WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 20, 2024 – 06:07 PM EDT

PDB ID	:	8TNN
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)

The following versions of software and data (see references ①) were used in the production of this report:

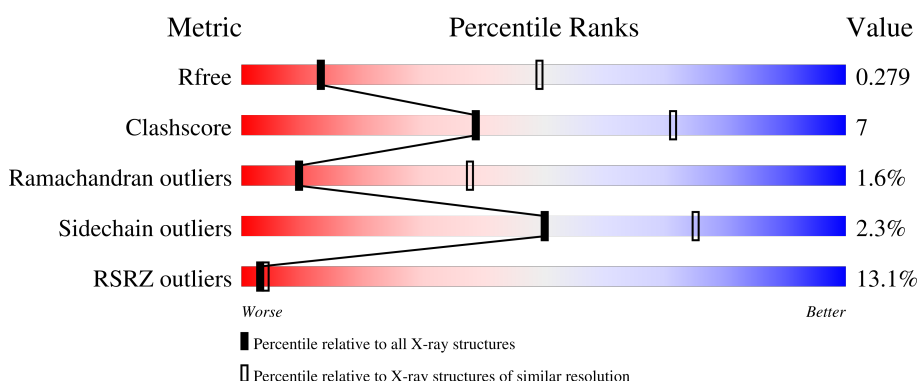|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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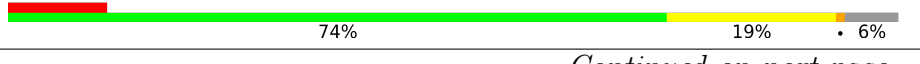*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.36 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	Percentile Ranks	Value
Rfree		0.279
Clashscore		7
Ramachandran outliers		1.6%
Sidechain outliers		2.3%
RSRZ outliers		13.1%

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 <=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	3% — 82% / 17% •
1	D	658	12% — 75% / 23% ••
2	B	112	6% — 73% / 22% •
2	E	112	16% — 58% / 22% • / 18%
3	C	191	11% — 74% / 19% • 6%

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Mol	Chain	Length	Quality of chain
3	F	191	17% 77% 14% 7%
4	G	213	15% 81% 15%
4	I	213	28% 81% 14%
5	H	234	14% 72% 18% 10%
5	J	234	23% 72% 18% 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 1535	C 971	N 257	O 302	S 5	0	0	0
5	J	212	Total 1543	C 966	N 265	O 308	S 4	0	0	0

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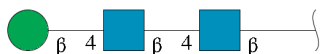
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	3	Total 39	C 22	N 2	O 15	0	0	0
6	T	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).
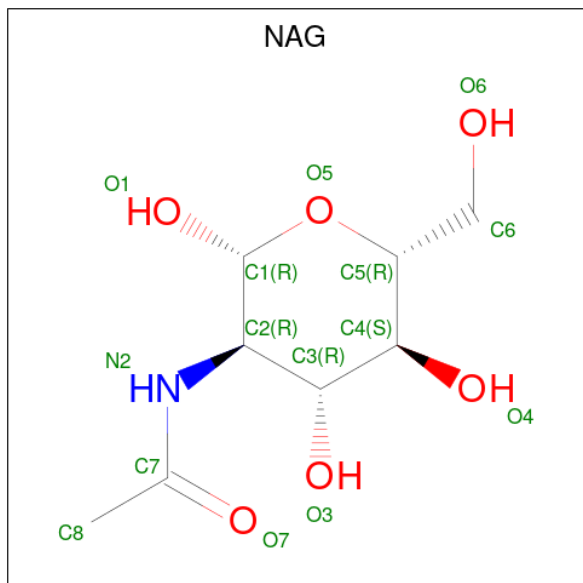
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 14	C 8	N 1	O 5	0	0
7	B	1	Total 14	C 8	N 1	O 5	0	0

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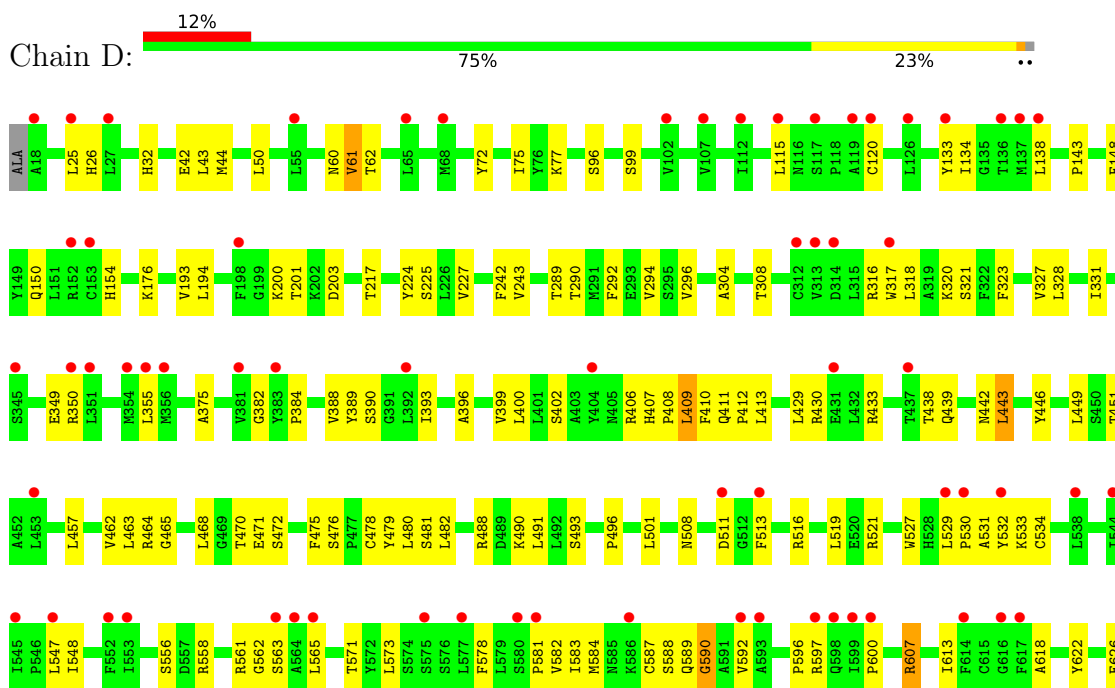| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total 14	C 8	N 1	O 5	0	0
7	C	1	Total 14	C 8	N 1	O 5	0	0
7	C	1	Total 14	C 8	N 1	O 5	0	0
7	D	1	Total 14	C 8	N 1	O 5	0	0
7	E	1	Total 14	C 8	N 1	O 5	0	0
7	E	1	Total 14	C 8	N 1	O 5	0	0

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.
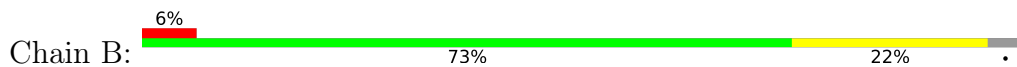
• Molecule 1: Envelope glycoprotein H

• Molecule 1: Envelope glycoprotein H

E629 T632 Y633 I634 T635 S636 Q637 E638 V639 Q640 I643 F649 D650 F651 D652 N653 H657 L661 T662 T663 V667 M668 E669 I670 A671 GLY LEU TYR

• Molecule 2: Envelope glycoprotein L

Chain B:

6%

73%   22%   •

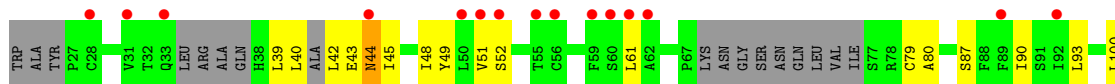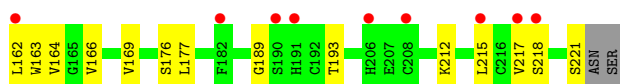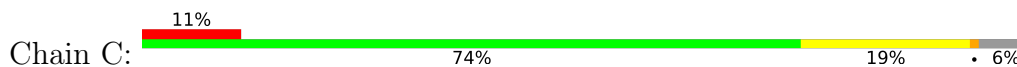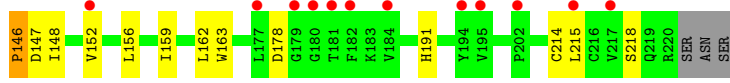TRP ALA Y26 Q33 I45 S46 D47 I48 Y49 N53 Q54 T55 C56 D57 G58 F59 S60 L61 A62 S63 L64 N65 G70 S71 N72 Q73 A80 N81 F89 I92 S96 S97 S98 T101 G102 H103 L123 N129 A132 TRP HIS ARG

