



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 11:07 PM EDT

PDB ID : 4J0M  
Title : Crystal structure of BRL1 (LRR) in complex with brassinolide  
Authors : Chai, J.; She, J.; Han, Z.; Zhou, B.  
Deposited on : 2013-01-31  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

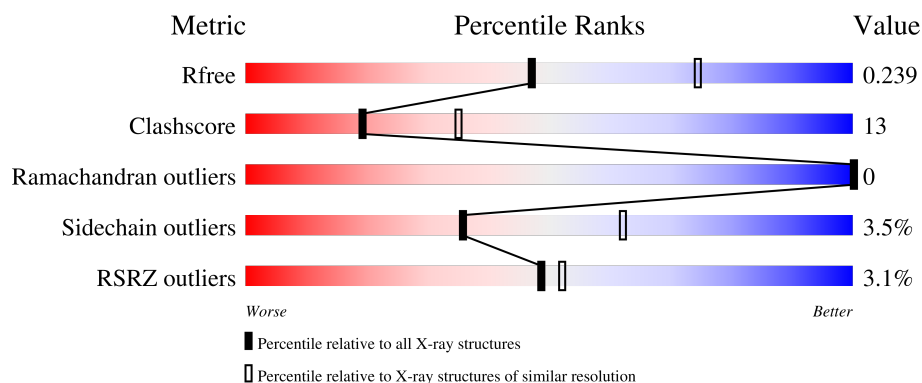
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	740	<div> <div>3%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	B	740	<div> <div>3%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>100%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 50%50%
2	J	2	 100%
2	K	2	 50%50%
3	D	6	 67%33%
3	I	6	 83%17%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11785 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.

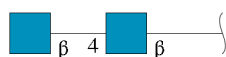
- Molecule 1 is a protein called Serine/threonine-protein kinase BRI1-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	0	0
			5455	3446	913	1067	29			
1	B	724	Total	C	N	O	S	0	0	0
			5455	3446	913	1067	29			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	759	HIS	-	expression tag	UNP Q9ZWC8
A	760	HIS	-	expression tag	UNP Q9ZWC8
A	761	HIS	-	expression tag	UNP Q9ZWC8
A	762	HIS	-	expression tag	UNP Q9ZWC8
A	763	HIS	-	expression tag	UNP Q9ZWC8
A	764	HIS	-	expression tag	UNP Q9ZWC8
B	759	HIS	-	expression tag	UNP Q9ZWC8
B	760	HIS	-	expression tag	UNP Q9ZWC8
B	761	HIS	-	expression tag	UNP Q9ZWC8
B	762	HIS	-	expression tag	UNP Q9ZWC8
B	763	HIS	-	expression tag	UNP Q9ZWC8
B	764	HIS	-	expression tag	UNP Q9ZWC8

- 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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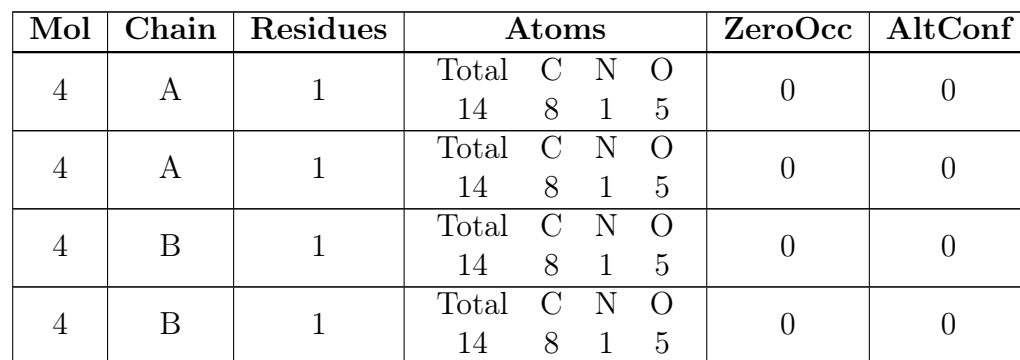
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-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	D	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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- The chemical structure of BLD (Bisdolide) is a complex polycyclic molecule. It features a central core with several fused and bridged rings. Key features include:
- Functional Groups:** Two hydroxyl groups (HO) are highlighted in red, attached to C23(R) and C22(S). A carboxylic acid group is present at the bottom, with a carbonyl oxygen (O=) and a hydroxyl group (OH) attached to C06.
  - Stereocenters:** Numerous chiral centers are indicated with wedged and dashed bonds. Labeled centers include C18, C17(R), C16, C15, C14(S), C13(S), C12, C11, C10(R), C09(S), C08(S), C07, C06, C05, C04, C03(S), C02(S), C01, C20(S), C21, C22(R), C23(R), C24(S), C25, C26, C27, and C28.
  - Ring System:** The structure includes a cyclohexane ring (C11-C16), a cyclopentane ring (C12-C16), and a cyclohexane ring (C01-C06). There are also several five-membered and six-membered rings formed by the bridging atoms.
  - Conformation:** The molecule is shown in a chair-like conformation for the cyclohexane rings, with various substituents in axial or equatorial positions.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			34	28	6		
5	B	1	Total	C	O	0	0
			34	28	6		

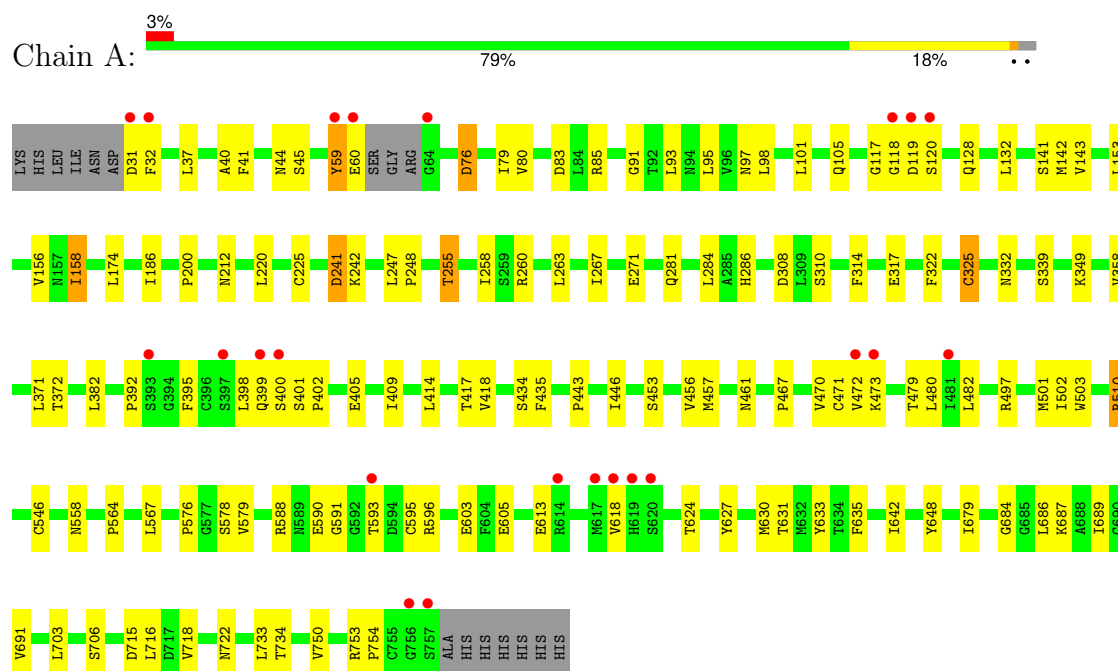
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total	O	0	0
			210	210		
6	B	201	Total	O	0	0
			201	201		

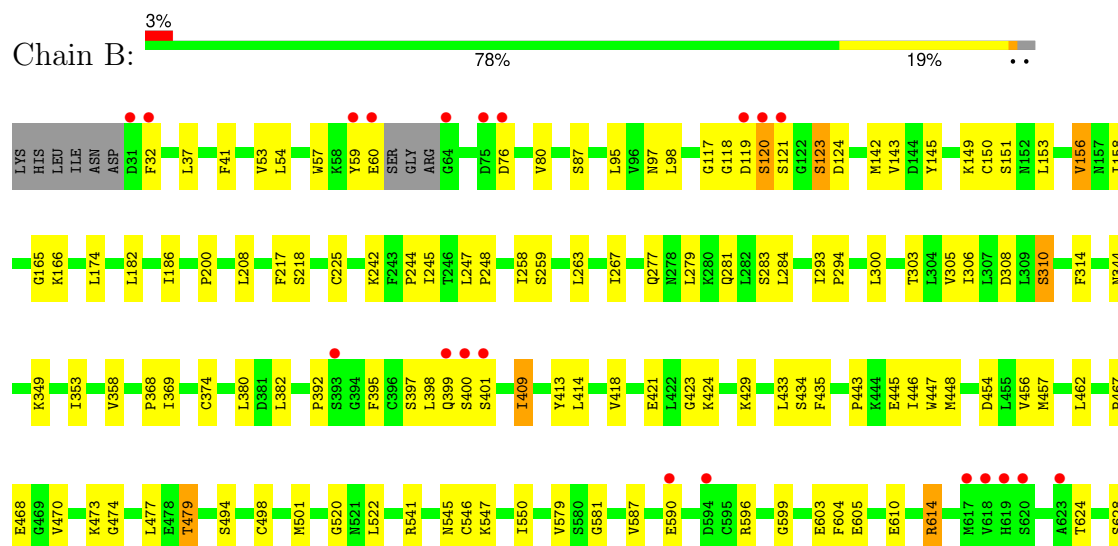
### 3 Residue-property plots [i](#)

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: Serine/threonine-protein kinase BRI1-like 1



#### • Molecule 1: Serine/threonine-protein kinase BRI1-like 1







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



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



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



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



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



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

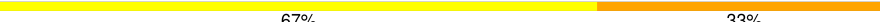


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%


  
MAG1  
MAG2

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

Chain D:  67% 33%

  
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain I:  83% 17%

  
MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.86Å 83.40Å 264.06Å 90.00° 97.24° 90.00°	Depositor
Resolution (Å)	29.83 – 2.50 29.83 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.83-2.50) 93.9 (29.83-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.32 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.187 , 0.239 0.188 , 0.239	Depositor DCC
$R_{free}$ test set	3786 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, MAN, BLD, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.43	0/5561	0.67	0/7559
1	B	0.42	0/5561	0.66	1/7559 (0.0%)
All	All	0.42	0/11122	0.66	1/15118 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	156	VAL	CB-CA-C	-5.11	101.69	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	120	SER	Peptide

### 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	5455	0	5391	144	0
1	B	5455	0	5390	133	1
2	C	28	0	25	2	0
2	E	28	0	24	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
3	D	72	0	55	7	0
3	I	72	0	54	1	0
4	A	28	0	26	2	0
4	B	28	0	26	0	0
5	A	34	0	48	5	0
5	B	34	0	48	5	0
6	A	210	0	0	8	0
6	B	201	0	0	11	0
All	All	11785	0	11212	291	1

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 13.

