



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:23 AM UTC

PDB ID : 8WEI / pdb\_00008wei  
Title : Crystal structure of Brassica napus MIK2 ectodomain (N393D mutant)  
Authors : Wan, L.H.; Hu, Y.X.; Wu, H.M.  
Deposited on : 2023-09-17  
Resolution : 2.71 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

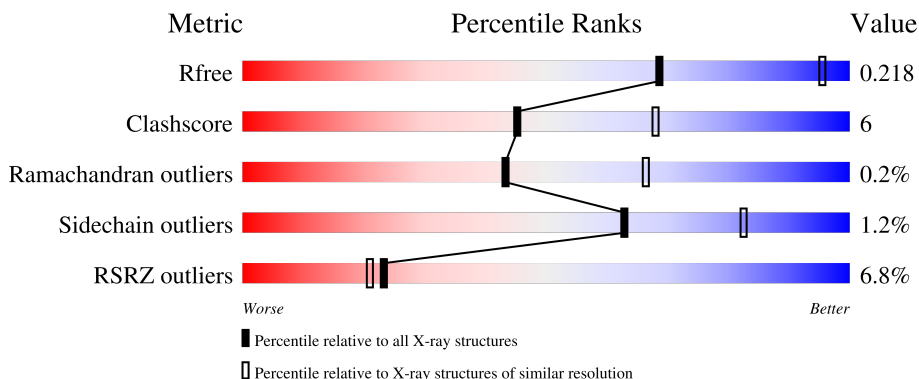
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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.



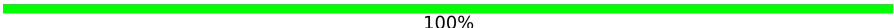
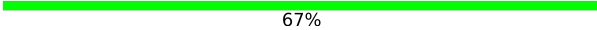
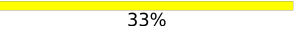
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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  $\geq 3$ , 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	702	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6%      78%      13%      8%</p>
2	B	2	<div style="width: 100%; height: 10px; background-color: green;"></div> <p style="text-align: center;">100%</p>
2	C	2	<div style="width: 100%; height: 10px; background-color: green;"></div> <p style="text-align: center;">100%</p>
2	E	2	<div style="display: flex; align-items: center;"> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">50%      50%</p>
3	D	4	<div style="width: 100%; height: 10px; background-color: green;"></div> <p style="text-align: center;">100%</p>

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Mol	Chain	Length	Quality of chain
4	F	3	 100%
5	G	3	 67%  33%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5445 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 MALE DISCOVERER 1-INTERACTING RECEPTOR-LIKE KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	644	4981	3145	840	981	15	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	ASP	ASN	engineered mutation	UNP A0A816I5A6
A	546	SER	THR	conflict	UNP A0A816I5A6
A	691	GLU	-	expression tag	UNP A0A816I5A6
A	692	PHE	-	expression tag	UNP A0A816I5A6
A	693	HIS	-	expression tag	UNP A0A816I5A6
A	694	HIS	-	expression tag	UNP A0A816I5A6
A	695	HIS	-	expression tag	UNP A0A816I5A6
A	696	HIS	-	expression tag	UNP A0A816I5A6
A	697	HIS	-	expression tag	UNP A0A816I5A6
A	698	HIS	-	expression tag	UNP A0A816I5A6
A	699	HIS	-	expression tag	UNP A0A816I5A6
A	700	HIS	-	expression tag	UNP A0A816I5A6
A	701	HIS	-	expression tag	UNP A0A816I5A6
A	702	HIS	-	expression tag	UNP A0A816I5A6

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



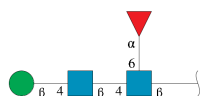
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

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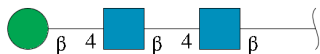
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



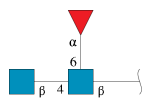
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 4 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
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

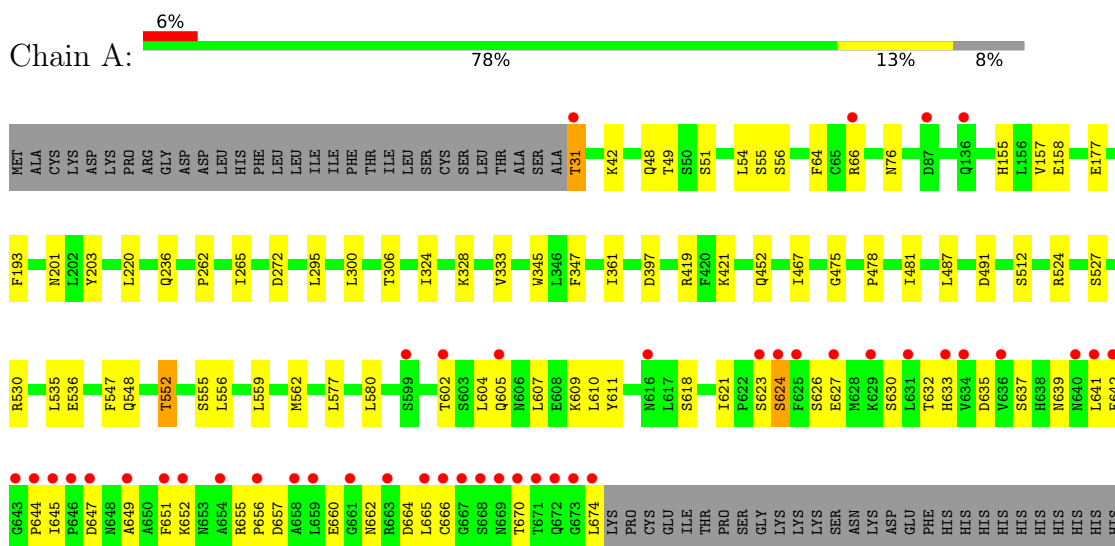
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	212	212	212	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: MALE DISCOVERER 1-INTERACTING RECEPTOR-LIKE KINASE 2



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

Chain B: 



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

Chain C: 



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

Chain E: 

MAG1  
MAG2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1  
MAG2  
BMA3  
FUC4

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

Chain F:  100%

MAG1  
MAG2  
BMA3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  67% 33%

MAG1  
MAG2  
FUC3

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.90Å 155.90Å 126.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.68 – 2.71 36.68 – 2.71	Depositor EDS
% Data completeness (in resolution range)	91.0 (36.68-2.71) 91.1 (36.68-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.72Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.199 , 0.216 0.200 , 0.218	Depositor DCC
$R_{free}$ test set	2212 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.18	0/5080	0.36	0/6909

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4981	0	4967	61	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
3	D	49	0	43	0	0
4	F	39	0	34	0	0
5	G	38	0	34	0	0
6	A	42	0	39	0	0
7	A	212	0	0	3	0
All	All	5445	0	5192	61	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 6.

