WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 08:18 PM JST

PDB ID	:	7WBQ
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 Delta variant spike glycoprotein in complex with its receptor human ACE2
Authors	:	Qi, J.; Han, P.
Deposited on	:	2021-12-17
Resolution	:	3.34 Å(reported)

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

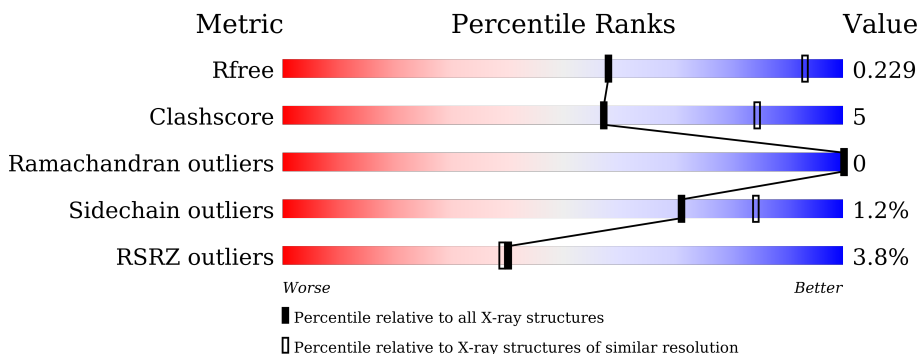|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.34 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		0.229
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		3.8%

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	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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	596	2% 87% 13%
1	C	596	3% 87% 13%
2	B	223	9% 75% 12% 13%
2	D	223	4% 76% 11% 13%
3	E	2	50% 50%
3	G	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	F	2	100%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 13025 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total 4862	C 3111	N 805	O 917	S 29	0	0	0
1	C	596	Total 4852	C 3105	N 801	O 917	S 29	0	0	0

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total 1548	C 991	N 261	O 288	S 8	0	0	0
2	D	194	Total 1541	C 986	N 260	O 287	S 8	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	452	ARG	LEU	variant	UNP P0DTC2
B	478	LYS	THR	engineered mutation	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	478	LYS	THR	engineered mutation	UNP P0DTC2

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total 28	C 16	N 2	O 10	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 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).
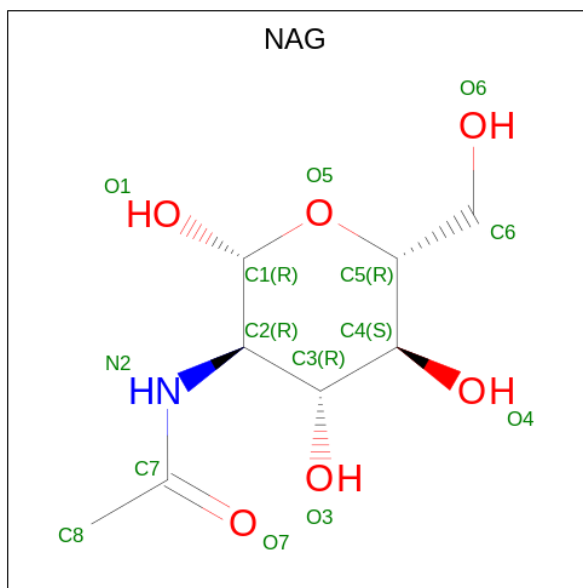
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Zn 1	0	0
6	C	1	Total 1	Zn 1	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: Angiotensin-converting enzyme 2
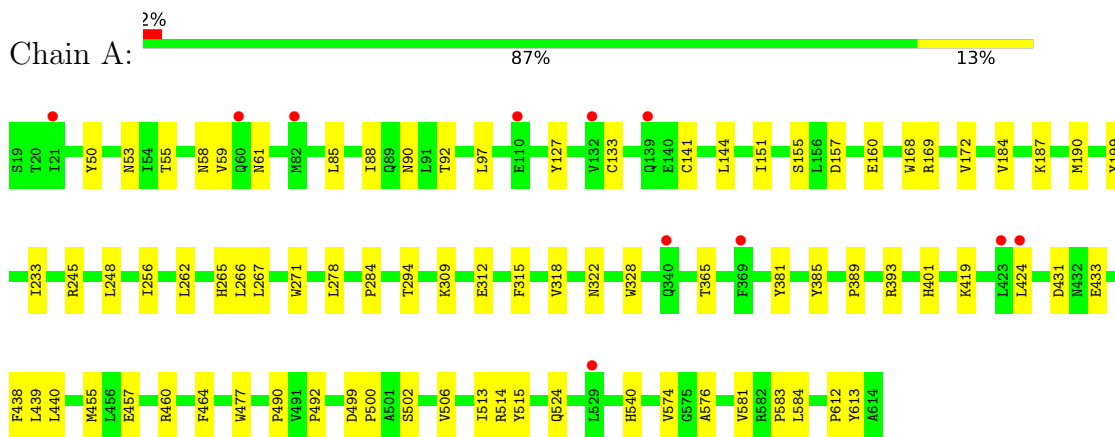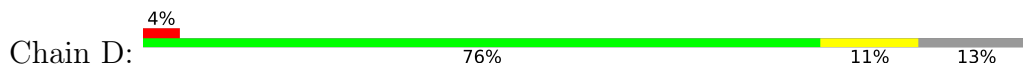
Chain A:

- Molecule 1: Angiotensin-converting enzyme 2

Chain C:

- Molecule 2: Spike protein S1

Chain B:

A435 S438 Y453 F456 Y473 E484 Y495 G502 Q506 P507 Y508 R509 V510 V511 V512 L513 S514 F515 E516 L517 A520 P521 A522 G526 P527 LYS LYS SER THR ASN LEU VAL LYS ASN LYS CYS VAL ASN PHE

• Molecule 2: Spike protein S1

Chain D:

4%

76%   11%   13%

ARG VAL GLN PRO THR GLU SER ILE VAL ARG PHE PRO ASN ILE T333 N334 F338 V350 V362 A363 D364 Y365 S366 V367 L368 Y369 N370 F377 K378 C379 V382 S383 P384 T385 K386 S399 F400 V401 E406 N422 N439 S443 G447 Y453 R454 L455 F456

Y489 Q498 G502 Q506 R509 V510 A520 P521 G526 PRO LYS LYS SER THR ASN LEU VAL LYS ASN LYS CYS VAL ASN PHE

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

Chain E: 50%   50%

NAG1 NAG2

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

Chain G: 50%   50%

NAG1 NAG2
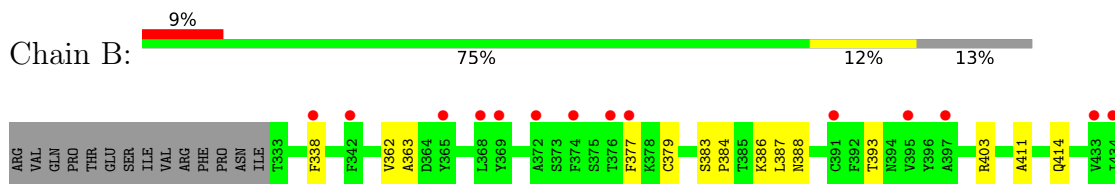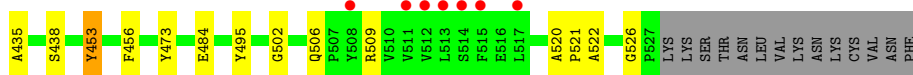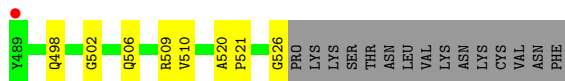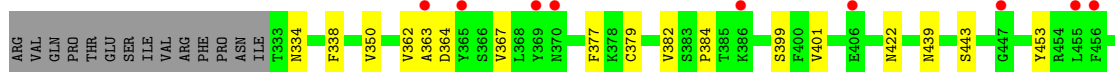
• Molecule 4: beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

NAG1 FUL2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.77Å 143.65Å 106.41Å 90.00° 95.29° 90.00°	Depositor
Resolution (Å)	44.70 – 3.34 49.71 – 3.34	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.70-3.34) 88.7 (49.71-3.34)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	0.30 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.19rc3_4028	Depositor
R, R_{free}	0.197 , 0.226 0.200 , 0.229	Depositor DCC
R_{free} test set	2000 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	88.8	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.8	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13025	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.26	0/4999	0.46	0/6792
1	C	0.26	0/4989	0.46	0/6781
2	B	0.27	0/1592	0.50	0/2165
2	D	0.27	0/1584	0.51	0/2153
All	All	0.26	0/13164	0.47	0/17891

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 ⓘ

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	4862	0	4634	48	0
1	C	4852	0	4611	47	0
2	B	1548	0	1467	17	0
2	D	1541	0	1456	12	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
4	F	24	0	22	1	0
5	A	56	0	52	0	0
5	C	70	0	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	14	0	13	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
All	All	13025	0	12370	124	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 5.

