



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:39 PM UTC

PDB ID : 8TNN / pdb_00008tnn
Title : Crystal structure of Epstein-Barr virus gH/gL/gp42 in complex with gp42 antibody A10
Authors : Bu, W.; Kumar, A.; Board, N.; Kim, J.; Dowdell, K.; Zhang, S.; Lei, Y.; Hostal, A.; Krogmann, T.; Wang, Y.; Pittaluga, S.; Marcotrigiano, J.; Cohen, J.I.
Deposited on : 2023-08-02
Resolution : 3.36 Å(reported)

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

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

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](#) ①) were used in the production of this report:

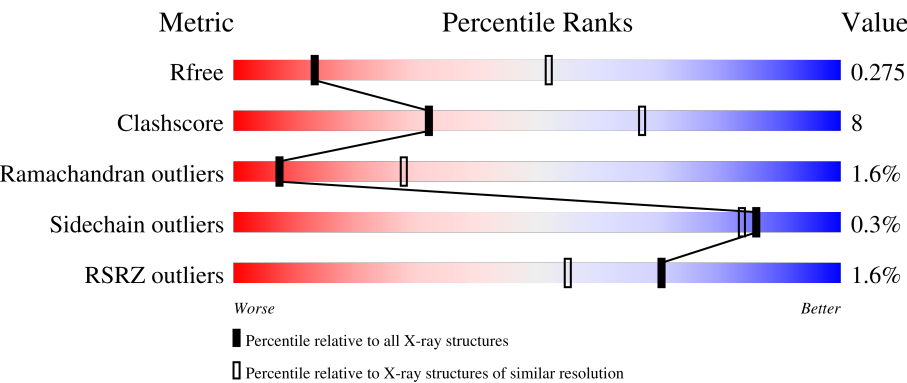
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 3.36 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	658	% 82%18%
1	D	658	2% 75%23%..
2	B	112	% 77%19%.
2	E	112	2% 61%21%18%
3	C	191	% 75%18%.6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	191	% 78% 14% 7%
4	G	213	82% 13%
4	I	213	5% 81% 15%
5	H	234	72% 17% 10%
5	J	234	4% 71% 19% 9%
6	L	3	33% 67%
6	T	3	33% 67%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 20293 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	658	Total	C	N	O	S	0	0	0
			5036	3225	832	949	30			
1	D	654	Total	C	N	O	S	0	0	0
			4952	3164	818	940	30			

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	S	0	0	0
			786	494	135	153	4			
2	E	92	Total	C	N	O	S	0	0	0
			675	422	113	136	4			

- Molecule 3 is a protein called Glycoprotein 42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	180	Total	C	N	O	S	0	0	0
			1408	913	228	256	11			
3	F	178	Total	C	N	O	S	0	0	0
			1383	899	220	253	11			

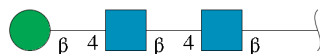
- Molecule 4 is a protein called A10 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	204	Total	C	N	O	S	0	0	0
			1400	865	241	290	4			
4	I	204	Total	C	N	O	S	0	0	0
			1385	850	240	292	3			

- Molecule 5 is a protein called A10 heavy chain.

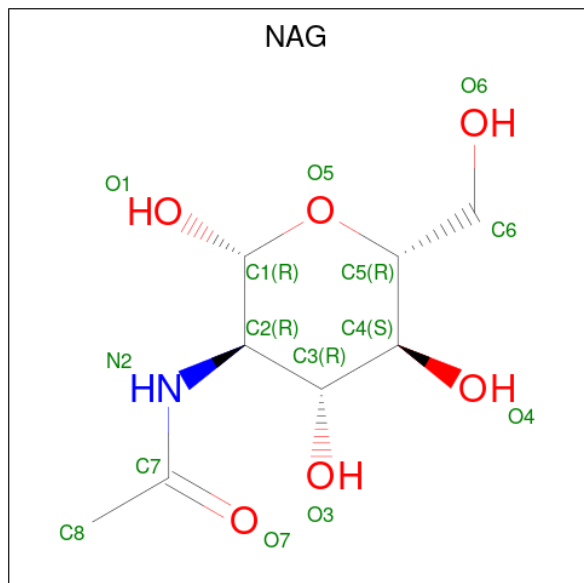
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	210	Total	C	N	O	S	0	0	0
			1535	971	257	302	5			
5	J	212	Total	C	N	O	S	0	0	0
			1543	966	265	308	4			

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



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



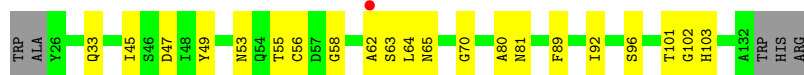
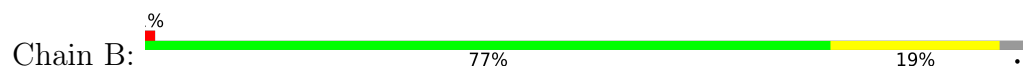
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

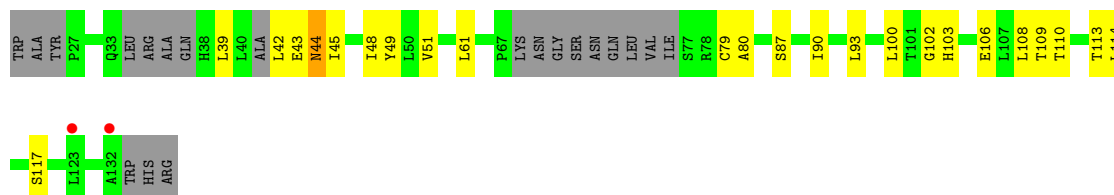
Continued from previous page...

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

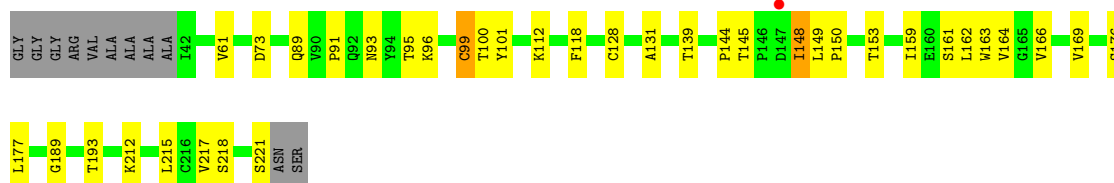
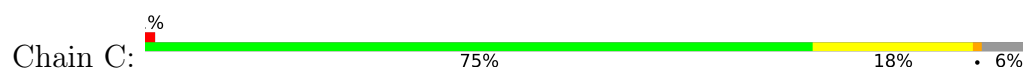
- Molecule 2: Envelope glycoprotein L



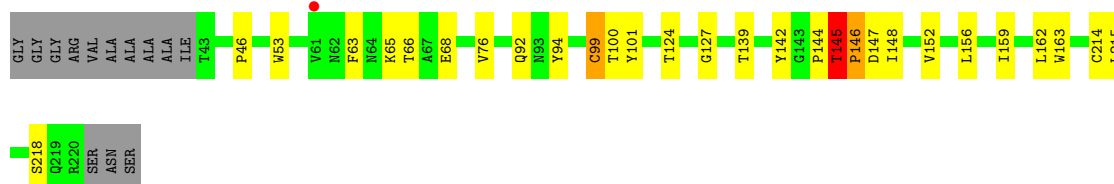
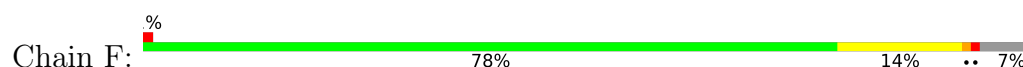
- Molecule 2: Envelope glycoprotein L



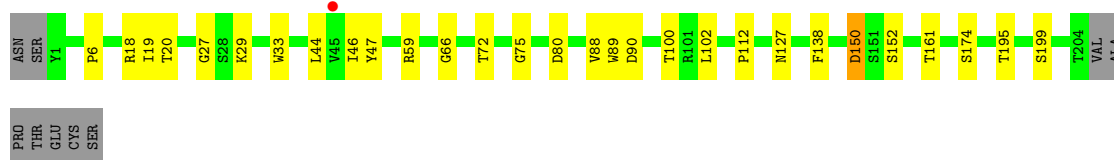
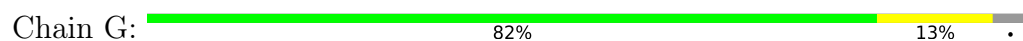
- Molecule 3: Glycoprotein 42



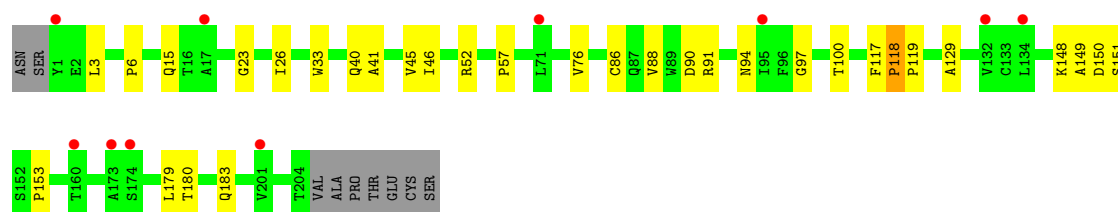
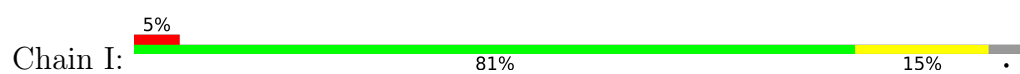
- Molecule 3: Glycoprotein 42



