



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2025 – 01:18 pm BST

PDB ID : 9S8Z / pdb_00009s8z
Title : Crystal structure of the BRI1 ectodomain from Arabidopsis thaliana in complex with 28-homobrassinolide.
Authors : Caregnato, A.; Hothorn, M.
Deposited on : 2025-08-05
Resolution : 2.35 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

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>.

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

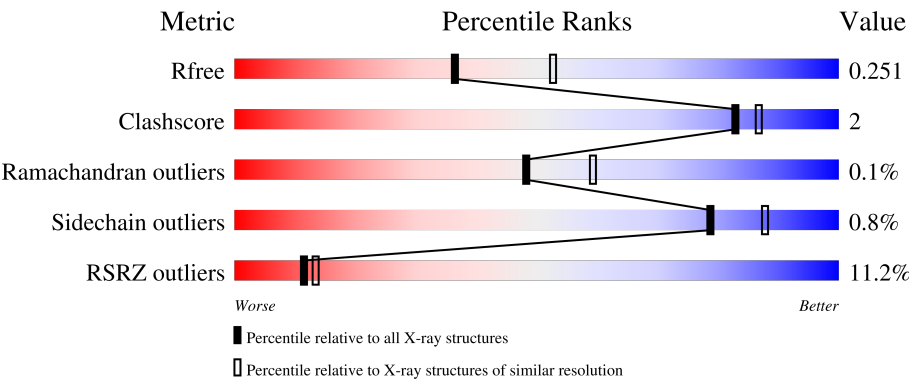
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

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 2.35 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.




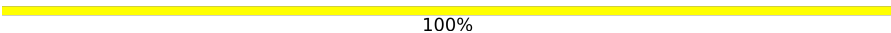

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	797	<div><div>10%</div><div>88%</div><div>5%</div><div>7%</div></div>
2	B	4	<div><div>25%</div><div>75%</div></div>
3	C	2	<div><div>50%</div><div>50%</div></div>
3	E	2	<div><div>100%</div></div>
3	H	2	<div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
4	D	7	 14%86%
5	F	5	 100%
6	G	3	 33%67%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 12058 atoms, of which 5972 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 Protein BRASSINOSTEROID INSENSITIVE 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	743	Total	C	H	N	O	S	0	0	0
			11214	3554	5586	934	1108	32			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	789	ALA	-	expression tag	UNP O22476
A	790	ALA	-	expression tag	UNP O22476
A	791	ALA	-	expression tag	UNP O22476
A	792	GLU	-	expression tag	UNP O22476
A	793	ASN	-	expression tag	UNP O22476
A	794	LEU	-	expression tag	UNP O22476
A	795	TYR	-	expression tag	UNP O22476
A	796	PHE	-	expression tag	UNP O22476
A	797	GLN	-	expression tag	UNP O22476

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



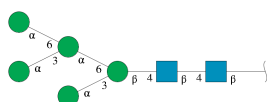
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

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



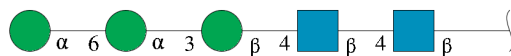
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
3	E	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
3	H	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

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



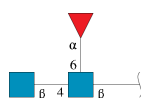
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total	C	H	N	O	0	0	0
			153	46	70	2	35			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



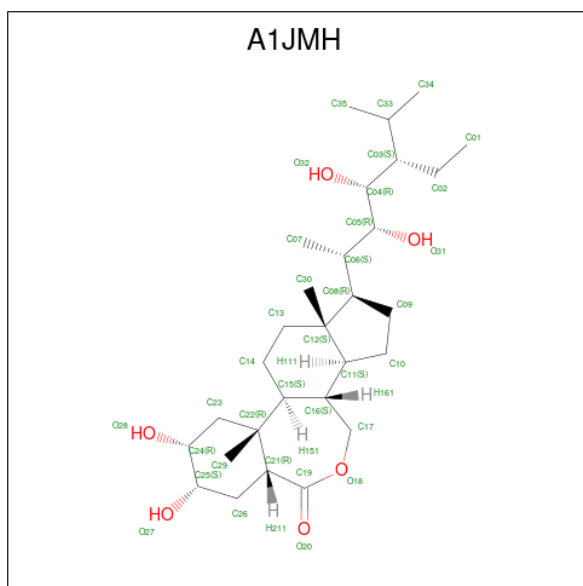
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	5	Total	C	H	N	O	0	0	0
			113	34	52	2	25			

- 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.



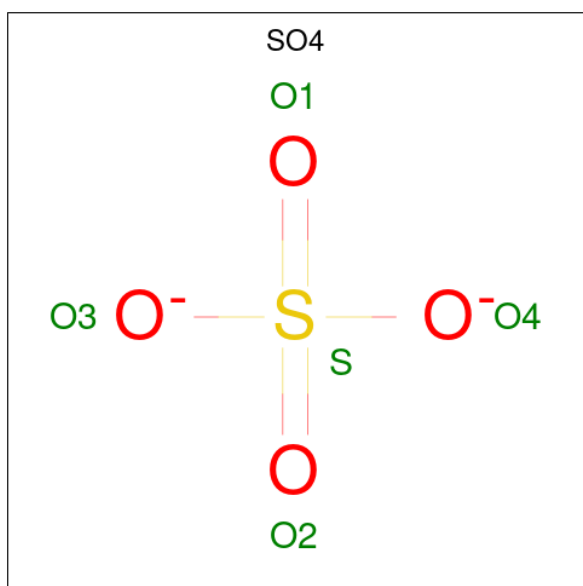
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	3	Total	C	H	N	O	0	0	0
			72	22	34	2	14			

- Molecule 7 is 28-homobrassinolide (CCD ID: A1JMH) (formula: $C_{29}H_{50}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			85	29	50	6		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

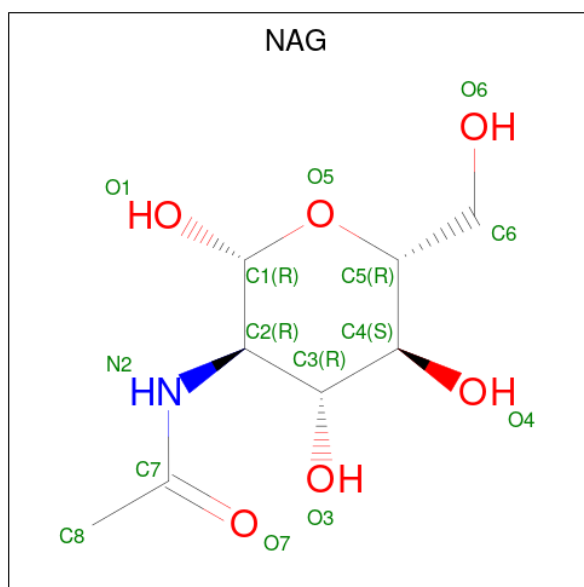


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Na	0	0
			1	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



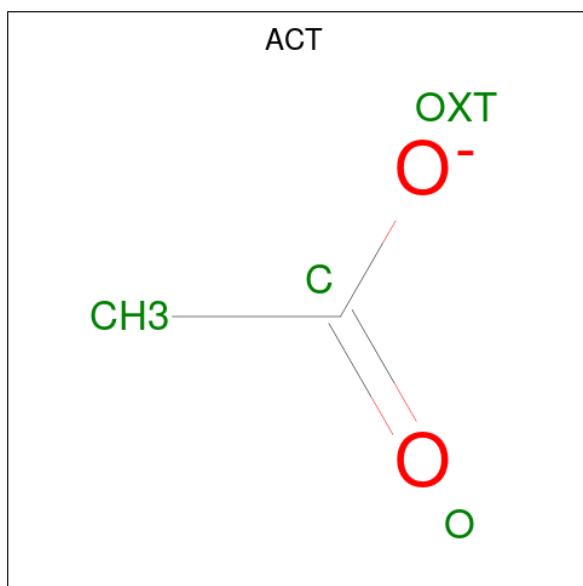
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 12 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 13 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	H	O	0	0
			10	2	6	2		
13	A	1	Total	C	H	O	0	0
			10	2	6	2		

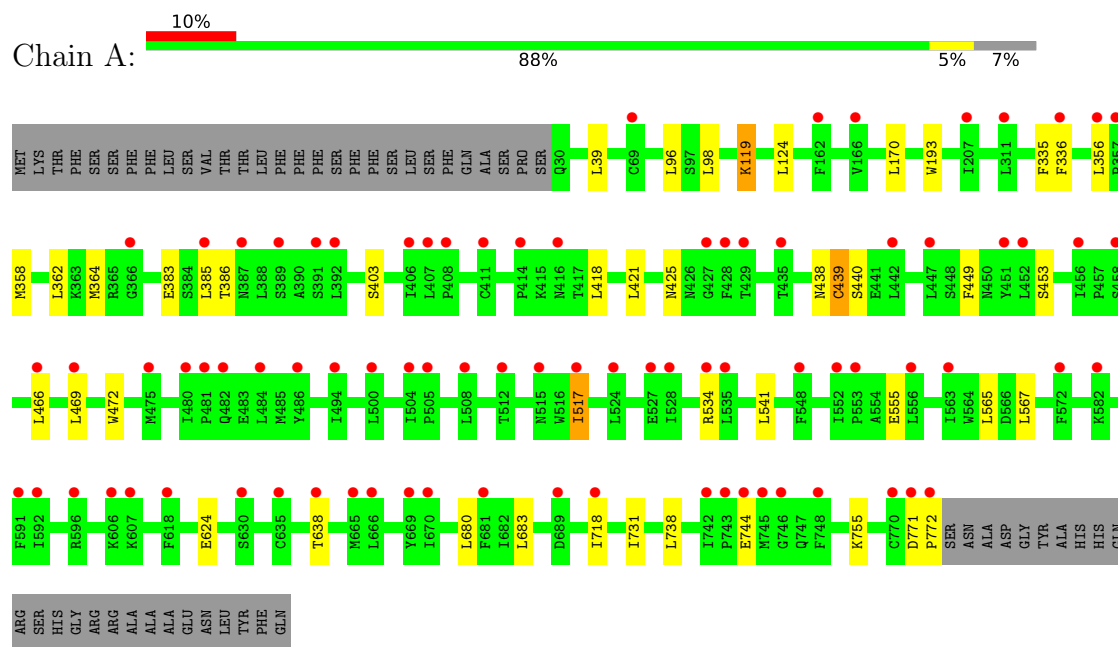
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	31	Total	O	0	0
			31	31		

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: Protein BRASSINOSTEROID INSENSITIVE 1



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



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




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

Chain E:  100%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain D:  14% 86%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-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
MAN4
MAN5

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

Chain G:  33% 67%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.08Å 66.73Å 121.60Å 90.00° 121.95° 90.00°	Depositor
Resolution (Å)	49.02 – 2.35 49.02 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.02-2.35) 87.6 (49.02-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.19 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.225 , 0.252 0.225 , 0.251	Depositor DCC
R_{free} test set	2424 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12058	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, FUC, NAG, A1JMH, GOL, NA, EDO, ACT, MAN, SO4

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	0.11	0/5737	0.29	0/7785

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	534	ARG	Sidechain

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	5628	5586	5585	26	0
2	B	50	43	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	25	25	0	0
3	E	28	25	25	0	0
3	H	28	25	25	1	0
4	D	83	70	70	0	0
5	F	61	52	52	0	0
6	G	38	34	34	0	0
7	A	35	50	0	1	0
8	A	15	0	0	0	0
9	A	1	0	0	0	0
10	A	42	39	39	0	0
11	A	6	8	8	0	0
12	A	4	3	3	0	0
13	A	8	12	12	0	0
14	A	31	0	0	0	0
All	All	6086	5972	5921	27	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 2.