All (61) 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:605:GLN:NE2	1:A:627:GLU:OE1	2.15	0.79
1:A:177:GLU:HG3	1:A:201:ASN:HB2	1.65	0.79
1:A:49:THR:HG22	1:A:51:SER:H	1.53	0.72
1:A:31:THR:OG1	1:A:76:ASN:O	2.07	0.71
1:A:562:MET:HE1	1:A:577:LEU:HD22	1.73	0.71
1:A:642:GLU:HB2	1:A:664:ASP:HB3	1.73	0.71
1:A:609:LYS:HG2	1:A:633:HIS:HB2	1.74	0.67
1:A:644:PRO:HA	1:A:666:CYS:HA	1.78	0.65
1:A:530:ARG:HD2	1:A:552:THR:HB	1.82	0.62
1:A:602:THR:O	1:A:605:GLN:NE2	2.33	0.62
1:A:333:VAL:HG11	1:A:361:ILE:HD12	1.81	0.62
1:A:666:CYS:SG	1:A:670:THR:OG1	2.58	0.61
1:A:524:ARG:HH21	1:A:548:GLN:HG2	1.68	0.59
1:A:157:VAL:HG23	1:A:158:GLU:HG3	1.83	0.59
1:A:639:ASN:O	1:A:662:ASN:HA	2.04	0.58
1:A:556:LEU:HB2	1:A:580:LEU:HD22	1.85	0.57
1:A:300:LEU:HB2	1:A:324:ILE:HG22	1.89	0.55
1:A:31:THR:HG23	1:A:64:PHE:HD2	1.74	0.53
1:A:655:ARG:HB3	1:A:656:PRO:HD2	1.91	0.53
1:A:662:ASN:HB2	1:A:665:LEU:HD11	1.92	0.51
1:A:155:HIS:NE2	1:A:177:GLU:OE1	2.26	0.50
1:A:201:ASN:HB3	1:A:203:TYR:CZ	2.47	0.50
1:A:602:THR:CG2	1:A:624:SER:HB3	2.42	0.49
1:A:306:THR:HG22	1:A:328:LYS:HB2	1.94	0.49
1:A:607:LEU:HD21	1:A:610:LEU:HB2	1.95	0.48
1:A:626:SER:HA	1:A:647:ASP:O	2.14	0.47
1:A:236:GLN:NE2	7:A:910:HOH:O	2.46	0.47
1:A:345:TRP:HB3	1:A:347:PHE:HE1	1.79	0.47
1:A:478:PRO:HG2	1:A:481:ILE:HG12	1.96	0.47
1:A:649:ALA:O	1:A:652:LYS:N	2.47	0.46
1:A:609:LYS:HB3	1:A:611:TYR:HE1	1.80	0.46
1:A:530:ARG:HG2	1:A:555:SER:OG	2.15	0.46
1:A:48:GLN:NE2	7:A:905:HOH:O	2.37	0.45
1:A:512:SER:HA	1:A:535:LEU:HA	1.98	0.45
1:A:524:ARG:HG2	1:A:547:PHE:HB2	1.98	0.45
1:A:272:ASP:HA	1:A:295:LEU:HA	1.99	0.45
1:A:193:PHE:O	1:A:220:LEU:HD21	2.17	0.44
1:A:42:LYS:HG3	1:A:54:LEU:HD23	1.99	0.44
1:A:604:LEU:HB3	1:A:607:LEU:HB2	1.99	0.44
1:A:621:ILE:HD13	1:A:641:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HG23	1:A:64:PHE:CD2	2.53	0.43
1:A:527:SER:O	1:A:530:ARG:HB2	2.19	0.43
1:A:630:SER:O	1:A:632:THR:HG23	2.18	0.43
1:A:345:TRP:HB3	1:A:347:PHE:CE1	2.54	0.42
1:A:536:GLU:HA	1:A:559:LEU:HA	2.01	0.42
1:A:657:ASP:HA	1:A:660:GLU:HG2	2.00	0.42
1:A:524:ARG:HH11	1:A:524:ARG:HB3	1.84	0.42
1:A:635:ASP:OD1	1:A:637:SER:OG	2.29	0.42
1:A:609:LYS:HB3	1:A:611:TYR:CE1	2.54	0.42
1:A:42:LYS:HE3	1:A:54:LEU:HB3	2.02	0.42
1:A:397:ASP:OD2	1:A:419:ARG:NH1	2.52	0.42
1:A:397:ASP:HA	1:A:421:LYS:O	2.19	0.42
1:A:645:ILE:HD13	1:A:651:PHE:HB3	2.01	0.42
1:A:262:PRO:HG2	1:A:265:ILE:HG12	2.02	0.42
1:A:487:LEU:HD12	1:A:487:LEU:HA	1.93	0.41
1:A:639:ASN:HB2	1:A:641:LEU:HD12	2.02	0.41
1:A:467:ILE:HG23	1:A:491:ASP:HB3	2.02	0.41
1:A:66:ARG:NH1	7:A:917:HOH:O	2.53	0.41
1:A:602:THR:HG21	1:A:624:SER:HB3	2.03	0.41
1:A:530:ARG:HD2	1:A:552:THR:O	2.20	0.41
1:A:452:GLN:HG2	1:A:475:GLY:HA3	2.02	0.40

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	642/702 (92%)	634 (99%)	7 (1%)	1 (0%)	43 66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	624	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	582/635 (92%)	575 (99%)	7 (1%)	63 82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	55	SER
1	A	56	SER
1	A	552	THR
1	A	618	SER
1	A	623	SER
1	A	674	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	59	ASN
1	A	176	HIS
1	A	201	ASN
1	A	236	GLN
1	A	256	ASN
1	A	294	ASN
1	A	352	HIS
1	A	411	ASN
1	A	440	ASN
1	A	446	ASN
1	A	489	GLN
1	A	496	ASN
1	A	517	ASN

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Mol	Chain	Res	Type
1	A	534	ASN
1	A	590	HIS
1	A	592	ASN
1	A	640	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

16 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	$\# Z  > 2$
2	NAG	B	1	1,2	14,14,15	0.23	0	17,19,21	0.59	0
2	NAG	B	2	2	14,14,15	0.41	0	17,19,21	0.57	0
2	NAG	C	1	1,2	14,14,15	0.20	0	17,19,21	0.52	0
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.52	0
3	NAG	D	1	1,3	14,14,15	0.55	0	17,19,21	0.57	0
3	NAG	D	2	3	14,14,15	0.30	0	17,19,21	0.38	0
3	BMA	D	3	3	11,11,12	0.77	0	15,15,17	0.77	0
3	FUC	D	4	3	10,10,11	0.85	0	14,14,16	0.73	0
2	NAG	E	1	1,2	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	E	2	2	14,14,15	0.58	0	17,19,21	1.64	4 (23%)
4	NAG	F	1	1,4	14,14,15	0.16	0	17,19,21	0.46	0
4	NAG	F	2	4	14,14,15	0.19	0	17,19,21	0.56	0
4	BMA	F	3	4	11,11,12	0.72	0	15,15,17	0.65	0
5	NAG	G	1	1,5	14,14,15	0.31	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	G	2	5	14,14,15	0.36	0	17,19,21	0.40	0
5	FUC	G	3	5	10,10,11	1.27	2 (20%)	14,14,16	1.19	2 (14%)

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
2	NAG	B	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3	FUC	C1-C2	2.29	1.57	1.52
5	G	3	FUC	C2-C3	2.12	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C2-N2-C7	4.77	129.29	122.90
2	E	2	NAG	C3-C4-C5	2.44	114.65	110.23
2	E	2	NAG	C1-C2-N2	2.41	114.23	110.43
2	E	2	NAG	C1-O5-C5	2.37	115.36	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	FUC	O5-C5-C4	2.32	113.73	109.55
5	G	3	FUC	C1-O5-C5	2.03	117.75	112.97

There are no chirality outliers.

All (30) torsion outliers are listed below:

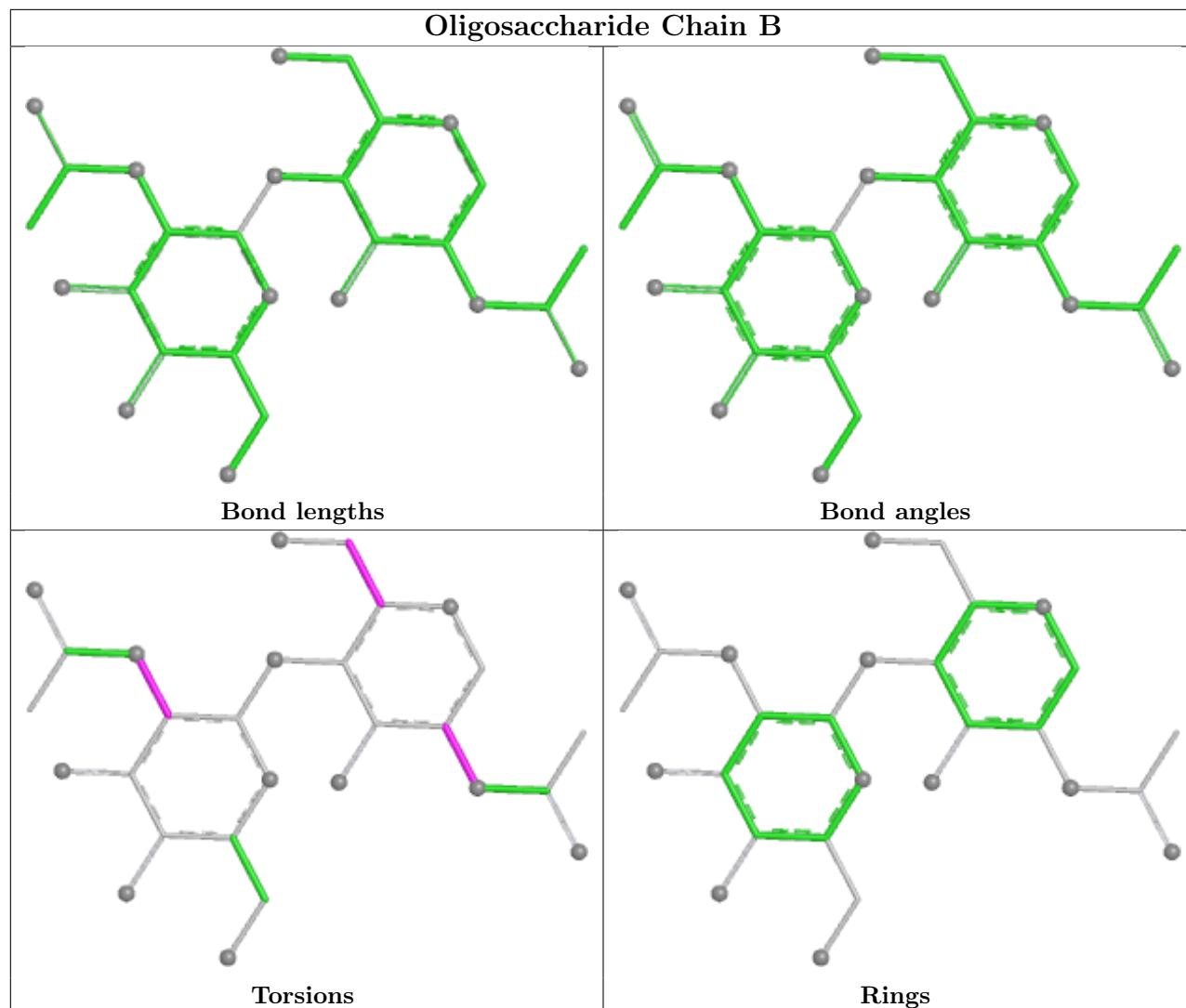
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C3-C2-N2-C7
2	B	1	NAG	C1-C2-N2-C7
2	B	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
4	F	1	NAG	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6