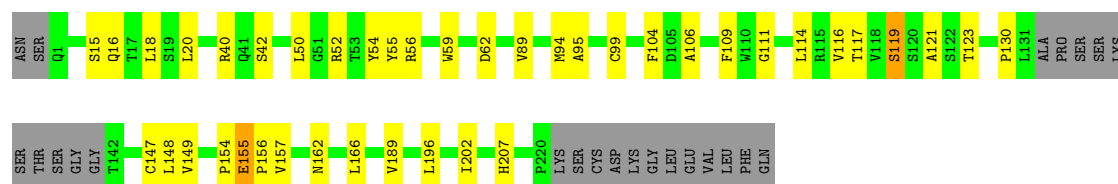
- Molecule 4: A10 light chain



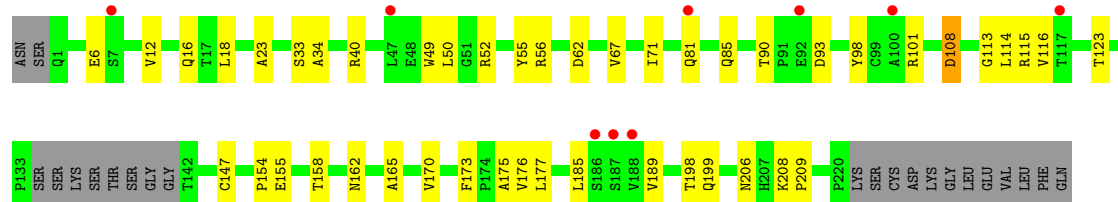
- Molecule 4: A10 light chain



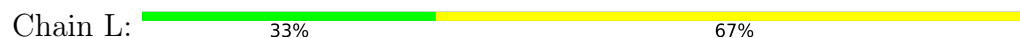
- Molecule 5: A10 heavy chain



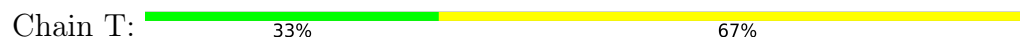
- Molecule 5: A10 heavy chain



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.75Å 138.96Å 316.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.83 – 3.36 45.83 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.83-3.36) 99.9 (45.83-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.234 , 0.281 0.233 , 0.275	Depositor DCC
R_{free} test set	2767 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	134.2	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 137.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20293	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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	0.22	1/5145 (0.0%)	0.44	0/7001
1	D	0.20	0/5056	0.49	0/6884
2	B	0.18	0/799	0.46	0/1089
2	E	0.27	0/682	0.47	0/924
3	C	0.15	0/1463	0.40	0/2018
3	F	0.14	0/1439	0.39	0/1988
4	G	0.14	0/1433	0.37	0/1977
4	I	0.19	0/1417	0.43	0/1957
5	H	0.15	0/1576	0.42	2/2168 (0.1%)
5	J	0.17	0/1582	0.42	0/2175
All	All	0.19	1/20592 (0.0%)	0.44	2/28181 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	GLY	CA-C	5.70	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	155	GLU	CA-C-N	5.11	139.26	127.00
5	H	155	GLU	C-N-CA	5.11	139.26	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	145	THR	Peptide

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	5036	0	4960	78	0
1	D	4952	0	4838	93	0
2	B	786	0	740	15	0
2	E	675	0	638	16	0
3	C	1408	0	1265	27	0
3	F	1383	0	1219	19	0
4	G	1400	0	1232	16	0
4	I	1385	0	1193	19	0
5	H	1535	0	1406	22	0
5	J	1543	0	1410	26	0
6	L	39	0	34	0	0
6	T	39	0	34	0	0
7	A	14	0	13	0	0
7	B	28	0	26	0	0
7	C	28	0	26	1	0
7	D	14	0	13	0	0
7	E	28	0	26	1	0
All	All	20293	0	19073	316	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 316 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:A:468:LEU:HD21	1:A:501:LEU:HD22	1.33	1.03
1:A:68:MET:HE3	2:B:81:ASN:HD21	1.35	0.91
1:A:617:PHE:HE1	1:A:663:THR:HG22	1.41	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ILE:HG22	3:C:150:PRO:HD2	1.61	0.82
1:A:59:ALA:HA	1:A:208:ARG:HH12	1.44	0.81

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	656/658 (100%)	605 (92%)	44 (7%)	7 (1%)	11	36
1	D	652/658 (99%)	593 (91%)	44 (7%)	15 (2%)	5	22
2	B	105/112 (94%)	90 (86%)	13 (12%)	2 (2%)	6	25
2	E	84/112 (75%)	73 (87%)	10 (12%)	1 (1%)	10	33
3	C	178/191 (93%)	162 (91%)	14 (8%)	2 (1%)	11	36
3	F	176/191 (92%)	154 (88%)	19 (11%)	3 (2%)	7	27
4	G	202/213 (95%)	184 (91%)	16 (8%)	2 (1%)	12	38
4	I	202/213 (95%)	178 (88%)	21 (10%)	3 (2%)	8	29
5	H	206/234 (88%)	183 (89%)	19 (9%)	4 (2%)	6	25
5	J	208/234 (89%)	184 (88%)	20 (10%)	4 (2%)	6	25
All	All	2669/2816 (95%)	2406 (90%)	220 (8%)	43 (2%)	7	28

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
2	B	102	GLY
1	D	530	PRO
1	D	562	GLY
1	D	573	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	542/562 (96%)	540 (100%)	2 (0%)	84	82
1	D	528/562 (94%)	528 (100%)	0	100	100
2	B	85/98 (87%)	85 (100%)	0	100	100
2	E	76/98 (78%)	75 (99%)	1 (1%)	61	70
3	C	152/169 (90%)	151 (99%)	1 (1%)	76	77
3	F	147/169 (87%)	146 (99%)	1 (1%)	76	77
4	G	137/178 (77%)	137 (100%)	0	100	100
4	I	133/178 (75%)	133 (100%)	0	100	100
5	H	163/205 (80%)	162 (99%)	1 (1%)	78	79
5	J	162/205 (79%)	161 (99%)	1 (1%)	78	79
All	All	2125/2424 (88%)	2118 (100%)	7 (0%)	86	84

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	39	LEU
3	F	99	CYS
5	J	147	CYS
5	H	147	CYS
3	C	99	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	239	HIS
1	D	589	GLN
1	D	344	GLN
3	F	86	HIS
2	B	30	HIS

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 ⓘ

6 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
6	NAG	L	1	1,6	14,14,15	1.25	1 (7%)	17,19,21	1.64	1 (5%)
6	NAG	L	2	6	14,14,15	0.91	1 (7%)	17,19,21	1.00	1 (5%)
6	BMA	L	3	6	11,11,12	0.92	0	15,15,17	0.61	0
6	NAG	T	1	1,6	14,14,15	0.96	2 (14%)	17,19,21	0.76	0
6	NAG	T	2	6	14,14,15	0.76	1 (7%)	17,19,21	1.72	1 (5%)
6	BMA	T	3	6	11,11,12	0.86	0	15,15,17	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	L	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
6	NAG	T	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	1/6/23/26	0/1/1/1
6	BMA	T	3	6	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1	NAG	O5-C1	4.44	1.51	1.43
6	L	2	NAG	C1-C2	2.79	1.56	1.52
6	T	2	NAG	O5-C1	2.58	1.48	1.43
6	T	1	NAG	O5-C1	2.58	1.48	1.43
6	T	1	NAG	C1-C2	2.23	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	2	NAG	C1-O5-C5	6.84	121.36	112.19
6	L	1	NAG	C1-O5-C5	6.59	121.02	112.19
6	L	2	NAG	C1-O5-C5	3.44	116.79	112.19

There are no chirality outliers.