All (27) 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:418:LEU:HD21	1:A:421:LEU:HD13	1.84	0.58
1:A:358:MET:HE3	1:A:362:LEU:HD11	1.86	0.57
7:A:801:A1JMH:O27	7:A:801:A1JMH:O20	2.25	0.54
1:A:438:ASN:O	1:A:440:SER:N	2.43	0.52
1:A:638:THR:HG21	3:H:1:NAG:H5	1.94	0.49
1:A:771:ASP:HB2	1:A:772:PRO:HD2	1.96	0.48
1:A:731:ILE:O	1:A:755:LYS:HG3	2.14	0.47
1:A:336:PHE:HB3	1:A:364:MET:CE	2.45	0.46
1:A:624:GLU:OE1	1:A:624:GLU:N	2.44	0.46
1:A:555:GLU:N	1:A:555:GLU:OE1	2.46	0.46
1:A:517:ILE:HG23	1:A:541:LEU:HD12	1.97	0.46
1:A:466:LEU:HD21	1:A:469:LEU:HB2	1.99	0.45
1:A:358:MET:HE3	1:A:362:LEU:CD1	2.48	0.44
1:A:425:ASN:HA	1:A:449:PHE:HB3	1.99	0.44
1:A:335:PHE:CD1	1:A:335:PHE:C	2.97	0.43
1:A:119:LYS:HD2	1:A:119:LYS:H	1.84	0.43
1:A:449:PHE:HE1	1:A:472:TRP:CH2	2.37	0.42
1:A:680:LEU:HD21	1:A:683:LEU:HB2	2.01	0.42
1:A:718:ILE:CG1	1:A:738:LEU:HD23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD13	1:A:193:TRP:CH2	2.55	0.41
1:A:358:MET:HE2	1:A:385:LEU:HA	2.02	0.41
1:A:565:LEU:HG	1:A:567:LEU:HD13	2.03	0.41
1:A:39:LEU:HD21	1:A:98:LEU:HD11	2.01	0.41
1:A:356:LEU:O	1:A:358:MET:N	2.52	0.41
1:A:383:GLU:O	1:A:386:THR:HG22	2.20	0.41
1:A:96:LEU:HD22	1:A:124:LEU:HD22	2.01	0.40
1:A:744:GLU:HG2	1:A:744:GLU:O	2.21	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	741/797 (93%)	688 (93%)	52 (7%)	1 (0%)	48 59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	CYS

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	656/702 (93%)	651 (99%)	5 (1%)	79 88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LYS
1	A	403	SER
1	A	439	CYS
1	A	453	SER
1	A	517	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	ASN
1	A	248	GLN
1	A	446	HIS
1	A	551	ASN
1	A	720	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

25 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	0.76	0	17,19,21	0.86	0
2	NAG	B	2	2	14,14,15	0.73	0	17,19,21	1.05	1 (5%)
2	BMA	B	3	2	11,11,12	0.85	0	15,15,17	2.24	5 (33%)
2	MAN	B	4	2	11,11,12	0.78	0	15,15,17	1.02	1 (6%)
3	NAG	C	1	1,3	14,14,15	0.68	0	17,19,21	1.06	1 (5%)
3	NAG	C	2	3	14,14,15	0.70	0	17,19,21	0.87	0
4	NAG	D	1	1,4	14,14,15	0.72	0	17,19,21	1.15	1 (5%)
4	NAG	D	2	4	14,14,15	0.73	0	17,19,21	1.09	1 (5%)
4	BMA	D	3	4	11,11,12	0.88	0	15,15,17	2.07	4 (26%)
4	MAN	D	4	4	11,11,12	0.75	0	15,15,17	0.99	0
4	MAN	D	5	4	11,11,12	0.69	0	15,15,17	1.27	1 (6%)
4	MAN	D	6	4	11,11,12	0.82	1 (9%)	15,15,17	1.00	0
4	MAN	D	7	4	11,11,12	0.73	0	15,15,17	1.07	1 (6%)
3	NAG	E	1	1,3	14,14,15	0.68	0	17,19,21	1.18	1 (5%)
3	NAG	E	2	3	14,14,15	0.78	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	F	1	1,5	14,14,15	0.69	0	17,19,21	1.81	3 (17%)
5	NAG	F	2	5	14,14,15	0.87	1 (7%)	17,19,21	2.37	4 (23%)
5	BMA	F	3	5	11,11,12	0.89	0	15,15,17	2.36	4 (26%)
5	MAN	F	4	5	11,11,12	0.64	0	15,15,17	1.46	1 (6%)
5	MAN	F	5	5	11,11,12	0.79	0	15,15,17	2.03	7 (46%)
6	NAG	G	1	6,1	14,14,15	0.70	0	17,19,21	1.27	1 (5%)
6	NAG	G	2	6	14,14,15	0.75	0	17,19,21	1.27	2 (11%)
6	FUC	G	3	6	10,10,11	0.81	0	14,14,16	0.95	0
3	NAG	H	1	1,3	14,14,15	0.69	0	17,19,21	1.00	0
3	NAG	H	2	3	14,14,15	0.69	0	17,19,21	1.12	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	2/2/19/22	0/1/1/1
4	MAN	D	7	4	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	1/2/19/22	0/1/1/1
5	MAN	F	4	5	-	1/2/19/22	0/1/1/1
5	MAN	F	5	5	-	1/2/19/22	0/1/1/1
6	NAG	G	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	FUC	G	3	6	-	-	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2	NAG	O5-C1	-2.17	1.40	1.43
3	E	2	NAG	C1-C2	2.09	1.55	1.52
4	D	6	MAN	O5-C1	-2.00	1.40	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	2	NAG	C1-C2-N2	-7.90	97.00	110.49
5	F	3	BMA	C1-O5-C5	6.42	120.89	112.19
2	B	3	BMA	C1-O5-C5	5.77	120.01	112.19
4	D	3	BMA	C1-O5-C5	5.49	119.64	112.19
5	F	4	MAN	C1-O5-C5	4.79	118.68	112.19
5	F	1	NAG	C1-O5-C5	4.70	118.56	112.19
4	D	5	MAN	C1-O5-C5	3.90	117.48	112.19
5	F	1	NAG	C2-N2-C7	3.69	128.16	122.90
2	B	3	BMA	C3-C4-C5	3.58	116.63	110.24
5	F	3	BMA	C1-C2-C3	3.40	113.85	109.67
5	F	5	MAN	O5-C1-C2	-3.35	105.60	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	1	NAG	C4-C3-C2	-3.34	106.12	111.02
5	F	3	BMA	O3-C3-C2	-3.24	103.78	109.99
5	F	5	MAN	C3-C4-C5	3.20	115.94	110.24
4	D	1	NAG	C2-N2-C7	3.17	127.42	122.90
5	F	2	NAG	C2-N2-C7	3.17	127.42	122.90
5	F	5	MAN	C2-C3-C4	3.14	116.33	110.89
6	G	2	NAG	O5-C1-C2	-3.06	106.46	111.29
4	D	3	BMA	C3-C4-C5	2.85	115.33	110.24
3	H	2	NAG	C2-N2-C7	2.84	126.94	122.90
4	D	3	BMA	O4-C4-C3	-2.71	104.08	110.35
4	D	7	MAN	C1-O5-C5	2.70	115.85	112.19
5	F	5	MAN	C1-O5-C5	2.68	115.82	112.19
3	E	2	NAG	O5-C1-C2	-2.60	107.18	111.29
5	F	1	NAG	O4-C4-C3	-2.59	104.35	110.35
3	H	2	NAG	O5-C1-C2	-2.58	107.22	111.29
2	B	3	BMA	O4-C4-C3	-2.51	104.54	110.35
3	C	1	NAG	C1-O5-C5	2.51	115.59	112.19
2	B	3	BMA	C2-C3-C4	2.47	115.16	110.89
6	G	2	NAG	C1-O5-C5	-2.44	108.88	112.19
2	B	4	MAN	C1-O5-C5	2.33	115.35	112.19
5	F	5	MAN	C1-C2-C3	2.28	112.47	109.67
3	E	1	NAG	C2-N2-C7	2.27	126.13	122.90
5	F	5	MAN	O3-C3-C2	-2.25	105.69	109.99
5	F	3	BMA	C2-C3-C4	2.22	114.73	110.89
5	F	2	NAG	C4-C3-C2	-2.21	107.78	111.02
4	D	2	NAG	O5-C1-C2	-2.20	107.81	111.29
2	B	2	NAG	C1-O5-C5	2.14	115.10	112.19
4	D	3	BMA	C2-C3-C4	2.08	114.49	110.89
2	B	3	BMA	O3-C3-C2	-2.07	106.02	109.99
5	F	5	MAN	O4-C4-C3	-2.03	105.66	110.35
5	F	2	NAG	C1-O5-C5	-2.01	109.47	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2