• Molecule 2: Envelope glycoprotein L

Chain E:
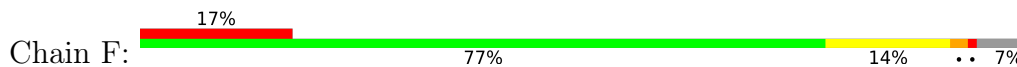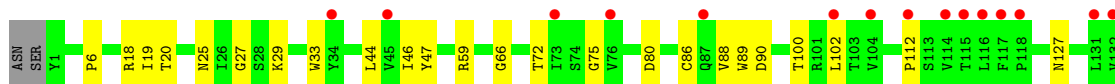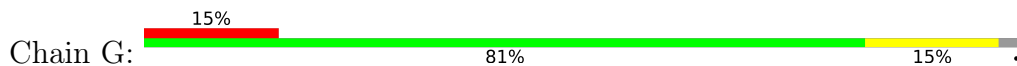
16%

58%   22%   •   18%

TRP ALA TYR P27 C28 V31 T32 Q33 LEU ARG ALA GLN H38 L39 L40 ALA L42 E43 N44 I45 I48 Y49 L50 V51 S52 T55 C56 F59 S60 L61 A62 P67 LYS ASN GLY SER ASN GLN LEU VAL ILE S77 R78 C79 A80 S87 F88 F89 I90 S91 I92 L93 L100

T101 G102 H103 E106 L107 L108 T109 T110 T113 L114 S117 F118 S119 V120 L123 A132 TRP HIS ARG

• Molecule 3: Glycoprotein 42

Chain C:

11%

74%   19%   •   6%

GLY GLY GLY ARG VAL ALA ALA ALA I42 V61 D73 Q89 V90 P91 Q92 N93 Y94 T95 K96 A97 N98 C99 T100 Y101 K112 C115 F116 Y117 F118 W125 C128 A131 T139 Y140 F141 Y142 G143 P144 T145 P146 D147 I148 L149 P150 T153 I159 E160 S161

L162 W163 V164 G165 V166 V169 S176 L177 F182 G189 S190 H191 C192 T193 H206 E207 C208 K212 L215 C216 V217 S218 S221 ASN SER

• Molecule 3: Glycoprotein 42

Chain F:

17%

77%   14%   • •   7%

GLY GLY GLY ARG VAL ALA ALA ALA ILE T43 W44 V45 P46 V52 W53 V61 N62 F63 N64 K65 T66 A67 E68 V76 K77 L78 H86 T87 F88 Q92 N93 Y94 C99 T100 F116 T124 W125 N126 G127 C128 F129 P137 C138 T139 Y140 F141 Y142 G143 P144 T145

P146 D147 I148 V152 L156 I159 L162 W163 L177 D178 D179 G180 T181 F182 K183 V184 H191 Y194 V195 P202 C214 L215 C216 V217 S218 Q219 R220 SER ASN SER

• Molecule 4: A10 light chain

Chain G:

15%

81%   15%   •

ASN SER Y1 P6 R18 I19 T20 N25 I26 G27 S28 K29 W33 Y34 L44 V45 I46 Y47 R59 G66 T72 I73 S74 G75 V76 D80 C86 Q87 V88 W89 D90 T100 R101 L102 T103 V104 P112 S113 V114 T115 L116 F117 P118 N127 L131 V132

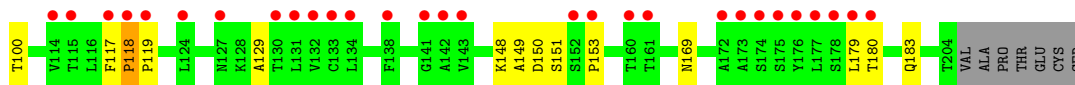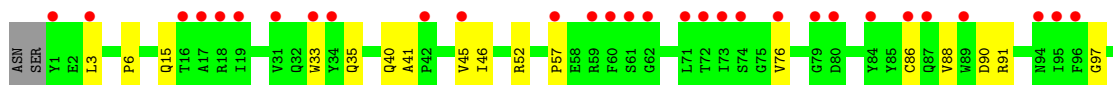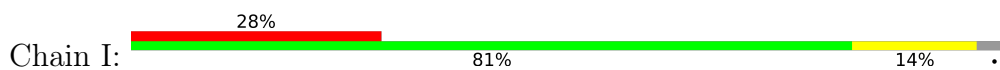C133 L134 I135 F138 V145 A146 W147 D150 V154 T161 S174 S175 Y176 L177 S178 W184 K185 S186 H187 C192 Q193 V194 T195 S199 T200 V201 E202 K203 T204 VAL ALA PRO THR GLU CYS SER

• Molecule 4: A10 light chain

Chain I:

28%

81% 14%

ASN SER Y1 E2 L3 P6 Q15 T16 A17 R18 I19 V31 Q32 W33 Y34 Q35 Q40 A41 P42 V45 I46 R52 P57 E58 R59 F60 S61 G62 L71 T72 I73 S74 G75 V76 G79 D80 Y84 Y85 C86 Q87 V88 W89 D90 R91 N94 I95 F96 G97

T100 V114 T115 L116 F117 P118 P119 L124 N127 K128 A129 T130 L131 V132 C133 L134 F138 G141 A142 V143 K148 A149 D150 S151 S152 P153 T160 T161 N169 A172 A173 S174 S175 Y176 L177 S178 L179 T180 Q183 T204 VAL ALA PRO THR GLU CYS SER
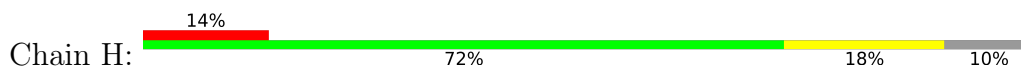
• Molecule 5: A10 heavy chain

Chain H:

14%

72% 18% 10%

ASN SER Q1 G10 S15 Q16 T17 L18 S19 L20 W36 R40 Q41 S42 P43 S44 L50 G51 R52 T53 Y54 Y55 R56 S57 K58 W59 Y60 Y61 D62 Q68 F82 Q85 V89 M94 A95 C99 F104 D105 A106 F109 W110 G111 L114 R115 V116 T117

V118 S119 T123 V128 F129 P130 L131 ALA PRO SER SER LYS SER THR SER GLY GLY T142 L145 G146 C147 L148 V149 P154 E155 P156 V157 W161 N162 S163 L166 L185 S186 S187 V188 V189 L196 T200 Y201 I202 C203 N204 V205 H207 V218 E219 P220 LYS SER

CYS ASP LYS GLY LEU GLU VAL LEU PHE GLN

• Molecule 5: A10 heavy chain

Chain J:

23%

72% 18% 9%

ASN SER Q1 L4 Q5 E6 S7 V12 Q16 T17 L18 A23 S33 A34 T35 W36 N37 R40 Q41 S42 L47 L50 G51 R52 T53 Y54 Y55 R56 D62 V67 I71 D76 Q81 Q85 Y98 C99 A100 R101 G102 D103 F104 D105 A106 F107 D108

G113 L114 R115 V116 T123 K124 G125 P126 S127 V128 F129 P130 L131 A132 P133 SER SER LYS SER THR SER GLY GLY T142 A143 A144 L145 G146 C147 L148 V149 K150 D151 Y152 F153 P154 E155 N162 A165 V170 H171 I172 F173 P174 A175 V176 L177 S184 L185 S186 S187 V188 V189 T190

V191 P192 S193 S194 S195 L196 G197 T198 Q199 C203 N204 V205 K208 P209 P220 LYS SER CYS ASP LYS GLY LEU GLU VAL LEU PHE GLN

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

Chain L:

33% 67%

NAG1 NAG2 BMA3

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

Chain T:

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 54.71 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.83-3.36) 99.9 (54.71-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.234 , 0.281 0.233 , 0.279	Depositor DCC
R_{free} test set	2764 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)	0.26 , 89.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.31	0/5145	0.54	0/7001
1	D	0.28	0/5056	0.56	0/6884
2	B	0.27	0/799	0.53	0/1089
2	E	0.29	0/682	0.54	0/924
3	C	0.28	0/1463	0.51	0/2018
3	F	0.27	0/1439	0.48	0/1988
4	G	0.26	0/1433	0.51	0/1977
4	I	0.27	0/1417	0.51	0/1957
5	H	0.25	0/1576	0.56	0/2168
5	J	0.26	0/1582	0.54	0/2175
All	All	0.28	0/20592	0.54	0/28181

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

There are no bond length outliers.

There are no bond angle outliers.

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	74	0
1	D	4952	0	4838	86	0
2	B	786	0	740	13	0
2	E	675	0	638	15	0
3	C	1408	0	1265	27	0
3	F	1383	0	1219	18	0
4	G	1400	0	1232	15	0
4	I	1385	0	1193	17	0
5	H	1535	0	1406	21	0
5	J	1543	0	1410	23	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	295	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 7.