The worst 5 of 291 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:B:120:SER:HB3	1:B:145:TYR:HB2	1.26	1.17
1:B:118:GLY:H	1:B:142:MET:HE3	1.06	1.15
1:A:95:LEU:HD22	1:A:142:MET:HE2	1.30	1.12
1:B:590:GLU:HG2	1:B:624:THR:HG21	1.25	1.12
1:A:510:ARG:HG2	1:A:510:ARG:HH11	1.06	1.11

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ASP:OD1	1:B:541:ARG:NH1[1_545]	1.99	0.21

## 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	720/740 (97%)	685 (95%)	35 (5%)	0	100	100
1	B	720/740 (97%)	693 (96%)	27 (4%)	0	100	100
All	All	1440/1480 (97%)	1378 (96%)	62 (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	627/641 (98%)	604 (96%)	23 (4%)	34	60
1	B	627/641 (98%)	606 (97%)	21 (3%)	38	64
All	All	1254/1282 (98%)	1210 (96%)	44 (4%)	36	62

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	186	ILE
1	B	409	ILE
1	B	225	CYS
1	B	353	ILE
1	B	479	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

26 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	C	1	2,1	14,14,15	0.51	0	17,19,21	1.67	1 (5%)
2	NAG	C	2	2	14,14,15	0.45	0	17,19,21	1.33	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.58	0	17,19,21	1.84	4 (23%)
3	NAG	D	2	3	14,14,15	1.90	4 (28%)	17,19,21	2.15	5 (29%)
3	BMA	D	3	3	11,11,12	1.09	1 (9%)	15,15,17	1.41	2 (13%)
3	MAN	D	4	3	11,11,12	1.42	3 (27%)	15,15,17	1.82	3 (20%)
3	MAN	D	5	3	11,11,12	3.96	1 (9%)	15,15,17	1.33	1 (6%)
3	MAN	D	6	3	11,11,12	2.03	5 (45%)	15,15,17	1.55	3 (20%)
2	NAG	E	1	2,1	14,14,15	1.93	3 (21%)	17,19,21	2.63	6 (35%)
2	NAG	E	2	2	14,14,15	1.66	3 (21%)	17,19,21	2.41	5 (29%)
2	NAG	F	1	2,1	14,14,15	0.59	0	17,19,21	0.74	0
2	NAG	F	2	2	14,14,15	0.47	0	17,19,21	0.89	2 (11%)
2	NAG	G	1	2,1	14,14,15	0.48	0	17,19,21	2.29	7 (41%)
2	NAG	G	2	2	14,14,15	0.47	0	17,19,21	1.07	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.51	0	17,19,21	1.77	1 (5%)
2	NAG	H	2	2	14,14,15	0.48	0	17,19,21	1.51	1 (5%)
3	NAG	I	1	1,3	14,14,15	2.06	7 (50%)	17,19,21	2.12	3 (17%)
3	NAG	I	2	3	14,14,15	2.31	6 (42%)	17,19,21	2.54	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	I	3	3	11,11,12	1.06	2 (18%)	15,15,17	1.31	2 (13%)
3	MAN	I	4	3	11,11,12	1.66	3 (27%)	15,15,17	1.70	3 (20%)
3	MAN	I	5	3	11,11,12	2.16	4 (36%)	15,15,17	2.96	4 (26%)
3	MAN	I	6	3	11,11,12	2.34	5 (45%)	15,15,17	1.38	2 (13%)
2	NAG	J	1	2,1	14,14,15	0.66	0	17,19,21	1.09	2 (11%)
2	NAG	J	2	2	14,14,15	0.56	0	17,19,21	1.24	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.64	0	17,19,21	1.03	1 (5%)
2	NAG	K	2	2	14,14,15	0.51	0	17,19,21	0.78	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
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
3	MAN	I	5	3	-	2/2/19/22	0/1/1/1
3	MAN	I	6	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	MAN	O6-C6	-12.91	0.88	1.42
3	I	2	NAG	O5-C1	-4.89	1.35	1.43
3	I	6	MAN	O5-C1	-4.44	1.36	1.43
3	I	1	NAG	O5-C1	-4.39	1.36	1.43
3	I	5	MAN	O5-C1	-4.06	1.36	1.43

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	O5-C1-C2	-7.80	99.22	111.29
3	I	5	MAN	C1-O5-C5	7.52	122.26	112.19
3	I	5	MAN	O5-C5-C6	-7.36	93.33	107.66
2	G	1	NAG	C1-O5-C5	6.93	121.48	112.19
2	H	1	NAG	C1-O5-C5	6.59	121.02	112.19

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	K	1	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 12 short contacts:

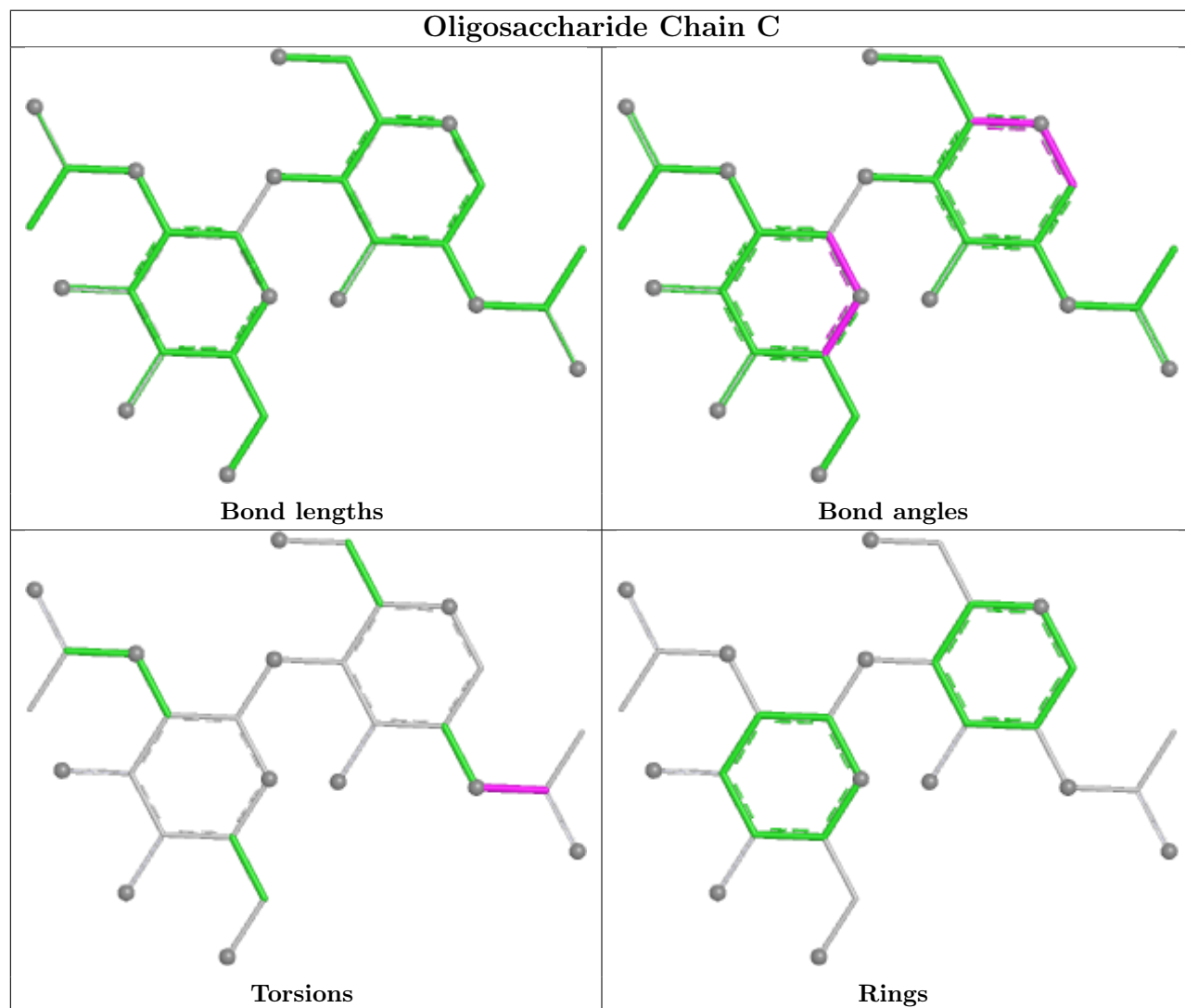
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
2	E	1	NAG	1	0
3	I	1	NAG	1	0