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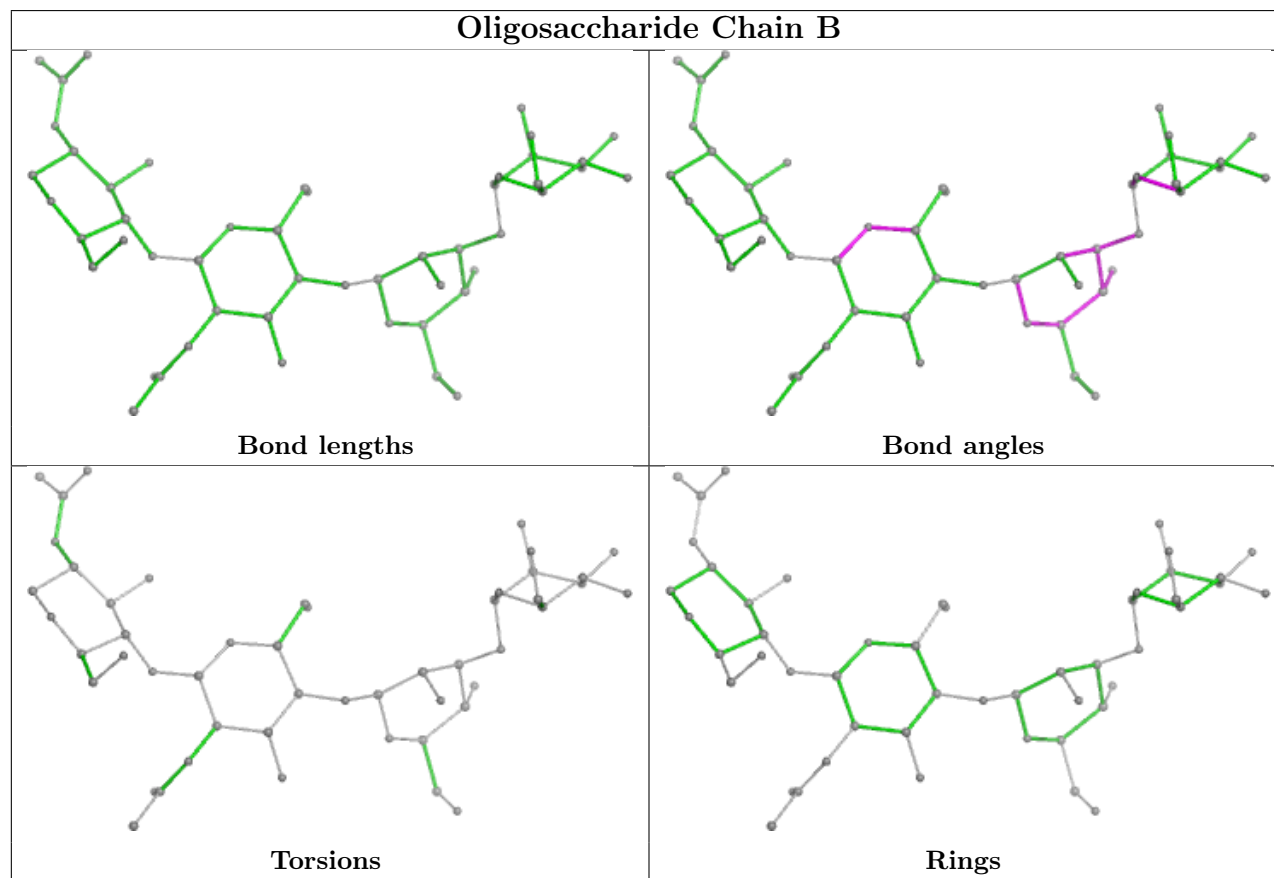
Mol	Chain	Res	Type	Atoms
5	F	1	NAG	O7-C7-N2-C2
5	F	5	MAN	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	F	4	MAN	O5-C5-C6-O6
4	D	6	MAN	O5-C5-C6-O6
4	D	6	MAN	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

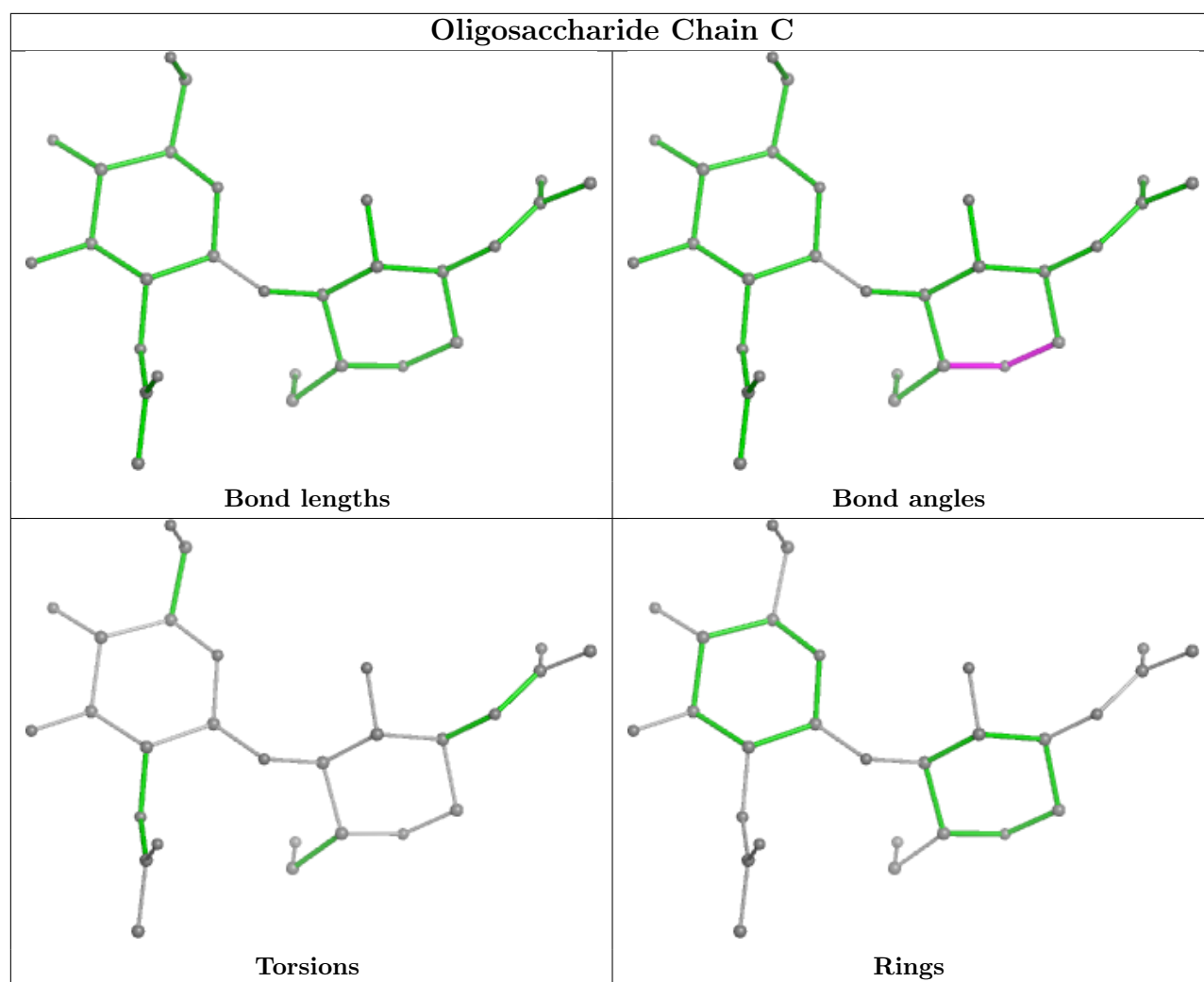
There are no ring outliers.

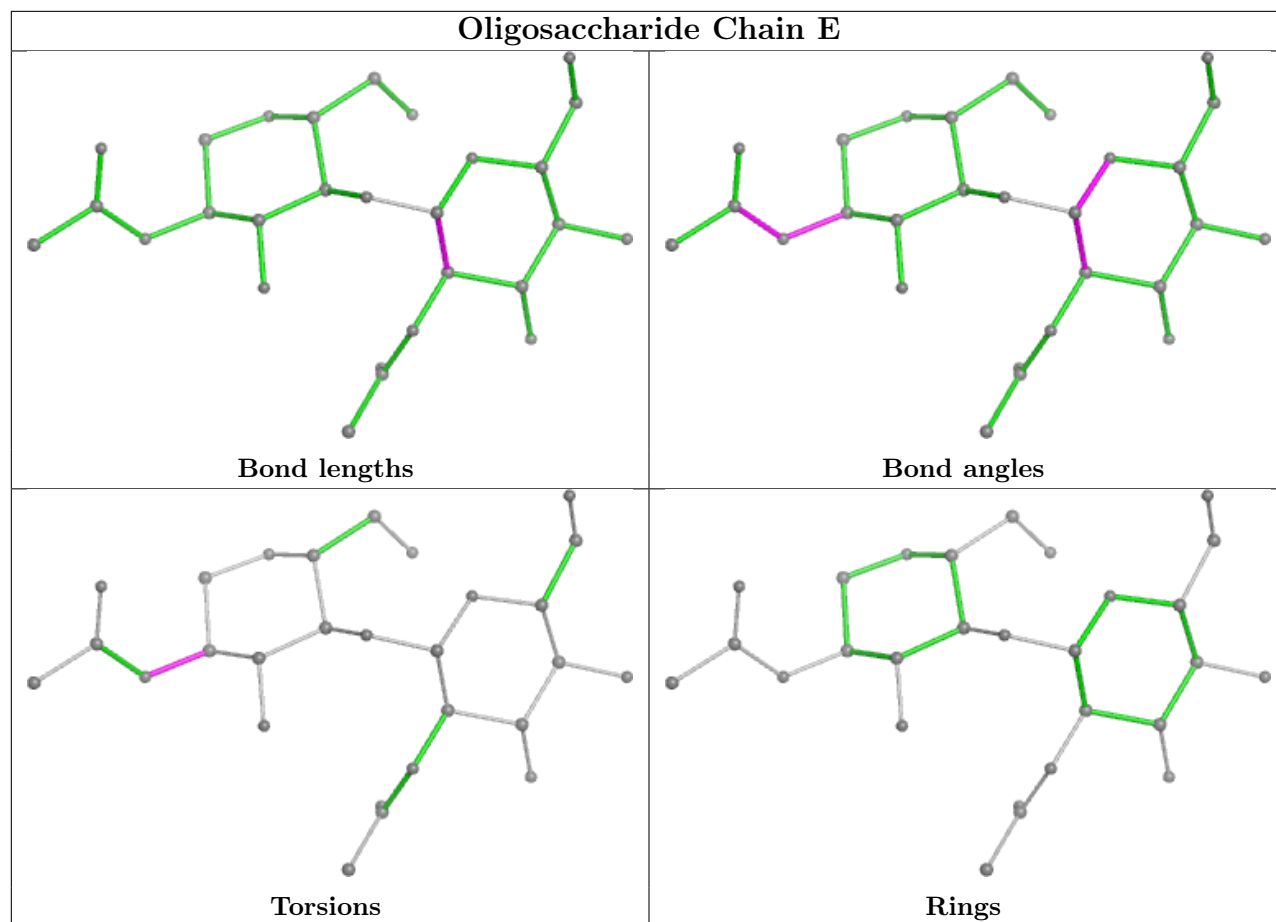
1 monomer is involved in 1 short contact:

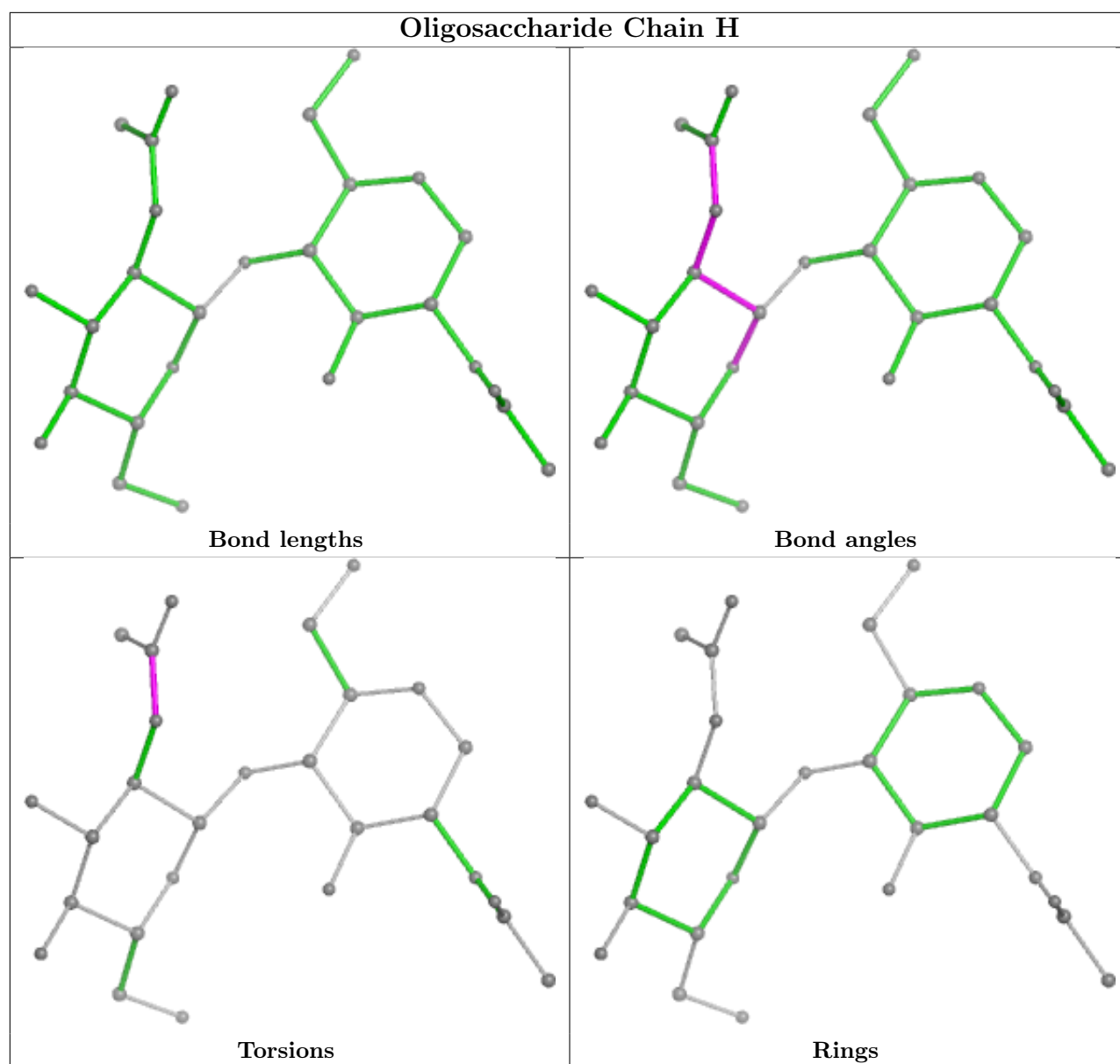
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0

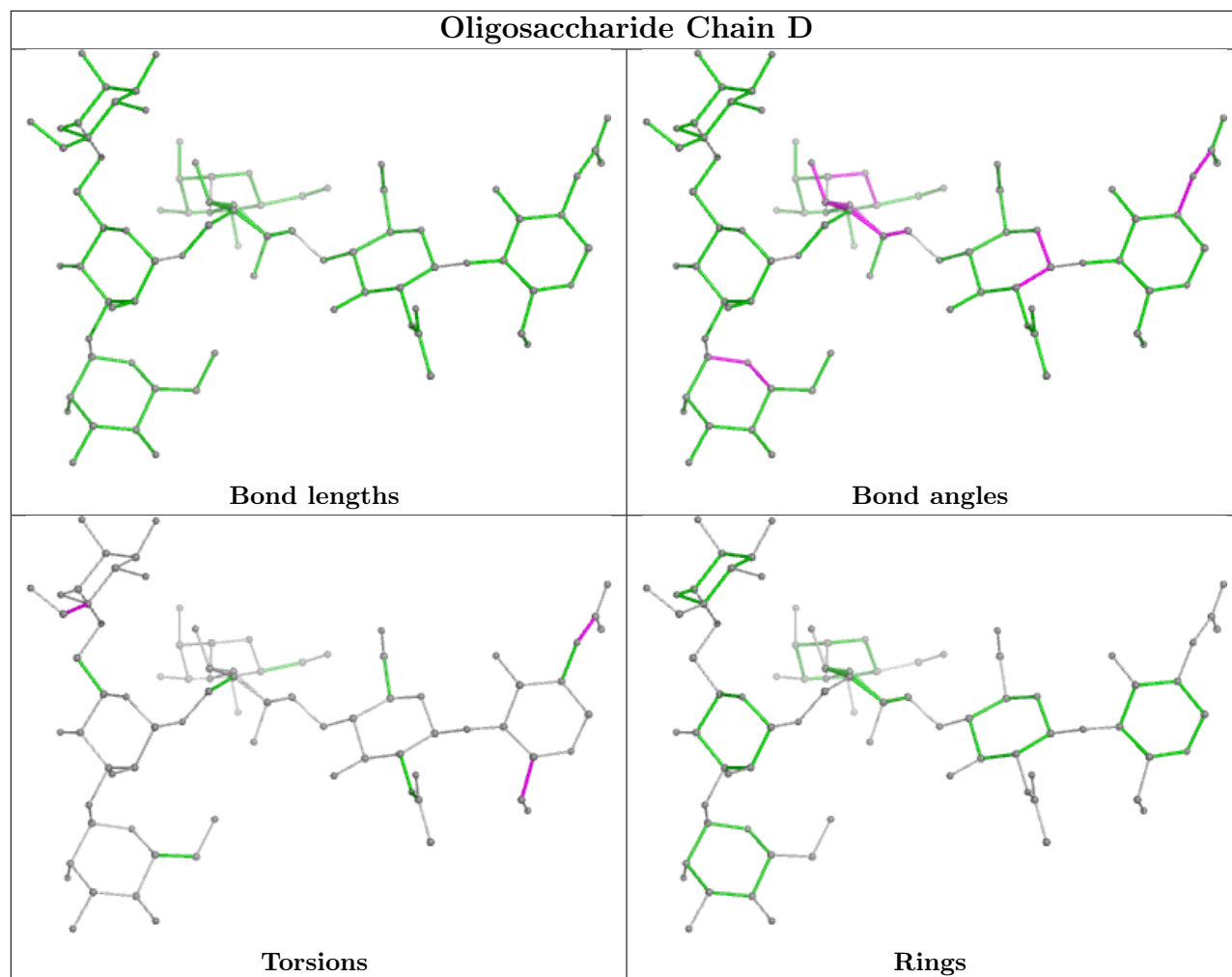
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



