



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:10 PM UTC

PDB ID : 6THG / pdb_00006thg
Title : Cedar Virus attachment glycoprotein (G) in complex with human ephrin-B1
Authors : Pryce, R.; Rissanen, I.; Harlos, K.; Bowden, T.
Deposited on : 2019-11-20
Resolution : 4.07 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

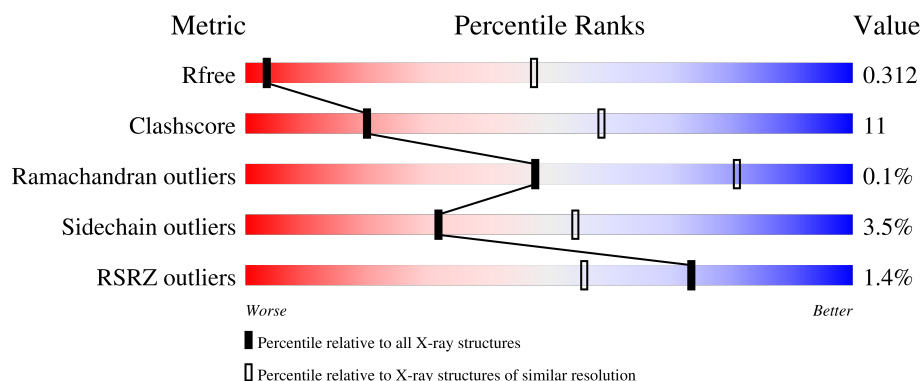
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.07 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.



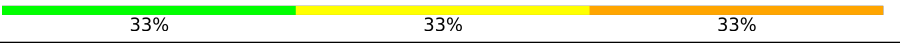
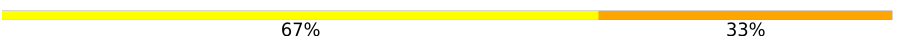
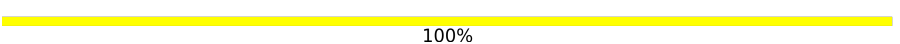
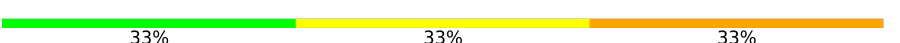
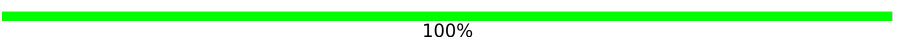
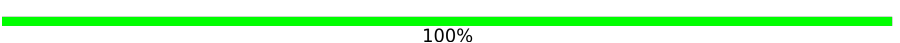
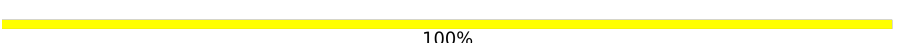
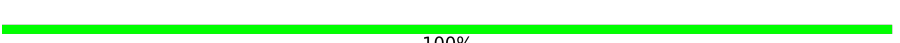
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1200 (4.36-3.80)
Clashscore	190562	1249 (4.36-3.80)
Ramachandran outliers	187476	1169 (4.36-3.80)
Sidechain outliers	187428	1158 (4.36-3.80)
RSRZ outliers	180081	1199 (4.36-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	426	0% 74% 23% ..
1	B	426	72% 25% ..
1	E	426	0% 72% 24% ..
1	G	426	2% 74% 23% ..
1	I	426	2% 69% 27% ..

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Mol	Chain	Length	Quality of chain
2	C	151	
2	D	151	
2	F	151	
2	H	151	
2	J	151	
3	K	3	
3	M	3	
3	N	3	
3	O	3	
3	Q	3	
3	U	3	
4	L	2	
4	P	2	
4	R	2	
4	S	2	
4	T	2	
4	V	2	
4	W	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22772 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 Attachment glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	419	Total	C	N	O	S	0	0	0
			3358	2131	555	648	24			
1	A	418	Total	C	N	O	S	0	0	0
			3351	2127	554	646	24			
1	E	415	Total	C	N	O	S	0	0	0
			3330	2113	550	643	24			
1	G	415	Total	C	N	O	S	0	0	0
			3330	2113	550	643	24			
1	I	417	Total	C	N	O	S	0	0	0
			3347	2125	553	645	24			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	GLU	-	expression tag	UNP A0A185KRV2
B	207	THR	-	expression tag	UNP A0A185KRV2
B	208	GLY	-	expression tag	UNP A0A185KRV2
B	623	GLY	-	expression tag	UNP A0A185KRV2
B	624	THR	-	expression tag	UNP A0A185KRV2
B	625	LYS	-	expression tag	UNP A0A185KRV2
B	626	HIS	-	expression tag	UNP A0A185KRV2
B	627	HIS	-	expression tag	UNP A0A185KRV2
B	628	HIS	-	expression tag	UNP A0A185KRV2
B	629	HIS	-	expression tag	UNP A0A185KRV2
B	630	HIS	-	expression tag	UNP A0A185KRV2
B	631	HIS	-	expression tag	UNP A0A185KRV2
A	206	GLU	-	expression tag	UNP A0A185KRV2
A	207	THR	-	expression tag	UNP A0A185KRV2
A	208	GLY	-	expression tag	UNP A0A185KRV2
A	623	GLY	-	expression tag	UNP A0A185KRV2
A	624	THR	-	expression tag	UNP A0A185KRV2
A	625	LYS	-	expression tag	UNP A0A185KRV2
A	626	HIS	-	expression tag	UNP A0A185KRV2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	627	HIS	-	expression tag	UNP A0A185KRV2
A	628	HIS	-	expression tag	UNP A0A185KRV2
A	629	HIS	-	expression tag	UNP A0A185KRV2
A	630	HIS	-	expression tag	UNP A0A185KRV2
A	631	HIS	-	expression tag	UNP A0A185KRV2
E	206	GLU	-	expression tag	UNP A0A185KRV2
E	207	THR	-	expression tag	UNP A0A185KRV2
E	208	GLY	-	expression tag	UNP A0A185KRV2
E	623	GLY	-	expression tag	UNP A0A185KRV2
E	624	THR	-	expression tag	UNP A0A185KRV2
E	625	LYS	-	expression tag	UNP A0A185KRV2
E	626	HIS	-	expression tag	UNP A0A185KRV2
E	627	HIS	-	expression tag	UNP A0A185KRV2
E	628	HIS	-	expression tag	UNP A0A185KRV2
E	629	HIS	-	expression tag	UNP A0A185KRV2
E	630	HIS	-	expression tag	UNP A0A185KRV2
E	631	HIS	-	expression tag	UNP A0A185KRV2
G	206	GLU	-	expression tag	UNP A0A185KRV2
G	207	THR	-	expression tag	UNP A0A185KRV2
G	208	GLY	-	expression tag	UNP A0A185KRV2
G	623	GLY	-	expression tag	UNP A0A185KRV2
G	624	THR	-	expression tag	UNP A0A185KRV2
G	625	LYS	-	expression tag	UNP A0A185KRV2
G	626	HIS	-	expression tag	UNP A0A185KRV2
G	627	HIS	-	expression tag	UNP A0A185KRV2
G	628	HIS	-	expression tag	UNP A0A185KRV2
G	629	HIS	-	expression tag	UNP A0A185KRV2
G	630	HIS	-	expression tag	UNP A0A185KRV2
G	631	HIS	-	expression tag	UNP A0A185KRV2
I	206	GLU	-	expression tag	UNP A0A185KRV2
I	207	THR	-	expression tag	UNP A0A185KRV2
I	208	GLY	-	expression tag	UNP A0A185KRV2
I	623	GLY	-	expression tag	UNP A0A185KRV2
I	624	THR	-	expression tag	UNP A0A185KRV2
I	625	LYS	-	expression tag	UNP A0A185KRV2
I	626	HIS	-	expression tag	UNP A0A185KRV2
I	627	HIS	-	expression tag	UNP A0A185KRV2
I	628	HIS	-	expression tag	UNP A0A185KRV2
I	629	HIS	-	expression tag	UNP A0A185KRV2
I	630	HIS	-	expression tag	UNP A0A185KRV2
I	631	HIS	-	expression tag	UNP A0A185KRV2

- Molecule 2 is a protein called Ephrin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	136	Total	C	N	O	S	0	0	0
			1089	695	186	201	7			
2	C	136	Total	C	N	O	S	0	0	0
			1076	686	183	200	7			
2	F	137	Total	C	N	O	S	0	0	0
			1084	690	184	203	7			
2	H	134	Total	C	N	O	S	0	0	0
			1063	679	180	197	7			
2	J	136	Total	C	N	O	S	0	0	0
			1076	686	183	200	7			

There are 60 discrepancies between the modelled and reference sequences:

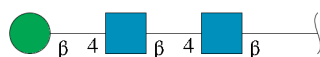
Chain	Residue	Modelled	Actual	Comment	Reference
D	26	GLU	-	expression tag	UNP P98172
D	27	THR	-	expression tag	UNP P98172
D	28	GLY	-	expression tag	UNP P98172
D	168	GLY	-	expression tag	UNP P98172
D	169	THR	-	expression tag	UNP P98172
D	170	LYS	-	expression tag	UNP P98172
D	171	HIS	-	expression tag	UNP P98172
D	172	HIS	-	expression tag	UNP P98172
D	173	HIS	-	expression tag	UNP P98172
D	174	HIS	-	expression tag	UNP P98172
D	175	HIS	-	expression tag	UNP P98172
D	176	HIS	-	expression tag	UNP P98172
C	26	GLU	-	expression tag	UNP P98172
C	27	THR	-	expression tag	UNP P98172
C	28	GLY	-	expression tag	UNP P98172
C	168	GLY	-	expression tag	UNP P98172
C	169	THR	-	expression tag	UNP P98172
C	170	LYS	-	expression tag	UNP P98172
C	171	HIS	-	expression tag	UNP P98172
C	172	HIS	-	expression tag	UNP P98172
C	173	HIS	-	expression tag	UNP P98172
C	174	HIS	-	expression tag	UNP P98172
C	175	HIS	-	expression tag	UNP P98172
C	176	HIS	-	expression tag	UNP P98172
F	26	GLU	-	expression tag	UNP P98172
F	27	THR	-	expression tag	UNP P98172
F	28	GLY	-	expression tag	UNP P98172
F	168	GLY	-	expression tag	UNP P98172
F	169	THR	-	expression tag	UNP P98172
F	170	LYS	-	expression tag	UNP P98172

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Chain	Residue	Modelled	Actual	Comment	Reference
F	171	HIS	-	expression tag	UNP P98172
F	172	HIS	-	expression tag	UNP P98172
F	173	HIS	-	expression tag	UNP P98172
F	174	HIS	-	expression tag	UNP P98172
F	175	HIS	-	expression tag	UNP P98172
F	176	HIS	-	expression tag	UNP P98172
H	26	GLU	-	expression tag	UNP P98172
H	27	THR	-	expression tag	UNP P98172
H	28	GLY	-	expression tag	UNP P98172
H	168	GLY	-	expression tag	UNP P98172
H	169	THR	-	expression tag	UNP P98172
H	170	LYS	-	expression tag	UNP P98172
H	171	HIS	-	expression tag	UNP P98172
H	172	HIS	-	expression tag	UNP P98172
H	173	HIS	-	expression tag	UNP P98172
H	174	HIS	-	expression tag	UNP P98172
H	175	HIS	-	expression tag	UNP P98172
H	176	HIS	-	expression tag	UNP P98172
J	26	GLU	-	expression tag	UNP P98172
J	27	THR	-	expression tag	UNP P98172
J	28	GLY	-	expression tag	UNP P98172
J	168	GLY	-	expression tag	UNP P98172
J	169	THR	-	expression tag	UNP P98172
J	170	LYS	-	expression tag	UNP P98172
J	171	HIS	-	expression tag	UNP P98172
J	172	HIS	-	expression tag	UNP P98172
J	173	HIS	-	expression tag	UNP P98172
J	174	HIS	-	expression tag	UNP P98172
J	175	HIS	-	expression tag	UNP P98172
J	176	HIS	-	expression tag	UNP P98172

- Molecule 3 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.



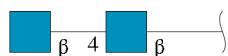
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

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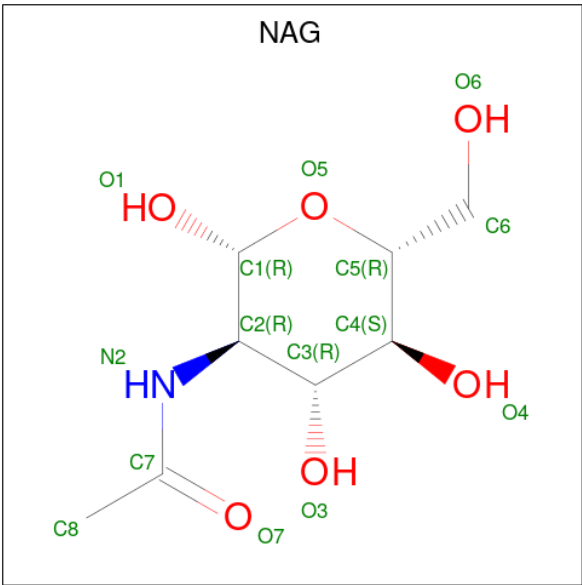
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	U	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	W	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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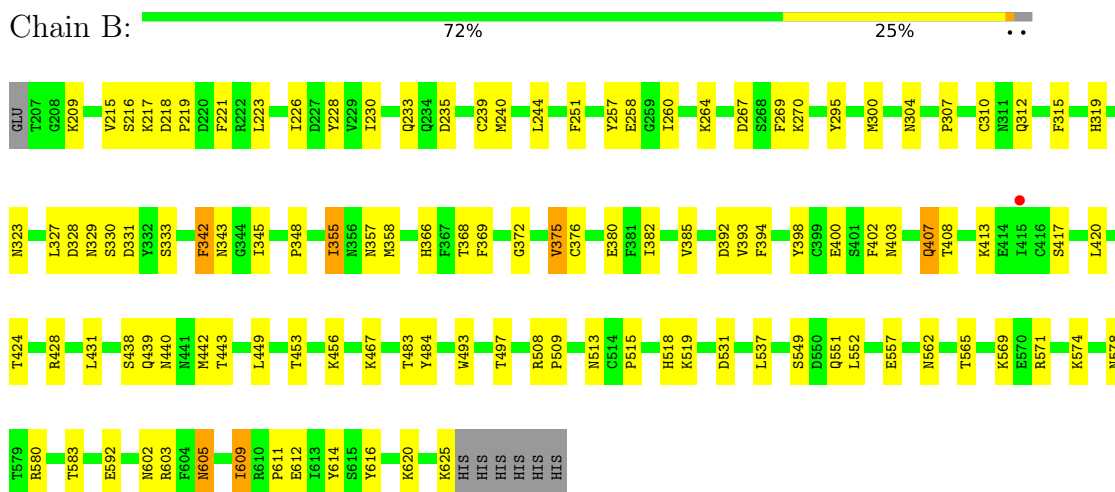
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		

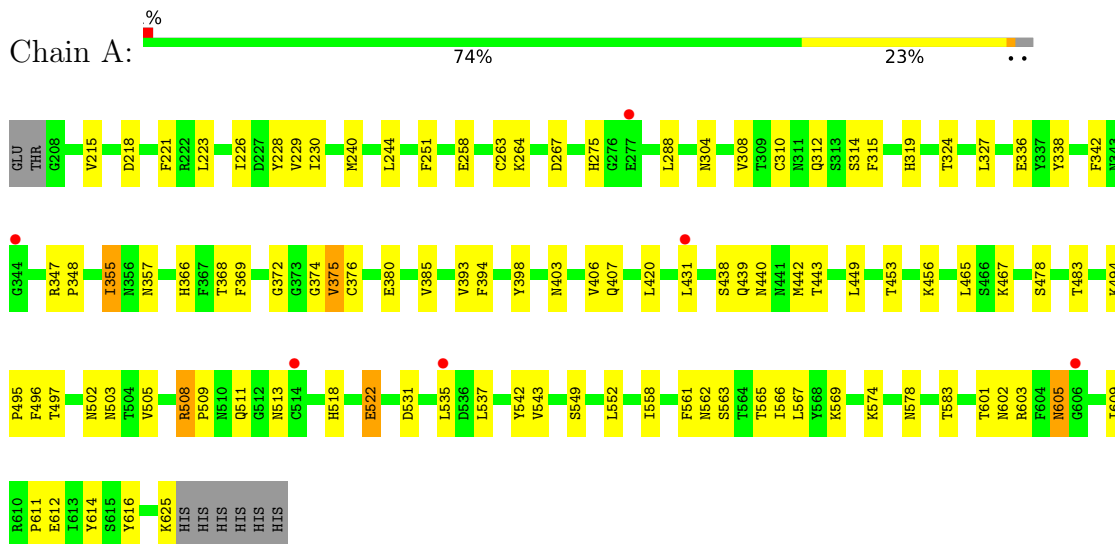
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Attachment glycoprotein

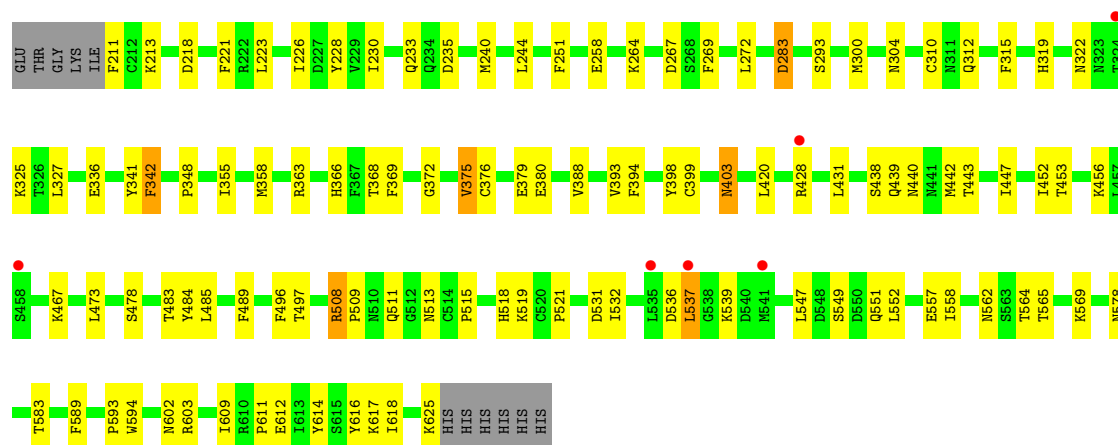


• Molecule 1: Attachment glycoprotein

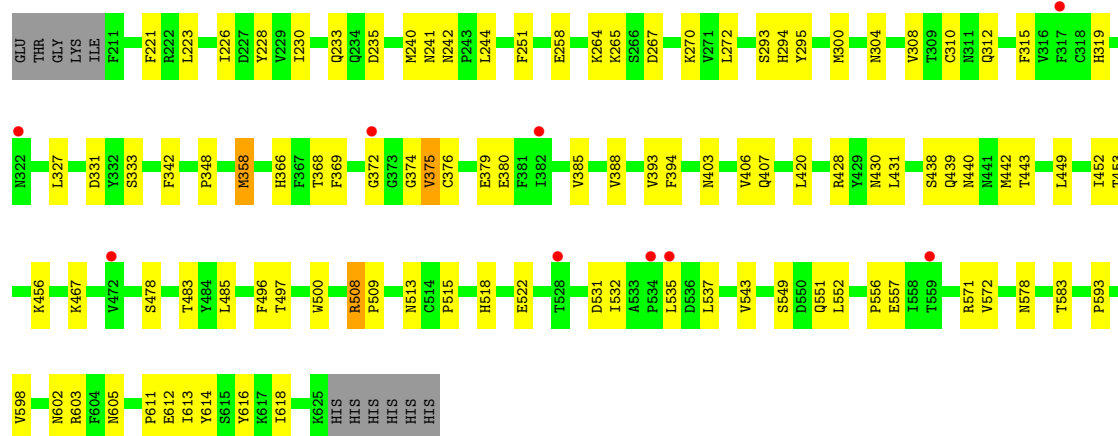
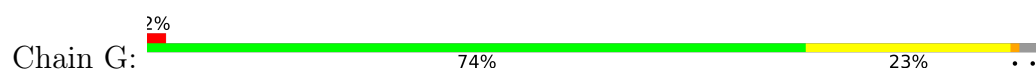


• Molecule 1: Attachment glycoprotein

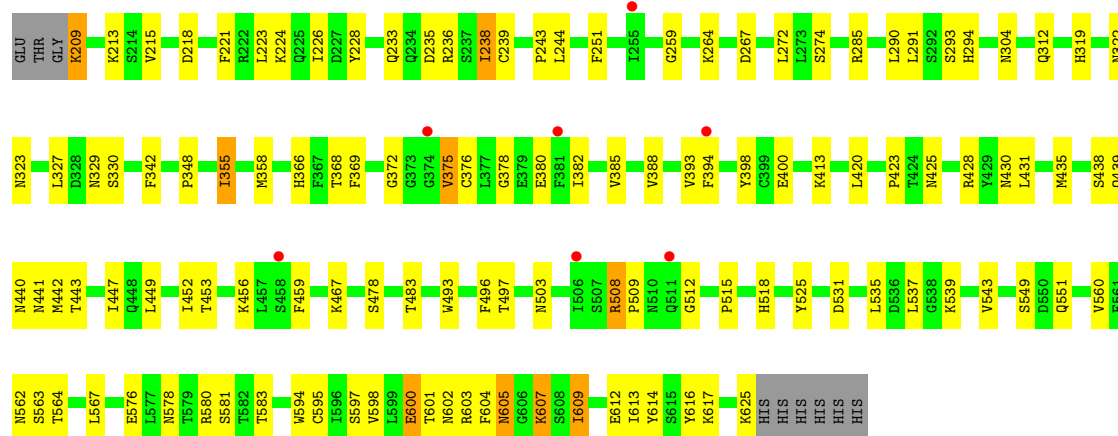




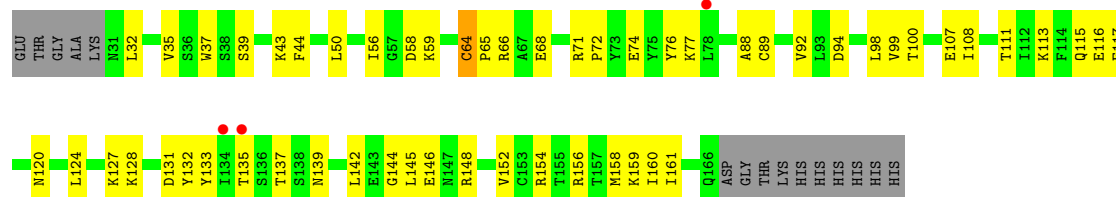
• Molecule 1: Attachment glycoprotein



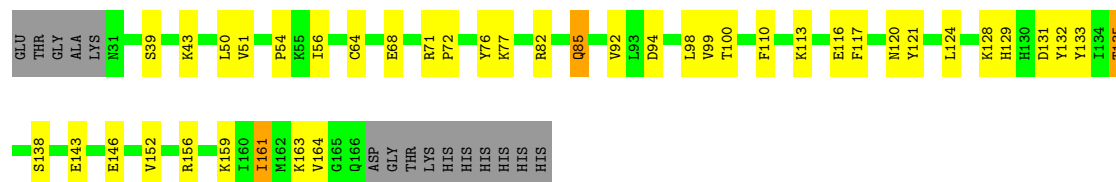
• Molecule 1: Attachment glycoprotein



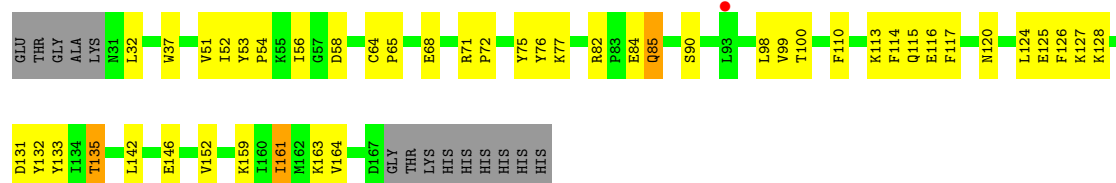
• Molecule 2: Ephrin-B1



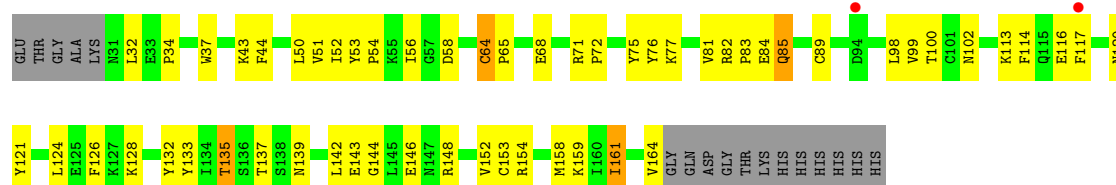
• Molecule 2: Ephrin-B1



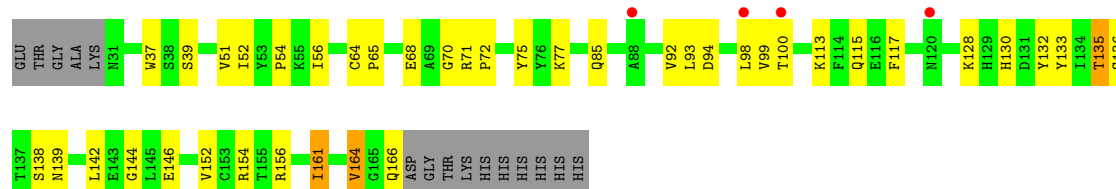
• Molecule 2: Ephrin-B1



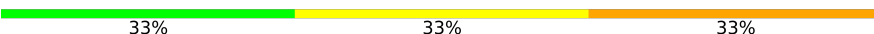
• Molecule 2: Ephrin-B1



• Molecule 2: Ephrin-B1



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

Chain K:  33% 33% 33%



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

Chain M:  33% 67%



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

Chain N:  67% 33%

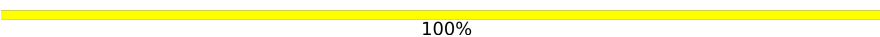


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  33% 67%

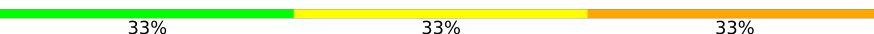


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

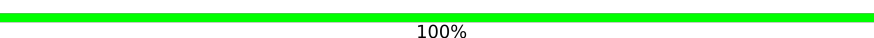


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  33% 33% 33%



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

Chain L:  100%



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

Chain P:  50% 50%

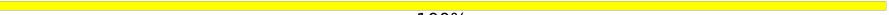


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



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

Chain S:  100%



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

Chain T:  50% 50%



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

Chain V:  100%



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

Chain W:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.80Å 138.44Å 235.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.22 – 4.07 69.22 – 4.07	Depositor EDS
% Data completeness (in resolution range)	99.6 (69.22-4.07) 99.6 (69.22-4.07)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 4.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.276 , 0.314 0.279 , 0.312	Depositor DCC
R_{free} test set	1475 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	118.1	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 137.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	22772	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/3434	0.53	0/4657
1	B	0.16	0/3441	0.54	0/4667
1	E	0.20	0/3413	0.55	0/4630
1	G	0.17	0/3413	0.52	0/4630
1	I	0.16	0/3430	0.51	1/4652 (0.0%)
2	C	0.13	0/1100	0.40	0/1487
2	D	0.14	0/1114	0.41	0/1505
2	F	0.13	0/1108	0.40	0/1498
2	H	0.13	0/1087	0.41	0/1470
2	J	0.15	0/1100	0.42	0/1487
All	All	0.16	0/22640	0.50	1/30683 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	604	PHE	N-CA-C	-5.98	101.67	110.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3351	0	3233	60	0
1	B	3358	0	3240	77	0
1	E	3330	0	3206	81	0
1	G	3330	0	3208	65	0
1	I	3347	0	3233	82	0
2	C	1076	0	1069	31	0
2	D	1089	0	1087	41	0
2	F	1084	0	1073	37	0
2	H	1063	0	1058	43	0
2	J	1076	0	1069	29	0
3	K	39	0	34	1	0
3	M	39	0	34	3	0
3	N	39	0	34	3	0
3	O	39	0	34	7	0
3	Q	39	0	34	1	0
3	U	39	0	34	1	0
4	L	28	0	25	0	0
4	P	28	0	25	2	0
4	R	28	0	25	0	0
4	S	28	0	25	2	0
4	T	28	0	25	1	0
4	V	28	0	25	0	0
4	W	28	0	25	1	0
5	A	56	0	52	1	0
5	B	42	0	39	0	0
5	D	14	0	13	1	0
5	E	14	0	13	1	0
5	F	14	0	13	1	0
5	G	42	0	39	2	0
5	H	14	0	13	1	0
5	I	28	0	26	4	0
5	J	14	0	13	2	0
All	All	22772	0	22076	512	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 11.