The worst 5 of 124 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:C:198:ASP:OD2	1:C:201:ASP:N	2.10	0.84
1:C:261:CYS:HB2	1:C:488:VAL:HB	1.70	0.72
1:A:438:PHE:CD2	1:A:540:HIS:HE1	2.08	0.72
1:A:438:PHE:CD2	1:A:540:HIS:CE1	2.80	0.69
1:C:132:VAL:HG11	1:C:167:SER:HB3	1.76	0.68

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	594/596 (100%)	578 (97%)	16 (3%)	0	100	100
1	C	594/596 (100%)	575 (97%)	19 (3%)	0	100	100
2	B	193/223 (86%)	182 (94%)	11 (6%)	0	100	100
2	D	192/223 (86%)	183 (95%)	9 (5%)	0	100	100
All	All	1573/1638 (96%)	1518 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	526/526 (100%)	520 (99%)	6 (1%)	73	86
1	C	524/526 (100%)	518 (99%)	6 (1%)	73	86
2	B	168/196 (86%)	166 (99%)	2 (1%)	71	84
2	D	167/196 (85%)	164 (98%)	3 (2%)	59	79
All	All	1385/1444 (96%)	1368 (99%)	17 (1%)	71	84

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	334	ASN
2	D	498[A]	GLN
2	B	453	TYR
1	C	133	CYS
1	C	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	540	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	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.43	0	17,19,21	1.08	2 (11%)
3	NAG	E	2	3	14,14,15	0.41	0	17,19,21	0.67	0
4	NAG	F	1	4,2	14,14,15	0.43	0	17,19,21	1.06	2 (11%)
4	FUL	F	2	4	10,10,11	1.73	2 (20%)	14,14,16	1.00	1 (7%)
3	NAG	G	1	3,1	14,14,15	0.42	0	17,19,21	0.97	1 (5%)
3	NAG	G	2	3	14,14,15	0.43	0	17,19,21	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
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
4	NAG	F	1	4,2	-	2/6/23/26	0/1/1/1
4	FUL	F	2	4	-	-	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	FUL	O5-C1	4.14	1.50	1.43
4	F	2	FUL	C2-C3	-2.44	1.48	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	NAG	C1-O5-C5	3.25	116.59	112.19
3	G	1	NAG	C1-O5-C5	2.72	115.88	112.19
4	F	2	FUL	C1-C2-C3	2.44	112.67	109.67
4	F	1	NAG	C1-O5-C5	2.25	115.24	112.19

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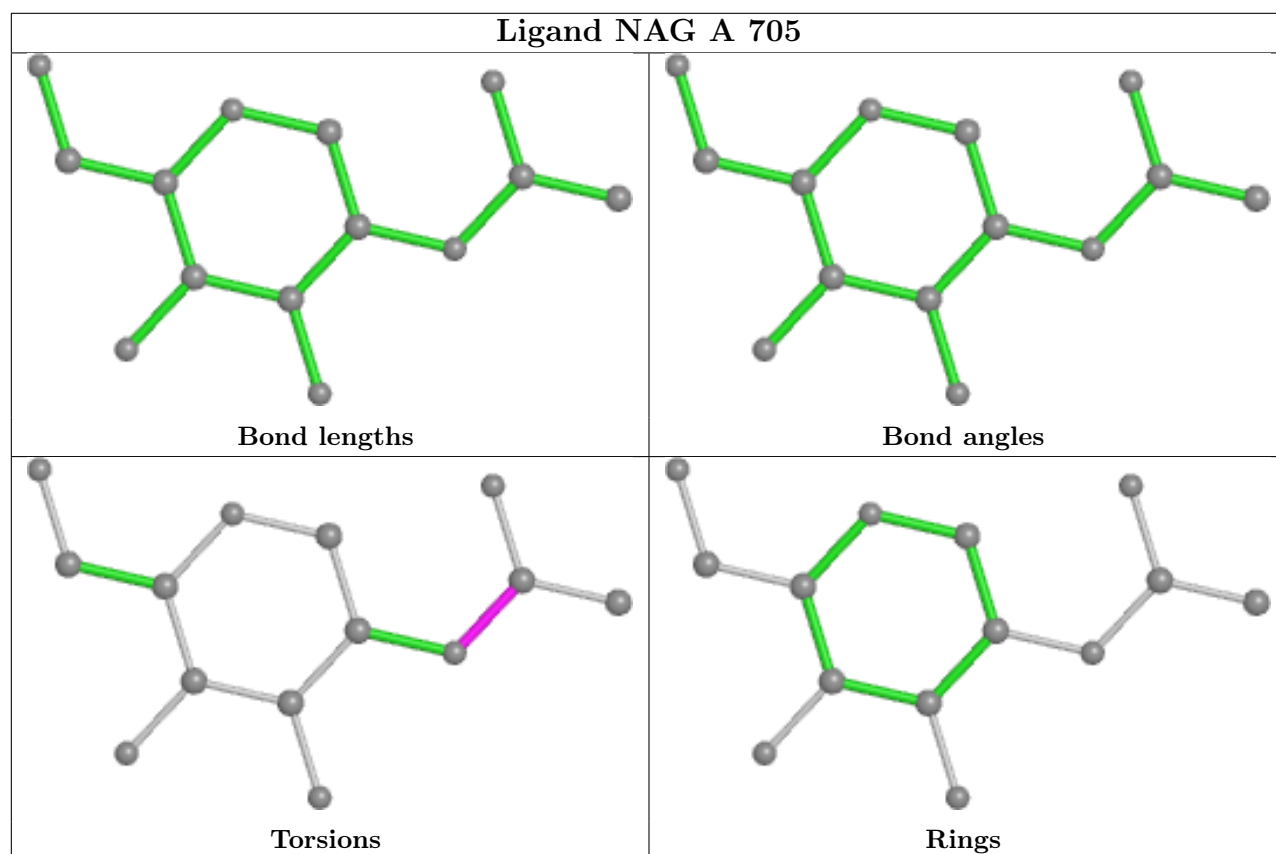| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	NAG	O5-C1-C2	-2.14	107.91	111.29

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

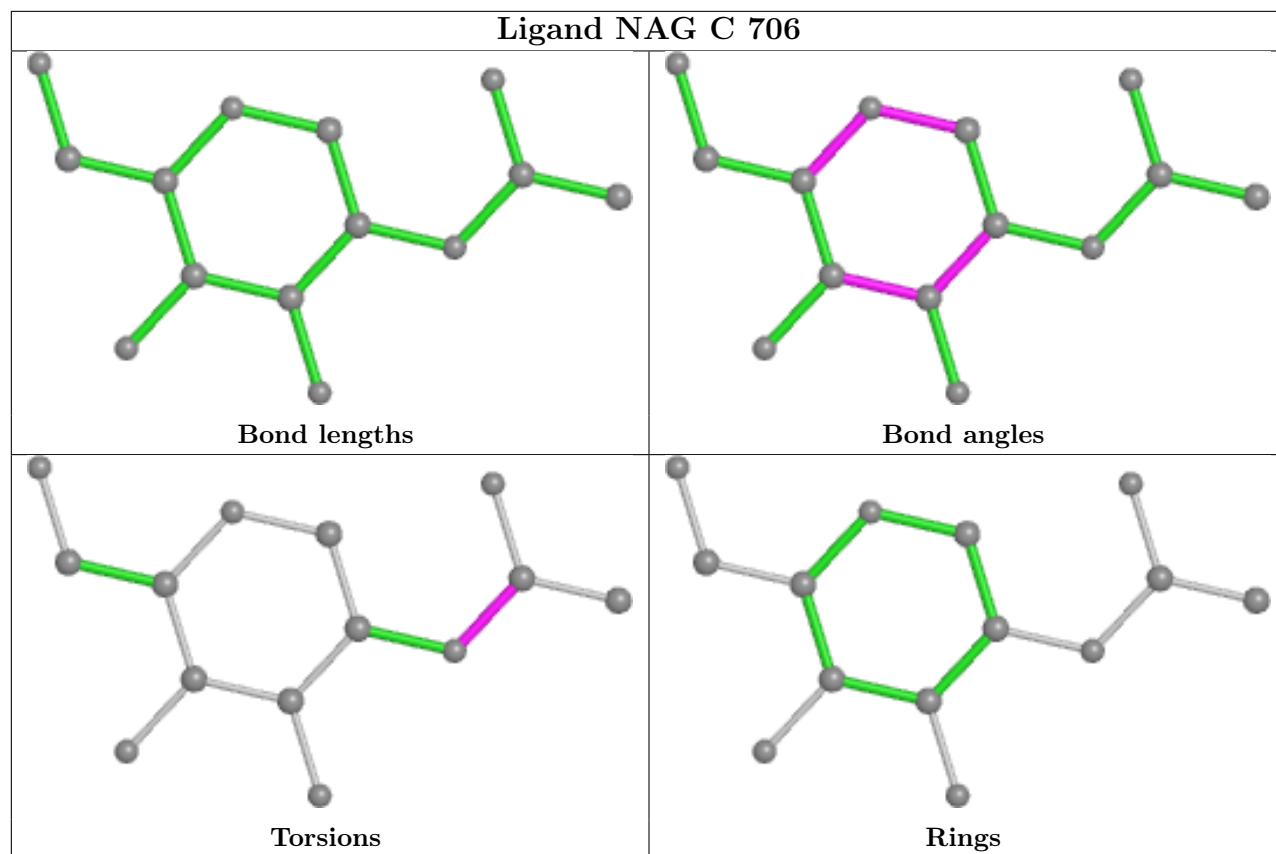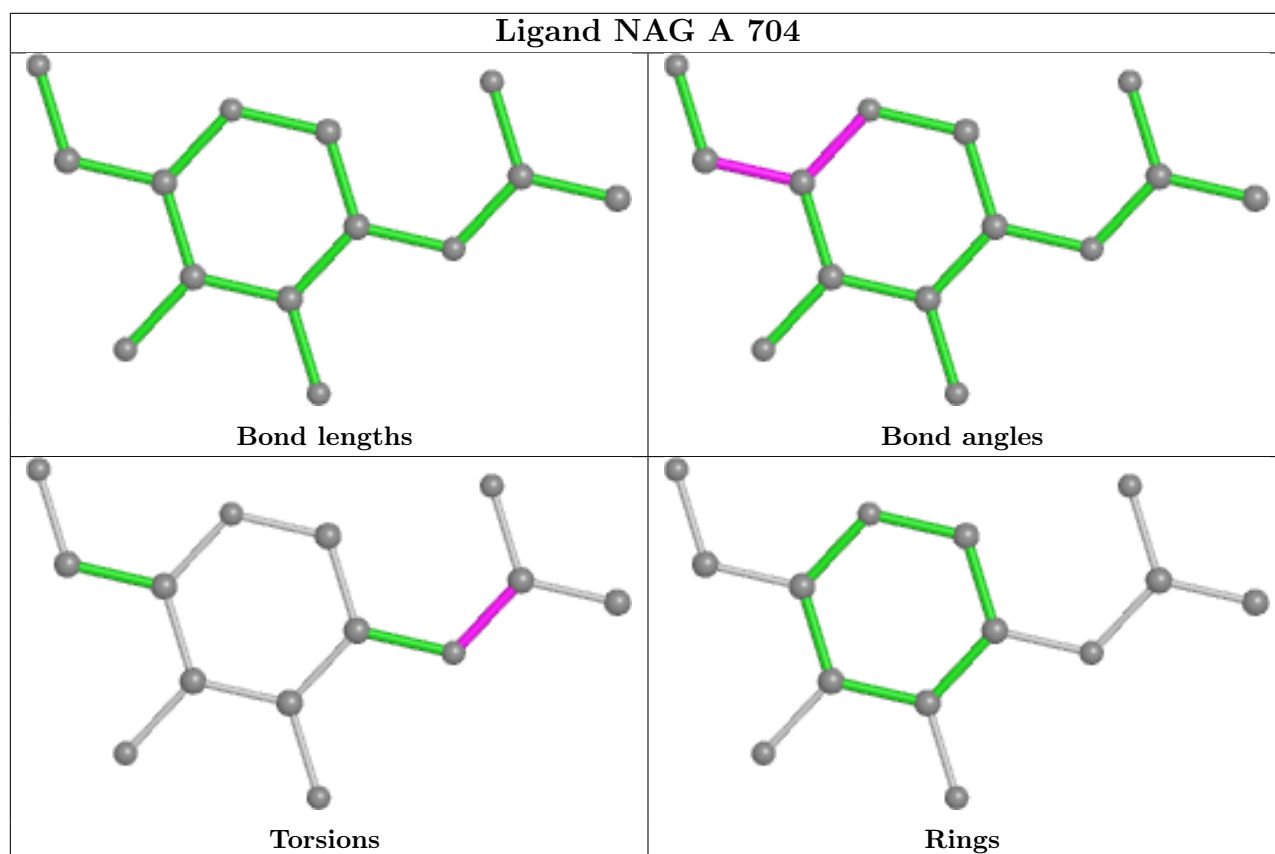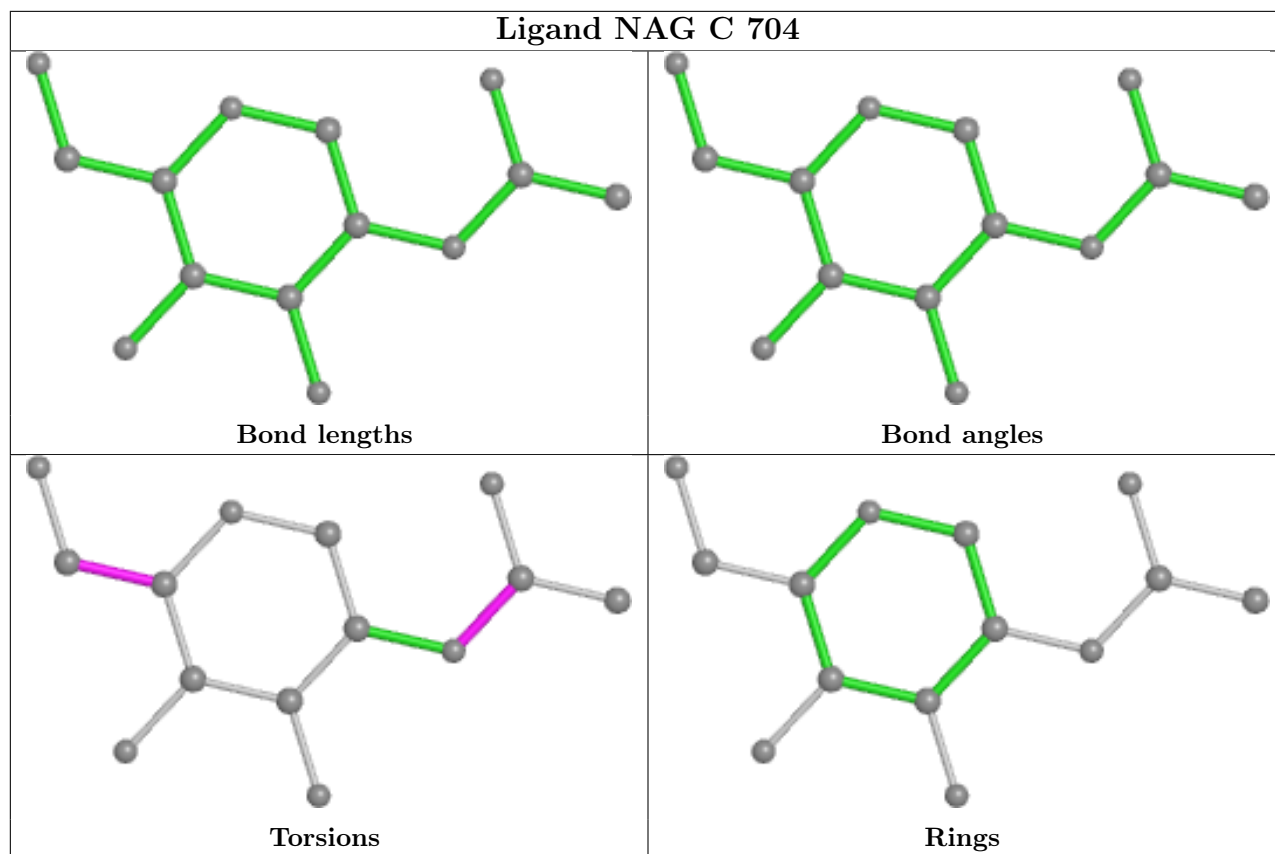| Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

