



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2025 – 01:15 pm BST

PDB ID : 9S87 / pdb\_00009s87  
Title : Crystal structure of the BRI1 ectodomain from Arabidopsis thaliana in complex with castasterone.  
Authors : Caregnato, A.; Hothorn, M.  
Deposited on : 2025-08-05  
Resolution : 2.14 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>.

---

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

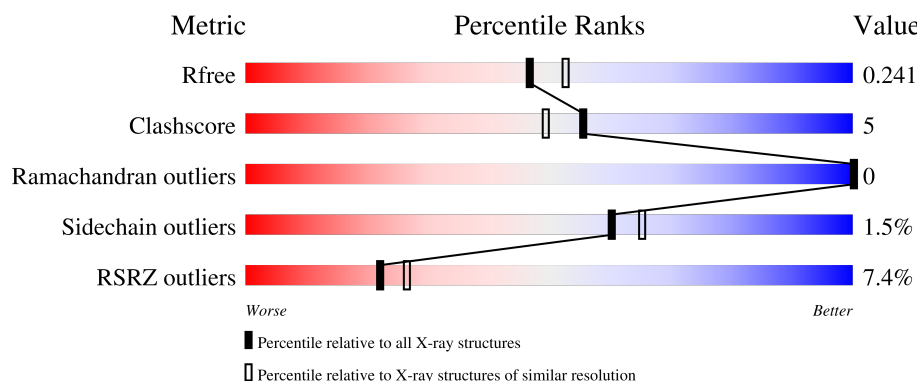
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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.




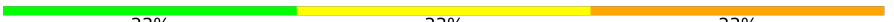

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3336 (2.16-2.12)
Clashscore	180529	3585 (2.16-2.12)
Ramachandran outliers	177936	3554 (2.16-2.12)
Sidechain outliers	177891	3553 (2.16-2.12)
RSRZ outliers	164620	3337 (2.16-2.12)

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	797	<div> <div>7%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
2	B	2	<div>100%</div>
2	E	2	<div>50%</div> <div>50%</div>
3	C	4	<div>100%</div>
4	D	5	<div>40%</div> <div>60%</div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	F	3	 100%
6	G	3	 33% 33% 33%
7	H	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	F	1	-	-	X	-

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 11926 atoms, of which 5722 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	742	Total	C	H	N	O	S	0	0	0
			11205	3549	5584	933	1107	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 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



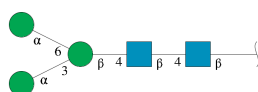
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 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.



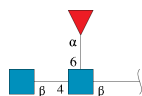
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

- Molecule 4 is an oligosaccharide called 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.



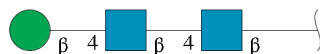
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	5	Total	C	H	N	O	0	0	0
			85	34	24	2	25			

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



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

- Molecule 6 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.



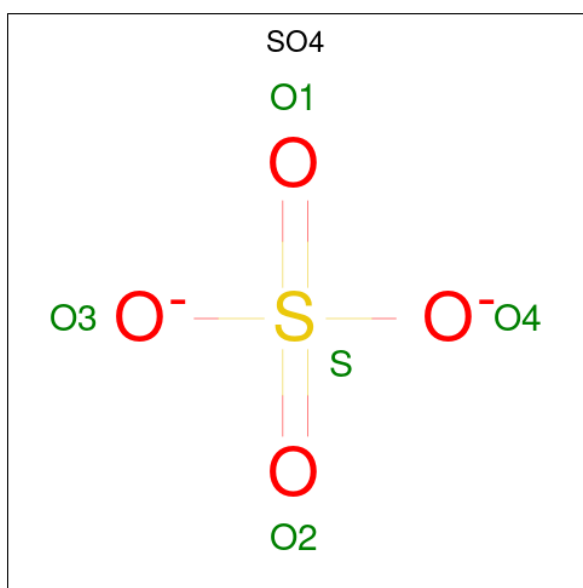
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



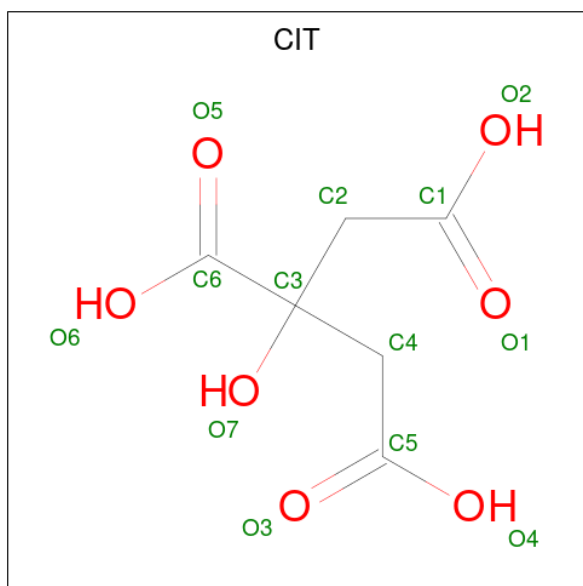
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
10	A	1	Total	C	N	O		0	0
			14	8	1	5			

Continued on next page...

Continued from previous page...

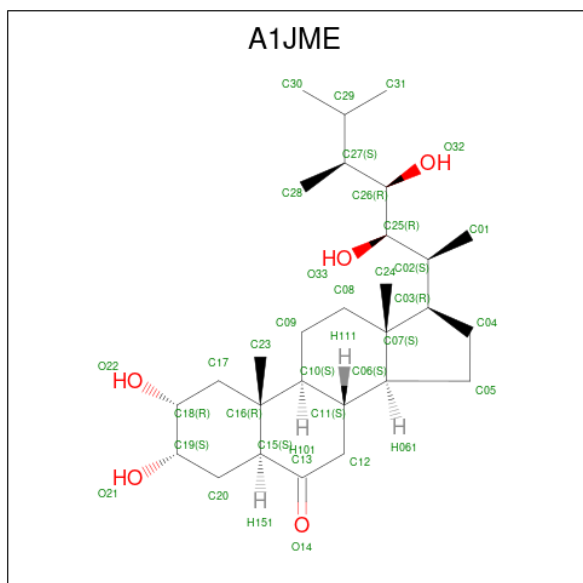
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	A	1	14	8	1	5	0	0

- Molecule 11 is CITRIC ACID (CCD ID: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
11	A	1	18	6	5	7	0	0

- Molecule 12 is Castasterone (CCD ID: A1JME) (formula:  $C_{28}H_{48}O_5$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			81	28	48	5		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	213	Total	O	0	0
			213	213		



Chain C:  100%

NAG1  
NAG2  
BMA3  
MAN4

- Molecule 4:  $\alpha$ -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:  40%  60%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5

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

Chain F:  100%

NAG1  
NAG2  
FUC3

- Molecule 6:  $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain G:  33%  33%  33%

NAG1  
NAG2  
BMA3

- Molecule 7:  $\alpha$ -L-fucopyranose-(1-6)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain H:  50%  50%

NAG1  
FUC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.40Å 66.90Å 120.43Å 90.00° 122.46° 90.00°	Depositor
Resolution (Å)	47.87 – 2.14 47.87 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.87-2.14) 88.7 (47.87-2.14)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.62 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.212 , 0.243 0.212 , 0.241	Depositor DCC
$R_{free}$ test set	3239 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 69.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11926	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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: FUC, EDO, BMA, CIT, NAG, SO4, A1JME, MAN

