



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2024 – 04:12 PM JST

PDB ID : 8WEF  
Title : Crystal structure of Brassica napus MIK2 ectodomain in complex with Fusarium oxysporum SCOOP  
Authors : Wan, L.H.; Hu, Y.X.; Wu, H.M.  
Deposited on : 2023-09-17  
Resolution : 2.80 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:

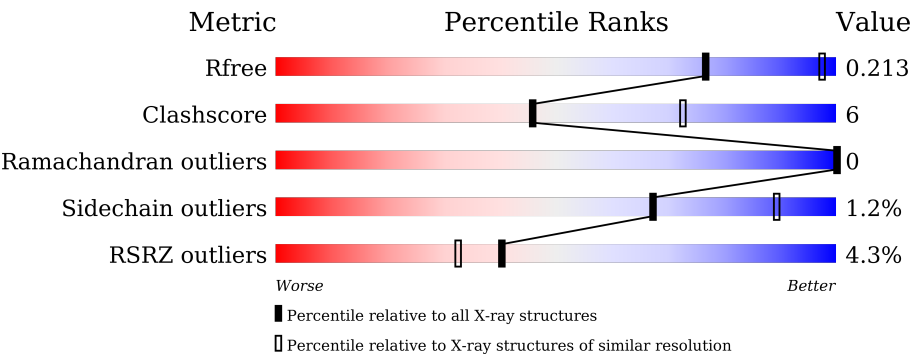
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

# 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 2.80 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.



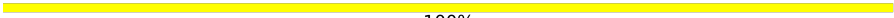


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	672	<div><div>3%</div><div></div><div>82%</div><div>14%</div><div>.</div></div>
2	C	13	<div><div>38%</div><div>15%</div><div>23%</div><div>62%</div></div>
3	B	3	<div><div>33%</div><div>67%</div></div>
4	D	2	<div><div>100%</div></div>
4	F	2	<div><div>50%</div><div>50%</div></div>
4	G	2	<div><div>50%</div><div>50%</div></div>

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Mol	Chain	Length	Quality of chain
4	H	2	 100%
5	E	4	 75% 25%
6	I	3	 67% 33%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5450 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
1	A	644	Total	C	N	O	S	0	0	0
			4981	3145	841	980	15			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 a protein called a SCOOP-like peptide from *F. oxysporum* f. sp. *conglutinans* strain Fo5176.

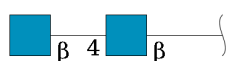
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			33	17	5	11			

- Molecule 3 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.



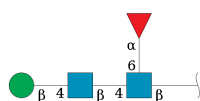
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



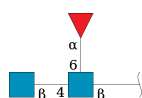
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.



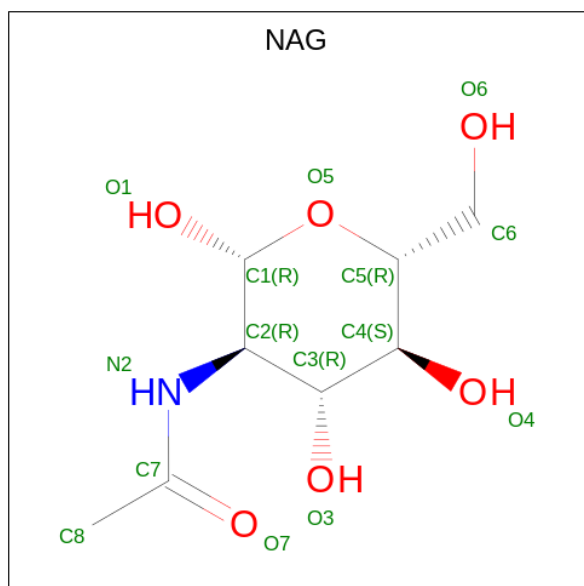
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 6 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
6	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

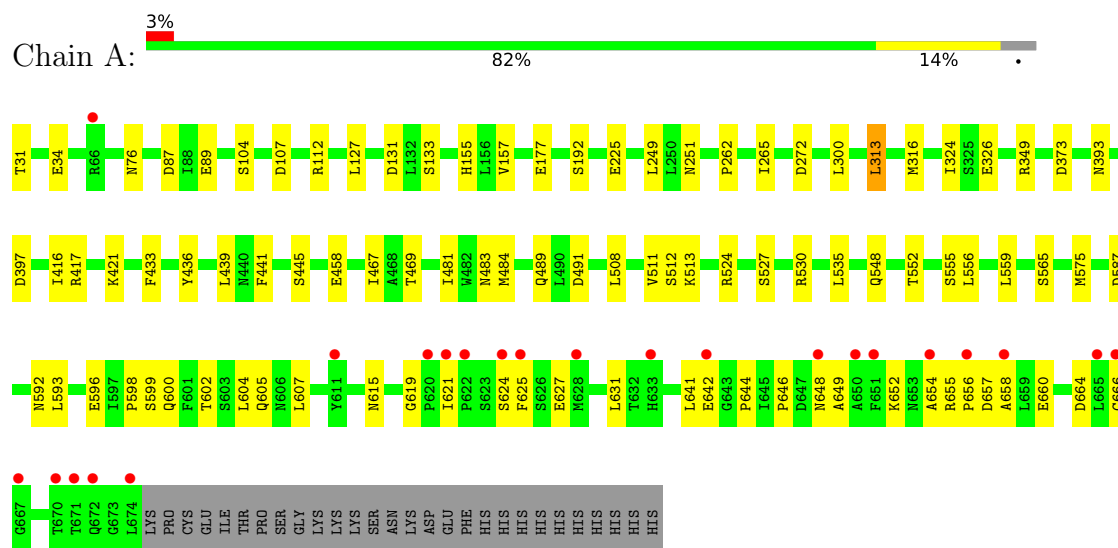
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	168	Total	O	0	0
			168	168		
8	C	2	Total	O	0	0
			2	2		

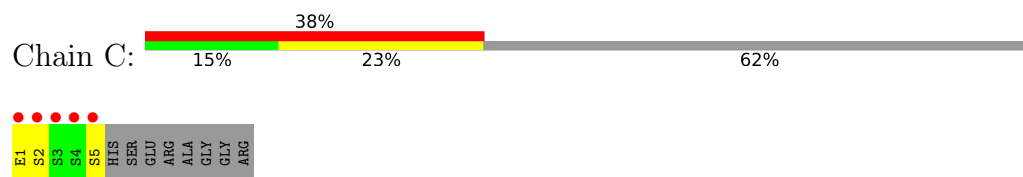
### 3 Residue-property plots

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: a SCOOP-like peptide from *F. oxysporum* f. sp. *conglutinans* strain Fo5176



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



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





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

Chain F:



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

Chain G:



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

Chain H:



- Molecule 5: 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 E:



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

Chain I:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.96Å 155.96Å 125.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.71 – 2.80 29.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.71-2.80) 98.6 (29.71-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.185 , 0.211 0.186 , 0.213	Depositor DCC
$R_{free}$ test set	2185 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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	0.27	0/5080	0.51	0/6909
2	C	0.30	0/32	0.38	0/41
All	All	0.27	0/5112	0.51	0/6950

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	4969	58	0
2	C	33	0	28	5	0
3	B	39	0	34	1	0
4	D	28	0	25	0	0
4	F	28	0	25	1	0
4	G	28	0	25	3	0
4	H	28	0	25	1	0
5	E	49	0	43	0	0
6	I	38	0	34	0	0
7	A	28	0	26	1	0
8	A	168	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	2	0	0	0	0
All	All	5450	0	5234	60	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 (60) 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:417:ARG:HB2	4:G:1:NAG:H62	1.54	0.87
1:A:657:ASP:HA	1:A:660:GLU:OE2	1.85	0.77
1:A:31:THR:OG1	1:A:76:ASN:O	2.01	0.76
1:A:300:LEU:HB2	1:A:324:ILE:HG22	1.68	0.74
1:A:416:ILE:HG22	4:G:1:NAG:H61	1.74	0.69
1:A:131:ASP:OD2	2:C:1:GLU:OE2	2.08	0.69
1:A:596:GLU:HG2	1:A:619:GLY:HA3	1.77	0.65
1:A:177:GLU:OE2	2:C:2:SER:HB2	1.97	0.64
1:A:251:ASN:ND2	2:C:5:SER:O	2.33	0.61
1:A:644:PRO:HA	1:A:666:CYS:HA	1.86	0.57
1:A:648:ASN:OD1	1:A:649:ALA:N	2.40	0.54
1:A:599:SER:O	1:A:602:THR:HG23	2.07	0.54
1:A:593:LEU:HD12	1:A:615:ASN:HD21	1.73	0.53
1:A:393:ASN:HD22	4:G:1:NAG:H83	1.74	0.53
1:A:107:ASP:HB2	3:B:1:NAG:H82	1.93	0.51
1:A:489:GLN:HG3	1:A:513:LYS:HB3	1.93	0.51
1:A:313:LEU:O	1:A:316:MET:HG3	2.12	0.50
1:A:436:TYR:HB3	1:A:439:LEU:HB2	1.94	0.50
1:A:642:GLU:HB2	1:A:664:ASP:HB3	1.92	0.50
1:A:481:ILE:O	1:A:484:MET:HG3	2.12	0.49
1:A:655:ARG:HB2	1:A:657:ASP:OD1	2.13	0.48
1:A:433:PHE:HB3	1:A:436:TYR:HE2	1.79	0.48
1:A:104:SER:HA	1:A:127:LEU:HA	1.96	0.47
1:A:648:ASN:O	1:A:652:LYS:HG3	2.14	0.47
1:A:467:ILE:HG23	1:A:491:ASP:HB3	1.95	0.47
1:A:421:LYS:HA	1:A:445:SER:O	2.15	0.47
1:A:575:MET:CE	1:A:598:PRO:HB3	2.45	0.47
1:A:89:GLU:OE1	1:A:112:ARG:NH1	2.47	0.47
1:A:133:SER:HB3	1:A:157:VAL:HG22	1.96	0.47
1:A:593:LEU:HD12	1:A:615:ASN:ND2	2.29	0.47
1:A:621:ILE:HG21	1:A:646:PRO:HD3	1.96	0.47
2:C:2:SER:O	2:C:2:SER:OG	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:ASP:OD2	4:H:1:NAG:N2	2.36	0.46
1:A:600:GLN:OE1	1:A:600:GLN:N	2.47	0.46
1:A:225:GLU:HG2	1:A:249:LEU:HB3	1.98	0.46
1:A:654:ALA:HB1	1:A:658:ALA:HB3	1.97	0.45
1:A:31:THR:HA	1:A:34:GLU:HB2	1.99	0.45
1:A:483:ASN:ND2	8:A:902:HOH:O	2.42	0.45
1:A:530:ARG:HD2	1:A:552:THR:HB	1.97	0.45
1:A:262:PRO:HG2	1:A:265:ILE:HG12	1.98	0.45
1:A:655:ARG:HB3	1:A:656:PRO:HD2	1.99	0.44
1:A:527:SER:O	1:A:530:ARG:HB2	2.18	0.43
1:A:604:LEU:HD23	1:A:607:LEU:HD12	2.00	0.43
1:A:155:HIS:CE1	2:C:2:SER:HB3	2.53	0.43
1:A:624:SER:O	1:A:625:PHE:HB2	2.19	0.43
1:A:192:SER:HA	7:A:802:NAG:H82	2.01	0.43
1:A:524:ARG:NH2	1:A:548:GLN:HG2	2.35	0.42
1:A:530:ARG:NH1	1:A:555:SER:OG	2.52	0.42
1:A:621:ILE:HD13	1:A:641:LEU:HD22	2.01	0.42
4:F:2:NAG:H83	4:F:2:NAG:H3	2.01	0.42
1:A:607:LEU:O	1:A:631:LEU:HD12	2.19	0.42
1:A:508:LEU:O	1:A:511:VAL:HG12	2.20	0.41
1:A:417:ARG:HG3	1:A:441:PHE:HB3	2.02	0.41
1:A:373:ASP:HB2	1:A:397:ASP:HB2	2.02	0.41
1:A:445:SER:HA	1:A:469:THR:O	2.21	0.41
1:A:605:GLN:HE22	1:A:627:GLU:HG2	1.86	0.41
1:A:512:SER:HA	1:A:535:LEU:HA	2.02	0.40
1:A:556:LEU:HB3	1:A:559:LEU:HB2	2.02	0.40
1:A:397:ASP:HA	1:A:421:LYS:O	2.21	0.40
1:A:458:GLU:HA	1:A:484:MET:SD	2.61	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	642/672 (96%)	633 (99%)	9 (1%)	0	100	100
2	C	3/13 (23%)	3 (100%)	0	0	100	100
All	All	645/685 (94%)	636 (99%)	9 (1%)	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	582/609 (96%)	575 (99%)	7 (1%)	67	89
2	C	5/10 (50%)	5 (100%)	0	100	100
All	All	587/619 (95%)	580 (99%)	7 (1%)	67	89

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

Mol	Chain	Res	Type
1	A	87	ASP
1	A	272	ASP
1	A	313	LEU
1	A	326	GLU
1	A	349	ARG
1	A	565	SER
1	A	592	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	582	GLN
1	A	614	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 ⓘ