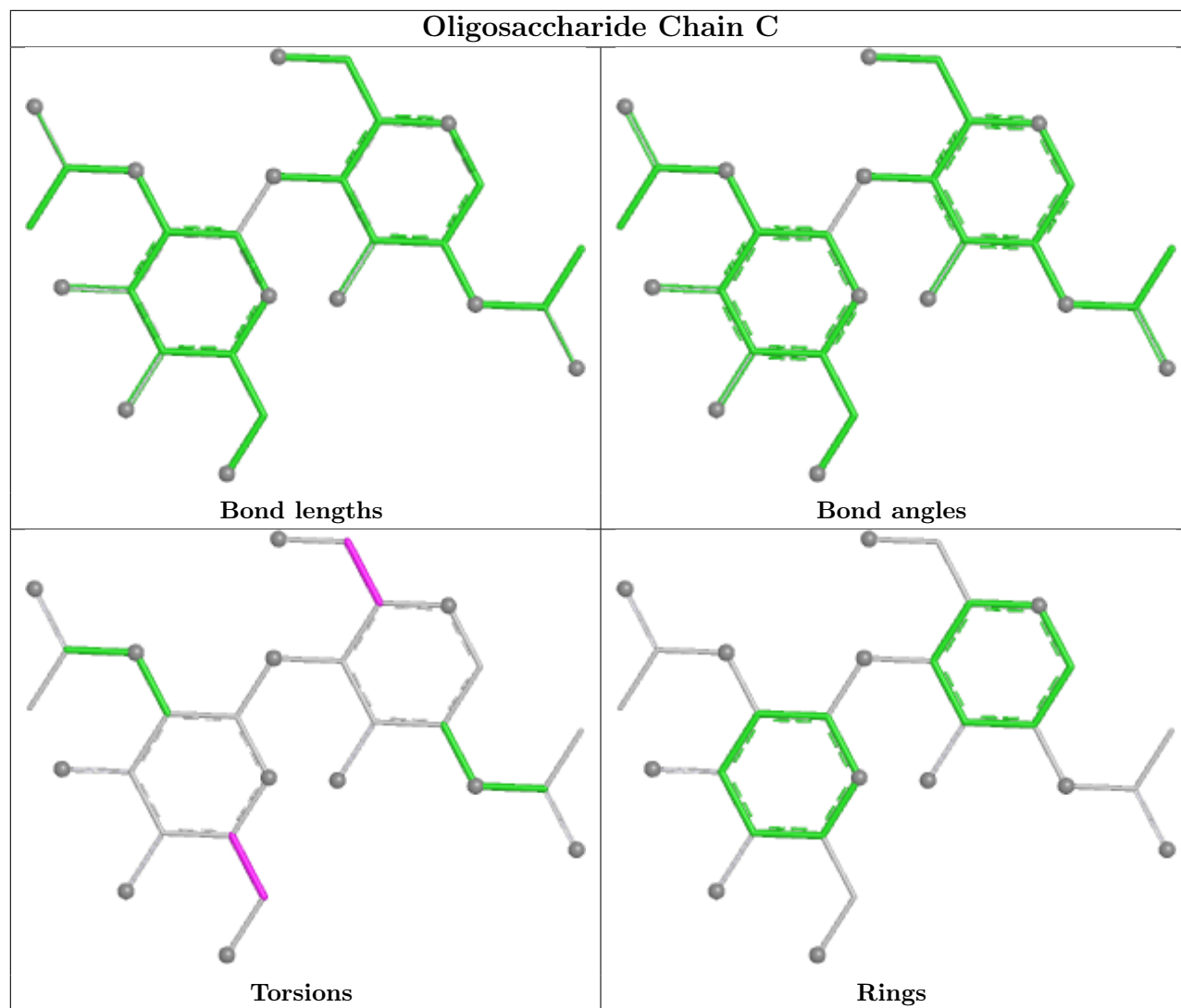
There are no ring outliers.

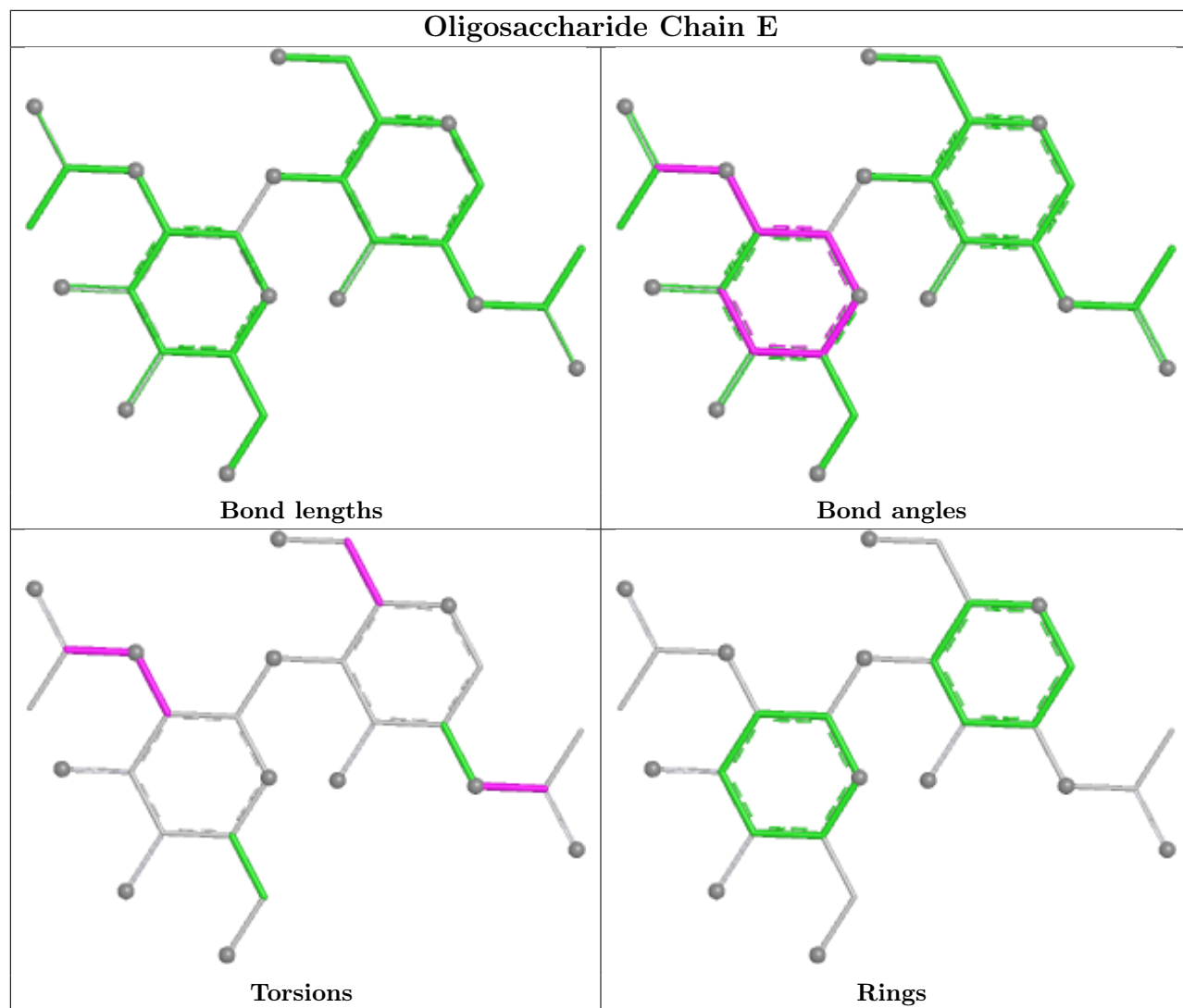
No monomer is involved in short contacts.