All (512) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:ASN:HB2	1:G:265:LYS:HZ2	1.27	1.00
1:B:209:LYS:H	2:H:34:PRO:HG2	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLN:OE1	1:B:442:MET:N	2.13	0.82
1:G:241:ASN:OD1	1:G:265:LYS:NZ	2.15	0.80
1:G:439:GLN:OE1	1:G:442:MET:N	2.14	0.79
2:F:56:ILE:HD11	2:F:128:LYS:HB2	1.65	0.79
1:G:230:ILE:HD13	1:G:611:PRO:HG2	1.65	0.78
1:I:439:GLN:OE1	1:I:442:MET:N	2.16	0.77
1:A:439:GLN:OE1	1:A:442:MET:N	2.17	0.77
1:E:325:LYS:NZ	2:H:83:PRO:O	2.17	0.77
1:E:439:GLN:OE1	1:E:442:MET:N	2.15	0.75
1:E:603:ARG:NH1	1:E:612:GLU:OE2	2.19	0.75
1:E:213:LYS:HD3	1:E:539:LYS:HG3	1.68	0.75
1:B:223:LEU:HD11	1:B:614:TYR:HB3	1.68	0.73
1:E:230:ILE:HD13	1:E:611:PRO:HG2	1.70	0.72
1:G:223:LEU:HD11	1:G:614:TYR:HB3	1.71	0.72
1:G:380:GLU:HG2	1:G:438:SER:HB3	1.71	0.71
1:I:581:SER:OG	1:I:600:GLU:OE2	2.03	0.70
2:C:56:ILE:HD11	2:C:128:LYS:HB2	1.74	0.70
2:D:88:ALA:O	2:D:154:ARG:NH2	2.25	0.70
1:B:440:ASN:O	1:B:443:THR:OG1	2.06	0.69
1:E:578:ASN:HD21	2:F:117:PHE:H	1.37	0.69
1:G:478:SER:O	1:G:508:ARG:NH2	2.24	0.69
1:E:609:ILE:HD11	2:F:116:GLU:HG2	1.74	0.69
2:D:135:THR:HG22	2:D:159:LYS:HB3	1.75	0.69
1:A:440:ASN:O	1:A:443:THR:OG1	2.09	0.69
1:E:578:ASN:HD22	1:E:602:ASN:HD22	1.42	0.68
1:A:407:GLN:OE1	1:A:407:GLN:N	2.26	0.68
1:I:578:ASN:HD21	2:J:117:PHE:HB2	1.59	0.68
1:I:233:GLN:HG2	1:I:238:ILE:HG12	1.76	0.68
1:A:567:LEU:HD22	3:O:1:NAG:H82	1.76	0.67
1:G:375:VAL:HG22	1:G:467:LYS:HG3	1.75	0.67
2:C:68:GLU:HB2	2:C:72:PRO:HD2	1.77	0.67
1:G:513:ASN:ND2	1:G:522:GLU:OE2	2.27	0.67
1:A:244:LEU:HD22	1:A:372:GLY:HA2	1.76	0.67
1:A:531:ASP:HB2	1:A:583:THR:HA	1.75	0.67
1:B:323:ASN:ND2	1:B:329:ASN:OD1	2.28	0.66
1:B:531:ASP:HB2	1:B:583:THR:HA	1.77	0.66
1:B:552:LEU:HD13	2:D:113:LYS:HB2	1.77	0.66
1:I:602:ASN:ND2	2:J:115:GLN:OE1	2.29	0.65
1:E:325:LYS:HZ3	2:H:84:GLU:HA	1.61	0.65
1:B:375:VAL:HG22	1:B:467:LYS:HG3	1.79	0.65
1:B:578:ASN:HD21	2:D:117:PHE:H	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:MET:HG2	1:B:258:GLU:HG2	1.79	0.65
1:I:453:THR:HB	1:I:497:THR:HG22	1.79	0.64
1:G:385:VAL:HG11	1:G:449:LEU:HD11	1.80	0.64
1:I:531:ASP:HB2	1:I:583:THR:HA	1.79	0.64
1:A:223:LEU:HD11	1:A:614:TYR:HB3	1.80	0.64
1:E:380:GLU:HG2	1:E:438:SER:HB3	1.79	0.63
1:B:269:PHE:HA	1:B:300:MET:HG2	1.79	0.63
1:I:609:ILE:HD11	2:J:117:PHE:CE2	2.33	0.63
2:H:43:LYS:HB3	2:H:50:LEU:HD13	1.81	0.63
2:D:56:ILE:HD11	2:D:128:LYS:HB2	1.80	0.63
1:I:244:LEU:HD22	1:I:372:GLY:HA2	1.80	0.63
1:I:213:LYS:HD3	1:I:539:LYS:HG3	1.80	0.62
1:E:223:LEU:HD11	1:E:614:TYR:HB3	1.79	0.62
5:D:201:NAG:H3	5:D:201:NAG:H83	1.82	0.62
2:H:89:CYS:SG	2:H:154:ARG:HG3	2.39	0.62
4:T:1:NAG:H3	4:T:1:NAG:H83	1.82	0.62
1:G:515:PRO:HB3	1:G:551:GLN:HG2	1.81	0.62
1:G:379:GLU:HG2	5:G:706:NAG:H62	1.82	0.62
1:G:221:PHE:HB3	1:G:616:TYR:HB2	1.80	0.61
2:C:76:TYR:HE2	2:C:152:VAL:HG21	1.65	0.61
1:E:342:PHE:HB3	1:E:348:PRO:HA	1.82	0.61
1:E:552:LEU:HD13	2:F:113:LYS:HB2	1.83	0.61
1:A:609:ILE:HD11	2:C:116:GLU:HG2	1.82	0.61
1:B:327:LEU:HD21	1:B:368:THR:HG23	1.82	0.61
1:G:552:LEU:HD13	2:H:113:LYS:HB2	1.82	0.61
2:D:98:LEU:HD23	2:D:99:VAL:HG12	1.83	0.60
1:A:240:MET:HG2	1:A:258:GLU:HG2	1.82	0.60
3:O:1:NAG:O7	3:O:1:NAG:O3	2.18	0.60
1:I:223:LEU:HD11	1:I:614:TYR:HB3	1.83	0.60
1:A:453:THR:HB	1:A:497:THR:HG22	1.81	0.60
1:A:230:ILE:HD13	1:A:611:PRO:HG2	1.84	0.60
1:E:327:LEU:HD21	1:E:368:THR:HG23	1.83	0.60
1:I:385:VAL:HG11	1:I:449:LEU:HD11	1.84	0.60
1:E:375:VAL:HG22	1:E:467:LYS:HG3	1.83	0.60
5:F:201:NAG:H83	5:F:201:NAG:H3	1.83	0.60
1:B:221:PHE:HB3	1:B:616:TYR:HB2	1.84	0.60
1:I:226:ILE:HG23	1:I:228:TYR:CZ	2.37	0.60
1:I:264:LYS:HB3	1:I:267:ASP:HB2	1.83	0.60
1:I:342:PHE:HB3	1:I:348:PRO:HA	1.84	0.60
2:F:77:LYS:NZ	2:F:146:GLU:OE2	2.34	0.60
1:E:394:PHE:HE1	1:E:431:LEU:HD22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:201:NAG:H83	5:J:201:NAG:H3	1.83	0.59
1:E:322:ASN:OD1	2:H:53:TYR:OH	2.19	0.59
1:G:264:LYS:HB3	1:G:267:ASP:HB2	1.84	0.59
1:I:221:PHE:HB3	1:I:616:TYR:HB2	1.84	0.59
3:N:1:NAG:O3	3:N:2:NAG:O5	2.18	0.59
1:G:531:ASP:HB2	1:G:583:THR:HA	1.85	0.59
1:A:229:VAL:HG21	1:A:288:LEU:HB2	1.85	0.59
1:I:603:ARG:NH1	1:I:612:GLU:OE2	2.35	0.59
1:G:453:THR:HB	1:G:497:THR:HG22	1.83	0.59
2:J:98:LEU:HD23	2:J:99:VAL:HG12	1.84	0.58
1:A:264:LYS:HB3	1:A:267:ASP:HB2	1.83	0.58
1:G:244:LEU:HD22	1:G:372:GLY:HA2	1.86	0.58
1:B:218:ASP:HB3	1:B:625:LYS:HG3	1.84	0.58
1:E:319:HIS:HD1	1:E:368:THR:HG22	1.68	0.58
1:A:380:GLU:HG2	1:A:438:SER:HB3	1.86	0.58
1:I:440:ASN:O	1:I:443:THR:OG1	2.17	0.58
1:G:440:ASN:O	1:G:443:THR:OG1	2.14	0.57
1:A:375:VAL:HG22	1:A:467:LYS:HG3	1.86	0.57
1:E:264:LYS:HB3	1:E:267:ASP:HB2	1.86	0.57
2:H:56:ILE:HD11	2:H:128:LYS:HB2	1.85	0.57
1:B:580:ARG:HB2	2:D:117:PHE:HB3	1.87	0.57
1:E:440:ASN:O	1:E:443:THR:OG1	2.11	0.57
4:W:1:NAG:H83	4:W:1:NAG:H3	1.85	0.57
1:E:319:HIS:ND1	1:E:368:THR:HG22	2.19	0.57
1:I:394:PHE:HE1	1:I:431:LEU:HD22	1.69	0.57
1:B:244:LEU:HD22	1:B:372:GLY:HA2	1.87	0.57
1:A:218:ASP:HB3	1:A:625:LYS:HG3	1.86	0.57
1:E:388:VAL:CG1	1:E:428:ARG:HD2	2.35	0.57
2:C:77:LYS:NZ	2:C:146:GLU:OE2	2.38	0.57
1:I:239:CYS:HA	1:I:609:ILE:HG23	1.87	0.57
2:C:77:LYS:HG3	2:C:100:THR:HG22	1.86	0.57
1:B:428:ARG:NH1	3:K:1:NAG:O6	2.38	0.57
1:A:342:PHE:HB3	1:A:348:PRO:HA	1.87	0.56
3:Q:2:NAG:O7	3:Q:2:NAG:O3	2.24	0.56
2:D:77:LYS:HG3	2:D:100:THR:HG22	1.88	0.56
1:I:425:ASN:OD1	1:I:428:ARG:N	2.38	0.56
1:I:578:ASN:ND2	2:J:117:PHE:HB2	2.20	0.56
5:H:201:NAG:H83	5:H:201:NAG:H3	1.86	0.56
1:I:509:PRO:HB3	1:I:549:SER:O	2.06	0.56
2:D:89:CYS:SG	2:D:154:ARG:HG3	2.46	0.56
1:E:453:THR:HB	1:E:497:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:ARG:HG3	2:D:158:MET:HG3	1.87	0.56
1:B:264:LYS:HB3	1:B:267:ASP:HB2	1.87	0.56
2:H:98:LEU:HD23	2:H:99:VAL:HG12	1.88	0.56
1:B:380:GLU:HG2	1:B:438:SER:HB3	1.88	0.55
1:A:327:LEU:HD21	1:A:368:THR:HG23	1.87	0.55
1:I:330:SER:O	1:I:428:ARG:NH2	2.38	0.55
1:B:304:ASN:HB3	1:B:369:PHE:O	2.07	0.55
2:D:139:ASN:HB2	2:D:144:GLY:HA3	1.87	0.55
2:J:92:VAL:HG23	2:J:94:ASP:H	1.70	0.55
1:B:453:THR:HB	1:B:497:THR:HG22	1.87	0.55
1:E:484:TYR:HE1	1:E:519:LYS:HG2	1.72	0.55
1:G:603:ARG:NH1	1:G:612:GLU:OE2	2.36	0.55
2:C:98:LEU:HD23	2:C:99:VAL:HG12	1.88	0.55
2:H:68:GLU:HB2	2:H:72:PRO:HD2	1.87	0.55
1:I:515:PRO:HB3	1:I:551:GLN:HG2	1.89	0.54
2:F:98:LEU:HD23	2:F:99:VAL:HG12	1.88	0.54
2:J:139:ASN:HB2	2:J:144:GLY:HA3	1.88	0.54
2:C:135:THR:HG23	2:C:159:LYS:HB3	1.89	0.54
1:A:394:PHE:HE1	1:A:431:LEU:HD22	1.72	0.54
2:F:135:THR:HG23	2:F:159:LYS:HB3	1.90	0.54
2:J:71:ARG:N	2:J:72:PRO:HD3	2.21	0.54
1:E:452:ILE:HA	1:E:496:PHE:HB3	1.89	0.54
2:H:76:TYR:HE2	2:H:152:VAL:HG21	1.71	0.54
1:E:240:MET:HG2	1:E:258:GLU:HG2	1.90	0.54
1:B:578:ASN:HD22	1:B:602:ASN:HD22	1.54	0.54
1:G:342:PHE:HB3	1:G:348:PRO:HA	1.88	0.54
1:G:578:ASN:HD21	2:H:117:PHE:H	1.54	0.54
1:B:319:HIS:ND1	1:B:368:THR:HG22	2.23	0.54
1:E:363:ARG:NH1	1:I:291:LEU:O	2.41	0.54
1:I:441:ASN:O	1:I:441:ASN:ND2	2.40	0.54
1:B:484:TYR:HE1	1:B:519:LYS:HG2	1.73	0.54
1:I:327:LEU:HD21	1:I:368:THR:HG23	1.89	0.54
2:H:37:TRP:O	2:H:65:PRO:HD3	2.08	0.54
1:B:239:CYS:SG	1:B:609:ILE:HG13	2.48	0.53
1:E:509:PRO:HB3	1:E:549:SER:O	2.08	0.53
1:G:327:LEU:HD21	1:G:368:THR:HG23	1.90	0.53
2:F:77:LYS:HG3	2:F:100:THR:HG22	1.90	0.53
1:E:283:ASP:N	1:E:283:ASP:OD1	2.38	0.53
1:G:388:VAL:CG1	1:G:428:ARG:HD2	2.39	0.53
1:I:435:MET:HE3	1:I:449:LEU:HD13	1.90	0.53
1:B:515:PRO:HB3	1:B:551:GLN:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:323:ASN:ND2	1:I:329:ASN:OD1	2.41	0.53
1:G:304:ASN:HB3	1:G:369:PHE:O	2.09	0.53
1:A:347:ARG:HH12	1:I:322:ASN:HD21	1.57	0.53
1:G:598:VAL:HG22	1:G:613:ILE:HG12	1.91	0.53
1:A:465:LEU:HD21	1:A:496:PHE:HZ	1.74	0.53
1:E:403:ASN:N	1:E:403:ASN:OD1	2.41	0.53
1:E:531:ASP:HB2	1:E:583:THR:HA	1.91	0.53
2:C:82:ARG:HE	2:C:85:GLN:HE21	1.57	0.53
2:D:43:LYS:HB3	2:D:50:LEU:HD13	1.91	0.53
1:I:251:PHE:CD1	1:I:312:GLN:HG2	2.43	0.53
3:M:1:NAG:O7	3:M:1:NAG:O3	2.26	0.52
1:G:556:PRO:HG2	1:G:572:VAL:HB	1.91	0.52
2:H:135:THR:HG23	2:H:159:LYS:HB3	1.92	0.52
2:J:77:LYS:NZ	2:J:146:GLU:OE2	2.42	0.52
1:E:244:LEU:HD22	1:E:372:GLY:HA2	1.91	0.52
1:G:578:ASN:HD21	2:H:117:PHE:HB2	1.74	0.52
3:U:2:NAG:O7	3:U:2:NAG:O3	2.24	0.52
2:F:68:GLU:HB2	2:F:72:PRO:HD2	1.91	0.52
1:G:452:ILE:HA	1:G:496:PHE:HB3	1.91	0.52
2:C:54:PRO:HG2	2:C:164:VAL:HG12	1.92	0.52
1:E:602:ASN:ND2	2:F:116:GLU:HB3	2.24	0.52
1:G:242:ASN:ND2	1:G:265:LYS:HE3	2.24	0.52
1:A:603:ARG:NH1	1:A:612:GLU:OE2	2.43	0.52
1:I:233:GLN:HG3	1:I:235:ASP:H	1.74	0.52
2:J:39:SER:O	2:J:156:ARG:NH2	2.42	0.52
1:B:330:SER:O	1:B:428:ARG:NH2	2.37	0.52
1:I:304:ASN:HB3	1:I:369:PHE:O	2.10	0.52
1:B:358:MET:HE3	1:B:449:LEU:HB2	1.91	0.52
2:J:130:HIS:H	2:J:164:VAL:HG22	1.73	0.52
2:D:66:ARG:HD3	2:D:107:GLU:HG2	1.92	0.51
1:A:602:ASN:ND2	2:C:116:GLU:HB3	2.25	0.51
1:B:251:PHE:CD1	1:B:312:GLN:HG2	2.45	0.51
1:B:230:ILE:HD13	1:B:611:PRO:HG2	1.91	0.51
1:B:385:VAL:HG11	1:B:449:LEU:HD11	1.92	0.51
1:G:388:VAL:HG11	1:G:428:ARG:HD2	1.91	0.51
1:I:601:THR:OG1	1:I:612:GLU:HG3	2.11	0.51
2:C:120:ASN:HD22	2:C:124:LEU:HD22	1.76	0.51
2:D:37:TRP:O	2:D:65:PRO:HD3	2.09	0.51
1:E:221:PHE:HB3	1:E:616:TYR:HB2	1.92	0.51
1:G:557:GLU:HG2	1:G:571:ARG:HA	1.93	0.51
1:A:221:PHE:HB3	1:A:616:TYR:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:609:ILE:CD1	2:F:116:GLU:HG2	2.39	0.51
1:I:512:GLY:HA2	2:J:99:VAL:HG23	1.93	0.51
2:H:32:LEU:HD13	2:H:58:ASP:HB3	1.93	0.51
1:A:535:LEU:HD11	1:A:543:VAL:HB	1.92	0.51
1:I:580:ARG:N	1:I:600:GLU:OE1	2.44	0.51
2:F:84:GLU:OE1	2:H:82:ARG:NH2	2.44	0.51
1:G:233:GLN:HG3	1:G:235:ASP:H	1.76	0.51
1:G:483:THR:HG22	1:G:518:HIS:O	2.10	0.51
1:A:385:VAL:HG11	1:A:449:LEU:HD11	1.93	0.51
1:E:398:TYR:CG	1:E:456:LYS:HG2	2.46	0.51
1:I:562:ASN:HB3	1:I:564:THR:H	1.76	0.51
2:C:39:SER:O	2:C:156:ARG:NH2	2.44	0.50
1:G:242:ASN:HB2	1:G:265:LYS:NZ	2.13	0.50
2:C:43:LYS:HB3	2:C:50:LEU:HD13	1.91	0.50
1:E:310:CYS:HB3	1:E:315:PHE:CE1	2.46	0.50
1:E:218:ASP:HB3	1:E:625:LYS:HG3	1.94	0.50
1:A:319:HIS:ND1	1:A:368:THR:HG22	2.27	0.50
1:E:515:PRO:HB3	1:E:551:GLN:HG2	1.93	0.50
2:F:52:ILE:HG22	2:F:54:PRO:HD3	1.94	0.50
2:H:71:ARG:N	2:H:72:PRO:HD3	2.27	0.50
1:A:578:ASN:HD21	2:C:117:PHE:HB2	1.77	0.50
1:G:593:PRO:HG2	1:G:618:ILE:HB	1.92	0.50
2:F:71:ARG:N	2:F:72:PRO:HD3	2.26	0.50
2:D:71:ARG:N	2:D:72:PRO:HD3	2.27	0.50
1:I:358:MET:HA	1:I:447:ILE:HG23	1.93	0.50
2:F:37:TRP:O	2:F:65:PRO:HD3	2.10	0.49
1:I:560:VAL:HG12	1:I:567:LEU:HD12	1.93	0.49
2:F:76:TYR:HE2	2:F:152:VAL:HG21	1.76	0.49
2:H:77:LYS:HG3	2:H:100:THR:HG22	1.95	0.49
3:N:1:NAG:O3	3:N:2:NAG:O6	2.27	0.49
1:I:598:VAL:HG22	1:I:613:ILE:HG12	1.94	0.49
1:B:407:GLN:OE1	1:B:407:GLN:N	2.45	0.49
2:F:116:GLU:O	2:F:125:GLU:HA	2.13	0.49
2:F:116:GLU:OE1	2:F:127:LYS:HG3	2.13	0.49
1:A:503:ASN:HA	1:A:563:SER:O	2.12	0.49
2:C:71:ARG:N	2:C:72:PRO:HD3	2.28	0.49
1:B:509:PRO:HB3	1:B:549:SER:O	2.13	0.49
1:A:263:CYS:SG	1:A:609:ILE:HD12	2.53	0.49
1:I:380:GLU:HG2	1:I:438:SER:HB3	1.94	0.49
1:B:300:MET:HE2	1:B:300:MET:HB3	1.71	0.48
1:E:226:ILE:HG23	1:E:228:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:578:ASN:ND2	2:F:117:PHE:HB2	2.28	0.48
1:E:388:VAL:HG13	1:E:428:ARG:HD2	1.95	0.48
1:B:513:ASN:CG	2:D:108:ILE:HD11	2.38	0.48
1:A:275:HIS:ND1	1:A:314:SER:OG	2.36	0.48
2:C:92:VAL:HG23	2:C:94:ASP:H	1.79	0.48
1:A:513:ASN:HB3	1:A:522:GLU:OE2	2.14	0.48
1:A:609:ILE:CD1	2:C:116:GLU:HG2	2.43	0.48
2:D:92:VAL:HG23	2:D:94:ASP:H	1.79	0.48
1:E:269:PHE:HA	1:E:300:MET:HG2	1.96	0.48
1:I:218:ASP:HB3	1:I:625:LYS:HG3	1.96	0.48
1:B:310:CYS:HB3	1:B:315:PHE:CE1	2.48	0.48
1:A:310:CYS:HB3	1:A:315:PHE:CE1	2.49	0.48
2:D:32:LEU:HB2	2:D:59:LYS:O	2.14	0.47
2:F:82:ARG:HD2	2:H:82:ARG:NH1	2.28	0.47
2:J:56:ILE:HD13	2:J:128:LYS:HD2	1.96	0.47
1:B:392:ASP:OD2	1:B:417:SER:OG	2.32	0.47
1:I:319:HIS:ND1	1:I:368:THR:HG22	2.28	0.47
1:I:375:VAL:HG22	1:I:467:LYS:HG3	1.95	0.47
2:C:131:ASP:HB3	2:C:133:TYR:HE1	1.79	0.47
1:E:379:GLU:HG2	5:E:701:NAG:O3	2.13	0.47
1:G:265:LYS:HA	1:G:265:LYS:HE2	1.97	0.47
2:J:52:ILE:HG22	2:J:54:PRO:HD3	1.96	0.47
1:B:394:PHE:HE1	1:B:431:LEU:HD22	1.79	0.47
1:E:394:PHE:CE1	1:E:431:LEU:HD22	2.50	0.47
2:D:152:VAL:HG13	2:D:156:ARG:HB3	1.97	0.47
1:E:304:ASN:HB3	1:E:369:PHE:O	2.15	0.47
1:I:382:ILE:HG21	1:I:493:TRP:CZ3	2.50	0.47
1:I:605:ASN:O	1:I:605:ASN:ND2	2.47	0.47
2:H:52:ILE:HG22	2:H:54:PRO:HD3	1.96	0.47
2:H:85:GLN:H	2:H:85:GLN:HG3	1.49	0.47
4:S:1:NAG:O7	4:S:1:NAG:O3	2.33	0.47
1:B:515:PRO:HD2	1:B:518:HIS:HB2	1.97	0.47
1:E:358:MET:HE2	1:E:447:ILE:HG21	1.97	0.47
2:H:135:THR:HG21	2:H:153:CYS:SG	2.55	0.47
1:B:217:LYS:HD3	1:B:217:LYS:HA	1.83	0.47
1:E:578:ASN:HD21	2:F:117:PHE:HB2	1.80	0.47
2:J:70:GLY:C	2:J:72:PRO:HD3	2.39	0.47
1:A:215:VAL:HG23	3:O:1:NAG:C8	2.46	0.46
2:H:75:TYR:CD2	2:H:142:LEU:HB3	2.51	0.46
2:F:131:ASP:HB3	2:F:133:TYR:HE1	1.81	0.46
1:A:347:ARG:NH1	1:I:322:ASN:HD21	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:ILE:HG23	1:E:358:MET:CE	2.45	0.46
1:E:478:SER:O	1:E:508:ARG:NH2	2.49	0.46
1:G:578:ASN:ND2	2:H:117:PHE:HB2	2.31	0.46
2:F:85:GLN:HB2	2:F:90:SER:O	2.16	0.46
3:M:1:NAG:O3	3:M:2:NAG:O5	2.21	0.46
1:A:478:SER:O	1:A:508:ARG:NH2	2.49	0.46
1:I:430:ASN:HB2	1:I:459:PHE:CE1	2.50	0.46
1:B:408:THR:HG21	2:D:142:LEU:HD22	1.97	0.46
1:A:567:LEU:CD2	3:O:1:NAG:H82	2.45	0.46
1:E:557:GLU:OE1	1:E:569:LYS:HD2	2.16	0.46
2:J:68:GLU:HB2	2:J:72:PRO:HD2	1.98	0.46
1:B:578:ASN:ND2	2:D:115:GLN:HB3	2.31	0.46
1:A:605:ASN:HD22	1:A:605:ASN:C	2.22	0.46
1:G:319:HIS:ND1	1:G:368:THR:HG22	2.31	0.46
1:I:355:ILE:H	1:I:355:ILE:HG13	1.28	0.46
2:H:77:LYS:NZ	2:H:146:GLU:OE2	2.49	0.46
1:B:342:PHE:HB3	1:B:348:PRO:HA	1.98	0.46
1:A:251:PHE:CD1	1:A:312:GLN:HG2	2.51	0.46
1:G:300:MET:HE2	1:G:300:MET:HB3	1.89	0.46
2:J:139:ASN:HB3	5:J:201:NAG:H82	1.98	0.46
1:A:505:VAL:HB	1:A:566:ILE:HG13	1.97	0.46
1:G:509:PRO:HB3	1:G:549:SER:O	2.16	0.46
2:C:138:SER:O	2:C:152:VAL:HG23	2.16	0.46
4:S:1:NAG:O3	4:S:2:NAG:O5	2.27	0.46
1:B:557:GLU:OE1	1:B:569:LYS:HD2	2.16	0.45
1:A:215:VAL:HG23	3:O:1:NAG:H81	1.97	0.45
1:I:272:LEU:HD11	1:I:293:SER:OG	2.15	0.45
2:D:32:LEU:HD13	2:D:58:ASP:HB3	1.98	0.45
1:B:574:LYS:H	1:B:574:LYS:HD2	1.82	0.45
1:E:578:ASN:HB3	1:E:602:ASN:HB3	1.99	0.45
1:B:574:LYS:HE3	1:A:574:LYS:HE3	1.99	0.45
1:G:331:ASP:OD2	1:G:333:SER:OG	2.26	0.45
1:G:394:PHE:HE1	1:G:431:LEU:HD22	1.81	0.45
1:A:552:LEU:HD13	2:C:113:LYS:HB2	1.98	0.45
1:G:251:PHE:CD1	1:G:312:GLN:HG2	2.51	0.45
2:F:114:PHE:HA	2:F:126:PHE:CD2	2.52	0.45
1:A:304:ASN:HB3	1:A:369:PHE:O	2.17	0.45
1:A:226:ILE:HG23	1:A:228:TYR:CZ	2.52	0.45
1:I:600:GLU:HG2	2:J:117:PHE:CE2	2.52	0.45
1:B:398:TYR:CG	1:B:456:LYS:HG2	2.52	0.45
1:A:483:THR:HG21	1:A:518:HIS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:576:GLU:OE1	2:J:113:LYS:NZ	2.31	0.45
1:G:452:ILE:HG13	1:G:496:PHE:HD2	1.81	0.45
3:N:1:NAG:HO3	3:N:2:NAG:HO6	1.61	0.45
1:B:215:VAL:HG23	3:M:1:NAG:C8	2.47	0.45
2:J:37:TRP:O	2:J:65:PRO:HD3	2.17	0.45
1:E:342:PHE:HD1	1:E:342:PHE:N	2.14	0.44
1:E:483:THR:HG21	1:E:518:HIS:HB3	1.99	0.44
1:I:224:LYS:HZ2	1:I:285:ARG:HD2	1.82	0.44
1:B:342:PHE:HD1	1:B:342:PHE:N	2.15	0.44
1:B:218:ASP:HB3	1:B:625:LYS:CG	2.47	0.44
2:D:39:SER:O	2:D:156:ARG:NH2	2.51	0.44
1:I:595:CYS:HB2	1:I:616:TYR:CE2	2.53	0.44
2:J:132:TYR:C	2:J:133:TYR:HD1	2.26	0.44
1:B:578:ASN:HD21	2:D:117:PHE:HB2	1.81	0.44
1:A:562:ASN:HB2	1:A:565:THR:O	2.17	0.44
1:I:215:VAL:HG23	5:I:704:NAG:H81	2.00	0.44
1:I:535:LEU:HD11	1:I:543:VAL:HB	1.98	0.44
2:F:75:TYR:CD2	2:F:142:LEU:HB3	2.52	0.44
1:B:240:MET:HA	1:B:257:TYR:O	2.17	0.44
1:G:240:MET:HG2	1:G:258:GLU:HG2	1.99	0.44
1:G:272:LEU:HD12	1:G:294:HIS:O	2.18	0.44
1:G:308:VAL:HG22	1:G:374:GLY:HA3	2.00	0.44
3:O:2:NAG:H3	3:O:3:BMA:H2	1.99	0.44
1:B:483:THR:HG21	1:B:518:HIS:HB3	2.00	0.44
1:B:557:GLU:HG2	1:B:571:ARG:HA	2.00	0.44
1:A:502:ASN:HB3	5:A:708:NAG:O5	2.17	0.44
2:H:114:PHE:HA	2:H:126:PHE:CD2	2.53	0.44
1:B:578:ASN:ND2	2:D:117:PHE:HB2	2.32	0.44
1:I:226:ILE:HG23	1:I:228:TYR:CE2	2.53	0.44
2:J:75:TYR:CD2	2:J:142:LEU:HB3	2.53	0.44
1:B:219:PRO:O	1:B:625:LYS:HE2	2.18	0.44
1:E:355:ILE:HG23	1:E:358:MET:HE3	1.99	0.44
1:I:605:ASN:HD22	1:I:605:ASN:N	2.14	0.44
2:D:64:CYS:SG	2:D:65:PRO:HD2	2.58	0.44
2:D:132:TYR:C	2:D:133:TYR:HD1	2.25	0.44
1:G:602:ASN:ND2	2:H:116:GLU:HB3	2.33	0.44
2:H:82:ARG:H	2:H:85:GLN:NE2	2.16	0.44
1:E:562:ASN:HB2	1:E:565:THR:O	2.17	0.43
1:G:407:GLN:HG2	2:H:102:ASN:ND2	2.33	0.43
1:I:319:HIS:HD1	1:I:368:THR:HG22	1.82	0.43
1:G:272:LEU:HD11	1:G:293:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:452:ILE:HA	1:I:496:PHE:HB3	1.99	0.43
2:J:77:LYS:HG3	2:J:100:THR:HG22	2.00	0.43
2:D:120:ASN:HD22	2:D:124:LEU:HD22	1.83	0.43
1:E:452:ILE:HG13	1:E:496:PHE:HD2	1.82	0.43
1:E:489:PHE:CE2	1:E:537:LEU:HD21	2.53	0.43
1:B:233:GLN:HG3	1:B:235:ASP:H	1.83	0.43
1:B:342:PHE:N	1:B:342:PHE:CD1	2.85	0.43
1:A:336:GLU:OE1	1:A:338:TYR:OH	2.17	0.43
1:I:378:GLY:O	5:I:701:NAG:H5	2.19	0.43
2:H:132:TYR:C	2:H:133:TYR:HD1	2.26	0.43
1:B:355:ILE:H	1:B:355:ILE:HG13	1.26	0.43
2:D:68:GLU:HB2	2:D:72:PRO:HD2	1.99	0.43
1:E:272:LEU:HD11	1:E:293:SER:OG	2.19	0.43
1:E:325:LYS:NZ	2:H:84:GLU:HA	2.33	0.43
1:E:342:PHE:N	1:E:342:PHE:CD1	2.85	0.43
1:E:593:PRO:HG2	1:E:618:ILE:HB	2.00	0.43
1:I:581:SER:H	1:I:600:GLU:CD	2.23	0.43
2:C:161:ILE:HD11	2:C:163:LYS:HE3	2.00	0.43
2:F:32:LEU:HD13	2:F:58:ASP:HB3	2.00	0.43
1:A:251:PHE:CE1	1:A:312:GLN:HG2	2.53	0.43
1:A:558:ILE:O	1:A:569:LYS:HA	2.19	0.43
2:H:120:ASN:HD22	2:H:124:LEU:HD22	1.84	0.43
2:J:51:VAL:HA	2:J:161:ILE:HG23	1.99	0.43
1:B:258:GLU:HB2	1:B:270:LYS:HB2	2.00	0.43
1:B:605:ASN:OD1	1:B:605:ASN:N	2.36	0.43
1:A:308:VAL:HG22	1:A:374:GLY:HA3	2.01	0.43
1:E:336:GLU:OE1	4:P:1:NAG:H82	2.18	0.43
1:G:394:PHE:CE1	1:G:431:LEU:HD22	2.54	0.43
1:G:456:LYS:HD2	1:G:500:TRP:CD1	2.54	0.43
1:I:483:THR:HG21	1:I:518:HIS:HB3	2.00	0.43
2:H:81:VAL:HB	2:H:85:GLN:OE1	2.19	0.43
1:B:270:LYS:HD3	1:B:295:TYR:CE1	2.53	0.43
1:B:562:ASN:HB2	1:B:565:THR:O	2.19	0.43
1:E:399:CYS:SG	1:E:521:PRO:HB3	2.59	0.43
1:I:400:GLU:OE2	1:I:413:LYS:HG3	2.19	0.43
1:A:601:THR:O	1:A:609:ILE:HG23	2.18	0.42
1:E:251:PHE:CE1	1:E:312:GLN:HG2	2.54	0.42
1:I:398:TYR:CG	1:I:456:LYS:HG2	2.54	0.42
1:I:478:SER:O	1:I:508:ARG:NH2	2.52	0.42
1:A:398:TYR:CG	1:A:456:LYS:HG2	2.54	0.42
1:E:578:ASN:ND2	2:F:117:PHE:H	2.10	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:294:HIS:CD2	1:I:348:PRO:HG3	2.54	0.42
2:C:51:VAL:HA	2:C:161:ILE:HG23	2.00	0.42
1:E:485:LEU:HD21	1:E:532:ILE:HD13	2.01	0.42
1:G:270:LYS:HD3	1:G:295:TYR:CE1	2.54	0.42
1:G:406:VAL:H	1:G:406:VAL:HG22	1.60	0.42
1:I:243:PRO:CD	1:I:600:GLU:HB3	2.49	0.42
2:F:53:TYR:HA	2:F:163:LYS:O	2.19	0.42
1:B:331:ASP:OD2	1:B:333:SER:OG	2.31	0.42
1:B:592:GLU:HG2	1:B:620:LYS:NZ	2.33	0.42
1:I:236:ARG:HG3	1:I:607:LYS:HB2	2.00	0.42
1:I:503:ASN:HA	1:I:563:SER:O	2.19	0.42
2:J:64:CYS:SG	2:J:65:PRO:HD2	2.59	0.42
1:B:602:ASN:ND2	2:D:116:GLU:HB3	2.34	0.42
1:I:567:LEU:CD2	5:I:704:NAG:H82	2.49	0.42
1:B:580:ARG:HB2	2:D:117:PHE:CG	2.54	0.42
1:E:509:PRO:CD	1:E:547:LEU:HB2	2.50	0.42
1:I:218:ASP:HB3	1:I:625:LYS:CG	2.49	0.42
2:F:115:GLN:O	2:F:126:PHE:HB2	2.20	0.42
1:I:209:LYS:HD2	1:I:213:LYS:NZ	2.34	0.42
2:C:129:HIS:N	2:C:164:VAL:HG23	2.35	0.42
2:C:132:TYR:C	2:C:133:TYR:HD1	2.28	0.42
2:F:132:TYR:C	2:F:133:TYR:HD1	2.28	0.42
2:J:135:THR:HG22	2:J:136:SER:H	1.85	0.42
2:D:137:THR:OG1	2:D:148:ARG:HA	2.20	0.42
2:D:142:LEU:HA	2:D:145:LEU:HB2	2.02	0.42
1:E:452:ILE:HG13	1:E:496:PHE:CD2	2.55	0.42
1:G:327:LEU:HD22	1:G:388:VAL:HG21	2.01	0.42
1:I:567:LEU:HD22	5:I:704:NAG:H82	2.02	0.42
2:H:54:PRO:HG2	2:H:164:VAL:HG12	2.01	0.42
1:G:428:ARG:NH1	1:G:430:ASN:OD1	2.53	0.42
2:H:64:CYS:SG	2:H:65:PRO:HD2	2.60	0.42
1:I:600:GLU:HG2	1:I:600:GLU:O	2.20	0.42
1:B:484:TYR:CE1	1:B:519:LYS:HG2	2.53	0.41
2:D:77:LYS:NZ	2:D:146:GLU:OE2	2.48	0.41
2:F:51:VAL:HA	2:F:161:ILE:HG23	2.01	0.41
3:O:1:NAG:HO3	3:O:1:NAG:C7	2.26	0.41
2:D:74:GLU:OE1	2:D:76:TYR:OH	2.25	0.41
1:E:388:VAL:HG11	1:E:428:ARG:HD2	2.01	0.41
1:E:511:GLN:HB3	2:F:110:PHE:CE2	2.55	0.41
1:E:562:ASN:HB3	1:E:564:THR:H	1.85	0.41
2:C:120:ASN:OD1	2:C:121:TYR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:138:SER:O	2:J:152:VAL:HG23	2.20	0.41
1:B:603:ARG:NH1	1:B:612:GLU:OE2	2.52	0.41
1:G:310:CYS:HB3	1:G:315:PHE:CE1	2.56	0.41
1:B:355:ILE:HG22	1:B:358:MET:SD	2.60	0.41
2:D:44:PHE:CD1	2:D:158:MET:HA	2.55	0.41
1:E:233:GLN:HG3	1:E:235:ASP:H	1.86	0.41
1:E:473:LEU:HB2	1:E:489:PHE:CE1	2.56	0.41
1:G:358:MET:HE2	1:G:449:LEU:HB2	2.02	0.41
2:D:74:GLU:HB3	2:D:76:TYR:HE1	1.85	0.41
1:A:511:GLN:HB3	2:C:110:PHE:CE2	2.56	0.41
1:E:594:TRP:CH2	1:E:617:LYS:HB2	2.56	0.41
1:G:226:ILE:HG23	1:G:228:TYR:CZ	2.56	0.41
1:I:594:TRP:CH2	1:I:617:LYS:HB2	2.55	0.41
2:F:85:GLN:H	2:F:85:GLN:HG3	1.64	0.41
1:B:244:LEU:HD13	1:B:307:PRO:HD3	2.03	0.41
2:D:116:GLU:OE1	2:D:127:LYS:HD2	2.21	0.41
1:G:452:ILE:HG13	1:G:496:PHE:CD2	2.55	0.41
1:G:513:ASN:ND2	2:H:100:THR:OG1	2.51	0.41
2:F:120:ASN:HD22	2:F:124:LEU:HD22	1.85	0.41
2:H:51:VAL:HA	2:H:161:ILE:HG23	2.02	0.41
2:H:137:THR:OG1	2:H:148:ARG:HA	2.21	0.41
1:A:542:TYR:HB2	1:A:561:PHE:CE1	2.55	0.41
1:E:300:MET:HE2	1:E:300:MET:HB3	1.81	0.41
2:H:44:PHE:CD1	2:H:158:MET:HA	2.56	0.41
1:B:382:ILE:HG21	1:B:493:TRP:CZ3	2.56	0.41
1:B:400:GLU:OE2	1:B:413:LYS:HG3	2.21	0.41
2:D:35:VAL:HG11	2:D:160:ILE:HD11	2.01	0.41
1:E:589:PHE:HB3	1:E:594:TRP:CD1	2.56	0.41
1:B:328:ASP:OD1	1:B:424:THR:OG1	2.38	0.41
1:E:578:ASN:HD21	2:F:117:PHE:N	2.10	0.41
1:I:274:SER:HB3	1:I:290:LEU:HD11	2.02	0.41
1:I:583:THR:O	1:I:597:SER:HA	2.21	0.41
2:F:161:ILE:HD11	2:F:163:LYS:HE3	2.02	0.41
2:J:93:LEU:HD23	2:J:93:LEU:HA	1.94	0.41
1:A:509:PRO:HB3	1:A:549:SER:O	2.21	0.41
1:E:513:ASN:ND2	2:F:100:THR:OG1	2.52	0.41
1:E:558:ILE:O	1:E:569:LYS:HA	2.21	0.41
1:G:535:LEU:HD11	1:G:543:VAL:HB	2.03	0.41
2:C:76:TYR:CE2	2:C:152:VAL:HG21	2.52	0.41
2:C:129:HIS:H	2:C:164:VAL:HG23	1.86	0.41
1:B:551:GLN:OE1	2:D:111:THR:N	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:ASP:HB3	2:D:133:TYR:CE1	2.56	0.40
1:I:238:ILE:HA	1:I:259:GLY:O	2.21	0.40
1:I:423:PRO:HB3	1:I:525:TYR:CD2	2.56	0.40
2:C:82:ARG:H	2:C:85:GLN:NE2	2.19	0.40
2:J:156:ARG:HA	2:J:156:ARG:HD2	1.93	0.40
2:C:85:GLN:H	2:C:85:GLN:HG3	1.57	0.40
1:E:211:PHE:HZ	1:E:536:ASP:HB2	1.86	0.40
5:G:705:NAG:O7	5:G:705:NAG:O3	2.33	0.40
2:H:139:ASN:HB2	2:H:144:GLY:HA3	2.03	0.40
1:B:402:PHE:HD1	1:B:402:PHE:HA	1.77	0.40
1:A:355:ILE:H	1:A:355:ILE:HG13	1.33	0.40
1:G:407:GLN:HG2	2:H:102:ASN:HD21	1.86	0.40
1:G:485:LEU:HD21	1:G:532:ILE:HD13	2.03	0.40
4:P:1:NAG:O7	4:P:1:NAG:H3	2.21	0.40
1:B:226:ILE:HG23	1:B:228:TYR:CZ	2.57	0.40
1:A:494:LYS:HA	1:A:495:PRO:HA	1.95	0.40
1:I:388:VAL:HG11	1:I:428:ARG:HE	1.86	0.40
2:H:120:ASN:OD1	2:H:121:TYR:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	416/426 (98%)	395 (95%)	21 (5%)	0	100	100
1	B	417/426 (98%)	396 (95%)	20 (5%)	1 (0%)	43	75
1	E	413/426 (97%)	393 (95%)	20 (5%)	0	100	100
1	G	413/426 (97%)	394 (95%)	19 (5%)	0	100	100
1	I	415/426 (97%)	395 (95%)	19 (5%)	1 (0%)	43	75
2	C	134/151 (89%)	114 (85%)	20 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	134/151 (89%)	114 (85%)	20 (15%)	0	100	100
2	F	135/151 (89%)	115 (85%)	20 (15%)	0	100	100
2	H	132/151 (87%)	112 (85%)	20 (15%)	0	100	100
2	J	134/151 (89%)	115 (86%)	19 (14%)	0	100	100
All	All	2743/2885 (95%)	2543 (93%)	198 (7%)	2 (0%)	48	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	ILE
1	I	607	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/398 (98%)	376 (96%)	14 (4%)	31	53
1	B	391/398 (98%)	374 (96%)	17 (4%)	26	49
1	E	388/398 (98%)	377 (97%)	11 (3%)	38	59
1	G	388/398 (98%)	378 (97%)	10 (3%)	40	61
1	I	390/398 (98%)	377 (97%)	13 (3%)	33	56
2	C	119/133 (90%)	114 (96%)	5 (4%)	26	49
2	D	121/133 (91%)	119 (98%)	2 (2%)	53	68
2	F	120/133 (90%)	115 (96%)	5 (4%)	26	49
2	H	118/133 (89%)	113 (96%)	5 (4%)	26	49
2	J	119/133 (90%)	113 (95%)	6 (5%)	22	45
All	All	2544/2655 (96%)	2456 (96%)	88 (4%)	32	54