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	0.13	0/5729	0.31	0/7773

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	5621	5584	5580	44	0
2	B	28	0	25	1	0
2	E	28	0	25	1	0
3	C	50	43	43	0	0
4	D	61	24	52	2	0
5	F	38	0	34	12	0
6	G	39	0	34	1	0
7	H	24	0	22	0	0
8	A	10	0	0	0	0
9	A	4	6	6	0	0
10	A	42	12	39	1	0
11	A	13	5	5	0	0
12	A	33	48	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	213	0	0	6	2
All	All	6204	5722	5865	54	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (54) 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:251:ASP:OD1	13:A:901:HOH:O	1.75	1.02
1:A:510:ASN:ND2	5:F:1:NAG:H83	1.97	0.79
1:A:284:PRO:O	13:A:902:HOH:O	2.10	0.69
5:F:1:NAG:H3	5:F:2:NAG:H2	1.77	0.65
1:A:392:LEU:O	1:A:417:THR:HG23	1.97	0.64
1:A:537:ASN:O	1:A:537:ASN:ND2	2.30	0.64
1:A:356:LEU:HD21	1:A:382:PRO:HD3	1.80	0.62
1:A:437:SER:OG	2:E:1:NAG:H82	2.01	0.60
1:A:263:ARG:NE	13:A:909:HOH:O	2.35	0.60
5:F:1:NAG:C3	5:F:2:NAG:H2	2.32	0.59
5:F:1:NAG:H61	5:F:3:FUC:O2	2.04	0.58
1:A:441:GLU:OE1	1:A:465:LYS:NZ	2.35	0.58
1:A:708:ASP:HB2	1:A:732:ASP:HB3	1.86	0.57
2:B:1:NAG:O4	2:B:2:NAG:O7	2.22	0.57
1:A:510:ASN:HD22	5:F:1:NAG:H83	1.66	0.56
1:A:592:ILE:HD12	1:A:593:ALA:N	2.21	0.55
1:A:695:PRO:O	1:A:698:VAL:HG22	2.07	0.55
1:A:275:ASN:HD22	4:D:1:NAG:H83	1.72	0.54
1:A:587:ILE:HD12	1:A:655:SER:HA	1.89	0.53
1:A:749:GLU:OE1	13:A:903:HOH:O	2.19	0.53
1:A:539:ALA:HB3	1:A:592:ILE:HG21	1.90	0.53
1:A:514:LEU:HD13	1:A:517:ILE:HD11	1.90	0.52
1:A:545:ASN:HD21	6:G:1:NAG:C1	2.22	0.52
1:A:515:ASN:HA	1:A:538:LEU:HA	1.91	0.51
1:A:698:VAL:HG21	1:A:722:MET:SD	2.50	0.51
5:F:1:NAG:H3	5:F:2:NAG:C2	2.41	0.50
1:A:356:LEU:HD23	1:A:356:LEU:H	1.76	0.50
1:A:499:ASP:OD1	1:A:523:ARG:NH1	2.37	0.49
1:A:166:VAL:O	1:A:166:VAL:HG13	2.14	0.48
1:A:425:ASN:HA	1:A:449:PHE:HB3	1.95	0.47
1:A:510:ASN:HD21	5:F:1:NAG:C1	2.27	0.47
5:F:1:NAG:H4	5:F:3:FUC:H3	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:2:NAG:H83	5:F:2:NAG:H3	1.96	0.46
1:A:233:ASN:HD22	10:A:804:NAG:H83	1.81	0.46
1:A:555:GLU:OE1	1:A:555:GLU:N	2.47	0.44
5:F:2:NAG:H82	5:F:2:NAG:C1	2.47	0.44
1:A:510:ASN:HD21	5:F:1:NAG:C2	2.30	0.44
1:A:692:GLY:O	1:A:715:ASP:N	2.42	0.44
1:A:557:GLY:O	1:A:583:GLN:HG2	2.17	0.44
4:D:2:NAG:H61	4:D:3:BMA:C1	2.49	0.43
1:A:548:PHE:HD1	13:A:904:HOH:O	2.02	0.42
1:A:273:LEU:C	1:A:273:LEU:HD23	2.45	0.42
1:A:750:THR:HG22	1:A:750:THR:O	2.19	0.42
1:A:437:SER:HA	1:A:463:LEU:HD21	2.01	0.41
5:F:1:NAG:C3	5:F:2:NAG:C2	2.94	0.41
1:A:684:ASN:OD1	1:A:708:ASP:OD1	2.38	0.41
1:A:334:PRO:HA	1:A:360:THR:HG21	2.02	0.41
1:A:638:THR:O	1:A:638:THR:HG23	2.20	0.41
1:A:238:ILE:HG23	1:A:239:PRO:HD2	2.03	0.41
1:A:548:PHE:HB3	13:A:904:HOH:O	2.20	0.41
1:A:202:LEU:HD21	1:A:205:LEU:HB2	2.02	0.40
1:A:650:PHE:CG	1:A:654:GLY:HA3	2.55	0.40
1:A:673:GLU:OE1	1:A:673:GLU:N	2.50	0.40
1:A:587:ILE:O	1:A:654:GLY:N	2.54	0.40

All (2) 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)
13:A:1004:HOH:O	13:A:1034:HOH:O[2_655]	2.08	0.12
13:A:1103:HOH:O	13:A:1107:HOH:O[2_656]	2.14	0.06

## 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	740/797 (93%)	694 (94%)	46 (6%)	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	655/702 (93%)	645 (98%)	10 (2%)	60	65

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	215	ASP
1	A	365	ARG
1	A	383	GLU
1	A	384	SER
1	A	598	VAL
1	A	603	ASP
1	A	646	THR
1	A	757	LEU
1	A	769	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	85	ASN
1	A	110	HIS
1	A	189	ASN
1	A	248	GLN
1	A	249	HIS
1	A	510	ASN
1	A	537	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	627	ASN
1	A	687	HIS
1	A	705	ASN

### 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 ⓘ

21 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	2,1	14,14,15	0.73	0	17,19,21	0.89	0
2	NAG	B	2	2	14,14,15	0.73	0	17,19,21	0.83	0
3	NAG	C	1	3,1	14,14,15	0.69	0	17,19,21	1.07	1 (5%)
3	NAG	C	2	3	14,14,15	0.74	0	17,19,21	1.79	4 (23%)
3	BMA	C	3	3	11,11,12	0.86	0	15,15,17	1.98	3 (20%)
3	MAN	C	4	3	11,11,12	0.72	0	15,15,17	1.12	1 (6%)
4	NAG	D	1	4,1	14,14,15	0.74	0	17,19,21	1.52	3 (17%)
4	NAG	D	2	4	14,14,15	0.70	0	17,19,21	2.18	6 (35%)
4	BMA	D	3	4	11,11,12	0.87	0	15,15,17	2.23	5 (33%)
4	MAN	D	4	4	11,11,12	0.86	1 (9%)	15,15,17	0.91	0
4	MAN	D	5	4	11,11,12	0.81	1 (9%)	15,15,17	0.91	0
2	NAG	E	1	2,1	14,14,15	0.67	0	17,19,21	1.06	2 (11%)
2	NAG	E	2	2	14,14,15	0.73	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	F	1	5	14,14,15	0.85	1 (7%)	17,19,21	1.84	3 (17%)
5	NAG	F	2	5	14,14,15	0.68	0	17,19,21	1.40	2 (11%)
5	FUC	F	3	5	10,10,11	0.99	1 (10%)	14,14,16	1.03	0
6	NAG	G	1	6	14,14,15	0.83	0	17,19,21	1.60	2 (11%)
6	NAG	G	2	6	14,14,15	0.76	0	17,19,21	0.68	0
6	BMA	G	3	6	11,11,12	0.87	0	15,15,17	2.85	6 (40%)
7	NAG	H	1	7,1	14,14,15	0.67	0	17,19,21	0.94	1 (5%)
7	FUC	H	2	7	10,10,11	0.79	0	14,14,16	0.97	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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	5/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
5	NAG	F	1	5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1
6	NAG	G	1	6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
7	NAG	H	1	7,1	-	0/6/23/26	0/1/1/1
7	FUC	H	2	7	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3	FUC	O5-C1	-2.54	1.39	1.43
4	D	4	MAN	O5-C1	-2.28	1.40	1.43
5	F	1	NAG	O5-C1	-2.17	1.40	1.43
4	D	5	MAN	O5-C1	-2.08	1.40	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	3	BMA	C1-O5-C5	8.69	123.97	112.19
4	D	3	BMA	C1-O5-C5	6.37	120.82	112.19
3	C	3	BMA	C1-O5-C5	5.59	119.76	112.19
5	F	1	NAG	O5-C1-C2	-5.45	102.69	111.29
3	C	2	NAG	C2-N2-C7	4.83	129.78	122.90
6	G	1	NAG	O5-C1-C2	-4.52	104.15	111.29
4	D	2	NAG	C1-O5-C5	4.43	118.20	112.19
4	D	1	NAG	C2-N2-C7	4.22	128.92	122.90
5	F	2	NAG	C2-N2-C7	4.14	128.80	122.90
4	D	2	NAG	O4-C4-C5	4.00	119.23	109.30
4	D	2	NAG	C2-N2-C7	3.66	128.12	122.90
6	G	3	BMA	C3-C4-C5	3.26	116.05	110.24
3	C	4	MAN	C1-O5-C5	2.92	116.16	112.19
4	D	2	NAG	C4-C3-C2	-2.88	106.80	111.02
5	F	1	NAG	C3-C4-C5	2.85	115.32	110.24
3	C	2	NAG	C1-O5-C5	2.81	116.01	112.19
3	C	3	BMA	C3-C4-C5	2.67	115.00	110.24
3	C	1	NAG	O5-C1-C2	-2.63	107.13	111.29
3	C	2	NAG	O5-C1-C2	-2.63	107.14	111.29
2	E	1	NAG	C1-O5-C5	2.52	115.61	112.19
6	G	3	BMA	C2-C3-C4	2.49	115.20	110.89
6	G	3	BMA	O4-C4-C3	-2.48	104.61	110.35
4	D	1	NAG	C1-O5-C5	2.43	115.49	112.19
4	D	3	BMA	O2-C2-C3	2.43	115.00	110.14
4	D	3	BMA	O4-C4-C3	-2.41	104.78	110.35
3	C	2	NAG	C8-C7-N2	2.38	120.13	116.10
4	D	3	BMA	O3-C3-C4	2.38	115.85	110.35
7	H	1	NAG	C1-O5-C5	2.37	115.40	112.19
5	F	2	NAG	O5-C1-C2	-2.34	107.60	111.29
6	G	3	BMA	O3-C3-C2	-2.31	105.56	109.99
6	G	3	BMA	O5-C5-C4	2.31	116.45	110.83
4	D	2	NAG	C3-C4-C5	-2.28	106.17	110.24
2	E	1	NAG	O5-C1-C2	-2.26	107.72	111.29
6	G	1	NAG	O4-C4-C3	-2.26	105.12	110.35
5	F	1	NAG	O4-C4-C5	-2.23	103.76	109.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	2.21	115.18	112.19
4	D	2	NAG	C8-C7-N2	2.15	119.75	116.10
4	D	1	NAG	C8-C7-N2	2.11	119.66	116.10
4	D	3	BMA	C2-C3-C4	2.09	114.51	110.89
3	C	3	BMA	C2-C3-C4	2.09	114.51	110.89