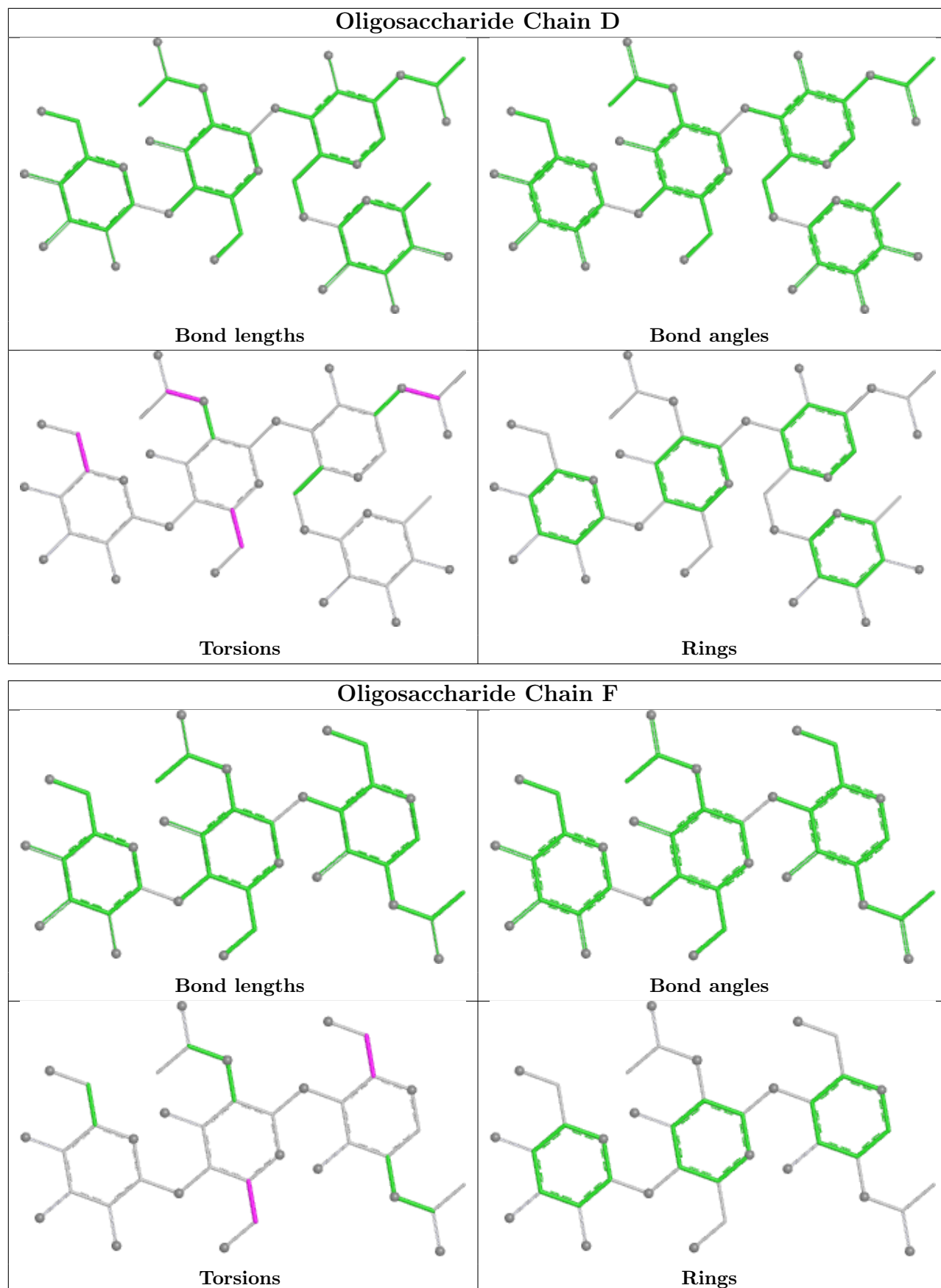
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

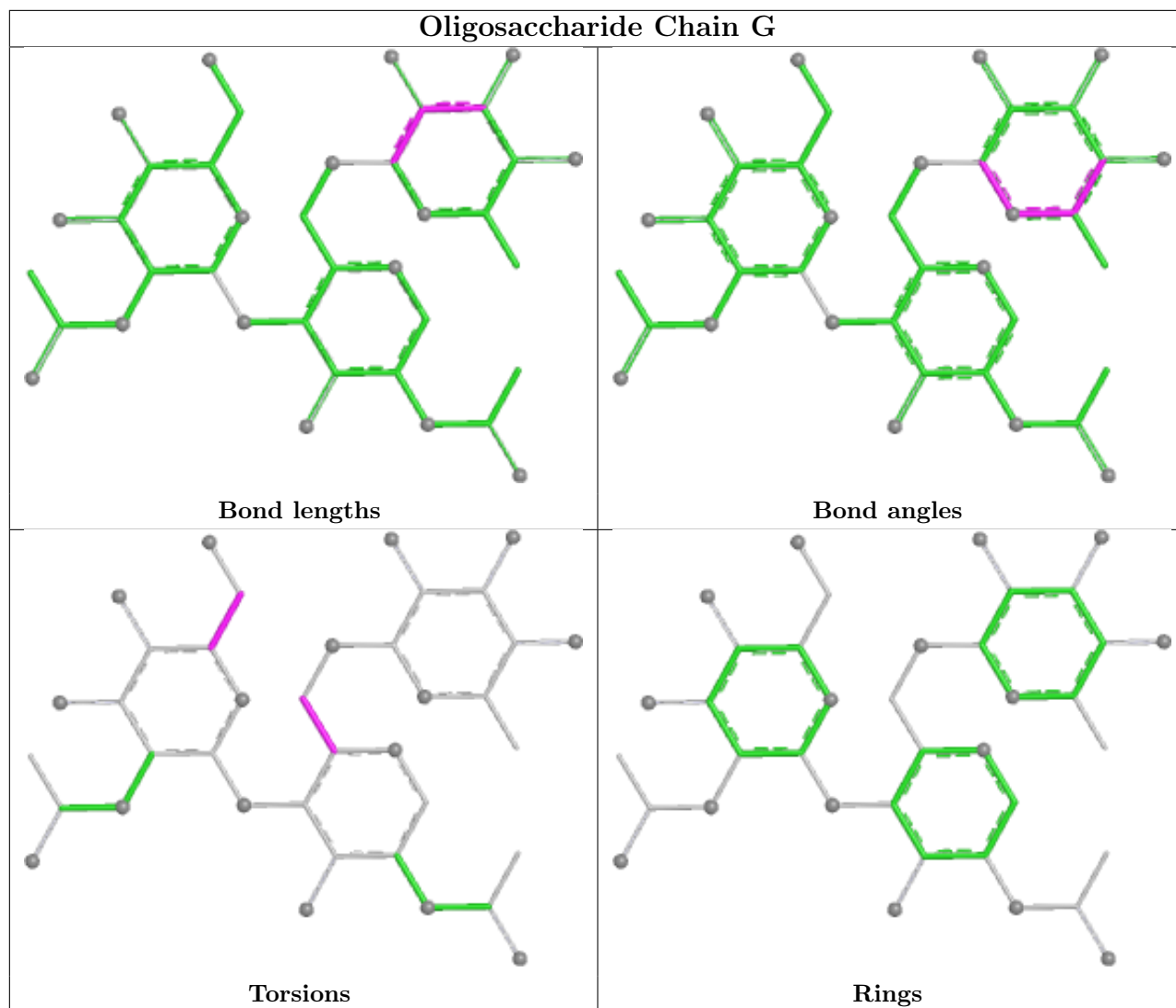
bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
6	NAG	A	802	1	14,14,15	0.60	0	17,19,21	0.65	1 (5%)
6	NAG	A	803	1	14,14,15	0.55	0	17,19,21	0.39	0
6	NAG	A	801	1	14,14,15	0.35	0	17,19,21	0.65	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	A	802	1	-	2/6/23/26	0/1/1/1
6	NAG	A	803	1	-	1/6/23/26	0/1/1/1
6	NAG	A	801	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	802	NAG	C1-O5-C5	2.09	114.98	112.19

There are no chirality outliers.