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	216	SER
1	B	260	ILE
1	B	342	PHE
1	B	343	ASN
1	B	355	ILE
1	B	357	ASN
1	B	366	HIS
1	B	375	VAL
1	B	376	CYS
1	B	393	VAL
1	B	403	ASN
1	B	407	GLN
1	B	420	LEU
1	B	508	ARG
1	B	537	LEU
1	B	605	ASN
1	B	609	ILE
2	D	64	CYS
2	D	161	ILE
1	A	324	THR
1	A	355	ILE
1	A	357	ASN
1	A	366	HIS
1	A	375	VAL
1	A	376	CYS
1	A	393	VAL
1	A	403	ASN
1	A	406	VAL
1	A	420	LEU
1	A	508	ARG
1	A	522	GLU
1	A	537	LEU
1	A	605	ASN
1	E	283	ASP
1	E	341	TYR
1	E	342	PHE
1	E	366	HIS
1	E	375	VAL
1	E	376	CYS
1	E	393	VAL
1	E	403	ASN
1	E	420	LEU
1	E	508	ARG

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Mol	Chain	Res	Type
1	E	537	LEU
1	G	358	MET
1	G	366	HIS
1	G	375	VAL
1	G	376	CYS
1	G	393	VAL
1	G	403	ASN
1	G	420	LEU
1	G	508	ARG
1	G	537	LEU
1	G	605	ASN
1	I	209	LYS
1	I	238	ILE
1	I	355	ILE
1	I	366	HIS
1	I	375	VAL
1	I	376	CYS
1	I	393	VAL
1	I	420	LEU
1	I	508	ARG
1	I	537	LEU
1	I	600	GLU
1	I	605	ASN
1	I	609	ILE
2	C	64	CYS
2	C	85	GLN
2	C	135	THR
2	C	143	GLU
2	C	161	ILE
2	F	64	CYS
2	F	85	GLN
2	F	135	THR
2	F	161	ILE
2	F	164	VAL
2	H	64	CYS
2	H	85	GLN
2	H	135	THR
2	H	143	GLU
2	H	161	ILE
2	J	85	GLN
2	J	135	THR
2	J	154	ARG

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Mol	Chain	Res	Type
2	J	161	ILE
2	J	164	VAL
2	J	166	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	578	ASN
1	B	602	ASN
2	D	31	ASN
2	D	41	ASN
1	A	233	GLN
1	A	241	ASN
1	A	242	ASN
1	A	396	HIS
1	A	450	ASN
1	A	578	ASN
1	A	602	ASN
1	E	396	HIS
1	E	578	ASN
1	E	602	ASN
1	G	233	GLN
1	G	242	ASN
1	G	578	ASN
1	G	602	ASN
1	I	294	HIS
1	I	323	ASN
1	I	329	ASN
1	I	450	ASN
1	I	578	ASN
1	I	605	ASN
2	C	31	ASN
2	C	102	ASN
2	F	147	ASN
2	J	102	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

32 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	K	1	1,3	14,14,15	0.63	0	17,19,21	0.92	1 (5%)
3	NAG	K	2	3	14,14,15	0.45	0	17,19,21	1.34	2 (11%)
3	BMA	K	3	3	11,11,12	0.82	0	15,15,17	0.75	0
4	NAG	L	1	1,4	14,14,15	0.17	0	17,19,21	0.54	0
4	NAG	L	2	4	14,14,15	0.31	0	17,19,21	0.40	0
3	NAG	M	1	1,3	14,14,15	0.88	2 (14%)	17,19,21	0.80	0
3	NAG	M	2	3	14,14,15	0.64	0	17,19,21	0.80	1 (5%)
3	BMA	M	3	3	11,11,12	0.52	0	15,15,17	0.98	1 (6%)
3	NAG	N	1	1,3	14,14,15	0.31	0	17,19,21	0.60	0
3	NAG	N	2	3	14,14,15	0.43	0	17,19,21	1.01	1 (5%)
3	BMA	N	3	3	11,11,12	0.69	0	15,15,17	1.00	1 (6%)
3	NAG	O	1	1,3	14,14,15	0.48	0	17,19,21	0.69	0
3	NAG	O	2	3	14,14,15	0.81	2 (14%)	17,19,21	0.73	1 (5%)
3	BMA	O	3	3	11,11,12	0.81	0	15,15,17	1.31	1 (6%)
4	NAG	P	1	1,4	14,14,15	0.39	0	17,19,21	0.82	1 (5%)
4	NAG	P	2	4	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	Q	1	1,3	14,14,15	0.25	0	17,19,21	0.80	1 (5%)
3	NAG	Q	2	3	14,14,15	0.32	0	17,19,21	0.71	0
3	BMA	Q	3	3	11,11,12	0.42	0	15,15,17	0.83	1 (6%)
4	NAG	R	1	1,4	14,14,15	0.34	0	17,19,21	0.49	0
4	NAG	R	2	4	14,14,15	0.27	0	17,19,21	0.41	0
4	NAG	S	1	1,4	14,14,15	0.59	0	17,19,21	0.64	0
4	NAG	S	2	4	14,14,15	0.67	0	17,19,21	0.53	0
4	NAG	T	1	1,4	14,14,15	0.57	0	17,19,21	1.35	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	T	2	4	14,14,15	0.35	0	17,19,21	0.31	0
3	NAG	U	1	1,3	14,14,15	0.25	0	17,19,21	1.05	2 (11%)
3	NAG	U	2	3	14,14,15	0.43	0	17,19,21	0.92	1 (5%)
3	BMA	U	3	3	11,11,12	0.64	0	15,15,17	0.74	0
4	NAG	V	1	1,4	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	V	2	4	14,14,15	0.31	0	17,19,21	0.54	0
4	NAG	W	1	2,4	14,14,15	0.67	1 (7%)	17,19,21	1.45	3 (17%)
4	NAG	W	2	4	14,14,15	0.40	0	17,19,21	0.49	0

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

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1	NAG	O5-C1	-2.29	1.39	1.43
4	W	1	NAG	C1-C2	2.27	1.55	1.52
3	M	1	NAG	C1-C2	2.17	1.55	1.52
3	O	2	NAG	O5-C1	2.13	1.47	1.43
3	O	2	NAG	C1-C2	2.06	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	1	NAG	C2-N2-C7	4.59	129.05	122.90
4	T	1	NAG	C2-N2-C7	4.44	128.85	122.90
3	K	2	NAG	C2-N2-C7	4.41	128.81	122.90
3	O	3	BMA	C1-O5-C5	4.16	117.76	112.19
3	U	1	NAG	O4-C4-C5	-3.11	101.67	109.32
3	N	3	BMA	C1-O5-C5	2.95	116.14	112.19
3	M	2	NAG	C1-O5-C5	2.64	115.72	112.19
3	K	2	NAG	O4-C4-C3	-2.50	104.49	110.38
3	U	1	NAG	O4-C4-C3	-2.47	104.56	110.38
3	N	2	NAG	O4-C4-C3	2.42	116.08	110.38
4	W	1	NAG	C1-O5-C5	2.38	115.37	112.19
3	U	2	NAG	O3-C3-C2	-2.34	104.54	109.40
3	Q	1	NAG	O4-C4-C5	-2.31	103.64	109.32
3	M	3	BMA	C1-O5-C5	2.26	115.22	112.19
4	W	1	NAG	C1-C2-N2	2.21	113.92	110.43
3	Q	3	BMA	C1-O5-C5	2.05	114.93	112.19
4	T	1	NAG	C1-C2-N2	2.03	113.63	110.43
4	P	1	NAG	C1-O5-C5	2.03	114.91	112.19
3	O	2	NAG	O4-C4-C5	2.01	114.27	109.32
3	K	1	NAG	C2-N2-C7	2.01	125.59	122.90

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	2	NAG	C3-C2-N2-C7
4	S	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	T	1	NAG	C8-C7-N2-C2
4	T	1	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
3	K	3	BMA	O5-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	P	1	NAG	C3-C2-N2-C7
3	M	3	BMA	O5-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
3	O	1	NAG	C1-C2-N2-C7
3	Q	2	NAG	C1-C2-N2-C7
4	S	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	V	2	NAG	C1-C2-N2-C7
4	W	2	NAG	C1-C2-N2-C7
4	V	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C3-C2-N2-C7
3	N	2	NAG	C3-C2-N2-C7
3	O	1	NAG	C3-C2-N2-C7
3	O	2	NAG	C3-C2-N2-C7
3	Q	2	NAG	C3-C2-N2-C7
4	S	2	NAG	C3-C2-N2-C7
4	W	2	NAG	C3-C2-N2-C7
4	V	2	NAG	O5-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C1-C2-N2-C7
4	W	1	NAG	C1-C2-N2-C7
3	U	2	NAG	C3-C2-N2-C7
4	L	2	NAG	C3-C2-N2-C7
4	S	1	NAG	C3-C2-N2-C7
4	T	1	NAG	C3-C2-N2-C7
4	V	2	NAG	C3-C2-N2-C7
4	W	1	NAG	C3-C2-N2-C7
4	R	1	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 22 short contacts:

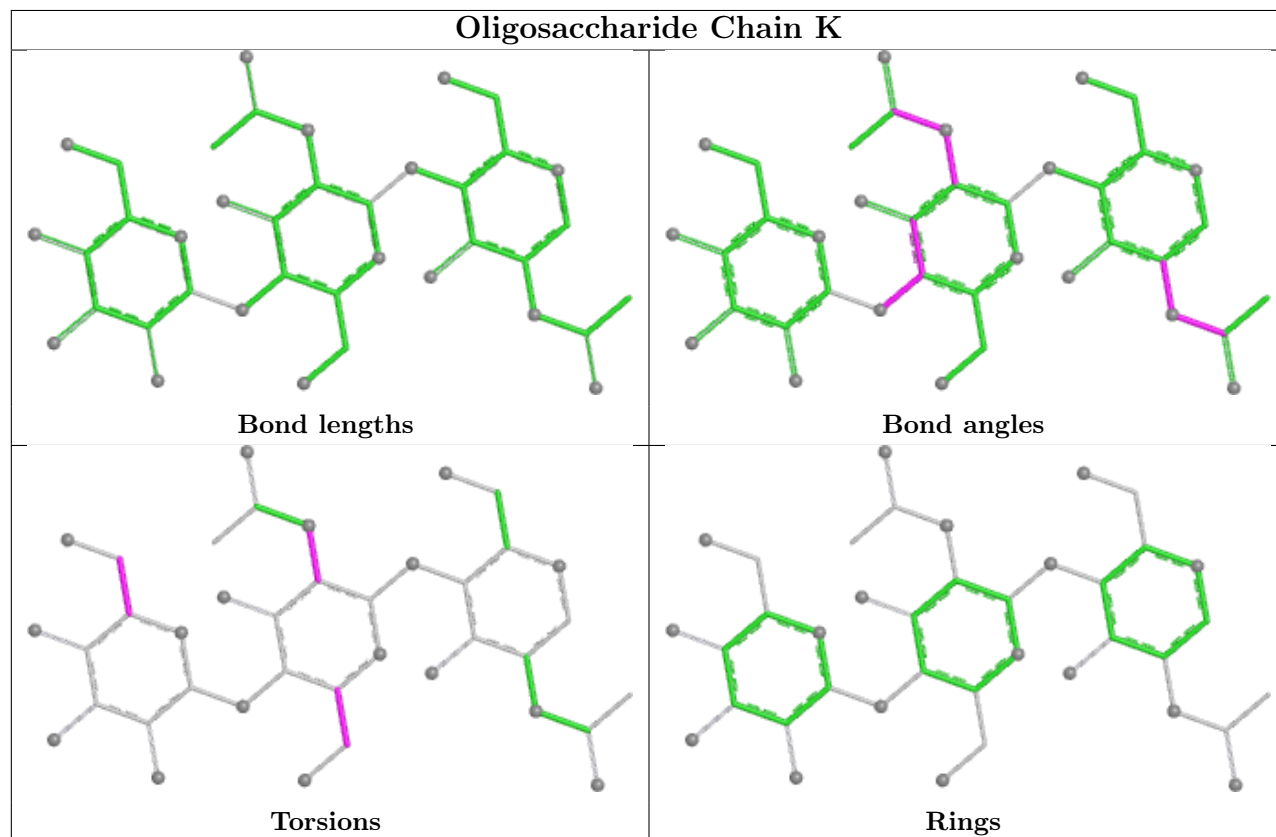
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1	NAG	2	0
4	S	2	NAG	1	0
3	O	3	BMA	1	0
3	M	2	NAG	1	0
3	N	1	NAG	3	0
3	N	2	NAG	3	0
3	O	2	NAG	1	0
3	M	1	NAG	3	0
3	Q	2	NAG	1	0
4	T	1	NAG	1	0
3	O	1	NAG	6	0
3	U	2	NAG	1	0
4	P	1	NAG	2	0
3	K	1	NAG	1	0