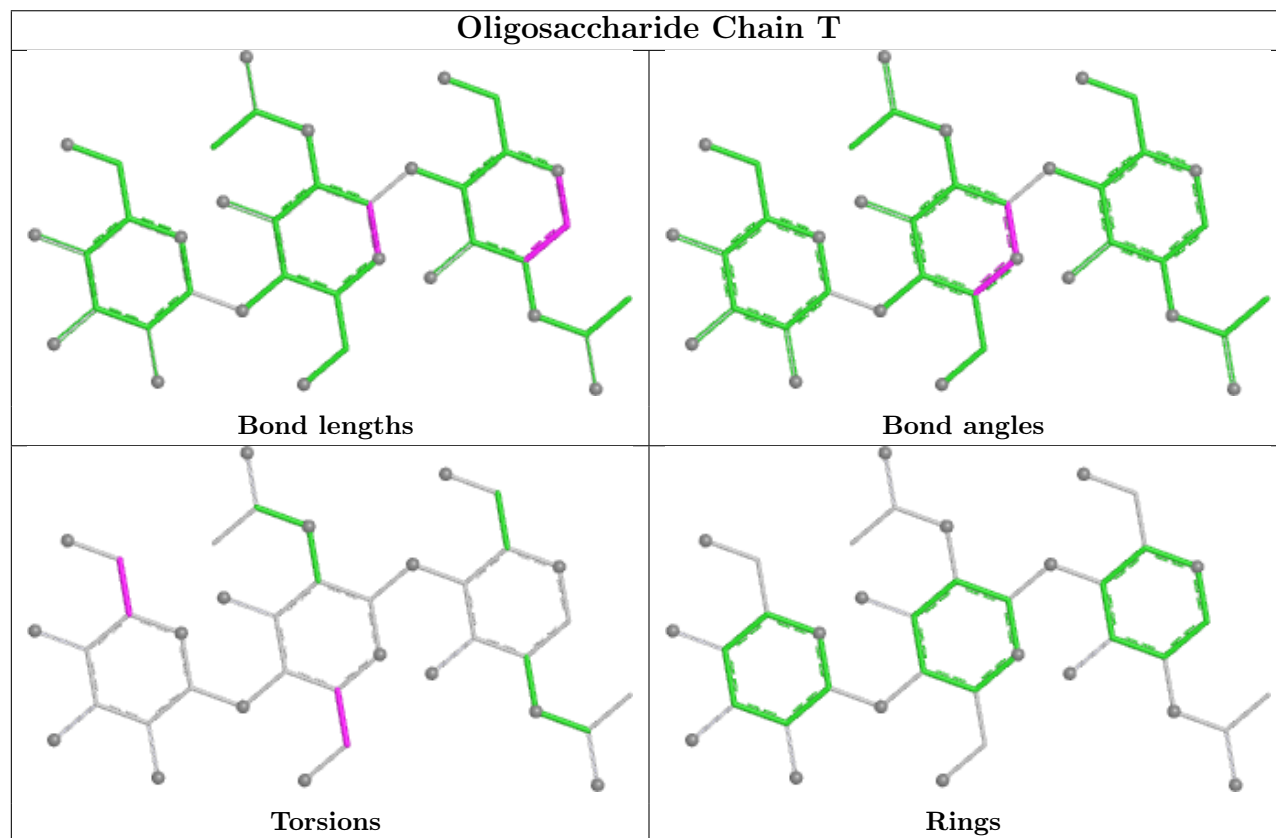
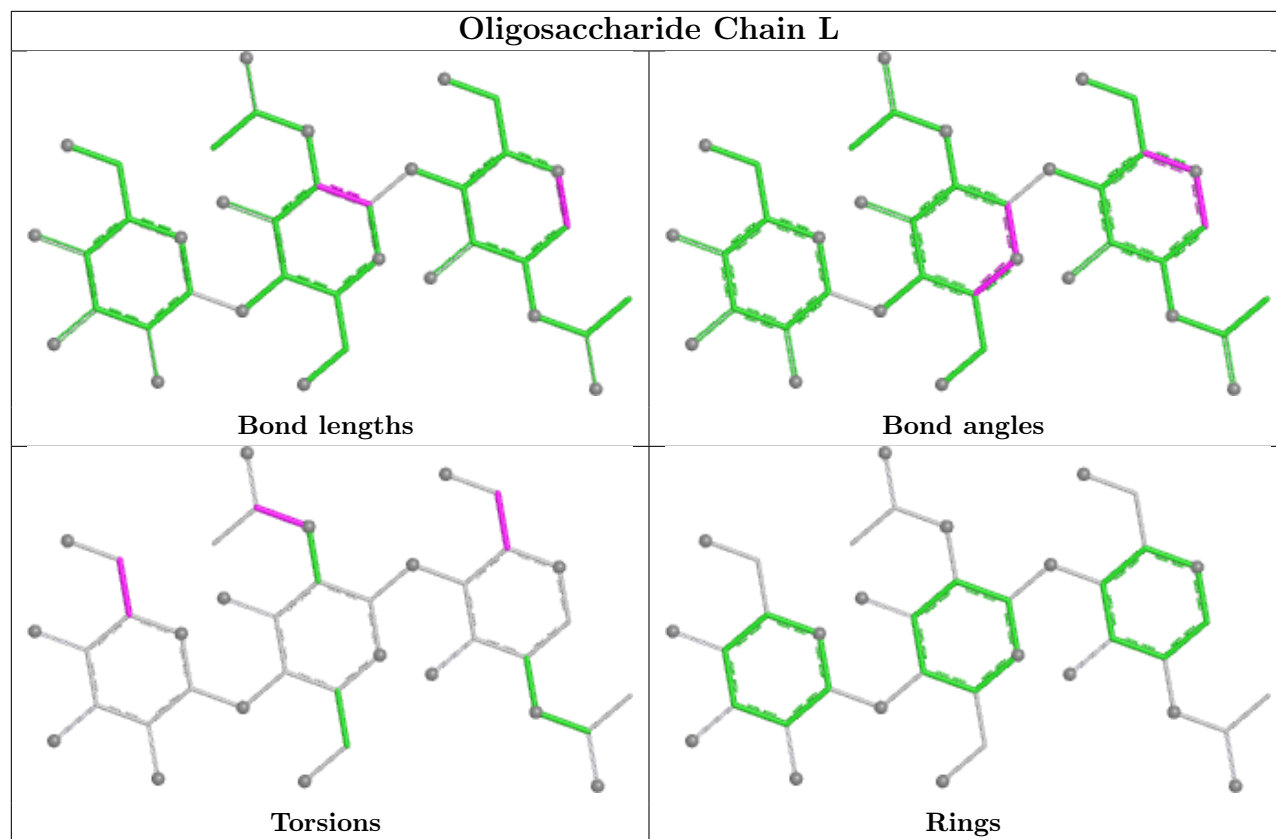
5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	3	BMA	O5-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
6	L	2	NAG	C8-C7-N2-C2
6	L	2	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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

8 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	$\# Z > 2$
7	NAG	B	202	2	14,14,15	0.35	0	17,19,21	0.52	0
7	NAG	B	201	2	14,14,15	0.45	0	17,19,21	0.47	0
7	NAG	D	701	1	14,14,15	0.51	0	17,19,21	0.49	0
7	NAG	C	301	3	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	E	201	2	14,14,15	0.70	1 (7%)	17,19,21	0.76	0
7	NAG	E	202	2	14,14,15	0.38	0	17,19,21	0.63	0
7	NAG	A	701	1	14,14,15	0.77	1 (7%)	17,19,21	0.62	0
7	NAG	C	302	3	14,14,15	0.42	0	17,19,21	0.48	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
7	NAG	B	202	2	-	0/6/23/26	0/1/1/1
7	NAG	B	201	2	-	2/6/23/26	0/1/1/1
7	NAG	D	701	1	-	4/6/23/26	0/1/1/1
7	NAG	C	301	3	-	1/6/23/26	0/1/1/1
7	NAG	E	201	2	-	0/6/23/26	0/1/1/1
7	NAG	E	202	2	-	4/6/23/26	0/1/1/1
7	NAG	A	701	1	-	2/6/23/26	0/1/1/1
7	NAG	C	302	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	701	NAG	C1-C2	2.72	1.56	1.52
7	E	201	NAG	O5-C1	-2.20	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