The worst 5 of 295 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:617:PHE:HE1	1:A:663:THR:HG22	1.41	0.86
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
1:D:468:LEU:HD21	1:D:501:LEU:HD22	1.63	0.78

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	656/658 (100%)	605 (92%)	44 (7%)	7 (1%)	14	46
1	D	652/658 (99%)	593 (91%)	44 (7%)	15 (2%)	6	31
2	B	105/112 (94%)	90 (86%)	13 (12%)	2 (2%)	8	34
2	E	84/112 (75%)	73 (87%)	10 (12%)	1 (1%)	13	44
3	C	178/191 (93%)	162 (91%)	14 (8%)	2 (1%)	14	46
3	F	176/191 (92%)	154 (88%)	19 (11%)	3 (2%)	9	36
4	G	202/213 (95%)	184 (91%)	16 (8%)	2 (1%)	15	49
4	I	202/213 (95%)	178 (88%)	21 (10%)	3 (2%)	10	39
5	H	206/234 (88%)	183 (89%)	19 (9%)	4 (2%)	8	34
5	J	208/234 (89%)	184 (88%)	20 (10%)	4 (2%)	8	34
All	All	2669/2816 (95%)	2406 (90%)	220 (8%)	43 (2%)	9	38

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%)	534 (98%)	8 (2%)	65	82
1	D	528/562 (94%)	515 (98%)	13 (2%)	47	73
2	B	85/98 (87%)	81 (95%)	4 (5%)	26	58
2	E	76/98 (78%)	71 (93%)	5 (7%)	16	47
3	C	152/169 (90%)	150 (99%)	2 (1%)	69	84
3	F	147/169 (87%)	142 (97%)	5 (3%)	37	66
4	G	137/178 (77%)	134 (98%)	3 (2%)	52	76
4	I	133/178 (75%)	131 (98%)	2 (2%)	65	82
5	H	163/205 (80%)	160 (98%)	3 (2%)	59	80
5	J	162/205 (79%)	159 (98%)	3 (2%)	57	79
All	All	2125/2424 (88%)	2077 (98%)	48 (2%)	50	75

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	40	LEU
3	F	178	ASP
2	E	52	SER
3	F	99	CYS
4	G	25	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	81	ASN
1	D	234	HIS
1	D	344	GLN

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	6,1	14,14,15	1.30	1 (7%)	17,19,21	1.62	1 (5%)
6	NAG	L	2	6	14,14,15	0.86	1 (7%)	17,19,21	0.99	1 (5%)
6	BMA	L	3	6	11,11,12	0.93	0	15,15,17	0.69	0
6	NAG	T	1	6,1	14,14,15	0.95	2 (14%)	17,19,21	0.75	0
6	NAG	T	2	6	14,14,15	0.78	1 (7%)	17,19,21	1.70	1 (5%)
6	BMA	T	3	6	11,11,12	0.88	0	15,15,17	0.66	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	6,1	-	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	6,1	-	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	4.65	1.51	1.43
6	T	2	NAG	O5-C1	2.70	1.48	1.43
6	T	1	NAG	O5-C1	2.70	1.48	1.43
6	L	2	NAG	C1-C2	2.55	1.56	1.52
6	T	1	NAG	C1-C2	2.04	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	2	NAG	C1-O5-C5	6.77	121.36	112.19
6	L	1	NAG	C1-O5-C5	6.52	121.02	112.19
6	L	2	NAG	C1-O5-C5	3.39	116.79	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

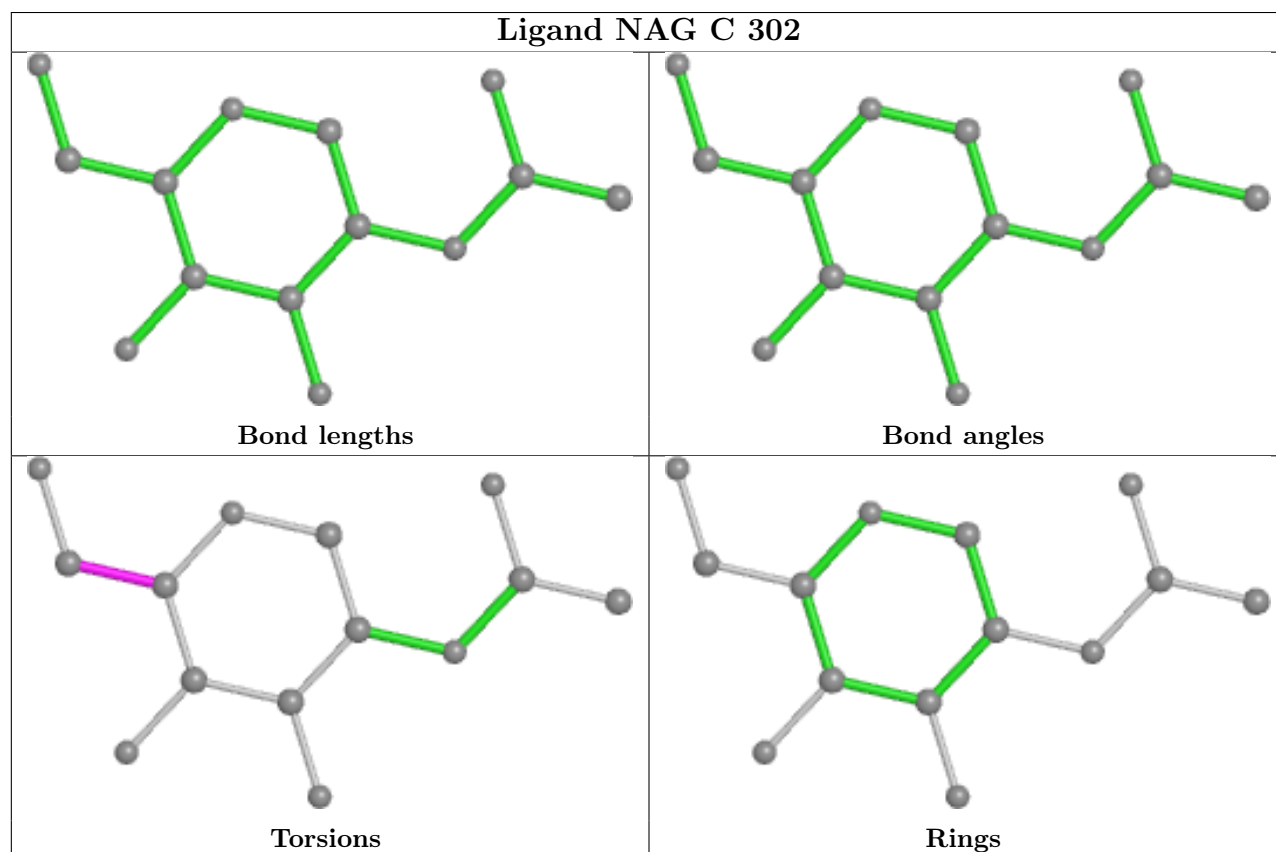| Mol	Chain	Res	Type	Atoms
6	L	1	NAG	C4-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	L	2	NAG	C8-C7-N2-C2
6	L	2	NAG	O7-C7-N2-C2
6	L	1	NAG	O5-C5-C6-O6

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.