18 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	B	1	3,1	14,14,15	0.39	0	17,19,21	0.61	0
3	NAG	B	2	3	14,14,15	0.23	0	17,19,21	0.52	0
3	BMA	B	3	3	11,11,12	0.90	1 (9%)	15,15,17	0.95	0
4	NAG	D	1	4,1	14,14,15	0.22	0	17,19,21	0.55	0
4	NAG	D	2	4	14,14,15	0.36	0	17,19,21	0.45	0
5	NAG	E	1	5,1	14,14,15	0.64	1 (7%)	17,19,21	0.48	0
5	NAG	E	2	5	14,14,15	0.27	0	17,19,21	0.39	0
5	BMA	E	3	5	11,11,12	0.86	0	15,15,17	0.83	0
5	FUC	E	4	5	10,10,11	0.74	0	14,14,16	0.79	0
4	NAG	F	1	4,1	14,14,15	0.22	0	17,19,21	0.36	0
4	NAG	F	2	4	14,14,15	0.56	0	17,19,21	1.56	4 (23%)
4	NAG	G	1	4,1	14,14,15	2.05	2 (14%)	17,19,21	2.20	1 (5%)
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	H	1	4,1	14,14,15	0.35	0	17,19,21	0.41	0
4	NAG	H	2	4	14,14,15	0.26	0	17,19,21	0.60	1 (5%)
6	NAG	I	1	6,1	14,14,15	0.30	0	17,19,21	0.49	0
6	NAG	I	2	6	14,14,15	0.31	0	17,19,21	0.42	0
6	FUC	I	3	6	10,10,11	1.07	1 (10%)	14,14,16	1.10	1 (7%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	O5-C1	7.10	1.55	1.43
4	G	1	NAG	C1-C2	2.78	1.56	1.52
5	E	1	NAG	O5-C1	-2.30	1.40	1.43
6	I	3	FUC	C2-C3	2.08	1.55	1.52
3	B	3	BMA	C1-C2	2.08	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C1-O5-C5	8.65	123.92	112.19
4	F	2	NAG	C2-N2-C7	4.45	129.24	122.90
4	F	2	NAG	C3-C4-C5	2.42	114.55	110.24
4	F	2	NAG	C1-O5-C5	2.41	115.45	112.19
4	F	2	NAG	C1-C2-N2	2.10	114.07	110.49
6	I	3	FUC	C1-O5-C5	2.02	117.36	112.78
4	H	2	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
4	H	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C3-C2-N2-C7

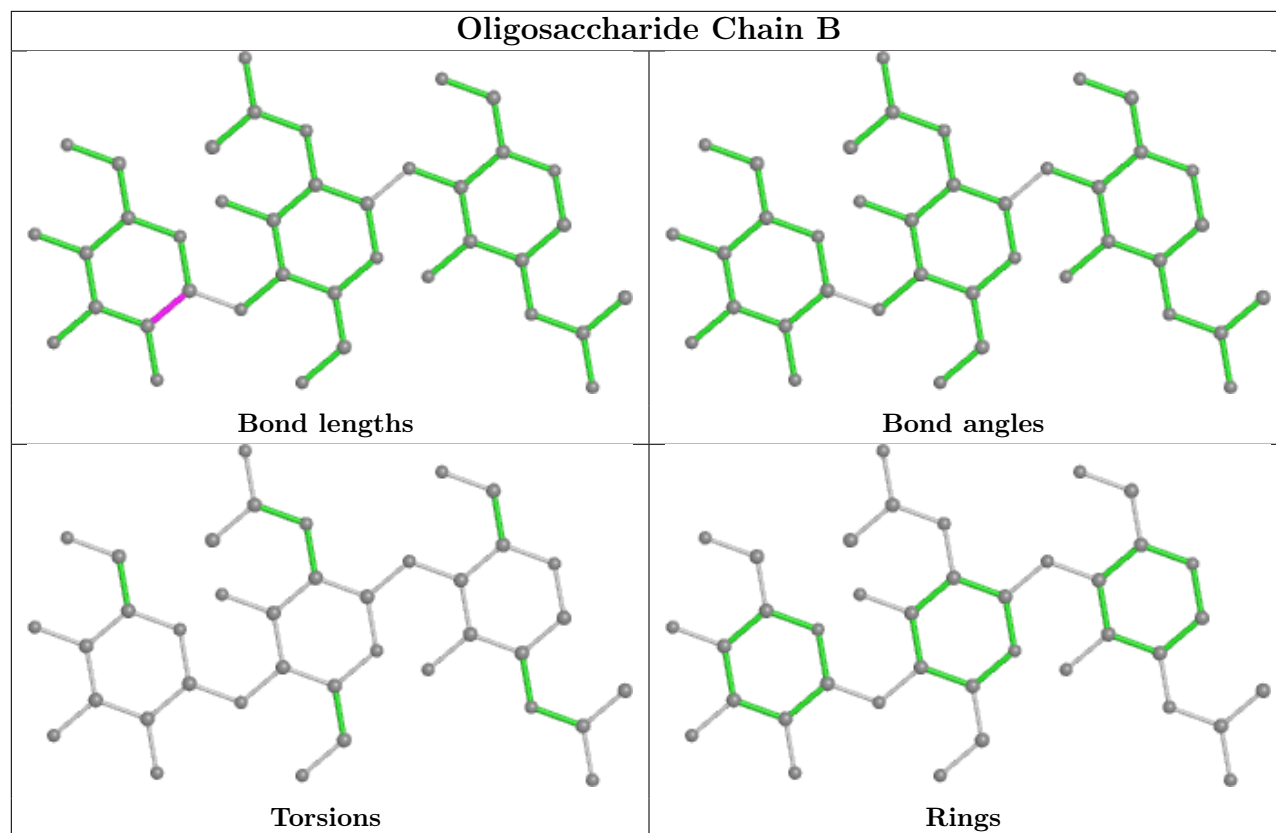
There are no ring outliers.