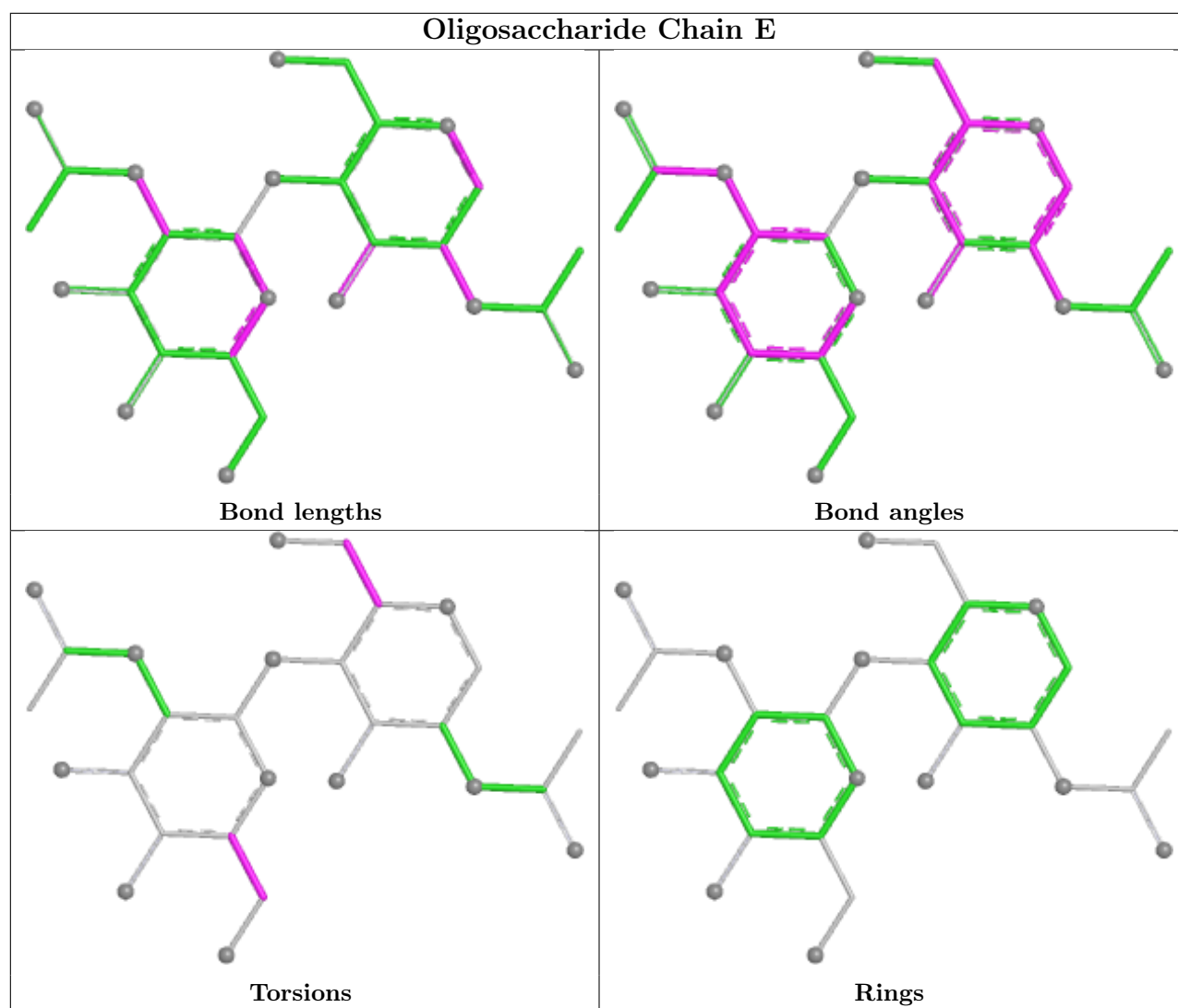
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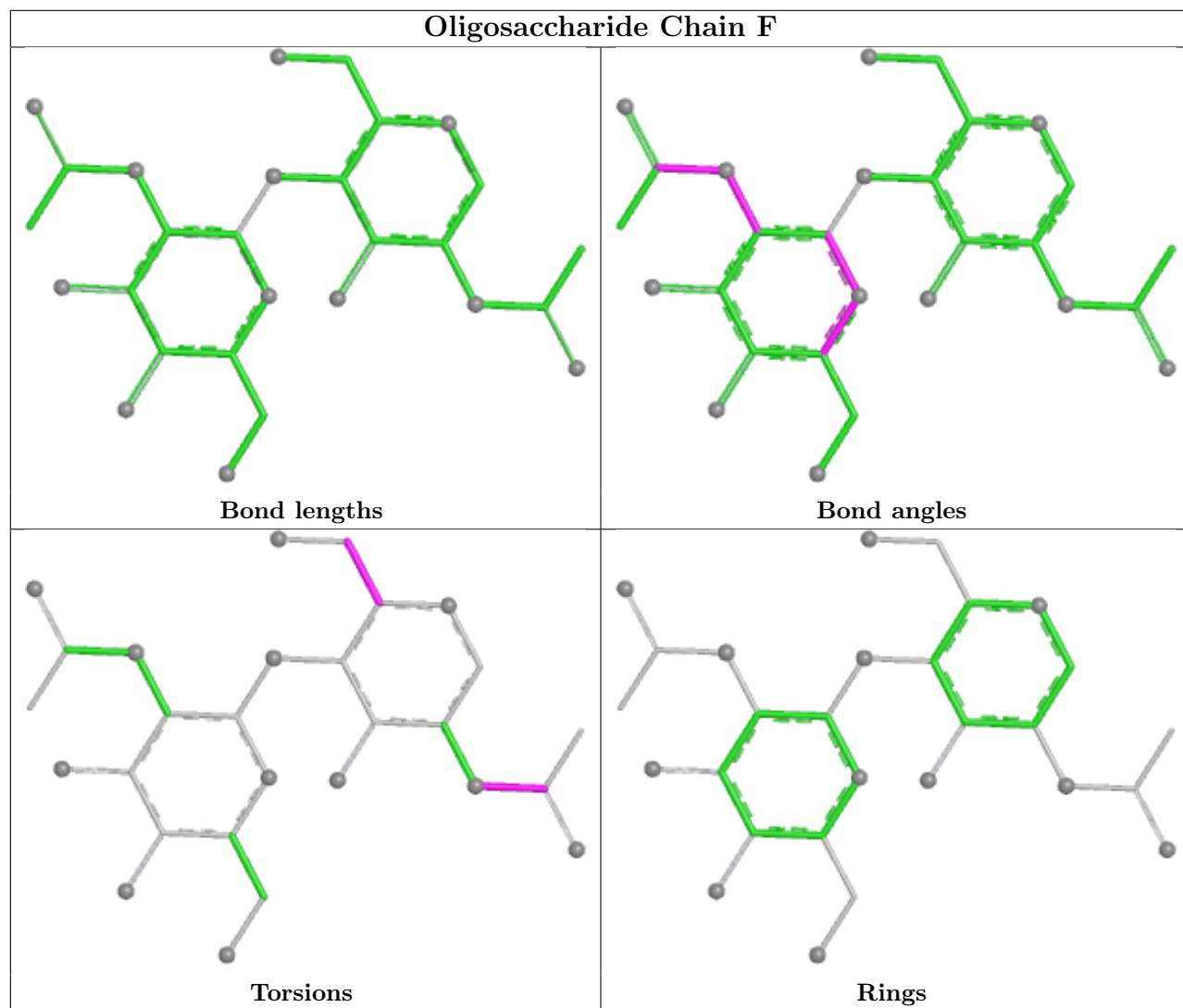
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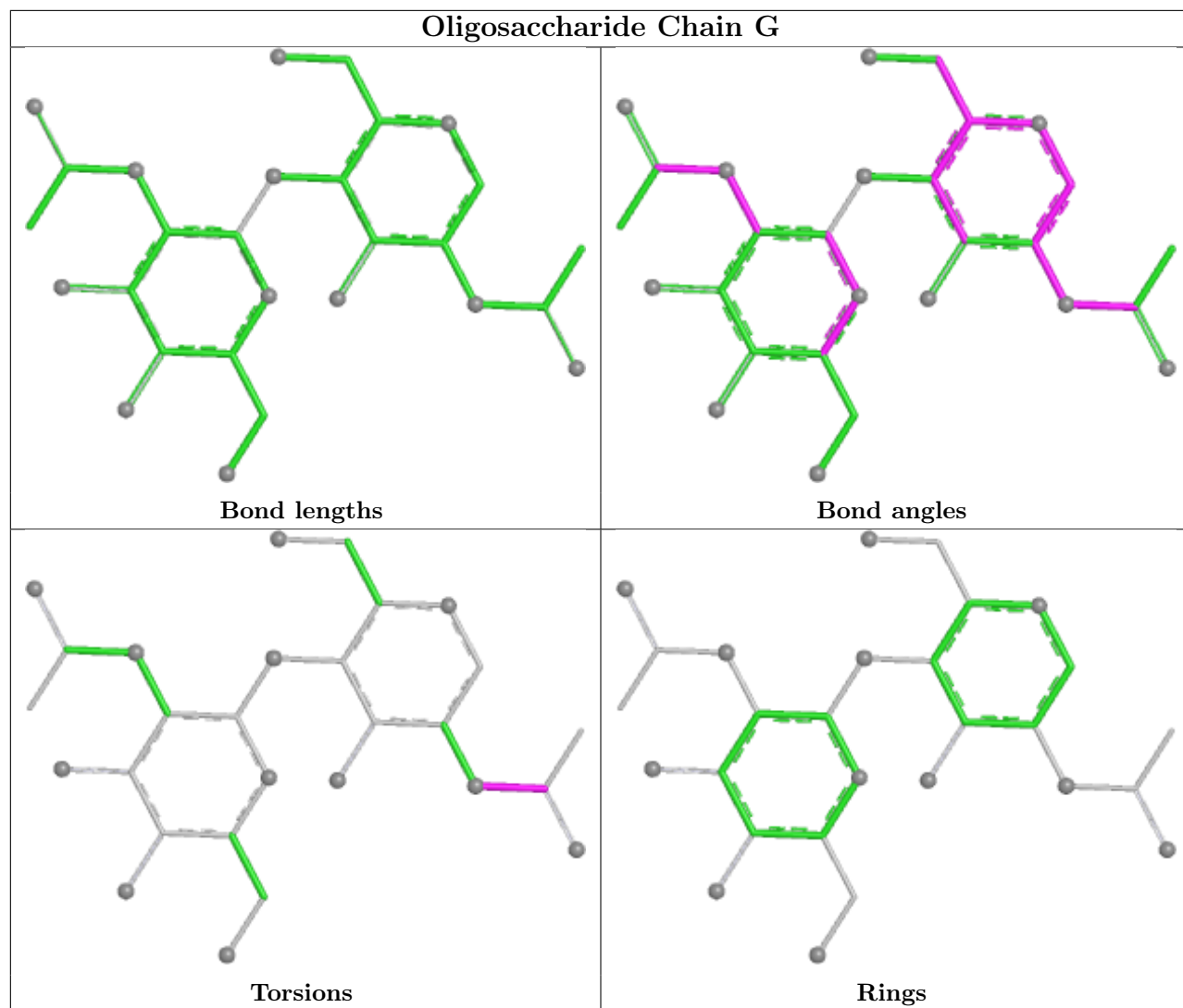
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	3	0
3	D	2	NAG	4	0
2	C	1	NAG	2	0
2	H	2	NAG	1	0