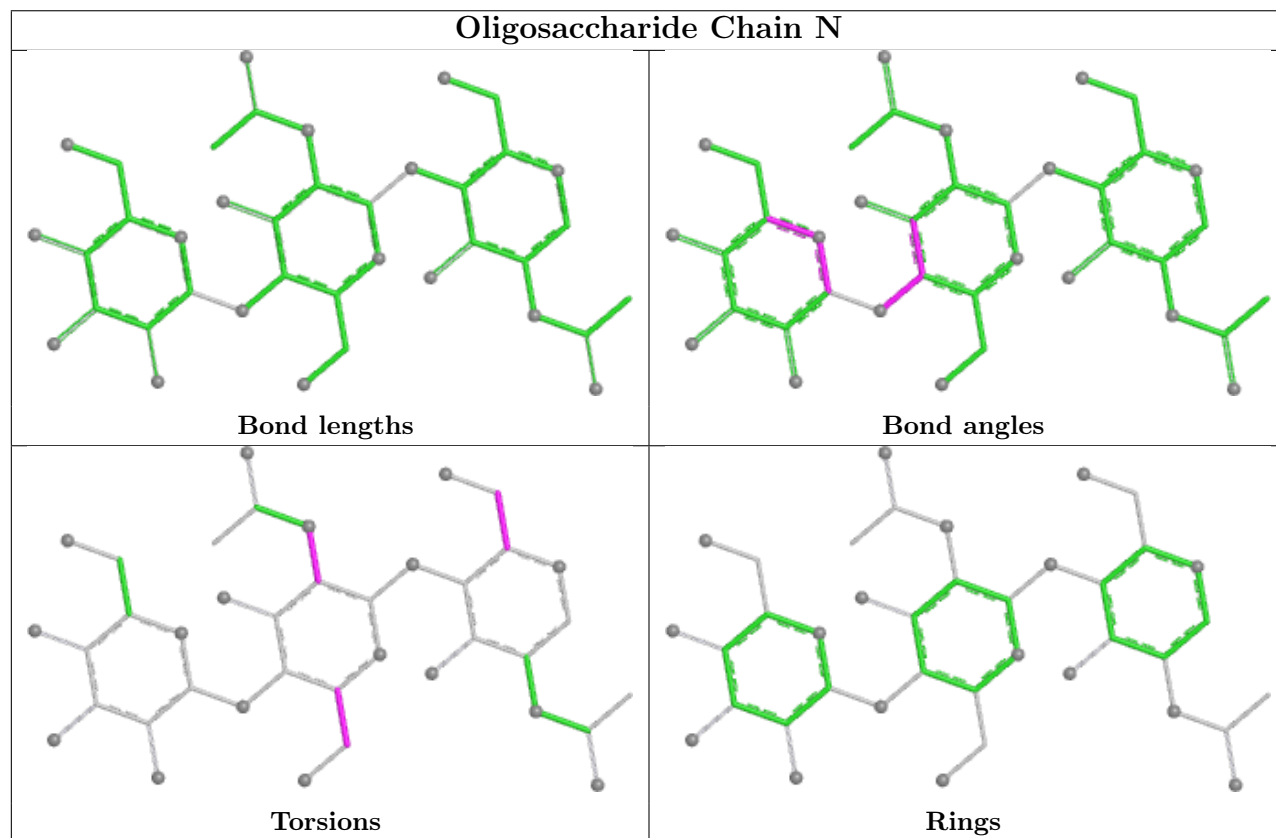
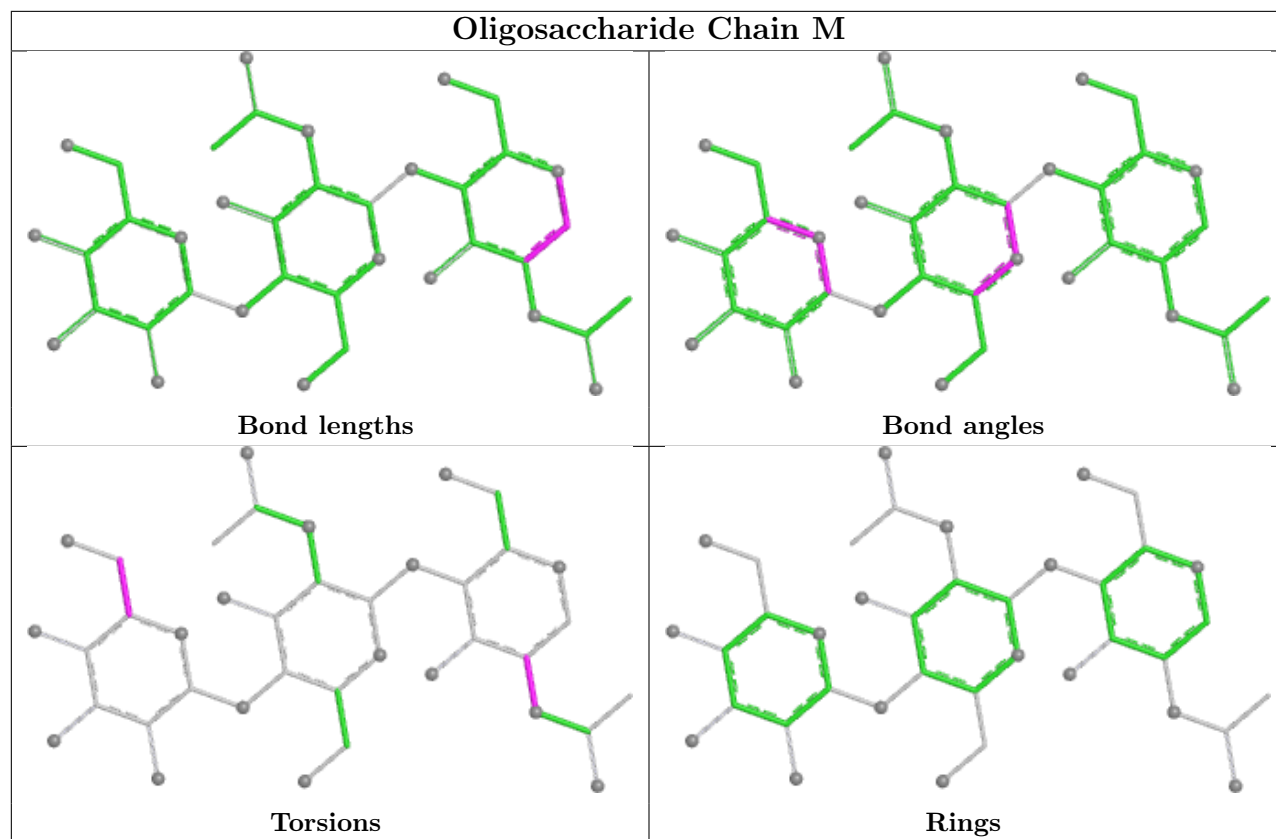
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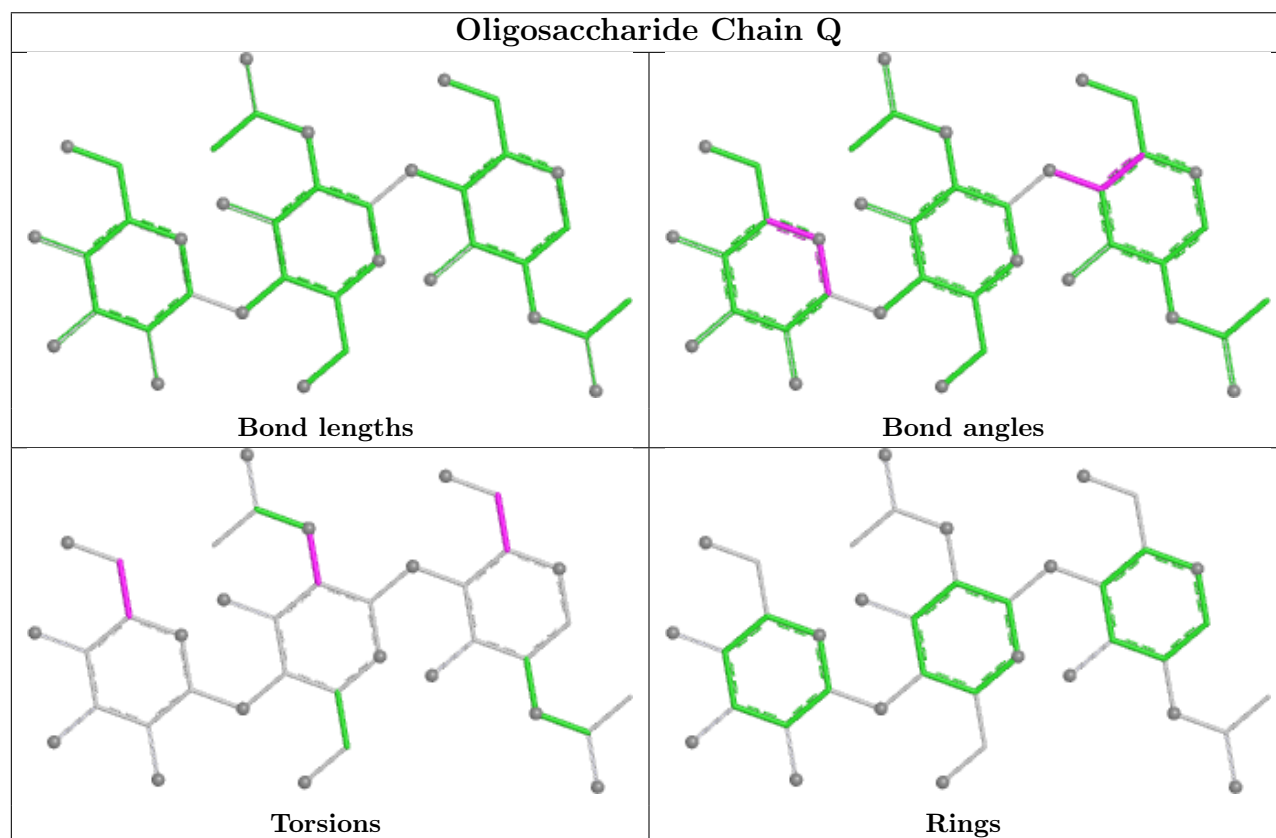
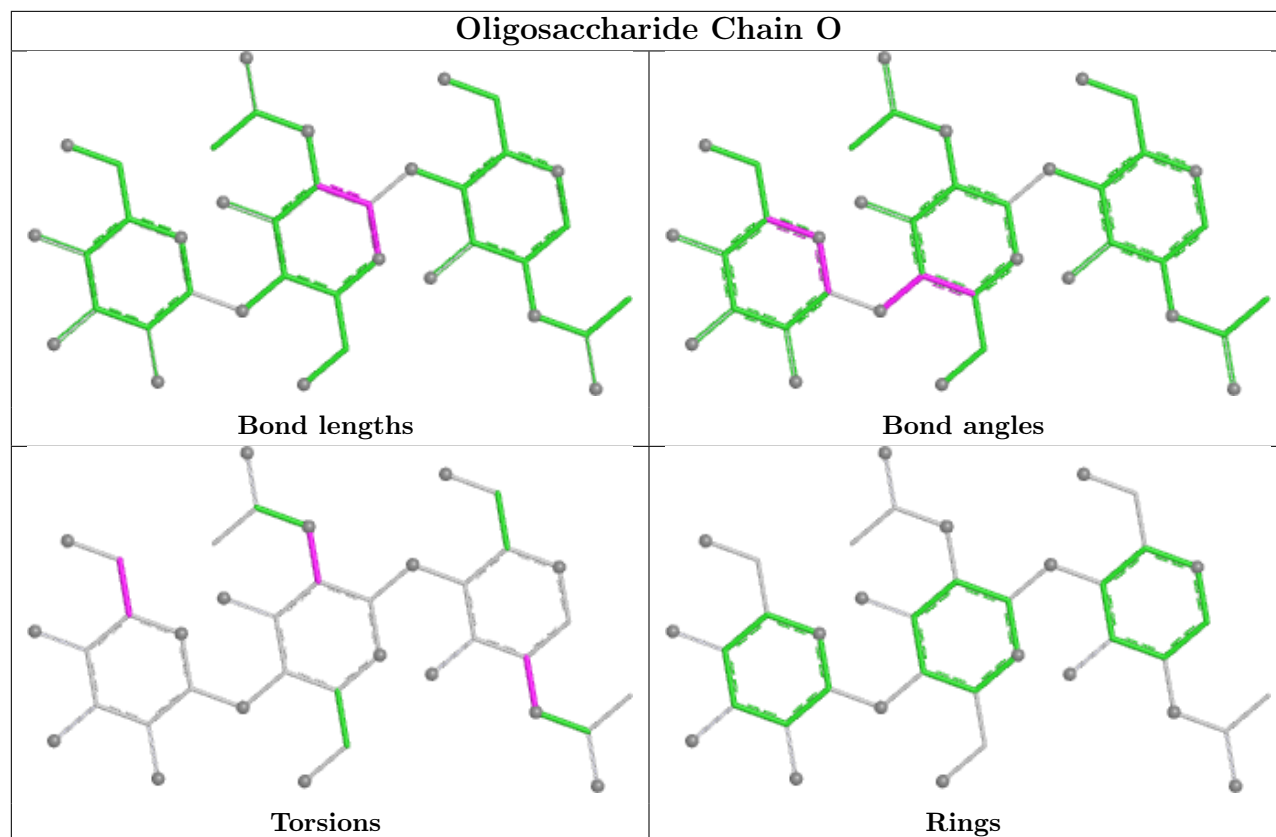
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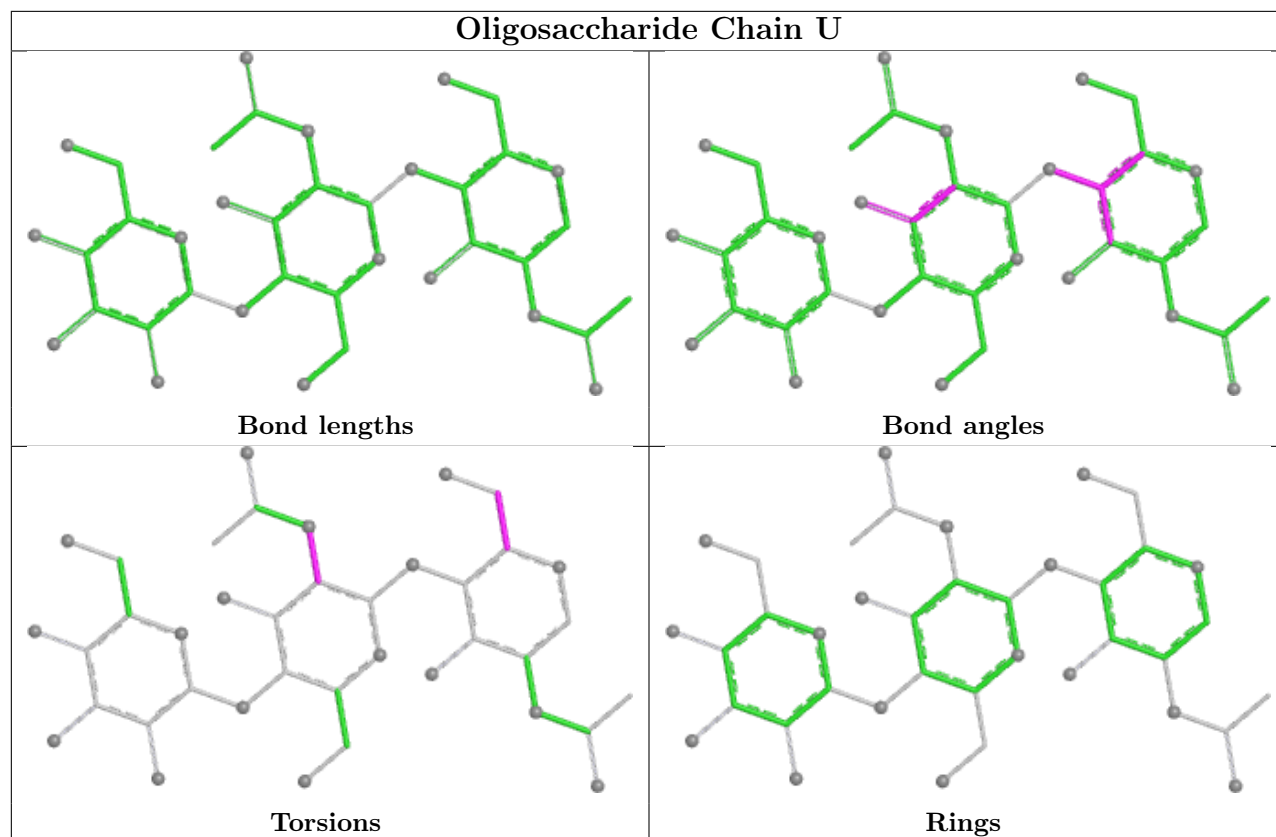
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	1	NAG	1	0

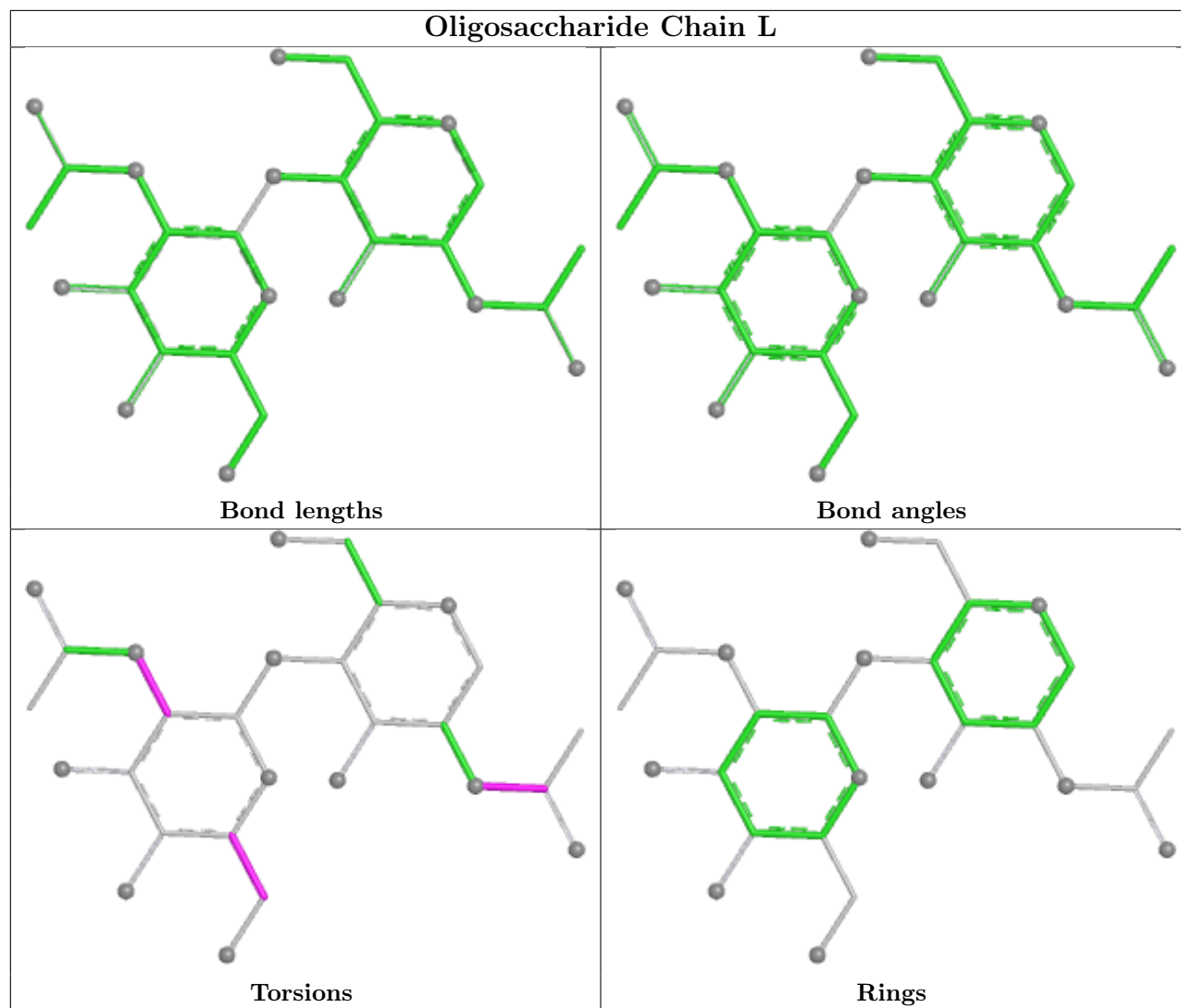
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