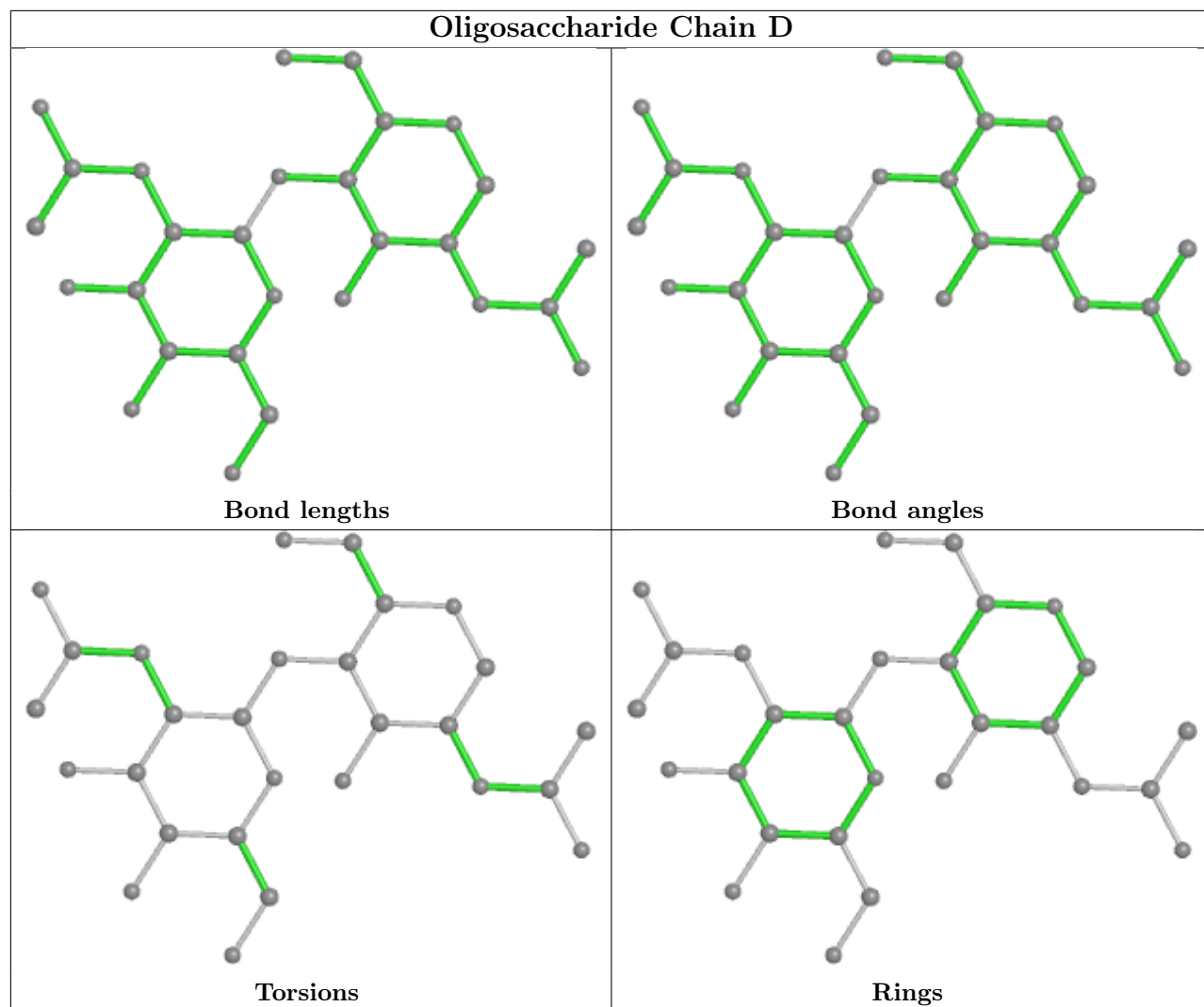
4 monomers are involved in 6 short contacts:

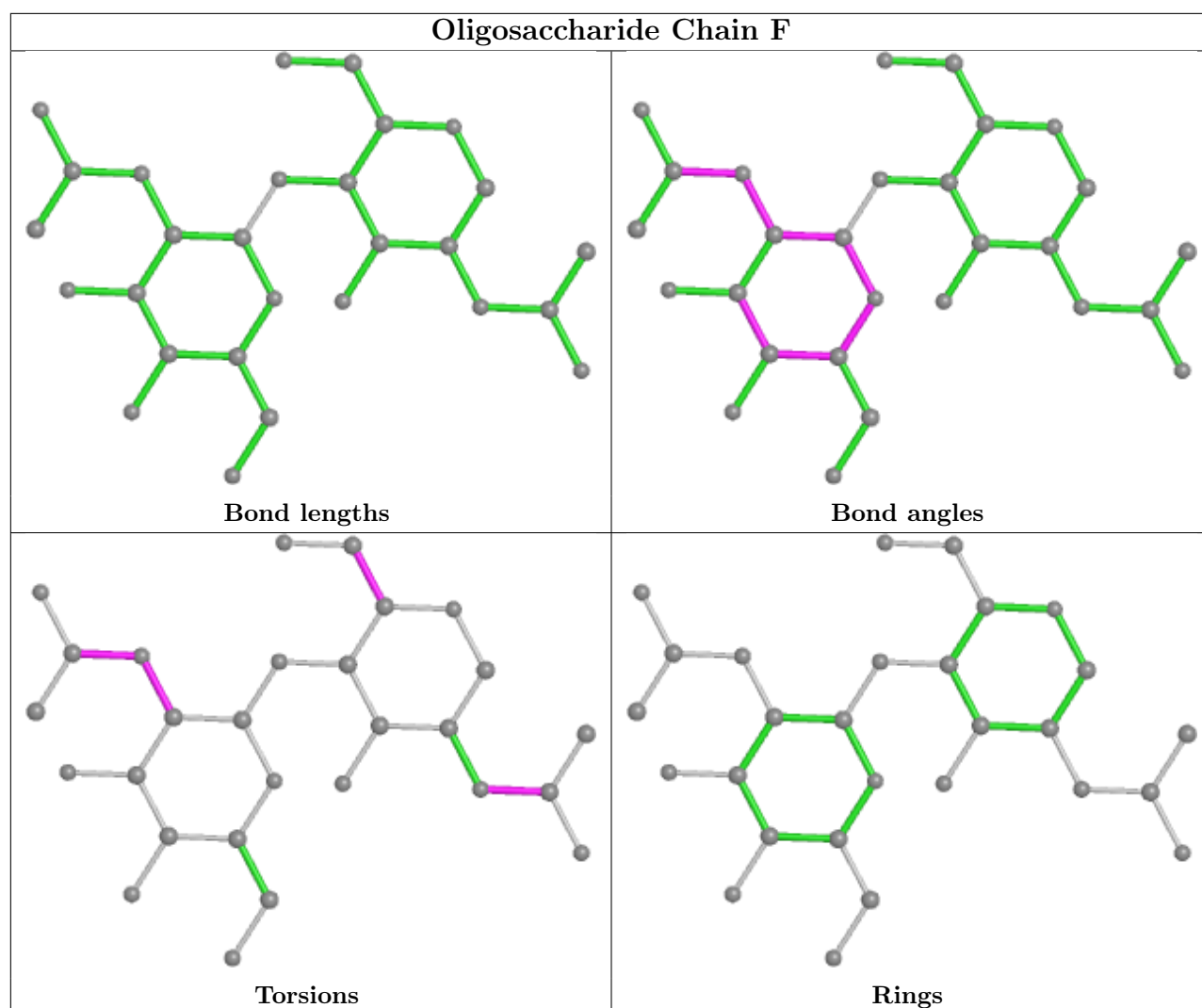
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	3	0
3	B	1	NAG	1	0
4	H	1	NAG	1	0
4	F	2	NAG	1	0