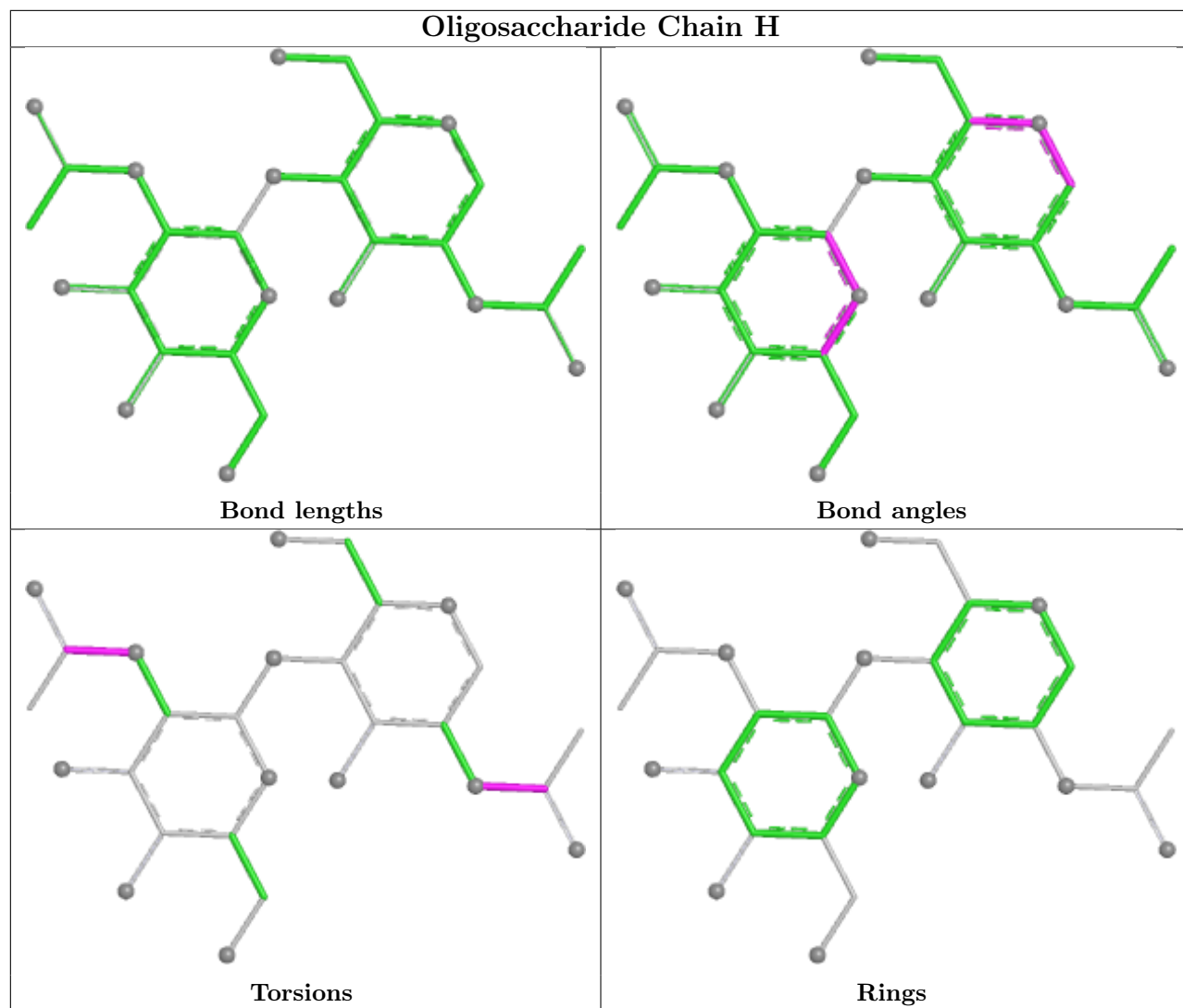
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