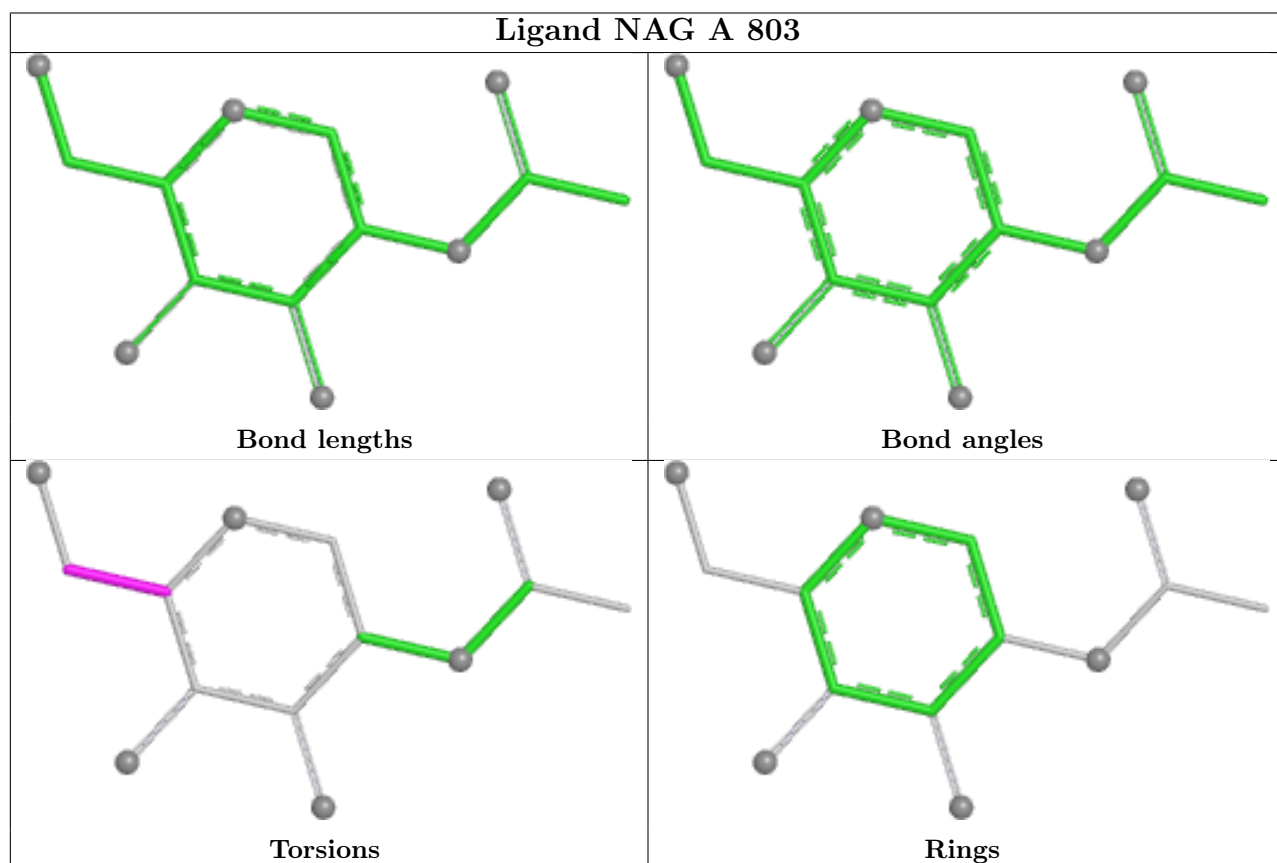
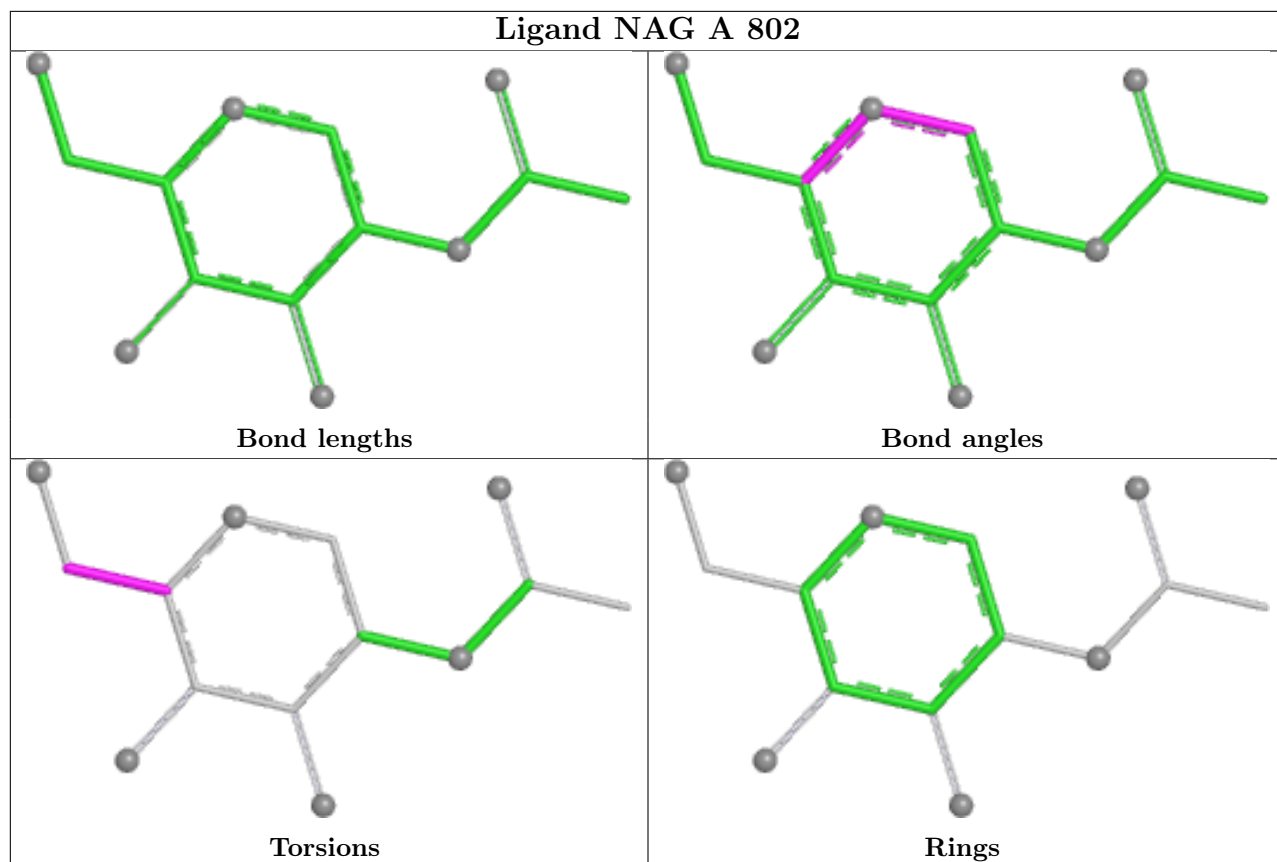
All (5) torsion outliers are listed below:

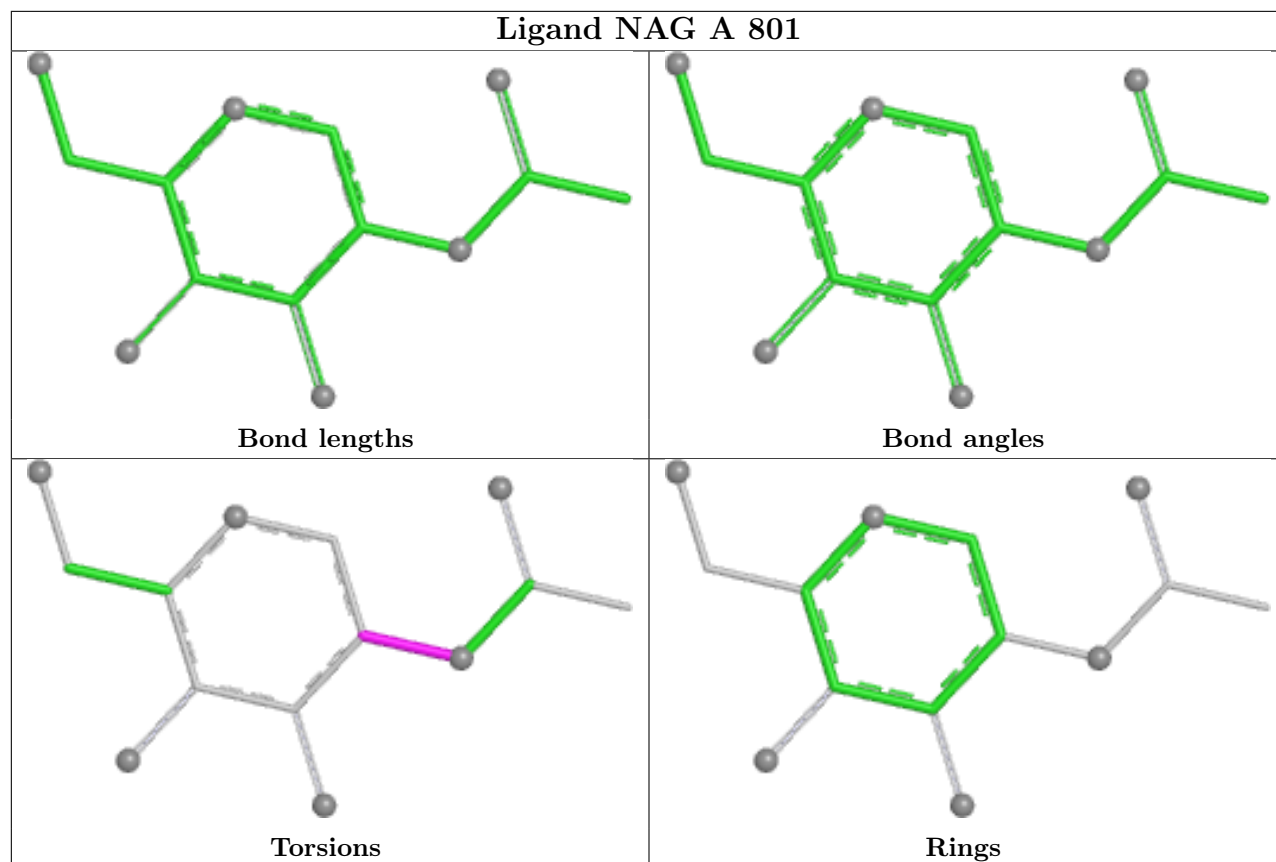
Mol	Chain	Res	Type	Atoms
6	A	802	NAG	O5-C5-C6-O6
6	A	803	NAG	O5-C5-C6-O6
6	A	801	NAG	C1-C2-N2-C7
6	A	801	NAG	C3-C2-N2-C7
6	A	802	NAG	C4-C5-C6-O6