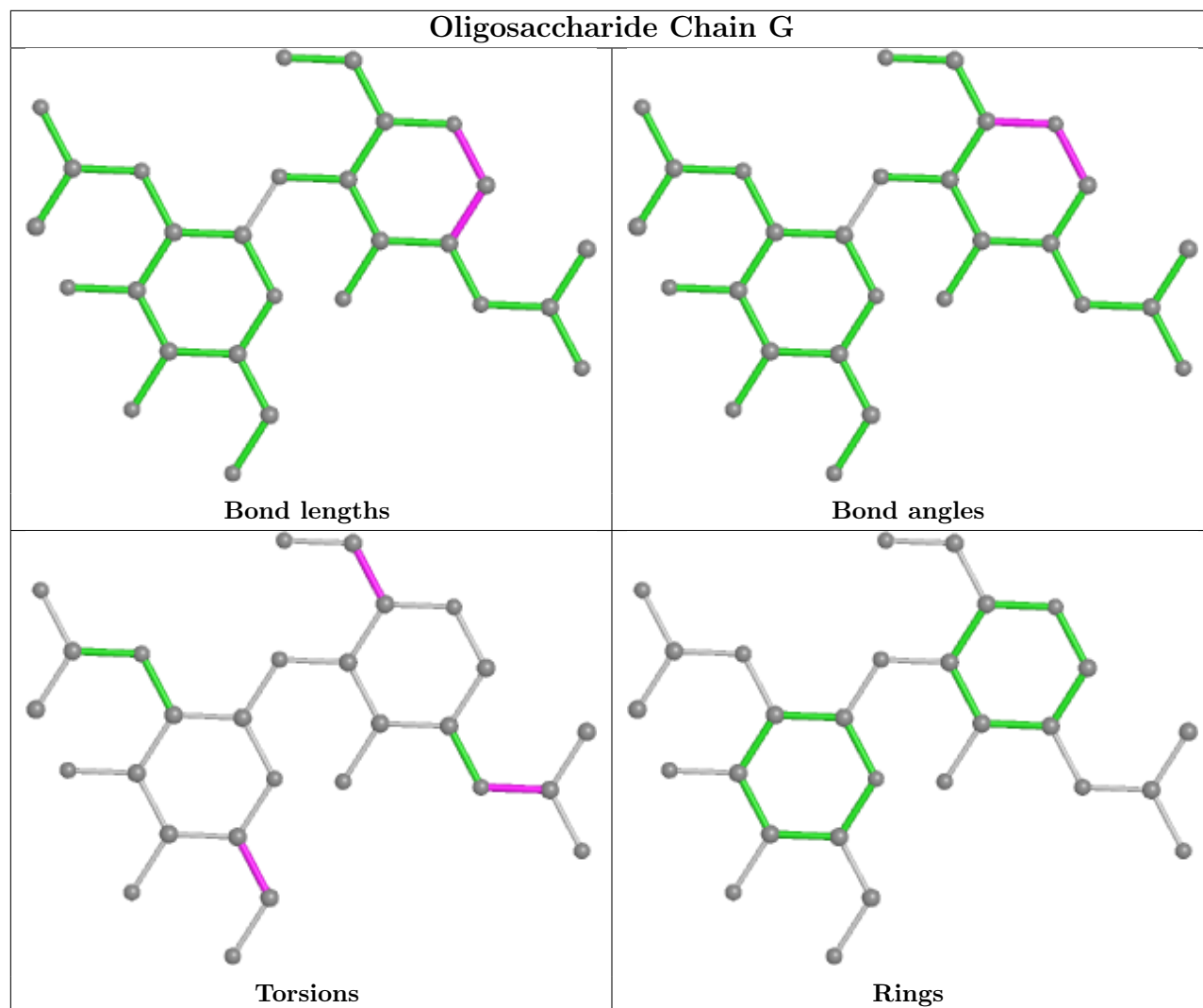
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