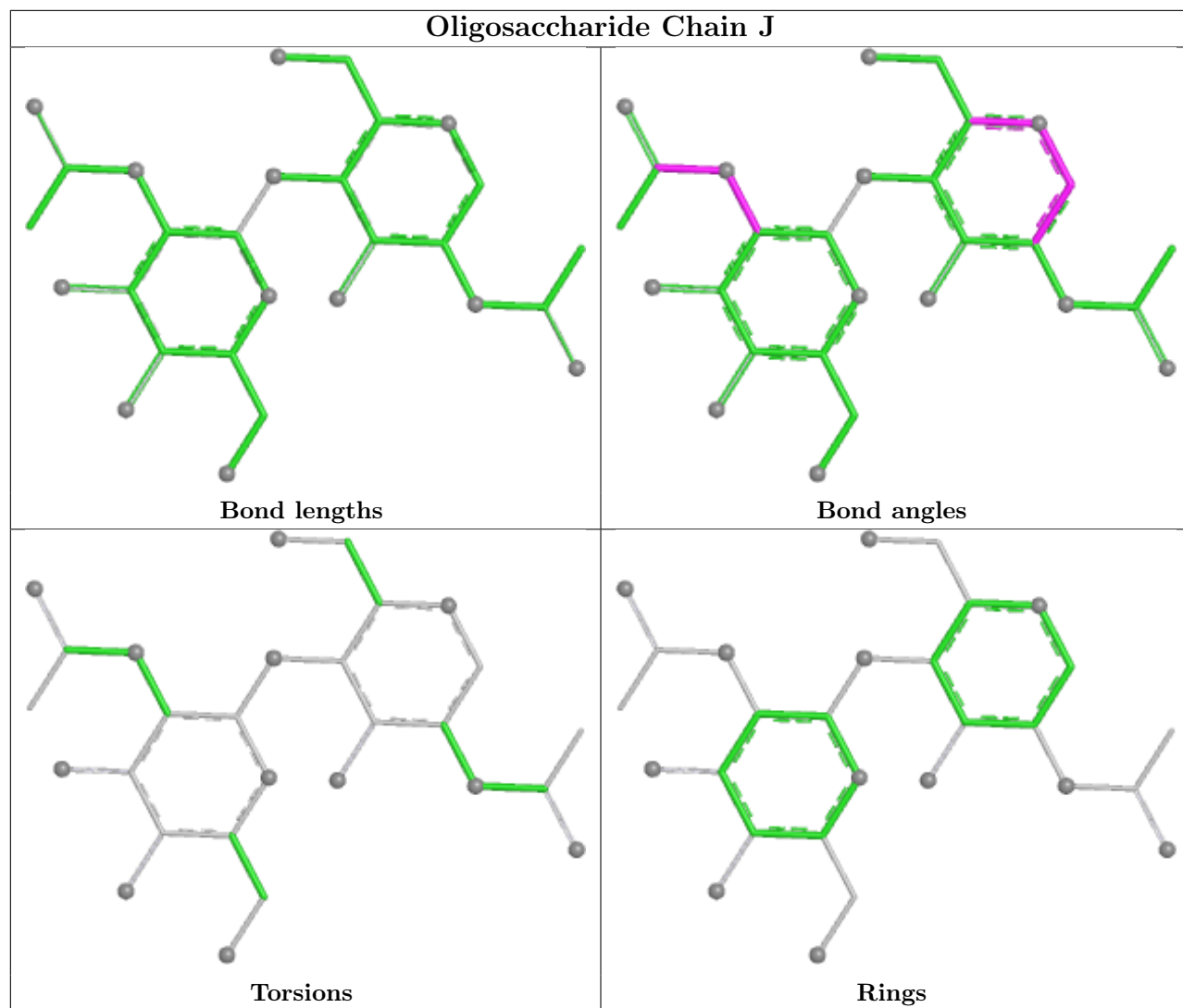


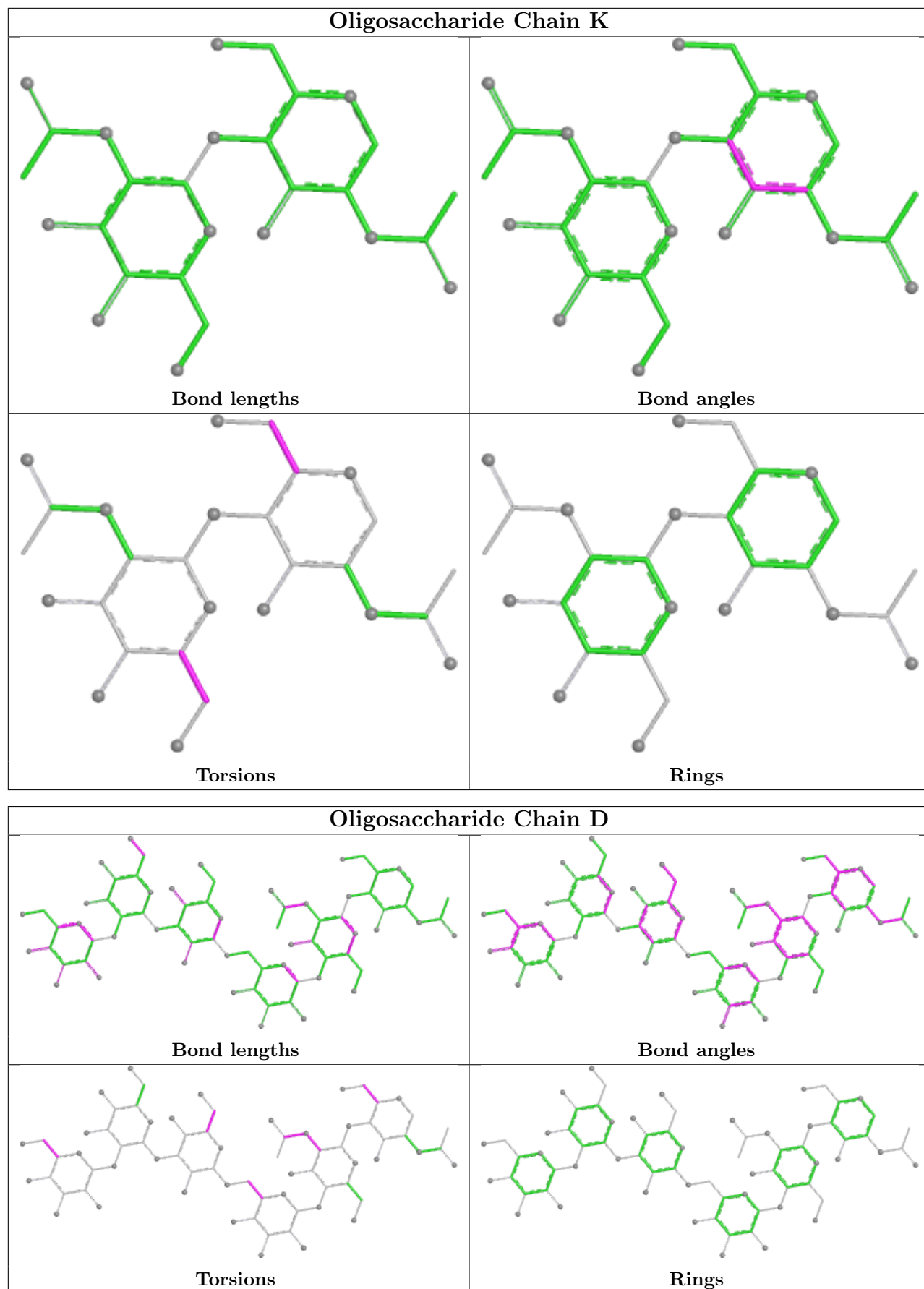




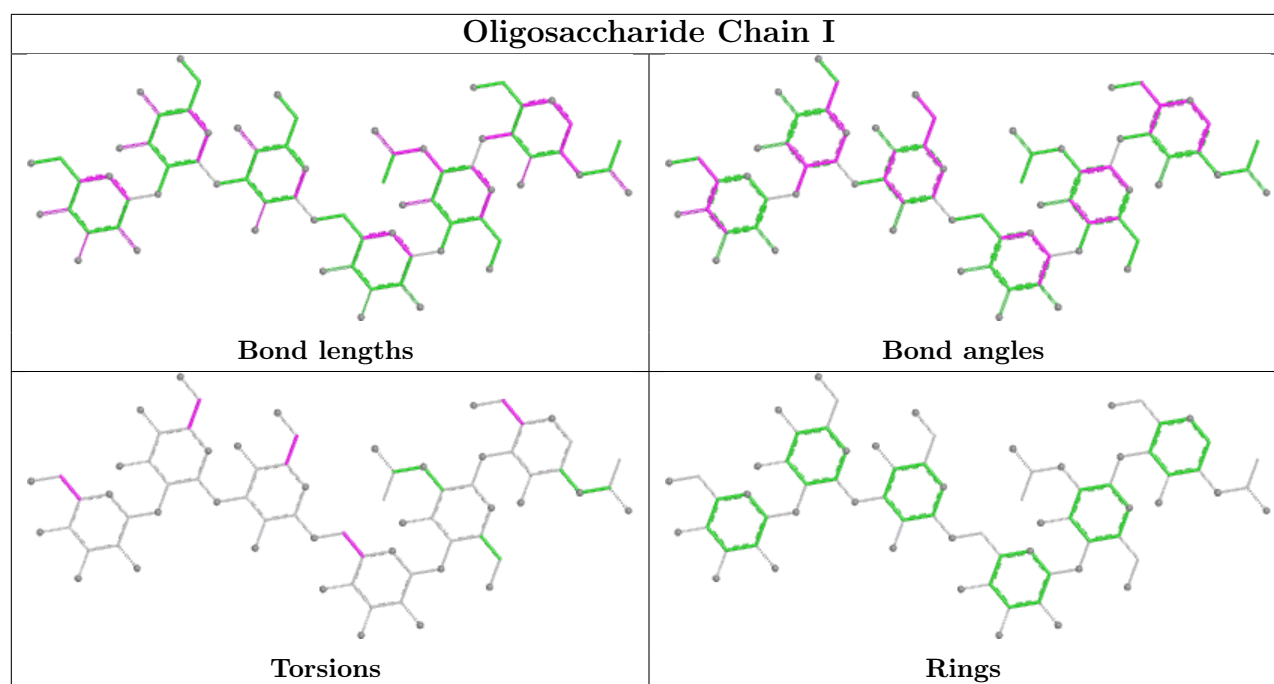












## 5.6 Ligand geometry [i](#)

6 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
4	NAG	A	815	1	14,14,15	0.51	0	17,19,21	1.32	2 (11%)
5	BLD	B	801	-	36,37,37	2.03	8 (22%)	49,59,59	2.67	19 (38%)
4	NAG	B	802	1	14,14,15	0.46	0	17,19,21	0.94	0
4	NAG	B	805	1	14,14,15	0.61	0	17,19,21	1.10	0
5	BLD	A	804	-	36,37,37	1.98	7 (19%)	49,59,59	2.80	20 (40%)
4	NAG	A	803	1	14,14,15	0.55	0	17,19,21	1.33	2 (11%)

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
4	NAG	A	815	1	-	5/6/23/26	0/1/1/1
5	BLD	B	801	-	-	2/20/85/85	0/4/4/4
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
4	NAG	B	805	1	-	0/6/23/26	0/1/1/1
5	BLD	A	804	-	-	1/20/85/85	0/4/4/4
4	NAG	A	803	1	-	0/6/23/26	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	BLD	O06-C06	6.72	1.38	1.21
5	A	804	BLD	O06-C06	6.60	1.37	1.21
5	B	801	BLD	O07-C07	-5.29	1.37	1.45
5	A	804	BLD	O07-C07	-5.22	1.37	1.45
5	A	804	BLD	C19-C10	-3.11	1.49	1.54

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	BLD	O07-C06-O06	-6.73	106.74	116.97
5	A	804	BLD	C19-C10-C05	-6.27	99.36	109.89
5	B	801	BLD	C18-C13-C12	-6.26	101.37	110.61
5	B	801	BLD	C12-C13-C17	6.24	125.79	116.60
5	A	804	BLD	C18-C13-C12	-6.13	101.57	110.61

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

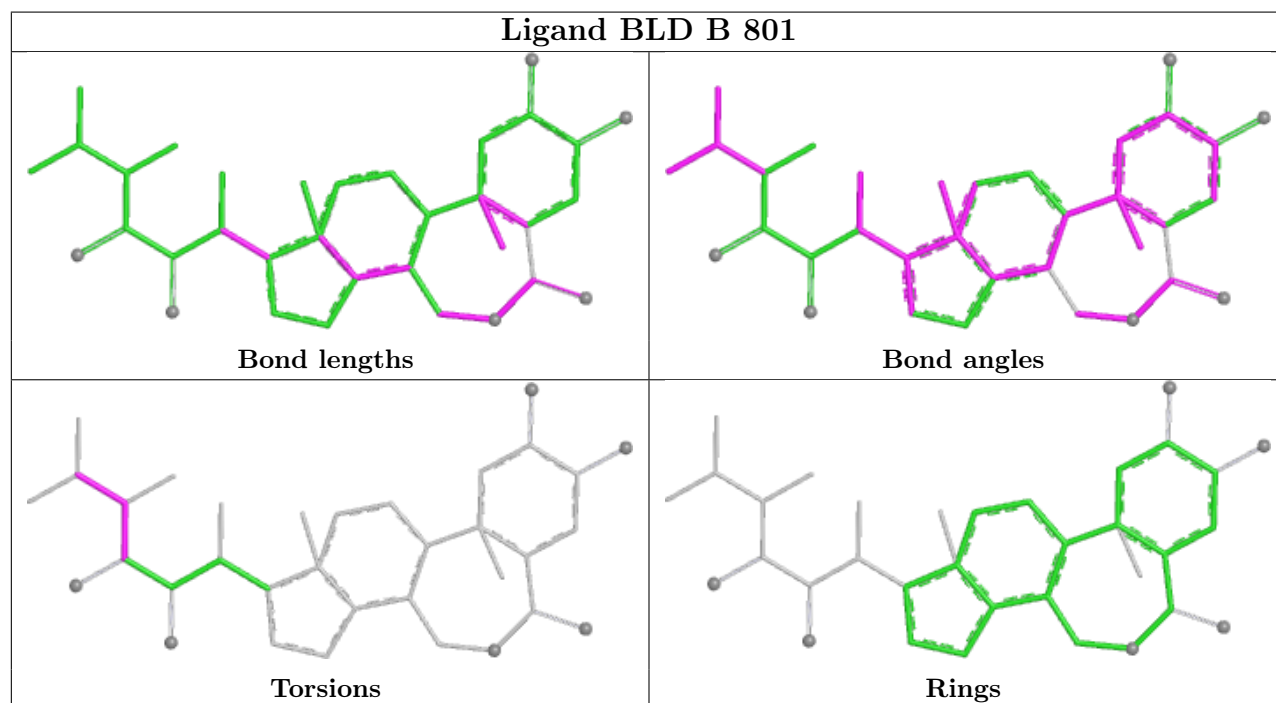
Mol	Chain	Res	Type	Atoms
4	A	815	NAG	C3-C2-N2-C7
4	A	815	NAG	C8-C7-N2-C2
4	A	815	NAG	O7-C7-N2-C2
5	A	804	BLD	C23-C24-C25-C27
5	B	801	BLD	C23-C24-C25-C27