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 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	644/702 (91%)	0.05	44 (6%) <span style="border: 1px solid red; padding: 2px;">23</span> <span style="border: 1px solid red; padding: 2px;">21</span>	23, 42, 103, 142	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	674	LEU	11.2
1	A	672	GLN	9.7
1	A	670	THR	8.2
1	A	671	THR	7.2
1	A	665	LEU	6.0
1	A	647	ASP	5.1
1	A	623	SER	4.9
1	A	673	GLY	4.5
1	A	656	PRO	4.5
1	A	652	LYS	4.2
1	A	658	ALA	4.1
1	A	627	GLU	4.1
1	A	645	ILE	4.0
1	A	668	SER	3.9
1	A	661	GLY	3.9
1	A	667	GLY	3.8
1	A	666	CYS	3.8
1	A	669	ASN	3.7
1	A	66	ARG	3.7
1	A	631	LEU	3.5
1	A	646	PRO	3.5
1	A	640	ASN	3.3
1	A	605	GLN	3.1
1	A	624	SER	3.1
1	A	651	PHE	3.1
1	A	654	ALA	3.0
1	A	649	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	625	PHE	2.9
1	A	633	HIS	2.8
1	A	599	SER	2.7
1	A	641	LEU	2.7
1	A	31	THR	2.6
1	A	616	ASN	2.6
1	A	602	THR	2.5
1	A	629	LYS	2.5
1	A	663	ARG	2.5
1	A	634	VAL	2.4
1	A	136	GLN	2.3
1	A	644	PRO	2.3
1	A	636	VAL	2.2
1	A	642	GLU	2.2
1	A	643	GLY	2.2
1	A	659	LEU	2.1
1	A	87	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

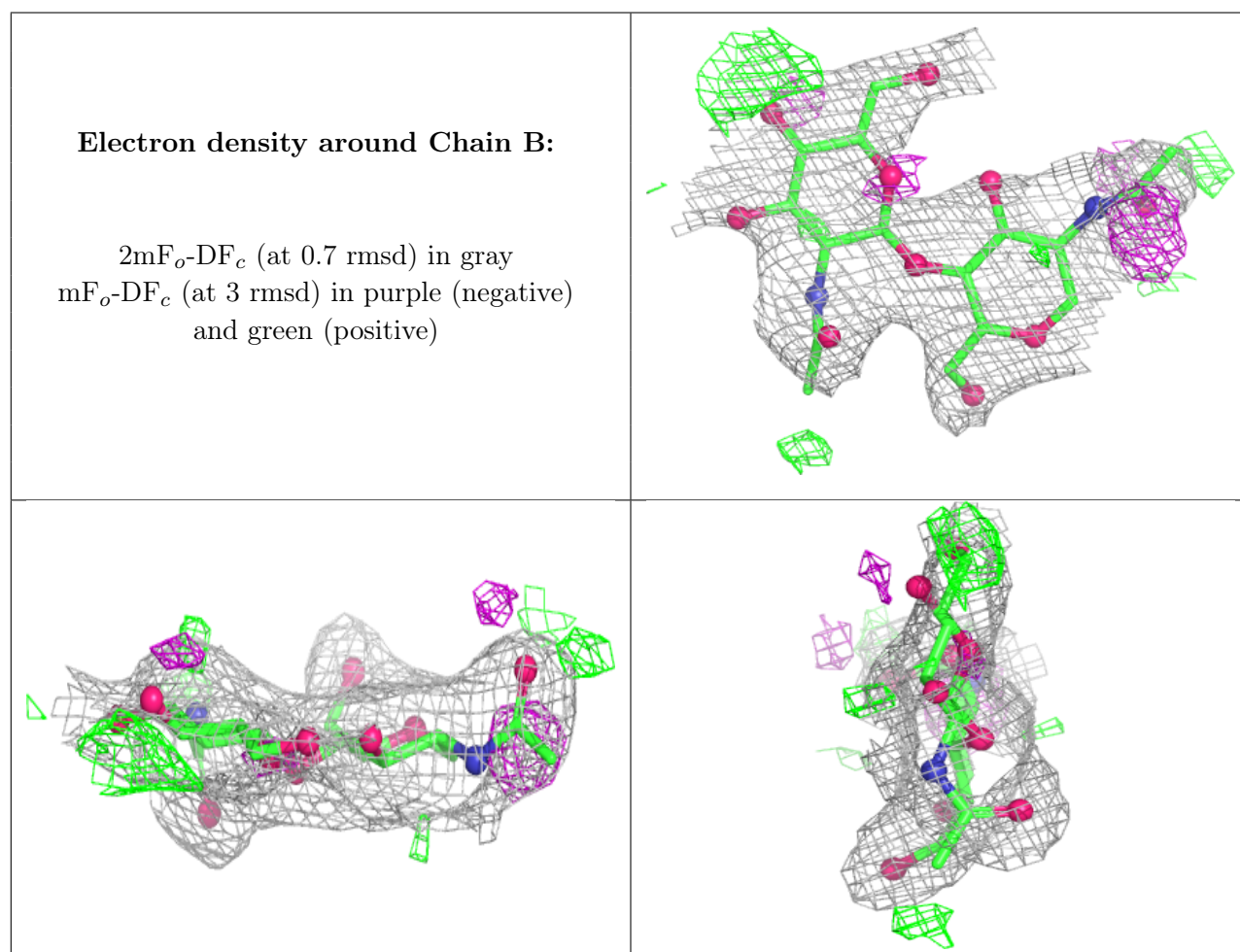
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	E	2	14/15	0.41	0.25	79,112,127,127	0
4	BMA	F	3	11/12	0.56	0.19	85,92,101,101	0
5	NAG	G	2	14/15	0.63	0.24	93,114,122,125	0
2	NAG	B	2	14/15	0.67	0.22	65,80,95,112	0
3	BMA	D	3	11/12	0.69	0.19	68,78,92,94	0
5	FUC	G	3	10/11	0.72	0.30	82,105,110,116	0
2	NAG	E	1	14/15	0.73	0.20	58,88,98,121	0
5	NAG	G	1	14/15	0.75	0.21	80,103,113,122	0
2	NAG	C	2	14/15	0.81	0.17	49,63,89,99	0
3	FUC	D	4	10/11	0.88	0.18	52,68,79,79	0
3	NAG	D	1	14/15	0.89	0.10	41,49,60,75	0

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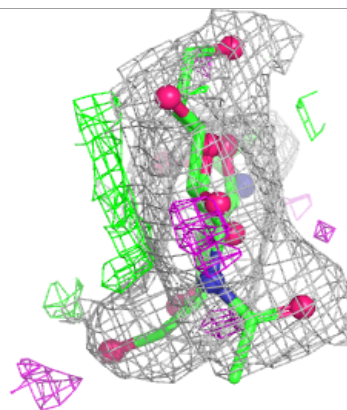
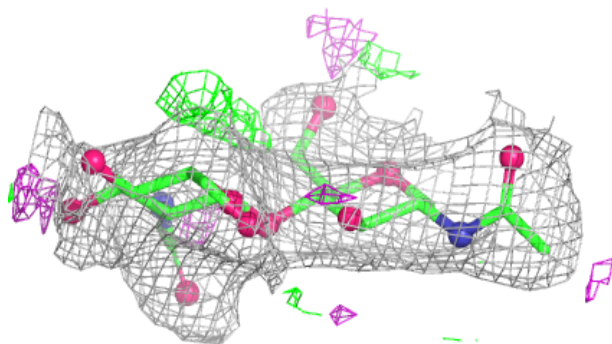
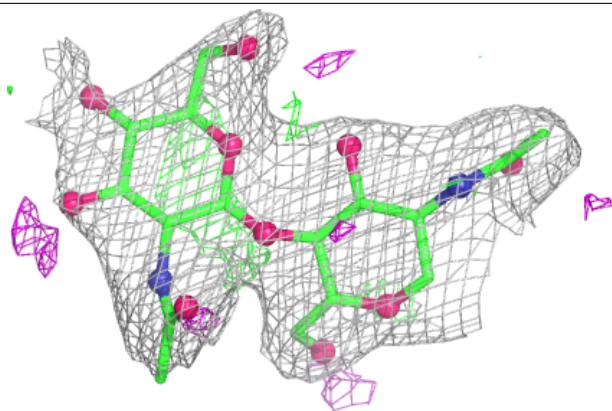
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	1	14/15	0.90	0.13	36,58,78,78	0
3	NAG	D	2	14/15	0.92	0.10	53,64,83,87	0
4	NAG	F	2	14/15	0.92	0.12	56,65,78,107	0
4	NAG	F	1	14/15	0.94	0.10	47,52,63,67	0
2	NAG	C	1	14/15	0.94	0.09	28,40,57,64	0

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.