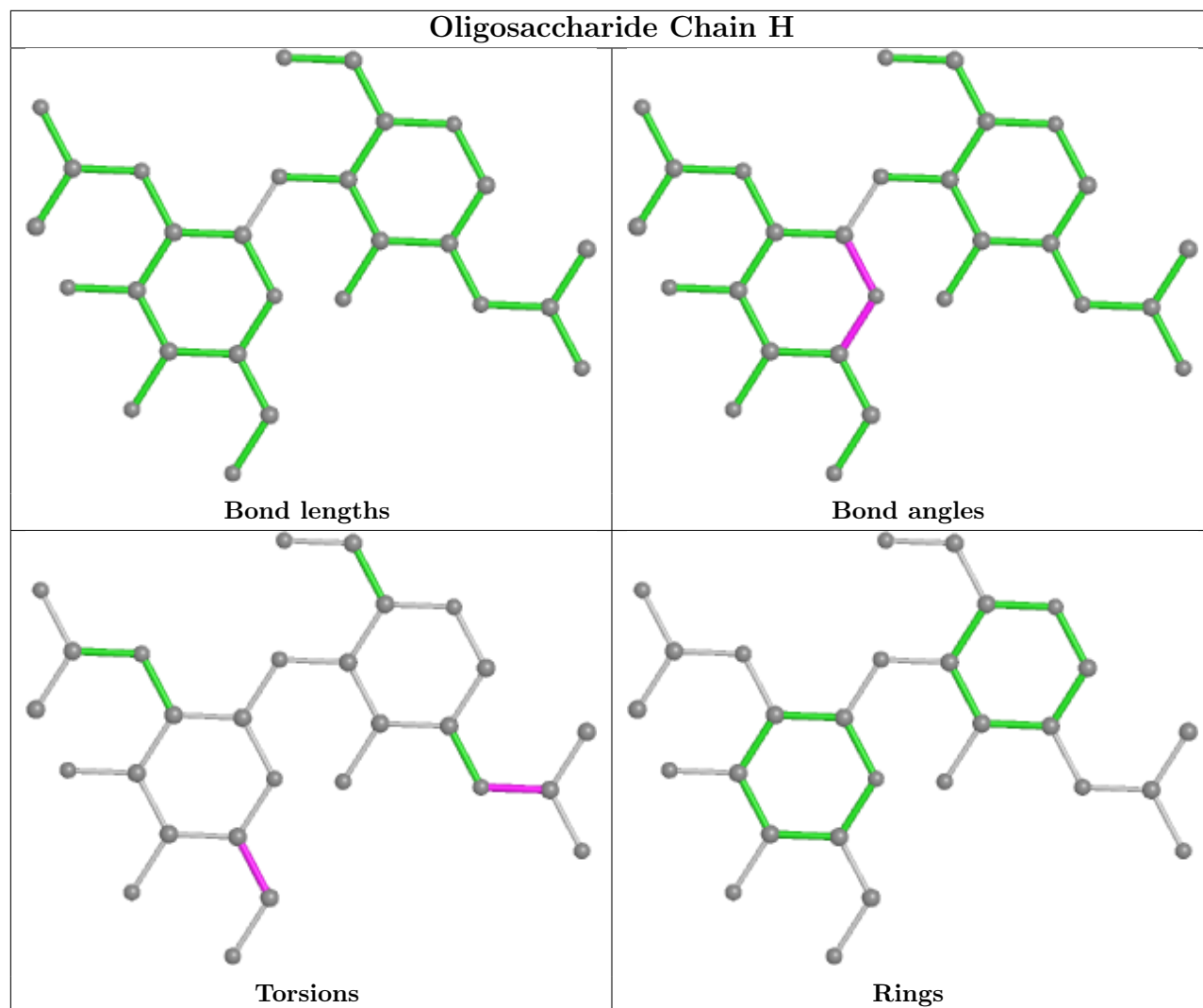


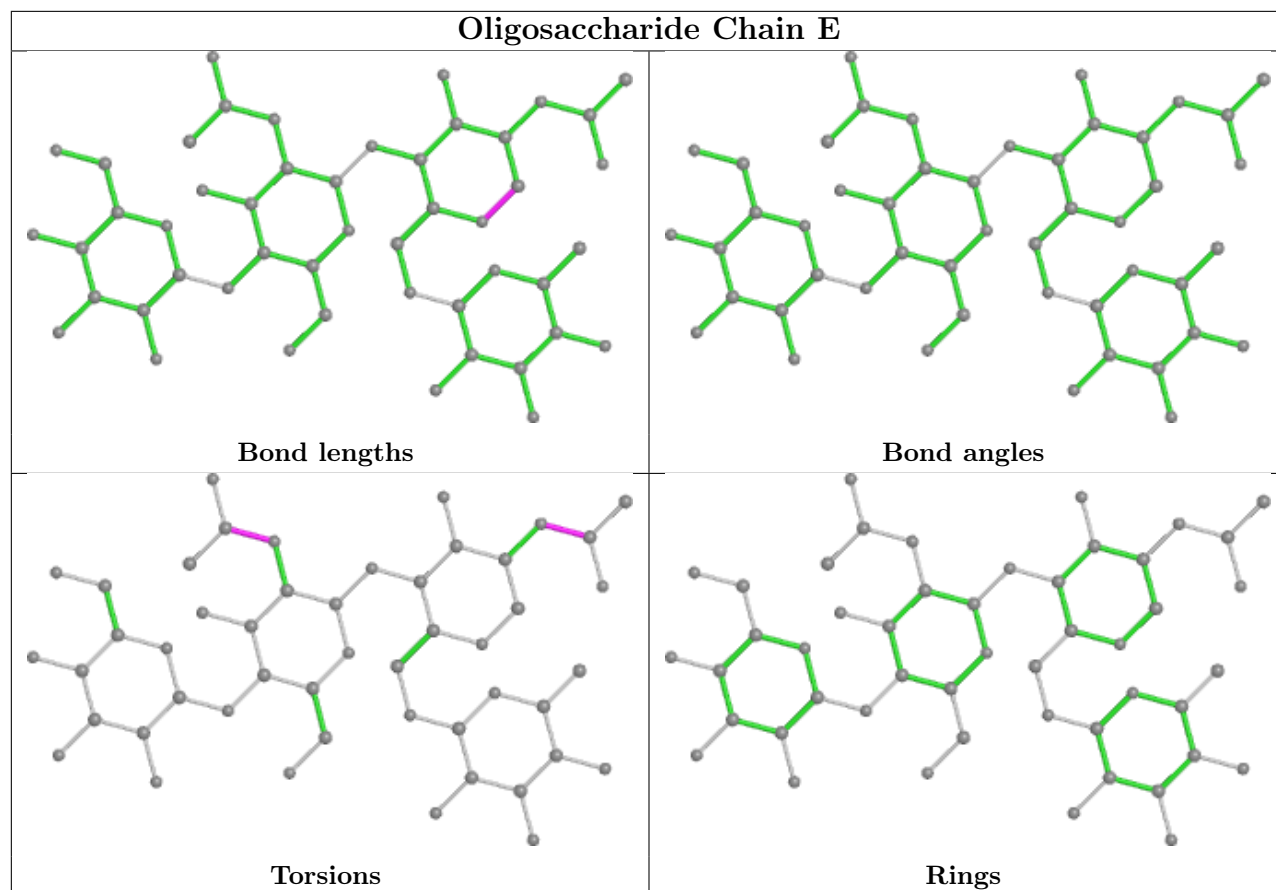


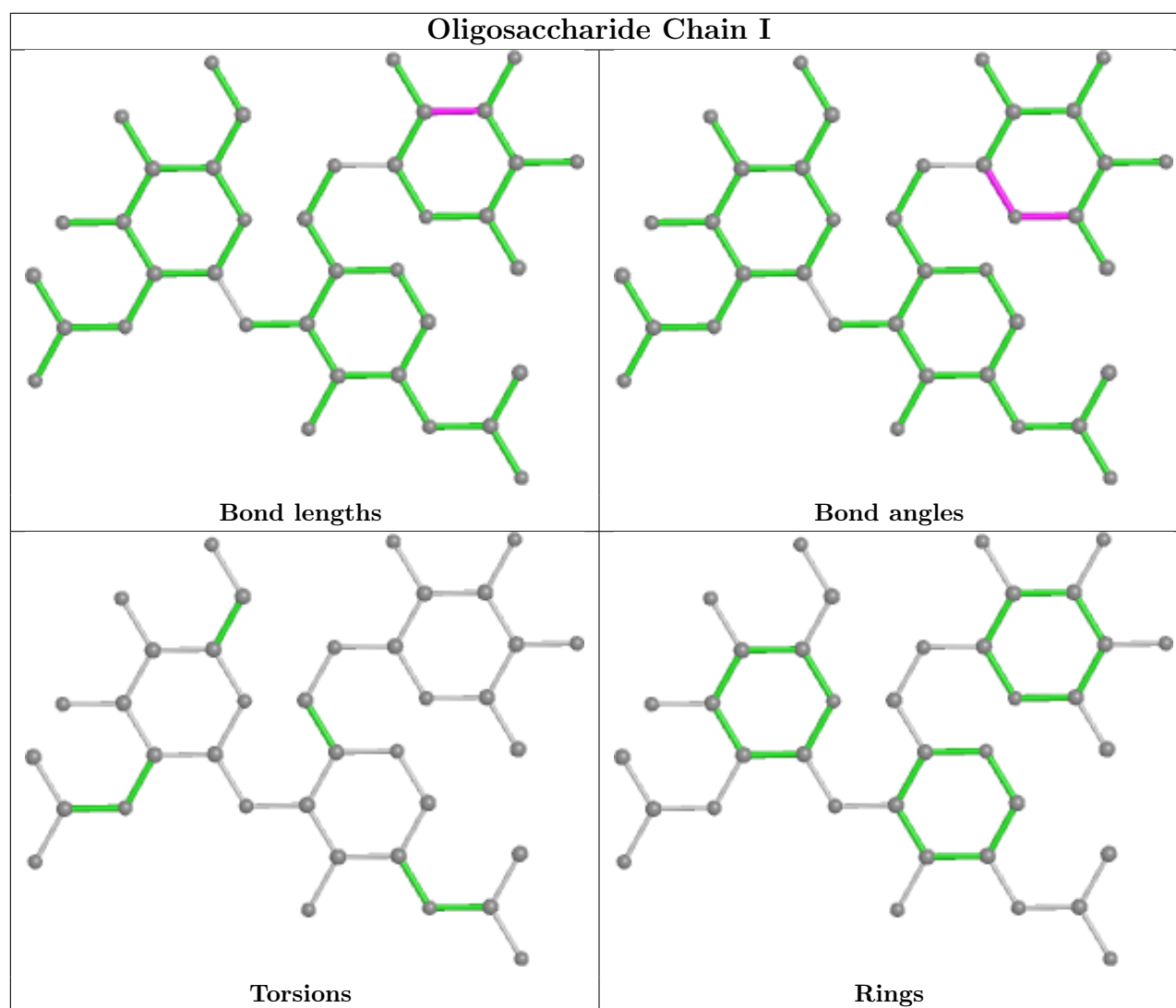












## 5.6 Ligand geometry [i](#)

2 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	A	801	1	14,14,15	0.36	0	17,19,21	0.60	0
