



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 10:46 PM EDT

PDB ID : 6TWV
Title : Crystal structure of the haemagglutinin mutant (Gln226Leu) from an H10N7 seal influenza virus isolated in Germany with human receptor analogue, 6'SLN
Authors : Zhang, J.; Xiong, X.; Purkiss, A.; Walker, P.; Gamblin, S.; Skehel, J.J.
Deposited on : 2020-01-13
Resolution : 2.55 Å (reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

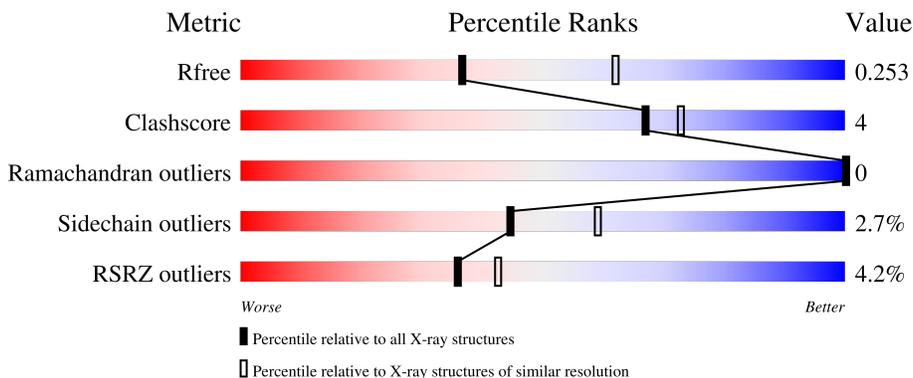
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

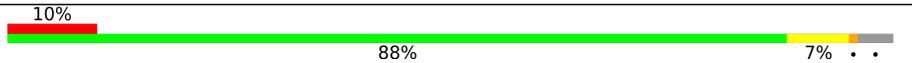
The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	325	
1	C	325	
1	E	325	
1	G	325	
1	I	325	

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Mol	Chain	Length	Quality of chain
1	K	325	 % 90% 8% .
2	B	177	 5% 82% 14% . .
2	D	177	 87% 10% .
2	F	177	 2% 89% 8% .
2	H	177	 % 88% 8% . .
2	J	177	 % 89% 8% .
2	L	177	 92% 5% . .
3	M	3	 33% 67%
3	O	3	 100%
3	P	3	 67% 33%
3	Q	3	 33% 33% 33%
4	N	2	 50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23356 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	318	2429	1508	438	467	16	0	1	0
1	E	313	2399	1485	436	462	16	0	1	0
1	K	319	2434	1511	441	466	16	0	0	0
1	A	315	2399	1492	430	461	16	0	1	0
1	G	318	2432	1509	440	467	16	0	1	0
1	I	319	2434	1511	441	466	16	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ASP	-	expression tag	UNP A0A0A7HR51
C	0	PRO	-	expression tag	UNP A0A0A7HR51
E	-1	ASP	-	expression tag	UNP A0A0A7HR51
E	0	PRO	-	expression tag	UNP A0A0A7HR51
K	-1	ASP	-	expression tag	UNP A0A0A7HR51
K	0	PRO	-	expression tag	UNP A0A0A7HR51
A	-1	ASP	-	expression tag	UNP A0A0A7HR51
A	0	PRO	-	expression tag	UNP A0A0A7HR51
G	-1	ASP	-	expression tag	UNP A0A0A7HR51
G	0	PRO	-	expression tag	UNP A0A0A7HR51
I	-1	ASP	-	expression tag	UNP A0A0A7HR51
I	0	PRO	-	expression tag	UNP A0A0A7HR51

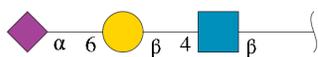
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	172	Total 1386	C 857	N 241	O 280	S 8	0	0	0
2	F	172	Total 1386	C 857	N 241	O 280	S 8	0	0	0
2	L	172	Total 1383	C 855	N 240	O 280	S 8	0	0	0
2	B	172	Total 1383	C 855	N 240	O 280	S 8	0	0	0
2	H	172	Total 1383	C 855	N 240	O 280	S 8	0	0	0
2	J	172	Total 1383	C 855	N 240	O 280	S 8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

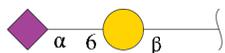
Chain	Residue	Modelled	Actual	Comment	Reference
D	177	LYS	-	expression tag	UNP A0A0A7HR51
F	177	LYS	-	expression tag	UNP A0A0A7HR51
L	177	LYS	-	expression tag	UNP A0A0A7HR51
B	177	LYS	-	expression tag	UNP A0A0A7HR51
H	177	LYS	-	expression tag	UNP A0A0A7HR51
J	177	LYS	-	expression tag	UNP A0A0A7HR51

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	M	3	Total 46	C 25	N 2	O 19	0	0	0
3	O	3	Total 46	C 25	N 2	O 19	0	0	0
3	P	3	Total 46	C 25	N 2	O 19	0	0	0
3	Q	3	Total 46	C 25	N 2	O 19	0	0	0

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose.

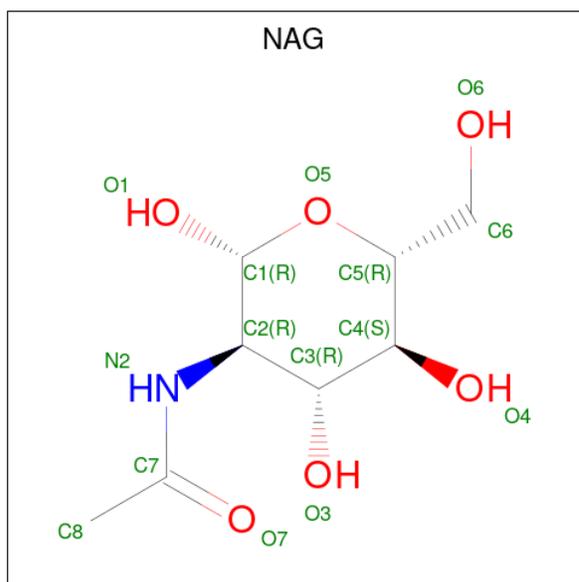


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	N	2	32	17	1	14	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		

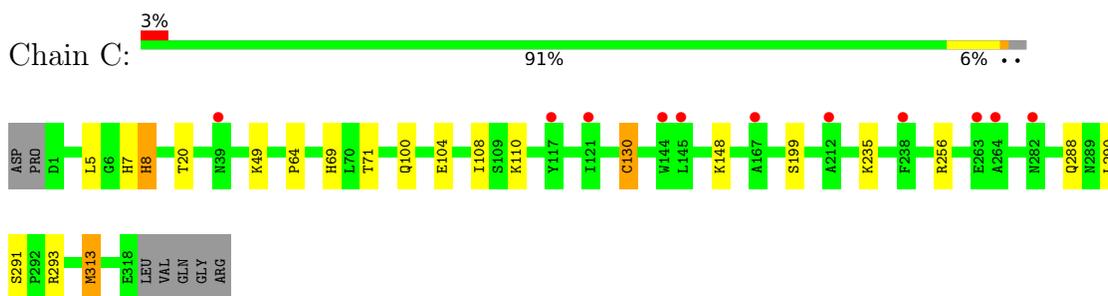
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	19	Total	O	0	0
			19	19		
7	D	21	Total	O	0	0
			21	21		
7	E	8	Total	O	0	0
			8	8		
7	F	11	Total	O	0	0
			11	11		
7	K	24	Total	O	0	0
			24	24		
7	L	15	Total	O	0	0
			15	15		
7	A	5	Total	O	0	0
			5	5		
7	B	12	Total	O	0	0
			12	12		
7	G	27	Total	O	0	0
			27	27		
7	H	11	Total	O	0	0
			11	11		
7	I	6	Total	O	0	0
			6	6		
7	J	8	Total	O	0	0
			8	8		

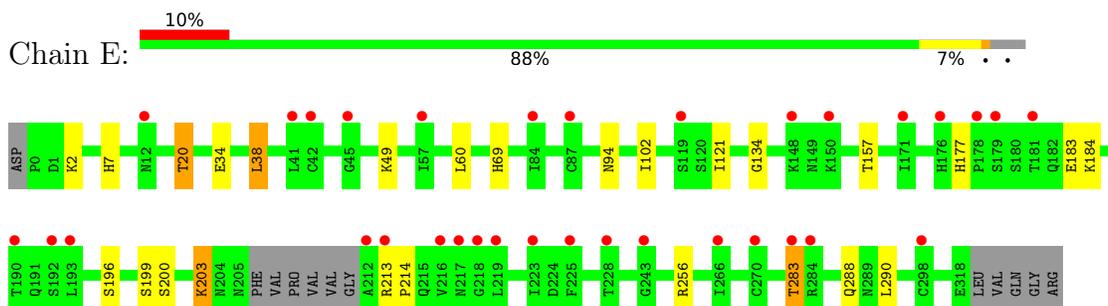
3 Residue-property plots [i](#)

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

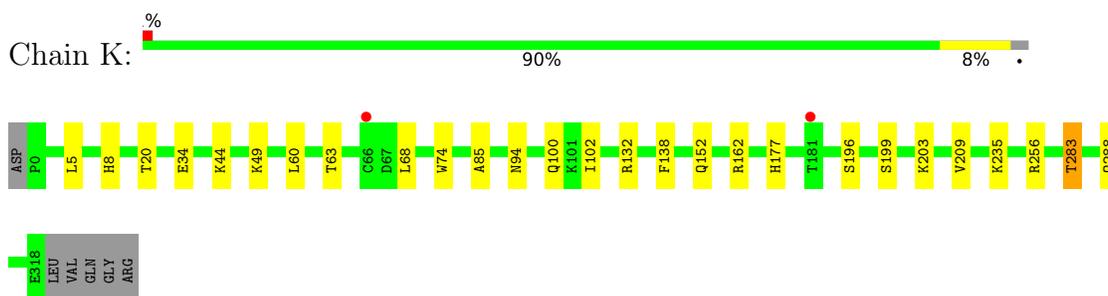
- Molecule 1: Hemagglutinin HA1



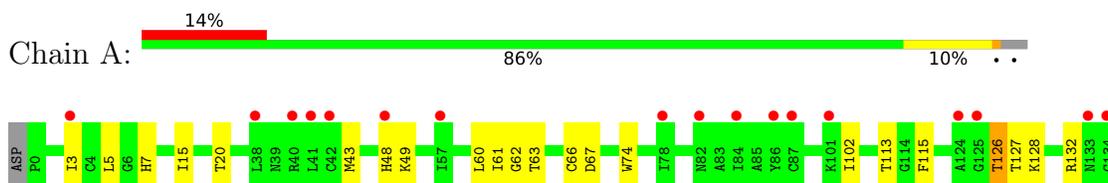
- Molecule 1: Hemagglutinin HA1

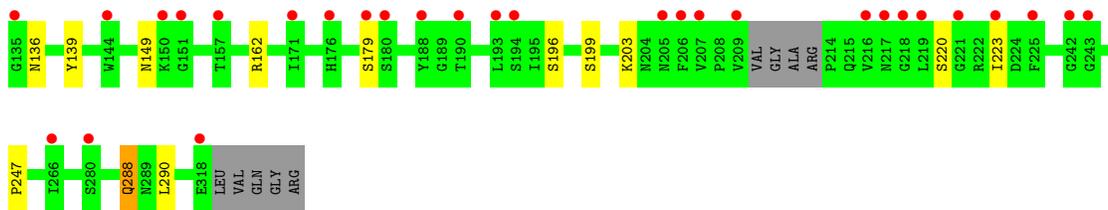


- Molecule 1: Hemagglutinin HA1

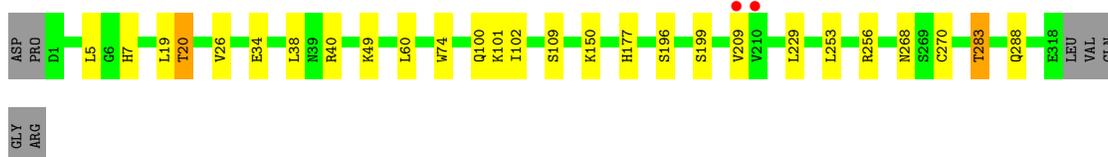


- Molecule 1: Hemagglutinin HA1

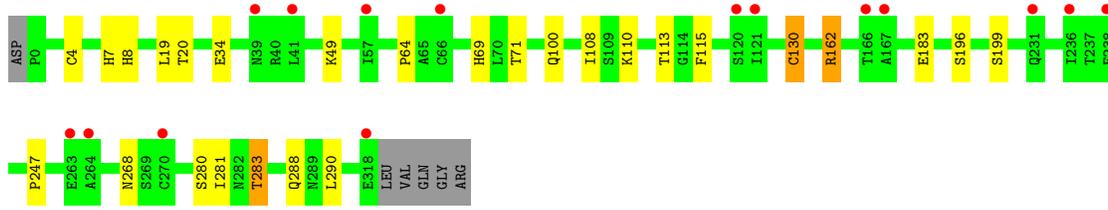




● Molecule 1: Hemagglutinin HA1



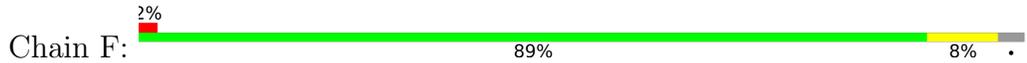
● Molecule 1: Hemagglutinin HA1



● Molecule 2: Hemagglutinin HA2



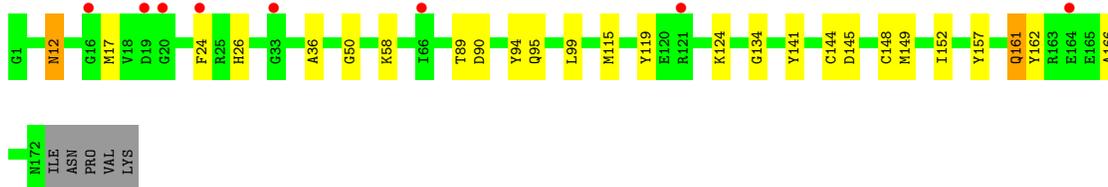
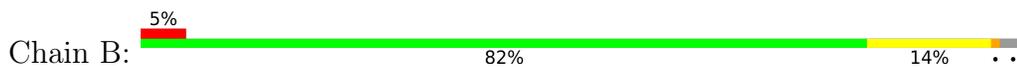
● Molecule 2: Hemagglutinin HA2



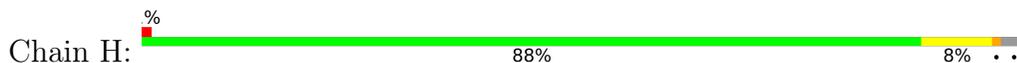
● Molecule 2: Hemagglutinin HA2



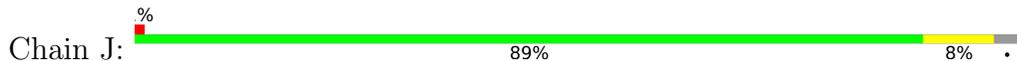
● Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  33% 33% 33%