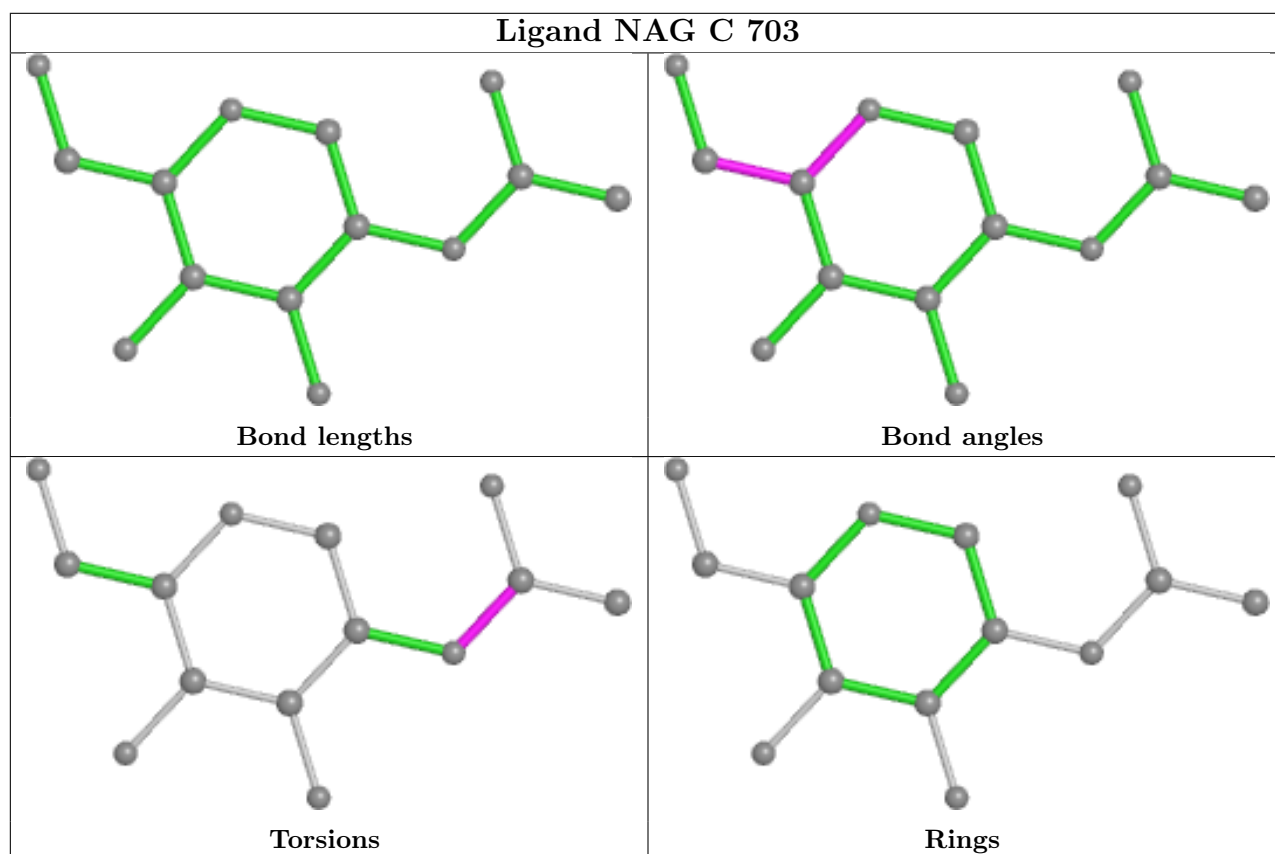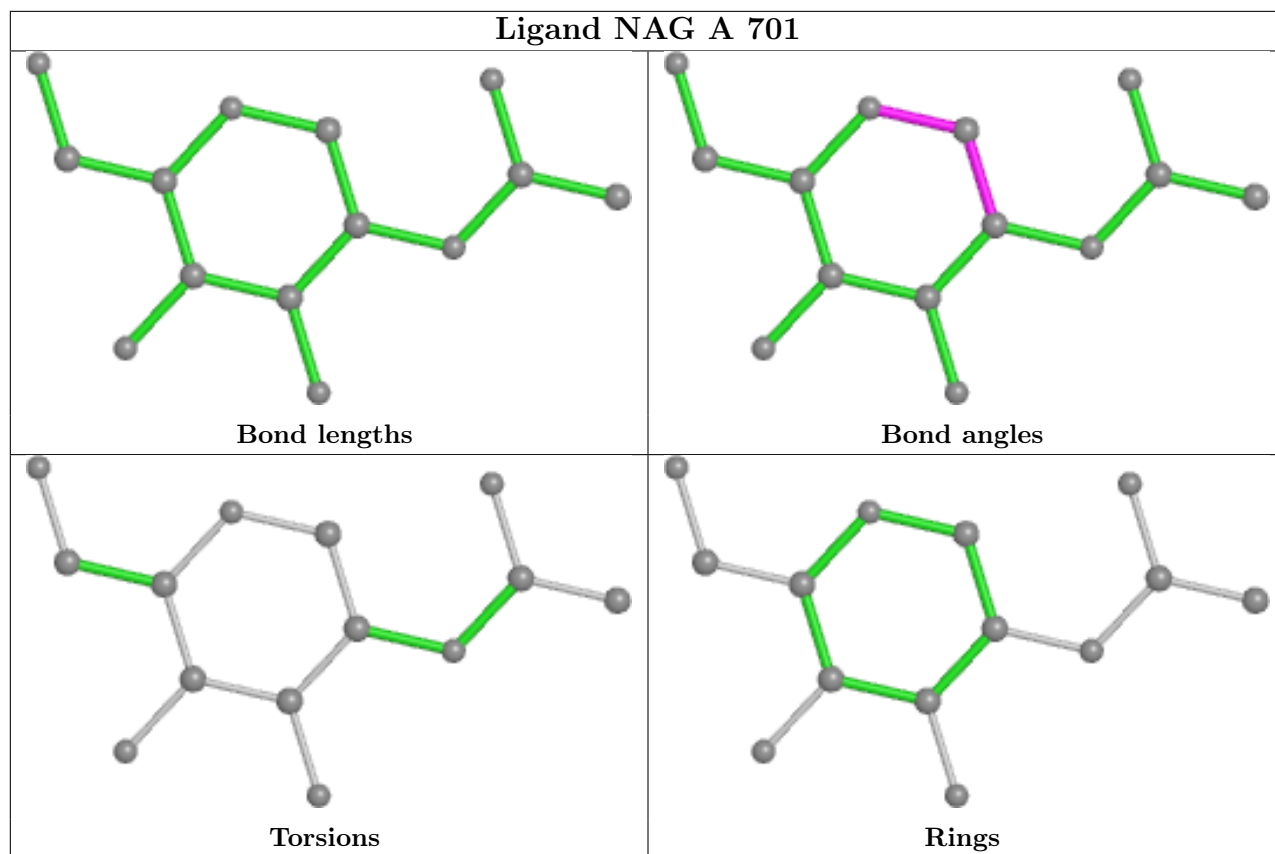| Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0
4	F	2	FUL	1	0