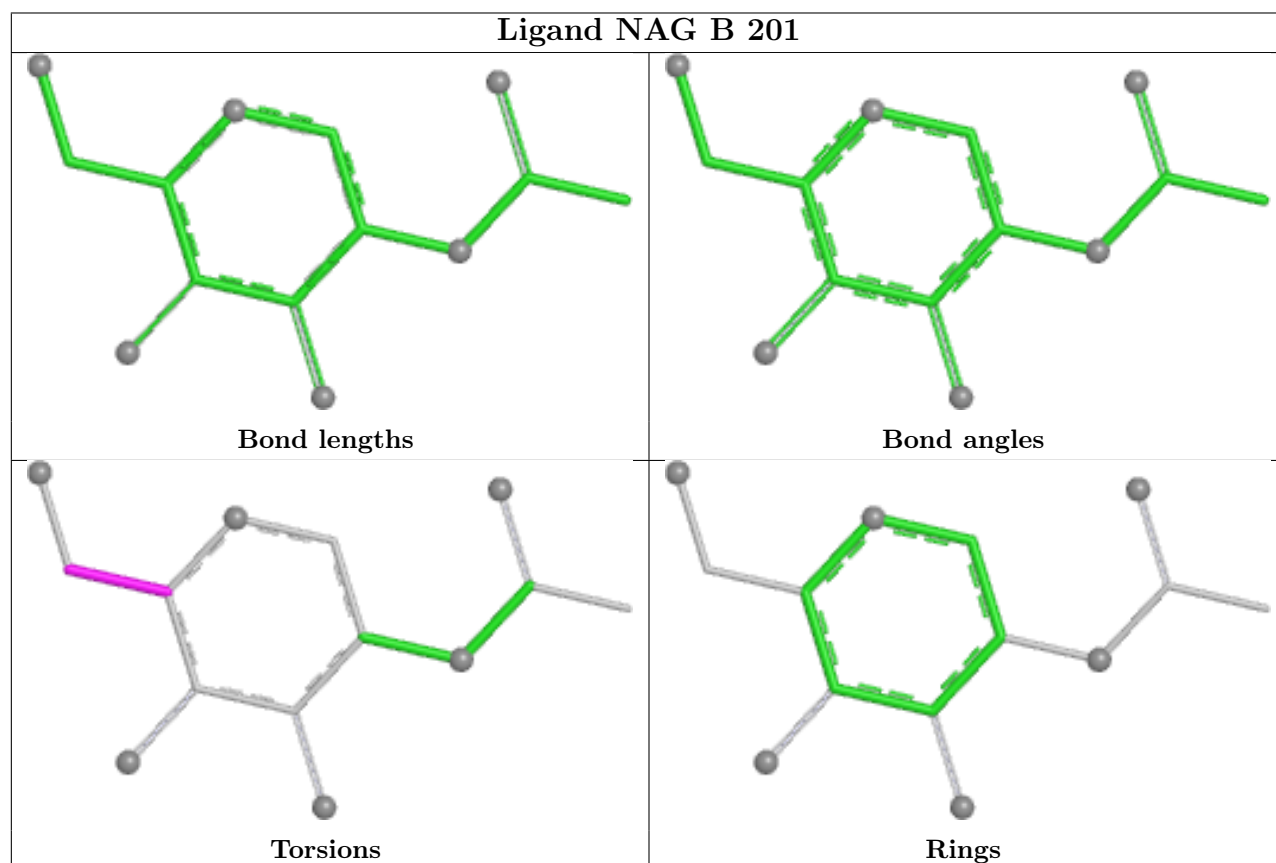
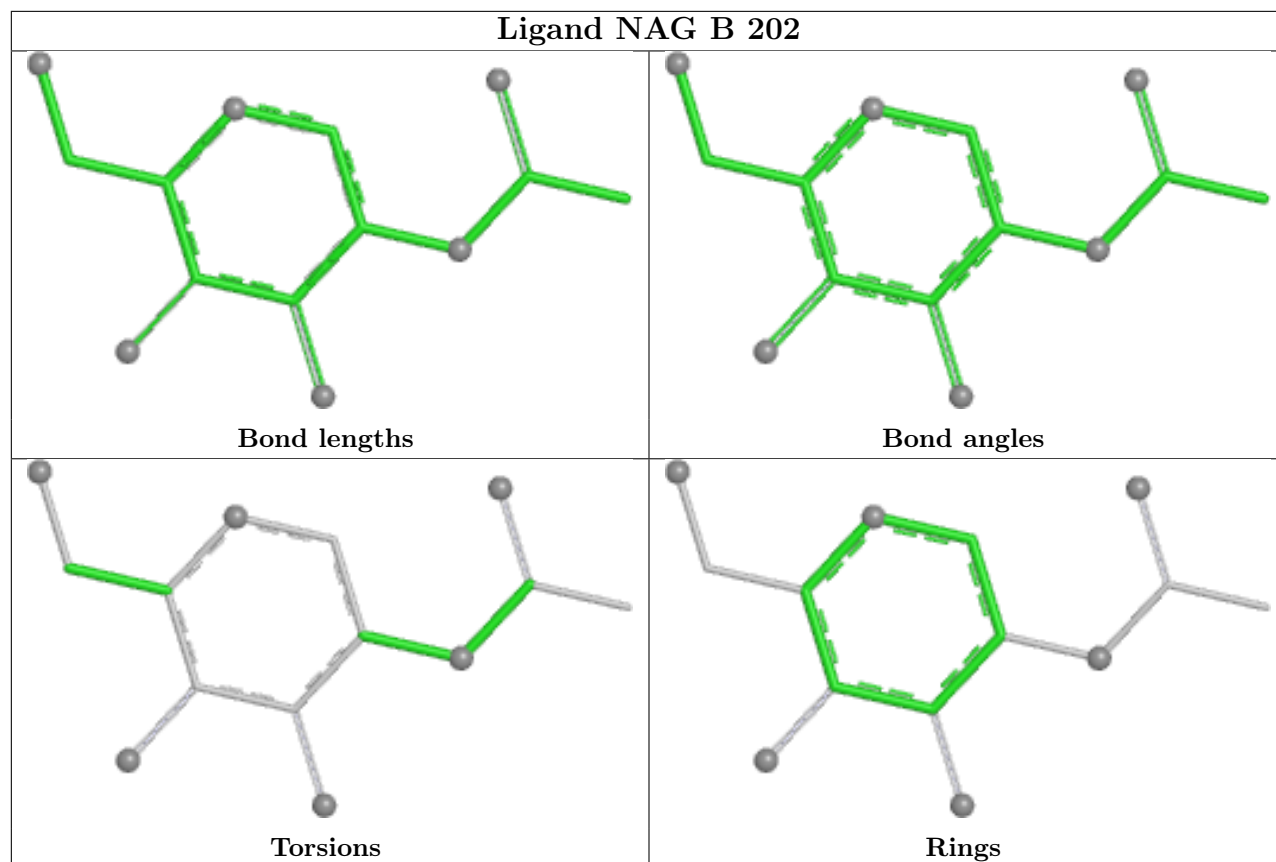
Mol	Chain	Res	Type	Atoms
7	D	701	NAG	C4-C5-C6-O6
7	C	302	NAG	O5-C5-C6-O6
7	D	701	NAG	O5-C5-C6-O6
7	E	202	NAG	O5-C5-C6-O6
7	C	302	NAG	C4-C5-C6-O6

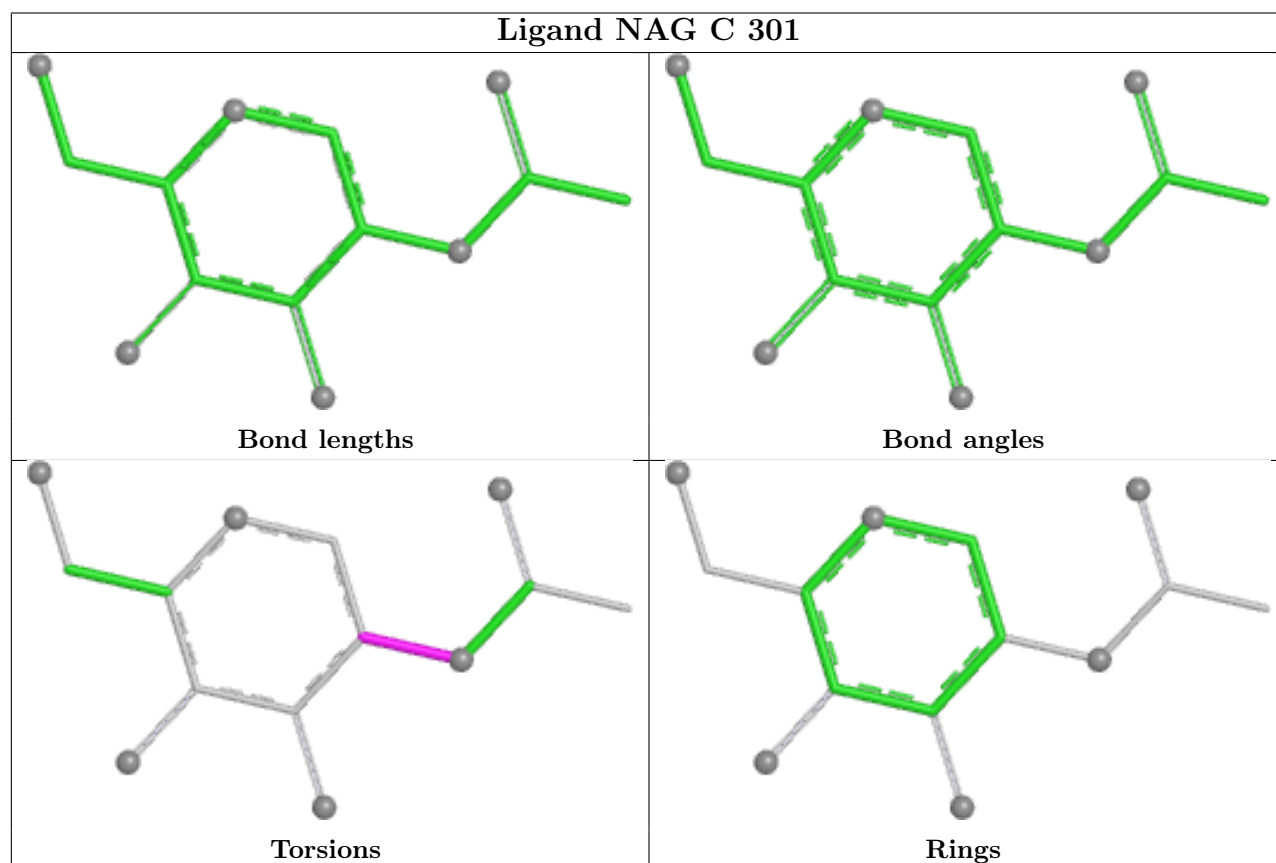
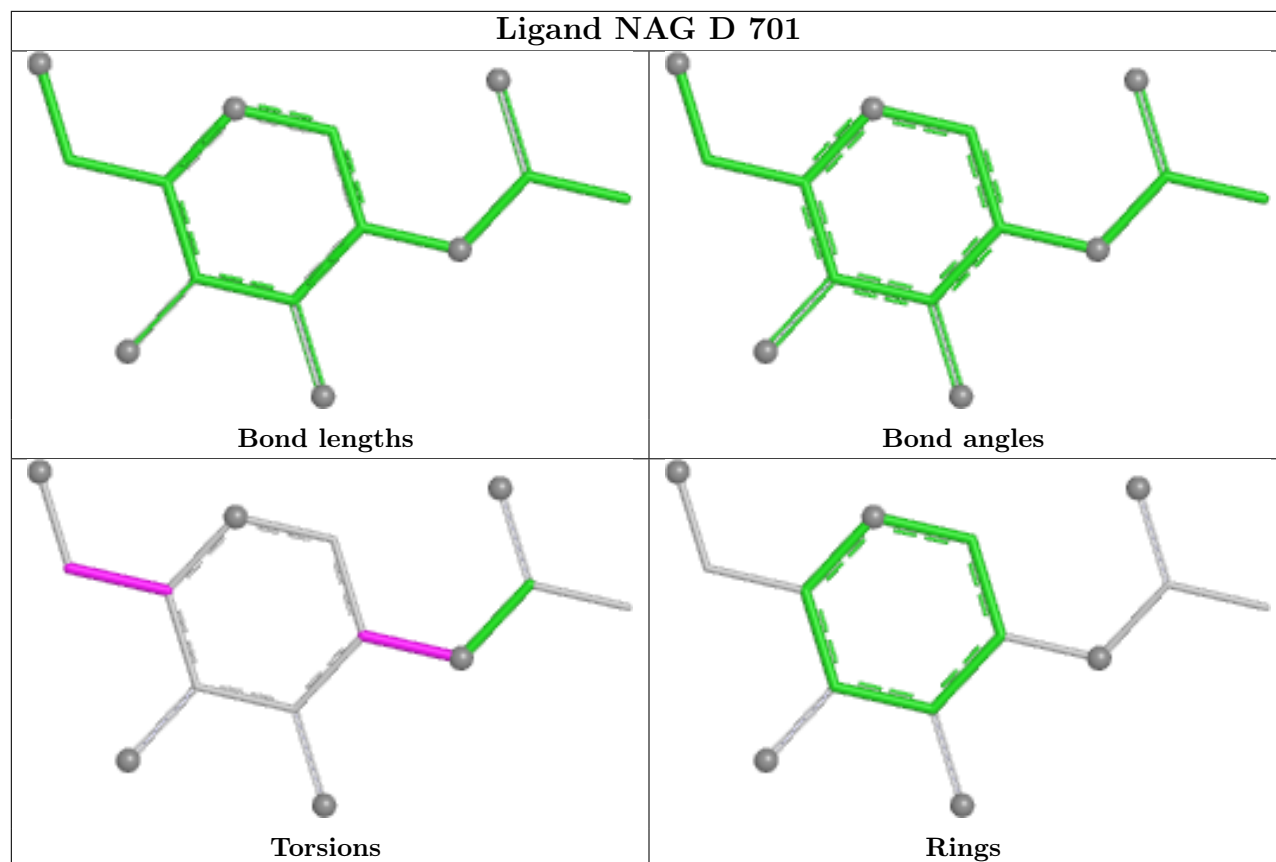
There are no ring outliers.