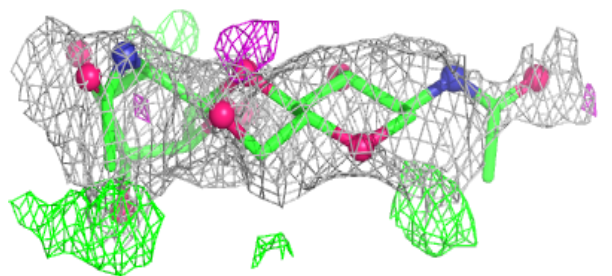
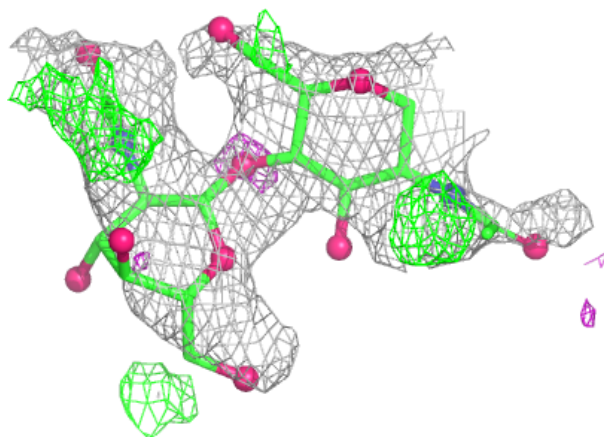


**Electron density around Chain C:**

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

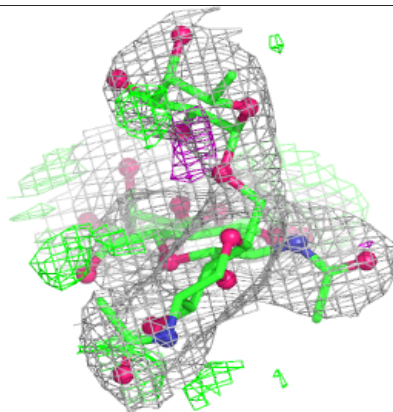
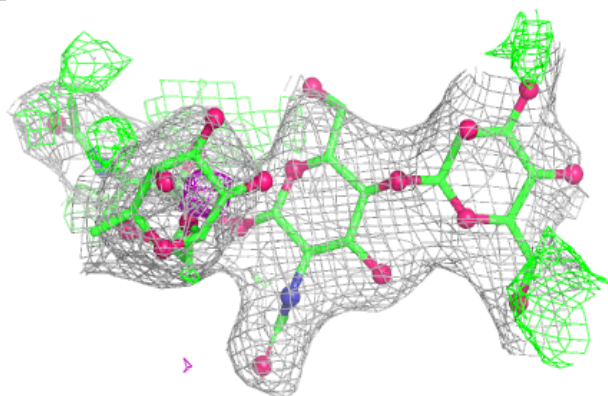
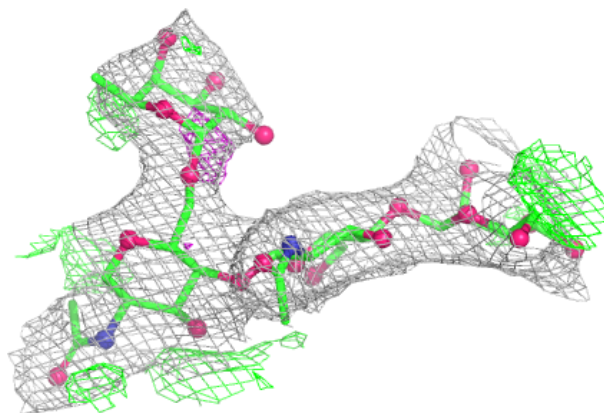
**Electron density around Chain E:**

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

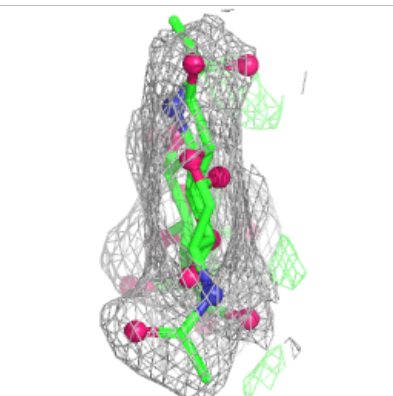
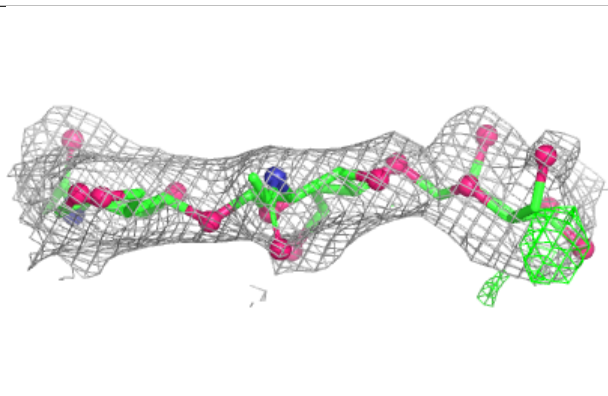
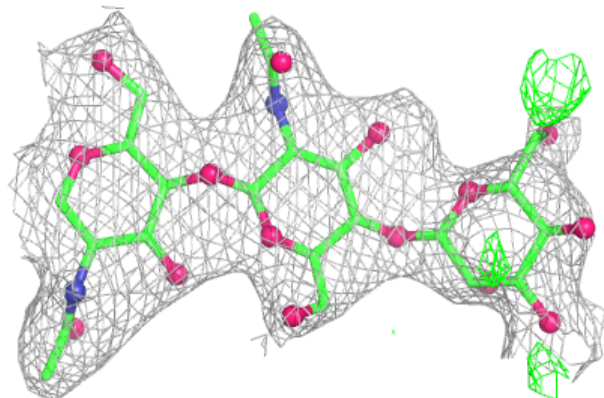