MAC1
GAL2
SIA3

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

Chain N:  50% 50%


GAL1
SIA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.53Å 217.74Å 150.30Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	65.08 – 2.55 65.08 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (65.08-2.55) 99.0 (65.08-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.55Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.236 , 0.256 0.234 , 0.253	Depositor DCC
R_{free} test set	6995 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtrriage
Anisotropy	0.574	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23356	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.85% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, SIA, NAG, CA

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	0.67	0/2451	0.75	0/3320
1	C	0.64	0/2481	0.75	0/3361
1	E	0.67	0/2449	0.76	0/3313
1	G	0.64	0/2484	0.74	0/3365
1	I	0.64	0/2484	0.74	0/3365
1	K	0.63	0/2484	0.74	0/3365
2	B	0.65	0/1408	0.72	0/1900
2	D	0.63	0/1411	0.71	0/1903
2	F	0.64	0/1411	0.72	0/1903
2	H	0.64	0/1408	0.71	0/1900
2	J	0.64	0/1408	0.71	0/1900
2	L	0.63	0/1408	0.73	0/1900
All	All	0.65	0/23287	0.74	0/31495

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2399	0	2349	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2429	0	2389	17	0
1	E	2399	0	2361	23	0
1	G	2432	0	2391	19	0
1	I	2434	0	2395	18	0
1	K	2434	0	2394	19	0
2	B	1383	0	1282	27	0
2	D	1386	0	1291	18	0
2	F	1386	0	1291	12	0
2	H	1383	0	1282	13	0
2	J	1383	0	1282	11	0
2	L	1383	0	1282	9	0
3	M	46	0	40	0	0
3	O	46	0	40	0	0
3	P	46	0	40	1	0
3	Q	46	0	40	1	0
4	N	32	0	28	2	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	14	0	13	1	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	D	14	0	13	0	0
6	F	14	0	13	0	0
6	G	14	0	13	0	0
6	H	14	0	13	0	0
6	J	14	0	13	0	0
6	K	14	0	13	0	0
6	L	14	0	13	0	0
7	A	5	0	0	0	0
7	B	12	0	0	1	0
7	C	19	0	0	0	0
7	D	21	0	0	1	0
7	E	8	0	0	0	0
7	F	11	0	0	0	0
7	G	27	0	0	1	0
7	H	11	0	0	0	0
7	I	6	0	0	0	0
7	J	8	0	0	0	0
7	K	24	0	0	0	0
7	L	15	0	0	0	0
All	All	23356	0	22307	176	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 4.

The worst 5 of 176 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:GLN:NE2	2:F:95:GLN:HE21	1.59	0.99
2:D:95:GLN:HE22	2:F:95:GLN:HE21	0.96	0.90
1:A:126:THR:CG2	1:A:136:ASN:HB3	2.03	0.89
2:B:145:ASP:O	2:B:148:CYS:SG	2.32	0.88
2:B:144:CYS:C	2:B:148:CYS:SG	2.52	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/325 (96%)	304 (97%)	8 (3%)	0	100	100
1	C	317/325 (98%)	308 (97%)	9 (3%)	0	100	100
1	E	310/325 (95%)	302 (97%)	8 (3%)	0	100	100
1	G	317/325 (98%)	310 (98%)	7 (2%)	0	100	100
1	I	317/325 (98%)	308 (97%)	9 (3%)	0	100	100
1	K	317/325 (98%)	310 (98%)	7 (2%)	0	100	100
2	B	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	D	170/177 (96%)	165 (97%)	5 (3%)	0	100	100
2	F	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	H	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	J	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	L	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
All	All	2910/3012 (97%)	2827 (97%)	83 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/275 (96%)	257 (97%)	8 (3%)	41	55
1	C	269/275 (98%)	262 (97%)	7 (3%)	46	61
1	E	266/275 (97%)	255 (96%)	11 (4%)	30	41
1	G	269/275 (98%)	261 (97%)	8 (3%)	41	55
1	I	269/275 (98%)	258 (96%)	11 (4%)	30	41
1	K	269/275 (98%)	259 (96%)	10 (4%)	34	46
2	B	145/151 (96%)	142 (98%)	3 (2%)	53	68
2	D	146/151 (97%)	144 (99%)	2 (1%)	67	79
2	F	146/151 (97%)	145 (99%)	1 (1%)	84	90
2	H	145/151 (96%)	142 (98%)	3 (2%)	53	68
2	J	145/151 (96%)	143 (99%)	2 (1%)	67	79
2	L	145/151 (96%)	143 (99%)	2 (1%)	67	79
All	All	2479/2556 (97%)	2411 (97%)	68 (3%)	44	59

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	20	THR
1	I	130	CYS
1	I	288	GLN
1	K	100	GLN
1	K	94	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	53	ASN

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Mol	Chain	Res	Type
1	I	94	ASN
1	I	7	HIS
1	I	153	ASN
1	E	177	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	M	1	3	15,15,15	0.58	0	21,21,21	1.64	5 (23%)
3	GAL	M	2	3	11,11,12	0.42	0	15,15,17	0.68	0
3	SIA	M	3	3	20,20,21	0.63	0	24,28,31	1.43	6 (25%)
4	GAL	N	1	4	12,12,12	0.57	0	17,17,17	0.84	0
4	SIA	N	2	4	20,20,21	0.62	0	24,28,31	1.28	4 (16%)
3	NAG	O	1	3	15,15,15	0.44	0	21,21,21	1.22	2 (9%)
3	GAL	O	2	3	11,11,12	0.37	0	15,15,17	1.21	2 (13%)
3	SIA	O	3	3	20,20,21	0.61	0	24,28,31	1.33	4 (16%)
3	NAG	P	1	3	15,15,15	0.47	0	21,21,21	0.88	1 (4%)
3	GAL	P	2	3	11,11,12	0.44	0	15,15,17	1.32	1 (6%)
3	SIA	P	3	3	20,20,21	0.69	0	24,28,31	1.33	5 (20%)
3	NAG	Q	1	3	15,15,15	0.58	0	21,21,21	1.65	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GAL	Q	2	3	11,11,12	0.42	0	15,15,17	0.77	0
3	SIA	Q	3	3	20,20,21	0.63	0	24,28,31	1.37	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	3	-	3/6/26/26	0/1/1/1
3	GAL	M	2	3	-	0/2/19/22	0/1/1/1
3	SIA	M	3	3	-	0/18/34/38	0/1/1/1
4	GAL	N	1	4	-	0/2/22/22	0/1/1/1
4	SIA	N	2	4	-	3/18/34/38	0/1/1/1
3	NAG	O	1	3	-	2/6/26/26	0/1/1/1
3	GAL	O	2	3	-	0/2/19/22	0/1/1/1
3	SIA	O	3	3	-	0/18/34/38	0/1/1/1
3	NAG	P	1	3	-	0/6/26/26	0/1/1/1
3	GAL	P	2	3	-	0/2/19/22	0/1/1/1
3	SIA	P	3	3	-	1/18/34/38	0/1/1/1
3	NAG	Q	1	3	-	3/6/26/26	0/1/1/1
3	GAL	Q	2	3	-	0/2/19/22	0/1/1/1
3	SIA	Q	3	3	-	2/18/34/38	0/1/1/1

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	2	GAL	C1-C2-C3	3.99	114.57	109.67
3	Q	1	NAG	O5-C1-C2	3.66	113.19	109.52
3	M	1	NAG	O5-C1-C2	3.45	112.98	109.52
3	M	1	NAG	C1-O5-C5	3.41	120.10	113.66
3	P	3	SIA	C6-C5-N5	-3.31	105.42	110.91

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	2	SIA	O6-C6-C7-O7
3	M	1	NAG	C8-C7-N2-C2

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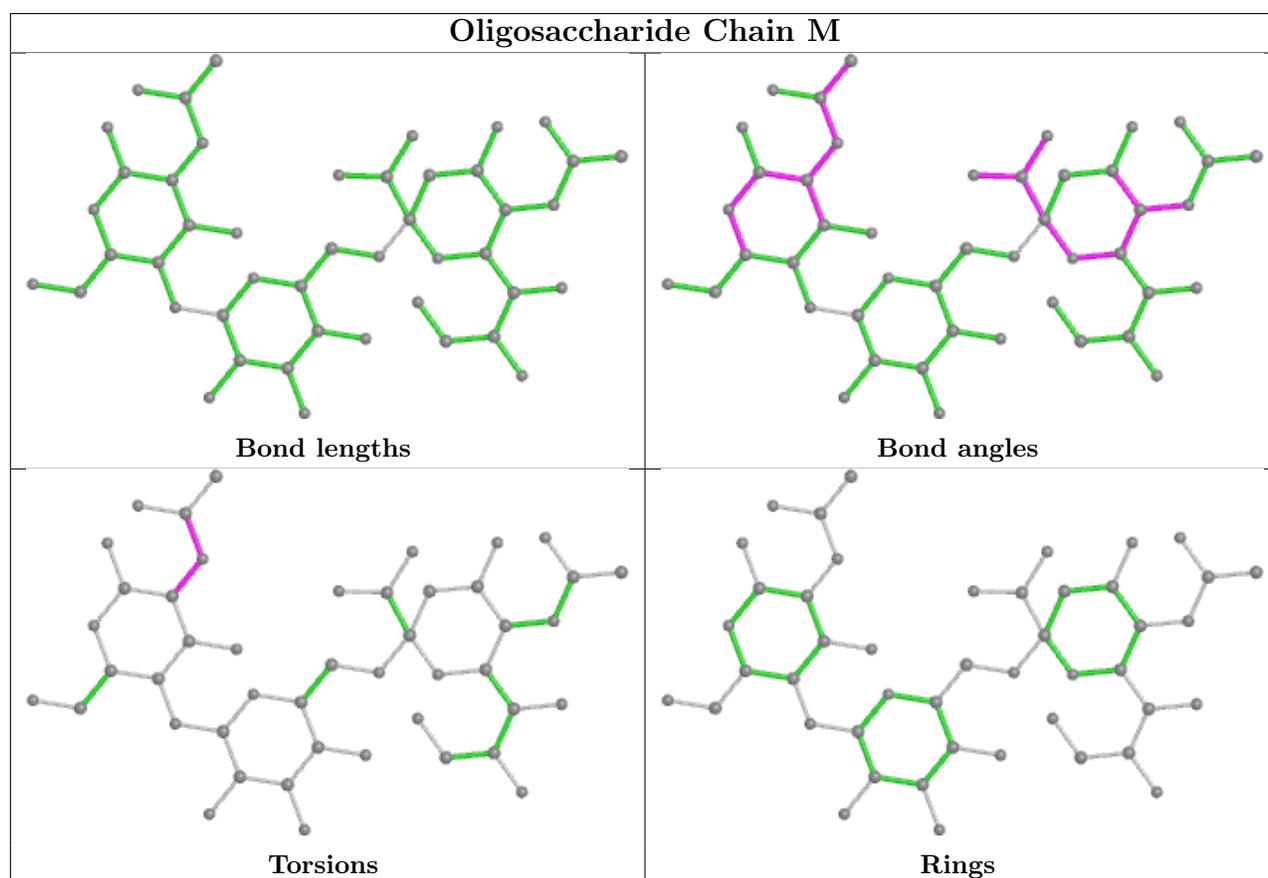
Mol	Chain	Res	Type	Atoms
3	M	1	NAG	O7-C7-N2-C2
3	O	1	NAG	C8-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2

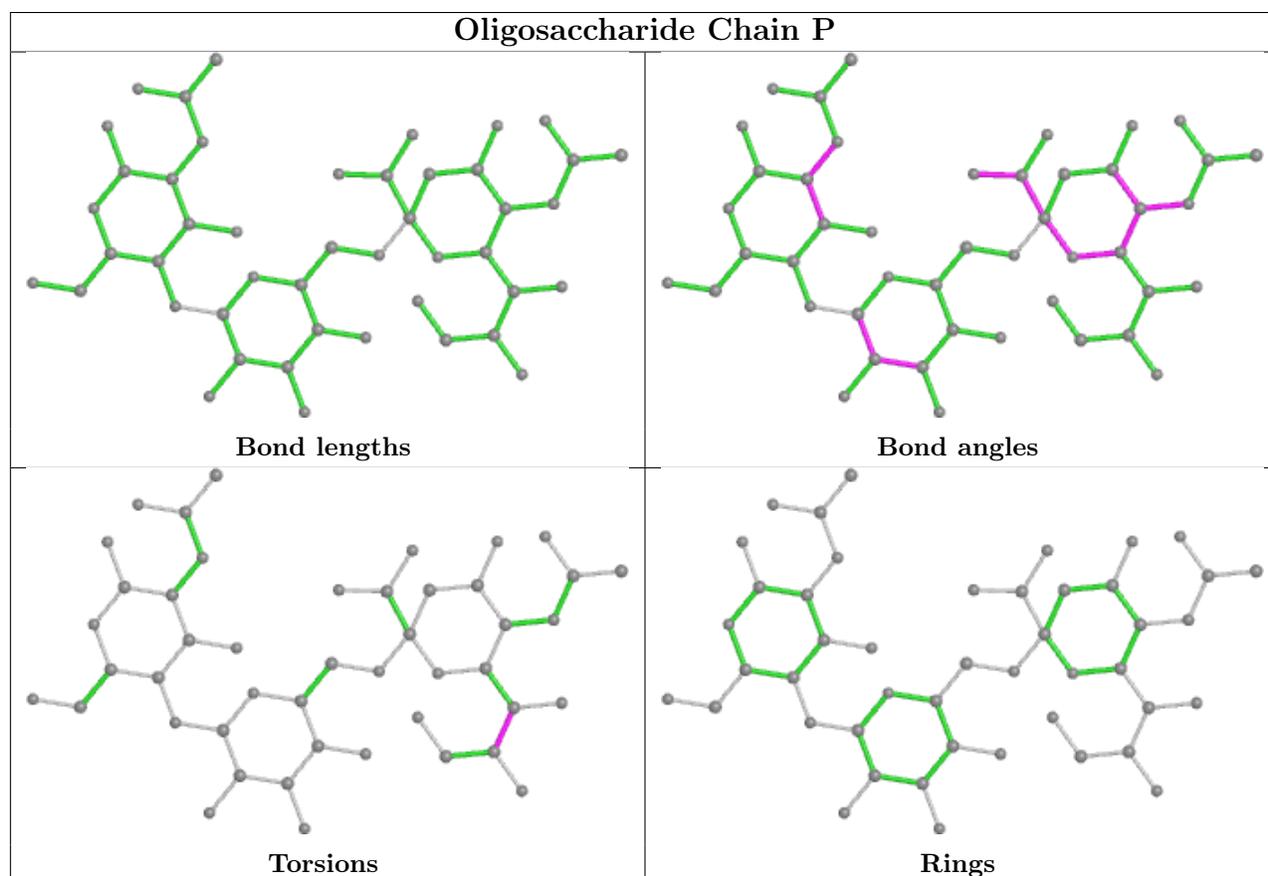
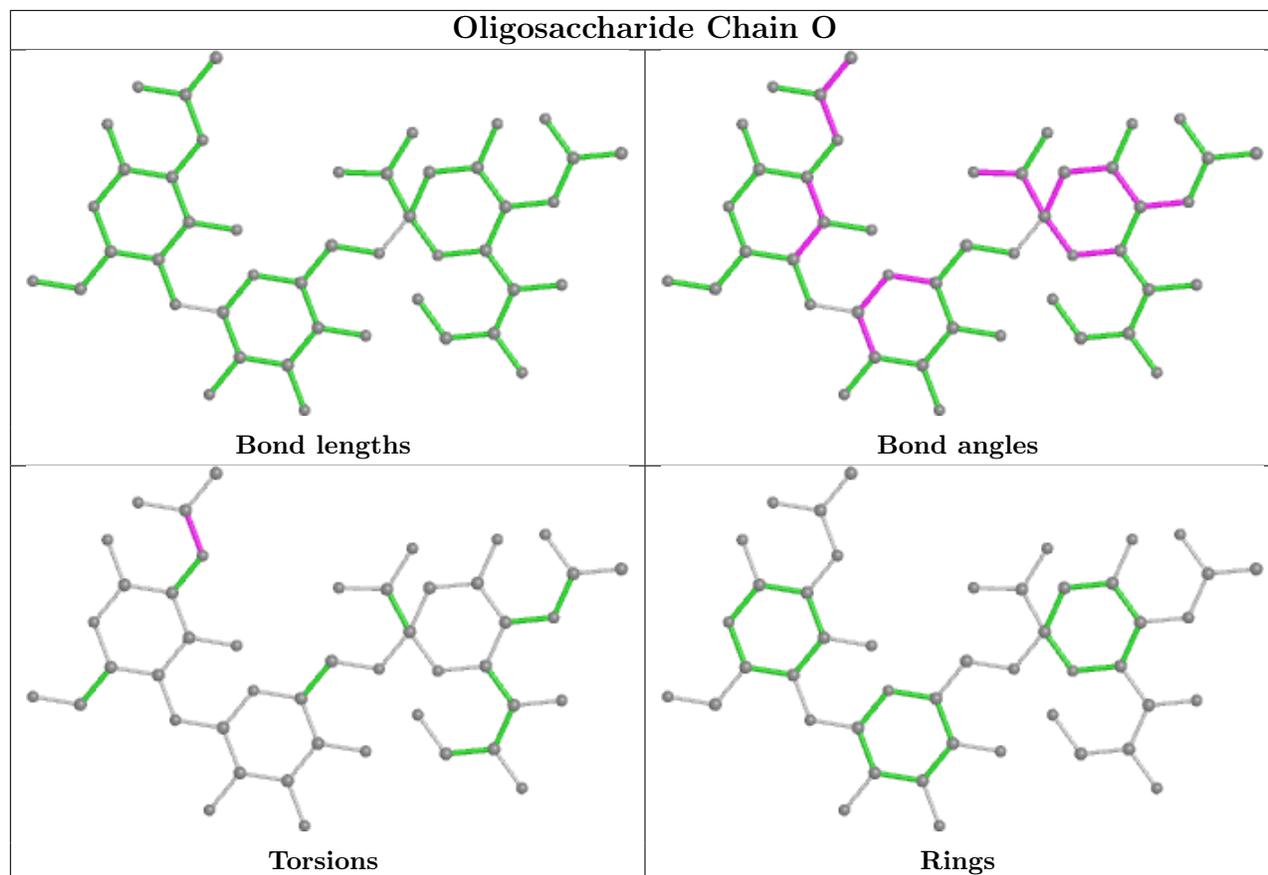
There are no ring outliers.

