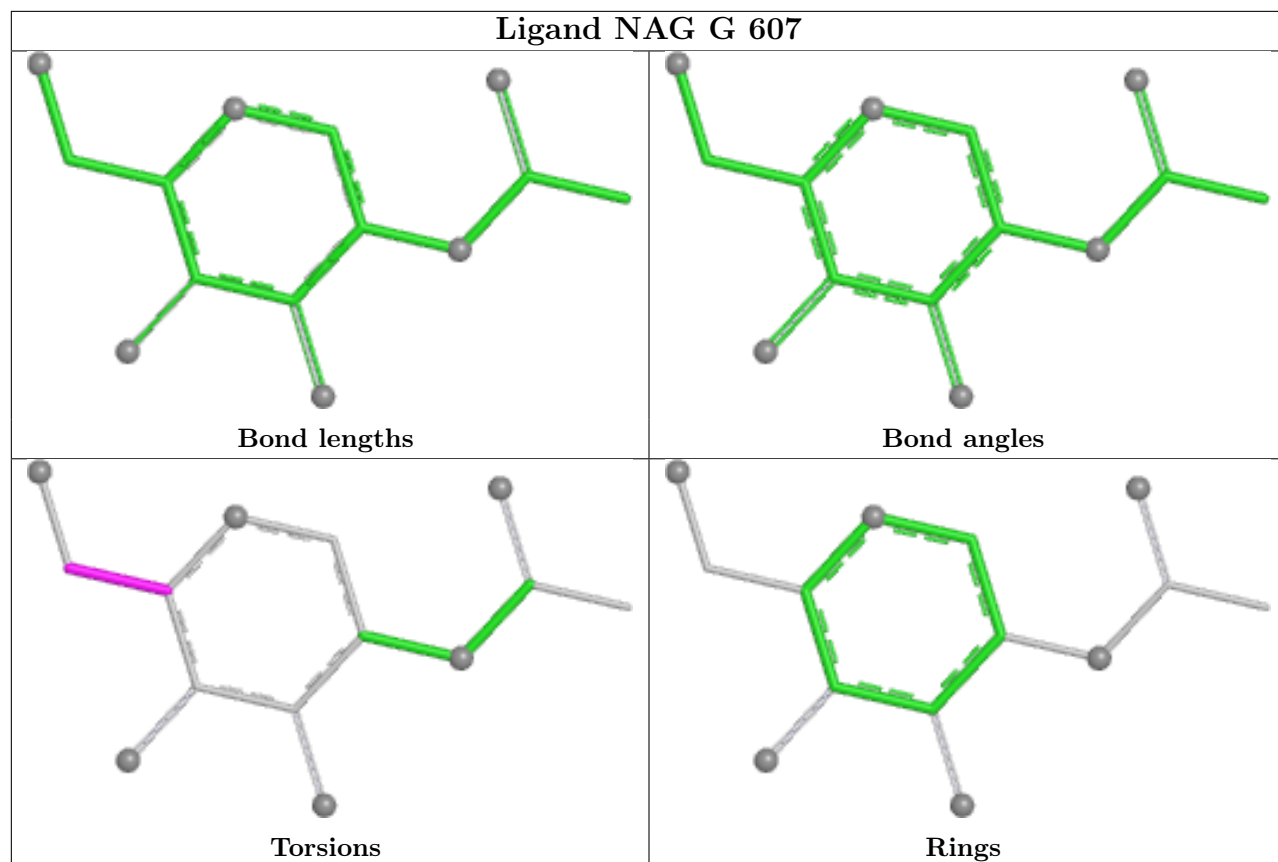
Ligand NAG M 602

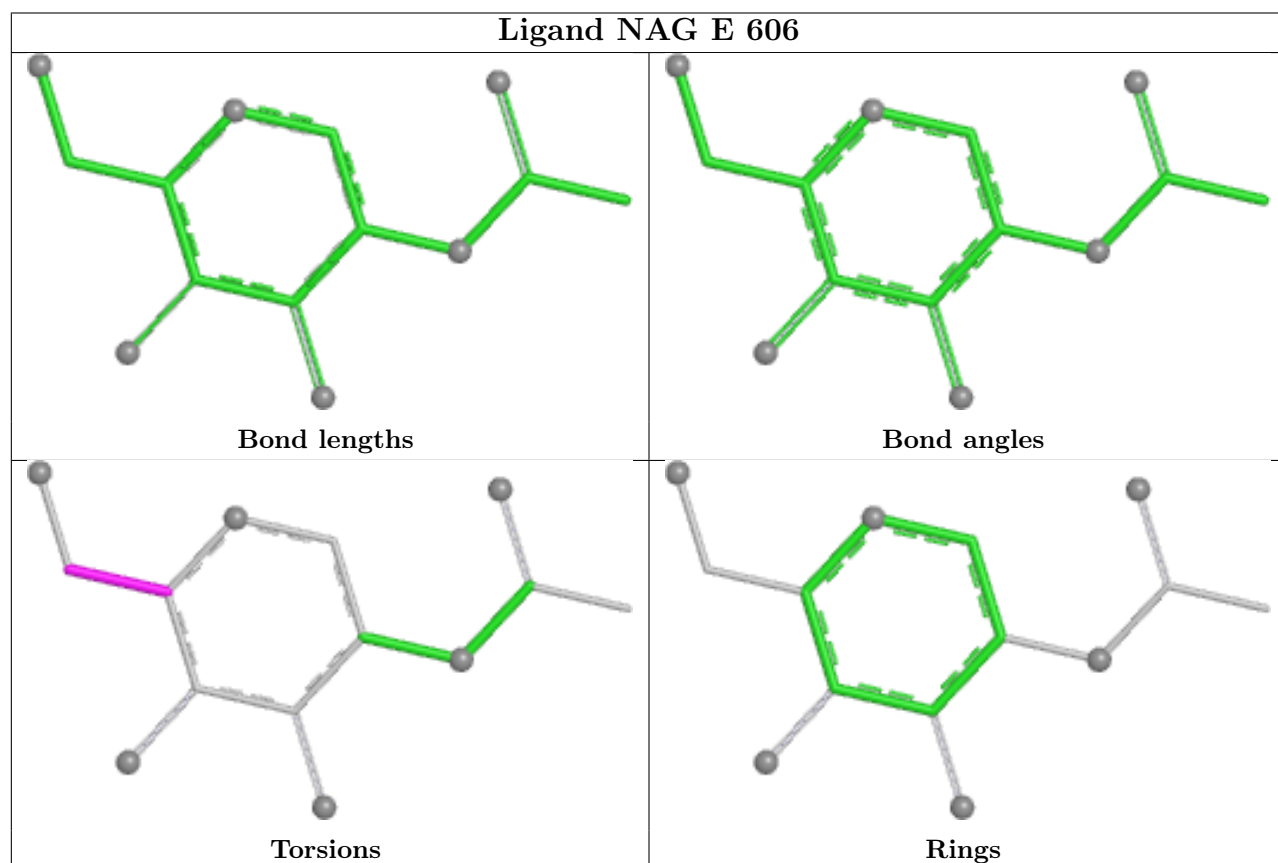
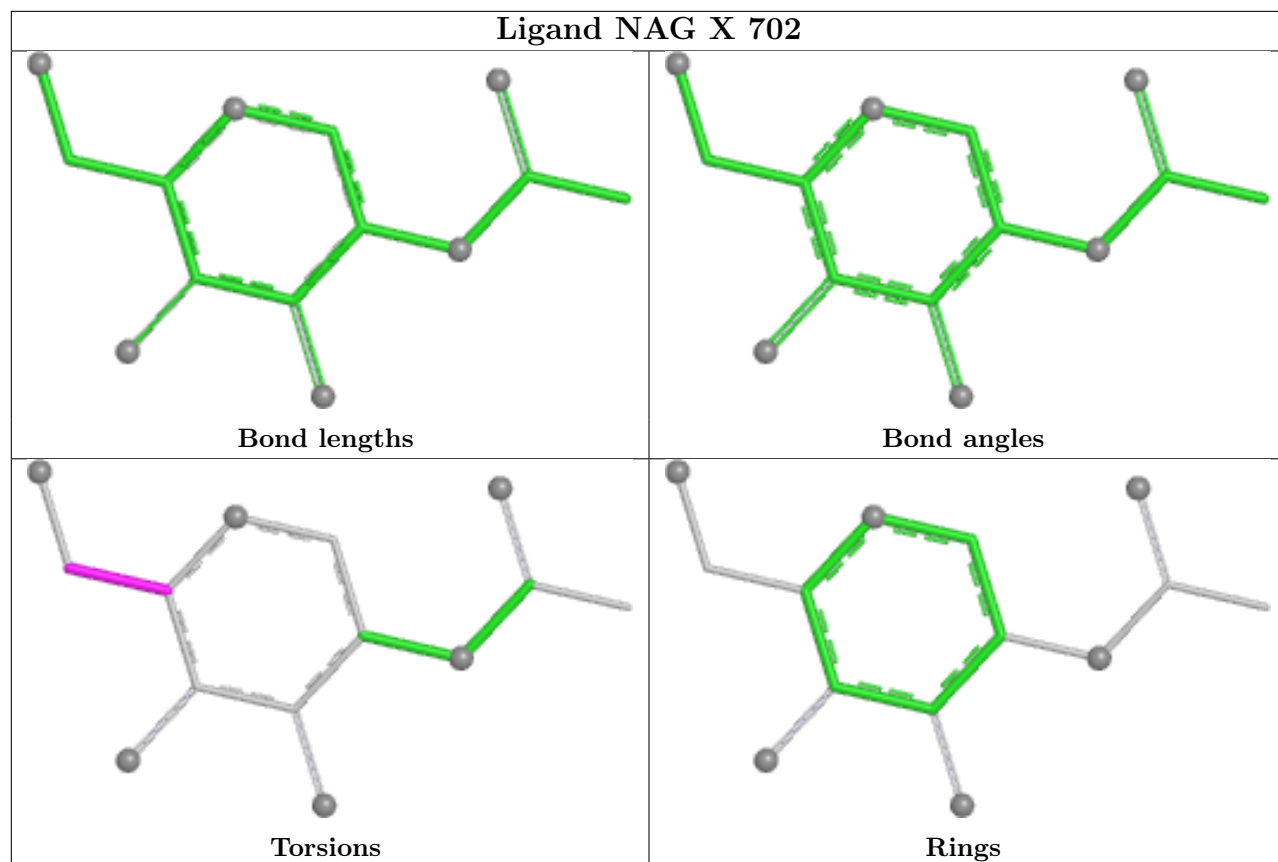


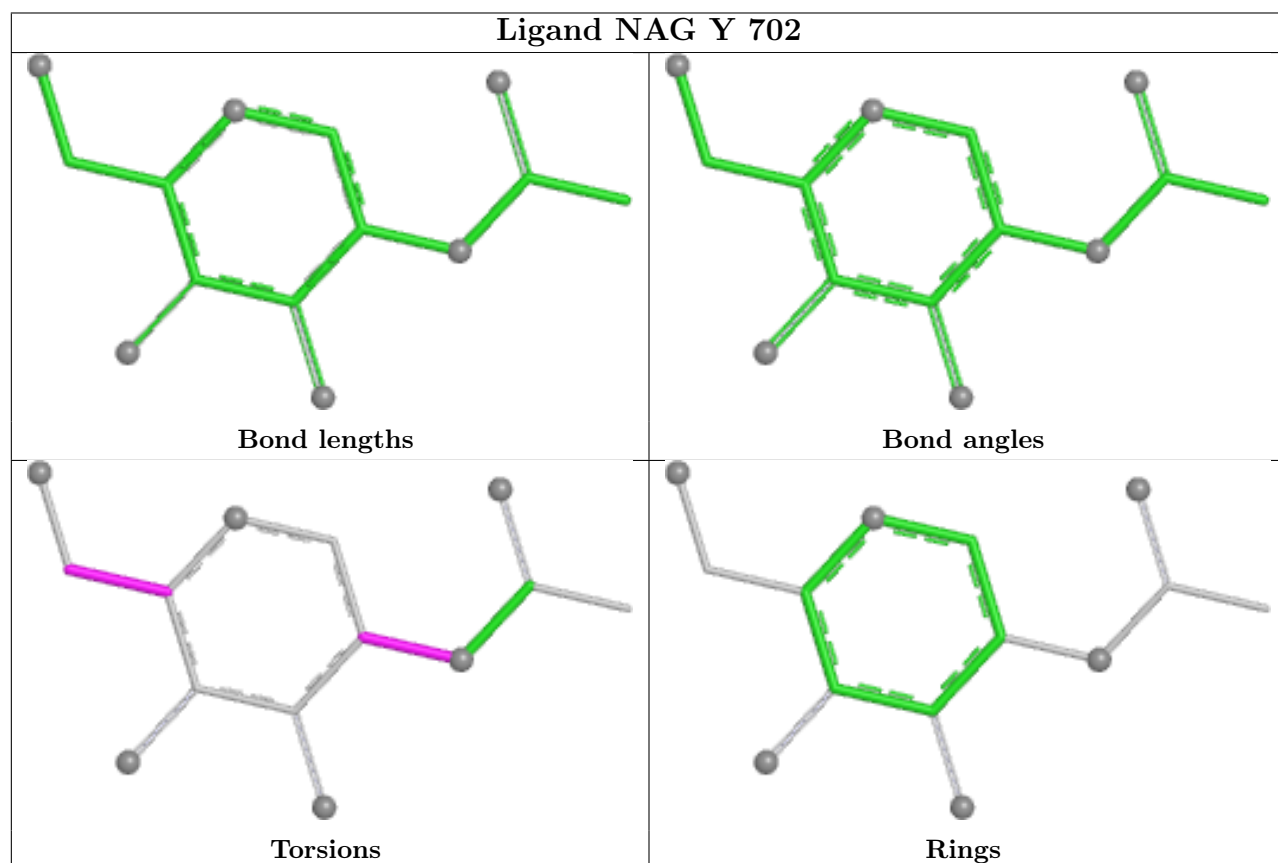
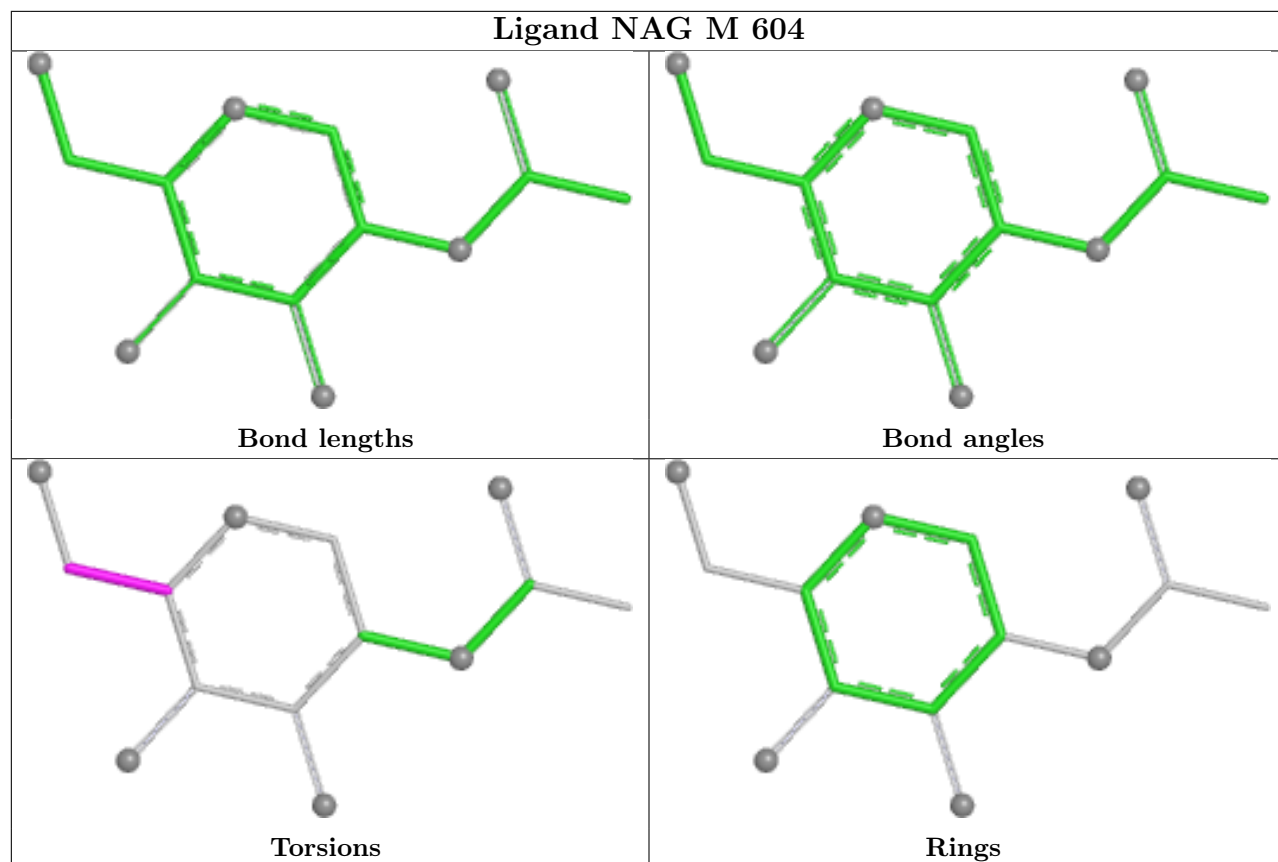
Ligand NAG E 603

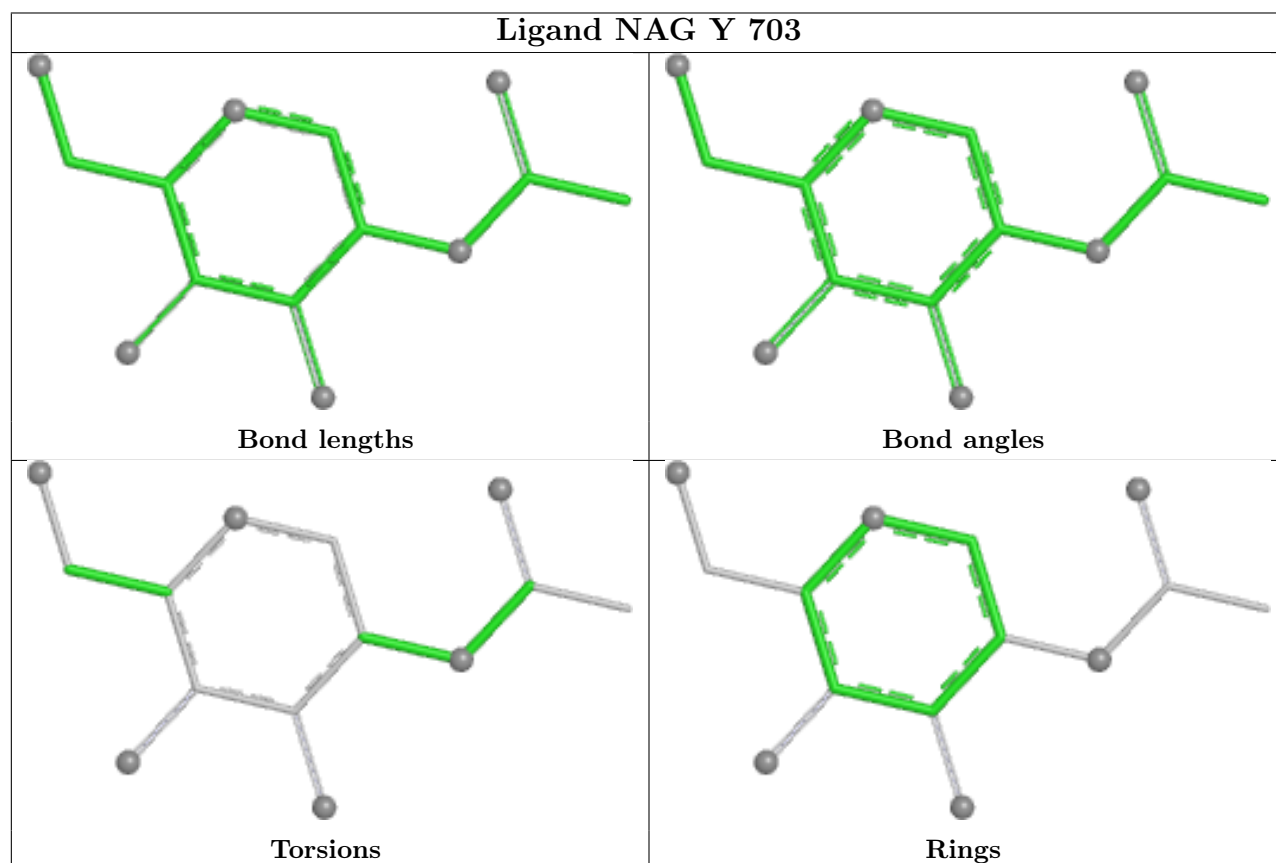
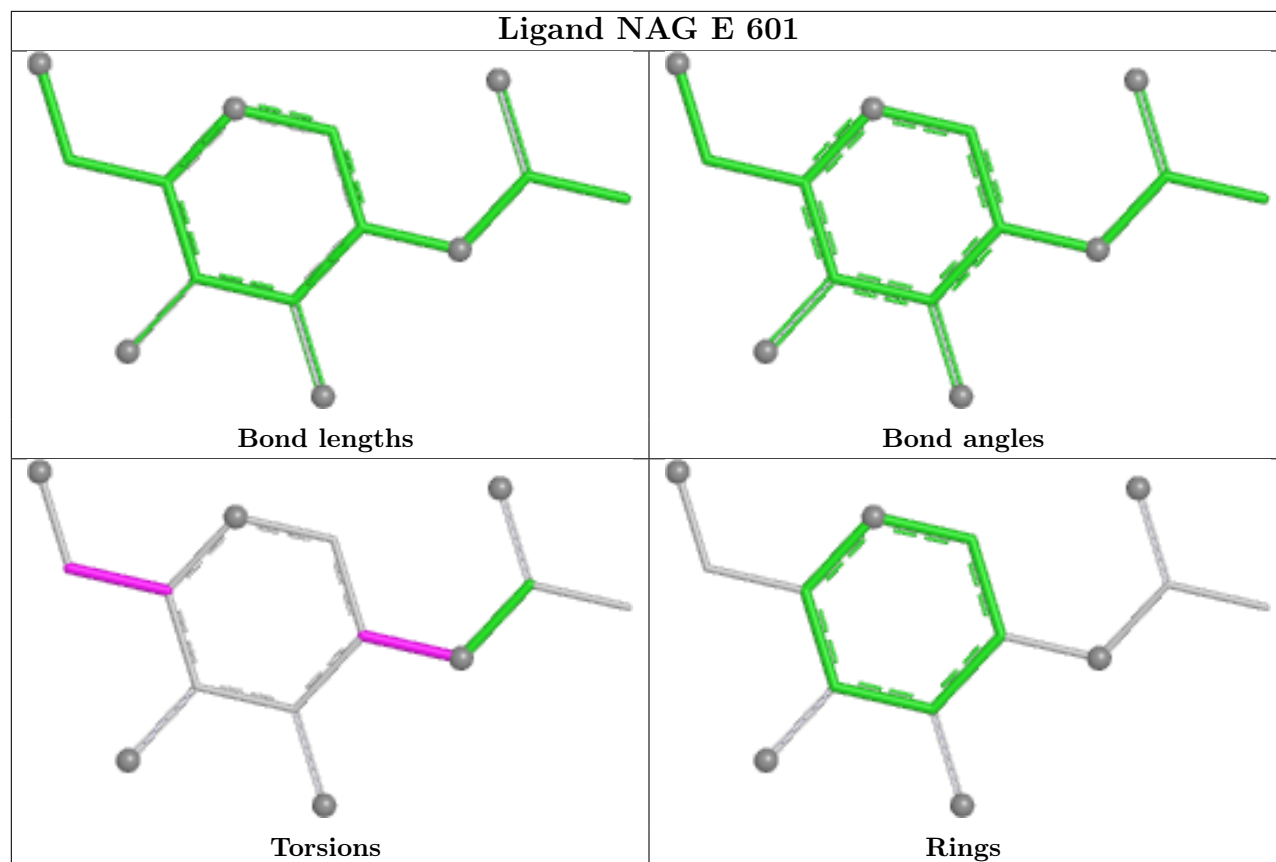