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain T

Bond lengths

Bond angles

Torsions

Rings
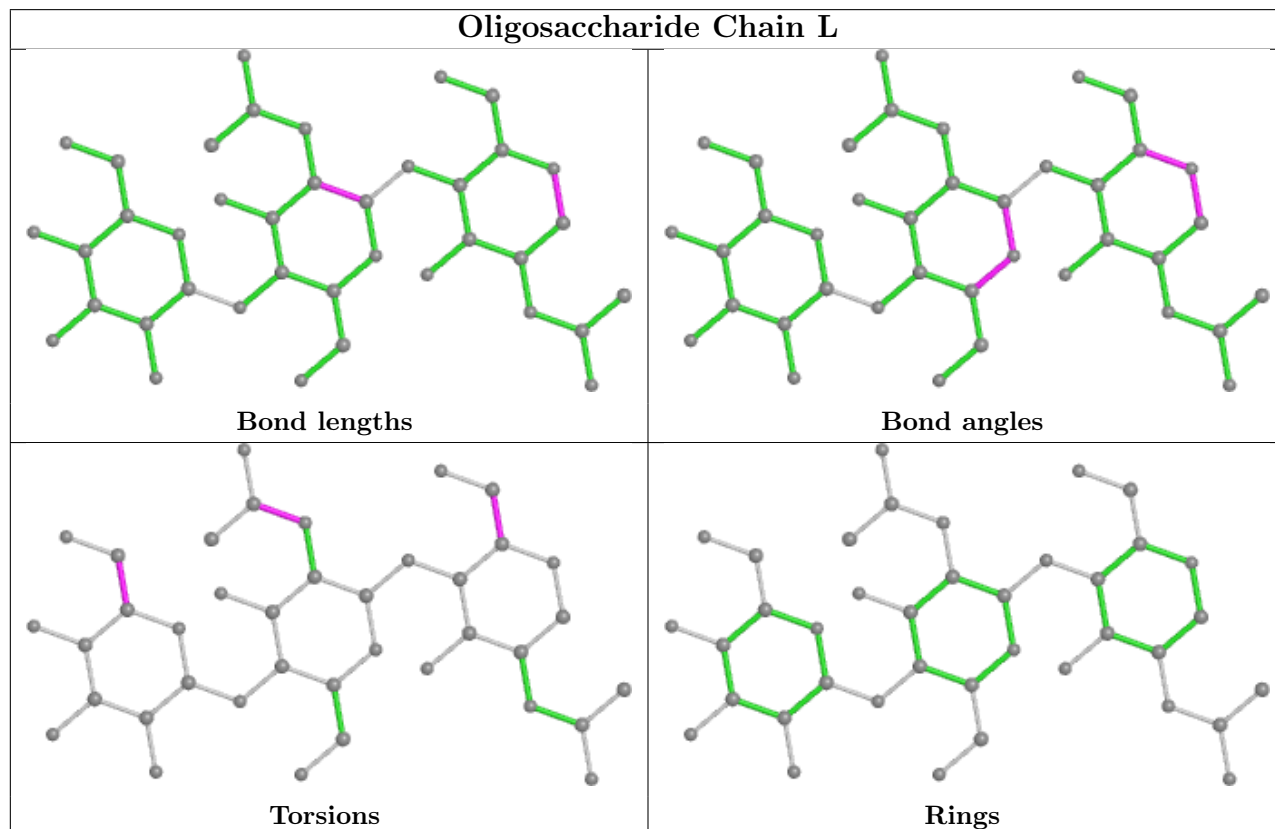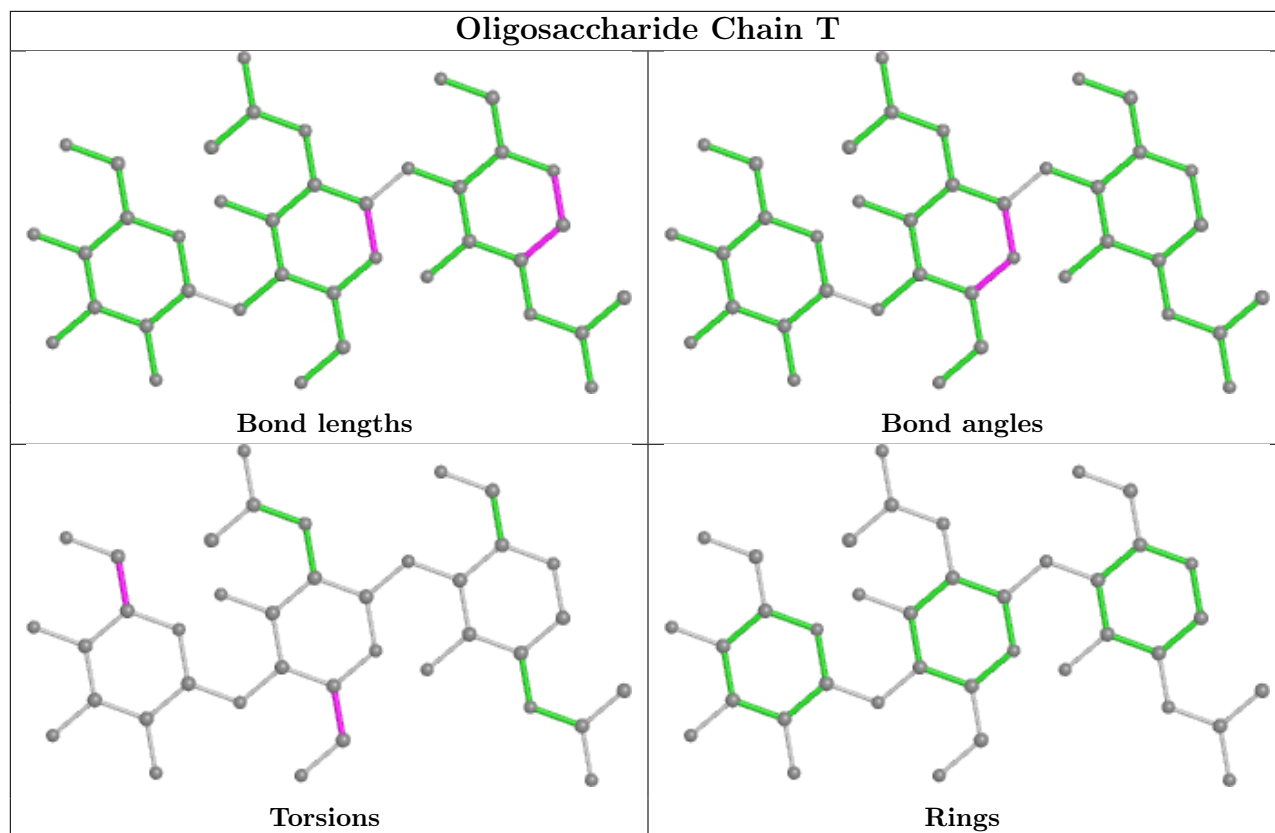
5.6 Ligand geometry ⓘ