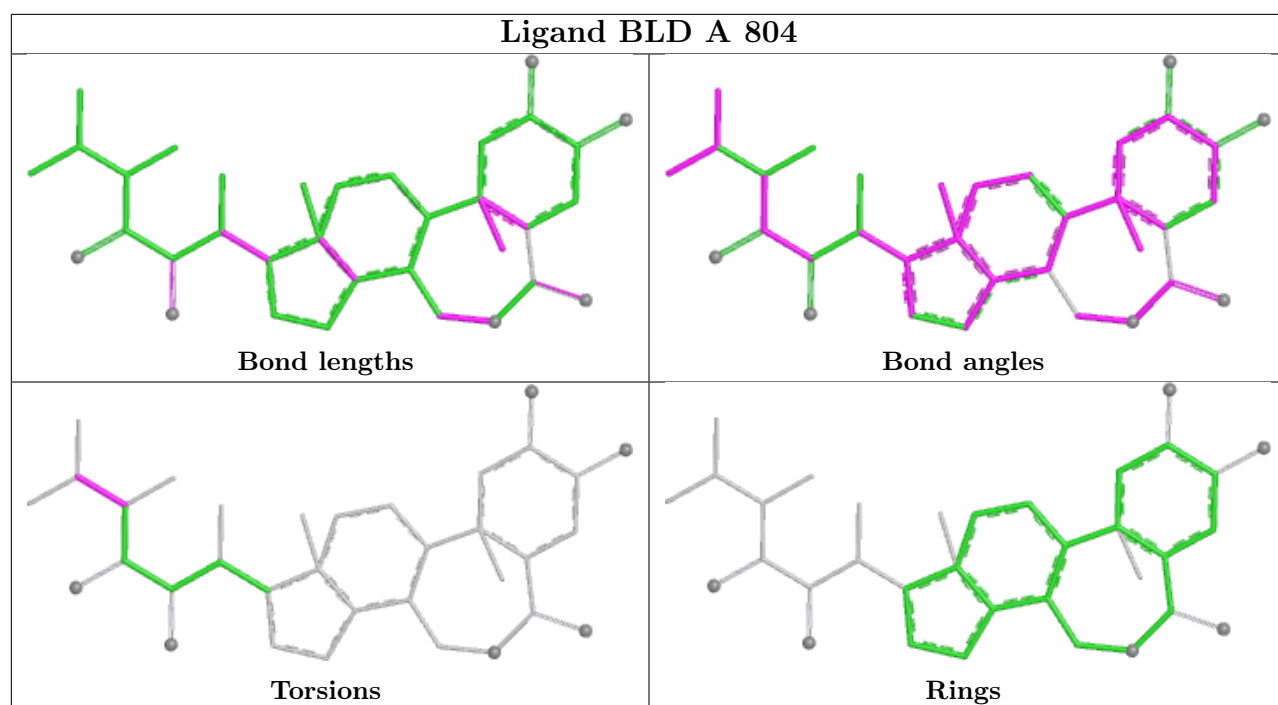
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	815	NAG	2	0
5	B	801	BLD	5	0
5	A	804	BLD	5	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	724/740 (97%)	-0.25	23 (3%) 47 51	11, 22, 48, 88	0
1	B	724/740 (97%)	-0.26	22 (3%) 50 53	12, 23, 50, 97	0
All	All	1448/1480 (97%)	-0.26	45 (3%) 49 52	11, 22, 49, 97	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	400	SER	10.3
1	A	400	SER	6.5
1	B	31	ASP	4.7
1	B	617	MET	4.6
1	A	619	HIS	4.5

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	H	2	14/15	0.83	0.39	49,68,74,77	0
2	NAG	H	1	14/15	0.85	0.25	40,50,57,58	0
2	NAG	C	1	14/15	0.86	0.30	25,41,51,52	0
2	NAG	G	1	14/15	0.86	0.23	28,41,47,52	0
3	MAN	D	4	11/12	0.86	0.17	18,23,25,27	0

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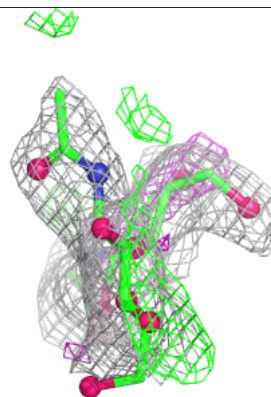
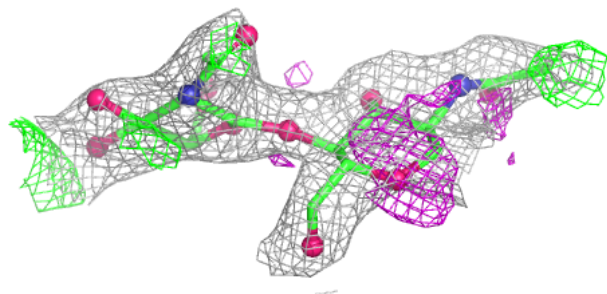
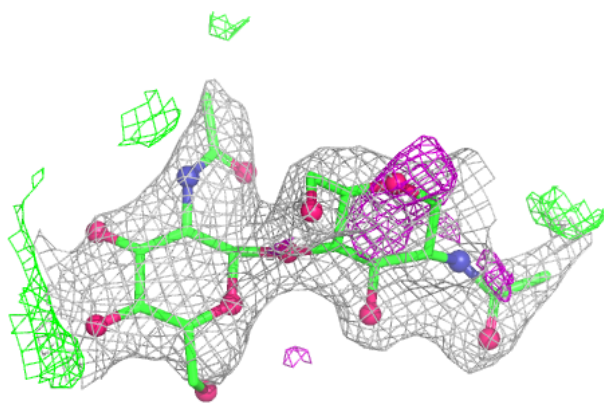
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	K	2	14/15	0.87	0.36	44,60,63,64	0
2	NAG	C	2	14/15	0.90	0.38	38,54,62,63	0
2	NAG	G	2	14/15	0.90	0.35	35,44,48,49	0
2	NAG	F	2	14/15	0.90	0.42	31,52,62,66	0
3	MAN	I	4	11/12	0.92	0.14	16,22,24,25	0
3	BMA	I	3	11/12	0.93	0.21	25,29,36,38	0
3	BMA	D	3	11/12	0.94	0.24	28,34,41,43	0
2	NAG	E	2	14/15	0.94	0.27	28,34,44,45	0
3	MAN	D	5	11/12	0.94	0.13	16,20,24,42	0
2	NAG	J	2	14/15	0.94	0.27	22,35,43,46	0
2	NAG	F	1	14/15	0.94	0.24	28,38,46,46	0
3	NAG	D	2	14/15	0.95	0.16	16,26,32,32	0
2	NAG	K	1	14/15	0.95	0.27	29,42,54,54	0
3	MAN	D	6	11/12	0.96	0.12	16,19,23,29	0
2	NAG	J	1	14/15	0.96	0.14	16,23,29,31	0
2	NAG	E	1	14/15	0.96	0.10	16,24,33,33	0
3	MAN	I	5	11/12	0.96	0.09	16,22,26,33	0
3	NAG	D	1	14/15	0.97	0.11	17,22,25,33	0
3	NAG	I	1	14/15	0.97	0.09	18,23,32,32	0
3	NAG	I	2	14/15	0.97	0.13	19,25,30,31	0
3	MAN	I	6	11/12	0.97	0.10	15,20,24,32	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.

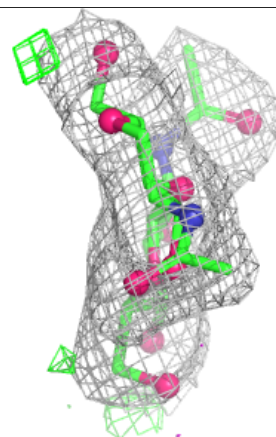
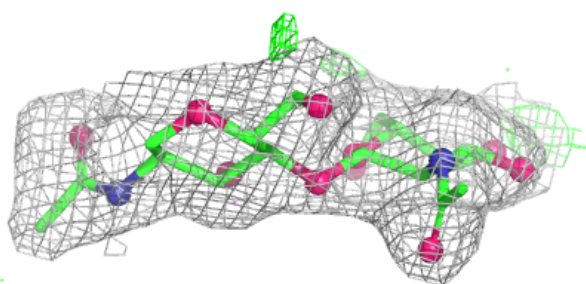
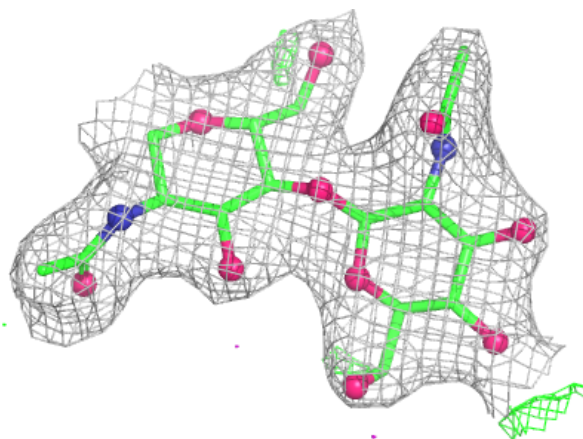
**Electron density around Chain C:**