There are no chirality outliers.

All (27) torsion outliers are listed below:

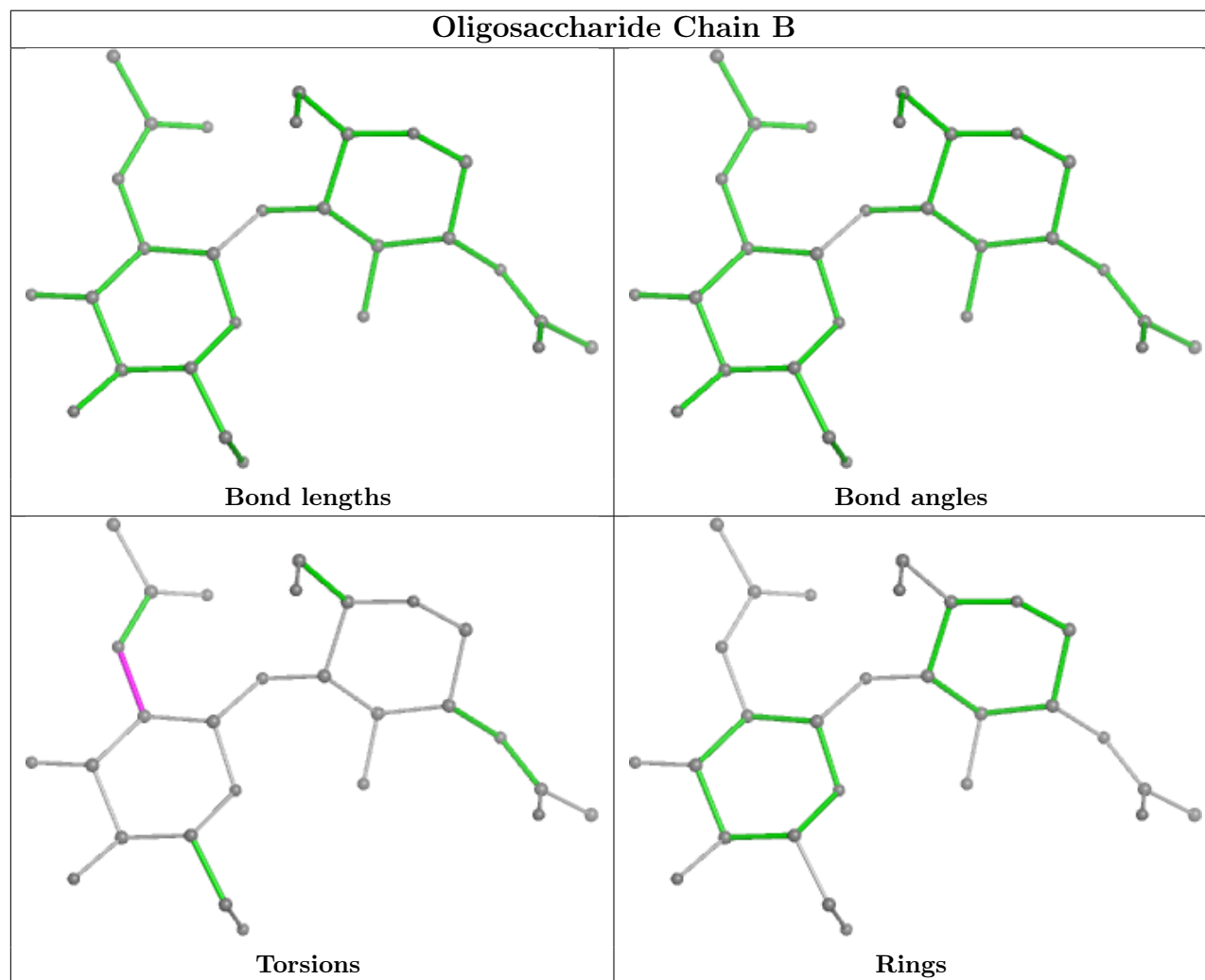
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C3-C2-N2-C7
4	D	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
5	F	2	NAG	C8-C7-N2-C2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

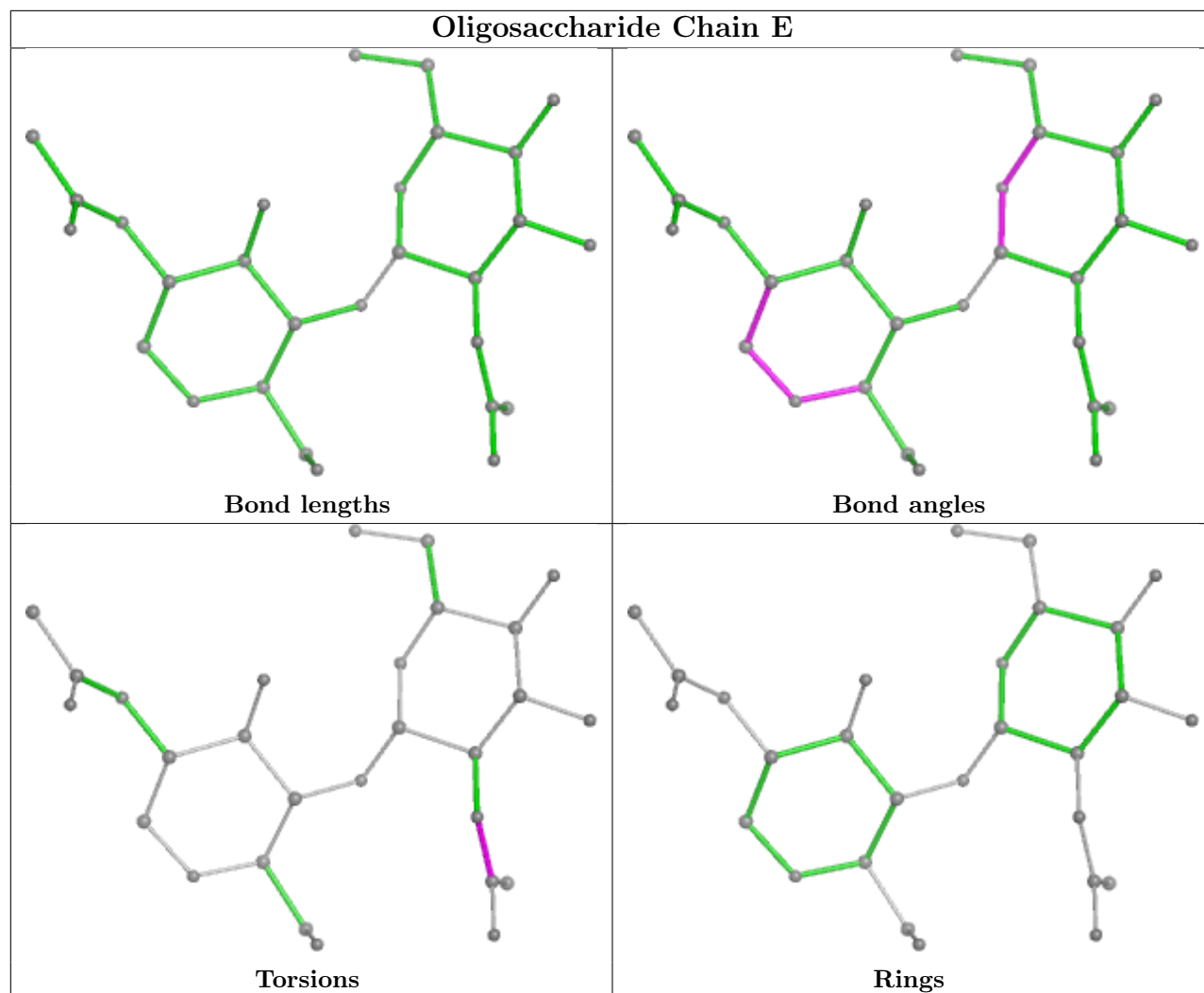
There are no ring outliers.