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 (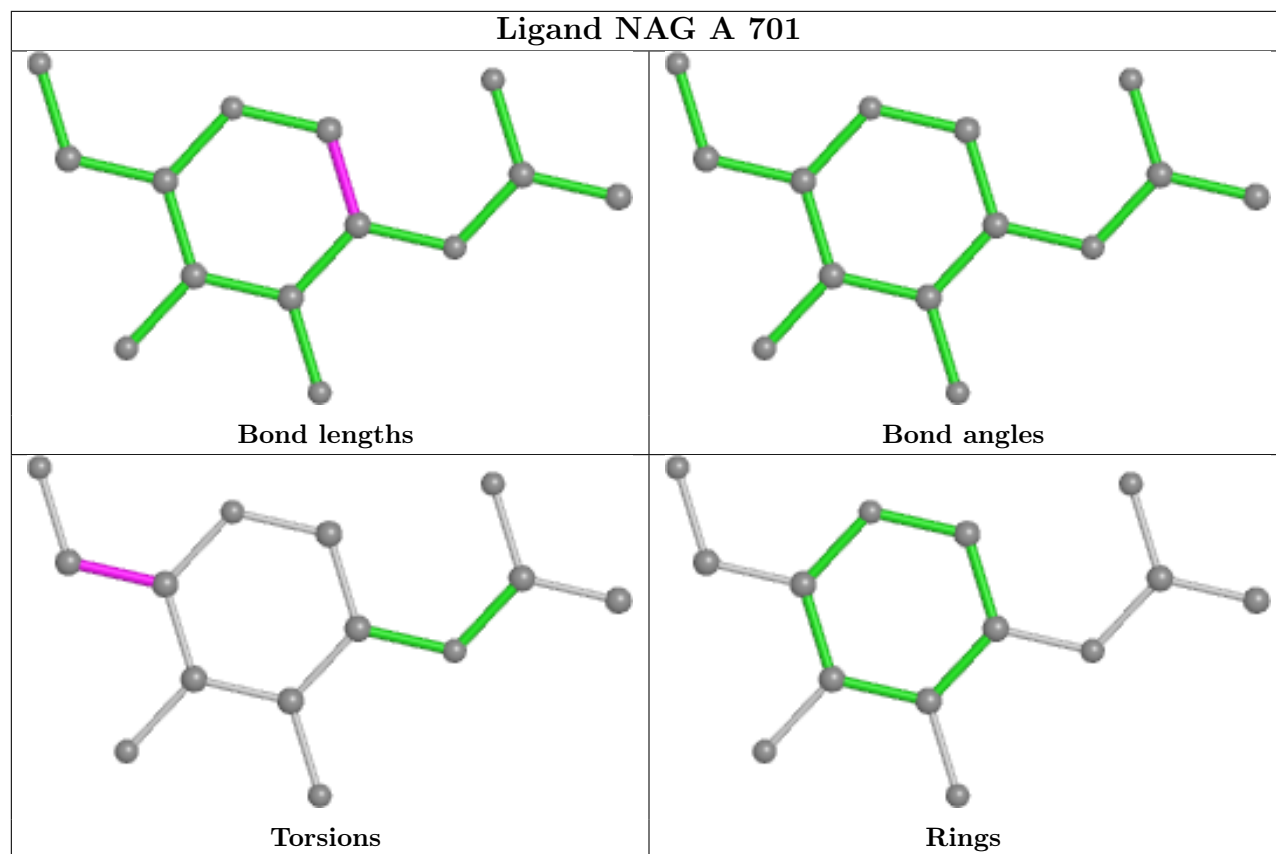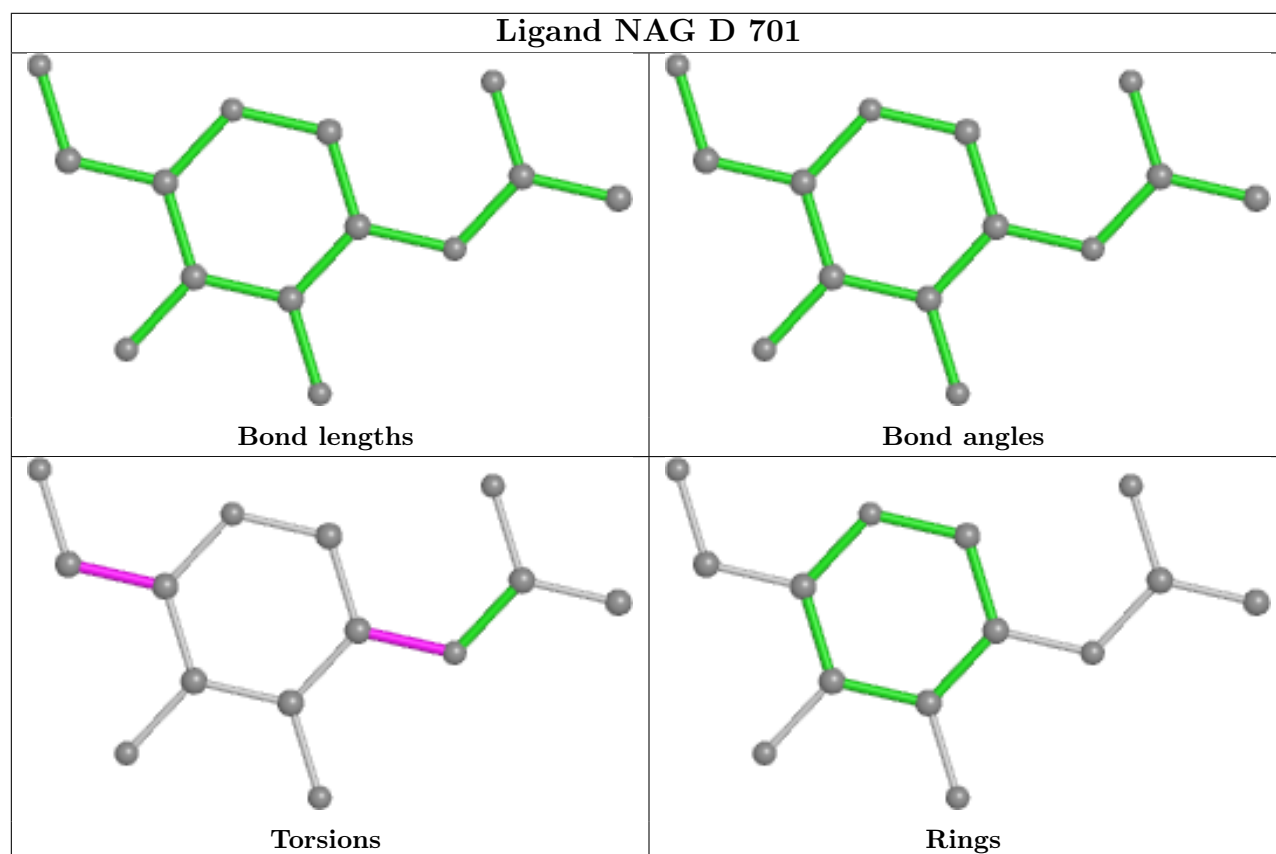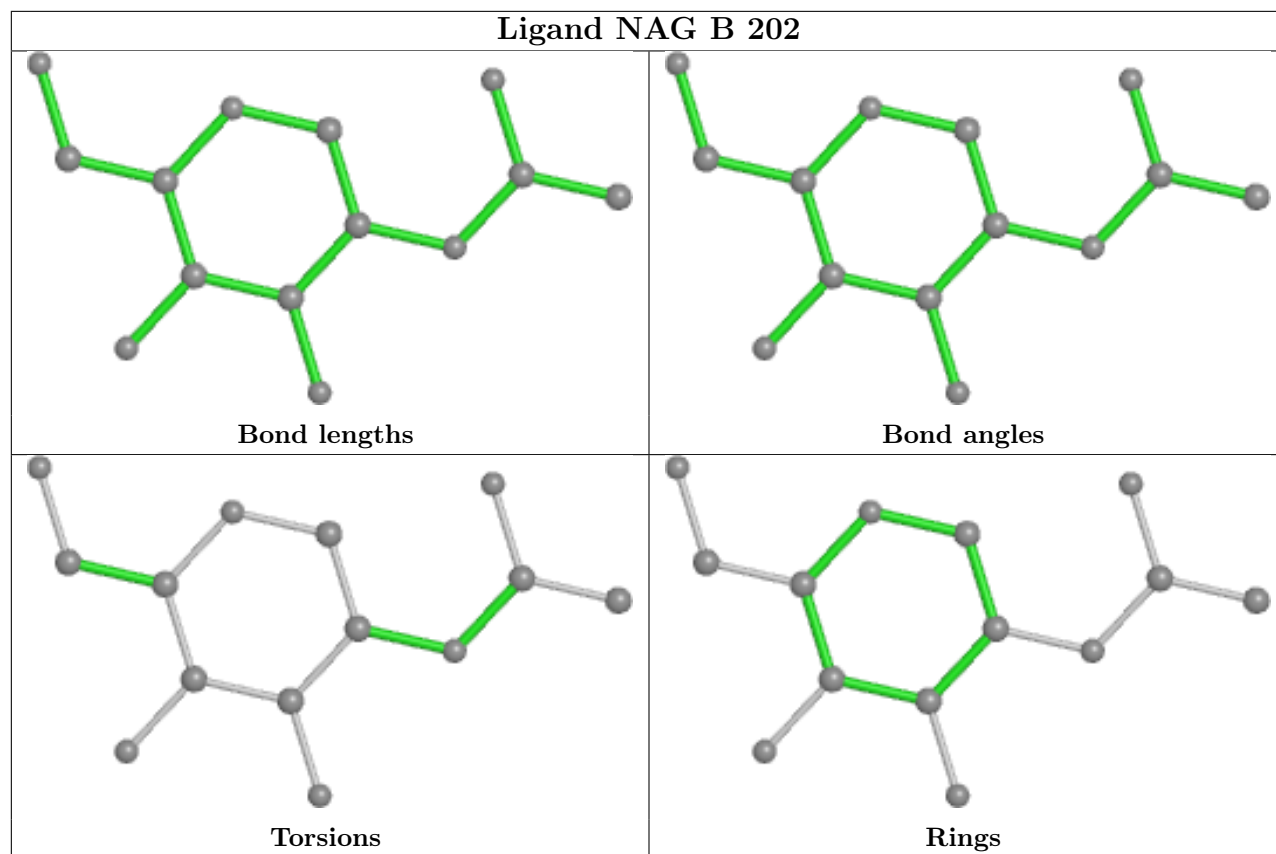or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
7	NAG	C	302	3	14,14,15	0.40	0	17,19,21	0.46	0
7	NAG	C	301	3	14,14,15	0.23	0	17,19,21	0.42	0
7	NAG	B	201	2	14,14,15	0.47	0	17,19,21	0.45	0
7	NAG	A	701	1	14,14,15	0.71	1 (7%)	17,19,21	0.61	0
7	NAG	E	202	2	14,14,15	0.36	0	17,19,21	0.61	0
7	NAG	B	202	2	14,14,15	0.33	0	17,19,21	0.50	0
7	NAG	D	701	1	14,14,15	0.48	0	17,19,21	0.46	0
7	NAG	E	201	2	14,14,15	0.72	1 (7%)	17,19,21	0.76	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	C	302	3	-	2/6/23/26	0/1/1/1
7	NAG	C	301	3	-	0/6/23/26	0/1/1/1
7	NAG	B	201	2	-	2/6/23/26	0/1/1/1
7	NAG	A	701	1	-	2/6/23/26	0/1/1/1
7	NAG	E	202	2	-	3/6/23/26	0/1/1/1
7	NAG	B	202	2	-	0/6/23/26	0/1/1/1
7	NAG	D	701	1	-	4/6/23/26	0/1/1/1
7	NAG	E	201	2	-	0/6/23/26	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	2.48	1.56	1.52
7	E	201	NAG	O5-C1	-2.32	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 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	C	302	NAG	1	0
7	E	202	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
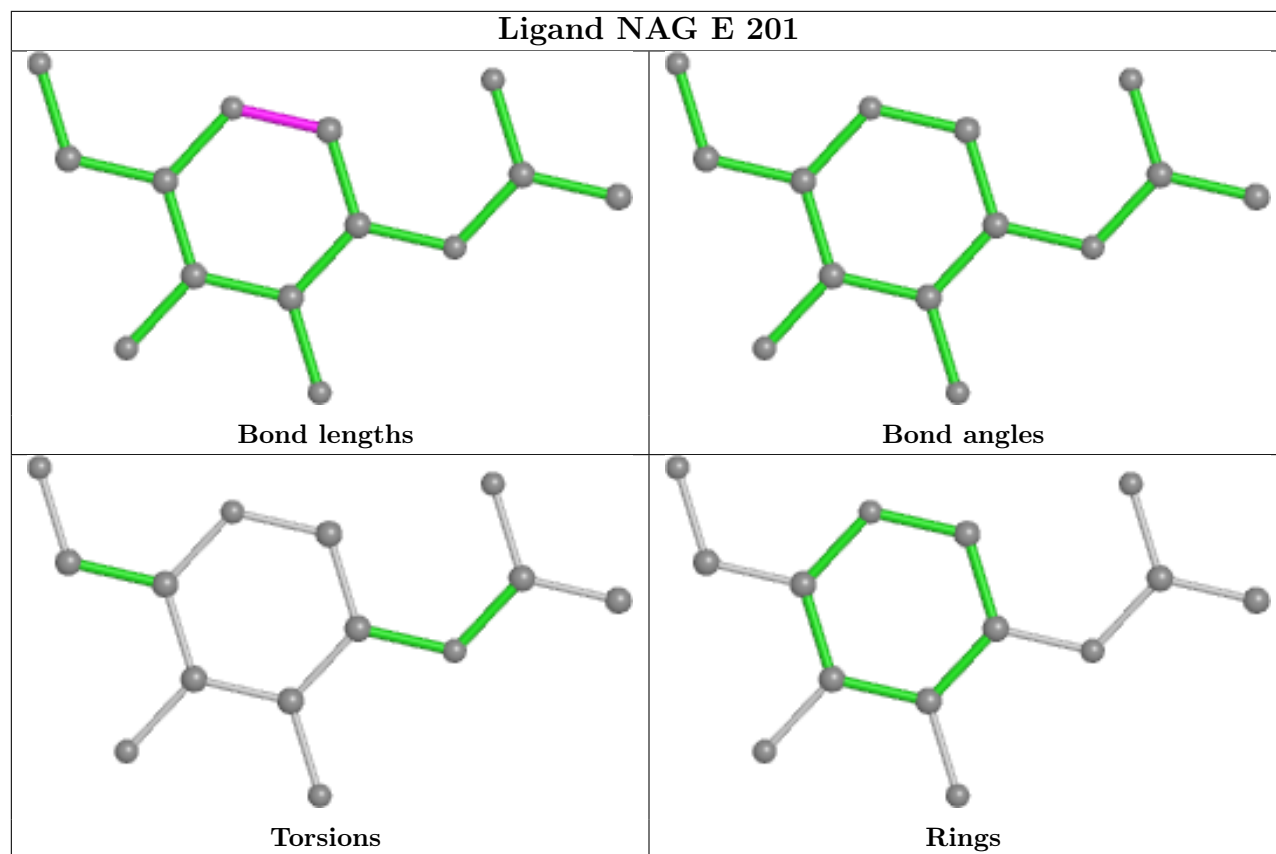
also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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 C 302