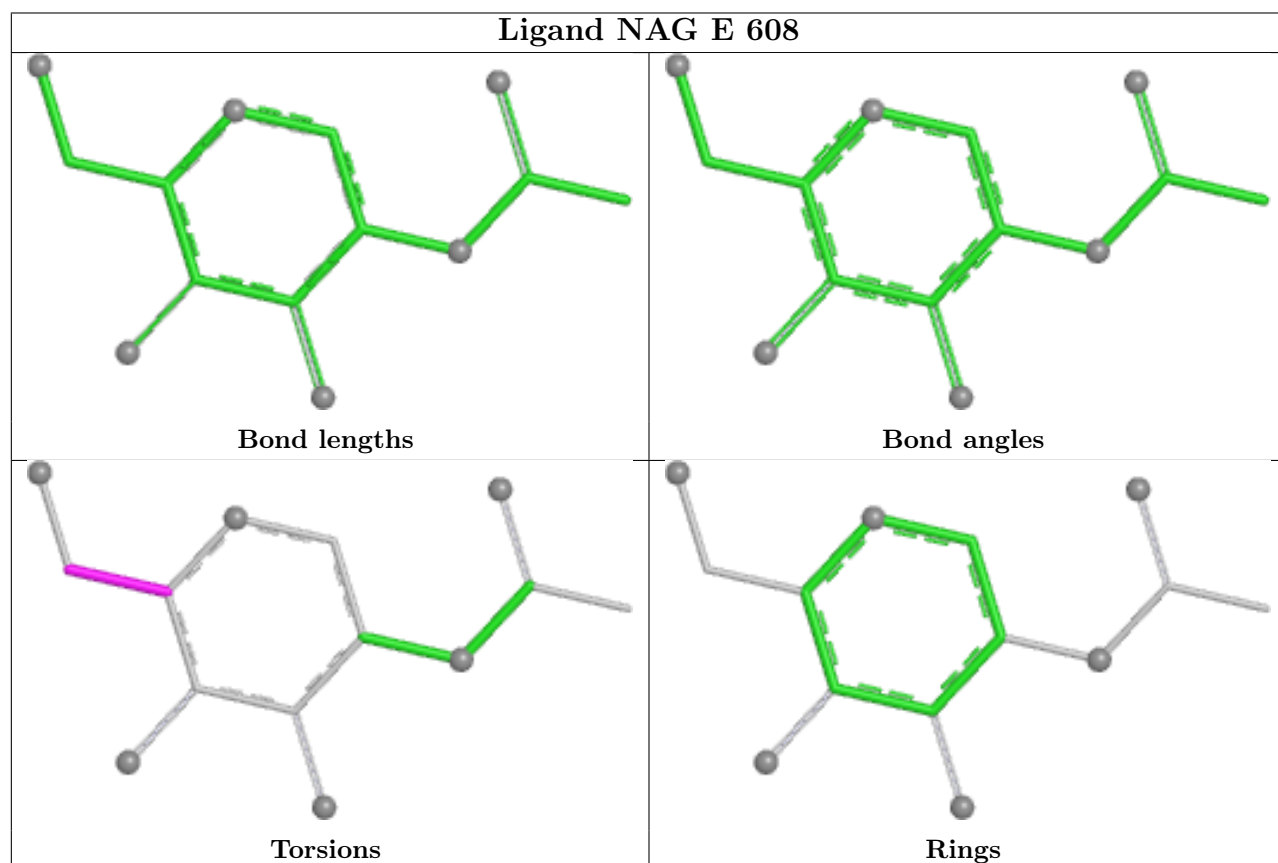
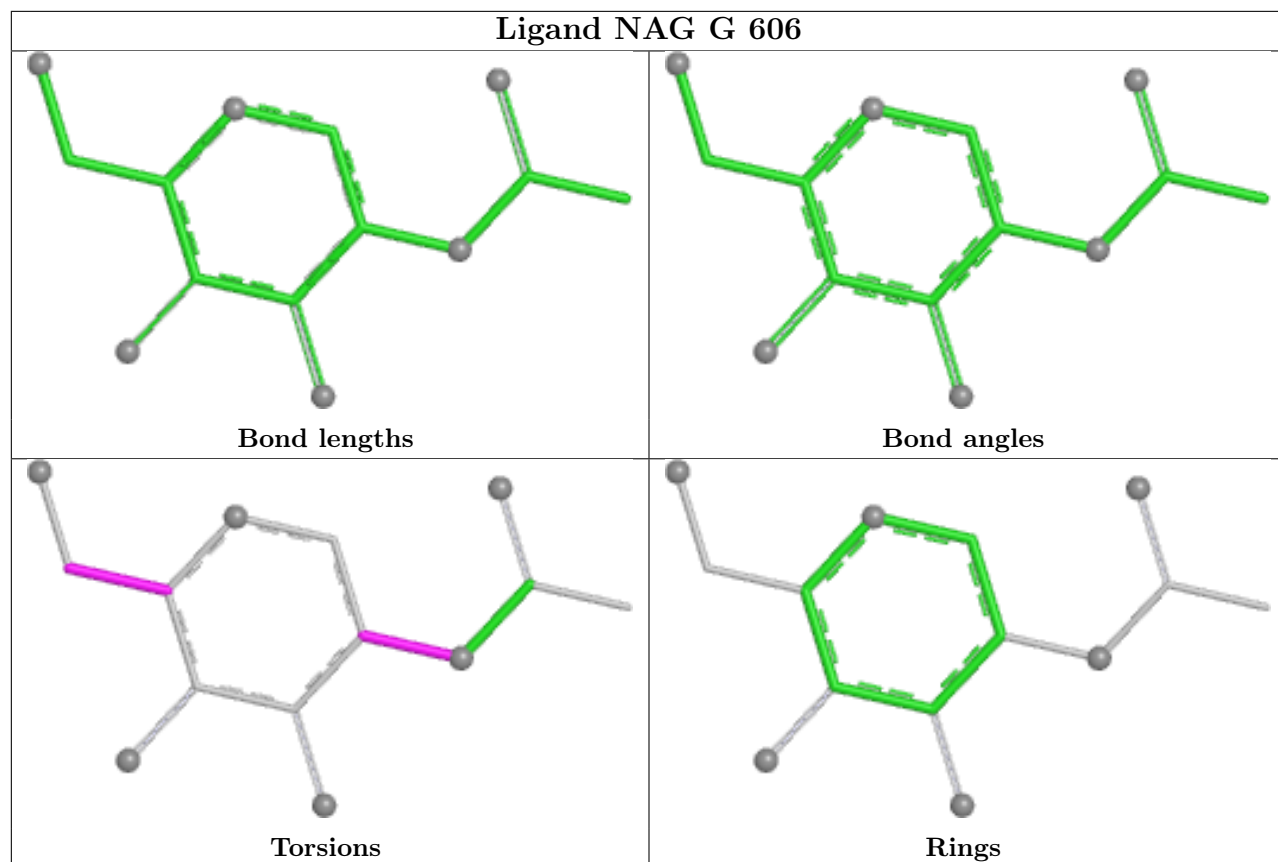




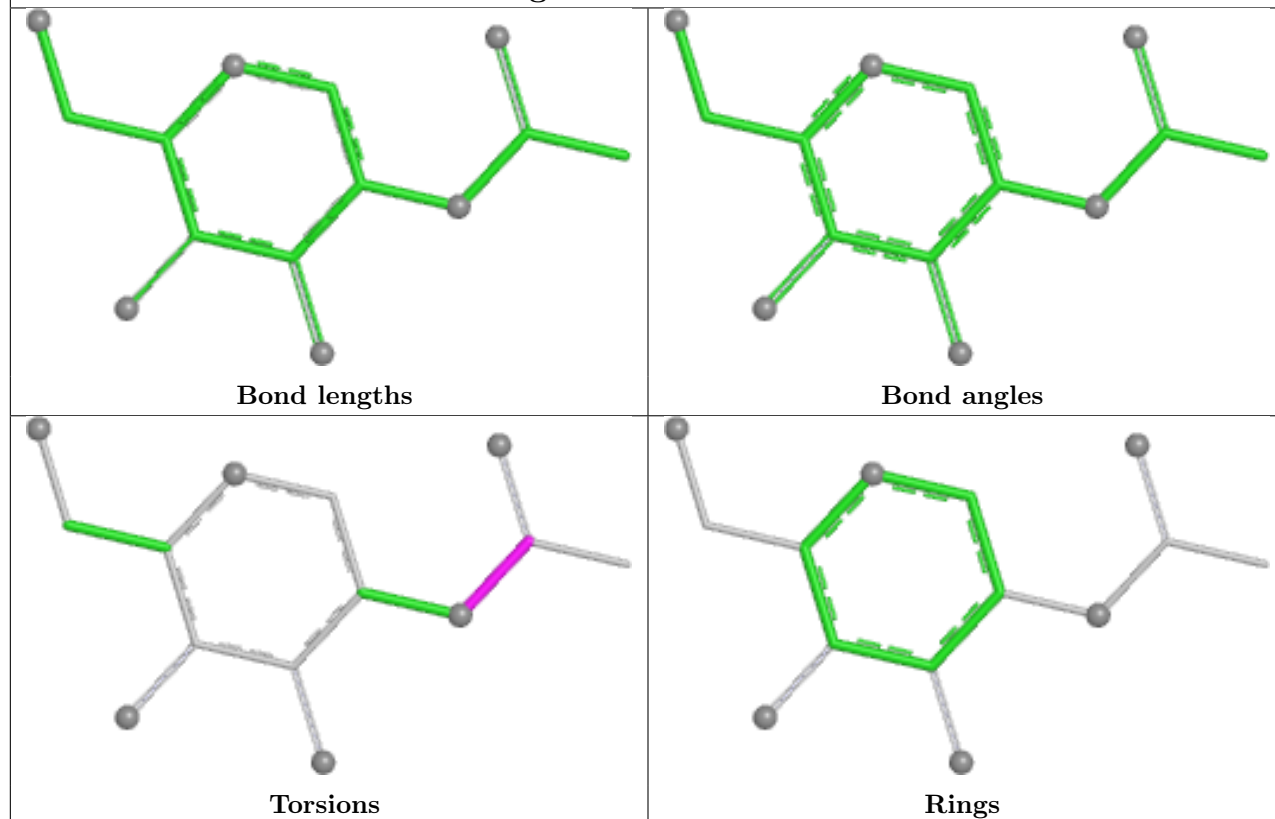




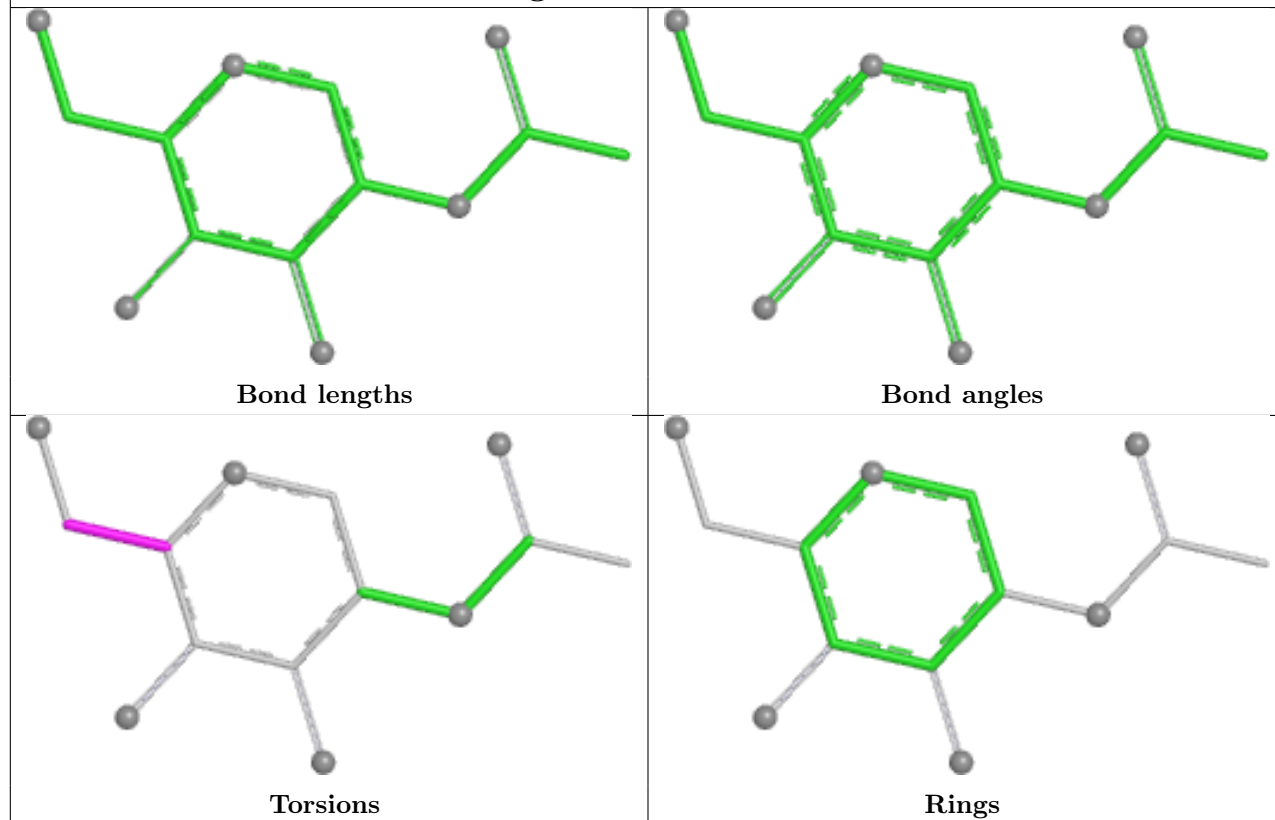


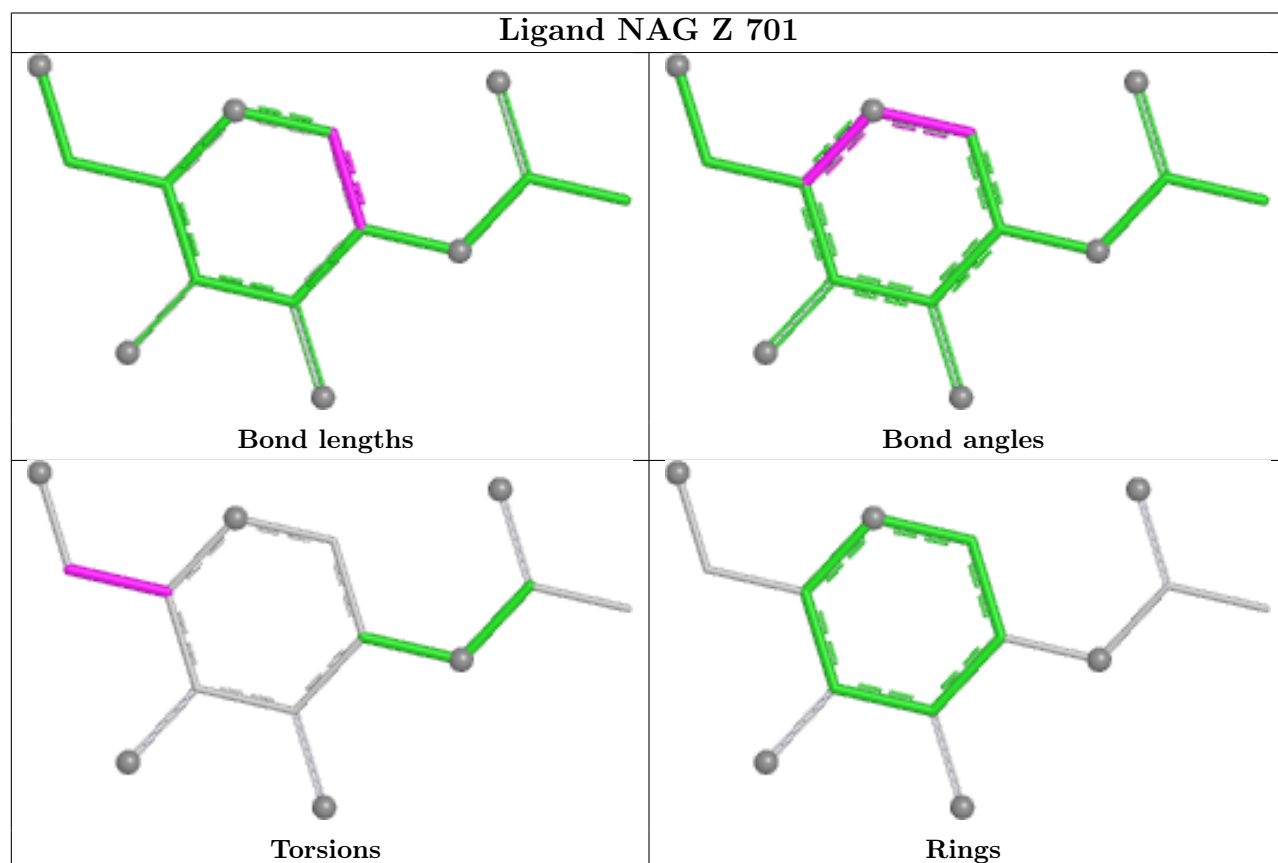
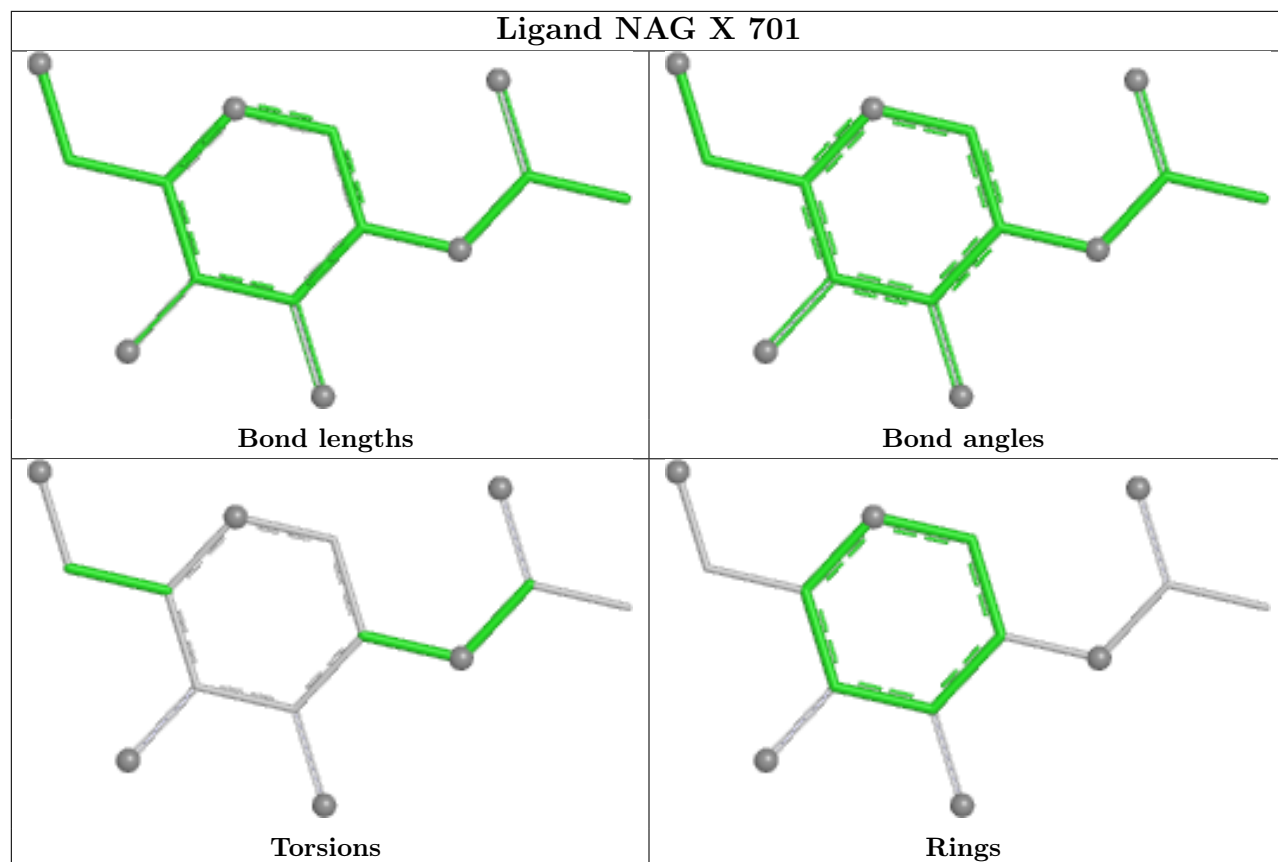