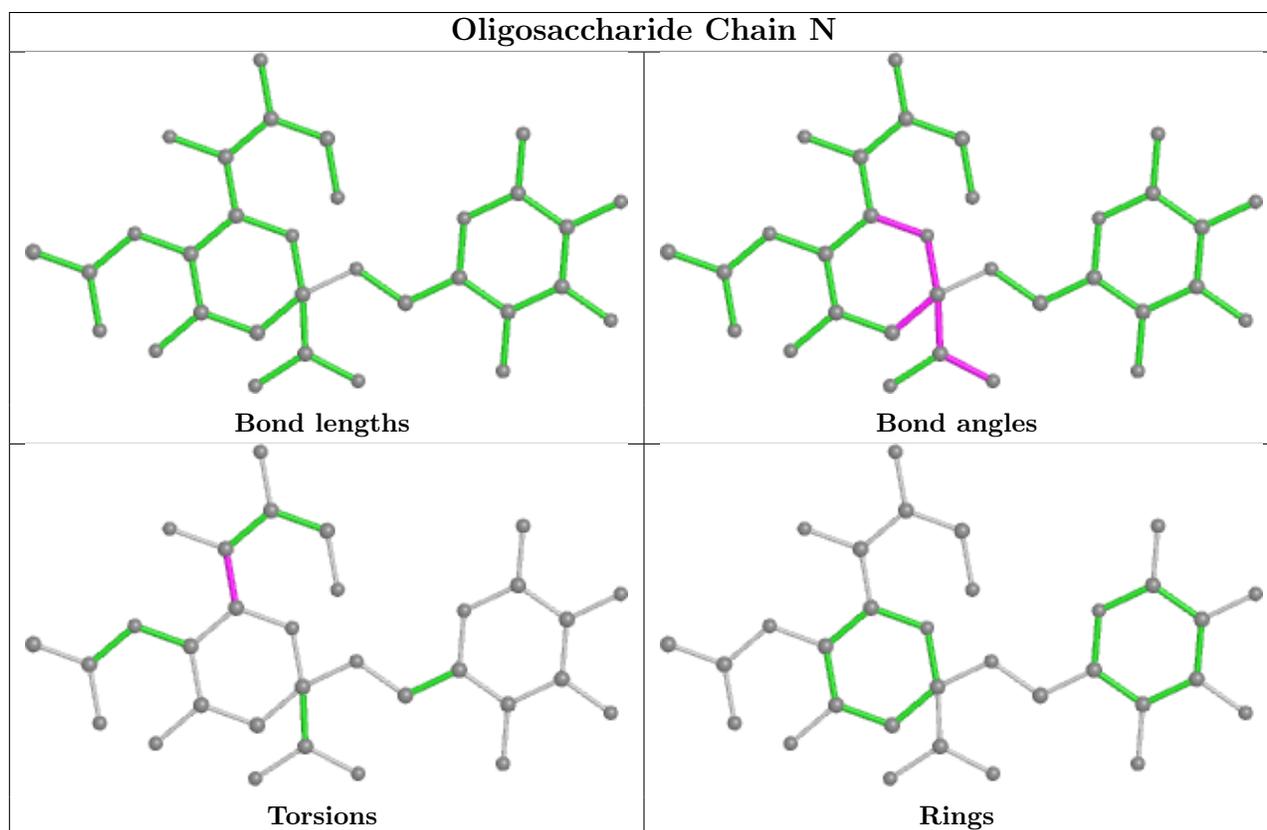
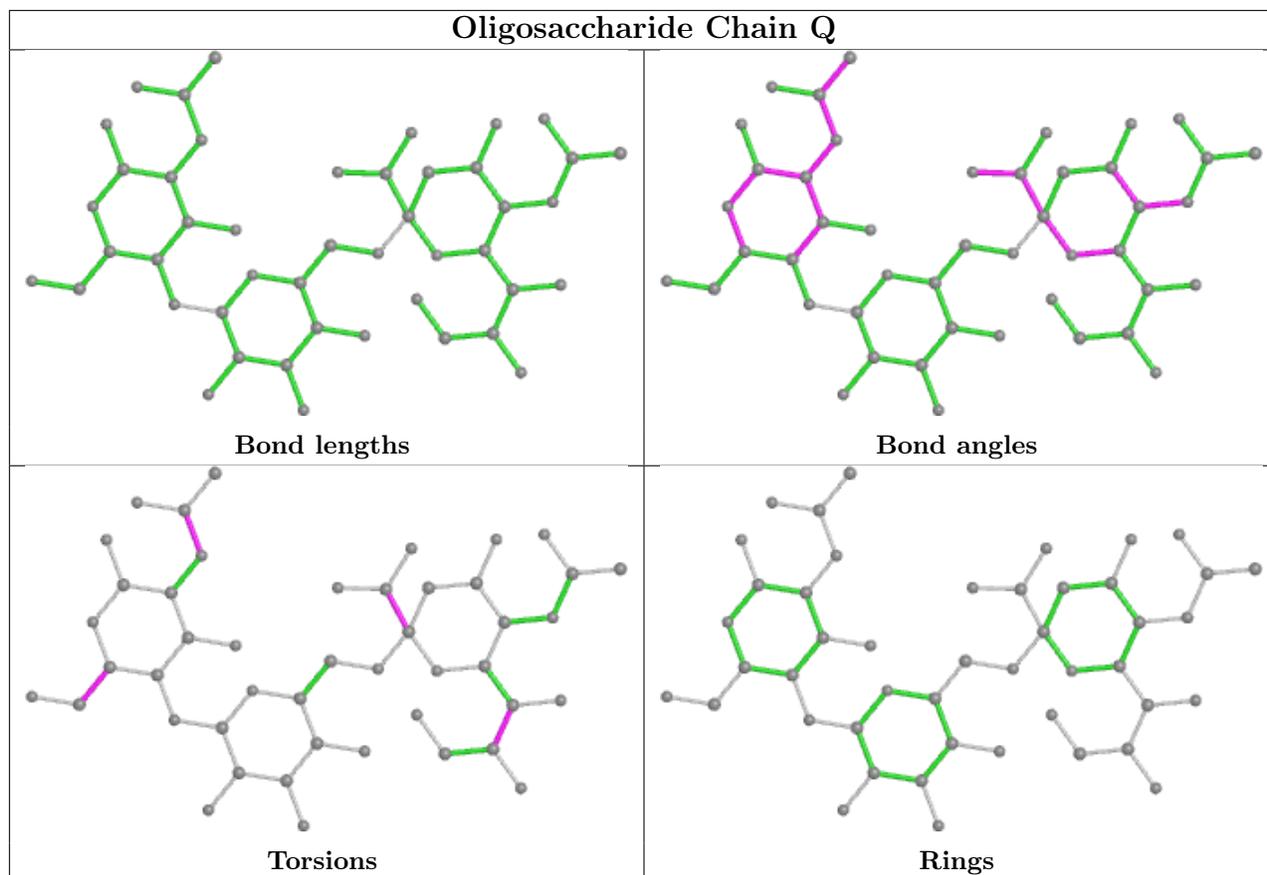
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	2	SIA	2	0
3	Q	3	SIA	1	0
3	P	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

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	H	201	2	14,14,15	0.31	0	17,19,21	1.07	1 (5%)
6	NAG	C	405	1	14,14,15	0.46	0	17,19,21	1.33	1 (5%)
6	NAG	F	201	2,5	14,14,15	0.49	0	17,19,21	1.04	1 (5%)
6	NAG	L	201	2	14,14,15	0.43	0	17,19,21	1.74	3 (17%)
6	NAG	A	401	1	14,14,15	0.59	0	17,19,21	1.90	3 (17%)
6	NAG	B	201	2,5	14,14,15	0.33	0	17,19,21	0.88	1 (5%)
6	NAG	G	401	1	14,14,15	0.39	0	17,19,21	1.06	1 (5%)
6	NAG	K	401	1	14,14,15	0.37	0	17,19,21	1.03	1 (5%)
6	NAG	J	201	2	14,14,15	0.33	0	17,19,21	1.66	1 (5%)
6	NAG	D	201	2	14,14,15	0.35	0	17,19,21	0.95	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	H	201	2	-	0/6/23/26	0/1/1/1
6	NAG	C	405	1	-	0/6/23/26	0/1/1/1
6	NAG	F	201	2,5	-	1/6/23/26	0/1/1/1
6	NAG	L	201	2	-	2/6/23/26	0/1/1/1
6	NAG	A	401	1	-	4/6/23/26	0/1/1/1
6	NAG	B	201	2,5	-	2/6/23/26	0/1/1/1
6	NAG	G	401	1	-	1/6/23/26	0/1/1/1
6	NAG	K	401	1	-	0/6/23/26	0/1/1/1
6	NAG	J	201	2	-	0/6/23/26	0/1/1/1
6	NAG	D	201	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	201	NAG	C1-O5-C5	6.01	120.34	112.19
6	L	201	NAG	C1-O5-C5	5.82	120.08	112.19
6	A	401	NAG	C2-N2-C7	4.57	129.41	122.90
6	C	405	NAG	C1-O5-C5	4.45	118.23	112.19
6	A	401	NAG	C8-C7-N2	3.74	122.43	116.10