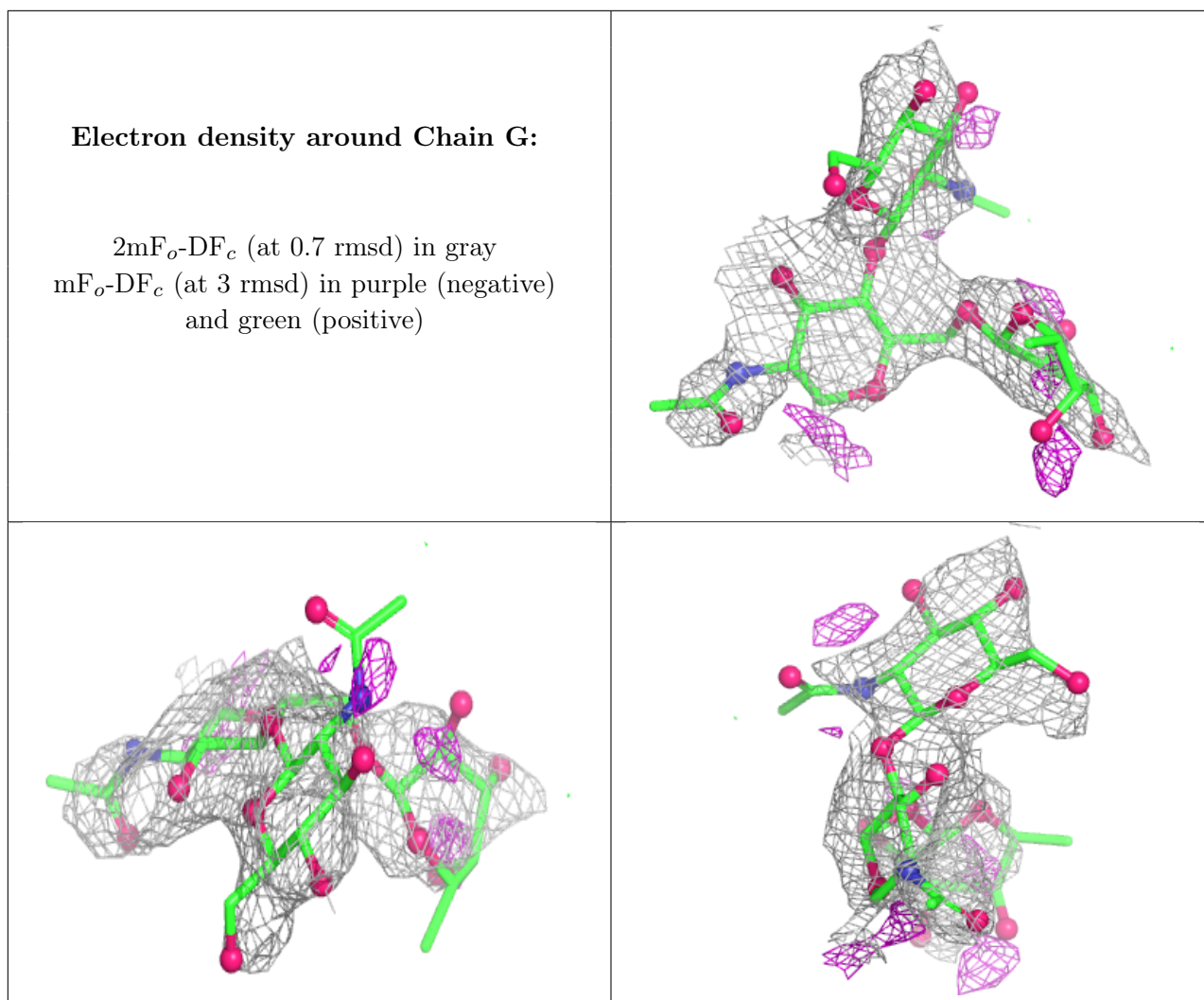
**Electron density around Chain D:**

$2mF_o-DF_c$  (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 [i](#)

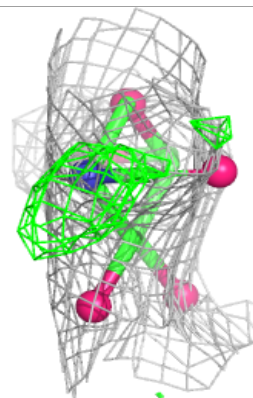
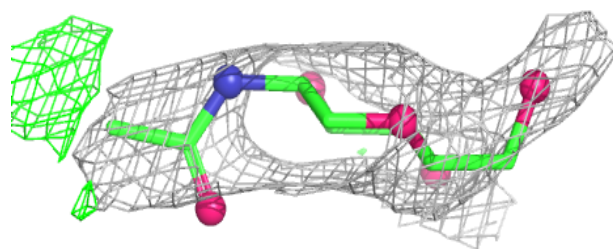
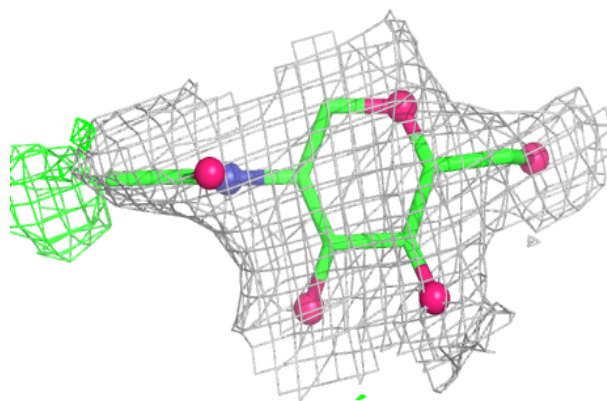
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	A	801	14/15	0.67	0.18	57,97,107,107	0
6	NAG	A	803	14/15	0.67	0.22	37,62,93,96	0
6	NAG	A	802	14/15	0.72	0.20	45,82,90,104	0

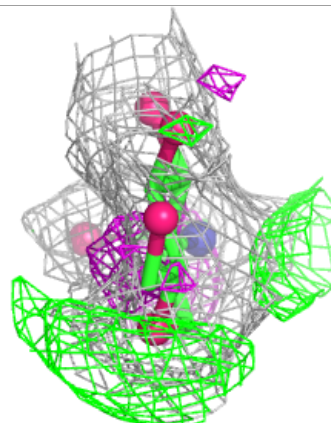
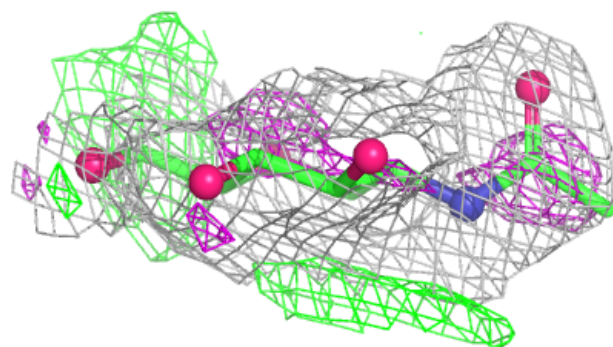
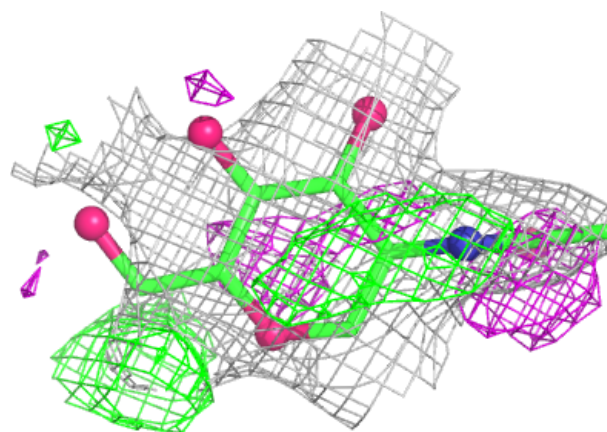
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

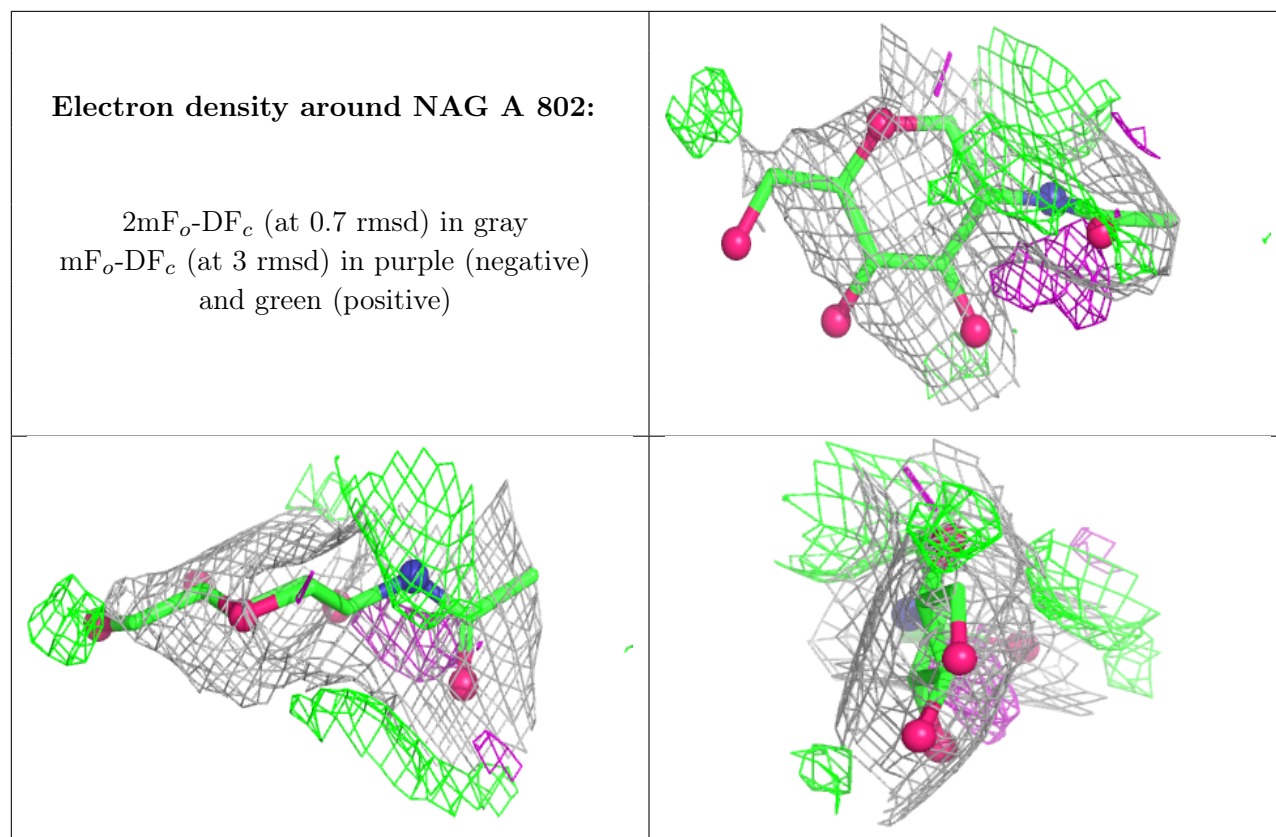
**Electron density around NAG A 801:**

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

**Electron density around NAG A 803:**

$2mF_o-DF_c$  (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.