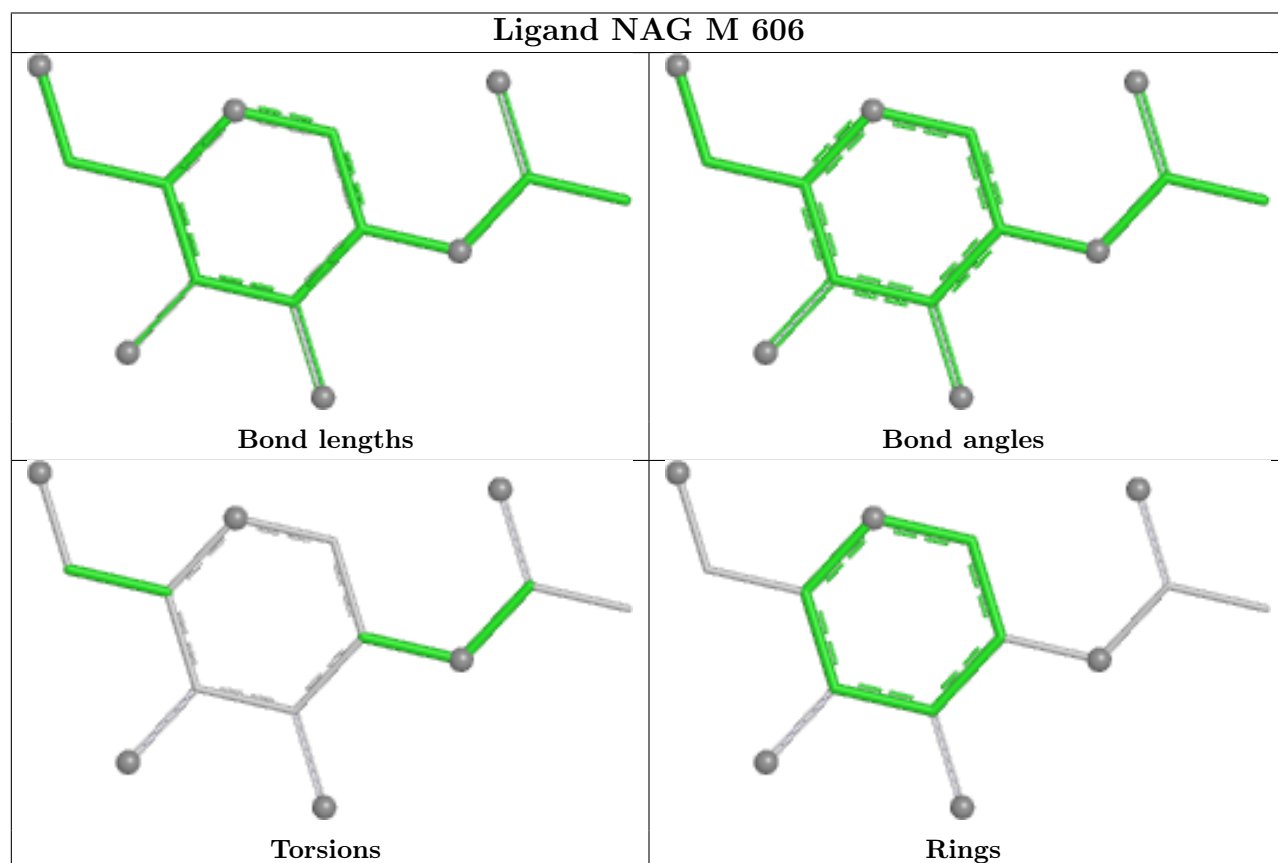
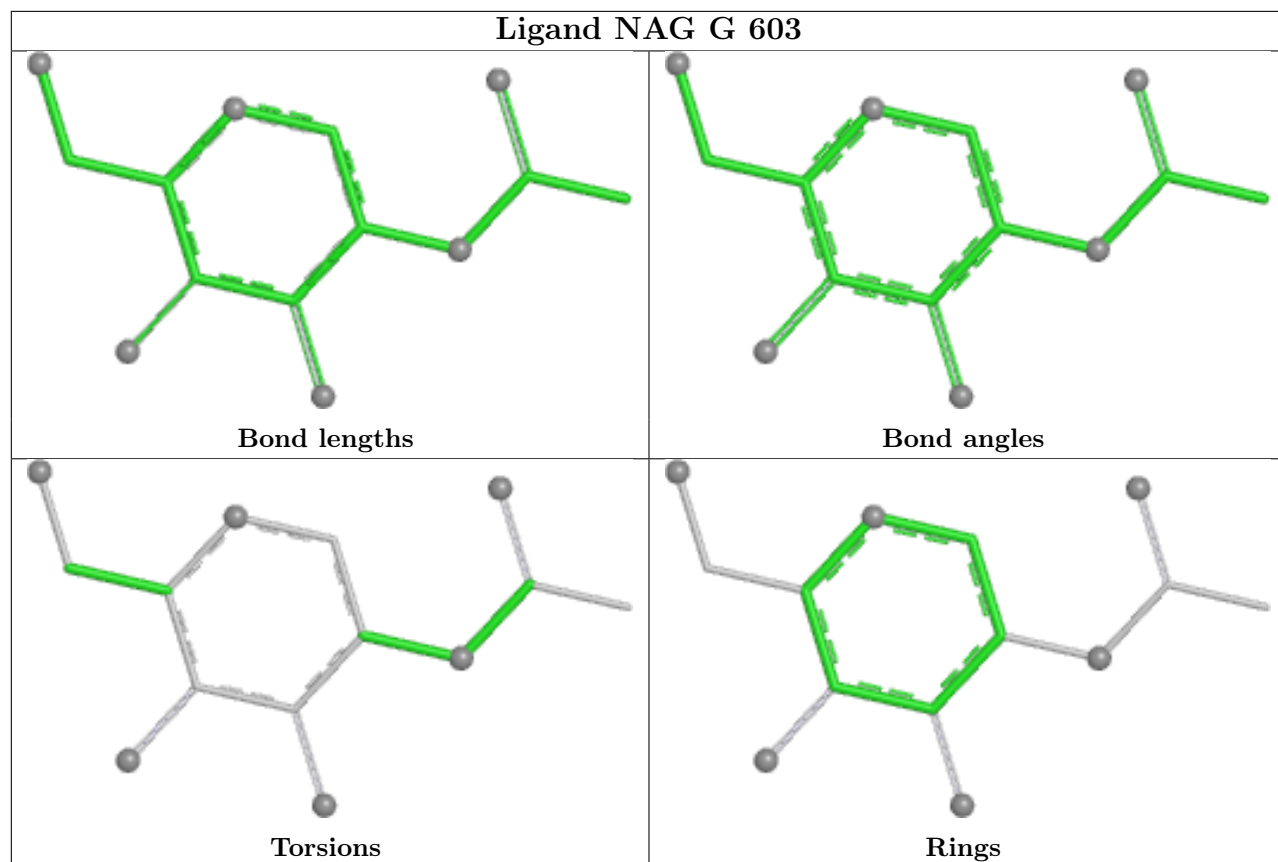
Ligand NAG Z 702



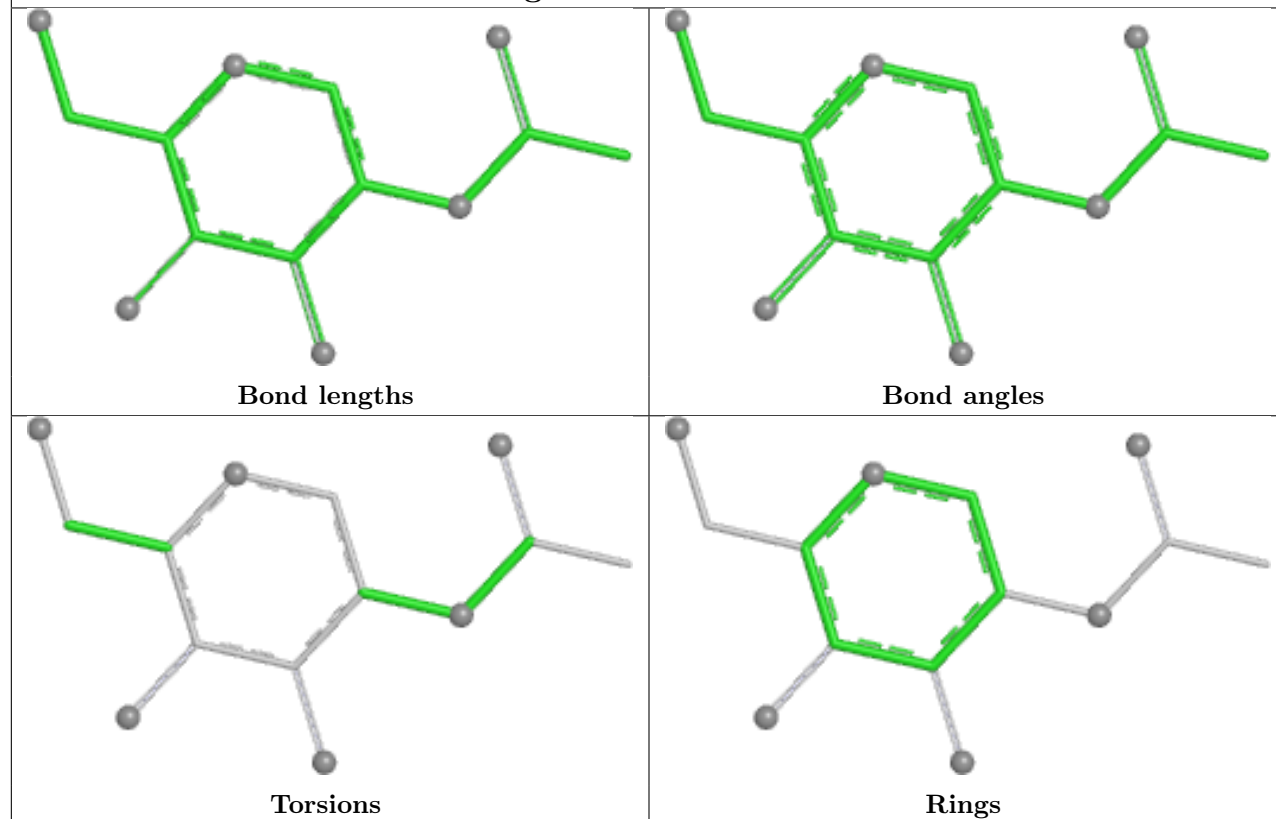
Ligand NAG E 604



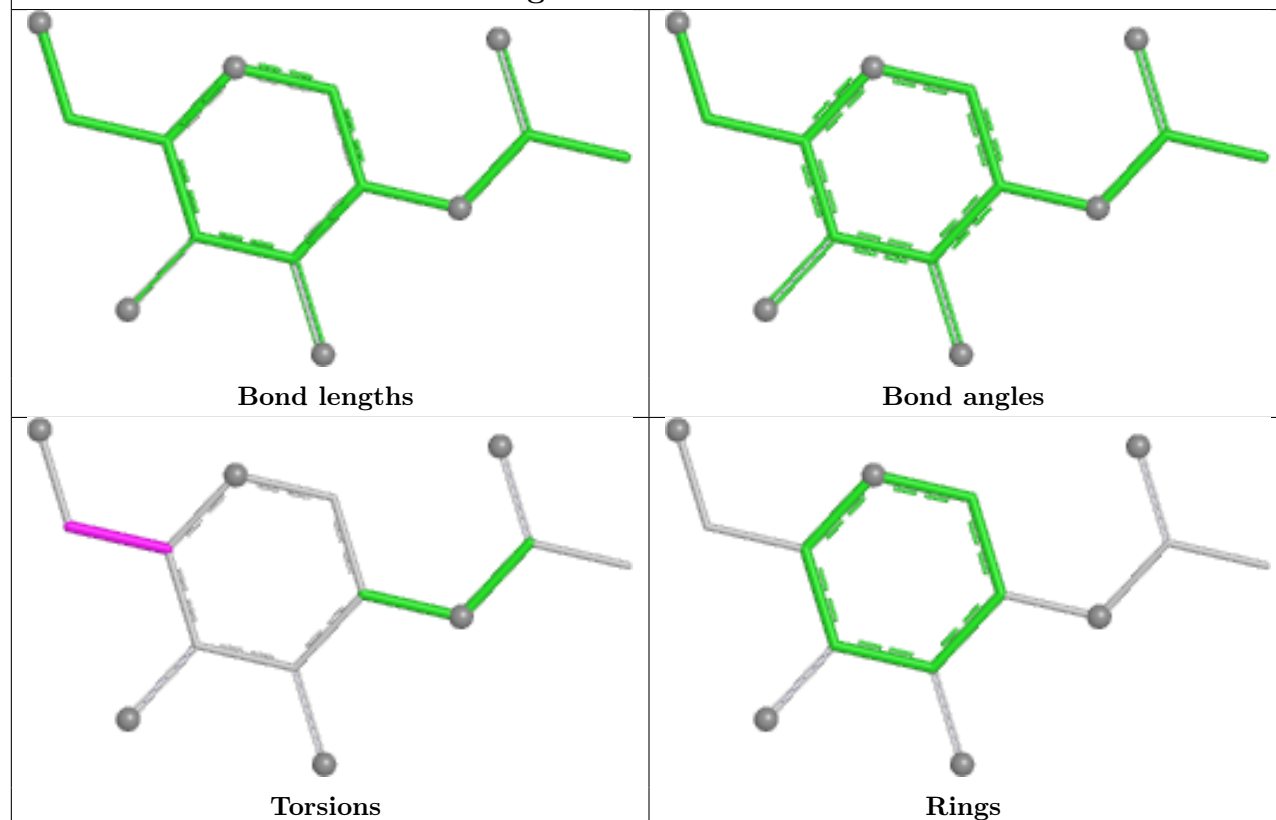


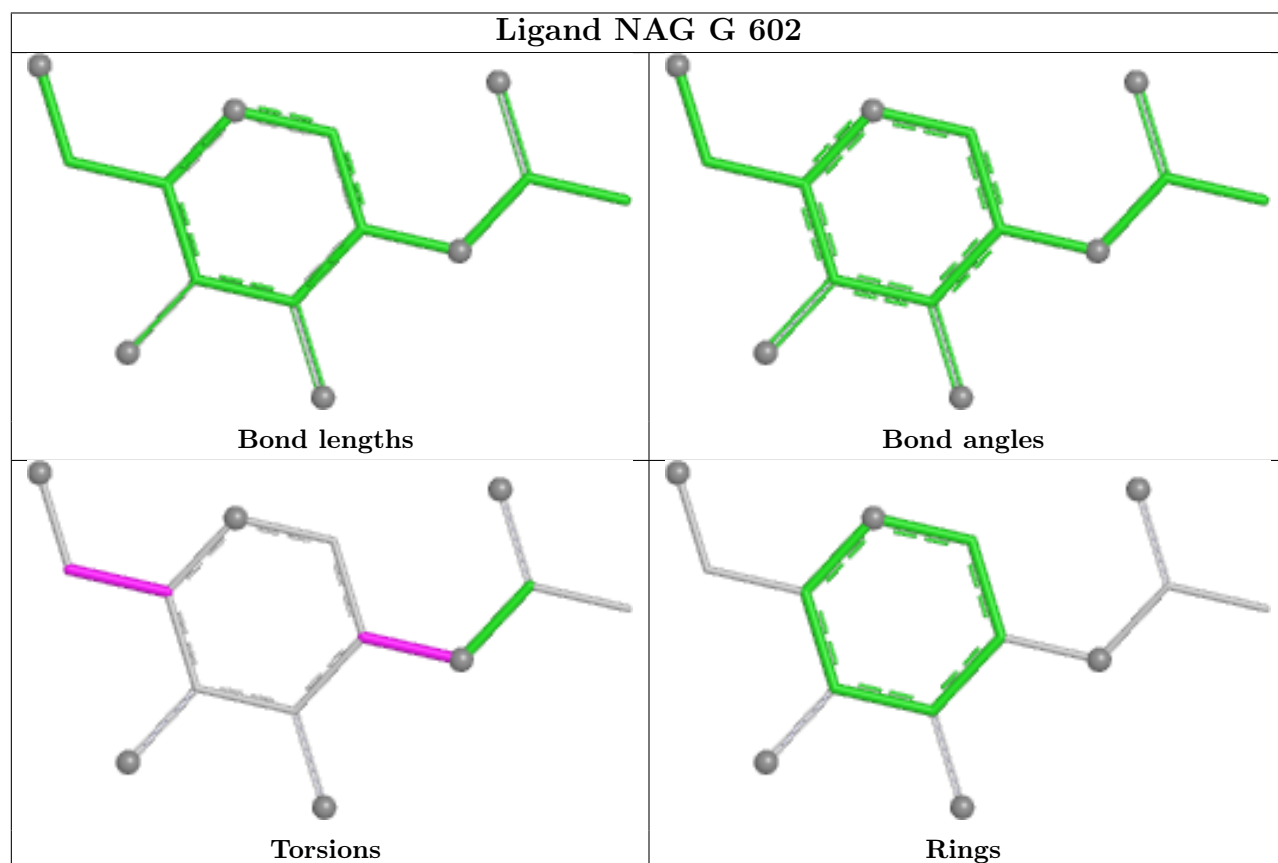
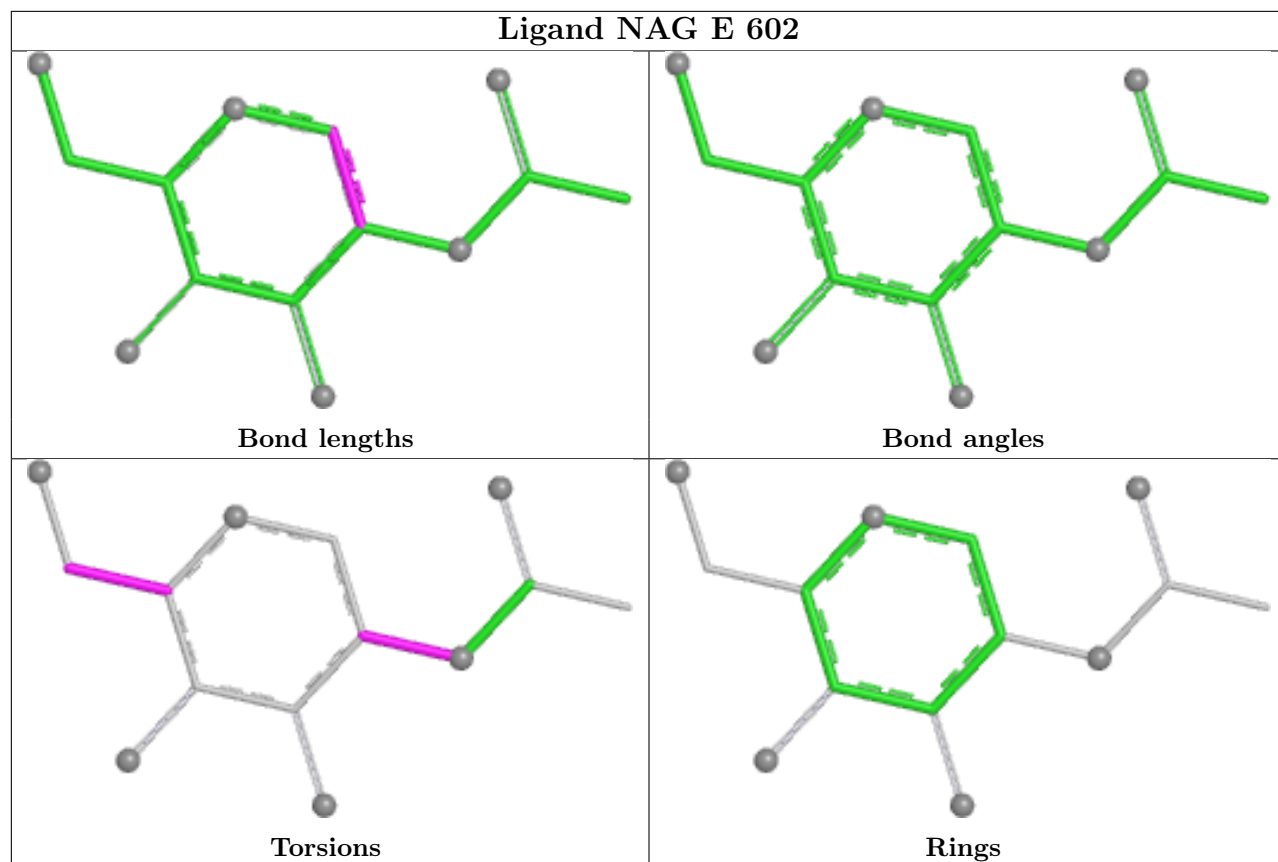