10 monomers are involved in 17 short contacts:

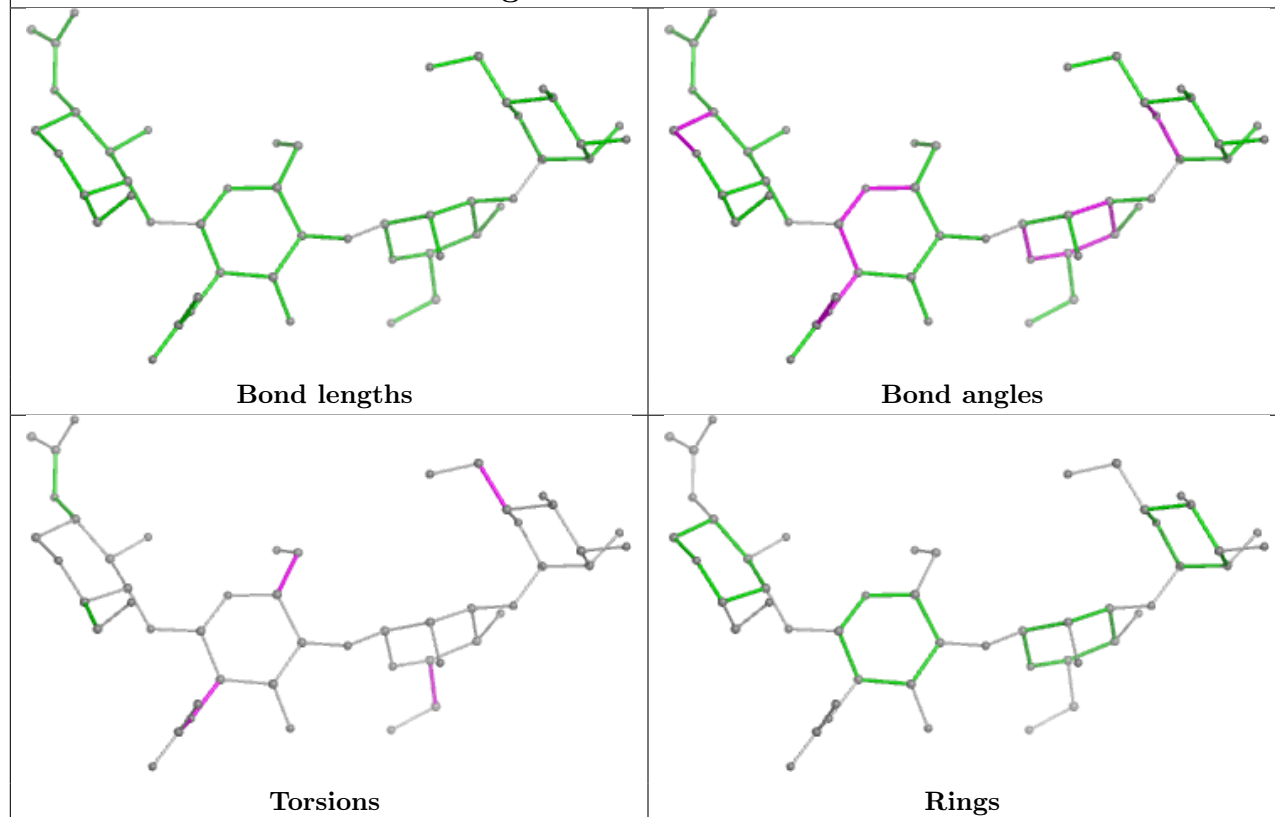
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
4	D	1	NAG	1	0
2	B	2	NAG	1	0
4	D	3	BMA	1	0
4	D	2	NAG	1	0
5	F	3	FUC	2	0
2	B	1	NAG	1	0
5	F	1	NAG	10	0
5	F	2	NAG	6	0
6	G	1	NAG	1	0