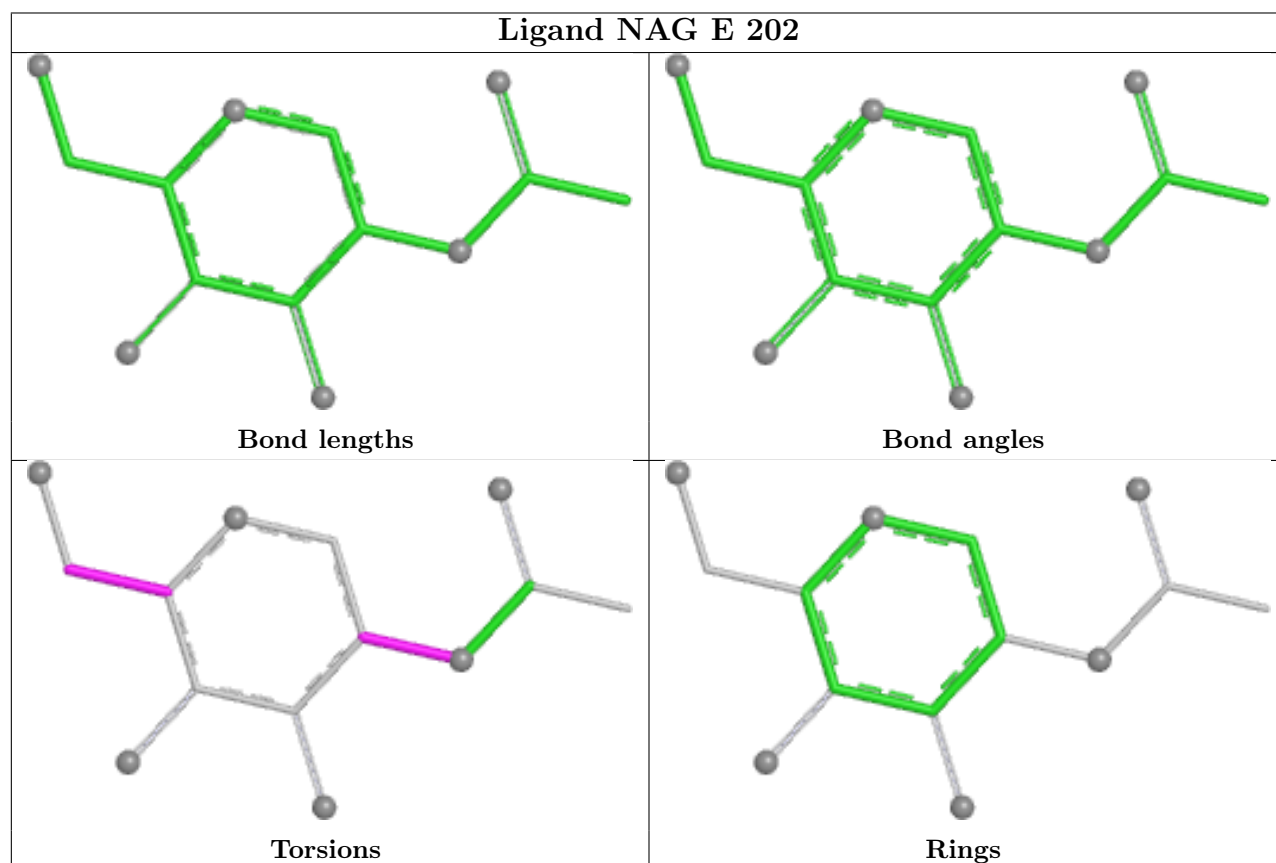
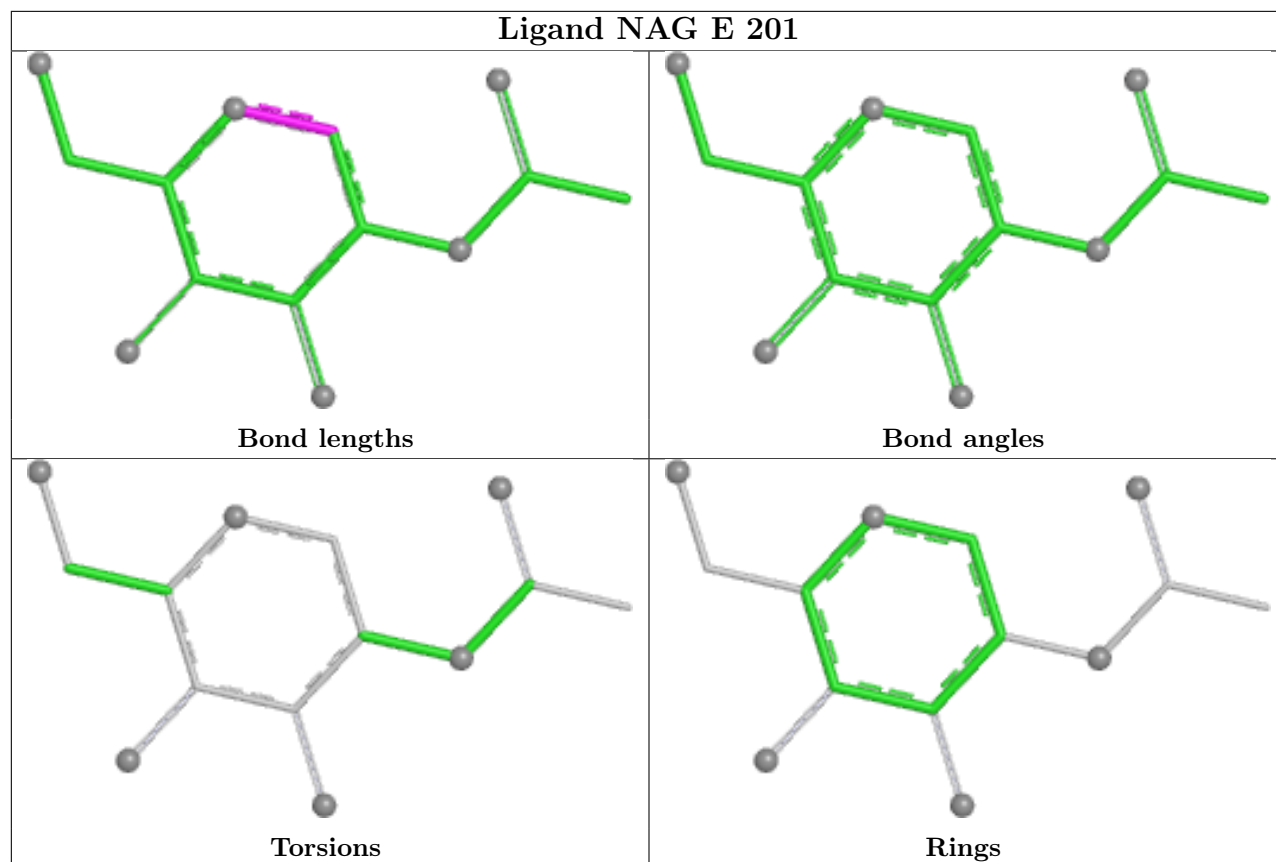
2 monomers are involved in 2 short contacts:

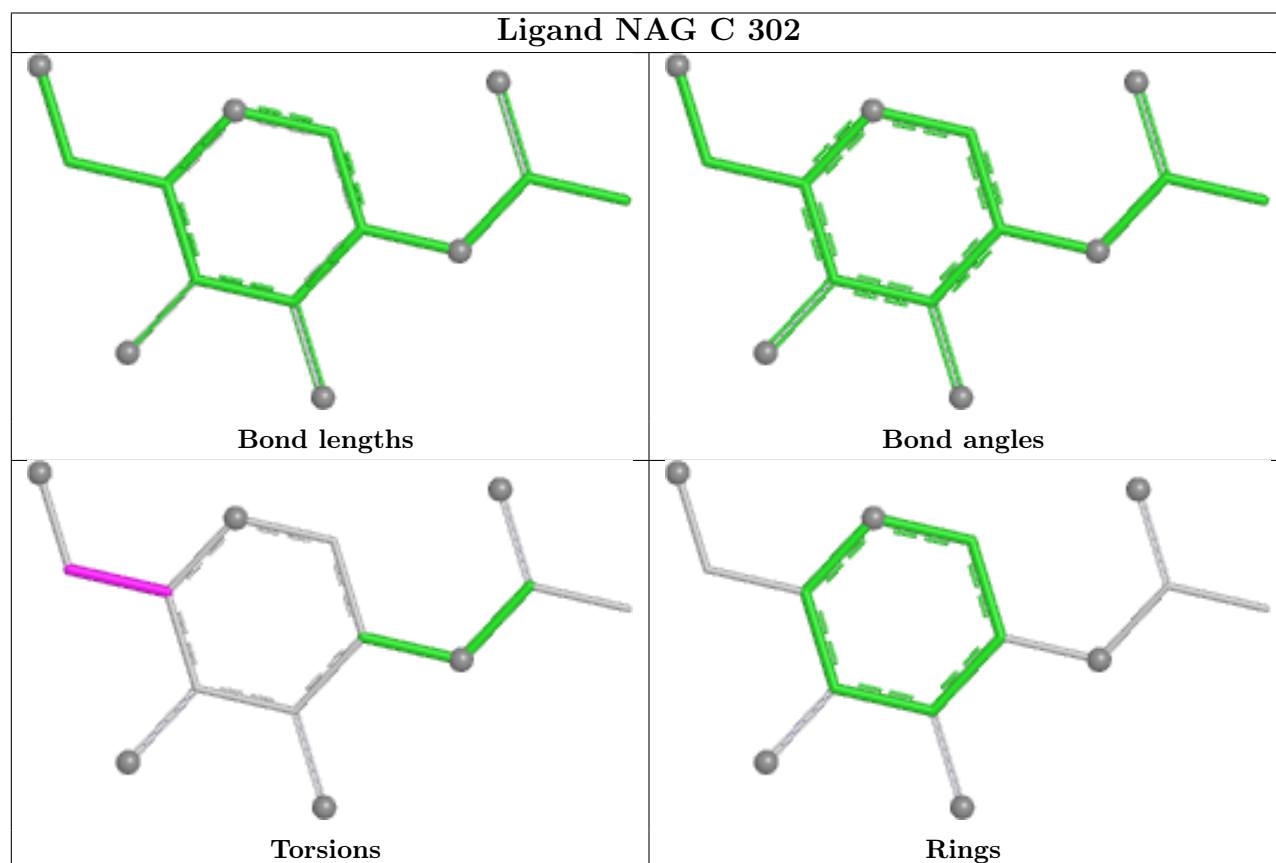
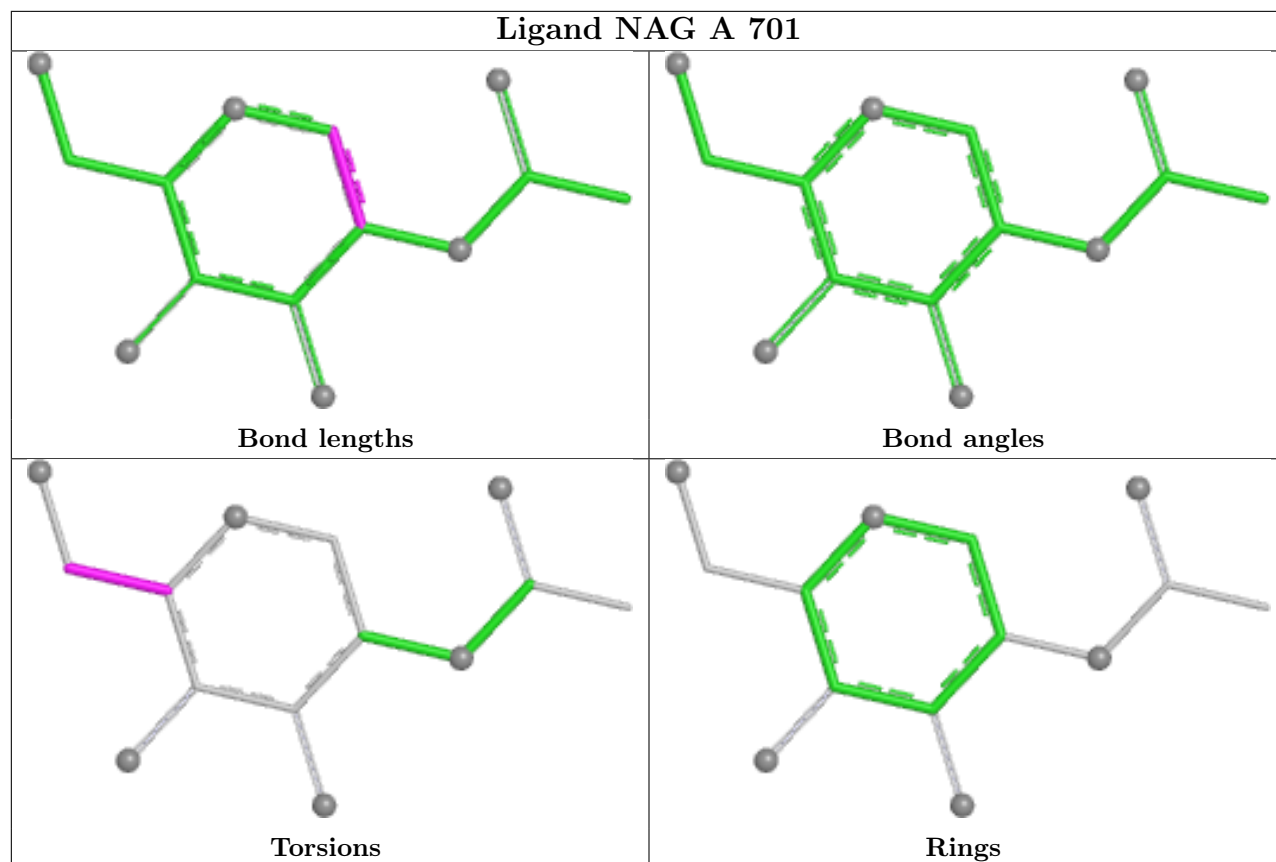
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	202	NAG	1	0
7	C	302	NAG	1	0

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	658/658 (100%)	-0.26	5 (0%) 82 71	74, 108, 172, 256	0
1	D	654/658 (99%)	-0.25	12 (1%) 67 51	87, 150, 228, 313	0
2	B	107/112 (95%)	-0.14	1 (0%) 81 69	91, 136, 213, 247	0
2	E	92/112 (82%)	-0.04	2 (2%) 62 46	111, 169, 216, 276	0
3	C	180/191 (94%)	-0.31	1 (0%) 85 75	87, 128, 173, 231	0
3	F	178/191 (93%)	-0.27	1 (0%) 85 75	105, 145, 196, 238	0
4	G	204/213 (95%)	-0.39	1 (0%) 87 78	121, 165, 224, 284	0
4	I	204/213 (95%)	0.08	10 (4%) 35 25	134, 190, 273, 301	0
5	H	210/234 (89%)	-0.25	0 100 100	123, 167, 230, 290	0
5	J	212/234 (90%)	-0.01	9 (4%) 40 28	122, 179, 247, 282	0
All	All	2699/2816 (95%)	-0.21	42 (1%) 70 55	74, 148, 228, 313	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	351	LEU	4.3
4	I	95	ILE	3.8
3	C	147	ASP	3.6
1	D	381	VAL	3.5
4	I	174	SER	3.5

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

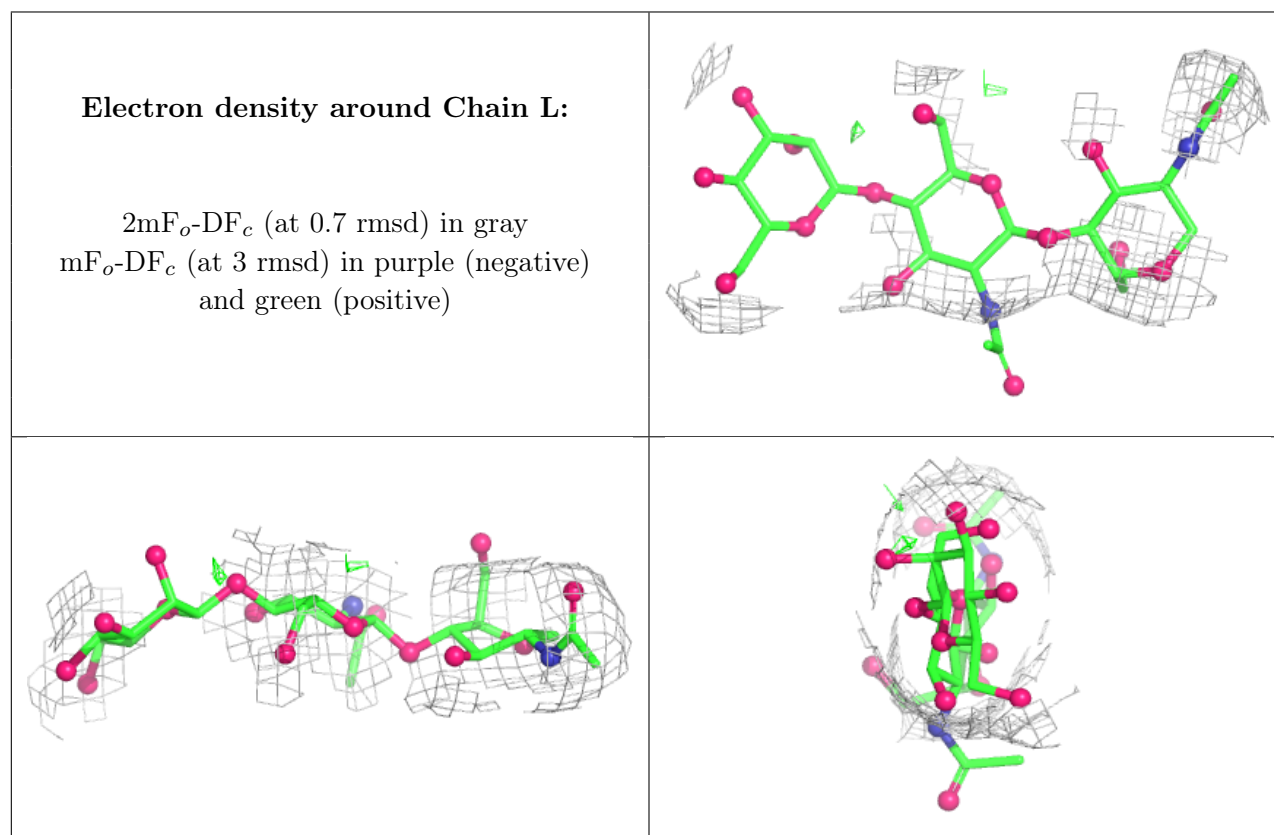
There are no non-standard protein/DNA/RNA residues in this entry.