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

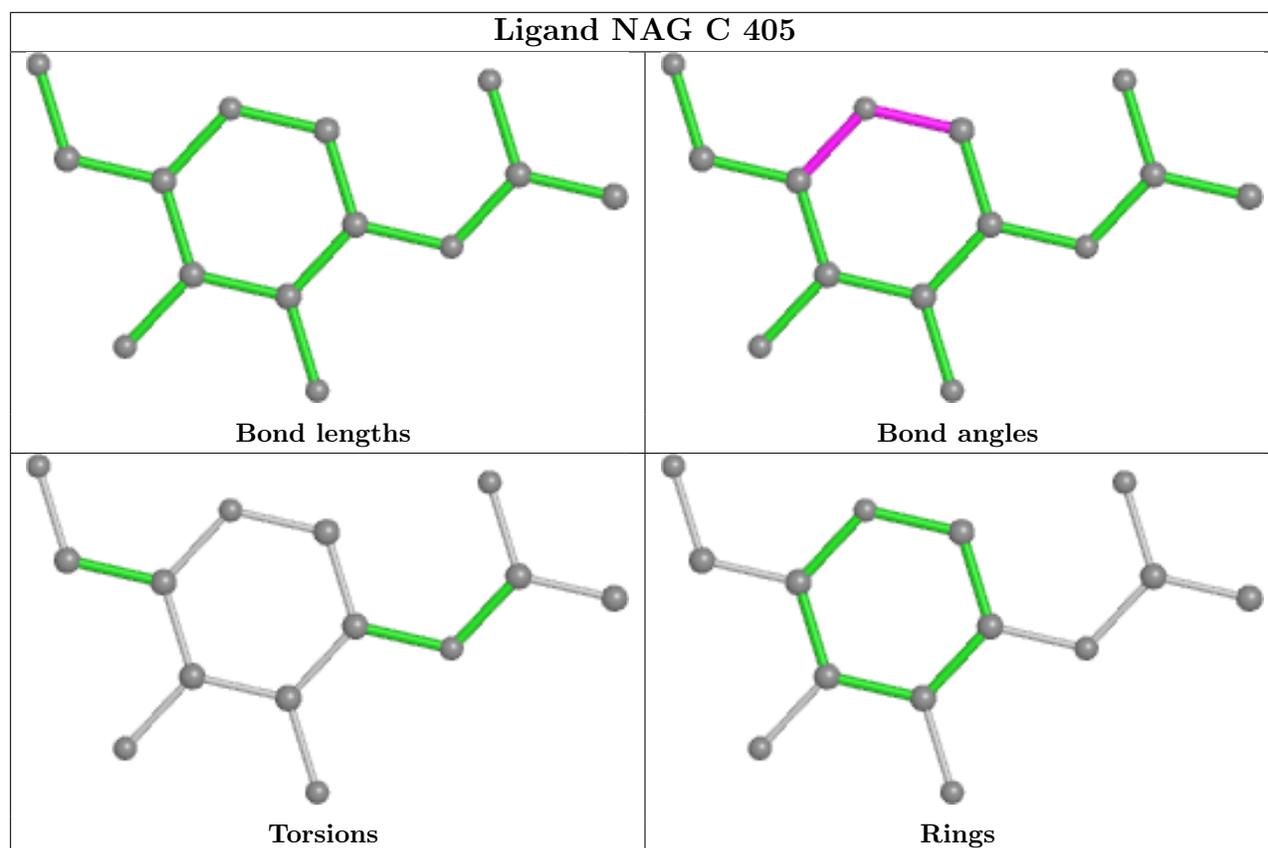
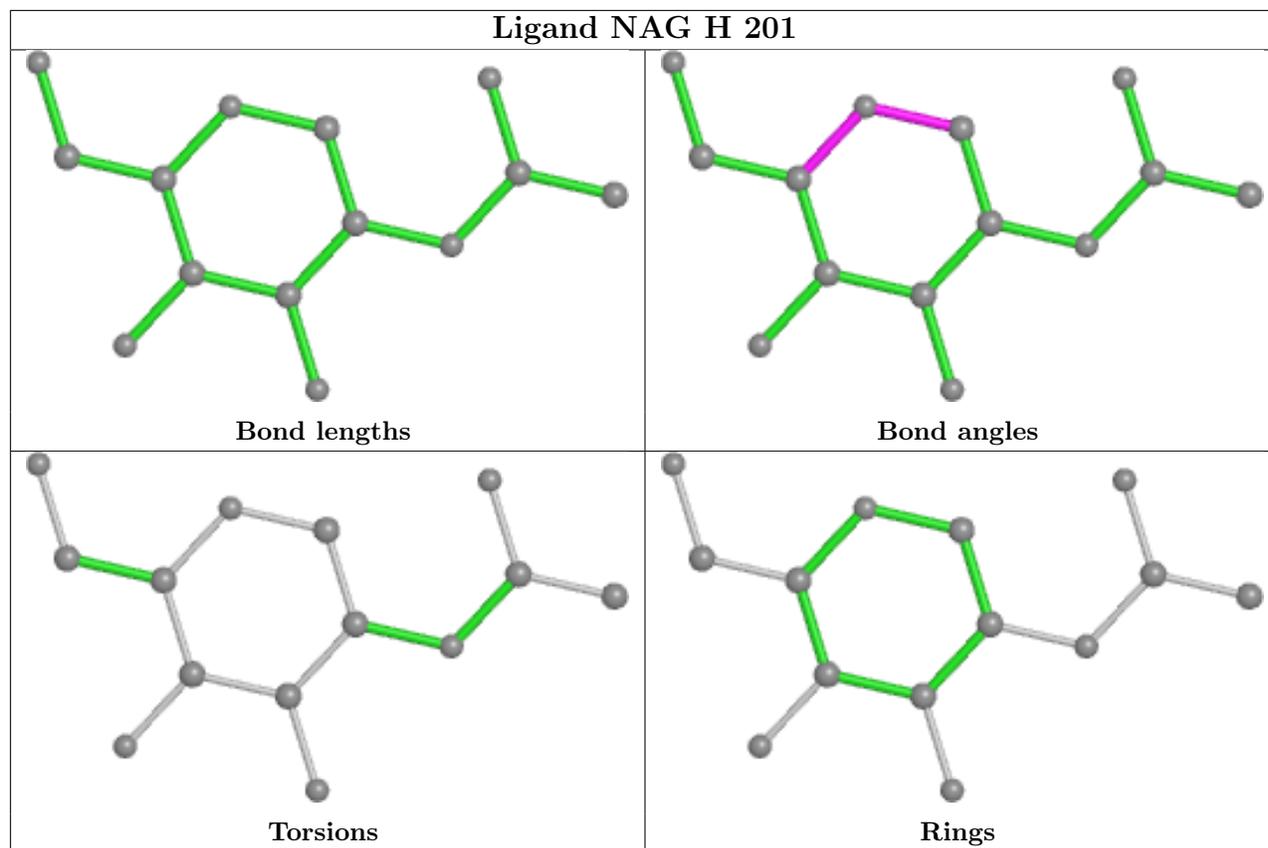
Mol	Chain	Res	Type	Atoms
6	L	201	NAG	O5-C5-C6-O6
6	A	401	NAG	C8-C7-N2-C2
6	A	401	NAG	O7-C7-N2-C2
6	D	201	NAG	O5-C5-C6-O6
6	D	201	NAG	C4-C5-C6-O6

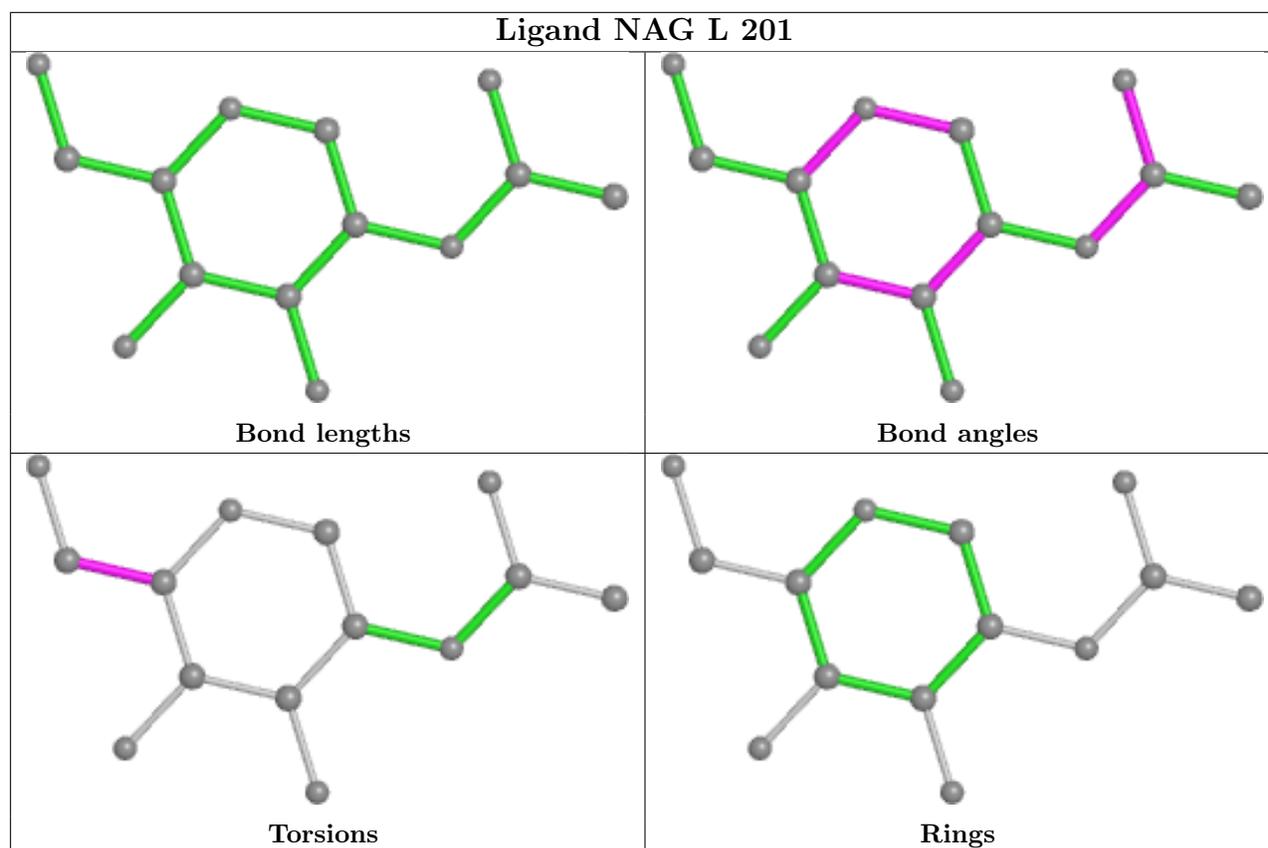
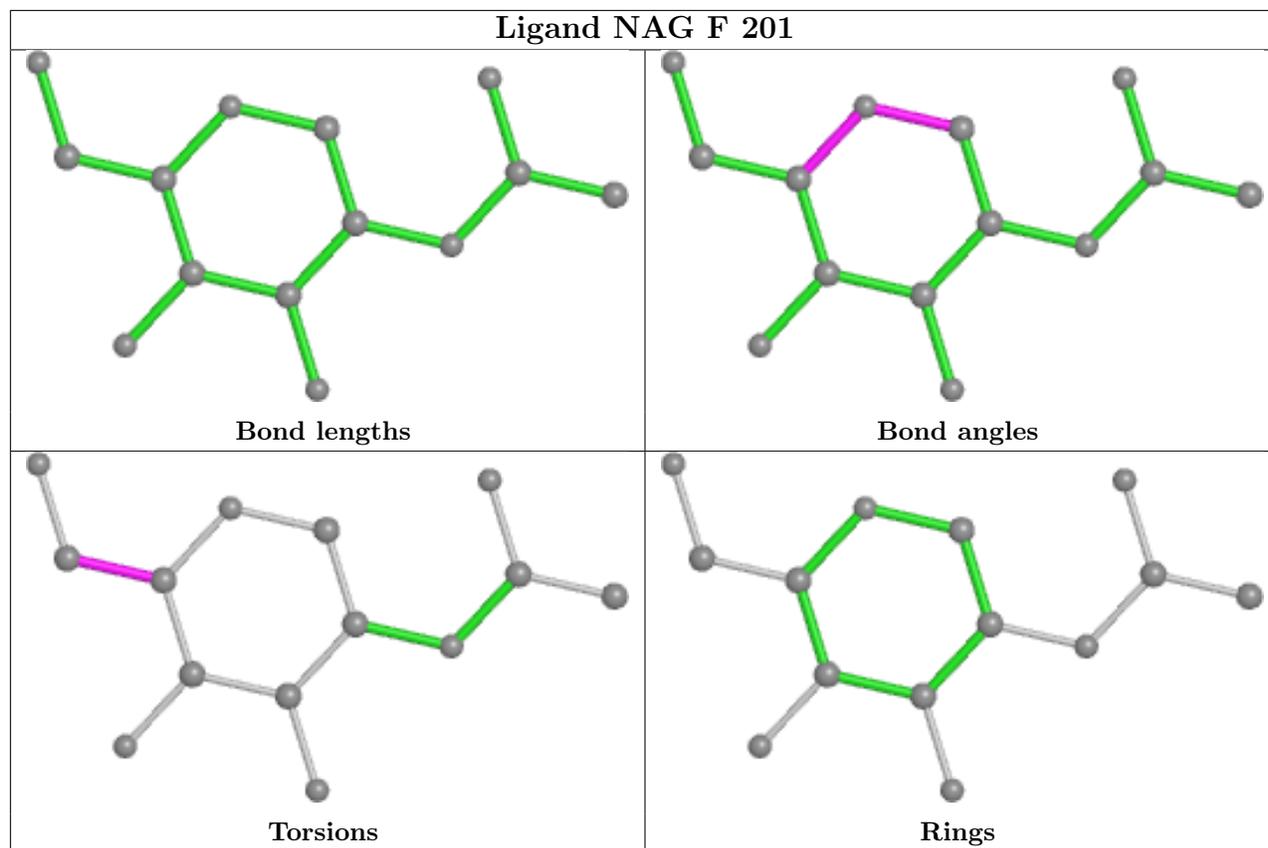
There are no ring outliers.

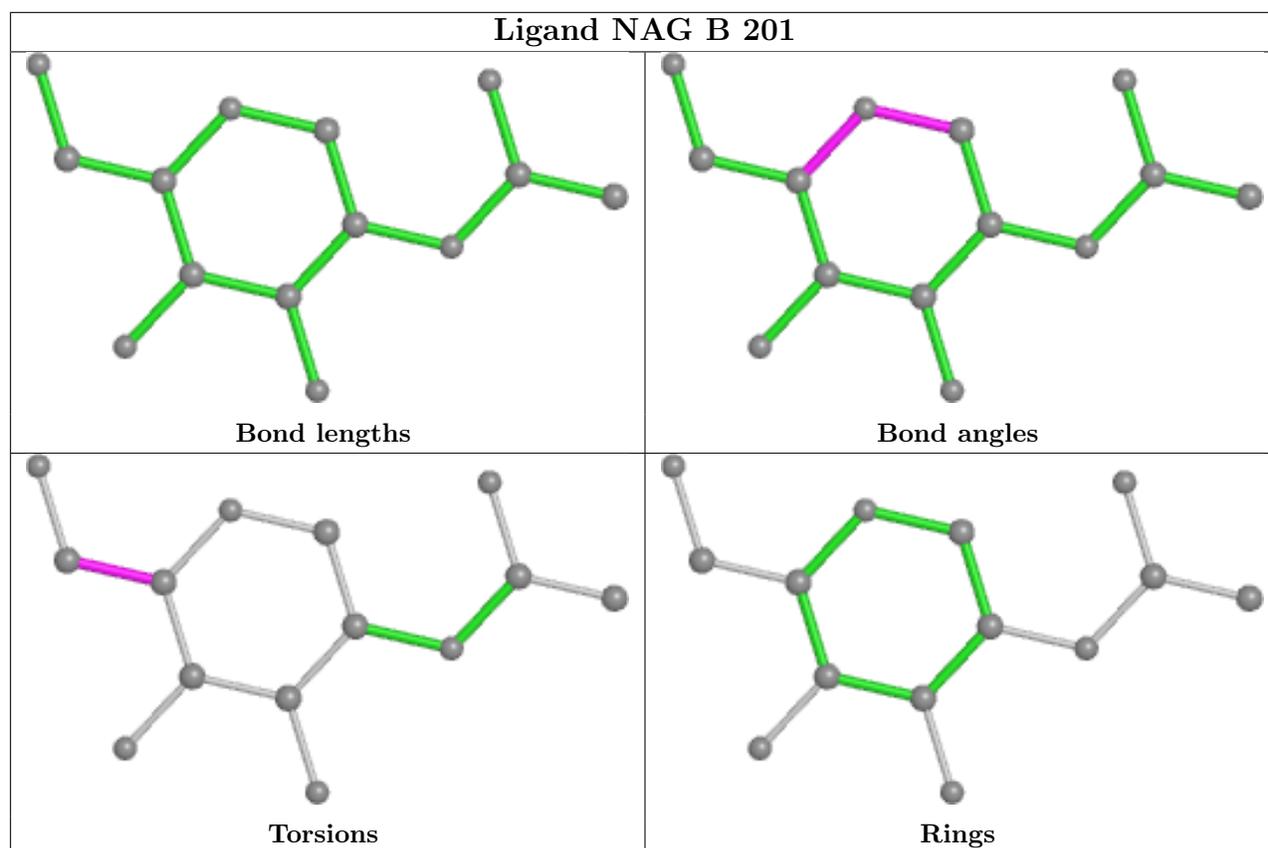
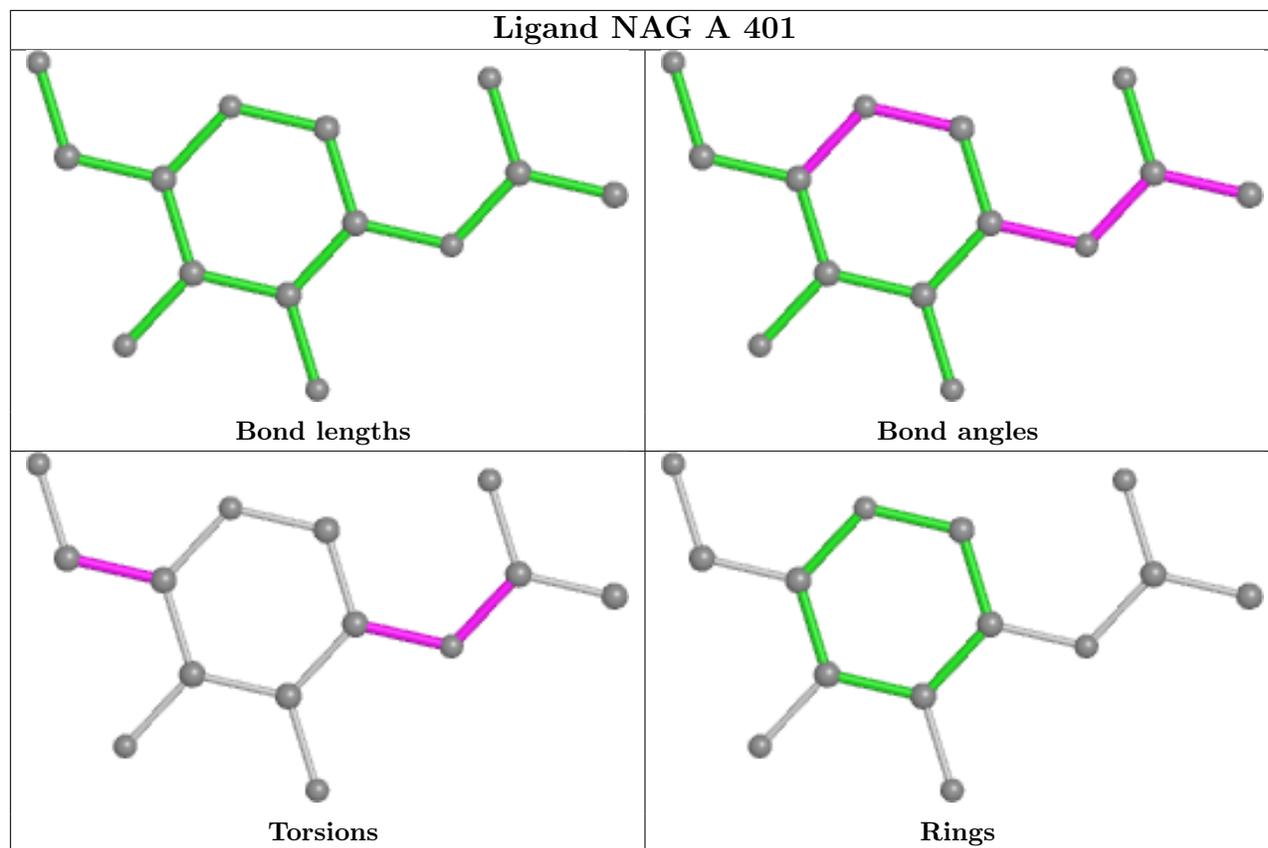
1 monomer is involved in 1 short contact:

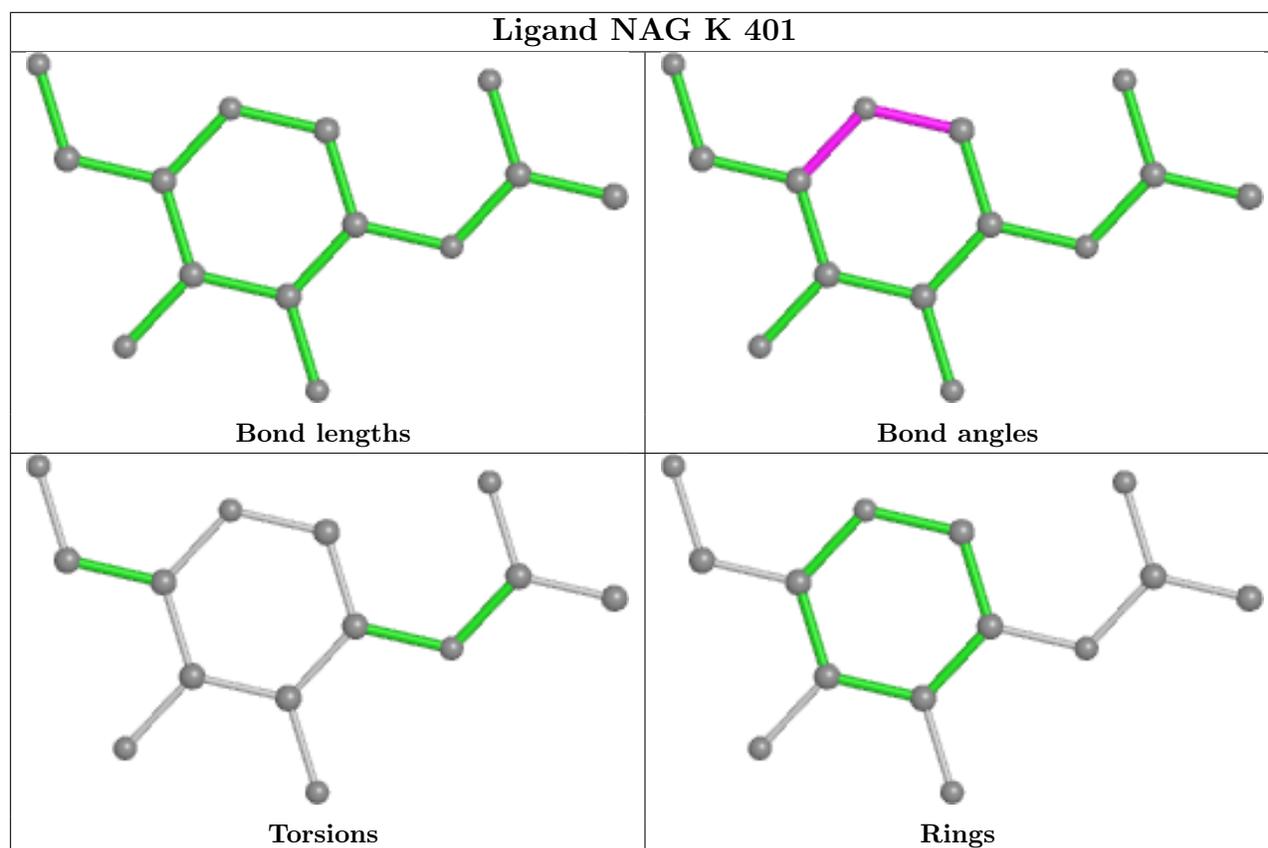
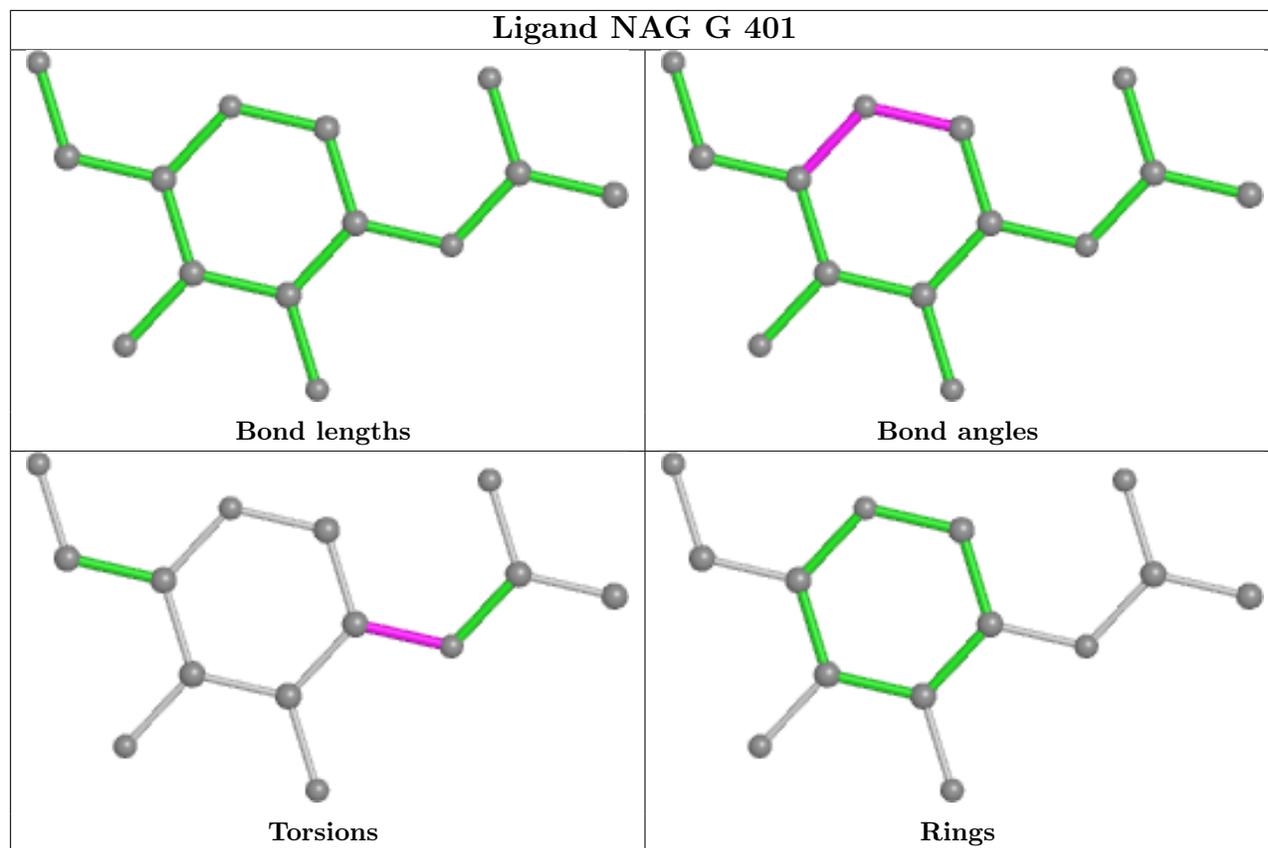
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	NAG	1	0

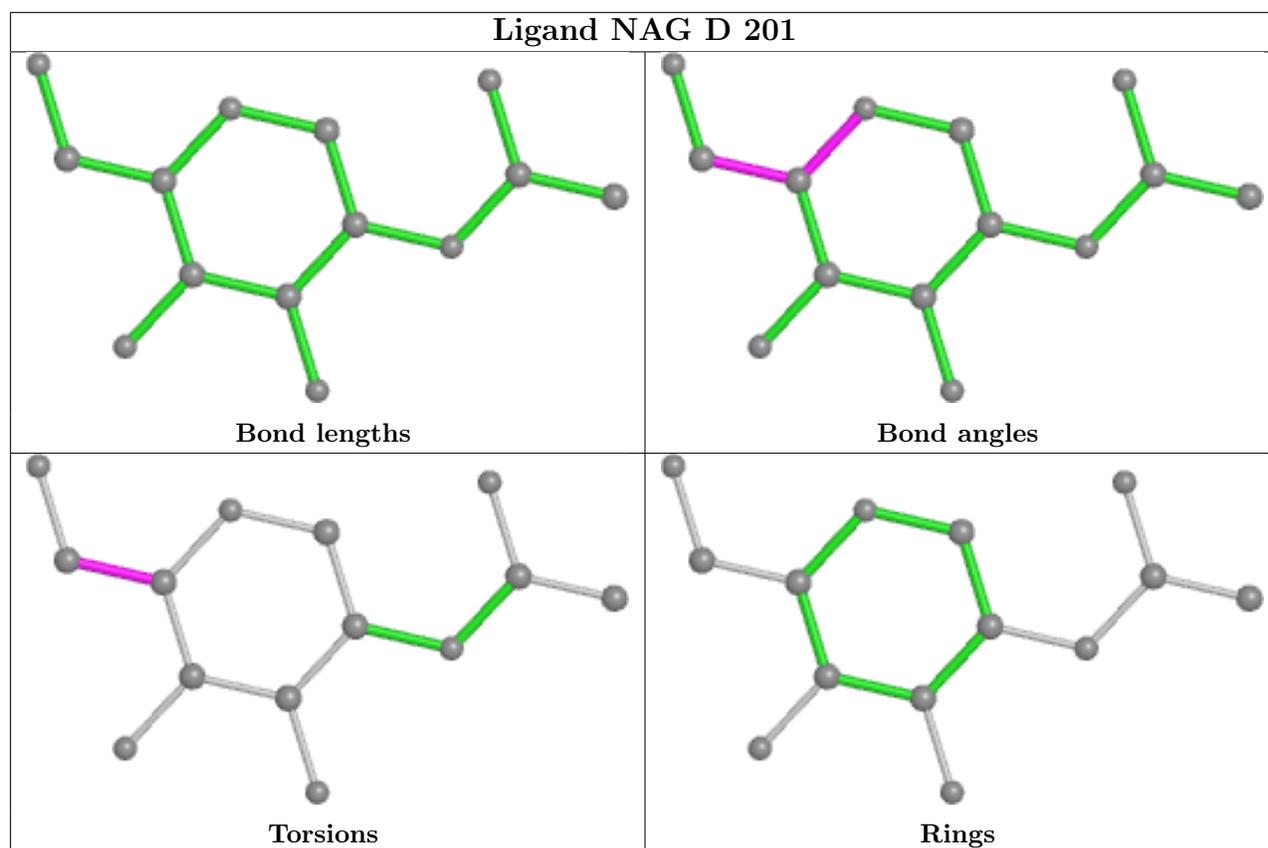
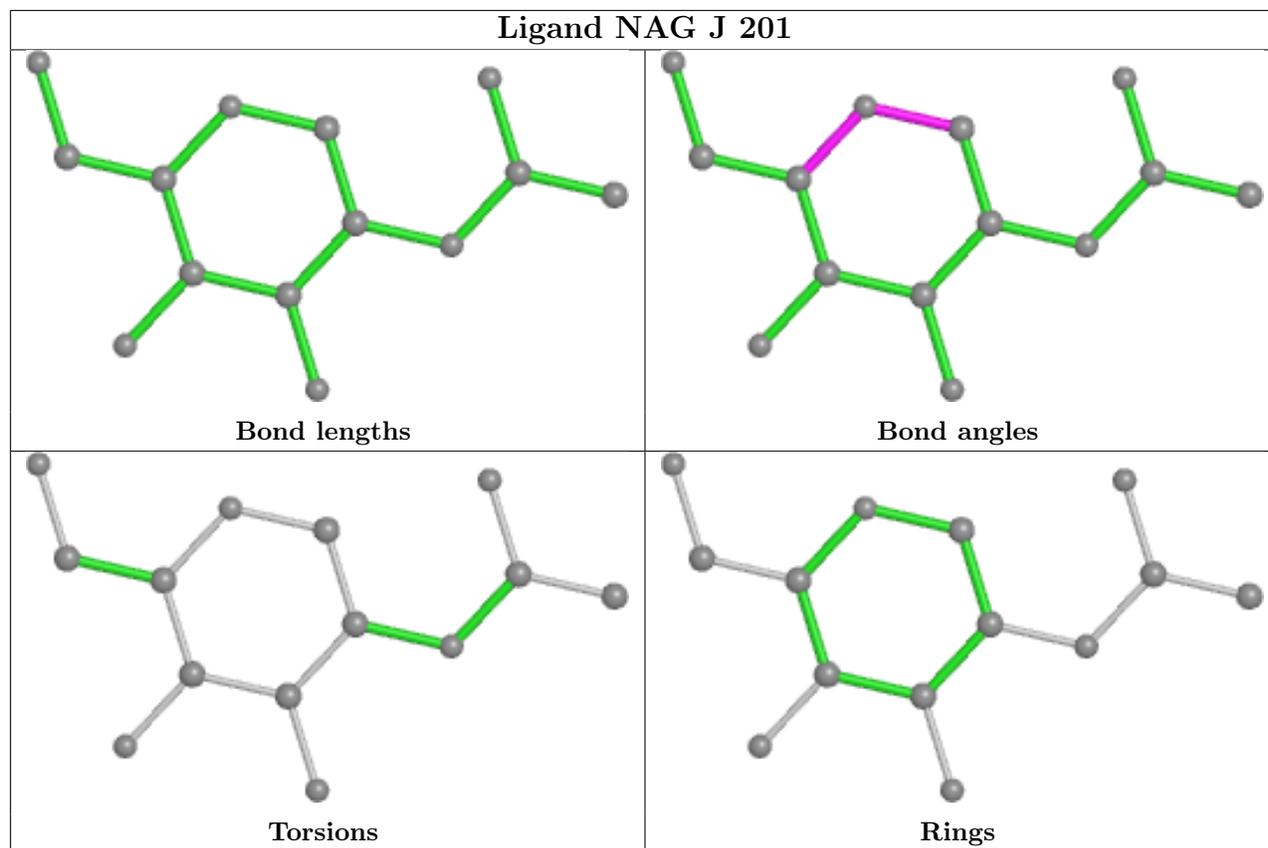
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	315/325 (96%)	0.87	46 (14%) 2 3	57, 91, 146, 179	0
1	C	318/325 (97%)	0.36	11 (3%) 44 51	43, 72, 104, 117	0
1	E	313/325 (96%)	0.68	33 (10%) 6 8	50, 83, 136, 184	0
1	G	318/325 (97%)	0.22	2 (0%) 89 92	47, 65, 94, 114	0
1	I	319/325 (98%)	0.53	15 (4%) 31 38	45, 80, 112, 129	0
1	K	319/325 (98%)	0.31	2 (0%) 89 92	44, 65, 94, 113	0
2	B	172/177 (97%)	0.54	8 (4%) 31 38	51, 80, 107, 119	0
2	D	172/177 (97%)	0.33	0 100 100	43, 60, 81, 106	0
2	F	172/177 (97%)	0.37	3 (1%) 70 76	45, 68, 98, 109	0
2	H	172/177 (97%)	0.35	2 (1%) 79 84	42, 71, 103, 127	0
2	J	172/177 (97%)	0.37	2 (1%) 79 84	43, 66, 93, 112	0
2	L	172/177 (97%)	0.26	0 100 100	44, 63, 90, 103	0
All	All	2934/3012 (97%)	0.45	124 (4%) 36 42	42, 73, 112, 184	0