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

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
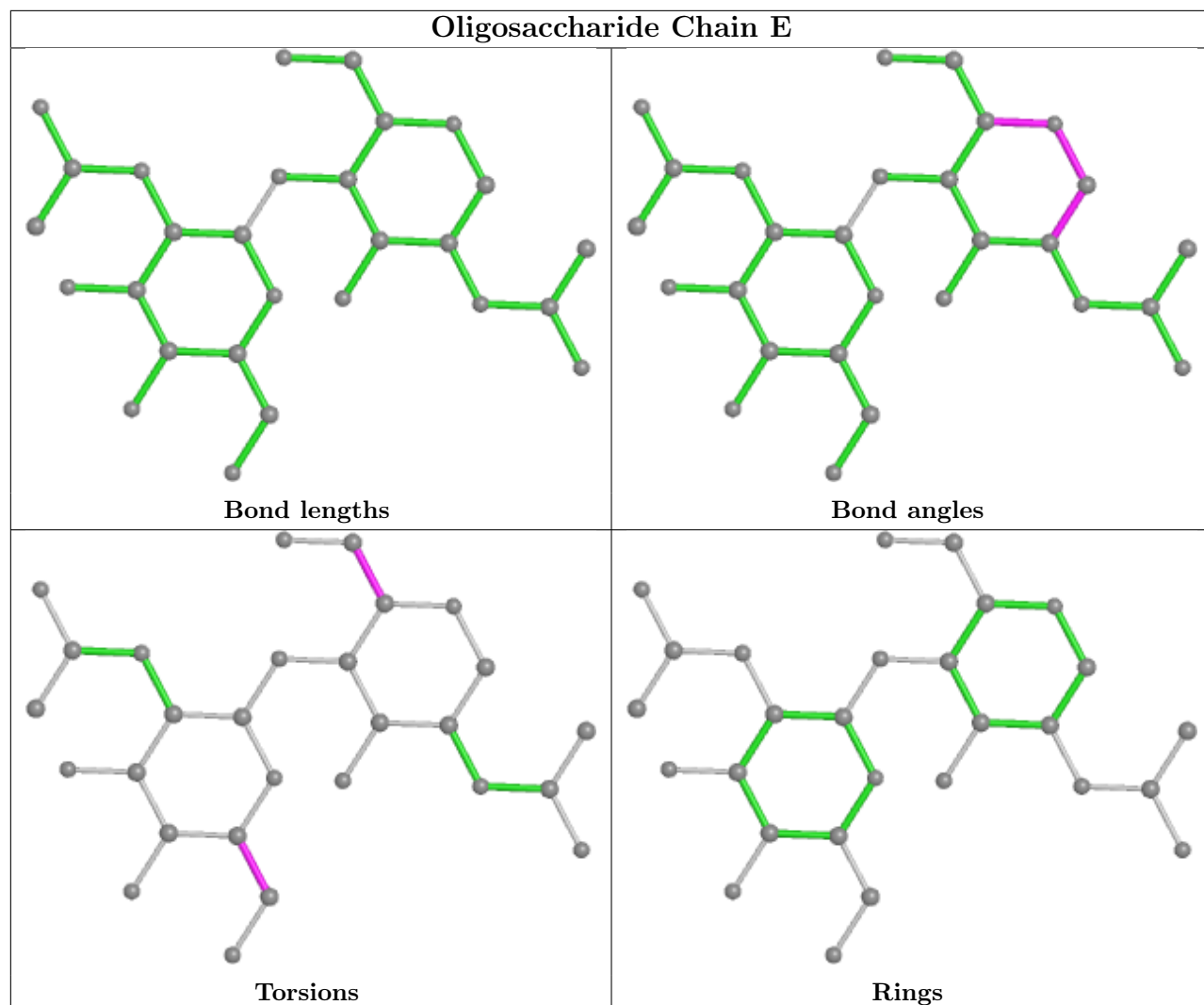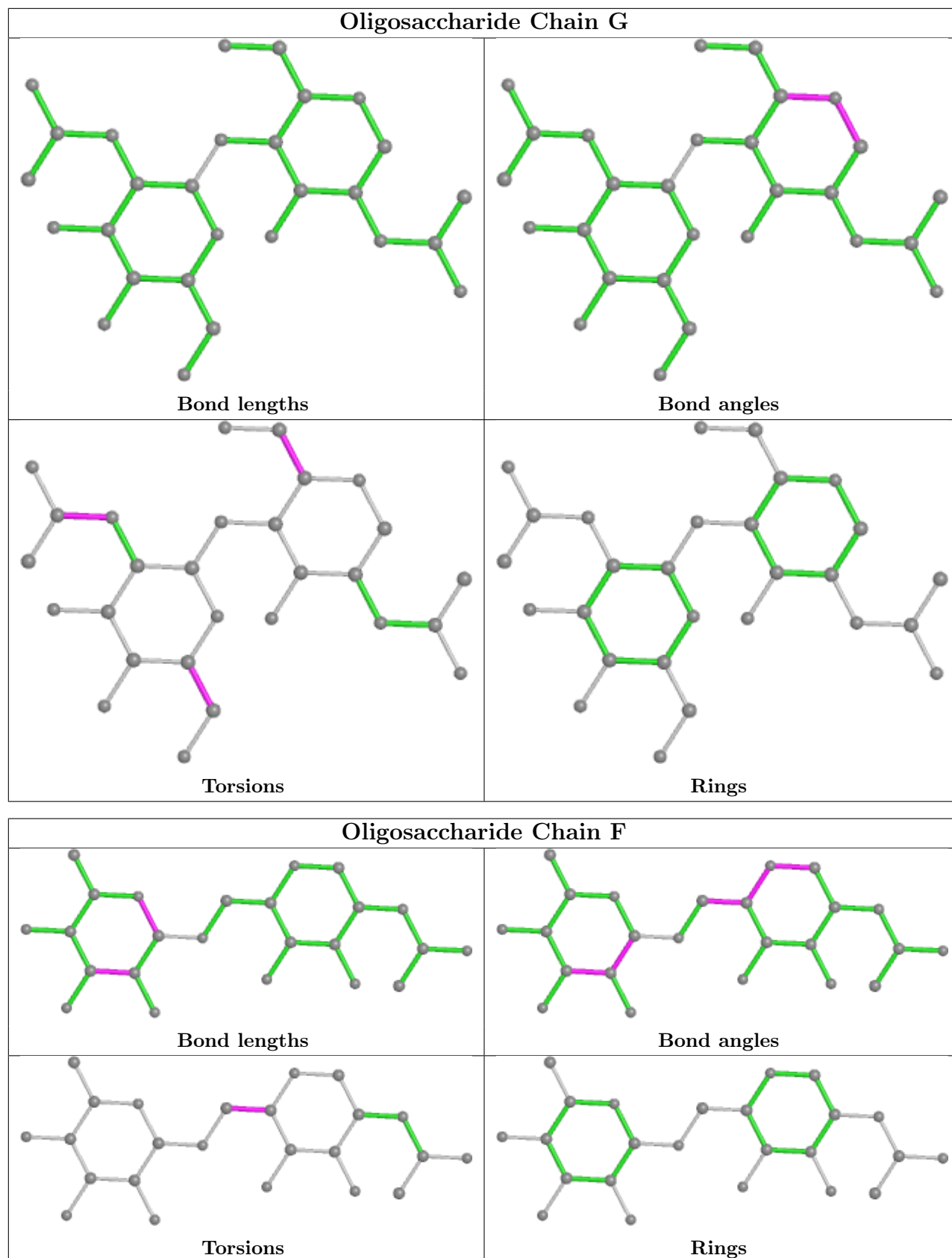
5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
5	NAG	A	703	1	14,14,15	0.37	0	17,19,21	0.61	0
5	NAG	A	705	1	14,14,15	0.33	0	17,19,21	0.63	0
5	NAG	C	706	1	14,14,15	0.32	0	17,19,21	1.05	2 (11%)
5	NAG	C	705	1	14,14,15	0.33	0	17,19,21	0.80	1 (5%)
5	NAG	C	704	1	14,14,15	0.31	0	17,19,21	0.78	0
5	NAG	A	704	1	14,14,15	0.48	0	17,19,21	1.17	1 (5%)
5	NAG	C	701	1	14,14,15	0.34	0	17,19,21	1.09	1 (5%)
5	NAG	D	601	2	14,14,15	0.29	0	17,19,21	0.88	1 (5%)
5	NAG	A	701	1	14,14,15	0.34	0	17,19,21	1.08	1 (5%)
5	NAG	C	703	1	14,14,15	0.38	0	17,19,21	0.96	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
5	NAG	A	703	1	-	2/6/23/26	0/1/1/1
5	NAG	A	705	1	-	2/6/23/26	0/1/1/1
5	NAG	C	706	1	-	2/6/23/26	0/1/1/1
5	NAG	C	705	1	-	3/6/23/26	0/1/1/1
5	NAG	C	704	1	-	3/6/23/26	0/1/1/1
5	NAG	A	704	1	-	1/6/23/26	0/1/1/1
5	NAG	C	701	1	-	2/6/23/26	0/1/1/1
5	NAG	D	601	2	-	4/6/23/26	0/1/1/1
5	NAG	A	701	1	-	0/6/23/26	0/1/1/1
5	NAG	C	703	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	704	NAG	O5-C5-C6	3.37	112.49	107.20
5	C	701	NAG	C1-O5-C5	3.17	116.49	112.19
5	A	701	NAG	O5-C1-C2	-2.81	106.85	111.29
5	C	705	NAG	C1-O5-C5	2.42	115.47	112.19
5	C	703	NAG	O5-C5-C6	2.41	110.98	107.20