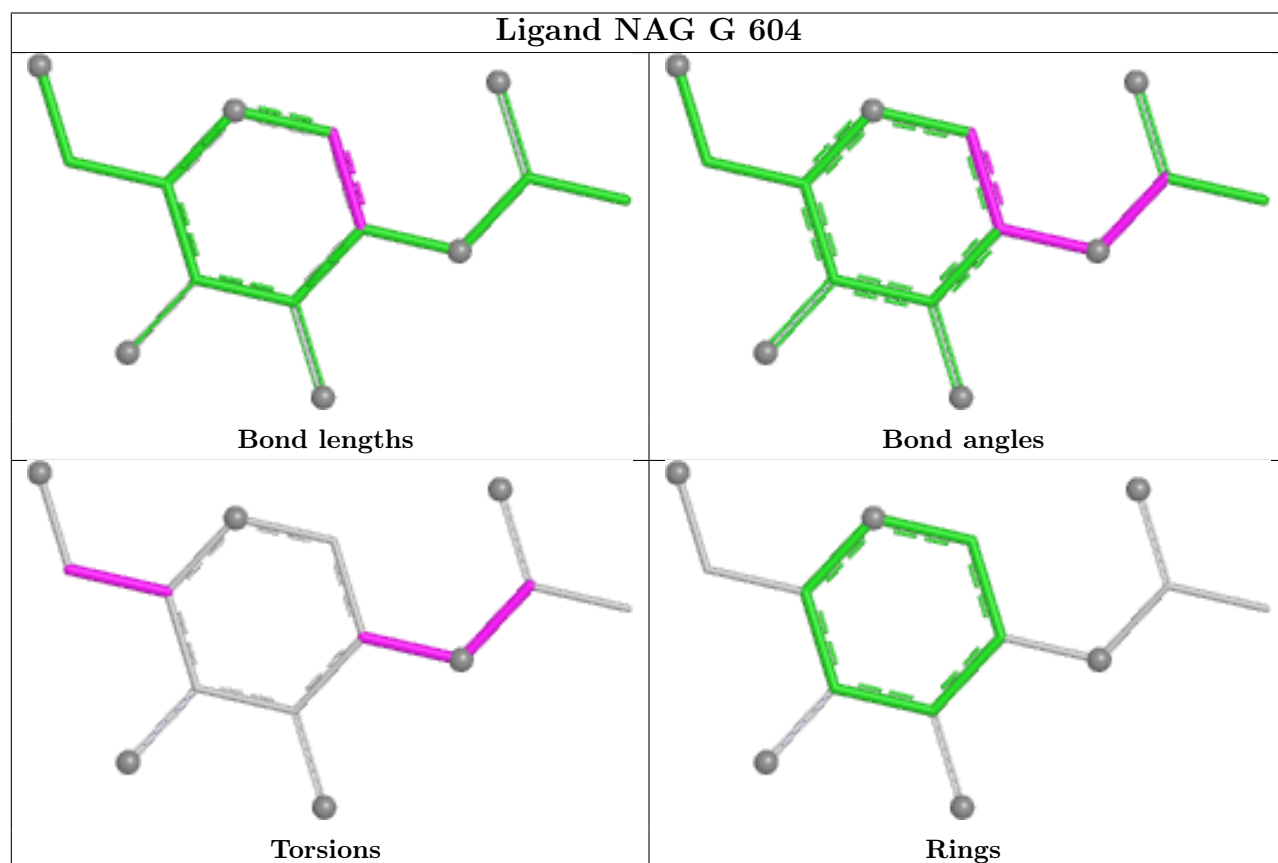
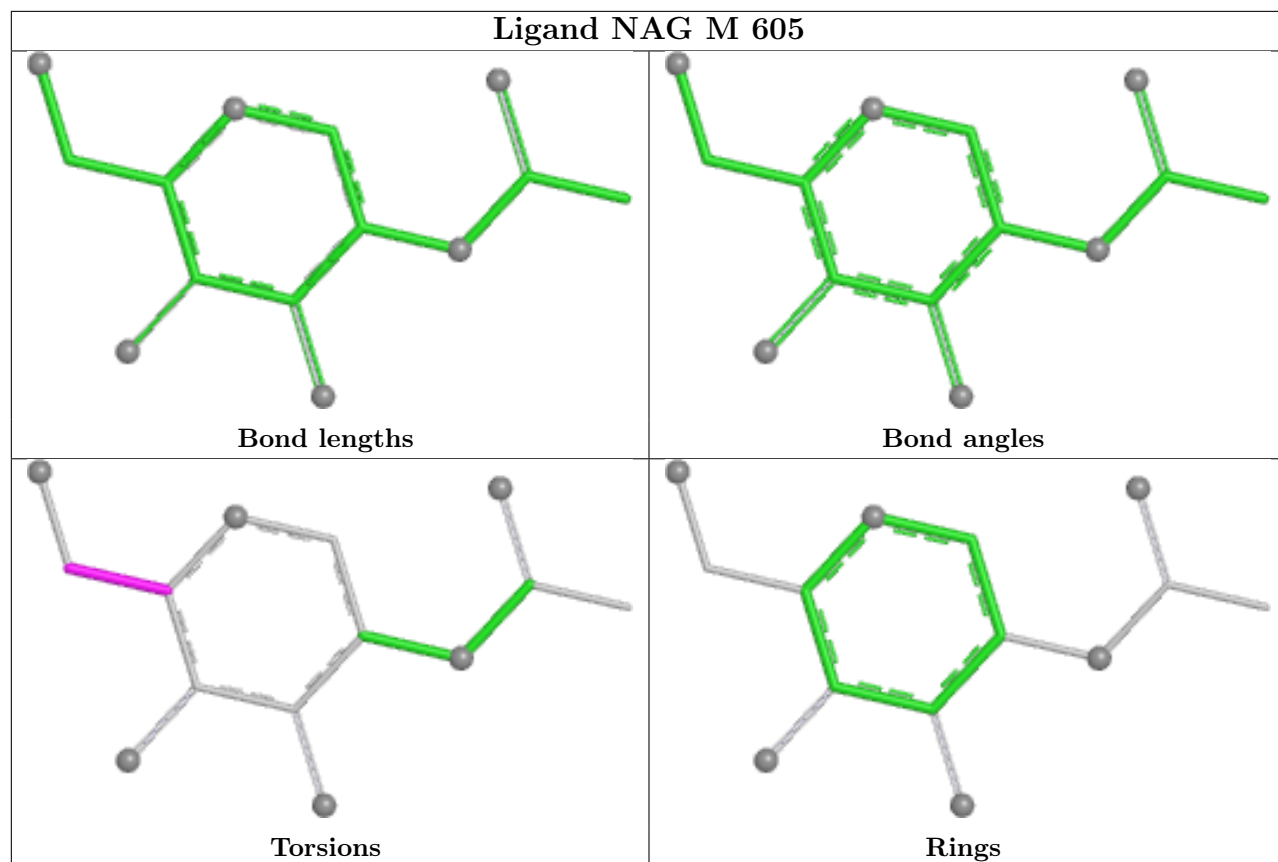
Ligand NAG M 603

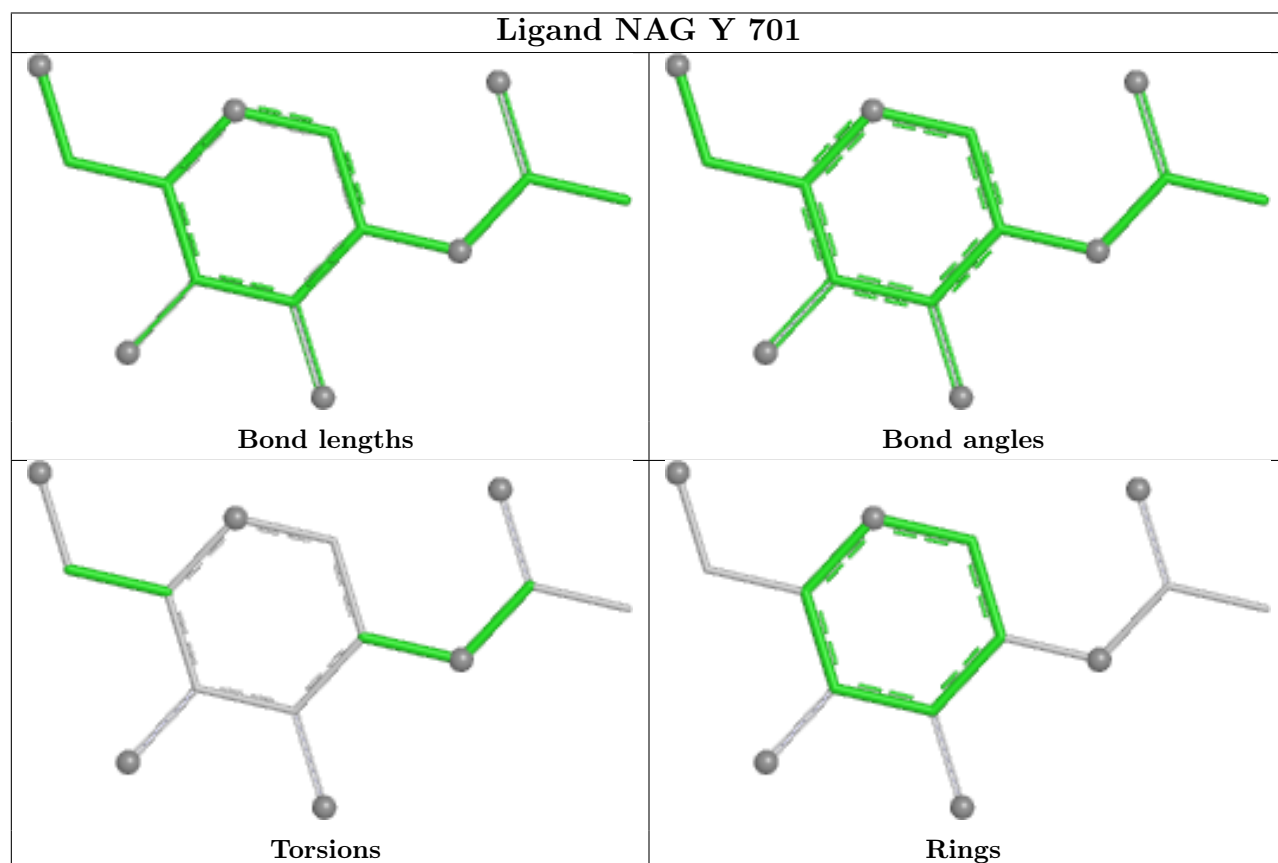
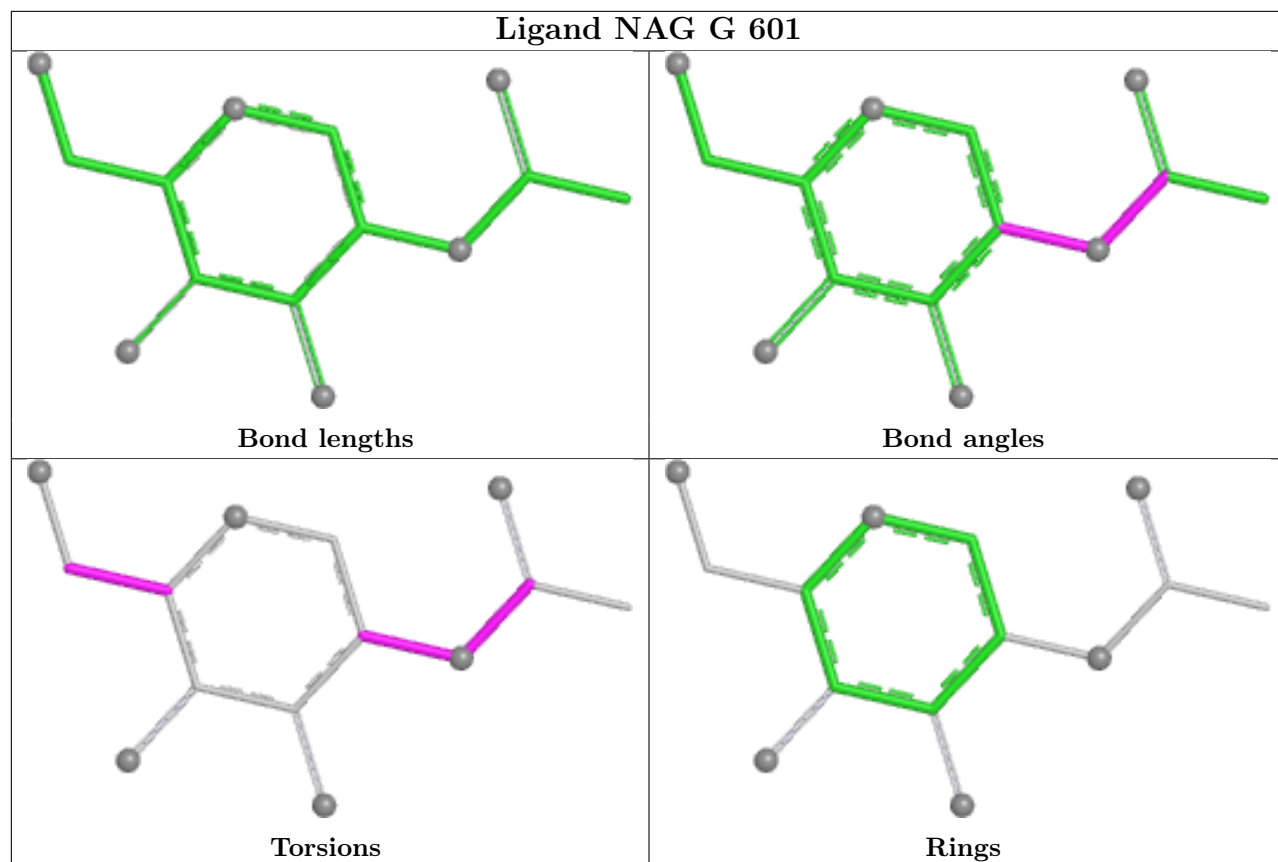


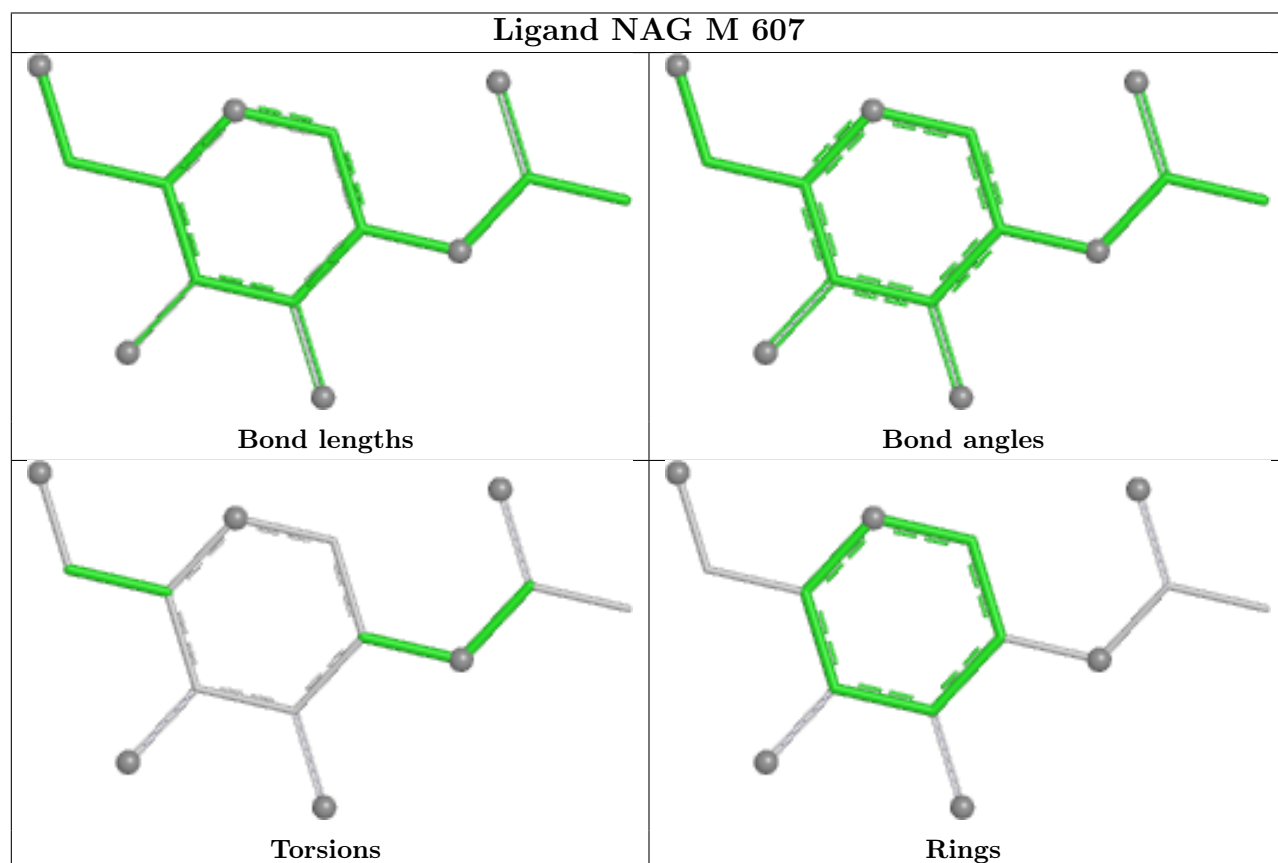
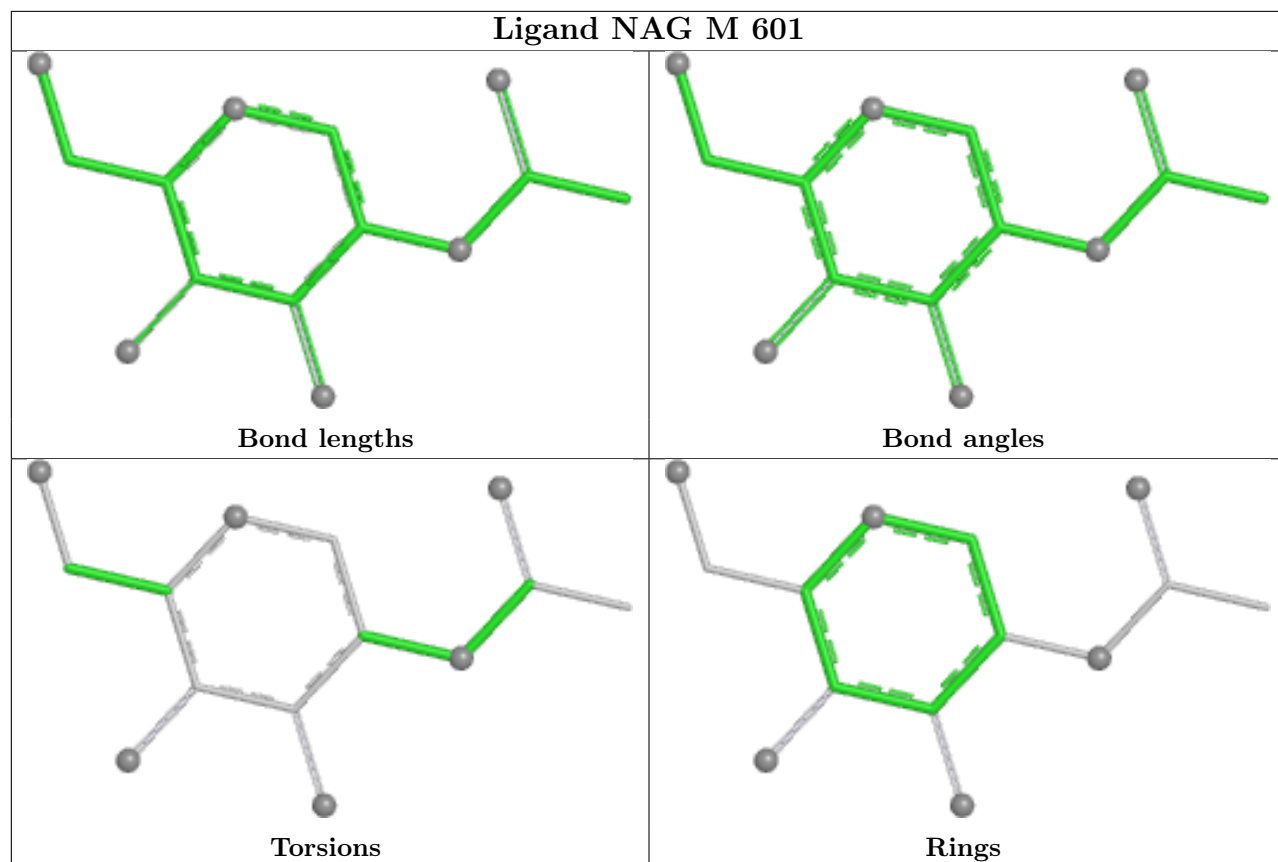
Ligand NAG G 605