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

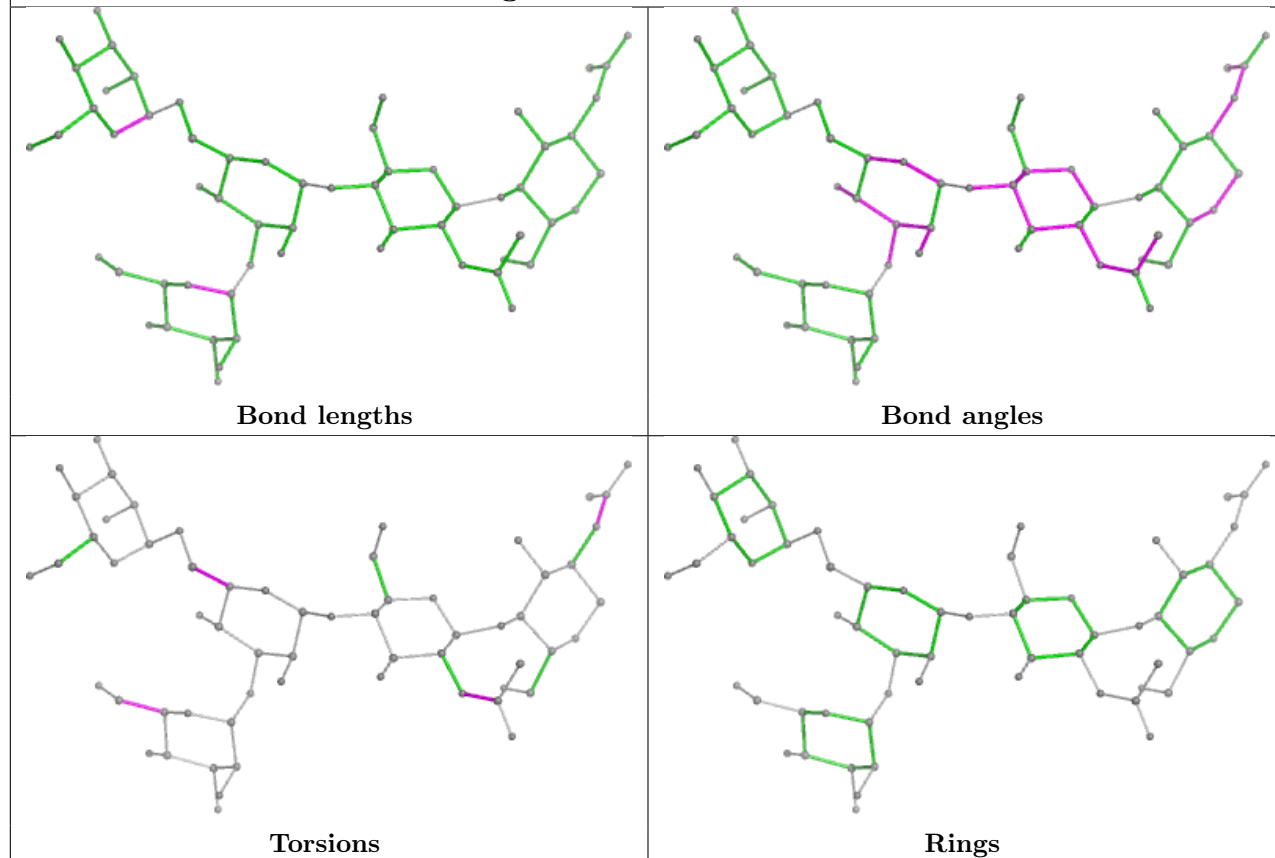


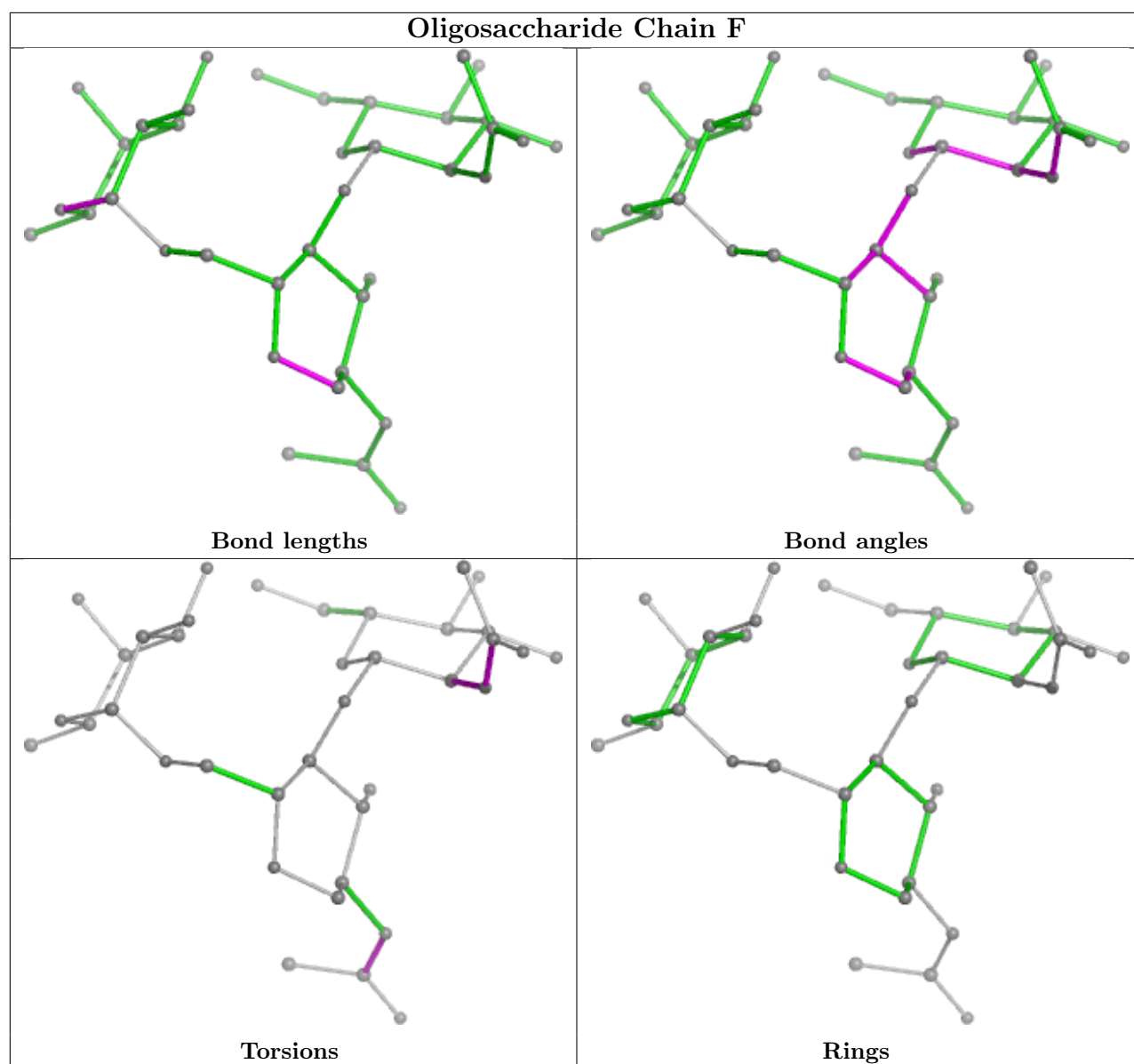


## Oligosaccharide Chain C

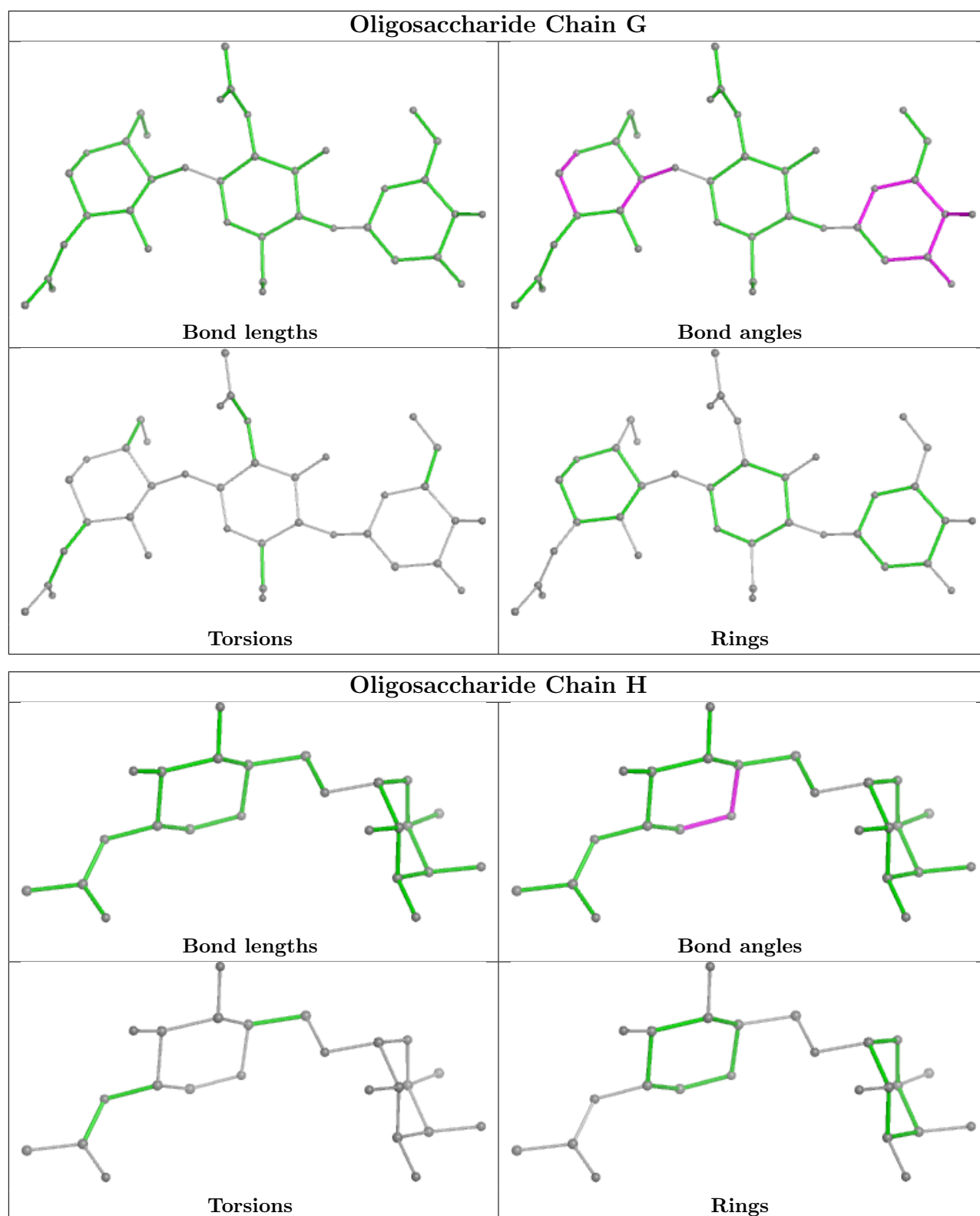


## Oligosaccharide Chain D









## 5.6 Ligand geometry [i](#)

8 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
10	NAG	A	804	1	14,14,15	0.70	0	17,19,21	1.27	1 (5%)
8	SO4	A	802	-	4,4,4	0.60	0	6,6,6	0.05	0
8	SO4	A	801	-	4,4,4	0.59	0	6,6,6	0.05	0
10	NAG	A	807	1	14,14,15	0.75	0	17,19,21	1.13	2 (11%)
10	NAG	A	806	1	14,14,15	0.83	0	17,19,21	1.02	1 (5%)
12	A1JME	A	808	-	36,36,36	1.74	10 (27%)	57,58,58	1.97	13 (22%)
9	EDO	A	803	-	3,3,3	0.28	0	2,2,2	0.21	0
11	CIT	A	805	-	12,12,12	1.36	1 (8%)	17,17,17	1.76	4 (23%)