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



**Electron density around Chain E:**

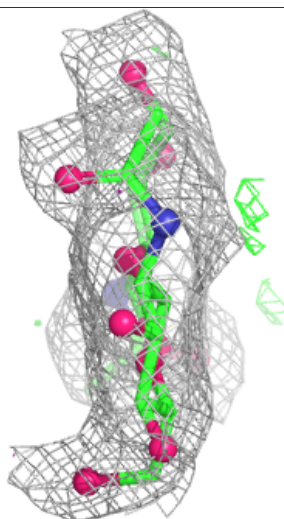
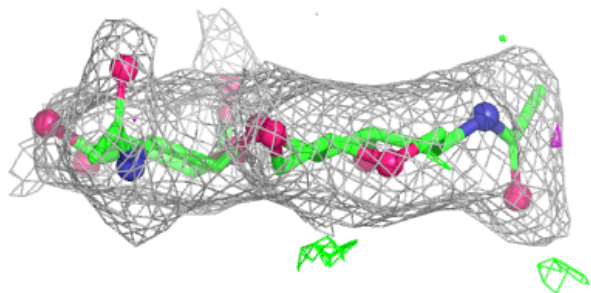
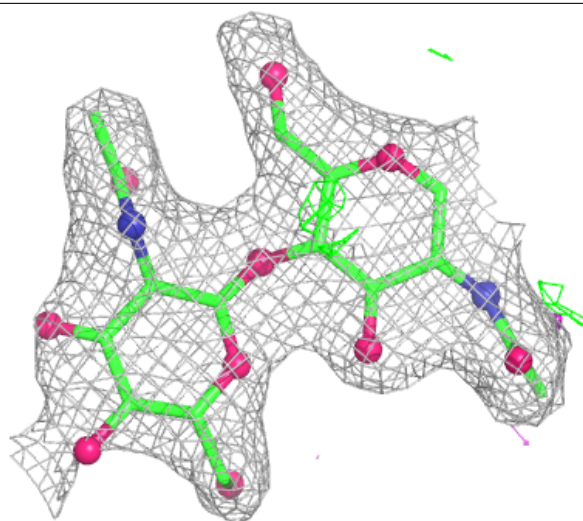
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





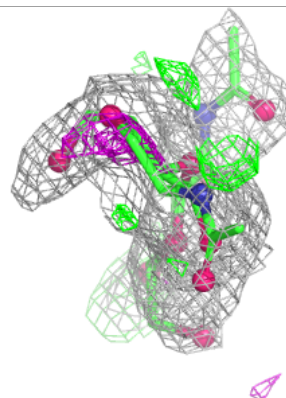
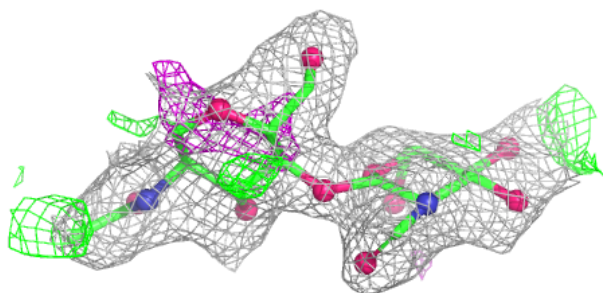
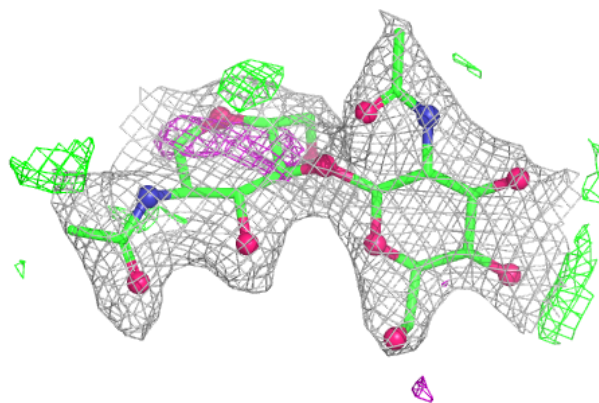
**Electron density around Chain F:**

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

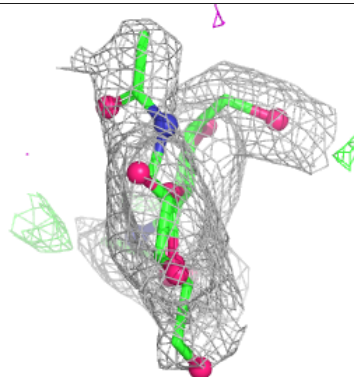
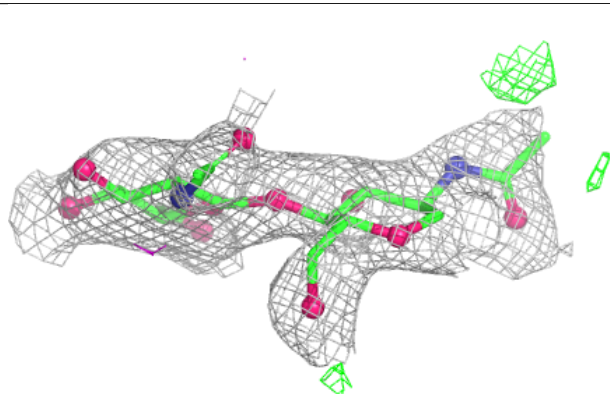
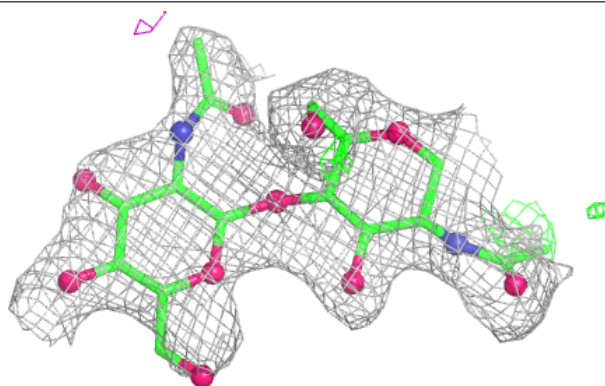


**Electron density around Chain G:**

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

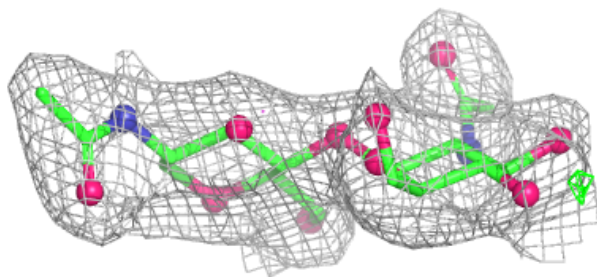
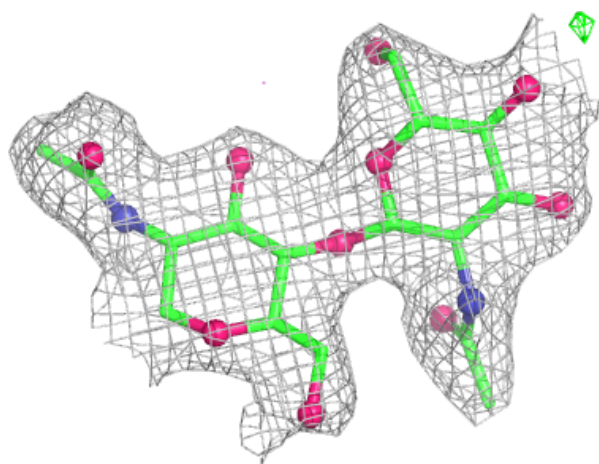
**Electron density around Chain H:**

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and green (positive)



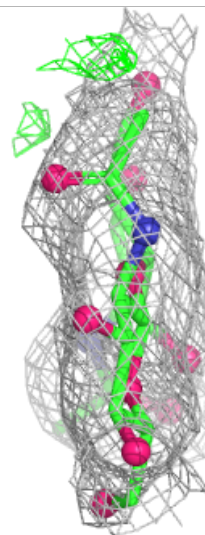
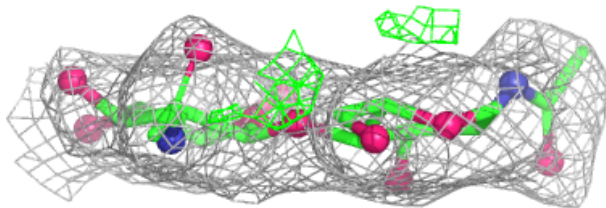
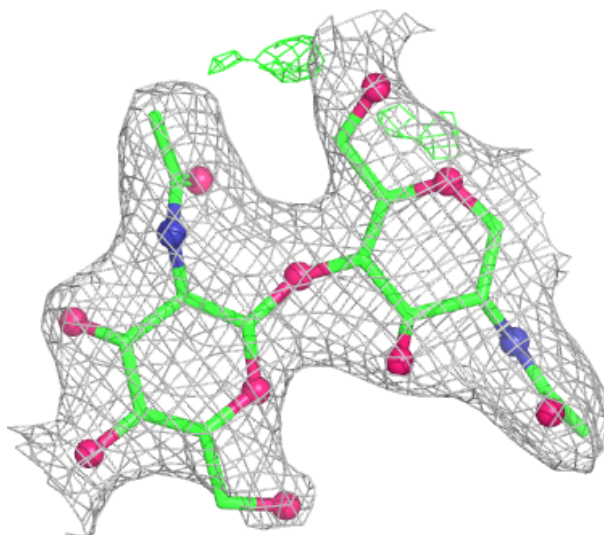
**Electron density around Chain J:**

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



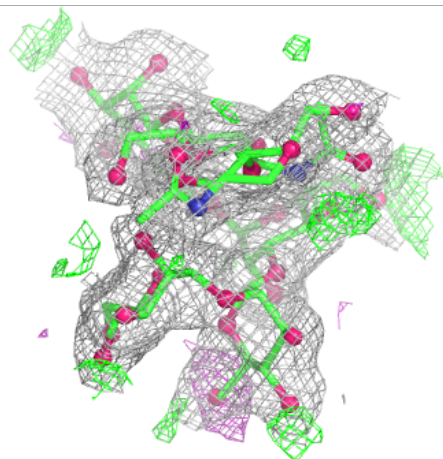
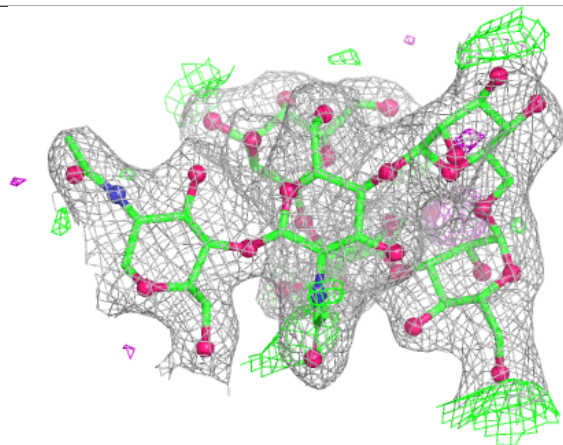
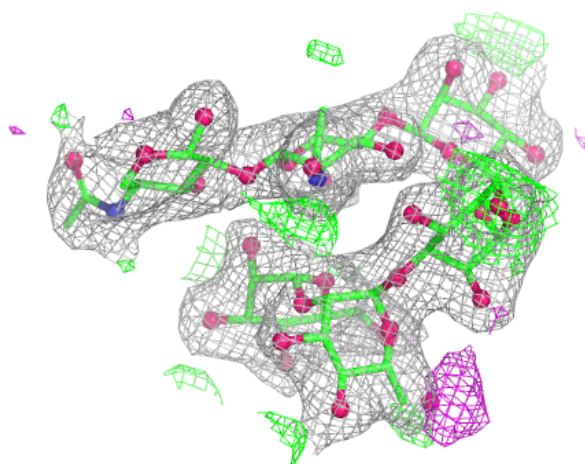
**Electron density around Chain K:**