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	216	VAL	7.7
1	E	219	LEU	7.0
1	A	225	PHE	5.6
1	A	223	ILE	5.4
1	I	120	SER	5.3

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

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

6.3 Carbohydrates

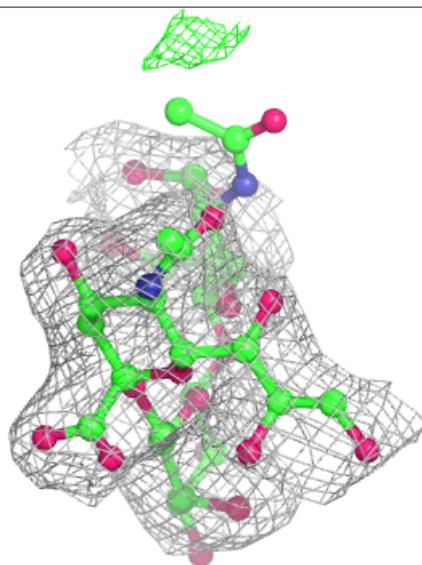
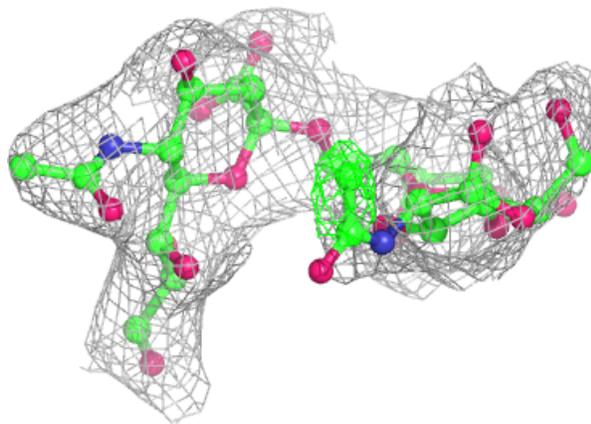
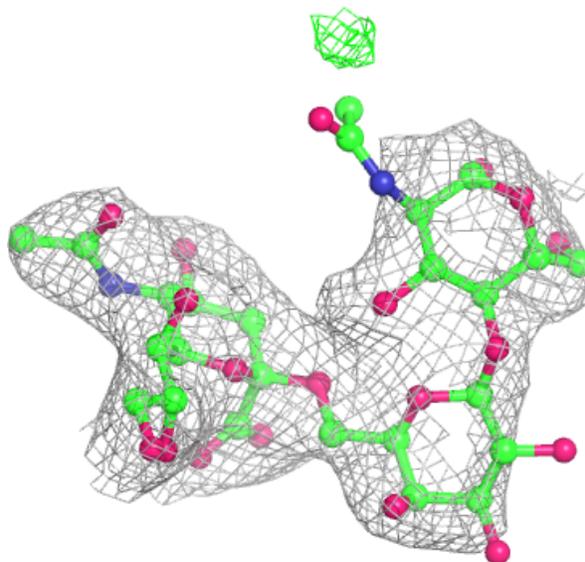
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	Q	1	15/15	0.58	0.33	154,163,169,170	0
3	NAG	P	1	15/15	0.60	0.33	136,152,156,156	0
3	NAG	M	1	15/15	0.68	0.27	130,144,153,154	0
3	NAG	O	1	15/15	0.77	0.31	144,153,155,156	0
3	GAL	P	2	11/12	0.85	0.15	95,114,129,136	0
4	GAL	N	1	12/12	0.85	0.30	123,130,134,134	0
3	GAL	O	2	11/12	0.86	0.15	110,123,130,131	0
4	SIA	N	2	20/21	0.86	0.22	101,113,121,126	0
3	GAL	M	2	11/12	0.89	0.18	95,116,132,133	0
3	GAL	Q	2	11/12	0.89	0.14	113,130,139,143	0
3	SIA	Q	3	20/21	0.91	0.15	81,91,104,106	0
3	SIA	O	3	20/21	0.92	0.16	73,78,100,101	0
3	SIA	P	3	20/21	0.95	0.14	69,74,82,82	0
3	SIA	M	3	20/21	0.95	0.15	68,77,87,88	0

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

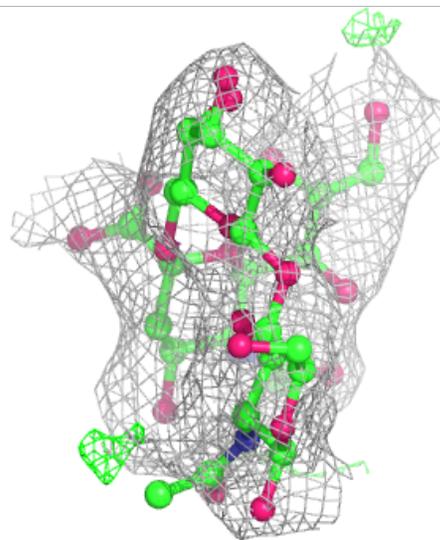
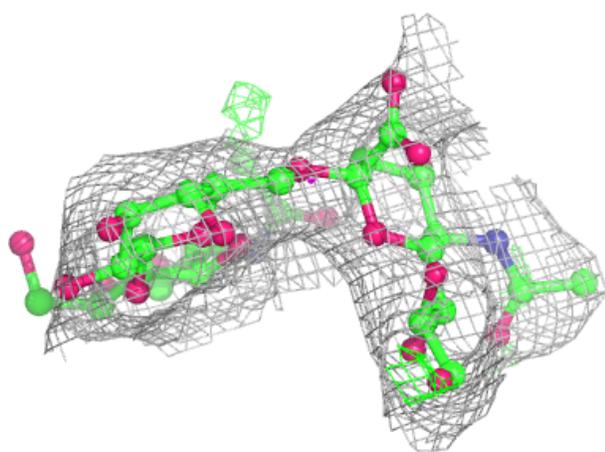
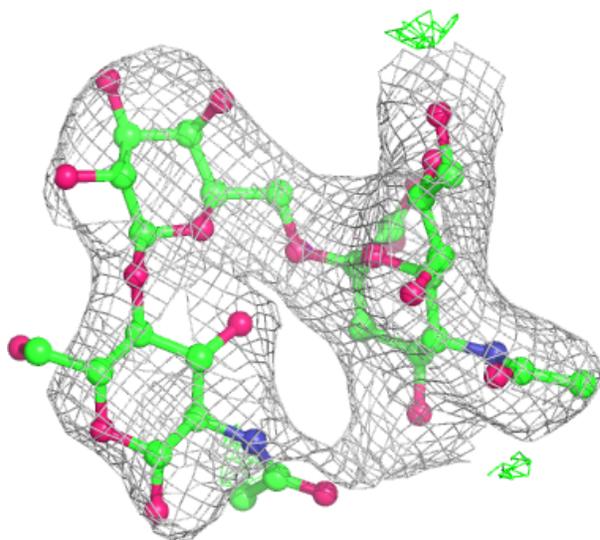
Electron density around Chain M:

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



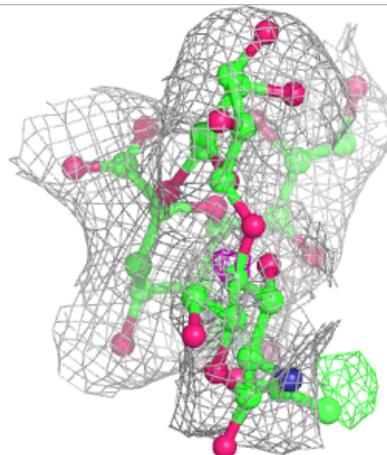
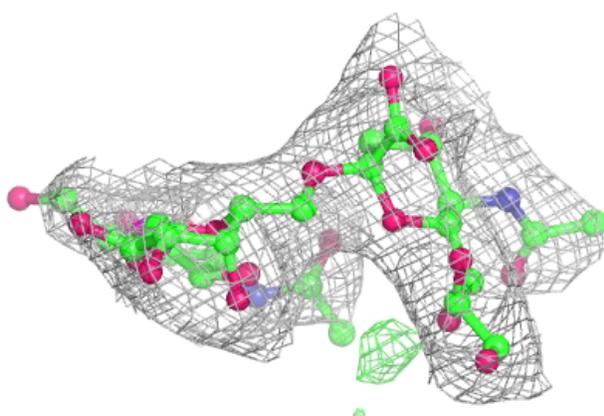
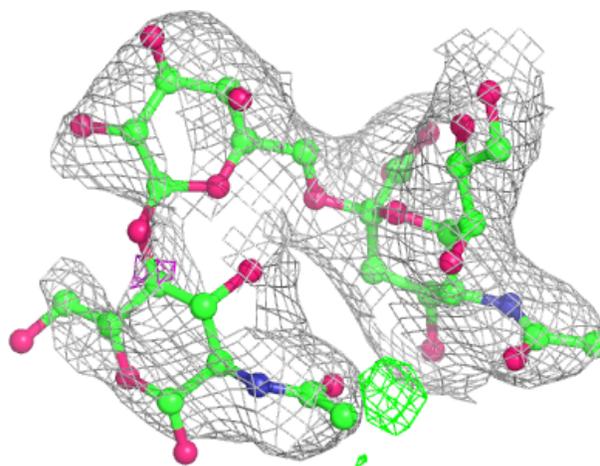
Electron density around Chain O:

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



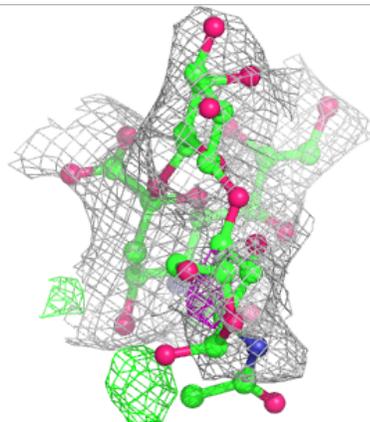
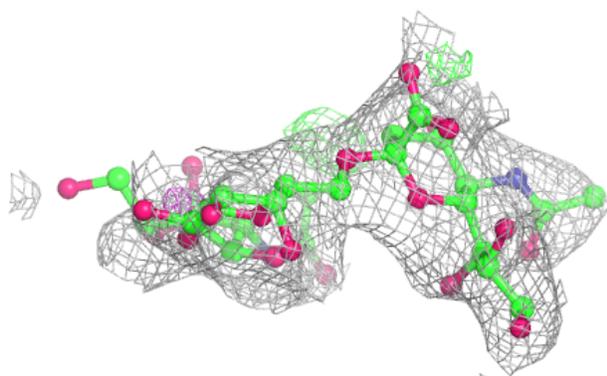
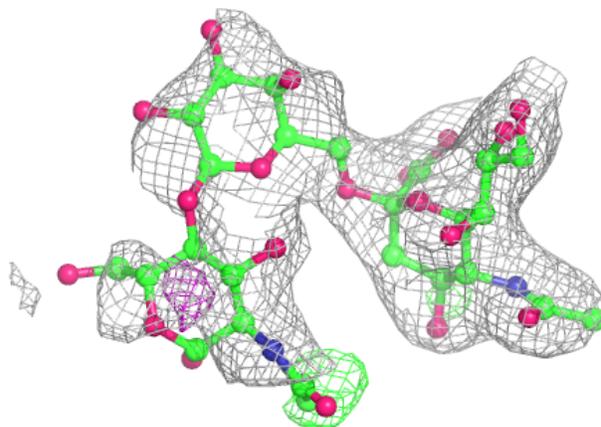
Electron density around Chain P:

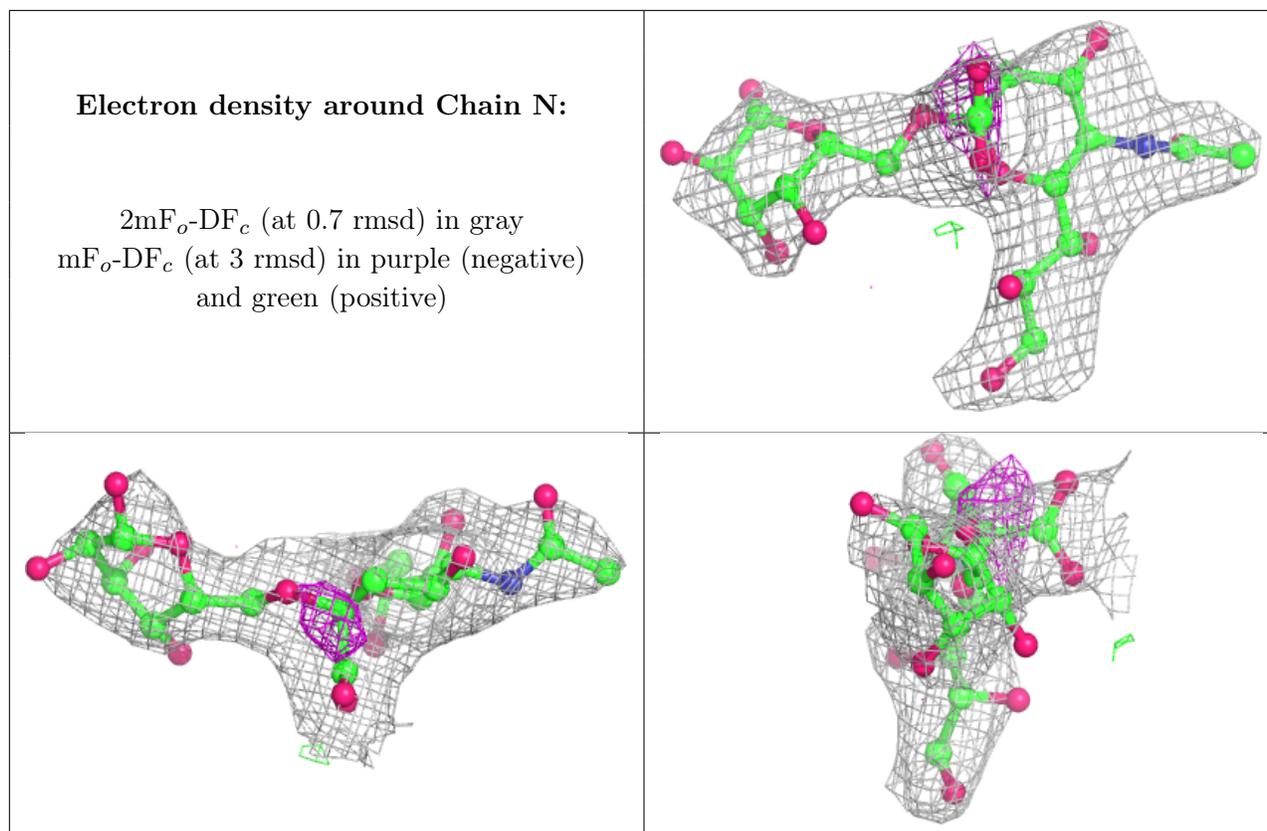
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Q:

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





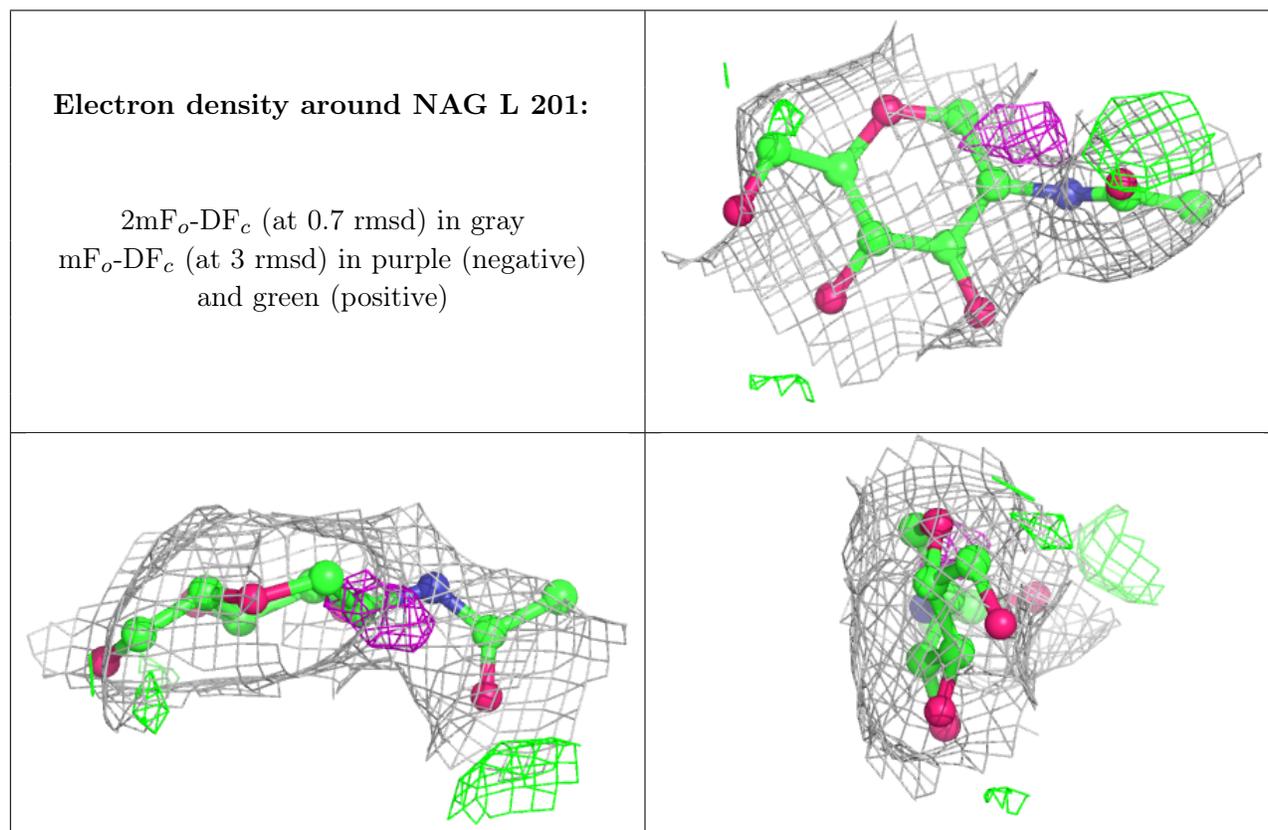
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	NAG	L	201	14/15	0.72	0.17	90,102,106,115	0
6	NAG	A	401	14/15	0.79	0.22	110,116,125,128	0
6	NAG	G	401	14/15	0.83	0.16	95,103,106,106	0
6	NAG	H	201	14/15	0.83	0.22	95,105,111,111	0
6	NAG	F	201	14/15	0.85	0.19	67,80,96,111	0
6	NAG	K	401	14/15	0.87	0.15	96,104,108,112	0
6	NAG	B	201	14/15	0.90	0.14	85,91,99,104	0
6	NAG	C	405	14/15	0.91	0.35	88,99,104,105	0
6	NAG	D	201	14/15	0.92	0.13	73,78,85,87	0
6	NAG	J	201	14/15	0.93	0.12	70,77,79,81	0
5	CA	C	404	1/1	0.98	0.16	75,75,75,75	0
5	CA	B	202	1/1	0.98	0.07	88,88,88,88	0

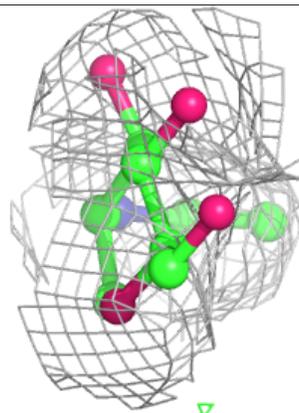
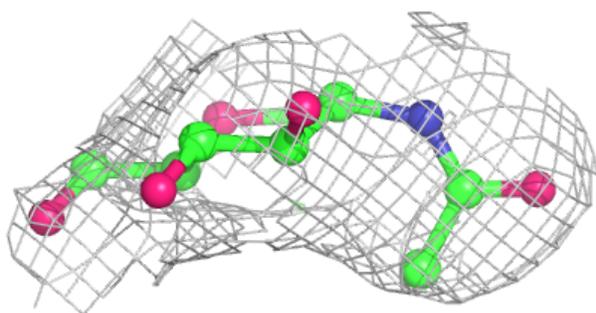
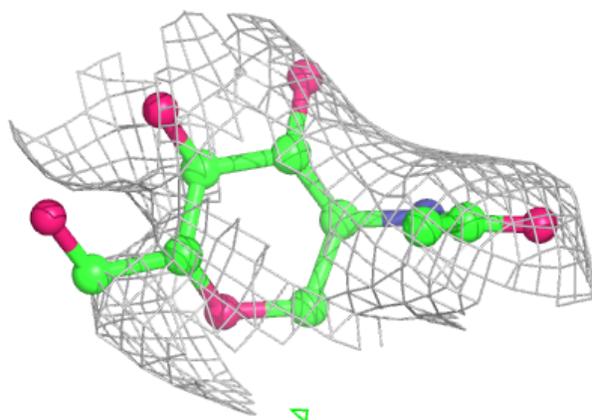
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



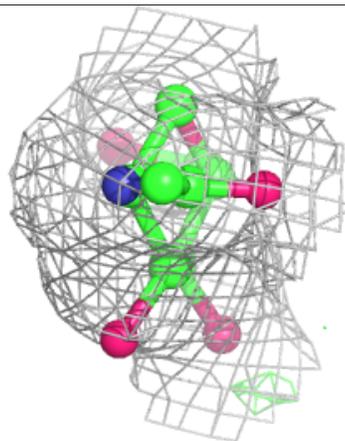
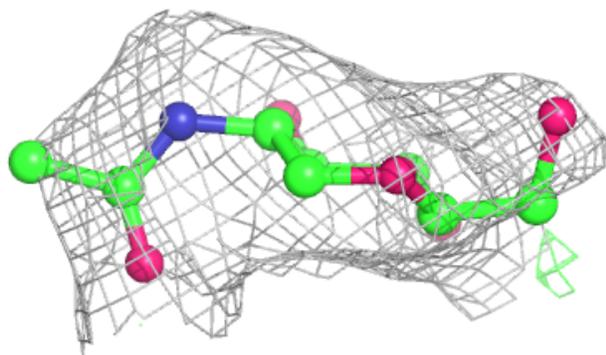
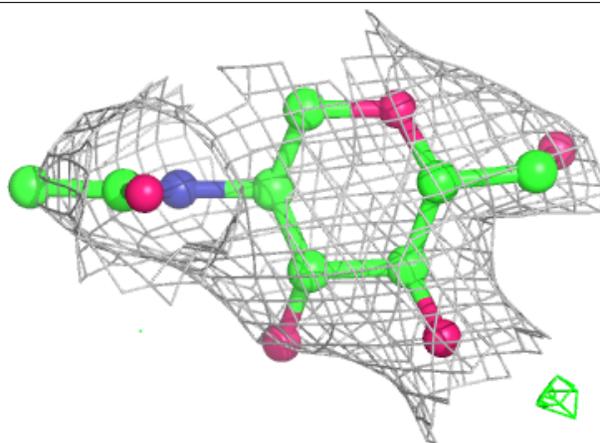
Electron density around NAG A 401:

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



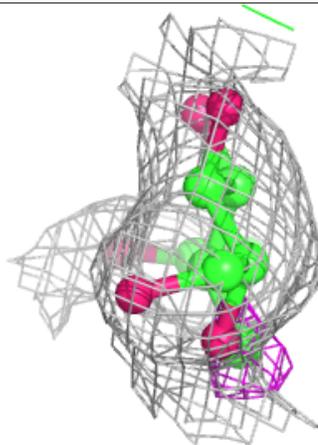
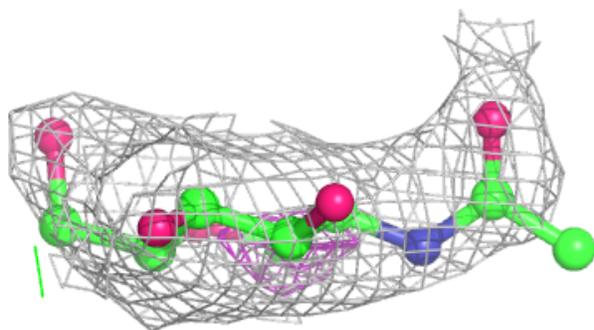
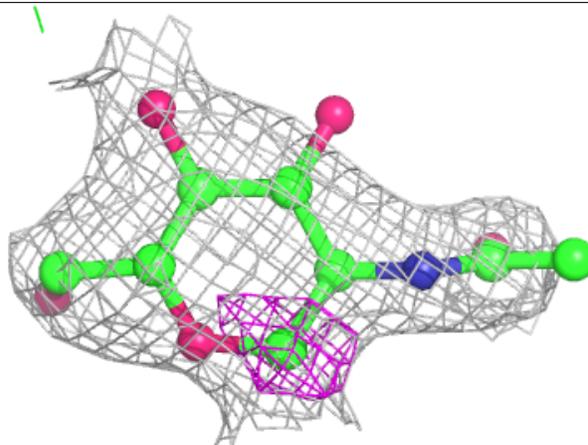
Electron density around NAG G 401:

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

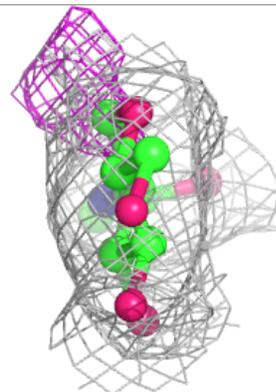
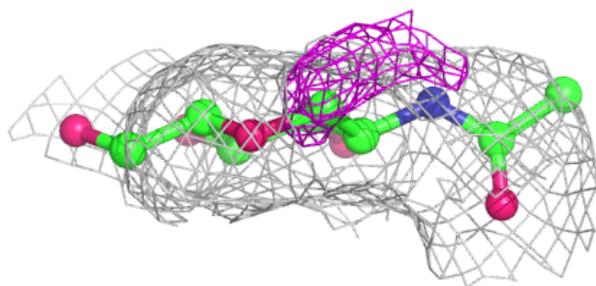
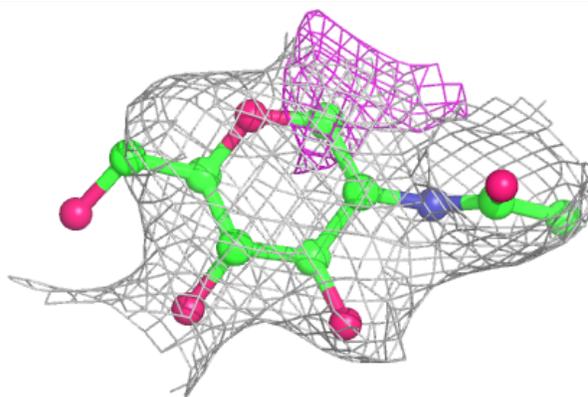


Electron density around NAG H 201:

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

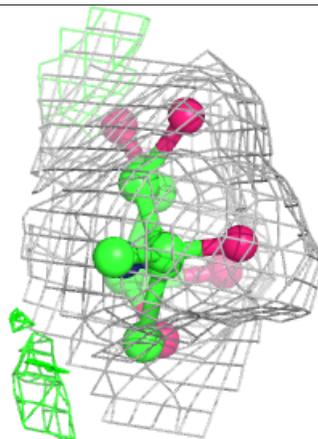
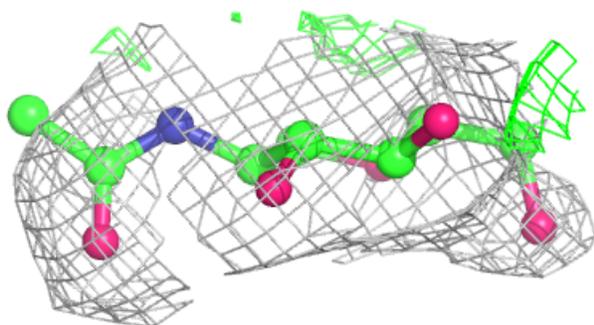
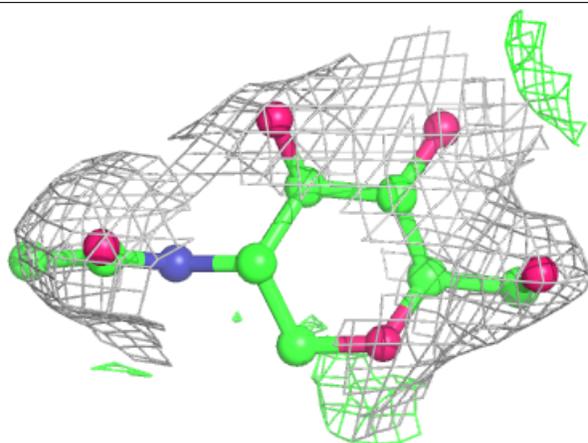
**Electron density around NAG F 201:**

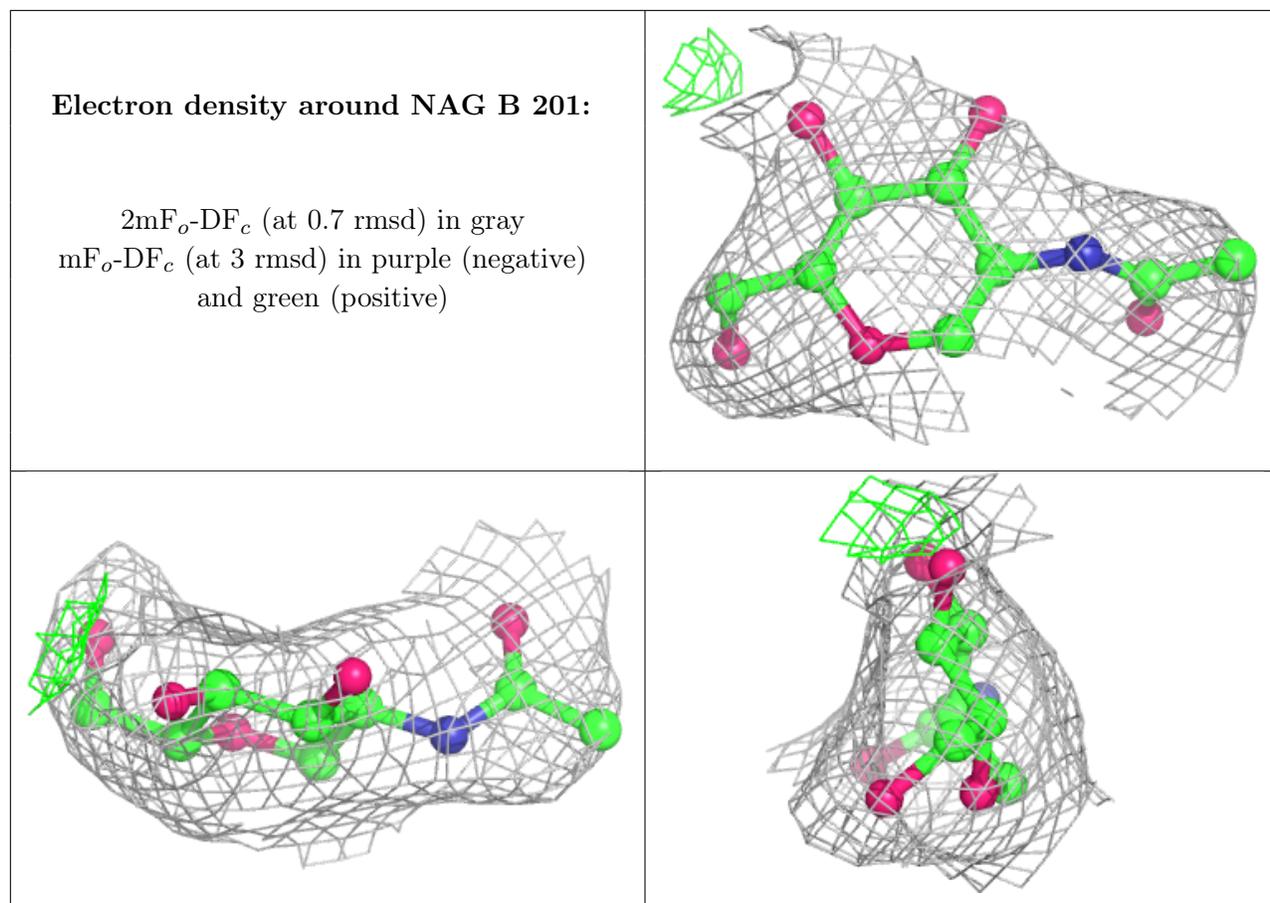
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAG K 401:

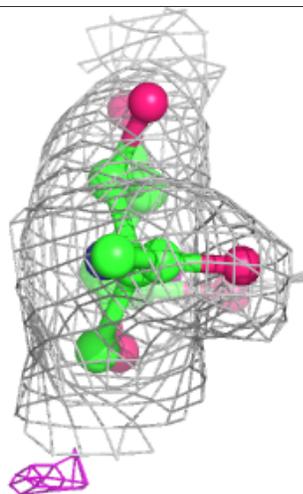
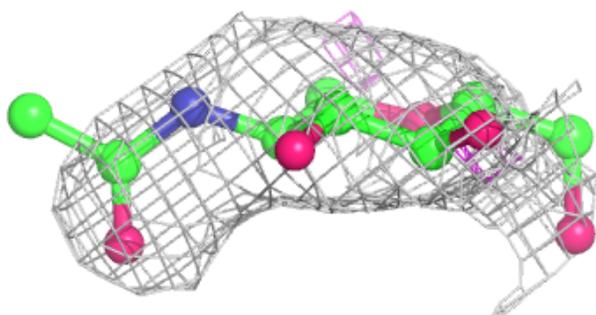
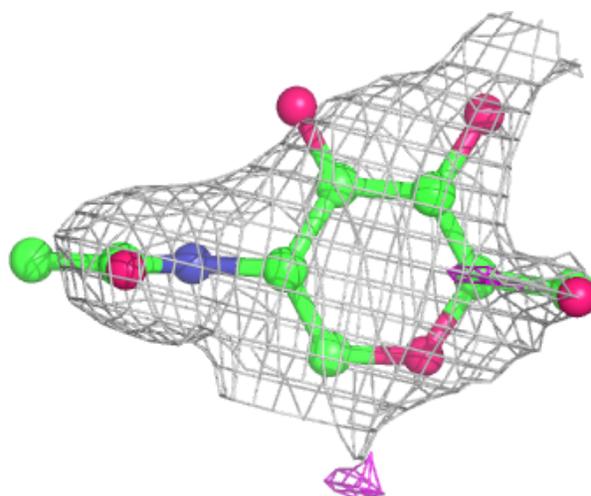
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

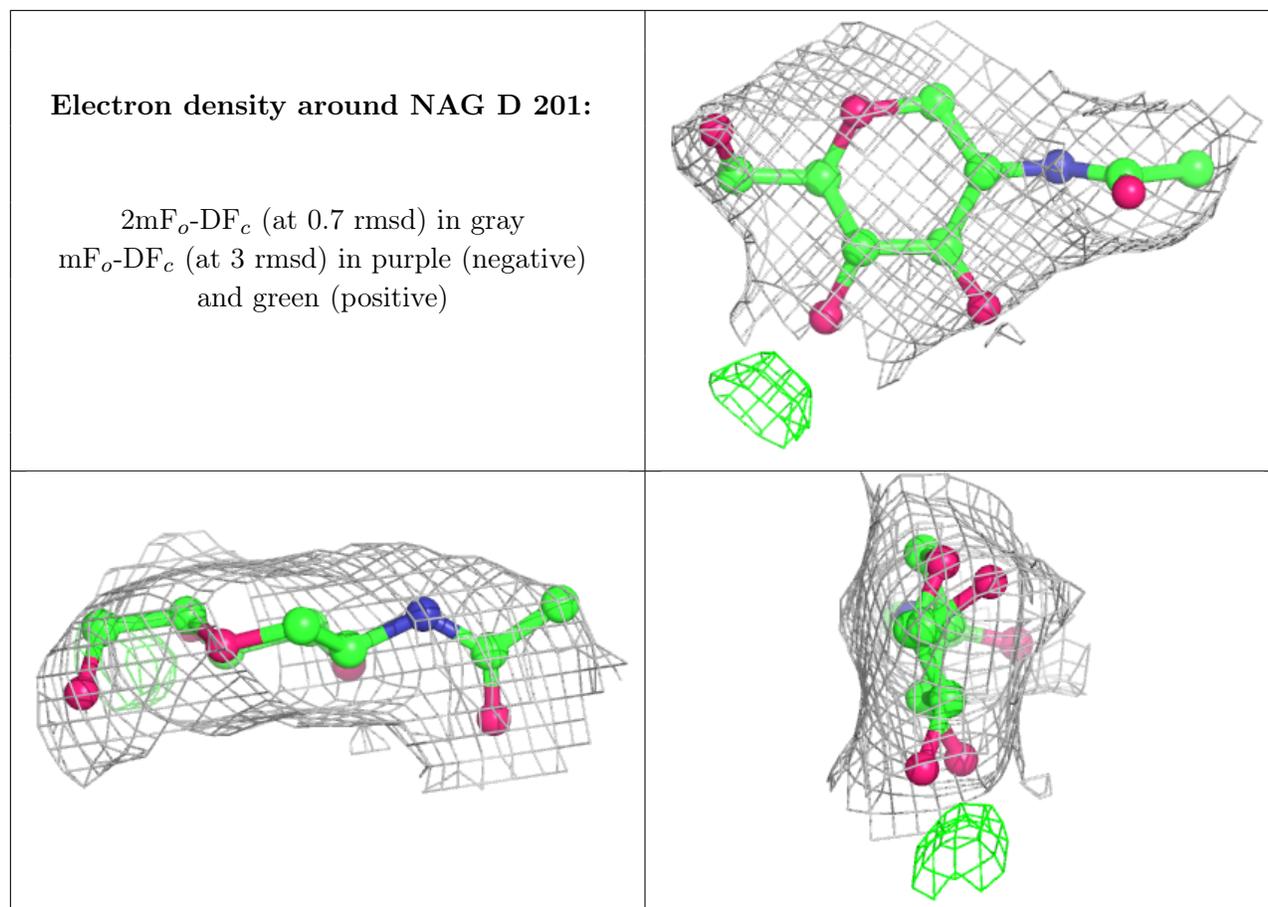


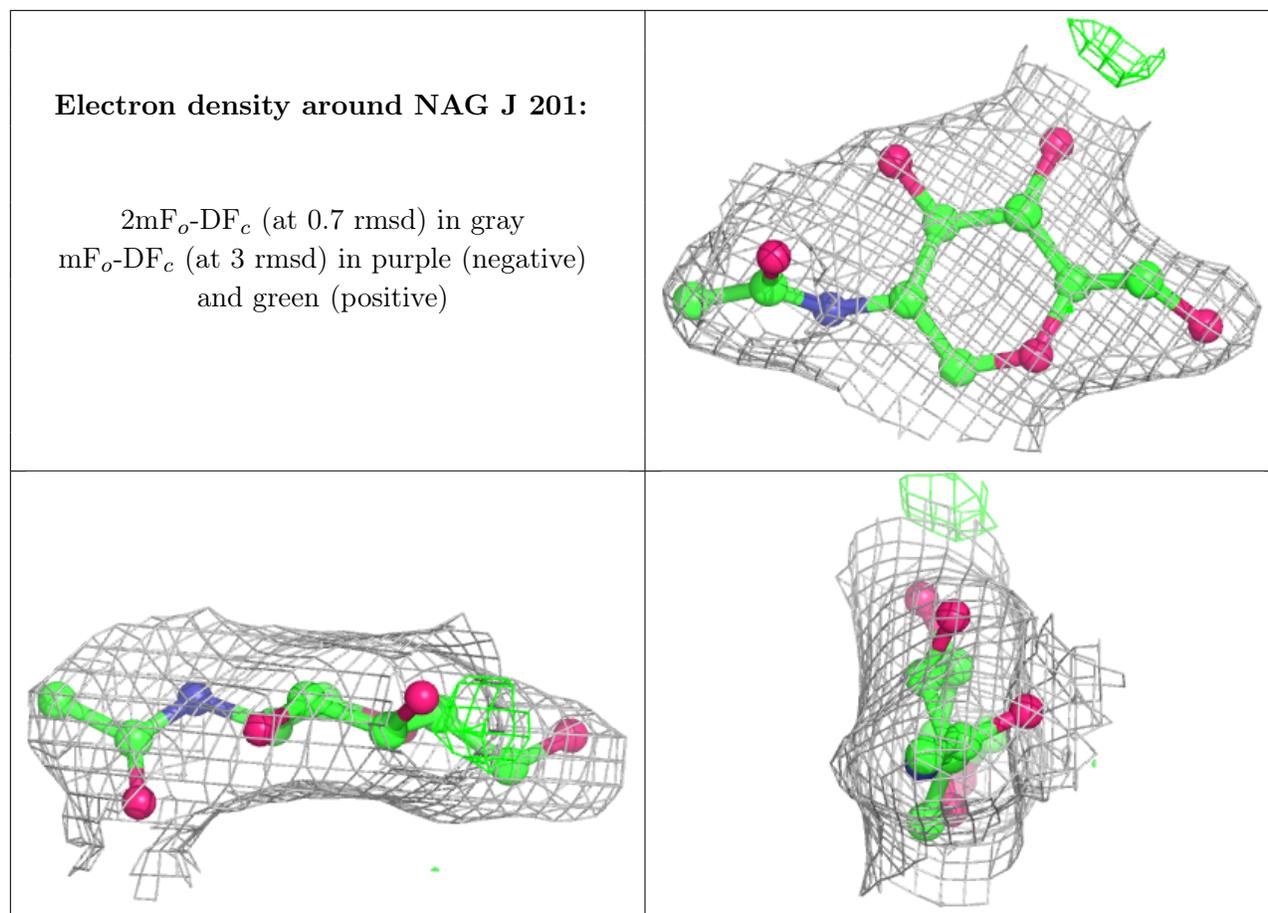


Electron density around NAG C 405:

$2mF_o-DF_c$ (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.