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	804	1	-	2/6/23/26	0/1/1/1
10	NAG	A	807	1	-	0/6/23/26	0/1/1/1
10	NAG	A	806	1	-	0/6/23/26	0/1/1/1
12	A1JME	A	808	-	-	1/20/84/84	0/4/4/4
9	EDO	A	803	-	-	1/1/1/1	-
11	CIT	A	805	-	-	0/16/16/16	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	808	A1JME	C16-C10	5.03	1.65	1.56
12	A	808	A1JME	C19-C18	3.37	1.57	1.52
11	A	805	CIT	C3-C6	3.18	1.56	1.53
12	A	808	A1JME	C07-C03	2.68	1.60	1.55
12	A	808	A1JME	C11-C10	2.66	1.58	1.53
12	A	808	A1JME	C26-C25	2.60	1.58	1.53
12	A	808	A1JME	C17-C16	2.52	1.58	1.54
12	A	808	A1JME	C08-C09	2.23	1.58	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	808	A1JME	C20-C19	2.23	1.56	1.52
12	A	808	A1JME	C11-C06	2.08	1.57	1.53
12	A	808	A1JME	O14-C13	2.03	1.25	1.21

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	808	A1JME	C09-C10-C16	7.67	122.75	113.91
12	A	808	A1JME	C12-C11-C06	-6.34	103.44	111.18
11	A	805	CIT	O5-C6-C3	-4.71	115.58	122.25
12	A	808	A1JME	C09-C10-C11	-4.39	105.43	111.75
12	A	808	A1JME	C08-C07-C03	3.72	122.14	116.57
10	A	804	NAG	C2-N2-C7	3.60	128.03	122.90
12	A	808	A1JME	C20-C15-C13	3.43	117.66	113.23
11	A	805	CIT	O6-C6-C3	3.20	118.61	113.05
12	A	808	A1JME	C24-C07-C08	-2.99	105.87	110.59
10	A	806	NAG	C1-O5-C5	2.93	116.16	112.19
10	A	807	NAG	C1-O5-C5	2.87	116.08	112.19
12	A	808	A1JME	C17-C16-C10	2.81	114.28	110.08
12	A	808	A1JME	C07-C03-C02	-2.79	115.68	118.89
11	A	805	CIT	O7-C3-C6	2.42	112.26	108.86
12	A	808	A1JME	O14-C13-C12	-2.35	118.16	122.08
12	A	808	A1JME	C12-C13-C15	2.30	118.83	115.35
12	A	808	A1JME	C23-C16-C17	-2.24	105.56	108.97
12	A	808	A1JME	C10-C11-C06	2.18	112.01	109.09
11	A	805	CIT	O1-C1-C2	-2.11	116.79	122.94
10	A	807	NAG	C4-C3-C2	-2.07	107.99	111.02
12	A	808	A1JME	C16-C15-C13	2.02	113.06	110.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

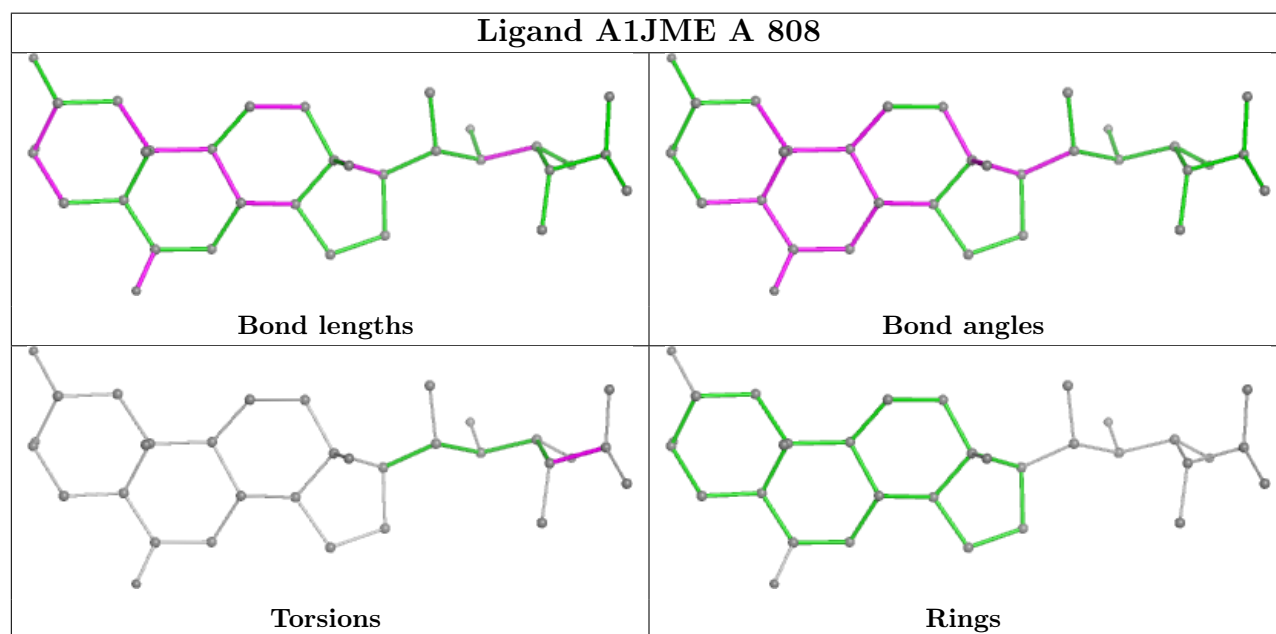
Mol	Chain	Res	Type	Atoms
10	A	804	NAG	C8-C7-N2-C2
10	A	804	NAG	O7-C7-N2-C2
9	A	803	EDO	O1-C1-C2-O2
12	A	808	A1JME	C28-C27-C29-C31

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	804	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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	742/797 (93%)	0.62	55 (7%) 22 26	56, 82, 125, 167	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	762	LEU	4.3
1	A	681	PHE	4.1
1	A	407	LEU	4.1
1	A	637	ILE	4.1
1	A	592	ILE	4.0
1	A	410	LEU	3.8
1	A	589	ALA	3.7
1	A	311	LEU	3.5
1	A	638	THR	3.5
1	A	166	VAL	3.4
1	A	750	THR	3.3
1	A	364	MET	3.3
1	A	636	ASN	3.2
1	A	362	LEU	3.2
1	A	718	ILE	3.2
1	A	361	LEU	3.2
1	A	642	TYR	3.0
1	A	741	PRO	3.0
1	A	386	THR	2.9
1	A	360	THR	2.9
1	A	365	ARG	2.9
1	A	591	PHE	2.7
1	A	698	VAL	2.7
1	A	162	PHE	2.7
1	A	728	LEU	2.6
1	A	409	ASN	2.6
1	A	435	THR	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	412	GLN	2.5
1	A	650	PHE	2.5
1	A	724	ALA	2.5
1	A	36	ILE	2.4
1	A	635	CYS	2.4
1	A	366	GLY	2.4
1	A	646	THR	2.4
1	A	123	SER	2.4
1	A	310	PHE	2.4
1	A	367	LEU	2.3
1	A	769	ARG	2.3
1	A	290	LEU	2.3
1	A	739	SER	2.3
1	A	406	ILE	2.3
1	A	725	LEU	2.3
1	A	342	LEU	2.2
1	A	639	SER	2.2
1	A	356	LEU	2.2
1	A	357	PRO	2.1
1	A	738	LEU	2.1
1	A	726	THR	2.1
1	A	408	PRO	2.1
1	A	605	MET	2.1
1	A	633	ASN	2.0
1	A	744	GLU	2.0
1	A	599	TYR	2.0
1	A	418	LEU	2.0
1	A	745	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