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and green (positive)

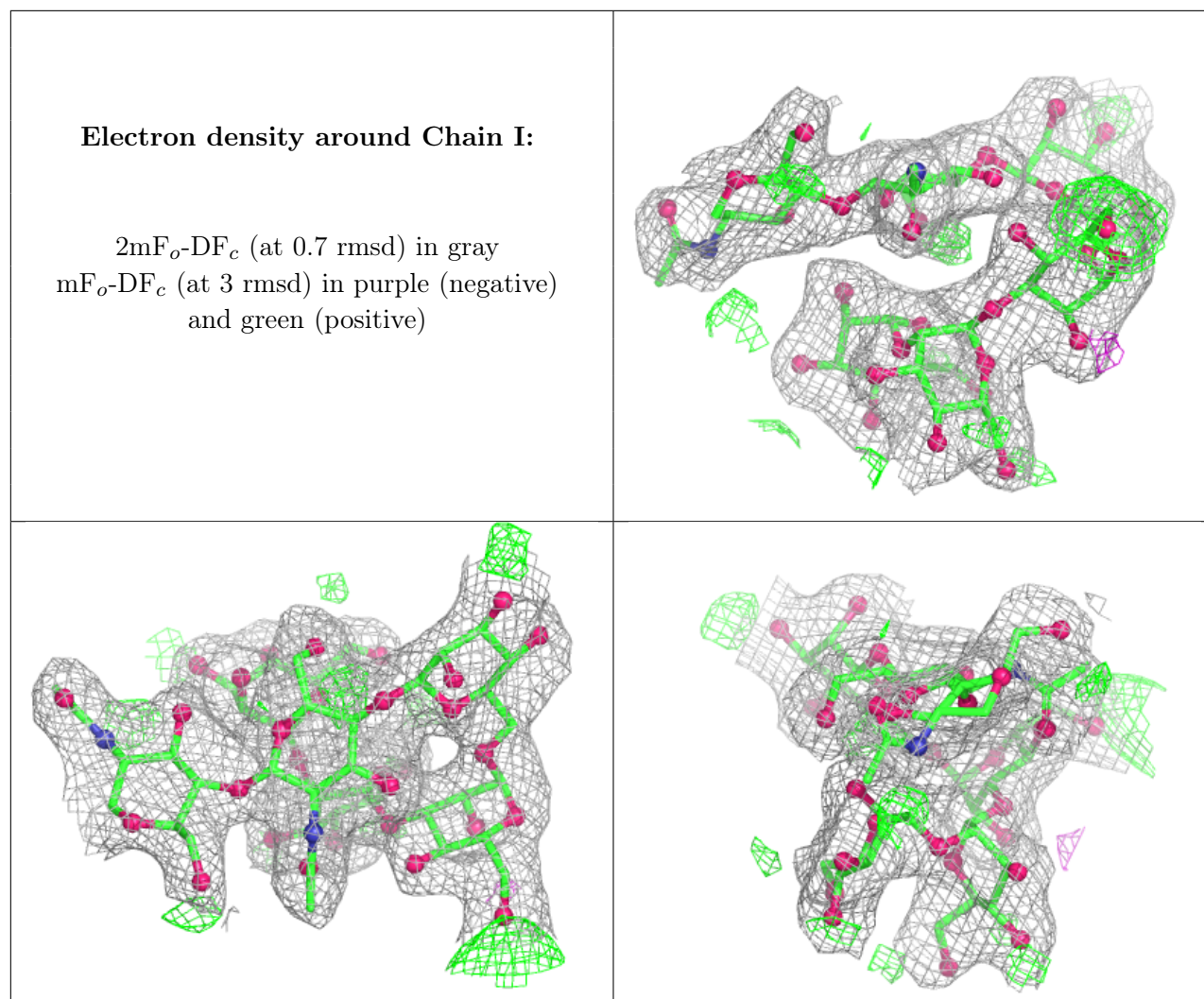


**Electron density around Chain D:**

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







## 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, 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.

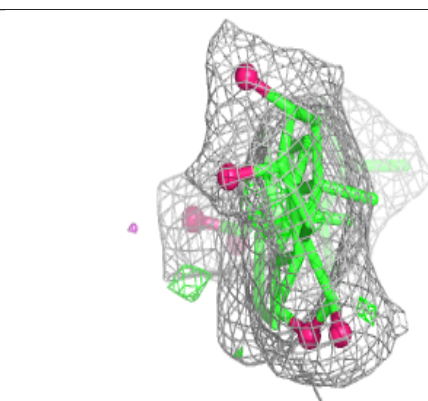
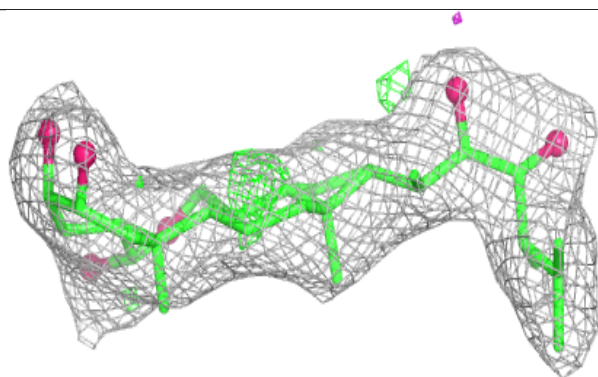
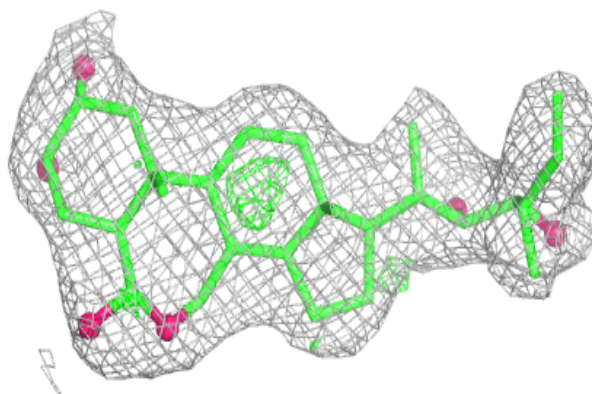
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	815	14/15	0.80	0.31	33,49,60,64	0
4	NAG	B	802	14/15	0.86	0.26	37,48,54,59	0
4	NAG	A	803	14/15	0.89	0.16	30,40,48,48	0
4	NAG	B	805	14/15	0.91	0.22	30,39,48,52	0
5	BLD	A	804	34/34	0.93	0.15	15,22,30,35	23
5	BLD	B	801	34/34	0.94	0.15	17,23,28,29	23

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.

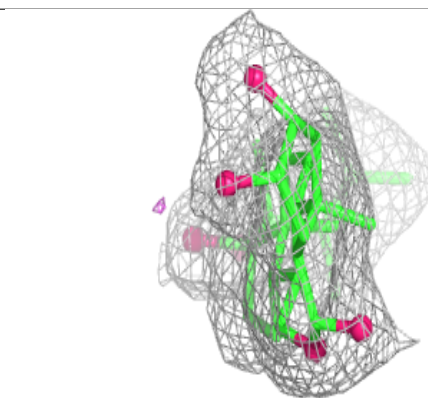
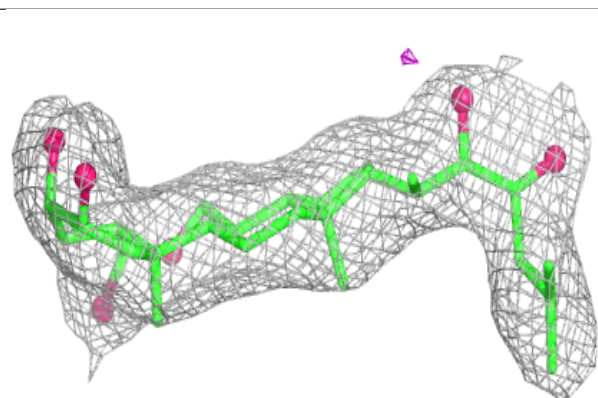
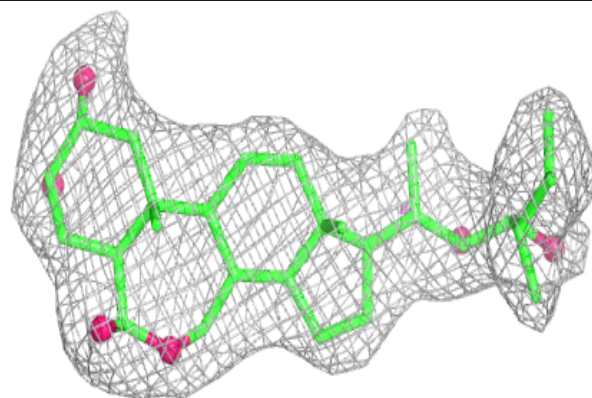
**Electron density around BLD A 804:**

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



**Electron density around BLD B 801:**

$2mF_o-DF_c$  (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.