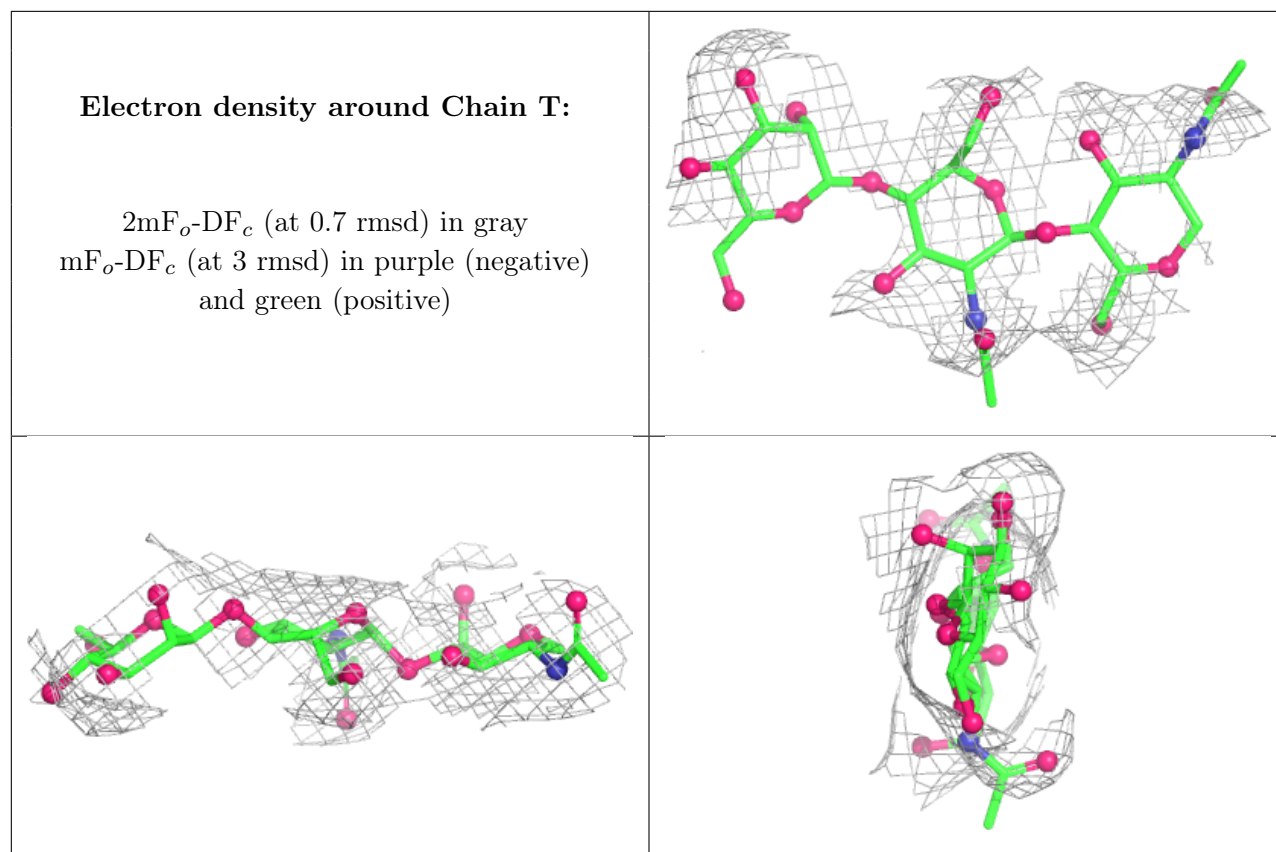
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
6	BMA	L	3	11/12	0.51	0.07	161,177,193,197	0
6	NAG	L	2	14/15	0.79	0.08	167,188,203,222	0
6	NAG	L	1	14/15	0.91	0.06	121,132,170,182	0
6	NAG	T	1	14/15	-	-	123,137,160,173	0
6	NAG	T	2	14/15	-	-	160,168,194,214	0
6	BMA	T	3	11/12	-	-	180,201,228,233	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.





6.4 Ligands [i](#)

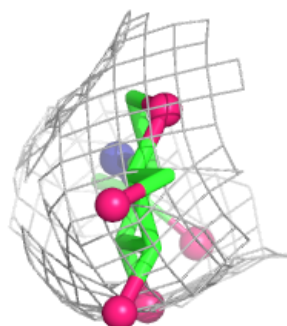
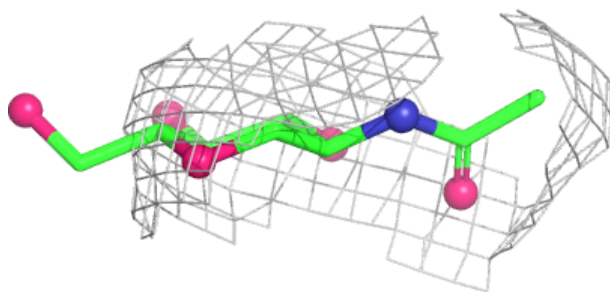
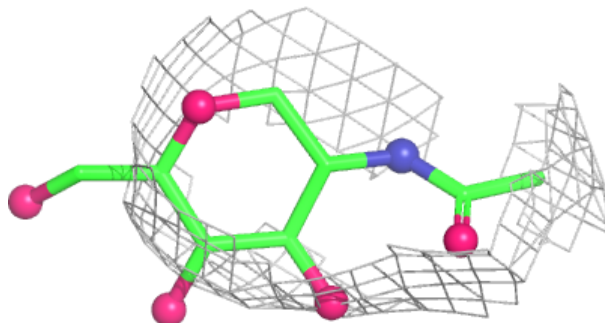
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	C	302	14/15	0.18	0.08	189,243,247,249	0
7	NAG	E	202	14/15	0.52	0.06	179,198,221,225	0
7	NAG	E	201	14/15	0.65	0.07	201,211,225,227	0
7	NAG	C	301	14/15	0.68	0.07	208,222,229,232	0
7	NAG	A	701	14/15	0.73	0.08	154,167,185,199	0
7	NAG	B	202	14/15	0.78	0.06	150,168,181,202	0
7	NAG	D	701	14/15	0.84	0.06	184,200,209,211	0
7	NAG	B	201	14/15	0.94	0.08	100,104,128,139	0

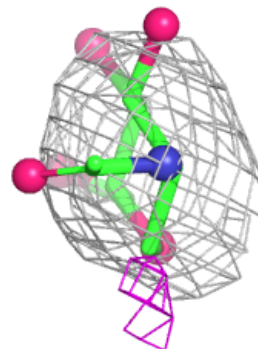
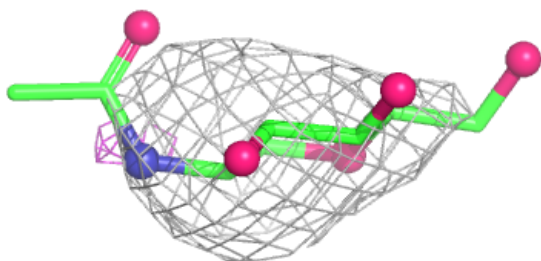
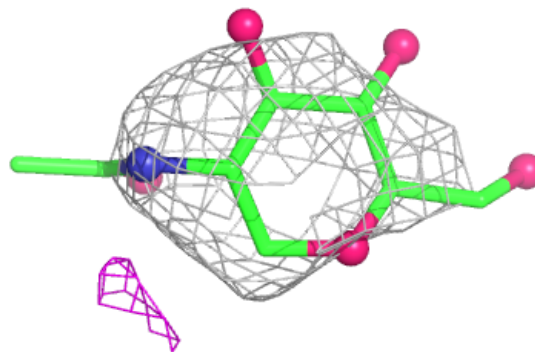
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG C 302:

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

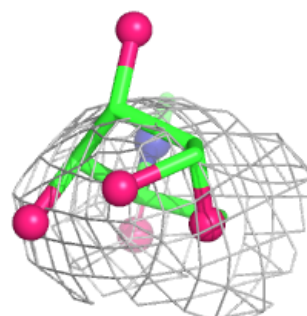
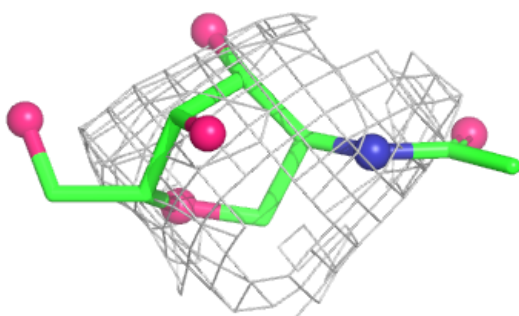
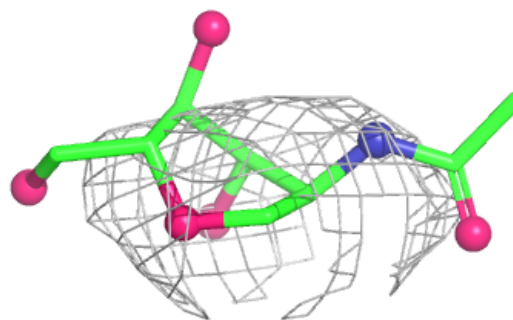
**Electron density around NAG E 202:**

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

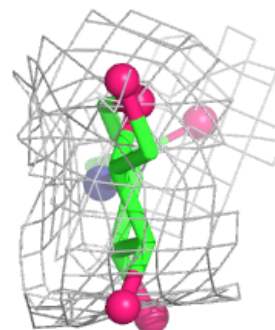
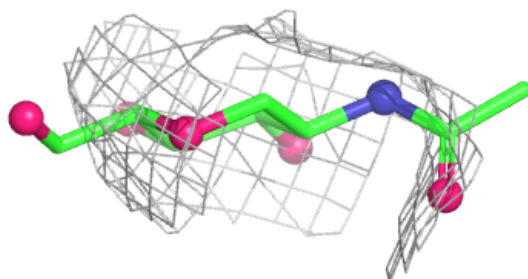
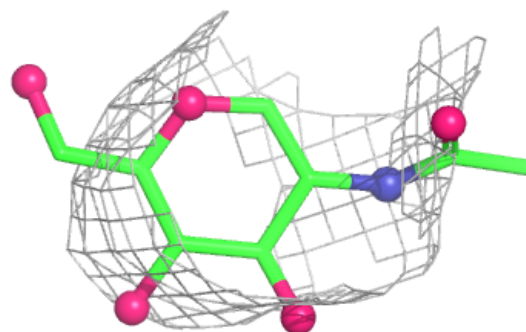


Electron density around NAG E 201:

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

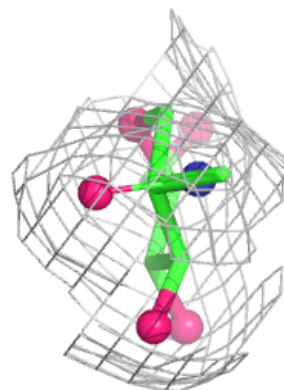
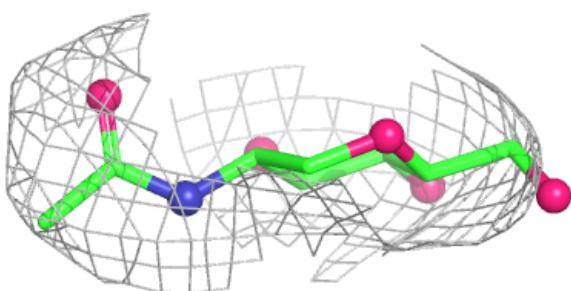
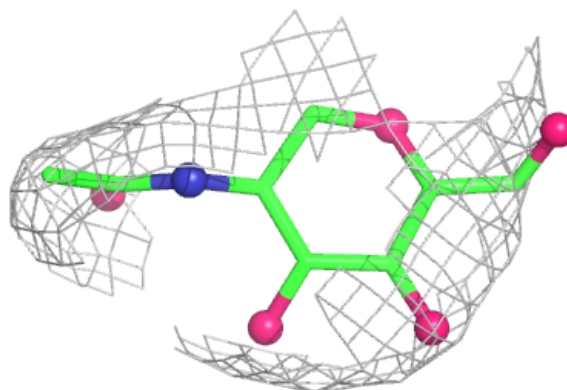
**Electron density around NAG C 301:**

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

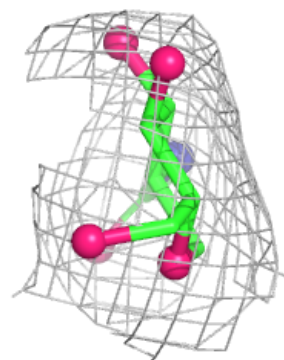
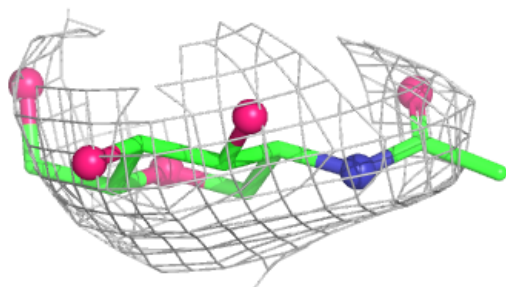
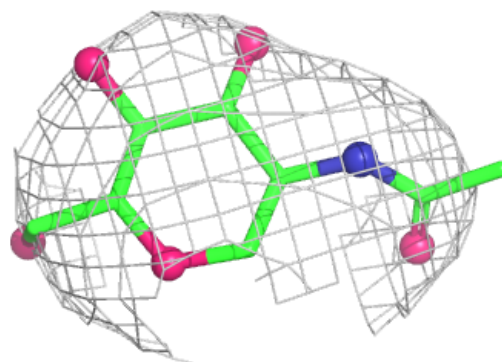


Electron density around NAG A 701:

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

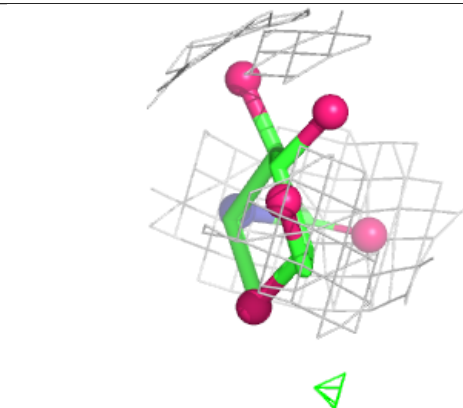
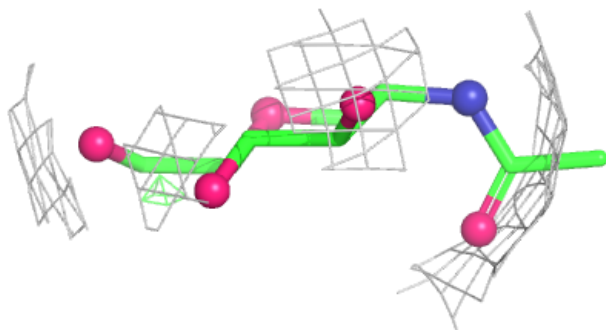
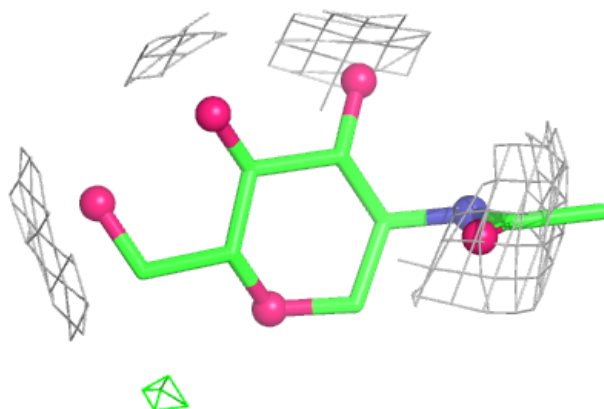
**Electron density around NAG B 202:**

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

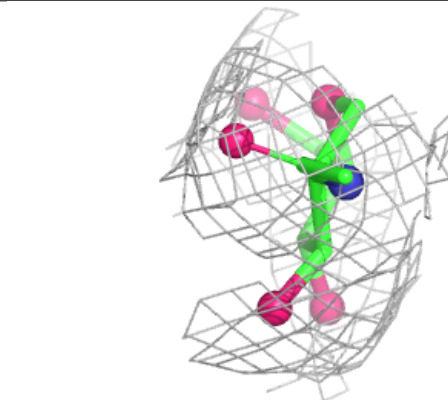
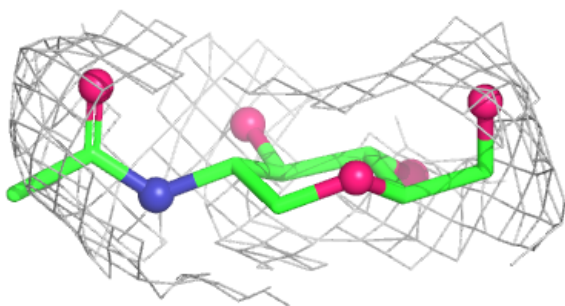
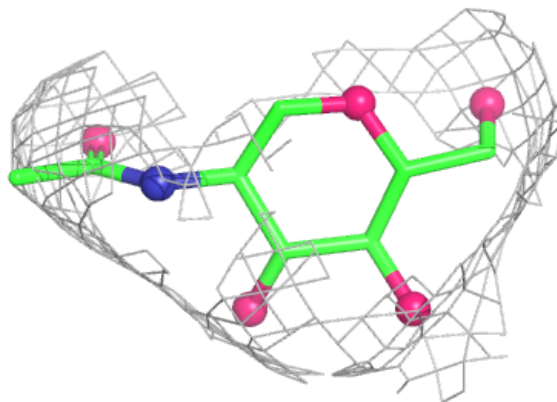


Electron density around NAG D 701:

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

**Electron density around NAG B 201:**

$2mF_o-DF_c$ (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.