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	703	NAG	C8-C7-N2-C2
5	A	703	NAG	O7-C7-N2-C2
5	C	704	NAG	C8-C7-N2-C2
5	C	704	NAG	O7-C7-N2-C2
5	D	601	NAG	C8-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 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 A 703

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 705

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 706

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 705

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 704

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 704

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 701

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG D 601

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG C 703

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(Å^2)	Q<0.9
1	A	596/596 (100%)	0.23	11 (1%)	68	67	73, 109, 158, 215	0
1	C	596/596 (100%)	0.32	18 (3%)	50	50	75, 118, 173, 214	0
2	B	195/223 (87%)	0.53	21 (10%)	5	5	80, 113, 188, 213	0
2	D	194/223 (86%)	0.42	10 (5%)	27	27	89, 127, 177, 200	0
All	All	1581/1638 (96%)	0.32	60 (3%)	40	39	73, 114, 174, 215	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	456	PHE	5.1
2	D	369	TYR	4.3
1	A	139	GLN	3.9
2	D	365	TYR	3.9
2	B	513	LEU	3.8

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   ⓘ

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	E	1	14/15	0.82	0.18	128,134,146,167	0
3	NAG	E	2	14/15	0.83	0.18	148,158,169,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	2	14/15	0.83	0.21	143,156,171,175	0
3	NAG	G	1	14/15	0.85	0.17	97,112,133,136	0
4	NAG	F	1	14/15	0.89	0.11	102,136,151,157	0
4	FUL	F	2	10/11	0.91	0.10	140,160,164,169	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 E:

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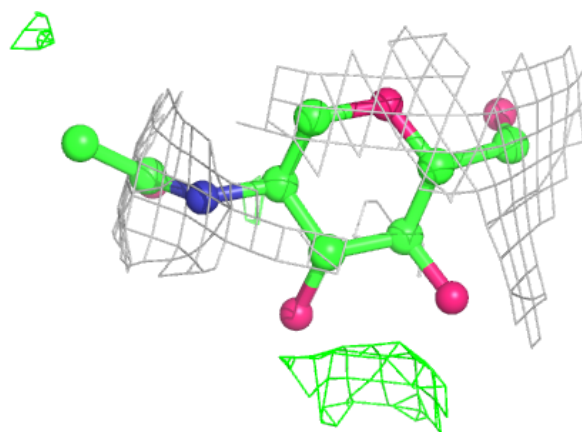and green (positive)
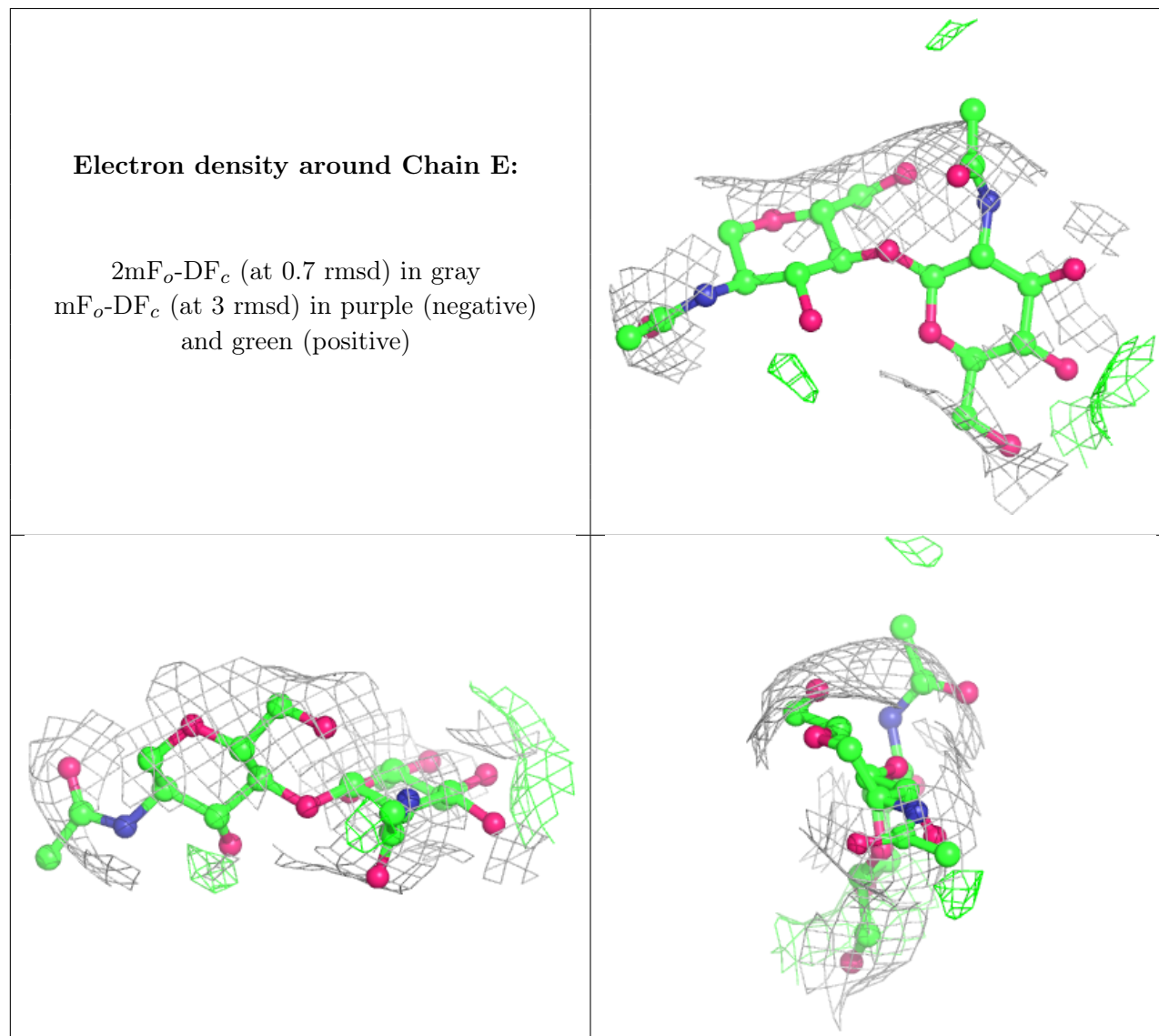
Electron density around Chain G:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
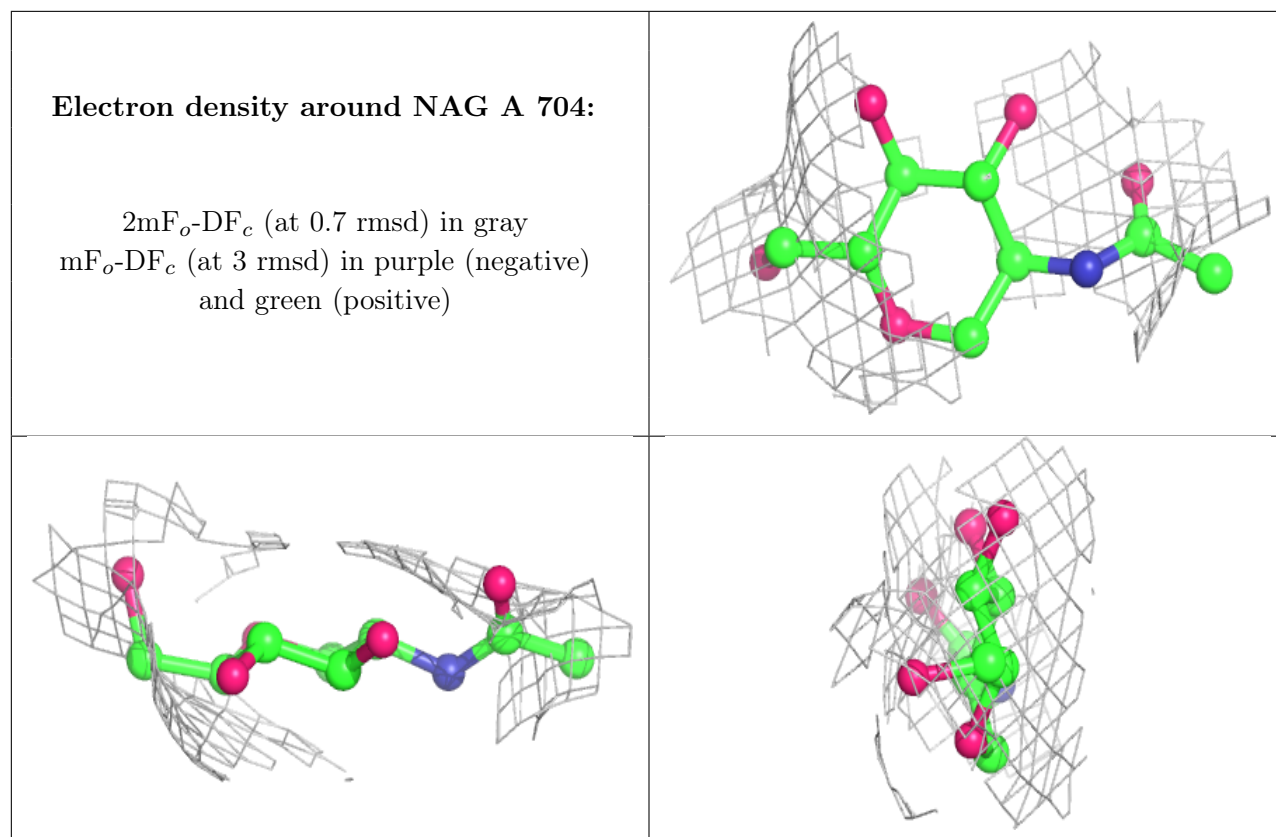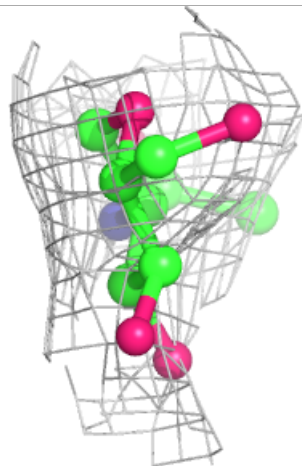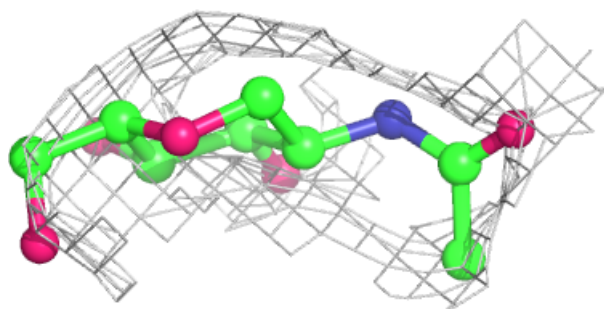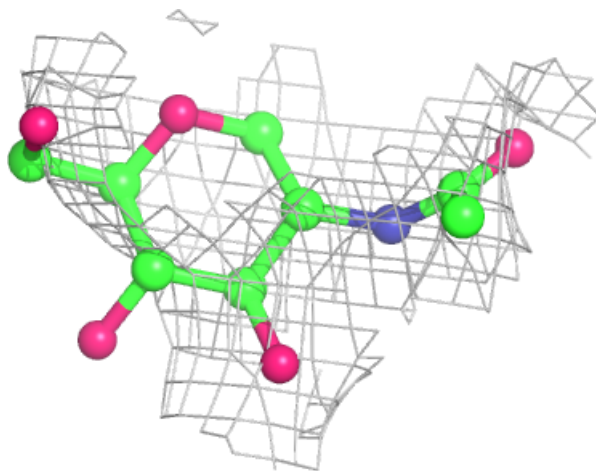mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
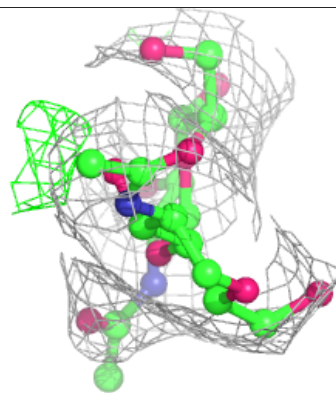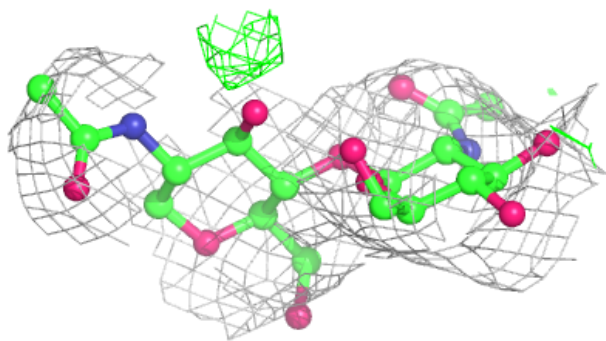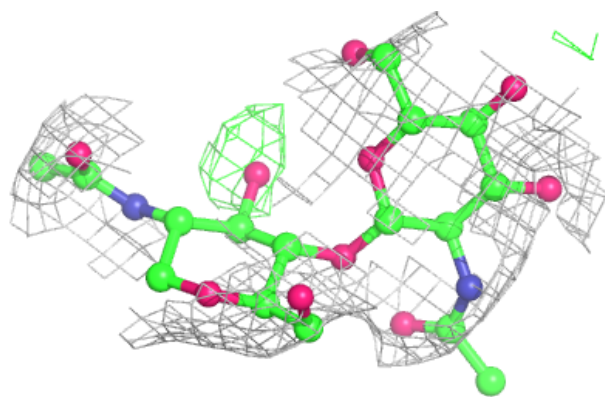
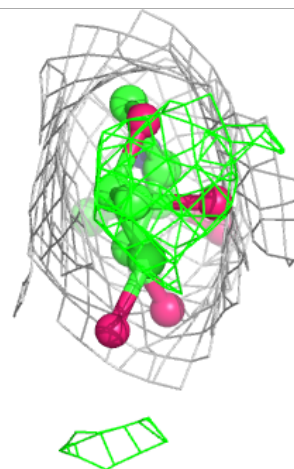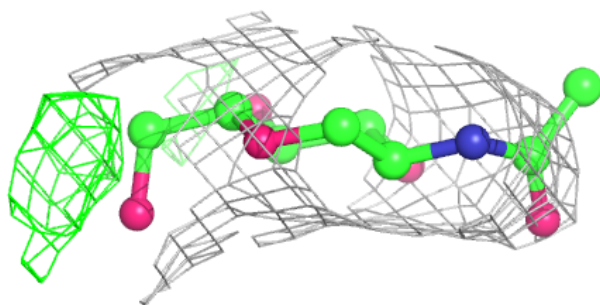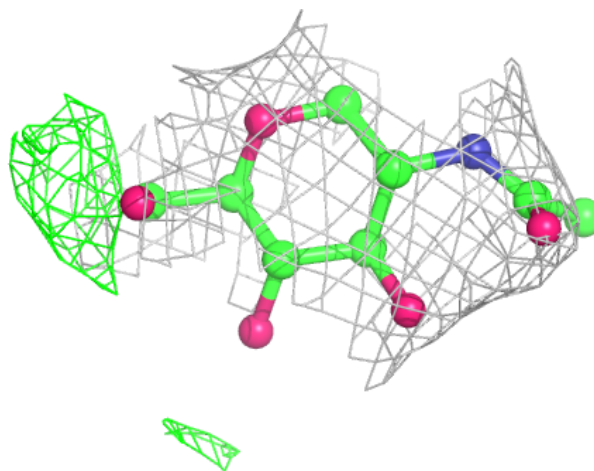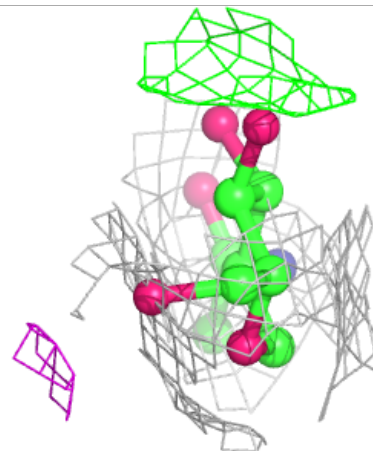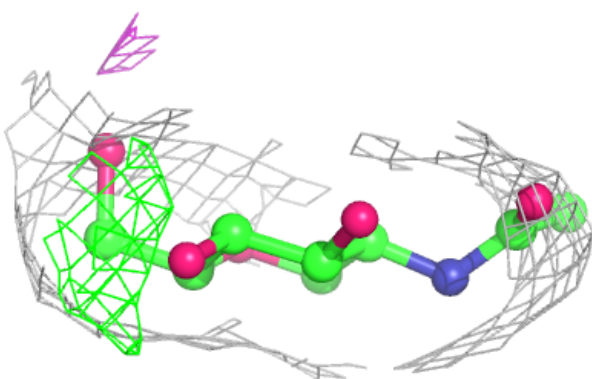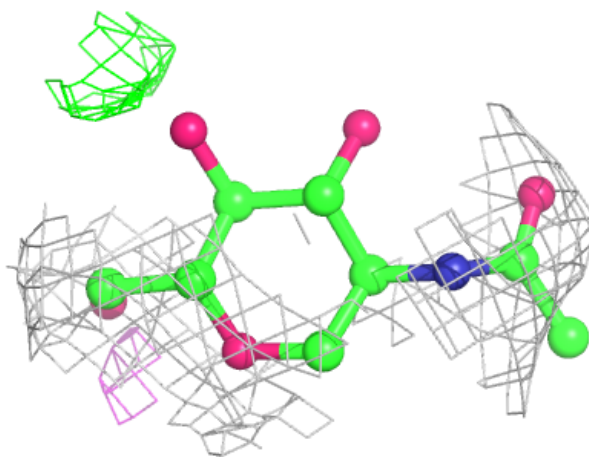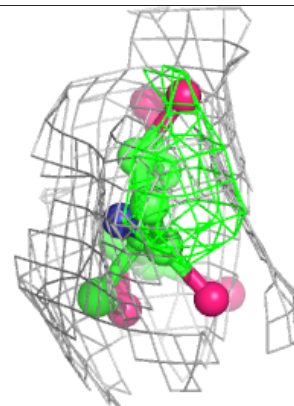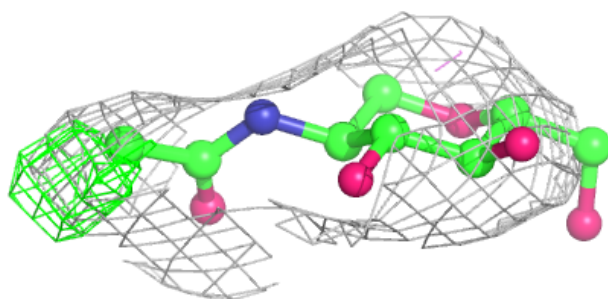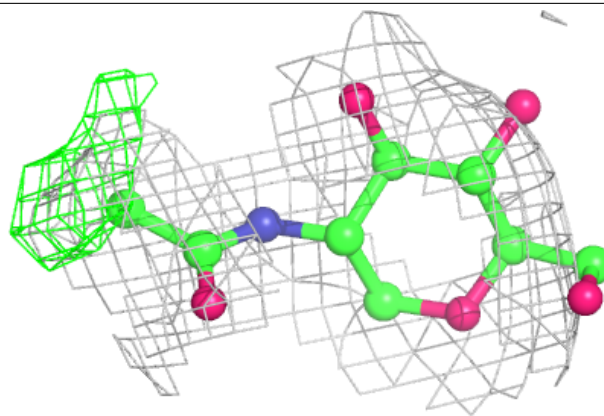**Electron density around Chain F:**