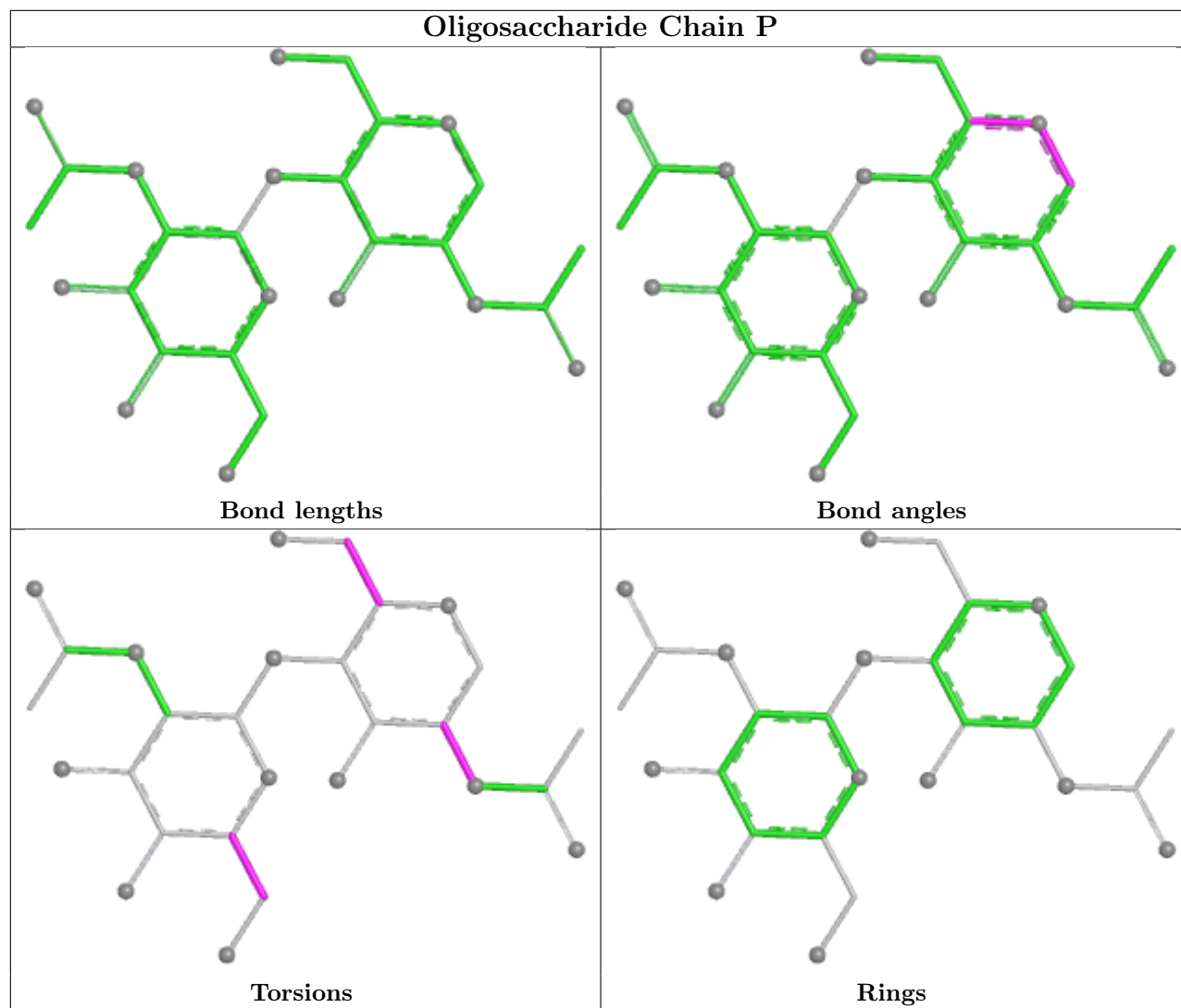


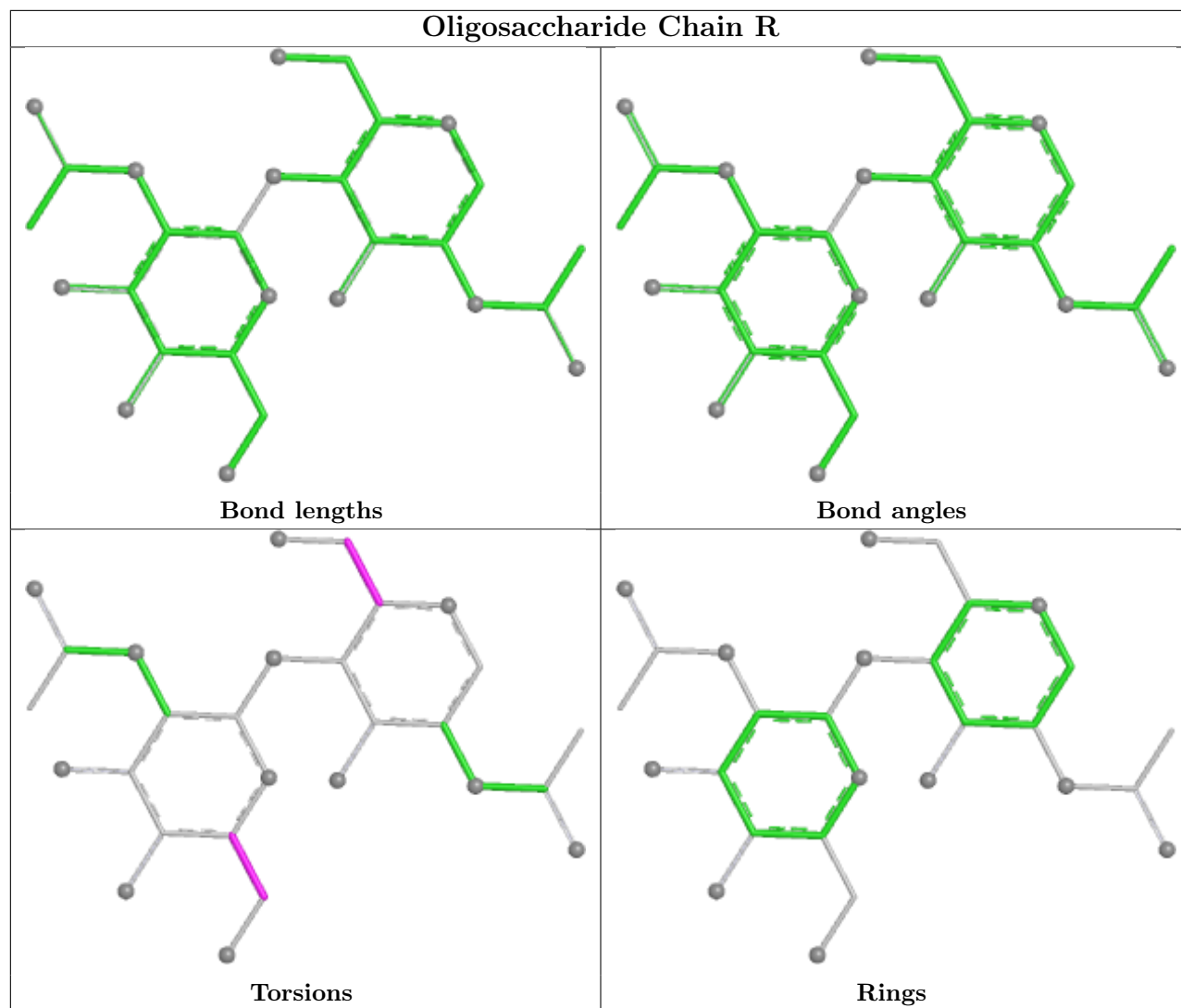


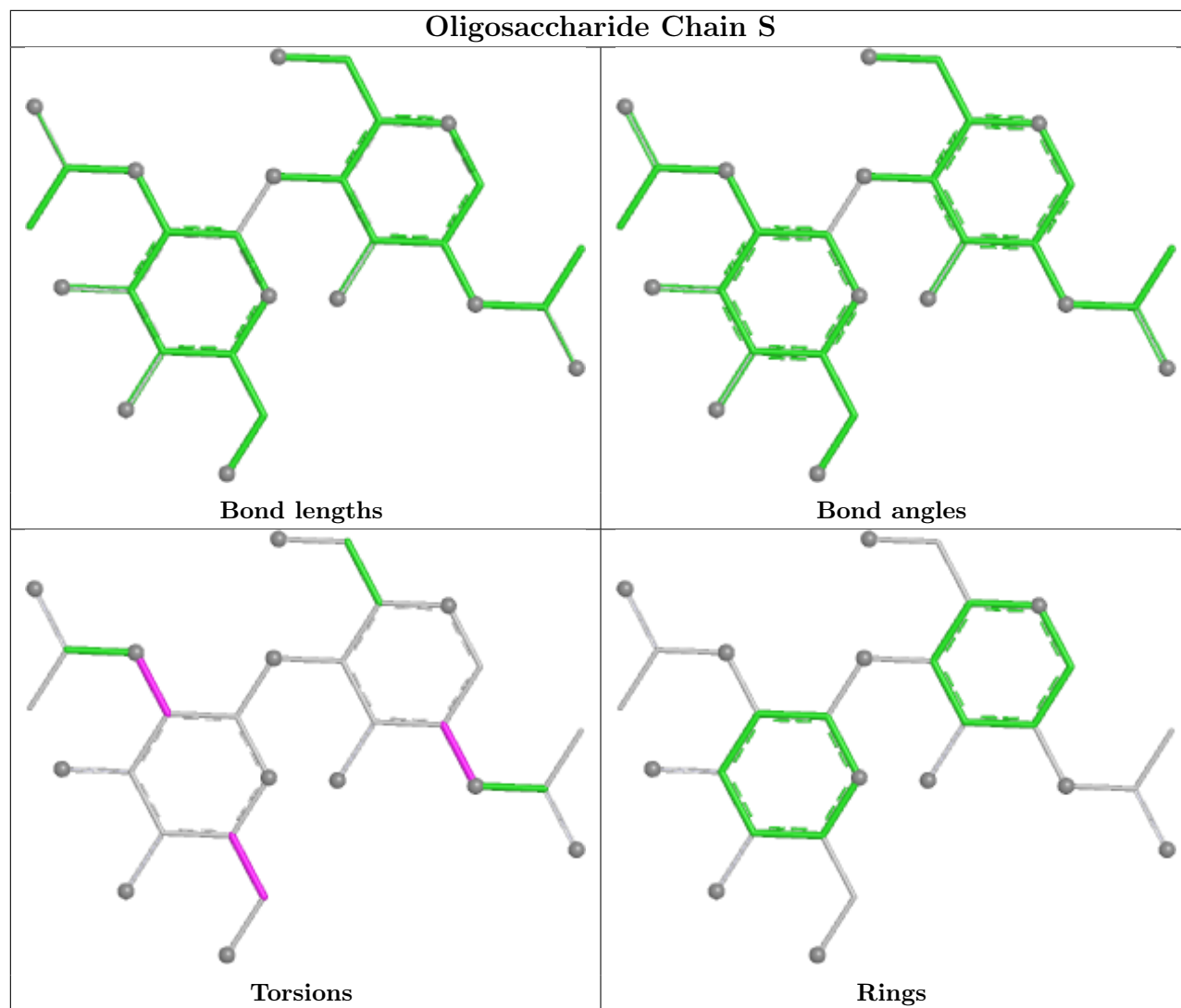


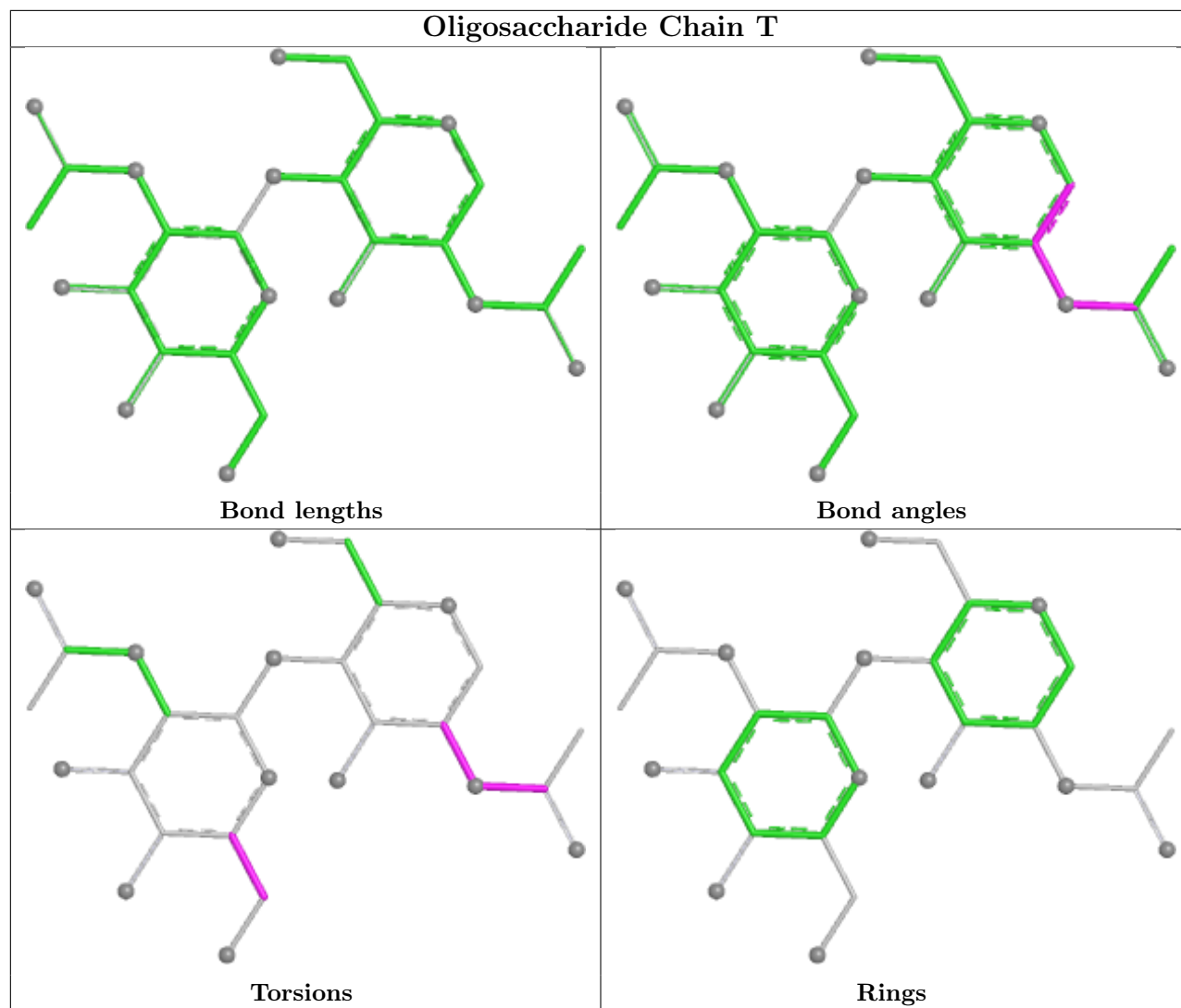


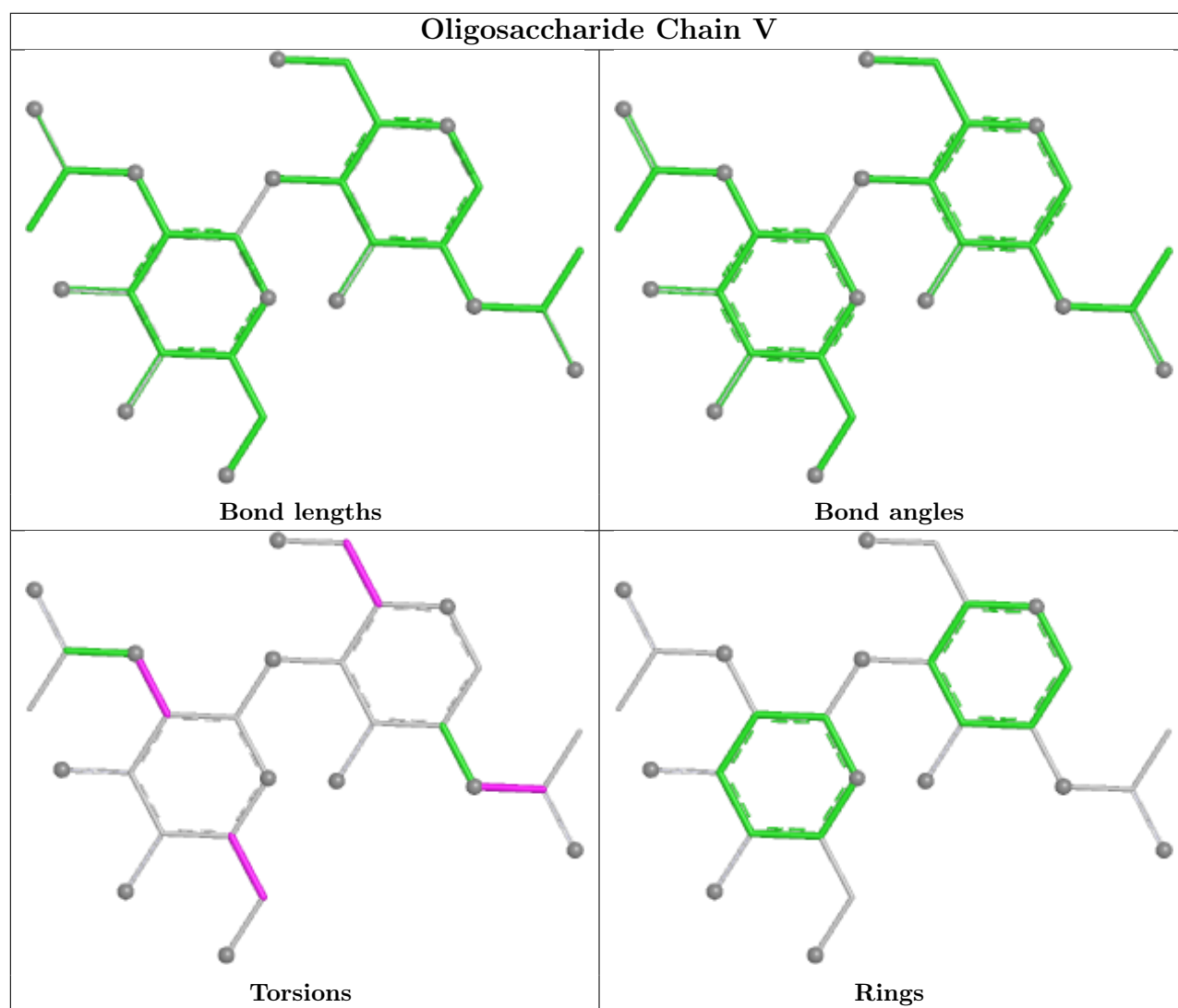


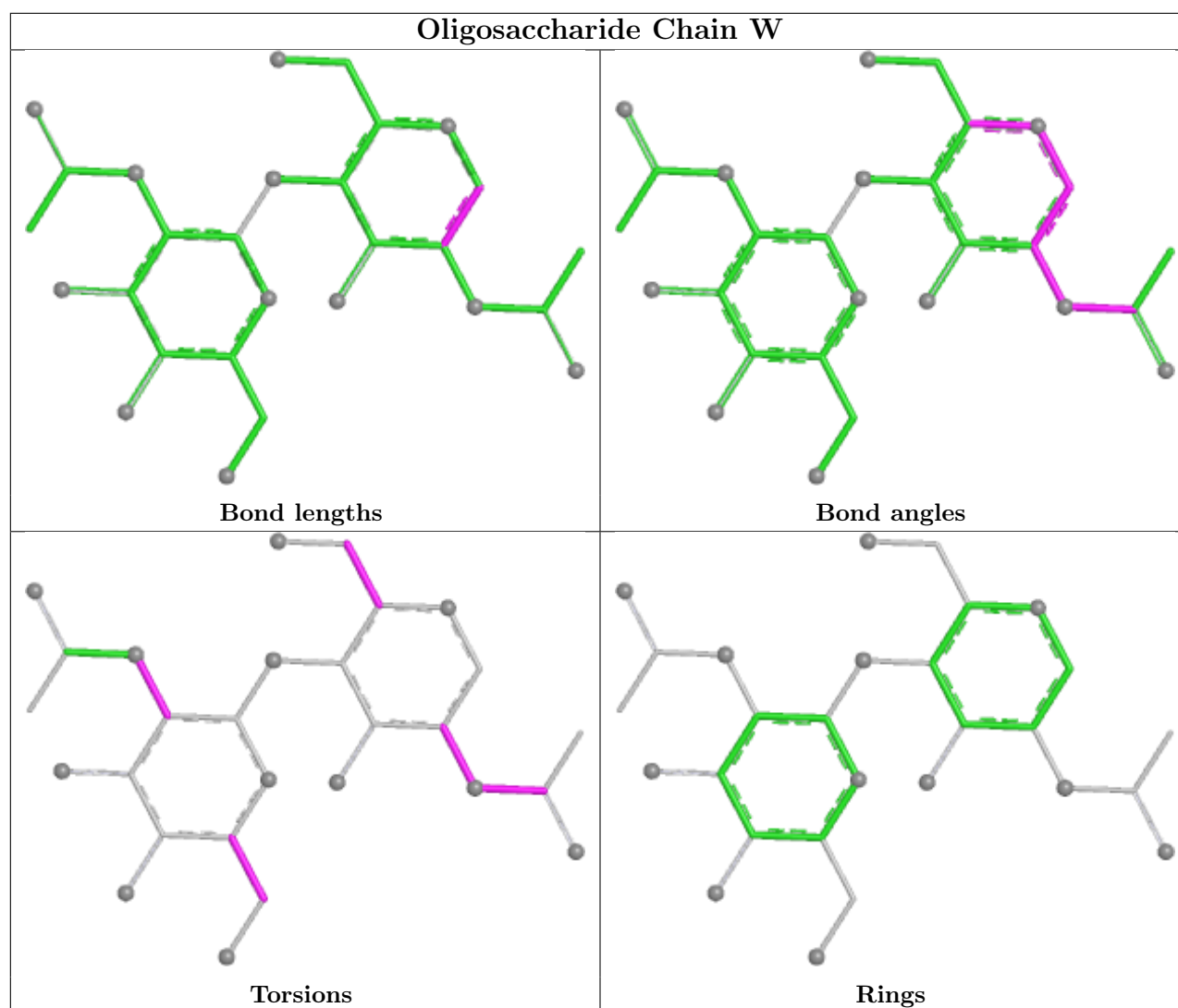












5.6 Ligand geometry [i](#)

17 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	$\# Z > 2$
5	NAG	E	701	1	14,14,15	0.21	0	17,19,21	0.73	0
5	NAG	I	704	1	14,14,15	0.32	0	17,19,21	0.50	0
5	NAG	F	201	2	14,14,15	0.61	0	17,19,21	1.36	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	706	1	14,14,15	0.17	0	17,19,21	0.55	0
5	NAG	B	711	1	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	G	701	1	14,14,15	0.25	0	17,19,21	0.73	1 (5%)
5	NAG	I	701	1	14,14,15	0.31	0	17,19,21	0.71	0
5	NAG	H	201	2	14,14,15	0.57	0	17,19,21	1.39	2 (11%)
5	NAG	A	708	1	14,14,15	0.63	1 (7%)	17,19,21	0.61	0
5	NAG	A	709	1	14,14,15	0.27	0	17,19,21	0.56	0
5	NAG	A	710	1	14,14,15	0.19	0	17,19,21	0.48	0
5	NAG	B	701	1	14,14,15	0.30	0	17,19,21	0.69	0
5	NAG	A	701	1	14,14,15	0.27	0	17,19,21	0.63	1 (5%)
5	NAG	J	201	2	14,14,15	0.59	0	17,19,21	1.37	2 (11%)
5	NAG	G	705	1	14,14,15	0.47	0	17,19,21	0.54	0
5	NAG	D	201	2	14,14,15	0.65	1 (7%)	17,19,21	1.38	2 (11%)
5	NAG	B	702	1	14,14,15	0.22	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	701	1	-	4/6/23/26	0/1/1/1
5	NAG	I	704	1	-	2/6/23/26	0/1/1/1
5	NAG	F	201	2	-	5/6/23/26	0/1/1/1
5	NAG	G	706	1	-	4/6/23/26	0/1/1/1
5	NAG	B	711	1	-	3/6/23/26	0/1/1/1
5	NAG	G	701	1	-	0/6/23/26	0/1/1/1
5	NAG	I	701	1	-	3/6/23/26	0/1/1/1
5	NAG	H	201	2	-	5/6/23/26	0/1/1/1
5	NAG	A	708	1	-	2/6/23/26	0/1/1/1
5	NAG	A	709	1	-	4/6/23/26	0/1/1/1
5	NAG	A	710	1	-	2/6/23/26	0/1/1/1
5	NAG	B	701	1	-	3/6/23/26	0/1/1/1
5	NAG	A	701	1	-	3/6/23/26	0/1/1/1
5	NAG	J	201	2	-	5/6/23/26	0/1/1/1
5	NAG	G	705	1	-	3/6/23/26	0/1/1/1
5	NAG	D	201	2	-	6/6/23/26	0/1/1/1
5	NAG	B	702	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	708	NAG	O5-C1	2.20	1.47	1.43
5	D	201	NAG	C1-C2	2.01	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	201	NAG	C2-N2-C7	4.53	128.98	122.90
5	H	201	NAG	C2-N2-C7	4.52	128.96	122.90
5	J	201	NAG	C2-N2-C7	4.52	128.95	122.90
5	F	201	NAG	C2-N2-C7	4.48	128.90	122.90
5	G	701	NAG	C1-O5-C5	2.47	115.50	112.19
5	H	201	NAG	C1-C2-N2	2.17	113.86	110.43
5	D	201	NAG	C1-O5-C5	2.12	115.03	112.19
5	A	701	NAG	C1-O5-C5	2.09	114.98	112.19
5	J	201	NAG	C1-C2-N2	2.07	113.70	110.43
5	F	201	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	701	NAG	O5-C5-C6-O6
5	A	708	NAG	C4-C5-C6-O6
5	A	709	NAG	O5-C5-C6-O6
5	E	701	NAG	C4-C5-C6-O6
5	D	201	NAG	O5-C5-C6-O6
5	G	706	NAG	O5-C5-C6-O6
5	A	708	NAG	O5-C5-C6-O6
5	I	704	NAG	O5-C5-C6-O6
5	A	709	NAG	C4-C5-C6-O6
5	G	706	NAG	C4-C5-C6-O6
5	G	705	NAG	O5-C5-C6-O6
5	D	201	NAG	C8-C7-N2-C2
5	D	201	NAG	O7-C7-N2-C2
5	A	701	NAG	C8-C7-N2-C2
5	A	701	NAG	O7-C7-N2-C2
5	F	201	NAG	C8-C7-N2-C2
5	F	201	NAG	O7-C7-N2-C2
5	H	201	NAG	C8-C7-N2-C2
5	H	201	NAG	O7-C7-N2-C2
5	J	201	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	J	201	NAG	O7-C7-N2-C2
5	I	704	NAG	C4-C5-C6-O6
5	A	710	NAG	O5-C5-C6-O6
5	A	710	NAG	C4-C5-C6-O6
5	D	201	NAG	C4-C5-C6-O6
5	J	201	NAG	O5-C5-C6-O6
5	B	701	NAG	O5-C5-C6-O6
5	B	702	NAG	O5-C5-C6-O6
5	G	705	NAG	C4-C5-C6-O6
5	B	711	NAG	O5-C5-C6-O6
5	F	201	NAG	O5-C5-C6-O6
5	H	201	NAG	O5-C5-C6-O6
5	I	701	NAG	O5-C5-C6-O6
5	A	701	NAG	O5-C5-C6-O6
5	B	701	NAG	C1-C2-N2-C7
5	B	711	NAG	C1-C2-N2-C7
5	A	709	NAG	C1-C2-N2-C7
5	E	701	NAG	C1-C2-N2-C7
5	I	701	NAG	C1-C2-N2-C7
5	B	701	NAG	C3-C2-N2-C7
5	D	201	NAG	C3-C2-N2-C7
5	G	706	NAG	C3-C2-N2-C7
5	I	701	NAG	C3-C2-N2-C7
5	J	201	NAG	C3-C2-N2-C7
5	D	201	NAG	C1-C2-N2-C7
5	G	706	NAG	C1-C2-N2-C7
5	F	201	NAG	C1-C2-N2-C7
5	H	201	NAG	C1-C2-N2-C7
5	J	201	NAG	C1-C2-N2-C7
5	B	711	NAG	C3-C2-N2-C7
5	A	709	NAG	C3-C2-N2-C7
5	E	701	NAG	C3-C2-N2-C7
5	G	705	NAG	C3-C2-N2-C7
5	F	201	NAG	C3-C2-N2-C7
5	H	201	NAG	C3-C2-N2-C7

There are no ring outliers.

10 monomers are involved in 13 short contacts:

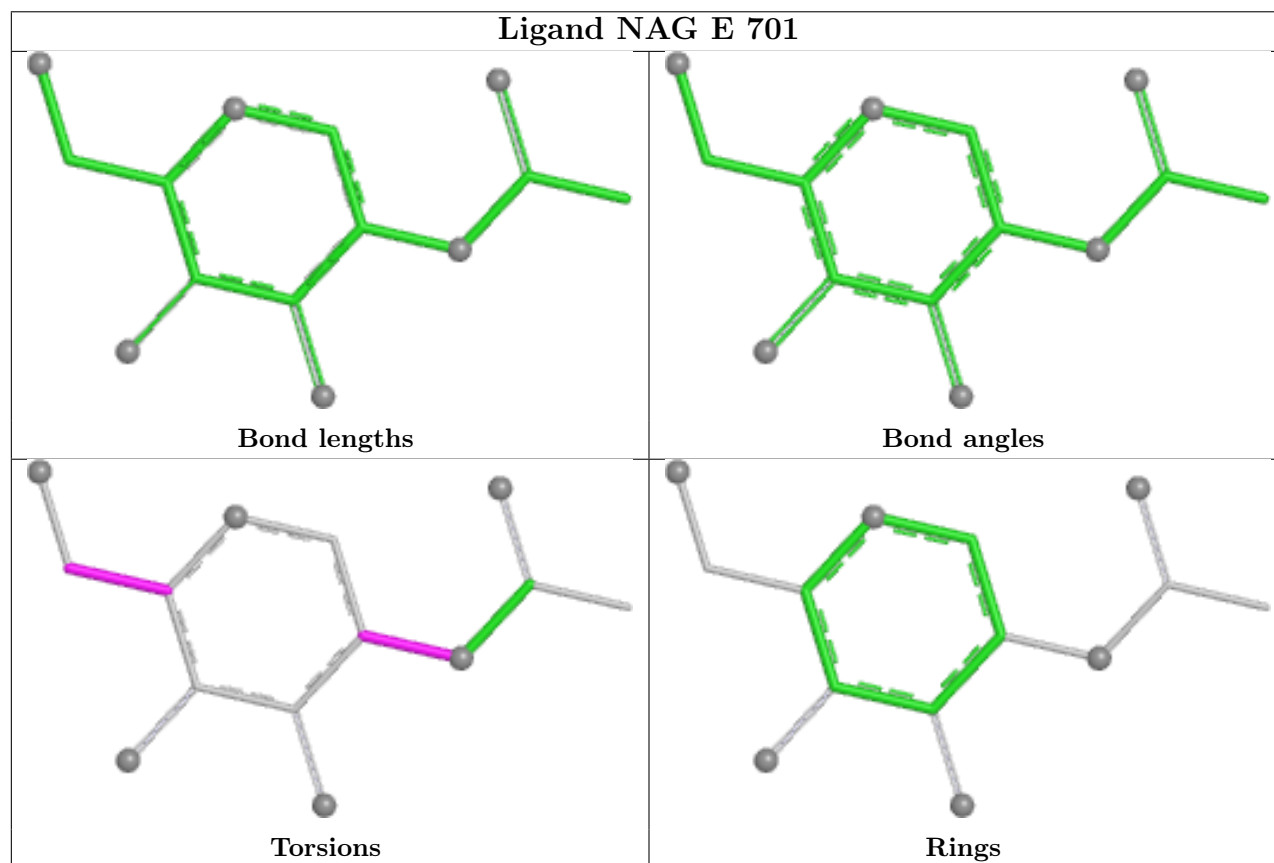
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	701	NAG	1	0
5	I	704	NAG	3	0

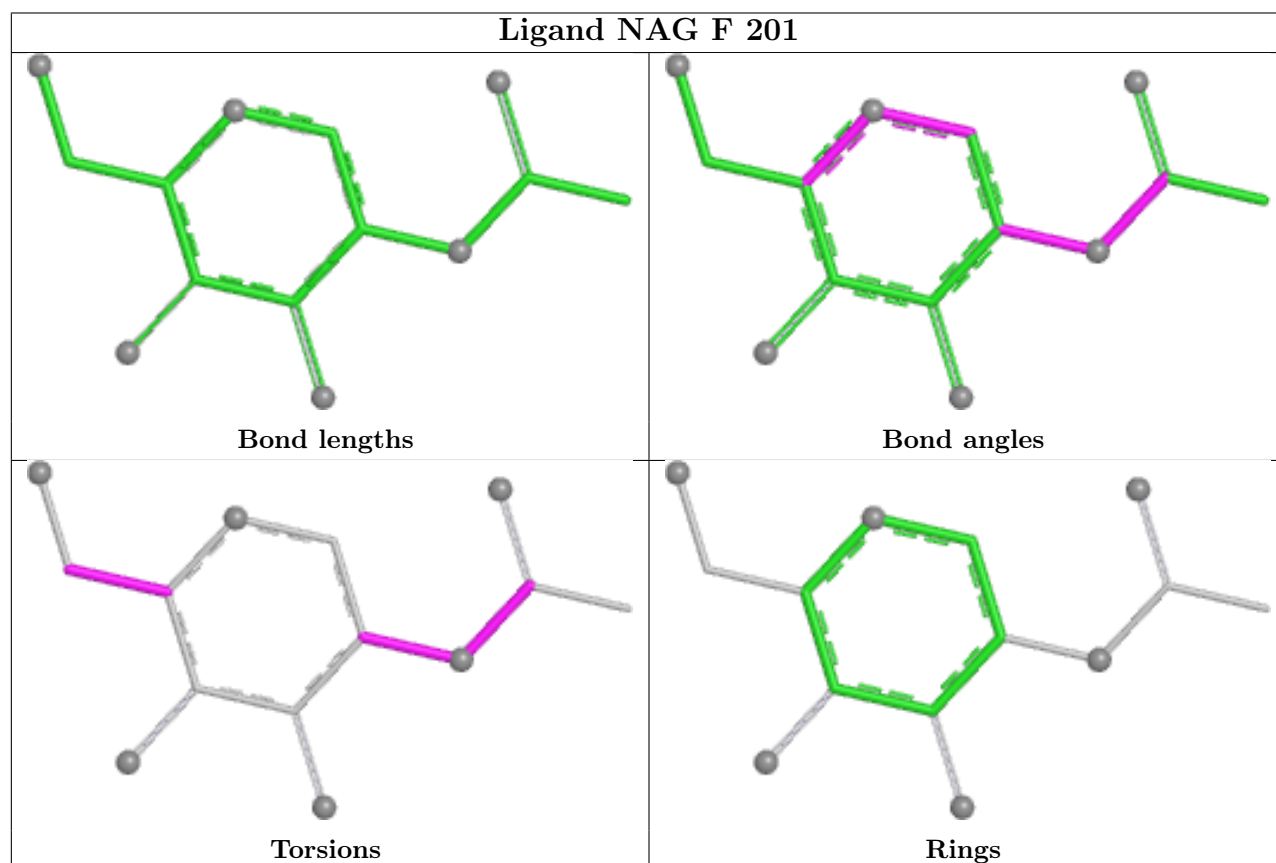
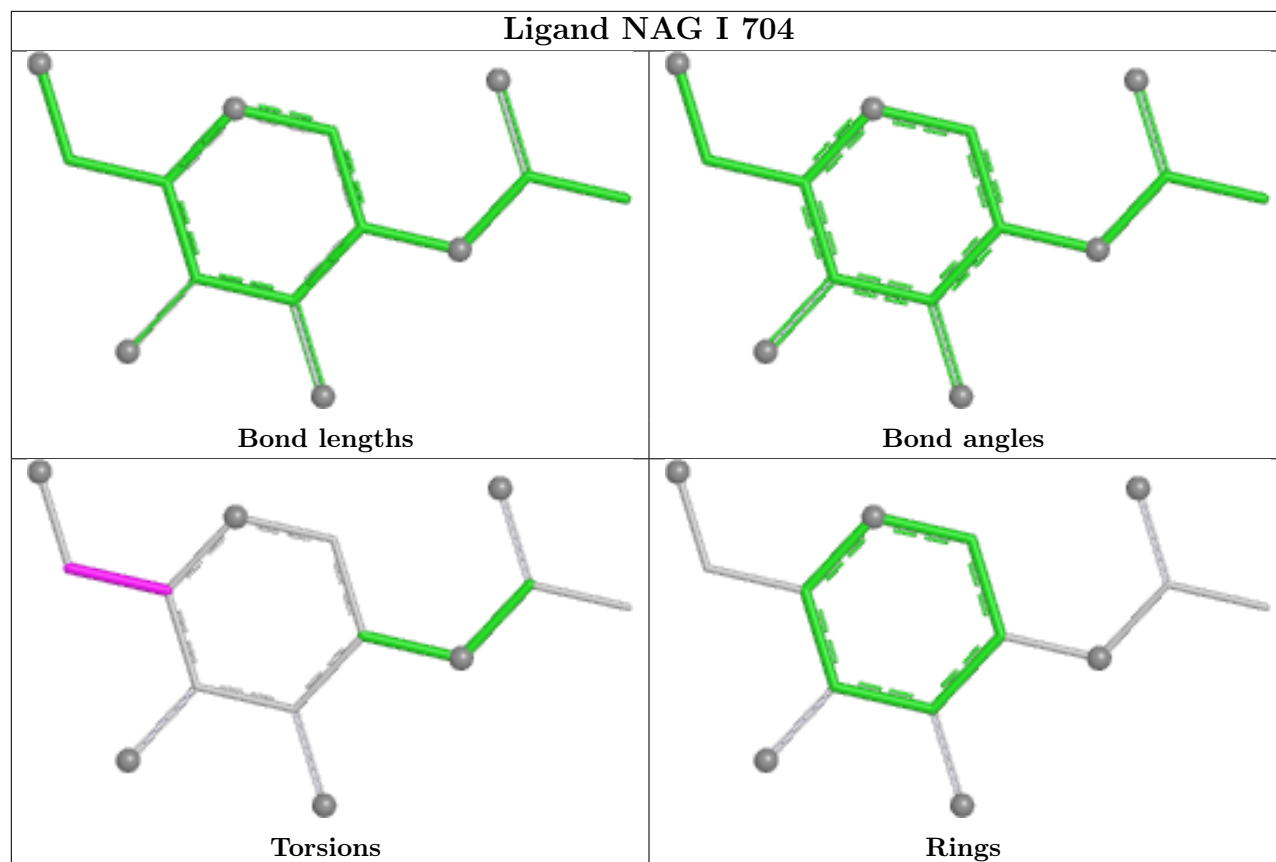
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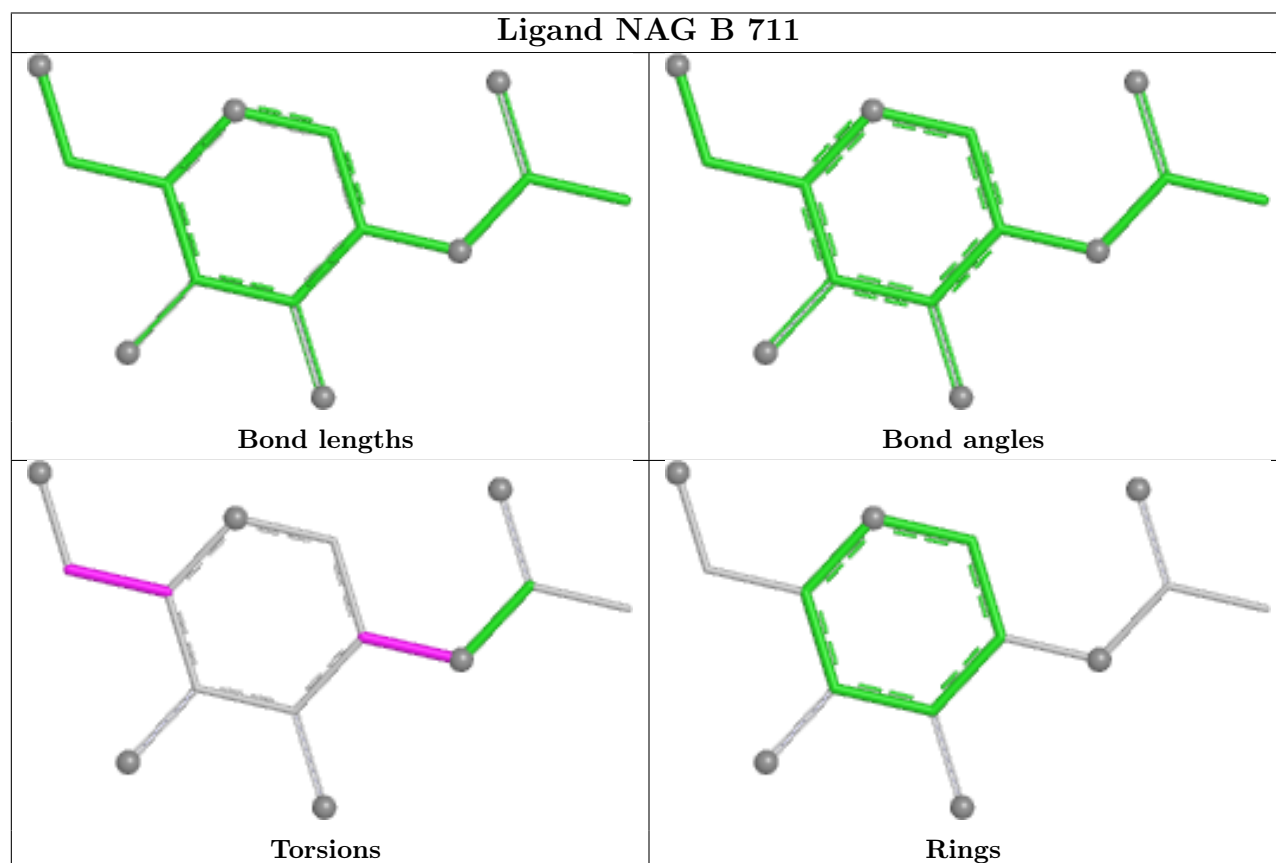
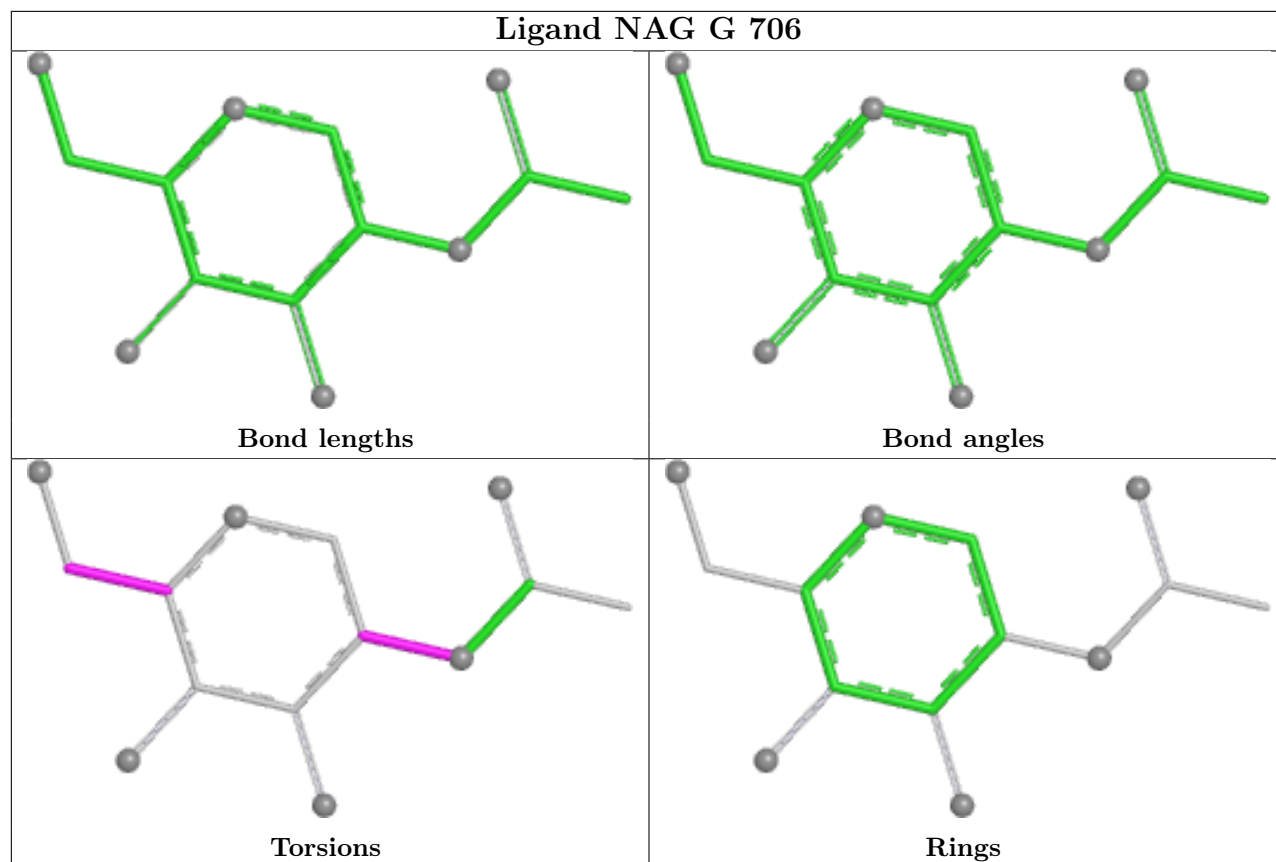
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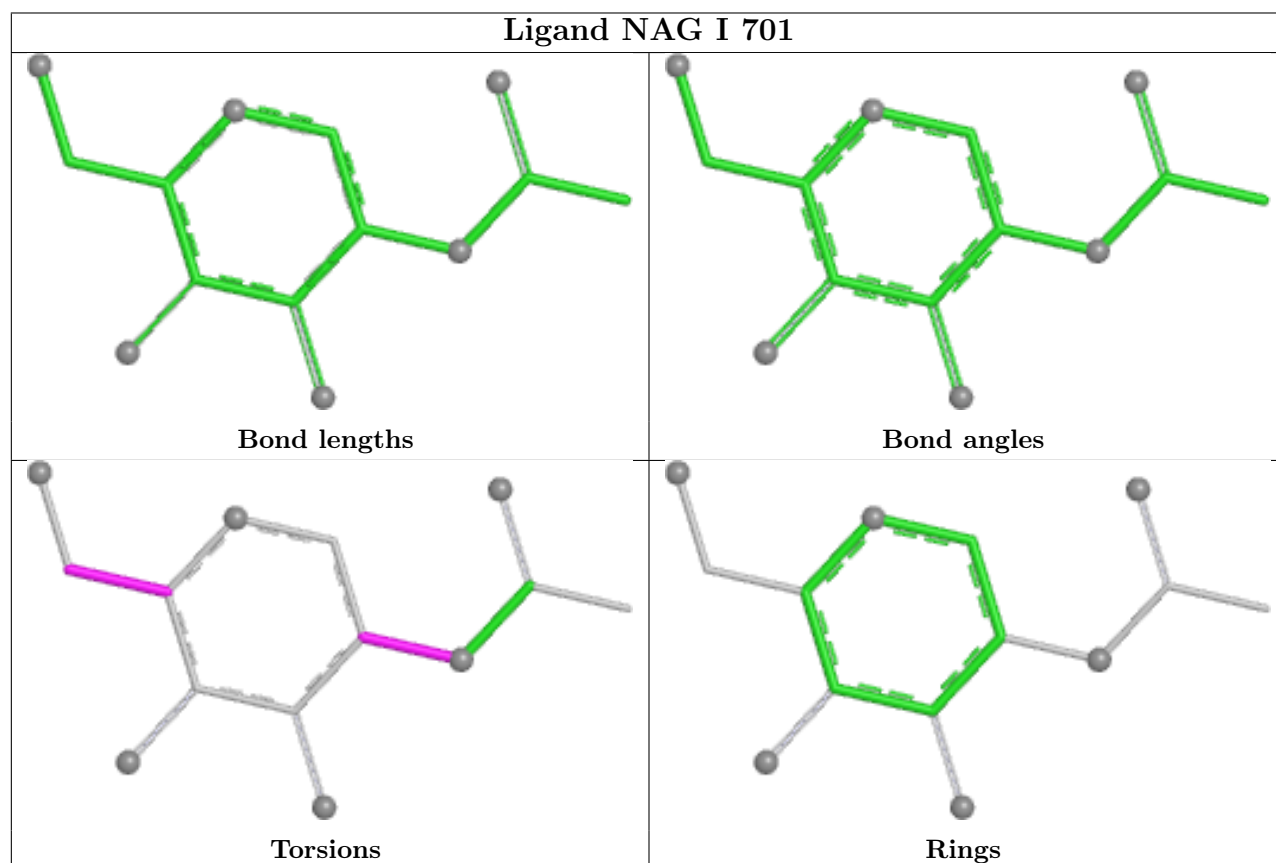
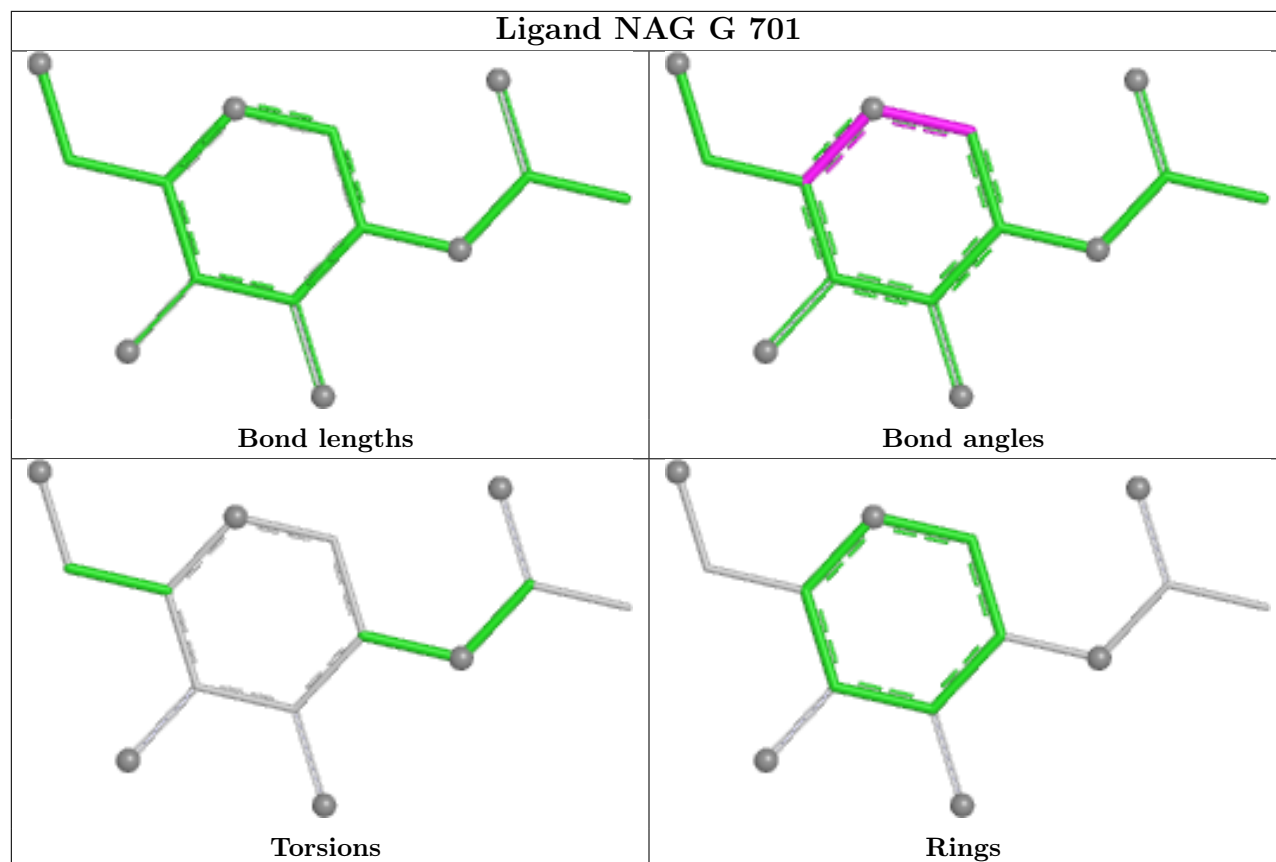
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	201	NAG	1	0
5	G	706	NAG	1	0
5	I	701	NAG	1	0
5	H	201	NAG	1	0
5	A	708	NAG	1	0
5	J	201	NAG	2	0
5	G	705	NAG	1	0
5	D	201	NAG	1	0