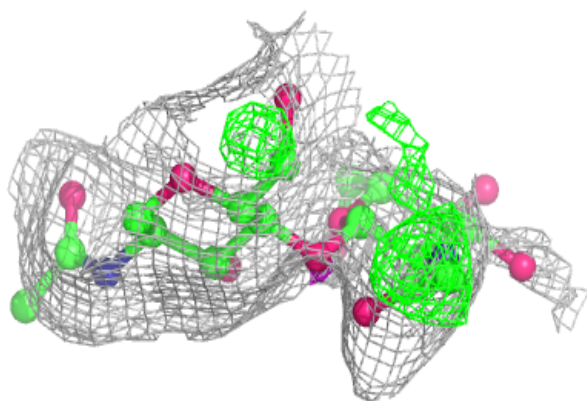
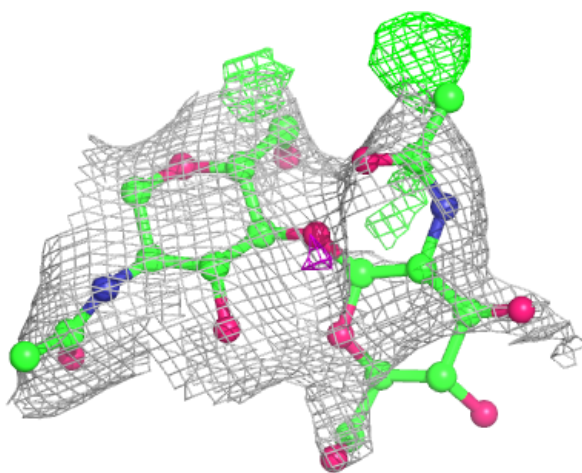
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	D	3	11/12	-0.14	0.22	220,238,246,252	0
4	MAN	D	4	11/12	0.07	0.23	207,224,228,232	0
4	MAN	D	5	11/12	0.24	0.19	181,212,219,220	0
5	FUC	F	3	10/11	0.31	0.19	146,150,159,161	0
5	NAG	F	2	14/15	0.37	0.24	154,161,165,175	0
2	NAG	E	1	14/15	0.49	0.18	99,137,143,148	0
4	NAG	D	2	14/15	0.50	0.36	141,209,270,420	0
2	NAG	E	2	14/15	0.55	0.18	127,144,150,150	0
5	NAG	F	1	14/15	0.59	0.20	116,136,150,160	0
2	NAG	B	2	14/15	0.61	0.17	125,136,145,153	0
3	MAN	C	4	11/12	0.62	0.10	161,172,205,209	0
3	BMA	C	3	11/12	0.68	0.09	137,160,188,196	0
6	BMA	G	3	11/12	0.71	0.15	93,103,113,123	0
7	NAG	H	1	14/15	0.71	0.16	101,108,114,116	0
3	NAG	C	2	14/15	0.74	0.16	80,115,136,138	0
2	NAG	B	1	14/15	0.84	0.13	104,118,133,144	0
4	NAG	D	1	14/15	0.87	0.18	62,89,123,145	0
6	NAG	G	2	14/15	0.87	0.16	74,80,86,95	0
7	FUC	H	2	10/11	0.87	0.13	109,121,126,127	0
6	NAG	G	1	14/15	0.88	0.19	68,71,76,78	0
3	NAG	C	1	14/15	0.91	0.12	57,69,84,90	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 B:**

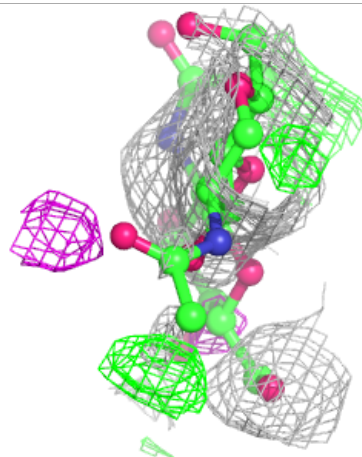
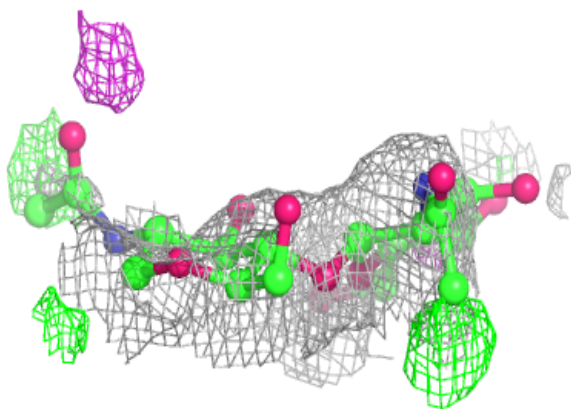
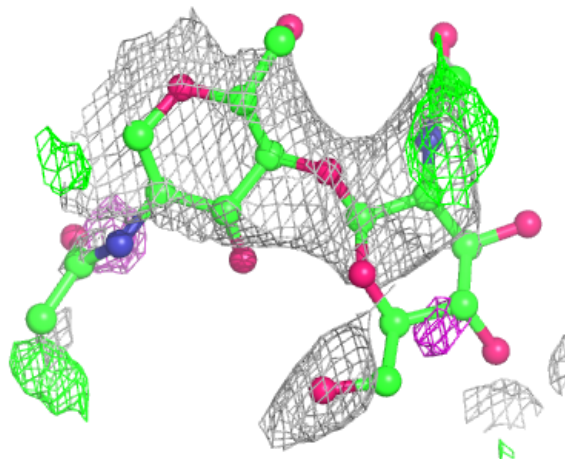
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





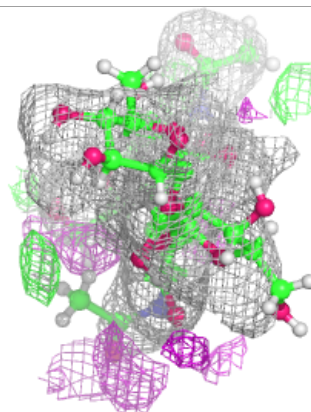
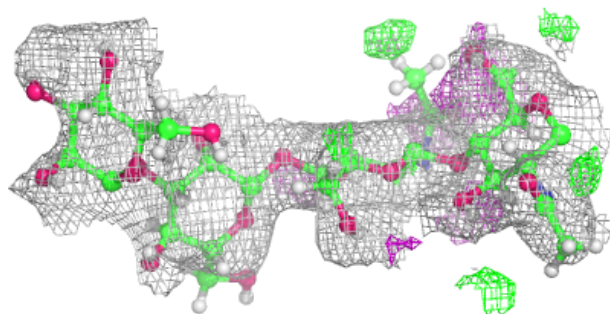
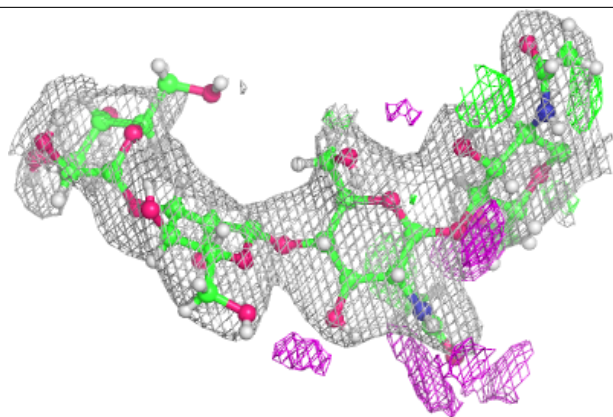
**Electron density around Chain E:**

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

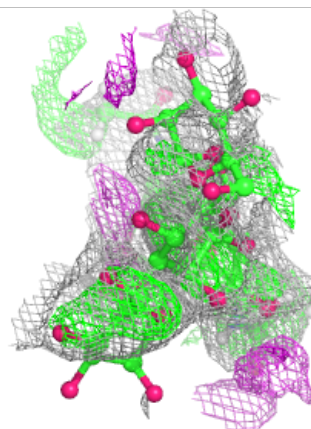
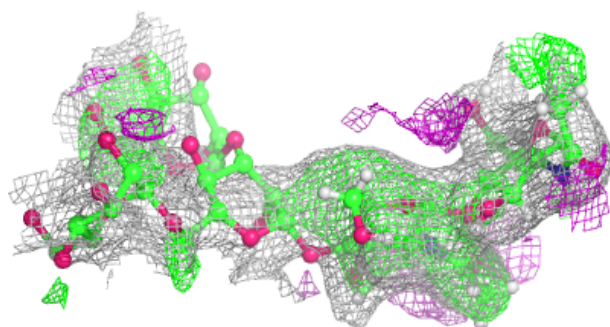
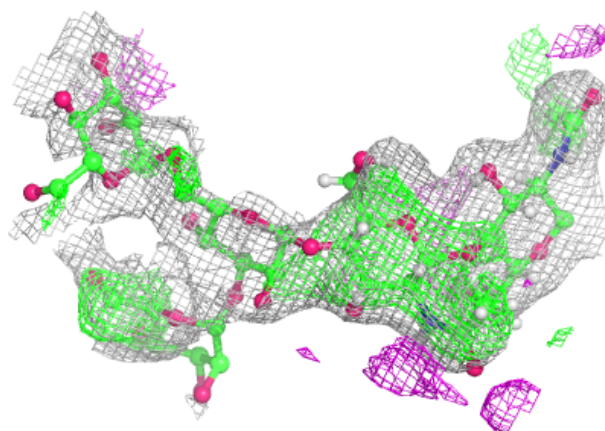