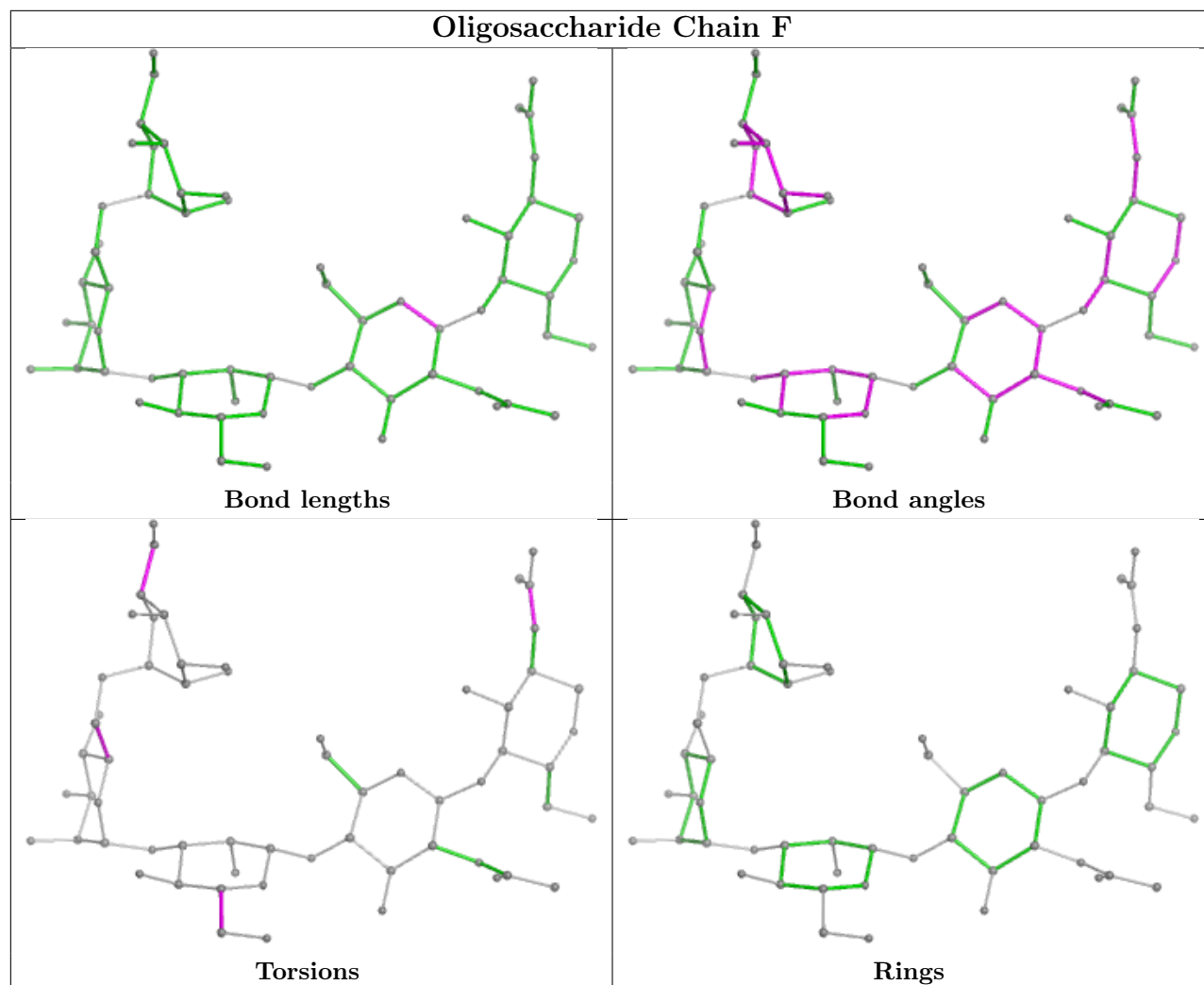


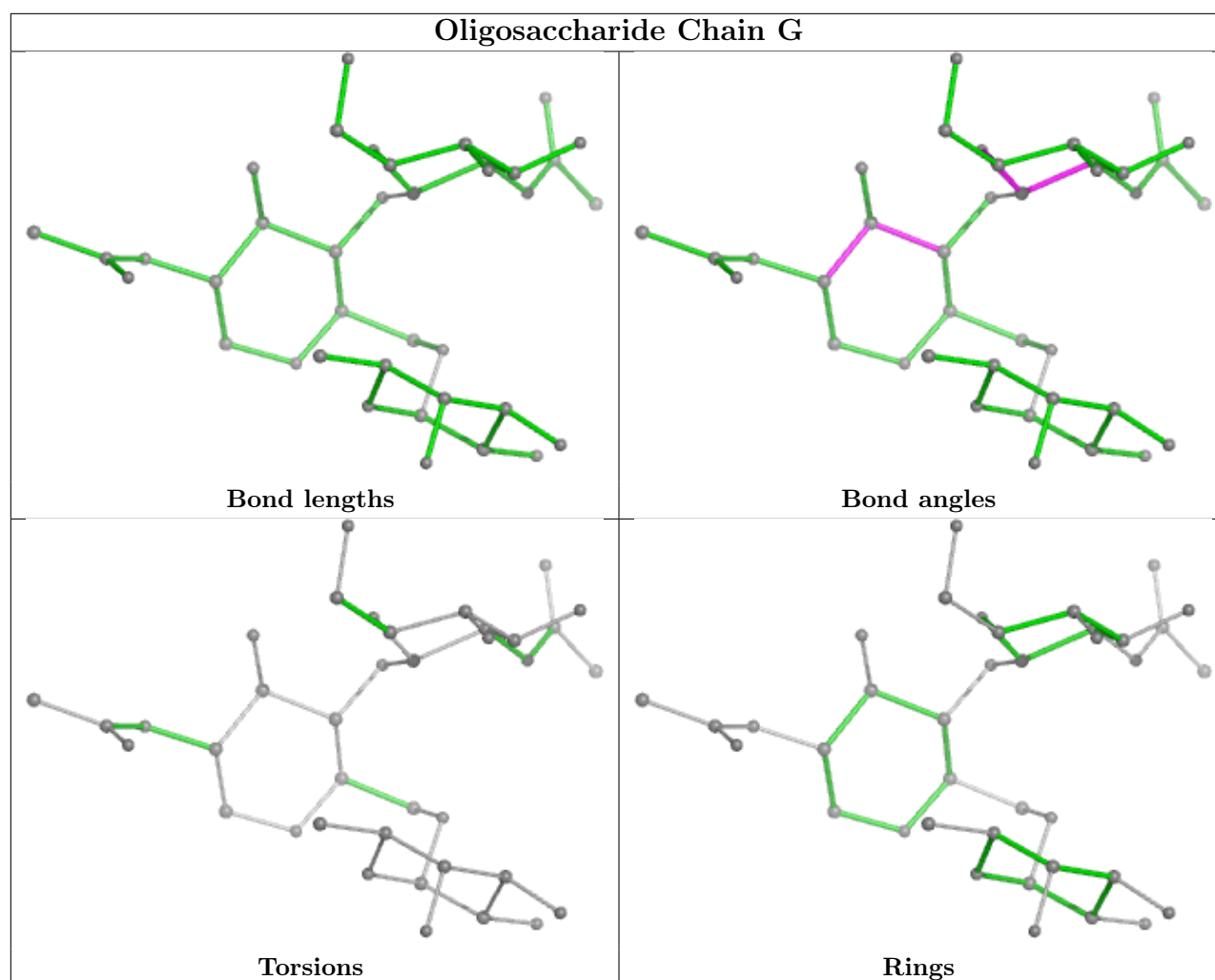






Oligosaccharide Chain F





5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	SO4	A	802	-	4,4,4	0.60	0	6,6,6	0.05	0
10	NAG	A	807	1	14,14,15	0.69	0	17,19,21	0.82	0
10	NAG	A	808	1	14,14,15	0.70	0	17,19,21	1.25	1 (5%)
7	A1JMH	A	801	-	37,38,38	2.07	11 (29%)	45,60,60	5.41	24 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	ACT	A	810	-	3,3,3	1.10	0	3,3,3	1.23	0
8	SO4	A	803	-	4,4,4	0.57	0	6,6,6	0.06	0
10	NAG	A	806	1	14,14,15	0.71	0	17,19,21	1.01	0
13	EDO	A	812	-	3,3,3	0.27	0	2,2,2	0.25	0
13	EDO	A	811	-	3,3,3	0.28	0	2,2,2	0.26	0
8	SO4	A	804	-	4,4,4	0.58	0	6,6,6	0.05	0
11	GOL	A	809	-	5,5,5	0.35	0	5,5,5	0.37	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
10	NAG	A	807	1	-	0/6/23/26	0/1/1/1
10	NAG	A	808	1	-	0/6/23/26	0/1/1/1
7	A1JMH	A	801	-	-	2/22/87/87	1/4/4/4
10	NAG	A	806	1	-	0/6/23/26	0/1/1/1
13	EDO	A	812	-	-	0/1/1/1	-
13	EDO	A	811	-	-	0/1/1/1	-
11	GOL	A	809	-	-	4/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	801	A1JMH	C06-C08	5.42	1.63	1.54
7	A	801	A1JMH	C13-C12	-4.99	1.45	1.54
7	A	801	A1JMH	O18-C17	-3.64	1.40	1.45
7	A	801	A1JMH	C12-C08	-3.27	1.48	1.55
7	A	801	A1JMH	C14-C15	-3.03	1.48	1.53
7	A	801	A1JMH	C10-C11	-2.85	1.48	1.54
7	A	801	A1JMH	C16-C15	-2.80	1.48	1.53
7	A	801	A1JMH	C16-C11	2.68	1.58	1.53
7	A	801	A1JMH	C05-C04	2.37	1.58	1.53
7	A	801	A1JMH	C09-C08	2.34	1.59	1.54
7	A	801	A1JMH	C03-C04	2.16	1.56	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	801	A1JMH	C07-C06-C08	16.68	142.31	112.74
7	A	801	A1JMH	C09-C08-C06	12.07	129.83	112.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	801	A1JMH	C11-C12-C08	10.84	112.91	100.07
7	A	801	A1JMH	C09-C08-C12	-10.74	90.90	103.84
7	A	801	A1JMH	C13-C14-C15	9.53	129.64	113.11
7	A	801	A1JMH	C10-C11-C16	-8.92	104.39	119.08
7	A	801	A1JMH	C12-C08-C06	-7.20	110.58	118.89
7	A	801	A1JMH	C08-C06-C05	-6.87	99.34	111.51
7	A	801	A1JMH	C14-C13-C12	-6.75	101.20	112.78
7	A	801	A1JMH	C17-O18-C19	-6.57	111.73	121.01
7	A	801	A1JMH	C29-C22-C21	-6.43	98.80	109.88
7	A	801	A1JMH	C30-C12-C13	-6.28	100.67	110.59
7	A	801	A1JMH	C10-C11-C12	-5.65	97.03	103.84
7	A	801	A1JMH	C07-C06-C05	-5.00	101.29	111.39
7	A	801	A1JMH	C11-C16-C15	-4.82	102.64	109.09
7	A	801	A1JMH	C30-C12-C08	-4.72	102.90	111.71
7	A	801	A1JMH	C29-C22-C23	4.25	115.41	108.97
7	A	801	A1JMH	C10-C09-C08	4.24	113.54	105.13
7	A	801	A1JMH	C14-C15-C16	-4.13	105.81	111.75
7	A	801	A1JMH	C21-C26-C25	3.64	117.01	111.90
7	A	801	A1JMH	C09-C10-C11	-2.95	99.28	105.13
7	A	801	A1JMH	O27-C25-C24	-2.53	104.61	110.22
7	A	801	A1JMH	O18-C19-O20	2.53	120.67	116.72
7	A	801	A1JMH	C23-C24-C25	-2.43	108.58	111.36
10	A	808	NAG	O5-C1-C2	-2.37	107.55	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	809	GOL	O1-C1-C2-C3
11	A	809	GOL	C1-C2-C3-O3
11	A	809	GOL	O2-C2-C3-O3
11	A	809	GOL	O1-C1-C2-O2
7	A	801	A1JMH	C05-C06-C08-C09
7	A	801	A1JMH	O31-C05-C06-C07