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG E 202

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG B 202

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG D 701

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG E 201

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	658/658 (100%)	0.44	19 (2%)	51	54	74, 108, 172, 256	0
1	D	654/658 (99%)	0.69	79 (12%)	4	4	87, 150, 228, 313	0
2	B	107/112 (95%)	0.47	7 (6%)	18	21	91, 136, 213, 247	0
2	E	92/112 (82%)	0.76	18 (19%)	1	1	111, 169, 216, 276	0
3	C	180/191 (94%)	0.52	21 (11%)	4	5	87, 128, 173, 231	0
3	F	178/191 (93%)	0.79	33 (18%)	1	1	105, 145, 196, 238	0
4	G	204/213 (95%)	0.71	32 (15%)	2	2	121, 165, 224, 284	0
4	I	204/213 (95%)	1.08	59 (28%)	0	0	134, 190, 273, 301	0
5	H	210/234 (89%)	0.61	32 (15%)	2	2	123, 167, 230, 290	0
5	J	212/234 (90%)	1.05	53 (25%)	0	0	122, 179, 247, 282	0
All	All	2699/2816 (95%)	0.67	353 (13%)	3	4	74, 148, 228, 313	0

The worst 5 of 353 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	17	ALA	9.0
4	I	174	SER	7.0
3	F	140	TYR	6.5
5	J	187	SER	5.9
4	G	186	SER	5.8

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

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
6	NAG	L	2	14/15	0.71	0.36	167,188,203,222	0
6	BMA	T	3	11/12	0.75	0.19	180,201,228,233	0
6	NAG	L	1	14/15	0.86	0.23	121,132,170,182	0
6	NAG	T	2	14/15	0.88	0.24	160,168,194,214	0
6	BMA	L	3	11/12	0.88	0.20	161,177,193,197	0
6	NAG	T	1	14/15	0.93	0.20	123,137,160,173	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 L:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
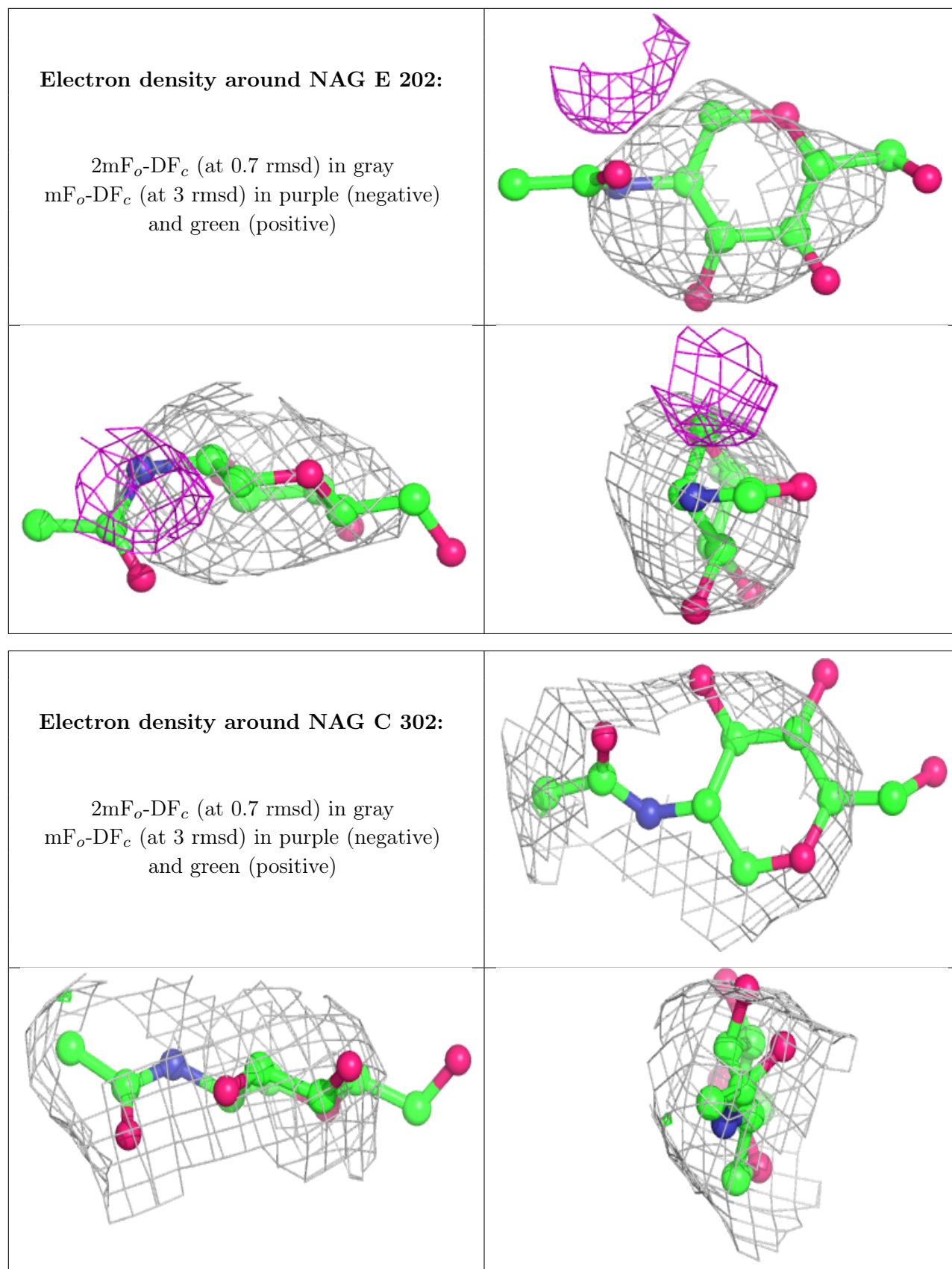$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
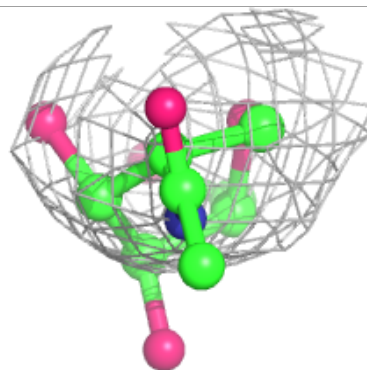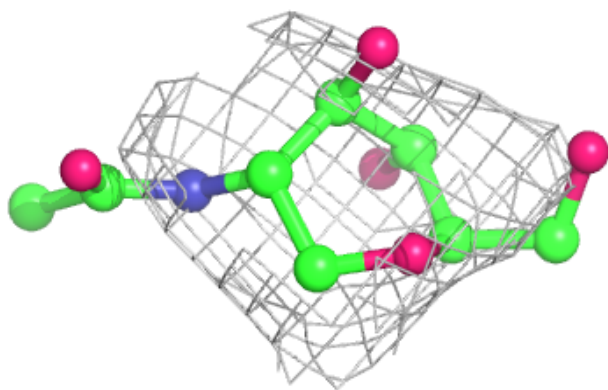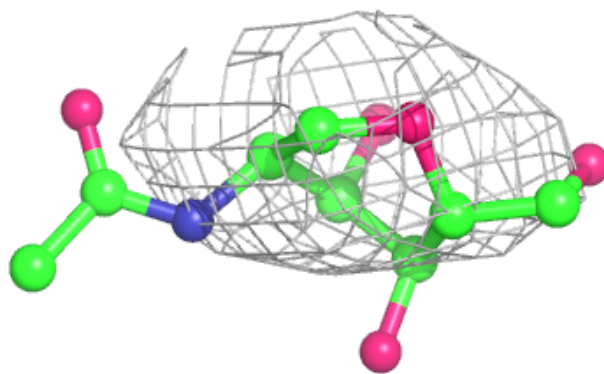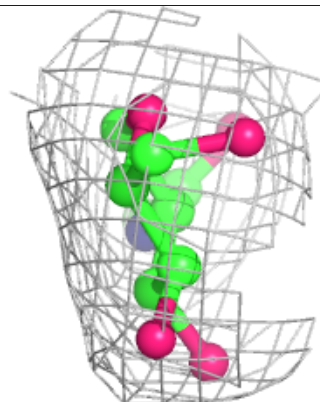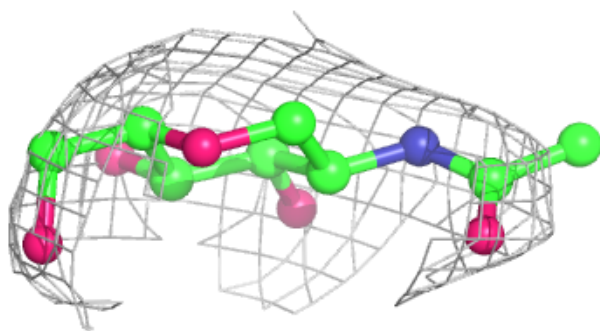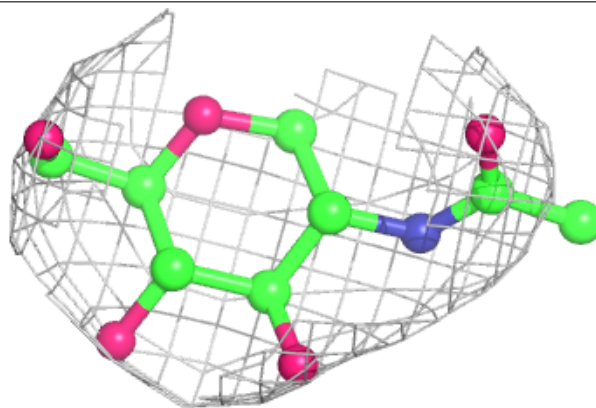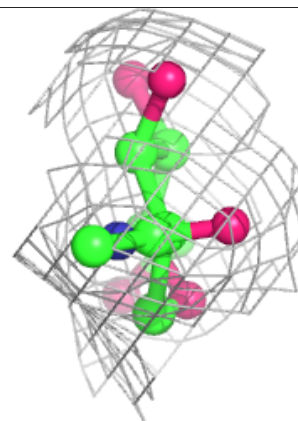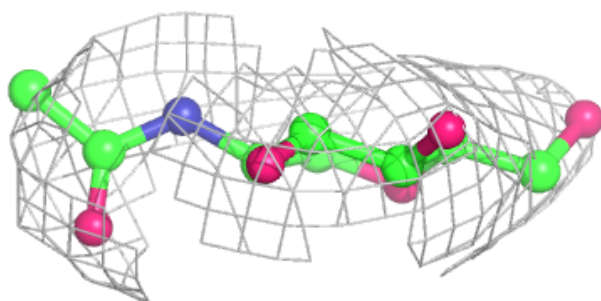
Electron density around Chain T:

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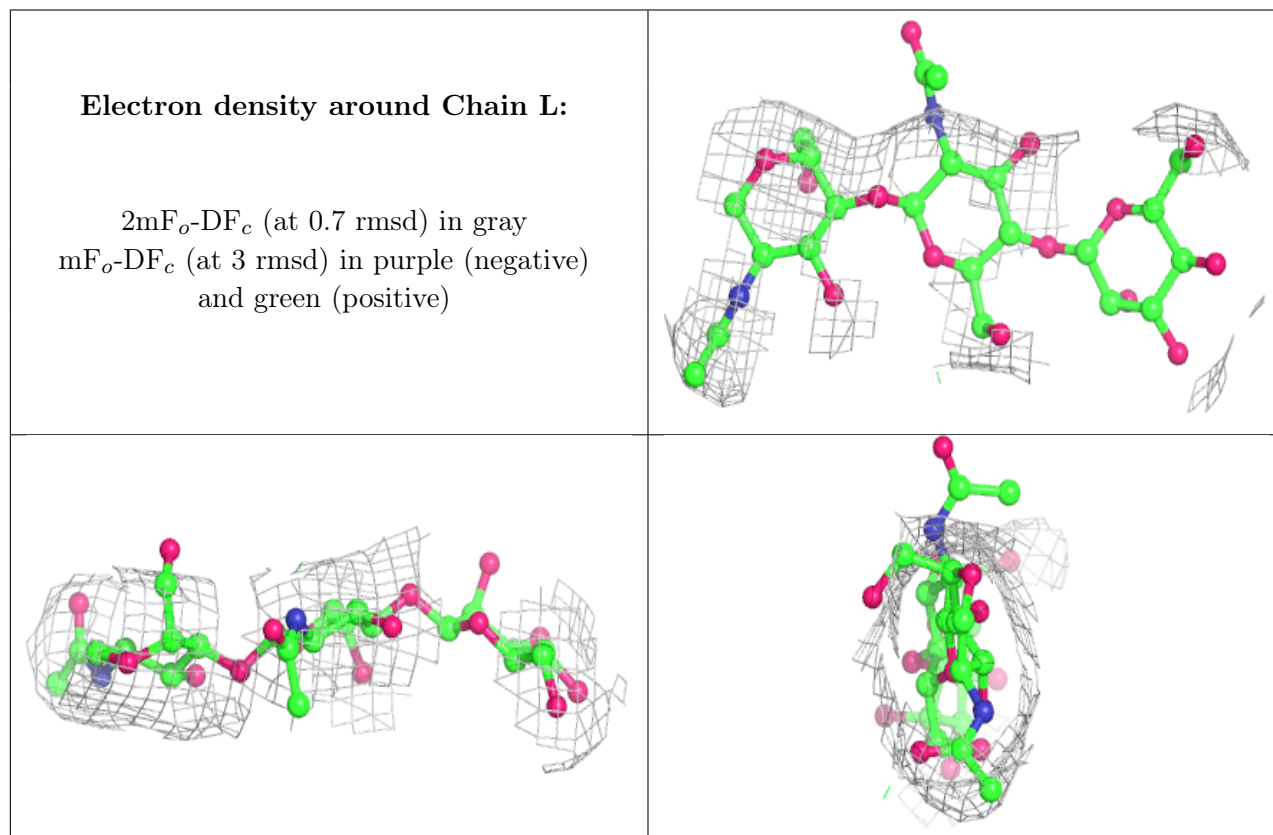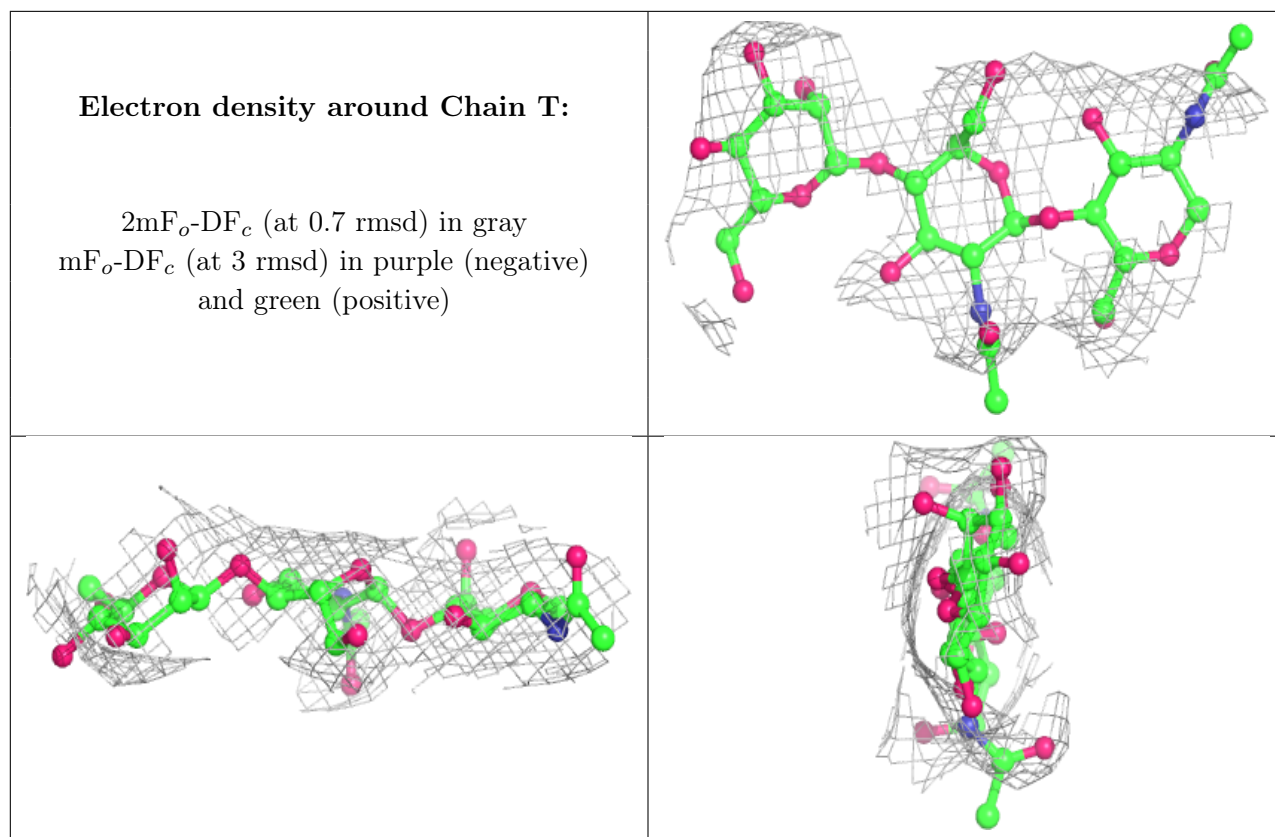
6.4　Ligands (i)