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	F	222/225 (98%)	0.26	7 (3%) 50 35	79, 119, 185, 222	0
1	H	222/225 (98%)	0.13	5 (2%) 61 43	71, 103, 145, 208	0
1	N	222/225 (98%)	0.46	3 (1%) 73 52	83, 123, 252, 272	0
2	I	205/210 (97%)	0.53	13 (6%) 26 22	81, 137, 179, 217	0
3	L	204/210 (97%)	0.35	8 (3%) 43 31	81, 112, 144, 186	0
3	O	205/210 (97%)	0.49	13 (6%) 26 22	87, 173, 239, 254	0
4	A	210/214 (98%)	0.26	4 (1%) 66 46	76, 158, 224, 235	0
4	C	210/214 (98%)	0.23	3 (1%) 73 52	77, 127, 224, 227	0
4	J	210/214 (98%)	0.38	6 (2%) 53 37	81, 156, 192, 206	0
5	E	447/474 (94%)	0.37	17 (3%) 44 32	66, 95, 152, 181	0
5	G	449/474 (94%)	0.25	11 (2%) 59 42	53, 81, 140, 177	0
5	M	449/474 (94%)	0.26	15 (3%) 49 34	61, 92, 141, 195	0
6	B	226/236 (95%)	0.21	4 (1%) 67 47	70, 131, 203, 212	0
6	D	226/236 (95%)	0.43	6 (2%) 56 39	72, 122, 237, 252	0
6	K	226/236 (95%)	0.42	15 (6%) 24 21	78, 138, 195, 210	0
7	X	129/153 (84%)	0.28	4 (3%) 51 35	68, 112, 169, 194	0
7	Y	129/153 (84%)	0.25	2 (1%) 70 49	62, 90, 136, 166	0
7	Z	129/153 (84%)	0.35	4 (3%) 51 35	70, 116, 164, 193	0
All	All	4320/4536 (95%)	0.32	140 (3%) 50 35	53, 109, 217, 272	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	G	473	GLY	6.4
3	O	82	GLU	5.7
1	N	24	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
5	E	195	ASN	4.8
7	Z	566	LEU	4.4
6	K	202	PRO	4.2
1	H	225	CYS	4.0
7	Y	518	VAL	4.0
6	K	11	LEU	4.0
4	A	15	LEU	3.7
6	K	27	GLY	3.7
2	I	13	GLY	3.7
3	O	112	ALA	3.7
4	J	15	LEU	3.6
2	I	14	SER	3.6
6	K	100(G)	PHE	3.5
5	E	473	GLY	3.5
1	F	150	LEU	3.5
1	F	225	CYS	3.5
1	N	159	VAL	3.4
5	M	186	GLU	3.4
5	M	341	THR	3.3
5	M	326	ILE	3.3
3	L	32	TYR	3.3
5	M	195	ASN	3.2
5	M	153	GLU	3.2
5	G	196	CYS	3.2
6	B	100(N)	TYR	3.2
5	E	333	VAL	3.2
5	M	73	ALA	3.2
6	D	150	VAL	3.2
7	Z	565	LEU	3.1
5	E	423	ILE	3.1
2	I	142	PRO	3.1
5	E	186(A)	ASN	3.0
5	M	186(A)	ASN	3.0
3	O	62	PHE	2.9
2	I	3	ALA	2.9
2	I	21	ILE	2.9
6	K	167	PRO	2.9
1	H	98	ARG	2.9
2	I	105	PHE	2.9
6	D	213	PRO	2.9
1	H	178	VAL	2.8
5	M	505	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
6	K	9	PRO	2.8
3	O	2	SER	2.8
4	J	107	SER	2.8
5	M	185	ASN	2.8
5	E	72	HIS	2.8
5	M	72	HIS	2.8
1	F	151	VAL	2.8
7	X	538	THR	2.8
4	J	75	ILE	2.7
4	J	119	PRO	2.7
7	Y	650	GLN	2.7
3	O	110	PRO	2.7
5	E	179	LEU	2.7
5	E	138	ILE	2.7
6	B	125	ALA	2.7
5	G	315	GLN	2.6
6	D	126	PRO	2.6
6	K	26	GLY	2.6
2	I	32	TYR	2.6
3	O	86	TYR	2.6
4	A	30	SER	2.6
5	E	68	VAL	2.6
6	K	2	VAL	2.6
3	O	159	GLY	2.6
1	H	224	SER	2.5
3	O	73	LEU	2.5
3	O	120	PRO	2.5
5	G	261	LEU	2.5
6	B	28	SER	2.5
3	L	212	CYS	2.5
4	J	133	VAL	2.5
7	X	567	LYS	2.5
6	K	12	VAL	2.5
6	D	149	PRO	2.4
4	C	62	PHE	2.4
7	Z	518	VAL	2.4
2	I	146	THR	2.4
6	K	213	PRO	2.4
5	E	73	ALA	2.4
5	G	72	HIS	2.4
7	Z	567	LYS	2.4
3	L	98	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
5	M	427	TRP	2.3
6	K	8	GLY	2.3
5	G	349	LEU	2.3
6	K	55	GLU	2.3
6	K	95	ALA	2.3
3	L	186	TRP	2.3
5	G	449	ILE	2.3
6	D	2	VAL	2.3
5	E	139	THR	2.3
3	L	3	ALA	2.3
3	L	71	ALA	2.3
1	F	137	SER	2.3
1	H	37	VAL	2.3
5	E	454	LEU	2.2
3	O	35	TRP	2.2
5	M	281	ALA	2.2
5	G	384	TYR	2.2
5	M	473	GLY	2.2
1	F	118	VAL	2.2
6	K	110	THR	2.2
2	I	186	TRP	2.2
4	A	19	ALA	2.2
1	F	88	SER	2.2
7	X	568	LEU	2.2
5	M	460	SER	2.2
3	L	106	VAL	2.2
3	O	113	ALA	2.1
6	B	25	SER	2.1
6	D	180	SER	2.1
4	A	67	PHE	2.1
3	L	27	SER	2.1
5	E	232	LYS	2.1
3	O	37	GLN	2.1
5	E	66	HIS	2.1
5	E	202	THR	2.1
4	J	157	ALA	2.1
3	O	21	ILE	2.1
5	E	115	SER	2.1
2	I	11	VAL	2.1
7	X	518	VAL	2.1
1	N	187	LEU	2.1
5	E	140	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	31	ASN	2.1
5	M	187	GLN	2.1
4	C	5	TYR	2.0
5	G	427	TRP	2.0
5	G	461	THR	2.0
1	F	149	CYS	2.0
2	I	88	CYS	2.0
2	I	207	VAL	2.0
5	G	38	VAL	2.0
6	K	126	PRO	2.0
4	C	131	THR	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	P	1	14/15	-	-	104,104,104,104	0
8	NAG	P	2	14/15	-	-	127,127,127,127	0
8	BMA	P	3	11/12	-	-	129,129,129,129	0
9	NAG	W	2	14/15	0.27	0.14	114,114,114,114	0
9	NAG	T	2	14/15	0.31	0.13	157,157,157,157	0
9	NAG	V	2	14/15	0.59	0.10	118,118,118,118	0
8	NAG	c	1	14/15	-	-	115,115,115,115	0
8	NAG	c	2	14/15	-	-	144,144,144,144	0
8	BMA	c	3	11/12	-	-	161,161,161,161	0
8	NAG	e	1	14/15	-	-	103,103,103,103	0
8	NAG	e	2	14/15	-	-	114,114,114,114	0
8	BMA	e	3	11/12	-	-	116,116,116,116	0
9	NAG	Q	1	14/15	-	-	109,109,109,109	0
9	NAG	Q	2	14/15	-	-	134,134,134,134	0
9	NAG	W	1	14/15	0.70	0.14	104,104,104,104	0
9	NAG	S	2	14/15	0.78	0.11	106,106,106,106	0
8	NAG	U	2	14/15	0.82	0.12	116,116,116,116	0

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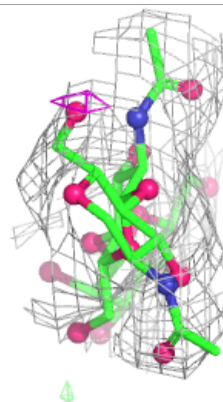
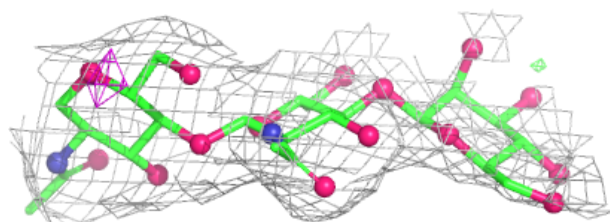
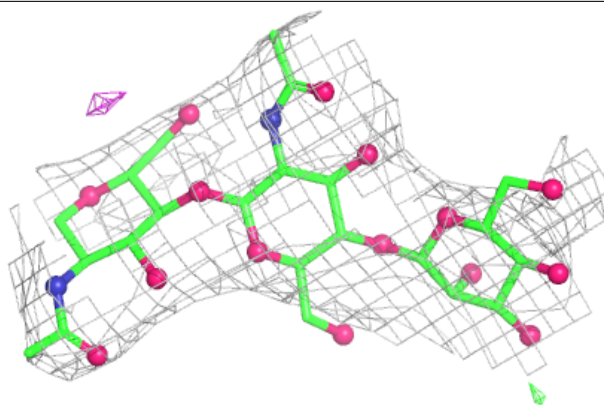
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	U	1	14/15	0.85	0.14	91,91,91,91	0
8	BMA	U	3	11/12	0.86	0.10	113,113,113,113	0
9	NAG	T	1	14/15	0.86	0.09	139,139,139,139	0
9	NAG	S	1	14/15	0.89	0.10	100,100,100,100	0
9	NAG	V	1	14/15	0.90	0.07	102,102,102,102	0
9	NAG	b	1	14/15	-	-	91,91,91,91	0
9	NAG	b	2	14/15	-	-	110,110,110,110	0
9	NAG	d	1	14/15	-	-	111,111,111,111	0
9	NAG	d	2	14/15	-	-	121,121,121,121	0
9	NAG	f	1	14/15	-	-	112,112,112,112	0
9	NAG	f	2	14/15	-	-	131,131,131,131	0
9	NAG	i	1	14/15	-	-	111,111,111,111	0
9	NAG	i	2	14/15	-	-	123,123,123,123	0
10	NAG	R	1	14/15	-	-	95,95,95,95	0
10	NAG	R	2	14/15	-	-	94,94,94,94	0
10	BMA	R	3	11/12	-	-	94,94,94,94	0
10	MAN	R	4	11/12	-	-	90,90,90,90	0
10	MAN	R	5	11/12	-	-	84,84,84,84	0
10	MAN	R	6	11/12	-	-	90,90,90,90	0
10	MAN	R	7	11/12	-	-	111,111,111,111	0
11	NAG	a	1	14/15	-	-	78,78,78,78	0
11	NAG	a	2	14/15	-	-	77,77,77,77	0
11	NAG	a	3	14/15	-	-	88,88,88,88	0
11	MAN	a	4	11/12	-	-	86,86,86,86	0
11	MAN	a	5	11/12	-	-	90,90,90,90	0
11	MAN	a	6	11/12	-	-	88,88,88,88	0
11	MAN	a	7	11/12	-	-	87,87,87,87	0
11	MAN	a	8	11/12	-	-	95,95,95,95	0
11	MAN	a	9	11/12	-	-	103,103,103,103	0
12	NAG	g	1	14/15	-	-	97,97,97,97	0
12	NAG	g	2	14/15	-	-	95,95,95,95	0
12	BMA	g	3	11/12	-	-	100,100,100,100	0
12	MAN	g	4	11/12	-	-	120,120,120,120	0
12	MAN	g	5	11/12	-	-	123,123,123,123	0
12	MAN	g	6	11/12	-	-	109,109,109,109	0
13	MAN	h	1	11/12	-	-	96,96,96,96	0
13	MAN	h	2	11/12	-	-	99,99,99,99	0
13	MAN	h	3	11/12	-	-	107,107,107,107	0

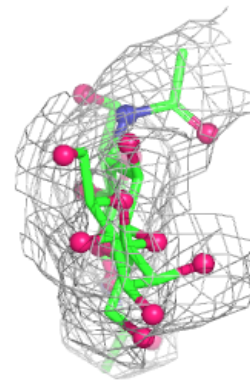
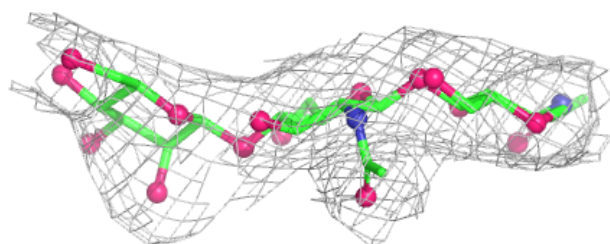
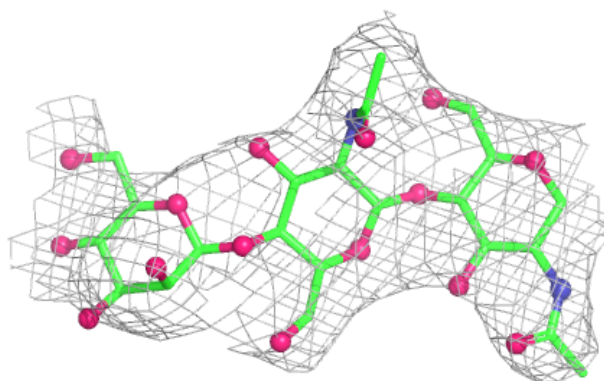
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain P:

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

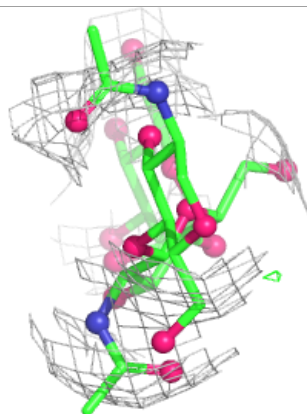
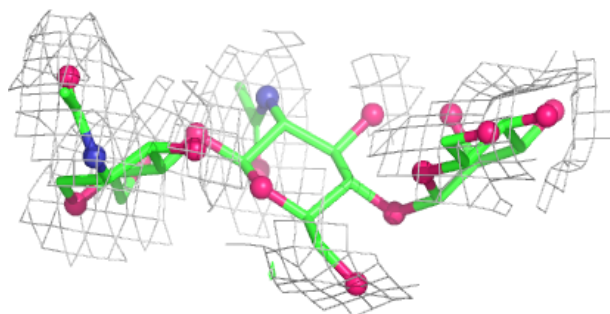
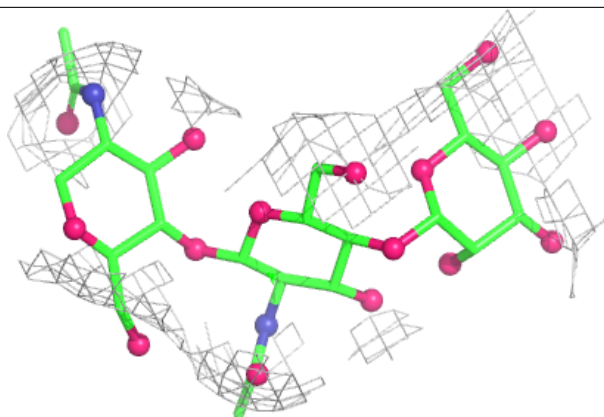
**Electron density around Chain U:**

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

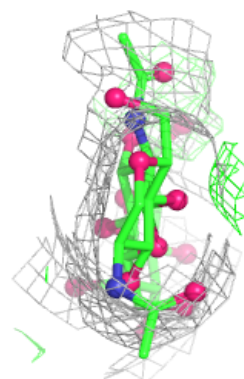
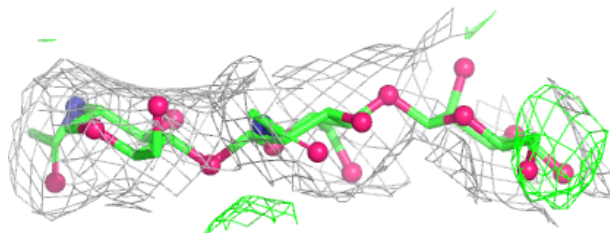
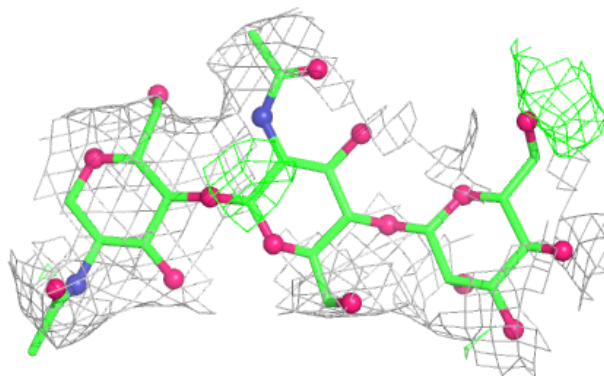


Electron density around Chain c:

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

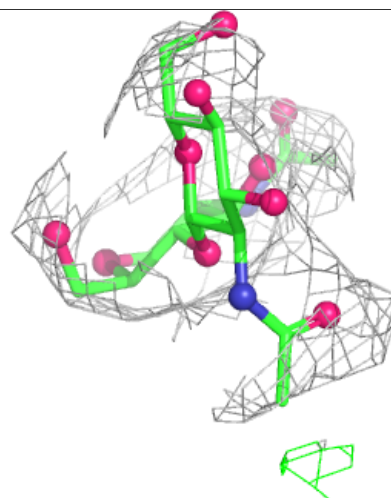
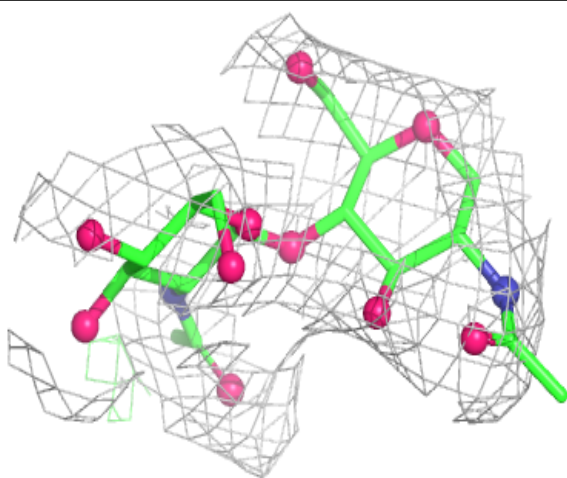
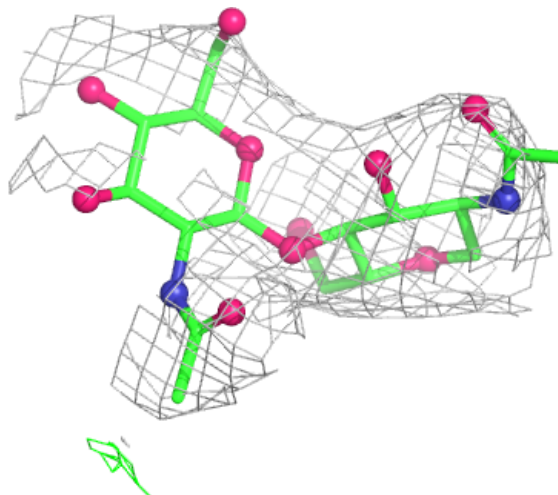
**Electron density around Chain e:**

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



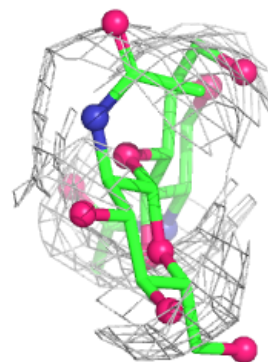
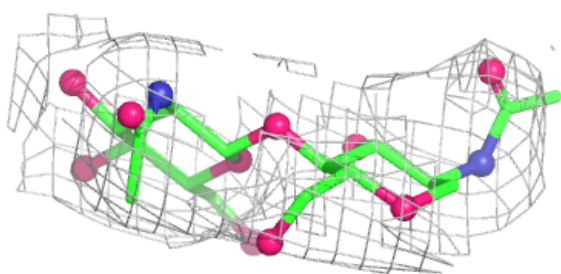
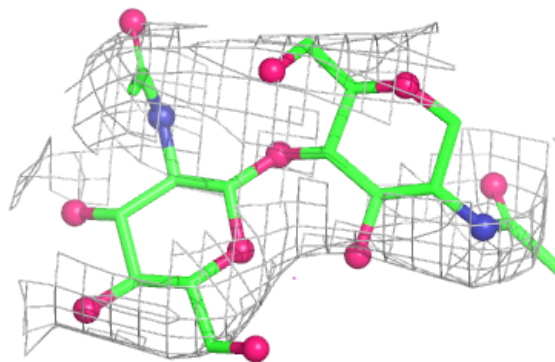
Electron density around Chain Q:

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

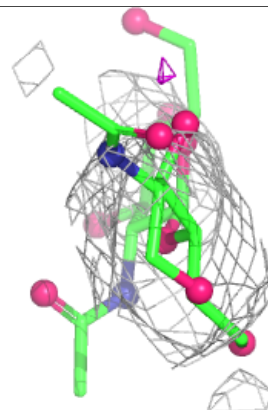
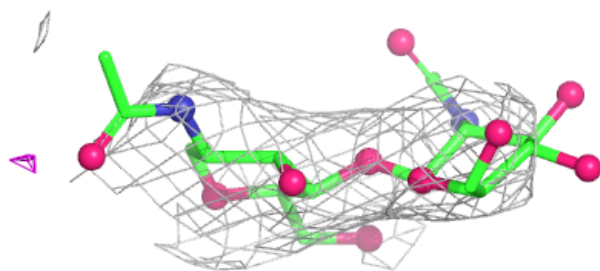
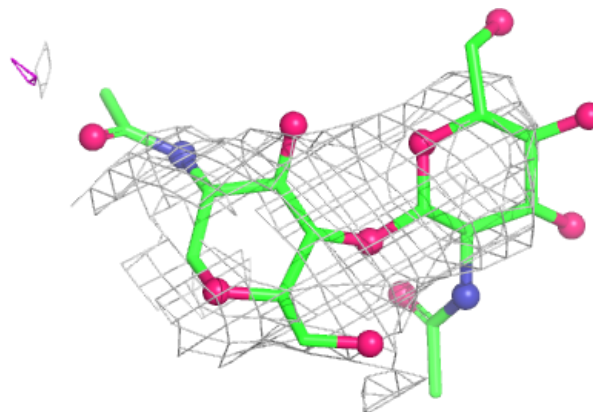


Electron density around Chain S:

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

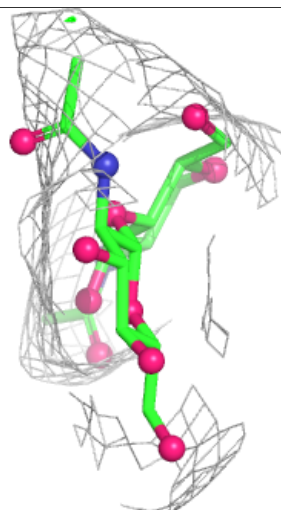
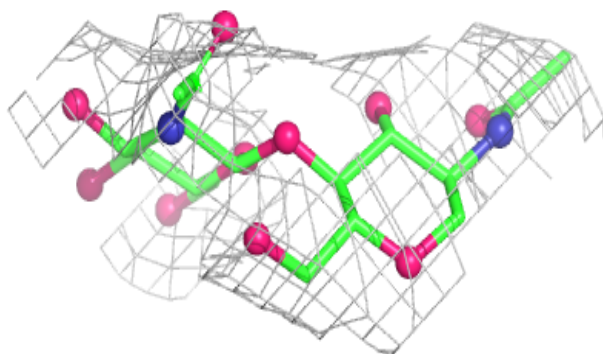
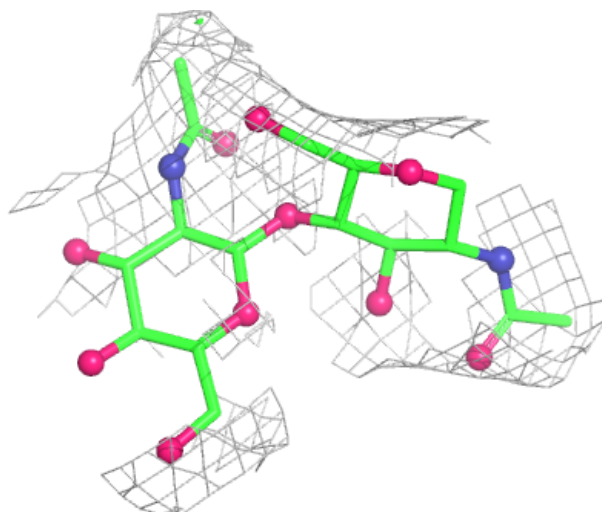
**Electron density around Chain T:**

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



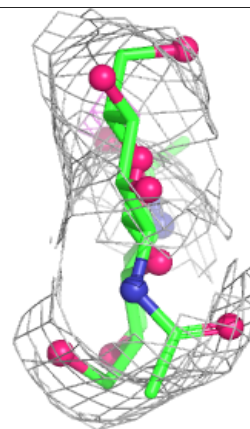
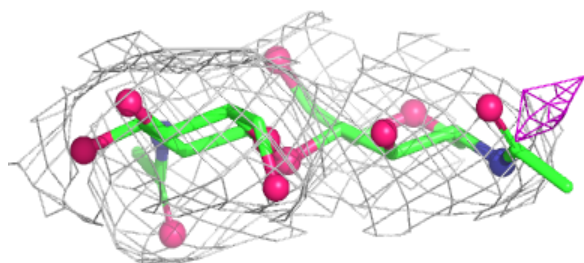
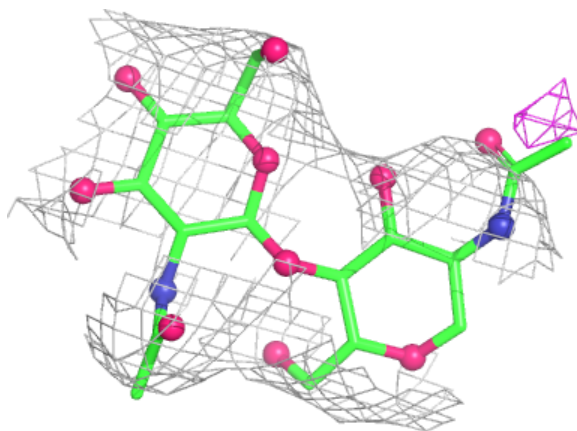
Electron density around Chain V:

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

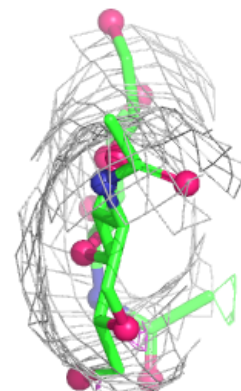
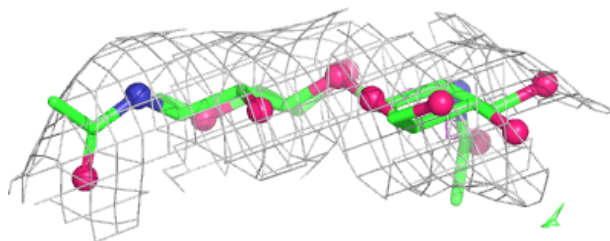
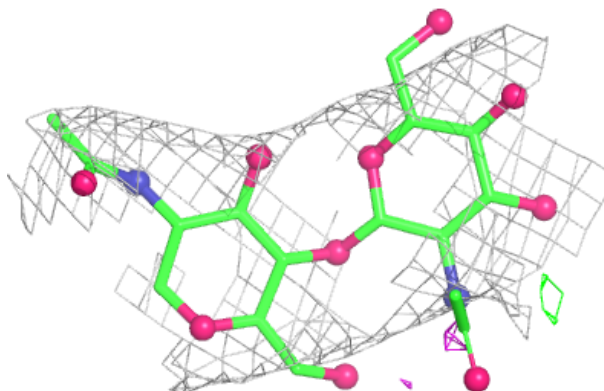


Electron density around Chain W:

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

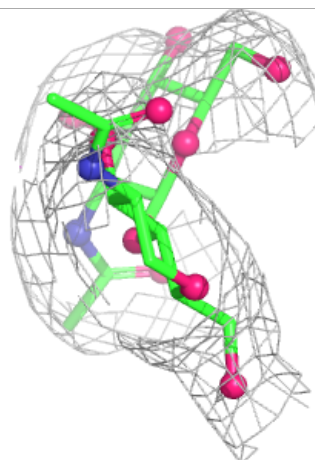
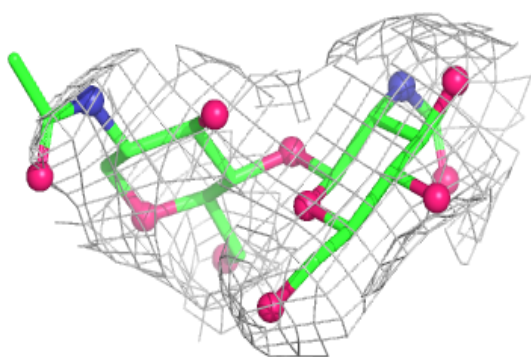
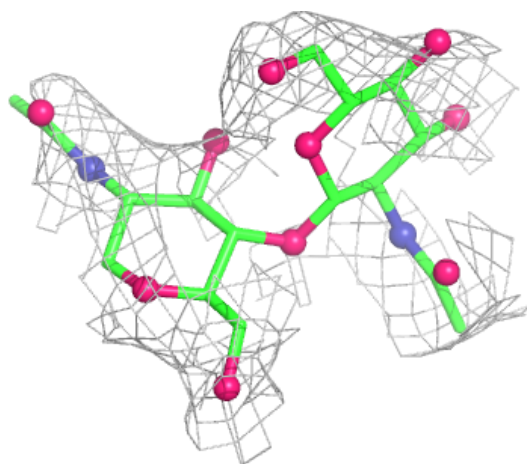
**Electron density around Chain b:**

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



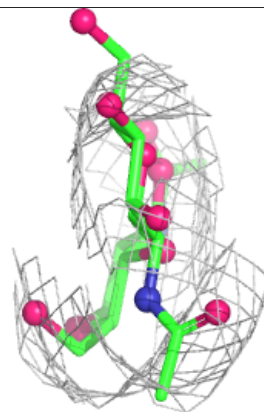
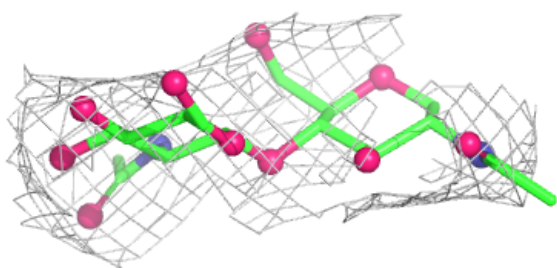
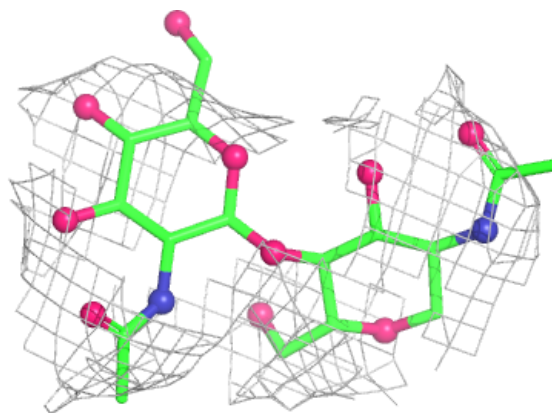
Electron density around Chain d:

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



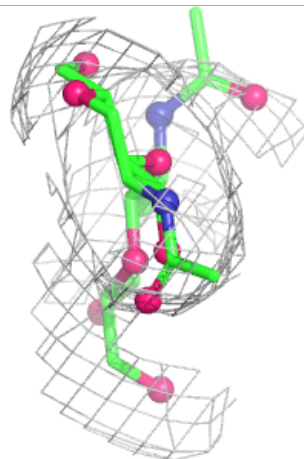
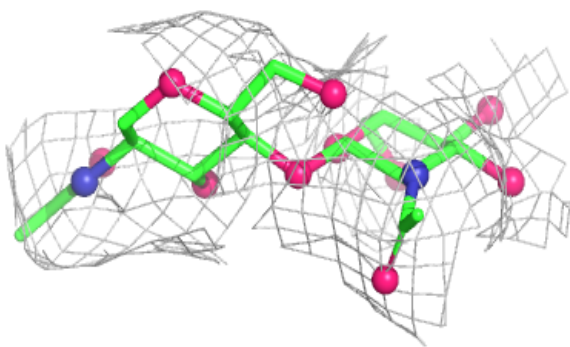
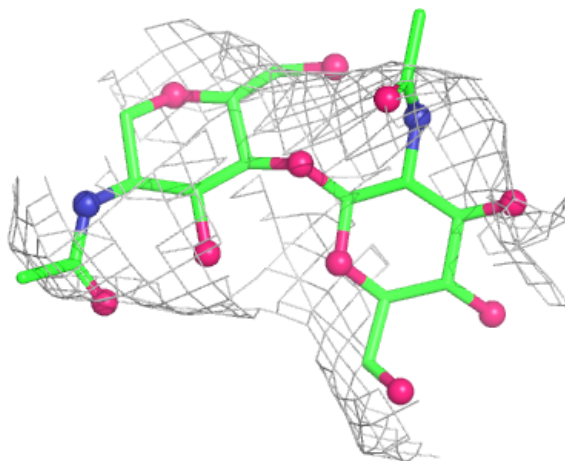
Electron density around Chain f:

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



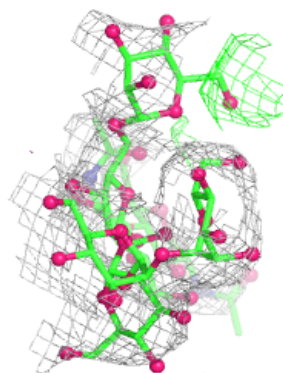
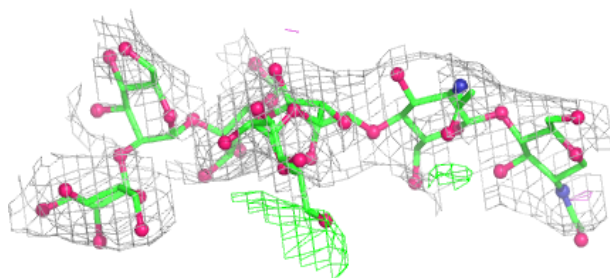
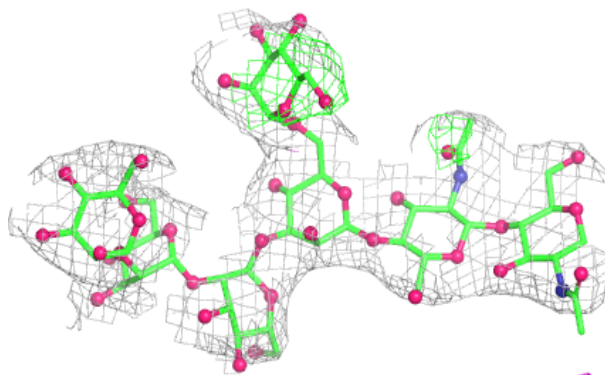
Electron density around Chain i:

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

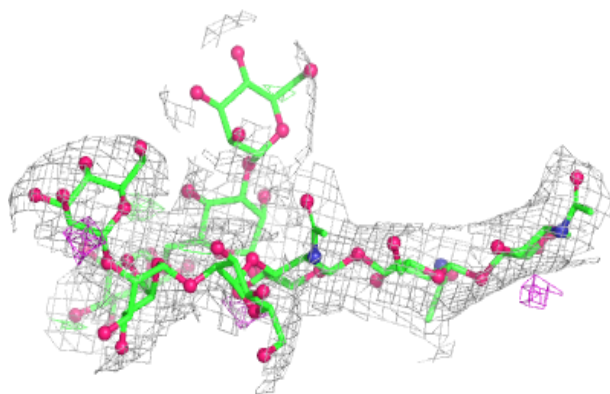
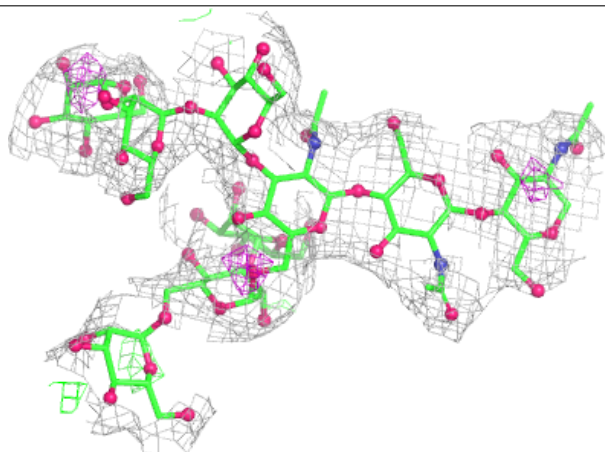


Electron density around Chain R:

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

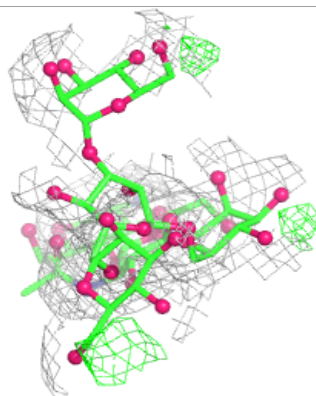
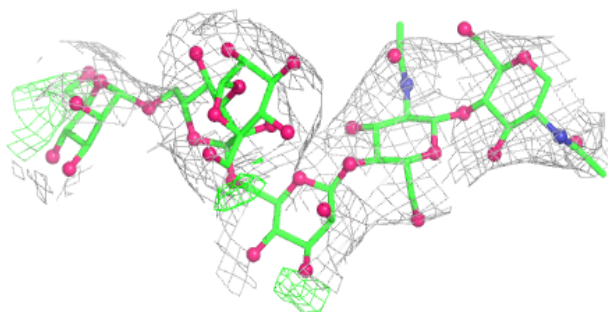
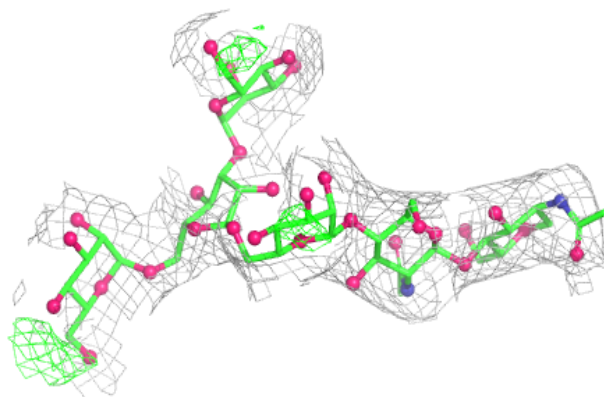
**Electron density around Chain a:**

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

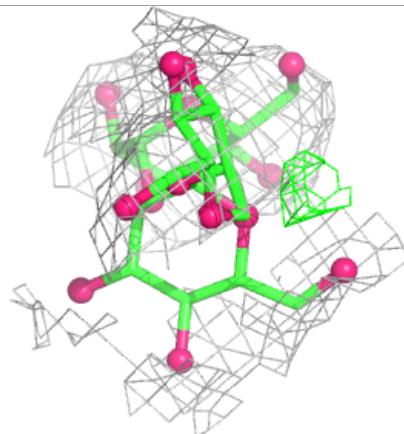
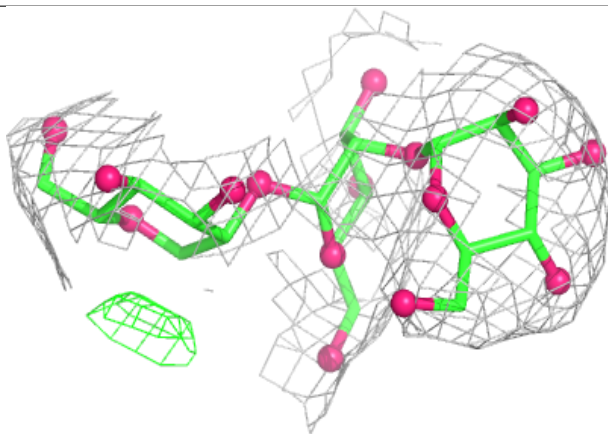
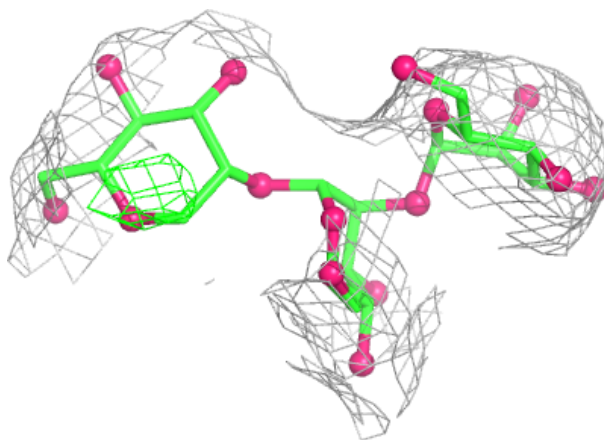


Electron density around Chain g:

$2mF_o-DF_c$ (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)



6.4 Ligands ⓘ

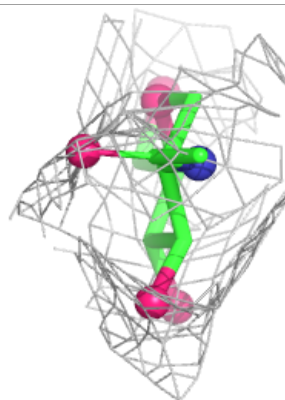
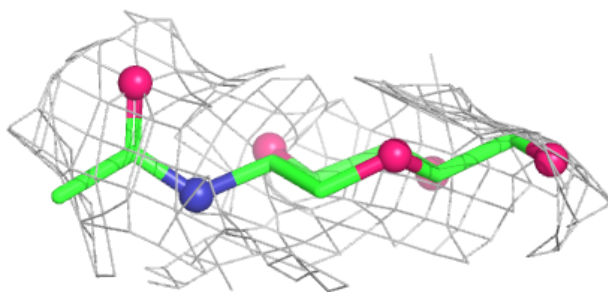
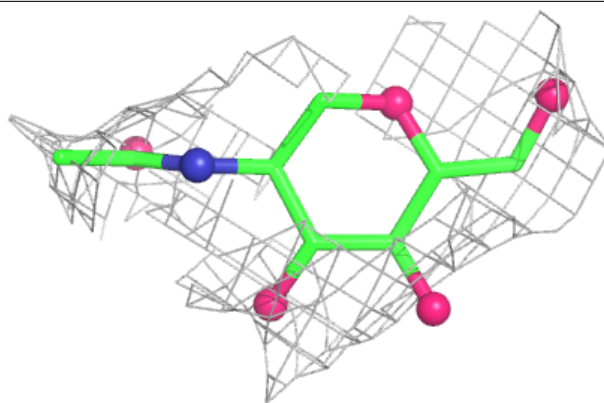
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	NAG	E	603	14/15	0.42	0.12	115,115,115,115	0
14	NAG	Z	702	14/15	0.42	0.12	198,198,198,198	0
14	NAG	X	702	14/15	0.43	0.13	152,152,152,152	0
14	NAG	E	606	14/15	0.43	0.15	135,135,135,135	0
14	NAG	E	607	14/15	0.48	0.10	144,144,144,144	0
14	NAG	M	601	14/15	0.50	0.11	131,131,131,131	0
14	NAG	M	608	14/15	0.53	0.16	124,124,124,124	0
14	NAG	G	605	14/15	0.54	0.10	126,126,126,126	0
14	NAG	Y	701	14/15	0.55	0.13	139,139,139,139	0
14	NAG	M	604	14/15	0.55	0.17	117,117,117,117	0
14	NAG	G	606	14/15	0.55	0.12	138,138,138,138	0
14	NAG	E	601	14/15	0.59	0.10	134,134,134,134	0
14	NAG	Y	703	14/15	0.61	0.12	140,140,140,140	0
14	NAG	G	602	14/15	0.64	0.12	123,123,123,123	0
14	NAG	X	701	14/15	0.64	0.15	159,159,159,159	0
14	NAG	G	604	14/15	0.67	0.13	106,106,106,106	0
14	NAG	M	607	14/15	0.72	0.13	109,109,109,109	0
14	NAG	M	606	14/15	0.73	0.12	147,147,147,147	0
14	NAG	E	605	14/15	0.75	0.14	107,107,107,107	0
14	NAG	Z	701	14/15	0.77	0.14	149,149,149,149	0
14	NAG	E	608	14/15	0.77	0.11	116,116,116,116	0
14	NAG	E	604	14/15	0.78	0.10	114,114,114,114	0
14	NAG	M	603	14/15	0.78	0.10	112,112,112,112	0
14	NAG	M	602	14/15	0.83	0.11	126,126,126,126	0
14	NAG	G	603	14/15	0.83	0.10	117,117,117,117	0
14	NAG	E	602	14/15	0.84	0.10	97,97,97,97	0
14	NAG	G	607	14/15	0.84	0.09	102,102,102,102	0
14	NAG	M	605	14/15	0.84	0.08	102,102,102,102	0
14	NAG	G	601	14/15	0.86	0.09	99,99,99,99	0
14	NAG	Y	702	14/15	0.87	0.12	101,101,101,101	0

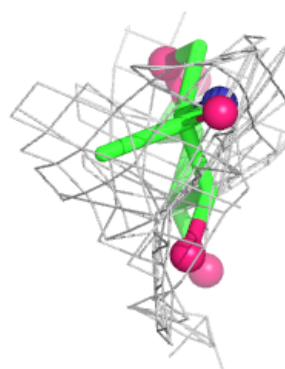
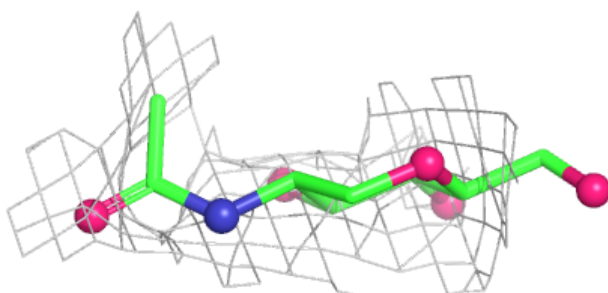
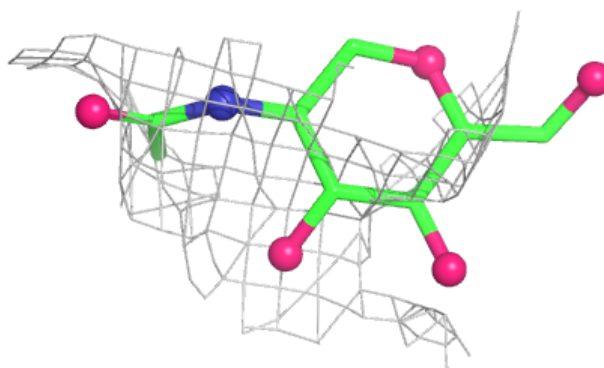
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG E 603:

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

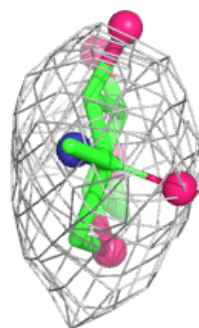
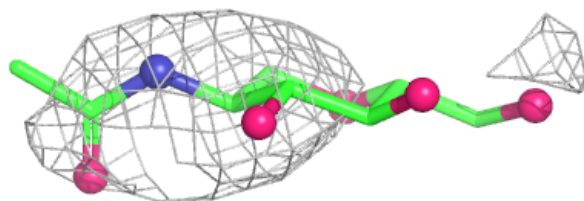
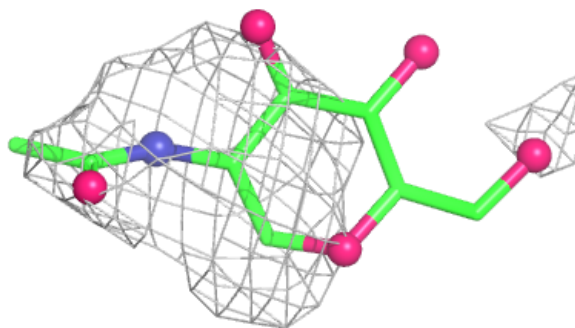
**Electron density around NAG Z 702:**