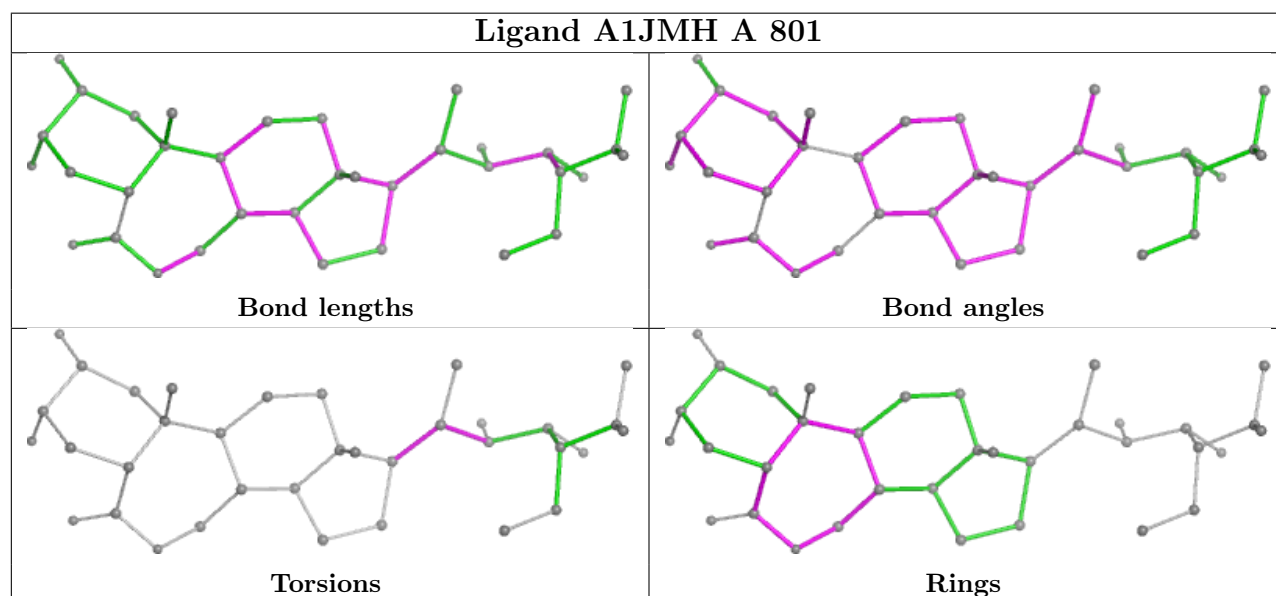
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	801	A1JMH	C15-C16-C17-C19-C21-C22-O18

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	801	A1JMH	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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	743/797 (93%)	0.82	83 (11%)	11 13	54, 97, 142, 180	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	VAL	4.4
1	A	669	TYR	4.2
1	A	681	PHE	4.1
1	A	447	LEU	3.7
1	A	515	ASN	3.7
1	A	553	PRO	3.7
1	A	481	PRO	3.6
1	A	772	PRO	3.6
1	A	744	GLU	3.5
1	A	552	ILE	3.5
1	A	480	ILE	3.4
1	A	356	LEU	3.4
1	A	505	PRO	3.4
1	A	572	PHE	3.4
1	A	665	MET	3.2
1	A	548	PHE	3.2
1	A	528	ILE	3.1
1	A	500	LEU	3.1
1	A	591	PHE	3.1
1	A	69	CYS	3.1
1	A	596	ARG	3.1
1	A	407	LEU	3.0
1	A	563	ILE	3.0
1	A	535	LEU	3.0
1	A	748	PHE	2.9
1	A	517	ILE	2.8
1	A	494	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	718	ILE	2.8
1	A	414	PRO	2.7
1	A	630	SER	2.7
1	A	504	ILE	2.6
1	A	389	SER	2.6
1	A	638	THR	2.6
1	A	635	CYS	2.6
1	A	357	PRO	2.6
1	A	162	PHE	2.5
1	A	406	ILE	2.5
1	A	534	ARG	2.5
1	A	311	LEU	2.5
1	A	484	LEU	2.5
1	A	442	LEU	2.5
1	A	452	LEU	2.5
1	A	482	GLN	2.5
1	A	527	GLU	2.5
1	A	743	PRO	2.5
1	A	475	MET	2.4
1	A	771	ASP	2.4
1	A	456	ILE	2.4
1	A	366	GLY	2.3
1	A	556	LEU	2.3
1	A	336	PHE	2.3
1	A	606	LYS	2.3
1	A	486	TYR	2.3
1	A	411	CYS	2.3
1	A	670	ILE	2.3
1	A	469	LEU	2.2
1	A	207	ILE	2.2
1	A	391	SER	2.2
1	A	524	LEU	2.2
1	A	745	MET	2.2
1	A	416	ASN	2.2
1	A	689	ASP	2.2
1	A	408	PRO	2.2
1	A	582	LYS	2.1
1	A	607	LYS	2.1
1	A	427	GLY	2.1
1	A	746	GLY	2.1
1	A	592	ILE	2.1
1	A	770	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	435	THR	2.1
1	A	458	SER	2.1
1	A	742	ILE	2.1
1	A	387	ASN	2.1
1	A	666	LEU	2.1
1	A	428	PHE	2.1
1	A	429	THR	2.1
1	A	451	TYR	2.0
1	A	385	LEU	2.0
1	A	392	LEU	2.0
1	A	512	THR	2.0
1	A	618	PHE	2.0
1	A	466	LEU	2.0
1	A	508	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

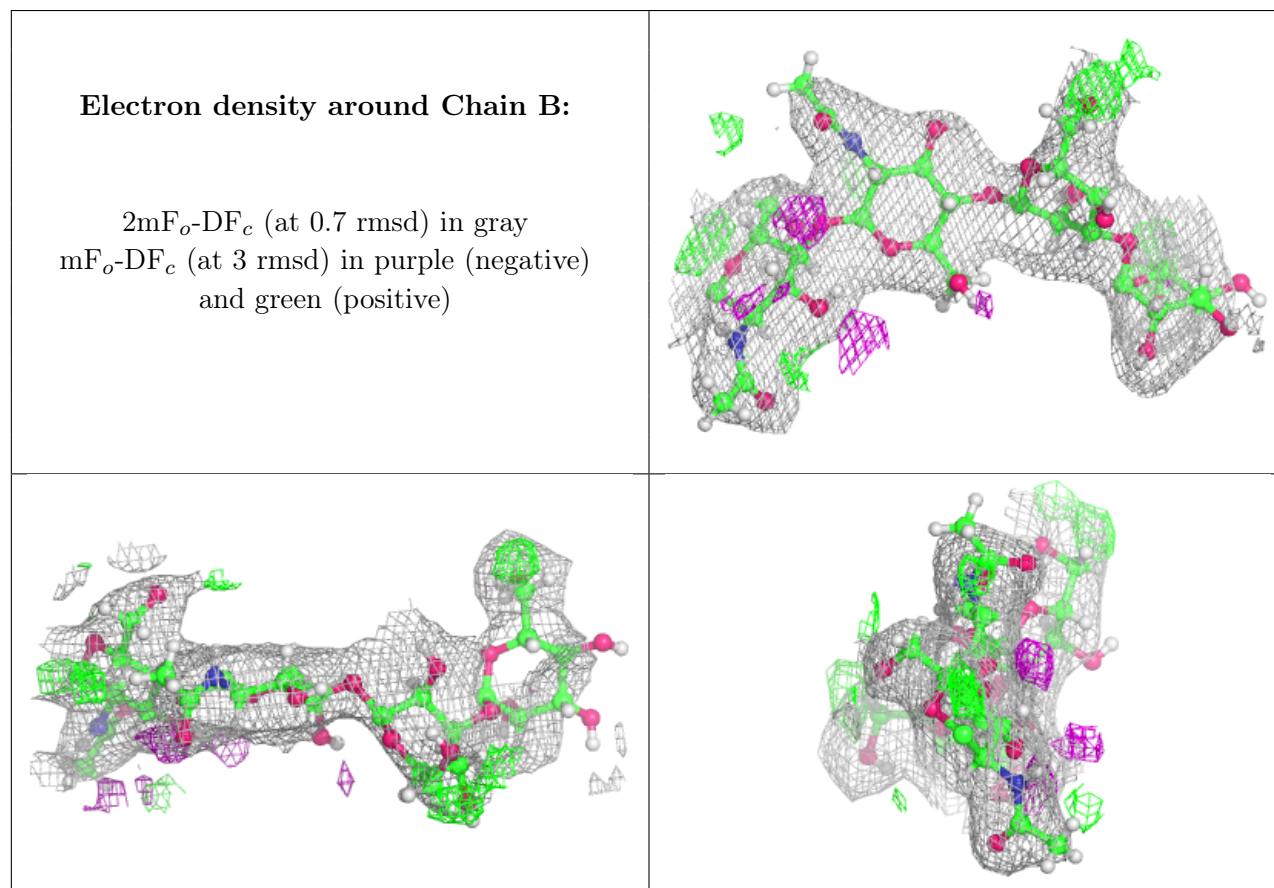
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	1	14/15	0.18	0.18	142,163,188,197	0
3	NAG	E	2	14/15	0.20	0.19	144,171,198,204	0
6	FUC	G	3	10/11	0.20	0.17	144,170,202,205	0
3	NAG	H	2	14/15	0.21	0.16	141,158,186,193	0
2	MAN	B	4	11/12	0.32	0.14	125,150,180,185	0
5	MAN	F	4	11/12	0.34	0.20	138,146,175,178	0
6	NAG	G	2	14/15	0.40	0.19	162,173,206,212	0
3	NAG	C	2	14/15	0.44	0.16	131,153,183,187	0
5	MAN	F	5	11/12	0.47	0.23	124,144,169,173	0
2	BMA	B	3	11/12	0.51	0.14	125,138,161,172	0
4	MAN	D	7	11/12	0.56	0.18	115,132,155,167	0
5	BMA	F	3	11/12	0.56	0.18	114,137,164,165	0
4	MAN	D	6	11/12	0.59	0.13	105,133,159,169	0
4	MAN	D	5	11/12	0.64	0.12	125,138,163,168	0