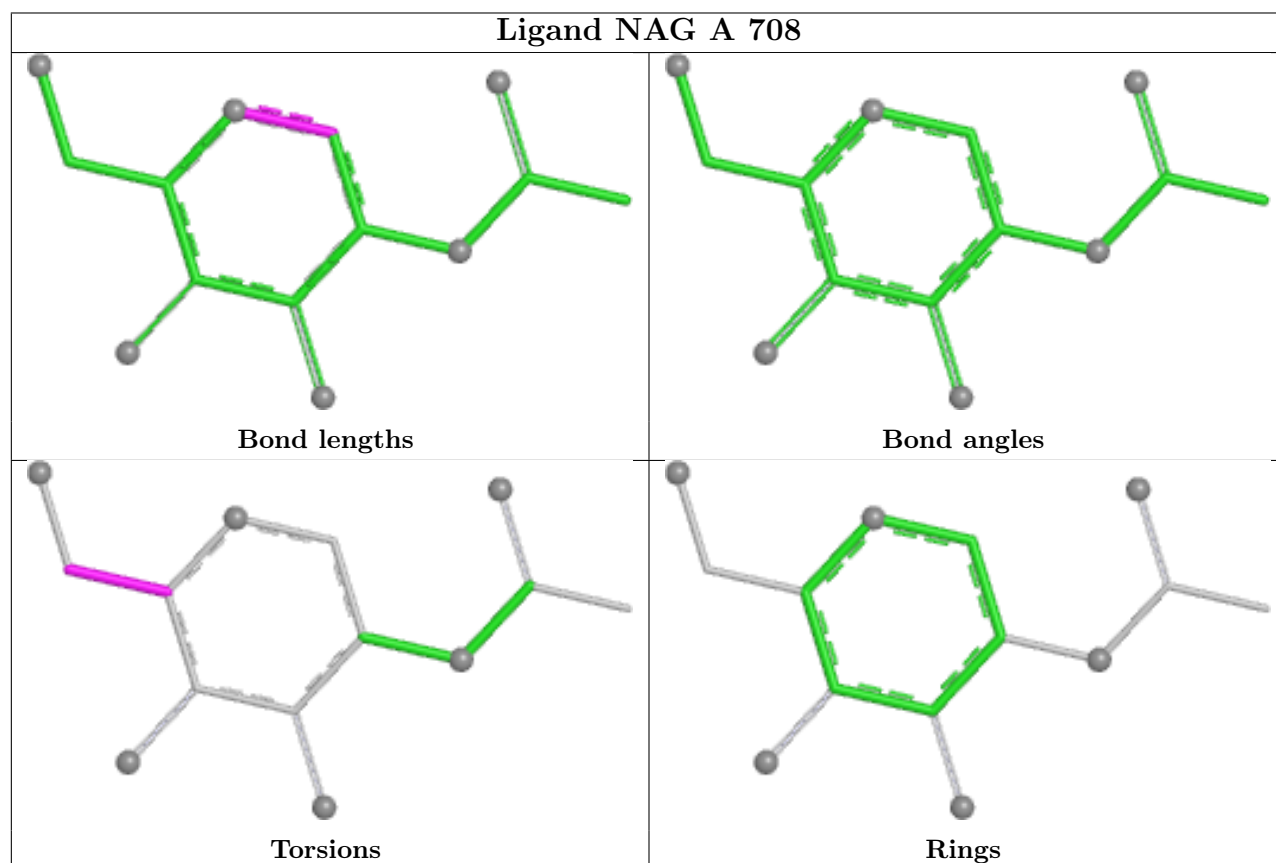
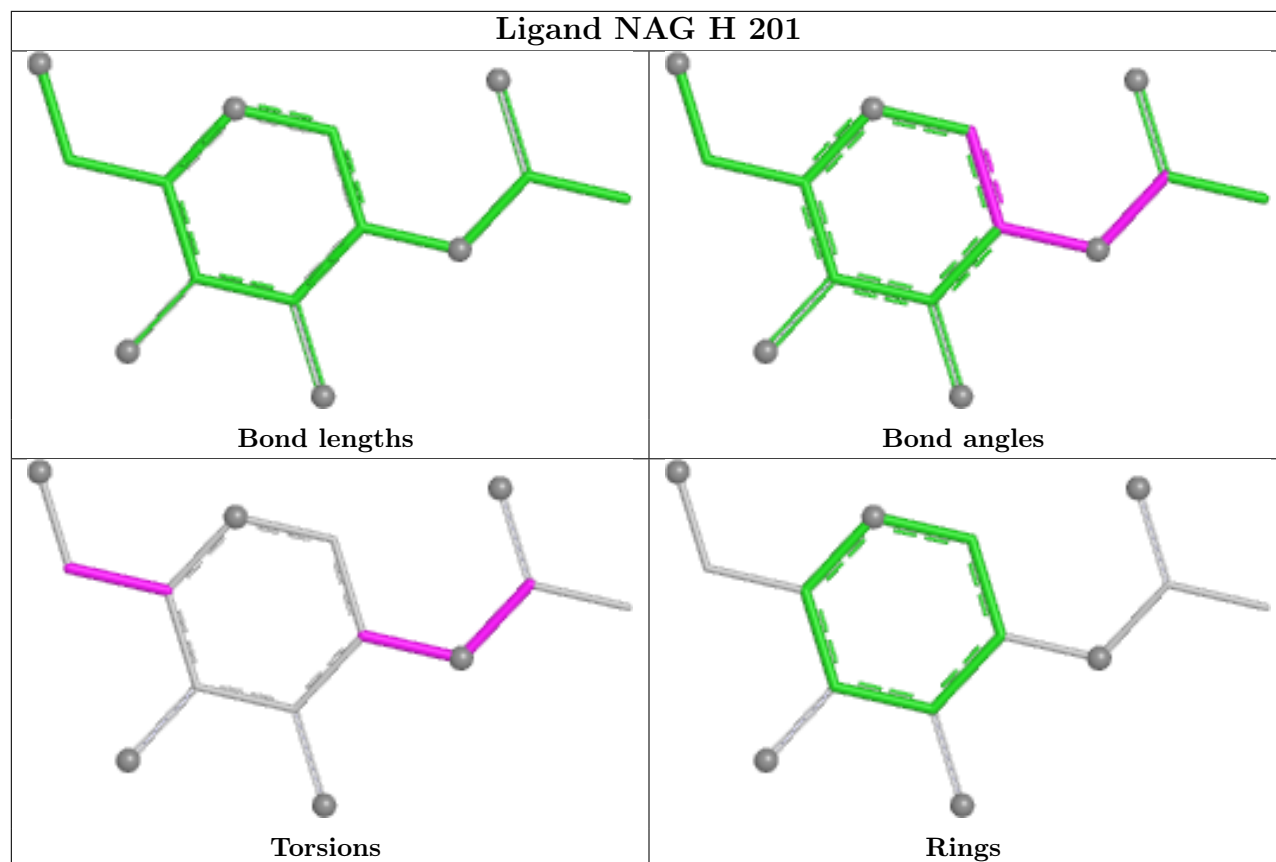
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

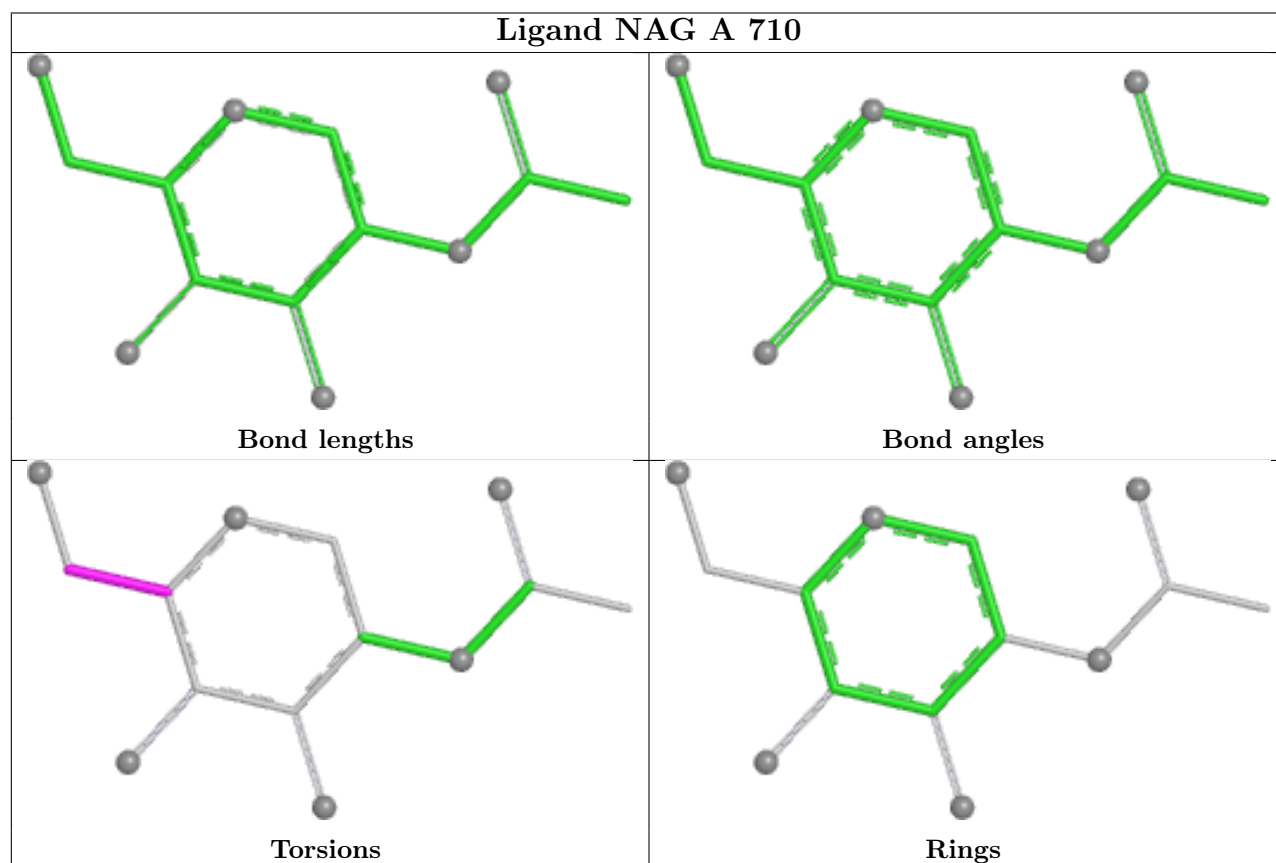
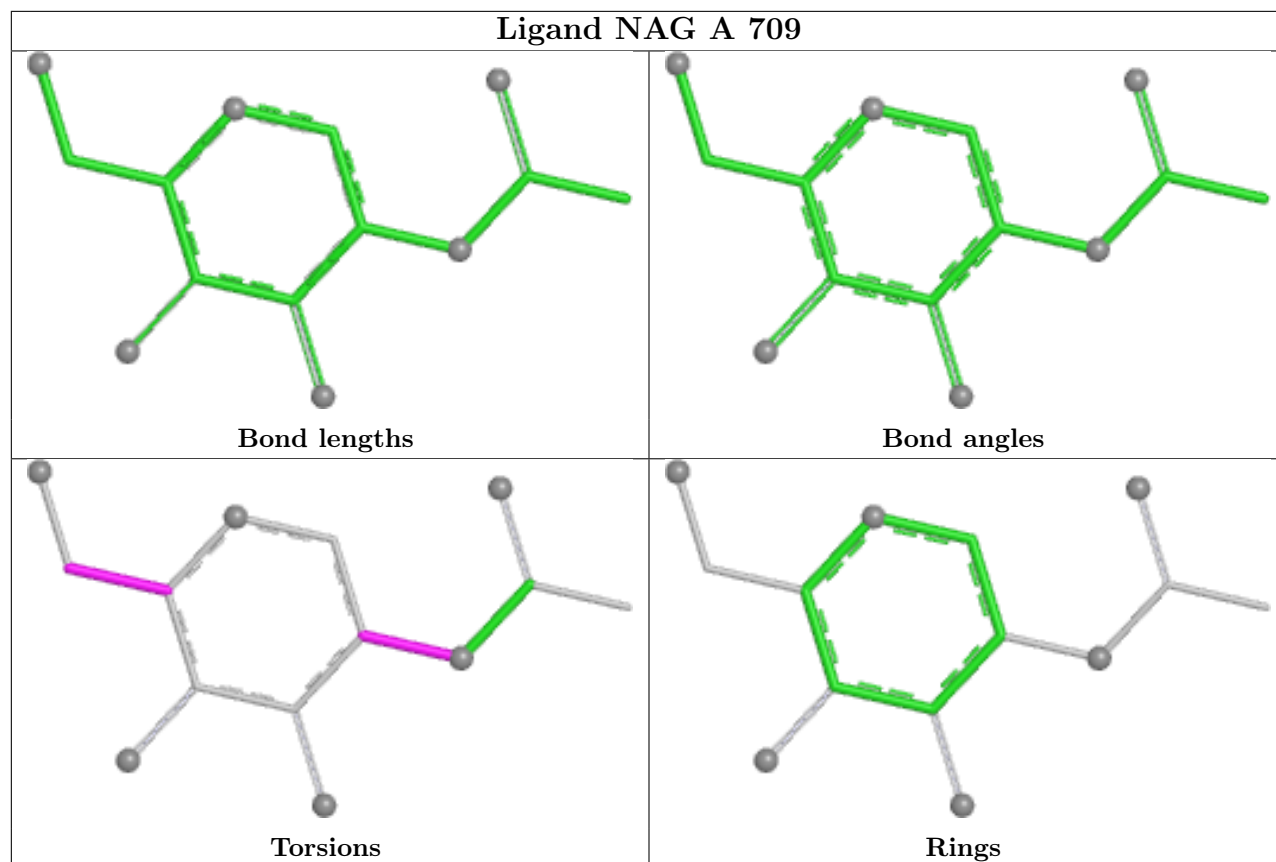


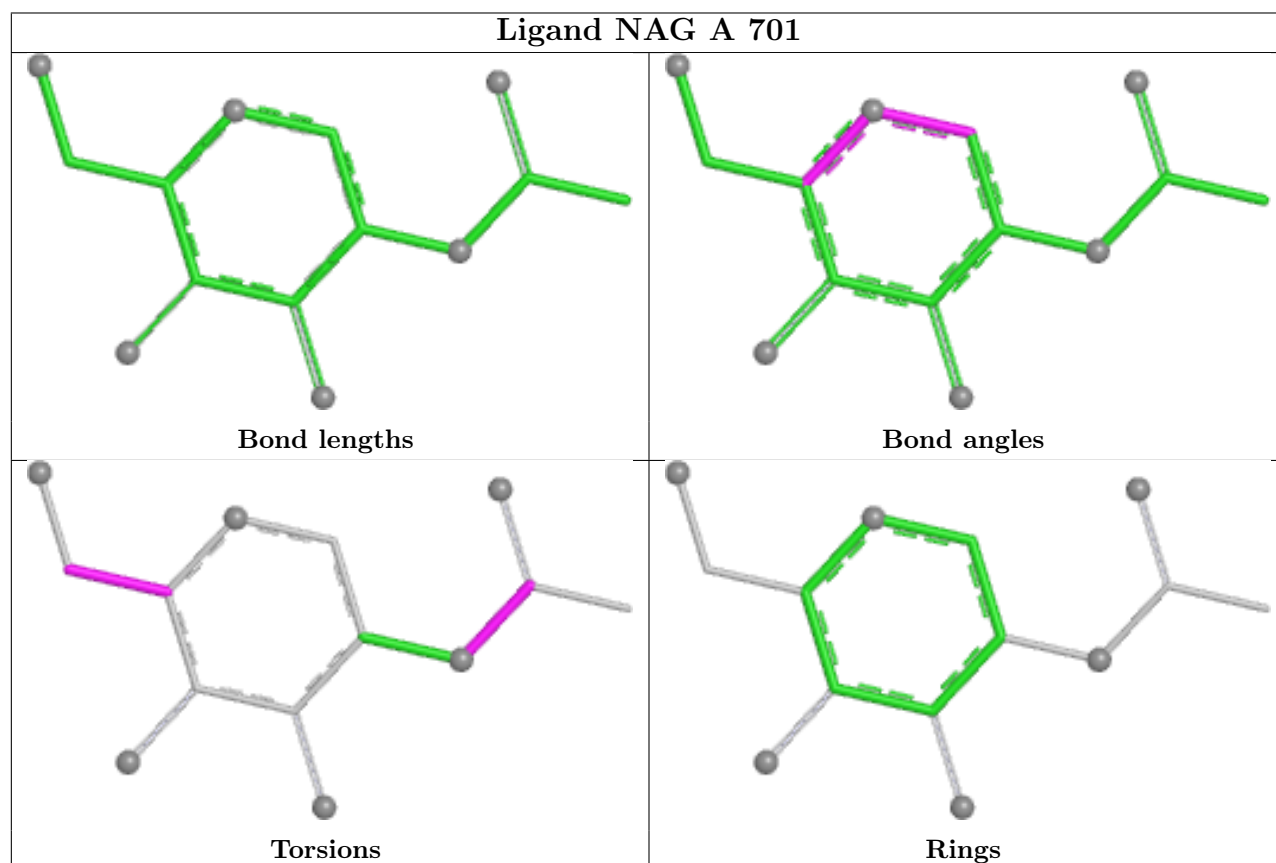
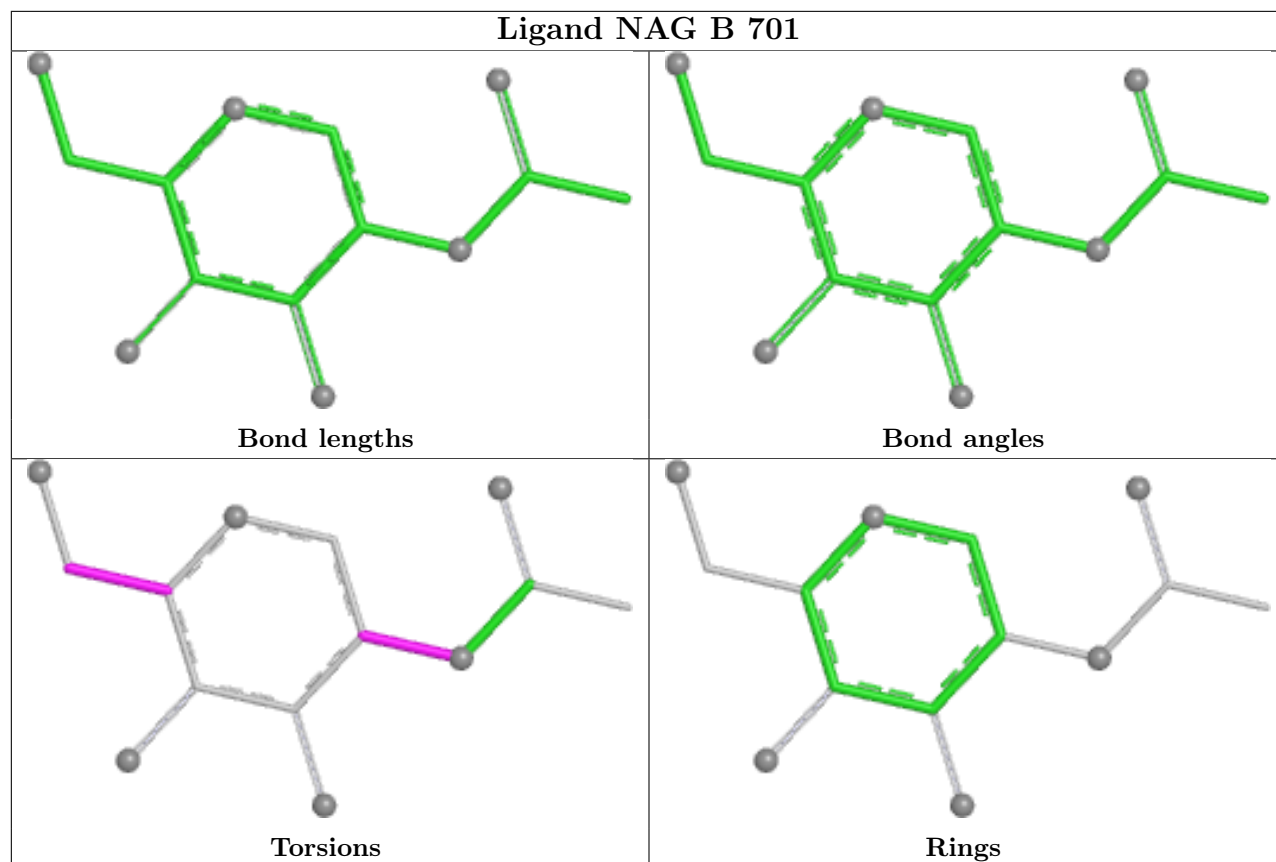