7	NAG	A	802	1	14,14,15	0.40	0	17,19,21	0.50	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	A	801	1	-	1/6/23/26	0/1/1/1
7	NAG	A	802	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

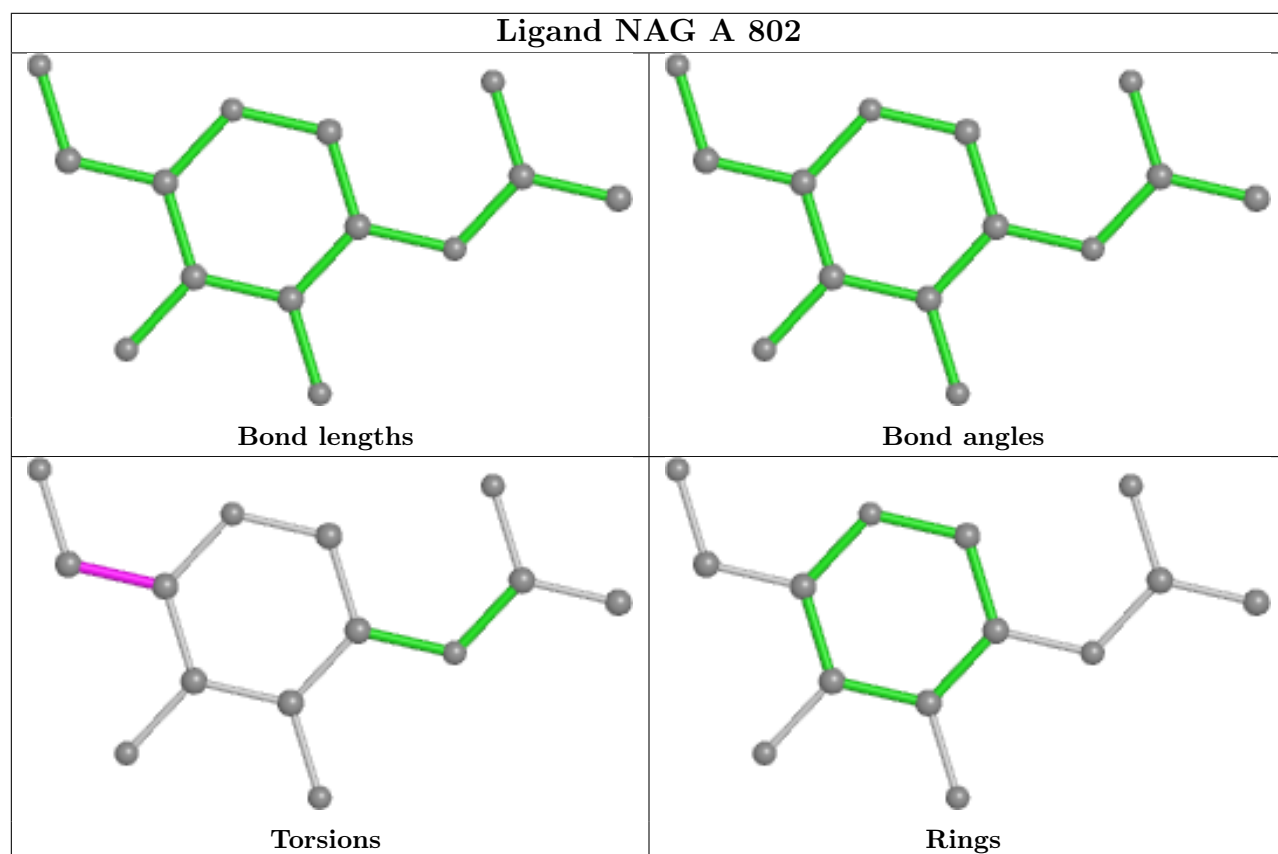
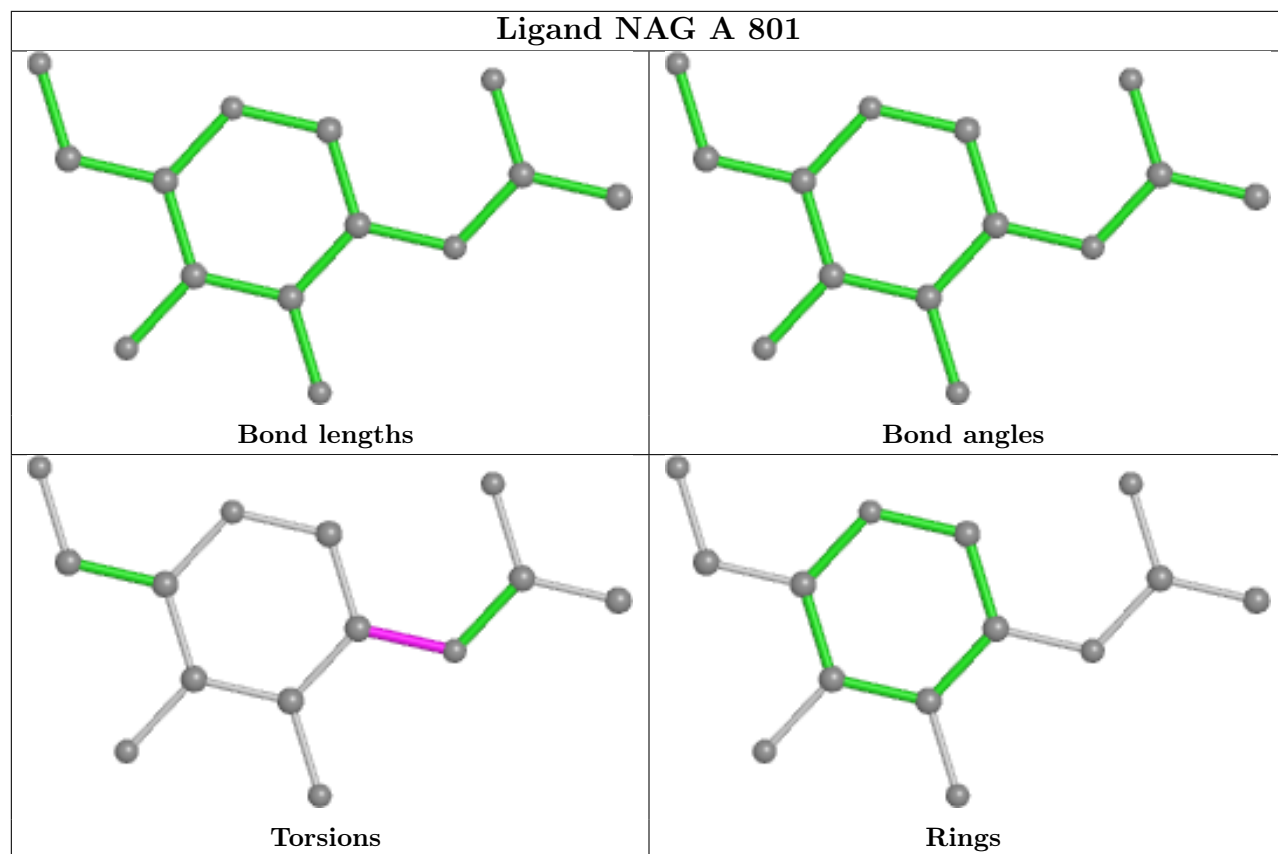
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	802	NAG	1	0