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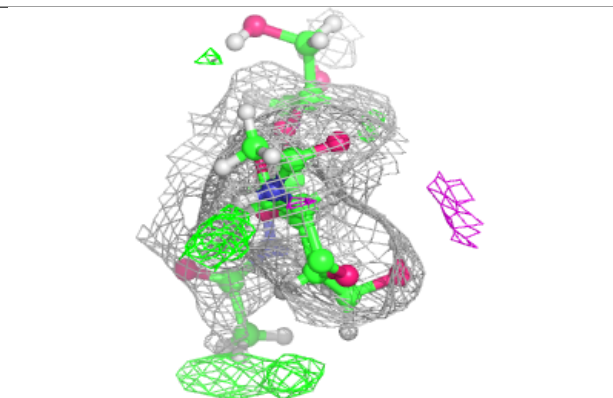
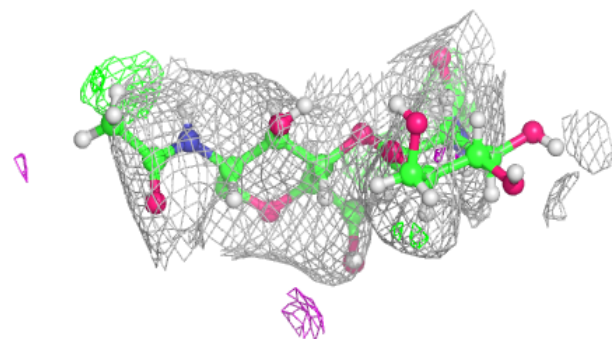
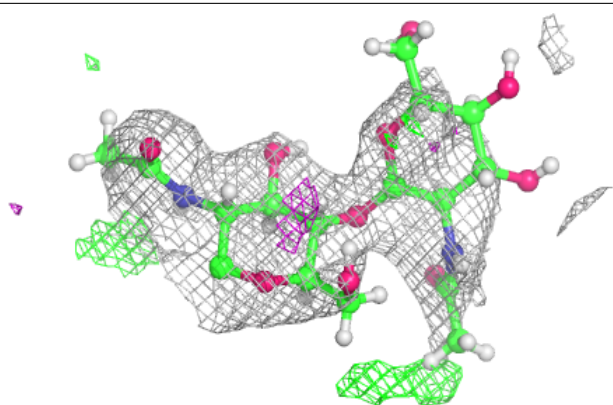
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	H	1	14/15	0.70	0.14	116,141,157,170	0
6	NAG	G	1	14/15	0.71	0.17	136,161,189,195	0
5	NAG	F	2	14/15	0.72	0.17	96,116,134,144	0
3	NAG	C	1	14/15	0.78	0.14	91,117,144,152	0
4	NAG	D	2	14/15	0.79	0.14	84,111,124,133	0
4	BMA	D	3	11/12	0.80	0.11	119,125,150,157	0
5	NAG	F	1	14/15	0.88	0.15	80,98,111,119	0
4	MAN	D	4	11/12	0.88	0.10	113,123,148,148	0
2	NAG	B	2	14/15	0.89	0.13	69,101,123,131	0
4	NAG	D	1	14/15	0.91	0.10	55,75,86,92	0
2	NAG	B	1	14/15	0.92	0.11	53,65,85,88	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.

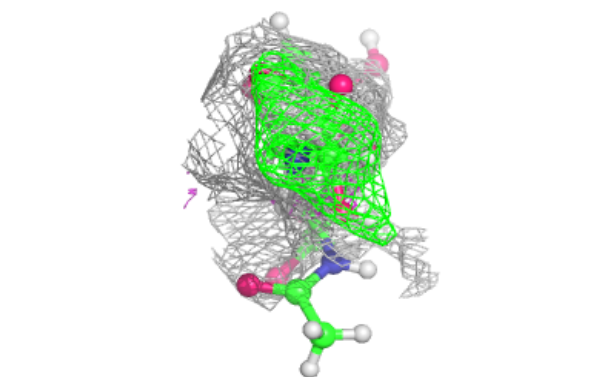
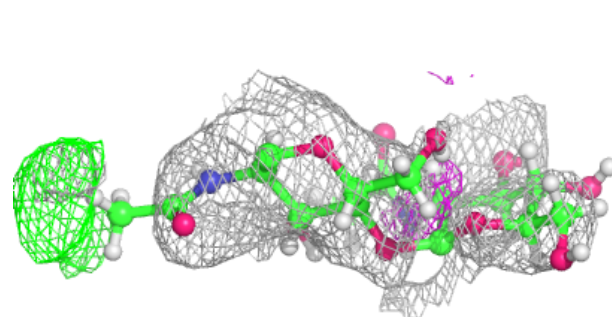
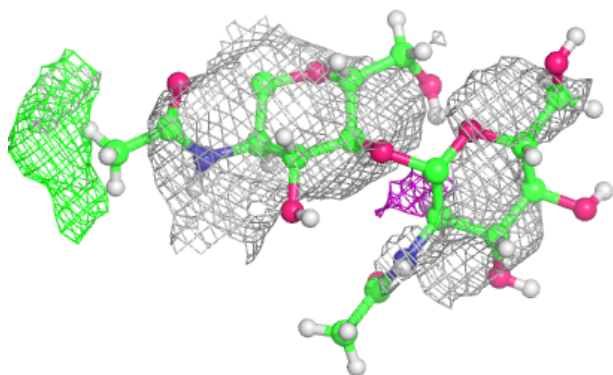


Electron density around Chain C:

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

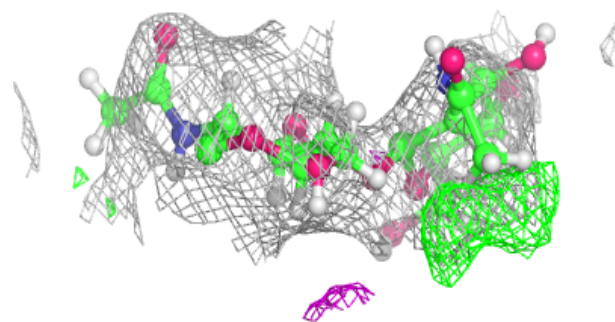
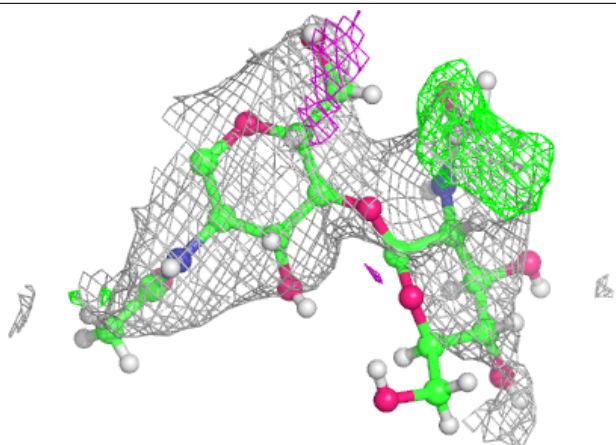
**Electron density around Chain E:**

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



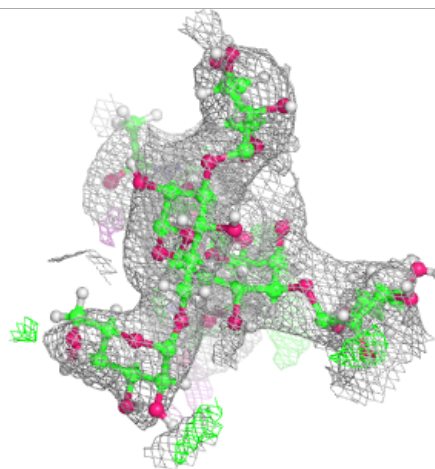
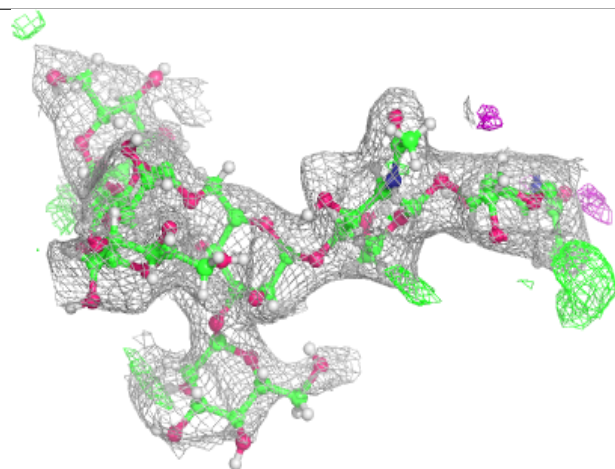
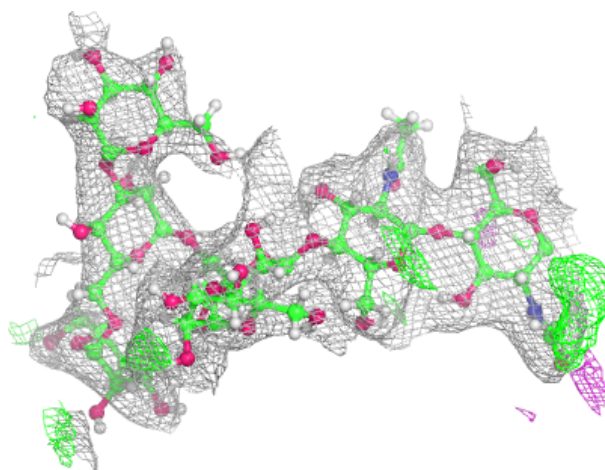
Electron density around Chain H:

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



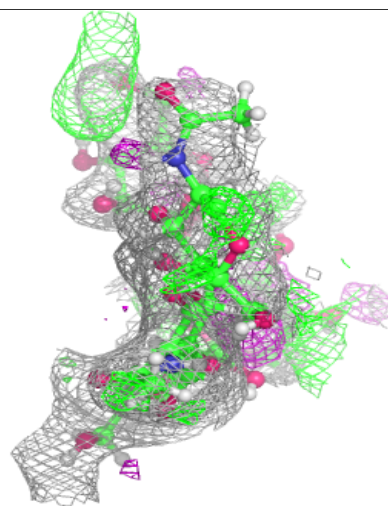
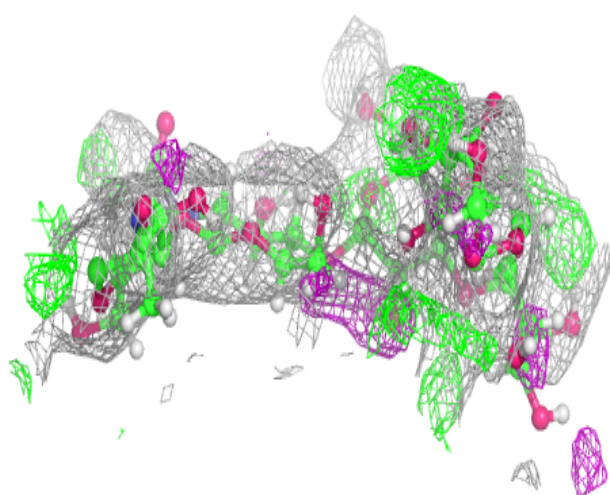
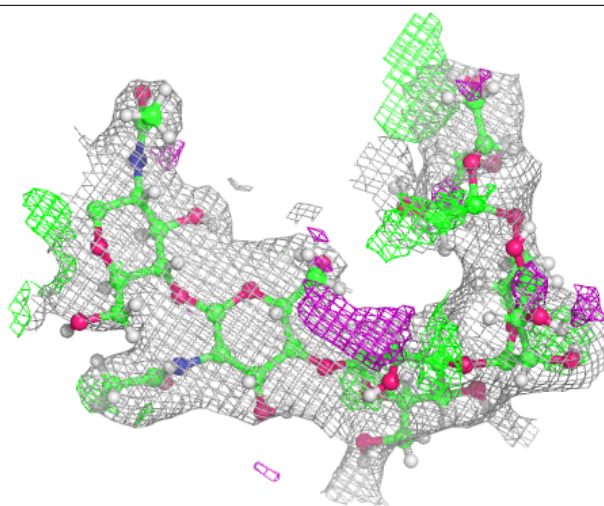
Electron density around Chain D:

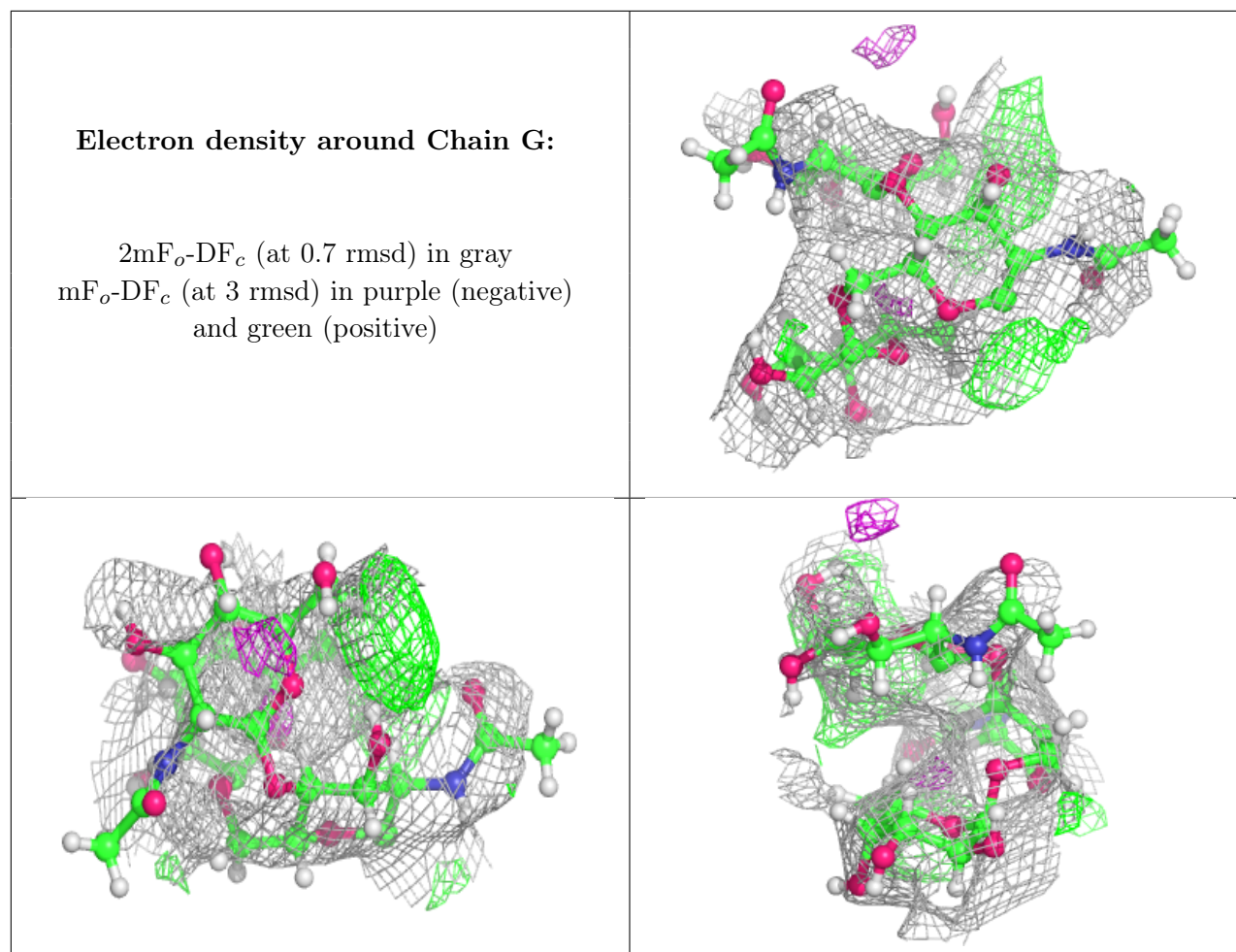
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

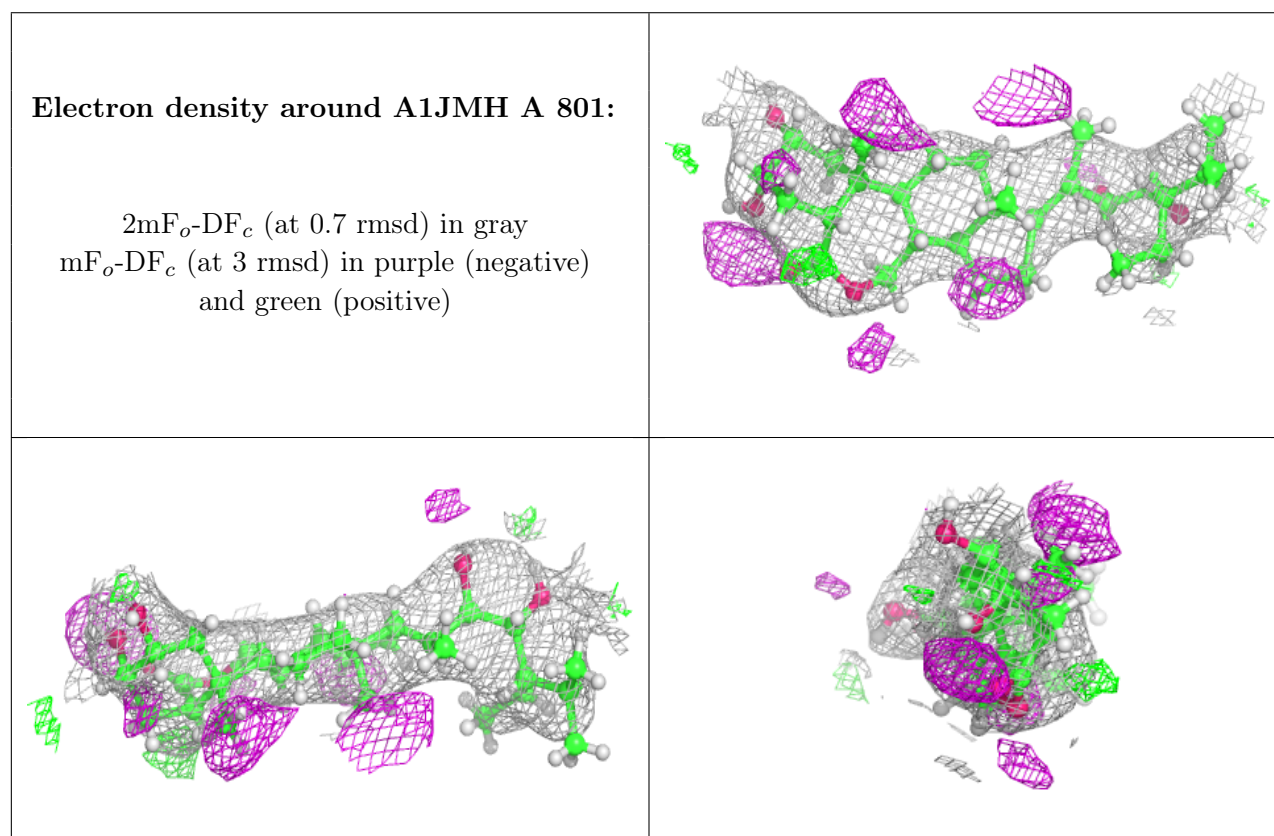
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	SO4	A	803	5/5	0.29	0.12	198,201,210,211	0
10	NAG	A	807	14/15	0.59	0.17	115,144,169,184	0
10	NAG	A	808	14/15	0.66	0.14	150,180,221,221	0
8	SO4	A	804	5/5	0.72	0.15	133,144,156,367	0
13	EDO	A	811	4/4	0.74	0.21	94,113,128,135	0
9	NA	A	805	1/1	0.79	0.33	331,331,331,331	0
8	SO4	A	802	5/5	0.79	0.11	118,122,136,195	0
12	ACT	A	810	4/4	0.85	0.25	71,91,110,110	0
13	EDO	A	812	4/4	0.85	0.18	95,114,128,139	0
11	GOL	A	809	6/6	0.87	0.20	85,107,128,128	0
10	NAG	A	806	14/15	0.87	0.12	101,115,138,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	A1JMH	A	801	35/35	0.91	0.15	68,95,114,116	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.