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

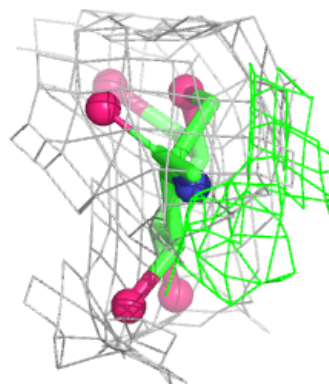
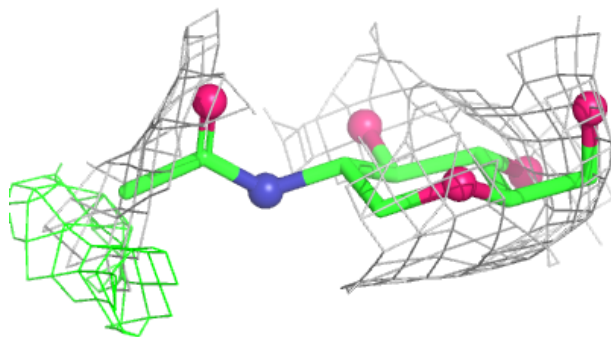
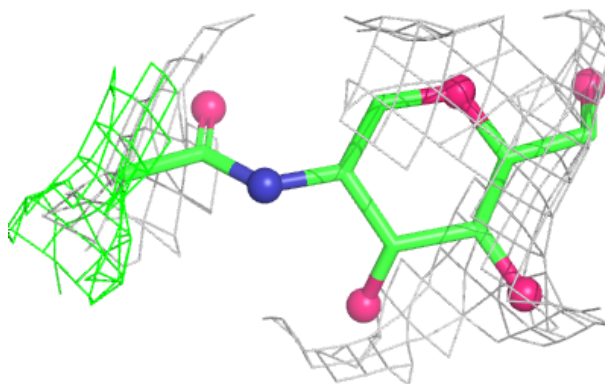


Electron density around NAG X 702:

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

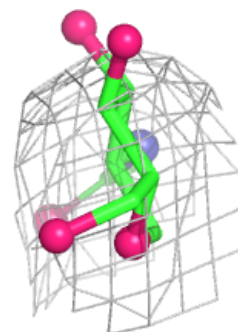
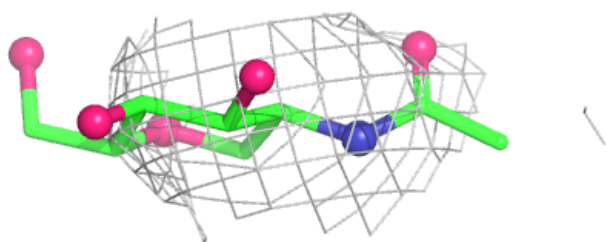
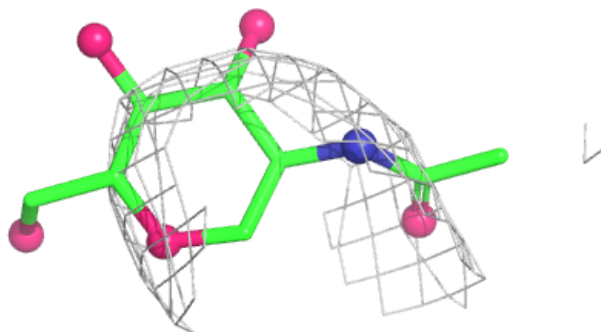
**Electron density around NAG E 606:**

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

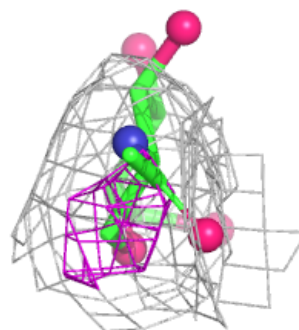
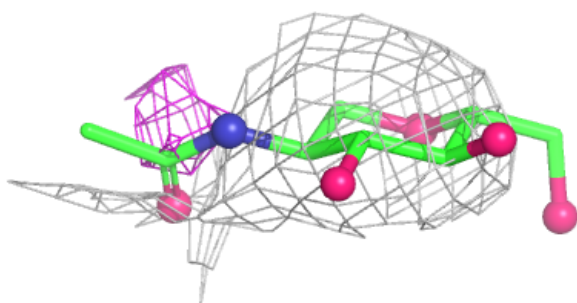
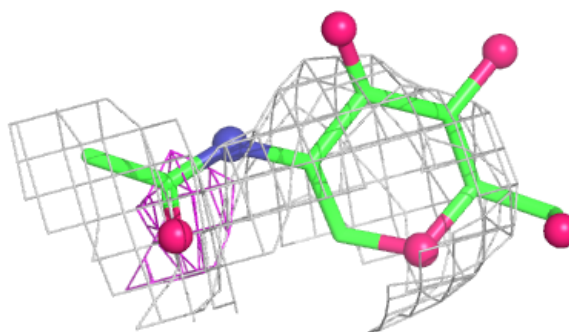


Electron density around NAG E 607:

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

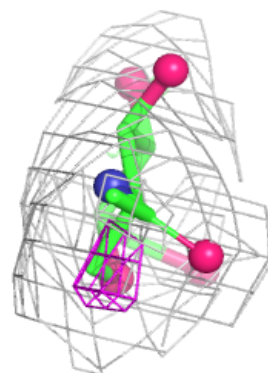
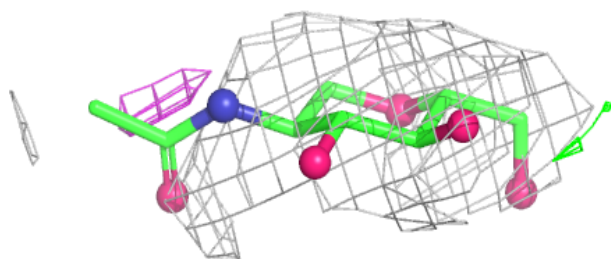
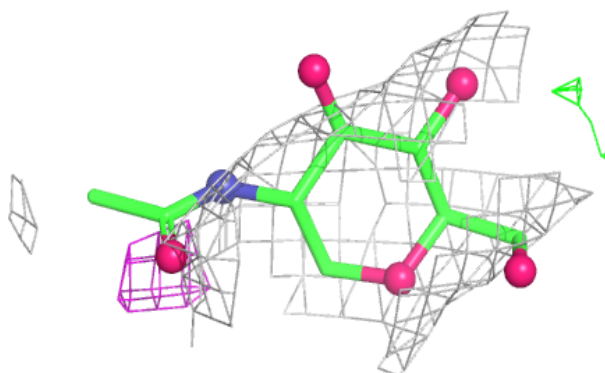
**Electron density around NAG M 601:**

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

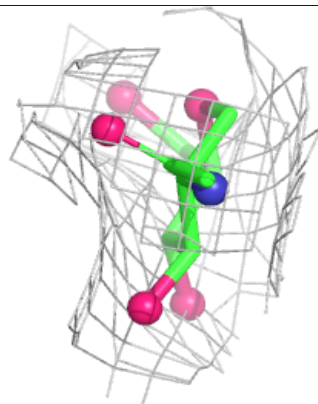
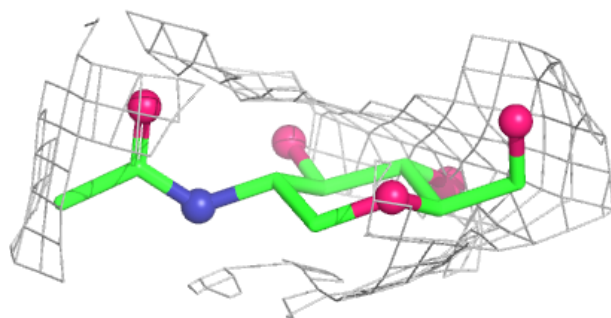
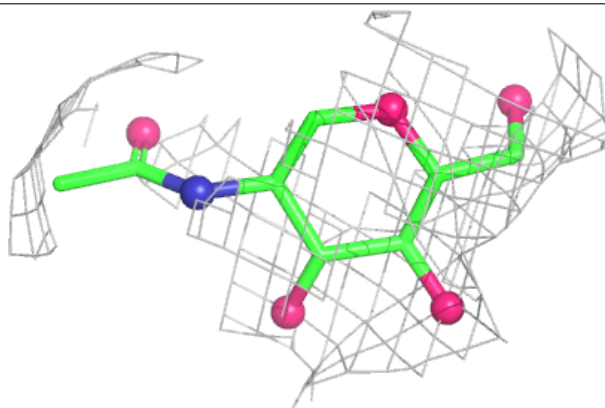


Electron density around NAG M 608:

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

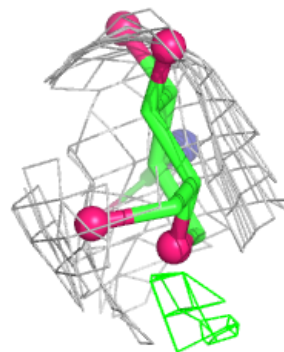
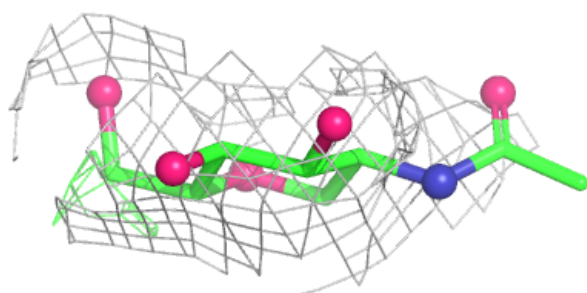
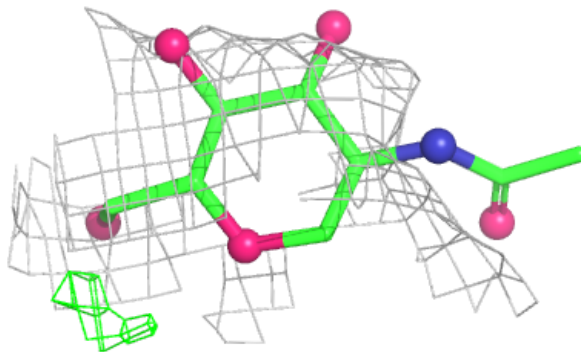
**Electron density around NAG G 605:**

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

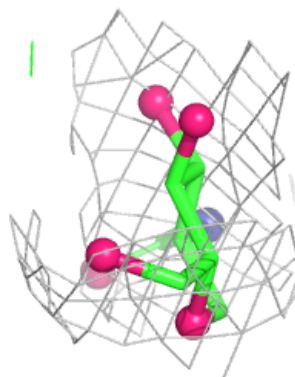
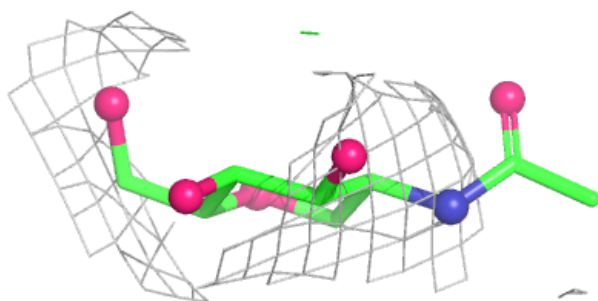
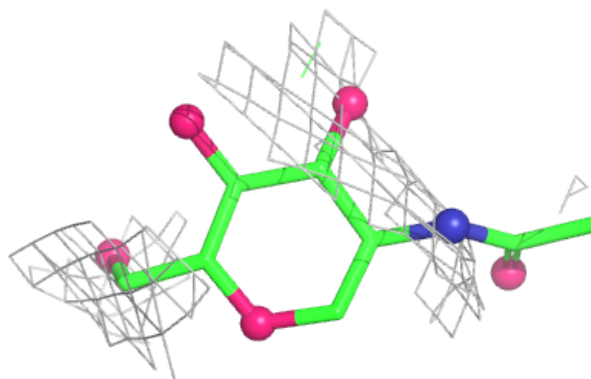


Electron density around NAG Y 701:

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

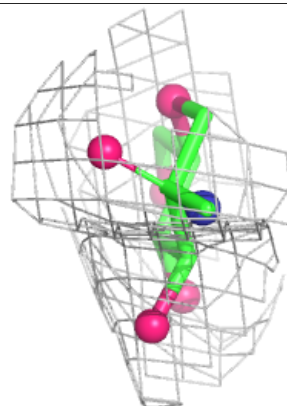
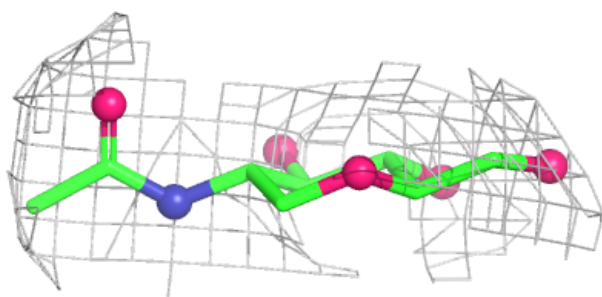
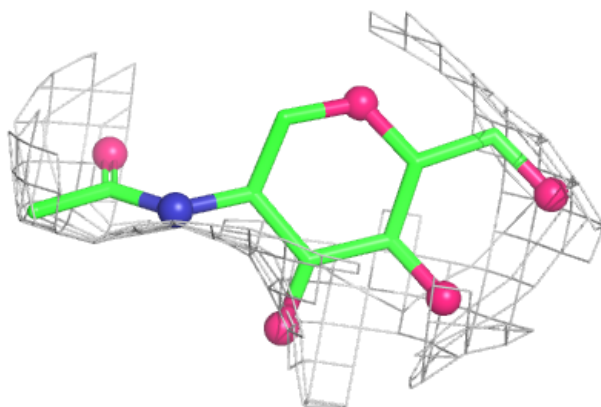
**Electron density around NAG M 604:**

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

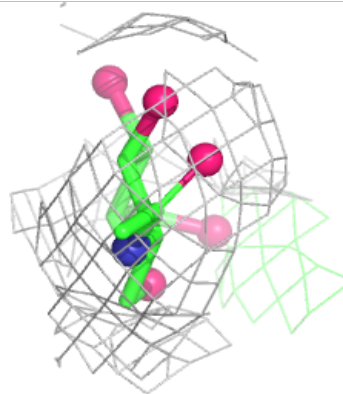
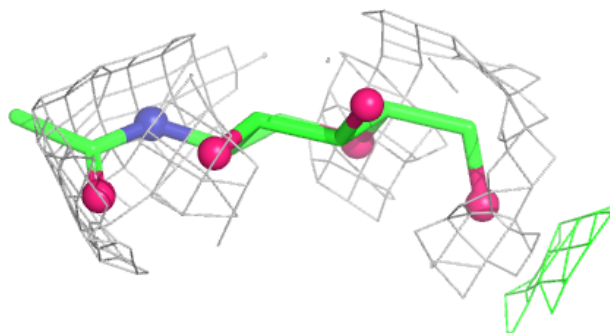
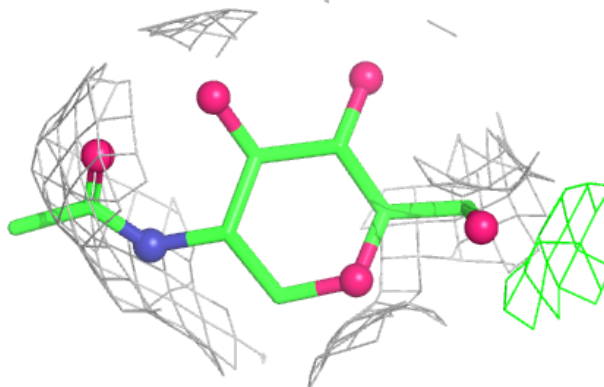


Electron density around NAG G 606:

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

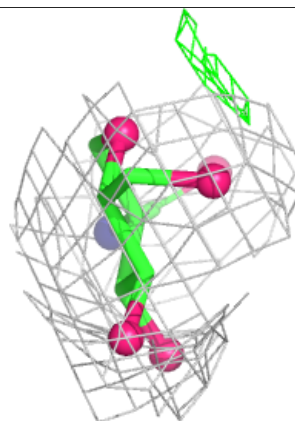
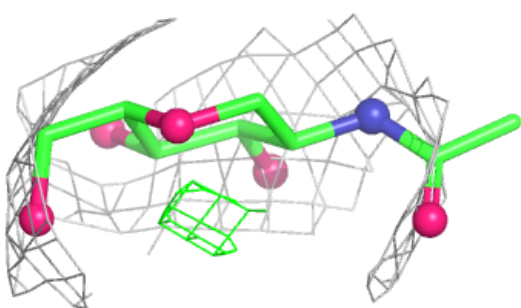
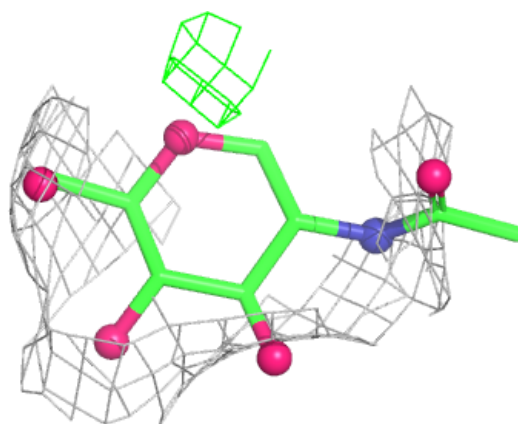
**Electron density around NAG E 601:**

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

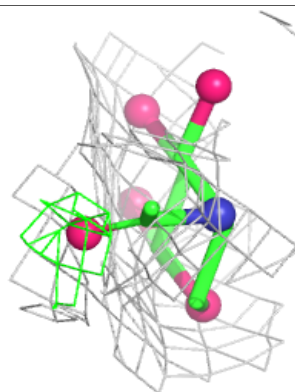
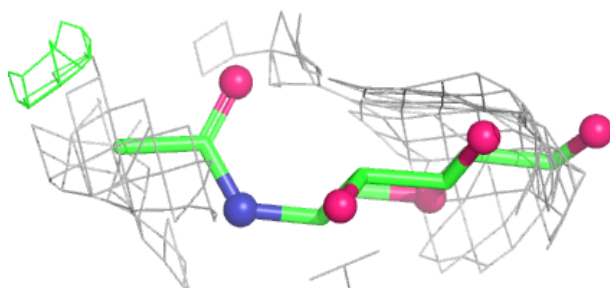
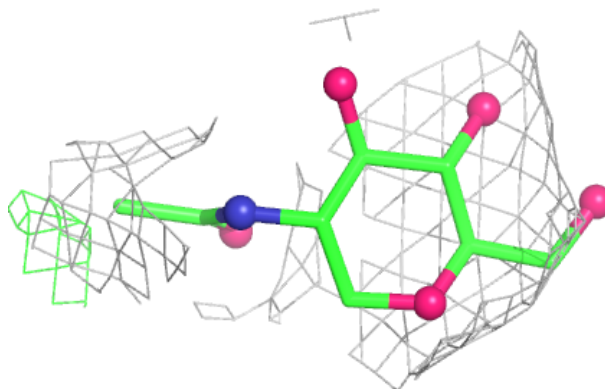


Electron density around NAG Y 703:

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

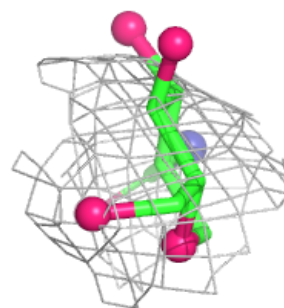
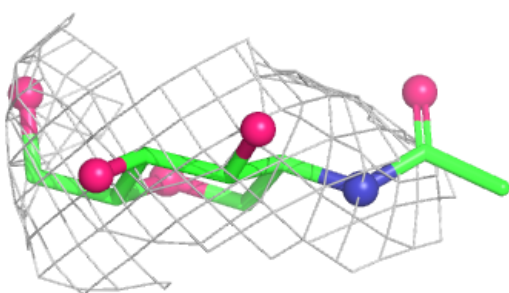
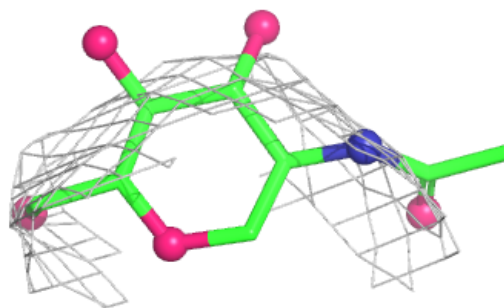
**Electron density around NAG G 602:**

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

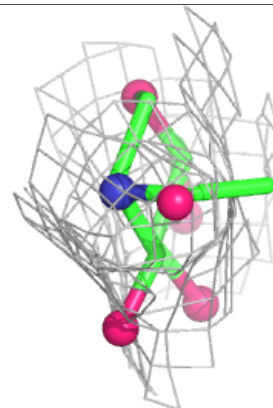
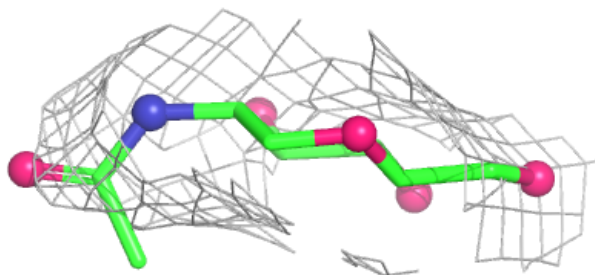
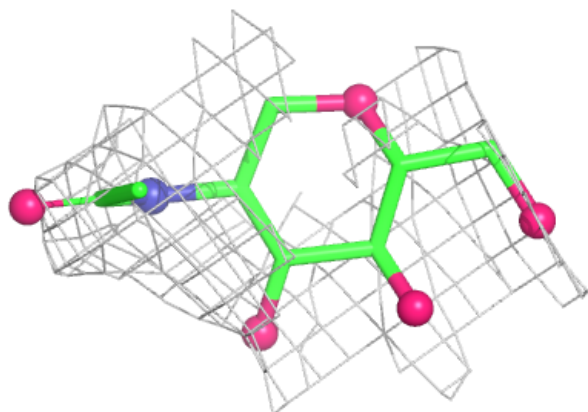


Electron density around NAG X 701:

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

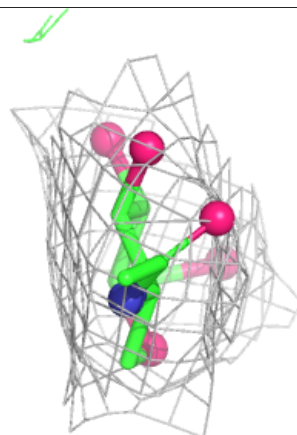
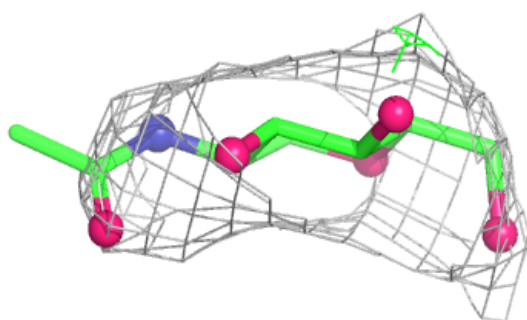
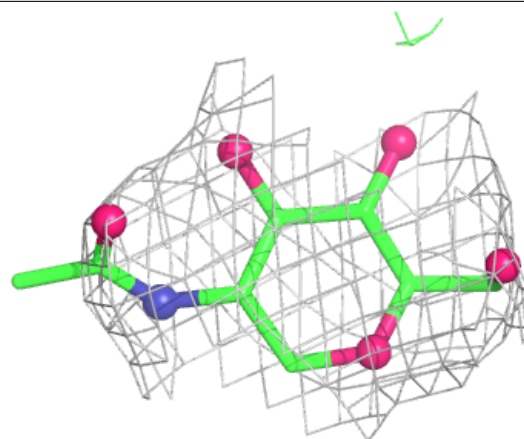
**Electron density around NAG G 604:**

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



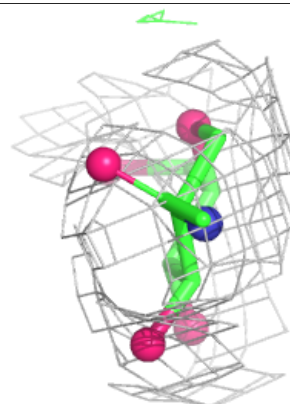
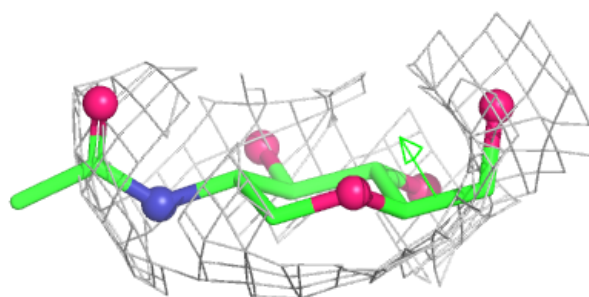
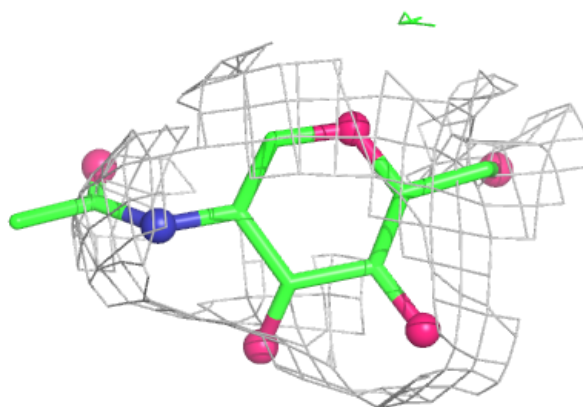
Electron density around NAG M 607:

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

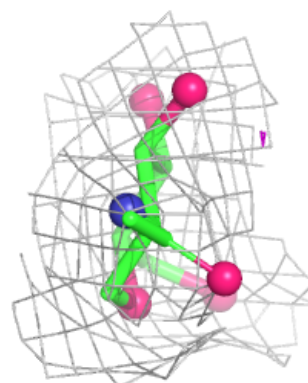
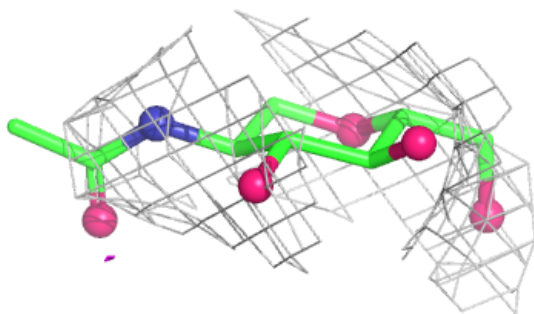
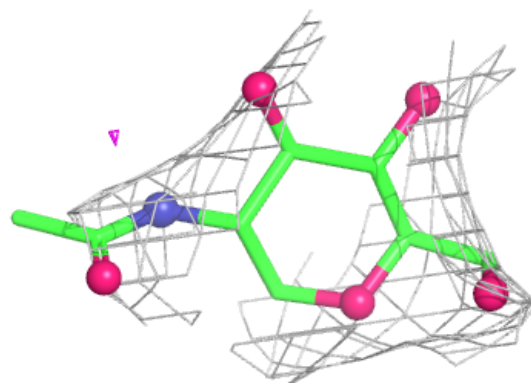


Electron density around NAG M 606:

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

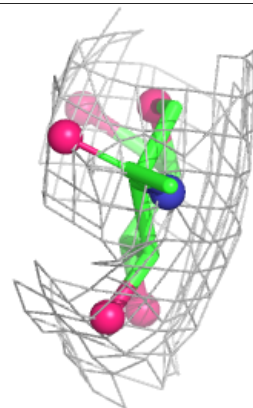
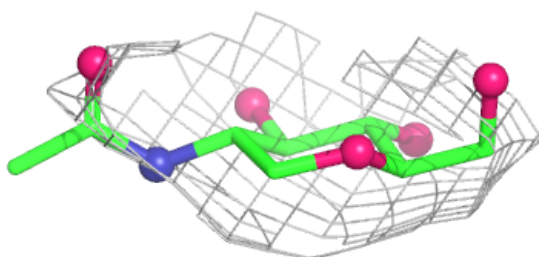
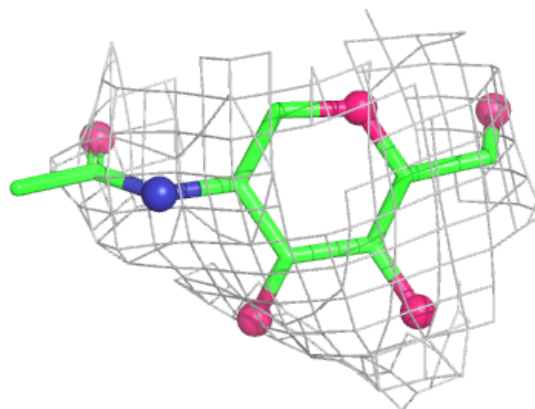
**Electron density around NAG E 605:**

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

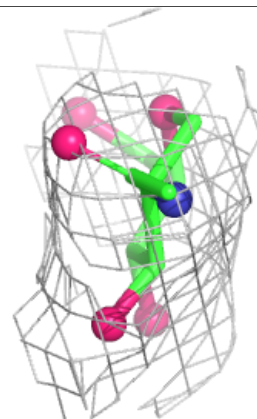
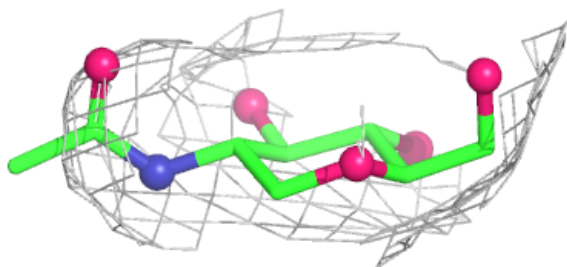
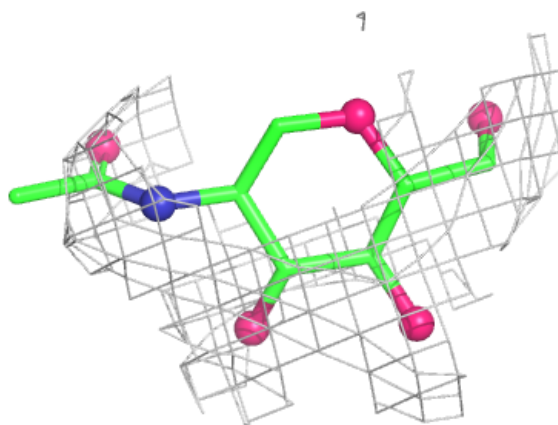


Electron density around NAG Z 701:

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

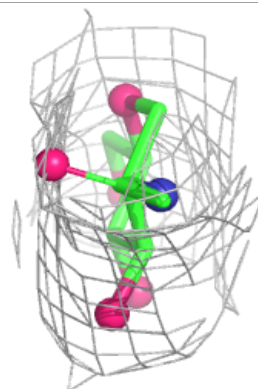
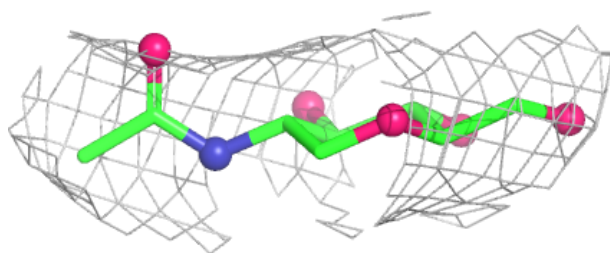
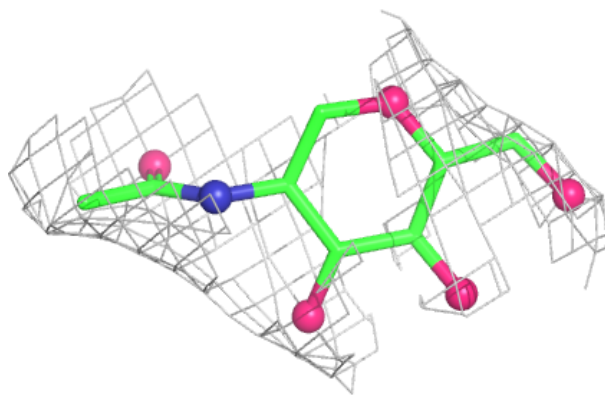
**Electron density around NAG E 608:**

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

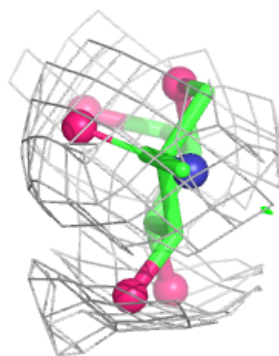
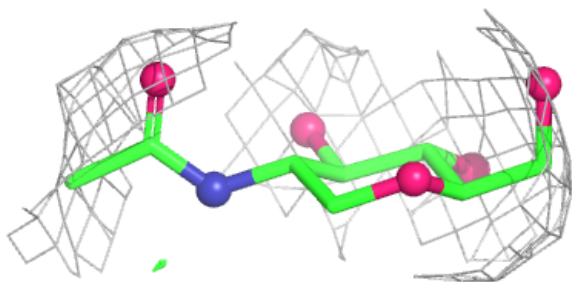
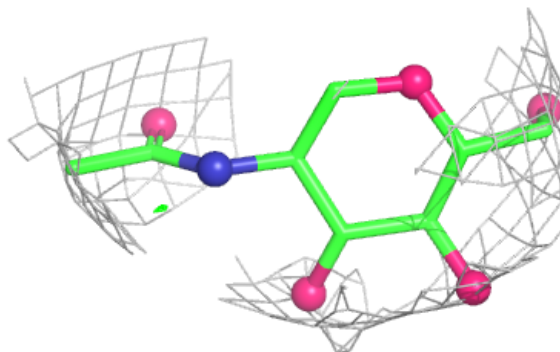


Electron density around NAG E 604:

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

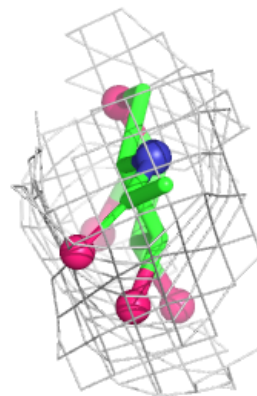
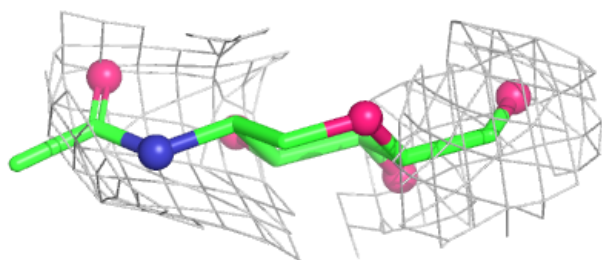
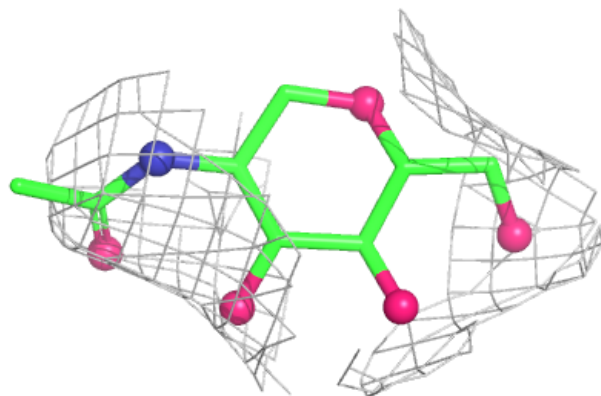
**Electron density around NAG M 603:**

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

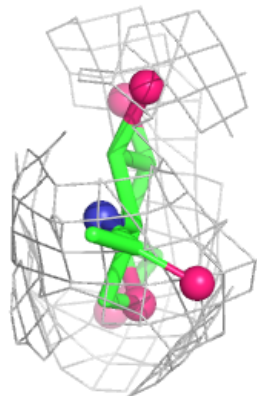
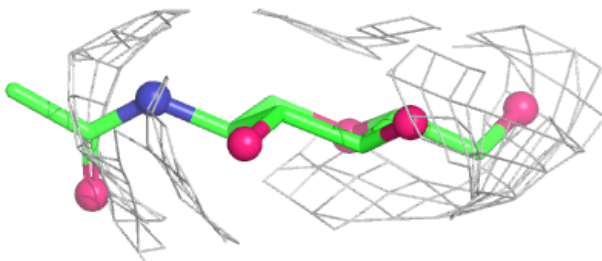
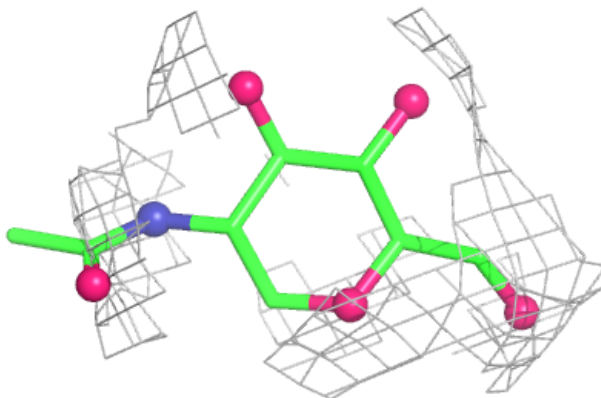


Electron density around NAG M 602:

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

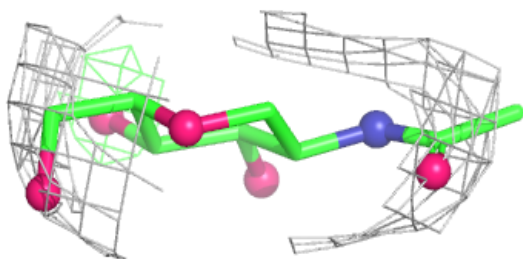
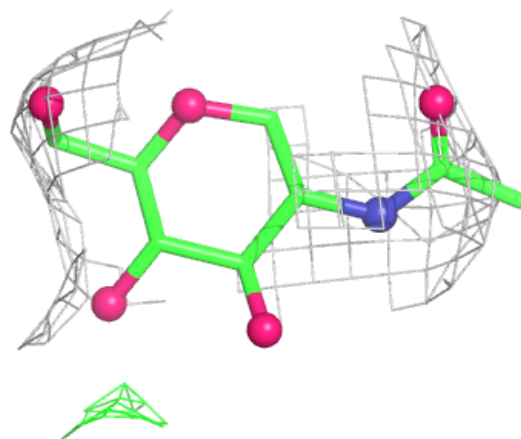
**Electron density around NAG G 603:**

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



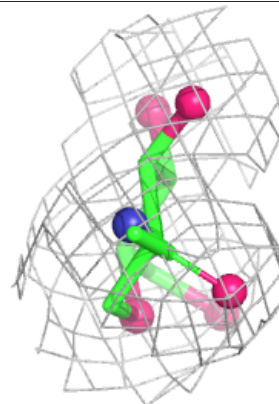
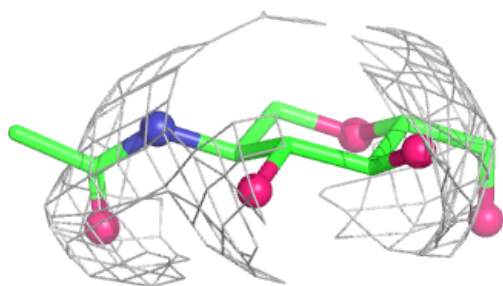
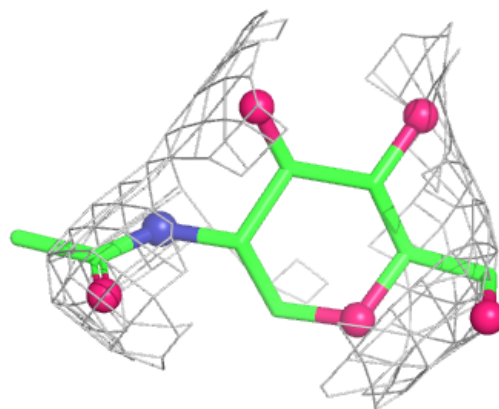
Electron density around NAG E 602:

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

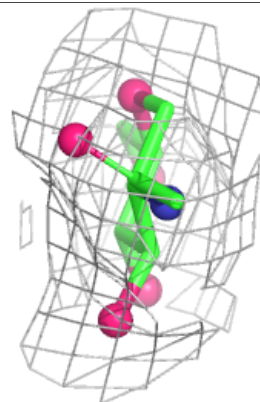
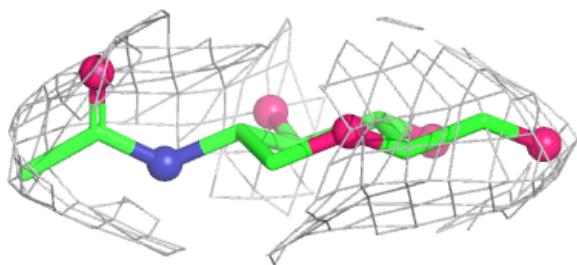
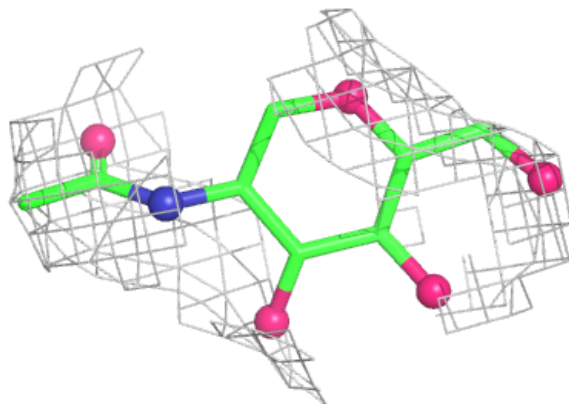


Electron density around NAG G 607:

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

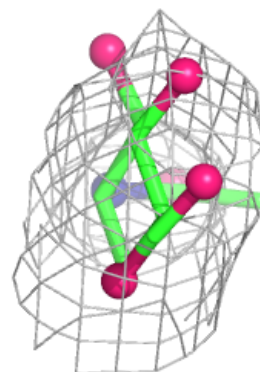
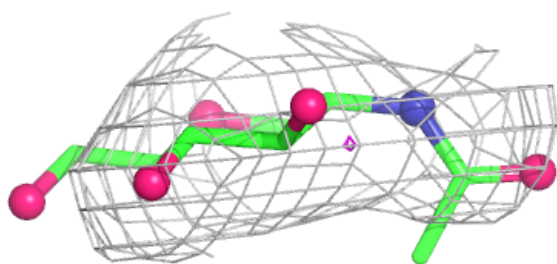
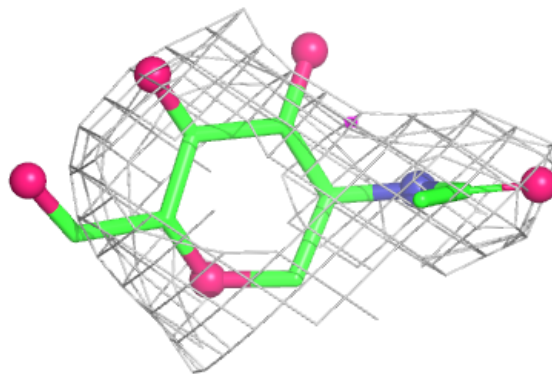
**Electron density around NAG M 605:**

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

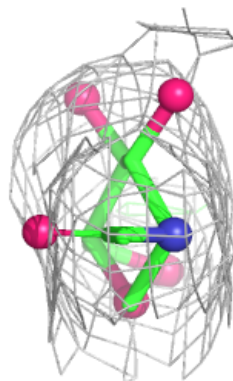
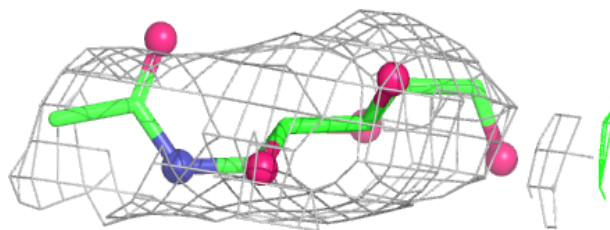
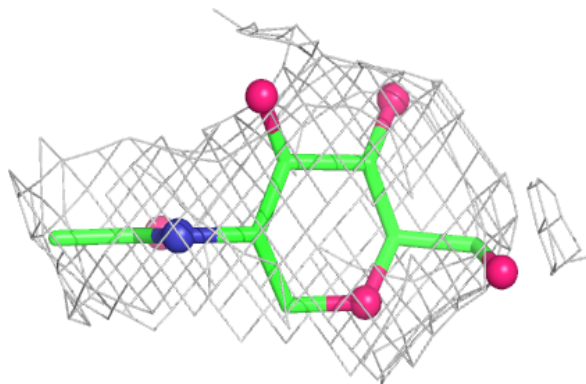


Electron density around NAG G 601:

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

**Electron density around NAG Y 702:**

$2mF_o - DF_c$ (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.