**Electron density around Chain C:**

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

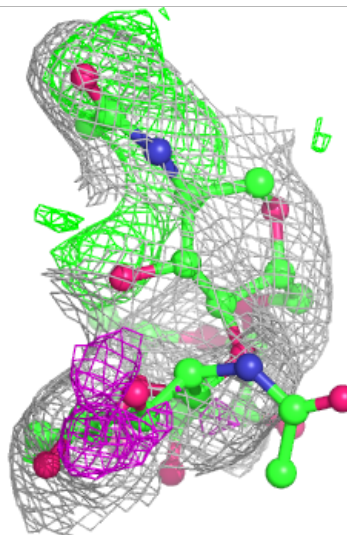
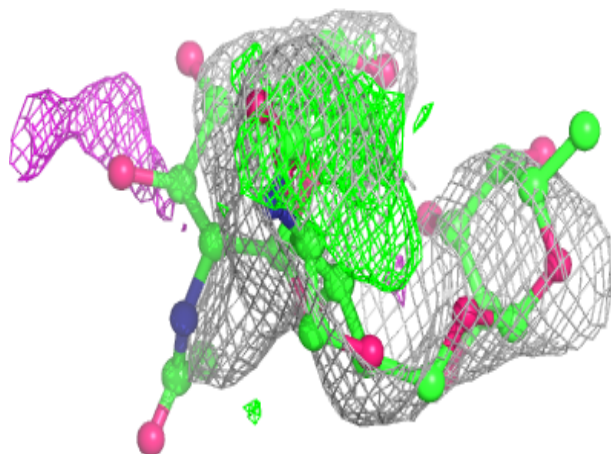
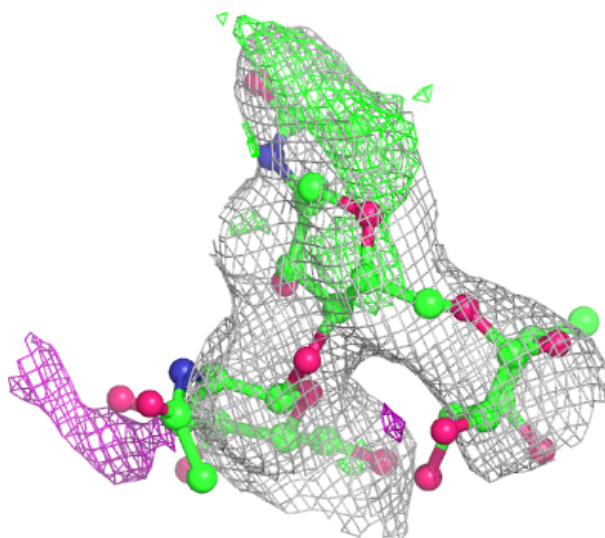
**Electron density around Chain D:**

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



**Electron density around Chain F:**

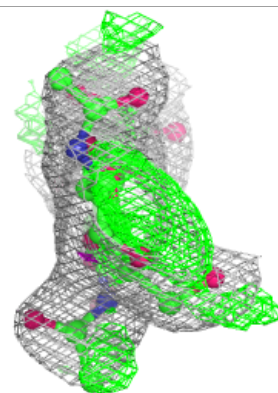
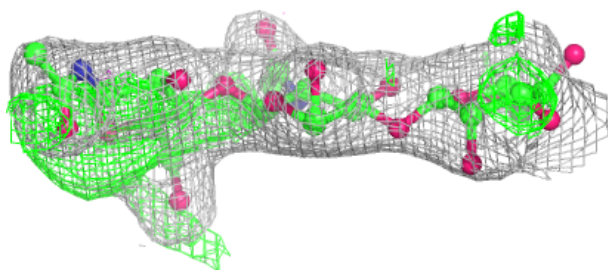
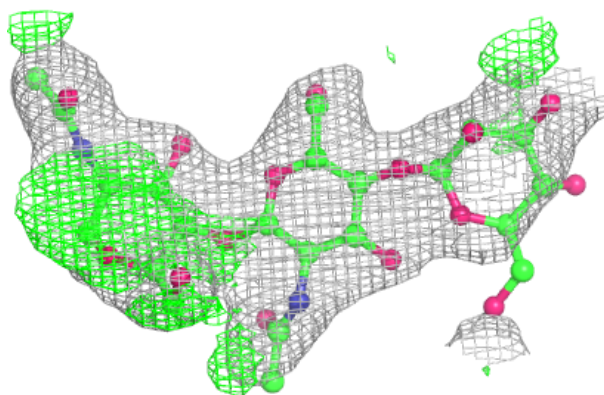
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



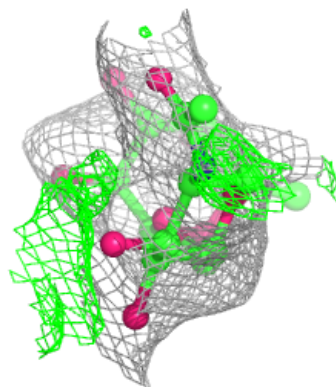
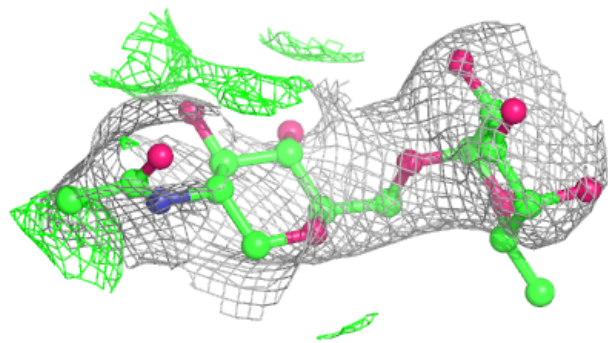
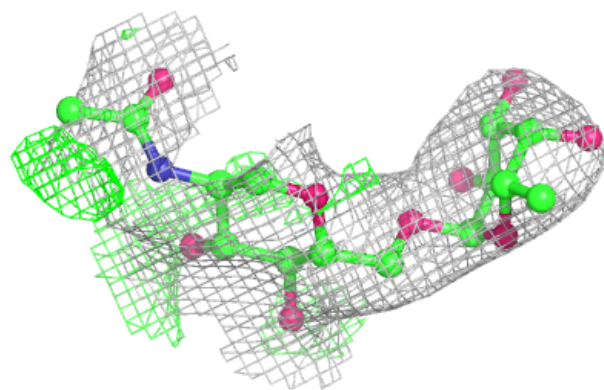


**Electron density around Chain G:**

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

**Electron density around Chain H:**

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



## 6.4 Ligands ⓘ

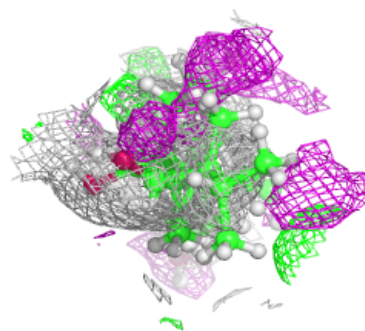
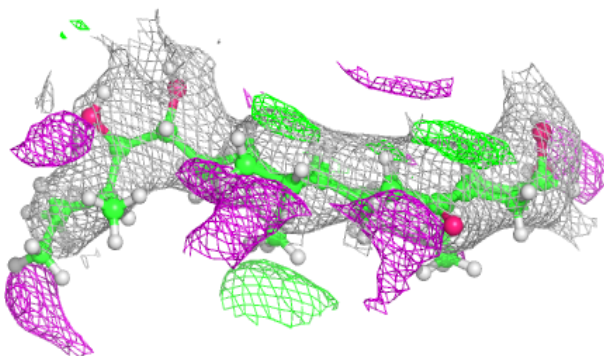
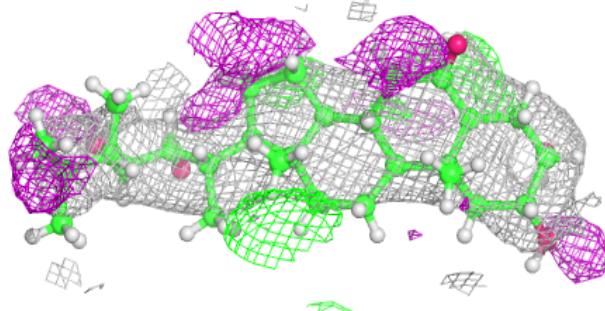
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	NAG	A	804	14/15	0.55	0.19	98,139,187,193	0
10	NAG	A	806	14/15	0.58	0.19	144,160,170,177	0
10	NAG	A	807	14/15	0.65	0.16	95,110,130,138	0
8	SO4	A	801	5/5	0.80	0.12	109,121,123,124	0
8	SO4	A	802	5/5	0.82	0.11	105,116,123,132	0
11	CIT	A	805	13/13	0.87	0.16	79,92,108,108	0
9	EDO	A	803	4/4	0.89	0.14	69,83,107,107	0
12	A1JME	A	808	33/33	0.91	0.18	75,100,122,124	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 A1JME A 808:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.