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





## 5.7 Other polymers

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, 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	644/672 (95%)	-0.42	23 (3%) 46 38	47, 68, 150, 201	0
2	C	5/13 (38%)	3.25	5 (100%) 0 0	103, 117, 129, 138	0
All	All	649/685 (94%)	-0.40	28 (4%) 40 32	47, 68, 150, 201	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	621	ILE	7.2
1	A	674	LEU	6.6
2	C	4	SER	5.2
1	A	620	PRO	4.6
1	A	671	THR	4.5
1	A	672	GLN	4.2
1	A	670	THR	4.1
1	A	648	ASN	3.9
1	A	665	LEU	3.7
1	A	622	PRO	3.4
1	A	656	PRO	3.3
1	A	66	ARG	3.2
2	C	5	SER	3.1
1	A	667	GLY	3.0
2	C	1	GLU	2.9
1	A	651	PHE	2.9
1	A	666	CYS	2.8
2	C	2	SER	2.8
1	A	628	MET	2.6
1	A	654	ALA	2.5
1	A	625	PHE	2.5
1	A	658	ALA	2.3
1	A	642	GLU	2.3
2	C	3	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	624	SER	2.1
1	A	650	ALA	2.1
1	A	611	TYR	2.0
1	A	633	HIS	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](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands [i](#)

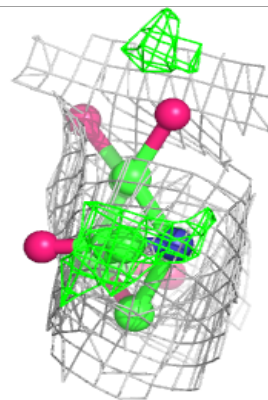
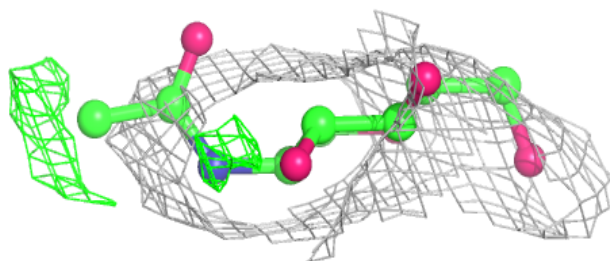
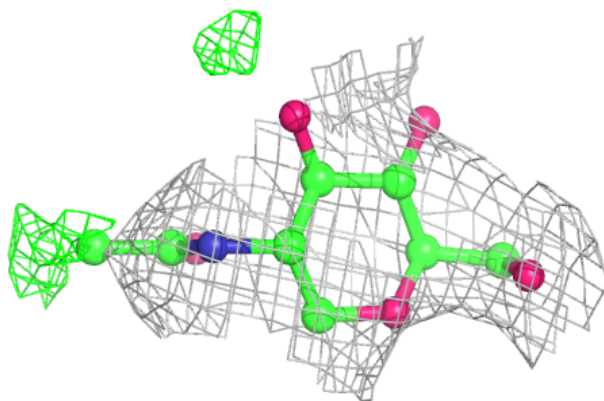
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	A	801	14/15	0.67	0.18	121,140,151,153	0
7	NAG	A	802	14/15	0.69	0.15	86,119,136,150	0

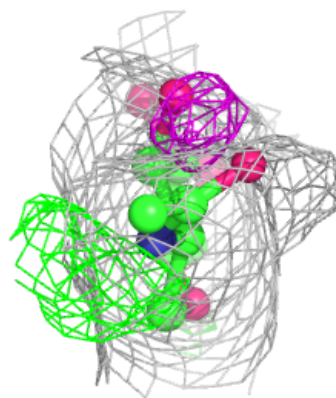
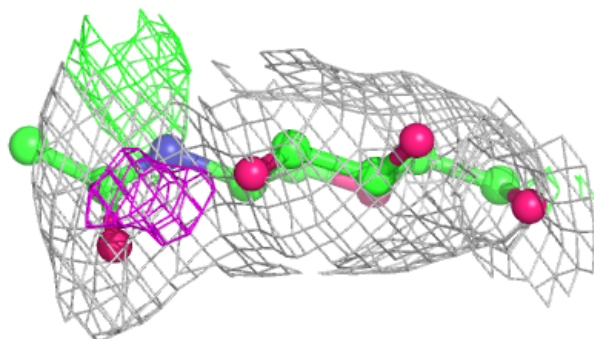
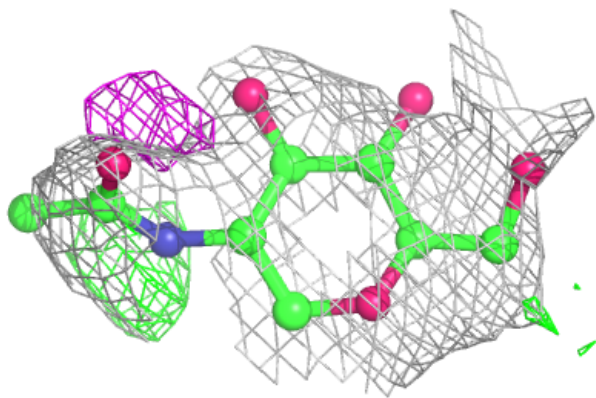
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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 802:**

$2mF_o-DF_c$  (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.