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	D	701	14/15	0.75	0.20	184,200,209,211	0
7	NAG	C	301	14/15	0.78	0.27	208,222,229,232	0
7	NAG	E	202	14/15	0.78	0.26	179,198,221,225	0
7	NAG	C	302	14/15	0.82	0.21	189,243,247,249	0
7	NAG	E	201	14/15	0.84	0.58	201,211,225,227	0
7	NAG	B	202	14/15	0.86	0.19	150,168,181,202	0
7	NAG	A	701	14/15	0.89	0.16	154,167,185,199	0
7	NAG	B	201	14/15	0.91	0.30	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 D 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
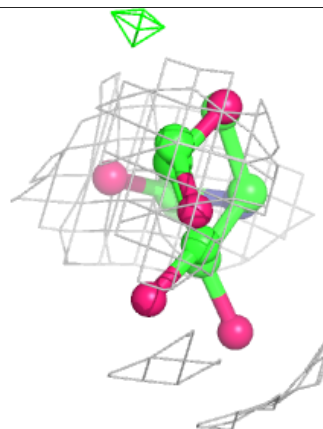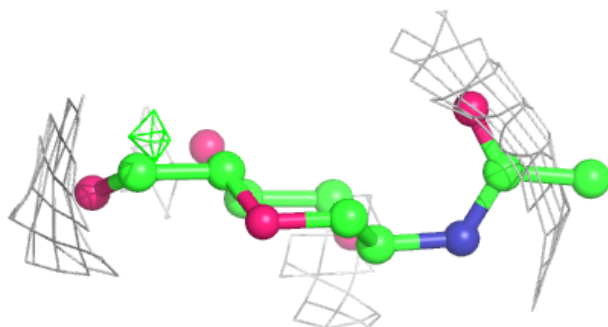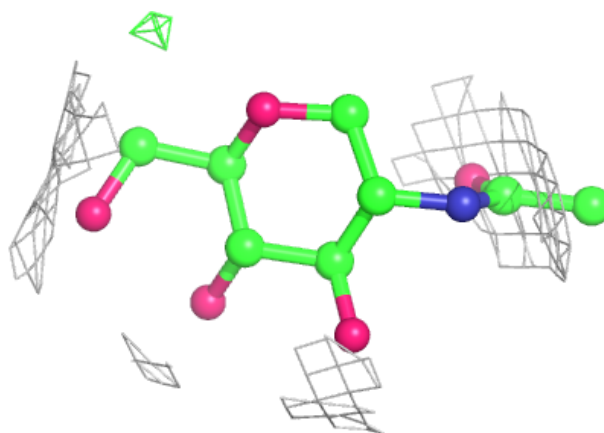
Electron density around NAG C 301:

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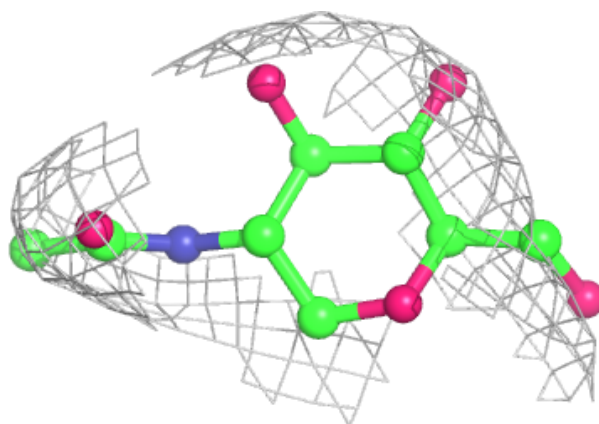$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAG E 202:

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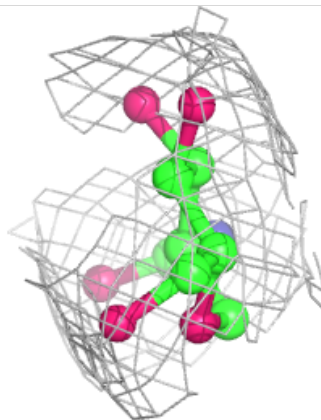and green (positive)

Electron density around NAG C 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
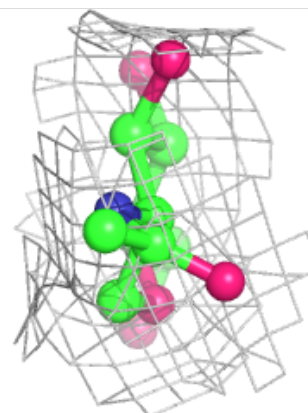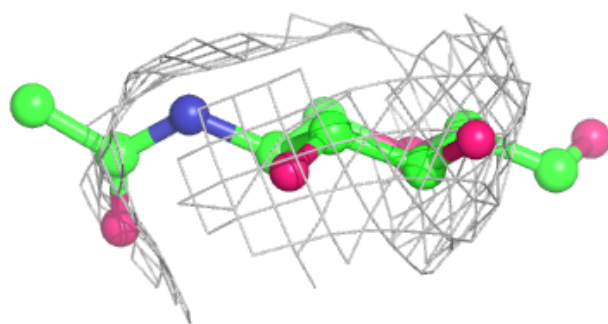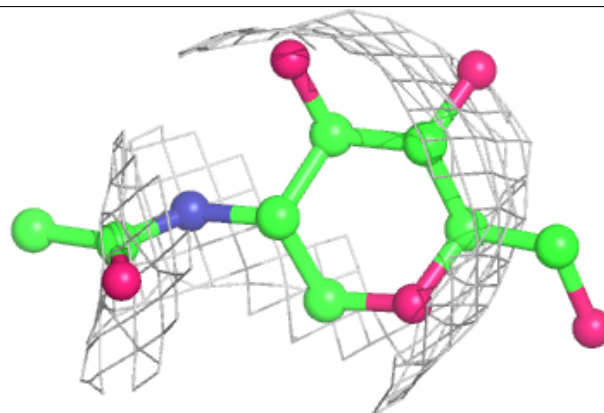
Electron density around NAG E 201:

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

Electron density around NAG B 202:

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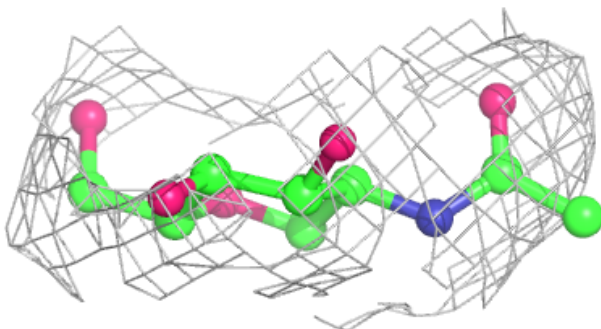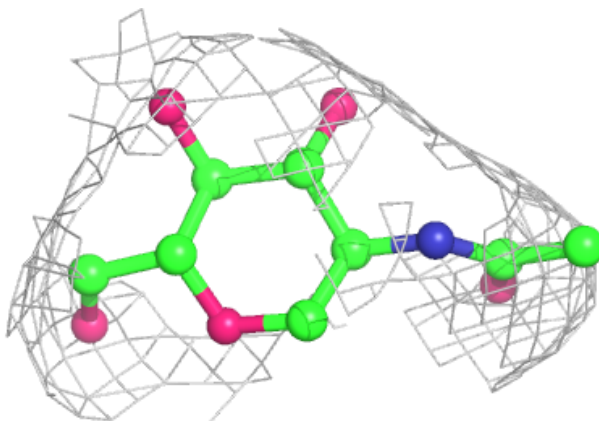mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAG B 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 ⓘ

There are no such residues in this entry.