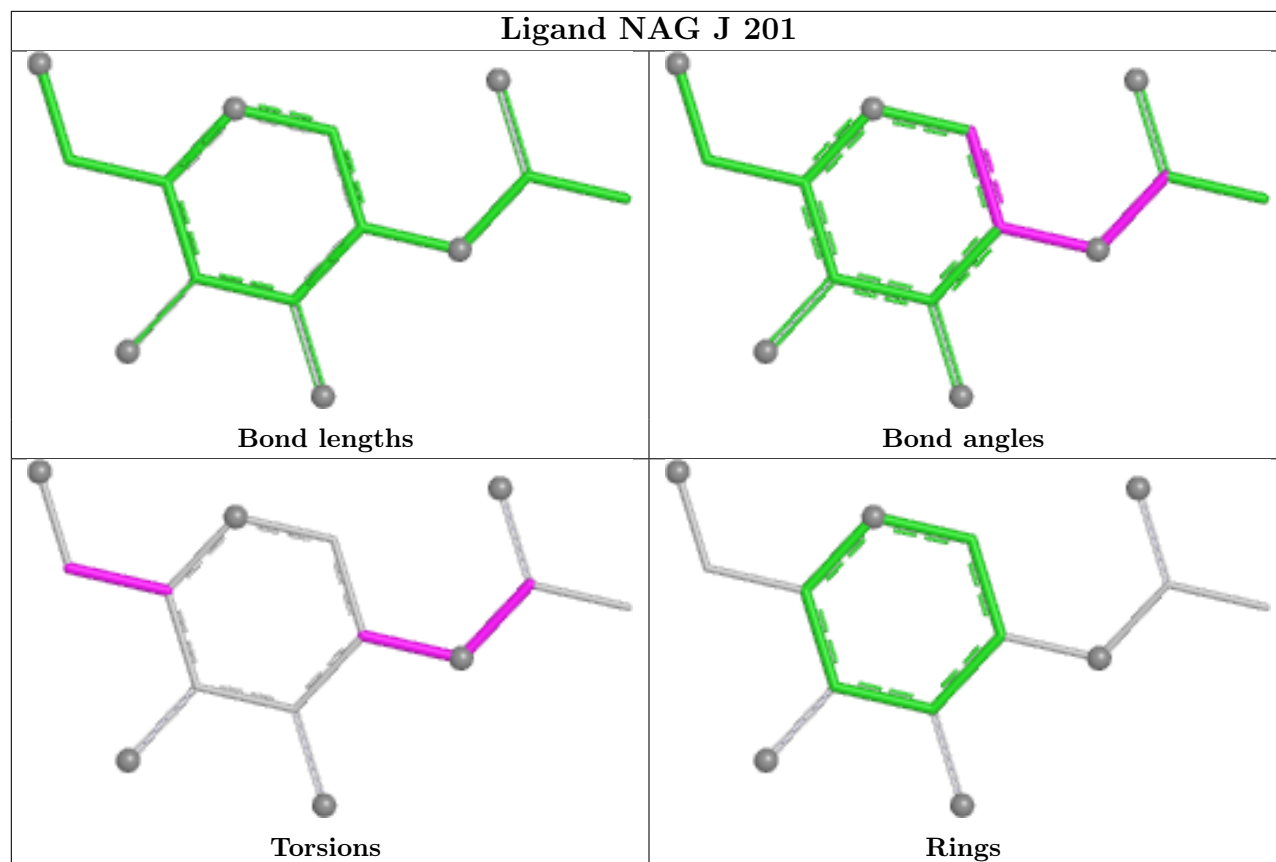




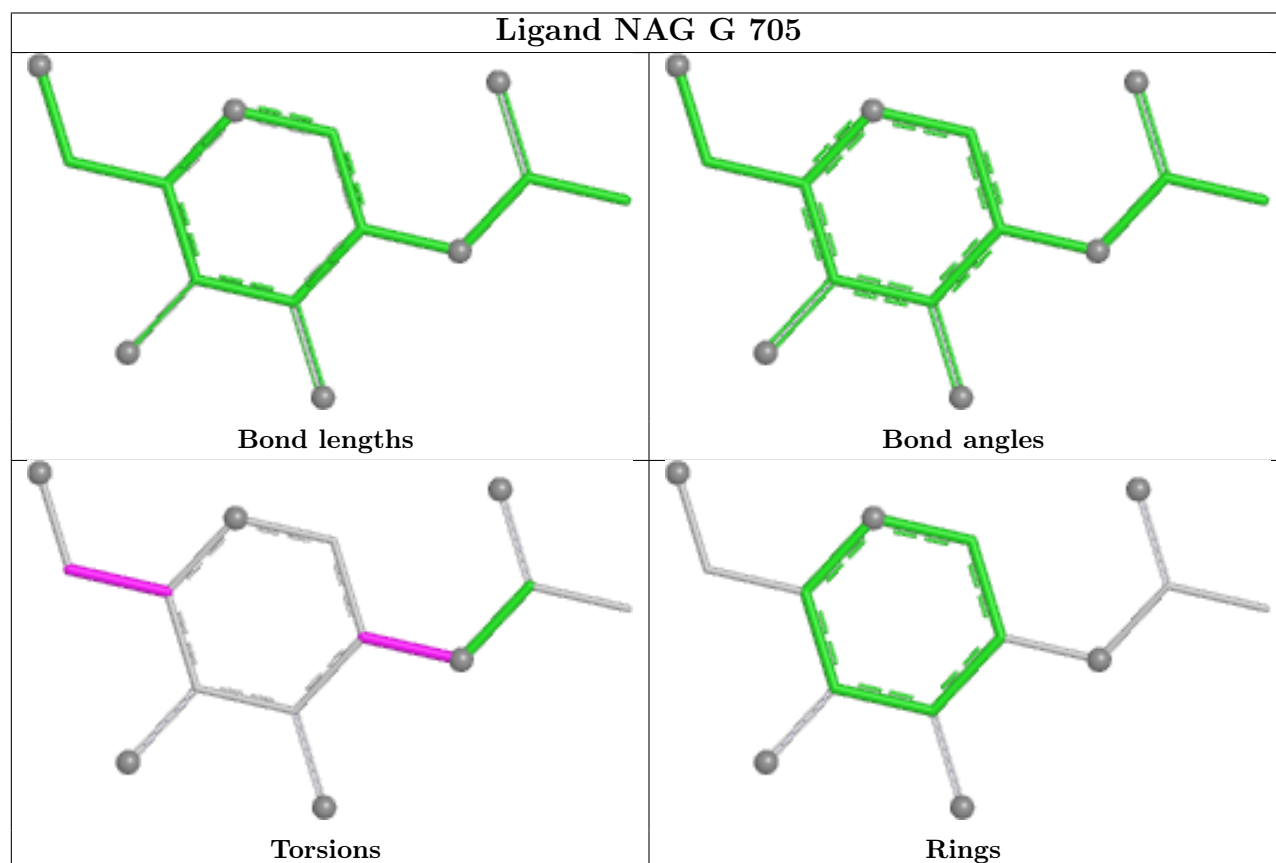


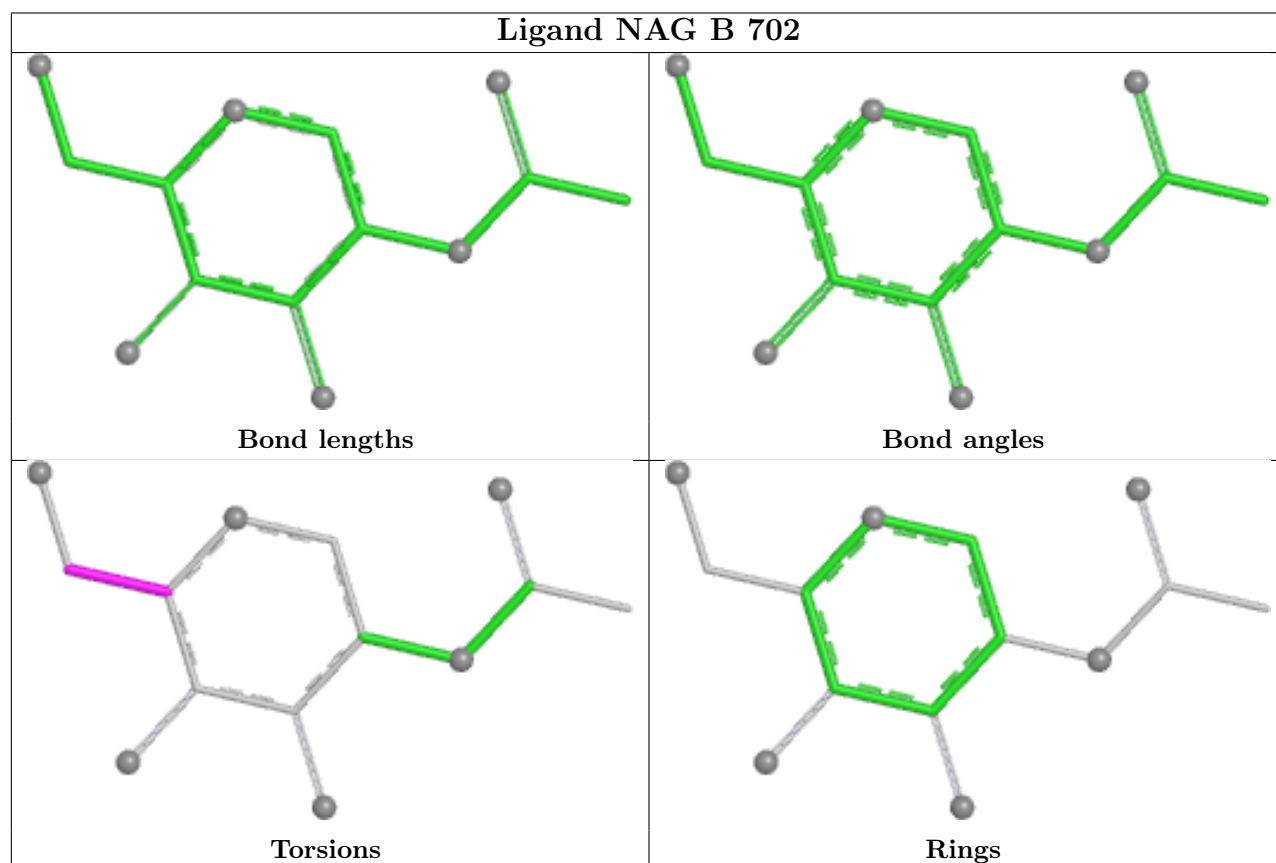
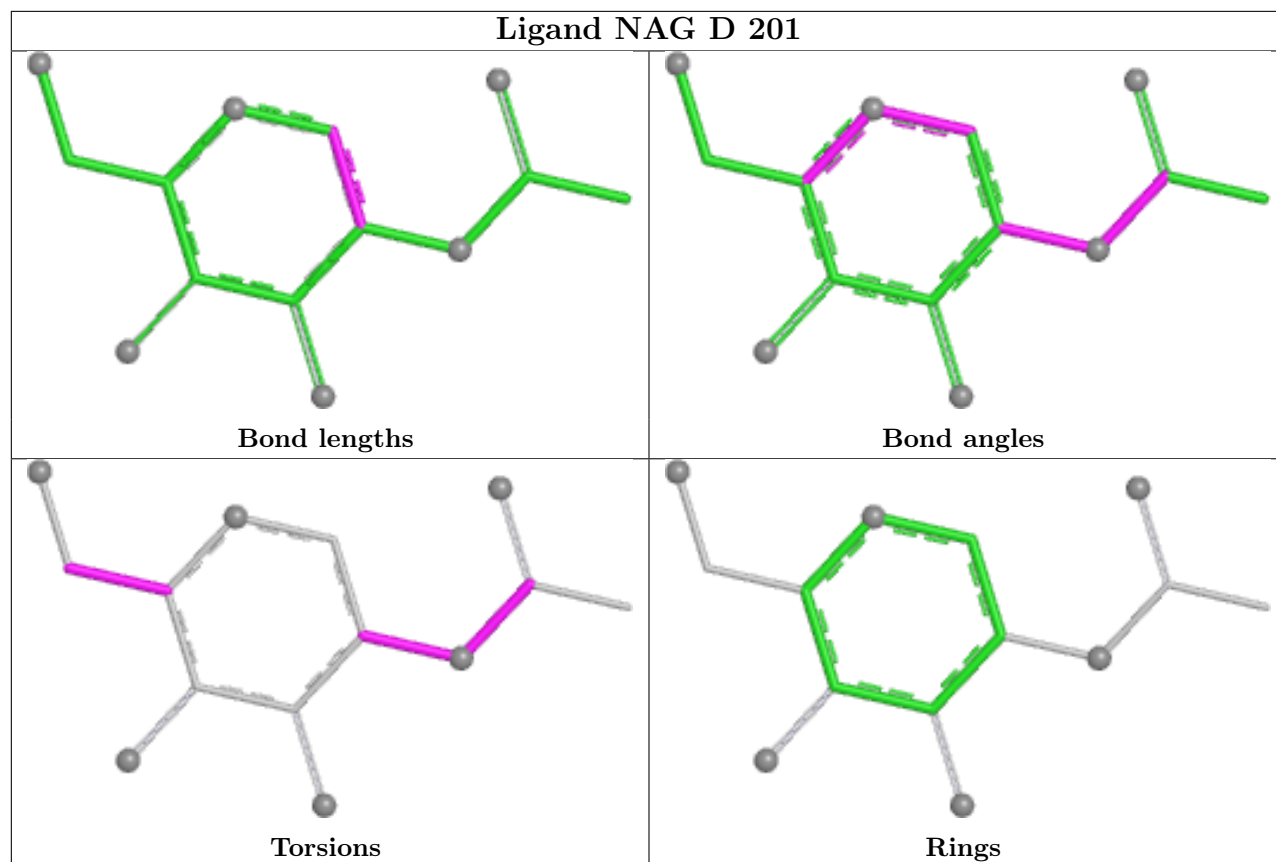


Ligand NAG J 201



Ligand NAG G 705





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	418/426 (98%)	0.22	6 (1%) 73 56	95, 129, 169, 190	0
1	B	419/426 (98%)	0.23	1 (0%) 91 82	81, 111, 146, 175	0
1	E	415/426 (97%)	0.28	6 (1%) 73 56	92, 121, 166, 193	0
1	G	415/426 (97%)	0.35	9 (2%) 62 47	124, 203, 253, 288	0
1	I	417/426 (97%)	0.38	7 (1%) 69 52	115, 177, 272, 369	0
2	C	136/151 (90%)	0.10	0 100 100	121, 164, 188, 200	0
2	D	136/151 (90%)	0.18	3 (2%) 62 47	98, 132, 160, 180	0
2	F	137/151 (90%)	0.24	1 (0%) 84 69	114, 149, 173, 212	0
2	H	134/151 (88%)	0.24	2 (1%) 72 54	98, 130, 159, 171	0
2	J	136/151 (90%)	0.46	4 (2%) 53 40	168, 198, 227, 239	0
All	All	2763/2885 (95%)	0.28	39 (1%) 73 56	81, 141, 232, 369	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	528	THR	3.9
1	G	382	ILE	3.4
2	D	134	ILE	3.3
1	I	374	GLY	3.0
1	A	344	GLY	2.9
2	D	135	THR	2.8
2	D	78	LEU	2.8
1	G	372	GLY	2.7
1	G	559	THR	2.7
1	E	535	LEU	2.7
1	A	606	GLY	2.7
2	H	94	ASP	2.6
1	A	431	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	506	ILE	2.6
1	A	535	LEU	2.6
1	A	277	GLU	2.6
1	G	317	PHE	2.5
1	I	255	ILE	2.5
2	J	98	LEU	2.5
1	G	534	PRO	2.4
1	I	394	PHE	2.4
1	E	428	ARG	2.4
2	F	93	LEU	2.3
1	E	324	THR	2.3
1	I	458	SER	2.3
1	I	381	PHE	2.3
1	E	541	MET	2.3
1	B	415	ILE	2.3
1	E	458	SER	2.3
1	G	322	ASN	2.2
1	A	514	CYS	2.2
1	G	535	LEU	2.2
1	G	472	VAL	2.2
2	J	88	ALA	2.1
2	H	117	PHE	2.1
1	E	537	LEU	2.1
2	J	120	ASN	2.1
1	I	511	GLN	2.0
2	J	100	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
3	BMA	O	3	11/12	-0.04	0.14	181,187,195,197	0
3	BMA	N	3	11/12	0.00	0.15	180,185,188,190	0

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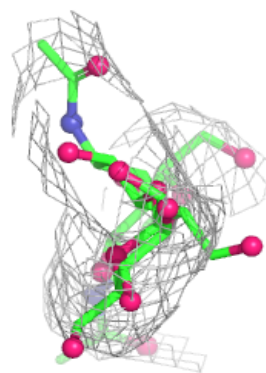
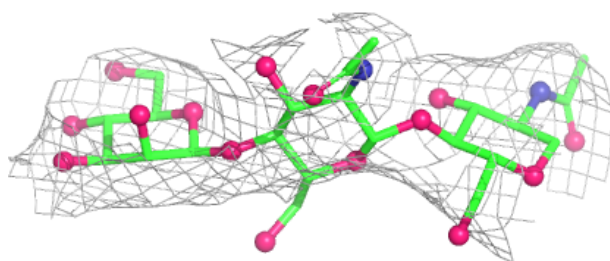
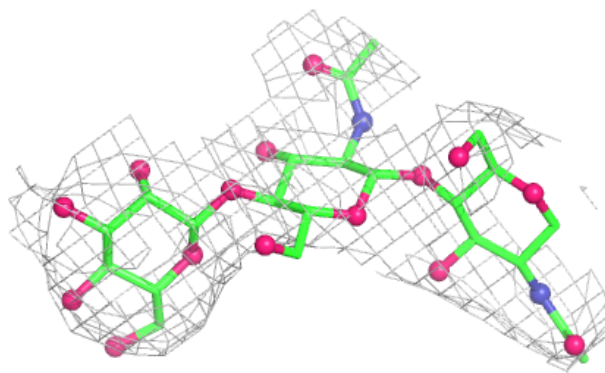
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	M	3	11/12	0.11	0.12	178,181,184,186	0
3	BMA	Q	3	11/12	0.29	0.15	151,154,157,157	0
4	NAG	T	2	14/15	0.36	0.14	176,181,191,194	0
4	NAG	S	2	14/15	0.37	0.18	188,194,197,200	0
3	BMA	U	3	11/12	0.49	0.11	265,269,275,276	0
3	NAG	M	2	14/15	0.63	0.17	157,162,167,167	0
3	BMA	K	3	11/12	0.65	0.09	166,170,174,176	0
3	NAG	K	2	14/15	0.66	0.14	159,163,165,167	0
4	NAG	P	2	14/15	0.66	0.14	153,154,156,156	0
4	NAG	T	1	14/15	0.67	0.11	176,179,183,184	0
3	NAG	U	1	14/15	0.67	0.10	238,243,251,251	0
4	NAG	W	2	14/15	0.68	0.10	157,178,193,197	0
3	NAG	U	2	14/15	0.70	0.12	243,259,271,272	0
4	NAG	S	1	14/15	0.70	0.13	172,174,176,176	0
4	NAG	V	2	14/15	0.73	0.11	203,211,219,224	0
4	NAG	L	1	14/15	0.73	0.10	122,130,139,140	0
3	NAG	O	1	14/15	0.75	0.13	151,159,167,171	0
4	NAG	L	2	14/15	0.77	0.09	133,138,143,146	0
4	NAG	W	1	14/15	0.80	0.10	169,177,183,185	0
3	NAG	O	2	14/15	0.80	0.09	163,168,172,173	0
4	NAG	V	1	14/15	0.83	0.10	191,201,204,205	0
4	NAG	R	2	14/15	0.83	0.08	149,156,167,168	0
3	NAG	N	2	14/15	0.84	0.11	165,168,173,174	0
4	NAG	P	1	14/15	0.84	0.10	128,131,133,134	0
3	NAG	M	1	14/15	0.84	0.11	137,139,141,141	0
3	NAG	Q	1	14/15	0.86	0.13	127,135,140,140	0
3	NAG	Q	2	14/15	0.87	0.12	143,151,159,160	0
3	NAG	N	1	14/15	0.87	0.10	140,144,147,148	0
4	NAG	R	1	14/15	0.89	0.09	135,143,153,154	0
3	NAG	K	1	14/15	0.92	0.10	118,123,127,127	0

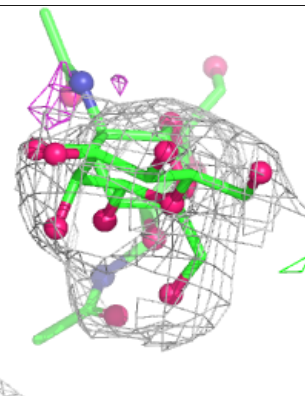
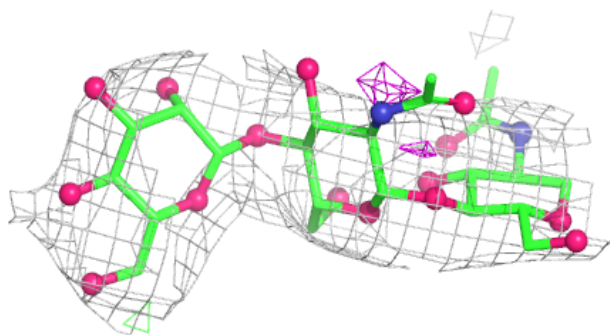
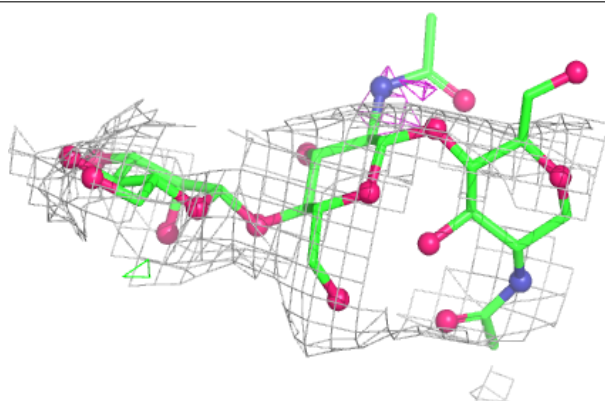
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain K:

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

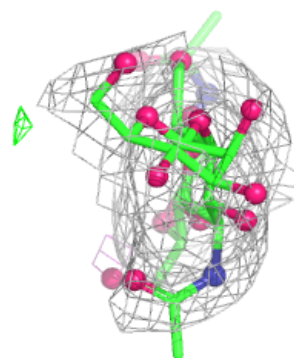
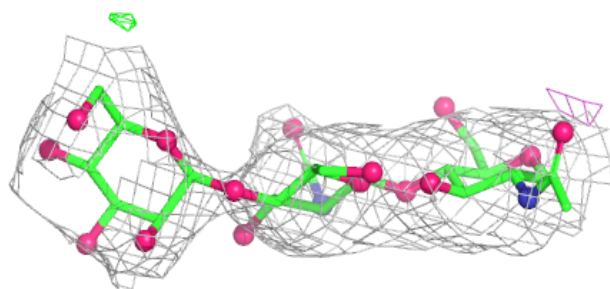
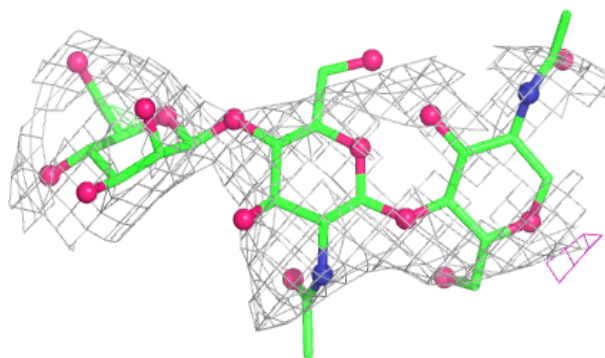
**Electron density around Chain M:**

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

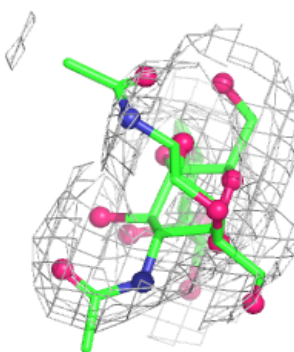
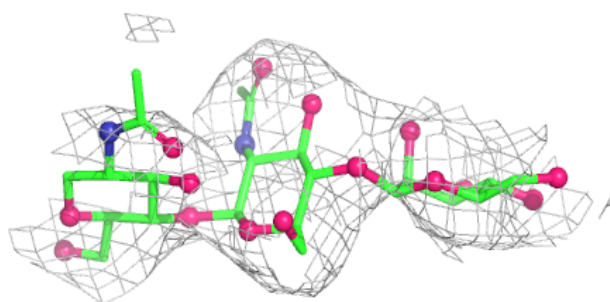
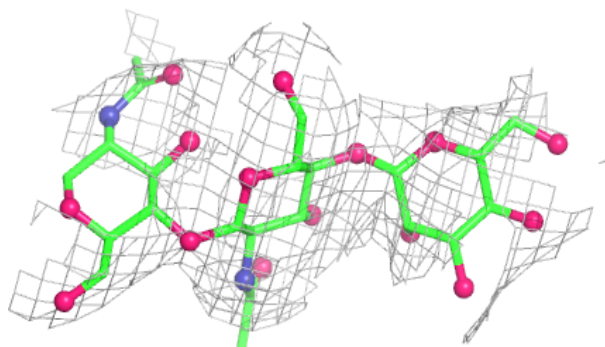


Electron density around Chain N:

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

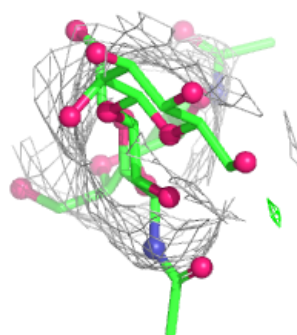
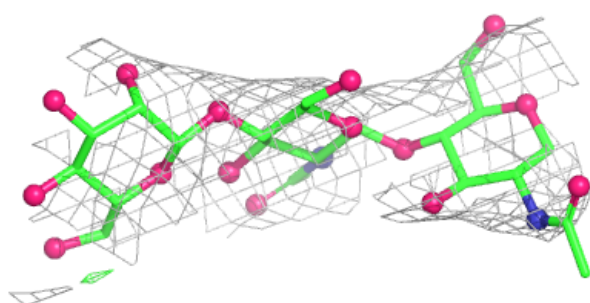
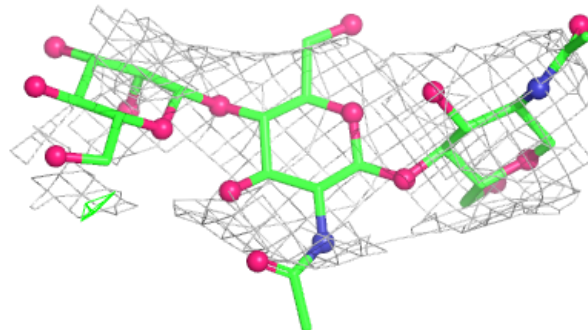
**Electron density around Chain O:**

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

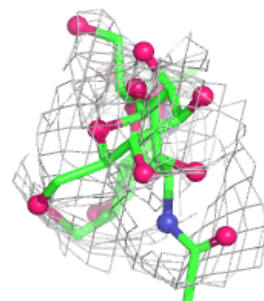
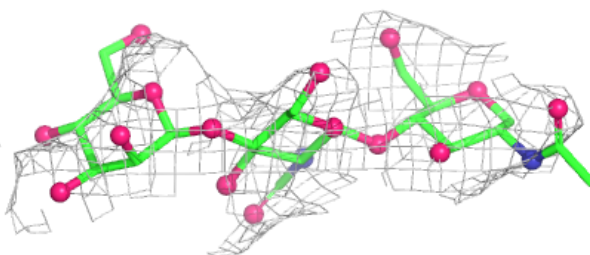


Electron density around Chain Q:

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and green (positive)

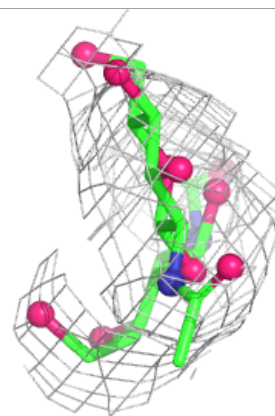
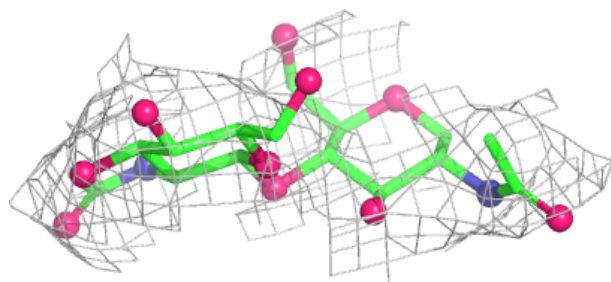
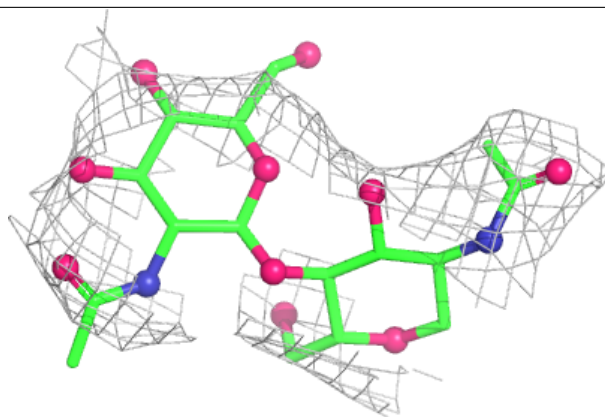
**Electron density around Chain U:**

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and green (positive)

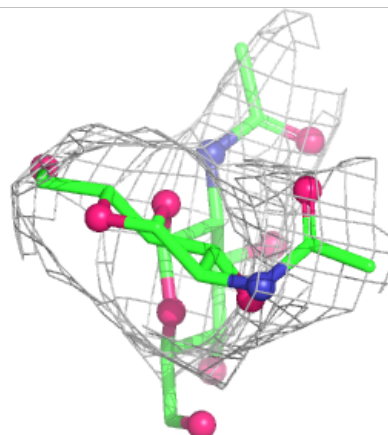
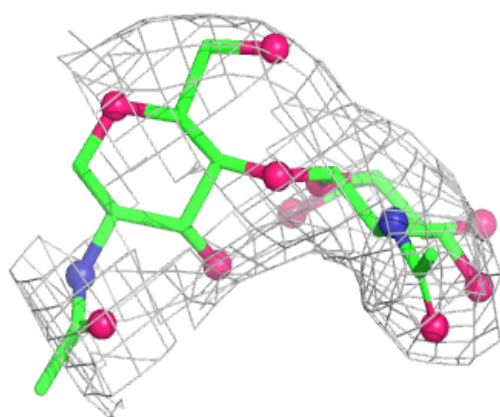
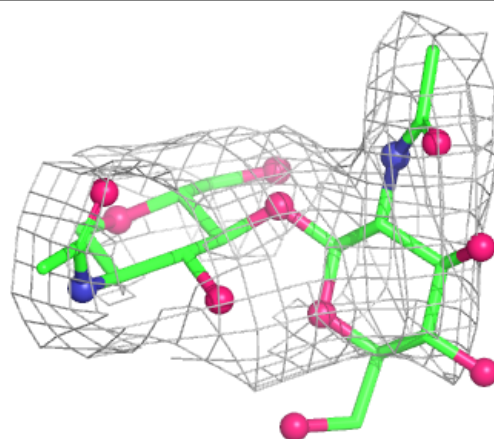


Electron density around Chain L:

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

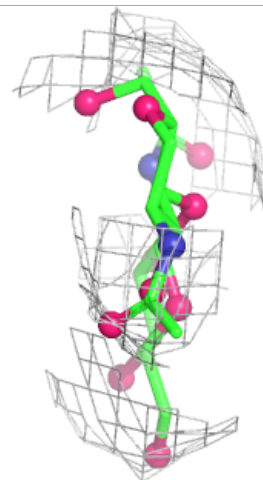
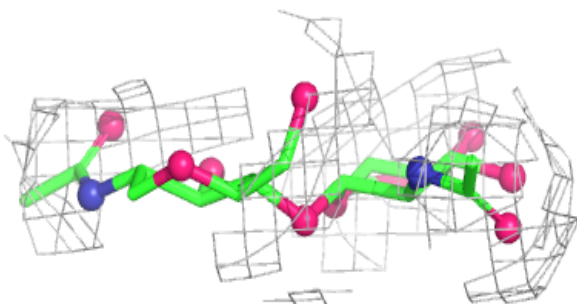
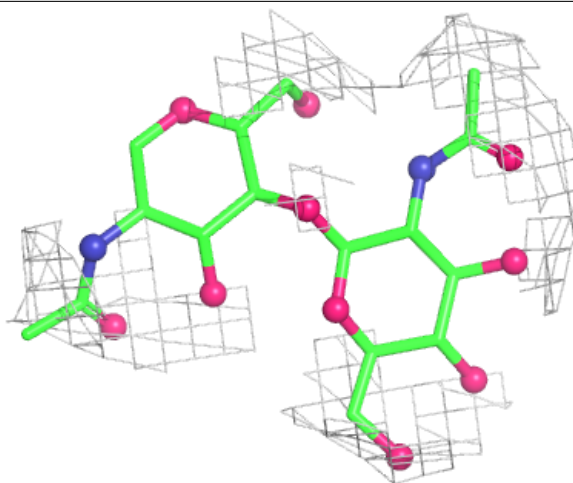
**Electron density around Chain P:**

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



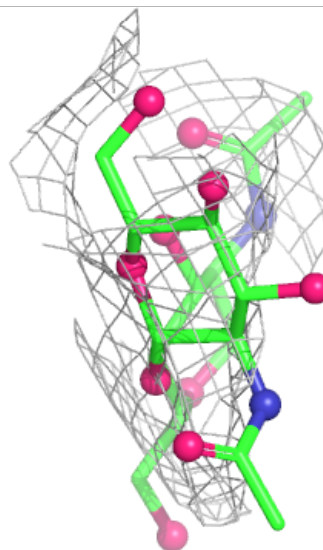
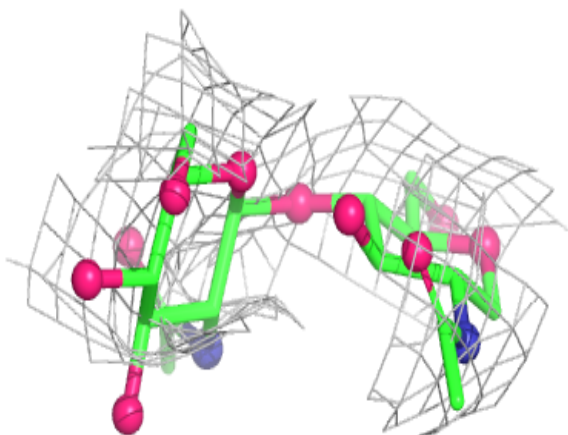
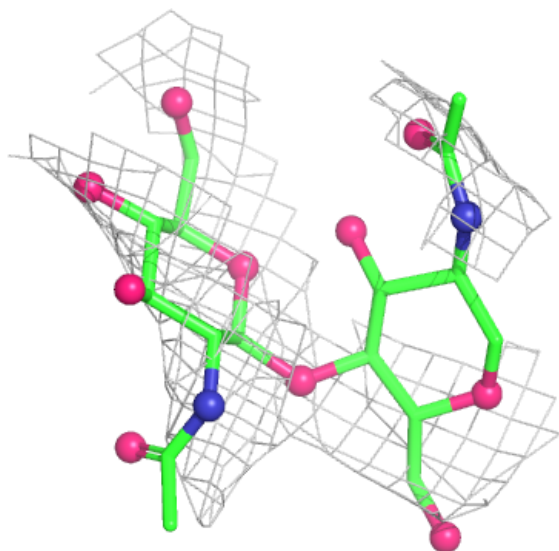
Electron density around Chain R:

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and green (positive)



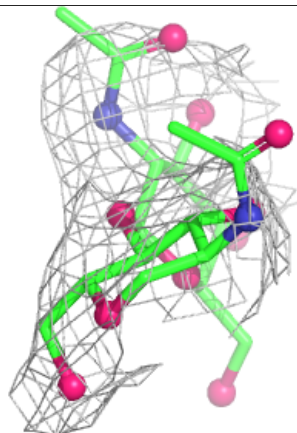
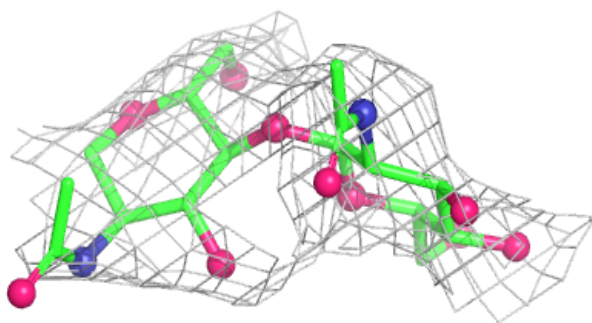
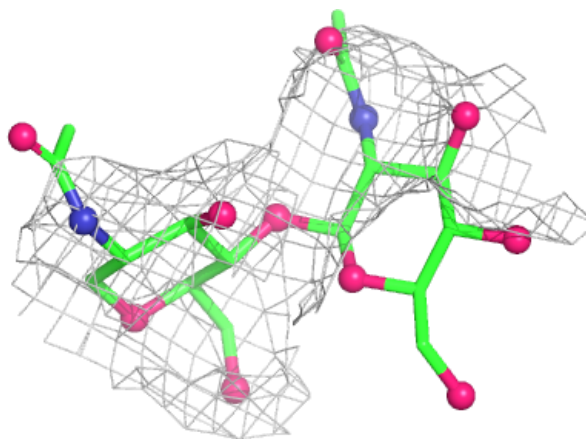
Electron density around Chain S:

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



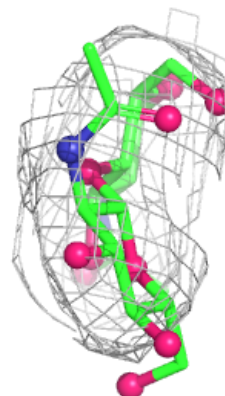
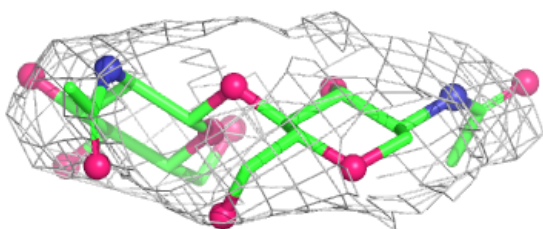
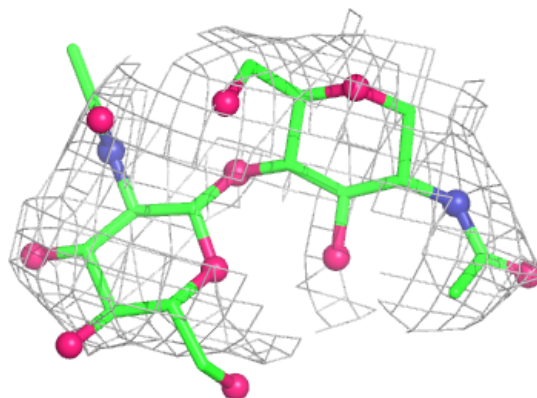
Electron density around Chain T:

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

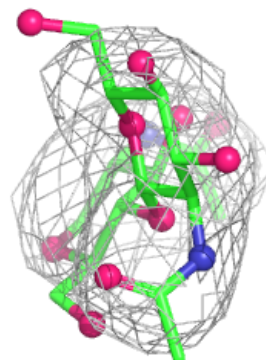
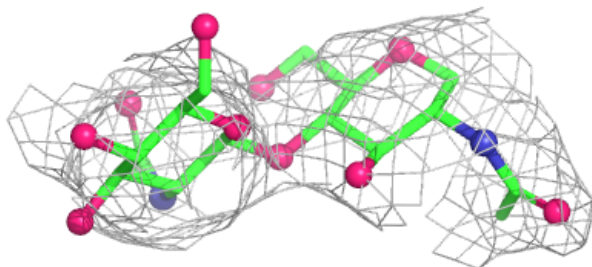
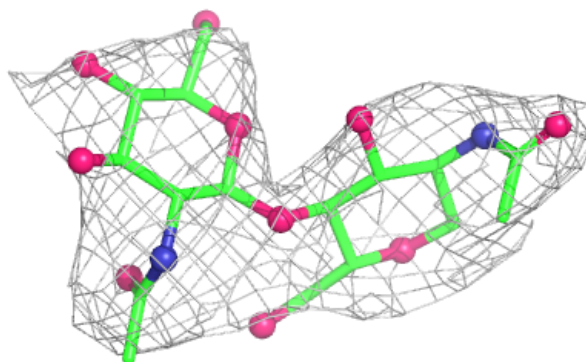


Electron density around Chain V:

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

**Electron density around Chain W:**

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



6.4 Ligands

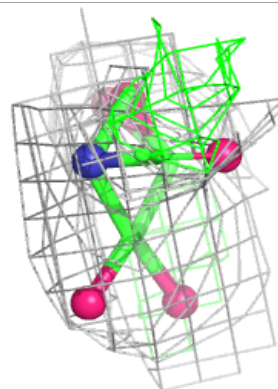
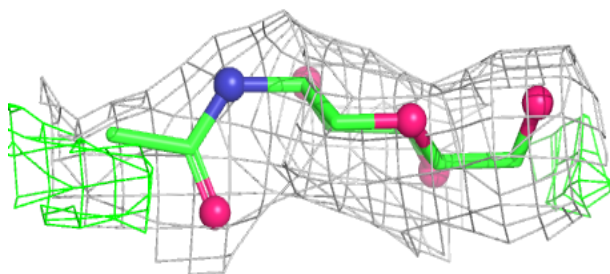
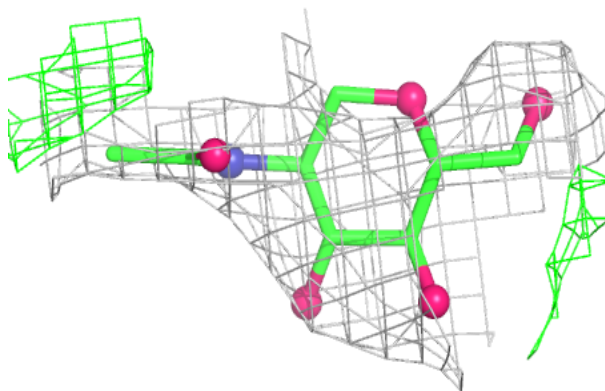
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	709	14/15	-0.10	0.18	167,181,187,191	0
5	NAG	B	711	14/15	0.13	0.16	182,186,190,195	0
5	NAG	G	706	14/15	0.52	0.12	259,266,274,275	0
5	NAG	A	710	14/15	0.61	0.12	183,186,188,191	0
5	NAG	A	701	14/15	0.61	0.12	142,151,167,172	0
5	NAG	J	201	14/15	0.63	0.14	200,206,210,210	0
5	NAG	B	702	14/15	0.67	0.12	152,156,161,161	0
5	NAG	G	705	14/15	0.67	0.12	204,210,218,222	0
5	NAG	A	708	14/15	0.68	0.10	157,165,170,173	0
5	NAG	I	704	14/15	0.69	0.11	219,241,256,258	0
5	NAG	D	201	14/15	0.73	0.10	149,157,167,169	0
5	NAG	B	701	14/15	0.78	0.12	140,145,148,150	0
5	NAG	F	201	14/15	0.80	0.08	164,167,171,172	0
5	NAG	H	201	14/15	0.80	0.09	140,154,162,166	0
5	NAG	E	701	14/15	0.80	0.11	142,144,145,146	0
5	NAG	I	701	14/15	0.84	0.12	160,163,164,167	0
5	NAG	G	701	14/15	0.85	0.12	177,187,195,195	0

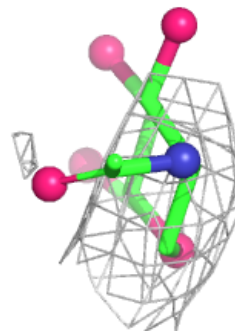
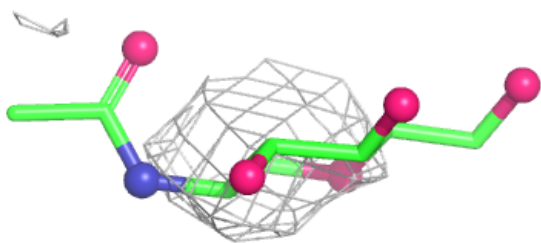
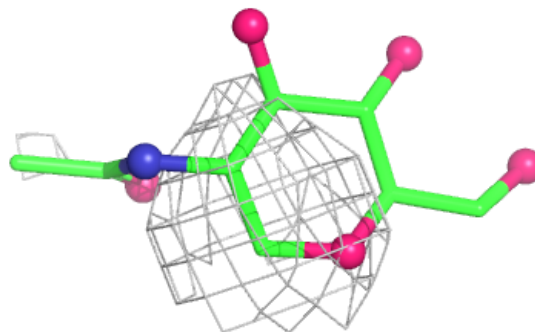
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 709:

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

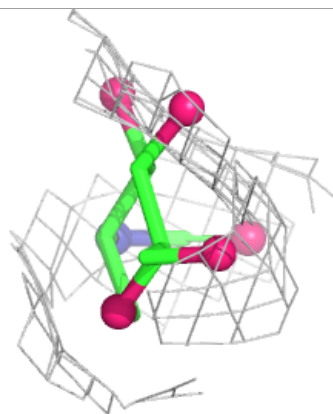
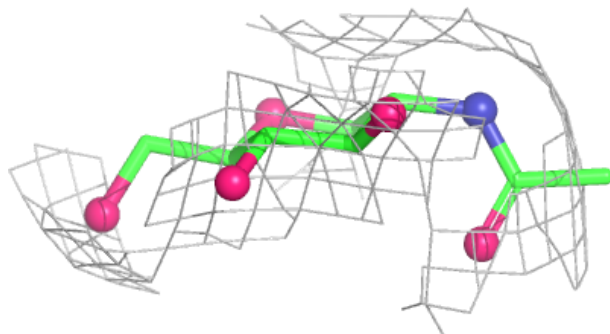
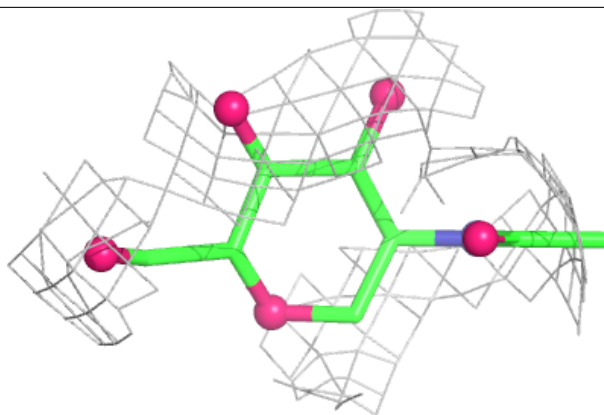
**Electron density around NAG B 711:**

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

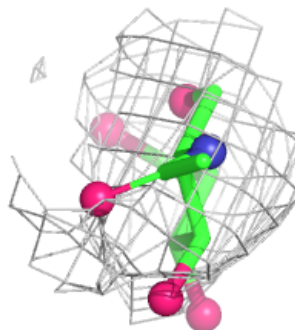
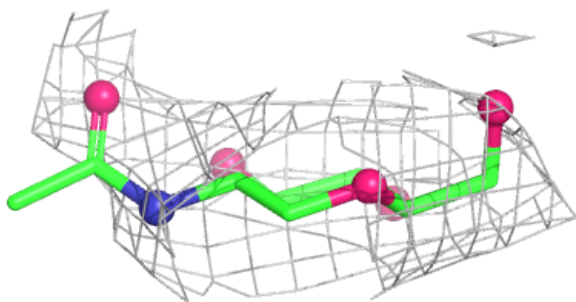


Electron density around NAG G 706:

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

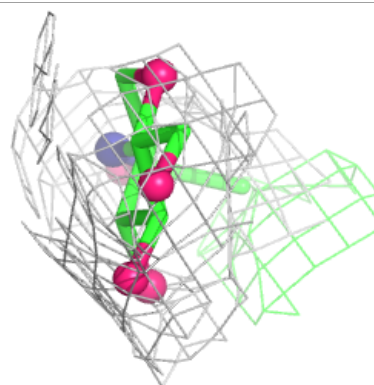
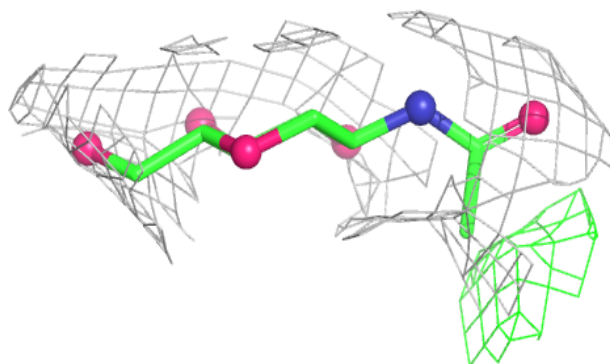
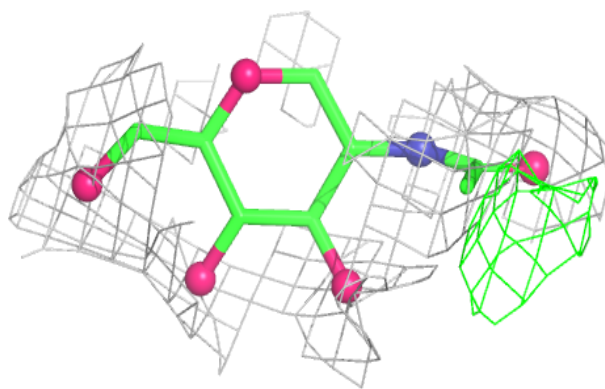
**Electron density around NAG A 710:**

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

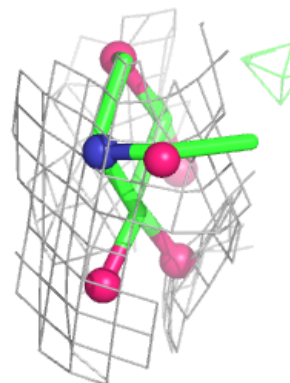
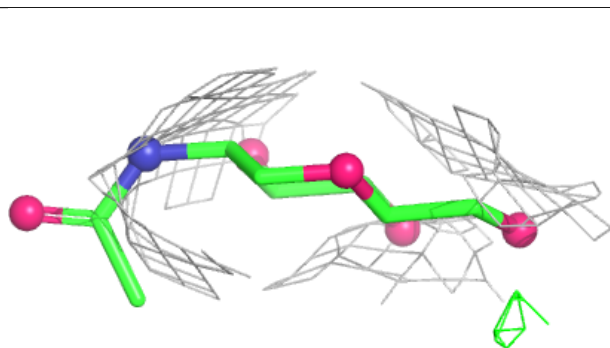
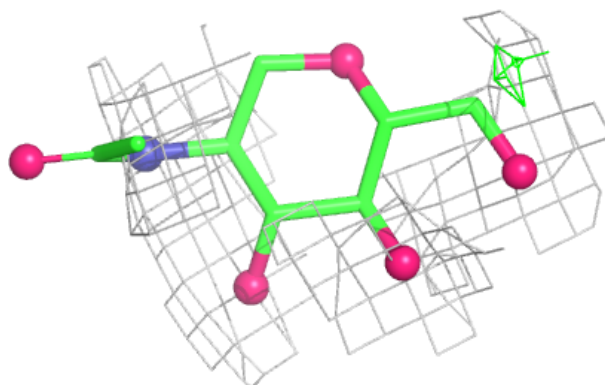


Electron density around NAG A 701:

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

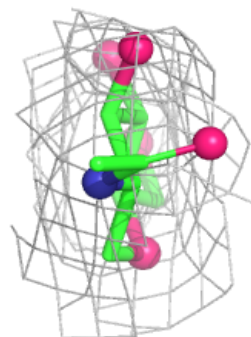
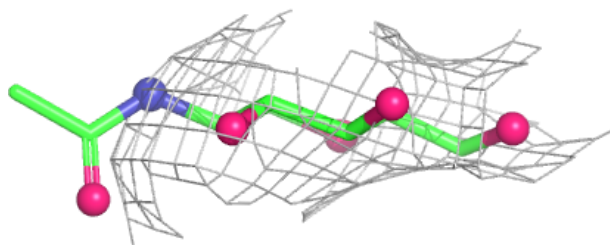
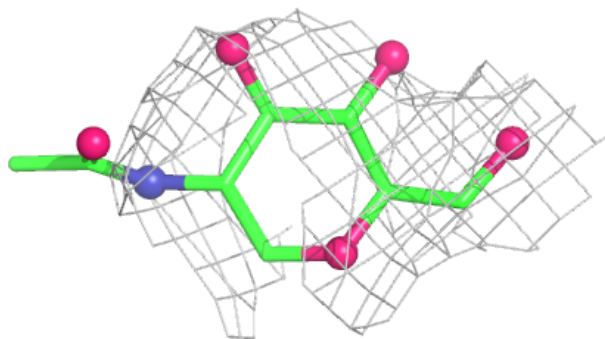
**Electron density around NAG J 201:**

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

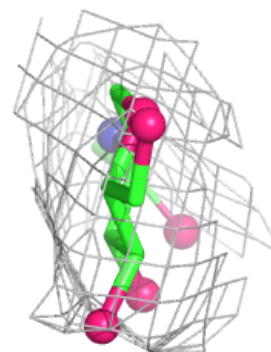
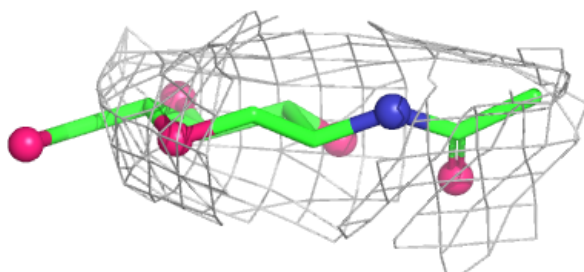
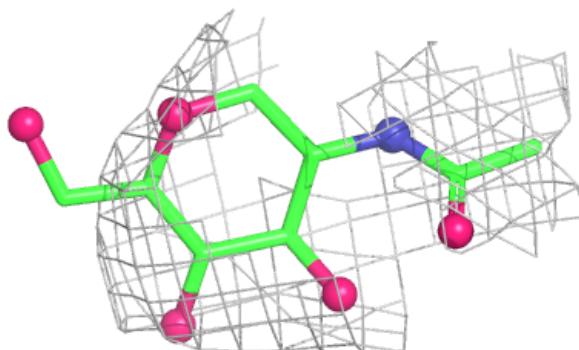


Electron density around NAG B 702:

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

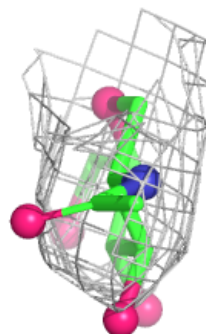
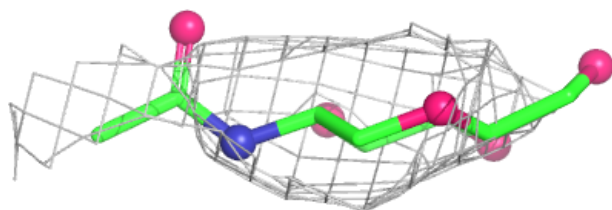
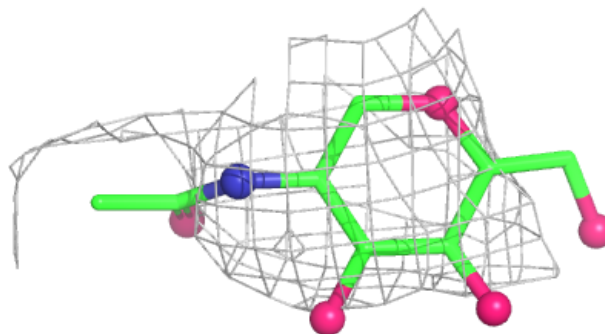
**Electron density around NAG G 705:**

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

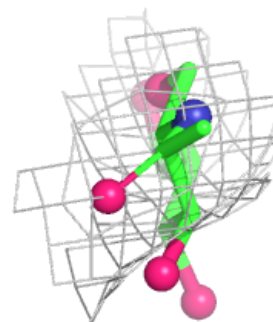
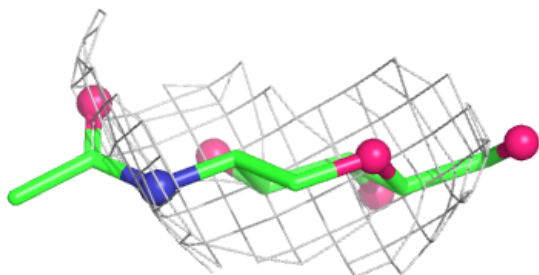
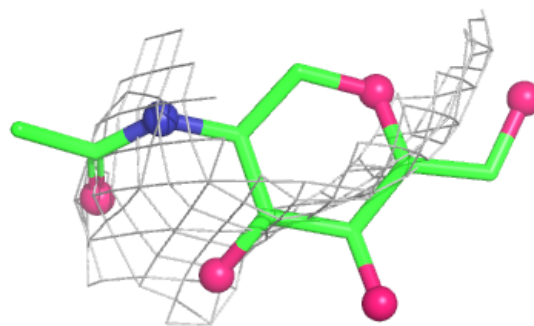


Electron density around NAG A 708:

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

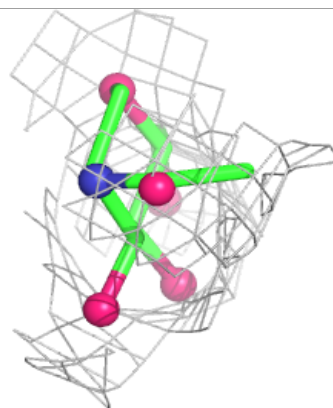
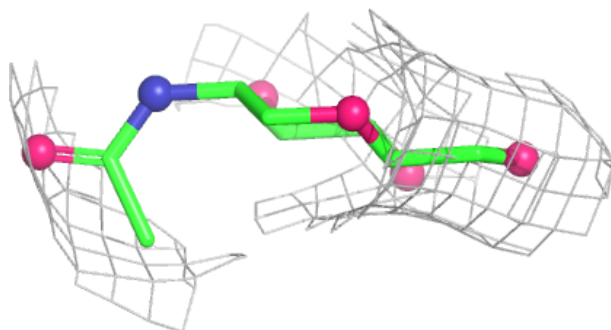
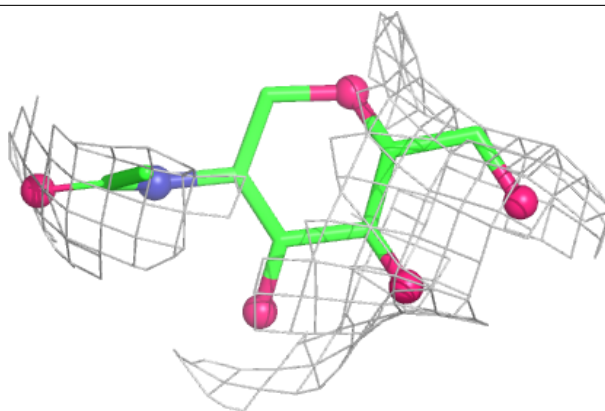
**Electron density around NAG I 704:**

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

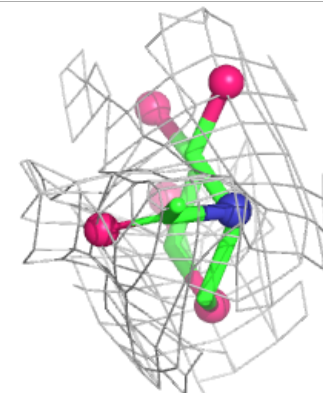
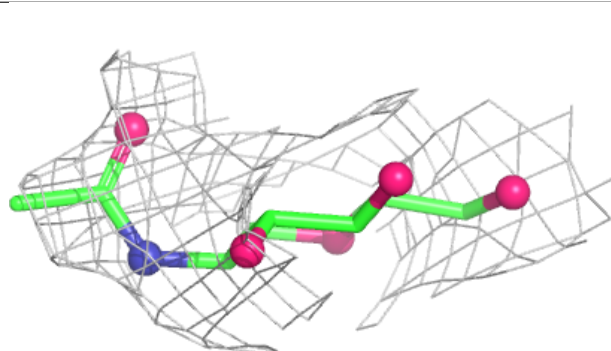
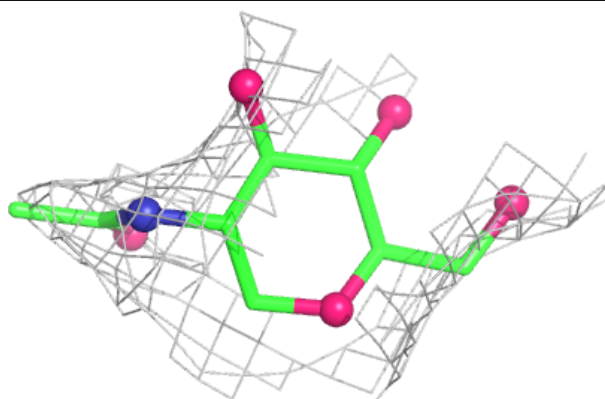


Electron density around NAG D 201:

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

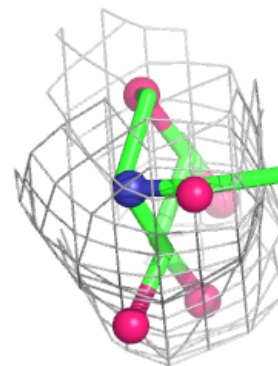
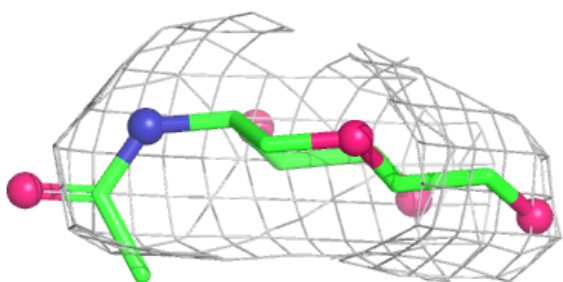
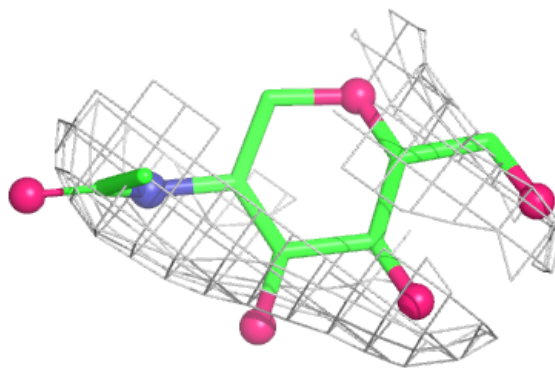
**Electron density around NAG B 701:**

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

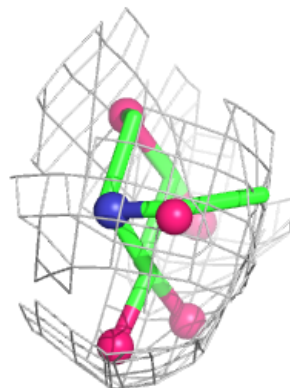
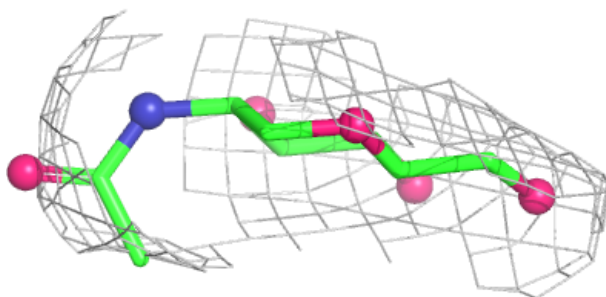
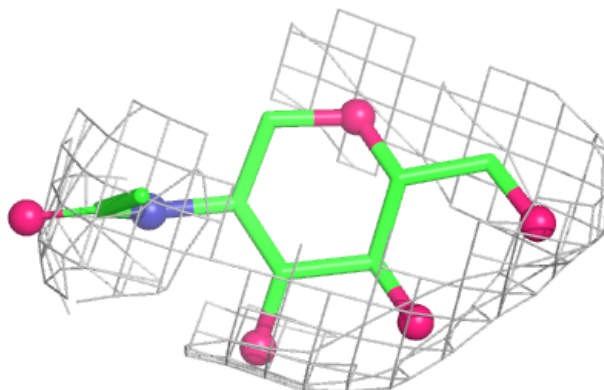


Electron density around NAG F 201:

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

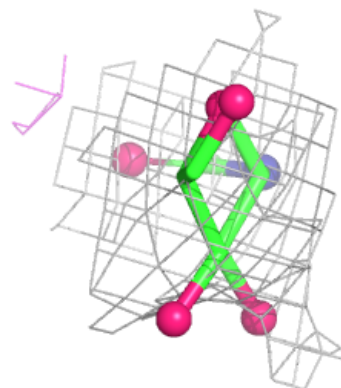
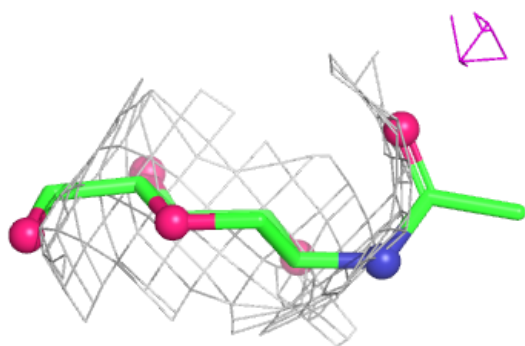
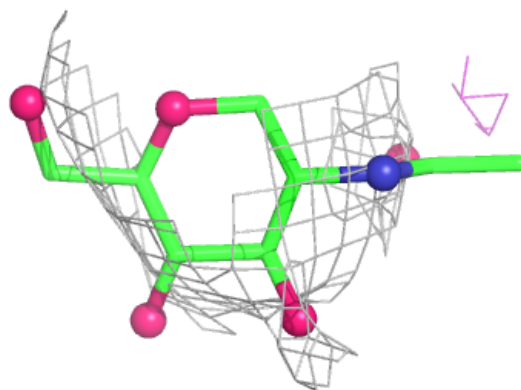
**Electron density around NAG H 201:**

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

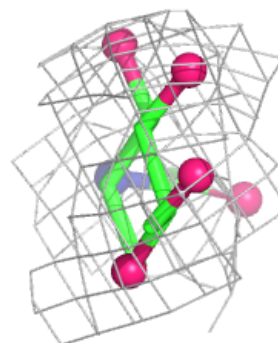
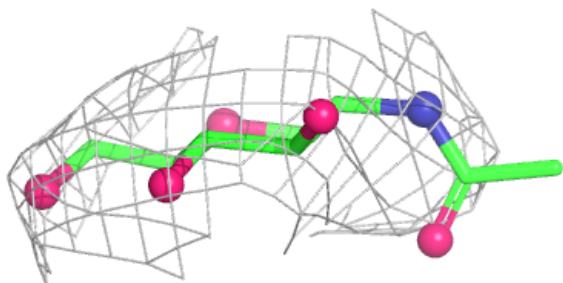
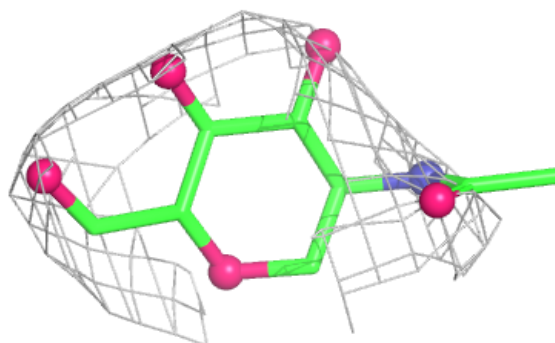


Electron density around NAG E 701:

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

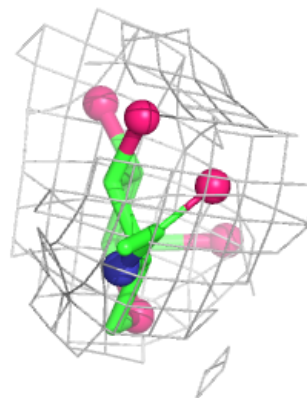
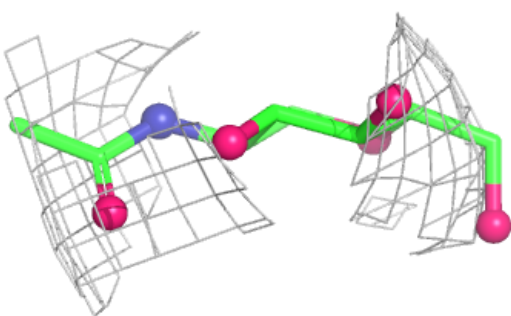
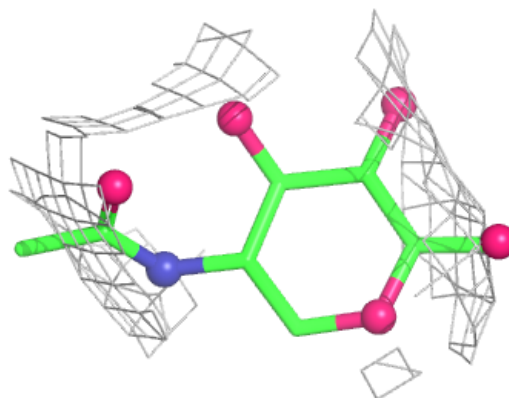
**Electron density around NAG I 701:**

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



Electron density around NAG G 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.