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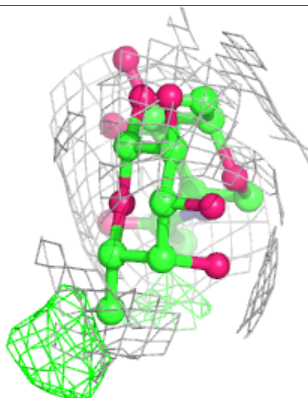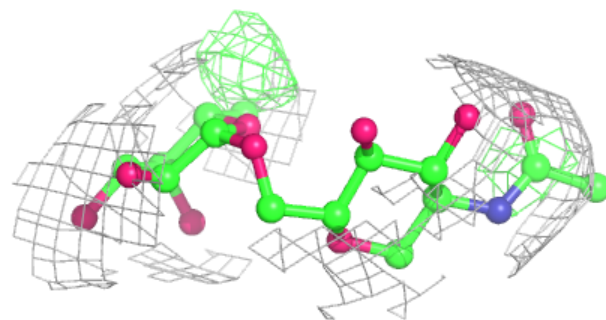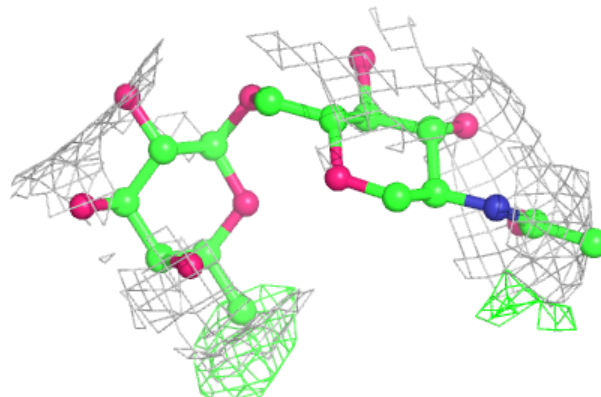
6.4   Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	C	701	14/15	0.56	0.37	142,166,182,185	0
5	NAG	A	701	14/15	0.58	0.33	162,185,198,198	0
5	NAG	C	705	14/15	0.59	0.39	151,170,175,187	0
5	NAG	C	706	14/15	0.63	0.25	110,150,172,174	0
5	NAG	A	704	14/15	0.71	0.22	146,161,174,178	0
5	NAG	C	704	14/15	0.72	0.35	165,184,200,210	0
5	NAG	D	601	14/15	0.73	0.22	126,141,148,152	0
5	NAG	A	703	14/15	0.75	0.24	137,155,175,194	0
5	NAG	A	705	14/15	0.84	0.31	102,159,177,194	0
5	NAG	C	703	14/15	0.84	0.23	112,143,159,159	0
6	ZN	C	702	1/1	0.84	0.28	99,99,99,99	0
6	ZN	A	702	1/1	0.85	0.36	111,111,111,111	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 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)
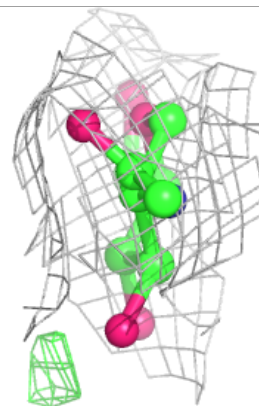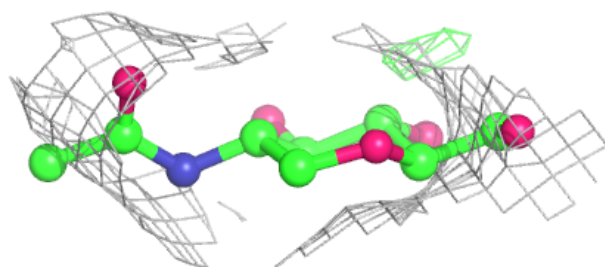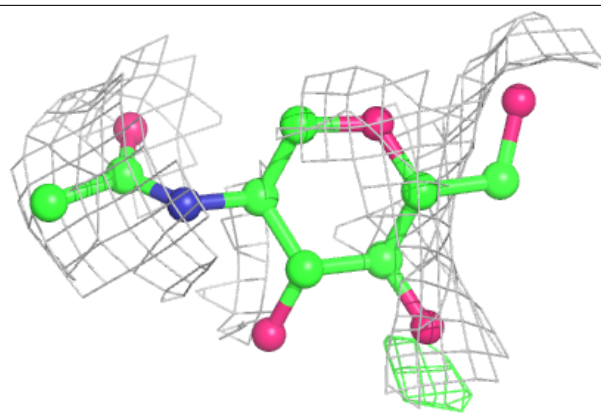
Electron density around NAG A 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
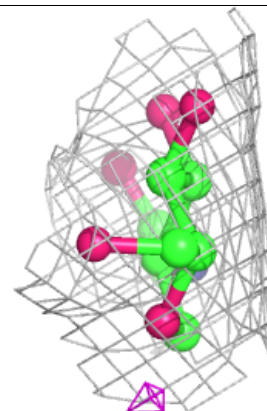$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
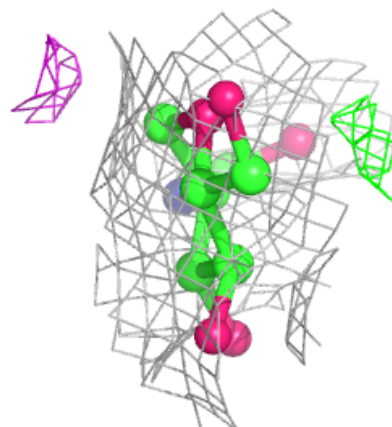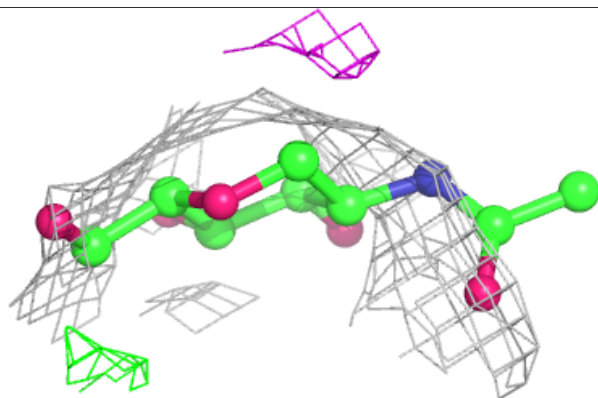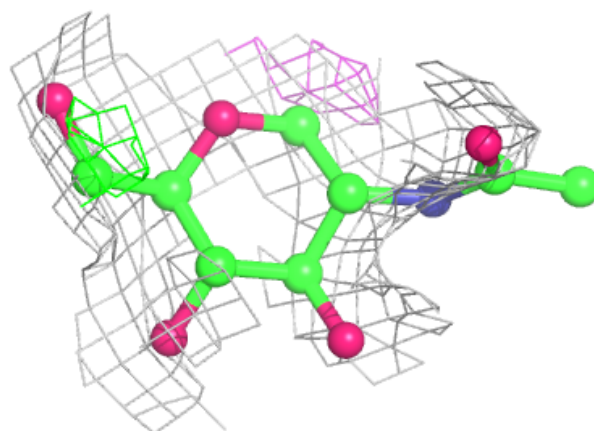
Electron density around NAG C 705:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
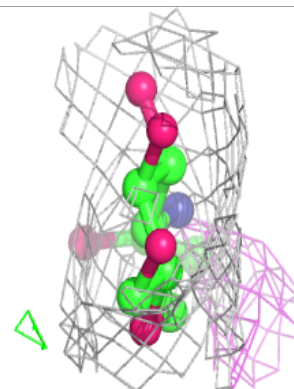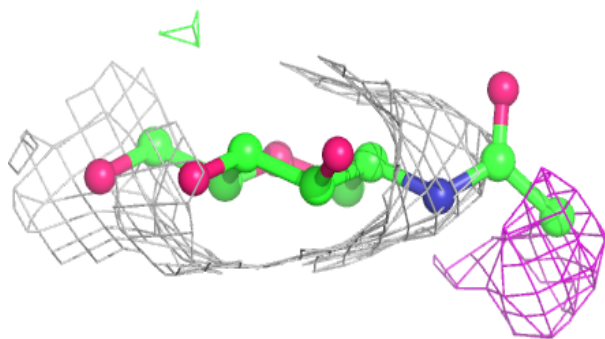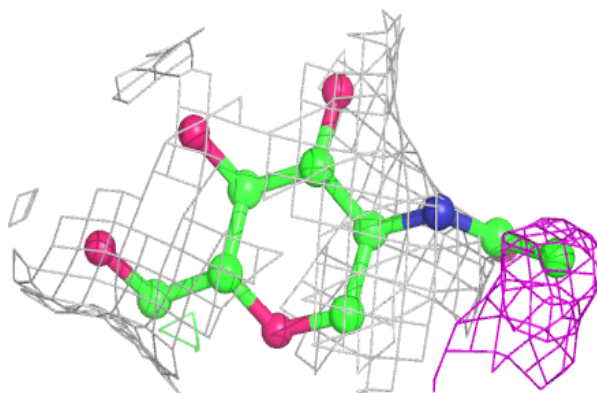
Electron density around NAG C 706:

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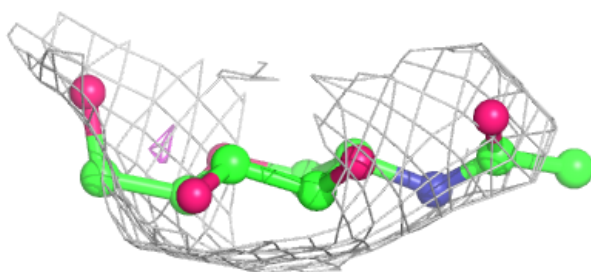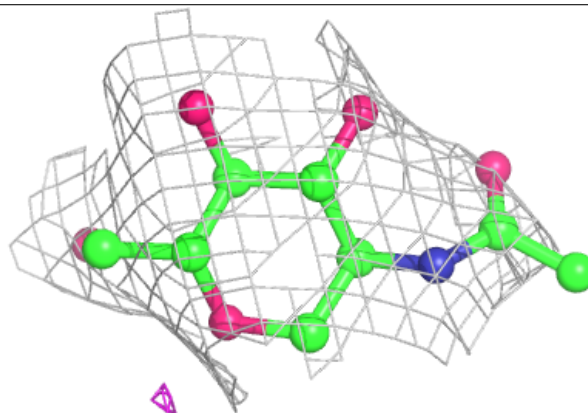$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAG A 704:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
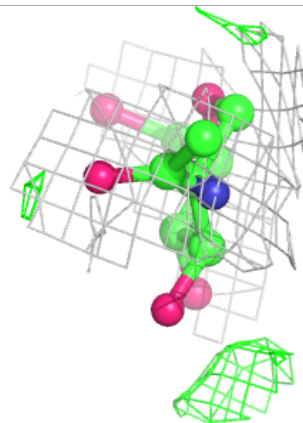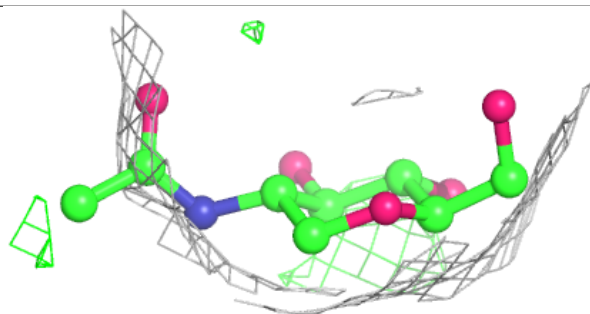
Electron density around NAG C 704:

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

Electron density around NAG D 601:

$2mF_o\text{-}DF_c$ (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 703:

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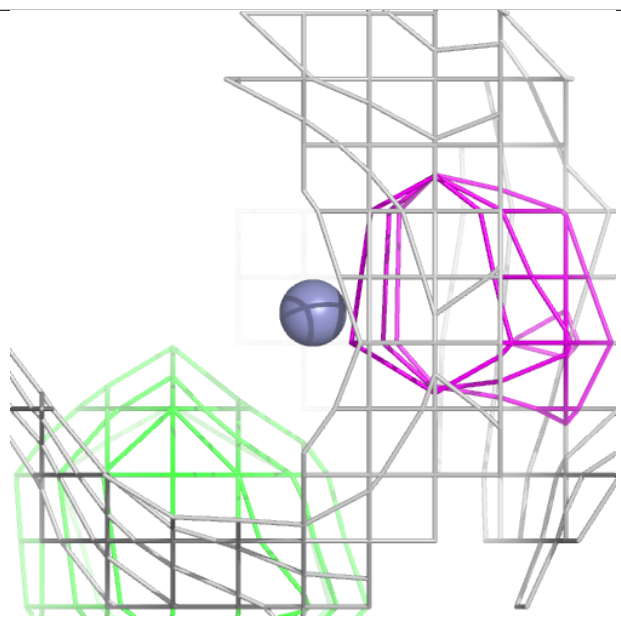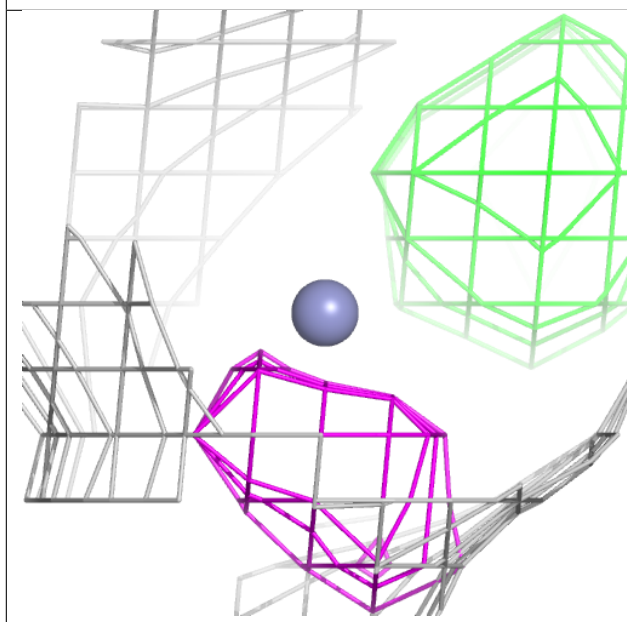$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAG A 705:

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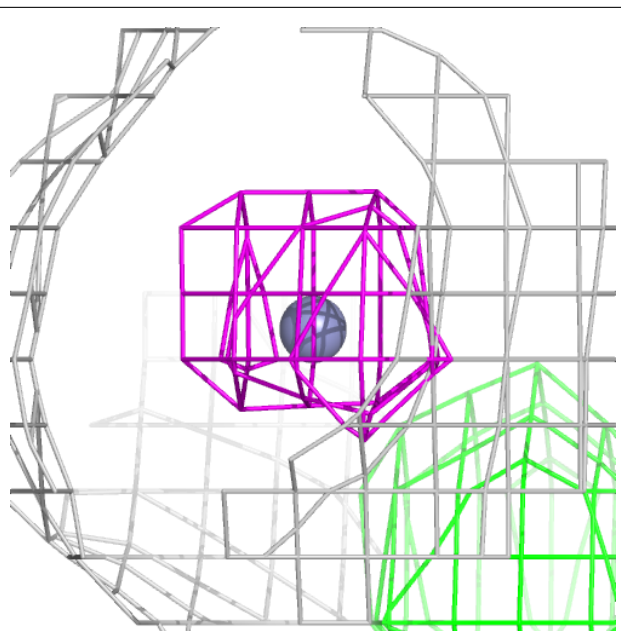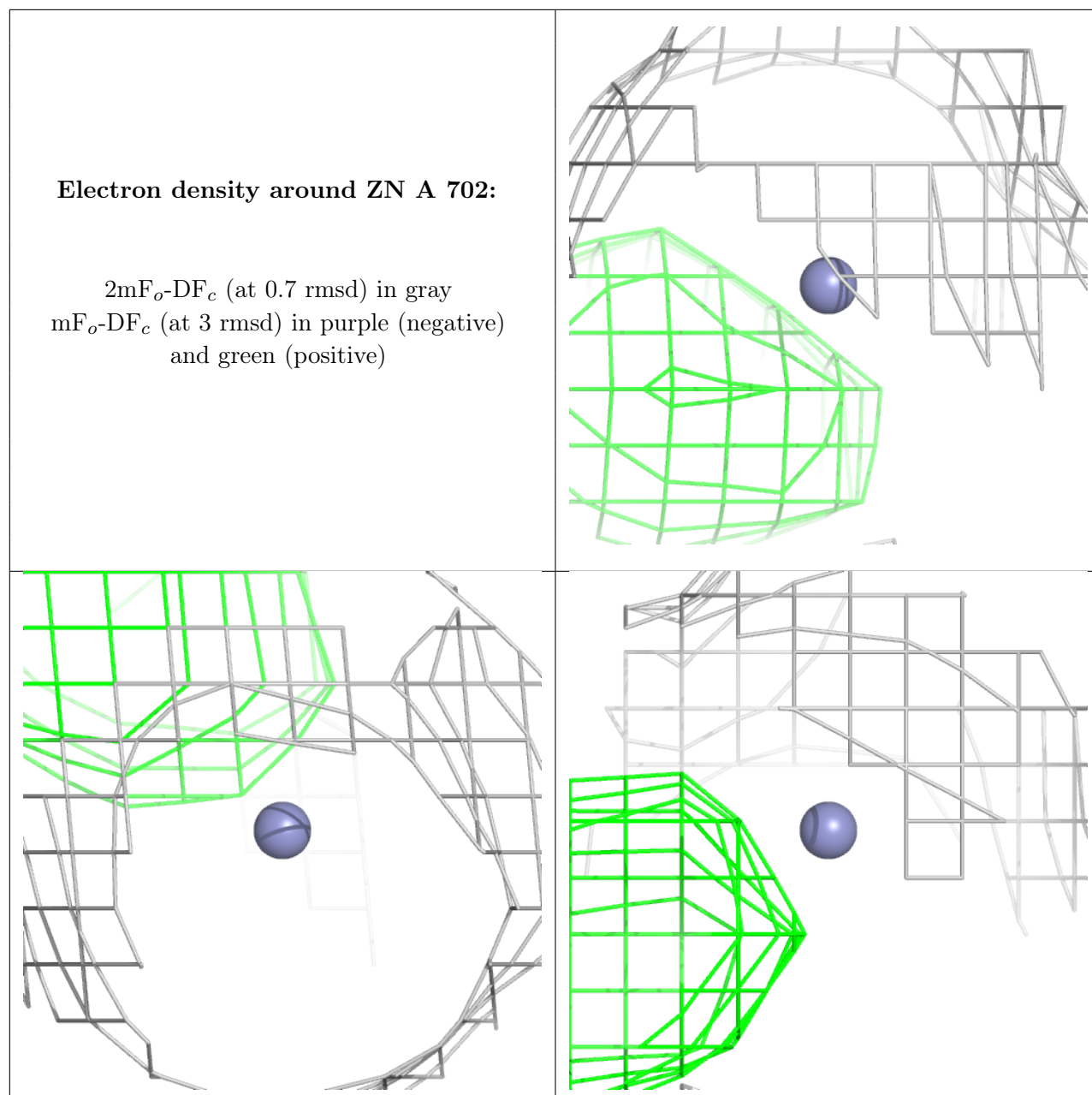and green (positive)

Electron density around NAG C 703:

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

Electron density around ZN C 702:

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

Electron density around ZN A 702:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.